



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:59 PM UTC

PDB ID : 2DPJ / pdb_00002dpj
Title : structure of hPoli with DNA and dTTP
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

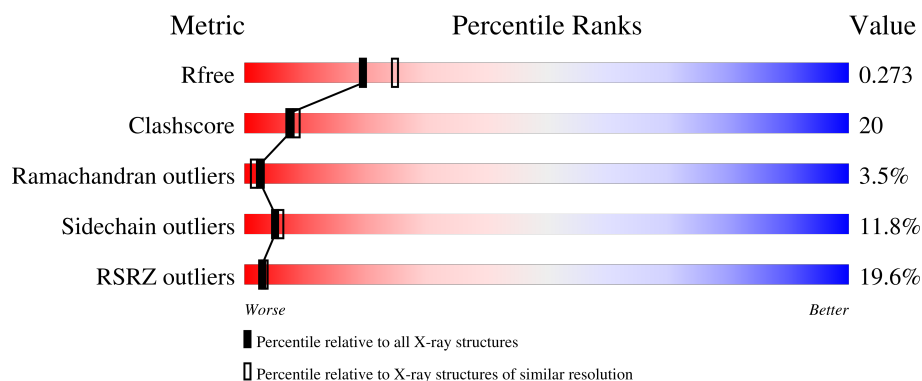
1 Overall quality at a glance

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 3357 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			

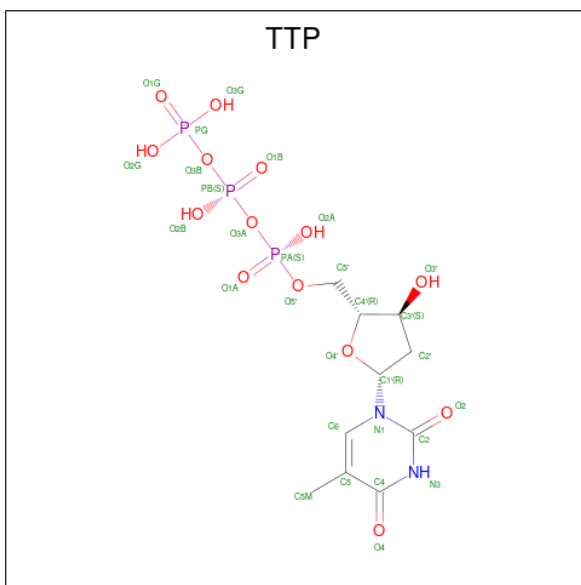
- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	373	Total	C	N	O	S	0	0	0
			2876	1809	504	542	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 THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



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

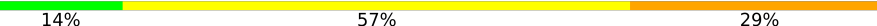
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	P	3	Total O 3 3	0	0
6	T	14	Total O 14 14	0	0
6	A	110	Total O 110 110	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.

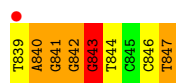
- Molecule 1: 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'

Chain P: 



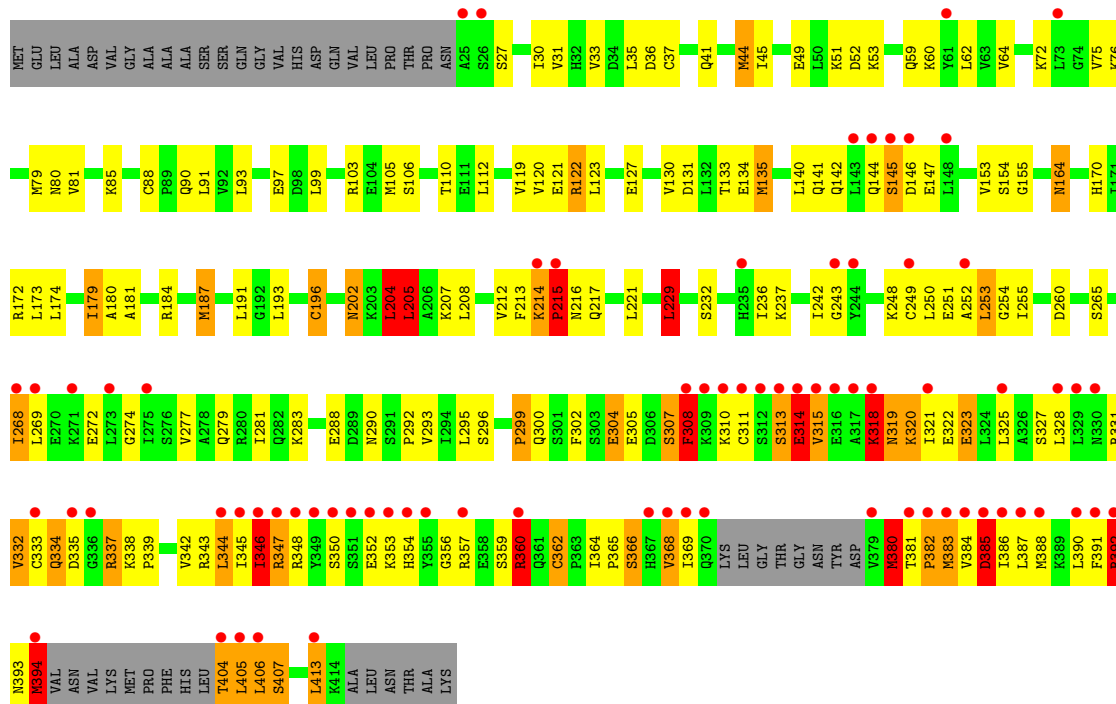
- Molecule 2: 5'-D(*TP*(EDA)P*GP*GP*GP*TP*CP*CP*T)-3'

