



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:16 AM UTC

PDB ID : 2FLP / pdb_00002flp
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

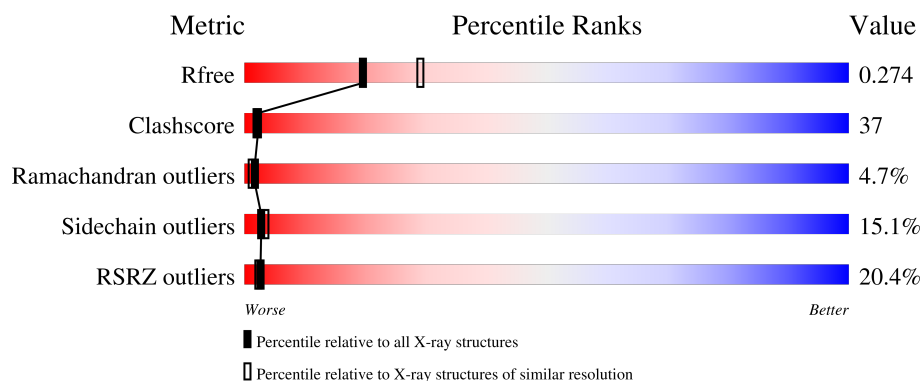
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	11	9% 45% 27% 9% 18%
2	P	7	14% 43% 43%
3	A	420	18% 34% 33% 17% • 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
1	T	9	Total	C	N	O	P	0	0	0
			183	88	32	55	8			

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

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

- Molecule 3 is a protein called DNA polymerase iota.

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

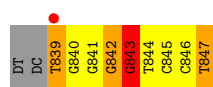
- Molecule 4 is water.

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

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.

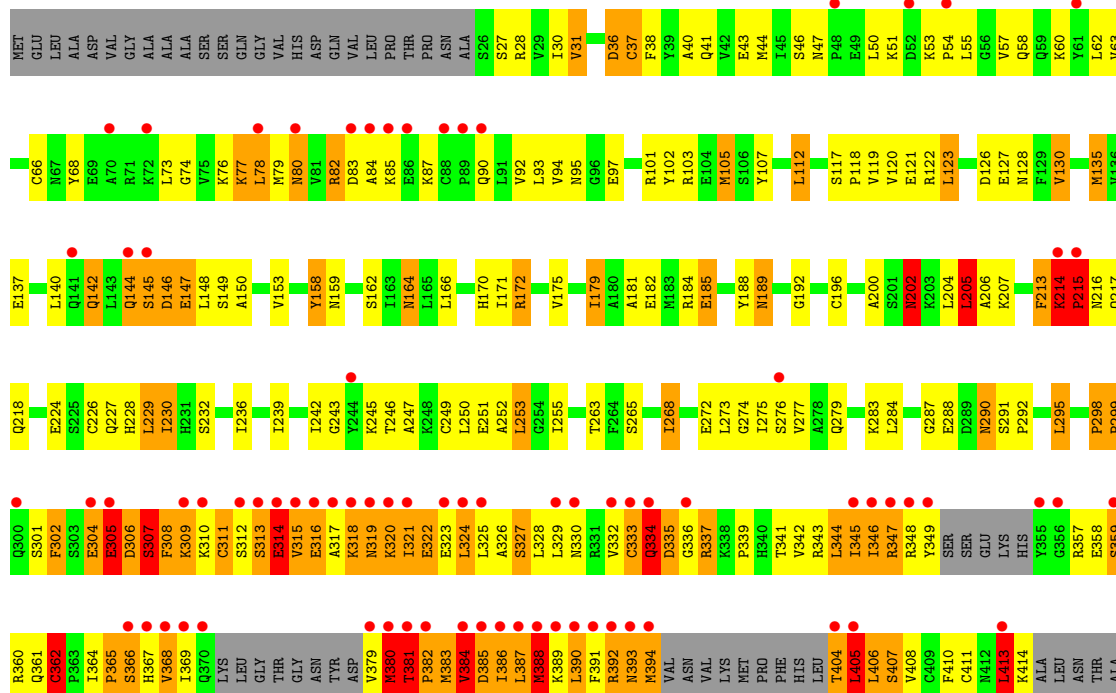
- Molecule 1: DNA template strand



- Molecule 2: DNA primer strand



- Molecule 3: DNA polymerase iota



LYS

4 Data and refinement statistics

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 36.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (36.51-2.40) 96.2 (36.51-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (9.73%)	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)	0.32 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	1.78	1/204 (0.5%)	2.65	19/314 (6.1%)
2	P	1.55	0/136	2.32	13/208 (6.2%)
3	A	3.29	165/2850 (5.8%)	1.89	97/3851 (2.5%)
All	All	3.16	166/3190 (5.2%)	1.97	129/4373 (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
1	T	0	1
3	A	0	3
All	All	0	4

