



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:23 AM UTC

PDB ID : 1TDC / pdb_00001tdc
Title : STRUCTURES OF THYMIDYLATE SYNTHASE WITH A C-TERMINAL DELETION: ROLE OF THE C-TERMINUS IN ALIGNMENT OF D/UMP AND CH₂H₄FOLATE
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Deposited on : 1993-02-15
Resolution : 2.65 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

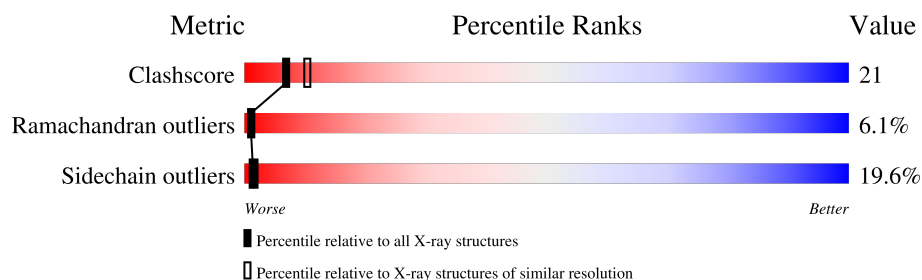
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	23% 40% 27% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	A	529	X	-	-	-

2 Entry composition [i](#)

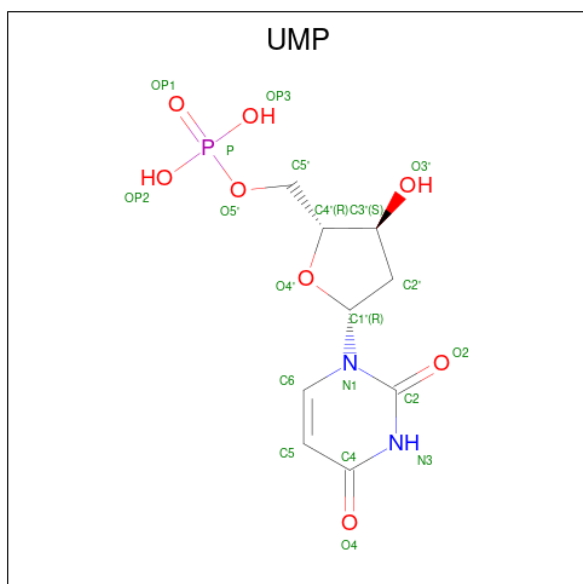
There are 2 unique types of molecules in this entry. The entry contains 2603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2583	1672	437	466	8			

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$).



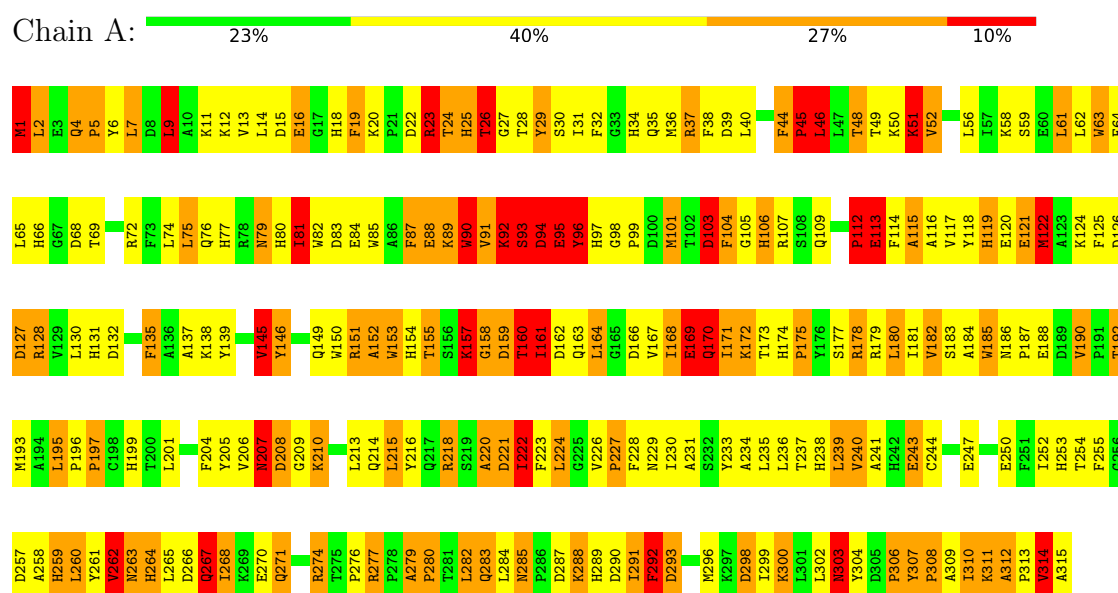
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.80Å 78.80Å 243.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.65	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.210 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2603	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	A	1.84	55/2667 (2.1%)	2.84	318/3624 (8.8%)

