



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:18 PM UTC

PDB ID : 2ALZ / pdb_00002alz
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 : 4-5-2 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

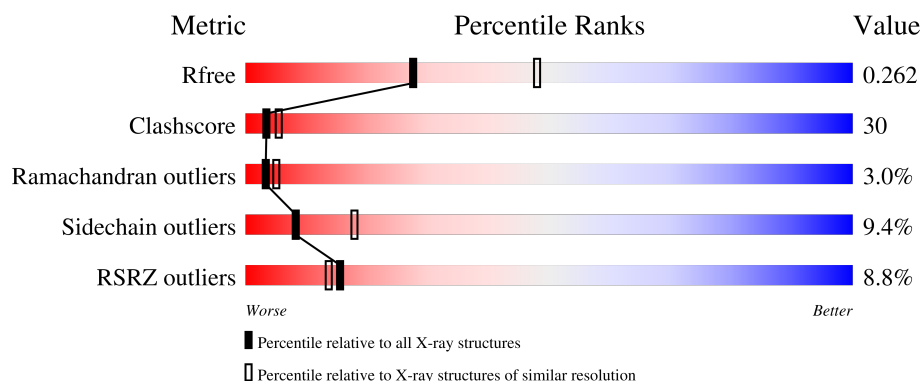
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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	11% 11% 22% 67%
2	P	7	29% 71%
3	A	390	8% 41% 38% 14% • •

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
1	T	9	Total	C	N	O	P	0	0	0
			183	88	32	55	8			

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

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

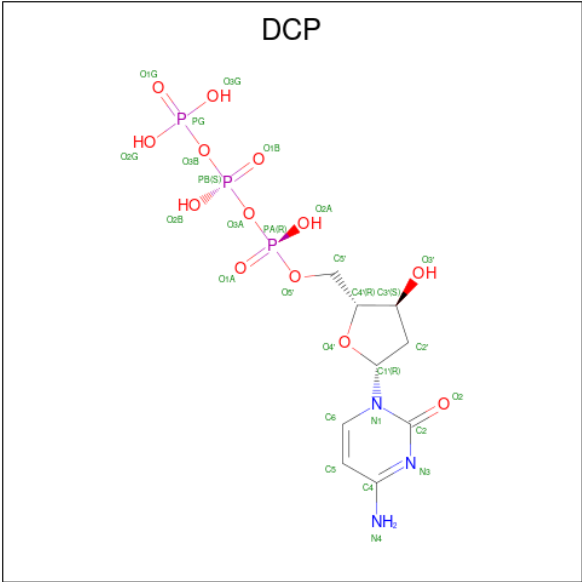
- Molecule 3 is a protein called DNA polymerase iota.

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

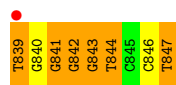
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	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		

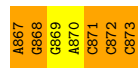
3 Residue-property plots

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.

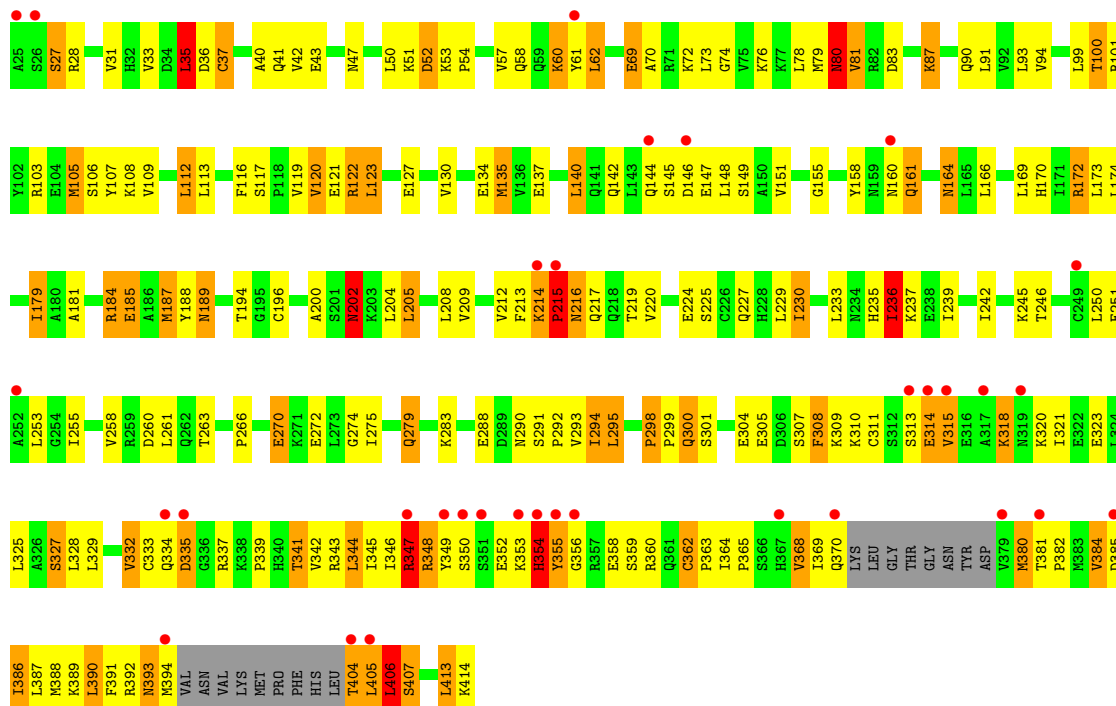
- Molecule 1: 5'-D(*TP*GP*GP*GP*GP*TP*CP*CP*T)-3'



