



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:43 AM UTC

PDB ID : 2DPI / pdb_00002dpi
Title : Ternary complex of hPoli with DNA and dCTP
Authors : Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on : 2006-05-12
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

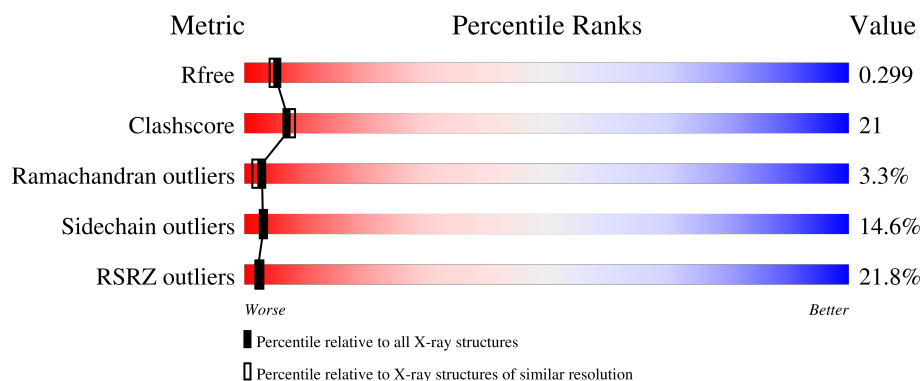
1 Overall quality at a glance

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	P	7	
2	T	9	
3	A	420	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3346 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 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	7	Total	C	N	O	P	0	0	0
			139	67	29	37	6			

- Molecule 2 is a DNA chain called 5'-D(*TP*(EDA)P*GP*GP*GP*TP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	9	Total	C	N	O	P	0	0	0
			184	90	32	54	8			

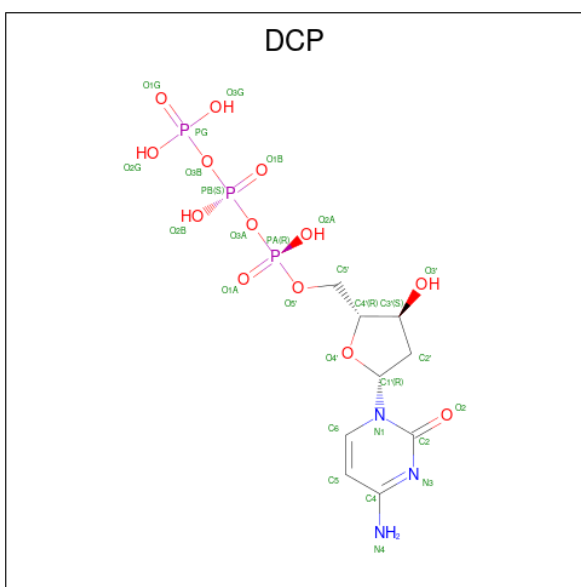
- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	372	Total	C	N	O	S	0	0	0
			2871	1806	503	541	21			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	3	Total O 3 3	0	0
6	T	12	Total O 12 12	0	0
6	A	107	Total O 107 107	0	0

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 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: 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'

Chain P: 



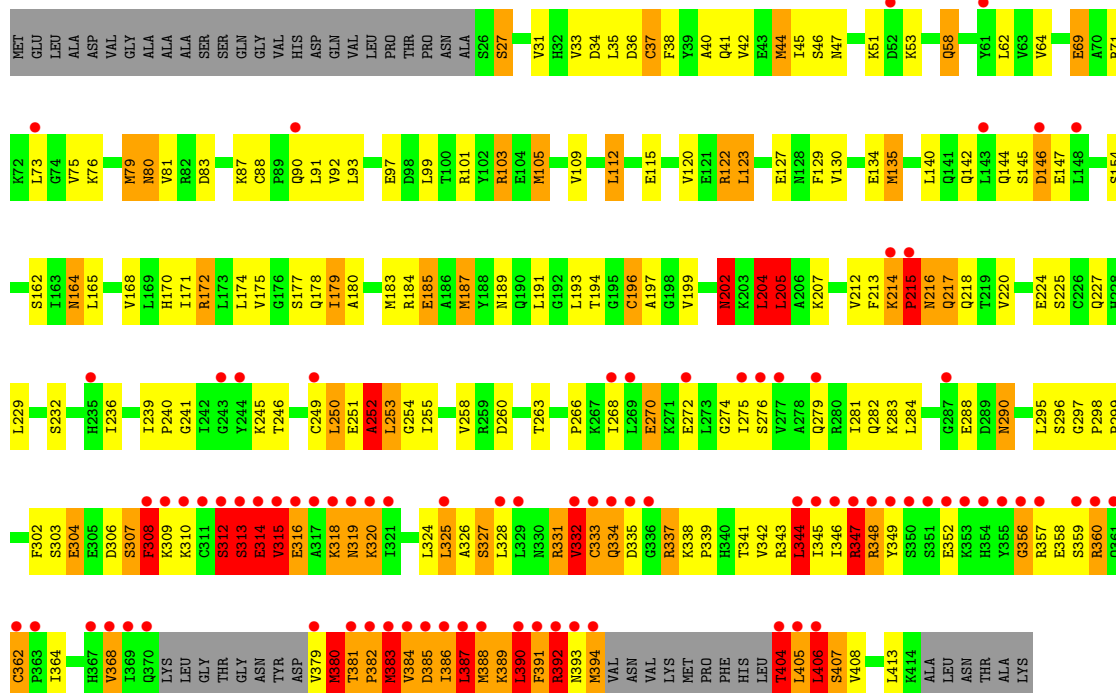
- Molecule 2: 5'-D(*TP*(EDA)P*GP*GP*GP*TP*CP*CP*T)-3'

Chain T: 



- Molecule 3: DNA polymerase iota

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.15Å 98.15Å 203.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.64 – 2.30 42.64 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (42.64-2.30) 98.6 (42.64-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.01 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.228 , 0.278 (Not available) , 0.299	Depositor DCC
R_{free} test set	2090 reflections (7.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3346	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	P	2.10	2/136 (1.5%)	3.44	26/208 (12.5%)
2	T	2.30	8/178 (4.5%)	3.34	26/271 (9.6%)
3	A	2.62	164/2909 (5.6%)	1.87	71/3927 (1.8%)
All	All	2.58	174/3223 (5.4%)	2.09	123/4406 (2.8%)

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	P	0	2
2	T	0	1
3	A	0	6
All	All	0	9