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	A	0	5

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	CA-CB	19.80	1.93	1.53
1	A	52	VAL	CA-CB	-13.48	1.44	1.54
1	A	216	TYR	CA-CB	-9.48	1.40	1.53
1	A	199	HIS	CD2-NE2	-8.51	1.28	1.37
1	A	1	MET	CB-CG	-8.19	1.27	1.52
1	A	183	SER	CA-C	-7.99	1.43	1.52
1	A	229	ASN	CA-CB	-7.73	1.40	1.53
1	A	50	LYS	CA-CB	-7.53	1.41	1.53
1	A	207	ASN	CA-CB	7.42	1.64	1.53
1	A	179	ARG	CA-CB	7.27	1.64	1.53
1	A	282	LEU	CA-CB	-7.21	1.43	1.53
1	A	34	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	247	GLU	CA-CB	-7.07	1.43	1.53
1	A	80	HIS	CD2-NE2	-7.05	1.30	1.37
1	A	253	HIS	CD2-NE2	-7.03	1.30	1.37
1	A	146	TYR	CA-CB	-7.01	1.42	1.53
1	A	264	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	231	ALA	CA-CB	-6.91	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	HIS	CG-ND1	-6.84	1.30	1.38
1	A	106	HIS	CD2-NE2	-6.80	1.30	1.37
1	A	196	PRO	CA-CB	-6.78	1.44	1.54
1	A	259	HIS	CD2-NE2	-6.77	1.30	1.37
1	A	289	HIS	CD2-NE2	-6.77	1.30	1.37
1	A	66	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	161	ILE	CA-CB	6.49	1.62	1.54
1	A	167	VAL	CA-CB	6.43	1.62	1.54
1	A	15	ASP	CA-CB	-6.42	1.45	1.54
1	A	82	TRP	CG-CD2	-6.42	1.32	1.43
1	A	276	PRO	CA-CB	-6.29	1.44	1.53
1	A	192	THR	CA-CB	6.25	1.60	1.53
1	A	126	ASP	CA-C	-6.07	1.44	1.52
1	A	131	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	238	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	266	ASP	CA-C	-5.79	1.45	1.52
1	A	153	TRP	CG-CD2	-5.69	1.33	1.43
1	A	168	ILE	CB-CG1	-5.61	1.42	1.53
1	A	117	VAL	CA-CB	5.60	1.61	1.54
1	A	169	GLU	CA-CB	5.53	1.63	1.53
1	A	186	ASN	CA-CB	-5.45	1.44	1.52
1	A	80	HIS	CG-ND1	-5.36	1.32	1.38
1	A	292	PHE	CA-C	5.34	1.59	1.52
1	A	150	TRP	CG-CD2	-5.33	1.34	1.43
1	A	18	HIS	CD2-NE2	-5.23	1.32	1.37
1	A	101	MET	CA-C	-5.21	1.45	1.52
1	A	199	HIS	CG-ND1	-5.19	1.32	1.38
1	A	39	ASP	CA-C	-5.16	1.46	1.52
1	A	163	GLN	CA-CB	-5.13	1.45	1.53
1	A	267	GLN	CD-NE2	-5.12	1.22	1.33
1	A	75	LEU	CA-C	-5.12	1.45	1.52
1	A	280	PRO	CA-CB	-5.05	1.46	1.53
1	A	77	HIS	CD2-NE2	-5.05	1.32	1.37
1	A	154	HIS	CD2-NE2	-5.05	1.32	1.37
1	A	179	ARG	CD-NE	5.04	1.53	1.46
1	A	179	ARG	NE-CZ	5.03	1.38	1.33
1	A	310	ILE	CA-CB	-5.03	1.48	1.54

