



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:42 PM UTC

PDB ID : 1VZA / pdb_00001vza
Title : THYMIDYLATE SYNTHASE E60D MUTANT BINARY COMPLEX WITH
2'-DEOXYURIDINE 5'-MONOPHOSPHATE (DUMP)
Authors : Birdsall, D.L.; Finer-Moore, J.; Stroud, R.M.
Deposited on : 1996-09-18
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

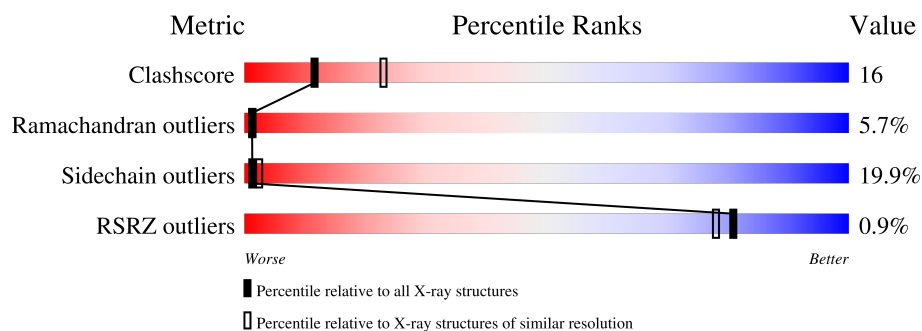
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	32% 40% 23% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3246 atoms, of which 608 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.

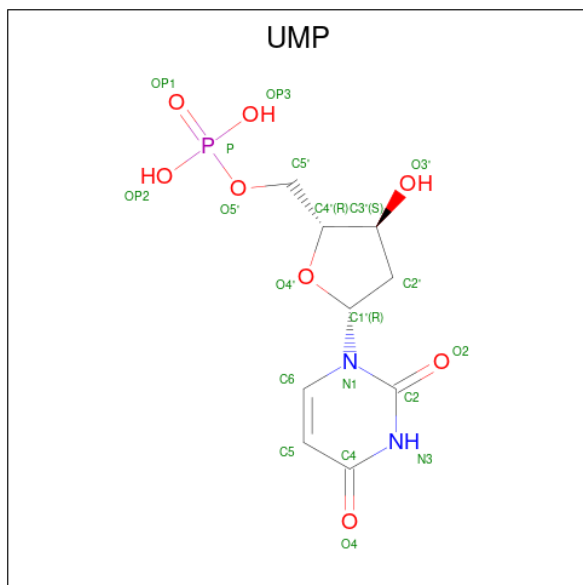
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	316	3138	1676	549	438	467	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLU	engineered mutation	UNP P00469
A	111	ALA	ASP	conflict	UNP P00469

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



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

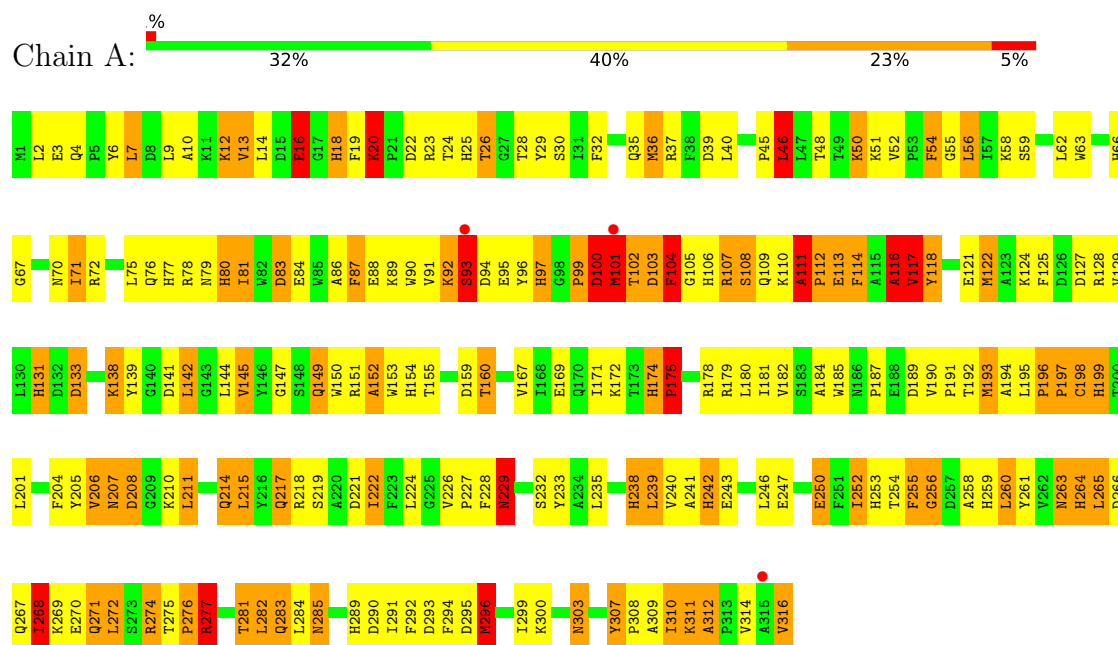
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	29	Total	H	O	0	0
			87	58	29		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.10Å 79.10Å 230.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 71.7 (15.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.210 , (Not available) 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3246	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	1.65	30/2673 (1.1%)	2.50	183/3633 (5.0%)