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	313	SER	CB-OG	64.87	2.71	1.42
3	A	318	LYS	CE-NZ	35.64	2.56	1.49
3	A	319	ASN	CG-ND2	34.24	2.05	1.33
3	A	314	GLU	C-O	33.08	1.65	1.24
3	A	319	ASN	CG-OD1	31.27	1.82	1.23
3	A	314	GLU	CA-CB	24.53	1.95	1.53
3	A	314	GLU	C-N	22.32	1.64	1.33
3	A	382	PRO	CA-C	22.32	1.84	1.52
3	A	320	LYS	CG-CD	20.81	2.14	1.52
3	A	390	LEU	C-O	20.51	1.50	1.24
3	A	314	GLU	CB-CG	17.81	2.05	1.52
3	A	405	LEU	C-O	16.38	1.44	1.24
3	A	381	THR	C-N	15.72	1.55	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	381	THR	C-O	15.60	1.44	1.24
3	A	214	LYS	CA-C	-13.67	1.35	1.52
3	A	322	GLU	CD-OE1	13.37	1.50	1.25
3	A	389	LYS	C-N	12.48	1.52	1.33
3	A	304	GLU	C-O	12.35	1.39	1.23
3	A	305	GLU	C-O	11.78	1.38	1.23
3	A	392	ARG	C-N	11.61	1.50	1.33
3	A	314	GLU	CD-OE2	11.37	1.47	1.25
3	A	306	ASP	CG-OD1	11.34	1.46	1.25
3	A	386	ILE	CA-CB	10.82	1.69	1.54
3	A	382	PRO	CA-CB	10.77	1.70	1.53
3	A	394	MET	CG-SD	10.77	2.07	1.80
3	A	385	ASP	C-O	10.73	1.36	1.24
3	A	383	MET	N-CA	10.53	1.59	1.46
3	A	348	ARG	CZ-NH1	10.41	1.47	1.32
3	A	389	LYS	N-CA	9.92	1.58	1.46
3	A	245	LYS	CA-CB	9.89	1.69	1.53
3	A	47	ASN	CA-C	9.88	1.63	1.52
3	A	384	VAL	CA-C	9.85	1.65	1.52
3	A	379	VAL	N-CA	9.84	1.65	1.46
3	A	242	ILE	CA-CB	9.79	1.64	1.53
3	A	388	MET	CA-C	9.16	1.65	1.52
3	A	321	ILE	CA-CB	-9.12	1.44	1.54
3	A	304	GLU	CA-C	9.11	1.63	1.52
3	A	392	ARG	CB-CG	9.02	1.79	1.52
3	A	218	GLN	CA-C	-9.01	1.41	1.52
3	A	105	MET	SD-CE	8.93	2.01	1.79
3	A	318	LYS	CB-CG	8.89	1.79	1.52
3	A	313	SER	C-O	8.86	1.35	1.24
3	A	382	PRO	CB-CG	8.86	1.94	1.49
3	A	159	ASN	N-CA	8.83	1.57	1.46
3	A	388	MET	C-O	8.80	1.35	1.24
3	A	324	LEU	N-CA	8.79	1.57	1.46
3	A	216	ASN	N-CA	8.63	1.65	1.46
3	A	385	ASP	CA-C	8.46	1.64	1.52
3	A	213	PHE	C-O	-8.24	1.14	1.24
3	A	305	GLU	C-N	8.21	1.44	1.33
3	A	346	ILE	CA-CB	8.18	1.67	1.55
3	A	158	TYR	C-O	8.09	1.34	1.24
3	A	205	LEU	CA-C	8.03	1.62	1.52
1	T	847	DT	C3'-O3'	8.00	1.66	1.42
