Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 08:11 PM EDT

PDB ID	:	2FLL
Title	:	Ternary complex of human DNA polymerase iota with DNA and dTTP
Authors	:	Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on	:	2006-01-06
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

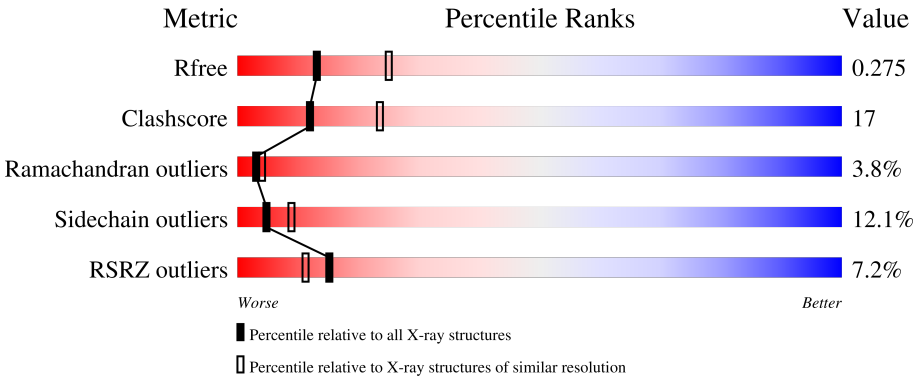
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	P	7	14% 71% 14%
2	T	11	9% 27% 45% 9% 18%
3	A	420	6% 45% 31% 10% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3309 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 DNA primer strand.

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 DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	9	Total	C	N	O	P	0	0	0
			182	88	32	54	8			

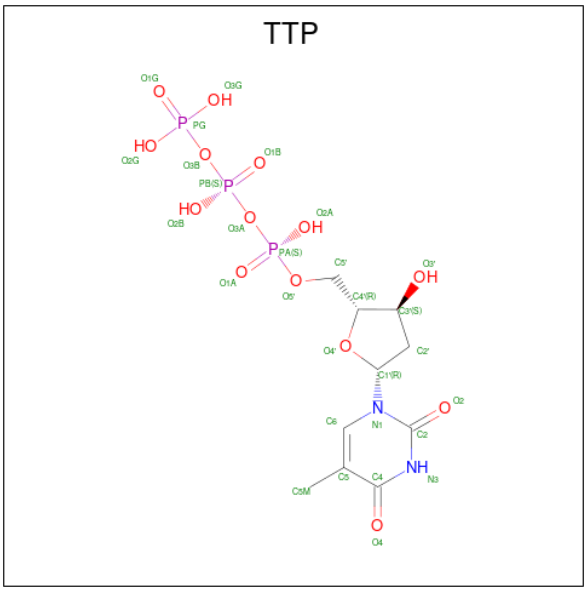
- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	373	Total	C	N	O	S	0	0	0
			2866	1802	502	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 THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



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

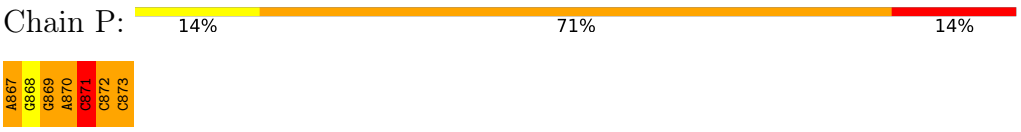
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	5	Total	O	0	0
			5	5		
6	A	86	Total	O	0	0
			86	86		

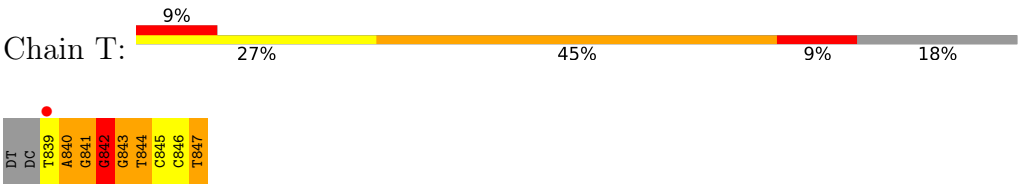
3 Residue-property plots (i)

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.

