Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2024 – 11:31 AM EST

PDB ID	:	2FLP
Title	:	Binary complex of the catalytic core of human DNA polymerase iota with DNA (template G)
Authors	:	Nair, D.T.; Johnson, R.E.; Prakash, L.; Prakash, S.; Aggarwal, A.K.
Deposited on	:	2006-01-06
Resolution	:	2.40 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:

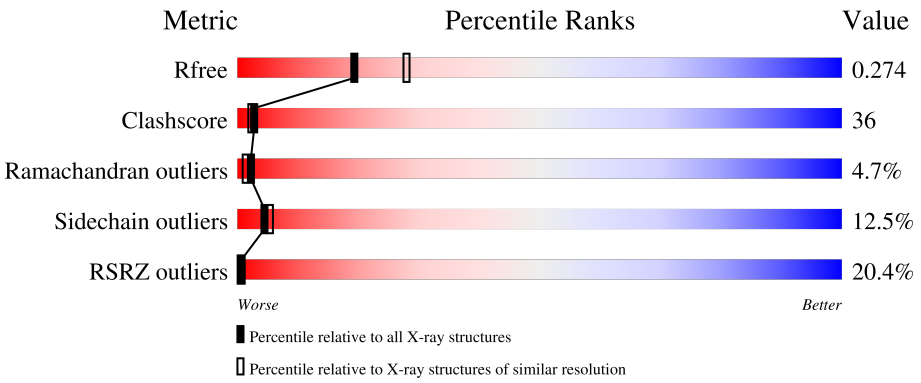
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	T	11	9%; 36%, 36%, 9%, 18%
2	P	7	57%, 43%
3	A	420	18%; 43%, 28%, 13%, •, 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3250 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
			Total	C	N	O	P			
1	T	9	183	88	32	55	8	0	0	0

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

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

- Molecule 3 is a protein called DNA polymerase iota.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	367	2813	1768	495	529	21	0	0	0

- Molecule 4 is water.

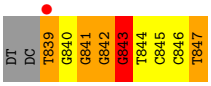
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	T	6	6	6	0	0
4	P	2	2	2	0	0
4	A	107	107	107	0	0

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 template strand

Chain T:

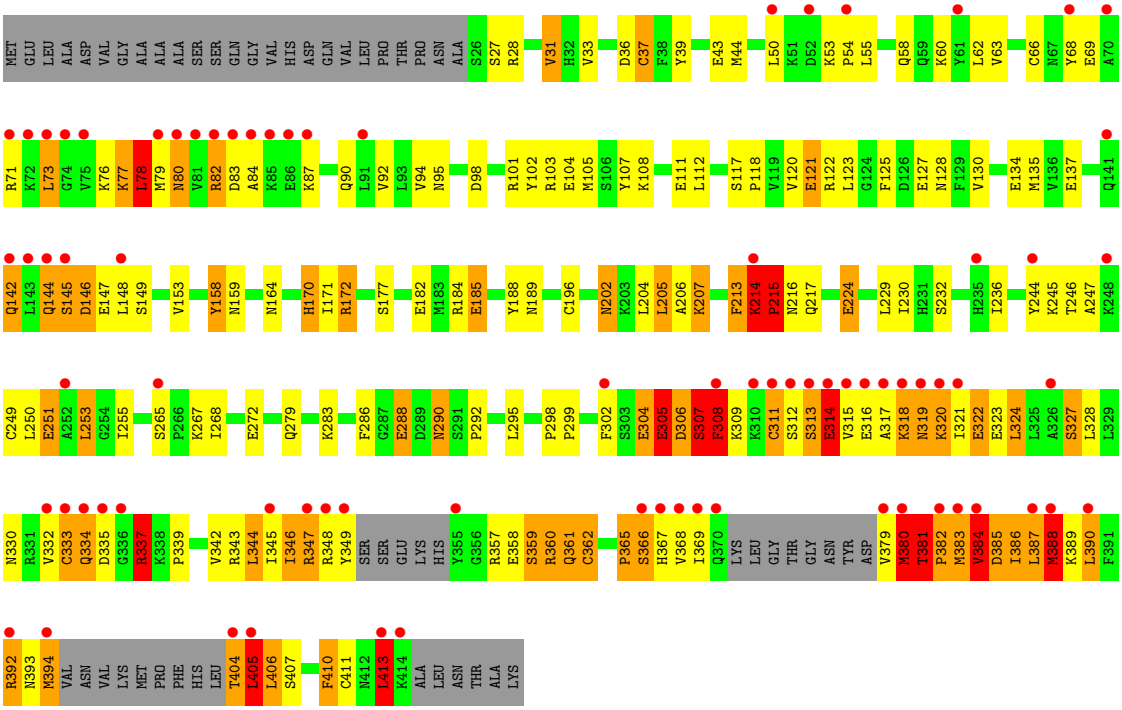


- Molecule 2: DNA primer strand

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	98.37Å 98.37Å 202.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.51 – 2.40 32.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (36.51-2.40) 96.2 (32.59-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.65 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.228 , 0.276 0.229 , 0.274	Depositor DCC
R_{free} test set	2280 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 71.2	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	3250	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 3.87% 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 (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	3.87	32/204 (15.7%)	3.78	52/314 (16.6%)
2	P	3.30	13/136 (9.6%)	3.58	24/208 (11.5%)
3	A	3.23	114/2850 (4.0%)	1.52	46/3851 (1.2%)
All	All	3.28	159/3190 (5.0%)	1.91	122/4373 (2.8%)