- 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 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.50) 98.1 (50.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.78 (at 2.45Å)	Xtriage
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 (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3305	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 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, DCP, 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	1.86	1/204 (0.5%)	2.94	31/314 (9.9%)
2	P	1.63	1/136 (0.7%)	2.76	17/208 (8.2%)
3	A	2.13	84/2912 (2.9%)	1.74	60/3930 (1.5%)
All	All	2.09	86/3252 (2.6%)	1.90	108/4452 (2.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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)
3	A	214	LYS	CA-C	-22.62	1.28	1.52
3	A	355	TYR	N-CA	10.84	1.60	1.46
3	A	184	ARG	CD-NE	-9.31	1.33	1.46
3	A	164	ASN	CA-C	-9.28	1.41	1.52
3	A	164	ASN	C-O	-8.94	1.13	1.24
3	A	216	ASN	N-CA	8.77	1.60	1.47
3	A	212	VAL	C-O	-8.75	1.13	1.24
3	A	151	VAL	CA-CB	-8.53	1.41	1.53
3	A	120	VAL	C-O	-8.46	1.14	1.24
3	A	103	ARG	CZ-NH2	8.40	1.44	1.33
3	A	292	PRO	CA-C	8.39	1.62	1.52
3	A	298	PRO	C-O	-8.30	1.15	1.24
3	A	109	VAL	C-O	-8.29	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	105	MET	CG-SD	8.16	2.01	1.80
3	A	298	PRO	CA-C	-8.01	1.44	1.52
3	A	122	ARG	CD-NE	-7.71	1.35	1.46
3	A	220	VAL	C-O	7.64	1.31	1.24
3	A	28	ARG	N-CA	-7.57	1.36	1.45
3	A	194	THR	CA-C	-7.49	1.43	1.52
3	A	209	VAL	C-O	-7.44	1.15	1.24
2	P	870	DA	O3'-P	7.37	1.72	1.61
3	A	255	ILE	CA-CB	-7.14	1.44	1.54
3	A	239	ILE	CA-C	7.05	1.60	1.52
3	A	260	ASP	C-O	-6.84	1.16	1.24
3	A	258	VAL	C-O	-6.76	1.15	1.24
3	A	119	VAL	CA-CB	6.66	1.61	1.53
3	A	134	GLU	CA-C	-6.64	1.44	1.52
3	A	407	SER	C-O	6.59	1.31	1.23
3	A	158	TYR	C-O	6.43	1.31	1.23
3	A	295	LEU	N-CA	6.42	1.54	1.46
3	A	202	ASN	C-O	6.38	1.31	1.23
3	A	189	ASN	N-CA	-6.35	1.38	1.46
3	A	54	PRO	C-O	-6.33	1.16	1.23
3	A	140	LEU	C-O	-6.28	1.15	1.24
3	A	200	ALA	C-O	-6.26	1.16	1.23
3	A	35	LEU	N-CA	6.18	1.53	1.45
3	A	209	VAL	N-CA	6.14	1.54	1.46
3	A	187	MET	SD-CE	-6.14	1.64	1.79
3	A	123	LEU	CA-C	6.07	1.59	1.52
3	A	169	LEU	N-CA	-6.07	1.38	1.46
3	A	227	GLN	CA-C	6.02	1.60	1.52
3	A	122	ARG	CG-CD	6.00	1.70	1.52
3	A	230	ILE	CA-CB	5.96	1.62	1.54
3	A	160	ASN	C-O	-5.91	1.14	1.24
3	A	233	LEU	CA-C	5.90	1.60	1.52
3	A	216	ASN	C-O	-5.88	1.15	1.23
3	A	363	PRO	C-O	-5.84	1.17	1.23
3	A	239	ILE	C-O	-5.84	1.17	1.24
3	A	27	SER	C-O	-5.74	1.17	1.23
3	A	123	LEU	N-CA	-5.63	1.39	1.46
3	A	406	LEU	CA-C	5.59	1.59	1.52
3	A	105	MET	N-CA	-5.58	1.39	1.46
3	A	135	MET	N-CA	5.56	1.52	1.46
3	A	258	VAL	CA-CB	5.55	1.62	1.54
3	A	57	VAL	N-CA	-5.47	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	122	ARG	NE-CZ	-5.47	1.27	1.33
3	A	384	VAL	CA-CB	-5.46	1.48	1.54
3	A	215	PRO	C-O	-5.45	1.16	1.24
3	A	263	THR	C-O	-5.44	1.16	1.24
3	A	173	LEU	CA-C	5.43	1.59	1.52
3	A	113	LEU	C-O	-5.41	1.17	1.24
3	A	155	GLY	CA-C	5.40	1.58	1.52
3	A	121	GLU	CA-C	5.40	1.59	1.52
3	A	108	LYS	N-CA	-5.38	1.39	1.46
3	A	181	ALA	CA-CB	5.32	1.61	1.53
3	A	42	VAL	CA-C	5.31	1.59	1.52
3	A	341	THR	CA-CB	-5.30	1.44	1.53
3	A	160	ASN	CA-C	5.29	1.61	1.52
3	A	245	LYS	C-O	-5.29	1.17	1.24
3	A	106	SER	C-O	-5.23	1.18	1.24
3	A	188	TYR	N-CA	-5.21	1.40	1.46
3	A	127	GLU	CD-OE1	5.19	1.35	1.25
3	A	117	SER	CB-OG	5.18	1.52	1.42
3	A	100	THR	CA-CB	5.17	1.61	1.53
3	A	161	GLN	N-CA	-5.17	1.39	1.46
3	A	219	THR	N-CA	-5.13	1.39	1.46
3	A	93	LEU	C-O	-5.12	1.17	1.23
3	A	41	GLN	CA-CB	5.12	1.61	1.53
3	A	261	LEU	C-O	-5.10	1.18	1.24
3	A	35	LEU	C-O	5.10	1.30	1.23
3	A	127	GLU	C-O	5.09	1.30	1.23
3	A	121	GLU	N-CA	-5.08	1.40	1.46
3	A	31	VAL	CA-CB	5.07	1.61	1.54
3	A	242	ILE	CA-CB	5.05	1.59	1.53
3	A	172	ARG	CD-NE	-5.03	1.39	1.46
1	T	844	DT	C5-C7	5.00	1.60	1.50