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASN	CA-CB-CG	21.73	134.33	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASP	CA-CB-CG	14.38	126.98	112.60
1	A	221	ASP	CA-CB-CG	11.77	124.37	112.60
1	A	63	TRP	N-CA-C	-10.25	99.65	111.03
1	A	103	ASP	O-C-N	10.14	136.08	122.59
1	A	179	ARG	N-CA-C	-10.06	98.62	112.30
1	A	51	LYS	N-CA-C	-9.95	93.02	109.24
1	A	179	ARG	NE-CZ-NH2	9.82	128.04	119.20
1	A	168	ILE	O-C-N	-9.74	112.42	121.87
1	A	288	LYS	N-CA-C	-9.66	96.18	110.48
1	A	255	PHE	CA-CB-CG	9.58	123.38	113.80
1	A	1	MET	N-CA-CB	-9.54	94.28	110.50
1	A	104	PHE	N-CA-C	9.41	122.53	111.71
1	A	289	HIS	CA-C-O	-9.34	107.90	118.55
1	A	137	ALA	N-CA-C	-9.25	101.15	111.14
1	A	168	ILE	CA-C-O	-9.23	111.35	120.95
1	A	36	MET	CA-CB-CG	9.11	132.32	114.10
1	A	30	SER	CA-CB-OG	9.10	129.29	111.10
1	A	117	VAL	N-CA-C	-9.02	101.61	110.72
1	A	103	ASP	CA-C-N	8.93	133.14	120.28
1	A	103	ASP	C-N-CA	8.93	133.14	120.28
1	A	263	ASN	OD1-CG-ND2	-8.90	113.70	122.60
1	A	74	LEU	N-CA-C	-8.87	101.56	111.14
1	A	4	GLN	OE1-CD-NE2	-8.81	113.78	122.60
1	A	192	THR	N-CA-C	-8.70	101.36	113.20
1	A	26	THR	CA-CB-OG1	-8.69	96.56	109.60
1	A	77	HIS	CA-CB-CG	-8.65	105.15	113.80
1	A	81	ILE	CB-CG1-CD1	-8.65	95.64	113.80
1	A	183	SER	CA-CB-OG	-8.55	94.01	111.10
1	A	138	LYS	N-CA-C	8.47	120.21	110.97
1	A	122	MET	CA-C-O	-8.41	112.24	120.90
1	A	178	ARG	CB-CG-CD	-8.37	92.06	111.30
1	A	1	MET	CB-CA-C	8.35	125.96	110.10
1	A	290	ASP	CA-CB-CG	8.34	120.94	112.60
1	A	157	LYS	N-CA-C	-8.33	93.06	110.80
1	A	107	ARG	N-CA-C	8.25	122.91	113.01
1	A	207	ASN	N-CA-C	-8.20	97.79	110.17
1	A	264	HIS	CA-CB-CG	8.20	122.00	113.80
1	A	50	LYS	N-CA-C	-8.16	95.86	108.76
1	A	235	LEU	N-CA-C	-8.14	100.74	111.24
1	A	285	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	A	7	LEU	CD1-CG-CD2	-8.01	93.17	110.80
1	A	237	THR	N-CA-C	-8.00	102.50	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	ASN	CB-CG-ND2	7.92	128.28	116.40
1	A	131	HIS	N-CA-C	7.91	124.52	114.31
1	A	122	MET	CG-SD-CE	-7.84	83.64	100.90
1	A	115	ALA	CA-C-O	-7.84	112.24	120.55
1	A	119	HIS	CA-C-N	-7.81	108.88	122.79
1	A	119	HIS	C-N-CA	-7.81	108.88	122.79
1	A	167	VAL	CA-C-O	-7.79	112.84	120.95
1	A	66	HIS	N-CA-C	-7.76	103.81	113.28
1	A	162	ASP	CA-C-O	-7.73	113.48	122.37
1	A	210	LYS	N-CA-C	7.72	121.70	109.50
1	A	215	LEU	O-C-N	-7.68	114.33	123.31
1	A	83	ASP	N-CA-C	7.63	120.56	111.33
1	A	160	THR	N-CA-CB	-7.58	97.27	111.00
1	A	35	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	A	170	GLN	CA-CB-CG	-7.51	99.08	114.10
1	A	207	ASN	OD1-CG-ND2	-7.47	115.13	122.60
1	A	26	THR	N-CA-C	7.45	126.66	110.80
1	A	44	PHE	CA-C-N	7.42	129.12	119.84
1	A	44	PHE	C-N-CA	7.42	129.12	119.84
1	A	166	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	226	VAL	CA-C-O	-7.30	110.17	119.95
1	A	26	THR	OG1-CB-CG2	7.28	123.86	109.30
1	A	287	ASP	CB-CA-C	7.28	121.98	109.24
1	A	291	ILE	CA-C-O	-7.26	111.71	120.78
1	A	1	MET	CA-CB-CG	-7.24	99.62	114.10
1	A	158	GLY	CA-C-O	-7.24	107.98	120.57
1	A	183	SER	O-C-N	7.21	131.88	123.30
1	A	199	HIS	CA-CB-CG	-7.18	106.62	113.80
1	A	271	GLN	CA-CB-CG	7.18	128.46	114.10
1	A	296	MET	CG-SD-CE	-7.18	85.10	100.90
1	A	25	HIS	CB-CG-CD2	-7.15	121.91	131.20
1	A	92	LYS	N-CA-C	-7.12	96.75	108.07
1	A	32	PHE	O-C-N	-7.10	115.03	123.27
1	A	229	ASN	N-CA-C	7.09	120.04	111.82
1	A	62	LEU	O-C-N	-7.08	113.18	122.39
1	A	298	ASP	CA-CB-CG	7.06	119.66	112.60
1	A	253	HIS	CA-C-O	-7.05	112.82	120.36