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	T	0	1
3	A	0	3
All	All	0	4

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	313	SER	CB-OG	99.73	2.71	1.42
3	A	318	LYS	CE-NZ	42.89	2.56	1.49
3	A	319	ASN	CG-ND2	28.92	2.05	1.32
3	A	314	GLU	CB-CG	28.28	2.05	1.52
3	A	319	ASN	CG-OD1	26.82	1.82	1.24
3	A	322	GLU	CD-OE1	22.82	1.50	1.25
3	A	314	GLU	C-O	22.27	1.65	1.23
3	A	314	GLU	CD-OE2	19.37	1.47	1.25
3	A	314	GLU	CA-CB	18.63	1.95	1.53
3	A	320	LYS	CG-CD	18.36	2.14	1.52
1	T	847	DT	C3'-O3'	17.47	1.66	1.44
3	A	382	PRO	CA-C	16.04	1.84	1.52
3	A	390	LEU	C-O	14.30	1.50	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	314	GLU	CD-OE1	13.08	1.40	1.25
3	A	314	GLU	C-N	13.02	1.64	1.34
1	T	847	DT	C5-C7	12.09	1.57	1.50
3	A	185	GLU	CD-OE2	11.89	1.38	1.25
3	A	381	THR	C-N	11.26	1.55	1.34
3	A	405	LEU	C-O	11.19	1.44	1.23
3	A	348	ARG	CZ-NH1	10.98	1.47	1.33
3	A	381	THR	C-O	10.97	1.44	1.23
1	T	844	DT	C5-C7	10.82	1.56	1.50
1	T	847	DT	C1'-N1	10.66	1.63	1.49
3	A	304	GLU	CD-OE1	10.62	1.37	1.25
2	P	871	DC	C3'-O3'	-10.60	1.30	1.44
3	A	394	MET	CG-SD	10.20	2.07	1.81
2	P	870	DA	C2-N3	10.12	1.42	1.33
3	A	392	ARG	CB-CG	9.98	1.79	1.52
3	A	304	GLU	CD-OE2	9.91	1.36	1.25
3	A	322	GLU	CG-CD	9.87	1.66	1.51
3	A	318	LYS	CB-CG	9.84	1.79	1.52
3	A	216	ASN	N-CA	9.53	1.65	1.46
3	A	306	ASP	CG-OD1	9.36	1.46	1.25
3	A	323	GLU	CD-OE2	9.30	1.35	1.25
3	A	379	VAL	N-CA	9.29	1.65	1.46
1	T	843	DG	C2-N3	9.03	1.40	1.32
3	A	327	SER	CB-OG	8.84	1.53	1.42
3	A	379	VAL	CA-CB	8.81	1.73	1.54
3	A	382	PRO	CB-CG	8.79	1.94	1.50
1	T	845	DC	C4-C5	8.68	1.49	1.43
3	A	382	PRO	CA-CB	8.67	1.70	1.53
1	T	842	DG	N3-C4	-8.63	1.29	1.35
2	P	871	DC	C2'-C1'	8.55	1.60	1.52
1	T	844	DT	P-O5'	8.49	1.68	1.59
3	A	304	GLU	C-O	8.46	1.39	1.23
1	T	839	DT	N1-C2	8.23	1.44	1.38
1	T	847	DT	C2'-C1'	8.12	1.60	1.52
3	A	288	GLU	CD-OE2	8.10	1.34	1.25
3	A	251	GLU	CD-OE1	8.04	1.34	1.25
1	T	839	DT	C1'-N1	7.90	1.59	1.49
1	T	841	DG	C2-N3	7.89	1.39	1.32
3	A	305	GLU	C-O	7.86	1.38	1.23
3	A	389	LYS	C-N	7.85	1.52	1.34
3	A	31	VAL	CB-CG2	7.84	1.69	1.52
1	T	842	DG	N7-C5	7.66	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	68	TYR	CG-CD1	7.56	1.49	1.39
2	P	869	DG	C5-C4	7.51	1.43	1.38
3	A	103	ARG	CZ-NH2	7.49	1.42	1.33
1	T	845	DC	N1-C6	7.44	1.41	1.37
3	A	392	ARG	CZ-NH1	7.36	1.42	1.33
3	A	392	ARG	CZ-NH2	7.36	1.42	1.33
3	A	279	GLN	CG-CD	7.28	1.67	1.51
3	A	232	SER	CB-OG	7.25	1.51	1.42
3	A	185	GLU	CD-OE1	7.25	1.33	1.25
3	A	323	GLU	CD-OE1	7.25	1.33	1.25
3	A	245	LYS	CA-CB	7.09	1.69	1.53
1	T	842	DG	P-O5'	7.07	1.66	1.59
3	A	104	GLU	CD-OE2	7.01	1.33	1.25
3	A	121	GLU	CG-CD	6.96	1.62	1.51
3	A	392	ARG	C-N	6.91	1.50	1.34
3	A	385	ASP	C-O	6.88	1.36	1.23
3	A	39	TYR	CG-CD1	-6.83	1.30	1.39
3	A	349	TYR	C-O	6.75	1.36	1.23
1	T	839	DT	C5'-C4'	6.74	1.58	1.51
3	A	305	GLU	CD-OE1	-6.73	1.18	1.25
3	A	383	MET	N-CA	6.71	1.59	1.46
1	T	845	DC	C5-C6	6.69	1.39	1.34
3	A	214	LYS	CA-C	-6.67	1.35	1.52
