W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:05 AM GMT

PDB ID	:	2FLN
Title	:	binary complex of catalytic core of human DNA polymerase iota with DNA (template A)
Authors	:	Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on	:	2006-01-06
Resolution	:	2.50 Å(reported)

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

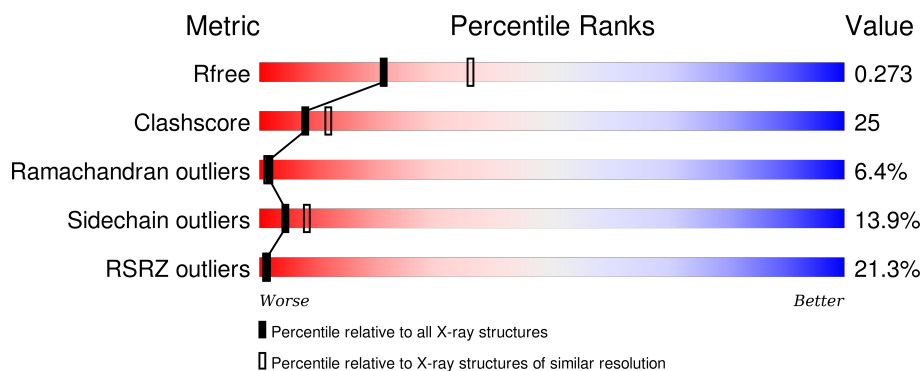|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	Percentile Ranks	Value
Rfree		0.273
Clashscore		25
Ramachandran outliers		6.4%
Sidechain outliers		13.9%
RSRZ outliers		21.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	T	11	45% 36% 18%
2	P	7	14% / 29% 71%
3	A	420	19% / 48% 26% 12% • 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3219 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 template strand.

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

- Molecule 2 is a DNA chain called DNA primer strand.

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

- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	366	Total 2797	C 1760	N 489	O 527	S 21	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total 95	O 95	0	0
4	P	3	Total 3	O 3	0	0
4	T	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
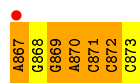
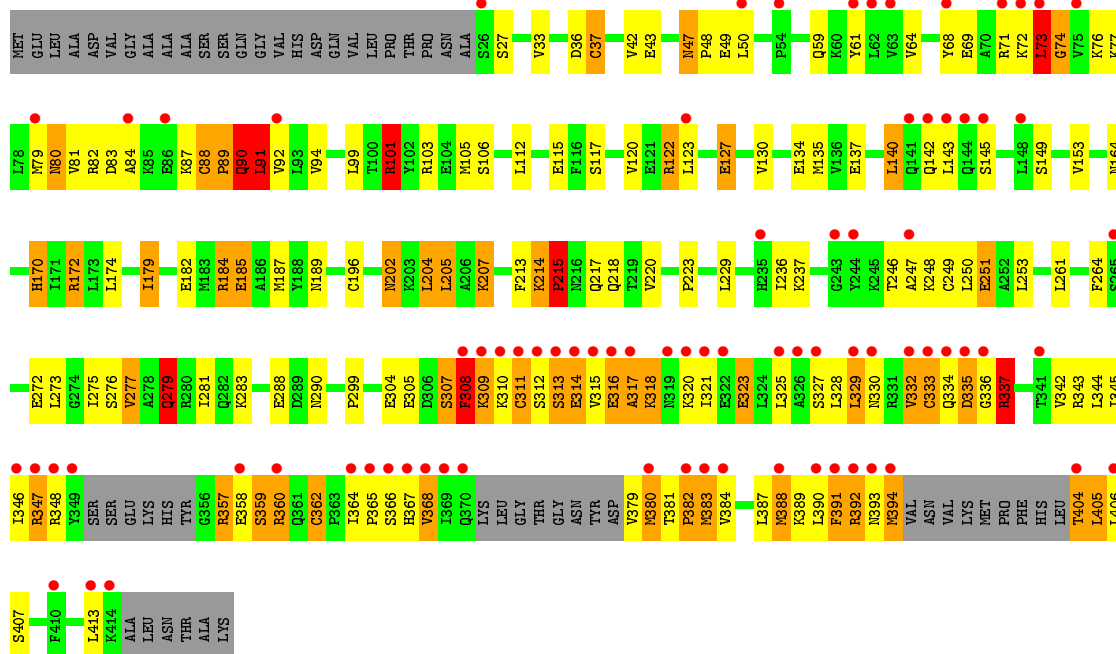• Molecule 1: DNA template strand

Chain T:

• Molecule 2: DNA primer strand

Chain P:

• Molecule 3: DNA polymerase iota

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.11Å 98.11Å 202.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.22 – 2.50 39.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (39.22-2.50) 95.7 (39.18-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.78 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.226 , 0.279 0.224 , 0.273	Depositor DCC
R_{free} test set	2065 reflections (11.56%)	DCC
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 81.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 20599 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3219	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 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	T	3.23	26/203 (12.8%)	4.27	55/312 (17.6%)
2	P	2.82	10/136 (7.4%)	4.07	44/208 (21.2%)
3	A	1.64	29/2835 (1.0%)	1.36	27/3835 (0.7%)
All	All	1.85	65/3174 (2.0%)	1.93	126/4355 (2.9%)

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
3	A	0	2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	382	PRO	N-CD	16.25	1.70	1.47
1	T	847	DT	C5-C7	12.34	1.57	1.50
1	T	847	DT	C3'-O3'	9.82	1.56	1.44
1	T	840	DA	N3-C4	-9.79	1.28	1.34
1	T	843	DG	O4'-C1'	-9.73	1.30	1.42
3	A	288	GLU	CD-OE2	9.70	1.36	1.25
1	T	839	DT	C5'-C4'	8.53	1.60	1.51
3	A	103	ARG	CZ-NH2	8.05	1.43	1.33
1	T	844	DT	C3'-O3'	-8.02	1.33	1.44
1	T	843	DG	P-O5'	7.78	1.67	1.59
1	T	847	DT	C5-C6	7.40	1.39	1.34
2	P	872	DC	P-O5'	7.24	1.67	1.59
3	A	33	VAL	CB-CG1	7.22	1.68	1.52
2	P	872	DC	C3'-O3'	-7.21	1.34	1.44
3	A	68	TYR	CD2-CE2	7.21	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	94	VAL	CB-CG2	-7.18	1.37	1.52
3	A	207	LYS	CE-NZ	-7.16	1.31	1.49
2	P	871	DC	N3-C4	6.96	1.38	1.33
3	A	103	ARG	CZ-NH1	6.84	1.42	1.33
1	T	844	DT	C5-C7	6.82	1.54	1.50
1	T	842	DG	C8-N7	6.80	1.35	1.30
2	P	871	DC	C5-C6	6.76	1.39	1.34
1	T	845	DC	C4'-C3'	6.72	1.60	1.53
3	A	134	GLU	CG-CD	6.70	1.61	1.51
2	P	870	DA	N7-C5	-6.67	1.35	1.39
1	T	847	DT	N1-C6	6.59	1.42	1.38
1	T	847	DT	C1'-N1	6.58	1.57	1.49
2	P	869	DG	N1-C2	6.58	1.43	1.37
3	A	182	GLU	CD-OE1	6.44	1.32	1.25
3	A	105	MET	CG-SD	6.33	1.97	1.81
1	T	841	DG	P-O5'	6.26	1.66	1.59
1	T	843	DG	C5'-C4'	-6.14	1.44	1.51
3	A	101	ARG	CG-CD	6.01	1.67	1.51
2	P	867	DA	N9-C4	5.99	1.41	1.37
3	A	251	GLU	CD-OE1	5.98	1.32	1.25
1	T	839	DT	C5-C7	5.97	1.53	1.50
3	A	185	GLU	CD-OE2	5.94	1.32	1.25
3	A	122	ARG	CD-NE	-5.87	1.36	1.46
3	A	127	GLU	CG-CD	5.80	1.60	1.51
3	A	69	GLU	CG-CD	5.79	1.60	1.51
1	T	842	DG	C3'-O3'	-5.77	1.36	1.44
3	A	134	GLU	CD-OE1	5.68	1.31	1.25
2	P	871	DC	O4'-C1'	-5.60	1.35	1.42
3	A	220	VAL	CB-CG2	5.48	1.64	1.52
3	A	299	PRO	CA-CB	5.46	1.64	1.53
3	A	115	GLU	CD-OE2	-5.44	1.19	1.25
1	T	843	DG	C4'-O4'	5.41	1.50	1.45
1	T	844	DT	C2'-C1'	5.40	1.57	1.52
1	T	843	DG	N3-C4	5.36	1.39	1.35
2	P	869	DG	P-O5'	5.33	1.65	1.59
1	T	843	DG	O5'-C5'	-5.32	1.28	1.42
1	T	843	DG	O3'-P	5.29	1.67	1.61
3	A	127	GLU	CD-OE2	-5.27	1.19	1.25
3	A	283	LYS	CB-CG	5.26	1.66	1.52
3	A	264	PHE	CD1-CE1	-5.26	1.28	1.39
3	A	214	LYS	CA-C	-5.25	1.39	1.52
1	T	844	DT	C4-O4	-5.24	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	845	DC	C2'-C1'	5.14	1.57	1.52
3	A	317	ALA	C-O	5.12	1.33	1.23
1	T	841	DG	N1-C2	5.11	1.41	1.37
2	P	871	DC	N1-C6	5.11	1.40	1.37
3	A	61	TYR	CD2-CE2	5.08	1.47	1.39
3	A	42	VAL	CB-CG2	-5.07	1.42	1.52
1	T	839	DT	C4'-O4'	5.03	1.50	1.45
3	A	218	GLN	CB-CG	-5.03	1.39	1.52

