



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:09 AM UTC

PDB ID : 1TDB / pdb_00001tdb
Title : STRUCTURES OF THYMIDYLATE SYNTHASE WITH A C-TERMINAL DELETION: ROLE OF THE C-TERMINUS IN ALIGNMENT OF D/UMP AND CH₂H₄FOLATE
Authors : Perry, K.M.; Carreras, C.W.; Chang, L.C.; Santi, D.V.; Stroud, R.M.
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

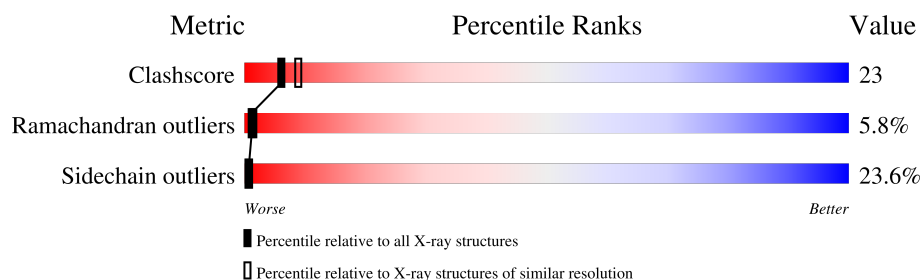
1 Overall quality at a glance

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	24% 37% 28% 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	UFP	A	529	X	-	-	-

2 Entry composition [i](#)

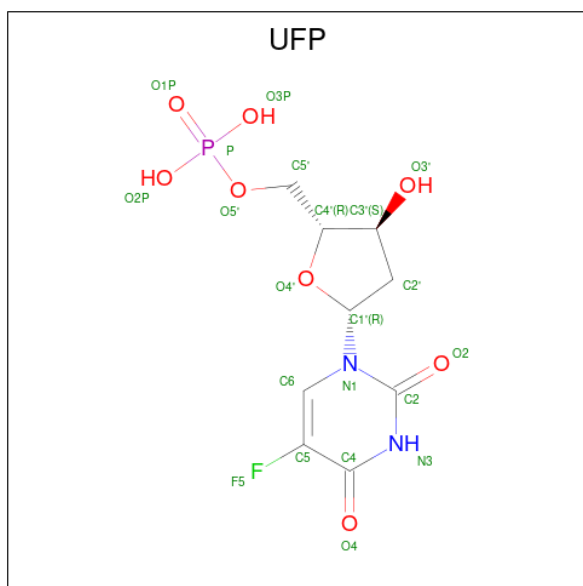
There are 3 unique types of molecules in this entry. The entry contains 2645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (CCD ID: UFP) (formula: C₉H₁₂FN₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0
			21	9	1	2	8	1	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total 41 O	0	0

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	2645	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

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: UFP

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	1.81	55/2667 (2.1%)	2.91	310/3624 (8.6%)

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	24	THR	CA-CB	8.92	1.65	1.53
1	A	167	VAL	CA-CB	8.90	1.68	1.54
1	A	154	HIS	CG-ND1	-8.68	1.28	1.38
1	A	253	HIS	CD2-NE2	-8.44	1.28	1.37
1	A	80	HIS	CD2-NE2	-8.34	1.28	1.37
1	A	264	HIS	CD2-NE2	-8.31	1.28	1.37
1	A	34	HIS	CD2-NE2	-8.19	1.28	1.37
1	A	259	HIS	CG-ND1	-7.58	1.29	1.38
1	A	174	HIS	CD2-NE2	-7.30	1.29	1.37
1	A	289	HIS	CD2-NE2	-7.30	1.29	1.37
1	A	18	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	192	THR	CA-CB	7.13	1.65	1.53
1	A	48	THR	CA-CB	7.06	1.64	1.54
1	A	199	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	80	HIS	CG-ND1	-6.79	1.30	1.38
1	A	282	LEU	CA-CB	-6.52	1.44	1.53
1	A	168	ILE	CA-CB	6.49	1.63	1.54
1	A	264	HIS	CG-ND1	-6.46	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	THR	CA-CB	6.34	1.63	1.53
1	A	259	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	146	TYR	CA-CB	-6.30	1.43	1.53
1	A	291	ILE	CA-CB	6.29	1.63	1.54
1	A	31	ILE	CA-CB	6.19	1.62	1.54
1	A	161	ILE	CA-CB	6.16	1.61	1.54
1	A	24	THR	CA-C	6.14	1.60	1.53
1	A	185	TRP	NE1-CE2	-6.12	1.30	1.37
1	A	72	ARG	CA-CB	6.03	1.62	1.53
1	A	77	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	264	HIS	CE1-NE2	-6.00	1.26	1.32
1	A	122	MET	CA-C	-5.93	1.45	1.52
1	A	169	GLU	CA-CB	5.91	1.62	1.53
1	A	131	HIS	CA-CB	5.85	1.63	1.53
1	A	179	ARG	CA-CB	5.83	1.62	1.53
1	A	131	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	66	HIS	CD2-NE2	-5.69	1.31	1.37
1	A	238	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	185	TRP	CG-CD2	-5.54	1.33	1.43
1	A	216	TYR	CA-CB	-5.53	1.45	1.53
1	A	154	HIS	CD2-NE2	-5.51	1.31	1.37
1	A	113	GLU	C-N	5.43	1.40	1.33
1	A	166	ASP	CA-CB	5.43	1.61	1.53
1	A	82	TRP	CG-CD2	-5.41	1.34	1.43
1	A	159	ASP	C-N	-5.37	1.26	1.33
1	A	66	HIS	CG-ND1	-5.33	1.32	1.38
1	A	150	TRP	CG-CD2	-5.31	1.34	1.43
1	A	229	ASN	CA-CB	-5.30	1.44	1.53
1	A	202	TYR	CA-CB	5.27	1.62	1.53
1	A	80	HIS	CB-CG	5.22	1.57	1.50
1	A	287	ASP	N-CA	-5.17	1.40	1.46
1	A	34	HIS	CG-ND1	-5.16	1.32	1.38
1	A	195	LEU	CA-CB	5.15	1.60	1.52
1	A	253	HIS	CG-ND1	-5.10	1.32	1.38
1	A	101	MET	CA-CB	-5.08	1.46	1.53
1	A	102	THR	CA-CB	5.04	1.59	1.53
1	A	106	HIS	CD2-NE2	-5.01	1.32	1.37