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	867	DA	O5'-C5'-C4'	14.43	132.44	110.80
3	A	355	TYR	N-CA-CB	14.06	134.25	110.49
1	T	842	DG	C4'-C3'-O3'	12.22	128.33	110.00
3	A	214	LYS	N-CA-CB	11.17	121.00	110.39
1	T	842	DG	C2'-C3'-O3'	-11.01	94.98	111.50
3	A	214	LYS	O-C-N	10.79	127.72	120.27
1	T	842	DG	O4'-C1'-N9	-10.15	93.17	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	349	TYR	N-CA-C	9.54	123.64	109.24
2	P	872	DC	C4'-C3'-O3'	9.43	124.15	110.00
3	A	215	PRO	CA-C-N	-9.15	109.15	123.24
3	A	215	PRO	C-N-CA	-9.15	109.15	123.24
1	T	844	DT	N3-C4-O4	-8.86	109.31	122.60
3	A	91	LEU	N-CA-C	8.79	122.52	109.59
1	T	844	DT	C4-C5-C6	-8.75	106.08	119.20
3	A	335	ASP	N-CA-C	-8.61	100.78	111.11
1	T	843	DG	C4'-C3'-C2'	-8.60	89.50	102.40
3	A	230	ILE	N-CA-C	-8.25	100.38	111.44
3	A	61	TYR	CA-C-N	-8.23	111.38	122.99
3	A	61	TYR	C-N-CA	-8.23	111.38	122.99
1	T	842	DG	C3'-C2'-C1'	8.00	113.60	101.60
2	P	872	DC	C2'-C3'-O3'	-7.99	99.52	111.50
3	A	315	VAL	N-CA-CB	-7.88	98.22	111.23
1	T	844	DT	C5'-C4'-C3'	-7.85	103.12	114.90
1	T	846	DC	O4'-C1'-N1	-7.85	96.62	108.40
3	A	116	PHE	N-CA-C	-7.78	102.74	111.14
3	A	215	PRO	N-CD-CG	-7.71	91.63	103.20
2	P	870	DA	C5'-C4'-O4'	-7.52	98.12	109.40
2	P	869	DG	P-O3'-C3'	-7.47	109.00	120.20
1	T	847	DT	C2'-C3'-O3'	7.46	122.68	111.50
3	A	279	GLN	N-CA-C	-7.39	103.73	112.89
3	A	407	SER	N-CA-C	7.36	120.05	108.79
1	T	839	DT	P-O3'-C3'	7.30	131.15	120.20
1	T	843	DG	C2'-C3'-O3'	-7.14	100.79	111.50
1	T	839	DT	C5'-C4'-C3'	7.09	125.53	114.90
3	A	105	MET	N-CA-C	-7.03	103.70	111.36
1	T	843	DG	O4'-C1'-C2'	-7.02	95.87	106.40
3	A	27	SER	N-CA-C	6.94	120.37	109.96
1	T	843	DG	O4'-C4'-C3'	6.91	115.76	105.40
2	P	872	DC	O4'-C4'-C3'	6.87	115.70	105.40
2	P	872	DC	C5'-C4'-C3'	-6.83	104.65	114.90
3	A	70	ALA	N-CA-C	6.82	118.72	111.28
1	T	843	DG	O4'-C1'-N9	-6.82	98.17	108.40
3	A	318	LYS	N-CA-C	-6.79	106.88	114.62
3	A	405	LEU	N-CA-C	6.77	119.46	109.24
2	P	867	DA	O4'-C1'-N9	6.74	118.51	108.40
1	T	840	DG	N1-C6-O6	-6.66	110.02	120.00
1	T	839	DT	O5'-C5'-C4'	6.64	120.76	110.80
3	A	300	GLN	N-CA-C	-6.61	104.84	113.17
1	T	840	DG	O3'-P-O5'	6.57	113.85	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	327	SER	CA-C-N	-6.53	111.72	120.54
3	A	327	SER	C-N-CA	-6.53	111.72	120.54
1	T	840	DG	C5-C6-O6	6.42	137.94	128.30
3	A	274	GLY	N-CA-C	-6.28	103.77	112.18