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	4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	HIS	CD2-NE2	-8.44	1.28	1.37
1	A	259	HIS	CD2-NE2	-8.09	1.28	1.37
1	A	259	HIS	CG-ND1	-7.75	1.29	1.38
1	A	199	HIS	CG-ND1	-6.97	1.30	1.38
1	A	253	HIS	CD2-NE2	-6.86	1.30	1.37
1	A	25	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	80	HIS	CD2-NE2	-6.52	1.30	1.37
1	A	181	ILE	CA-CB	-6.52	1.46	1.54
1	A	229	ASN	CA-CB	-6.44	1.43	1.53
1	A	242	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	264	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	153	TRP	CG-CD2	-5.98	1.32	1.43
1	A	12	LYS	CA-CB	-5.78	1.44	1.53
1	A	185	TRP	CG-CD2	-5.76	1.33	1.43
1	A	78	ARG	NE-CZ	5.76	1.39	1.33
1	A	238	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	66	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	207	ASN	CA-CB	-5.51	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	HIS	CD2-NE2	-5.50	1.31	1.37
1	A	233	TYR	CA-CB	-5.42	1.44	1.53
1	A	219	SER	CA-CB	-5.40	1.44	1.53
1	A	106	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	14	LEU	CA-CB	-5.16	1.45	1.53
1	A	131	HIS	CD2-NE2	-5.16	1.32	1.37
1	A	14	LEU	CB-CG	-5.12	1.43	1.53
1	A	78	ARG	CA-CB	5.08	1.61	1.53
1	A	217	GLN	CA-CB	-5.07	1.46	1.53
1	A	235	LEU	CA-CB	-5.06	1.44	1.53
1	A	167	VAL	CA-CB	-5.02	1.48	1.54
1	A	80	HIS	CG-ND1	-5.02	1.32	1.38

