Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 07:47 PM EST

PDB ID	:	1TDC
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

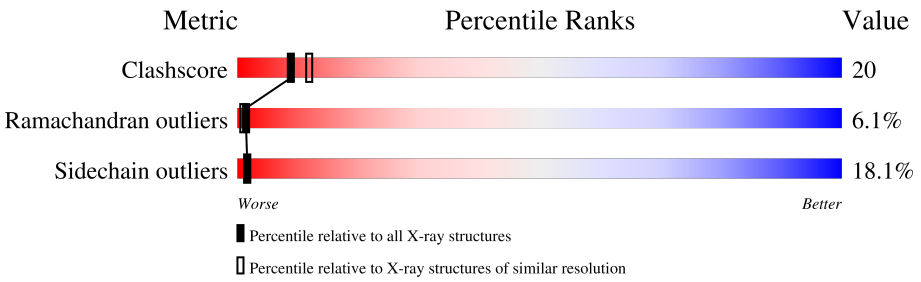
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	315	37% 40% 16% 7%

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)

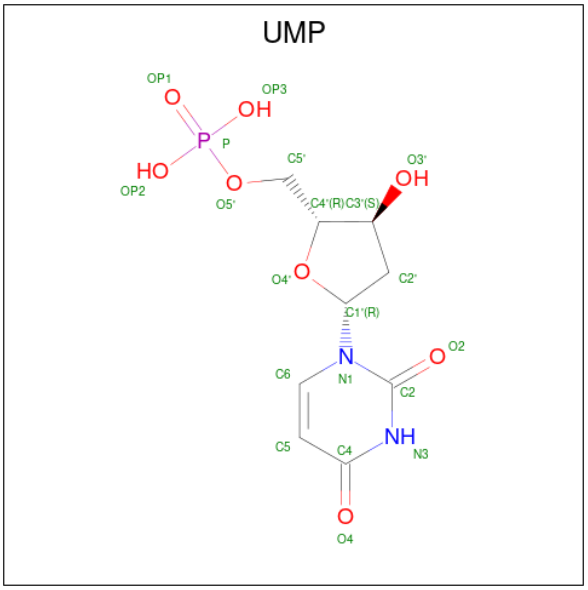
There are 2 unique types of molecules in this entry. The entry contains 2603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	315	2583	1672	437	466	8	0	0	0

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



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

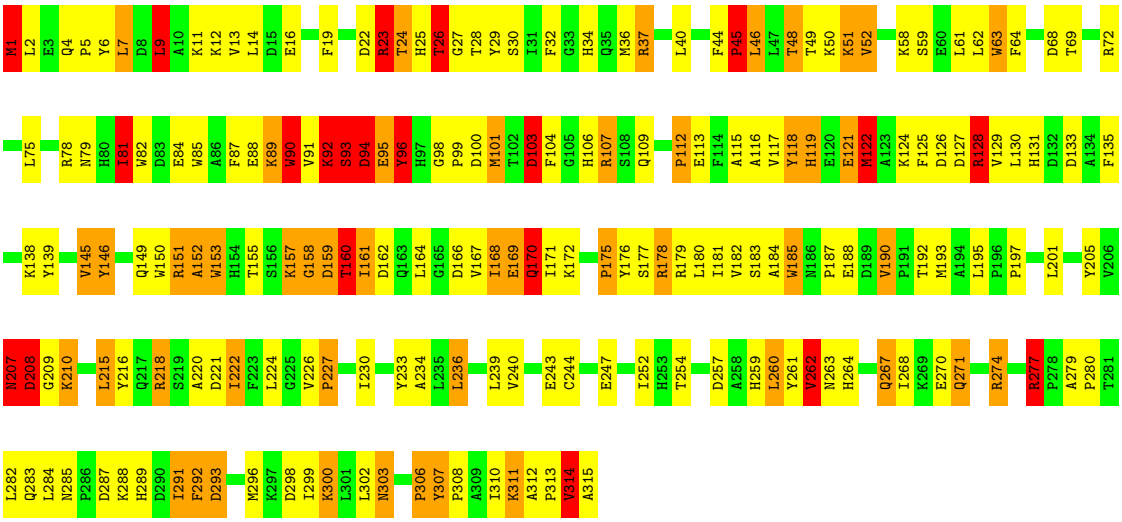
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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