1	T	847	DT	C3'-C2'	6.64	1.60	1.52
1	T	840	DG	C2-N3	6.63	1.38	1.32
3	A	122	ARG	CD-NE	-6.62	1.35	1.46
3	A	184	ARG	CD-NE	-6.58	1.35	1.46
3	A	102	TYR	CG-CD2	6.53	1.47	1.39
3	A	290	ASN	CB-CG	6.51	1.66	1.51
2	P	872	DC	P-O5'	6.46	1.66	1.59
3	A	392	ARG	NE-CZ	6.45	1.41	1.33
3	A	348	ARG	NE-CZ	6.42	1.41	1.33
3	A	348	ARG	CB-CG	6.42	1.69	1.52
3	A	108	LYS	CD-CE	6.41	1.67	1.51
2	P	869	DG	P-O5'	6.37	1.66	1.59
3	A	386	ILE	CA-CB	6.36	1.69	1.54
3	A	188	TYR	CG-CD2	6.35	1.47	1.39
3	A	388	MET	C-O	6.29	1.35	1.23
3	A	177	SER	CB-OG	6.29	1.50	1.42
3	A	111	GLU	CD-OE2	6.28	1.32	1.25
3	A	134	GLU	CD-OE1	6.28	1.32	1.25
3	A	286	PHE	CE1-CZ	6.25	1.49	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	117	SER	CB-OG	6.24	1.50	1.42
3	A	313	SER	C-O	6.21	1.35	1.23
3	A	389	LYS	N-CA	6.18	1.58	1.46
3	A	134	GLU	CG-CD	6.13	1.61	1.51
2	P	869	DG	N7-C5	6.09	1.43	1.39
1	T	847	DT	C4'-C3'	6.07	1.59	1.53
3	A	306	ASP	CB-CG	6.01	1.64	1.51
2	P	871	DC	O4'-C1'	-5.96	1.35	1.42
3	A	358	GLU	CD-OE1	5.93	1.32	1.25
2	P	868	DG	C6-N1	5.91	1.43	1.39
3	A	182	GLU	CD-OE2	5.88	1.32	1.25
3	A	251	GLU	CD-OE2	5.80	1.32	1.25
1	T	840	DG	N9-C8	5.79	1.42	1.37
1	T	843	DG	O5'-C5'	-5.78	1.27	1.42
3	A	286	PHE	CD1-CE1	5.77	1.50	1.39
3	A	182	GLU	CD-OE1	5.75	1.31	1.25
3	A	111	GLU	CG-CD	5.74	1.60	1.51
3	A	158	TYR	C-O	5.69	1.34	1.23
2	P	870	DA	C6-N1	5.68	1.39	1.35
1	T	847	DT	N1-C6	5.68	1.42	1.38
3	A	348	ARG	CZ-NH2	5.67	1.40	1.33
3	A	320	LYS	CB-CG	5.63	1.67	1.52
3	A	135	MET	CB-CG	-5.61	1.33	1.51
3	A	68	TYR	CE1-CZ	5.61	1.45	1.38
3	A	255	ILE	CB-CG2	5.61	1.70	1.52
3	A	159	ASN	N-CA	5.60	1.57	1.46
3	A	324	LEU	N-CA	5.60	1.57	1.46
3	A	118	PRO	CA-CB	5.53	1.64	1.53
2	P	872	DC	C2'-C1'	5.52	1.57	1.52
3	A	172	ARG	CZ-NH2	5.51	1.40	1.33
1	T	843	DG	C4'-O4'	5.51	1.50	1.45
3	A	348	ARG	CG-CD	5.51	1.65	1.51
3	A	102	TYR	CD2-CE2	-5.50	1.31	1.39
3	A	346	ILE	CA-CB	5.49	1.67	1.54
1	T	839	DT	C3'-C2'	5.48	1.58	1.52
1	T	841	DG	O3'-P	-5.46	1.54	1.61
1	T	842	DG	N9-C8	5.46	1.41	1.37
3	A	172	ARG	CZ-NH1	5.45	1.40	1.33
3	A	307	SER	CB-OG	5.43	1.49	1.42
1	T	844	DT	C4-C5	5.41	1.49	1.45
3	A	244	TYR	CE2-CZ	5.38	1.45	1.38
3	A	125	PHE	CD2-CE2	5.38	1.50	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	206	ALA	CA-CB	5.36	1.63	1.52
2	P	870	DA	N9-C4	-5.35	1.34	1.37
3	A	316	GLU	C-O	5.33	1.33	1.23
3	A	153	VAL	N-CA	-5.31	1.35	1.46
3	A	267	LYS	CD-CE	5.31	1.64	1.51
3	A	410	PHE	CB-CG	-5.29	1.42	1.51
3	A	384	VAL	C-O	5.28	1.33	1.23
3	A	28	ARG	CZ-NH1	5.26	1.39	1.33
1	T	844	DT	C3'-O3'	-5.25	1.37	1.44
3	A	224	GLU	CD-OE2	5.23	1.31	1.25
3	A	68	TYR	CE2-CZ	5.20	1.45	1.38
1	T	843	DG	C2'-C1'	5.15	1.57	1.52
3	A	87	LYS	CE-NZ	5.14	1.61	1.49
1	T	844	DT	C4'-O4'	5.13	1.50	1.45
3	A	33	VAL	CB-CG1	5.10	1.63	1.52
3	A	318	LYS	CD-CE	5.10	1.64	1.51
2	P	869	DG	N9-C8	5.09	1.41	1.37
1	T	847	DT	C5'-C4'	5.05	1.56	1.51
3	A	213	PHE	CE2-CZ	5.02	1.46	1.37
3	A	308	PHE	CB-CG	5.02	1.59	1.51