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	98.06Å 98.06Å 203.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.76 – 2.30 36.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (36.76-2.30) 93.9 (36.76-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.14 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.238 , 0.277 0.232 , 0.273	Depositor DCC
R_{free} test set	2085 reflections (7.88%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.4	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	0.92	EDS
Total number of atoms	3357	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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, 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	1.40	1/136 (0.7%)	2.71	13/208 (6.2%)
2	T	1.79	4/178 (2.2%)	2.72	21/271 (7.7%)
3	A	2.01	68/2914 (2.3%)	1.57	35/3934 (0.9%)
All	All	1.98	73/3228 (2.3%)	1.73	69/4413 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	T	0	1
3	A	0	3
All	All	0	4

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	313	SER	CB-OG	19.76	1.81	1.42
3	A	319	ASN	C-O	14.94	1.41	1.24
3	A	214	LYS	CA-C	-13.98	1.35	1.52
3	A	318	LYS	CE-NZ	11.80	1.84	1.49
3	A	385	ASP	CG-OD1	9.36	1.43	1.25
3	A	394	MET	SD-CE	-9.32	1.56	1.79
3	A	64	VAL	CA-CB	9.11	1.66	1.54
3	A	242	ILE	CA-CB	8.92	1.64	1.53
3	A	207	LYS	CE-NZ	-8.59	1.23	1.49
3	A	103	ARG	CZ-NH2	8.17	1.44	1.33
3	A	385	ASP	C-O	7.71	1.33	1.24
3	A	75	VAL	CA-CB	7.36	1.63	1.54
3	A	122	ARG	CD-NE	-7.34	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	319	ASN	C-N	7.09	1.43	1.33
3	A	338	LYS	CA-CB	7.03	1.63	1.53
3	A	382	PRO	CA-C	6.86	1.61	1.52
3	A	179	ILE	CG1-CD1	-6.80	1.25	1.51
3	A	122	ARG	CG-CD	6.63	1.72	1.52
3	A	212	VAL	C-O	-6.58	1.16	1.24
3	A	290	ASN	CA-C	6.52	1.61	1.52
3	A	394	MET	CG-SD	6.40	1.96	1.80
3	A	216	ASN	N-CA	6.37	1.60	1.46
3	A	180	ALA	CA-C	-6.36	1.44	1.52
3	A	105	MET	CG-SD	6.26	1.96	1.80
3	A	187	MET	SD-CE	-6.20	1.64	1.79
3	A	313	SER	C-O	6.20	1.31	1.24
3	A	193	LEU	C-O	6.11	1.31	1.24
3	A	382	PRO	N-CD	6.06	1.56	1.47
3	A	45	ILE	C-O	-6.01	1.17	1.24
3	A	196	CYS	C-O	5.99	1.31	1.23
3	A	205	LEU	CA-C	5.99	1.60	1.52
3	A	121	GLU	CA-C	5.98	1.60	1.52
3	A	191	LEU	C-O	-5.96	1.16	1.24
3	A	392	ARG	C-O	5.94	1.31	1.24
3	A	260	ASP	N-CA	5.92	1.53	1.46
3	A	31	VAL	CA-C	5.89	1.59	1.52
2	T	843	DG	P-O5'	5.82	1.72	1.60
3	A	383	MET	C-O	5.77	1.31	1.24
3	A	313	SER	C-N	5.76	1.41	1.33
3	A	127	GLU	C-O	5.67	1.31	1.24
3	A	413	LEU	C-O	5.66	1.31	1.23
3	A	75	VAL	N-CA	5.65	1.53	1.46
3	A	319	ASN	CG-OD1	5.61	1.34	1.23
3	A	346	ILE	CA-CB	5.57	1.63	1.54
3	A	360	ARG	CA-C	-5.55	1.46	1.52
3	A	134	GLU	CA-C	-5.52	1.45	1.52
1	P	872	DC	P-OP2	-5.48	1.37	1.48
3	A	255	ILE	CA-CB	-5.47	1.47	1.53
3	A	321	ILE	CB-CG1	5.46	1.64	1.53
3	A	110	THR	C-O	-5.46	1.17	1.24
2	T	841	DG	P-O5'	5.45	1.71	1.60
3	A	214	LYS	CE-NZ	-5.44	1.33	1.49
3	A	232	SER	CA-C	5.40	1.60	1.52
3	A	119	VAL	CA-CB	5.37	1.59	1.53
3	A	164	ASN	CA-C	-5.33	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	174	LEU	CG-CD2	-5.28	1.35	1.52
3	A	64	VAL	C-O	-5.24	1.18	1.24
3	A	381	THR	CA-C	5.24	1.58	1.52
3	A	155	GLY	CA-C	5.22	1.58	1.52
2	T	843	DG	O4'-C1'	-5.18	1.31	1.41
3	A	207	LYS	CA-C	5.18	1.59	1.52
3	A	181	ALA	CA-CB	5.14	1.61	1.53
3	A	173	LEU	C-O	5.12	1.30	1.24
3	A	187	MET	CG-SD	5.12	1.93	1.80
3	A	362	CYS	CA-CB	5.10	1.61	1.54
3	A	133	THR	CA-C	5.09	1.59	1.52
3	A	292	PRO	CG-CD	5.08	1.68	1.50
3	A	44	MET	SD-CE	-5.08	1.66	1.79
3	A	315	VAL	C-O	5.07	1.30	1.24
3	A	296	SER	C-O	-5.04	1.18	1.24
3	A	93	LEU	C-O	-5.04	1.18	1.24
3	A	392	ARG	C-N	5.04	1.40	1.33
2	T	843	DG	O5'-C5'	-5.02	1.27	1.42