Chain A: 37% 40% 16% 7%



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.39	14/2667 (0.5%)	2.38	152/3624 (4.2%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	CA-CB	17.77	1.93	1.53
1	A	1	MET	CB-CG	-7.33	1.27	1.51
1	A	82	TRP	CG-CD2	-6.74	1.32	1.43
1	A	63	TRP	CD2-CE2	-6.31	1.33	1.41
1	A	153	TRP	CG-CD2	-5.97	1.33	1.43
1	A	216	TYR	CA-CB	-5.95	1.40	1.53
1	A	50	LYS	CA-CB	-5.77	1.41	1.53
1	A	153	TRP	CD1-NE1	-5.60	1.28	1.38
1	A	150	TRP	CG-CD2	-5.58	1.34	1.43
1	A	146	TYR	CA-CB	-5.26	1.42	1.53
1	A	185	TRP	CD2-CE2	-5.20	1.35	1.41
1	A	185	TRP	CG-CD2	-5.13	1.34	1.43
1	A	52	VAL	CA-CB	-5.09	1.44	1.54
1	A	247	GLU	CA-CB	-5.01	1.43	1.53

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	ARG	NE-CZ-NH2	15.47	128.04	120.30
1	A	151	ARG	NE-CZ-NH2	-14.09	113.25	120.30
1	A	233	TYR	CB-CG-CD1	-12.61	113.44	121.00
1	A	151	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	A	307	TYR	CB-CG-CD1	-11.60	114.04	121.00
1	A	36	MET	CA-CB-CG	11.19	132.32	113.30
1	A	103	ASP	CA-C-N	-11.00	93.00	117.20
1	A	185	TRP	CD1-CG-CD2	10.67	114.84	106.30
1	A	122	MET	CG-SD-CE	-10.35	83.64	100.20
1	A	78	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	A	274	ARG	NE-CZ-NH1	10.13	125.37	120.30
1	A	207	ASN	CA-CB-CG	9.52	134.33	113.40
1	A	37	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	A	296	MET	CG-SD-CE	-9.44	85.10	100.20
1	A	63	TRP	CD1-CG-CD2	9.25	113.70	106.30
1	A	150	TRP	CD1-CG-CD2	9.09	113.57	106.30
1	A	1	MET	N-CA-CB	-9.07	94.28	110.60
1	A	153	TRP	CD1-CG-CD2	8.86	113.38	106.30
1	A	233	TYR	CB-CG-CD2	8.48	126.09	121.00
1	A	103	ASP	O-C-N	8.36	136.08	122.70
1	A	216	TYR	CB-CG-CD2	-8.32	116.01	121.00
1	A	128	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	168	ILE	CA-C-N	8.24	135.33	117.20
1	A	90	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	A	150	TRP	CE2-CD2-CG	-8.22	100.73	107.30
1	A	1	MET	CA-CB-CG	-8.05	99.62	113.30
1	A	201	LEU	CA-CB-CG	8.01	133.72	115.30
1	A	90	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	A	185	TRP	CE2-CD2-CG	-7.91	100.97	107.30
1	A	153	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	A	1	MET	CB-CA-C	7.78	125.96	110.40
1	A	63	TRP	CG-CD1-NE1	-7.52	102.58	110.10
1	A	178	ARG	CB-CG-CD	-7.52	92.06	111.60
1	A	82	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	A	90	TRP	CB-CG-CD1	-7.21	117.63	127.00
1	A	277	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	289	HIS	CA-C-N	7.10	132.81	117.20
1	A	236	LEU	CA-CB-CG	7.04	131.50	115.30
1	A	185	TRP	CG-CD1-NE1	-7.02	103.08	110.10