3	A	122	ARG	CD-NE	-7.89	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	388	MET	SD-CE	7.87	1.99	1.79
3	A	184	ARG	CD-NE	-7.84	1.35	1.46
3	A	384	VAL	C-O	7.82	1.33	1.24
3	A	189	ASN	C-O	-7.81	1.15	1.24
3	A	314	GLU	CD-OE1	7.73	1.40	1.25
3	A	291	SER	CA-C	7.72	1.61	1.52
3	A	118	PRO	CA-CB	7.69	1.64	1.53
3	A	392	ARG	NE-CZ	7.63	1.41	1.33
3	A	348	ARG	NE-CZ	7.59	1.41	1.33
3	A	380	MET	SD-CE	7.50	1.98	1.79
3	A	263	THR	C-O	-7.48	1.14	1.24
3	A	153	VAL	N-CA	-7.41	1.35	1.46
3	A	316	GLU	C-O	7.37	1.33	1.24
3	A	230	ILE	CA-CB	7.33	1.63	1.54
3	A	405	LEU	N-CA	7.23	1.55	1.46
3	A	179	ILE	CG1-CD1	-7.20	1.23	1.51
3	A	103	ARG	CZ-NH2	7.18	1.42	1.33
3	A	298	PRO	CA-C	-7.16	1.45	1.52
3	A	393	ASN	C-N	7.14	1.43	1.33
3	A	30	ILE	CA-CB	7.13	1.64	1.54
3	A	364	ILE	CA-CB	-7.09	1.45	1.54
3	A	41	GLN	CA-C	-7.08	1.43	1.52
3	A	392	ARG	CZ-NH2	7.05	1.42	1.33
3	A	392	ARG	CZ-NH1	7.05	1.42	1.32
3	A	185	GLU	CD-OE2	7.04	1.38	1.25
3	A	307	SER	N-CA	7.03	1.54	1.45
3	A	379	VAL	CA-CB	6.96	1.73	1.54
3	A	307	SER	C-O	6.89	1.32	1.23
3	A	390	LEU	N-CA	6.87	1.55	1.46
3	A	295	LEU	C-O	-6.87	1.15	1.24
3	A	206	ALA	CA-CB	6.67	1.63	1.53
3	A	299	PRO	CA-CB	6.65	1.62	1.53
3	A	381	THR	CA-CB	6.63	1.64	1.53
3	A	408	VAL	CA-C	6.63	1.60	1.52
3	A	230	ILE	CG1-CD1	6.58	1.77	1.51
3	A	405	LEU	C-N	6.54	1.42	1.33
3	A	382	PRO	C-N	6.47	1.42	1.33
3	A	140	LEU	C-O	-6.46	1.16	1.24
3	A	226	CYS	C-O	6.42	1.31	1.24
3	A	135	MET	CB-CG	-6.36	1.33	1.52
3	A	349	TYR	C-O	6.31	1.36	1.23
3	A	389	LYS	CA-C	6.31	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	188	TYR	N-CA	-6.31	1.38	1.46
3	A	304	GLU	CD-OE1	6.30	1.37	1.25
3	A	279	GLN	CG-CD	6.30	1.67	1.52
3	A	321	ILE	C-O	6.29	1.32	1.24
3	A	385	ASP	C-N	6.25	1.41	1.33
3	A	392	ARG	CA-C	6.22	1.60	1.52
3	A	381	THR	N-CA	6.20	1.54	1.46
3	A	181	ALA	CA-CB	6.18	1.62	1.53
3	A	162	SER	N-CA	6.16	1.53	1.46
3	A	164	ASN	CA-C	-6.12	1.45	1.53
3	A	345	ILE	CA-CB	-6.05	1.45	1.54
3	A	130	VAL	N-CA	-6.05	1.39	1.46