All (310) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASP	CA-CB-CG	19.30	131.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	VAL	O-C-N	16.08	140.14	122.61
1	A	303	ASN	OD1-CG-ND2	-13.87	108.73	122.60
1	A	93	SER	N-CA-C	12.43	126.72	110.43
1	A	166	ASP	CA-CB-CG	12.13	124.73	112.60
1	A	204	PHE	CA-CB-CG	11.91	125.72	113.80
1	A	170	GLN	OE1-CD-NE2	-11.74	110.86	122.60
1	A	207	ASN	CA-CB-CG	11.38	123.98	112.60
1	A	24	THR	N-CA-C	-11.22	94.53	111.81
1	A	290	ASP	CA-C-O	11.04	132.39	120.58
1	A	293	ASP	N-CA-CB	-11.01	95.21	111.51
1	A	157	LYS	N-CA-C	-10.66	88.09	110.80
1	A	303	ASN	CA-CB-CG	10.59	123.19	112.60
1	A	169	GLU	N-CA-C	-10.57	99.05	112.90
1	A	109	GLN	N-CA-C	-10.42	99.88	111.14
1	A	189	ASP	CA-CB-CG	10.40	123.00	112.60
1	A	208	ASP	CA-CB-CG	-10.35	102.25	112.60
1	A	167	VAL	CA-C-O	-10.15	109.58	120.64
1	A	32	PHE	CA-CB-CG	-9.80	104.00	113.80
1	A	293	ASP	CA-CB-CG	9.75	122.35	112.60
1	A	208	ASP	N-CA-C	9.59	131.23	110.80
1	A	235	LEU	N-CA-C	-9.45	100.53	112.90
1	A	160	THR	N-CA-CB	-9.39	96.00	110.65
1	A	263	ASN	OD1-CG-ND2	-9.37	113.23	122.60
1	A	102	THR	CA-C-O	9.33	130.24	120.54
1	A	188	GLU	CA-CB-CG	9.29	132.68	114.10
1	A	59	SER	N-CA-C	-9.08	101.36	111.07
1	A	182	VAL	N-CA-C	-8.98	95.55	108.48
1	A	289	HIS	CB-CG-CD2	-8.92	119.61	131.20
1	A	307	TYR	N-CA-C	-8.80	100.00	110.13
1	A	155	THR	N-CA-CB	-8.73	97.16	110.42
1	A	62	LEU	N-CA-C	-8.68	101.29	112.23
1	A	72	ARG	CB-CG-CD	8.48	130.81	111.30
1	A	169	GLU	CA-CB-CG	8.47	131.04	114.10
1	A	71	ILE	N-CA-CB	-8.46	99.03	110.54
1	A	17	GLY	CA-C-N	-8.40	111.13	122.72
1	A	17	GLY	C-N-CA	-8.40	111.13	122.72
1	A	15	ASP	CA-CB-CG	-8.39	104.20	112.60
1	A	205	TYR	N-CA-C	8.37	121.09	108.46
1	A	253	HIS	N-CA-C	-8.31	95.69	109.07
1	A	91	VAL	CA-CB-CG2	-8.31	96.28	110.40
1	A	207	ASN	OD1-CG-ND2	-8.24	114.36	122.60
1	A	106	HIS	CA-CB-CG	8.24	122.04	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	303	ASN	CB-CG-ND2	8.13	128.59	116.40
1	A	95	GLU	CB-CG-CD	8.12	126.41	112.60
1	A	151	ARG	N-CA-C	8.12	122.03	112.93
1	A	313	PRO	N-CA-CB	8.12	110.10	103.36
1	A	196	PRO	N-CA-C	8.05	120.52	110.70
1	A	211	LEU	N-CA-C	8.04	122.54	109.59
1	A	16	GLU	CA-CB-CG	-8.03	98.05	114.10
1	A	167	VAL	N-CA-CB	8.03	123.14	110.54
1	A	285	ASN	CA-CB-CG	-7.99	104.61	112.60
1	A	74	LEU	CA-C-O	-7.95	112.51	120.70
1	A	167	VAL	CB-CA-C	-7.95	100.45	112.05
1	A	174	HIS	CB-CG-CD2	-7.94	120.88	131.20
1	A	77	HIS	CA-CB-CG	-7.90	105.90	113.80
1	A	185	TRP	N-CA-C	7.88	120.89	108.67
1	A	267	GLN	N-CA-C	7.79	120.86	111.82
1	A	60	GLU	O-C-N	-7.73	112.07	122.43
1	A	25	HIS	CA-CB-CG	-7.69	106.11	113.80
1	A	94	ASP	O-C-N	7.68	132.81	122.59
1	A	292	PHE	CA-CB-CG	7.63	121.43	113.80
1	A	244	CYS	N-CA-C	7.57	122.09	113.01
1	A	128	ARG	CA-C-N	7.55	131.18	120.53
1	A	128	ARG	C-N-CA	7.55	131.18	120.53
1	A	215	LEU	N-CA-C	7.44	121.03	108.02
1	A	118	TYR	N-CA-C	-7.43	102.87	110.97
1	A	42	LYS	CA-CB-CG	7.42	128.95	114.10
1	A	94	ASP	CA-C-N	7.42	135.72	121.54
1	A	94	ASP	C-N-CA	7.42	135.72	121.54
1	A	109	GLN	CB-CA-C	7.42	122.62	110.90
1	A	289	HIS	CA-CB-CG	-7.42	106.38	113.80
1	A	71	ILE	CB-CA-C	7.41	122.15	112.14
1	A	226	VAL	CA-C-O	-7.34	110.11	119.95
1	A	24	THR	CA-C-N	7.30	135.49	121.54
1	A	24	THR	C-N-CA	7.30	135.49	121.54
1	A	293	ASP	CB-CA-C	7.30	124.00	111.45