3	A	332	VAL	CB-CA-C	-6.27	103.83	112.04
1	T	839	DT	N1-C1'-C2'	6.26	122.89	113.50
3	A	258	VAL	CB-CA-C	-6.23	102.50	112.16
2	P	871	DC	C4'-C3'-O3'	6.21	119.31	110.00
1	T	842	DG	O3'-P-O5'	6.12	113.19	104.00
2	P	868	DG	O3'-P-O5'	-6.04	94.95	104.00
3	A	172	ARG	NE-CZ-NH1	-6.01	115.49	121.50
3	A	355	TYR	N-CA-C	-6.00	98.01	110.80
3	A	208	LEU	N-CA-C	-6.00	104.82	111.36
1	T	844	DT	C5-C6-N1	5.96	131.74	122.80
2	P	872	DC	C1'-O4'-C4'	-5.95	100.77	109.70
3	A	122	ARG	NE-CZ-NH2	-5.91	113.88	119.20
3	A	291	SER	CA-C-O	5.91	124.67	119.71
3	A	406	LEU	N-CA-C	5.83	119.04	109.72
3	A	87	LYS	N-CA-C	-5.80	106.37	113.50
3	A	386	ILE	N-CA-C	-5.78	104.88	110.42
3	A	294	ILE	N-CA-C	5.77	118.24	109.12
3	A	135	MET	CG-SD-CE	-5.75	88.25	100.90
3	A	215	PRO	O-C-N	-5.75	114.88	122.64
3	A	393	ASN	N-CA-C	-5.74	104.87	112.34
3	A	166	LEU	N-CA-C	-5.73	105.95	113.17
3	A	214	LYS	CA-C-O	-5.72	113.87	119.13
1	T	843	DG	C1'-O4'-C4'	-5.59	101.31	109.70
3	A	246	THR	OG1-CB-CG2	-5.59	98.13	109.30
3	A	242	ILE	CA-C-N	-5.58	117.46	122.43
3	A	242	ILE	C-N-CA	-5.58	117.46	122.43
1	T	842	DG	N9-C1'-C2'	-5.58	105.14	113.50
2	P	868	DG	N1-C6-O6	5.57	128.36	120.00
3	A	236	ILE	CB-CG1-CD1	-5.56	102.12	113.80
3	A	260	ASP	N-CA-C	-5.56	105.12	111.07
2	P	872	DC	C3'-C2'-C1'	5.56	109.93	101.60
1	T	847	DT	C4'-C3'-O3'	5.51	118.26	110.00
3	A	214	LYS	CB-CG-CD	-5.50	98.64	111.30
3	A	40	ALA	CA-C-O	-5.43	114.66	120.42
3	A	103	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	T	842	DG	C5'-C4'-O4'	-5.41	101.28	109.40
3	A	179	ILE	CB-CA-C	-5.39	104.86	112.14
3	A	122	ARG	CG-CD-NE	-5.37	100.20	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	869	DG	O4'-C1'-N9	5.35	116.43	108.40
3	A	149	SER	N-CA-C	-5.34	106.76	113.28
3	A	270	GLU	N-CA-C	-5.33	104.71	111.11
2	P	867	DA	O4'-C4'-C3'	-5.32	97.42	105.40
3	A	293	VAL	N-CA-C	-5.32	100.66	108.54
3	A	74	GLY	N-CA-C	5.31	121.83	114.92
2	P	867	DA	C1'-O4'-C4'	5.30	117.65	109.70
1	T	841	DG	O3'-P-O5'	5.30	111.94	104.00
3	A	80	ASN	N-CA-C	-5.25	103.46	110.55
3	A	122	ARG	CD-NE-CZ	5.23	131.73	124.40
1	T	842	DG	O4'-C1'-C2'	-5.22	98.56	106.40
1	T	846	DC	O3'-P-O5'	-5.18	96.23	104.00
1	T	844	DT	N3-C4-C5	5.17	122.56	114.80
3	A	60	LYS	CB-CA-C	-5.17	110.63	116.63
3	A	235	HIS	CA-C-O	-5.17	114.96	120.75
3	A	389	LYS	N-CA-C	-5.16	105.73	111.36
2	P	871	DC	C5'-C4'-C3'	-5.05	107.33	114.90