1	A	289	HIS	CA-C-N	-7.05	112.78	122.30
1	A	289	HIS	C-N-CA	-7.05	112.78	122.30
1	A	4	GLN	CG-CD-NE2	7.01	126.92	116.40
1	A	81	ILE	CB-CA-C	-7.00	100.91	112.26
1	A	306	PRO	O-C-N	6.98	131.42	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	N-CA-C	-6.98	104.73	113.18
1	A	239	LEU	N-CA-C	-6.96	102.01	112.04
1	A	166	ASP	CA-C-O	-6.95	111.62	120.31
1	A	119	HIS	CA-CB-CG	-6.93	106.87	113.80
1	A	132	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	37	ARG	O-C-N	-6.85	114.51	123.21
1	A	18	HIS	N-CA-C	-6.85	98.09	109.46
1	A	287	ASP	N-CA-CB	-6.80	100.55	110.47
1	A	307	TYR	N-CA-CB	6.79	117.80	109.59
1	A	19	PHE	N-CA-C	-6.76	99.51	110.20
1	A	231	ALA	N-CA-C	-6.75	104.87	113.23
1	A	96	TYR	CA-C-N	6.73	133.64	122.33
1	A	96	TYR	C-N-CA	6.73	133.64	122.33
1	A	82	TRP	CD2-CE2-CZ2	-6.68	115.72	122.40
1	A	172	LYS	CA-C-O	-6.67	113.82	120.82
1	A	48	THR	O-C-N	-6.67	114.01	122.34
1	A	93	SER	N-CA-C	6.67	125.00	110.80
1	A	87	PHE	N-CA-C	-6.64	104.44	112.54
1	A	179	ARG	CA-CB-CG	6.62	127.35	114.10
1	A	65	LEU	N-CA-C	6.62	120.94	112.34
1	A	151	ARG	NE-CZ-NH2	-6.61	113.25	119.20
1	A	250	GLU	N-CA-C	6.55	120.37	109.95
1	A	303	ASN	OD1-CG-ND2	-6.50	116.10	122.60
1	A	218	ARG	CA-C-O	-6.47	112.78	120.10
1	A	306	PRO	CA-C-O	-6.47	113.61	122.15
1	A	228	PHE	CA-CB-CG	6.46	120.26	113.80
1	A	213	LEU	CA-C-O	-6.44	112.62	120.54
1	A	44	PHE	CB-CA-C	6.43	117.22	109.31
1	A	174	HIS	CB-CG-CD2	-6.40	122.89	131.20
1	A	215	LEU	CD1-CG-CD2	-6.40	96.73	110.80
1	A	96	TYR	CA-CB-CG	-6.36	102.45	113.90
1	A	207	ASN	N-CA-CB	6.35	120.73	110.51
1	A	50	LYS	O-C-N	-6.34	116.37	123.48
1	A	2	LEU	CA-C-O	-6.32	114.36	121.00
1	A	195	LEU	CA-C-N	6.31	126.88	120.38
1	A	195	LEU	C-N-CA	6.31	126.88	120.38
1	A	199	HIS	CB-CG-CD2	-6.30	123.00	131.20
1	A	160	THR	CA-CB-OG1	-6.27	100.19	109.60
1	A	186	ASN	OD1-CG-ND2	6.27	128.87	122.60
1	A	214	GLN	O-C-N	-6.24	115.11	123.23
1	A	241	ALA	N-CA-C	-6.21	104.51	111.28
1	A	106	HIS	CA-CB-CG	-6.20	107.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	CB-CG-CD	-6.20	97.03	111.30
1	A	289	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	A	311	LYS	O-C-N	6.19	130.29	123.04
1	A	314	VAL	CB-CA-C	6.19	121.44	111.29
1	A	90	TRP	CB-CG-CD1	-6.18	117.63	126.90
1	A	312	ALA	CA-C-N	6.17	126.14	119.78
1	A	312	ALA	C-N-CA	6.17	126.14	119.78
1	A	243	GLU	CA-C-O	-6.17	113.39	120.24
1	A	137	ALA	CA-C-O	-6.16	114.36	120.70
1	A	77	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	A	36	MET	CA-C-O	-6.14	113.24	120.60
1	A	265	LEU	N-CA-C	6.13	118.75	111.33
1	A	210	LYS	CA-CB-CG	6.12	126.34	114.10
1	A	49	THR	N-CA-CB	-6.12	101.13	110.92
1	A	114	PHE	N-CA-CB	6.11	119.10	110.12
1	A	170	GLN	CG-CD-NE2	6.11	125.56	116.40
1	A	164	LEU	CB-CA-C	-6.10	101.26	110.90
1	A	36	MET	N-CA-C	-6.10	98.70	109.06
1	A	91	VAL	CA-C-O	6.10	128.40	120.78
1	A	188	GLU	CA-CB-CG	6.09	126.29	114.10
1	A	312	ALA	O-C-N	-6.06	114.35	121.32
1	A	309	ALA	CA-C-N	-6.05	115.25	123.12
1	A	309	ALA	C-N-CA	-6.05	115.25	123.12
1	A	97	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	A	34	HIS	CA-C-O	-6.03	114.26	120.89
1	A	210	LYS	CB-CG-CD	-6.01	97.48	111.30
1	A	88	GLU	O-C-N	-6.01	115.78	122.03
1	A	253	HIS	CA-CB-CG	6.00	119.80	113.80
1	A	243	GLU	N-CA-C	-5.97	104.35	111.69
1	A	259	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	A	271	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	285	ASN	CA-CB-CG	-5.96	106.64	112.60