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	214	LYS	CA-C	-21.16	1.26	1.52
3	A	392	ARG	C-O	20.58	1.51	1.24
3	A	44	MET	SD-CE	-18.09	1.34	1.79
3	A	338	LYS	CA-CB	13.72	1.73	1.53
3	A	314	GLU	N-CA	12.97	1.62	1.46
3	A	394	MET	SD-CE	-12.37	1.48	1.79
3	A	387	LEU	C-O	12.20	1.38	1.24
1	P	867	DA	O3'-P	11.95	1.79	1.61
3	A	384	VAL	N-CA	11.67	1.60	1.46
3	A	122	ARG	CD-NE	-11.66	1.29	1.46
3	A	391	PHE	CA-C	11.58	1.68	1.52
3	A	122	ARG	NE-CZ	-11.18	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	383	MET	CA-C	10.90	1.66	1.52
3	A	386	ILE	CA-CB	10.67	1.65	1.54
3	A	105	MET	CG-SD	10.52	2.07	1.80
3	A	103	ARG	CZ-NH2	10.42	1.47	1.33
3	A	298	PRO	C-O	-10.17	1.13	1.24
2	T	847	DT	C3'-O3'	9.92	1.72	1.42
3	A	260	ASP	N-CA	9.86	1.58	1.46
3	A	258	VAL	C-O	-9.81	1.12	1.24
3	A	313	SER	CB-OG	9.63	1.61	1.42
3	A	381	THR	CA-CB	9.41	1.68	1.54
3	A	315	VAL	C-N	9.36	1.45	1.33
3	A	187	MET	SD-CE	-9.31	1.56	1.79
3	A	212	VAL	C-O	-9.22	1.13	1.24
3	A	302	PHE	C-O	9.12	1.34	1.23
3	A	179	ILE	CG1-CD1	-9.11	1.16	1.51
3	A	179	ILE	CA-CB	-9.09	1.43	1.54
3	A	216	ASN	N-CA	9.06	1.66	1.46
3	A	255	ILE	CA-CB	-9.06	1.43	1.53
3	A	320	LYS	N-CA	8.96	1.57	1.46
3	A	383	MET	N-CA	8.89	1.56	1.46
3	A	140	LEU	C-O	-8.71	1.13	1.24
3	A	199	VAL	CA-CB	-8.43	1.44	1.54
3	A	383	MET	SD-CE	-8.36	1.58	1.79
3	A	122	ARG	CG-CD	8.28	1.77	1.52
3	A	45	ILE	C-O	-8.23	1.14	1.24
3	A	245	LYS	C-O	-8.21	1.14	1.24
3	A	344	LEU	CA-C	-8.18	1.42	1.52
3	A	239	ILE	CA-C	8.03	1.61	1.52
3	A	42	VAL	C-O	-7.99	1.14	1.24
3	A	184	ARG	CD-NE	-7.99	1.35	1.46
3	A	315	VAL	C-O	7.94	1.33	1.24
3	A	189	ASN	CG-OD1	7.93	1.38	1.23
3	A	385	ASP	C-O	7.91	1.33	1.24
3	A	263	THR	C-O	-7.72	1.13	1.24
2	T	843	DG	P-OP2	-7.67	1.33	1.48
3	A	168	VAL	CA-C	7.60	1.63	1.52
3	A	383	MET	C-O	7.50	1.32	1.24
3	A	392	ARG	C-N	7.48	1.45	1.33
3	A	40	ALA	CA-C	-7.45	1.43	1.52
3	A	185	GLU	C-O	-7.44	1.15	1.24
3	A	380	MET	SD-CE	-7.38	1.61	1.79
2	T	843	DG	P-O5'	7.23	1.75	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	394	MET	CG-SD	7.22	1.98	1.80
3	A	319	ASN	CG-ND2	7.19	1.48	1.33
3	A	390	LEU	C-O	7.15	1.32	1.24
3	A	217	GLN	N-CA	-7.14	1.36	1.46
3	A	406	LEU	C-O	-7.14	1.14	1.24
2	T	843	DG	O5'-C5'	-6.92	1.22	1.42
3	A	258	VAL	CA-CB	-6.88	1.45	1.54
3	A	382	PRO	CA-C	-6.85	1.42	1.52
3	A	388	MET	CG-SD	6.83	1.97	1.80
3	A	390	LEU	CA-C	6.82	1.61	1.52
3	A	281	ILE	C-O	-6.79	1.15	1.24
3	A	193	LEU	C-O	6.79	1.32	1.24
3	A	241	GLY	C-O	-6.76	1.16	1.24
3	A	314	GLU	CA-C	6.69	1.61	1.52
3	A	315	VAL	CA-CB	6.69	1.63	1.54
3	A	207	LYS	CE-NZ	-6.67	1.29	1.49
3	A	405	LEU	N-CA	6.64	1.54	1.45
3	A	205	LEU	CA-C	6.61	1.61	1.52
3	A	215	PRO	N-CA	6.58	1.55	1.47
3	A	129	PHE	N-CA	-6.49	1.38	1.45
3	A	75	VAL	N-CA	6.49	1.54	1.46
3	A	93	LEU	C-O	-6.46	1.16	1.24
3	A	92	VAL	CA-C	6.45	1.60	1.52
3	A	189	ASN	C-O	-6.42	1.16	1.24
3	A	385	ASP	CA-CB	6.41	1.63	1.53
3	A	252	ALA	CA-CB	-6.34	1.42	1.53
3	A	387	LEU	CA-C	6.33	1.61	1.52
3	A	91	LEU	C-O	-6.33	1.16	1.24
3	A	97	GLU	N-CA	-6.33	1.38	1.46
3	A	212	VAL	N-CA	6.25	1.53	1.46
3	A	282	GLN	CG-CD	6.23	1.67	1.52
3	A	112	LEU	CG-CD2	-6.20	1.32	1.52