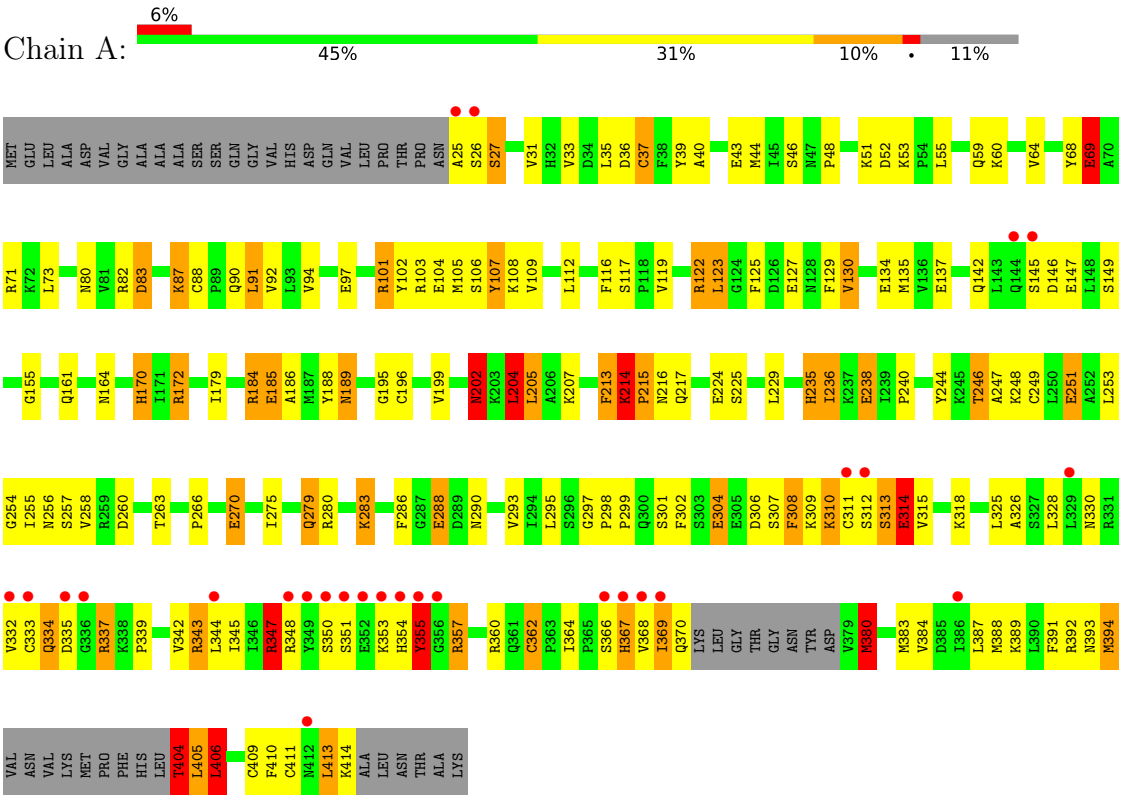
• Molecule 1: DNA primer strand



• Molecule 2: DNA template strand



• Molecule 3: DNA polymerase iota



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.33Å 98.33Å 202.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 39.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (50.00-2.60) 94.2 (39.72-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.29 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.277 0.219 , 0.275	Depositor DCC
R_{free} test set	1450 reflections (7.84%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3309	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TTP, 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	P	3.94	22/136 (16.2%)	3.71	32/208 (15.4%)
2	T	4.48	44/203 (21.7%)	3.39	34/312 (10.9%)
3	A	1.97	85/2904 (2.9%)	1.42	27/3922 (0.7%)
All	All	2.32	151/3243 (4.7%)	1.80	93/4442 (2.1%)