1	A	158	GLY	CA-C-O	-7.01	107.98	120.60
1	A	262	VAL	CA-CB-CG2	-6.96	100.46	110.90
1	A	107	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	63	TRP	CE2-CD2-CG	-6.87	101.81	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	THR	N-CA-CB	-6.86	97.27	110.30
1	A	271	GLN	CA-CB-CG	6.85	128.46	113.40
1	A	190	VAL	CA-CB-CG2	-6.72	100.81	110.90
1	A	30	SER	CA-CB-OG	6.70	129.29	111.20
1	A	51	LYS	N-CA-C	-6.66	93.02	111.00
1	A	157	LYS	N-CA-C	-6.64	93.06	111.00
1	A	244	CYS	CA-CB-SG	-6.64	102.05	114.00
1	A	311	LYS	CA-C-N	-6.62	102.63	117.20
1	A	185	TRP	CG-CD2-CE3	6.57	139.81	133.90
1	A	62	LEU	CA-CB-CG	6.55	130.38	115.30
1	A	81	ILE	CB-CG1-CD1	-6.52	95.64	113.90
1	A	170	GLN	CA-CB-CG	-6.51	99.08	113.40
1	A	32	PHE	CA-C-N	6.51	129.22	116.20
1	A	314	VAL	CA-CB-CG2	-6.44	101.23	110.90
1	A	168	ILE	O-C-N	-6.42	112.42	122.70
1	A	277	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	183	SER	CA-CB-OG	-6.37	94.01	111.20
1	A	179	ARG	CA-CB-CG	6.34	127.35	113.40
1	A	157	LYS	CA-C-N	-6.26	103.68	116.20
1	A	116	ALA	N-CA-CB	6.23	118.82	110.10
1	A	1	MET	CG-SD-CE	6.22	110.16	100.20
1	A	94	ASP	CA-C-N	-6.18	103.60	117.20
1	A	293	ASP	CA-CB-CG	6.17	126.98	113.40
1	A	96	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	A	117	VAL	CA-CB-CG1	-6.13	101.70	110.90
1	A	85	TRP	CD1-CG-CD2	6.12	111.20	106.30
1	A	26	THR	OG1-CB-CG2	6.03	123.86	110.00
1	A	85	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	A	85	TRP	CE2-CD2-CG	-5.99	102.51	107.30
1	A	117	VAL	CA-CB-CG2	5.96	119.84	110.90
1	A	167	VAL	CA-C-N	5.95	130.30	117.20
1	A	62	LEU	O-C-N	-5.95	113.18	122.70
1	A	26	THR	CA-CB-OG1	-5.92	96.56	109.00
1	A	37	ARG	CA-C-N	5.92	130.22	117.20
1	A	24	THR	CA-CB-CG2	-5.90	104.14	112.40
1	A	210	LYS	CA-CB-CG	5.88	126.34	113.40
1	A	119	HIS	CB-CA-C	-5.88	98.64	110.40
1	A	100	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	188	GLU	CA-CB-CG	5.86	126.29	113.40
1	A	262	VAL	CA-CB-CG1	5.85	119.67	110.90
1	A	289	HIS	CA-C-O	-5.81	107.90	120.10
1	A	26	THR	N-CA-C	5.80	126.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	TRP	CE2-CD2-CG	-5.80	102.66	107.30
1	A	287	ASP	CB-CA-C	5.79	121.98	110.40
1	A	7	LEU	CD1-CG-CD2	-5.78	93.17	110.50
1	A	247	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	A	9	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	A	93	SER	CA-C-N	-5.76	104.53	117.20
1	A	96	TYR	CA-CB-CG	-5.76	102.45	113.40
1	A	24	THR	N-CA-C	-5.75	95.49	111.00
1	A	63	TRP	CA-CB-CG	5.75	124.62	113.70
1	A	183	SER	O-C-N	5.74	131.88	122.70
