



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:20 AM UTC

PDB ID : 1T3N / pdb_00001t3n
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 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

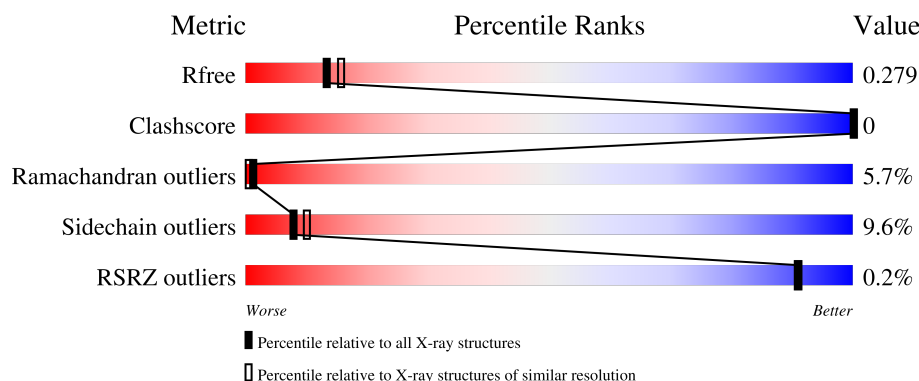
1 Overall quality at a glance

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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	29% 57% 14%
1	2-T	14	29% 57% 14%
2	1-P	13	15% 85%
2	2-P	13	15% 85%
3	1-A	388	% 85% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1-B	388	 81% 15% . .
3	2-A	388	 85% 12% .
3	2-B	388	 81% 15% . .

2 Entry composition

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			

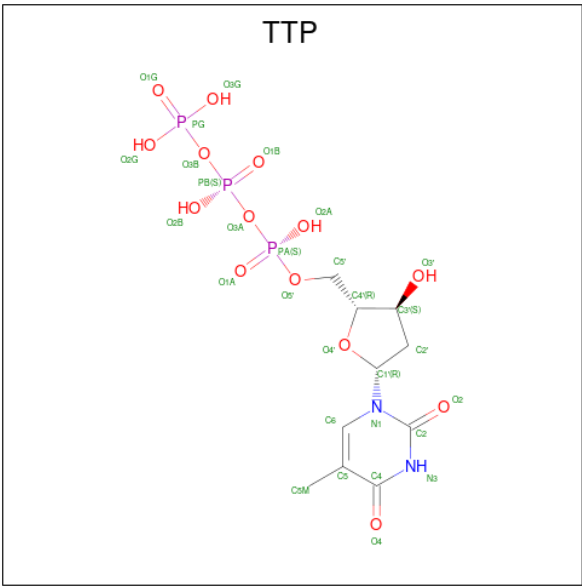
- Molecule 3 is a protein called polymerase (DNA directed) iota.

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 (CCD ID: 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 (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



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



- Molecule 1: Template DNA strand



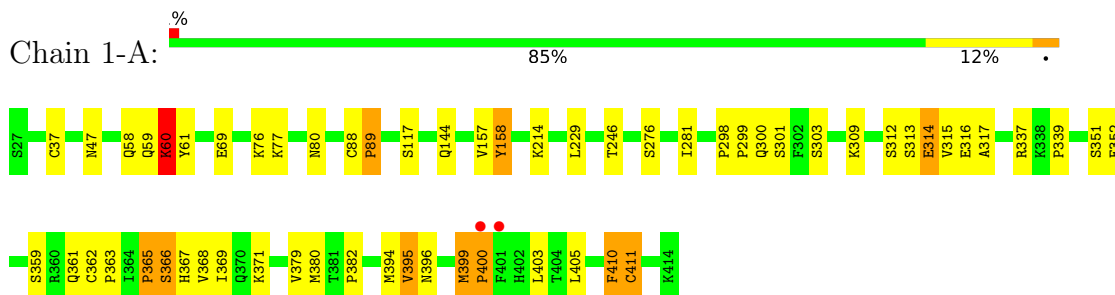
- Molecule 2: Primer DNA strand



- Molecule 2: Primer DNA strand

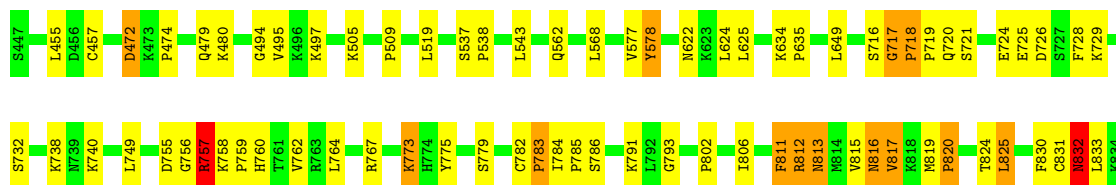


- Molecule 3: polymerase (DNA directed) iota



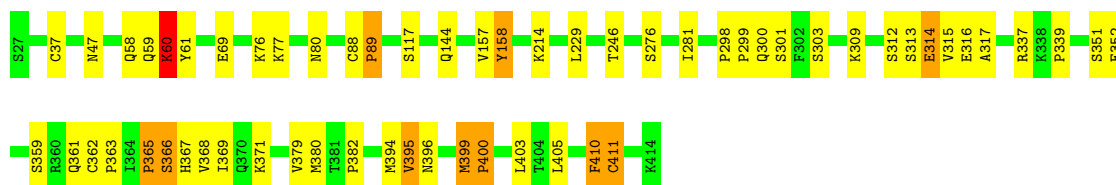
- Molecule 3: polymerase (DNA directed) iota

Chain 1-B:  81% 15% ..