1	A	15	ASP	N-CA-C	7.28	123.42	113.37
1	A	314	VAL	CA-C-N	7.28	134.80	121.70
1	A	314	VAL	C-N-CA	7.28	134.80	121.70
1	A	69	THR	CA-CB-OG1	-7.25	98.73	109.60
1	A	149	GLN	OE1-CD-NE2	-7.24	115.36	122.60
1	A	10	ALA	N-CA-C	-7.23	104.59	113.41
1	A	130	LEU	N-CA-C	7.22	120.19	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	VAL	N-CA-CB	-7.18	103.46	112.15
1	A	199	HIS	CA-CB-CG	-7.17	106.63	113.80
1	A	50	LYS	CA-C-O	-7.16	113.24	121.26
1	A	94	ASP	N-CA-C	7.16	126.05	110.80
1	A	161	ILE	CB-CG1-CD1	7.13	128.78	113.80
1	A	305	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	160	THR	CB-CA-C	7.06	121.88	110.16
1	A	46	LEU	CA-C-O	7.04	128.11	120.43
1	A	86	ALA	N-CA-C	-7.03	104.98	113.97
1	A	239	LEU	CD1-CG-CD2	-7.01	95.37	110.80
1	A	254	THR	N-CA-C	-7.00	98.52	109.72
1	A	169	GLU	N-CA-CB	6.94	120.73	110.33
1	A	109	GLN	N-CA-CB	-6.93	100.02	110.07
1	A	107	ARG	CA-CB-CG	6.92	127.94	114.10
1	A	217	GLN	N-CA-C	-6.92	97.24	108.52
1	A	131	HIS	CB-CG-CD2	-6.91	122.22	131.20
1	A	103	ASP	CA-C-N	6.87	134.67	121.54
1	A	103	ASP	C-N-CA	6.87	134.67	121.54
1	A	179	ARG	CA-CB-CG	6.86	127.82	114.10
1	A	282	LEU	N-CA-C	-6.86	98.06	109.24
1	A	135	PHE	O-C-N	6.85	129.96	122.15
1	A	263	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	176	TYR	N-CA-C	6.84	120.29	112.57
1	A	139	TYR	O-C-N	6.82	132.10	122.41
1	A	22	ASP	CA-C-N	6.82	134.56	121.54
1	A	22	ASP	C-N-CA	6.82	134.56	121.54
1	A	185	TRP	CG-CD2-CE3	6.75	140.65	133.90
1	A	264	HIS	CB-CG-CD2	-6.71	122.48	131.20
1	A	248	VAL	CA-CB-CG2	-6.71	98.99	110.40
1	A	116	ALA	O-C-N	-6.70	113.36	122.33
1	A	21	PRO	O-C-N	-6.69	117.98	122.73
1	A	226	VAL	N-CA-C	6.68	123.31	108.88
1	A	82	TRP	CD2-CE2-CZ2	-6.65	115.75	122.40
1	A	1	MET	CA-CB-CG	-6.63	100.85	114.10
1	A	263	ASN	CB-CG-ND2	6.62	126.33	116.40
1	A	102	THR	CB-CA-C	6.61	121.36	110.78
1	A	206	VAL	CA-C-O	6.60	129.27	120.69
1	A	211	LEU	CA-C-O	6.54	127.64	120.71
1	A	211	LEU	O-C-N	-6.52	114.93	123.21
1	A	18	HIS	CB-CA-C	6.52	120.51	109.75
1	A	222	ILE	N-CA-CB	-6.50	102.95	110.55
1	A	7	LEU	N-CA-C	6.49	120.29	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	A	242	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	A	229	ASN	N-CA-C	6.44	119.12	111.71
1	A	103	ASP	CA-C-O	6.44	129.56	122.03
1	A	161	ILE	N-CA-CB	-6.41	103.38	111.46
1	A	156	SER	N-CA-C	-6.41	98.09	108.41
1	A	91	VAL	CA-CB-CG1	6.40	121.27	110.40
1	A	174	HIS	N-CA-C	6.38	123.90	109.81
1	A	146	TYR	CA-C-O	-6.36	114.35	120.90
1	A	134	ALA	CA-C-N	6.33	129.28	120.29
1	A	134	ALA	C-N-CA	6.33	129.28	120.29
1	A	185	TRP	CB-CG-CD1	-6.31	117.43	126.90
1	A	150	TRP	CG-CD2-CE3	6.28	140.18	133.90
1	A	289	HIS	CB-CG-ND1	6.24	132.05	122.70
1	A	243	GLU	CA-C-O	-6.23	114.28	120.70
1	A	190	VAL	N-CA-CB	6.20	119.88	111.21
1	A	85	TRP	CE2-CD2-CG	-6.19	99.77	107.20
1	A	34	HIS	CB-CG-CD2	-6.18	123.16	131.20
1	A	104	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	205	TYR	CA-C-O	6.18	127.29	120.31
1	A	153	TRP	CB-CA-C	-6.17	101.48	110.06
1	A	154	HIS	CA-CB-CG	-6.17	107.63	113.80
1	A	6	TYR	O-C-N	6.16	128.44	122.03
1	A	121	GLU	CB-CG-CD	6.16	123.07	112.60
1	A	92	LYS	N-CA-C	-6.15	97.69	110.80
1	A	311	LYS	CG-CD-CE	6.14	125.42	111.30
1	A	190	VAL	O-C-N	-6.13	114.11	121.10
1	A	242	HIS	CA-CB-CG	6.13	119.93	113.80