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	HIS	CA-CB-CG	-13.60	100.20	113.80
1	A	106	HIS	CA-CB-CG	-13.36	100.44	113.80
1	A	229	ASN	OD1-CG-ND2	-11.29	111.31	122.60
1	A	290	ASP	CA-CB-CG	-10.81	101.78	112.60
1	A	284	LEU	N-CA-C	-10.47	90.89	108.26
1	A	7	LEU	N-CA-C	-10.28	100.04	111.14
1	A	54	PHE	CA-CB-CG	10.27	124.07	113.80
1	A	228	PHE	CA-CB-CG	10.04	123.84	113.80
1	A	97	HIS	CA-CB-CG	-9.90	103.90	113.80
1	A	29	TYR	N-CA-C	-9.90	93.11	109.24
1	A	141	ASP	N-CA-C	-9.77	92.60	108.52
1	A	114	PHE	CA-CB-CG	-9.58	104.22	113.80
1	A	169	GLU	CA-CB-CG	-9.54	95.01	114.10
1	A	314	VAL	N-CA-C	-9.42	97.42	109.58
1	A	63	TRP	N-CA-C	-9.35	101.06	111.07
1	A	149	GLN	N-CA-C	-9.34	100.01	111.40
1	A	293	ASP	CA-CB-CG	-9.29	103.31	112.60
1	A	107	ARG	N-CA-C	-9.16	92.48	108.23
1	A	99	PRO	N-CA-C	9.02	131.06	112.47
1	A	90	TRP	O-C-N	8.90	132.97	122.20
1	A	46	LEU	N-CA-C	-8.62	95.15	109.46
1	A	174	HIS	CA-CB-CG	8.54	122.34	113.80
1	A	226	VAL	CA-C-O	-8.32	111.78	118.85
1	A	118	TYR	CA-C-O	-8.04	112.56	121.00
1	A	2	LEU	N-CA-CB	-7.87	98.10	110.22
1	A	84	GLU	CA-C-O	-7.81	110.04	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	CYS	CA-C-O	7.80	128.90	120.55
1	A	104	PHE	CA-CB-CG	7.72	121.52	113.80
1	A	159	ASP	N-CA-CB	-7.64	97.81	110.65
1	A	78	ARG	CB-CG-CD	7.60	128.78	111.30
1	A	195	LEU	N-CA-C	-7.56	94.66	109.10
1	A	205	TYR	CA-C-O	-7.38	110.98	119.98
1	A	116	ALA	CA-C-O	-7.35	110.00	120.51
1	A	229	ASN	CB-CG-ND2	7.30	127.36	116.40
1	A	152	ALA	CA-C-O	7.23	130.84	120.51
1	A	30	SER	N-CA-C	7.21	120.89	109.50
1	A	23	ARG	CA-CB-CG	7.19	128.47	114.10
1	A	172	LYS	N-CA-C	-7.17	101.99	111.24
1	A	35	GLN	OE1-CD-NE2	-7.16	115.44	122.60
1	A	114	PHE	N-CA-C	7.14	121.63	112.34
1	A	108	SER	N-CA-C	-7.07	95.75	110.80
1	A	214	GLN	CA-CB-CG	-7.00	100.09	114.10
1	A	263	ASN	CA-CB-CG	7.00	119.60	112.60
1	A	70	ASN	CA-C-O	7.00	127.92	120.36
1	A	258	ALA	O-C-N	-6.96	115.40	123.27
1	A	292	PHE	CA-CB-CG	-6.95	106.85	113.80
1	A	174	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	A	274	ARG	CA-CB-CG	-6.93	100.24	114.10
1	A	254	THR	CA-CB-OG1	-6.93	99.21	109.60
1	A	18	HIS	N-CA-C	-6.93	99.31	110.32
1	A	239	LEU	N-CA-C	6.93	118.48	111.07
1	A	309	ALA	N-CA-C	6.85	119.79	110.55
1	A	14	LEU	O-C-N	6.83	129.96	122.11
1	A	149	GLN	OE1-CD-NE2	-6.83	115.77	122.60
1	A	266	ASP	CA-C-O	6.71	128.19	120.00
1	A	250	GLU	CA-C-O	-6.69	113.82	121.58
1	A	221	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	253	HIS	CA-C-O	-6.67	113.13	120.33
1	A	233	TYR	CA-CB-CG	-6.60	102.01	113.90
1	A	199	HIS	N-CA-C	-6.60	97.04	108.52
1	A	271	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	A	99	PRO	N-CA-CB	-6.49	96.44	103.25