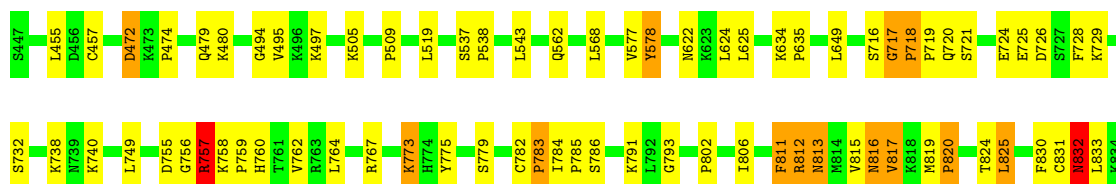
- Molecule 3: polymerase (DNA directed) iota

Chain 2-A:  85% 12% .



- Molecule 3: polymerase (DNA directed) iota

Chain 2-B:  81% 15% ..



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	4842 reflections (9.75%)	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 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TTP, MG, 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	1-T	0.48	0/308	1.67	9/472 (1.9%)
1	2-T	0.48	0/308	1.67	9/472 (1.9%)
2	1-P	0.68	0/285	1.97	20/440 (4.5%)
2	2-P	0.68	0/285	1.97	20/440 (4.5%)
3	1-A	0.65	5/2908 (0.2%)	1.28	49/3946 (1.2%)
3	1-B	0.85	10/2928 (0.3%)	1.39	53/3975 (1.3%)
3	2-A	0.65	5/2908 (0.2%)	1.28	49/3946 (1.2%)
3	2-B	0.85	10/2928 (0.3%)	1.39	53/3975 (1.3%)
All	All	0.74	30/12858 (0.2%)	1.39	262/17666 (1.5%)

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

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	832	ASN	N-CA	11.49	1.61	1.46
3	2-B	832	ASN	N-CA	11.49	1.61	1.46
3	1-B	816	ASN	C-O	-9.40	1.11	1.24
3	2-B	816	ASN	C-O	-9.40	1.11	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-B	817	VAL	CA-C	-9.34	1.40	1.52
3	2-B	817	VAL	CA-C	-9.34	1.40	1.52
3	1-B	832	ASN	CA-C	8.95	1.64	1.52
3	2-B	832	ASN	CA-C	8.95	1.64	1.52
3	1-B	721	SER	N-CA	7.64	1.55	1.46
3	2-B	721	SER	N-CA	7.64	1.55	1.46
3	1-B	720	GLN	CA-C	7.58	1.63	1.52
3	2-B	720	GLN	CA-C	7.58	1.63	1.52
3	1-A	395	VAL	CA-C	-7.09	1.43	1.52
3	2-A	395	VAL	CA-C	-7.09	1.43	1.52
3	1-A	300	GLN	CA-C	-6.51	1.44	1.52
3	2-A	300	GLN	CA-C	-6.51	1.44	1.52
3	1-B	816	ASN	CA-C	6.43	1.61	1.52
3	2-B	816	ASN	CA-C	6.43	1.61	1.52
3	1-A	301	SER	N-CA	-6.04	1.38	1.45
3	2-A	301	SER	N-CA	-6.04	1.38	1.45
3	1-B	817	VAL	N-CA	5.94	1.53	1.46
3	2-B	817	VAL	N-CA	5.94	1.53	1.46
3	1-B	816	ASN	C-N	5.93	1.41	1.33
3	2-B	816	ASN	C-N	5.93	1.41	1.33
3	1-A	60	LYS	CB-CG	-5.78	1.35	1.52
3	2-A	60	LYS	CB-CG	-5.78	1.35	1.52
3	1-A	60	LYS	C-O	-5.62	1.16	1.24
3	2-A	60	LYS	C-O	-5.62	1.16	1.24
3	1-B	784	ILE	CA-C	5.06	1.58	1.52
3	2-B	784	ILE	CA-C	5.06	1.58	1.52