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	847	DT	C4-C5-C6	-18.63	106.82	118.00
1	T	844	DT	C4-C5-C6	-17.24	107.66	118.00
1	T	844	DT	N3-C4-C5	17.06	125.44	115.20
1	T	844	DT	C4-C5-C7	15.53	128.32	119.00
2	P	870	DA	O4'-C4'-C3'	12.76	113.66	106.00
2	P	870	DA	O4'-C1'-N9	12.52	116.77	108.00
1	T	839	DT	C4-C5-C7	12.44	126.46	119.00
1	T	847	DT	N3-C4-C5	12.15	122.49	115.20
1	T	847	DT	C6-C5-C7	11.80	129.98	122.90
3	A	337	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	T	847	DT	O4'-C4'-C3'	11.28	112.77	106.00
2	P	867	DA	O4'-C1'-N9	10.60	115.42	108.00
2	P	869	DG	P-O3'-C3'	-10.35	107.28	119.70
1	T	847	DT	C5-C6-N1	10.18	129.81	123.70
2	P	867	DA	O4'-C4'-C3'	-10.15	99.91	106.00
1	T	840	DA	O5'-P-OP1	-10.08	96.62	105.70
1	T	844	DT	N3-C4-O4	-9.86	113.98	119.90
2	P	871	DC	N1-C2-O2	-9.82	113.01	118.90
2	P	870	DA	O5'-P-OP2	-9.63	97.03	105.70
2	P	867	DA	P-O3'-C3'	9.60	131.22	119.70
1	T	839	DT	O4'-C4'-C3'	-9.33	100.40	106.00
1	T	841	DG	C5-C6-N1	9.31	116.16	111.50
3	A	215	PRO	N-CD-CG	-9.14	89.48	103.20
2	P	867	DA	C8-N9-C4	-9.00	102.20	105.80
1	T	843	DG	N1-C6-O6	-8.73	114.66	119.90
1	T	841	DG	N7-C8-N9	-8.71	108.75	113.10
2	P	872	DC	O4'-C4'-C3'	8.67	111.20	106.00
1	T	846	DC	O4'-C1'-N1	-8.64	101.95	108.00
3	A	103	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	T	839	DT	C6-C5-C7	-8.63	117.72	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	184	ARG	NE-CZ-NH2	-8.60	116.00	120.30
3	A	172	ARG	NE-CZ-NH1	-8.46	116.07	120.30
2	P	871	DC	N3-C2-O2	8.38	127.77	121.90
1	T	843	DG	O4'-C1'-N9	-8.36	102.15	108.00
1	T	839	DT	O4'-C1'-C2'	-8.20	99.34	105.90
1	T	844	DT	C5-C6-N1	8.13	128.58	123.70
1	T	839	DT	O5'-C5'-C4'	8.09	131.22	111.00
1	T	841	DG	C5-N7-C8	7.98	108.29	104.30
3	A	337	ARG	NE-CZ-NH2	-7.97	116.31	120.30
2	P	872	DC	N1-C2-O2	-7.72	114.27	118.90
1	T	843	DG	C4'-C3'-C2'	-7.67	96.20	103.10
3	A	329	LEU	CB-CG-CD2	-7.59	98.09	111.00
3	A	122	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	T	841	DG	C6-N1-C2	-7.55	120.57	125.10
1	T	843	DG	C3'-C2'-C1'	7.42	111.41	102.50
1	T	847	DT	C4'-C3'-O3'	7.34	128.05	109.70
2	P	870	DA	C2-N3-C4	-7.31	106.94	110.60
1	T	844	DT	C5-C4-O4	-7.21	119.85	124.90
3	A	143	LEU	CB-CG-CD1	-7.20	98.76	111.00
1	T	843	DG	C5-C6-N1	7.17	115.09	111.50
2	P	867	DA	N7-C8-N9	7.17	117.39	113.80
1	T	845	DC	OP1-P-O3'	-7.15	89.48	105.20
3	A	101	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	T	840	DA	O4'-C1'-N9	-7.10	103.03	108.00
1	T	843	DG	C8-N9-C4	-7.04	103.58	106.40
2	P	868	DG	O4'-C1'-N9	7.03	112.92	108.00
1	T	847	DT	C4-C5-C7	6.99	123.19	119.00
1	T	839	DT	C5'-C4'-C3'	6.94	126.59	114.10
1	T	844	DT	C2-N3-C4	-6.84	123.09	127.20
2	P	867	DA	O4'-C1'-C2'	-6.82	100.44	105.90
3	A	172	ARG	CG-CD-NE	-6.70	97.72	111.80
1	T	843	DG	N9-C4-C5	6.63	108.05	105.40
2	P	867	DA	C1'-O4'-C4'	6.62	116.72	110.10
