



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 10:14 AM EDT

PDB ID : 2ALZ
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 : 2005-08-08
Resolution : 2.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

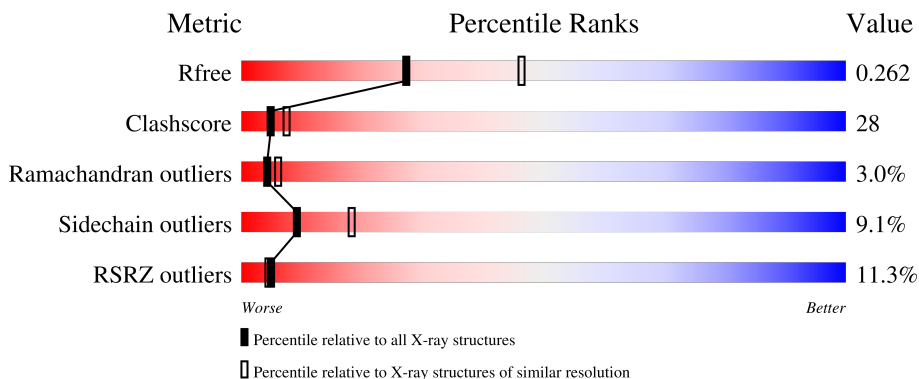
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	T	9	
2	P	7	
3	A	390	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3305 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(*TP*GP*GP*GP*GP*TP*CP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	9	183	88	32	55	8	0	0	0

- Molecule 2 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'.

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

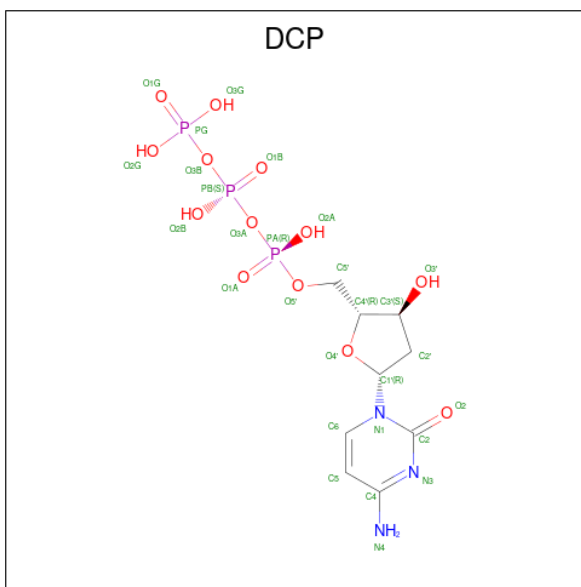
- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	373	2874	1808	504	541	21	0	0	0

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

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

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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

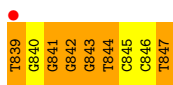
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	5	Total	O	0	0
			5	5		
6	P	4	Total	O	0	0
			4	4		
6	A	70	Total	O	0	0
			70	70		

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.

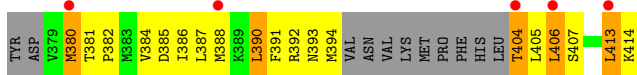
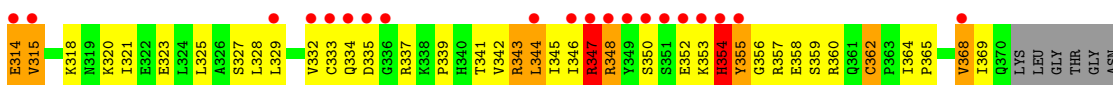
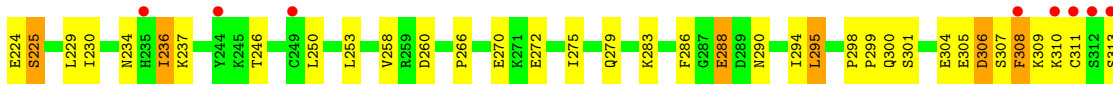
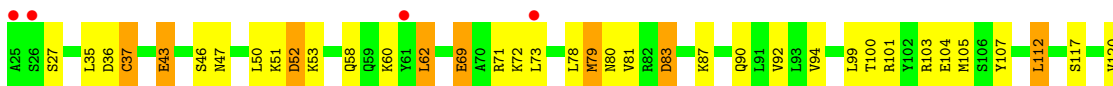
- Molecule 1: 5'-D(*TP*GP*GP*GP*GP*TP*CP*CP*T)-3'



- Molecule 2: 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'



- Molecule 3: DNA polymerase iota



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.11Å 98.11Å 202.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 39.18 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.50) 98.1 (39.18-2.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.78 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.228 , 0.272 0.228 , 0.262	Depositor DCC
R_{free} test set	2163 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtrriage
Anisotropy	0.202	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3305	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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: DCP, DOC, MG

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	T	3.93	38/204 (18.6%)	5.18	73/314 (23.2%)
2	P	3.26	18/136 (13.2%)	4.43	42/208 (20.2%)
3	A	1.67	30/2912 (1.0%)	1.36	26/3930 (0.7%)
All	All	1.98	86/3252 (2.6%)	2.11	141/4452 (3.2%)

