



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:00 PM GMT

PDB ID : 2DPI
Title : Ternary complex of hPoli with DNA and dCTP
Authors : Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on : 2006-05-12
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

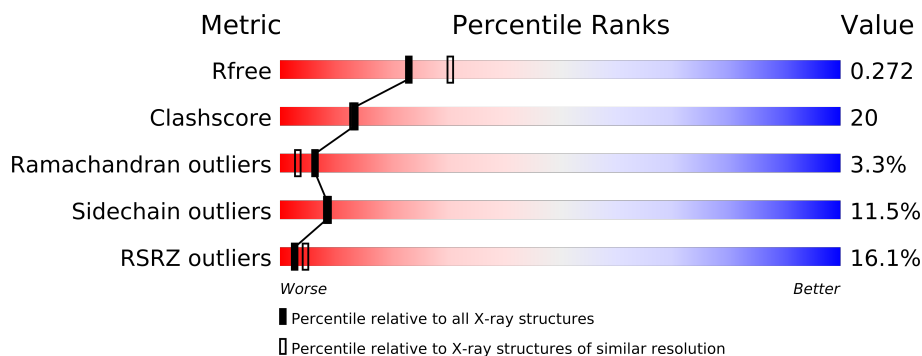
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	P	7	
2	T	9	
3	A	420	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	A	872	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3346 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called 5'-D(*AP*GP*GP*AP*CP*CP*(DOC))-3'.

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

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

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

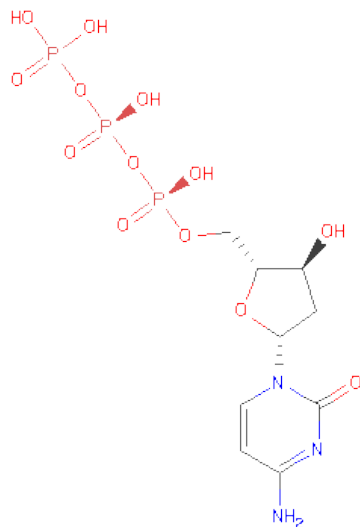
- Molecule 3 is a protein called DNA polymerase iota.

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

- Molecule 4 is MAGNESIUM ION (three-letter code: 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 (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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

- Molecule 6 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.15Å 98.15Å 203.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.64 – 2.30 41.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (42.64-2.30) 98.6 (41.60-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.01 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.228 , 0.278 0.225 , 0.272	Depositor DCC
R_{free} test set	2063 reflections (7.90%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 26492 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3346	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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

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	3.99	26/136 (19.1%)	5.48	60/208 (28.8%)
2	T	4.53	36/178 (20.2%)	4.88	68/271 (25.1%)
3	A	2.04	79/2909 (2.7%)	1.58	51/3927 (1.3%)
All	All	2.35	141/3223 (4.4%)	2.26	179/4406 (4.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	2
2	T	0	1
3	A	0	6
All	All	0	9