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	867	DA	O5'-C5'-C4'	19.82	140.53	110.80
2	T	842	DG	C4'-C3'-O3'	10.83	126.25	110.00
2	T	843	DG	N9-C1'-C2'	-9.99	98.52	113.50
2	T	839	DT	C5'-C4'-O4'	9.55	123.72	109.40
1	P	872	DC	C4'-C3'-O3'	9.49	124.24	110.00
2	T	842	DG	C2'-C3'-O3'	-8.66	98.51	111.50
2	T	839	DT	O5'-C5'-C4'	8.49	123.54	110.80
3	A	215	PRO	N-CD-CG	-8.49	90.47	103.20
2	T	844	DT	C5'-C4'-C3'	-8.22	102.56	114.90
2	T	843	DG	O4'-C1'-C2'	-8.11	94.24	106.40
1	P	872	DC	C2'-C3'-O3'	-7.97	99.54	111.50
3	A	215	PRO	CA-C-N	-7.88	110.51	123.04
3	A	215	PRO	C-N-CA	-7.88	110.51	123.04
3	A	302	PHE	N-CA-C	-7.64	95.58	108.26
3	A	407	SER	N-CA-C	7.60	120.72	109.24
3	A	268	ILE	CA-C-N	7.50	130.19	120.44
3	A	268	ILE	C-N-CA	7.50	130.19	120.44
2	T	843	DG	C4'-C3'-C2'	-7.48	91.17	102.40
3	A	320	LYS	N-CA-C	-7.44	102.33	111.33
3	A	215	PRO	O-C-N	-7.07	113.10	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	122	ARG	CG-CD-NE	-7.00	96.61	112.00
3	A	311	CYS	N-CA-C	6.92	120.98	112.54
2	T	847	DT	C4'-C3'-O3'	6.82	120.23	110.00
3	A	308	PHE	N-CA-C	-6.81	96.29	110.80
1	P	870	DA	O4'-C1'-N9	6.78	118.57	108.40
3	A	319	ASN	O-C-N	6.71	129.82	122.11
3	A	405	LEU	N-CA-C	6.64	119.31	108.55
3	A	385	ASP	N-CA-C	6.46	119.31	111.82
3	A	332	VAL	CB-CA-C	-6.46	103.42	112.14
2	T	844	DT	N1-C1'-C2'	-6.41	103.89	113.50
2	T	846	DC	O3'-P-O5'	-6.32	94.52	104.00
1	P	870	DA	O4'-C4'-C3'	6.17	114.66	105.40
1	P	869	DG	P-O3'-C3'	-6.05	111.12	120.20
3	A	141	GLN	N-CA-C	-6.02	105.89	113.18
3	A	252	ALA	N-CA-C	-5.95	104.61	112.34
3	A	274	GLY	N-CA-C	-5.90	104.27	112.18
2	T	842	DG	C5'-C4'-C3'	-5.84	106.13	114.90
3	A	229	LEU	N-CA-C	-5.81	104.87	111.14
2	T	843	DG	C3'-C2'-C1'	5.81	110.31	101.60
1	P	870	DA	C5'-C4'-O4'	-5.74	100.80	109.40
2	T	842	DG	O4'-C1'-C2'	-5.71	97.84	106.40
3	A	269	LEU	N-CA-C	5.68	117.15	111.07
3	A	253	LEU	N-CA-C	5.68	119.20	112.72
3	A	204	LEU	CB-CA-C	-5.68	101.73	110.81
3	A	366	SER	N-CA-C	5.65	117.44	111.28
2	T	842	DG	C5'-C4'-O4'	-5.64	100.93	109.40
3	A	323	GLU	CB-CA-C	-5.64	101.95	110.92
2	T	842	DG	C3'-C2'-C1'	5.63	110.04	101.60
2	T	842	DG	O4'-C1'-N9	-5.62	99.98	108.40
3	A	103	ARG	NH1-CZ-NH2	5.59	126.56	119.30
2	T	842	DG	N9-C1'-C2'	-5.48	105.28	113.50
3	A	214	LYS	CA-C-O	-5.42	112.73	120.16
1	P	872	DC	C3'-C2'-C1'	5.38	109.67	101.60
1	P	867	DA	C1'-O4'-C4'	5.36	117.73	109.70
2	T	843	DG	C4-N9-C1'	-5.35	118.98	127.00
2	T	843	DG	C4'-C3'-O3'	5.33	118.00	110.00
3	A	279	GLN	N-CA-C	-5.29	106.33	112.89
3	A	300	GLN	N-CA-C	-5.29	106.88	113.38
1	P	872	DC	N1-C1'-C2'	-5.26	105.61	113.50
3	A	299	PRO	CB-CA-C	-5.25	104.35	111.12
3	A	214	LYS	N-CA-CB	5.24	119.69	110.37
1	P	869	DG	O4'-C1'-N9	5.21	116.21	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	871	DC	C4'-C3'-O3'	5.16	117.74	110.00
3	A	232	SER	N-CA-C	-5.14	106.26	112.54
3	A	243	GLY	N-CA-C	5.14	119.62	112.57
2	T	843	DG	C8-N9-C1'	5.13	134.69	127.00
3	A	293	VAL	N-CA-C	-5.12	102.13	108.89
3	A	41	GLN	N-CA-CB	5.12	117.56	109.94
1	P	871	DC	C5'-C4'-O4'	-5.07	101.80	109.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	346	ILE	Peptide
3	A	380	MET	Peptide
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	1	1
2	T	184	0	104	10	1
3	A	2876	0	2899	125	0
4	A	2	0	0	0	0
5	A	29	0	13	1	0
6	A	110	0	0	4	0
6	P	3	0	0	0	0
6	T	14	0	0	1	0
All	All	3357	0	3095	129	1