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	844	DT	C4-C5-C7	18.14	129.88	119.00
2	P	870	DA	O4'-C1'-N9	16.06	119.24	108.00
2	P	867	DA	O4'-C1'-N9	15.30	118.71	108.00
3	A	122	ARG	NE-CZ-NH2	-13.75	113.43	120.30
3	A	306	ASP	CB-CG-OD1	12.61	129.65	118.30
1	T	847	DT	C4-C5-C6	-12.43	110.54	118.00
1	T	839	DT	N3-C4-O4	12.09	127.15	119.90
2	P	870	DA	O4'-C4'-C3'	11.77	113.06	106.00
1	T	847	DT	N3-C4-C5	11.22	121.93	115.20
1	T	843	DG	O4'-C4'-C3'	10.50	112.30	106.00
3	A	318	LYS	CD-CE-NZ	-10.41	87.75	111.70
1	T	847	DT	O4'-C4'-C3'	10.12	112.07	106.00
1	T	840	DG	C5'-C4'-C3'	-10.01	96.09	114.10
2	P	871	DC	O4'-C4'-C3'	9.89	111.93	106.00
2	P	867	DA	O4'-C4'-C3'	-9.51	100.29	106.00
3	A	172	ARG	CG-CD-NE	-9.36	92.15	111.80
1	T	844	DT	C4-C5-C6	-9.21	112.48	118.00
2	P	867	DA	C5-C6-N1	9.13	122.27	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	844	DT	N3-C4-O4	-8.97	114.52	119.90
2	P	867	DA	C8-N9-C4	-8.90	102.24	105.80
1	T	844	DT	C6-C5-C7	-8.79	117.62	122.90
3	A	319	ASN	OD1-CG-ND2	8.75	142.03	121.90
3	A	215	PRO	N-CD-CG	-8.72	90.12	103.20
1	T	839	DT	C5-C4-O4	-8.66	118.84	124.90
3	A	382	PRO	N-CD-CG	-8.64	90.24	103.20
3	A	382	PRO	CA-CB-CG	-8.62	87.63	104.00
1	T	839	DT	C2-N1-C1'	8.30	131.49	118.20
1	T	839	DT	N3-C2-O2	-8.18	117.39	122.30
3	A	314	GLU	O-C-N	8.04	135.56	122.70
1	T	840	DG	C5-C6-N1	7.99	115.49	111.50
2	P	868	DG	N1-C6-O6	7.97	124.68	119.90
3	A	253	LEU	CA-CB-CG	-7.96	96.99	115.30
2	P	871	DC	O4'-C1'-N1	7.86	113.50	108.00
3	A	122	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	T	839	DT	P-O3'-C3'	7.79	129.05	119.70
3	A	306	ASP	CB-CG-OD2	-7.70	111.37	118.30
2	P	867	DA	C1'-O4'-C4'	7.51	117.61	110.10
1	T	847	DT	O4'-C1'-C2'	7.47	111.88	105.90
3	A	323	GLU	OE1-CD-OE2	7.42	132.20	123.30
1	T	847	DT	C4'-C3'-O3'	7.35	128.06	109.70
3	A	348	ARG	NE-CZ-NH2	-7.32	116.64	120.30
3	A	319	ASN	CB-CG-OD1	-7.31	106.98	121.60
3	A	122	ARG	CG-CD-NE	-7.25	96.57	111.80
1	T	845	DC	OP1-P-O3'	-7.16	89.44	105.20
1	T	839	DT	C6-N1-C1'	-7.07	109.79	120.40
1	T	841	DG	C6-N1-C2	-7.04	120.87	125.10
1	T	840	DG	C6-N1-C2	-7.04	120.88	125.10
1	T	846	DC	C6-N1-C2	-7.02	117.49	120.30
1	T	847	DT	C6-C5-C7	6.98	127.09	122.90
1	T	845	DC	N3-C4-N4	-6.95	113.14	118.00
1	T	847	DT	N3-C4-O4	-6.93	115.74	119.90
1	T	843	DG	C4'-C3'-C2'	-6.93	96.86	103.10
2	P	872	DC	O4'-C1'-N1	6.91	112.84	108.00
1	T	844	DT	P-O3'-C3'	-6.74	111.61	119.70
1	T	840	DG	C2-N3-C4	6.71	115.26	111.90
2	P	869	DG	P-O3'-C3'	-6.63	111.74	119.70
2	P	867	DA	C6-N1-C2	-6.56	114.67	118.60
3	A	184	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	T	844	DT	C1'-O4'-C4'	-6.48	103.62	110.10
1	T	839	DT	N1-C2-O2	6.44	128.25	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	870	DA	C6-N1-C2	-6.37	114.78	118.60
2	P	867	DA	N1-C6-N6	-6.35	114.79	118.60
3	A	207	LYS	CD-CE-NZ	-6.30	97.21	111.70
1	T	843	DG	C5-C6-N1	6.28	114.64	111.50
3	A	172	ARG	NE-CZ-NH1	-6.27	117.17	120.30
3	A	390	LEU	CA-C-N	-6.25	103.46	117.20
1	T	845	DC	OP2-P-O3'	6.21	118.86	105.20
3	A	382	PRO	CB-CG-CD	-6.20	82.34	106.50
1	T	844	DT	O4'-C4'-C3'	6.18	109.71	106.00
1	T	843	DG	N1-C6-O6	-6.18	116.19	119.90
1	T	845	DC	C4-C5-C6	-6.16	114.32	117.40
2	P	867	DA	N7-C8-N9	6.15	116.87	113.80
3	A	73	LEU	CA-CB-CG	6.13	129.41	115.30
3	A	380	MET	C-N-CA	6.12	137.00	121.70
3	A	305	GLU	N-CA-CB	-6.06	99.69	110.60
2	P	869	DG	C2-N3-C4	-6.00	108.90	111.90
1	T	841	DG	C5-C6-O6	-5.99	125.00	128.60
1	T	840	DG	C8-N9-C4	-5.95	104.02	106.40
1	T	847	DT	C5'-C4'-O4'	-5.93	98.04	109.30
3	A	413	LEU	CA-CB-CG	5.92	128.92	115.30
2	P	870	DA	N7-C8-N9	5.90	116.75	113.80
3	A	311	CYS	CB-CA-C	-5.90	98.60	110.40
3	A	103	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	T	844	DT	N3-C4-C5	5.80	118.68	115.20
2	P	872	DC	O4'-C4'-C3'	5.69	109.42	106.00
1	T	842	DG	C4'-C3'-O3'	5.66	123.84	109.70
3	A	122	ARG	CD-NE-CZ	5.65	131.50	123.60
3	A	337	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	A	28	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	A	246	THR	OG1-CB-CG2	-5.56	97.20	110.00
1	T	847	DT	C4-C5-C7	5.55	122.33	119.00
3	A	78	LEU	CB-CG-CD1	5.54	120.43	111.00
3	A	388	MET	N-CA-C	5.54	125.97	111.00
1	T	845	DC	N3-C4-C5	5.54	124.11	121.90
3	A	392	ARG	CG-CD-NE	-5.52	100.22	111.80
1	T	840	DG	C5'-C4'-O4'	5.51	119.77	109.30
3	A	388	MET	CG-SD-CE	-5.50	91.40	100.20
3	A	390	LEU	CB-CG-CD1	-5.49	101.67	111.00
1	T	843	DG	C6-N1-C2	-5.48	121.81	125.10
1	T	839	DT	N1-C1'-C2'	5.47	123.00	112.60
3	A	253	LEU	CB-CG-CD1	-5.47	101.70	111.00
2	P	870	DA	OP2-P-O3'	5.47	117.23	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	847	DT	C5-C6-N1	5.42	126.95	123.70
3	A	214	LYS	CA-CB-CG	5.41	125.30	113.40
3	A	215	PRO	C-N-CA	-5.38	108.24	121.70
1	T	842	DG	P-O5'-C5'	5.38	129.51	120.90
1	T	847	DT	O5'-P-OP2	5.36	117.13	110.70
2	P	867	DA	O5'-C5'-C4'	5.35	124.38	111.00
3	A	68	TYR	CA-CB-CG	-5.26	103.40	113.40
2	P	868	DG	N1-C2-N3	-5.23	120.76	123.90
1	T	846	DC	C4'-C3'-C2'	5.20	107.78	103.10
1	T	839	DT	C6-N1-C2	-5.17	118.71	121.30
3	A	380	MET	O-C-N	5.14	130.93	122.70
2	P	867	DA	O4'-C1'-C2'	-5.14	101.79	105.90
3	A	98	ASP	CB-CG-OD2	5.09	122.88	118.30
3	A	304	GLU	OE1-CD-OE2	5.08	129.40	123.30
1	T	840	DG	N7-C8-N9	5.05	115.63	113.10
2	P	868	DG	C8-N9-C4	-5.04	104.38	106.40
3	A	360	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	T	842	DG	N3-C4-N9	-5.03	122.98	126.00
3	A	348	ARG	NE-CZ-NH1	5.02	122.81	120.30
3	A	69	GLU	OE1-CD-OE2	-5.02	117.28	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	213	PHE	Peptide
3	A	305	GLU	Peptide
3	A	388	MET	Peptide
1	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	T	183	0	104	9	2
2	P	139	0	79	2	2
3	A	2813	0	2813	212	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	107	0	0	8	0
4	P	2	0	0	0	0
4	T	6	0	0	0	0
All	All	3250	0	2996	219	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 36.