2	P	870	DA	C5'-C4'-O4'	-6.52	96.92	109.30
2	P	868	DG	C6-C5-N7	-6.48	126.51	130.40
3	A	122	ARG	CG-CD-NE	-6.42	98.32	111.80
3	A	74	GLY	N-CA-C	6.38	129.05	113.10
1	T	843	DG	C2-N3-C4	6.28	115.04	111.90
1	T	842	DG	C4'-C3'-O3'	6.26	125.34	109.70
1	T	847	DT	C5-C4-O4	-6.25	120.52	124.90
2	P	872	DC	O4'-C1'-C2'	6.21	110.87	105.90
2	P	871	DC	O5'-P-OP2	-6.20	100.12	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	870	DA	OP1-P-O3'	6.19	118.82	105.20
3	A	71	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	T	844	DT	O4'-C1'-N1	6.18	112.33	108.00
1	T	845	DC	O4'-C1'-C2'	6.13	110.81	105.90
1	T	843	DG	O4'-C1'-C2'	-6.12	101.01	105.90
2	P	867	DA	C6-N1-C2	-6.08	114.95	118.60
2	P	872	DC	O5'-P-OP1	-6.07	100.24	105.70
1	T	839	DT	C2-N1-C1'	6.05	127.89	118.20
3	A	279	GLN	CB-CA-C	5.99	122.39	110.40
1	T	847	DT	O4'-C1'-N1	5.95	112.17	108.00
2	P	868	DG	C4-C5-N7	5.92	113.17	110.80
1	T	847	DT	O5'-P-OP2	5.86	117.73	110.70
2	P	872	DC	C4'-C3'-O3'	5.81	124.23	109.70
3	A	335	ASP	CB-CG-OD1	5.79	123.52	118.30
1	T	841	DG	N1-C6-O6	-5.73	116.46	119.90
3	A	73	LEU	CB-CG-CD2	5.71	120.70	111.00
1	T	846	DC	C4'-C3'-C2'	5.66	108.19	103.10
2	P	872	DC	C5'-C4'-O4'	-5.63	98.60	109.30
2	P	871	DC	C5-C4-N4	-5.54	116.32	120.20
1	T	842	DG	N1-C2-N2	5.54	121.18	116.20
1	T	846	DC	C4-C5-C6	5.54	120.17	117.40
2	P	871	DC	C4'-C3'-O3'	5.54	123.54	109.70
1	T	839	DT	C6-N1-C1'	-5.52	112.13	120.40
2	P	871	DC	N3-C4-N4	5.50	121.85	118.00
2	P	867	DA	C5-C6-N1	5.47	120.44	117.70
2	P	869	DG	OP2-P-O3'	5.45	117.20	105.20
2	P	869	DG	C6-N1-C2	-5.45	121.83	125.10
1	T	846	DC	N3-C4-C5	-5.43	119.73	121.90
3	A	140	LEU	CB-CG-CD1	-5.41	101.80	111.00
3	A	69	GLU	OE1-CD-OE2	-5.40	116.82	123.30
2	P	867	DA	N3-C4-C5	-5.40	123.02	126.80
3	A	88	CYS	N-CA-C	5.39	125.56	111.00
2	P	868	DG	P-O5'-C5'	5.37	129.50	120.90
2	P	867	DA	C5'-C4'-C3'	5.33	123.69	114.10
1	T	840	DA	C3'-C2'-C1'	5.32	108.89	102.50
1	T	842	DG	OP2-P-O3'	5.29	116.85	105.20
3	A	246	THR	OG1-CB-CG2	-5.29	97.83	110.00
3	A	223	PRO	N-CD-CG	5.29	111.13	103.20
2	P	868	DG	O3'-P-O5'	-5.28	93.96	104.00
3	A	91	LEU	CA-CB-CG	5.27	127.43	115.30
2	P	869	DG	C8-N9-C4	-5.24	104.31	106.40
2	P	868	DG	N9-C4-C5	-5.23	103.31	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	842	DG	C5'-C4'-O4'	-5.23	99.37	109.30
2	P	872	DC	O4'-C1'-N1	5.21	111.65	108.00
1	T	839	DT	C5'-C4'-O4'	5.19	119.17	109.30
2	P	870	DA	C5-N7-C8	-5.18	101.31	103.90
3	A	336	GLY	N-CA-C	-5.18	100.16	113.10
3	A	179	ILE	CA-CB-CG1	5.16	120.81	111.00
1	T	847	DT	C3'-C2'-C1'	5.15	108.68	102.50
2	P	867	DA	O5'-C5'-C4'	5.08	123.70	111.00
2	P	870	DA	N1-C6-N6	5.05	121.63	118.60
2	P	869	DG	O4'-C1'-N9	5.05	111.53	108.00
3	A	204	LEU	CB-CG-CD2	5.02	119.54	111.00
3	A	215	PRO	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	309	LYS	Peptide