3	A	284	LEU	N-CA	-6.20	1.38	1.46
3	A	382	PRO	N-CD	6.18	1.56	1.47
3	A	38	PHE	CB-CG	-6.16	1.36	1.50
3	A	227	GLN	CA-C	6.16	1.60	1.52
3	A	134	GLU	CA-C	-6.16	1.44	1.52
3	A	220	VAL	CA-CB	-6.15	1.46	1.54
3	A	392	ARG	N-CA	6.14	1.54	1.46
3	A	341	THR	CA-C	-6.12	1.45	1.52
3	A	384	VAL	CA-C	6.09	1.60	1.52
3	A	382	PRO	N-CA	6.08	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	71	ARG	CA-C	6.04	1.61	1.52
3	A	196	CYS	C-O	6.03	1.31	1.23
3	A	164	ASN	CA-C	-6.00	1.45	1.53
3	A	123	LEU	N-CA	-5.99	1.39	1.46
3	A	360	ARG	C-O	5.95	1.31	1.24
3	A	27	SER	CA-C	5.93	1.60	1.52
3	A	342	VAL	C-O	5.91	1.29	1.24
3	A	101	ARG	CD-NE	5.87	1.54	1.46
3	A	37	CYS	CA-C	-5.87	1.45	1.52
3	A	214	LYS	CE-NZ	-5.86	1.31	1.49
3	A	178	GLN	C-O	-5.83	1.17	1.24
2	T	844	DT	O3'-P	5.79	1.69	1.61
3	A	290	ASN	CA-C	5.79	1.60	1.52
3	A	172	ARG	CD-NE	-5.79	1.38	1.46
3	A	347	ARG	CA-C	5.78	1.60	1.52
3	A	180	ALA	CA-C	-5.77	1.45	1.52
3	A	380	MET	CA-C	-5.77	1.45	1.52
3	A	162	SER	CA-CB	5.76	1.62	1.53
3	A	290	ASN	CG-ND2	5.75	1.45	1.33
3	A	202	ASN	CG-OD1	5.75	1.34	1.23
3	A	390	LEU	N-CA	5.75	1.53	1.46
3	A	135	MET	C-O	-5.70	1.17	1.24
3	A	105	MET	SD-CE	-5.69	1.65	1.79
3	A	408	VAL	CA-CB	-5.67	1.47	1.54
3	A	58	GLN	CD-OE1	5.64	1.34	1.23
3	A	276	SER	C-O	-5.64	1.17	1.24
3	A	207	LYS	CA-C	5.62	1.60	1.52
3	A	174	LEU	CG-CD2	-5.61	1.34	1.52
2	T	845	DC	C4'-C3'	5.61	1.64	1.52
3	A	306	ASP	CG-OD1	5.59	1.35	1.25
3	A	41	GLN	CA-C	-5.58	1.45	1.52
3	A	115	GLU	C-O	-5.56	1.17	1.24
3	A	296	SER	N-CA	5.56	1.53	1.46
3	A	298	PRO	CA-C	-5.55	1.47	1.52
3	A	122	ARG	CZ-NH1	-5.54	1.25	1.32
3	A	187	MET	CG-SD	5.54	1.94	1.80
3	A	364	ILE	CA-CB	-5.54	1.47	1.54
3	A	224	GLU	CA-C	-5.53	1.45	1.52
3	A	38	PHE	N-CA	5.52	1.52	1.46
3	A	282	GLN	N-CA	-5.52	1.39	1.46
3	A	313	SER	N-CA	5.50	1.53	1.46
2	T	843	DG	O4'-C1'	-5.47	1.30	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	389	LYS	N-CA	5.45	1.53	1.46
3	A	194	THR	C-O	-5.44	1.17	1.23
3	A	341	THR	CA-CB	-5.43	1.42	1.54
3	A	303	SER	CA-C	-5.42	1.45	1.52
3	A	178	GLN	CG-CD	5.38	1.65	1.52
3	A	127	GLU	C-O	5.35	1.30	1.23
3	A	313	SER	C-O	5.35	1.30	1.24
3	A	191	LEU	C-O	-5.32	1.17	1.24
3	A	383	MET	CG-SD	5.31	1.94	1.80
3	A	225	SER	CA-CB	5.30	1.61	1.53
3	A	341	THR	C-O	-5.30	1.17	1.23
3	A	384	VAL	C-N	5.30	1.40	1.33
3	A	171	ILE	CA-CB	5.27	1.60	1.54
3	A	225	SER	N-CA	5.27	1.52	1.46
3	A	47	ASN	N-CA	-5.23	1.40	1.46
3	A	183	MET	CG-SD	5.22	1.93	1.80
3	A	385	ASP	CB-CG	5.21	1.65	1.52
3	A	386	ILE	C-O	5.18	1.29	1.24
3	A	177	SER	C-N	-5.18	1.26	1.33
3	A	218	GLN	C-O	-5.17	1.17	1.23
3	A	120	VAL	CA-C	-5.14	1.46	1.52
3	A	313	SER	CA-CB	5.14	1.61	1.53
1	P	867	DA	C5'-C4'	5.13	1.62	1.52
3	A	46	SER	C-O	-5.12	1.18	1.24
3	A	324	LEU	N-CA	5.11	1.52	1.46
3	A	386	ILE	C-N	5.11	1.40	1.33
3	A	297	GLY	CA-C	5.10	1.59	1.51
3	A	197	ALA	CA-CB	-5.08	1.43	1.54
3	A	240	PRO	C-N	-5.07	1.28	1.34
3	A	319	ASN	CG-OD1	5.05	1.33	1.23
3	A	134	GLU	CD-OE1	5.04	1.34	1.25
3	A	202	ASN	C-O	5.03	1.29	1.23
3	A	165	LEU	C-O	-5.03	1.16	1.24
3	A	387	LEU	CG-CD1	-5.01	1.36	1.52
2	T	841	DG	P-O5'	5.00	1.70	1.60
3	A	314	GLU	CD-OE2	5.00	1.34	1.25