3	A	301	SER	CA-C	5.98	1.59	1.52
3	A	277	VAL	CA-CB	5.96	1.61	1.54
3	A	188	TYR	CA-C	5.93	1.60	1.52
3	A	386	ILE	C-O	5.93	1.31	1.24
3	A	202	ASN	CG-OD1	5.93	1.34	1.23
3	A	304	GLU	CD-OE2	5.90	1.36	1.25
3	A	322	GLU	CG-CD	5.88	1.66	1.52
3	A	306	ASP	N-CA	5.86	1.53	1.46
3	A	40	ALA	N-CA	5.84	1.53	1.46
3	A	348	ARG	CB-CG	5.81	1.69	1.52
3	A	227	GLN	N-CA	5.80	1.53	1.46
3	A	327	SER	CB-OG	5.80	1.53	1.42
3	A	384	VAL	C-N	5.78	1.41	1.33
3	A	321	ILE	C-N	5.69	1.42	1.33
3	A	276	SER	C-O	-5.68	1.17	1.24
3	A	46	SER	C-O	-5.65	1.17	1.24
3	A	279	GLN	CA-C	5.64	1.60	1.52
3	A	383	MET	C-N	5.64	1.41	1.33
3	A	227	GLN	CA-C	5.62	1.60	1.52
3	A	389	LYS	C-O	5.60	1.31	1.24
3	A	290	ASN	CB-CG	5.59	1.66	1.52
3	A	309	LYS	CA-C	5.57	1.59	1.52
3	A	322	GLU	CA-C	-5.55	1.45	1.52
3	A	164	ASN	C-O	-5.55	1.17	1.24
3	A	323	GLU	CD-OE2	5.54	1.35	1.25
3	A	31	VAL	CA-C	5.51	1.59	1.52
3	A	309	LYS	CA-CB	5.51	1.61	1.53
3	A	189	ASN	CG-OD1	5.48	1.33	1.23
3	A	200	ALA	CA-CB	-5.48	1.45	1.53
3	A	97	GLU	N-CA	5.39	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	57	VAL	CA-CB	5.39	1.60	1.54
3	A	311	CYS	C-N	5.38	1.41	1.33
3	A	123	LEU	CA-C	5.37	1.58	1.53
3	A	348	ARG	CZ-NH2	5.36	1.40	1.33
3	A	255	ILE	CB-CG2	5.36	1.70	1.52
3	A	393	ASN	C-O	5.32	1.30	1.24
3	A	192	GLY	CA-C	5.31	1.58	1.51
3	A	164	ASN	CG-ND2	5.30	1.44	1.33
3	A	51	LYS	CA-CB	5.28	1.61	1.53
3	A	172	ARG	CZ-NH1	5.28	1.40	1.32
3	A	287	GLY	C-O	-5.28	1.17	1.24
3	A	119	VAL	N-CA	-5.26	1.39	1.47
3	A	172	ARG	CZ-NH2	5.21	1.40	1.33
3	A	393	ASN	CA-C	5.19	1.59	1.52
3	A	182	GLU	CA-C	5.15	1.59	1.52
3	A	93	LEU	CA-C	-5.14	1.46	1.52
3	A	117	SER	C-O	-5.13	1.17	1.24
3	A	228	HIS	C-O	5.11	1.29	1.24
3	A	28	ARG	CZ-NH1	5.10	1.39	1.32
3	A	150	ALA	CA-C	5.10	1.59	1.52
3	A	320	LYS	CB-CG	5.10	1.67	1.52
3	A	239	ILE	CA-C	5.09	1.58	1.52
3	A	31	VAL	CB-CG2	5.08	1.69	1.52
3	A	36	ASP	CA-C	5.08	1.59	1.52
3	A	229	LEU	N-CA	5.07	1.52	1.46
3	A	284	LEU	CA-C	5.04	1.59	1.52
3	A	386	ILE	C-N	5.01	1.40	1.33