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	181	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	5	0	0	0	0
All	All	3305	0	3090	190	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 30.

All (190) 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:HZ1	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:405:LEU:C	3:A:406:LEU:HD23	2.10	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:202:ASN:HD22	3:A:202:ASN:C	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:325:LEU:HD11	3:A:387:LEU:HD11	1.71	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:392:ARG:C	3:A:394:MET:N	2.46	0.68
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
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:327:SER:O	3:A:328:LEU:C	2.35	0.65
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: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: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:112:LEU:C	3:A:112:LEU:HD23	2.26	0.60
3:A:347:ARG:O	3:A:404:THR:N	2.34	0.60
3:A:386:ILE:C	3:A:390:LEU:HD12	2.27	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:392:ARG:C	3:A:394:MET:H	2.09	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:325:LEU:HD23	3:A:380:MET:HE3	1.84	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:237:LYS:O	3:A:237:LYS:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:76:LYS:HB2	3:A:79:MET:HE3	1.87	0.56
3:A:294:ILE:HG22	3:A:295:LEU:N	2.19	0.56
3:A:392:ARG:O	3:A:393:ASN:C	2.47	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
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:36:ASP:O	3:A:37:CYS:C	2.51	0.53
3:A:72:LYS:NZ	6:A:1015:HOH:O	2.40	0.53
3:A:334:GLN:O	3:A:335:ASP:C	2.50	0.53
3:A:51:LYS:C	3:A:53:LYS:H	2.16	0.53
3:A:308:PHE:CE1	3:A:405:LEU:HA	2.43	0.53
3:A:184:ARG:HA	3:A:187:MET:HE3	1.90	0.53
3:A:353:LYS:C	3:A:355:TYR:H	2.15	0.53
3:A:382:PRO:O	3:A:385:ASP:N	2.42	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:388:MET:CE	3:A:391:PHE:HD1	2.24	0.51
3:A:112:LEU:C	3:A:112:LEU:CD2	2.84	0.51
3:A:318:LYS:HB2	3:A:388:MET:HE1	1.91	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:202:ASN:C	3:A:202:ASN:ND2	2.63	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:135:MET:HE2	3:A:179:ILE:HD12	1.92	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:332:VAL:O	3:A:333:CYS:C	2.55	0.49
3:A:392:ARG:O	3:A:394:MET:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:161:GLN:NE2	3:A:224:GLU:HB2	2.28	0.49
3:A:304:GLU:HG2	3:A:328:LEU:HD21	1.95	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: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:353:LYS:C	3:A:355:TYR:N	2.70	0.47
3:A:202:ASN:ND2	3:A:205:LEU:H	2.12	0.47
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.44	0.47
3:A:144:GLN:HG2	3:A:147:GLU:CD	2.39	0.47
3:A:313:SER:O	3:A:314:GLU:HB2	2.14	0.47
3:A:309:LYS:C	3:A:310:LYS:HG3	2.41	0.46
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
3:A:62:LEU:HD23	3:A:79:MET:O	2.16	0.46
3:A:318:LYS:HD2	3:A:388:MET:HE2	1.97	0.46
3:A:335:ASP:CG	3:A:337:ARG:HH11	2.23	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:388:MET:HE3	3:A:391:PHE:HD1	1.81	0.46
3:A:406:LEU:HD23	3:A:406:LEU:N	2.30	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:352:GLU:C	3:A:354:HIS:H	2.23	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:33:VAL:CG1	3:A:187:MET:HE1	2.47	0.45
3:A:335:ASP:CG	3:A:337:ARG:NH1	2.74	0.45
3:A:105:MET:CA	3:A:105:MET:HE2	2.47	0.45
3:A:360:ARG:HG2	3:A:394:MET:SD	2.57	0.45
3:A:33:VAL:HG11	3:A:187:MET:HE1	1.99	0.45
3:A:51:LYS:C	3:A:52:ASP:OD1	2.60	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:364:ILE:O	3:A:365:PRO:C	2.60	0.44
3:A:99:LEU:O	3:A:100:THR:C	2.58	0.44
3:A:341:THR:HG22	3:A:342:VAL:N	2.33	0.44
3:A:380:MET:HE2	3:A:384:VAL:HG23	2.00	0.44
1:T:839:DT:C7	3:A:78:LEU:HD13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:251:GLU:C	3:A:253:LEU:N	2.74	0.43
3:A:140:LEU:HD23	3:A:140:LEU:HA	1.89	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:80:ASN:HD22	3:A:83:ASP:CG	2.27	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:385:ASP:O	3:A:386:ILE:C	2.59	0.42
3:A:36:ASP:OD1	3:A:215:PRO:O	2.37	0.42
3:A:80:ASN:ND2	3:A:83:ASP:CG	2.77	0.42
3:A:344:LEU:C	3:A:345:ILE:HG13	2.43	0.42
3:A:43:GLU:OE1	3:A:101:ARG:NH2	2.53	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: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:105:MET:HE2	3:A:105:MET:HA	2.03	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: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:290:ASN:OD1	3:A:290:ASN:C	2.64	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
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: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%)	3 5