All (219) 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:392:ARG:CG	3:A:392:ARG:CB	1.79	1.58
3:A:318:LYS:CB	3:A:318:LYS:CG	1.79	1.57
3:A:230:ILE:CD1	3:A:230:ILE:CG1	1.77	1.55
3:A:105:MET:SD	3:A:105:MET:CE	2.01	1.48
3:A:382:PRO:C	3:A:382:PRO:CA	1.84	1.46
3:A:314:GLU:CB	3:A:314:GLU:CA	1.94	1.43
3:A:382:PRO:CG	3:A:382:PRO:CB	1.93	1.43
3:A:394:MET:CG	3:A:394:MET:SD	2.07	1.42
1:T:847:DT:O3'	1:T:847:DT:C3'	1.66	1.41
3:A:314:GLU:O	3:A:314:GLU:C	1.65	1.35
3:A:314:GLU:CB	3:A:314:GLU:CG	2.05	1.32
3:A:318:LYS:HE3	3:A:384:VAL:CG1	1.59	1.30
3:A:320:LYS:CG	3:A:320:LYS:CD	2.14	1.24
3:A:388:MET:O	3:A:392:ARG:NH1	1.72	1.22
3:A:319:ASN:CG	3:A:319:ASN:OD1	1.83	1.18
3:A:189:ASN:HB3	4:A:914:HOH:O	1.46	1.15
3:A:319:ASN:CG	3:A:319:ASN:ND2	2.05	1.10
3:A:388:MET:CE	3:A:392:ARG:HH12	1.65	1.08
3:A:347:ARG:CG	3:A:404:THR:HG23	1.85	1.06
3:A:347:ARG:HG3	3:A:404:THR:HG23	1.06	1.03
3:A:380:MET:CE	3:A:384:VAL:CG2	2.39	1.01
3:A:308:PHE:CD2	3:A:320:LYS:NZ	2.28	1.00
3:A:381:THR:HB	3:A:382:PRO:HD2	1.42	0.99
3:A:388:MET:HE3	3:A:392:ARG:HH12	1.25	0.99
3:A:318:LYS:O	3:A:321:ILE:HB	1.65	0.96
3:A:318:LYS:HE3	3:A:384:VAL:HG11	1.47	0.95
3:A:318:LYS:HE3	3:A:384:VAL:HG13	1.47	0.94
3:A:388:MET:HE3	3:A:392:ARG:NH1	1.84	0.92
3:A:367:HIS:CD2	3:A:368:VAL:N	2.37	0.91
3:A:381:THR:HB	3:A:382:PRO:CD	2.00	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:137:GLU:HG2	3:A:172:ARG:HH12	1.36	0.91
3:A:158:TYR:O	4:A:999:HOH:O	1.87	0.90
3:A:347:ARG:HG3	3:A:404:THR:CG2	1.99	0.89
3:A:388:MET:CE	3:A:392:ARG:NH1	2.36	0.85
3:A:392:ARG:CB	3:A:392:ARG:CD	2.55	0.85
3:A:380:MET:O	3:A:383:MET:HB2	1.76	0.85
3:A:388:MET:HE2	3:A:392:ARG:HH22	1.43	0.83
3:A:318:LYS:CE	3:A:384:VAL:CG1	2.51	0.83
3:A:62:LEU:HD13	3:A:78:LEU:HD23	1.58	0.83
3:A:367:HIS:NE2	3:A:368:VAL:HG13	1.93	0.83
3:A:367:HIS:CD2	3:A:368:VAL:HG13	2.13	0.83
3:A:137:GLU:HG2	3:A:172:ARG:NH1	1.93	0.82
3:A:304:GLU:HG3	3:A:328:LEU:HG	1.60	0.81
3:A:388:MET:C	3:A:392:ARG:HH11	1.84	0.81
3:A:367:HIS:CD2	3:A:368:VAL:CG1	2.64	0.80
3:A:290:ASN:ND2	4:A:905:HOH:O	2.14	0.80
3:A:292:PRO:O	4:A:929:HOH:O	2.00	0.79
3:A:344:LEU:HD11	3:A:387:LEU:HD22	1.65	0.79
3:A:367:HIS:NE2	3:A:368:VAL:CG1	2.46	0.79
3:A:164:ASN:H	3:A:170:HIS:HD2	1.30	0.78
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.12	0.78
3:A:253:LEU:HD12	3:A:253:LEU:N	1.99	0.78
3:A:387:LEU:HA	3:A:390:LEU:HD12	1.66	0.78
3:A:253:LEU:HD12	3:A:253:LEU:H	1.51	0.76
3:A:344:LEU:CD1	3:A:387:LEU:HD22	2.16	0.76
3:A:380:MET:HE2	3:A:384:VAL:HG21	1.68	0.75
3:A:236:ILE:HD12	3:A:250:LEU:HD13	1.69	0.74
3:A:230:ILE:CD1	3:A:230:ILE:CB	2.63	0.73
3:A:388:MET:HE2	3:A:392:ARG:NH2	2.04	0.73
3:A:43:GLU:OE1	3:A:101:ARG:NH2	2.23	0.72
3:A:347:ARG:HD3	3:A:405:LEU:CB	2.19	0.72
3:A:302:PHE:CE1	3:A:413:LEU:HD11	2.25	0.71
3:A:202:ASN:C	3:A:202:ASN:HD22	1.93	0.71
3:A:367:HIS:HD2	3:A:368:VAL:N	1.88	0.70
3:A:62:LEU:HD13	3:A:78:LEU:CD2	2.21	0.70
3:A:318:LYS:CE	3:A:384:VAL:HG11	2.19	0.70
3:A:392:ARG:CG	3:A:392:ARG:CA	2.70	0.70
3:A:405:LEU:O	3:A:406:LEU:CD2	2.39	0.70
3:A:318:LYS:CE	3:A:318:LYS:NZ	2.56	0.69
3:A:380:MET:CE	3:A:384:VAL:HG23	2.20	0.69
3:A:380:MET:HE1	3:A:384:VAL:CG2	2.20	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:137:GLU:CG	3:A:172:ARG:HH12	2.03	0.69