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 20.

All (129) 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:318:LYS:CE	3:A:318:LYS:NZ	1.84	1.38
3:A:313:SER:CB	3:A:313:SER:OG	1.81	1.27
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.21	1.08
2:T:842:DG:H2''	2:T:843:DG:H5'	1.44	0.97
3:A:249:CYS:O	3:A:253:LEU:HD12	1.69	0.93
3:A:308:PHE:O	3:A:308:PHE:HD1	1.49	0.92
3:A:308:PHE:O	3:A:308:PHE:CD1	2.22	0.91
3:A:344:LEU:CD1	3:A:387:LEU:HD22	2.02	0.88
3:A:392:ARG:C	3:A:394:MET:H	1.83	0.85
3:A:76:LYS:HB2	3:A:79:MET:HE3	1.62	0.80
3:A:365:PRO:O	3:A:368:VAL:HG22	1.85	0.77
3:A:392:ARG:C	3:A:394:MET:N	2.40	0.75
3:A:331:ARG:HD2	6:A:1014:HOH:O	1.87	0.73
3:A:347:ARG:NH1	3:A:404:THR:OG1	2.21	0.73
3:A:319:ASN:O	3:A:322:GLU:N	2.22	0.72
3:A:391:PHE:O	3:A:394:MET:HB2	1.88	0.72
2:T:841:DG:OP2	3:A:307:SER:HB2	1.89	0.72
3:A:405:LEU:C	3:A:406:LEU:HD23	2.15	0.71
3:A:343:ARG:HD2	3:A:345:ILE:HD11	1.72	0.71
3:A:335:ASP:OD2	3:A:337:ARG:HD3	1.91	0.70
2:T:841:DG:H2''	2:T:842:DG:H5''	1.72	0.69
3:A:382:PRO:O	3:A:383:MET:C	2.35	0.69
3:A:325:LEU:HD23	3:A:380:MET:HE3	1.76	0.67
3:A:318:LYS:HB2	3:A:388:MET:CE	2.24	0.67
3:A:392:ARG:O	3:A:394:MET:N	2.28	0.67
3:A:283:LYS:HE3	3:A:288:GLU:OE1	1.96	0.66
3:A:386:ILE:O	3:A:390:LEU:HD12	1.96	0.65
3:A:164:ASN:H	3:A:170:HIS:HD2	1.42	0.65
3:A:344:LEU:HD11	3:A:387:LEU:CD2	2.12	0.65
3:A:332:VAL:CG1	3:A:339:PRO:HD3	2.26	0.65
3:A:44:MET:HE3	3:A:51:LYS:HA	1.78	0.64
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.79	0.64
3:A:394:MET:C	6:A:989:HOH:O	2.41	0.64
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.82	0.62
3:A:346:ILE:HG22	3:A:406:LEU:HD22	1.81	0.62
3:A:305:GLU:HG3	3:A:407:SER:HB3	1.81	0.61
3:A:335:ASP:CG	3:A:337:ARG:HH11	2.08	0.60
2:T:840:EDA:H5''	3:A:60:LYS:HB2	1.82	0.60
3:A:347:ARG:HD3	3:A:404:THR:OG1	2.01	0.60
3:A:196:CYS:SG	3:A:214:LYS:O	2.59	0.60
3:A:335:ASP:OD2	3:A:337:ARG:NH1	2.35	0.60
3:A:304:GLU:O	3:A:407:SER:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:388:MET:HE3	3:A:388:MET:HA	1.85	0.58
3:A:251:GLU:C	3:A:253:LEU:N	2.57	0.58
3:A:365:PRO:HB2	3:A:368:VAL:HG13	1.85	0.58
3:A:184:ARG:HA	3:A:187:MET:HE3	1.85	0.58
3:A:359:SER:O	3:A:360:ARG:HD3	2.05	0.57
3:A:237:LYS:O	3:A:237:LYS:HD3	2.04	0.57
3:A:318:LYS:HB2	3:A:388:MET:HE1	1.85	0.57
3:A:404:THR:HA	6:A:994:HOH:O	2.05	0.56
3:A:51:LYS:C	3:A:53:LYS:H	2.12	0.56
3:A:352:GLU:O	3:A:354:HIS:N	2.38	0.56
3:A:347:ARG:NH1	3:A:404:THR:HG1	2.04	0.56
3:A:318:LYS:O	3:A:319:ASN:C	2.50	0.55
3:A:202:ASN:HD22	3:A:202:ASN:C	2.15	0.54
3:A:380:MET:O	3:A:384:VAL:HG23	2.06	0.54
3:A:388:MET:O	3:A:391:PHE:HB3	2.08	0.54
3:A:308:PHE:HZ	3:A:406:LEU:HG	1.72	0.54
3:A:332:VAL:HG13	3:A:339:PRO:HD3	1.89	0.53
3:A:313:SER:O	3:A:314:GLU:OE2	2.26	0.53
3:A:36:ASP:OD1	3:A:215:PRO:O	2.28	0.52
3:A:347:ARG:HD3	3:A:404:THR:HG23	1.91	0.52
3:A:36:ASP:O	3:A:37:CYS:C	2.53	0.52