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	P	0	1
3	A	0	2
All	All	0	3

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	844	DT	C5-C7	17.34	1.60	1.50
1	T	847	DT	C5-C7	14.51	1.58	1.50
2	P	872	DC	C3'-O3'	-10.51	1.30	1.44
1	T	847	DT	C3'-O3'	10.45	1.57	1.44
1	T	844	DT	C5-C6	9.72	1.41	1.34
1	T	845	DC	N1-C6	-9.69	1.31	1.37
3	A	214	LYS	CA-C	-9.54	1.28	1.52
2	P	872	DC	C4'-O4'	9.39	1.54	1.45
1	T	843	DG	N7-C5	-9.28	1.33	1.39
2	P	870	DA	O3'-P	9.21	1.72	1.61
2	P	871	DC	C3'-O3'	-8.97	1.32	1.44
3	A	103	ARG	CZ-NH2	8.71	1.44	1.33
3	A	127	GLU	CD-OE1	8.69	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	844	DT	C3'-O3'	-8.52	1.32	1.44
1	T	842	DG	C3'-O3'	-8.24	1.33	1.44
1	T	843	DG	O4'-C1'	-8.16	1.32	1.42
3	A	117	SER	CB-OG	7.89	1.52	1.42
1	T	843	DG	P-O5'	7.79	1.67	1.59
3	A	184	ARG	CD-NE	-7.79	1.33	1.46
3	A	105	MET	CG-SD	7.69	2.01	1.81
1	T	843	DG	C2'-C1'	7.64	1.59	1.52
2	P	871	DC	O4'-C1'	-7.40	1.33	1.42
3	A	122	ARG	CG-CD	7.40	1.70	1.51
1	T	844	DT	C4-C5	7.32	1.51	1.45
1	T	844	DT	C2'-C1'	7.23	1.59	1.52
1	T	845	DC	P-O5'	7.15	1.67	1.59
2	P	870	DA	C2'-C1'	6.96	1.59	1.52
3	A	216	ASN	N-CA	6.96	1.60	1.46
3	A	355	TYR	N-CA	6.91	1.60	1.46
1	T	844	DT	C1'-N1	6.89	1.58	1.49
1	T	839	DT	C3'-O3'	6.85	1.52	1.44
3	A	46	SER	CB-OG	-6.73	1.33	1.42
2	P	870	DA	N9-C8	-6.67	1.32	1.37
3	A	134	GLU	CD-OE1	6.61	1.32	1.25
3	A	151	VAL	CA-CB	-6.48	1.41	1.54
3	A	258	VAL	CB-CG2	-6.47	1.39	1.52
3	A	122	ARG	CD-NE	-6.47	1.35	1.46
1	T	841	DG	C5-C4	-6.41	1.33	1.38
1	T	846	DC	C4-N4	6.26	1.39	1.33
1	T	845	DC	N3-C4	-6.18	1.29	1.33
2	P	871	DC	C4-N4	-6.17	1.28	1.33
1	T	842	DG	C2-N2	6.12	1.40	1.34
1	T	844	DT	N1-C2	-6.05	1.33	1.38
3	A	185	GLU	CG-CD	6.05	1.61	1.51
1	T	842	DG	N7-C5	-6.03	1.35	1.39
2	P	870	DA	P-O5'	6.03	1.65	1.59
2	P	867	DA	C5-C4	-6.01	1.34	1.38
1	T	840	DG	C6-N1	-5.99	1.35	1.39
2	P	869	DG	N7-C5	5.99	1.42	1.39
1	T	840	DG	N7-C5	-5.96	1.35	1.39
3	A	92	VAL	CB-CG2	5.93	1.65	1.52
3	A	225	SER	CB-OG	5.93	1.50	1.42
3	A	134	GLU	CG-CD	5.91	1.60	1.51
3	A	286	PHE	CE2-CZ	5.89	1.48	1.37
1	T	841	DG	C6-N1	5.87	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	839	DT	C5'-C4'	5.84	1.57	1.51
3	A	213	PHE	CD2-CE2	5.77	1.50	1.39
1	T	845	DC	C4-N4	5.73	1.39	1.33
1	T	841	DG	P-OP1	-5.72	1.39	1.49
2	P	868	DG	C2-N3	-5.71	1.28	1.32
3	A	94	VAL	CB-CG1	-5.70	1.40	1.52
1	T	843	DG	P-OP2	-5.64	1.39	1.49
1	T	843	DG	C8-N7	-5.64	1.27	1.30
2	P	872	DC	P-O5'	5.64	1.65	1.59
3	A	134	GLU	CD-OE2	5.63	1.31	1.25
2	P	870	DA	C6-N1	-5.63	1.31	1.35
1	T	844	DT	N1-C6	5.61	1.42	1.38
3	A	104	GLU	CG-CD	5.56	1.60	1.51
3	A	43	GLU	CD-OE1	5.55	1.31	1.25
1	T	846	DC	N1-C6	-5.52	1.33	1.37
2	P	870	DA	C8-N7	-5.50	1.27	1.31
3	A	286	PHE	CD1-CE1	5.49	1.50	1.39
2	P	869	DG	C6-N1	5.42	1.43	1.39
1	T	847	DT	C2'-C1'	5.38	1.57	1.52
3	A	288	GLU	CG-CD	5.38	1.60	1.51
1	T	844	DT	O3'-P	5.37	1.67	1.61
3	A	189	ASN	CB-CG	5.31	1.63	1.51
2	P	872	DC	C2-O2	-5.24	1.19	1.24
3	A	212	VAL	C-O	-5.23	1.13	1.23
2	P	872	DC	P-OP2	-5.17	1.40	1.49
1	T	843	DG	O3'-P	5.16	1.67	1.61
3	A	288	GLU	CD-OE2	5.12	1.31	1.25
1	T	842	DG	C6-O6	-5.12	1.19	1.24
1	T	843	DG	O5'-C5'	-5.10	1.29	1.42
1	T	842	DG	C2-N3	5.08	1.36	1.32
3	A	234	ASN	CB-CG	5.06	1.62	1.51