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	867	DA	O5'-C5'-C4'	19.26	139.69	110.80
2	T	842	DG	C4'-C3'-O3'	14.76	132.15	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	847	DT	C4'-C3'-O3'	13.61	130.41	110.00
3	A	387	LEU	N-CA-C	13.47	127.63	111.33
3	A	383	MET	N-CA-C	13.31	125.32	111.07
3	A	389	LYS	N-CA-C	-12.35	96.50	111.69
3	A	215	PRO	O-C-N	-12.04	106.39	122.64
2	T	843	DG	C4'-C3'-C2'	-11.31	85.43	102.40
1	P	872	DC	C4'-C3'-O3'	10.73	126.10	110.00
1	P	870	DA	O4'-C4'-C3'	10.11	120.57	105.40
2	T	839	DT	O5'-C5'-C4'	-10.05	95.72	110.80
3	A	215	PRO	CA-C-N	-9.58	107.81	123.04
3	A	215	PRO	C-N-CA	-9.58	107.81	123.04
2	T	843	DG	N9-C1'-C2'	-9.54	99.19	113.50
3	A	405	LEU	N-CA-C	9.54	124.57	109.50
2	T	842	DG	C2'-C3'-O3'	-9.08	97.88	111.50
3	A	381	THR	N-CA-C	-8.92	101.26	113.57
2	T	843	DG	C4'-C3'-O3'	8.89	123.33	110.00
3	A	386	ILE	N-CA-C	-8.77	101.11	110.23
3	A	215	PRO	N-CD-CG	-8.73	90.11	103.20
2	T	843	DG	C2'-C3'-O3'	-8.63	98.56	111.50
2	T	843	DG	C3'-C2'-C1'	8.49	114.33	101.60
3	A	214	LYS	CA-C-O	-8.45	108.59	120.16
2	T	843	DG	O4'-C4'-C3'	8.39	117.99	105.40
2	T	843	DG	O4'-C1'-C2'	-8.33	93.91	106.40
2	T	842	DG	C3'-C2'-C1'	8.29	114.04	101.60
2	T	842	DG	P-O5'-C5'	8.14	132.21	120.00
1	P	869	DG	O4'-C1'-N9	8.06	120.49	108.40
3	A	407	SER	N-CA-C	8.02	121.58	108.99
3	A	254	GLY	N-CA-C	8.02	125.97	115.47
2	T	846	DC	O3'-P-O5'	-7.95	92.07	104.00
3	A	404	THR	CA-C-N	7.91	134.97	122.62
3	A	404	THR	C-N-CA	7.91	134.97	122.62
2	T	842	DG	C5'-C4'-C3'	-7.80	103.21	114.90
3	A	279	GLN	N-CA-C	-7.76	103.27	112.89
2	T	844	DT	C5'-C4'-C3'	-7.72	103.32	114.90
2	T	839	DT	C5'-C4'-C3'	-7.71	103.33	114.90
1	P	867	DA	O4'-C4'-C3'	-7.63	93.95	105.40
3	A	214	LYS	N-CA-CB	7.56	123.83	110.37
1	P	871	DC	C4'-C3'-O3'	7.55	121.32	110.00
3	A	390	LEU	N-CA-C	7.54	120.45	111.33
3	A	349	TYR	N-CA-C	7.53	120.75	108.26
3	A	392	ARG	CA-C-N	-7.44	107.43	122.31
3	A	392	ARG	C-N-CA	-7.44	107.43	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	253	LEU	N-CA-C	7.44	121.95	113.02
3	A	122	ARG	CG-CD-NE	-7.42	95.67	112.00
3	A	393	ASN	N-CA-C	-7.38	104.36	113.15
1	P	867	DA	C5'-C4'-C3'	7.37	125.96	114.90
1	P	869	DG	P-O3'-C3'	-7.36	109.16	120.20
1	P	867	DA	O4'-C1'-N9	7.19	119.19	108.40
3	A	308	PHE	N-CA-C	-7.17	95.53	110.80
3	A	406	LEU	N-CA-C	7.06	120.91	109.40
1	P	872	DC	C2'-C3'-O3'	-6.79	101.32	111.50
3	A	381	THR	O-C-N	6.77	127.56	120.92
1	P	870	DA	C4'-C3'-O3'	6.75	120.12	110.00
1	P	872	DC	C3'-C2'-C1'	6.68	111.62	101.60
2	T	843	DG	O4'-C1'-N9	-6.60	98.50	108.40
3	A	381	THR	CB-CA-C	6.55	123.83	111.64
3	A	122	ARG	NE-CZ-NH2	-6.54	113.31	119.20
3	A	217	GLN	N-CA-CB	-6.49	100.37	111.21
3	A	302	PHE	N-CA-C	-6.49	97.49	108.26
1	P	870	DA	C2'-C3'-O3'	6.48	121.21	111.50
1	P	870	DA	C5'-C4'-O4'	-6.46	99.71	109.40
3	A	27	SER	N-CA-C	6.43	119.05	109.59
1	P	867	DA	C1'-O4'-C4'	6.39	119.28	109.70
2	T	847	DT	C4'-C3'-C2'	-6.37	92.84	102.40
1	P	867	DA	C4'-C3'-O3'	6.37	119.55	110.00
3	A	204	LEU	CB-CA-C	-6.36	100.63	110.81
2	T	842	DG	O4'-C1'-C2'	-6.36	96.86	106.40
1	P	870	DA	O5'-P-OP2	-6.35	88.94	108.00
3	A	316	GLU	N-CA-C	-6.35	100.96	111.37
3	A	175	VAL	N-CA-C	-6.34	104.15	110.62
3	A	268	ILE	N-CA-C	-6.30	104.36	110.72
1	P	870	DA	C1'-O4'-C4'	-6.30	100.25	109.70
1	P	870	DA	O4'-C1'-N9	6.19	117.69	108.40
3	A	326	ALA	N-CA-C	-6.16	104.49	111.14
2	T	843	DG	O5'-C5'-C4'	6.14	120.01	110.80
3	A	103	ARG	NH1-CZ-NH2	6.11	127.24	119.30
3	A	135	MET	CG-SD-CE	-6.10	87.47	100.90
1	P	870	DA	C4'-C3'-C2'	-6.07	93.30	102.40
3	A	250	LEU	N-CA-C	-6.06	104.79	111.82
2	T	846	DC	C5'-C4'-C3'	-6.03	105.86	114.90
2	T	839	DT	C4'-C3'-O3'	5.98	118.98	110.00
2	T	844	DT	C4'-C3'-O3'	5.98	118.97	110.00
3	A	332	VAL	CB-CA-C	-5.97	104.24	111.88
3	A	327	SER	CB-CA-C	-5.82	101.67	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	384	VAL	CB-CA-C	-5.80	101.78	111.29
3	A	312	SER	CA-C-O	-5.75	115.64	122.13
3	A	232	SER	N-CA-C	-5.75	105.77	112.89
3	A	274	GLY	N-CA-C	-5.73	106.20	112.04
2	T	842	DG	O4'-C1'-N9	-5.70	99.86	108.40
3	A	383	MET	CB-CA-C	-5.66	101.99	110.88
1	P	871	DC	C5'-C4'-C3'	-5.66	106.41	114.90
3	A	179	ILE	CB-CA-C	-5.63	104.53	112.14
3	A	331	ARG	CA-C-N	5.61	127.84	120.60
3	A	331	ARG	C-N-CA	5.61	127.84	120.60
3	A	386	ILE	N-CA-CB	5.48	116.37	110.62
2	T	847	DT	P-O5'-C5'	5.46	128.19	120.00
3	A	101	ARG	CG-CD-NE	5.46	124.01	112.00
3	A	216	ASN	N-CA-C	-5.40	97.34	108.53
1	P	870	DA	O5'-C5'-C4'	5.39	118.89	110.80
3	A	313	SER	CA-C-N	5.37	131.80	121.54
3	A	313	SER	C-N-CA	5.37	131.80	121.54
3	A	383	MET	O-C-N	5.37	127.60	122.07
3	A	325	LEU	N-CA-C	5.34	117.11	111.28
3	A	347	ARG	N-CA-C	5.32	116.74	109.18
3	A	154	SER	CA-CB-OG	-5.30	100.50	111.10
3	A	240	PRO	CA-C-N	-5.28	117.70	123.30
3	A	240	PRO	C-N-CA	-5.28	117.70	123.30
3	A	380	MET	N-CA-C	-5.28	105.42	111.07
3	A	391	PHE	N-CA-CB	-5.25	102.14	110.22
3	A	214	LYS	O-C-N	5.24	127.35	121.32
3	A	270	GLU	N-CA-C	-5.18	105.64	111.28
1	P	871	DC	O4'-C4'-C3'	5.16	113.13	105.40
1	P	872	DC	O4'-C4'-C3'	5.16	113.13	105.40
3	A	109	VAL	N-CA-C	5.16	115.37	110.42
1	P	870	DA	P-O5'-C5'	-5.15	112.28	120.00
3	A	172	ARG	NE-CZ-NH2	-5.14	114.58	119.20
3	A	44	MET	N-CA-C	5.12	116.86	111.28
3	A	385	ASP	N-CA-CB	5.08	117.33	109.91
1	P	870	DA	C3'-C2'-C1'	5.08	109.22	101.60
3	A	64	VAL	N-CA-C	-5.01	104.82	111.09
3	A	103	ARG	NE-CZ-NH2	-5.01	114.69	119.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	299	PRO	Mainchain
3	A	313	SER	Peptide
3	A	380	MET	Peptide
3	A	383	MET	Peptide
3	A	390	LEU	Peptide
1	P	868	DG	Sidechain
1	P	871	DC	Sidechain
2	T	843	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	P	139	0	79	2	2
2	T	184	0	104	7	2
3	A	2871	0	2894	126	0
4	A	2	0	0	0	0
5	A	28	0	12	0	0
6	A	107	0	0	4	0
6	P	3	0	0	1	0
6	T	12	0	0	0	0
All	All	3346	0	3089	133	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 21.