1	A	79	ASN	O-C-N	-6.48	115.61	123.19
1	A	277	ARG	O-C-N	-6.46	116.49	121.14
1	A	285	ASN	N-CA-C	6.41	118.92	109.50
1	A	19	PHE	CA-C-O	-6.39	113.63	120.92
1	A	4	GLN	CG-CD-NE2	6.37	125.95	116.40
1	A	128	ARG	N-CA-C	-6.36	104.27	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	MET	N-CA-C	6.35	124.33	110.80
1	A	25	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	A	289	HIS	CB-CG-CD2	-6.29	123.03	131.20
1	A	26	THR	N-CA-C	-6.28	100.04	109.96
1	A	122	MET	CG-SD-CE	-6.26	87.13	100.90
1	A	192	THR	CA-CB-OG1	-6.26	100.21	109.60
1	A	274	ARG	CB-CG-CD	6.25	125.67	111.30
1	A	178	ARG	CA-CB-CG	-6.25	101.61	114.10
1	A	242	HIS	CA-CB-CG	6.24	120.04	113.80
1	A	309	ALA	O-C-N	-6.23	115.75	122.85
1	A	303	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	102	THR	O-C-N	6.21	130.85	122.59
1	A	97	HIS	CA-C-O	6.21	128.40	120.57
1	A	67	GLY	CA-C-O	6.21	125.87	119.10
1	A	242	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	A	77	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	A	39	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	124	LYS	N-CA-C	-6.11	104.63	111.28
1	A	160	THR	N-CA-CB	-6.10	100.43	110.68
1	A	153	TRP	N-CA-C	-6.10	99.22	108.67
1	A	154	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	293	ASP	N-CA-C	6.07	120.68	113.16
1	A	13	VAL	N-CA-C	-6.07	104.72	110.42
1	A	238	HIS	CB-CG-CD2	-6.06	123.33	131.20
1	A	159	ASP	CA-C-N	6.04	131.51	122.99
1	A	159	ASP	C-N-CA	6.04	131.51	122.99
1	A	133	ASP	CA-C-O	-6.04	114.02	120.42
1	A	182	VAL	O-C-N	-6.00	116.88	123.18
1	A	228	PHE	N-CA-CB	-5.98	101.35	110.33
1	A	178	ARG	CB-CG-CD	5.94	124.95	111.30
1	A	254	THR	CA-CB-CG2	5.92	120.57	110.50
1	A	263	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	267	GLN	N-CA-C	-5.88	104.77	111.07
1	A	36	MET	CA-C-O	-5.88	114.76	121.40
1	A	145	VAL	N-CA-CB	-5.87	101.51	112.36
1	A	294	PHE	CA-C-O	5.84	127.93	121.56
1	A	2	LEU	N-CA-C	5.84	118.43	111.71
1	A	22	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	299	ILE	O-C-N	-5.82	116.76	122.99
1	A	272	LEU	N-CA-C	5.82	119.85	112.87
1	A	100	ASP	N-CA-C	-5.79	98.46	110.80
1	A	206	VAL	N-CA-C	-5.76	100.27	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	CYS	N-CA-C	5.75	118.42	111.40
1	A	281	THR	O-C-N	-5.74	114.73	122.94
1	A	59	SER	N-CA-C	-5.73	104.94	111.07
1	A	147	GLY	O-C-N	-5.73	116.69	122.19
1	A	268	ILE	N-CA-CB	-5.72	104.16	110.51
1	A	151	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	A	222	ILE	CB-CA-C	-5.70	103.33	112.16
1	A	159	ASP	N-CA-C	5.68	118.52	109.65
1	A	2	LEU	O-C-N	-5.67	115.59	122.22
1	A	16	GLU	CA-C-O	5.67	125.30	119.97
1	A	93	SER	O-C-N	5.66	130.82	123.07