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	842	DG	O4'-C1'-N9	-21.18	93.17	108.00
1	T	844	DT	C4-C5-C6	-19.87	106.08	118.00
1	T	844	DT	N3-C4-O4	-17.65	109.31	119.90
1	T	844	DT	C4-C5-C7	17.38	129.43	119.00
1	T	840	DG	N1-C6-O6	-16.47	110.02	119.90
1	T	843	DG	O4'-C4'-C3'	16.26	115.76	106.00
1	T	846	DC	O4'-C1'-N1	-16.25	96.62	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	872	DC	O4'-C4'-C3'	16.17	115.70	106.00
1	T	840	DG	C5-C6-O6	15.56	137.94	128.60
1	T	843	DG	C4'-C3'-C2'	-15.11	89.50	103.10
2	P	867	DA	O4'-C1'-N9	15.01	118.51	108.00
2	P	867	DA	O4'-C4'-C3'	-14.31	97.42	106.00
2	P	868	DG	N1-C6-O6	14.10	128.36	119.90
1	T	843	DG	O4'-C1'-N9	-14.04	98.17	108.00
1	T	844	DT	C5-C6-N1	13.40	131.74	123.70
3	A	355	TYR	N-CA-CB	13.14	134.25	110.60
3	A	122	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	T	842	DG	C4-C5-N7	-12.74	105.70	110.80
2	P	870	DA	N1-C2-N3	12.60	135.60	129.30
1	T	843	DG	O4'-C1'-C2'	-12.54	95.87	105.90
1	T	844	DT	N3-C4-C5	12.27	122.56	115.20
2	P	869	DG	O4'-C1'-N9	12.04	116.43	108.00
1	T	846	DC	N3-C4-C5	-11.91	117.13	121.90
1	T	845	DC	N3-C4-C5	-11.68	117.23	121.90
2	P	868	DG	C5-C6-O6	-11.68	121.59	128.60
1	T	841	DG	C5-C6-N1	11.64	117.32	111.50
2	P	870	DA	C2-N3-C4	-11.61	104.80	110.60
1	T	842	DG	N9-C4-C5	11.40	109.96	105.40
1	T	839	DT	O4'-C4'-C3'	-10.81	99.51	106.00
1	T	841	DG	C6-N1-C2	-10.79	118.63	125.10
1	T	841	DG	C2-N3-C4	10.09	116.94	111.90
2	P	870	DA	O4'-C4'-C3'	10.02	112.01	106.00
1	T	840	DG	C8-N9-C4	-9.97	102.41	106.40
3	A	172	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	T	839	DT	P-O3'-C3'	9.54	131.15	119.70
2	P	872	DC	C1'-O4'-C4'	-9.33	100.77	110.10
2	P	869	DG	O4'-C4'-C3'	-9.30	100.42	106.00
2	P	870	DA	O5'-P-OP2	-9.27	97.36	105.70
1	T	842	DG	C3'-C2'-C1'	9.25	113.60	102.50
2	P	869	DG	C2-N3-C4	9.25	116.52	111.90
2	P	871	DC	O4'-C1'-N1	9.18	114.42	108.00
1	T	842	DG	O4'-C1'-C2'	-9.17	98.56	105.90
1	T	844	DT	C6-N1-C2	-9.04	116.78	121.30
1	T	843	DG	C5-N7-C8	8.98	108.79	104.30
2	P	868	DG	N3-C2-N2	-8.96	113.63	119.90
2	P	869	DG	P-O3'-C3'	-8.92	109.00	119.70
1	T	843	DG	C1'-O4'-C4'	-8.79	101.31	110.10
2	P	867	DA	O5'-C5'-C4'	8.58	132.44	111.00
1	T	843	DG	C4-C5-N7	-8.54	107.38	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	847	DT	N3-C4-C5	8.52	120.31	115.20
1	T	847	DT	C4-C5-C6	-8.50	112.90	118.00
1	T	842	DG	C5-N7-C8	8.47	108.53	104.30
3	A	103	ARG	NE-CZ-NH1	-8.46	116.07	120.30
2	P	870	DA	C6-N1-C2	-8.41	113.55	118.60
2	P	868	DG	N1-C2-N2	8.36	123.72	116.20
1	T	846	DC	C2-N3-C4	8.27	124.03	119.90
1	T	842	DG	O4'-C4'-C3'	8.10	110.86	106.00
1	T	845	DC	C5-C4-N4	8.05	125.84	120.20
1	T	845	DC	C4-C5-C6	7.97	121.38	117.40
1	T	842	DG	C4'-C3'-C2'	-7.96	95.94	103.10
2	P	867	DA	C5-C6-N6	-7.86	117.41	123.70
2	P	870	DA	O4'-C1'-C2'	7.84	112.17	105.90
1	T	843	DG	C8-N9-C4	-7.84	103.27	106.40
1	T	842	DG	C6-C5-N7	7.82	135.09	130.40
2	P	871	DC	OP1-P-OP2	-7.79	107.91	119.60
2	P	871	DC	O4'-C4'-C3'	7.79	110.67	106.00
3	A	184	ARG	NE-CZ-NH2	-7.78	116.41	120.30
3	A	215	PRO	N-CD-CG	-7.71	91.63	103.20
1	T	847	DT	N3-C4-O4	-7.59	115.34	119.90
2	P	867	DA	C1'-O4'-C4'	7.55	117.65	110.10
3	A	135	MET	CG-SD-CE	-7.47	88.25	100.20
1	T	842	DG	C4'-C3'-O3'	7.45	128.33	109.70
1	T	842	DG	C6-N1-C2	-7.42	120.65	125.10
2	P	872	DC	C4'-C3'-C2'	-7.39	96.45	103.10