All (133) 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:A:122:ARG:CD	3:A:122:ARG:CG	1.77	1.57
3:A:105:MET:CG	3:A:105:MET:SD	2.07	1.42
2:T:847:DT:O3'	2:T:847:DT:C3'	1.72	1.37
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.33	1.10
3:A:383:MET:O	3:A:387:LEU:HG	1.54	1.06
3:A:380:MET:C	3:A:382:PRO:HD2	1.86	0.99
3:A:308:PHE:O	3:A:308:PHE:HD1	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:122:ARG:CG	3:A:122:ARG:NE	2.29	0.95
3:A:348:ARG:NH1	3:A:358:GLU:OE2	2.02	0.93
3:A:379:VAL:C	3:A:382:PRO:HD2	1.94	0.92
3:A:381:THR:N	3:A:382:PRO:CD	2.35	0.88
2:T:842:DG:H2''	2:T:843:DG:H5'	1.54	0.86
3:A:283:LYS:HE3	3:A:288:GLU:OE1	1.77	0.84
3:A:381:THR:N	3:A:382:PRO:HD2	1.93	0.84
3:A:344:LEU:CD1	3:A:387:LEU:HD22	2.08	0.83
3:A:249:CYS:O	3:A:253:LEU:HD12	1.79	0.83
3:A:80:ASN:ND2	3:A:83:ASP:CG	2.37	0.81
3:A:122:ARG:CD	3:A:122:ARG:CB	2.59	0.80
3:A:380:MET:C	3:A:382:PRO:CD	2.57	0.78
3:A:379:VAL:O	3:A:382:PRO:HD2	1.83	0.77
3:A:308:PHE:O	3:A:308:PHE:CD1	2.35	0.76
2:T:847:DT:O3'	2:T:847:DT:H3'	1.85	0.76
2:T:841:DG:OP2	3:A:307:SER:HB2	1.86	0.75
3:A:331:ARG:HD2	6:A:1014:HOH:O	1.86	0.74
3:A:344:LEU:HD11	3:A:387:LEU:CD2	2.16	0.74
3:A:348:ARG:NH1	3:A:358:GLU:CD	2.46	0.74
3:A:348:ARG:NH1	3:A:358:GLU:OE1	2.22	0.72
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.19	0.72
3:A:80:ASN:HD21	3:A:83:ASP:CG	1.98	0.71
3:A:304:GLU:O	3:A:407:SER:HB2	1.92	0.70
3:A:76:LYS:HB2	3:A:79:MET:HE3	1.74	0.69
3:A:405:LEU:C	3:A:406:LEU:HD23	2.18	0.69
3:A:325:LEU:HD11	3:A:387:LEU:HD11	1.74	0.68
3:A:347:ARG:HD3	3:A:404:THR:HG23	1.78	0.66
3:A:312:SER:O	3:A:312:SER:OG	2.08	0.65
3:A:325:LEU:HD11	3:A:387:LEU:CD1	2.27	0.65
3:A:390:LEU:O	3:A:394:MET:HG3	1.96	0.65
3:A:385:ASP:O	3:A:386:ILE:C	2.39	0.65
3:A:345:ILE:HG12	3:A:359:SER:HB3	1.80	0.64
3:A:196:CYS:SG	3:A:214:LYS:O	2.57	0.62
3:A:308:PHE:CE1	3:A:405:LEU:HA	2.34	0.62
3:A:379:VAL:O	3:A:382:PRO:CD	2.47	0.62
3:A:202:ASN:HD22	3:A:202:ASN:C	2.06	0.62
3:A:392:ARG:C	3:A:394:MET:H	2.07	0.62
3:A:389:LYS:O	3:A:392:ARG:N	2.30	0.61
3:A:270:GLU:OE2	3:A:275:ILE:HD12	2.01	0.61
3:A:388:MET:O	3:A:391:PHE:HB3	2.01	0.60
3:A:379:VAL:O	3:A:382:PRO:CG	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:841:DG:H2''	2:T:842:DG:H5''	1.86	0.57
3:A:379:VAL:C	3:A:382:PRO:CD	2.72	0.57
3:A:343:ARG:HD2	3:A:345:ILE:HD11	1.87	0.57
3:A:347:ARG:NH1	3:A:404:THR:OG1	2.28	0.56
3:A:251:GLU:O	3:A:252:ALA:C	2.47	0.56
3:A:164:ASN:H	3:A:170:HIS:HD2	1.53	0.56
3:A:251:GLU:O	3:A:253:LEU:N	2.38	0.56
3:A:249:CYS:O	3:A:253:LEU:CD1	2.54	0.55
3:A:315:VAL:O	3:A:316:GLU:C	2.49	0.55
3:A:368:VAL:HG21	3:A:383:MET:CE	2.37	0.55
3:A:347:ARG:HD3	3:A:404:THR:CG2	2.37	0.54
3:A:346:ILE:HG22	3:A:406:LEU:HD22	1.89	0.54
3:A:380:MET:O	3:A:381:THR:C	2.51	0.53
3:A:105:MET:CG	3:A:105:MET:CE	2.83	0.53
3:A:290:ASN:ND2	6:A:913:HOH:O	2.42	0.53
3:A:360:ARG:HG2	3:A:394:MET:SD	2.48	0.53
3:A:380:MET:HE2	3:A:384:VAL:HG23	1.89	0.53
3:A:387:LEU:O	3:A:391:PHE:HB2	2.07	0.53
3:A:380:MET:CE	3:A:384:VAL:CG2	2.86	0.53
3:A:251:GLU:C	3:A:253:LEU:N	2.66	0.52
3:A:202:ASN:ND2	3:A:205:LEU:H	2.07	0.52
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.90	0.52
3:A:360:ARG:HG2	3:A:394:MET:CG	2.40	0.52
2:T:847:DT:C3'	2:T:847:DT:HO3'	2.15	0.52
3:A:392:ARG:C	3:A:394:MET:N	2.66	0.51
3:A:360:ARG:HG2	3:A:394:MET:HG2	1.93	0.51
1:P:868:DG:N7	6:P:914:HOH:O	2.34	0.51
3:A:105:MET:SD	3:A:105:MET:CB	2.94	0.51
3:A:343:ARG:HG2	3:A:344:LEU:N	2.24	0.51
3:A:308:PHE:HZ	3:A:406:LEU:HG	1.77	0.50
3:A:36:ASP:O	3:A:37:CYS:C	2.55	0.50
3:A:80:ASN:HD22	3:A:83:ASP:CG	2.19	0.50
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.94	0.50
3:A:362:CYS:SG	3:A:390:LEU:HD11	2.52	0.50
3:A:58:GLN:NE2	6:A:996:HOH:O	2.46	0.49
3:A:347:ARG:HB2	3:A:356:GLY:O	2.13	0.48
3:A:332:VAL:HG13	3:A:339:PRO:HD3	1.95	0.48
3:A:196:CYS:HA	3:A:217:GLN:O	2.14	0.48
3:A:283:LYS:HE2	3:A:288:GLU:HB3	1.95	0.48
3:A:379:VAL:O	3:A:382:PRO:HG2	2.13	0.47
3:A:105:MET:CE	3:A:105:MET:CB	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:112:LEU:C	3:A:112:LEU:HD23	2.40	0.47
3:A:103:ARG:CZ	3:A:331:ARG:NH1	2.77	0.47
3:A:344:LEU:HD13	3:A:390:LEU:HB3	1.97	0.47
3:A:380:MET:O	3:A:382:PRO:N	2.48	0.47
3:A:406:LEU:HD23	3:A:406:LEU:N	2.30	0.47
3:A:386:ILE:C	3:A:390:LEU:HD12	2.41	0.46
3:A:73:LEU:HD22	3:A:88:CYS:SG	2.56	0.46
3:A:105:MET:CE	3:A:105:MET:HB2	2.46	0.45
3:A:348:ARG:CZ	3:A:358:GLU:OE2	2.61	0.45
3:A:380:MET:O	3:A:383:MET:HB2	2.16	0.45
3:A:236:ILE:HG21	3:A:236:ILE:HD13	1.72	0.45
3:A:334:GLN:HE21	3:A:334:GLN:HB3	1.63	0.45
3:A:404:THR:OG1	3:A:405:LEU:N	2.49	0.45
3:A:380:MET:C	3:A:382:PRO:N	2.73	0.45
3:A:44:MET:HE3	3:A:51:LYS:HA	2.00	0.44
3:A:270:GLU:OE2	3:A:275:ILE:CD1	2.65	0.44
3:A:315:VAL:O	3:A:318:LYS:HB3	2.17	0.44
3:A:31:VAL:HG12	3:A:130:VAL:HB	1.99	0.43
3:A:122:ARG:HD3	6:A:957:HOH:O	2.18	0.43
3:A:135:MET:HE2	3:A:179:ILE:HD12	2.00	0.43
3:A:144:GLN:HG3	3:A:147:GLU:HG2	2.00	0.43
3:A:327:SER:O	3:A:328:LEU:C	2.61	0.43
3:A:332:VAL:HG12	3:A:333:CYS:N	2.33	0.43
3:A:335:ASP:CG	3:A:337:ARG:HH11	2.25	0.43
3:A:266:PRO:O	3:A:270:GLU:HB2	2.18	0.42
3:A:344:LEU:C	3:A:345:ILE:HG13	2.43	0.42
2:T:842:DG:H4'	3:A:99:LEU:HD12	2.02	0.42
3:A:391:PHE:O	3:A:394:MET:HB2	2.19	0.42
3:A:359:SER:O	3:A:360:ARG:HD3	2.18	0.42
3:A:103:ARG:CZ	3:A:331:ARG:CZ	2.98	0.41
3:A:51:LYS:C	3:A:53:LYS:H	2.28	0.41
3:A:214:LYS:N	3:A:215:PRO:CD	2.82	0.41
3:A:335:ASP:OD2	3:A:337:ARG:NH1	2.53	0.41
3:A:389:LYS:HA	3:A:392:ARG:HD2	2.01	0.41
3:A:368:VAL:HG21	3:A:383:MET:HE2	2.01	0.41
3:A:204:LEU:HD13	3:A:205:LEU:HD13	2.02	0.41
3:A:144:GLN:O	3:A:146:ASP:N	2.53	0.41
3:A:382:PRO:CG	3:A:383:MET:H	2.33	0.41
3:A:308:PHE:CD1	3:A:404:THR:O	2.74	0.41
1:P:869:DG:O5'	1:P:869:DG:H2'	2.21	0.40
3:A:380:MET:CE	3:A:384:VAL:HG22	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:33:VAL:CG1	3:A:187:MET:HE1	2.51	0.40
3:A:69:GLU:O	3:A:73:LEU:CD1	2.69	0.40
3:A:34:ASP:OD2	3:A:34:ASP:C	2.64	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:P:867:DA:O5'	2:T:847:DT:O3'[10_665]	0.70	1.50
1:P:867:DA:C5'	2:T:847:DT:O3'[10_665]	1.75	0.45