1	A	300	LYS	CA-CB-CG	5.69	125.93	113.40
1	A	179	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
1	A	207	ASN	N-CA-CB	5.63	120.73	110.60
1	A	50	LYS	N-CA-C	-5.61	95.86	111.00
1	A	37	ARG	CB-CG-CD	-5.60	97.03	111.60
1	A	116	ALA	CB-CA-C	-5.59	101.71	110.10
1	A	218	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	176	TYR	CB-CG-CD1	-5.59	117.65	121.00
1	A	257	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	287	ASP	N-CA-CB	-5.59	100.55	110.60
1	A	72	ARG	CG-CD-NE	5.56	123.48	111.80
1	A	226	VAL	CA-C-N	5.54	132.60	117.10
1	A	287	ASP	CB-CG-OD2	5.51	123.25	118.30
1	A	288	LYS	N-CA-C	-5.49	96.18	111.00
1	A	82	TRP	CD2-CE2-CZ2	-5.49	115.72	122.30
1	A	96	TYR	CA-C-N	-5.48	105.14	117.20
1	A	133	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	306	PRO	O-C-N	5.45	131.42	122.70
1	A	101	MET	CA-CB-CG	-5.44	104.05	113.30
1	A	48	THR	O-C-N	-5.43	114.01	122.70
1	A	210	LYS	CB-CG-CD	-5.43	97.48	111.60
1	A	179	ARG	CG-CD-NE	5.41	123.17	111.80
1	A	314	VAL	CA-CB-CG1	5.41	119.02	110.90
1	A	122	MET	CA-C-N	5.40	129.08	117.20
1	A	167	VAL	CA-CB-CG2	5.40	118.99	110.90
1	A	37	ARG	CB-CA-C	-5.37	99.67	110.40
1	A	90	TRP	NE1-CE2-CZ2	-5.36	124.50	130.40
1	A	49	THR	CA-CB-CG2	-5.35	104.91	112.40
1	A	81	ILE	CB-CA-C	-5.34	100.91	111.60
1	A	129	VAL	CG1-CB-CG2	-5.30	102.41	110.90
1	A	215	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	A	138	LYS	CB-CG-CD	-5.30	97.83	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	291	ILE	CA-C-N	5.28	128.82	117.20
1	A	314	VAL	CB-CA-C	5.28	121.44	111.40
1	A	92	LYS	N-CA-C	-5.28	96.75	111.00
1	A	208	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	128	ARG	CA-CB-CG	5.27	125.00	113.40
1	A	216	TYR	CD1-CG-CD2	5.27	123.70	117.90
1	A	185	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	A	121	GLU	CA-CB-CG	5.25	124.95	113.40
1	A	118	TYR	CB-CG-CD1	-5.24	117.85	121.00
1	A	215	LEU	O-C-N	-5.23	114.33	122.70
1	A	162	ASP	CA-C-N	5.21	128.66	117.20
1	A	158	GLY	CA-C-N	5.20	128.64	117.20
1	A	93	SER	N-CA-C	5.18	125.00	111.00
1	A	254	THR	CA-CB-CG2	-5.13	105.22	112.40
1	A	119	HIS	C-N-CA	-5.13	108.88	121.70
1	A	218	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	37	ARG	O-C-N	-5.12	114.51	122.70
1	A	45	PRO	CA-N-CD	-5.10	104.36	111.50
1	A	34	HIS	CA-C-N	5.10	128.42	117.20
1	A	166	ASP	CA-C-N	5.10	128.41	117.20
1	A	58	LYS	CB-CG-CD	-5.05	98.46	111.60
1	A	82	TRP	CE2-CD2-CE3	5.02	124.72	118.70
1	A	131	HIS	N-CA-C	5.01	124.52	111.00
1	A	82	TRP	CB-CG-CD2	-5.00	120.09	126.60
1	A	257	ASP	CA-C-N	5.00	128.21	117.20