1	T	843	DG	N9-C4-C5	7.32	108.33	105.40
2	P	870	DA	O4'-C1'-N9	7.25	113.08	108.00
1	T	847	DT	C2-N3-C4	-7.13	122.92	127.20
1	T	842	DG	C5-C6-N1	7.06	115.03	111.50
1	T	842	DG	C8-N9-C4	-6.96	103.62	106.40
1	T	844	DT	N1-C2-N3	6.81	118.69	114.60
1	T	840	DG	O5'-P-OP2	-6.79	99.59	105.70
1	T	844	DT	O4'-C1'-N1	-6.67	103.33	108.00
1	T	840	DG	N7-C8-N9	6.52	116.36	113.10
3	A	343	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	T	847	DT	C4'-C3'-C2'	-6.44	97.30	103.10
1	T	842	DG	N1-C6-O6	-6.40	116.06	119.90
1	T	847	DT	O4'-C4'-C3'	6.36	109.82	106.00
1	T	839	DT	C5'-C4'-C3'	6.35	125.53	114.10
1	T	843	DG	N1-C6-O6	-6.30	116.12	119.90
1	T	841	DG	N3-C2-N2	6.21	124.24	119.90
1	T	840	DG	N9-C4-C5	6.20	107.88	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	872	DC	C3'-C2'-C1'	6.20	109.93	102.50
2	P	869	DG	N3-C4-C5	-6.17	125.52	128.60
2	P	867	DA	N1-C6-N6	6.16	122.30	118.60
1	T	844	DT	C5'-C4'-C3'	-6.10	103.12	114.10
3	A	315	VAL	N-CA-CB	-6.04	98.22	111.50
3	A	71	ARG	NE-CZ-NH1	6.01	123.31	120.30
3	A	205	LEU	CB-CG-CD1	5.97	121.16	111.00
1	T	841	DG	C8-N9-C4	-5.92	104.03	106.40
2	P	870	DA	C5'-C4'-O4'	-5.88	98.12	109.30
1	T	845	DC	O4'-C1'-N1	-5.86	103.90	108.00
3	A	83	ASP	CB-CG-OD2	5.82	123.54	118.30
2	P	870	DA	N9-C4-C5	-5.82	103.47	105.80
3	A	122	ARG	CD-NE-CZ	5.81	131.73	123.60
2	P	868	DG	C5-N7-C8	-5.80	101.40	104.30
2	P	870	DA	C8-N9-C4	5.79	108.12	105.80
2	P	872	DC	C4'-C3'-O3'	5.78	124.15	109.70
3	A	214	LYS	N-CA-CB	5.78	121.00	110.60
3	A	343	ARG	NE-CZ-NH1	5.71	123.16	120.30
3	A	306	ASP	CB-CG-OD1	5.69	123.42	118.30
1	T	841	DG	C5-C6-O6	-5.69	125.19	128.60
2	P	867	DA	O4'-C1'-C2'	-5.68	101.36	105.90
1	T	847	DT	N3-C2-O2	-5.67	118.90	122.30
3	A	167	ASP	CB-CG-OD2	5.67	123.40	118.30
2	P	869	DG	C6-N1-C2	-5.65	121.71	125.10
3	A	52	ASP	CB-CG-OD2	5.61	123.34	118.30
1	T	844	DT	OP1-P-OP2	-5.58	111.22	119.60
3	A	172	ARG	NE-CZ-NH2	5.55	123.07	120.30
3	A	260	ASP	CB-CG-OD1	5.54	123.29	118.30
2	P	870	DA	OP1-P-O3'	5.54	117.38	105.20
3	A	122	ARG	CG-CD-NE	-5.53	100.20	111.80
1	T	839	DT	N1-C1'-C2'	5.42	122.89	112.60
2	P	870	DA	OP2-P-O3'	5.41	117.11	105.20
3	A	295	LEU	CB-CG-CD2	5.37	120.13	111.00
3	A	204	LEU	CA-CB-CG	5.35	127.61	115.30
1	T	842	DG	C2'-C3'-O3'	-5.34	94.98	112.60
1	T	843	DG	C2-N3-C4	5.34	114.57	111.90
1	T	844	DT	C2-N3-C4	-5.28	124.03	127.20
2	P	872	DC	O4'-C1'-N1	-5.27	104.31	108.00
2	P	872	DC	C5'-C4'-C3'	-5.25	104.65	114.10
1	T	845	DC	N3-C2-O2	-5.24	118.23	121.90
1	T	840	DG	O3'-P-O5'	5.18	113.85	104.00
3	A	246	THR	OG1-CB-CG2	-5.16	98.13	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	841	DG	O4'-C1'-C2'	5.16	110.03	105.90
1	T	839	DT	N3-C4-O4	5.08	122.95	119.90
2	P	867	DA	C5-C6-N1	5.07	120.23	117.70
2	P	872	DC	O5'-P-OP1	-5.07	101.14	105.70
3	A	139	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	T	843	DG	N3-C4-C5	-5.05	126.08	128.60
3	A	215	PRO	C-N-CA	-5.02	109.15	121.70
1	T	844	DT	O4'-C1'-C2'	-5.00	101.90	105.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	354	HIS	Peptide
2	P	871	DC	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	T	183	0	104	9	1
2	P	139	0	77	3	1
3	A	2874	0	2897	166	0
4	A	2	0	0	0	0
5	A	28	0	12	0	0
6	A	70	0	0	6	0
6	P	4	0	0	0	0
6	T	5	0	0	0	0
All	All	3305	0	3090	175	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 28.