1	A	179	ARG	N-CA-C	-6.11	104.00	112.30
1	A	77	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	208	ASP	N-CA-CB	-6.09	100.19	110.49
1	A	131	HIS	CB-CG-ND1	6.09	131.83	122.70
1	A	169	GLU	CB-CG-CD	6.09	122.95	112.60
1	A	6	TYR	N-CA-CB	6.08	118.79	109.91
1	A	69	THR	CA-CB-CG2	6.08	120.84	110.50
1	A	203	GLN	O-C-N	-6.07	116.12	123.16
1	A	93	SER	CA-C-O	6.06	128.54	121.87
1	A	124	LYS	CA-C-N	6.04	128.30	120.44
1	A	124	LYS	C-N-CA	6.04	128.30	120.44
1	A	83	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	221	ASP	CA-CB-CG	6.03	118.62	112.60
1	A	243	GLU	O-C-N	-6.02	115.59	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASN	N-CA-C	-6.01	101.30	110.14
1	A	132	ASP	CA-C-O	6.00	128.13	120.57
1	A	97	HIS	CB-CG-CD2	-6.00	123.41	131.20
1	A	37	ARG	CA-CB-CG	5.99	126.09	114.10
1	A	22	ASP	CA-C-O	-5.96	111.99	120.51
1	A	96	TYR	CA-CB-CG	-5.96	103.17	113.90
1	A	72	ARG	CA-C-O	-5.93	114.56	120.90
1	A	123	ALA	CA-C-O	-5.91	114.29	120.55
1	A	179	ARG	O-C-N	-5.91	114.17	122.26
1	A	25	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	170	GLN	CG-CD-NE2	5.88	125.22	116.40
1	A	214	GLN	O-C-N	-5.88	116.62	123.27
1	A	42	LYS	N-CA-CB	-5.87	101.45	110.20
1	A	70	ASN	N-CA-C	5.86	118.50	109.07
1	A	252	ILE	CA-CB-CG2	-5.85	100.55	110.50
1	A	259	HIS	CA-CB-CG	5.85	119.65	113.80
1	A	111	ASP	CA-C-N	5.84	127.14	119.84
1	A	111	ASP	C-N-CA	5.84	127.14	119.84
1	A	89	LYS	CA-C-N	-5.83	110.61	120.58
1	A	89	LYS	C-N-CA	-5.83	110.61	120.58
1	A	311	LYS	N-CA-C	5.81	119.38	110.20
1	A	180	LEU	CA-CB-CG	5.80	136.61	116.30
1	A	292	PHE	CA-C-O	5.79	126.50	119.49
1	A	18	HIS	N-CA-C	-5.78	99.81	109.24
1	A	215	LEU	O-C-N	-5.78	115.49	123.12
1	A	18	HIS	CB-CG-ND1	5.76	131.34	122.70
1	A	175	PRO	N-CA-C	5.75	124.32	112.47
1	A	197	PRO	O-C-N	-5.74	114.90	122.64
1	A	9	LEU	CA-CB-CG	5.71	136.29	116.30
1	A	306	PRO	N-CA-C	5.71	120.18	111.34
1	A	226	VAL	CA-C-N	5.70	126.97	119.84
1	A	226	VAL	C-N-CA	5.70	126.97	119.84
1	A	35	GLN	N-CA-C	-5.69	100.86	109.85
1	A	87	PHE	N-CA-C	-5.68	105.85	112.89
1	A	209	GLY	O-C-N	-5.68	115.13	122.34
1	A	59	SER	CA-CB-OG	5.66	122.43	111.10
1	A	145	VAL	O-C-N	-5.66	115.50	122.57
1	A	103	ASP	O-C-N	5.66	129.64	122.57
1	A	153	TRP	N-CA-CB	5.65	118.55	109.28
1	A	82	TRP	CE2-CD2-CE3	5.65	124.45	118.80
1	A	234	ALA	N-CA-C	-5.64	106.35	113.18
1	A	78	ARG	CA-CB-CG	-5.64	102.82	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	MET	CA-CB-CG	5.64	125.38	114.10
1	A	230	ILE	CA-CB-CG1	-5.62	100.84	110.40
1	A	77	HIS	CE1-NE2-CD2	5.62	114.62	109.00
1	A	38	PHE	CB-CA-C	-5.62	100.25	109.80
1	A	212	SER	CA-C-O	-5.62	114.59	121.78
1	A	159	ASP	CA-CB-CG	-5.61	106.99	112.60
1	A	282	LEU	CA-C-O	-5.60	114.33	120.43
1	A	3	GLU	CA-CB-CG	5.59	125.28	114.10
1	A	270	GLU	O-C-N	-5.58	116.10	122.08
1	A	85	TRP	CD1-CG-CD2	5.58	115.23	106.30
1	A	240	VAL	CA-C-O	-5.58	114.44	120.47
1	A	6	TYR	N-CA-C	-5.53	104.94	110.97
1	A	37	ARG	N-CA-C	5.52	118.63	110.46
1	A	236	LEU	O-C-N	5.50	127.74	122.07
1	A	311	LYS	CA-C-O	5.50	127.32	121.05
1	A	34	HIS	O-C-N	-5.48	115.30	122.59
1	A	197	PRO	N-CA-CB	-5.48	97.50	103.25
1	A	314	VAL	CA-CB-CG2	-5.48	101.09	110.40
1	A	131	HIS	CA-C-N	-5.47	114.87	123.13
1	A	131	HIS	C-N-CA	-5.47	114.87	123.13
1	A	91	VAL	N-CA-C	-5.47	97.97	109.34