3:A:302:PHE:HE1	3:A:413:LEU:HD11	1.55	0.69
3:A:388:MET:HB3	3:A:392:ARG:NH1	2.09	0.68
3:A:405:LEU:C	3:A:406:LEU:HD23	2.14	0.68
3:A:318:LYS:HD2	3:A:388:MET:SD	2.33	0.68
3:A:388:MET:HE2	3:A:392:ARG:HH12	1.53	0.67
3:A:388:MET:C	3:A:392:ARG:NH1	2.42	0.67
3:A:366:SER:O	3:A:369:ILE:HB	1.95	0.67
1:T:841:DG:H2"	1:T:842:DG:H5"	1.76	0.67
1:T:847:DT:O3'	1:T:847:DT:H3'	1.86	0.66
3:A:50:LEU:HD22	3:A:92:VAL:HG11	1.76	0.66
3:A:382:PRO:HG2	3:A:383:MET:H	1.60	0.66
3:A:380:MET:HE1	3:A:384:VAL:HG22	1.78	0.65
3:A:388:MET:CE	3:A:392:ARG:HH22	2.10	0.65
3:A:80:ASN:O	3:A:84:ALA:HB3	1.97	0.65
3:A:318:LYS:O	3:A:321:ILE:CB	2.44	0.64
3:A:390:LEU:O	3:A:394:MET:HG3	1.97	0.64
3:A:366:SER:HA	3:A:369:ILE:HD12	1.78	0.64
3:A:312:SER:OG	3:A:317:ALA:HB3	1.98	0.64
3:A:27:SER:HB3	4:A:981:HOH:O	1.96	0.64
3:A:405:LEU:O	3:A:406:LEU:HD23	1.98	0.63
3:A:249:CYS:O	3:A:253:LEU:HD12	1.99	0.63
1:T:842:DG:H2"	1:T:843:DG:H5'	1.80	0.62
3:A:185:GLU:OE1	3:A:189:ASN:ND2	2.33	0.62
3:A:202:ASN:ND2	3:A:205:LEU:H	1.98	0.62
3:A:105:MET:CE	3:A:105:MET:HB2	2.30	0.61
3:A:388:MET:HE2	3:A:392:ARG:NH1	2.11	0.61
3:A:305:GLU:HG3	3:A:407:SER:HB3	1.81	0.61
3:A:318:LYS:O	3:A:321:ILE:N	2.31	0.61
3:A:367:HIS:CD2	3:A:368:VAL:HG12	2.36	0.60
3:A:142:GLN:HA	3:A:142:GLN:NE2	2.17	0.60
3:A:196:CYS:SG	3:A:214:LYS:O	2.60	0.60
3:A:367:HIS:CD2	3:A:368:VAL:H	2.18	0.60
3:A:382:PRO:O	3:A:385:ASP:N	2.35	0.60
3:A:202:ASN:HD21	3:A:205:LEU:H	1.51	0.59
3:A:318:LYS:O	3:A:318:LYS:HG2	2.04	0.58
1:T:847:DT:C3'	1:T:847:DT:HO3'	2.10	0.58
3:A:318:LYS:HE2	3:A:322:GLU:OE1	2.04	0.57
3:A:50:LEU:CD2	3:A:92:VAL:HG11	2.35	0.57
3:A:313:SER:O	3:A:314:GLU:OE2	2.22	0.57
3:A:112:LEU:O	3:A:112:LEU:HD23	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:142:GLN:NE2	3:A:142:GLN:CA	2.67	0.56
3:A:318:LYS:HE3	3:A:384:VAL:HG12	1.74	0.56
3:A:330:ASN:O	3:A:333:CYS:HB3	2.05	0.56
3:A:405:LEU:O	3:A:406:LEU:HD22	2.06	0.56
3:A:318:LYS:CG	3:A:318:LYS:CA	2.77	0.55
3:A:62:LEU:CD1	3:A:78:LEU:HD23	2.35	0.55
3:A:80:ASN:C	3:A:82:ARG:H	2.10	0.55
3:A:249:CYS:O	3:A:253:LEU:CD1	2.55	0.55
3:A:388:MET:HE2	3:A:392:ARG:CZ	2.37	0.55
3:A:388:MET:CE	3:A:392:ARG:NH2	2.69	0.54
3:A:345:ILE:HG22	3:A:346:ILE:N	2.22	0.54
3:A:361:GLN:OE1	4:A:946:HOH:O	2.18	0.54
3:A:144:GLN:OE1	3:A:146:ASP:CB	2.55	0.54
3:A:36:ASP:OD1	3:A:215:PRO:O	2.26	0.54
3:A:308:PHE:CE1	3:A:312:SER:HB2	2.42	0.54
3:A:164:ASN:H	3:A:170:HIS:CD2	2.19	0.54
1:T:841:DG:OP2	3:A:307:SER:HB2	2.07	0.54
3:A:214:LYS:N	3:A:215:PRO:CD	2.71	0.53
3:A:308:PHE:HE2	3:A:320:LYS:HD2	1.72	0.53
3:A:394:MET:CG	3:A:394:MET:CE	2.85	0.53
3:A:79:MET:HE3	3:A:84:ALA:HA	1.90	0.53
3:A:308:PHE:HB2	3:A:311:CYS:SG	2.48	0.53
3:A:362:CYS:HB3	3:A:390:LEU:HD21	1.92	0.52
3:A:283:LYS:HE2	3:A:288:GLU:OE1	2.09	0.52
3:A:308:PHE:CE2	3:A:320:LYS:HD2	2.45	0.52
3:A:367:HIS:CD2	3:A:367:HIS:C	2.83	0.52
3:A:388:MET:CE	3:A:392:ARG:CZ	2.88	0.52
3:A:381:THR:CB	3:A:382:PRO:HD2	2.28	0.51
3:A:388:MET:HB3	3:A:392:ARG:HH12	1.75	0.51
3:A:367:HIS:CE1	4:A:1036:HOH:O	2.62	0.51
3:A:112:LEU:HD23	3:A:112:LEU:C	2.30	0.51
3:A:105:MET:CE	3:A:105:MET:CB	2.89	0.50
3:A:302:PHE:HE1	3:A:413:LEU:CD1	2.24	0.50
3:A:380:MET:HE3	3:A:384:VAL:HG23	1.94	0.50
3:A:202:ASN:C	3:A:202:ASN:ND2	2.60	0.50