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 (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	104	0
2	A	20	0	10	1	0
All	All	2603	0	2497	104	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 20.

All (104) 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: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: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: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: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:101:MET:HE2	1:A:118:TYR:HA	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:151:ARG:O	1:A:152:ALA:HB2	2.19	0.42
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:291:ILE:O	1:A:292:PHE:C	2.58	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: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%)	226 (82%)	50 (18%)	1 1

All (50) 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	81	ILE
1	A	88	GLU
1	A	89	LYS
1	A	90	TRP
1	A	92	LYS
1	A	96	TYR
1	A	103	ASP
1	A	107	ARG
1	A	122	MET
1	A	126	ASP
1	A	128	ARG
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	207	ASN
1	A	208	ASP
1	A	210	LYS
1	A	215	LEU

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Mol	Chain	Res	Type
1	A	227	PRO
1	A	239	LEU
1	A	252	ILE
1	A	260	LEU
1	A	261	TYR
1	A	262	VAL
1	A	267	GLN
1	A	270	GLU
1	A	277	ARG
1	A	284	LEU
1	A	303	ASN
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	149	GLN
1	A	170	GLN
1	A	207	ASN
1	A	229	ASN
1	A	303	ASN

5.3.3 RNA (i)

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 monosaccharides 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	UMP	A	529	-	21,21,21	1.63	4 (19%)	31,31,31	2.70	9 (29%)

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	3/10/22/22	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	-4.11	1.28	1.38
2	A	529	UMP	P-O5'	-2.91	1.50	1.60
2	A	529	UMP	P-OP2	-2.73	1.44	1.54
2	A	529	UMP	C2-N3	-2.71	1.33	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	529	UMP	C2'-C1'-N1	8.52	133.40	113.77
2	A	529	UMP	C1'-N1-C6	-6.24	109.23	121.55
2	A	529	UMP	O4'-C1'-N1	6.08	118.73	107.86
2	A	529	UMP	C1'-N1-C2	4.97	127.42	117.64
2	A	529	UMP	O2-C2-N3	-2.48	116.88	121.50
2	A	529	UMP	O4-C4-N3	2.42	122.86	119.31
2	A	529	UMP	OP2-P-O5'	-2.27	100.70	106.73
2	A	529	UMP	N3-C2-N1	2.22	117.83	114.89
2	A	529	UMP	OP3-P-OP1	2.18	119.23	110.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	529	UMP	C1'

All (3) 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
2	A	529	UMP	O4'-C4'-C5'-O5'

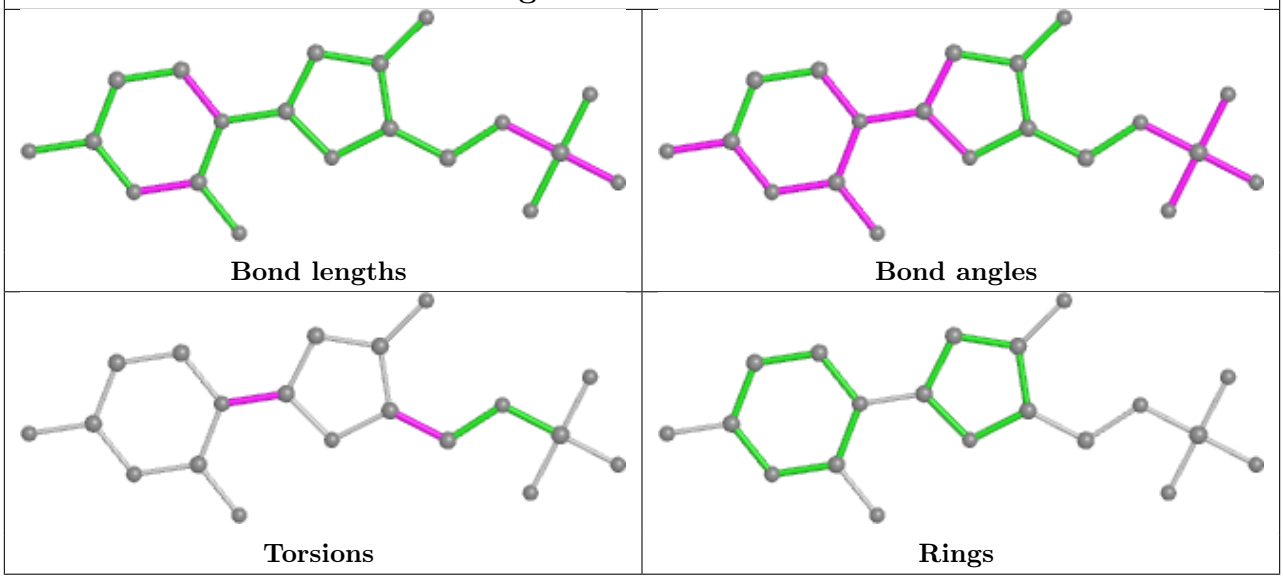
There are no ring outliers.

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 then 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.

Ligand UMP A 529



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.