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
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%)	290 (91%)	30 (9%)	8 18

All (30) 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	80	ASN
3	A	81	VAL
3	A	94	VAL
3	A	112	LEU
3	A	123	LEU
3	A	142	GLN
3	A	145	SER
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	236	ILE
3	A	308	PHE
3	A	344	LEU
3	A	347	ARG
3	A	348	ARG
3	A	362	CYS
3	A	368	VAL
3	A	370	GLN
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	58	GLN
3	A	80	ASN
3	A	128	ASN
3	A	142	GLN
3	A	170	HIS
3	A	202	ASN
3	A	216	ASN
3	A	262	GLN
3	A	279	GLN

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Mol	Chain	Res	Type
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 ⓘ

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	1,2	16,19,20	2.38	6 (37%)	20,26,29	1.88	6 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	P	873	1,2	-	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'	-5.95	1.29	1.42
2	P	873	DOC	C2'-C1'	3.70	1.60	1.52
2	P	873	DOC	O4'-C4'	3.34	1.51	1.44
2	P	873	DOC	C1'-N1	3.09	1.55	1.48
2	P	873	DOC	C3'-C2'	-2.45	1.47	1.54
2	P	873	DOC	O5'-C5'	2.17	1.50	1.44

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	873	DOC	C4-N3-C2	3.42	125.65	120.26
2	P	873	DOC	O4'-C1'-N1	-3.11	102.34	107.86
2	P	873	DOC	O2-C2-N1	2.70	124.20	118.90
2	P	873	DOC	C5-C4-N4	2.62	125.22	120.63
2	P	873	DOC	N4-C4-N3	-2.59	113.28	117.91
2	P	873	DOC	O4'-C4'-C5'	2.15	113.21	109.34

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 [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	1.53	5 (17%)	41,45,45	1.67	9 (21%)

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	-	5/22/34/34	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	DCP	PA-O3A	4.03	1.63	1.59
5	A	875	DCP	C6-C5	3.17	1.42	1.35
5	A	875	DCP	PA-O1A	-2.73	1.41	1.50
5	A	875	DCP	O4'-C4'	-2.55	1.39	1.45
5	A	875	DCP	C4-N3	2.34	1.39	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	875	DCP	O2B-PB-O3A	4.55	119.58	107.27
5	A	875	DCP	O3A-PA-O1A	-3.67	99.67	110.70
5	A	875	DCP	O3G-PG-O2G	2.90	118.69	107.80
5	A	875	DCP	C5-C4-N4	2.71	125.38	120.63
5	A	875	DCP	C1'-N1-C6	2.63	126.70	121.53
5	A	875	DCP	O3A-PB-O1B	-2.47	103.28	110.70
5	A	875	DCP	C5-C4-N3	-2.44	117.21	121.32
5	A	875	DCP	O2B-PB-O1B	-2.36	101.48	112.44
5	A	875	DCP	C4'-O4'-C1'	2.31	114.99	109.51

There are no chirality outliers.