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	847	DT	C3'-O3'	21.88	1.72	1.44
2	T	843	DG	P-O5'	15.17	1.75	1.59
1	P	867	DA	O3'-P	14.93	1.79	1.61
3	A	313	SER	CB-OG	14.74	1.61	1.42
3	A	392	ARG	C-O	14.69	1.51	1.23
2	T	844	DT	C3'-O3'	-11.45	1.29	1.44
2	T	839	DT	C3'-O3'	-11.38	1.29	1.44
3	A	103	ARG	CZ-NH2	10.72	1.47	1.33
2	T	841	DG	P-O5'	10.71	1.70	1.59
2	T	845	DC	C4'-C3'	10.61	1.64	1.53
1	P	867	DA	N7-C5	-10.60	1.32	1.39
2	T	839	DT	C2-N3	10.31	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	214	LYS	CA-C	-10.30	1.26	1.52
2	T	844	DT	C2-N3	10.29	1.46	1.37
1	P	867	DA	C5'-C4'	10.15	1.62	1.51
3	A	122	ARG	CG-CD	10.14	1.77	1.51
3	A	216	ASN	N-CA	10.01	1.66	1.46
3	A	105	MET	CG-SD	9.96	2.07	1.81
3	A	122	ARG	CD-NE	-9.72	1.29	1.46
2	T	845	DC	C2'-C1'	9.71	1.62	1.52
3	A	122	ARG	NE-CZ	-9.46	1.20	1.33
2	T	843	DG	O4'-C1'	-9.45	1.30	1.42
1	P	872	DC	C4'-O4'	9.43	1.54	1.45
2	T	843	DG	P-OP2	-9.31	1.33	1.49
2	T	843	DG	N1-C2	9.30	1.45	1.37
1	P	868	DG	C2'-C1'	9.17	1.61	1.52
3	A	338	LYS	CA-CB	8.76	1.73	1.53
3	A	38	PHE	CB-CG	-8.75	1.36	1.51
1	P	871	DC	C3'-O3'	-8.56	1.32	1.44
3	A	134	GLU	CD-OE1	8.44	1.34	1.25
3	A	314	GLU	CD-OE2	8.37	1.34	1.25
1	P	872	DC	C3'-O3'	-8.33	1.33	1.44
3	A	314	GLU	N-CA	8.29	1.62	1.46
2	T	843	DG	N7-C5	-8.22	1.34	1.39
2	T	843	DG	O5'-C5'	-8.11	1.22	1.42
1	P	870	DA	C2'-C1'	8.09	1.60	1.52
2	T	847	DT	C4'-C3'	8.04	1.61	1.53
3	A	387	LEU	C-O	7.97	1.38	1.23
3	A	207	LYS	CE-NZ	-7.88	1.29	1.49
3	A	44	MET	SD-CE	-7.77	1.34	1.77
2	T	843	DG	C3'-C2'	-7.67	1.43	1.52
1	P	870	DA	C4'-O4'	7.67	1.52	1.45
1	P	871	DC	O4'-C1'	-7.59	1.33	1.42
1	P	871	DC	C2'-C1'	7.43	1.59	1.52
2	T	842	DG	C6-O6	-7.41	1.17	1.24
1	P	872	DC	P-O5'	7.33	1.67	1.59
3	A	384	VAL	N-CA	7.29	1.60	1.46
2	T	844	DT	O3'-P	7.24	1.69	1.61
3	A	282	GLN	CG-CD	7.21	1.67	1.51
2	T	845	DC	P-O5'	7.03	1.66	1.59
3	A	270	GLU	CD-OE2	7.02	1.33	1.25
2	T	845	DC	N1-C6	-6.94	1.32	1.37
3	A	408	VAL	CB-CG2	6.94	1.67	1.52
3	A	214	LYS	CE-NZ	-6.91	1.31	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	305	GLU	CD-OE2	-6.88	1.18	1.25
1	P	869	DG	N3-C4	-6.87	1.30	1.35
1	P	870	DA	P-O5'	6.84	1.66	1.59
1	P	871	DC	P-O5'	6.83	1.66	1.59
3	A	394	MET	CG-SD	6.79	1.98	1.81
3	A	251	GLU	CD-OE1	6.72	1.33	1.25
3	A	184	ARG	CD-NE	-6.70	1.35	1.46
3	A	189	ASN	CG-OD1	6.66	1.38	1.24
3	A	162	SER	CA-CB	6.60	1.62	1.52
1	P	872	DC	C4-C5	-6.58	1.37	1.43
3	A	303	SER	CB-OG	-6.58	1.33	1.42
2	T	847	DT	N1-C6	-6.50	1.33	1.38
2	T	846	DC	C2-N3	6.50	1.41	1.35
3	A	46	SER	CB-OG	-6.43	1.33	1.42
3	A	388	MET	CG-SD	6.42	1.97	1.81
3	A	107	TYR	CD2-CE2	6.39	1.49	1.39
3	A	305	GLU	CD-OE1	-6.39	1.18	1.25
3	A	385	ASP	CB-CG	6.35	1.65	1.51
3	A	288	GLU	CD-OE2	6.34	1.32	1.25
3	A	134	GLU	CD-OE2	6.30	1.32	1.25
3	A	322	GLU	CD-OE1	6.30	1.32	1.25
3	A	178	GLN	CG-CD	6.28	1.65	1.51
3	A	410	PHE	CD1-CE1	6.27	1.51	1.39
3	A	117	SER	CB-OG	6.21	1.50	1.42
3	A	319	ASN	CG-ND2	6.20	1.48	1.32
3	A	122	ARG	CZ-NH1	-6.20	1.25	1.33
3	A	382	PRO	N-CD	6.11	1.56	1.47
1	P	868	DG	N9-C8	6.08	1.42	1.37
2	T	847	DT	C5'-C4'	6.08	1.58	1.51
2	T	843	DG	C6-N1	6.05	1.43	1.39
3	A	185	GLU	CG-CD	6.00	1.60	1.51
1	P	869	DG	N9-C8	6.00	1.42	1.37
2	T	845	DC	C4-N4	5.97	1.39	1.33
3	A	391	PHE	CA-C	5.96	1.68	1.52
3	A	260	ASP	N-CA	5.92	1.58	1.46
2	T	841	DG	N3-C4	-5.89	1.31	1.35
3	A	322	GLU	CG-CD	5.89	1.60	1.51
2	T	842	DG	C2-N3	5.86	1.37	1.32
3	A	313	SER	CA-CB	5.83	1.61	1.52
3	A	213	PHE	CB-CG	5.83	1.61	1.51
3	A	225	SER	CA-CB	5.78	1.61	1.52
1	P	869	DG	N1-C2	-5.74	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	276	SER	CB-OG	5.73	1.49	1.42
3	A	302	PHE	C-O	5.73	1.34	1.23
1	P	867	DA	C5-C6	-5.71	1.35	1.41
1	P	867	DA	C4'-C3'	5.71	1.59	1.53
1	P	869	DG	N7-C5	5.70	1.42	1.39
2	T	841	DG	C6-N1	5.70	1.43	1.39
1	P	869	DG	O3'-P	5.64	1.68	1.61
3	A	381	THR	CA-CB	5.64	1.68	1.53
3	A	258	VAL	C-O	-5.61	1.12	1.23
3	A	283	LYS	CD-CE	5.59	1.65	1.51
3	A	264	PHE	CD1-CE1	-5.57	1.28	1.39
2	T	841	DG	C2-N3	5.57	1.37	1.32
1	P	870	DA	N9-C4	-5.55	1.34	1.37
2	T	841	DG	P-OP2	-5.50	1.39	1.49
3	A	320	LYS	N-CA	5.49	1.57	1.46
2	T	847	DT	C5-C6	-5.48	1.30	1.34
3	A	232	SER	CB-OG	5.47	1.49	1.42
3	A	207	LYS	CD-CE	5.45	1.64	1.51
3	A	209	VAL	CB-CG1	-5.44	1.41	1.52
2	T	847	DT	N1-C2	-5.43	1.33	1.38
2	T	843	DG	C5'-C4'	-5.37	1.45	1.51
3	A	212	VAL	C-O	-5.36	1.13	1.23
3	A	315	VAL	C-O	5.35	1.33	1.23
3	A	112	LEU	CG-CD2	-5.34	1.32	1.51
3	A	140	LEU	C-O	-5.34	1.13	1.23
3	A	383	MET	N-CA	5.30	1.56	1.46
1	P	868	DG	C6-O6	5.30	1.28	1.24
3	A	383	MET	CA-C	5.28	1.66	1.52
1	P	867	DA	C4'-O4'	5.24	1.50	1.45
3	A	127	GLU	CD-OE1	5.22	1.31	1.25
3	A	394	MET	SD-CE	-5.22	1.48	1.77
2	T	844	DT	C2'-C1'	5.19	1.57	1.52
3	A	138	LYS	CD-CE	5.19	1.64	1.51
3	A	385	ASP	C-O	5.17	1.33	1.23
3	A	187	MET	CG-SD	5.17	1.94	1.81
2	T	839	DT	C2'-C1'	5.13	1.57	1.52
3	A	179	ILE	CA-CB	-5.11	1.43	1.54
3	A	382	PRO	CA-C	-5.09	1.42	1.52
3	A	298	PRO	C-O	-5.08	1.13	1.23
3	A	263	THR	C-O	-5.07	1.13	1.23
3	A	199	VAL	CA-CB	-5.07	1.44	1.54
2	T	846	DC	C4'-C3'	5.07	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	392	ARG	C-N	5.06	1.45	1.34
3	A	302	PHE	CB-CG	-5.02	1.42	1.51
3	A	288	GLU	CG-CD	5.02	1.59	1.51