2:T:842:DG:H2''	2:T:843:DG:C5'	2.29	0.52
2:T:840:EDA:H8	3:A:59:GLN:OE1	2.10	0.52
3:A:406:LEU:HD23	3:A:406:LEU:N	2.24	0.52
2:T:841:DG:OP1	3:A:97:GLU:HG2	2.09	0.51
3:A:202:ASN:ND2	3:A:205:LEU:H	2.08	0.51
3:A:221:LEU:HD22	3:A:229:LEU:HD12	1.92	0.51
3:A:380:MET:HE2	3:A:384:VAL:HG22	1.94	0.50
3:A:214:LYS:HB2	3:A:215:PRO:HD3	1.93	0.50
3:A:343:ARG:HG2	3:A:344:LEU:N	2.26	0.50
3:A:304:GLU:HG2	3:A:328:LEU:HD21	1.94	0.50
3:A:332:VAL:HG11	3:A:339:PRO:HD3	1.94	0.50
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.42	0.49
2:T:842:DG:H4'	3:A:99:LEU:HD12	1.94	0.49
3:A:388:MET:CE	3:A:388:MET:HA	2.41	0.49
3:A:135:MET:HE2	3:A:179:ILE:HD12	1.94	0.49
3:A:388:MET:HE1	3:A:391:PHE:CD1	2.48	0.49
3:A:362:CYS:SG	3:A:390:LEU:HD11	2.53	0.48
3:A:59:GLN:O	3:A:60:LYS:HB2	2.13	0.48
3:A:112:LEU:C	3:A:112:LEU:HD23	2.39	0.48
2:T:840:EDA:C5'	3:A:60:LYS:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:88:CYS:SG	3:A:91:LEU:HB2	2.53	0.48
3:A:51:LYS:O	3:A:53:LYS:N	2.47	0.47
3:A:265:SER:OG	3:A:268:ILE:HG13	2.15	0.47
3:A:299:PRO:O	3:A:337:ARG:NH2	2.44	0.47
3:A:72:LYS:NZ	6:A:949:HOH:O	2.42	0.47
3:A:325:LEU:HD23	3:A:380:MET:CE	2.43	0.47
2:T:840:EDA:H5''	3:A:60:LYS:CB	2.44	0.47
3:A:319:ASN:O	3:A:322:GLU:CB	2.63	0.47
3:A:313:SER:OG	3:A:314:GLU:N	2.37	0.46
3:A:327:SER:O	3:A:328:LEU:C	2.57	0.46
3:A:335:ASP:CG	3:A:337:ARG:NH1	2.73	0.46
3:A:153:VAL:HG22	3:A:154:SER:N	2.31	0.46
3:A:106:SER:OG	3:A:122:ARG:NH2	2.44	0.46
3:A:347:ARG:O	3:A:404:THR:N	2.49	0.46
3:A:33:VAL:CG1	3:A:187:MET:HE1	2.46	0.45
3:A:76:LYS:HB2	3:A:79:MET:CE	2.39	0.45
3:A:320:LYS:O	3:A:323:GLU:HB2	2.17	0.45
3:A:346:ILE:HA	3:A:405:LEU:O	2.17	0.45
3:A:196:CYS:HA	3:A:217:GLN:O	2.17	0.45
3:A:364:ILE:HG22	3:A:369:ILE:HG13	1.99	0.44
3:A:204:LEU:HD13	3:A:205:LEU:HD13	2.00	0.44
3:A:164:ASN:H	3:A:170:HIS:CD2	2.28	0.44
3:A:204:LEU:HD22	3:A:208:LEU:CD1	2.47	0.44
3:A:388:MET:CE	3:A:391:PHE:CD1	3.01	0.44
3:A:345:ILE:HG12	3:A:359:SER:HB3	2.00	0.43
3:A:386:ILE:C	3:A:390:LEU:HD12	2.43	0.43
3:A:120:VAL:HG22	3:A:130:VAL:HG22	2.00	0.43
3:A:272:GLU:HG3	3:A:272:GLU:O	2.18	0.43
3:A:325:LEU:HD11	3:A:387:LEU:HD11	1.99	0.43
3:A:30:ILE:HD13	3:A:131:ASP:HA	2.00	0.43
3:A:251:GLU:O	3:A:254:GLY:N	2.42	0.43
3:A:49:GLU:O	3:A:53:LYS:HD2	2.19	0.42
3:A:33:VAL:HG11	3:A:187:MET:HE1	2.02	0.42
3:A:382:PRO:O	3:A:385:ASP:N	2.53	0.42
3:A:140:LEU:HA	3:A:140:LEU:HD23	1.73	0.42
3:A:236:ILE:HD13	3:A:236:ILE:HG21	1.65	0.42
3:A:364:ILE:HG23	3:A:368:VAL:CG2	2.50	0.42
3:A:251:GLU:C	3:A:253:LEU:H	2.26	0.41
3:A:268:ILE:O	3:A:272:GLU:HB2	2.20	0.41
1:P:873:DOC:C2'	5:A:875:TTP:HM52	2.51	0.41
3:A:144:GLN:O	3:A:146:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:144:GLN:HG3	3:A:147:GLU:HG2	2.01	0.41
6:T:957:HOH:O	3:A:122:ARG:HD3	2.21	0.40
3:A:318:LYS:HG2	3:A:319:ASN:N	2.36	0.40
3:A:277:VAL:O	3:A:281:ILE:HG12	2.21	0.40
3:A:248:LYS:HD3	3:A:248:LYS:HA	1.90	0.40