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	319	ASN	OD1-CG-ND2	19.43	142.03	122.60
1	T	840	DG	C5'-C4'-C3'	-12.54	96.09	114.90
1	T	847	DT	C4'-C3'-O3'	12.04	128.06	110.00
3	A	311	CYS	N-CA-C	11.39	123.70	111.28
3	A	324	LEU	N-CA-C	-11.31	98.70	111.82
3	A	314	GLU	O-C-N	9.75	135.56	122.59
3	A	388	MET	N-CA-C	9.73	125.97	112.45
3	A	215	PRO	CA-C-N	-9.31	108.24	123.04
3	A	215	PRO	C-N-CA	-9.31	108.24	123.04
1	T	842	DG	C4'-C3'-O3'	9.23	123.84	110.00
2	P	867	DA	O5'-C5'-C4'	9.05	124.38	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	172	ARG	CG-CD-NE	-9.02	92.15	112.00
3	A	382	PRO	CA-CB-CG	-8.88	87.63	104.50
3	A	215	PRO	N-CD-CG	-8.72	90.12	103.20
3	A	382	PRO	N-CD-CG	-8.64	90.24	103.20
3	A	380	MET	O-C-N	8.56	130.93	122.03
2	P	871	DC	C4'-C3'-O3'	8.18	122.26	110.00
3	A	326	ALA	N-CA-C	-8.15	101.98	111.03
1	T	839	DT	C2-N1-C1'	8.09	131.49	119.35
3	A	159	ASN	N-CA-C	-7.92	99.98	111.30
3	A	305	GLU	CA-C-N	-7.83	111.92	122.72
3	A	305	GLU	C-N-CA	-7.83	111.92	122.72
3	A	389	LYS	CA-C-O	-7.78	111.31	120.10
2	P	872	DC	C4'-C3'-O3'	7.64	121.46	110.00
1	T	847	DT	C5'-C4'-O4'	-7.58	98.04	109.40
3	A	318	LYS	CD-CE-NZ	-7.55	87.75	111.90
3	A	382	PRO	CB-CG-CD	-7.43	82.34	106.10
3	A	381	THR	O-C-N	7.42	129.85	121.32
3	A	311	CYS	CB-CA-C	-7.35	98.60	110.79
3	A	362	CYS	N-CA-C	7.31	116.73	108.25
3	A	253	LEU	N-CA-C	7.30	121.84	113.15
3	A	158	TYR	CA-C-N	-7.28	110.94	123.25
3	A	158	TYR	C-N-CA	-7.28	110.94	123.25
2	P	870	DA	O4'-C1'-N9	7.23	119.24	108.40
3	A	166	LEU	N-CA-C	-7.22	104.33	113.72
3	A	305	GLU	CA-C-O	-7.11	112.48	120.66
3	A	74	GLY	N-CA-C	7.09	123.52	115.08
3	A	122	ARG	CG-CD-NE	-7.01	96.57	112.00
3	A	326	ALA	O-C-N	6.92	129.51	122.03
1	T	840	DG	C5'-C4'-O4'	6.91	119.77	109.40
3	A	319	ASN	CB-CG-OD1	-6.91	106.98	120.80
3	A	311	CYS	CA-C-N	-6.90	111.71	121.99
3	A	311	CYS	C-N-CA	-6.90	111.71	121.99
2	P	867	DA	O4'-C1'-N9	6.88	118.71	108.40
3	A	179	ILE	N-CA-C	-6.82	104.12	110.53
1	T	840	DG	C2'-C3'-O3'	6.74	121.60	111.50
1	T	842	DG	N9-C1'-C2'	-6.67	103.50	113.50
3	A	252	ALA	N-CA-C	-6.65	104.10	111.82
3	A	314	GLU	CB-CG-CD	-6.64	101.31	112.60
3	A	306	ASP	N-CA-C	6.63	120.05	109.24
3	A	392	ARG	N-CA-C	6.60	118.55	111.36
3	A	38	PHE	N-CA-C	6.54	119.00	111.02
3	A	382	PRO	N-CA-C	-6.53	103.20	113.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	390	LEU	CA-C-O	6.46	127.42	119.79
3	A	345	ILE	N-CA-C	6.43	119.03	108.99
3	A	102	TYR	N-CA-C	-6.42	104.36	111.36
3	A	122	ARG	NE-CZ-NH2	-6.42	113.43	119.20
1	T	839	DT	C6-N1-C1'	-6.37	109.79	119.35
3	A	389	LYS	N-CA-C	6.35	119.01	111.71
3	A	313	SER	CA-CB-OG	-6.35	98.40	111.10
1	T	842	DG	P-O5'-C5'	6.34	129.51	120.00
1	T	839	DT	N1-C1'-C2'	6.33	123.00	113.50
3	A	305	GLU	N-CA-CB	-6.25	99.69	111.00