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	870	DA	O4'-C4'-C3'	24.28	120.57	106.00
1	P	867	DA	O4'-C4'-C3'	-20.08	93.95	106.00
2	T	843	DG	O4'-C4'-C3'	19.98	117.99	106.00
2	T	843	DG	C4'-C3'-C2'	-19.63	85.43	103.10
1	P	870	DA	O5'-P-OP2	-18.13	88.94	110.70
1	P	869	DG	O4'-C1'-N9	17.84	120.49	108.00
1	P	867	DA	O4'-C1'-N9	15.98	119.19	108.00
2	T	843	DG	O4'-C1'-C2'	-14.98	93.91	105.90
3	A	122	ARG	NE-CZ-NH2	-13.98	113.31	120.30
1	P	870	DA	O4'-C1'-N9	13.84	117.69	108.00
2	T	846	DC	N3-C4-C5	-13.72	116.41	121.90
2	T	843	DG	O4'-C1'-N9	-13.57	98.50	108.00
1	P	869	DG	C8-N9-C4	-12.25	101.50	106.40
2	T	841	DG	C8-N9-C4	-12.12	101.55	106.40
1	P	871	DC	O4'-C4'-C3'	11.89	113.13	106.00
1	P	872	DC	O4'-C4'-C3'	11.89	113.13	106.00
2	T	842	DG	O4'-C1'-N9	-11.63	99.86	108.00
1	P	868	DG	C5-C6-O6	-11.56	121.66	128.60
1	P	867	DA	O5'-C5'-C4'	11.48	139.69	111.00
1	P	869	DG	N1-C6-O6	-11.46	113.02	119.90
3	A	172	ARG	NE-CZ-NH2	-11.45	114.58	120.30
2	T	847	DT	C4'-C3'-C2'	-11.40	92.84	103.10
3	A	385	ASP	CB-CG-OD2	11.35	128.51	118.30
2	T	842	DG	O4'-C1'-C2'	-11.29	96.86	105.90
3	A	103	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	P	870	DA	C4'-C3'-C2'	-10.89	93.30	103.10
2	T	841	DG	N7-C8-N9	10.80	118.50	113.10
1	P	868	DG	N1-C6-O6	10.67	126.30	119.90
2	T	844	DT	N1-C2-N3	10.32	120.79	114.60
2	T	839	DT	N1-C2-N3	10.29	120.77	114.60
3	A	215	PRO	O-C-N	-10.20	106.39	122.70
1	P	869	DG	N9-C4-C5	10.06	109.42	105.40
2	T	843	DG	C3'-C2'-C1'	9.86	114.33	102.50
1	P	870	DA	C1'-O4'-C4'	-9.85	100.25	110.10
2	T	842	DG	C3'-C2'-C1'	9.62	114.04	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	847	DT	O4'-C4'-C3'	9.58	111.75	106.00
2	T	842	DG	O4'-C4'-C3'	9.41	111.65	106.00
2	T	842	DG	C8-N9-C4	-9.36	102.66	106.40
3	A	306	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	P	867	DA	C1'-O4'-C4'	9.18	119.28	110.10
2	T	844	DT	C6-C5-C7	-9.08	117.45	122.90
2	T	839	DT	C6-C5-C7	-9.02	117.49	122.90
2	T	842	DG	C4'-C3'-O3'	8.98	132.15	109.70
2	T	841	DG	C5-N7-C8	-8.92	99.84	104.30
2	T	839	DT	C2-N3-C4	-8.89	121.86	127.20
2	T	844	DT	C2-N3-C4	-8.87	121.88	127.20
3	A	172	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	P	871	DC	OP1-P-OP2	-8.87	106.30	119.60
1	P	869	DG	P-O3'-C3'	-8.79	109.16	119.70
3	A	215	PRO	N-CD-CG	-8.73	90.11	103.20
3	A	306	ASP	CB-CG-OD1	8.68	126.11	118.30
3	A	52	ASP	CB-CG-OD2	8.58	126.02	118.30
2	T	847	DT	C2-N3-C4	-8.52	122.09	127.20
3	A	331	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	P	868	DG	O4'-C1'-C2'	8.42	112.64	105.90
2	T	847	DT	N1-C2-N3	8.35	119.61	114.60
2	T	845	DC	N3-C4-C5	-8.34	118.57	121.90
2	T	847	DT	C4'-C3'-O3'	8.28	130.41	109.70
1	P	870	DA	O4'-C1'-C2'	8.21	112.47	105.90
1	P	871	DC	O5'-P-OP1	-8.03	98.47	105.70
3	A	135	MET	CG-SD-CE	-7.96	87.47	100.20
3	A	184	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	P	867	DA	C8-N9-C4	-7.94	102.62	105.80
2	T	844	DT	C6-N1-C2	-7.73	117.44	121.30
1	P	867	DA	O4'-C1'-C2'	-7.70	99.74	105.90
3	A	122	ARG	CG-CD-NE	-7.68	95.67	111.80
1	P	869	DG	N7-C8-N9	7.64	116.92	113.10
2	T	839	DT	C6-N1-C2	-7.64	117.48	121.30
1	P	872	DC	C3'-C2'-C1'	7.60	111.62	102.50
3	A	343	ARG	NE-CZ-NH2	-7.54	116.53	120.30
2	T	846	DC	C6-N1-C2	-7.50	117.30	120.30
1	P	870	DA	C2-N3-C4	-7.49	106.85	110.60
1	P	869	DG	OP2-P-O3'	7.49	121.67	105.20
1	P	871	DC	O5'-P-OP2	-7.44	99.01	105.70
2	T	842	DG	N9-C4-C5	7.44	108.38	105.40
3	A	73	LEU	CB-CG-CD1	7.39	123.56	111.00
3	A	214	LYS	N-CA-CB	7.35	123.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	847	DT	O4'-C1'-N1	-7.26	102.92	108.00