All (1) 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]	1.91	0.29

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	A	367/420 (87%)	329 (90%)	25 (7%)	13 (4%)	3 1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	308	PHE
3	A	314	GLU
3	A	315	VAL
3	A	333	CYS
3	A	353	LYS
3	A	52	ASP
3	A	215	PRO
3	A	334	GLN
3	A	337	ARG
3	A	350	SER
3	A	393	ASN

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Mol	Chain	Res	Type
3	A	145	SER
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%)	283 (88%)	38 (12%)	5 6

All (38) 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	80	ASN
3	A	81	VAL
3	A	85	LYS
3	A	90	GLN
3	A	123	LEU
3	A	135	MET
3	A	142	GLN
3	A	145	SER
3	A	172	ARG
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	229	LEU
3	A	295	LEU
3	A	304	GLU
3	A	307	SER
3	A	310	LYS
3	A	314	GLU
3	A	318	LYS
3	A	334	GLN
3	A	342	VAL

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Mol	Chain	Res	Type
3	A	344	LEU
3	A	347	ARG
3	A	348	ARG
3	A	357	ARG
3	A	360	ARG
3	A	366	SER
3	A	368	VAL
3	A	380	MET
3	A	385	ASP
3	A	392	ARG
3	A	394	MET
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	$\# Z > 2$
1	DOC	P	873	1,2	16,19,20	2.08	5 (31%)	20,26,29	2.00	5 (25%)
2	EDA	T	840	2	23,26,27	2.05	9 (39%)	29,38,41	2.41	11 (37%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	840	EDA	C2-N1	4.75	1.42	1.37
1	P	873	DOC	O4'-C4'	4.28	1.52	1.44
1	P	873	DOC	C2'-C1'	4.07	1.60	1.52
1	P	873	DOC	C3'-C2'	-3.91	1.43	1.54
2	T	840	EDA	C5-N7	-3.84	1.31	1.39
2	T	840	EDA	O5'-C5'	-3.31	1.34	1.44
2	T	840	EDA	C5-C6	-2.97	1.35	1.44
2	T	840	EDA	C4-N9	-2.80	1.30	1.38
1	P	873	DOC	O4'-C1'	-2.64	1.36	1.42
2	T	840	EDA	C2'-C1'	2.59	1.59	1.52
1	P	873	DOC	C1'-N1	2.36	1.54	1.48
2	T	840	EDA	C10-N1	-2.34	1.34	1.38
2	T	840	EDA	C8-N9	-2.24	1.32	1.37
2	T	840	EDA	C11-N6	-2.13	1.34	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	873	DOC	C4'-O4'-C1'	-6.15	104.01	109.81
2	T	840	EDA	O4'-C1'-N9	-5.65	97.83	107.86
2	T	840	EDA	N1-C6-N6	-4.65	107.83	111.19
2	T	840	EDA	C10-N1-C2	4.59	135.29	129.82
2	T	840	EDA	C11-N6-C6	4.07	109.11	105.08
2	T	840	EDA	C2-N3-C4	3.84	120.07	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	873	DOC	O4'-C4'-C3'	3.74	110.96	104.81
2	T	840	EDA	C4'-O4'-C1'	-3.15	102.02	109.51
2	T	840	EDA	C2'-C1'-N9	3.14	121.66	113.81
2	T	840	EDA	O4'-C4'-C3'	2.92	112.32	105.65
2	T	840	EDA	C11-C10-N1	2.77	108.50	105.78
2	T	840	EDA	N1-C2-N3	-2.71	120.02	124.61
1	P	873	DOC	O4'-C4'-C5'	2.66	114.14	109.34
2	T	840	EDA	C5-C4-N3	-2.46	123.65	127.27
1	P	873	DOC	O4'-C1'-N1	-2.25	103.87	107.86
1	P	873	DOC	C2'-C1'-N1	-2.12	108.39	112.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	873	DOC	1	0
2	T	840	EDA	4	0

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	TTP	A	875	4	29,30,30	1.67	7 (24%)	43,47,47	2.23	12 (27%)