3:A:383:MET:O	3:A:384:VAL:C	2.50	0.50
3:A:382:PRO:HG2	3:A:383:MET:N	2.25	0.50
3:A:107:TYR:OH	3:A:299:PRO:HG3	2.12	0.49
3:A:265:SER:OG	3:A:268:ILE:HG13	2.12	0.49
3:A:318:LYS:HG2	3:A:318:LYS:C	2.33	0.49
3:A:318:LYS:CG	3:A:318:LYS:C	2.81	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:318:LYS:C	3:A:321:ILE:H	2.16	0.49
3:A:413:LEU:HD22	3:A:413:LEU:H	1.78	0.49
3:A:413:LEU:H	3:A:413:LEU:CD2	2.26	0.48
3:A:367:HIS:NE2	3:A:368:VAL:HG12	2.26	0.48
3:A:170:HIS:HE1	3:A:224:GLU:OE2	1.97	0.48
2:P:872:DC:H2"	2:P:873:DOC:H6	1.96	0.48
3:A:148:LEU:C	3:A:148:LEU:HD23	2.33	0.48
1:T:839:DT:H73	3:A:78:LEU:HD13	1.96	0.48
3:A:55:LEU:O	3:A:66:CYS:HA	2.14	0.48
3:A:335:ASP:OD2	3:A:337:ARG:NH1	2.46	0.47
1:T:839:DT:C7	3:A:78:LEU:HD13	2.44	0.47
3:A:318:LYS:HD2	3:A:388:MET:CG	2.45	0.47
3:A:339:PRO:HG3	3:A:410:PHE:CD2	2.50	0.47
3:A:31:VAL:HG12	3:A:130:VAL:HB	1.96	0.47
3:A:127:GLU:OE1	3:A:207:LYS:HE3	2.15	0.47
3:A:80:ASN:O	3:A:84:ALA:CB	2.62	0.46
3:A:247:ALA:O	3:A:251:GLU:HG3	2.15	0.46
3:A:343:ARG:HD2	3:A:345:ILE:HD11	1.98	0.46
3:A:344:LEU:O	3:A:359:SER:HA	2.16	0.46
3:A:382:PRO:C	3:A:382:PRO:N	2.62	0.46
3:A:236:ILE:CD1	3:A:250:LEU:HD13	2.44	0.46
3:A:314:GLU:CB	3:A:314:GLU:CD	2.80	0.46
3:A:365:PRO:O	3:A:368:VAL:N	2.42	0.46
3:A:31:VAL:CG1	3:A:130:VAL:HB	2.46	0.46
3:A:236:ILE:HD13	3:A:236:ILE:HG21	1.64	0.46
3:A:318:LYS:CG	3:A:388:MET:SD	3.04	0.45
3:A:298:PRO:HA	3:A:299:PRO:HD3	1.81	0.45
3:A:44:MET:HE1	4:A:954:HOH:O	2.16	0.45
3:A:388:MET:O	3:A:392:ARG:HD2	2.16	0.45
3:A:36:ASP:O	3:A:37:CYS:C	2.54	0.45
3:A:308:PHE:O	3:A:308:PHE:CD1	2.70	0.45
3:A:62:LEU:CD1	3:A:78:LEU:CD2	2.93	0.44
3:A:308:PHE:CE2	3:A:320:LYS:NZ	2.60	0.44
3:A:380:MET:CE	3:A:384:VAL:HG21	2.25	0.44
3:A:60:LYS:HD3	3:A:60:LYS:HA	1.75	0.44
3:A:324:LEU:HD13	3:A:407:SER:HA	1.99	0.44
3:A:388:MET:CB	3:A:392:ARG:HH12	2.30	0.44
3:A:120:VAL:HG22	3:A:130:VAL:HG22	2.00	0.44
3:A:268:ILE:O	3:A:272:GLU:HB2	2.18	0.44
3:A:388:MET:CB	3:A:392:ARG:NH1	2.80	0.43
3:A:318:LYS:HG3	3:A:388:MET:SD	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:76:LYS:O	3:A:77:LYS:C	2.56	0.43
3:A:105:MET:HB2	3:A:105:MET:HE3	1.97	0.43
1:T:839:DT:H73	3:A:78:LEU:CB	2.48	0.43
3:A:318:LYS:CG	3:A:318:LYS:O	2.67	0.43
3:A:121:GLU:O	3:A:128:ASN:HA	2.19	0.43
3:A:318:LYS:HA	3:A:321:ILE:HD12	2.01	0.43
3:A:360:ARG:HG2	3:A:394:MET:SD	2.59	0.42
3:A:80:ASN:HB3	3:A:83:ASP:H	1.83	0.42
3:A:147:GLU:H	3:A:147:GLU:HG2	1.52	0.42
3:A:318:LYS:HD2	3:A:388:MET:HG3	2.01	0.42
3:A:94:VAL:HG12	3:A:95:ASN:N	2.35	0.42
3:A:215:PRO:HD2	3:A:217:GLN:NE2	2.33	0.42
3:A:365:PRO:O	3:A:368:VAL:HG22	2.19	0.42
3:A:384:VAL:HG23	3:A:384:VAL:H	1.56	0.42
3:A:345:ILE:HG22	3:A:346:ILE:H	1.84	0.42
3:A:80:ASN:C	3:A:82:ARG:N	2.72	0.42
3:A:170:HIS:CE1	3:A:224:GLU:OE2	2.73	0.41
3:A:308:PHE:HB2	3:A:311:CYS:HB2	2.02	0.41
3:A:405:LEU:C	3:A:406:LEU:CD2	2.86	0.41
3:A:63:VAL:O	3:A:63:VAL:HG12	2.19	0.41
3:A:386:ILE:O	3:A:390:LEU:HG	2.20	0.41
3:A:171:ILE:HD12	3:A:171:ILE:HG23	1.88	0.41
3:A:380:MET:HE2	3:A:380:MET:HB3	1.83	0.41
3:A:53:LYS:HA	3:A:54:PRO:HD3	1.65	0.41
2:P:872:DC:C2'	2:P:873:DOC:OP2	2.59	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:T:847:DT:O3'	2:P:867:DA:O5'[10_665]	1.55	0.65
1:T:847:DT:O3'	2:P:867:DA:C5'[10_665]	2.14	0.06