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	831	CYS	N-CA-C	16.84	136.67	109.72
3	2-B	831	CYS	N-CA-C	16.84	136.67	109.72
1	1-T	15	DC	C2'-C3'-O3'	14.74	133.62	111.50
1	2-T	15	DC	C2'-C3'-O3'	14.74	133.62	111.50
3	1-A	60	LYS	CB-CG-CD	-14.14	78.77	111.30
3	2-A	60	LYS	CB-CG-CD	-14.14	78.77	111.30
3	1-B	757	ARG	CB-CG-CD	11.61	138.00	111.30
3	2-B	757	ARG	CB-CG-CD	11.61	138.00	111.30
1	1-T	13	DT	C2'-C3'-O3'	11.37	128.55	111.50
1	2-T	13	DT	C2'-C3'-O3'	11.37	128.55	111.50
3	1-B	758	LYS	N-CA-C	11.28	125.87	110.31
3	2-B	758	LYS	N-CA-C	11.28	125.87	110.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	831	CYS	CA-C-N	10.65	141.88	121.54
3	1-B	831	CYS	C-N-CA	10.65	141.88	121.54
3	2-B	831	CYS	CA-C-N	10.65	141.88	121.54
3	2-B	831	CYS	C-N-CA	10.65	141.88	121.54
2	1-P	12	DC	C2'-C3'-O3'	10.59	127.39	111.50
2	2-P	12	DC	C2'-C3'-O3'	10.59	127.39	111.50
3	1-A	362	CYS	N-CA-C	10.33	117.26	108.07
3	2-A	362	CYS	N-CA-C	10.33	117.26	108.07
3	1-B	811	PHE	CA-C-N	10.22	141.06	121.54
3	1-B	811	PHE	C-N-CA	10.22	141.06	121.54
3	2-B	811	PHE	CA-C-N	10.22	141.06	121.54
3	2-B	811	PHE	C-N-CA	10.22	141.06	121.54
2	1-P	11	DC	C4'-C3'-O3'	10.22	125.33	110.00
2	2-P	11	DC	C4'-C3'-O3'	10.22	125.33	110.00
3	1-A	394	MET	CA-C-N	10.06	140.08	121.97
3	1-A	394	MET	C-N-CA	10.06	140.08	121.97
3	2-A	394	MET	CA-C-N	10.06	140.08	121.97
3	2-A	394	MET	C-N-CA	10.06	140.08	121.97
3	1-B	816	ASN	CA-C-N	-9.80	104.34	121.97
3	1-B	816	ASN	C-N-CA	-9.80	104.34	121.97
3	2-B	816	ASN	CA-C-N	-9.80	104.34	121.97
3	2-B	816	ASN	C-N-CA	-9.80	104.34	121.97
3	1-B	817	VAL	N-CA-C	9.68	129.47	109.34
3	2-B	817	VAL	N-CA-C	9.68	129.47	109.34
2	1-P	7	DA	C2'-C3'-O3'	9.47	125.70	111.50
2	2-P	7	DA	C2'-C3'-O3'	9.47	125.70	111.50
3	1-A	411	CYS	CA-C-N	9.08	138.88	121.54
3	1-A	411	CYS	C-N-CA	9.08	138.88	121.54
3	2-A	411	CYS	CA-C-N	9.08	138.88	121.54
3	2-A	411	CYS	C-N-CA	9.08	138.88	121.54
3	1-B	718	PRO	N-CA-C	9.07	121.76	110.70
3	2-B	718	PRO	N-CA-C	9.07	121.76	110.70
1	1-T	13	DT	C4'-C3'-O3'	9.01	123.52	110.00
1	2-T	13	DT	C4'-C3'-O3'	9.01	123.52	110.00
3	1-A	399	MET	CA-C-N	8.97	131.06	119.84
3	1-A	399	MET	C-N-CA	8.97	131.06	119.84
3	2-A	399	MET	CA-C-N	8.97	131.06	119.84
3	2-A	399	MET	C-N-CA	8.97	131.06	119.84
3	1-A	214	LYS	N-CA-C	8.94	124.91	112.75
3	2-A	214	LYS	N-CA-C	8.94	124.91	112.75
3	1-B	756	GLY	CA-C-N	8.92	138.57	121.54
3	1-B	756	GLY	C-N-CA	8.92	138.57	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-B	756	GLY	CA-C-N	8.92	138.57	121.54
3	2-B	756	GLY	C-N-CA	8.92	138.57	121.54
3	1-A	214	LYS	CA-C-N	-8.83	108.81	119.84
3	1-A	214	LYS	C-N-CA	-8.83	108.81	119.84
3	2-A	214	LYS	CA-C-N	-8.83	108.81	119.84
3	2-A	214	LYS	C-N-CA	-8.83	108.81	119.84
3	1-B	764	LEU	N-CA-C	-8.78	93.73	108.75
3	2-B	764	LEU	N-CA-C	-8.78	93.73	108.75
2	1-P	3	DG	C2'-C3'-O3'	8.77	124.65	111.50
2	2-P	3	DG	C2'-C3'-O3'	8.77	124.65	111.50
2	1-P	3	DG	C5'-C4'-C3'	-8.45	102.22	114.90
2	2-P	3	DG	C5'-C4'-C3'	-8.45	102.22	114.90
2	1-P	7	DA	C4'-C3'-O3'	8.28	122.42	110.00
2	2-P	7	DA	C4'-C3'-O3'	8.28	122.42	110.00
3	1-B	757	ARG	CA-CB-CG	8.16	130.43	114.10
3	2-B	757	ARG	CA-CB-CG	8.16	130.43	114.10
3	1-B	819	MET	N-CA-C	8.01	122.61	109.79
3	2-B	819	MET	N-CA-C	8.01	122.61	109.79
2	1-P	3	DG	C4'-C3'-O3'	7.88	121.82	110.00
2	2-P	3	DG	C4'-C3'-O3'	7.88	121.82	110.00
3	1-A	403	LEU	N-CA-C	-7.74	103.97	113.41
3	2-A	403	LEU	N-CA-C	-7.74	103.97	113.41
3	1-B	817	VAL	CA-C-O	-7.70	111.16	120.78
3	2-B	817	VAL	CA-C-O	-7.70	111.16	120.78
2	1-P	11	DC	O3'-P-O5'	-7.64	92.55	104.00
2	2-P	11	DC	O3'-P-O5'	-7.64	92.55	104.00
3	1-B	832	ASN	CA-C-N	7.58	136.01	121.54
3	1-B	832	ASN	C-N-CA	7.58	136.01	121.54
3	2-B	832	ASN	CA-C-N	7.58	136.01	121.54
3	2-B	832	ASN	C-N-CA	7.58	136.01	121.54
3	1-A	410	PHE	N-CA-C	-7.52	103.70	113.17
3	2-A	410	PHE	N-CA-C	-7.52	103.70	113.17