1	A	196	PRO	CA-C-N	5.65	125.62	120.03
1	A	196	PRO	C-N-CA	5.65	125.62	120.03
1	A	35	GLN	CA-C-O	-5.65	114.17	120.66
1	A	307	TYR	N-CA-C	-5.62	102.50	109.64
1	A	294	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	13	VAL	CB-CA-C	-5.59	104.66	111.87
1	A	290	ASP	N-CA-C	-5.58	101.12	109.15
1	A	81	ILE	CB-CA-C	-5.58	104.74	111.88
1	A	154	HIS	CA-CB-CG	-5.57	108.23	113.80
1	A	295	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	81	ILE	CA-CB-CG2	-5.55	101.06	110.50
1	A	232	SER	N-CA-C	-5.54	105.15	111.14
1	A	113	GLU	CB-CG-CD	5.52	121.99	112.60
1	A	150	TRP	N-CA-C	5.52	118.22	111.82
1	A	174	HIS	N-CA-CB	5.51	120.17	110.37
1	A	255	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	283	GLN	N-CA-C	-5.48	98.62	108.48
1	A	270	GLU	O-C-N	-5.45	116.36	122.03
1	A	86	ALA	N-CA-C	-5.44	105.00	111.69
1	A	48	THR	N-CA-C	-5.43	106.82	113.50
1	A	252	ILE	O-C-N	-5.42	117.33	123.18
1	A	241	ALA	CA-C-O	-5.42	115.11	120.80
1	A	13	VAL	N-CA-CB	5.41	116.77	110.65
1	A	102	THR	CA-C-N	5.40	131.85	121.54
1	A	102	THR	C-N-CA	5.40	131.85	121.54
1	A	50	LYS	CB-CA-C	-5.39	104.04	110.94
1	A	179	ARG	CB-CG-CD	5.38	123.68	111.30
1	A	12	LYS	CA-C-O	-5.37	114.83	120.63
1	A	195	LEU	N-CA-CB	5.37	119.18	110.05
1	A	80	HIS	CB-CG-CD2	-5.34	124.26	131.20
1	A	35	GLN	N-CA-C	-5.33	100.35	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ALA	O-C-N	-5.33	115.19	121.32
1	A	169	GLU	CA-C-O	-5.32	114.34	120.24
1	A	117	VAL	N-CA-C	5.30	120.36	109.34
1	A	193	MET	O-C-N	5.26	130.07	123.23
1	A	211	LEU	O-C-N	-5.24	117.19	123.06
1	A	51	LYS	O-C-N	5.23	129.44	122.95
1	A	196	PRO	N-CA-C	-5.23	104.32	110.70
1	A	292	PHE	O-C-N	5.23	130.06	122.43
1	A	87	PHE	CB-CA-C	-5.18	102.53	110.81
1	A	182	VAL	N-CA-C	-5.16	100.95	108.17
1	A	10	ALA	CB-CA-C	-5.15	102.10	110.85
1	A	4	GLN	CA-C-O	-5.13	113.36	118.34
1	A	101	MET	CG-SD-CE	-5.13	89.61	100.90
1	A	20	LYS	N-CA-C	-5.13	102.39	110.14
1	A	111	ALA	N-CA-C	5.13	121.14	109.81
1	A	174	HIS	CB-CA-C	-5.12	100.09	110.17
1	A	155	THR	CA-CB-OG1	-5.11	101.93	109.60
1	A	311	LYS	CB-CG-CD	5.11	123.05	111.30
1	A	189	ASP	N-CA-C	5.11	119.64	113.41
1	A	175	PRO	CB-CA-C	5.10	118.07	110.88
1	A	295	ASP	N-CA-C	-5.09	100.40	109.06
1	A	35	GLN	CB-CG-CD	-5.08	103.96	112.60
1	A	142	LEU	CA-C-O	5.08	125.23	119.18
1	A	309	ALA	N-CA-CB	-5.07	102.74	110.45
1	A	101	MET	N-CA-C	5.06	121.57	110.80
1	A	310	ILE	O-C-N	-5.04	117.58	122.97
1	A	160	THR	CA-CB-OG1	-5.04	102.05	109.60
1	A	185	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	A	18	HIS	CA-CB-CG	5.02	118.82	113.80
1	A	208	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	195	LEU	CA-C-O	-5.01	114.98	119.59