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	182	0	104	10	1
2	P	139	0	79	4	1
3	A	2797	0	2781	140	0
4	A	95	0	0	4	0
4	P	3	0	0	0	0
4	T	3	0	0	0	0
All	All	3219	0	2964	152	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 25.

All (152) 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:382:PRO:CD	3:A:382:PRO:N	1.70	1.45
3:A:87:LYS:O	3:A:88:CYS:SG	1.98	1.21
3:A:392:ARG:O	3:A:394:MET:N	1.83	1.10
3:A:347:ARG:HD3	3:A:405:LEU:CB	1.80	1.10
3:A:320:LYS:O	3:A:323:GLU:HB2	1.51	1.08
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.31	1.06
3:A:347:ARG:HG2	3:A:404:THR:HG23	1.35	1.03
3:A:347:ARG:CG	3:A:404:THR:HG23	1.93	0.97
3:A:89:PRO:O	3:A:91:LEU:N	1.98	0.97
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.52	0.92
3:A:347:ARG:CD	3:A:405:LEU:CB	2.50	0.89
3:A:379:VAL:O	3:A:382:PRO:HD2	1.72	0.89
3:A:247:ALA:O	3:A:251:GLU:HG3	1.74	0.88
3:A:47:ASN:C	3:A:47:ASN:HD22	1.76	0.87
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.56	0.86
1:T:841:DG:H2"	1:T:842:DG:H5"	1.61	0.81
3:A:82:ARG:O	3:A:84:ALA:N	2.14	0.79
3:A:82:ARG:C	3:A:84:ALA:H	1.82	0.79
3:A:120:VAL:HG22	3:A:130:VAL:HG22	1.68	0.75
1:T:842:DG:C2'	1:T:843:DG:H5'	2.16	0.75
3:A:249:CYS:SG	3:A:273:LEU:HD21	2.27	0.75
3:A:325:LEU:HB3	3:A:380:MET:HE3	1.68	0.74
3:A:308:PHE:HB2	3:A:311:CYS:HB2	1.68	0.74
2:P:872:DC:H2"	2:P:873:DOC:H5"	1.70	0.74
3:A:392:ARG:C	3:A:394:MET:H	1.89	0.72
1:T:842:DG:H2'	1:T:843:DG:H5'	1.70	0.71
3:A:47:ASN:HD21	3:A:49:GLU:HB2	1.53	0.71
3:A:388:MET:O	3:A:391:PHE:HB3	1.93	0.69
3:A:47:ASN:ND2	3:A:47:ASN:C	2.46	0.69
3:A:47:ASN:ND2	3:A:47:ASN:O	2.16	0.69
3:A:82:ARG:C	3:A:84:ALA:N	2.46	0.69
3:A:164:ASN:H	3:A:170:HIS:HD2	1.42	0.68
3:A:202:ASN:C	3:A:202:ASN:HD22	1.99	0.66
3:A:308:PHE:O	3:A:308:PHE:HD1	1.78	0.66
3:A:196:CYS:SG	3:A:214:LYS:O	2.53	0.65
3:A:344:LEU:O	3:A:359:SER:HA	1.96	0.65
3:A:137:GLU:HG2	3:A:172:ARG:NH1	2.12	0.65
3:A:335:ASP:OD2	3:A:337:ARG:HB2	1.98	0.64
3:A:236:ILE:CD1	3:A:250:LEU:HD13	2.25	0.64
3:A:172:ARG:HD3	4:A:981:HOH:O	1.97	0.63
3:A:335:ASP:OD2	3:A:337:ARG:HD3	1.99	0.63
3:A:36:ASP:OD1	3:A:215:PRO:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:389:LYS:HA	3:A:392:ARG:HD2	1.81	0.62
3:A:236:ILE:HD12	3:A:250:LEU:CD1	2.27	0.62
3:A:137:GLU:HG2	3:A:172:ARG:HH12	1.65	0.62