All (5) torsion outliers are listed below:

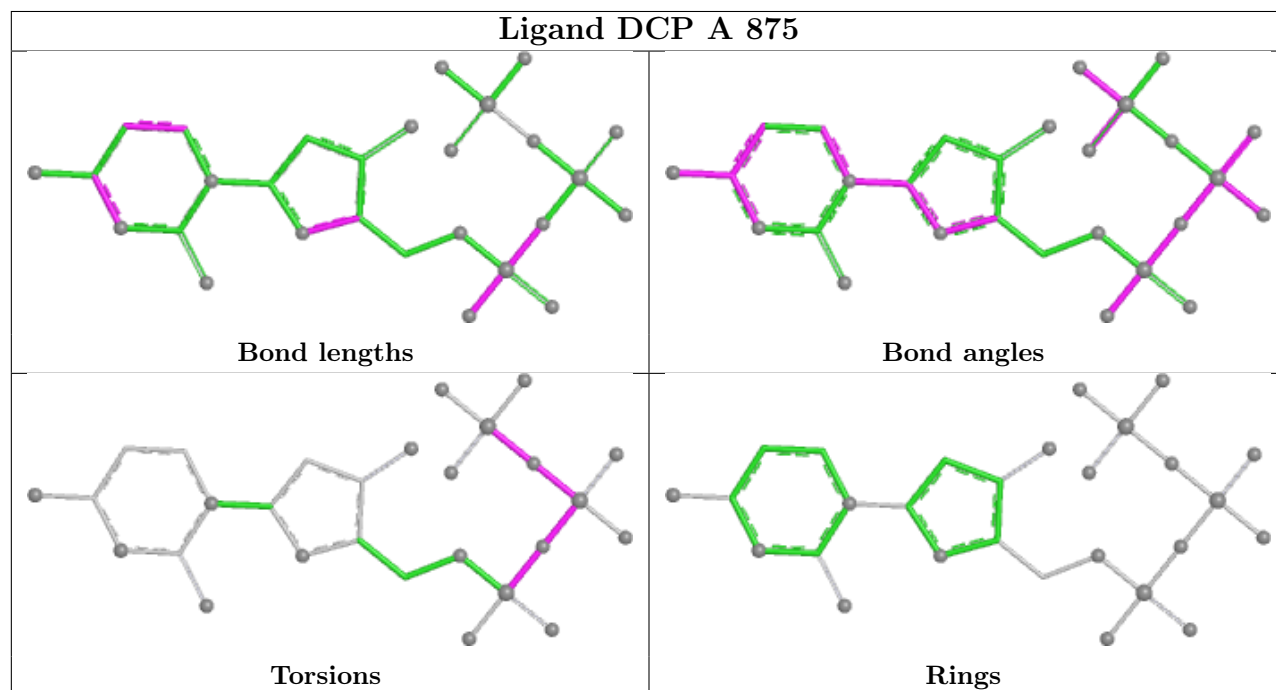
Mol	Chain	Res	Type	Atoms
5	A	875	DCP	PG-O3B-PB-O1B
5	A	875	DCP	PB-O3B-PG-O2G
5	A	875	DCP	PA-O3A-PB-O1B
5	A	875	DCP	PA-O3A-PB-O2B
5	A	875	DCP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	9/9 (100%)	-0.03	1 (11%) 10 8	19, 26, 35, 87	0
2	P	6/7 (85%)	-0.17	0 100 100	27, 32, 37, 41	0
3	A	373/390 (95%)	0.40	33 (8%) 15 14	6, 37, 78, 99	0
All	All	388/406 (95%)	0.38	34 (8%) 15 14	6, 36, 78, 99	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	379	VAL	5.0
3	A	353	LYS	4.7
3	A	25	ALA	4.3
3	A	354	HIS	4.3
3	A	355	TYR	4.2
3	A	405	LEU	4.2
3	A	381	THR	4.0
3	A	146	ASP	3.8
3	A	349	TYR	3.5
3	A	214	LYS	3.5
3	A	394	MET	3.4
3	A	350	SER	3.4
3	A	351	SER	3.1
3	A	249	CYS	3.1
3	A	385	ASP	3.1
1	T	839	DT	3.0
3	A	313	SER	3.0
3	A	367	HIS	2.9
3	A	314	GLU	2.9
3	A	356	GLY	2.7
3	A	370	GLN	2.6
3	A	317	ALA	2.5
3	A	160	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	61	TYR	2.3
3	A	144	GLN	2.3
3	A	315	VAL	2.2
3	A	26	SER	2.2
3	A	347	ARG	2.1
3	A	215	PRO	2.1
3	A	404	THR	2.1
3	A	334	GLN	2.0
3	A	252	ALA	2.0
3	A	319	ASN	2.0
3	A	335	ASP	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	0.06	10,20,27,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