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	359/420 (86%)	315 (88%)	27 (8%)	17 (5%)	2 1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	145	SER
3	A	146	ASP
3	A	333	CYS
3	A	334	GLN
3	A	366	SER
3	A	381	THR
3	A	405	LEU
3	A	77	LYS
3	A	215	PRO
3	A	314	GLU
3	A	393	ASN
3	A	308	PHE
3	A	315	VAL
3	A	337	ARG
3	A	37	CYS
3	A	384	VAL
3	A	365	PRO

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	312/376 (83%)	273 (88%)	39 (12%)	4 5

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

Mol	Chain	Res	Type
3	A	58	GLN
3	A	71	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	73	LEU
3	A	78	LEU
3	A	80	ASN
3	A	82	ARG
3	A	90	GLN
3	A	123	LEU
3	A	142	GLN
3	A	144	GLN
3	A	145	SER
3	A	149	SER
3	A	170	HIS
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	214	LYS
3	A	229	LEU
3	A	295	LEU
3	A	306	ASP
3	A	307	SER
3	A	309	LYS
3	A	314	GLU
3	A	327	SER
3	A	332	VAL
3	A	334	GLN
3	A	342	VAL
3	A	344	LEU
3	A	347	ARG
3	A	357	ARG
3	A	359	SER
3	A	361	GLN
3	A	362	CYS
3	A	380	MET
3	A	387	LEU
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	142	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	170	HIS
3	A	202	ASN
3	A	217	GLN
3	A	262	GLN
3	A	279	GLN
3	A	340	HIS
3	A	367	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DOC	P	873	1,2	16,19,20	1.66	3 (18%)	20,26,29	1.93	3 (15%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	873	DOC	C2'-C1'	4.23	1.61	1.51
2	P	873	DOC	O4'-C4'	3.03	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	873	DOC	O4'-C1'	-2.21	1.37	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	873	DOC	C2'-C1'-N1	-4.79	103.33	112.40
2	P	873	DOC	O4'-C4'-C3'	4.32	111.98	104.80
2	P	873	DOC	C4'-O4'-C1'	-3.99	106.04	109.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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 monosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	314:GLU	C	315:VAL	N	1.64

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%)	0.71	1 (11%) 5 4	32, 34, 64, 101	0
2	P	6/7 (85%)	0.20	0 100 100	32, 41, 44, 53	0
3	A	367/420 (87%)	1.06	77 (20%) 1 0	9, 39, 89, 101	0
All	All	382/438 (87%)	1.04	78 (20%) 1 0	9, 39, 89, 101	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	355	TYR	12.0
3	A	313	SER	10.2
3	A	349	TYR	9.1
3	A	319	ASN	8.6
3	A	84	ALA	6.8
3	A	348	ARG	6.7
3	A	244	TYR	6.4
3	A	333	CYS	6.0
3	A	315	VAL	5.7
3	A	388	MET	5.4
3	A	314	GLU	5.4
3	A	335	ASP	5.4
3	A	317	ALA	5.3
3	A	332	VAL	5.3
3	A	310	LYS	5.2
3	A	86	GLU	5.2
3	A	82	ARG	5.2
1	T	839	DT	5.2
3	A	368	VAL	5.1
3	A	144	GLN	5.1
3	A	143	LEU	5.0
3	A	72	LYS	4.6
3	A	83	ASP	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	311	CYS	4.5
3	A	320	LYS	4.4
3	A	414	LYS	4.4
3	A	54	PRO	4.2
3	A	145	SER	4.2
3	A	74	GLY	4.1
3	A	336	GLY	4.0
3	A	73	LEU	3.8
3	A	347	ARG	3.7
3	A	379	VAL	3.7
3	A	367	HIS	3.7
3	A	392	ARG	3.7
3	A	382	PRO	3.3
3	A	85	LYS	3.2
3	A	312	SER	3.2
3	A	80	ASN	3.2
3	A	71	ARG	3.0
3	A	370	GLN	3.0
3	A	404	THR	3.0
3	A	316	GLU	2.9
3	A	380	MET	2.9
3	A	91	LEU	2.8
3	A	318	LYS	2.8
3	A	52	ASP	2.8
3	A	70	ALA	2.8
3	A	148	LEU	2.8
3	A	384	VAL	2.7
3	A	383	MET	2.6
3	A	366	SER	2.6
3	A	387	LEU	2.6
3	A	68	TYR	2.6
3	A	61	TYR	2.5
3	A	390	LEU	2.5
3	A	345	ILE	2.4
3	A	79	MET	2.4
3	A	405	LEU	2.4
3	A	369	ILE	2.4
3	A	326	ALA	2.4
3	A	142	GLN	2.4
3	A	75	VAL	2.3
3	A	235	HIS	2.3
3	A	413	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	321	ILE	2.3
3	A	302	PHE	2.3
3	A	81	VAL	2.2
3	A	214	LYS	2.2
3	A	252	ALA	2.2
3	A	334	GLN	2.2
3	A	394	MET	2.2
3	A	308	PHE	2.2
3	A	248	LYS	2.1
3	A	141	GLN	2.1
3	A	265	SER	2.0
3	A	50	LEU	2.0
3	A	87	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DOC	P	873	18/19	0.93	0.18	27,34,39,42	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.