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	2
3	A	0	2
All	All	0	6

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	844	DT	C5-C7	17.14	1.60	1.50
1	P	869	DG	N7-C5	15.94	1.48	1.39
2	T	840	DA	N7-C5	-15.46	1.29	1.39
2	T	843	DG	O4'-C1'	-15.05	1.24	1.42
2	T	839	DT	N1-C6	13.71	1.47	1.38
2	T	847	DT	C5-C7	13.50	1.58	1.50
1	P	872	DC	N3-C4	11.20	1.41	1.33
1	P	872	DC	O4'-C1'	-10.83	1.29	1.42
2	T	840	DA	C6-N1	10.63	1.43	1.35
2	T	844	DT	N3-C4	-9.97	1.30	1.38
1	P	870	DA	C2'-C1'	9.74	1.62	1.52
1	P	867	DA	N7-C5	-9.27	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	868	DG	N3-C4	9.27	1.42	1.35
3	A	103	ARG	CZ-NH2	8.88	1.44	1.33
2	T	847	DT	O4'-C1'	-8.82	1.31	1.42
1	P	871	DC	C3'-O3'	-8.71	1.32	1.44
2	T	846	DC	C2'-C1'	8.65	1.60	1.52
2	T	839	DT	O3'-P	8.64	1.71	1.61
1	P	872	DC	C3'-O3'	-8.59	1.32	1.44
1	P	872	DC	P-O5'	8.51	1.68	1.59
2	T	845	DC	O4'-C1'	-8.38	1.32	1.42
3	A	288	GLU	CD-OE2	8.27	1.34	1.25
3	A	186	ALA	CA-CB	-8.23	1.35	1.52
3	A	94	VAL	CB-CG2	-7.94	1.36	1.52
3	A	39	TYR	CB-CG	7.79	1.63	1.51
1	P	871	DC	O3'-P	7.66	1.70	1.61
3	A	185	GLU	CD-OE2	7.61	1.34	1.25
2	T	840	DA	N9-C8	-7.54	1.31	1.37
1	P	871	DC	O4'-C1'	-7.51	1.33	1.42
3	A	214	LYS	CA-C	-7.46	1.33	1.52
2	T	841	DG	C5-C4	-7.45	1.33	1.38
2	T	843	DG	C4'-O4'	7.42	1.52	1.45
3	A	189	ASN	CB-CG	7.42	1.68	1.51
3	A	304	GLU	CD-OE1	7.39	1.33	1.25
3	A	310	LYS	CA-CB	7.24	1.69	1.53
2	T	846	DC	N3-C4	7.23	1.39	1.33
3	A	39	TYR	CD2-CE2	-7.21	1.28	1.39
3	A	25	ALA	CA-CB	7.21	1.67	1.52
3	A	389	LYS	CA-CB	7.19	1.69	1.53
1	P	867	DA	C4'-O4'	7.14	1.52	1.45
3	A	286	PHE	CD1-CE1	7.13	1.53	1.39
3	A	184	ARG	CD-NE	-7.06	1.34	1.46
2	T	844	DT	O3'-P	7.05	1.69	1.61
3	A	405	LEU	CA-CB	-6.92	1.37	1.53
2	T	839	DT	C3'-O3'	6.89	1.52	1.44
3	A	64	VAL	CB-CG1	6.89	1.67	1.52
3	A	216	ASN	N-CA	6.87	1.60	1.46
3	A	283	LYS	CE-NZ	6.78	1.66	1.49
2	T	843	DG	C2'-C1'	6.75	1.59	1.52
3	A	134	GLU	CD-OE1	6.64	1.32	1.25
2	T	841	DG	C5'-C4'	-6.59	1.44	1.51
2	T	846	DC	C5-C6	6.59	1.39	1.34
3	A	380	MET	CG-SD	6.57	1.98	1.81
3	A	302	PHE	CD1-CE1	6.56	1.52	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	104	GLU	CD-OE2	6.54	1.32	1.25
1	P	870	DA	C4'-O4'	6.51	1.51	1.45
3	A	107	TYR	CD2-CE2	-6.50	1.29	1.39
3	A	248	LYS	CD-CE	6.47	1.67	1.51
3	A	116	PHE	C-O	-6.43	1.11	1.23
3	A	297	GLY	N-CA	-6.40	1.36	1.46
3	A	129	PHE	CD1-CE1	6.39	1.52	1.39
3	A	117	SER	CB-OG	6.34	1.50	1.42
3	A	155	GLY	CA-C	6.30	1.61	1.51
2	T	840	DA	P-O5'	6.25	1.66	1.59
2	T	842	DG	C4'-O4'	6.22	1.51	1.45
3	A	108	LYS	CE-NZ	6.20	1.64	1.49
3	A	290	ASN	CB-CG	6.17	1.65	1.51
3	A	286	PHE	CE2-CZ	6.16	1.49	1.37
3	A	293	VAL	CB-CG1	-6.12	1.40	1.52
1	P	872	DC	C2-N3	-6.08	1.30	1.35
2	T	839	DT	C4'-C3'	6.06	1.59	1.53
1	P	872	DC	C3'-C2'	-6.06	1.45	1.52
3	A	82	ARG	CA-CB	6.04	1.67	1.53