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	A	875	4	-	3/22/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	TTP	C4-C5	-3.90	1.38	1.44
5	A	875	TTP	O4'-C1'	3.65	1.50	1.42
5	A	875	TTP	C6-C5	3.40	1.40	1.34
5	A	875	TTP	PA-O1A	-2.70	1.41	1.50
5	A	875	TTP	C1'-N1	-2.67	1.41	1.48
5	A	875	TTP	C2'-C3'	-2.53	1.46	1.52
5	A	875	TTP	C5'-C4'	-2.15	1.45	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	875	TTP	N3-C2-N1	5.86	122.52	114.89
5	A	875	TTP	C4-N3-C2	-5.17	120.56	127.34
5	A	875	TTP	C6-N1-C2	-5.14	116.19	121.30
5	A	875	TTP	O2-C2-N1	-4.62	116.78	122.80
5	A	875	TTP	O2B-PB-O3A	4.01	118.12	107.27
5	A	875	TTP	C1'-N1-C6	3.72	126.99	120.74
5	A	875	TTP	C5-C4-N3	3.60	118.45	115.32
5	A	875	TTP	O2A-PA-O3A	-2.94	99.33	107.27
5	A	875	TTP	C2'-C3'-C4'	2.64	108.15	102.80
5	A	875	TTP	O3A-PB-O1B	-2.53	103.09	110.70
5	A	875	TTP	O4-C4-C5	-2.43	122.14	124.92
5	A	875	TTP	O3G-PG-O2G	2.37	116.71	107.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

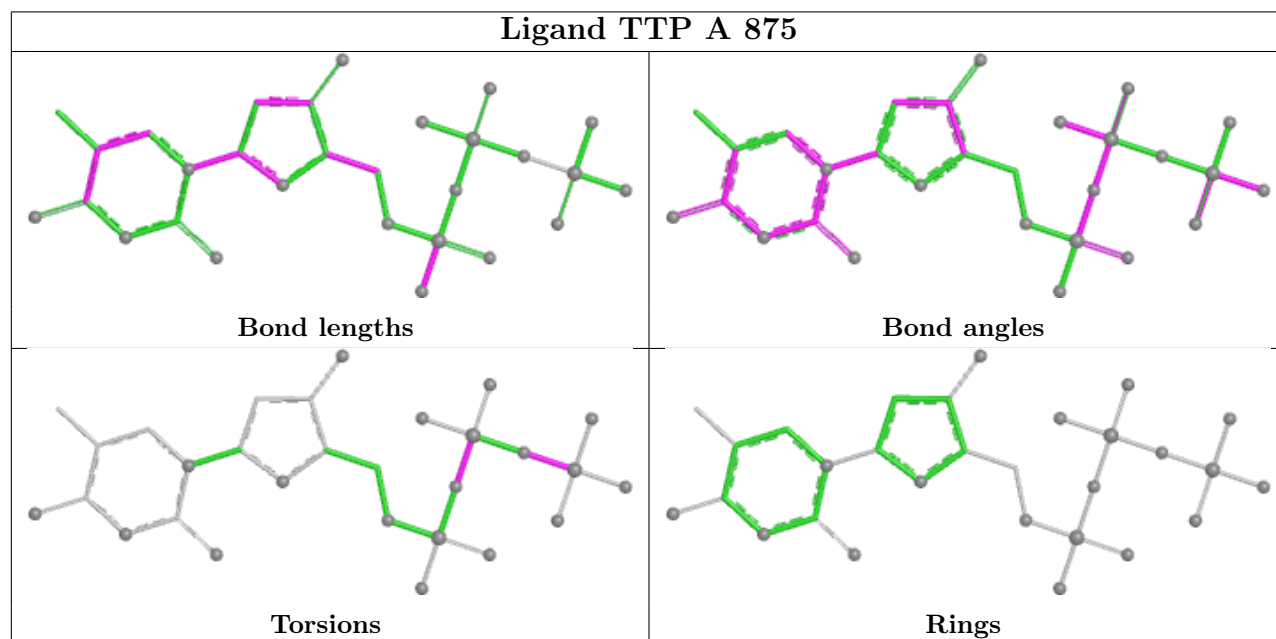
Mol	Chain	Res	Type	Atoms
5	A	875	TTP	PB-O3B-PG-O2G
5	A	875	TTP	PA-O3A-PB-O2B
5	A	875	TTP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	875	TTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	T	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	839:DT	O3'	840:EDA	P	1.35
1	T	840:EDA	O3'	841:DG	P	1.35