1	A	255	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	102	THR	CA-C-N	5.44	130.14	122.46
1	A	102	THR	C-N-CA	5.44	130.14	122.46
1	A	35	GLN	OE1-CD-NE2	-5.44	117.16	122.60
1	A	186	ASN	CA-C-N	5.42	125.76	119.47
1	A	186	ASN	C-N-CA	5.42	125.76	119.47
1	A	289	HIS	N-CA-C	5.41	121.29	114.31
1	A	155	THR	CB-CA-C	5.41	120.73	110.51
1	A	102	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	18	HIS	O-C-N	-5.40	117.17	123.27
1	A	287	ASP	N-CA-CB	-5.38	102.21	110.12
1	A	222	ILE	O-C-N	5.38	127.18	121.91
1	A	16	GLU	O-C-N	5.38	127.63	121.93
1	A	135	PHE	CA-CB-CG	5.38	119.17	113.80
1	A	154	HIS	ND1-CG-CD2	5.37	111.47	106.10
1	A	302	LEU	CD1-CG-CD2	-5.37	98.99	110.80
1	A	220	ALA	O-C-N	5.37	129.54	123.42
1	A	74	LEU	CB-CA-C	-5.36	102.43	110.90
1	A	132	ASP	N-CA-C	5.36	118.47	107.69
1	A	21	PRO	N-CA-C	-5.36	101.85	110.74
1	A	72	ARG	NE-CZ-NH2	5.36	124.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	LEU	N-CA-C	-5.35	106.60	113.23
1	A	181	ILE	N-CA-C	-5.34	100.55	108.45
1	A	286	PRO	CA-C-N	5.33	127.42	120.28
1	A	286	PRO	C-N-CA	5.33	127.42	120.28
1	A	61	LEU	N-CA-C	-5.32	105.53	112.23
1	A	269	LYS	CB-CA-C	-5.32	102.30	110.81
1	A	162	ASP	N-CA-CB	-5.31	102.43	110.35
1	A	73	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	281	THR	N-CA-CB	-5.30	102.25	110.57
1	A	178	ARG	CA-C-O	5.27	126.07	119.59
1	A	256	GLY	N-CA-C	-5.27	100.69	113.18
1	A	17	GLY	CA-C-O	5.26	129.72	120.57
1	A	289	HIS	CA-C-O	-5.26	112.93	118.77
1	A	1	MET	N-CA-CB	-5.25	101.58	110.50
1	A	160	THR	N-CA-C	-5.24	99.87	108.41
1	A	60	GLU	N-CA-C	5.23	118.92	112.54
1	A	25	HIS	CB-CG-ND1	5.23	130.55	122.70
1	A	174	HIS	CB-CG-ND1	5.21	130.52	122.70
1	A	248	VAL	CA-C-O	-5.21	114.26	121.51
1	A	251	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	98	GLY	N-CA-C	5.20	122.95	112.34
1	A	2	LEU	N-CA-C	5.20	117.03	111.36
1	A	45	PRO	N-CA-C	5.20	123.17	112.47
1	A	301	LEU	N-CA-C	-5.19	101.24	109.76
1	A	244	CYS	CA-C-O	5.19	125.80	119.05
1	A	148	SER	CA-CB-OG	5.18	121.47	111.10
1	A	229	ASN	O-C-N	5.17	128.28	122.22
1	A	64	PHE	O-C-N	-5.17	116.51	122.09
1	A	133	ASP	N-CA-C	5.16	121.80	110.80
1	A	166	ASP	CA-C-O	-5.16	115.58	121.00
1	A	122	MET	O-C-N	5.15	127.65	122.09
1	A	71	ILE	CA-C-O	-5.15	115.59	120.95
1	A	190	VAL	CG1-CB-CG2	-5.15	99.47	110.80
1	A	105	GLY	O-C-N	5.15	127.13	122.19
1	A	174	HIS	CA-C-N	5.14	126.27	119.84
1	A	174	HIS	C-N-CA	5.14	126.27	119.84
1	A	205	TYR	O-C-N	-5.14	117.87	123.52
1	A	261	TYR	CA-C-O	-5.13	115.54	121.19
1	A	229	ASN	CA-C-N	5.13	127.48	120.46
1	A	229	ASN	C-N-CA	5.13	127.48	120.46
1	A	6	TYR	CA-C-O	-5.12	115.62	121.00
1	A	220	ALA	CA-C-N	5.12	129.94	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ALA	C-N-CA	5.12	129.94	122.41
1	A	277	ARG	O-C-N	-5.11	115.44	121.32
1	A	285	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	193	MET	O-C-N	5.11	129.60	123.16
1	A	148	SER	O-C-N	-5.10	116.58	122.09
1	A	214	GLN	N-CA-C	5.08	117.52	109.24
1	A	153	TRP	CE2-CD2-CG	-5.08	101.11	107.20
1	A	109	GLN	CB-CG-CD	5.07	121.21	112.60
1	A	37	ARG	CA-C-O	-5.05	115.48	121.89
1	A	72	ARG	O-C-N	-5.04	116.84	122.09
1	A	18	HIS	CA-C-N	-5.04	115.72	122.42
1	A	18	HIS	C-N-CA	-5.04	115.72	122.42
1	A	199	HIS	N-CA-C	-5.04	100.30	108.41
1	A	135	PHE	N-CA-C	-5.02	105.89	111.36
1	A	94	ASP	CA-C-O	5.02	127.69	120.51