3	A	102	TYR	CG-CD2	6.03	1.47	1.39
3	A	27	SER	C-O	-6.02	1.11	1.23
3	A	147	GLU	CG-CD	6.02	1.60	1.51
3	A	362	CYS	CB-SG	-6.02	1.72	1.82
2	T	843	DG	P-O5'	5.99	1.65	1.59
1	P	867	DA	C6-N6	-5.97	1.29	1.33
2	T	845	DC	C3'-O3'	5.96	1.51	1.44
2	T	844	DT	C3'-O3'	-5.93	1.36	1.44
2	T	844	DT	P-OP1	-5.92	1.38	1.49
2	T	839	DT	C5'-C4'	5.90	1.57	1.51
3	A	258	VAL	CB-CG2	-5.89	1.40	1.52
2	T	839	DT	O5'-C5'	5.86	1.56	1.42
2	T	840	DA	N9-C4	-5.86	1.34	1.37
3	A	213	PHE	CG-CD2	5.85	1.47	1.38
2	T	842	DG	C4'-C3'	-5.84	1.46	1.52
3	A	122	ARG	CZ-NH1	-5.83	1.25	1.33
3	A	263	THR	C-O	-5.83	1.12	1.23
1	P	872	DC	P-OP2	-5.82	1.39	1.49
3	A	355	TYR	CA-CB	5.82	1.66	1.53
3	A	225	SER	CB-OG	5.82	1.49	1.42
2	T	839	DT	C2-N3	5.78	1.42	1.37
3	A	199	VAL	CA-CB	-5.70	1.42	1.54
2	T	840	DA	N3-C4	5.69	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	845	DC	C4-C5	5.66	1.47	1.43
2	T	844	DT	N1-C2	-5.65	1.33	1.38
3	A	172	ARG	CZ-NH2	5.61	1.40	1.33
3	A	44	MET	SD-CE	-5.60	1.46	1.77
1	P	871	DC	C3'-C2'	-5.60	1.45	1.52
3	A	279	GLN	CG-CD	5.55	1.63	1.51
3	A	109	VAL	CA-CB	-5.54	1.43	1.54
3	A	40	ALA	CA-CB	-5.54	1.40	1.52
3	A	172	ARG	CD-NE	-5.52	1.37	1.46
2	T	842	DG	O3'-P	-5.51	1.54	1.61
3	A	257	SER	CB-OG	-5.51	1.35	1.42
2	T	839	DT	N3-C4	5.51	1.43	1.38
3	A	283	LYS	CD-CE	5.50	1.65	1.51
3	A	288	GLU	CD-OE1	5.46	1.31	1.25
3	A	255	ILE	CA-CB	-5.45	1.42	1.54
2	T	846	DC	P-OP1	-5.43	1.39	1.49
3	A	251	GLU	CD-OE2	5.42	1.31	1.25
3	A	105	MET	CG-SD	5.41	1.95	1.81
2	T	846	DC	C3'-C2'	5.40	1.58	1.52
3	A	125	PHE	CG-CD2	-5.40	1.30	1.38
3	A	130	VAL	CB-CG2	-5.37	1.41	1.52
3	A	188	TYR	CD2-CE2	-5.36	1.31	1.39
3	A	104	GLU	CG-CD	5.35	1.59	1.51
2	T	839	DT	O4'-C1'	5.32	1.48	1.42
3	A	238	GLU	CG-CD	5.32	1.59	1.51
1	P	871	DC	C1'-N1	5.32	1.56	1.49
3	A	244	TYR	CG-CD2	5.31	1.46	1.39
3	A	280	ARG	CZ-NH2	5.31	1.40	1.33
3	A	304	GLU	CD-OE2	5.30	1.31	1.25
2	T	839	DT	N1-C2	5.29	1.42	1.38
3	A	46	SER	CB-OG	-5.29	1.35	1.42
1	P	872	DC	C5-C6	-5.28	1.30	1.34
3	A	33	VAL	CB-CG2	-5.28	1.41	1.52
1	P	871	DC	N1-C2	-5.27	1.34	1.40
2	T	844	DT	C5-C6	5.27	1.38	1.34
3	A	256	ASN	CB-CG	5.26	1.63	1.51
3	A	188	TYR	CE2-CZ	-5.25	1.31	1.38
3	A	404	THR	CA-CB	5.22	1.67	1.53
3	A	125	PHE	CE2-CZ	-5.21	1.27	1.37
3	A	270	GLU	CG-CD	5.20	1.59	1.51
3	A	122	ARG	CD-NE	-5.20	1.37	1.46
3	A	215	PRO	N-CA	5.20	1.56	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	847	DT	C3'-O3'	5.18	1.50	1.44
3	A	69	GLU	CG-CD	5.17	1.59	1.51
3	A	410	PHE	CE1-CZ	-5.16	1.27	1.37
3	A	125	PHE	CE1-CZ	5.14	1.47	1.37
3	A	409	CYS	CB-SG	-5.14	1.73	1.81
3	A	103	ARG	CG-CD	5.12	1.64	1.51
3	A	314	GLU	CB-CG	5.12	1.61	1.52
3	A	101	ARG	CG-CD	5.08	1.64	1.51
3	A	254	GLY	C-O	-5.08	1.15	1.23
3	A	202	ASN	CA-CB	-5.06	1.40	1.53
1	P	869	DG	O3'-P	5.04	1.67	1.61
3	A	213	PHE	C-O	-5.04	1.13	1.23
2	T	842	DG	C2-N3	-5.00	1.28	1.32