All (175) 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:365:PRO:O	3:A:368:VAL:HG22	1.46	1.14
3:A:347:ARG:CD	3:A:404:THR:HG23	1.81	1.11
3:A:347:ARG:HD3	3:A:404:THR:HG23	1.12	1.09
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.10	1.07
1:T:841:DG:H2''	1:T:842:DG:H5''	1.32	1.05
3:A:347:ARG:HD3	3:A:404:THR:CG2	1.86	1.04
3:A:365:PRO:HB2	3:A:368:VAL:HG13	1.44	0.99
3:A:391:PHE:O	3:A:394:MET:HB2	1.63	0.98
3:A:365:PRO:HB2	3:A:368:VAL:CG1	1.96	0.95
3:A:308:PHE:HD2	3:A:320:LYS:HZ2	1.01	0.94
3:A:344:LEU:HD11	3:A:387:LEU:CD2	1.97	0.94
3:A:308:PHE:O	3:A:308:PHE:HD1	1.52	0.91
3:A:388:MET:O	3:A:391:PHE:HB3	1.72	0.90
3:A:137:GLU:HG2	3:A:172:ARG:HH12	1.38	0.88
1:T:842:DG:H2''	1:T:843:DG:H5'	1.57	0.86
3:A:384:VAL:O	3:A:388:MET:HG2	1.77	0.84
3:A:308:PHE:HD2	3:A:320:LYS:NZ	1.73	0.84
3:A:364:ILE:HG22	3:A:369:ILE:HG13	1.60	0.83
3:A:335:ASP:OD2	3:A:337:ARG:HD3	1.79	0.82
3:A:335:ASP:OD2	3:A:337:ARG:NH1	2.12	0.81
3:A:90:GLN:N	3:A:90:GLN:OE1	2.12	0.81
3:A:308:PHE:O	3:A:308:PHE:CD1	2.34	0.81
3:A:347:ARG:CG	3:A:404:THR:HG23	2.14	0.77
3:A:196:CYS:SG	3:A:214:LYS:O	2.43	0.76
3:A:344:LEU:CD1	3:A:387:LEU:HD22	2.05	0.76
3:A:308:PHE:CD2	3:A:320:LYS:NZ	2.48	0.75
3:A:325:LEU:HD11	3:A:387:LEU:CD1	2.17	0.74
3:A:283:LYS:HE3	3:A:288:GLU:OE1	1.88	0.74
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.67	0.74
3:A:344:LEU:HD21	3:A:387:LEU:HD13	1.71	0.72
3:A:325:LEU:HD11	3:A:387:LEU:HD11	1.71	0.72
3:A:202:ASN:HD22	3:A:202:ASN:C	1.93	0.72
3:A:405:LEU:C	3:A:406:LEU:HD23	2.10	0.72
3:A:309:LYS:HD3	3:A:404:THR:OG1	1.91	0.70
3:A:347:ARG:NH1	3:A:404:THR:OG1	2.23	0.70
3:A:347:ARG:HG2	3:A:404:THR:CG2	2.22	0.70
3:A:337:ARG:NH2	3:A:413:LEU:HG	2.07	0.70
3:A:347:ARG:HG2	3:A:404:THR:HG23	1.76	0.68
1:T:841:DG:H2''	1:T:842:DG:C5'	2.19	0.67
3:A:343:ARG:HD2	3:A:345:ILE:HD11	1.78	0.66
3:A:137:GLU:HG2	3:A:172:ARG:NH1	2.09	0.66
3:A:214:LYS:HB2	3:A:215:PRO:HD3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:364:ILE:HG23	3:A:368:VAL:CG2	2.25	0.66
1:T:841:DG:C2'	1:T:842:DG:H5''	2.19	0.66
3:A:365:PRO:HB2	3:A:368:VAL:HG11	1.78	0.66
3:A:320:LYS:O	3:A:323:GLU:HB2	1.97	0.65
3:A:353:LYS:O	3:A:355:TYR:N	2.29	0.65
3:A:347:ARG:NH1	3:A:404:THR:HG1	1.94	0.64
3:A:392:ARG:C	3:A:394:MET:N	2.46	0.64
3:A:300:GLN:NE2	6:A:1011:HOH:O	2.31	0.63
3:A:321:ILE:O	3:A:325:LEU:HD13	1.99	0.62
3:A:388:MET:HE3	3:A:391:PHE:HD1	1.63	0.62
3:A:381:THR:OG1	3:A:382:PRO:CD	2.48	0.62
3:A:290:ASN:ND2	6:A:902:HOH:O	2.15	0.62
3:A:107:TYR:OH	3:A:299:PRO:HG3	2.00	0.62
3:A:172:ARG:HD3	6:A:912:HOH:O	2.00	0.61
3:A:386:ILE:O	3:A:390:LEU:HD12	2.01	0.61
3:A:299:PRO:O	3:A:337:ARG:NH2	2.33	0.61
3:A:318:LYS:HB2	3:A:388:MET:HE1	1.83	0.60
3:A:327:SER:O	3:A:328:LEU:C	2.35	0.60
3:A:347:ARG:O	3:A:404:THR:N	2.34	0.60
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.82	0.60
3:A:381:THR:OG1	3:A:382:PRO:HD3	2.02	0.59
1:T:844:DT:OP2	3:A:301:SER:OG	2.19	0.59
3:A:308:PHE:HB2	3:A:311:CYS:HB2	1.85	0.59
3:A:405:LEU:O	3:A:406:LEU:HD23	2.02	0.58
3:A:309:LYS:CD	3:A:404:THR:OG1	2.50	0.58
3:A:332:VAL:HG11	3:A:339:PRO:HD3	1.86	0.58
3:A:325:LEU:O	3:A:329:LEU:HD13	2.04	0.58
1:T:842:DG:H2''	1:T:843:DG:C5'	2.32	0.58
3:A:184:ARG:HA	3:A:187:MET:HE3	1.85	0.57
3:A:237:LYS:O	3:A:237:LYS:HD3	2.05	0.56
3:A:325:LEU:HD23	3:A:380:MET:HE3	1.86	0.56
3:A:47:ASN:HB3	3:A:50:LEU:HD12	1.88	0.56
3:A:283:LYS:CE	3:A:288:GLU:OE1	2.54	0.56
3:A:253:LEU:HD12	3:A:253:LEU:N	2.21	0.56
3:A:392:ARG:C	3:A:394:MET:H	2.09	0.56
3:A:294:ILE:HG22	3:A:295:LEU:N	2.19	0.56
3:A:112:LEU:C	3:A:112:LEU:HD23	2.26	0.55
3:A:386:ILE:C	3:A:390:LEU:HD12	2.27	0.55
3:A:120:VAL:HG22	3:A:130:VAL:HG22	1.88	0.55
3:A:347:ARG:HH11	3:A:404:THR:HG1	1.52	0.55
1:T:839:DT:H72	3:A:78:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:69:GLU:OE1	3:A:69:GLU:HA	2.06	0.54
3:A:73:LEU:HD23	3:A:90:GLN:NE2	2.23	0.54
3:A:345:ILE:HG12	3:A:359:SER:HB3	1.89	0.54
3:A:72:LYS:NZ	6:A:1015:HOH:O	2.40	0.53