3:A:347:ARG:HG3	3:A:404:THR:HG23	1.79	0.62
3:A:325:LEU:HD11	3:A:387:LEU:CD1	2.30	0.61
3:A:253:LEU:HD12	3:A:253:LEU:N	2.15	0.61
3:A:325:LEU:HD11	3:A:387:LEU:HD12	1.84	0.60
3:A:333:CYS:O	3:A:335:ASP:N	2.35	0.60
3:A:79:MET:CE	3:A:84:ALA:HB2	2.33	0.59
3:A:318:LYS:O	3:A:321:ILE:HB	2.03	0.59
3:A:405:LEU:O	3:A:406:LEU:HD23	2.04	0.58
3:A:318:LYS:O	3:A:318:LYS:HG2	2.00	0.57
3:A:117:SER:OG	4:A:907:HOH:O	2.17	0.57
1:T:842:DG:H2"	1:T:843:DG:C5'	2.34	0.57
3:A:202:ASN:ND2	3:A:205:LEU:H	2.02	0.57
1:T:842:DG:C2'	1:T:843:DG:C5'	2.82	0.56
3:A:36:ASP:O	3:A:37:CYS:C	2.43	0.56
1:T:841:DG:OP2	3:A:307:SER:HB2	2.06	0.55
3:A:275:ILE:HG13	3:A:279:GLN:NE2	2.22	0.55
3:A:112:LEU:HD23	3:A:112:LEU:C	2.26	0.55
3:A:345:ILE:HA	3:A:358:GLU:O	2.06	0.55
3:A:327:SER:O	3:A:328:LEU:C	2.45	0.54
3:A:308:PHE:CD1	3:A:308:PHE:O	2.60	0.54
3:A:43:GLU:OE1	3:A:101:ARG:NH2	2.40	0.54
3:A:275:ILE:HG23	3:A:276:SER:N	2.23	0.54
3:A:308:PHE:HB2	3:A:311:CYS:CB	2.39	0.53
2:P:872:DC:H2"	2:P:873:DOC:C5'	2.36	0.53
1:T:842:DG:H2"	1:T:843:DG:H5"	1.91	0.52
3:A:348:ARG:NH1	3:A:358:GLU:OE1	2.42	0.52
3:A:320:LYS:HA	3:A:323:GLU:HG3	1.92	0.52
3:A:343:ARG:HG2	3:A:344:LEU:N	2.24	0.52
3:A:304:GLU:HG3	3:A:328:LEU:CG	2.35	0.52
3:A:342:VAL:HG21	3:A:387:LEU:HD21	1.94	0.50
3:A:275:ILE:CG1	3:A:279:GLN:NE2	2.75	0.49
3:A:80:ASN:O	3:A:84:ALA:HB3	2.12	0.49
3:A:202:ASN:HD21	3:A:205:LEU:H	1.59	0.49
3:A:87:LYS:C	3:A:88:CYS:SG	2.85	0.49
3:A:76:LYS:HG2	3:A:77:LYS:N	2.27	0.49
3:A:76:LYS:HG2	3:A:77:LYS:H	1.76	0.49
3:A:379:VAL:C	3:A:382:PRO:HD2	2.30	0.48
3:A:261:LEU:HD12	3:A:261:LEU:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:79:MET:CE	3:A:84:ALA:CB	2.90	0.48
3:A:290:ASN:ND2	4:A:900:HOH:O	2.33	0.48
3:A:321:ILE:HD12	3:A:391:PHE:CD1	2.48	0.48
3:A:388:MET:HE3	3:A:388:MET:HA	1.95	0.48
3:A:89:PRO:O	3:A:90:GLN:C	2.52	0.48
3:A:79:MET:HE3	3:A:84:ALA:HB2	1.95	0.48
3:A:321:ILE:O	3:A:325:LEU:HD13	2.14	0.47
3:A:79:MET:HE2	3:A:84:ALA:CB	2.44	0.47
3:A:79:MET:HE2	3:A:84:ALA:HB2	1.96	0.47
3:A:89:PRO:C	3:A:91:LEU:N	2.66	0.47
3:A:316:GLU:O	3:A:318:LYS:N	2.48	0.47
3:A:392:ARG:C	3:A:394:MET:N	2.56	0.47
3:A:365:PRO:O	3:A:368:VAL:HG13	2.15	0.46
3:A:325:LEU:HB3	3:A:380:MET:CE	2.42	0.46
2:P:869:DG:H2"	2:P:870:DA:OP2	2.14	0.46
3:A:185:GLU:OE1	3:A:189:ASN:ND2	2.48	0.46
3:A:214:LYS:N	3:A:215:PRO:CD	2.78	0.46