3	1-A	394	MET	O-C-N	7.38	132.32	122.43
3	2-A	394	MET	O-C-N	7.38	132.32	122.43
2	1-P	11	DC	C2'-C3'-O3'	7.22	122.33	111.50
2	2-P	11	DC	C2'-C3'-O3'	7.22	122.33	111.50
3	1-B	820	PRO	CA-C-N	-7.14	110.27	123.05
3	1-B	820	PRO	C-N-CA	-7.14	110.27	123.05
3	2-B	820	PRO	CA-C-N	-7.14	110.27	123.05
3	2-B	820	PRO	C-N-CA	-7.14	110.27	123.05
3	1-B	634	LYS	N-CA-C	7.10	125.50	109.81
3	2-B	634	LYS	N-CA-C	7.10	125.50	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	60	LYS	CA-CB-CG	7.08	128.26	114.10
3	2-A	60	LYS	CA-CB-CG	7.08	128.26	114.10
3	1-A	300	GLN	CA-C-O	6.84	126.57	119.05
3	2-A	300	GLN	CA-C-O	6.84	126.57	119.05
2	1-P	4	DG	C5'-C4'-C3'	-6.83	104.65	114.90
2	2-P	4	DG	C5'-C4'-C3'	-6.83	104.65	114.90
2	1-P	11	DC	N1-C1'-C2'	-6.76	103.36	113.50
2	2-P	11	DC	N1-C1'-C2'	-6.76	103.36	113.50
2	1-P	6	DA	C2'-C3'-O3'	6.72	121.58	111.50
2	2-P	6	DA	C2'-C3'-O3'	6.72	121.58	111.50
2	1-P	12	DC	N1-C1'-C2'	6.72	123.58	113.50
2	2-P	12	DC	N1-C1'-C2'	6.72	123.58	113.50
2	1-P	5	DG	C4'-C3'-O3'	6.64	119.97	110.00
2	2-P	5	DG	C4'-C3'-O3'	6.64	119.97	110.00
3	1-A	59	GLN	N-CA-C	-6.62	98.11	108.90
3	2-A	59	GLN	N-CA-C	-6.62	98.11	108.90
3	1-B	820	PRO	CB-CA-C	-6.46	105.52	111.40
3	2-B	820	PRO	CB-CA-C	-6.46	105.52	111.40
1	1-T	6	DG	C5'-C4'-C3'	-6.38	105.34	114.90
1	2-T	6	DG	C5'-C4'-C3'	-6.38	105.34	114.90
3	1-A	60	LYS	N-CA-C	6.37	124.36	110.80
3	2-A	60	LYS	N-CA-C	6.37	124.36	110.80
3	1-B	816	ASN	N-CA-C	6.32	123.09	113.61
3	2-B	816	ASN	N-CA-C	6.32	123.09	113.61
3	1-B	831	CYS	O-C-N	6.28	131.36	123.19
3	2-B	831	CYS	O-C-N	6.28	131.36	123.19
3	1-A	316	GLU	N-CA-C	6.23	124.07	110.80
3	2-A	316	GLU	N-CA-C	6.23	124.07	110.80
3	1-B	724	GLU	CA-C-N	-6.19	113.95	122.93
3	1-B	724	GLU	C-N-CA	-6.19	113.95	122.93
3	2-B	724	GLU	CA-C-N	-6.19	113.95	122.93
3	2-B	724	GLU	C-N-CA	-6.19	113.95	122.93
3	1-A	300	GLN	N-CA-C	-6.14	105.74	113.72
3	2-A	300	GLN	N-CA-C	-6.14	105.74	113.72
3	1-A	59	GLN	CA-C-O	6.14	126.99	120.36
3	2-A	59	GLN	CA-C-O	6.14	126.99	120.36
3	1-A	47	ASN	CA-C-N	6.06	127.42	119.84
3	1-A	47	ASN	C-N-CA	6.06	127.42	119.84
3	2-A	47	ASN	CA-C-N	6.06	127.42	119.84
3	2-A	47	ASN	C-N-CA	6.06	127.42	119.84
3	1-B	760	HIS	N-CA-C	-6.03	105.50	112.92
3	2-B	760	HIS	N-CA-C	-6.03	105.50	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	157	VAL	N-CA-C	-5.99	99.24	107.99
3	2-A	157	VAL	N-CA-C	-5.99	99.24	107.99
3	1-B	578	TYR	N-CA-C	5.96	123.49	110.80
3	1-B	729	LYS	N-CA-C	5.96	119.40	111.30
3	2-B	578	TYR	N-CA-C	5.96	123.49	110.80
3	2-B	729	LYS	N-CA-C	5.96	119.40	111.30
3	1-B	784	ILE	N-CA-CB	-5.89	102.96	111.21
3	2-B	784	ILE	N-CA-CB	-5.89	102.96	111.21
3	1-A	117	SER	CA-C-N	5.88	125.58	119.05
3	1-A	117	SER	C-N-CA	5.88	125.58	119.05
3	2-A	117	SER	CA-C-N	5.88	125.58	119.05
3	2-A	117	SER	C-N-CA	5.88	125.58	119.05
2	1-P	7	DA	N9-C1'-C2'	-5.76	104.85	113.50
2	2-P	7	DA	N9-C1'-C2'	-5.76	104.85	113.50
3	1-A	303	SER	N-CA-C	5.75	118.12	110.53
3	2-A	303	SER	N-CA-C	5.75	118.12	110.53
3	1-A	58	GLN	CA-C-N	5.68	130.99	122.99
3	1-A	58	GLN	C-N-CA	5.68	130.99	122.99
3	2-A	58	GLN	CA-C-N	5.68	130.99	122.99
3	2-A	58	GLN	C-N-CA	5.68	130.99	122.99
3	1-B	537	SER	CA-C-N	5.65	125.76	119.32
3	1-B	537	SER	C-N-CA	5.65	125.76	119.32
3	2-B	537	SER	CA-C-N	5.65	125.76	119.32
3	2-B	537	SER	C-N-CA	5.65	125.76	119.32
3	1-B	832	ASN	N-CA-C	5.64	122.81	110.80
3	2-B	832	ASN	N-CA-C	5.64	122.81	110.80
2	1-P	5	DG	C5'-C4'-C3'	-5.59	106.52	114.90
2	2-P	5	DG	C5'-C4'-C3'	-5.59	106.52	114.90
1	1-T	10	DC	C5'-C4'-C3'	-5.58	106.52	114.90
3	1-B	538	PRO	N-CA-C	5.58	122.07	113.75
1	2-T	10	DC	C5'-C4'-C3'	-5.58	106.52	114.90
3	2-B	538	PRO	N-CA-C	5.58	122.07	113.75
2	1-P	7	DA	C5'-C4'-C3'	-5.58	106.53	114.90
2	2-P	7	DA	C5'-C4'-C3'	-5.58	106.53	114.90
3	1-B	568	LEU	N-CA-C	-5.54	106.50	113.20
3	2-B	568	LEU	N-CA-C	-5.54	106.50	113.20