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	867	DA	O4'-C4'-C3'	-15.30	96.82	106.00
2	T	840	DA	C8-N9-C4	-13.47	100.41	105.80
2	T	844	DT	C4-C5-C7	12.27	126.36	119.00
2	T	844	DT	C4-C5-C6	-12.02	110.79	118.00
1	P	867	DA	O4'-C1'-N9	11.71	116.20	108.00
3	A	357	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	P	870	DA	O4'-C4'-C3'	10.96	112.58	106.00
2	T	840	DA	OP1-P-OP2	-10.84	103.35	119.60
2	T	847	DT	O4'-C4'-C3'	10.78	112.47	106.00
2	T	843	DG	C4'-C3'-C2'	-10.62	93.54	103.10
2	T	842	DG	C3'-C2'-C1'	10.61	115.23	102.50
3	A	343	ARG	NE-CZ-NH1	10.36	125.48	120.30
2	T	839	DT	P-O3'-C3'	10.01	131.71	119.70
2	T	840	DA	N7-C8-N9	9.75	118.67	113.80
3	A	343	ARG	NE-CZ-NH2	-9.34	115.63	120.30
3	A	184	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	P	867	DA	C8-N9-C4	-9.25	102.10	105.80
3	A	184	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	P	869	DG	P-O3'-C3'	-8.76	109.19	119.70
2	T	842	DG	O4'-C1'-C2'	-8.74	98.91	105.90
2	T	839	DT	O4'-C1'-N1	8.71	114.10	108.00
1	P	867	DA	C1'-O4'-C4'	8.67	118.77	110.10
1	P	871	DC	N3-C4-C5	-8.58	118.47	121.90
1	P	870	DA	N1-C2-N3	8.43	133.51	129.30
3	A	71	ARG	NE-CZ-NH1	8.13	124.36	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	867	DA	O5'-C5'-C4'	8.06	131.16	111.00
2	T	843	DG	O4'-C1'-C2'	-7.79	99.67	105.90
1	P	867	DA	C6-N1-C2	-7.78	113.93	118.60
3	A	122	ARG	NE-CZ-NH2	-7.74	116.43	120.30
3	A	71	ARG	NE-CZ-NH2	-7.70	116.45	120.30
2	T	842	DG	C4'-C3'-C2'	-7.69	96.18	103.10
1	P	872	DC	O4'-C4'-C3'	7.68	110.61	106.00
1	P	867	DA	N1-C6-N6	-7.66	114.01	118.60
1	P	871	DC	C2-N3-C4	7.64	123.72	119.90
1	P	870	DA	C2-N3-C4	-7.47	106.87	110.60
1	P	870	DA	C5-N7-C8	-7.46	100.17	103.90
2	T	842	DG	O4'-C4'-C3'	7.44	110.47	106.00
2	T	846	DC	O4'-C1'-N1	-7.43	102.80	108.00
3	A	357	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	T	844	DT	C5-C6-N1	7.40	128.14	123.70
2	T	847	DT	C4'-C3'-C2'	-7.40	96.44	103.10
1	P	870	DA	N1-C6-N6	7.22	122.93	118.60
1	P	871	DC	O4'-C4'-C3'	7.09	110.25	106.00
2	T	847	DT	C4'-C3'-O3'	7.05	127.32	109.70
2	T	840	DA	N9-C4-C5	6.97	108.59	105.80
1	P	867	DA	P-O3'-C3'	6.96	128.06	119.70
2	T	839	DT	OP1-P-O3'	6.93	120.45	105.20
3	A	122	ARG	NE-CZ-NH1	6.90	123.75	120.30
3	A	394	MET	CB-CA-C	-6.83	96.73	110.40
2	T	844	DT	C5'-C4'-C3'	-6.82	101.82	114.10
1	P	872	DC	C4'-C3'-O3'	6.75	126.58	109.70
3	A	69	GLU	OE1-CD-OE2	-6.71	115.25	123.30
3	A	147	GLU	OE1-CD-OE2	-6.65	115.32	123.30
2	T	839	DT	N3-C4-C5	6.60	119.16	115.20
1	P	867	DA	O4'-C1'-C2'	-6.49	100.70	105.90
3	A	204	LEU	CA-CB-CG	6.40	130.01	115.30
3	A	347	ARG	CB-CA-C	6.35	123.10	110.40
2	T	843	DG	O4'-C4'-C3'	6.25	109.75	106.00
2	T	839	DT	C5-C4-O4	-6.20	120.56	124.90
1	P	870	DA	C5-C6-N6	-6.11	118.81	123.70
1	P	869	DG	C8-N9-C4	6.09	108.84	106.40
2	T	839	DT	O4'-C1'-C2'	6.09	110.77	105.90
1	P	870	DA	OP2-P-O3'	6.06	118.54	105.20
1	P	871	DC	C4'-C3'-O3'	6.04	124.80	109.70
3	A	360	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	P	870	DA	O4'-C1'-C2'	6.03	110.72	105.90
2	T	847	DT	C4-C5-C6	-5.95	114.43	118.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	839	DT	OP2-P-O3'	5.93	118.25	105.20
1	P	867	DA	N9-C4-C5	5.91	108.16	105.80
3	A	347	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	A	337	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	T	845	DC	OP1-P-O3'	-5.82	92.39	105.20
3	A	215	PRO	N-CD-CG	-5.78	94.54	103.20
3	A	260	ASP	CB-CG-OD1	5.72	123.45	118.30
1	P	870	DA	N7-C8-N9	5.69	116.64	113.80
2	T	847	DT	C4-C5-C7	5.66	122.40	119.00
2	T	846	DC	OP1-P-OP2	5.64	128.05	119.60
2	T	840	DA	N1-C2-N3	-5.61	126.49	129.30
1	P	870	DA	C1'-O4'-C4'	-5.61	104.49	110.10
3	A	347	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	T	842	DG	C4'-C3'-O3'	5.47	123.37	109.70
1	P	870	DA	C4-C5-N7	5.46	113.43	110.70
3	A	172	ARG	CG-CD-NE	-5.33	100.62	111.80
1	P	872	DC	C5-C6-N1	5.29	123.64	121.00
1	P	870	DA	N9-C4-C5	-5.24	103.70	105.80
2	T	847	DT	O4'-C1'-C2'	5.22	110.07	105.90
3	A	270	GLU	OE1-CD-OE2	-5.16	117.11	123.30
3	A	204	LEU	CB-CG-CD2	5.08	119.64	111.00
1	P	868	DG	N3-C2-N2	-5.07	116.35	119.90
3	A	215	PRO	CA-C-N	5.04	128.29	117.20
3	A	406	LEU	CB-CG-CD1	5.02	119.54	111.00
3	A	306	ASP	CB-CG-OD1	5.01	122.81	118.30
2	T	841	DG	N7-C8-N9	-5.00	110.60	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	68	TYR	Sidechain
1	P	871	DC	Sidechain
1	P	872	DC	Sidechain
2	T	842	DG	Sidechain
2	T	843	DG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	139	0	77	4	2
2	T	182	0	103	7	2
3	A	2866	0	2888	103	0
4	A	2	0	0	0	0
5	A	29	0	13	0	0
6	A	86	0	0	3	0
6	T	5	0	0	0	0
All	All	3309	0	3081	108	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (108) 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:391:PHE:O	3:A:394:MET:HB2	1.62	0.97
1:P:871:DC:OP1	3:A:246:THR:HG22	1.66	0.93