1	P	869	DG	N3-C2-N2	7.25	124.98	119.90
1	P	870	DA	C5-N7-C8	-7.17	100.31	103.90
3	A	337	ARG	NE-CZ-NH1	7.15	123.88	120.30
3	A	103	ARG	NH1-CZ-NH2	7.12	127.24	119.40
2	T	842	DG	P-O5'-C5'	7.07	132.21	120.90
2	T	843	DG	N9-C1'-C2'	-7.06	99.19	112.60
2	T	845	DC	C4-C5-C6	7.04	120.92	117.40
2	T	846	DC	O4'-C1'-N1	-7.03	103.08	108.00
3	A	304	GLU	OE1-CD-OE2	6.95	131.64	123.30
1	P	870	DA	OP2-P-O3'	6.93	120.44	105.20
2	T	844	DT	N1-C2-O2	-6.84	117.63	123.10
2	T	846	DC	C4-C5-C6	6.82	120.81	117.40
1	P	872	DC	O4'-C1'-N1	-6.79	103.24	108.00
2	T	841	DG	O5'-P-OP1	-6.76	99.61	105.70
2	T	839	DT	N1-C2-O2	-6.74	117.71	123.10
2	T	842	DG	C5-C6-N1	6.73	114.87	111.50
2	T	842	DG	C4'-C3'-C2'	-6.71	97.06	103.10
3	A	343	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	P	869	DG	C5-N7-C8	-6.60	101.00	104.30
1	P	867	DA	C5'-C4'-C3'	6.59	125.96	114.10
2	T	847	DT	C6-N1-C2	-6.58	118.01	121.30
1	P	872	DC	C4'-C3'-O3'	6.56	126.10	109.70
2	T	843	DG	O5'-P-OP2	-6.37	99.97	105.70
3	A	98	ASP	CB-CG-OD2	6.36	124.02	118.30
1	P	869	DG	N3-C4-N9	-6.33	122.20	126.00
3	A	83	ASP	CB-CG-OD2	6.31	123.98	118.30
3	A	357	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	T	846	DC	O3'-P-O5'	-6.28	92.07	104.00
2	T	846	DC	C2-N3-C4	6.28	123.04	119.90
3	A	123	LEU	CB-CG-CD2	6.27	121.66	111.00
2	T	843	DG	N3-C4-N9	-6.24	122.25	126.00
2	T	843	DG	N9-C4-C5	6.17	107.87	105.40
3	A	387	LEU	N-CA-C	6.16	127.63	111.00
2	T	839	DT	O5'-C5'-C4'	-6.11	95.72	111.00
2	T	844	DT	OP2-P-O3'	6.08	118.57	105.20
1	P	870	DA	N1-C2-N3	6.08	132.34	129.30
1	P	870	DA	OP1-P-O3'	6.07	118.56	105.20
2	T	842	DG	C5'-C4'-C3'	-6.05	103.21	114.10
1	P	868	DG	N9-C4-C5	-6.01	103.00	105.40
2	T	844	DT	C5'-C4'-C3'	-5.99	103.32	114.10
2	T	839	DT	C5'-C4'-C3'	-5.99	103.33	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	868	DG	C4-C5-N7	5.98	113.19	110.80
3	A	382	PRO	CA-C-N	-5.94	104.14	117.20
1	P	868	DG	N3-C2-N2	-5.91	115.76	119.90
2	T	844	DT	O4'-C1'-C2'	-5.89	101.19	105.90
2	T	839	DT	O4'-C1'-C2'	-5.87	101.20	105.90
1	P	867	DA	C6-C5-N7	-5.83	128.22	132.30
3	A	101	ARG	CG-CD-NE	5.81	124.01	111.80
3	A	308	PHE	N-CA-C	-5.73	95.53	111.00
3	A	392	ARG	C-N-CA	-5.71	107.43	121.70
1	P	870	DA	OP1-P-OP2	5.70	128.15	119.60
3	A	217	GLN	N-CA-CB	-5.68	100.37	110.60
2	T	843	DG	P-O3'-C3'	5.67	126.50	119.70
1	P	867	DA	C4-C5-C6	5.65	119.82	117.00
2	T	845	DC	C3'-C2'-C1'	-5.64	95.74	102.50
1	P	870	DA	C3'-C2'-C1'	5.60	109.22	102.50
1	P	868	DG	O4'-C1'-N9	5.58	111.90	108.00
3	A	215	PRO	C-N-CA	-5.56	107.81	121.70
3	A	324	LEU	CB-CG-CD1	5.55	120.43	111.00
2	T	841	DG	C6-N1-C2	-5.50	121.80	125.10
3	A	214	LYS	CA-C-O	-5.48	108.59	120.10
3	A	347	ARG	CB-CA-C	5.48	121.36	110.40
3	A	126	ASP	CB-CG-OD2	5.48	123.23	118.30
1	P	868	DG	C3'-C2'-C1'	-5.46	95.94	102.50
2	T	843	DG	C4'-C3'-O3'	5.45	123.33	109.70
1	P	872	DC	C1'-O4'-C4'	-5.44	104.66	110.10
1	P	868	DG	C1'-O4'-C4'	-5.41	104.69	110.10
2	T	842	DG	N1-C2-N2	-5.41	111.33	116.20
1	P	870	DA	P-O5'-C5'	-5.39	112.28	120.90
2	T	842	DG	N1-C6-O6	-5.38	116.67	119.90
3	A	389	LYS	N-CA-C	-5.37	96.50	111.00
1	P	872	DC	C5-C4-N4	-5.33	116.47	120.20
1	P	869	DG	C5-C6-O6	5.32	131.79	128.60
2	T	844	DT	C3'-C2'-C1'	5.31	108.87	102.50
2	T	839	DT	C3'-C2'-C1'	5.31	108.87	102.50
3	A	404	THR	C-N-CA	5.31	134.97	121.70
3	A	383	MET	N-CA-C	5.30	125.32	111.00
1	P	868	DG	C6-C5-N7	-5.30	127.22	130.40
3	A	258	VAL	CG1-CB-CG2	-5.29	102.44	110.90
3	A	139	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	P	871	DC	N1-C2-O2	-5.27	115.74	118.90
2	T	847	DT	C6-C5-C7	-5.25	119.75	122.90