3	1-A	315	VAL	CA-C-N	5.52	132.09	121.54
3	1-A	315	VAL	C-N-CA	5.52	132.09	121.54
3	2-A	315	VAL	CA-C-N	5.52	132.09	121.54
3	2-A	315	VAL	C-N-CA	5.52	132.09	121.54
3	1-B	811	PHE	O-C-N	5.51	130.21	123.21
3	2-B	811	PHE	O-C-N	5.51	130.21	123.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-P	12	DC	C4'-C3'-O3'	5.48	118.22	110.00
2	2-P	12	DC	C4'-C3'-O3'	5.48	118.22	110.00
1	1-T	13	DT	N1-C1'-C2'	-5.46	105.31	113.50
1	2-T	13	DT	N1-C1'-C2'	-5.46	105.31	113.50
3	1-B	813	ASN	N-CA-C	5.46	117.98	109.52
3	2-B	813	ASN	N-CA-C	5.46	117.98	109.52
3	1-A	315	VAL	N-CA-C	5.44	120.66	109.34
3	2-A	315	VAL	N-CA-C	5.44	120.66	109.34
1	1-T	8	DG	C5'-C4'-C3'	-5.40	106.80	114.90
1	2-T	8	DG	C5'-C4'-C3'	-5.40	106.80	114.90
3	1-B	819	MET	C-N-CD	-5.39	102.91	125.00
3	2-B	819	MET	C-N-CD	-5.39	102.91	125.00
3	1-B	757	ARG	N-CA-CB	5.36	119.56	110.49
3	2-B	757	ARG	N-CA-CB	5.36	119.56	110.49
3	1-A	317	ALA	N-CA-C	-5.36	106.79	113.38
3	2-A	317	ALA	N-CA-C	-5.36	106.79	113.38
3	1-A	369	ILE	N-CA-C	5.34	116.06	110.62
3	2-A	369	ILE	N-CA-C	5.34	116.06	110.62
3	1-A	59	GLN	CB-CA-C	5.31	119.43	109.71
3	2-A	59	GLN	CB-CA-C	5.31	119.43	109.71
3	1-A	69	GLU	N-CA-C	-5.31	106.97	113.50
3	2-A	69	GLU	N-CA-C	-5.31	106.97	113.50
3	1-B	782	CYS	CB-CA-C	-5.30	101.84	109.63
3	2-B	782	CYS	CB-CA-C	-5.30	101.84	109.63
3	1-A	312	SER	N-CA-C	5.28	116.22	107.73
3	2-A	312	SER	N-CA-C	5.28	116.22	107.73
2	1-P	6	DA	C4'-C3'-O3'	5.26	117.90	110.00
2	2-P	6	DA	C4'-C3'-O3'	5.26	117.90	110.00
3	1-B	755	ASP	CA-C-N	-5.26	112.96	121.05
3	1-B	755	ASP	C-N-CA	-5.26	112.96	121.05
3	2-B	755	ASP	CA-C-N	-5.26	112.96	121.05
3	2-B	755	ASP	C-N-CA	-5.26	112.96	121.05
3	1-A	158	TYR	N-CA-C	5.25	121.99	110.80
3	2-A	158	TYR	N-CA-C	5.25	121.99	110.80
3	1-B	820	PRO	CA-N-CD	-5.25	104.66	112.00
3	2-B	820	PRO	CA-N-CD	-5.25	104.66	112.00
3	1-A	59	GLN	O-C-N	5.24	129.54	123.30
3	2-A	59	GLN	O-C-N	5.24	129.54	123.30
3	1-A	58	GLN	N-CA-C	5.23	117.48	109.07
3	2-A	58	GLN	N-CA-C	5.23	117.48	109.07
3	1-B	479	GLN	N-CA-C	-5.20	100.93	109.40
3	2-B	479	GLN	N-CA-C	-5.20	100.93	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	365	PRO	N-CA-C	5.19	119.23	111.14
3	2-A	365	PRO	N-CA-C	5.19	119.23	111.14
3	1-A	59	GLN	CA-C-N	5.13	131.33	121.54
3	1-A	59	GLN	C-N-CA	5.13	131.33	121.54
3	2-A	59	GLN	CA-C-N	5.13	131.33	121.54
3	2-A	59	GLN	C-N-CA	5.13	131.33	121.54
3	1-B	824	THR	N-CA-C	-5.12	101.50	109.24
3	2-B	824	THR	N-CA-C	-5.12	101.50	109.24
3	1-A	366	SER	CA-C-N	5.12	131.31	121.54
3	1-A	366	SER	C-N-CA	5.12	131.31	121.54
3	1-B	577	VAL	N-CA-C	-5.12	99.80	107.37
3	2-A	366	SER	CA-C-N	5.12	131.31	121.54
3	2-A	366	SER	C-N-CA	5.12	131.31	121.54
3	2-B	577	VAL	N-CA-C	-5.12	99.80	107.37
3	1-A	400	PRO	N-CA-CB	5.09	108.60	103.25
3	2-A	400	PRO	N-CA-CB	5.09	108.60	103.25
3	1-B	717	GLY	CA-C-N	-5.08	115.15	120.38
3	1-B	717	GLY	C-N-CA	-5.08	115.15	120.38
3	2-B	717	GLY	CA-C-N	-5.08	115.15	120.38
3	2-B	717	GLY	C-N-CA	-5.08	115.15	120.38
3	1-B	505	LYS	N-CA-C	-5.07	106.35	112.54
3	2-B	505	LYS	N-CA-C	-5.07	106.35	112.54
3	1-B	773	LYS	N-CA-C	5.05	121.55	110.80
3	2-B	773	LYS	N-CA-C	5.05	121.55	110.80
3	1-A	365	PRO	CA-C-N	5.04	129.96	123.00
3	1-A	365	PRO	C-N-CA	5.04	129.96	123.00
3	2-A	365	PRO	CA-C-N	5.04	129.96	123.00
3	2-A	365	PRO	C-N-CA	5.04	129.96	123.00
2	1-P	5	DG	N9-C1'-C2'	-5.04	105.94	113.50
3	1-A	362	CYS	CB-CA-C	-5.04	104.61	110.76
2	2-P	5	DG	N9-C1'-C2'	-5.04	105.94	113.50
3	2-A	362	CYS	CB-CA-C	-5.04	104.61	110.76
3	1-B	820	PRO	O-C-N	-5.03	118.05	122.93
3	2-B	820	PRO	O-C-N	-5.03	118.05	122.93
1	1-T	6	DG	N9-C1'-C2'	-5.03	105.96	113.50
1	1-T	11	DC	C5'-C4'-C3'	-5.03	107.36	114.90
1	2-T	6	DG	N9-C1'-C2'	-5.03	105.96	113.50
1	2-T	11	DC	C5'-C4'-C3'	-5.03	107.36	114.90
3	1-B	783	PRO	CA-N-CD	-5.01	104.99	112.00
3	2-B	783	PRO	CA-N-CD	-5.01	104.99	112.00