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	A	366/420 (87%)	328 (90%)	26 (7%)	12 (3%)	3 2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	314	GLU
3	A	315	VAL
3	A	337	ARG
3	A	252	ALA
3	A	308	PHE
3	A	352	GLU
3	A	146	ASP
3	A	215	PRO
3	A	310	LYS
3	A	333	CYS
3	A	272	GLU
3	A	356	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	321/376 (85%)	274 (85%)	47 (15%)	3 3

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	27	SER
3	A	35	LEU
3	A	62	LEU
3	A	69	GLU
3	A	79	MET
3	A	80	ASN
3	A	81	VAL
3	A	87	LYS
3	A	90	GLN
3	A	123	LEU
3	A	142	GLN
3	A	145	SER
3	A	172	ARG
3	A	185	GLU
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	216	ASN
3	A	229	LEU
3	A	246	THR
3	A	295	LEU
3	A	304	GLU
3	A	307	SER
3	A	308	PHE
3	A	309	LYS
3	A	312	SER
3	A	313	SER
3	A	314	GLU
3	A	318	LYS
3	A	319	ASN

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Mol	Chain	Res	Type
3	A	320	LYS
3	A	332	VAL
3	A	334	GLN
3	A	344	LEU
3	A	347	ARG
3	A	348	ARG
3	A	357	ARG
3	A	362	CYS
3	A	368	VAL
3	A	380	MET
3	A	383	MET
3	A	387	LEU
3	A	390	LEU
3	A	392	ARG
3	A	404	THR
3	A	406	LEU
3	A	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	80	ASN
3	A	170	HIS
3	A	202	ASN
3	A	216	ASN
3	A	256	ASN
3	A	262	GLN
3	A	279	GLN
3	A	330	ASN
3	A	334	GLN

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	EDA	T	840	2	23,26,27	2.48	11 (47%)	29,38,41	2.88	12 (41%)
1	DOC	P	873	2,1	16,19,20	2.34	7 (43%)	20,26,29	2.13	5 (25%)