2:T:841:DG:H2"	2:T:842:DG:H5"	1.52	0.91
3:A:283:LYS:HE3	3:A:288:GLU:OE1	1.73	0.88
3:A:367:HIS:N	3:A:367:HIS:ND1	2.32	0.78
3:A:405:LEU:C	3:A:406:LEU:HD23	2.04	0.78
3:A:308:PHE:HB2	3:A:311:CYS:HB2	1.69	0.75
3:A:335:ASP:OD2	3:A:337:ARG:NH1	2.21	0.73
3:A:413:LEU:N	3:A:413:LEU:CD2	2.52	0.73
3:A:172:ARG:HD3	6:A:912:HOH:O	1.89	0.72
3:A:325:LEU:HD11	3:A:387:LEU:HD11	1.72	0.72
3:A:413:LEU:N	3:A:413:LEU:HD23	2.06	0.71
3:A:202:ASN:HD22	3:A:202:ASN:C	1.94	0.70
3:A:137:GLU:HG2	3:A:172:ARG:HH12	1.58	0.68
3:A:249:CYS:O	3:A:253:LEU:HD12	1.92	0.68
3:A:73:LEU:HD12	3:A:73:LEU:N	2.09	0.67
3:A:119:VAL:HB	6:A:1054:HOH:O	1.94	0.67
3:A:406:LEU:HD23	3:A:406:LEU:N	2.11	0.66
3:A:283:LYS:CE	3:A:288:GLU:OE1	2.43	0.66
3:A:342:VAL:HG21	3:A:387:LEU:HD21	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:344:LEU:HD11	3:A:387:LEU:CD2	2.26	0.65
3:A:325:LEU:HD11	3:A:387:LEU:CD1	2.28	0.62
3:A:137:GLU:HG2	3:A:172:ARG:NH1	2.15	0.62
3:A:202:ASN:HD21	3:A:205:LEU:H	1.49	0.61
3:A:347:ARG:HD3	3:A:404:THR:HG23	1.83	0.60
3:A:88:CYS:SG	3:A:90:GLN:O	2.59	0.60
3:A:202:ASN:ND2	3:A:205:LEU:H	2.00	0.60
1:P:871:DC:OP1	3:A:246:THR:CG2	2.45	0.59
3:A:283:LYS:HE2	3:A:288:GLU:HB3	1.86	0.57
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.86	0.57
3:A:413:LEU:HD23	3:A:413:LEU:H	1.65	0.57
3:A:238:GLU:O	3:A:240:PRO:HD3	2.05	0.56
3:A:337:ARG:HG2	3:A:414:LYS:C	2.26	0.56
3:A:73:LEU:HD12	3:A:73:LEU:H	1.70	0.56
3:A:368:VAL:HG21	3:A:383:MET:CE	2.36	0.55
3:A:369:ILE:O	3:A:369:ILE:HG22	2.06	0.55
2:T:840:DA:OP1	3:A:309:LYS:HE3	2.08	0.53
2:T:841:DG:C2'	2:T:842:DG:H5"	2.32	0.53
3:A:347:ARG:HG2	3:A:404:THR:HG23	1.92	0.52
3:A:332:VAL:CG1	3:A:339:PRO:HD3	2.40	0.52
3:A:161:GLN:NE2	3:A:224:GLU:HB2	2.25	0.51
3:A:189:ASN:HB3	6:A:1028:HOH:O	2.11	0.51
3:A:392:ARG:C	3:A:394:MET:H	2.15	0.50
3:A:325:LEU:O	3:A:326:ALA:C	2.46	0.50
3:A:137:GLU:CG	3:A:172:ARG:HH12	2.25	0.50
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.94	0.49
3:A:196:CYS:SG	3:A:214:LYS:O	2.71	0.49
3:A:266:PRO:O	3:A:270:GLU:HB2	2.13	0.49
2:T:840:DA:H1'	3:A:59:GLN:OE1	2.13	0.48
3:A:83:ASP:O	3:A:87:LYS:HB2	2.14	0.48
3:A:275:ILE:HG12	3:A:279:GLN:NE2	2.27	0.48
3:A:299:PRO:O	3:A:337:ARG:NH2	2.47	0.48
3:A:60:LYS:HZ2	3:A:97:GLU:CD	2.18	0.48
3:A:380:MET:CE	3:A:384:VAL:HG22	2.43	0.48
3:A:170:HIS:HE1	3:A:224:GLU:OE2	1.97	0.47
3:A:202:ASN:C	3:A:202:ASN:ND2	2.62	0.47
3:A:164:ASN:H	3:A:170:HIS:HD2	1.61	0.47
3:A:308:PHE:HB2	3:A:311:CYS:CB	2.42	0.47
3:A:73:LEU:N	3:A:73:LEU:CD1	2.77	0.47
3:A:69:GLU:O	3:A:73:LEU:CD1	2.62	0.47
3:A:344:LEU:HD11	3:A:387:LEU:HD23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:112:LEU:C	3:A:112:LEU:HD23	2.36	0.46
3:A:350:SER:OG	3:A:351:SER:N	2.47	0.46
2:T:844:DT:OP2	3:A:301:SER:OG	2.33	0.46
3:A:106:SER:OG	3:A:122:ARG:NH2	2.48	0.46
3:A:404:THR:O	3:A:405:LEU:CB	2.60	0.46
3:A:235:HIS:HD2	3:A:238:GLU:OE2	1.99	0.45
3:A:184:ARG:HD2	3:A:195:GLY:O	2.17	0.45
3:A:308:PHE:CZ	3:A:405:LEU:HA	2.52	0.45
3:A:43:GLU:OE1	3:A:101:ARG:NH2	2.51	0.44
3:A:51:LYS:C	3:A:53:LYS:H	2.20	0.44
3:A:55:LEU:HD12	3:A:92:VAL:O	2.17	0.44
3:A:170:HIS:CE1	3:A:224:GLU:OE2	2.71	0.44
3:A:308:PHE:CD1	3:A:308:PHE:O	2.69	0.44
3:A:73:LEU:H	3:A:73:LEU:CD1	2.31	0.44
3:A:330:ASN:O	3:A:333:CYS:HB3	2.18	0.44
1:P:873:DOC:OP1	3:A:207:LYS:NZ	2.41	0.44
3:A:388:MET:O	3:A:391:PHE:HB3	2.18	0.44
3:A:88:CYS:O	3:A:91:LEU:HB2	2.17	0.43
3:A:204:LEU:HD13	3:A:205:LEU:HD13	2.00	0.43
3:A:353:LYS:O	3:A:355:TYR:N	2.52	0.43
3:A:196:CYS:HA	3:A:217:GLN:O	2.18	0.43
3:A:283:LYS:HE2	3:A:288:GLU:CB	2.47	0.43
2:T:844:DT:O5'	2:T:844:DT:H2'	2.18	0.43
3:A:369:ILE:C	3:A:370:GLN:CG	2.86	0.43
3:A:31:VAL:HG12	3:A:130:VAL:HB	1.99	0.43
3:A:275:ILE:HG12	3:A:279:GLN:HE21	1.83	0.43
3:A:135:MET:HE2	3:A:179:ILE:HD12	2.01	0.43
3:A:384:VAL:O	3:A:388:MET:HG2	2.19	0.43
3:A:364:ILE:O	3:A:364:ILE:HG22	2.18	0.42
3:A:298:PRO:HA	3:A:299:PRO:HD3	1.84	0.42
2:T:840:DA:N3	2:T:840:DA:H2'	2.35	0.42
3:A:405:LEU:O	3:A:406:LEU:HD23	2.19	0.42
3:A:247:ALA:O	3:A:251:GLU:HG3	2.20	0.42
3:A:308:PHE:CE1	3:A:405:LEU:HA	2.55	0.42
3:A:392:ARG:C	3:A:394:MET:N	2.73	0.42
3:A:123:LEU:O	3:A:127:GLU:HB2	2.20	0.41
3:A:369:ILE:O	3:A:369:ILE:CG2	2.67	0.41
3:A:236:ILE:H	3:A:236:ILE:HG12	1.60	0.41
3:A:334:GLN:HE21	3:A:334:GLN:HB3	1.51	0.41
3:A:342:VAL:CG2	3:A:387:LEU:HD21	2.49	0.41
3:A:343:ARG:HD2	3:A:345:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:36:ASP:O	3:A:37:CYS:C	2.60	0.41
3:A:270:GLU:HG2	3:A:275:ILE:HG13	2.03	0.41
3:A:283:LYS:HD2	3:A:283:LYS:HA	1.88	0.40
1:P:869:DG:H2"	1:P:870:DA:H5'	2.03	0.40
3:A:318:LYS:HB2	3:A:388:MET:CE	2.51	0.40
3:A:107:TYR:OH	3:A:299:PRO:HG3	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:867:DA:O5'	2:T:847:DT:O3'[10_665]	1.65	0.55
1:P:867:DA:C5'	2:T:847:DT:O3'[10_665]	2.02	0.18