3:A:112:LEU:HD23	3:A:112:LEU:O	2.15	0.46
3:A:360:ARG:HG2	3:A:394:MET:CG	2.45	0.46
3:A:346:ILE:O	3:A:357:ARG:HA	2.14	0.46
3:A:380:MET:HE2	3:A:384:VAL:HG23	1.97	0.46
3:A:135:MET:CE	3:A:179:ILE:HD12	2.46	0.46
3:A:90:GLN:O	3:A:91:LEU:C	2.54	0.46
1:T:841:DG:H2"	1:T:842:DG:C5'	2.41	0.45
3:A:127:GLU:OE1	3:A:207:LYS:HE3	2.16	0.45
3:A:80:ASN:C	3:A:82:ARG:H	2.19	0.45
1:T:842:DG:H2"	1:T:843:DG:H5'	1.95	0.45
3:A:275:ILE:HG13	3:A:279:GLN:HE21	1.81	0.44
3:A:305:GLU:HG3	3:A:407:SER:HB3	1.99	0.44
3:A:275:ILE:CG2	3:A:276:SER:N	2.81	0.44
1:T:842:DG:H4'	3:A:99:LEU:HD12	2.00	0.44
3:A:196:CYS:HA	3:A:217:GLN:O	2.18	0.44
3:A:184:ARG:HA	3:A:187:MET:HE2	1.99	0.44
3:A:248:LYS:HD3	3:A:248:LYS:HA	1.72	0.44
3:A:202:ASN:C	3:A:202:ASN:ND2	2.66	0.43
3:A:153:VAL:HG23	3:A:174:LEU:HD22	2.00	0.43
3:A:347:ARG:HD2	3:A:405:LEU:CB	2.43	0.43
3:A:364:ILE:HG22	3:A:364:ILE:O	2.17	0.43
3:A:275:ILE:CG1	3:A:279:GLN:HE22	2.31	0.43
3:A:72:LYS:C	3:A:74:GLY:H	2.22	0.43
3:A:404:THR:O	3:A:405:LEU:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:325:LEU:HD11	3:A:387:LEU:HD11	2.01	0.43
3:A:59:GLN:OE1	3:A:64:VAL:HG11	2.19	0.43
3:A:346:ILE:HG22	3:A:406:LEU:CD2	2.49	0.42
3:A:344:LEU:HD21	3:A:387:LEU:HD13	2.01	0.42
3:A:277:VAL:O	3:A:281:ILE:HG23	2.19	0.42
3:A:332:VAL:HG12	3:A:333:CYS:N	2.35	0.42
3:A:360:ARG:HD3	3:A:360:ARG:HA	1.92	0.42
3:A:273:LEU:O	3:A:277:VAL:HB	2.20	0.42
3:A:312:SER:C	3:A:314:GLU:H	2.23	0.42
3:A:367:HIS:CD2	3:A:368:VAL:HG12	2.55	0.42
3:A:406:LEU:HD23	3:A:406:LEU:HA	1.85	0.42
3:A:164:ASN:H	3:A:170:HIS:CD2	2.29	0.41
3:A:172:ARG:CD	4:A:981:HOH:O	2.65	0.41
3:A:140:LEU:HD23	3:A:140:LEU:HA	1.91	0.41
3:A:364:ILE:HG12	3:A:383:MET:CE	2.51	0.41
3:A:106:SER:OG	3:A:122:ARG:NH2	2.45	0.41
3:A:318:LYS:HG3	3:A:388:MET:CE	2.51	0.41
3:A:50:LEU:CD2	3:A:92:VAL:HG11	2.50	0.41
3:A:237:LYS:HD3	3:A:237:LYS:O	2.20	0.41
3:A:362:CYS:HB3	3:A:390:LEU:HD21	2.02	0.41
3:A:80:ASN:C	3:A:82:ARG:N	2.74	0.41
3:A:214:LYS:HE3	3:A:214:LYS:HB3	1.81	0.41
3:A:342:VAL:HB	3:A:364:ILE:HD11	2.03	0.41
3:A:236:ILE:HD13	3:A:236:ILE:HG21	1.51	0.41
3:A:88:CYS:O	3:A:89:PRO:O	2.39	0.40
3:A:90:GLN:O	3:A:91:LEU:O	2.39	0.40
2:P:871:DC:H2"	2:P:872:DC:H5'	2.03	0.40
3:A:164:ASN:N	3:A:170:HIS:HD2	2.15	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]	1.82	0.38