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	EDA	T	840	2	-	3/7/21/22	0/4/4/4
1	DOC	P	873	2,1	-	0/7/18/19	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	840	EDA	C2-N1	5.00	1.42	1.37
2	T	840	EDA	O5'-C5'	-4.56	1.31	1.44
1	P	873	DOC	C3'-C2'	-4.47	1.41	1.54
2	T	840	EDA	C5-N7	-4.29	1.30	1.39
1	P	873	DOC	C2'-C1'	4.19	1.61	1.52
2	T	840	EDA	C5-C6	-3.68	1.33	1.44
1	P	873	DOC	O4'-C1'	-3.63	1.34	1.42
2	T	840	EDA	C11-N6	-3.20	1.31	1.38
1	P	873	DOC	C4-N3	3.19	1.40	1.34
2	T	840	EDA	C2'-C3'	-3.17	1.44	1.52
1	P	873	DOC	C1'-N1	2.72	1.54	1.48
2	T	840	EDA	C2'-C1'	2.70	1.59	1.52
2	T	840	EDA	C4-N9	-2.68	1.31	1.38
1	P	873	DOC	O4'-C4'	2.63	1.49	1.44
2	T	840	EDA	C10-N1	-2.35	1.34	1.38
2	T	840	EDA	C6-N6	-2.33	1.29	1.33
2	T	840	EDA	C2-N3	2.30	1.34	1.30
1	P	873	DOC	O5'-C5'	-2.17	1.37	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	840	EDA	N1-C6-N6	-7.53	105.74	111.19
2	T	840	EDA	C11-N6-C6	7.07	112.07	105.08
1	P	873	DOC	C4'-O4'-C1'	-5.36	104.75	109.81
2	T	840	EDA	C2-N3-C4	4.76	121.87	112.53
2	T	840	EDA	C5-C4-N3	-3.99	121.40	127.27
1	P	873	DOC	O4'-C4'-C5'	3.90	116.38	109.34
1	P	873	DOC	O4'-C4'-C3'	3.89	111.21	104.81
2	T	840	EDA	N1-C2-N3	-3.84	118.12	124.61
2	T	840	EDA	C10-N1-C2	3.61	134.11	129.82
1	P	873	DOC	C2'-C1'-N1	-3.49	105.78	112.40
2	T	840	EDA	C5'-C4'-C3'	-3.28	96.30	114.64
2	T	840	EDA	C4'-O4'-C1'	-3.25	101.79	109.51
2	T	840	EDA	O4'-C4'-C3'	2.89	112.25	105.65
2	T	840	EDA	O4'-C4'-C5'	2.88	118.56	109.33
2	T	840	EDA	C10-C11-N6	-2.66	107.25	110.74
1	P	873	DOC	C5-C6-N1	2.04	125.15	121.84
2	T	840	EDA	N9-C4-N3	2.02	131.51	126.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	840	EDA	C3'-C4'-C5'-O5'
2	T	840	EDA	O4'-C4'-C5'-O5'
2	T	840	EDA	C2'-C1'-N9-C4

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DCP	A	875	4	28,29,29	2.46	13 (46%)	41,45,45	1.45	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
5	DCP	A	875	4	-	3/22/34/34	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	DCP	PB-O3B	6.21	1.66	1.59
5	A	875	DCP	PB-O3A	-4.74	1.54	1.59
5	A	875	DCP	PA-O3A	4.13	1.64	1.59
5	A	875	DCP	O4'-C1'	3.37	1.49	1.42
5	A	875	DCP	C4-N3	3.14	1.40	1.34
5	A	875	DCP	C3'-C4'	3.11	1.61	1.53
5	A	875	DCP	C2'-C1'	3.01	1.60	1.52
5	A	875	DCP	C5-C4	-2.70	1.36	1.42
5	A	875	DCP	O2-C2	2.57	1.28	1.23
5	A	875	DCP	PA-O2A	2.34	1.66	1.55
5	A	875	DCP	PG-O1G	2.34	1.57	1.50
5	A	875	DCP	O3'-C3'	2.04	1.47	1.43
5	A	875	DCP	C1'-N1	2.01	1.53	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	875	DCP	O2B-PB-O3A	3.60	117.01	107.27
5	A	875	DCP	O2A-PA-O5'	2.77	120.11	107.57
5	A	875	DCP	O2B-PB-O3B	2.73	114.65	107.27
5	A	875	DCP	O2A-PA-O3A	-2.50	100.52	107.27
5	A	875	DCP	C5-C6-N1	2.19	125.40	121.84
5	A	875	DCP	C1'-N1-C6	2.17	125.81	121.53
5	A	875	DCP	O2G-PG-O1G	-2.09	102.67	110.83

There are no chirality outliers.

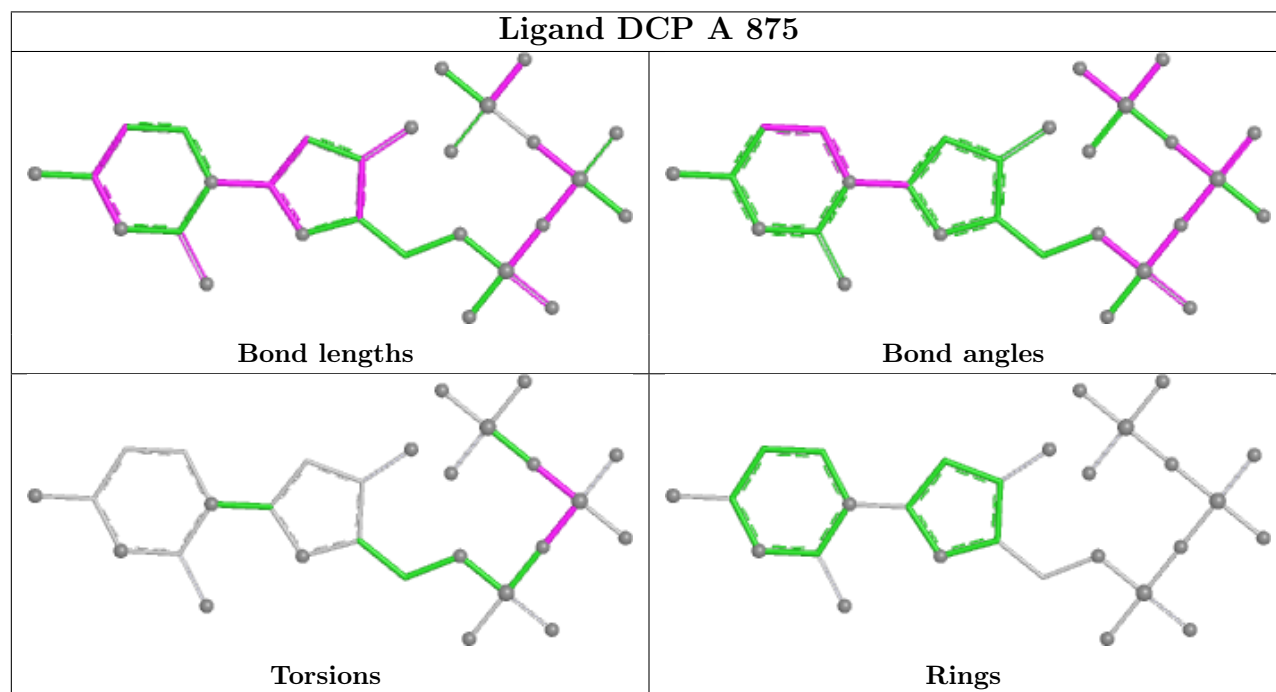
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	875	DCP	PA-O3A-PB-O2B
5	A	875	DCP	PG-O3B-PB-O1B
5	A	875	DCP	PA-O3A-PB-O1B

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	T	2
1	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	867:DA	O3'	868:DG	P	1.79
1	T	839:DT	O3'	840:EDA	P	1.34
1	T	840:EDA	O3'	841:DG	P	1.32