3	A	380	MET	CA-C-N	6.23	137.00	121.80
3	A	380	MET	C-N-CA	6.23	137.00	121.80
1	T	845	DC	OP1-P-O3'	-6.19	89.44	108.00
3	A	407	SER	N-CA-C	6.09	118.55	108.99
3	A	246	THR	OG1-CB-CG2	-6.05	97.20	109.30
3	A	304	GLU	CA-C-N	-5.94	113.10	122.73
3	A	304	GLU	C-N-CA	-5.94	113.10	122.73
3	A	273	LEU	N-CA-C	-5.91	105.83	114.39
1	T	839	DT	P-O3'-C3'	5.90	129.05	120.20
1	T	846	DC	O3'-P-O5'	-5.86	95.21	104.00
3	A	68	TYR	CA-CB-CG	-5.83	103.40	113.90
1	T	847	DT	C4-C5-C6	-5.77	110.54	119.20
1	T	844	DT	P-O3'-C3'	-5.72	111.61	120.20
3	A	279	GLN	N-CA-C	-5.67	105.85	112.89
3	A	335	ASP	N-CA-C	-5.66	105.11	111.28
2	P	869	DG	P-O3'-C3'	-5.64	111.74	120.20
3	A	323	GLU	N-CA-C	5.63	117.50	111.36
2	P	872	DC	C5'-C4'-C3'	-5.62	106.48	114.90
3	A	214	LYS	CA-CB-CG	5.60	125.30	114.10
3	A	243	GLY	N-CA-C	5.59	120.80	112.41
2	P	869	DG	C5'-C4'-C3'	-5.58	106.53	114.90
2	P	871	DC	N1-C1'-C2'	-5.57	105.15	113.50
3	A	68	TYR	N-CA-C	5.54	118.03	111.33
3	A	253	LEU	CA-CB-CG	-5.52	96.99	116.30
3	A	379	VAL	CA-C-N	5.50	127.92	120.65
3	A	379	VAL	C-N-CA	5.50	127.92	120.65
2	P	869	DG	C2'-C3'-O3'	5.50	119.76	111.50
3	A	334	GLN	N-CA-C	5.49	122.48	110.80
2	P	872	DC	N1-C1'-C2'	-5.48	105.28	113.50
3	A	126	ASP	N-CA-C	5.47	119.52	112.41
3	A	383	MET	CA-C-N	-5.41	112.24	121.97
3	A	383	MET	C-N-CA	-5.41	112.24	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	843	DG	C4'-C3'-O3'	5.40	118.10	110.00
1	T	844	DT	N3-C4-O4	-5.39	114.52	122.60
3	A	392	ARG	CG-CD-NE	-5.36	100.22	112.00
3	A	298	PRO	CA-C-N	5.34	125.26	119.76
3	A	298	PRO	C-N-CA	5.34	125.26	119.76
3	A	310	LYS	CA-C-N	5.33	127.43	120.28
3	A	310	LYS	C-N-CA	5.33	127.43	120.28
3	A	40	ALA	N-CA-C	-5.29	105.59	111.36
3	A	414	LYS	CA-C-O	5.28	129.78	120.80
2	P	867	DA	C1'-O4'-C4'	5.27	117.61	109.70
3	A	299	PRO	CA-C-O	-5.27	115.33	121.34
3	A	322	GLU	CB-CG-CD	-5.24	103.70	112.60
1	T	844	DT	C5'-C4'-C3'	-5.23	107.05	114.90
3	A	214	LYS	CA-C-O	-5.23	113.00	120.16
3	A	216	ASN	N-CA-C	-5.22	97.73	108.53
3	A	314	GLU	CA-C-N	-5.22	112.58	121.97
3	A	314	GLU	C-N-CA	-5.22	112.58	121.97
3	A	358	GLU	N-CA-C	5.22	118.06	109.72
3	A	336	GLY	N-CA-C	-5.20	100.85	113.18
3	A	341	THR	OG1-CB-CG2	-5.18	98.94	109.30
3	A	392	ARG	CB-CG-CD	-5.18	99.39	111.30
3	A	175	VAL	N-CA-C	-5.12	105.55	110.72
3	A	380	MET	N-CA-C	5.12	116.55	110.97
2	P	870	DA	O4'-C4'-C3'	5.11	113.06	105.40
3	A	302	PHE	CB-CA-C	-5.09	102.81	110.24
3	A	413	LEU	N-CA-C	5.08	117.26	110.35
3	A	122	ARG	CD-NE-CZ	5.07	131.50	124.40
3	A	381	THR	CA-C-N	-5.07	113.97	119.24
3	A	381	THR	C-N-CA	-5.07	113.97	119.24
3	A	232	SER	N-CA-C	-5.05	106.38	112.54
3	A	390	LEU	O-C-N	5.05	129.10	122.33
3	A	389	LYS	O-C-N	5.05	128.13	122.22
3	A	391	PHE	N-CA-C	5.03	116.58	111.14
3	A	274	GLY	N-CA-C	-5.02	106.40	112.48