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	358/420 (85%)	303 (85%)	32 (9%)	23 (6%)	2 1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	83	ASP
3	A	89	PRO
3	A	90	GLN
3	A	91	LEU
3	A	145	SER
3	A	308	PHE
3	A	315	VAL
3	A	317	ALA
3	A	333	CYS
3	A	334	GLN
3	A	366	SER
3	A	393	ASN
3	A	215	PRO
3	A	337	ARG
3	A	405	LEU
3	A	313	SER
3	A	323	GLU
3	A	73	LEU
3	A	310	LYS
3	A	37	CYS
3	A	316	GLU
3	A	81	VAL
3	A	277	VAL

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	309/376 (82%)	266 (86%)	43 (14%)	4 8

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	27	SER
3	A	47	ASN
3	A	48	PRO
3	A	73	LEU
3	A	80	ASN
3	A	90	GLN
3	A	91	LEU
3	A	101	ARG
3	A	123	LEU
3	A	142	GLN
3	A	149	SER
3	A	170	HIS
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	229	LEU
3	A	272	GLU
3	A	279	GLN
3	A	307	SER
3	A	308	PHE
3	A	309	LYS
3	A	311	CYS
3	A	313	SER
3	A	314	GLU
3	A	318	LYS
3	A	329	LEU
3	A	330	ASN
3	A	332	VAL
3	A	347	ARG
3	A	357	ARG

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Mol	Chain	Res	Type
3	A	359	SER
3	A	360	ARG
3	A	362	CYS
3	A	368	VAL
3	A	380	MET
3	A	381	THR
3	A	383	MET
3	A	388	MET
3	A	391	PHE
3	A	392	ARG
3	A	394	MET
3	A	404	THR
3	A	413	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	ASN
3	A	170	HIS
3	A	202	ASN
3	A	262	GLN
3	A	279	GLN
3	A	393	ASN

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	11,19,20	1.51	1 (9%)	14,26,29	1.87	4 (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
2	DOC	P	873	1,2	-	0/3/18/19	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	873	DOC	O4'-C1'	-3.10	1.35	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	873	DOC	C2'-C1'-N1	-2.46	107.51	112.49
2	P	873	DOC	O4'-C4'-C3'	2.71	109.24	104.69
2	P	873	DOC	C3'-C2'-C1'	3.59	106.72	102.71
2	P	873	DOC	O4'-C4'-C5'	3.78	115.12	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	9/11 (81%)	0.82	0	100	100	29, 33, 46, 74	0
2	P	6/7 (85%)	1.14	1 (16%)	2	2	39, 49, 50, 55	0
3	A	366/420 (87%)	1.34	80 (21%)	1	1	7, 39, 90, 100	0
All	All	381/438 (86%)	1.32	81 (21%)	1	1	7, 39, 90, 100	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	313	SER	9.9
3	A	312	SER	7.9
3	A	311	CYS	7.0
3	A	244	TYR	6.9
3	A	329	LEU	6.6
3	A	336	GLY	6.5
3	A	388	MET	6.1
3	A	368	VAL	6.1
3	A	335	ASP	5.4
3	A	319	ASN	5.2
3	A	349	TYR	5.1
3	A	348	ARG	5.0
3	A	73	LEU	4.7
3	A	72	LYS	4.7
3	A	310	LYS	4.6
3	A	320	LYS	4.6
3	A	391	PHE	4.6
3	A	142	GLN	4.6
3	A	333	CYS	4.5
3	A	26	SER	4.5
3	A	394	MET	4.3
3	A	321	ILE	4.2
3	A	314	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
3	A	317	ALA	4.0
3	A	243	GLY	4.0
3	A	327	SER	4.0
3	A	71	ARG	3.9
3	A	326	ALA	3.8
3	A	366	SER	3.8
3	A	84	ALA	3.8
3	A	369	ILE	3.8
3	A	61	TYR	3.8
3	A	404	THR	3.7
3	A	380	MET	3.7
3	A	308	PHE	3.6
3	A	143	LEU	3.4
3	A	346	ILE	3.3
3	A	75	VAL	3.3
3	A	392	ARG	3.3
3	A	309	LYS	3.2
3	A	364	ILE	3.1
3	A	315	VAL	3.1
3	A	406	LEU	3.1
3	A	367	HIS	3.0
3	A	365	PRO	3.0
3	A	370	GLN	2.9
3	A	316	GLU	2.8
3	A	144	GLN	2.8
3	A	347	ARG	2.8
3	A	145	SER	2.8
3	A	235	HIS	2.7
3	A	79	MET	2.7
3	A	382	PRO	2.6
3	A	360	ARG	2.6
3	A	50	LEU	2.6
3	A	384	VAL	2.6
3	A	334	GLN	2.6
3	A	63	VAL	2.5
3	A	330	ASN	2.5
3	A	322	GLU	2.5
3	A	332	VAL	2.5
3	A	62	LEU	2.5
3	A	68	TYR	2.5
3	A	141	GLN	2.4
3	A	148	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	413	LEU	2.4
3	A	358	GLU	2.3
3	A	265	SER	2.3
3	A	86	GLU	2.3
3	A	390	LEU	2.2
3	A	341	THR	2.2
3	A	92	VAL	2.2
2	P	867	DA	2.1
3	A	383	MET	2.1
3	A	414	LYS	2.1
3	A	393	ASN	2.1
3	A	247	ALA	2.0
3	A	54	PRO	2.0
3	A	123	LEU	2.0
3	A	410	PHE	2.0
3	A	325	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	DOC	P	873	18/19	0.92	0.21	-	23,31,38,39	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.