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Peptide
1	A	176	TYR	Sidechain
1	A	304	TYR	Sidechain
1	A	312	ALA	Peptide
1	A	98	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2583	0	2487	115	0
2	A	21	0	9	2	0
3	A	41	0	0	2	0
All	All	2645	0	2496	115	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 23.

All (115) 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:65:LEU:HD13	1:A:291:ILE:HG12	1.51	0.90
1:A:29:TYR:HE1	1:A:262:VAL:HG23	1.39	0.86
1:A:6:TYR:HA	1:A:36:MET:HE2	1.59	0.83
1:A:90:TRP:CH2	1:A:95:GLU:HB3	2.15	0.81
1:A:91:VAL:HG21	1:A:101:MET:HB2	1.61	0.81
1:A:90:TRP:HA	1:A:90:TRP:CE3	2.18	0.76
1:A:86:ALA:HB2	1:A:142:LEU:HD21	1.69	0.73
1:A:40:LEU:HD21	1:A:234:ALA:HB1	1.70	0.72
1:A:127:ASP:HA	1:A:130:LEU:HD12	1.71	0.72
1:A:74:LEU:HB3	1:A:79:ASN:HB3	1.72	0.71
1:A:65:LEU:HB3	1:A:292:PHE:HD1	1.55	0.71
1:A:90:TRP:HA	1:A:90:TRP:HE3	1.57	0.70
1:A:120:GLU:O	1:A:124:LYS:HG3	1.91	0.69
1:A:12:LYS:O	1:A:16:GLU:HB2	1.93	0.69
1:A:87:PHE:CE1	1:A:122:MET:HA	2.27	0.69
1:A:177:SER:HB3	1:A:180:LEU:HD13	1.74	0.68
1:A:23:ARG:HG3	1:A:261:TYR:HE1	1.58	0.67
1:A:264:HIS:HE1	1:A:315:ALA:HA	1.60	0.66
1:A:264:HIS:CE1	1:A:315:ALA:HA	2.32	0.65
1:A:28:THR:CG2	1:A:259:HIS:HB2	2.29	0.63
1:A:51:LYS:HZ3	1:A:304:TYR:HE2	1.49	0.60
1:A:83:ASP:HB3	1:A:122:MET:HE1	1.83	0.60
1:A:72:ARG:HG3	1:A:129:VAL:O	2.01	0.60
1:A:46:LEU:HD12	1:A:301:LEU:HD21	1.84	0.60
1:A:72:ARG:HH22	1:A:133:ASP:HA	1.67	0.59
1:A:122:MET:O	1:A:125:PHE:HB3	2.03	0.59
1:A:204:PHE:CD2	1:A:213:LEU:HD12	2.38	0.58
1:A:223:PHE:CE2	1:A:224:LEU:HD23	2.38	0.58
1:A:6:TYR:HD1	1:A:7:LEU:HD12	1.68	0.58
1:A:90:TRP:CH2	1:A:135:PHE:HE2	2.22	0.58
1:A:54:PHE:HA	1:A:57:ILE:HD12	1.86	0.57
1:A:65:LEU:CD1	1:A:291:ILE:HG12	2.30	0.57
1:A:92:LYS:HD2	1:A:93:SER:H	1.70	0.57
1:A:222:ILE:HB	1:A:259:HIS:O	2.04	0.57
1:A:21:PRO:HB2	1:A:25:HIS:ND1	2.20	0.56
1:A:59:SER:HB2	1:A:79:ASN:ND2	2.21	0.56
1:A:218:ARG:HH22	2:A:529:UFP:P	2.29	0.56
1:A:193:MET:HB2	1:A:196:PRO:HD3	1.88	0.56
1:A:107:ARG:HB2	1:A:114:PHE:CE2	2.41	0.56
1:A:156:SER:O	1:A:157:LYS:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HD23	1:A:299:ILE:HG23	1.88	0.56
1:A:220:ALA:HA	2:A:529:UFP:O2	2.05	0.55
1:A:101:MET:SD	1:A:101:MET:N	2.79	0.55
1:A:177:SER:HB3	1:A:180:LEU:CD1	2.36	0.55
1:A:13:VAL:HG21	1:A:222:ILE:HD13	1.90	0.54
1:A:38:PHE:HZ	1:A:230:ILE:HD13	1.71	0.54
1:A:224:LEU:HG	1:A:264:HIS:NE2	2.23	0.54
1:A:163:GLN:O	1:A:167:VAL:HG22	2.07	0.53
1:A:271:GLN:HA	1:A:274:ARG:HG3	1.91	0.53
1:A:114:PHE:HA	1:A:117:VAL:HG22	1.91	0.52
1:A:84:GLU:HA	1:A:87:PHE:HB3	1.94	0.50
1:A:2:LEU:HD12	1:A:42:LYS:HB3	1.93	0.49
1:A:38:PHE:CZ	1:A:230:ILE:HD13	2.47	0.49
1:A:271:GLN:HB3	1:A:310:ILE:HD11	1.94	0.49
1:A:222:ILE:HD12	1:A:259:HIS:C	2.37	0.49
1:A:180:LEU:HD23	1:A:204:PHE:HB2	1.95	0.49
1:A:163:GLN:CB	1:A:182:VAL:HG13	2.42	0.49