2	T	847	DT	N1-C2-O2	-5.24	118.91	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	872	DC	C4-C5-C6	5.21	120.00	117.40
2	T	844	DT	P-O3'-C3'	-5.18	113.48	119.70
3	A	329	LEU	CB-CG-CD1	5.18	119.80	111.00
3	A	254	GLY	N-CA-C	5.15	125.97	113.10
1	P	872	DC	C4'-C3'-C2'	-5.12	98.50	103.10
2	T	843	DG	C1'-O4'-C4'	-5.10	105.00	110.10
3	A	167	ASP	CB-CG-OD2	5.08	122.88	118.30
3	A	384	VAL	CB-CA-C	-5.06	101.78	111.40
3	A	216	ASN	N-CA-C	-5.06	97.34	111.00
1	P	870	DA	C5'-C4'-O4'	-5.05	99.71	109.30
1	P	869	DG	OP1-P-OP2	5.04	127.16	119.60
3	A	204	LEU	CB-CA-C	-5.04	100.63	110.20
2	T	842	DG	N3-C2-N2	5.04	123.42	119.90
3	A	405	LEU	N-CA-C	5.03	124.57	111.00
3	A	390	LEU	CB-CG-CD2	-5.01	102.47	111.00
3	A	205	LEU	CB-CG-CD1	5.01	119.51	111.00
1	P	869	DG	C4'-C3'-C2'	-5.00	98.60	103.10
3	A	302	PHE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	299	PRO	Mainchain
3	A	313	SER	Peptide
3	A	380	MET	Peptide
3	A	383	MET	Peptide
3	A	390	LEU	Peptide
1	P	868	DG	Sidechain
1	P	871	DC	Sidechain
2	T	843	DG	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	139	0	79	2	2
2	T	184	0	104	7	2
3	A	2871	0	2894	122	0
4	A	2	0	0	0	0
5	A	28	0	12	0	0
6	A	107	0	0	4	0
6	P	3	0	0	1	0
6	T	12	0	0	0	0
All	All	3346	0	3089	129	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:122:ARG:CD	3:A:122:ARG:CG	1.77	1.57
3:A:105:MET:SD	3:A:105:MET:CG	2.07	1.42
2:T:847:DT:O3'	2:T:847:DT:C3'	1.72	1.37
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.33	1.10
3:A:383:MET:O	3:A:387:LEU:HG	1.54	1.06
3:A:308:PHE:O	3:A:308:PHE:HD1	1.47	0.97
3:A:122:ARG:CG	3:A:122:ARG:NE	2.29	0.95
3:A:380:MET:C	3:A:382:PRO:HD2	1.86	0.95
3:A:348:ARG:NH1	3:A:358:GLU:OE2	2.02	0.93
3:A:381:THR:N	3:A:382:PRO:CD	2.35	0.88
2:T:842:DG:H2''	2:T:843:DG:H5'	1.54	0.86
3:A:379:VAL:C	3:A:382:PRO:HD2	1.94	0.86
3:A:283:LYS:HE3	3:A:288:GLU:OE1	1.77	0.84
3:A:381:THR:N	3:A:382:PRO:HD2	1.93	0.84
3:A:344:LEU:CD1	3:A:387:LEU:HD22	2.08	0.83
3:A:249:CYS:O	3:A:253:LEU:HD12	1.79	0.83
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.12	0.80
3:A:122:ARG:CB	3:A:122:ARG:CD	2.59	0.80
3:A:379:VAL:O	3:A:382:PRO:HD2	1.83	0.77
3:A:80:ASN:ND2	3:A:83:ASP:CG	2.37	0.77
3:A:308:PHE:CD1	3:A:308:PHE:O	2.35	0.76
2:T:847:DT:H3'	2:T:847:DT:O3'	1.85	0.76
2:T:841:DG:OP2	3:A:307:SER:HB2	1.86	0.75
3:A:331:ARG:HD2	6:A:1014:HOH:O	1.86	0.74
3:A:344:LEU:HD11	3:A:387:LEU:CD2	2.16	0.74
3:A:380:MET:C	3:A:382:PRO:CD	2.57	0.73
3:A:348:ARG:NH1	3:A:358:GLU:OE1	2.22	0.72
3:A:304:GLU:O	3:A:407:SER:HB2	1.92	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:348:ARG:NH1	3:A:358:GLU:CD	2.46	0.68
3:A:325:LEU:HD11	3:A:387:LEU:HD11	1.74	0.68
3:A:312:SER:O	3:A:312:SER:OG	2.08	0.67
3:A:347:ARG:HD3	3:A:404:THR:HG23	1.78	0.66
3:A:80:ASN:HD21	3:A:83:ASP:CG	1.98	0.66
3:A:325:LEU:HD11	3:A:387:LEU:CD1	2.27	0.65
3:A:390:LEU:O	3:A:394:MET:HG3	1.96	0.65
3:A:345:ILE:HG12	3:A:359:SER:HB3	1.80	0.64
3:A:405:LEU:C	3:A:406:LEU:HD23	2.18	0.64
3:A:308:PHE:CE1	3:A:405:LEU:HA	2.34	0.62
3:A:196:CYS:SG	3:A:214:LYS:O	2.57	0.62
3:A:379:VAL:O	3:A:382:PRO:CD	2.47	0.62
3:A:389:LYS:O	3:A:392:ARG:N	2.30	0.61
3:A:270:GLU:OE2	3:A:275:ILE:HD12	2.01	0.61
3:A:385:ASP:O	3:A:386:ILE:C	2.39	0.60
3:A:388:MET:O	3:A:391:PHE:HB3	2.01	0.60
3:A:202:ASN:C	3:A:202:ASN:HD22	2.06	0.59
3:A:379:VAL:O	3:A:382:PRO:CG	2.51	0.58
3:A:392:ARG:C	3:A:394:MET:H	2.07	0.57
2:T:841:DG:H2''	2:T:842:DG:H5''	1.86	0.57
3:A:343:ARG:HD2	3:A:345:ILE:HD11	1.87	0.57
3:A:347:ARG:NH1	3:A:404:THR:OG1	2.28	0.56
3:A:164:ASN:H	3:A:170:HIS:HD2	1.53	0.56