1	A	271	GLN	CG-CD-NE2	5.96	125.33	116.40
1	A	182	VAL	O-C-N	-5.94	116.76	123.18
1	A	274	ARG	O-C-N	-5.94	116.08	122.85
1	A	255	PHE	N-CA-C	5.93	119.14	109.24
1	A	257	ASP	CA-C-O	-5.93	114.58	120.98
1	A	82	TRP	CE2-CD2-CE3	5.92	124.72	118.80
1	A	300	LYS	CA-CB-CG	5.91	125.93	114.10
1	A	94	ASP	O-C-N	5.91	130.45	122.59
1	A	185	TRP	CG-CD2-CE3	5.91	139.81	133.90
1	A	18	HIS	CB-CG-CD2	-5.90	123.53	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	PHE	N-CA-C	-5.90	104.85	111.28
1	A	160	THR	CB-CA-C	5.89	121.02	109.35
1	A	314	VAL	N-CA-CB	-5.89	101.50	111.23
1	A	46	LEU	N-CA-C	-5.88	100.08	109.96
1	A	105	GLY	N-CA-C	-5.87	105.69	112.50
1	A	63	TRP	CG-CD1-NE1	-5.86	102.58	110.20
1	A	138	LYS	CB-CG-CD	-5.86	97.83	111.30
1	A	262	VAL	CA-CB-CG2	-5.85	100.46	110.40
1	A	93	SER	CA-C-O	5.85	128.87	120.51
1	A	237	THR	CA-CB-OG1	-5.84	100.84	109.60
1	A	155	THR	N-CA-CB	-5.83	100.90	110.41
1	A	23	ARG	CA-C-O	-5.83	112.17	120.51
1	A	127	ASP	N-CA-C	-5.82	105.94	113.16
1	A	258	ALA	O-C-N	-5.82	116.59	123.22
1	A	119	HIS	CB-CG-CD2	-5.81	123.64	131.20
1	A	63	TRP	CA-CB-CG	5.80	124.62	113.60
1	A	120	GLU	N-CA-C	-5.80	106.25	113.55
1	A	155	THR	O-C-N	-5.78	116.59	123.06
1	A	222	ILE	N-CA-C	5.78	121.36	109.34
1	A	24	THR	N-CA-C	-5.77	95.49	107.67
1	A	135	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	293	ASP	CA-C-N	5.75	133.20	122.74
1	A	293	ASP	C-N-CA	5.75	133.20	122.74
1	A	9	LEU	CA-C-O	-5.74	114.46	120.55
1	A	128	ARG	CB-CA-C	-5.72	102.08	110.95
1	A	206	VAL	O-C-N	-5.72	115.67	122.77
1	A	279	ALA	CA-C-N	5.71	126.98	119.84
1	A	279	ALA	C-N-CA	5.71	126.98	119.84
1	A	94	ASP	CA-C-N	5.71	132.44	121.54
1	A	94	ASP	C-N-CA	5.71	132.44	121.54
1	A	180	LEU	CD1-CG-CD2	-5.71	98.24	110.80
1	A	160	THR	N-CA-C	-5.69	99.73	109.24
1	A	223	PHE	N-CA-C	5.68	117.33	111.03
1	A	95	GLU	N-CA-C	-5.66	98.75	110.80
1	A	190	VAL	O-C-N	-5.66	114.65	121.10
1	A	190	VAL	CA-CB-CG2	-5.64	100.81	110.40
1	A	261	TYR	CA-C-O	-5.64	114.84	121.16
1	A	72	ARG	CA-C-O	-5.64	114.57	120.55
1	A	75	LEU	CA-C-N	-5.63	113.49	122.66
1	A	75	LEU	C-N-CA	-5.63	113.49	122.66
1	A	76	GLN	CG-CD-NE2	-5.61	107.98	116.40
1	A	58	LYS	CA-C-O	-5.59	114.63	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	LYS	CB-CG-CD	-5.58	98.46	111.30
1	A	238	HIS	CA-CB-CG	5.57	119.37	113.80
1	A	204	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	117	VAL	CA-CB-CG2	5.55	119.84	110.40
1	A	7	LEU	CA-C-O	-5.55	112.77	119.49
1	A	173	THR	O-C-N	-5.54	114.88	122.46
1	A	1	MET	CA-C-N	5.53	127.95	120.65
1	A	1	MET	C-N-CA	5.53	127.95	120.65
1	A	74	LEU	CA-C-O	-5.53	115.00	120.70
1	A	107	ARG	O-C-N	-5.53	114.83	122.46
1	A	80	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	A	154	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	A	116	ALA	N-CA-CB	5.51	118.82	110.28
1	A	34	HIS	O-C-N	-5.50	117.31	123.48
1	A	81	ILE	N-CA-C	5.50	117.97	111.09
1	A	25	HIS	CB-CG-ND1	5.49	130.94	122.70
1	A	185	TRP	CG-CD1-NE1	-5.48	103.08	110.20
1	A	30	SER	CA-C-O	-5.47	115.03	121.44
1	A	146	TYR	N-CA-C	5.47	117.25	111.28
1	A	45	PRO	CA-N-CD	-5.46	104.36	112.00
1	A	79	ASN	N-CA-C	-5.46	98.32	107.99
1	A	262	VAL	CA-CB-CG1	5.46	119.67	110.40
1	A	128	ARG	CA-CB-CG	5.45	125.00	114.10
1	A	38	PHE	N-CA-C	-5.45	100.14	109.24
1	A	48	THR	OG1-CB-CG2	5.43	120.15	109.30
1	A	114	PHE	CB-CA-C	-5.43	101.78	110.79
1	A	121	GLU	CA-CB-CG	5.42	124.95	114.10
1	A	85	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	A	112	PRO	N-CA-C	-5.41	101.33	112.47