1:A:202:TYR:HA	1:A:214:GLN:O	2.13	0.48
1:A:6:TYR:CD1	1:A:7:LEU:HD12	2.49	0.48
1:A:224:LEU:HD12	1:A:315:ALA:HB2	1.96	0.48
1:A:295:ASP:O	1:A:298:ASP:HB2	2.14	0.48
1:A:163:GLN:HB2	1:A:182:VAL:HG13	1.95	0.48
1:A:264:HIS:HE1	1:A:315:ALA:O	1.96	0.47
1:A:239:LEU:HD23	1:A:291:ILE:HB	1.97	0.47
1:A:90:TRP:HH2	1:A:95:GLU:HB3	1.72	0.47
1:A:107:ARG:HA	1:A:110:LYS:HG2	1.97	0.47
1:A:35:GLN:HA	1:A:254:THR:HA	1.97	0.47
1:A:50:LYS:HE3	3:A:321:HOH:O	2.14	0.47
1:A:72:ARG:NH2	1:A:133:ASP:HA	2.29	0.47
1:A:86:ALA:HB2	1:A:142:LEU:CD2	2.44	0.46
1:A:152:ALA:CB	1:A:160:THR:HG23	2.45	0.46
1:A:29:TYR:CE1	1:A:262:VAL:HG23	2.31	0.46
1:A:96:TYR:OH	1:A:101:MET:SD	2.74	0.46
1:A:185:TRP:CE2	1:A:190:VAL:HG21	2.51	0.46
1:A:121:GLU:HA	1:A:124:LYS:HD2	1.97	0.46
1:A:257:ASP:OD1	1:A:259:HIS:ND1	2.48	0.46
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.81	0.46
1:A:205:TYR:O	1:A:211:LEU:HA	2.16	0.45
1:A:174:HIS:O	1:A:176:TYR:N	2.49	0.45
1:A:28:THR:HG22	1:A:259:HIS:HB2	1.96	0.45
1:A:186:ASN:O	1:A:190:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:MET:CB	1:A:196:PRO:HD3	2.46	0.45
1:A:193:MET:HE1	1:A:197:PRO:HD3	1.98	0.45
1:A:214:GLN:OE1	1:A:252:ILE:HB	2.17	0.45
1:A:23:ARG:HG3	1:A:261:TYR:CE1	2.45	0.44
1:A:107:ARG:HB2	1:A:114:PHE:CD2	2.53	0.44
1:A:23:ARG:HB3	1:A:24:THR:H	1.64	0.44
1:A:106:HIS:HB2	3:A:356:HOH:O	2.17	0.44
1:A:89:LYS:HA	1:A:92:LYS:HB2	2.00	0.43
1:A:152:ALA:HB1	1:A:160:THR:HG23	2.00	0.43
1:A:171:ILE:O	1:A:175:PRO:HD3	2.18	0.43
1:A:274:ARG:CZ	1:A:307:TYR:HB3	2.48	0.43
1:A:225:GLY:O	1:A:228:PHE:HB2	2.18	0.43
1:A:19:PHE:CD1	1:A:19:PHE:C	2.96	0.43
1:A:13:VAL:HG21	1:A:222:ILE:CD1	2.49	0.43
1:A:121:GLU:HA	1:A:124:LYS:CD	2.48	0.42
1:A:146:TYR:N	1:A:146:TYR:CD1	2.85	0.42
1:A:291:ILE:HD13	1:A:292:PHE:N	2.33	0.42
1:A:35:GLN:NE2	1:A:214:GLN:HE22	2.18	0.42
1:A:89:LYS:NZ	1:A:139:TYR:O	2.52	0.42
1:A:12:LYS:HE3	1:A:12:LYS:HB3	1.88	0.42
1:A:118:TYR:O	1:A:122:MET:HB3	2.19	0.42
1:A:62:LEU:HD13	1:A:62:LEU:HA	1.74	0.42
1:A:282:LEU:HD11	1:A:299:ILE:HG21	2.01	0.42
1:A:65:LEU:HB3	1:A:292:PHE:CD1	2.44	0.41
1:A:223:PHE:CD2	1:A:224:LEU:HD23	2.56	0.41
1:A:169:GLU:O	1:A:173:THR:HG23	2.21	0.41
1:A:199:HIS:HB3	1:A:215:LEU:HD21	2.02	0.41
1:A:18:HIS:O	1:A:29:TYR:HA	2.22	0.40
1:A:101:MET:HE2	1:A:118:TYR:HA	2.04	0.40
1:A:153:TRP:CH2	1:A:186:ASN:HB2	2.55	0.40
1:A:186:ASN:OD1	1:A:188:GLU:HB3	2.21	0.40
1:A:224:LEU:HD22	1:A:224:LEU:HA	1.91	0.40
1:A:86:ALA:HA	1:A:89:LYS:NZ	2.36	0.40
1:A:91:VAL:HG21	1:A:101:MET:CB	2.42	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%)	259 (83%)	36 (12%)	18 (6%)	1 1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	112	PRO
1	A	133	ASP
1	A	157	LYS
1	A	158	GLY
1	A	175	PRO
1	A	208	ASP
1	A	23	ARG
1	A	84	GLU
1	A	95	GLU
1	A	83	ASP
1	A	104	PHE
1	A	152	ALA
1	A	197	PRO
1	A	17	GLY
1	A	25	HIS
1	A	45	PRO
1	A	225	GLY