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	THR	Mainchain
1	A	111	ALA	Peptide
1	A	312	ALA	Peptide
1	A	6	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	2589	549	2497	82	0
2	A	20	1	11	0	0
3	A	29	58	0	0	0
All	All	2638	608	2508	82	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 16.

All (82) 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:101:MET:SD	1:A:118:TYR:HA	2.18	0.84
1:A:55:GLY:HA2	1:A:58:LYS:NZ	2.04	0.72
1:A:199:HIS:HB3	1:A:215:LEU:HD21	1.72	0.72
1:A:24:THR:HG21	1:A:316:VAL:HB	1.73	0.70
1:A:274:ARG:HG2	1:A:307:TYR:CE2	2.26	0.70
1:A:72:ARG:HG2	1:A:76:GLN:NE2	2.06	0.70
1:A:210:LYS:HA	1:A:247:GLU:O	1.92	0.70
1:A:87:PHE:HD2	1:A:122:MET:SD	2.18	0.67
1:A:274:ARG:NH2	1:A:310:ILE:HD11	2.09	0.67
1:A:260:LEU:HD21	1:A:268:ILE:HG13	1.75	0.66
1:A:87:PHE:CE2	1:A:122:MET:HA	2.31	0.65
1:A:92:LYS:HE2	1:A:93:SER:HA	1.79	0.64
1:A:93:SER:HB3	1:A:139:TYR:OH	1.96	0.64
1:A:55:GLY:HA2	1:A:58:LYS:HZ3	1.62	0.64
1:A:117:VAL:HG23	1:A:118:TYR:H	1.62	0.64
1:A:101:MET:HG3	1:A:121:GLU:HG2	1.80	0.63
1:A:114:PHE:O	1:A:118:TYR:HB3	1.98	0.63
1:A:12:LYS:O	1:A:16:GLU:HG2	1.99	0.61
1:A:87:PHE:HE2	1:A:122:MET:HA	1.66	0.60
1:A:37:ARG:HD3	1:A:250:GLU:OE1	2.03	0.59
1:A:190:VAL:HG23	1:A:191:PRO:HD3	1.83	0.59
1:A:13:VAL:HB	1:A:260:LEU:HD12	1.85	0.59
1:A:92:LYS:HE2	1:A:93:SER:CA	2.32	0.58
1:A:122:MET:O	1:A:125:PHE:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:MET:HE3	1:A:121:GLU:HB2	1.85	0.57
1:A:71:ILE:HD11	1:A:142:LEU:HD11	1.87	0.57
1:A:101:MET:SD	1:A:118:TYR:CA	2.92	0.57
1:A:71:ILE:O	1:A:75:LEU:HG	2.05	0.56
1:A:311:LYS:HD3	1:A:312:ALA:C	2.30	0.56
1:A:204:PHE:CD2	1:A:211:LEU:HD21	2.40	0.56
1:A:138:LYS:NZ	1:A:139:TYR:CE2	2.74	0.56
1:A:271:GLN:O	1:A:274:ARG:HB2	2.06	0.56
1:A:100:ASP:HB3	1:A:114:PHE:CZ	2.41	0.55
1:A:40:LEU:HB3	1:A:238:HIS:HE1	1.73	0.53
1:A:87:PHE:HE2	1:A:122:MET:CA	2.21	0.53
1:A:87:PHE:CD2	1:A:122:MET:SD	3.01	0.52
1:A:116:ALA:O	1:A:118:TYR:N	2.42	0.52
1:A:101:MET:HE1	1:A:117:VAL:HB	1.90	0.52
1:A:125:PHE:O	1:A:129:VAL:HG23	2.10	0.52
1:A:214:GLN:HG3	1:A:252:ILE:HB	1.91	0.52
1:A:229:ASN:HD22	1:A:229:ASN:N	2.08	0.52
1:A:24:THR:HG21	1:A:316:VAL:CB	2.39	0.52
1:A:32:PHE:HA	1:A:256:GLY:O	2.11	0.51
1:A:46:LEU:HD11	1:A:54:PHE:HB2	1.94	0.50
1:A:107:ARG:HB2	1:A:112:PRO:HD3	1.93	0.49
1:A:110:LYS:O	1:A:111:ALA:HB3	2.13	0.49
1:A:72:ARG:HG2	1:A:76:GLN:HE22	1.78	0.48
1:A:131:HIS:O	1:A:133:ASP:N	2.47	0.48
1:A:204:PHE:HB3	1:A:211:LEU:HD11	1.95	0.47
1:A:265:LEU:O	1:A:269:LYS:HG3	2.15	0.47
1:A:224:LEU:HD12	1:A:264:HIS:CE1	2.50	0.46
1:A:88:GLU:O	1:A:91:VAL:HG12	2.15	0.46
1:A:87:PHE:CE1	1:A:91:VAL:HB	2.49	0.46
1:A:103:ASP:O	1:A:104:PHE:C	2.59	0.45
1:A:198:CYS:HA	1:A:218:ARG:HH11	1.81	0.45
1:A:91:VAL:HG23	1:A:96:TYR:CE1	2.51	0.45
1:A:56:LEU:HD23	1:A:81:ILE:HD11	1.99	0.45
1:A:93:SER:O	1:A:95:GLU:N	2.50	0.45
1:A:54:PHE:HZ	1:A:282:LEU:HD11	1.83	0.44
1:A:20:LYS:O	1:A:28:THR:OG1	2.36	0.44
1:A:62:LEU:HD12	1:A:296:MET:HG3	1.99	0.44
1:A:36:MET:HE3	1:A:255:PHE:HZ	1.83	0.44
1:A:190:VAL:HG12	1:A:196:PRO:HB3	2.00	0.44
1:A:100:ASP:HB3	1:A:114:PHE:HZ	1.80	0.44
1:A:198:CYS:O	1:A:217:GLN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:NH1	1:A:114:PHE:CZ	2.86	0.43
1:A:184:ALA:O	1:A:197:PRO:HG3	2.18	0.43
1:A:207:ASN:OD1	1:A:208:ASP:N	2.52	0.43
1:A:95:GLU:O	1:A:97:HIS:N	2.52	0.42
1:A:37:ARG:HH11	1:A:250:GLU:CD	2.27	0.42
1:A:91:VAL:HG22	1:A:91:VAL:O	2.19	0.42
1:A:87:PHE:CD2	1:A:122:MET:HA	2.54	0.42
1:A:277:ARG:NH1	1:A:307:TYR:CE1	2.87	0.42
1:A:54:PHE:O	1:A:58:LYS:HG3	2.21	0.41
1:A:80:HIS:HB3	1:A:83:ASP:HB2	2.02	0.41
1:A:171:ILE:O	1:A:175:PRO:HB3	2.20	0.41
1:A:72:ARG:HG2	1:A:76:GLN:HE21	1.81	0.41
1:A:204:PHE:CZ	1:A:240:VAL:HG21	2.55	0.41
1:A:283:GLN:NE2	1:A:300:LYS:NZ	2.69	0.41
1:A:83:ASP:OD2	1:A:122:MET:SD	2.79	0.41
1:A:122:MET:HE2	1:A:122:MET:HB2	1.88	0.41
1:A:261:TYR:HB2	1:A:264:HIS:ND1	2.35	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	314/316 (99%)	253 (81%)	43 (14%)	18 (6%)	1 1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	99	PRO
1	A	101	MET
1	A	105	GLY