1	A	117	VAL	CA-C-O	-5.41	115.12	120.85
1	A	31	ILE	O-C-N	-5.40	117.30	122.97
1	A	167	VAL	O-C-N	-5.40	116.63	121.87
1	A	37	ARG	CB-CA-C	-5.40	99.67	109.38
1	A	150	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	A	314	VAL	CA-CB-CG2	-5.39	101.23	110.40
1	A	244	CYS	CA-CB-SG	-5.37	102.05	114.40
1	A	186	ASN	CB-CG-ND2	-5.36	108.36	116.40
1	A	126	ASP	CA-C-N	-5.36	112.68	122.38
1	A	126	ASP	C-N-CA	-5.36	112.68	122.38
1	A	157	LYS	CA-C-N	5.35	131.90	121.41
1	A	157	LYS	C-N-CA	5.35	131.90	121.41
1	A	262	VAL	CA-C-O	-5.35	115.38	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	TRP	N-CA-C	-5.35	105.89	112.90
1	A	106	HIS	CB-CG-CD2	-5.34	124.25	131.20
1	A	185	TRP	CD1-CG-CD2	5.33	114.84	106.30
1	A	167	VAL	CA-C-N	-5.33	113.16	120.46
1	A	167	VAL	C-N-CA	-5.33	113.16	120.46
1	A	85	TRP	N-CA-C	-5.33	105.55	111.36
1	A	31	ILE	CA-C-O	-5.32	116.03	121.67
1	A	36	MET	N-CA-CB	-5.31	101.63	111.13
1	A	23	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	A	197	PRO	O-C-N	-5.29	116.63	123.03
1	A	90	TRP	O-C-N	5.29	127.59	122.09
1	A	119	HIS	CB-CA-C	-5.28	98.64	110.21
1	A	126	ASP	CA-C-O	-5.28	114.38	120.24
1	A	233	TYR	O-C-N	-5.28	115.17	122.46
1	A	221	ASP	N-CA-CB	-5.28	102.96	110.46
1	A	282	LEU	CA-C-O	-5.28	114.52	120.43
1	A	292	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	247	GLU	CA-C-O	-5.27	115.03	121.88
1	A	304	TYR	N-CA-C	-5.26	101.21	109.25
1	A	5	PRO	CB-CA-C	5.25	120.41	112.21
1	A	253	HIS	N-CA-C	-5.25	100.17	108.73
1	A	31	ILE	CB-CG1-CD1	-5.22	102.83	113.80
1	A	72	ARG	CG-CD-NE	5.22	123.48	112.00
1	A	119	HIS	CG-CD2-NE2	-5.21	101.99	107.20
1	A	220	ALA	CB-CA-C	-5.21	102.64	110.24
1	A	90	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	A	29	TYR	N-CA-C	-5.20	99.94	108.41
1	A	185	TRP	CE2-CD2-CG	-5.19	100.97	107.20
1	A	16	GLU	CA-C-O	5.18	125.49	119.32
1	A	153	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	179	ARG	O-C-N	-5.18	115.16	122.26
1	A	163	GLN	N-CA-C	5.16	117.57	111.33
1	A	37	ARG	CA-C-O	-5.15	115.25	120.71
1	A	113	GLU	N-CA-C	5.15	119.72	113.38
1	A	103	ASP	CA-CB-CG	-5.14	107.46	112.60
1	A	39	ASP	N-CA-C	-5.13	99.43	108.20
1	A	179	ARG	CB-CG-CD	5.12	123.08	111.30
1	A	157	LYS	O-C-N	5.12	129.40	122.59
1	A	117	VAL	CA-CB-CG1	-5.12	101.70	110.40
1	A	76	GLN	OE1-CD-NE2	5.11	127.71	122.60
1	A	265	LEU	O-C-N	-5.11	116.70	122.12
1	A	25	HIS	CA-CB-CG	-5.11	108.69	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	LYS	CG-CD-CE	-5.10	99.57	111.30
1	A	308	PRO	CA-N-CD	-5.10	104.86	112.00
1	A	207	ASN	O-C-N	-5.09	116.02	122.43
1	A	171	ILE	N-CA-C	-5.08	104.63	111.44
1	A	158	GLY	N-CA-C	5.08	125.22	113.18
1	A	179	ARG	CG-CD-NE	5.08	123.17	112.00
1	A	314	VAL	CA-CB-CG1	5.07	119.02	110.40
1	A	9	LEU	N-CA-C	-5.07	105.75	111.28
1	A	186	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	127	ASP	CB-CA-C	5.06	119.12	110.01
1	A	126	ASP	CA-CB-CG	-5.06	107.54	112.60
1	A	167	VAL	CA-CB-CG2	5.05	118.99	110.40
1	A	131	HIS	O-C-N	-5.05	116.78	122.34
1	A	26	THR	CA-CB-CG2	5.04	119.07	110.50
1	A	145	VAL	O-C-N	-5.04	116.27	122.57
1	A	229	ASN	CB-CG-ND2	5.03	123.94	116.40
1	A	49	THR	CB-CA-C	5.03	119.11	111.02
1	A	75	LEU	CB-CA-C	-5.03	102.14	110.68
1	A	101	MET	CA-CB-CG	-5.03	104.05	114.10
1	A	255	PHE	O-C-N	-5.02	117.15	123.27
1	A	303	ASN	CA-C-O	5.01	127.25	121.28
1	A	254	THR	N-CA-C	-5.01	101.98	109.95
1	A	285	ASN	O-C-N	-5.01	117.56	121.47