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%)	211 (76%)	65 (24%)	1 1

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	5	PRO
1	A	7	LEU
1	A	9	LEU
1	A	15	ASP
1	A	16	GLU
1	A	23	ARG
1	A	24	THR
1	A	36	MET
1	A	42	LYS
1	A	46	LEU
1	A	61	LEU
1	A	62	LEU
1	A	69	THR
1	A	71	ILE
1	A	84	GLU
1	A	89	LYS
1	A	90	TRP
1	A	92	LYS
1	A	94	ASP
1	A	100	ASP
1	A	103	ASP
1	A	104	PHE
1	A	113	GLU
1	A	118	TYR
1	A	120	GLU
1	A	122	MET
1	A	127	ASP
1	A	133	ASP
1	A	142	LEU
1	A	145	VAL
1	A	157	LYS
1	A	160	THR
1	A	161	ILE
1	A	162	ASP
1	A	164	LEU
1	A	169	GLU
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	172	LYS
1	A	180	LEU
1	A	192	THR
1	A	195	LEU
1	A	197	PRO
1	A	201	LEU
1	A	210	LYS
1	A	215	LEU
1	A	222	ILE
1	A	224	LEU
1	A	236	LEU
1	A	239	LEU
1	A	240	VAL
1	A	247	GLU
1	A	252	ILE
1	A	257	ASP
1	A	265	LEU
1	A	267	GLN
1	A	268	ILE
1	A	270	GLU
1	A	281	THR
1	A	283	GLN
1	A	290	ASP
1	A	291	ILE
1	A	299	ILE
1	A	306	PRO
1	A	311	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	35	GLN
1	A	170	GLN
1	A	207	ASN
1	A	238	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	UFP	A	529	-	22,22,22	2.08	8 (36%)	32,33,33	2.43	13 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UFP	A	529	-	1/1/4/4	3/10/22/22	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	529	UFP	P-O5'	-3.68	1.48	1.60
2	A	529	UFP	P-O2P	-3.47	1.41	1.54
2	A	529	UFP	P-O1P	-3.27	1.40	1.50
2	A	529	UFP	C6-C5	3.07	1.37	1.33
2	A	529	UFP	F5-C5	-2.96	1.29	1.35
2	A	529	UFP	C3'-C4'	2.87	1.60	1.53
2	A	529	UFP	P-O3P	-2.79	1.44	1.54
2	A	529	UFP	O4'-C4'	2.22	1.49	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	529	UFP	O4'-C1'-N1	8.40	122.76	107.86
2	A	529	UFP	C2'-C1'-N1	4.75	125.69	113.81
2	A	529	UFP	F5-C5-C4	4.35	120.28	116.47
2	A	529	UFP	C5-C4-N3	3.08	115.46	112.64
2	A	529	UFP	C1'-N1-C6	-2.60	116.37	120.74
2	A	529	UFP	O3P-P-O5'	-2.60	99.89	106.67
2	A	529	UFP	F5-C5-C6	-2.44	118.93	120.99
2	A	529	UFP	C3'-C2'-C1'	2.44	108.56	102.60
2	A	529	UFP	C4-N3-C2	-2.32	124.30	127.34
2	A	529	UFP	O4-C4-C5	2.21	127.57	125.69
2	A	529	UFP	O2P-P-O5'	-2.17	101.00	106.67
2	A	529	UFP	O3P-P-O1P	2.16	119.26	110.83
2	A	529	UFP	C6-C5-C4	-2.15	120.61	122.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	529	UFP	C1'

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	529	UFP	C2'-C1'-N1-C2
2	A	529	UFP	C2'-C1'-N1-C6
2	A	529	UFP	O4'-C4'-C5'-O5'

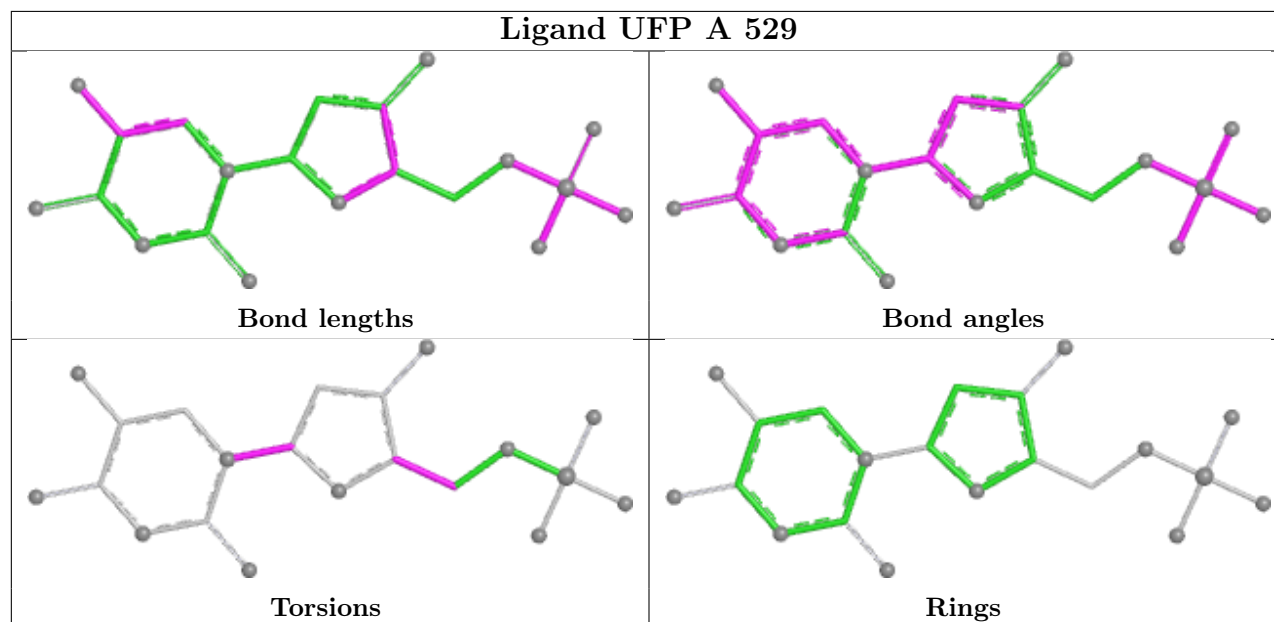
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	529	UFP	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.