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, 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	P	6/7 (85%)	-0.09	0 100 100	22, 27, 33, 35	0
2	T	8/9 (88%)	-0.01	1 (12%) 8 9	17, 20, 25, 77	0
3	A	372/420 (88%)	1.03	83 (22%) 2 2	5, 32, 74, 96	0
All	All	386/436 (88%)	0.99	84 (21%) 2 2	5, 31, 74, 96	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	349	TYR	8.1
3	A	354	HIS	6.7
3	A	355	TYR	6.4
3	A	312	SER	6.2
3	A	315	VAL	6.1
3	A	314	GLU	6.0
3	A	317	ALA	6.0
3	A	391	PHE	5.8
3	A	383	MET	5.8
3	A	353	LYS	5.6
3	A	379	VAL	5.6
3	A	382	PRO	5.5
3	A	390	LEU	5.3
3	A	387	LEU	5.3
3	A	381	THR	5.0
3	A	384	VAL	4.8
3	A	335	ASP	4.6
3	A	357	ARG	4.5
3	A	350	SER	4.4
3	A	244	TYR	4.4
3	A	310	LYS	4.4
3	A	394	MET	4.4
3	A	316	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
3	A	392	ARG	4.1
3	A	370	GLN	4.1
3	A	309	LYS	4.0
3	A	336	GLY	4.0
3	A	348	ARG	3.9
3	A	318	LYS	3.9
3	A	351	SER	3.9
3	A	311	CYS	3.8
2	T	839	DT	3.8
3	A	313	SER	3.8
3	A	385	ASP	3.6
3	A	406	LEU	3.6
3	A	368	VAL	3.6
3	A	249	CYS	3.6
3	A	243	GLY	3.5
3	A	268	ILE	3.5
3	A	235	HIS	3.5
3	A	404	THR	3.5
3	A	269	LEU	3.3
3	A	325	LEU	3.3
3	A	369	ILE	3.2
3	A	352	GLU	3.2
3	A	386	ILE	3.2
3	A	329	LEU	3.2
3	A	388	MET	3.2
3	A	405	LEU	3.1
3	A	367	HIS	3.1
3	A	148	LEU	3.1
3	A	360	ARG	3.0
3	A	321	ILE	3.0
3	A	347	ARG	3.0
3	A	308	PHE	2.9
3	A	214	LYS	2.9
3	A	346	ILE	2.9
3	A	332	VAL	2.8
3	A	90	GLN	2.8
3	A	320	LYS	2.7
3	A	143	LEU	2.7
3	A	328	LEU	2.7
3	A	319	ASN	2.7
3	A	344	LEU	2.6
3	A	345	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	277	VAL	2.5
3	A	334	GLN	2.5
3	A	73	LEU	2.4
3	A	276	SER	2.4
3	A	146	ASP	2.3
3	A	287	GLY	2.3
3	A	333	CYS	2.3
3	A	272	GLU	2.3
3	A	393	ASN	2.2
3	A	279	GLN	2.2
3	A	361	GLN	2.1
3	A	52	ASP	2.1
3	A	275	ILE	2.1
3	A	356	GLY	2.1
3	A	359	SER	2.1
3	A	215	PRO	2.1
3	A	363	PRO	2.0
3	A	61	TYR	2.0
3	A	362	CYS	2.0

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	EDA	T	840	23/24	0.92	0.10	18,30,52,59	0
1	DOC	P	873	18/19	0.97	0.08	13,18,26,26	0

6.3 Carbohydrates [i](#)

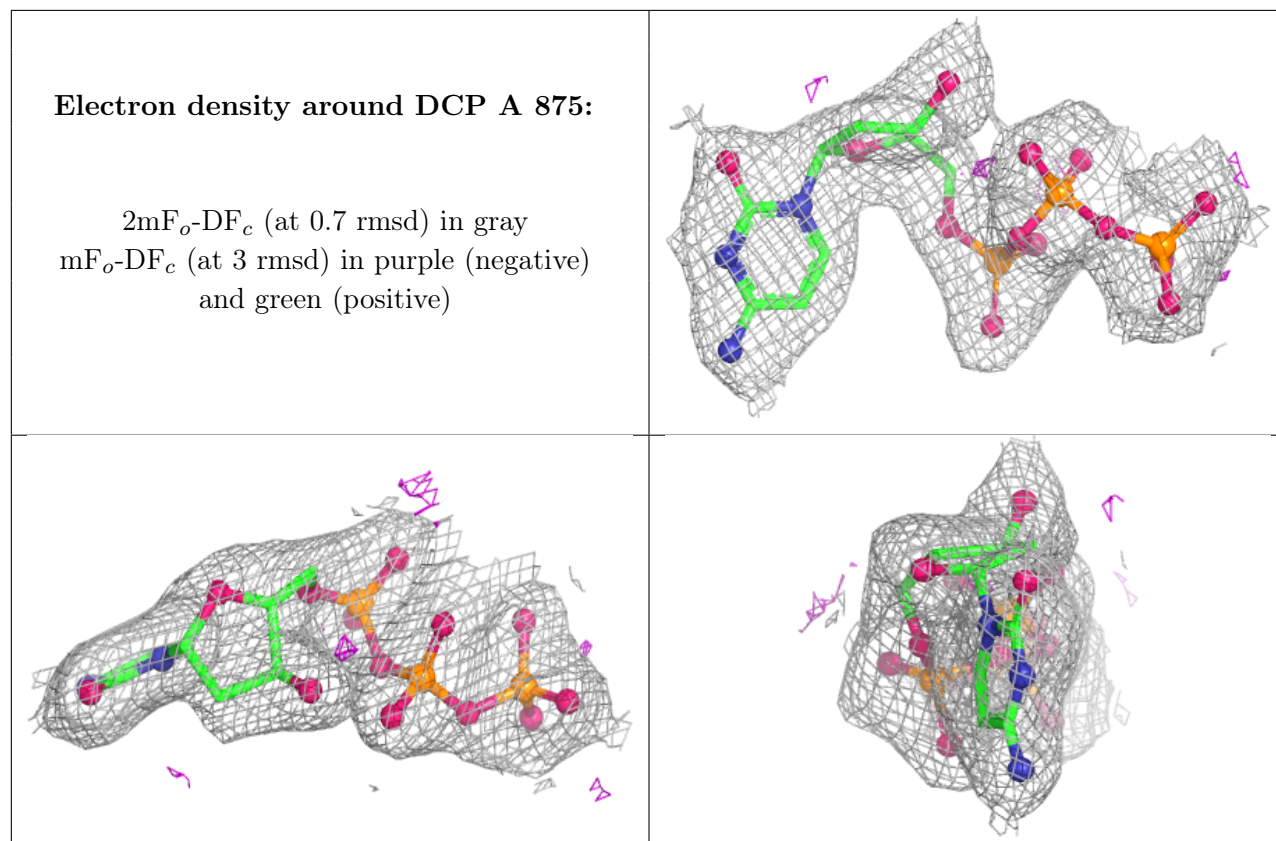
There are no oligosaccharides in this entry.

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	A	872	1/1	0.83	0.23	68,68,68,68	0
4	MG	A	871	1/1	0.92	0.05	20,20,20,20	0
5	DCP	A	875	28/28	0.96	0.07	13,20,25,26	0

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.