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASP	Mainchain
1	A	307	TYR	Sidechain
1	A	312	ALA	Peptide
1	A	314	VAL	Mainchain
1	A	96	TYR	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	A	2583	0	2487	108	0
2	A	20	0	10	1	0
All	All	2603	0	2497	108	0

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 21.

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CA	1:A:1:MET:CB	1.93	1.42
1:A:1:MET:CA	1:A:1:MET:CG	2.48	0.91
1:A:177:SER:HB3	1:A:180:LEU:HD13	1.58	0.85
1:A:185:TRP:CE3	1:A:197:PRO:HD2	2.22	0.75
1:A:59:SER:HB2	1:A:79:ASN:HD22	1.53	0.74
1:A:1:MET:CB	1:A:1:MET:N	2.50	0.73
1:A:127:ASP:HA	1:A:130:LEU:HD12	1.71	0.72
1:A:92:LYS:HD2	1:A:93:SER:HB2	1.73	0.70
1:A:84:GLU:HA	1:A:87:PHE:HB3	1.74	0.69
1:A:205:TYR:HE1	1:A:207:ASN:ND2	1.92	0.67
1:A:101:MET:HE3	1:A:118:TYR:HA	1.76	0.67
1:A:243:GLU:OE1	1:A:291:ILE:HG12	1.94	0.67
1:A:285:ASN:HB2	1:A:298:ASP:HB3	1.77	0.66
1:A:220:ALA:HA	2:A:529:UMP:O2	1.97	0.63
1:A:121:GLU:HA	1:A:124:LYS:HG3	1.82	0.61
1:A:13:VAL:HG21	1:A:222:ILE:CD1	2.31	0.60
1:A:153:TRP:O	1:A:160:THR:HA	2.01	0.59
1:A:101:MET:SD	1:A:101:MET:N	2.75	0.59
1:A:101:MET:HE2	1:A:121:GLU:HB3	1.86	0.58
1:A:1:MET:CA	1:A:1:MET:HG2	2.33	0.58
1:A:291:ILE:HG13	1:A:292:PHE:H	1.68	0.57
1:A:260:LEU:HD21	1:A:268:ILE:HG21	1.85	0.57
1:A:236:LEU:O	1:A:240:VAL:HG13	2.04	0.57
1:A:104:PHE:CD2	1:A:118:TYR:HE1	2.23	0.56
1:A:197:PRO:O	1:A:218:ARG:HD3	2.04	0.56
1:A:184:ALA:O	1:A:197:PRO:HG2	2.04	0.56
1:A:185:TRP:HE3	1:A:197:PRO:HD2	1.70	0.56
1:A:155:THR:HG21	1:A:161:ILE:HD13	1.88	0.56
1:A:89:LYS:O	1:A:92:LYS:HB3	2.06	0.55
1:A:291:ILE:O	1:A:293:ASP:N	2.39	0.55
1:A:23:ARG:HD3	1:A:26:THR:HG21	1.89	0.54
1:A:90:TRP:CZ3	1:A:95:GLU:HB3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HG3	1:A:170:GLN:HE21	1.73	0.54
1:A:45:PRO:HB2	1:A:230:ILE:HG22	1.92	0.52
1:A:104:PHE:CD2	1:A:118:TYR:CE1	2.97	0.52
1:A:181:ILE:HG22	1:A:182:VAL:N	2.25	0.52
1:A:291:ILE:HG13	1:A:292:PHE:N	2.24	0.52
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.45	0.52
1:A:224:LEU:HD11	1:A:314:VAL:HA	1.92	0.52
1:A:28:THR:HG23	1:A:259:HIS:HB2	1.92	0.52
1:A:177:SER:HB3	1:A:180:LEU:CD1	2.33	0.52
1:A:118:TYR:HD2	1:A:119:HIS:ND1	2.09	0.51
1:A:283:GLN:OE1	1:A:300:LYS:HB2	2.09	0.51
1:A:128:ARG:HB3	1:A:135:PHE:CD2	2.46	0.51
1:A:4:GLN:N	1:A:5:PRO:HD2	2.26	0.51
1:A:112:PRO:HB2	1:A:113:GLU:OE2	2.11	0.51
1:A:89:LYS:NZ	1:A:139:TYR:O	2.45	0.50
1:A:157:LYS:HB3	1:A:157:LYS:HZ2	1.76	0.50
1:A:23:ARG:CB	1:A:26:THR:HB	2.43	0.49
1:A:51:LYS:HG2	1:A:306:PRO:HG3	1.93	0.49
1:A:48:THR:HB	1:A:277:ARG:HB2	1.95	0.49
1:A:93:SER:HB3	1:A:94:ASP:OD2	2.14	0.48
1:A:279:ALA:HB1	1:A:280:PRO:HD2	1.94	0.48
1:A:121:GLU:OE1	1:A:124:LYS:HD2	2.13	0.48
1:A:267:GLN:OE1	1:A:313:PRO:HD2	2.13	0.48
1:A:90:TRP:CH2	1:A:95:GLU:HB3	2.49	0.48
1:A:271:GLN:HB3	1:A:310:ILE:HD11	1.95	0.48
1:A:274:ARG:NH2	1:A:308:PRO:HG2	2.28	0.48
1:A:6:TYR:HD2	1:A:7:LEU:HD12	1.79	0.47
1:A:69:THR:HG22	1:A:145:VAL:HG23	1.96	0.47
1:A:13:VAL:HG21	1:A:222:ILE:HD13	1.97	0.47
1:A:291:ILE:O	1:A:292:PHE:C	2.58	0.46
1:A:101:MET:HE3	1:A:118:TYR:CA	2.43	0.46
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.73	0.45
1:A:282:LEU:HD11	1:A:299:ILE:HG23	1.99	0.45
1:A:19:PHE:CZ	1:A:27:GLY:HA2	2.52	0.45
1:A:29:TYR:CE2	1:A:262:VAL:HG23	2.52	0.45
1:A:91:VAL:HG11	1:A:101:MET:O	2.17	0.45
1:A:98:GLY:HA3	1:A:99:PRO:HD3	1.76	0.44
1:A:207:ASN:O	1:A:209:GLY:N	2.50	0.44
1:A:1:MET:HG2	1:A:1:MET:HA	1.99	0.44
1:A:61:LEU:O	1:A:64:PHE:HB2	2.19	0.43
1:A:121:GLU:HA	1:A:124:LYS:CG	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HB3	1:A:303:ASN:ND2	2.33	0.43
1:A:303:ASN:ND2	1:A:303:ASN:N	2.67	0.43
1:A:122:MET:O	1:A:125:PHE:HB3	2.19	0.43
1:A:106:HIS:O	1:A:109:GLN:HB2	2.17	0.43
1:A:171:ILE:HG12	1:A:180:LEU:HD21	2.00	0.43
1:A:205:TYR:HE1	1:A:207:ASN:HD22	1.64	0.43
1:A:164:LEU:HD13	1:A:292:PHE:HE1	1.84	0.42
1:A:44:PHE:HB3	1:A:280:PRO:HG2	2.02	0.42
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.84	0.42
1:A:92:LYS:O	1:A:96:TYR:HB2	2.20	0.42
1:A:121:GLU:O	1:A:124:LYS:HB2	2.20	0.42
1:A:168:ILE:HG21	1:A:168:ILE:HD13	1.66	0.42
1:A:178:ARG:HH11	1:A:178:ARG:HD2	1.61	0.42
1:A:221:ASP:HA	1:A:259:HIS:CD2	2.55	0.42
1:A:46:LEU:CD2	1:A:52:VAL:HB	2.50	0.42
1:A:81:ILE:HG22	1:A:81:ILE:O	2.19	0.42
1:A:23:ARG:HB3	1:A:26:THR:HB	2.00	0.42
1:A:44:PHE:HA	1:A:45:PRO:HD2	1.85	0.42
1:A:121:GLU:CD	1:A:124:LYS:HD2	2.45	0.42
1:A:29:TYR:HE2	1:A:262:VAL:HG23	1.83	0.41
1:A:40:LEU:HD21	1:A:234:ALA:HB1	2.02	0.41
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.85	0.41
1:A:89:LYS:HE2	1:A:89:LYS:HB2	1.95	0.41
1:A:87:PHE:CG	1:A:122:MET:SD	3.14	0.41
1:A:7:LEU:O	1:A:11:LYS:HG3	2.20	0.41
1:A:151:ARG:O	1:A:152:ALA:HB2	2.19	0.41
1:A:9:LEU:O	1:A:13:VAL:HG23	2.21	0.41
1:A:7:LEU:HD12	1:A:7:LEU:N	2.35	0.41
1:A:128:ARG:HB3	1:A:135:PHE:HD2	1.83	0.41
1:A:146:TYR:HA	1:A:149:GLN:HE21	1.86	0.41
1:A:264:HIS:HE1	1:A:315:ALA:HA	1.86	0.41
1:A:153:TRP:HB3	1:A:161:ILE:HB	2.03	0.40
1:A:46:LEU:HD21	1:A:52:VAL:HB	2.03	0.40
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.74	0.40
1:A:115:ALA:O	1:A:118:TYR:HB3	2.21	0.40