3:A:251:GLU:O	3:A:253:LEU:N	2.38	0.56
3:A:249:CYS:O	3:A:253:LEU:CD1	2.54	0.55
3:A:368:VAL:HG21	3:A:383:MET:CE	2.37	0.55
3:A:347:ARG:HD3	3:A:404:THR:CG2	2.37	0.54
3:A:346:ILE:HG22	3:A:406:LEU:HD22	1.89	0.54
3:A:379:VAL:C	3:A:382:PRO:CD	2.72	0.54
3:A:105:MET:CE	3:A:105:MET:CG	2.83	0.53
3:A:290:ASN:ND2	6:A:913:HOH:O	2.42	0.53
3:A:360:ARG:HG2	3:A:394:MET:SD	2.48	0.53
3:A:387:LEU:O	3:A:391:PHE:HB2	2.07	0.53
3:A:202:ASN:ND2	3:A:205:LEU:H	2.07	0.52
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.90	0.52
3:A:360:ARG:HG2	3:A:394:MET:CG	2.40	0.52
2:T:847:DT:HO3'	2:T:847:DT:C3'	2.15	0.52
3:A:380:MET:CE	3:A:384:VAL:CG2	2.86	0.51
3:A:251:GLU:O	3:A:252:ALA:C	2.47	0.51
3:A:360:ARG:HG2	3:A:394:MET:HG2	1.93	0.51
3:A:105:MET:SD	3:A:105:MET:CB	2.94	0.51
1:P:868:DG:N7	6:P:914:HOH:O	2.34	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:343:ARG:HG2	3:A:344:LEU:N	2.24	0.51
3:A:315:VAL:O	3:A:316:GLU:C	2.49	0.50
3:A:308:PHE:HZ	3:A:406:LEU:HG	1.77	0.50
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.94	0.50
3:A:362:CYS:SG	3:A:390:LEU:HD11	2.52	0.50
3:A:392:ARG:C	3:A:394:MET:N	2.66	0.49
3:A:58:GLN:NE2	6:A:996:HOH:O	2.46	0.49
3:A:380:MET:O	3:A:381:THR:C	2.51	0.49
3:A:347:ARG:HB2	3:A:356:GLY:O	2.13	0.48
3:A:332:VAL:HG13	3:A:339:PRO:HD3	1.95	0.48
3:A:196:CYS:HA	3:A:217:GLN:O	2.14	0.48
3:A:283:LYS:HE2	3:A:288:GLU:HB3	1.95	0.48
3:A:380:MET:HE2	3:A:384:VAL:HG23	1.92	0.47
3:A:379:VAL:O	3:A:382:PRO:HG2	2.13	0.47
3:A:251:GLU:C	3:A:253:LEU:N	2.66	0.47
3:A:105:MET:CE	3:A:105:MET:CB	2.92	0.47
3:A:344:LEU:HD13	3:A:390:LEU:HB3	1.97	0.47
3:A:103:ARG:CZ	3:A:331:ARG:NH1	2.77	0.47
3:A:380:MET:O	3:A:382:PRO:N	2.48	0.47
3:A:406:LEU:N	3:A:406:LEU:HD23	2.30	0.47
3:A:80:ASN:HD22	3:A:83:ASP:CG	2.19	0.46
3:A:73:LEU:HD22	3:A:88:CYS:SG	2.56	0.46
3:A:105:MET:HB2	3:A:105:MET:CE	2.46	0.45
3:A:36:ASP:O	3:A:37:CYS:C	2.55	0.45
3:A:348:ARG:CZ	3:A:358:GLU:OE2	2.61	0.45
3:A:380:MET:O	3:A:383:MET:HB2	2.16	0.45
3:A:236:ILE:HD13	3:A:236:ILE:HG21	1.72	0.45
3:A:76:LYS:HB2	3:A:79:MET:HE3	1.99	0.45
3:A:334:GLN:HB3	3:A:334:GLN:HE21	1.63	0.45
3:A:404:THR:OG1	3:A:405:LEU:N	2.49	0.45
3:A:76:LYS:HB2	3:A:79:MET:CE	2.47	0.44
3:A:380:MET:N	3:A:382:PRO:HD2	2.33	0.44
3:A:270:GLU:OE2	3:A:275:ILE:CD1	2.65	0.44
3:A:315:VAL:O	3:A:318:LYS:HB3	2.17	0.44
3:A:122:ARG:HD3	6:A:957:HOH:O	2.18	0.43
3:A:31:VAL:HG12	3:A:130:VAL:HB	1.99	0.43
3:A:144:GLN:HG3	3:A:147:GLU:HG2	2.00	0.43
3:A:184:ARG:HA	3:A:187:MET:HE2	2.00	0.43
3:A:332:VAL:HG12	3:A:333:CYS:N	2.33	0.43
3:A:266:PRO:O	3:A:270:GLU:HB2	2.18	0.42
2:T:842:DG:H4'	3:A:99:LEU:HD12	2.02	0.42
3:A:112:LEU:HD23	3:A:112:LEU:C	2.40	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:391:PHE:O	3:A:394:MET:HB2	2.19	0.42
3:A:359:SER:O	3:A:360:ARG:HD3	2.18	0.42
3:A:103:ARG:CZ	3:A:331:ARG:CZ	2.98	0.41
3:A:368:VAL:HG21	3:A:383:MET:HE2	2.03	0.41
3:A:389:LYS:HA	3:A:392:ARG:HD2	2.01	0.41
3:A:214:LYS:N	3:A:215:PRO:CD	2.82	0.41
3:A:335:ASP:OD2	3:A:337:ARG:NH1	2.53	0.41
3:A:386:ILE:C	3:A:390:LEU:HD12	2.41	0.41
3:A:204:LEU:HD13	3:A:205:LEU:HD13	2.02	0.41
3:A:144:GLN:O	3:A:146:ASP:N	2.53	0.41
3:A:382:PRO:CG	3:A:383:MET:H	2.33	0.41
3:A:308:PHE:CD1	3:A:404:THR:O	2.74	0.41
3:A:380:MET:CE	3:A:384:VAL:HG22	2.50	0.40
1:P:869:DG:H2'	1:P:869:DG:O5'	2.21	0.40
3:A:69:GLU:O	3:A:73:LEU:CD1	2.69	0.40
3:A:202:ASN:C	3:A:202:ASN:ND2	2.74	0.40
3:A:380:MET:C	3:A:382:PRO:N	2.73	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:867:DA:O5'	2:T:847:DT:O3'[10.665]	0.70	1.50
1:P:867:DA:C5'	2:T:847:DT:O3'[10.665]	1.75	0.45