All (2) chirality outliers are listed below:

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

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	1-B	816	ASN	Mainchain
2	1-P	1	DG	Sidechain
2	1-P	2	DG	Sidechain
2	1-P	8	DG	Sidechain
1	1-T	16	DC	Sidechain
1	1-T	17	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
3	2-B	816	ASN	Mainchain
2	2-P	1	DG	Sidechain
2	2-P	2	DG	Sidechain
2	2-P	8	DG	Sidechain
1	2-T	16	DC	Sidechain
1	2-T	17	DC	Sidechain
1	2-T	5	DA	Sidechain
1	2-T	6	DG	Sidechain
1	2-T	7	DG	Sidechain
1	2-T	8	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	1-T	277	0	159	0	0
1	2-T	277	0	159	0	0
2	1-P	270	0	145	0	0
2	2-P	270	0	145	0	0
3	1-A	2868	0	2764	0	0
3	1-B	2886	0	2789	0	0
3	2-A	2868	0	2764	0	0

Continued on next page...

Continued from previous page...

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

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	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

All (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
3	1-A	309	LYS
3	1-A	314	GLU
3	1-A	351	SER
3	1-A	352	GLU
3	1-A	395	VAL
3	1-A	396	ASN
3	1-A	399	MET
3	1-A	400	PRO
3	1-A	411	CYS
3	1-B	480	LYS
3	1-B	635	PRO
3	1-B	773	LYS
3	1-B	779	SER
3	1-B	812	ARG
3	1-B	815	VAL
3	1-B	825	LEU
3	1-B	832	ASN
3	1-B	833	LEU
3	2-A	60	LYS
3	2-A	61	TYR
3	2-A	76	LYS
3	2-A	80	ASN
3	2-A	89	PRO
3	2-A	309	LYS
3	2-A	314	GLU
3	2-A	351	SER
3	2-A	352	GLU
3	2-A	395	VAL
3	2-A	396	ASN
3	2-A	399	MET
3	2-A	400	PRO
3	2-A	411	CYS
3	2-B	480	LYS
3	2-B	635	PRO
3	2-B	773	LYS
3	2-B	779	SER
3	2-B	812	ARG
3	2-B	815	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-B	825	LEU
3	2-B	832	ASN
3	2-B	833	LEU
3	1-A	77	LYS
3	1-A	380	MET
3	1-B	717	GLY
3	1-B	718	PRO
3	1-B	738	LYS
3	2-A	77	LYS
3	2-A	380	MET
3	2-B	717	GLY
3	2-B	718	PRO
3	2-B	738	LYS
3	1-A	37	CYS
3	1-A	158	TYR
3	1-B	457	CYS
3	1-B	472	ASP
3	1-B	474	PRO
3	1-B	817	VAL
3	2-A	37	CYS
3	2-B	457	CYS
3	2-B	472	ASP
3	2-B	474	PRO
3	2-B	817	VAL
3	1-A	88	CYS
3	1-A	367	HIS
3	1-A	405	LEU
3	1-B	578	TYR
3	1-B	775	TYR
3	1-B	793	GLY
3	2-A	88	CYS
3	2-A	158	TYR
3	2-A	367	HIS
3	2-A	405	LEU
3	2-B	578	TYR
3	2-B	775	TYR
3	2-B	793	GLY
3	2-B	757	ARG
3	1-B	757	ARG
3	1-B	494	GLY
3	1-B	509	PRO
3	2-B	494	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-B	509	PRO
3	1-B	495	VAL
3	2-B	495	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	1-A	299/353 (85%)	276 (92%)	23 (8%)	12	16
3	1-B	304/353 (86%)	269 (88%)	35 (12%)	5	6
3	2-A	299/353 (85%)	276 (92%)	23 (8%)	12	16
3	2-B	304/353 (86%)	269 (88%)	35 (12%)	5	6
All	All	1206/1412 (85%)	1090 (90%)	116 (10%)	8	10