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%)	0.01	0 100 100	26, 31, 37, 39	0
2	T	8/9 (88%)	0.14	1 (12%) 8 9	20, 22, 25, 88	0
3	A	373/420 (88%)	0.83	75 (20%) 3 3	8, 37, 79, 97	0
All	All	387/436 (88%)	0.81	76 (19%) 3 3	8, 36, 79, 97	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	25	ALA	8.6
3	A	354	HIS	7.3
3	A	349	TYR	7.1
3	A	353	LYS	5.9
3	A	379	VAL	5.5
3	A	312	SER	5.4
3	A	317	ALA	5.4
3	A	350	SER	5.0
3	A	382	PRO	4.6
3	A	355	TYR	4.6
3	A	249	CYS	4.5
3	A	313	SER	4.4
3	A	315	VAL	4.4
2	T	839	DT	4.3
3	A	336	GLY	4.1
3	A	381	THR	4.0
3	A	351	SER	4.0
3	A	73	LEU	3.9
3	A	309	LYS	3.9
3	A	214	LYS	3.8
3	A	310	LYS	3.7
3	A	385	ASP	3.6
3	A	244	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
3	A	269	LEU	3.5
3	A	311	CYS	3.5
3	A	394	MET	3.5
3	A	357	ARG	3.5
3	A	335	ASP	3.3
3	A	369	ILE	3.3
3	A	348	ARG	3.2
3	A	243	GLY	3.1
3	A	344	LEU	3.1
3	A	275	ILE	3.1
3	A	333	CYS	3.1
3	A	368	VAL	3.1
3	A	360	ARG	3.0
3	A	383	MET	3.0
3	A	405	LEU	3.0
3	A	235	HIS	3.0
3	A	316	GLU	3.0
3	A	370	GLN	2.9
3	A	387	LEU	2.9
3	A	406	LEU	2.9
3	A	404	THR	2.9
3	A	145	SER	2.8
3	A	330	ASN	2.8
3	A	314	GLU	2.8
3	A	329	LEU	2.7
3	A	386	ILE	2.7
3	A	391	PHE	2.7
3	A	146	ASP	2.6
3	A	268	ILE	2.6
3	A	143	LEU	2.6
3	A	308	PHE	2.6
3	A	273	LEU	2.6
3	A	215	PRO	2.6
3	A	61	TYR	2.5
3	A	367	HIS	2.5
3	A	347	ARG	2.4
3	A	26	SER	2.4
3	A	148	LEU	2.4
3	A	328	LEU	2.4
3	A	318	LYS	2.3
3	A	384	VAL	2.3
3	A	346	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	144	GLN	2.2
3	A	390	LEU	2.2
3	A	271	LYS	2.2
3	A	252	ALA	2.2
3	A	345	ILE	2.2
3	A	352	GLU	2.2
3	A	325	LEU	2.1
3	A	392	ARG	2.1
3	A	321	ILE	2.1
3	A	388	MET	2.1
3	A	413	LEU	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	EDA	T	840	23/24	0.90	0.12	24,38,61,65	0
1	DOC	P	873	18/19	0.97	0.08	15,18,27,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

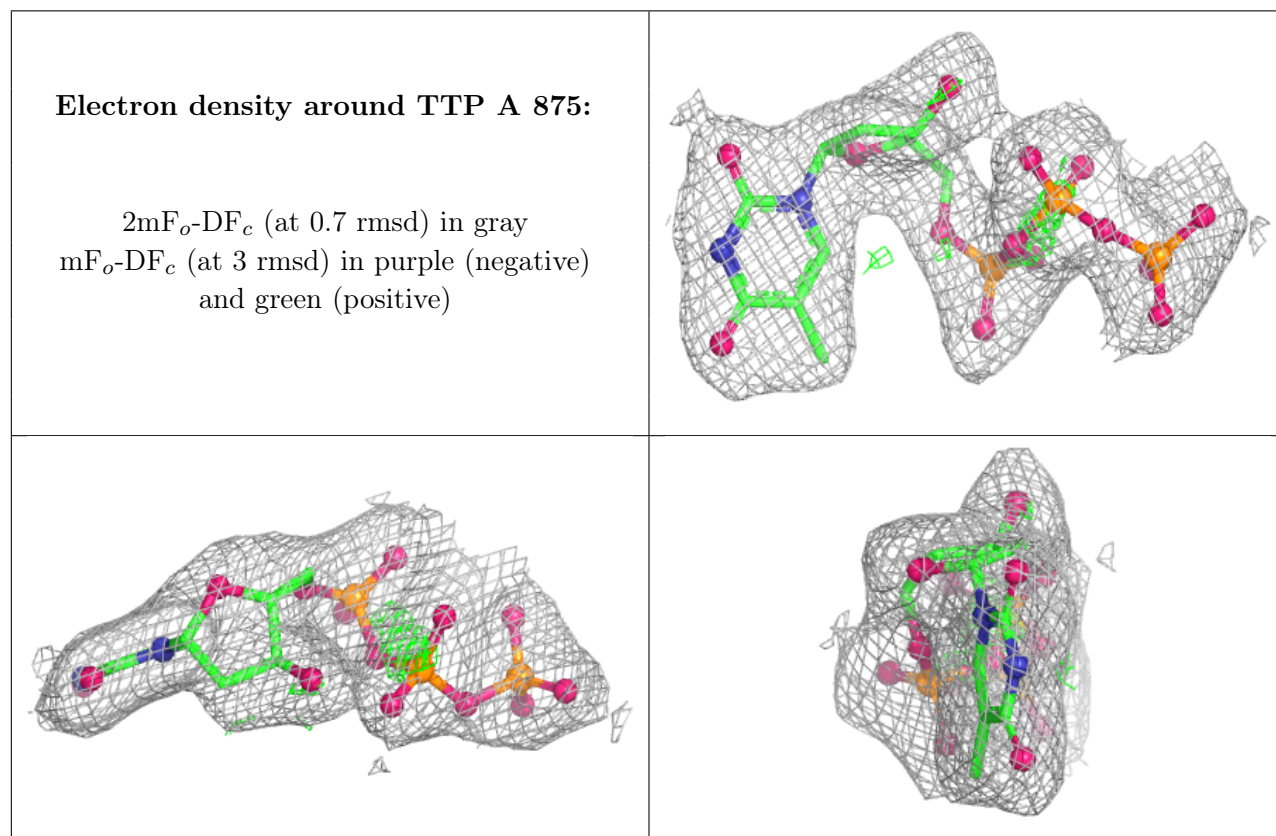
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
4	MG	A	872	1/1	0.79	0.31	78,78,78,78	0
4	MG	A	871	1/1	0.96	0.04	18,18,18,18	0
5	TTP	A	875	29/29	0.96	0.08	13,18,22,24	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.