5.3 Torsion angles

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	366/420 (87%)	328 (90%)	26 (7%)	12 (3%)	6 3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	314	GLU

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	321/376 (85%)	284 (88%)	37 (12%)	8 8

All (37) 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	87	LYS
3	A	90	GLN
3	A	123	LEU
3	A	126	ASP
3	A	142	GLN
3	A	145	SER
3	A	170	HIS
3	A	172	ARG
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	229	LEU

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Mol	Chain	Res	Type
3	A	295	LEU
3	A	307	SER
3	A	308	PHE
3	A	312	SER
3	A	313	SER
3	A	318	LYS
3	A	320	LYS
3	A	334	GLN
3	A	344	LEU
3	A	347	ARG
3	A	348	ARG
3	A	357	ARG
3	A	362	CYS
3	A	380	MET
3	A	385	ASP
3	A	387	LEU
3	A	390	LEU
3	A	404	THR
3	A	406	LEU
3	A	413	LEU

Some 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	170	HIS
3	A	202	ASN
3	A	262	GLN
3	A	279	GLN
3	A	334	GLN
3	A	340	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	17,19,20	1.99	5 (29%)	20,26,29	4.02	8 (40%)
2	EDA	T	840	2	24,26,27	2.23	8 (33%)	32,38,41	2.39	10 (31%)