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	367/420 (87%)	322 (88%)	31 (8%)	14 (4%)	3 4

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	310	LYS
3	A	313	SER
3	A	314	GLU
3	A	315	VAL
3	A	354	HIS
3	A	355	TYR
3	A	37	CYS
3	A	52	ASP
3	A	215	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	146	ASP
3	A	308	PHE
3	A	393	ASN
3	A	334	GLN
3	A	369	ILE

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	321/376 (85%)	282 (88%)	39 (12%)	5 9

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	26	SER
3	A	27	SER
3	A	35	LEU
3	A	48	PRO
3	A	69	GLU
3	A	80	ASN
3	A	83	ASP
3	A	87	LYS
3	A	91	LEU
3	A	123	LEU
3	A	142	GLN
3	A	145	SER
3	A	149	SER
3	A	170	HIS
3	A	185	GLU
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	214	LYS
3	A	229	LEU
3	A	235	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	236	ILE
3	A	246	THR
3	A	295	LEU
3	A	307	SER
3	A	312	SER
3	A	313	SER
3	A	314	GLU
3	A	347	ARG
3	A	348	ARG
3	A	357	ARG
3	A	362	CYS
3	A	366	SER
3	A	367	HIS
3	A	380	MET
3	A	404	THR
3	A	406	LEU
3	A	411	CYS
3	A	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	ASN
3	A	80	ASN
3	A	170	HIS
3	A	202	ASN
3	A	235	HIS
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	$\#\|Z\| > 2$
1	DOC	P	873	1,2	16,19,20	2.63	6 (37%)	20,26,29	2.12	8 (40%)

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	-	2/7/18/19	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	873	DOC	O4'-C1'	-5.51	1.30	1.42
1	P	873	DOC	C1'-N1	5.03	1.61	1.48
1	P	873	DOC	O5'-C5'	-3.73	1.35	1.44
1	P	873	DOC	C6-C5	-3.69	1.26	1.35
1	P	873	DOC	C2-N1	-3.12	1.33	1.40
1	P	873	DOC	C3'-C2'	-2.61	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	873	DOC	C2'-C1'-N1	-4.43	104.00	112.40
1	P	873	DOC	O4'-C1'-C2'	-3.76	102.60	106.67
1	P	873	DOC	C4'-O4'-C1'	2.97	112.61	109.81
1	P	873	DOC	C5-C6-N1	2.77	126.45	121.81
1	P	873	DOC	C4-N3-C2	2.48	124.26	120.25
1	P	873	DOC	O4'-C4'-C5'	2.38	113.43	109.52
1	P	873	DOC	N1-C2-N3	-2.16	114.88	118.81
1	P	873	DOC	C6-C5-C4	-2.00	114.28	117.50

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	P	873	DOC	O4'-C4'-C5'-O5'
1	P	873	DOC	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TTP	A	875	4	26,30,30	2.14	8 (30%)	39,47,47	2.39	11 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TTP	A	875	4	-	4/22/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	TTP	C5M-C5	-6.38	1.34	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	875	TTP	C4-N3	-4.49	1.30	1.38
5	A	875	TTP	C6-C5	3.04	1.39	1.34
5	A	875	TTP	C5'-C4'	-2.95	1.42	1.51
5	A	875	TTP	O4-C4	2.94	1.29	1.23
5	A	875	TTP	PA-O1A	-2.56	1.41	1.50
5	A	875	TTP	O5'-C5'	2.17	1.53	1.44
5	A	875	TTP	C3'-C4'	-2.17	1.47	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	875	TTP	C6-N1-C2	-7.42	113.79	121.30
5	A	875	TTP	N3-C2-N1	6.02	122.89	114.89
5	A	875	TTP	C1'-N1-C6	5.74	130.67	120.77
5	A	875	TTP	O5'-C5'-C4'	3.57	121.29	108.99
5	A	875	TTP	C4-N3-C2	-3.50	122.82	127.35
5	A	875	TTP	C5-C4-N3	3.49	118.29	115.31
5	A	875	TTP	O2-C2-N3	-3.22	115.50	121.50
5	A	875	TTP	PB-O3A-PA	-2.69	123.61	132.83
5	A	875	TTP	C5M-C5-C4	2.25	121.24	118.77
5	A	875	TTP	C2'-C1'-N1	-2.18	108.75	113.77
5	A	875	TTP	O4'-C4'-C5'	2.05	116.13	109.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

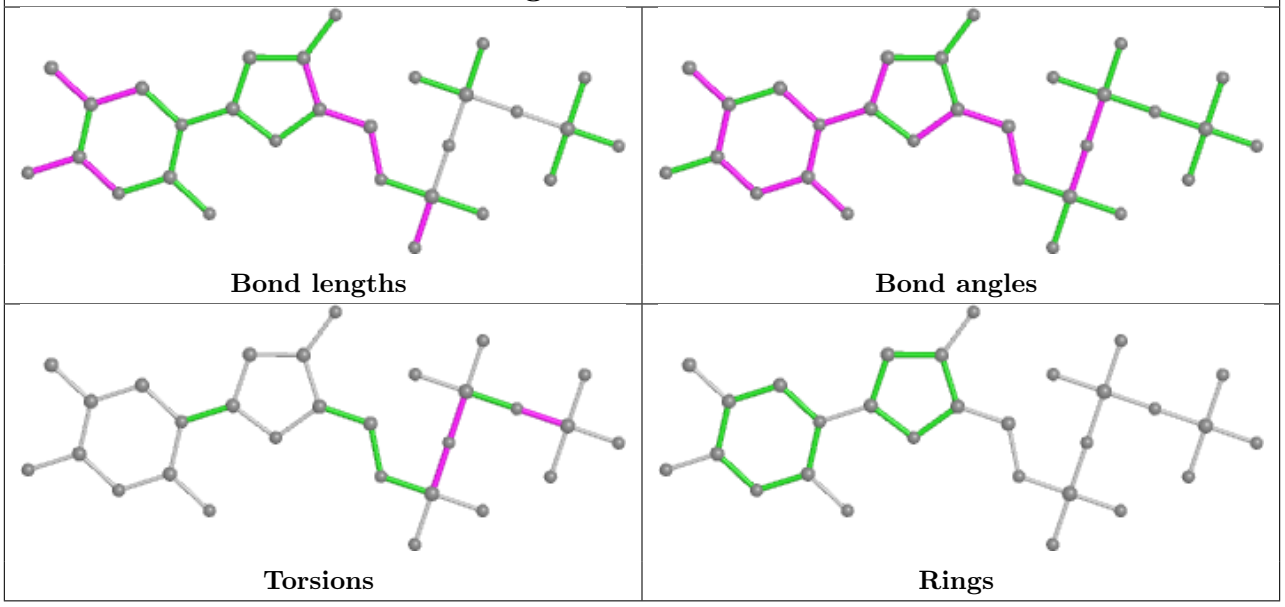
There are no ring outliers.