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	T	843	DG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	218	0
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	225	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 37.

All (225) 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:382:PRO:C	3:A:382:PRO:CA	1.84	1.50
3:A:105:MET:SD	3:A:105:MET:CE	2.01	1.48
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	1.38
3:A:388:MET:HE3	3:A:392:ARG:NH1	1.43	1.33
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:319:ASN:CG	3:A:319:ASN:OD1	1.83	1.22
3:A:388:MET:O	3:A:392:ARG:NH1	1.72	1.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.15
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: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: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
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:388:MET:HE2	3:A:392:ARG:HH22	1.37	0.89
3:A:347:ARG:HG3	3:A:404:THR:CG2	1.99	0.89
3:A:388:MET:C	3:A:392:ARG:HH11	1.84	0.86
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: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: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:380:MET:HE1	3:A:384:VAL:CG2	2.12	0.78
3:A:164:ASN:H	3:A:170:HIS:HD2	1.30	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:202:ASN:C	3:A:202:ASN:HD22	1.93	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:405:LEU:C	3:A:406:LEU:HD23	2.14	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:43:GLU:OE1	3:A:101:ARG:NH2	2.23	0.72
3:A:388:MET:C	3:A:392:ARG:NH1	2.42	0.72
3:A:347:ARG:HD3	3:A:405:LEU:CB	2.19	0.72
3:A:388:MET:CE	3:A:392:ARG:NH1	2.36	0.71
3:A:302:PHE:CE1	3:A:413:LEU:HD11	2.25	0.71
3:A:380:MET:HE2	3:A:384:VAL:CG2	2.19	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:388:MET:HE3	3:A:392:ARG:HH12	0.70	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: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:318:LYS:HD2	3:A:388:MET:SD	2.33	0.68
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:CE	3:A:384:VAL:HG21	2.25	0.65
3:A:80:ASN:O	3:A:84:ALA:HB3	1.97	0.65
3:A:388:MET:HE3	3:A:392:ARG:CZ	2.25	0.64
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
3:A:388:MET:CE	3:A:392:ARG:HH22	2.10	0.62
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:380:MET:HE1	3:A:384:VAL:HG22	1.81	0.62
3:A:105:MET:CE	3:A:105:MET:HB2	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:MET:HE2	3:A:179:ILE:HD12	1.82	0.59
3:A:318:LYS:O	3:A:318:LYS:HG2	2.04	0.58
3:A:80:ASN:C	3:A:82:ARG:H	2.10	0.58
3:A:318:LYS:HE2	3:A:322:GLU:OE1	2.04	0.57
1:T:847:DT:C3'	1:T:847:DT:HO3'	2.10	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
3:A:142:GLN:NE2	3:A:142:GLN:CA	2.67	0.56
3:A:367:HIS:CD2	3:A:367:HIS:C	2.83	0.56
3:A:388:MET:HE2	3:A:392:ARG:NH2	2.15	0.56
3:A:388:MET:CE	3:A:392:ARG:NH2	2.69	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:112:LEU:HD23	3:A:112:LEU:C	2.30	0.56
3:A:380:MET:HE2	3:A:384:VAL:HG21	1.86	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:249:CYS:O	3:A:253:LEU:CD1	2.55	0.55
3:A:383:MET:O	3:A:384:VAL:C	2.50	0.55
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:202:ASN:C	3:A:202:ASN:ND2	2.60	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:380:MET:CE	3:A:384:VAL:HG22	2.32	0.54
3:A:214:LYS:N	3:A:215:PRO:CD	2.71	0.53
3:A:314:GLU:CB	3:A:314:GLU:CD	2.80	0.53
3:A:318:LYS:CG	3:A:318:LYS:C	2.81	0.53
3:A:318:LYS:C	3:A:321:ILE:H	2.16	0.53
3:A:308:PHE:HE2	3:A:320:LYS:HD2	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:318:LYS:HG2	3:A:318:LYS:C	2.33	0.53
3:A:394:MET:CG	3:A:394:MET:CE	2.85	0.53
3:A:308:PHE:HB2	3:A:311:CYS:SG	2.48	0.53
3:A:148:LEU:C	3:A:148:LEU:HD23	2.33	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: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: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:382:PRO:C	3:A:382:PRO:N	2.62	0.50
3:A:382:PRO:HG2	3:A:383:MET:N	2.25	0.50
3:A:36:ASP:O	3:A:37:CYS:C	2.54	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: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:76:LYS:O	3:A:77:LYS:C	2.56	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
3:A:79:MET:HE3	3:A:84:ALA:HA	1.95	0.47
3:A:388:MET:CE	3:A:392:ARG:CZ	2.88	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:380:MET:HE2	3:A:384:VAL:HG23	1.91	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:380:MET:HE1	3:A:384:VAL:HG21	1.94	0.46
3:A:344:LEU:O	3:A:359:SER:HA	2.16	0.46
3:A:380:MET:HE2	3:A:380:MET:HB3	1.62	0.46
3:A:236:ILE:CD1	3:A:250:LEU:HD13	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:365:PRO:O	3:A:368:VAL:N	2.42	0.46
3:A:405:LEU:C	3:A:406:LEU:CD2	2.86	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:388:MET:O	3:A:392:ARG:HD2	2.16	0.45
3:A:308:PHE:O	3:A:308:PHE:CD1	2.70	0.45
3:A:44:MET:HE1	4:A:954:HOH:O	2.17	0.44
3:A:80:ASN:C	3:A:82:ARG:N	2.72	0.44
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:137:GLU:CD	3:A:172:ARG:HH12	2.26	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
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:105:MET:HB2	3:A:105:MET:HE2	1.99	0.42
3:A:384:VAL:O	3:A:385:ASP:C	2.63	0.42
3:A:315:VAL:O	3:A:316:GLU:C	2.62	0.42
3:A:345:ILE:HG22	3:A:346:ILE:H	1.84	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:312:SER:O	3:A:313:SER:C	2.62	0.41
3:A:53:LYS:HA	3:A:54:PRO:HD3	1.65	0.41
3:A:381:THR:C	3:A:382:PRO:C	2.89	0.40
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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	265 (85%)	47 (15%)	3 3