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1-A	60	LYS
3	1-A	89	PRO
3	1-A	144	GLN
3	1-A	229	LEU
3	1-A	246	THR
3	1-A	276	SER
3	1-A	281	ILE
3	1-A	298	PRO
3	1-A	299	PRO
3	1-A	313	SER
3	1-A	314	GLU
3	1-A	337	ARG
3	1-A	339	PRO
3	1-A	359	SER
3	1-A	361	GLN
3	1-A	363	PRO
3	1-A	365	PRO
3	1-A	366	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1-A	368	VAL
3	1-A	371	LYS
3	1-A	379	VAL
3	1-A	382	PRO
3	1-A	410	PHE
3	1-B	455	LEU
3	1-B	472	ASP
3	1-B	497	LYS
3	1-B	519	LEU
3	1-B	543	LEU
3	1-B	562	GLN
3	1-B	622	ASN
3	1-B	624	LEU
3	1-B	625	LEU
3	1-B	649	LEU
3	1-B	716	SER
3	1-B	719	PRO
3	1-B	725	GLU
3	1-B	726	ASP
3	1-B	728	PHE
3	1-B	732	SER
3	1-B	740	LYS
3	1-B	749	LEU
3	1-B	757	ARG
3	1-B	759	PRO
3	1-B	762	VAL
3	1-B	767	ARG
3	1-B	783	PRO
3	1-B	785	PRO
3	1-B	786	SER
3	1-B	791	LYS
3	1-B	802	PRO
3	1-B	806	ILE
3	1-B	811	PHE
3	1-B	812	ARG
3	1-B	813	ASN
3	1-B	820	PRO
3	1-B	825	LEU
3	1-B	830	PHE
3	1-B	832	ASN
3	2-A	60	LYS
3	2-A	89	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-A	144	GLN
3	2-A	229	LEU
3	2-A	246	THR
3	2-A	276	SER
3	2-A	281	ILE
3	2-A	298	PRO
3	2-A	299	PRO
3	2-A	313	SER
3	2-A	314	GLU
3	2-A	337	ARG
3	2-A	339	PRO
3	2-A	359	SER
3	2-A	361	GLN
3	2-A	363	PRO
3	2-A	365	PRO
3	2-A	366	SER
3	2-A	368	VAL
3	2-A	371	LYS
3	2-A	379	VAL
3	2-A	382	PRO
3	2-A	410	PHE
3	2-B	455	LEU
3	2-B	472	ASP
3	2-B	497	LYS
3	2-B	519	LEU
3	2-B	543	LEU
3	2-B	562	GLN
3	2-B	622	ASN
3	2-B	624	LEU
3	2-B	625	LEU
3	2-B	649	LEU
3	2-B	716	SER
3	2-B	719	PRO
3	2-B	725	GLU
3	2-B	726	ASP
3	2-B	728	PHE
3	2-B	732	SER
3	2-B	740	LYS
3	2-B	749	LEU
3	2-B	757	ARG
3	2-B	759	PRO
3	2-B	762	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-B	767	ARG
3	2-B	783	PRO
3	2-B	785	PRO
3	2-B	786	SER
3	2-B	791	LYS
3	2-B	802	PRO
3	2-B	806	ILE
3	2-B	811	PHE
3	2-B	812	ARG
3	2-B	813	ASN
3	2-B	820	PRO
3	2-B	825	LEU
3	2-B	830	PHE
3	2-B	832	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
3	1-A	47	ASN
3	1-A	59	GLN
3	1-A	95	ASN
3	1-A	161	GLN
3	1-A	170	HIS
3	1-A	227	GLN
3	1-A	262	GLN
3	1-A	367	HIS
3	1-A	370	GLN
3	1-B	478	GLN
3	1-B	487	ASN
3	1-B	562	GLN
3	1-B	590	HIS
3	1-B	622	ASN
3	1-B	636	ASN
3	1-B	638	GLN
3	1-B	676	ASN
3	1-B	682	GLN
3	1-B	699	GLN
3	1-B	813	ASN
3	2-A	47	ASN
3	2-A	59	GLN
3	2-A	95	ASN
3	2-A	161	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2-A	170	HIS
3	2-A	227	GLN
3	2-A	262	GLN
3	2-A	330	ASN
3	2-A	367	HIS
3	2-A	370	GLN
3	2-B	478	GLN
3	2-B	487	ASN
3	2-B	562	GLN
3	2-B	590	HIS
3	2-B	622	ASN
3	2-B	636	ASN
3	2-B	638	GLN
3	2-B	676	ASN
3	2-B	682	GLN
3	2-B	699	GLN
3	2-B	813	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1,2	16,19,20	0.78	0	20,26,29	0.78	1 (5%)
2	DOC	1-P	13	1,2	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	1,2	-	0/7/18/19	0/2/2/2
2	DOC	1-P	13	1,2	-	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(°)	Ideal(°)
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.

No monomer is involved in short contacts.

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	2-B	902	4	29,30,30	5.40	13 (44%)	43,47,47	2.50	15 (34%)
5	TTP	1-B	902	4	29,30,30	5.38	12 (41%)	43,47,47	2.52	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	2-B	902	4	-	3/22/34/34	0/2/2/2
5	TTP	1-B	902	4	-	3/22/34/34	0/2/2/2

All (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
5	1-B	902	TTP	PB-O3B	7.91	1.68	1.59
5	1-B	902	TTP	PB-O3A	7.83	1.67	1.59
5	2-B	902	TTP	PB-O3B	7.67	1.67	1.59
5	1-B	902	TTP	O4-C4	5.26	1.33	1.23
5	2-B	902	TTP	O4-C4	5.17	1.33	1.23
5	1-B	902	TTP	PA-O5'	-4.93	1.40	1.59
5	1-B	902	TTP	PA-O1A	-4.90	1.33	1.50
5	2-B	902	TTP	C1'-N1	4.84	1.60	1.48
5	2-B	902	TTP	PA-O5'	-4.81	1.40	1.59
5	2-B	902	TTP	PA-O1A	-4.79	1.34	1.50
5	1-B	902	TTP	C1'-N1	4.78	1.60	1.48
5	1-B	902	TTP	O5'-C5'	4.63	1.62	1.44
5	2-B	902	TTP	O5'-C5'	4.53	1.61	1.44
5	2-B	902	TTP	C6-C5	4.46	1.41	1.34
5	1-B	902	TTP	C6-C5	4.40	1.41	1.34
5	1-B	902	TTP	C2-N1	2.83	1.42	1.38
5	2-B	902	TTP	C2-N1	2.80	1.42	1.38
5	1-B	902	TTP	PG-O1G	2.40	1.57	1.50
5	2-B	902	TTP	PG-O1G	2.33	1.57	1.50
5	2-B	902	TTP	PB-O1B	2.04	1.57	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	1-B	902	TTP	C4-N3-C2	-5.35	120.32	127.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2-B	902	TTP	C6-N1-C2	-5.24	116.08	121.30
5	2-B	902	TTP	C4-N3-C2	-5.15	120.59	127.34
5	2-B	902	TTP	C1'-N1-C6	4.68	128.61	120.74
5	1-B	902	TTP	C1'-N1-C6	4.63	128.52	120.74
5	1-B	902	TTP	C2'-C1'-N1	-4.37	102.89	113.81
5	2-B	902	TTP	C2'-C1'-N1	-4.06	103.66	113.81
5	1-B	902	TTP	O2-C2-N3	-3.89	114.31	121.49
5	2-B	902	TTP	O2-C2-N3	-3.77	114.54	121.49
5	1-B	902	TTP	O2A-PA-O5'	3.42	123.06	107.57
5	2-B	902	TTP	O2A-PA-O5'	3.42	123.06	107.57
5	1-B	902	TTP	C6-C5-C4	-3.35	115.26	118.02
5	2-B	902	TTP	C5M-C5-C4	3.31	122.32	118.78
5	2-B	902	TTP	C6-C5-C4	-2.91	115.62	118.02
5	1-B	902	TTP	C5M-C5-C4	2.81	121.78	118.78
5	2-B	902	TTP	O5'-C5'-C4'	2.66	118.05	108.99
5	1-B	902	TTP	O5'-C5'-C4'	2.65	118.01	108.99
5	1-B	902	TTP	O4-C4-N3	-2.47	115.48	120.11
5	1-B	902	TTP	O2A-PA-O1A	-2.36	101.47	112.44
5	2-B	902	TTP	O2A-PA-O1A	-2.34	101.54	112.44
5	2-B	902	TTP	O4-C4-N3	-2.34	115.72	120.11
5	2-B	902	TTP	O3A-PB-O1B	-2.21	104.06	110.70
5	1-B	902	TTP	O3G-PG-O3B	2.18	111.94	104.64
5	2-B	902	TTP	O3G-PG-O3B	2.18	111.93	104.64
5	1-B	902	TTP	O3A-PB-O1B	-2.14	104.27	110.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