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	-	0/5/18/19	0/2/2/2
2	EDA	T	840	2	-	0/6/21/22	0/1/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	840	EDA	C6-N6	-4.55	1.29	1.33
2	T	840	EDA	C4-N9	-4.46	1.31	1.37
2	T	840	EDA	C5-C6	-4.35	1.33	1.40
1	P	873	DOC	C3'-C2'	-4.19	1.41	1.54
1	P	873	DOC	O4'-C1'	-3.47	1.34	1.42
1	P	873	DOC	C2'-C1'	3.42	1.61	1.51
2	T	840	EDA	C2-N1	3.10	1.42	1.38
2	T	840	EDA	C2'-C3'	-2.90	1.44	1.52
1	P	873	DOC	C4-N3	2.71	1.40	1.35
2	T	840	EDA	C5-N7	-2.61	1.30	1.40
2	T	840	EDA	C2'-C1'	2.60	1.59	1.52
1	P	873	DOC	O4'-C4'	2.31	1.49	1.44
2	T	840	EDA	C10-N1	-2.17	1.34	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	873	DOC	C4'-O4'-C1'	-12.71	104.75	110.05
1	P	873	DOC	C6-C5-C4	-6.89	114.61	117.47
2	T	840	EDA	C11-N6-C6	6.45	112.07	103.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	840	EDA	C2-N1-C6	-5.79	118.57	122.22
1	P	873	DOC	C2-N3-C4	5.13	123.00	115.57
1	P	873	DOC	O4'-C4'-C5'	4.80	116.38	109.67
2	T	840	EDA	N6-C6-N1	-4.73	105.74	112.70
1	P	873	DOC	O4'-C4'-C3'	3.81	111.21	104.80
1	P	873	DOC	C5-C6-N1	3.48	125.15	121.21
1	P	873	DOC	C2'-C1'-N1	-3.44	105.78	112.66
2	T	840	EDA	N3-C4-N9	3.37	131.51	125.43
2	T	840	EDA	C2-N3-C4	3.30	121.87	116.23
2	T	840	EDA	C4'-O4'-C1'	-3.02	101.79	109.44
1	P	873	DOC	P-O5'-C5'	-3.02	111.40	123.19
2	T	840	EDA	C5'-C4'-C3'	-2.95	96.30	114.76
2	T	840	EDA	O4'-C4'-C3'	2.60	112.25	105.66
2	T	840	EDA	O4'-C4'-C5'	2.58	118.56	109.36
2	T	840	EDA	C10-N1-C2	2.30	134.11	130.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	29,29,29	1.87	9 (31%)	42,45,45	1.80	10 (23%)

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	-	0/19/34/34	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	DCP	PB-O3B	3.50	1.66	1.59
5	A	875	DCP	O4'-C1'	3.16	1.49	1.42
5	A	875	DCP	PB-O3A	-3.03	1.54	1.59
5	A	875	DCP	C2'-C1'	2.90	1.60	1.52
5	A	875	DCP	C3'-C4'	2.84	1.61	1.53
5	A	875	DCP	C4-N3	2.66	1.40	1.35
5	A	875	DCP	PA-O2A	2.50	1.66	1.55
5	A	875	DCP	O2-C2	2.41	1.28	1.23
5	A	875	DCP	PA-O3A	2.26	1.64	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	875	DCP	C6-C5-C4	-6.06	114.95	117.47
5	A	875	DCP	C2-N3-C4	4.17	121.61	115.57
5	A	875	DCP	C5-C6-N1	3.70	125.40	121.21
5	A	875	DCP	C6-N1-C1'	2.78	125.81	119.35
5	A	875	DCP	C2-N1-C1'	-2.70	116.10	119.25
5	A	875	DCP	O2B-PB-O3A	2.50	117.01	105.14
5	A	875	DCP	O2G-PG-O1G	-2.38	102.67	110.44
5	A	875	DCP	O2A-PA-O5'	2.30	120.11	108.51
5	A	875	DCP	PB-O3B-PG	-2.27	125.03	131.68
5	A	875	DCP	O2B-PB-O3B	2.00	114.65	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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	P	7/7 (100%)	0.16	0 100 100	19, 26, 33, 35	0
2	T	9/9 (100%)	0.47	1 (11%) 6 9	17, 20, 34, 77	0
3	A	372/420 (88%)	0.77	62 (16%) 2 4	5, 32, 74, 96	0
All	All	388/436 (88%)	0.75	63 (16%) 2 4	5, 31, 74, 96	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	355	TYR	19.7
3	A	354	HIS	16.4
3	A	352	GLU	9.3
3	A	353	LYS	8.6
3	A	383	MET	6.9
3	A	349	TYR	6.7
3	A	311	CYS	6.3
3	A	348	ARG	6.2
3	A	391	PHE	6.1
3	A	350	SER	6.0
3	A	312	SER	5.6
3	A	244	TYR	5.6
3	A	356	GLY	5.5
3	A	314	GLU	5.1
3	A	351	SER	4.8
3	A	368	VAL	4.8
3	A	310	LYS	4.5
3	A	336	GLY	4.4
3	A	387	LEU	4.4
3	A	145	SER	4.2
3	A	268	ILE	4.2
3	A	315	VAL	4.0
3	A	309	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
3	A	249	CYS	3.7
3	A	367	HIS	3.5
3	A	333	CYS	3.4
3	A	385	ASP	3.4
3	A	370	GLN	3.4
3	A	252	ALA	3.3
3	A	273	LEU	3.3
3	A	382	PRO	3.3
3	A	384	VAL	3.1
3	A	406	LEU	3.1
3	A	82	ARG	3.1
3	A	335	ASP	2.9
3	A	329	LEU	2.8
3	A	392	ARG	2.8
3	A	390	LEU	2.8
3	A	235	HIS	2.8
3	A	313	SER	2.8
3	A	267	LYS	2.7
3	A	317	ALA	2.7
3	A	52	ASP	2.7
3	A	61	TYR	2.6
3	A	50	LEU	2.5
3	A	148	LEU	2.5
2	T	839	DT	2.5
3	A	366	SER	2.5
3	A	73	LEU	2.4
3	A	90	GLN	2.4
3	A	269	LEU	2.3
3	A	319	ASN	2.3
3	A	26	SER	2.3
3	A	279	GLN	2.3
3	A	388	MET	2.2
3	A	276	SER	2.1
3	A	272	GLU	2.1
3	A	334	GLN	2.1
3	A	264	PHE	2.1
3	A	325	LEU	2.1
3	A	53	LYS	2.0
3	A	254	GLY	2.0
3	A	293	VAL	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	DOC	P	873	18/19	0.18	2.00	13,18,26,26	0
2	EDA	T	840	23/24	0.14	-0.45	18,30,52,59	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	A	872	1/1	0.22	6.15	68,68,68,68	0
5	DCP	A	875	28/28	0.12	-0.21	13,20,25,26	0
4	MG	A	871	1/1	0.06	-1.63	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.