3:A:308:PHE:CE1	3:A:405:LEU:HA	2.43	0.53
3:A:382:PRO:O	3:A:385:ASP:N	2.42	0.52
3:A:202:ASN:C	3:A:202:ASN:ND2	2.63	0.52
3:A:332:VAL:CG1	3:A:339:PRO:HD3	2.38	0.52
3:A:364:ILE:CG2	3:A:369:ILE:HG13	2.38	0.52
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.40	0.52
3:A:388:MET:CE	3:A:391:PHE:HD1	2.24	0.51
2:P:867:DA:H1'	2:P:868:DG:H5'	1.93	0.51
3:A:318:LYS:O	3:A:321:ILE:HB	2.11	0.51
3:A:392:ARG:O	3:A:393:ASN:C	2.47	0.51
3:A:345:ILE:HG22	3:A:346:ILE:N	2.24	0.51
3:A:294:ILE:CG2	3:A:295:LEU:N	2.74	0.50
3:A:266:PRO:O	3:A:270:GLU:HB2	2.11	0.50
3:A:347:ARG:CG	3:A:404:THR:CG2	2.84	0.50
3:A:362:CYS:HB3	3:A:390:LEU:HD21	1.94	0.50
3:A:364:ILE:HG23	3:A:368:VAL:HG23	1.93	0.50
3:A:305:GLU:HG3	3:A:407:SER:HB3	1.92	0.50
3:A:144:GLN:HG3	3:A:147:GLU:HG2	1.94	0.49
3:A:83:ASP:O	3:A:87:LYS:HB2	2.12	0.49
3:A:112:LEU:HD23	3:A:112:LEU:O	2.13	0.49
3:A:392:ARG:O	3:A:394:MET:N	2.46	0.49
3:A:36:ASP:O	3:A:37:CYS:C	2.51	0.49
3:A:161:GLN:NE2	3:A:224:GLU:HB2	2.28	0.49
3:A:334:GLN:O	3:A:335:ASP:C	2.50	0.49
3:A:304:GLU:HG2	3:A:328:LEU:HD21	1.95	0.48
3:A:51:LYS:C	3:A:53:LYS:H	2.16	0.48
3:A:275:ILE:HG12	3:A:279:GLN:NE2	2.27	0.48
3:A:137:GLU:CG	3:A:172:ARG:HH12	2.18	0.48
3:A:337:ARG:HH21	3:A:413:LEU:HG	1.76	0.48
3:A:353:LYS:C	3:A:355:TYR:H	2.15	0.48
3:A:51:LYS:O	3:A:53:LYS:N	2.46	0.48
3:A:364:ILE:CG2	3:A:368:VAL:CG2	2.91	0.48
3:A:202:ASN:ND2	3:A:205:LEU:H	2.12	0.47
3:A:313:SER:O	3:A:314:GLU:HB2	2.14	0.47
3:A:380:MET:HE2	3:A:384:VAL:HG23	1.97	0.47
3:A:214:LYS:HE3	3:A:214:LYS:HB3	1.79	0.46
1:T:843:DG:C8	1:T:844:DT:H72	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:62:LEU:HD23	3:A:79:MET:O	2.16	0.46
3:A:364:ILE:HG22	3:A:369:ILE:CG1	2.40	0.46
3:A:387:LEU:O	3:A:391:PHE:N	2.45	0.46
3:A:406:LEU:HD23	3:A:406:LEU:N	2.30	0.46
3:A:112:LEU:C	3:A:112:LEU:CD2	2.84	0.46
3:A:283:LYS:HE2	3:A:288:GLU:HB3	1.98	0.46
3:A:164:ASN:H	3:A:170:HIS:HD2	1.63	0.45
3:A:343:ARG:HG2	3:A:344:LEU:N	2.30	0.45
3:A:202:ASN:HD21	3:A:205:LEU:H	1.64	0.45
3:A:347:ARG:CD	3:A:404:THR:CG2	2.66	0.45
3:A:360:ARG:HG2	3:A:394:MET:SD	2.57	0.45
3:A:148:LEU:O	3:A:148:LEU:HD23	2.17	0.45
3:A:185:GLU:OE1	3:A:189:ASN:ND2	2.50	0.44
3:A:332:VAL:O	3:A:333:CYS:C	2.55	0.44
3:A:341:THR:HG22	3:A:342:VAL:N	2.33	0.44
1:T:839:DT:C7	3:A:78:LEU:HD13	2.48	0.44
3:A:140:LEU:HD23	3:A:140:LEU:HA	1.89	0.43
3:A:353:LYS:C	3:A:355:TYR:N	2.70	0.43
3:A:144:GLN:HG2	3:A:147:GLU:OE2	2.19	0.43
3:A:298:PRO:HB2	3:A:337:ARG:NH1	2.33	0.43
3:A:381:THR:OG1	3:A:382:PRO:HD2	2.19	0.43
3:A:304:GLU:HG2	3:A:328:LEU:CD2	2.49	0.43
3:A:362:CYS:CB	3:A:390:LEU:HD21	2.49	0.43
3:A:335:ASP:OD2	3:A:337:ARG:CD	2.61	0.42
3:A:144:GLN:HG2	3:A:147:GLU:CD	2.39	0.42
3:A:36:ASP:OD1	3:A:215:PRO:O	2.37	0.42
3:A:43:GLU:OE1	3:A:101:ARG:NH2	2.53	0.42
3:A:99:LEU:O	3:A:100:THR:C	2.58	0.42
3:A:147:GLU:HG2	3:A:147:GLU:H	1.54	0.42
3:A:348:ARG:NH1	3:A:358:GLU:OE1	2.53	0.42
3:A:309:LYS:C	3:A:310:LYS:HG3	2.41	0.41
3:A:364:ILE:HG23	3:A:368:VAL:HG21	2.01	0.41
3:A:275:ILE:HG12	3:A:279:GLN:HE21	1.85	0.41
3:A:122:ARG:HD3	6:A:988:HOH:O	2.19	0.41
3:A:413:LEU:O	3:A:414:LYS:HG2	2.20	0.41
3:A:335:ASP:CG	3:A:337:ARG:HH11	2.23	0.41
3:A:137:GLU:OE2	3:A:172:ARG:NH2	2.49	0.41
3:A:283:LYS:HE2	3:A:288:GLU:CB	2.51	0.41
3:A:352:GLU:C	3:A:354:HIS:H	2.23	0.41
2:P:872:DC:H2''	2:P:873:DOC:H6	2.03	0.41
3:A:225:SER:HA	6:A:960:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:35:LEU:HA	3:A:35:LEU:HD12	1.88	0.41
3:A:60:LYS:HE2	3:A:307:SER:HB3	2.03	0.41
3:A:387:LEU:O	3:A:391:PHE:HB2	2.21	0.41
3:A:58:GLN:OE1	3:A:81:VAL:HG21	2.21	0.40
3:A:170:HIS:O	3:A:174:LEU:HG	2.21	0.40
3:A:335:ASP:CG	3:A:337:ARG:NH1	2.74	0.40
3:A:196:CYS:HA	3:A:217:GLN:O	2.21	0.40
3:A:298:PRO:HA	3:A:299:PRO:HD3	1.95	0.40
2:P:867:DA:C1'	2:P:868:DG:H5'	2.51	0.40
3:A:230:ILE:HD12	3:A:230:ILE:HA	1.98	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:T:847:DT:O3'	2:P:867:DA:O5'[10_665]	1.80	0.40