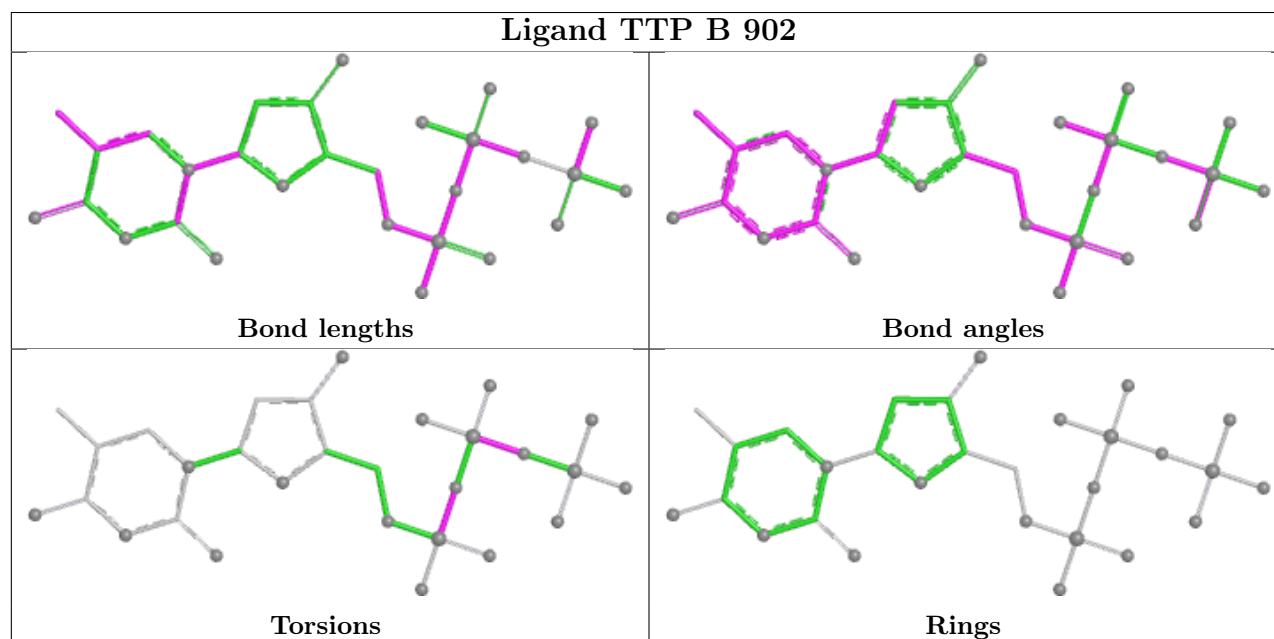
Mol	Chain	Res	Type	Atoms
5	1-B	902	TTP	PG-O3B-PB-O2B
5	2-B	902	TTP	PG-O3B-PB-O2B
5	1-B	902	TTP	PB-O3A-PA-O1A
5	2-B	902	TTP	PB-O3A-PA-O1A
5	1-B	902	TTP	PB-O3A-PA-O2A
5	2-B	902	TTP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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, 95th 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%)	-1.50	0 100 100	21, 25, 30, 35	14 (100%)
1	2-T	0/14	-	-	-	-
2	1-P	12/13 (92%)	-1.42	0 100 100	24, 29, 35, 36	12 (100%)
2	2-P	0/13	-	-	-	-
3	1-A	388/388 (100%)	-0.87	2 (0%) 87 87	9, 25, 50, 50	388 (100%)
3	1-B	388/388 (100%)	-0.88	0 100 100	11, 25, 50, 50	388 (100%)
3	2-A	0/388	-	-	-	-
3	2-B	0/388	-	-	-	-
All	All	802/1606 (49%)	-0.90	2 (0%) 91 91	9, 25, 50, 50	802 (100%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	1-A	400	PRO	4.2
3	1-A	401	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DOC	1-P	13	18/19	1.00	0.02	25,30,37,37	18
2	DOC	2-P	13	18/19	-	-	25,31,34,36	18

6.3 Carbohydrates [i](#)

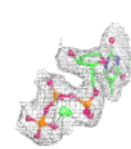
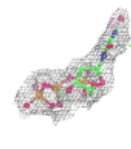
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	1-B	901	1/1	0.98	0.03	35,35,35,35	1
4	MG	2-B	901	1/1	-	-	35,35,35,35	1
5	TTP	1-B	902	29/29	0.99	0.03	28,31,37,38	29
5	TTP	2-B	902	29/29	-	-	27,33,36,38	29

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TTP B 902: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers ⓘ

There are no such residues in this entry.