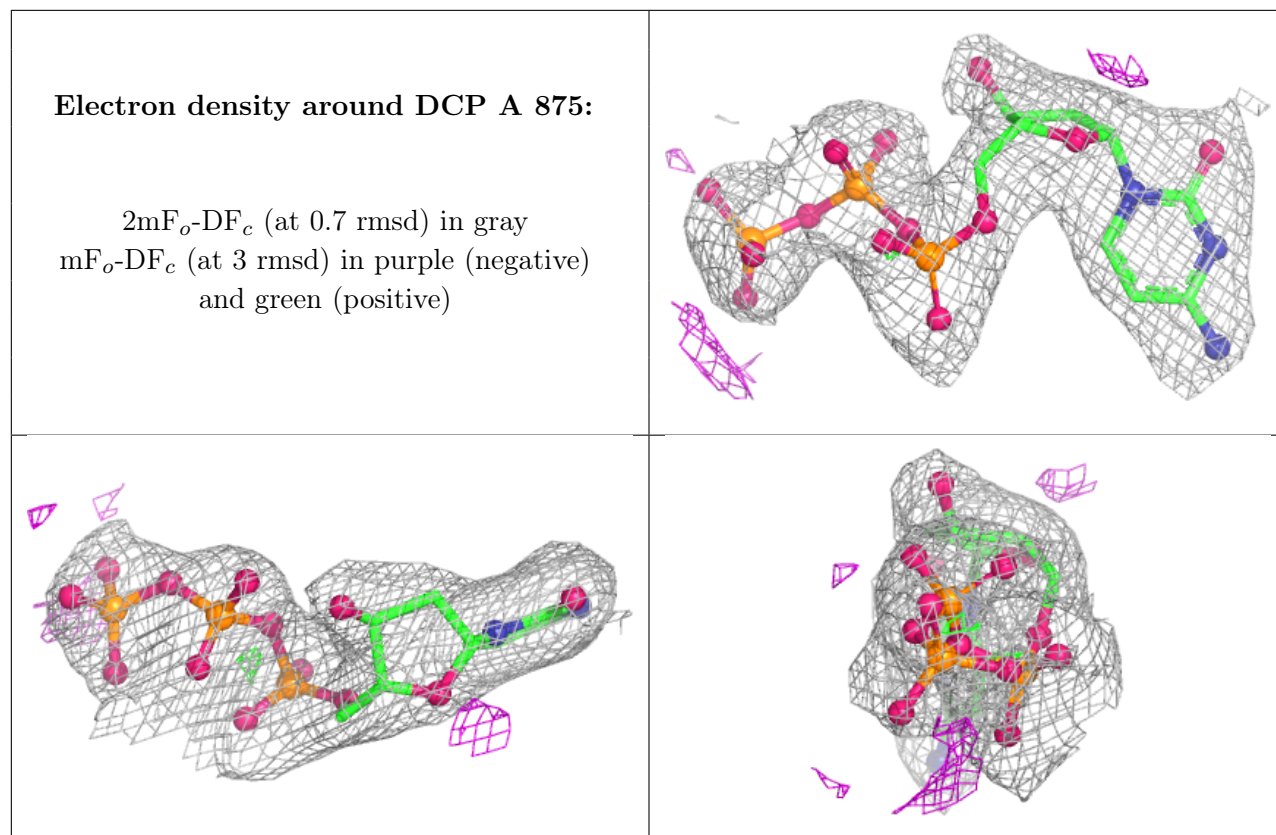
6.4 Ligands [i](#)

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	0.89	0.11	57,57,57,57	0
5	DCP	A	875	28/28	0.98	0.06	14,20,25,27	0
4	MG	A	871	1/1	0.99	0.09	12,12,12,12	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 ⓘ

There are no such residues in this entry.