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	58	GLN
3	A	73	LEU
3	A	78	LEU
3	A	80	ASN
3	A	82	ARG
3	A	85	LYS
3	A	87	LYS
3	A	90	GLN
3	A	112	LEU
3	A	123	LEU
3	A	142	GLN
3	A	144	GLN
3	A	145	SER
3	A	147	GLU
3	A	149	SER
3	A	202	ASN
3	A	204	LEU
3	A	205	LEU
3	A	214	LYS
3	A	229	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	268	ILE
3	A	275	ILE
3	A	295	LEU
3	A	305	GLU
3	A	306	ASP
3	A	307	SER
3	A	309	LYS
3	A	314	GLU
3	A	325	LEU
3	A	327	SER
3	A	329	LEU
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	362	CYS
3	A	368	VAL
3	A	380	MET
3	A	381	THR
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	128	ASN
3	A	142	GLN
3	A	159	ASN
3	A	170	HIS
3	A	202	ASN
3	A	216	ASN
3	A	217	GLN
3	A	262	GLN
3	A	279	GLN
3	A	334	GLN
3	A	367	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	412	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	16,19,20	1.69	3 (18%)	20,26,29	1.94	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'	4.31	1.61	1.52
2	P	873	DOC	O4'-C4'	3.12	1.50	1.44
2	P	873	DOC	O4'-C1'	-2.23	1.37	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	873	DOC	C2'-C1'-N1	-4.79	103.33	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	873	DOC	O4'-C4'-C3'	4.36	111.98	104.81
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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	T	9/11 (81%)	0.34	1 (11%) 10 7	32, 34, 64, 101	0
2	P	6/7 (85%)	0.11	0 100 100	32, 41, 44, 53	0
3	A	367/420 (87%)	0.84	77 (20%) 2 2	9, 39, 89, 101	0
All	All	382/438 (87%)	0.82	78 (20%) 3 2	9, 39, 89, 101	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	317	ALA	7.1
3	A	349	TYR	6.9
3	A	379	VAL	6.9
3	A	355	TYR	6.5
3	A	405	LEU	6.1
3	A	315	VAL	5.7
3	A	318	LYS	5.6
3	A	381	THR	5.5
3	A	319	ASN	5.5
3	A	391	PHE	5.3
3	A	388	MET	5.2
3	A	316	GLU	5.1
3	A	382	PRO	5.1
3	A	386	ILE	4.7
3	A	313	SER	4.6
3	A	144	GLN	4.6
3	A	314	GLU	4.6
3	A	83	ASP	4.3
3	A	385	ASP	4.3
3	A	392	ARG	4.3
3	A	321	ILE	4.0
3	A	89	PRO	4.0
3	A	276	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	347	ARG	3.7
3	A	384	VAL	3.7
3	A	345	ILE	3.7
3	A	404	THR	3.7
3	A	346	ILE	3.6
3	A	394	MET	3.6
3	A	84	ALA	3.4
3	A	334	GLN	3.3
3	A	368	VAL	3.3
3	A	333	CYS	3.2
3	A	389	LYS	3.2
3	A	214	LYS	3.1
3	A	244	TYR	3.1
3	A	332	VAL	3.1
3	A	348	ARG	3.1
3	A	359	SER	3.0
3	A	356	GLY	3.0
3	A	215	PRO	2.9
3	A	320	LYS	2.9
3	A	300	GLN	2.9
3	A	413	LEU	2.9
3	A	309	LYS	2.8
3	A	367	HIS	2.8
1	T	839	DT	2.8
3	A	70	ALA	2.8
3	A	324	LEU	2.7
3	A	393	ASN	2.7
3	A	304	GLU	2.7
3	A	329	LEU	2.7
3	A	52	ASP	2.6
3	A	310	LYS	2.6
3	A	86	GLU	2.5
3	A	85	LYS	2.5
3	A	48	PRO	2.5
3	A	369	ILE	2.5
3	A	54	PRO	2.4
3	A	312	SER	2.3
3	A	141	GLN	2.3
3	A	387	LEU	2.3
3	A	61	TYR	2.3
3	A	370	GLN	2.3
3	A	145	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	390	LEU	2.3
3	A	78	LEU	2.2
3	A	323	GLU	2.2
3	A	330	ASN	2.2
3	A	88	CYS	2.2
3	A	325	LEU	2.2
3	A	305	GLU	2.2
3	A	72	LYS	2.2
3	A	90	GLN	2.2
3	A	80	ASN	2.2
3	A	336	GLY	2.1
3	A	380	MET	2.1
3	A	366	SER	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	0.91	0.11	27,34,39,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.