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 then 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.

Ligand TTP A 875



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

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	P	6/7 (85%)	-0.26	0 100 100	24, 38, 44, 44	0
2	T	9/11 (81%)	0.28	1 (11%) 5 3	29, 33, 51, 90	0
3	A	373/420 (88%)	0.09	27 (7%) 15 11	15, 43, 84, 102	0
All	All	388/438 (88%)	0.09	28 (7%) 15 11	15, 42, 84, 102	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	25	ALA	10.6
3	A	356	GLY	8.6
3	A	354	HIS	5.8
3	A	332	VAL	5.6
3	A	355	TYR	5.5
3	A	368	VAL	5.5
3	A	353	LYS	5.2
3	A	349	TYR	4.9
3	A	351	SER	4.9
3	A	350	SER	4.5
3	A	335	ASP	3.5
3	A	344	LEU	3.1
3	A	352	GLU	3.1
3	A	348	ARG	3.1
2	T	839	DT	2.8
3	A	311	CYS	2.8
3	A	333	CYS	2.7
3	A	412	ASN	2.7
3	A	26	SER	2.6
3	A	145	SER	2.5
3	A	366	SER	2.4
3	A	367	HIS	2.4
3	A	336	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	329	LEU	2.3
3	A	369	ILE	2.3
3	A	312	SER	2.2
3	A	144	GLN	2.1
3	A	386	ILE	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
1	DOC	P	873	18/19	0.97	0.19	11,25,41,43	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

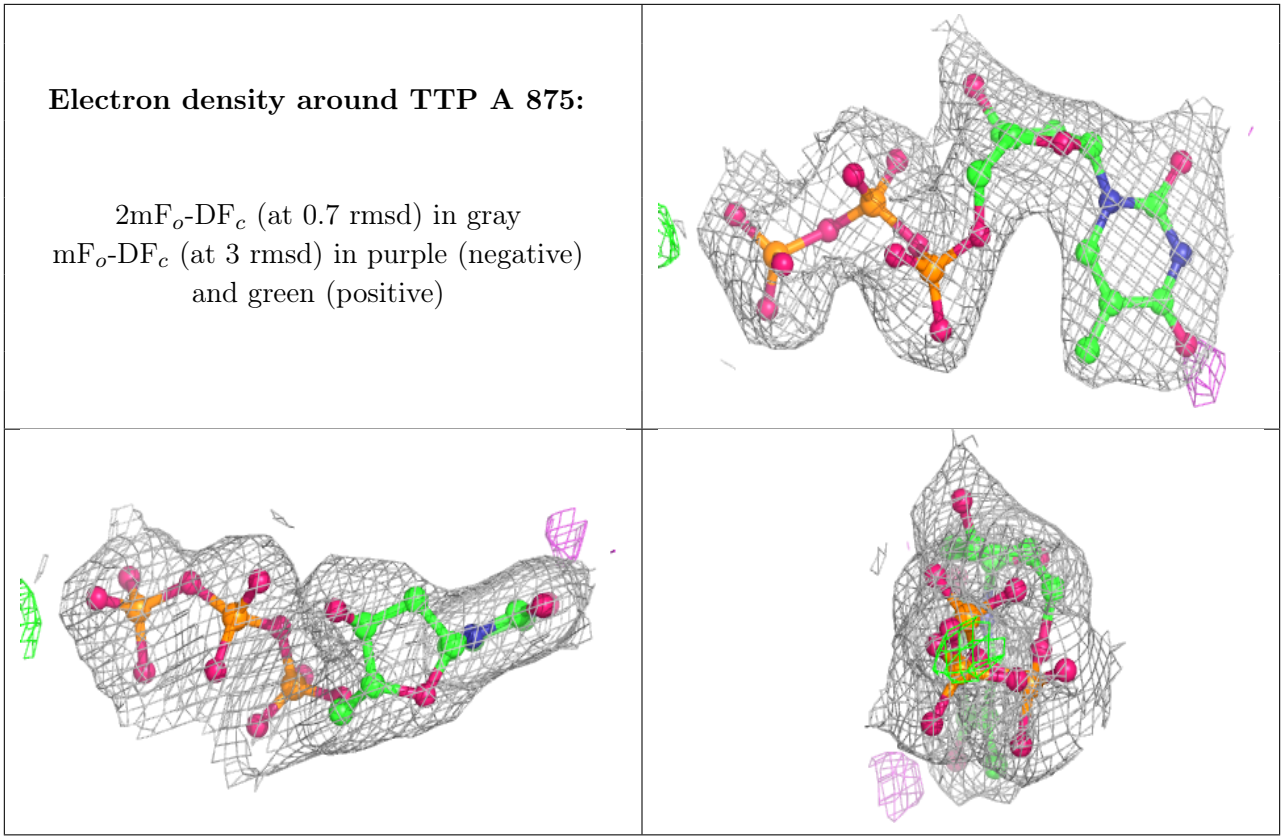
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.75	0.56	102,102,102,102	0
4	MG	A	871	1/1	0.98	0.16	3,3,3,3	0
5	TTP	A	875	29/29	0.99	0.16	17,21,24,27	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.

Electron density around TTP A 875:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.