There are no symmetry-related clashes.

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
1	A	313/315 (99%)	258 (82%)	36 (12%)	19 (6%)	1 1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	93	SER
1	A	112	PRO
1	A	158	GLY
1	A	208	ASP
1	A	292	PHE
1	A	22	ASP
1	A	23	ARG
1	A	25	HIS
1	A	95	GLU
1	A	103	ASP
1	A	152	ALA
1	A	45	PRO
1	A	94	ASP
1	A	159	ASP
1	A	175	PRO
1	A	263	ASN
1	A	222	ILE
1	A	227	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
1	A	276/277 (100%)	222 (80%)	54 (20%)	1 2

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LEU
1	A	9	LEU
1	A	12	LYS
1	A	16	GLU
1	A	23	ARG
1	A	24	THR
1	A	37	ARG
1	A	46	LEU
1	A	51	LYS
1	A	61	LEU
1	A	81	ILE
1	A	88	GLU
1	A	89	LYS
1	A	90	TRP
1	A	92	LYS
1	A	103	ASP
1	A	113	GLU
1	A	122	MET
1	A	145	VAL
1	A	157	LYS
1	A	159	ASP
1	A	160	THR
1	A	161	ILE
1	A	169	GLU
1	A	170	GLN
1	A	172	LYS
1	A	175	PRO
1	A	187	PRO
1	A	190	VAL
1	A	192	THR
1	A	193	MET
1	A	195	LEU
1	A	201	LEU
1	A	207	ASN
1	A	208	ASP
1	A	210	LYS
1	A	215	LEU

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	227	PRO
1	A	239	LEU
1	A	240	VAL
1	A	252	ILE
1	A	260	LEU
1	A	262	VAL
1	A	267	GLN
1	A	268	ILE
1	A	270	GLU
1	A	277	ARG
1	A	283	GLN
1	A	284	LEU
1	A	288	LYS
1	A	303	ASN
1	A	311	LYS

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

Mol	Chain	Res	Type
1	A	35	GLN
1	A	66	HIS
1	A	149	GLN
1	A	170	GLN
1	A	174	HIS
1	A	207	ASN
1	A	285	ASN
1	A	303	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand 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	UMP	A	529	-	21,21,21	1.67	4 (19%)	30,31,31	2.69	9 (30%)

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	UMP	A	529	-	1/1/4/4	2/10/22/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	529	UMP	C6-N1	-4.21	1.28	1.38
2	A	529	UMP	P-O5'	-3.00	1.50	1.60
2	A	529	UMP	P-OP2	-2.82	1.44	1.54
2	A	529	UMP	C2-N3	-2.77	1.33	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	529	UMP	C2'-C1'-N1	7.83	133.40	113.81
2	A	529	UMP	C1'-N1-C6	-6.25	109.23	121.53
2	A	529	UMP	O4'-C1'-N1	6.12	118.73	107.86
2	A	529	UMP	C1'-N1-C2	4.99	127.42	117.66
2	A	529	UMP	O2-C2-N3	-2.50	116.88	121.49
2	A	529	UMP	O4-C4-N3	2.48	122.86	119.27
2	A	529	UMP	OP2-P-O5'	-2.29	100.70	106.67
2	A	529	UMP	N3-C2-N1	2.26	117.83	114.89
2	A	529	UMP	OP3-P-OP1	2.16	119.23	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	529	UMP	C1'

All (2) torsion outliers are listed below:

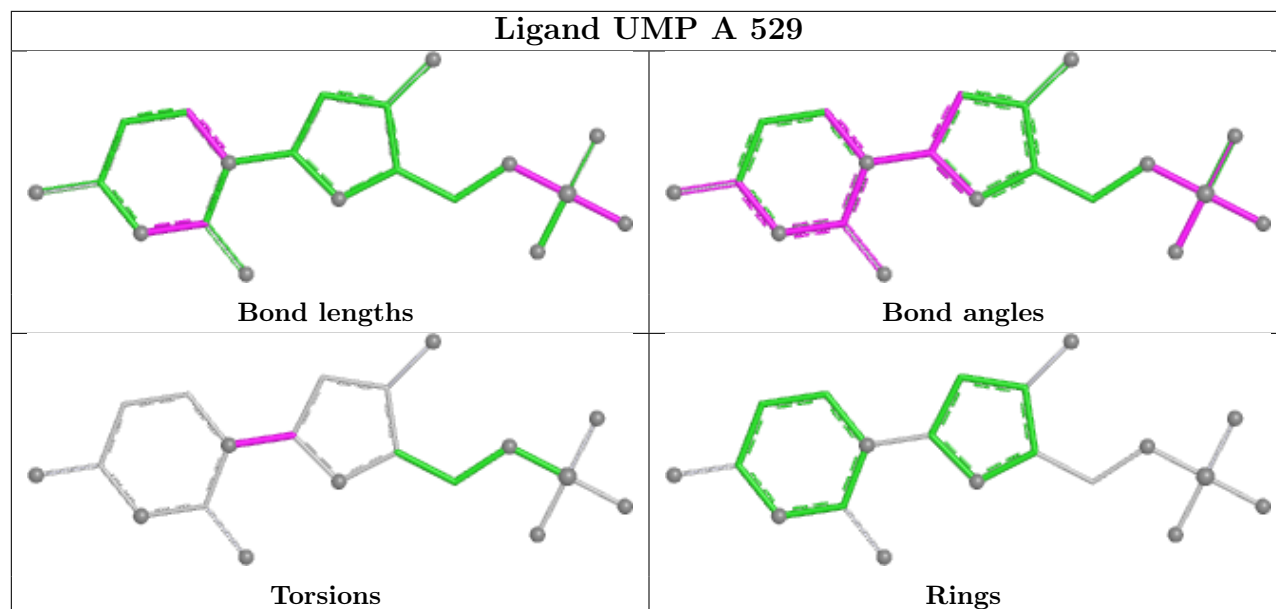
Mol	Chain	Res	Type	Atoms
2	A	529	UMP	C2'-C1'-N1-C2
2	A	529	UMP	C2'-C1'-N1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	529	UMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.