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	367/390 (94%)	324 (88%)	32 (9%)	11 (3%)	4 6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	314	GLU
3	A	350	SER
3	A	52	ASP
3	A	215	PRO
3	A	315	VAL
3	A	354	HIS

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Mol	Chain	Res	Type
3	A	37	CYS
3	A	347	ARG
3	A	356	GLY
3	A	146	ASP
3	A	272	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	320/354 (90%)	291 (91%)	29 (9%)	9 18

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	27	SER
3	A	62	LEU
3	A	69	GLU
3	A	79	MET
3	A	80	ASN
3	A	112	LEU
3	A	123	LEU
3	A	126	ASP
3	A	142	GLN
3	A	145	SER
3	A	170	HIS
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	229	LEU
3	A	236	ILE
3	A	306	ASP
3	A	308	PHE
3	A	344	LEU
3	A	347	ARG
3	A	348	ARG

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Mol	Chain	Res	Type
3	A	357	ARG
3	A	362	CYS
3	A	368	VAL
3	A	380	MET
3	A	390	LEU
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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	80	ASN
3	A	142	GLN
3	A	170	HIS
3	A	202	ASN
3	A	262	GLN
3	A	279	GLN
3	A	334	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	DOC	P	873	2,1	16,19,20	2.36	6 (37%)	20,26,29	1.91	7 (35%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	P	873	2,1	-	0/7/18/19	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	873	DOC	O4'-C1'	-5.91	1.29	1.42
2	P	873	DOC	C2'-C1'	3.64	1.60	1.51
2	P	873	DOC	O4'-C4'	3.25	1.51	1.44
2	P	873	DOC	C1'-N1	2.99	1.55	1.48
2	P	873	DOC	C3'-C2'	-2.43	1.47	1.54
2	P	873	DOC	O5'-C5'	2.26	1.50	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	873	DOC	C4-N3-C2	3.34	125.65	120.25
2	P	873	DOC	O4'-C1'-N1	-3.09	102.34	107.86
2	P	873	DOC	C5-C4-N4	2.95	125.22	120.57
2	P	873	DOC	N4-C4-N3	-2.67	113.28	117.97
2	P	873	DOC	O2-C2-N1	2.57	124.20	118.89
2	P	873	DOC	O4'-C4'-C5'	2.25	113.21	109.52
2	P	873	DOC	O4'-C1'-C2'	-2.11	104.38	106.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	873	DOC	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	25,29,29	1.37	4 (16%)	37,45,45	1.43	6 (16%)

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	-	4/22/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	DCP	C6-C5	3.18	1.42	1.35
5	A	875	DCP	PA-O1A	-2.69	1.41	1.50
5	A	875	DCP	O4'-C4'	-2.54	1.39	1.45
5	A	875	DCP	C4-N3	2.31	1.39	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	875	DCP	C5-C4-N4	3.05	125.38	120.57
5	A	875	DCP	O3G-PG-O2G	2.89	118.69	107.64
5	A	875	DCP	C1'-N1-C6	2.61	126.70	121.55
5	A	875	DCP	C5-C4-N3	-2.42	117.21	121.33
5	A	875	DCP	C4'-O4'-C1'	2.29	114.99	109.45
5	A	875	DCP	O2B-PB-O1B	-2.18	101.48	112.24

There are no chirality outliers.

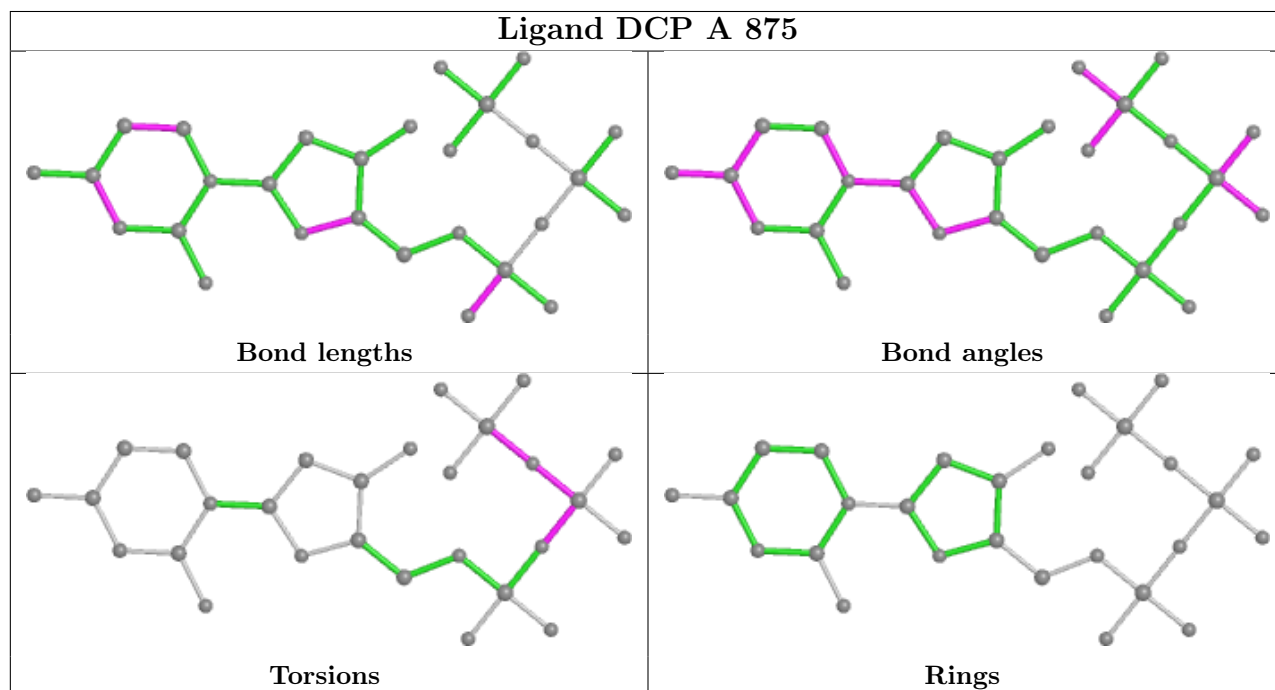
All (4) torsion outliers are listed below:

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

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	T	9/9 (100%)	0.31	1 (11%) 5 5	19, 26, 35, 87	0
2	P	6/7 (85%)	-0.07	0 100 100	27, 32, 37, 41	0
3	A	373/390 (95%)	0.42	43 (11%) 4 4	6, 37, 78, 99	0
All	All	388/406 (95%)	0.41	44 (11%) 5 4	6, 36, 78, 99	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	355	TYR	10.4
3	A	354	HIS	10.3
3	A	25	ALA	7.9
3	A	353	LYS	5.4
3	A	348	ARG	4.9
3	A	352	GLU	4.9
3	A	351	SER	4.7
3	A	26	SER	4.6
3	A	349	TYR	4.4
3	A	333	CYS	4.3
3	A	311	CYS	4.1
3	A	312	SER	4.0
3	A	314	GLU	4.0
3	A	350	SER	3.8
3	A	148	LEU	3.4
3	A	404	THR	3.4
3	A	368	VAL	3.4
3	A	335	ASP	3.1
3	A	413	LEU	3.1
3	A	336	GLY	3.0
3	A	310	LYS	3.0
3	A	249	CYS	2.9
3	A	73	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	A	142	GLN	2.8
3	A	332	VAL	2.8
3	A	144	GLN	2.7
3	A	61	TYR	2.7
3	A	380	MET	2.6
3	A	235	HIS	2.6
3	A	244	TYR	2.6
3	A	347	ARG	2.5
3	A	334	GLN	2.5
3	A	344	LEU	2.5
3	A	308	PHE	2.4
3	A	388	MET	2.4
3	A	406	LEU	2.4
3	A	214	LYS	2.3
3	A	346	ILE	2.3
3	A	315	VAL	2.2
3	A	145	SER	2.2
3	A	313	SER	2.1
3	A	143	LEU	2.1
1	T	839	DT	2.1
3	A	329	LEU	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	DOC	P	873	18/19	0.98	0.19	10,20,27,32	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

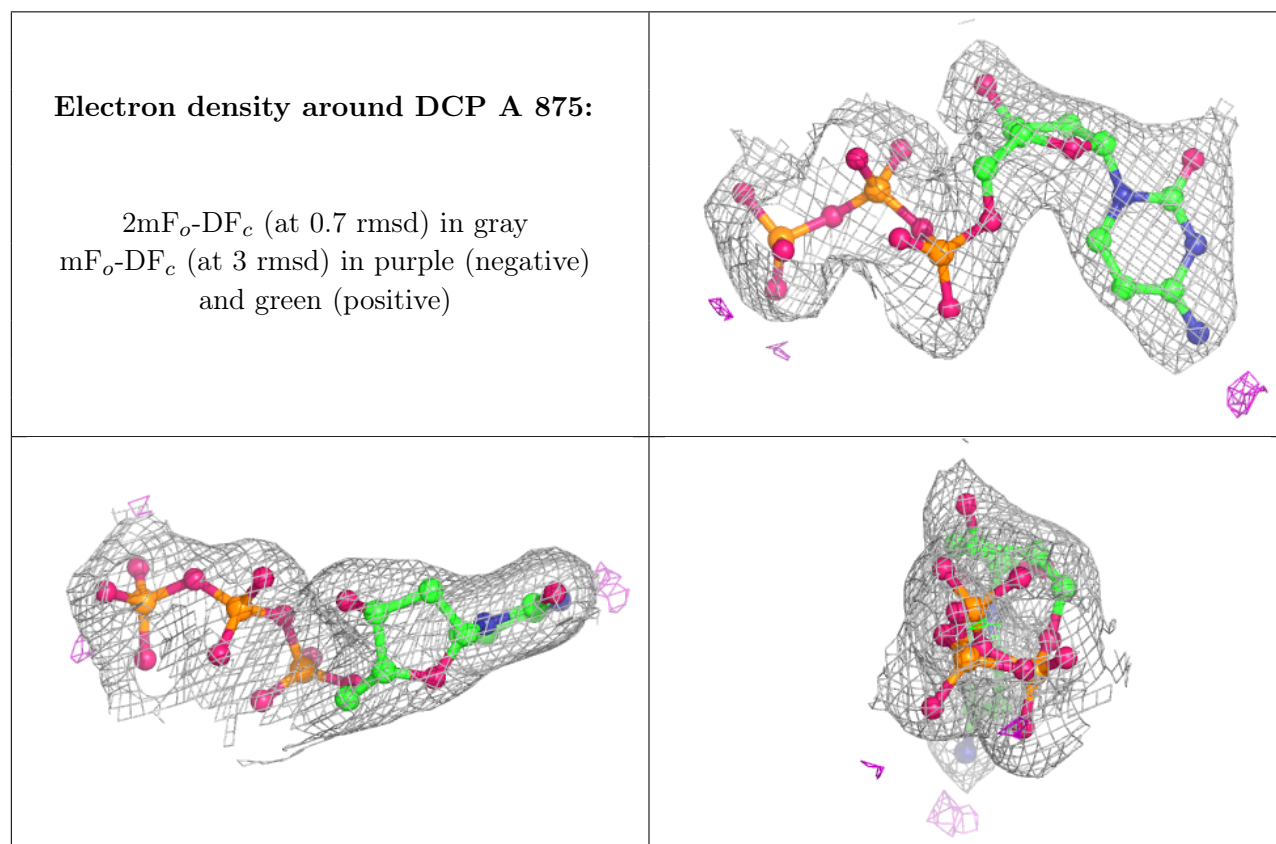
6.4 Ligands [i](#)

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	0.78	0.22	57,57,57,57	0
4	MG	A	871	1/1	0.99	0.15	12,12,12,12	0
5	DCP	A	875	28/28	0.99	0.14	14,20,25,27	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.