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Mol	Chain	Res	Type
1	A	108	SER
1	A	111	ALA
1	A	117	VAL
1	A	296	MET
1	A	308	PRO
1	A	103	ASP
1	A	112	PRO
1	A	116	ALA
1	A	104	PHE
1	A	152	ALA
1	A	194	ALA
1	A	242	HIS
1	A	256	GLY
1	A	276	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	277/277 (100%)	222 (80%)	55 (20%)	1 2

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	7	LEU
1	A	9	LEU
1	A	16	GLU
1	A	18	HIS
1	A	20	LYS
1	A	26	THR
1	A	45	PRO
1	A	46	LEU
1	A	50	LYS
1	A	52	VAL
1	A	56	LEU

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Mol	Chain	Res	Type
1	A	71	ILE
1	A	83	ASP
1	A	89	LYS
1	A	92	LYS
1	A	93	SER
1	A	100	ASP
1	A	109	GLN
1	A	113	GLU
1	A	127	ASP
1	A	138	LYS
1	A	144	LEU
1	A	145	VAL
1	A	149	GLN
1	A	160	THR
1	A	174	HIS
1	A	175	PRO
1	A	180	LEU
1	A	187	PRO
1	A	193	MET
1	A	197	PRO
1	A	201	LEU
1	A	206	VAL
1	A	215	LEU
1	A	222	ILE
1	A	227	PRO
1	A	229	ASN
1	A	239	LEU
1	A	243	GLU
1	A	246	LEU
1	A	260	LEU
1	A	263	ASN
1	A	265	LEU
1	A	268	ILE
1	A	272	LEU
1	A	275	THR
1	A	276	PRO
1	A	277	ARG
1	A	281	THR
1	A	282	LEU
1	A	285	ASN
1	A	291	ILE
1	A	303	ASN

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Mol	Chain	Res	Type
1	A	316	VAL

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	238	HIS
1	A	271	GLN
1	A	283	GLN
1	A	289	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	UMP	A	317	-	21,21,21	1.44	3 (14%)	30,31,31	1.81	8 (26%)

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	317	-	-	2/10/22/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	UMP	C6-C5	3.45	1.43	1.35
2	A	317	UMP	C2-N1	3.16	1.43	1.38
2	A	317	UMP	P-OP3	-2.04	1.47	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	UMP	O4'-C1'-N1	5.90	118.34	107.86
2	A	317	UMP	C1'-N1-C6	-3.04	115.56	121.53
2	A	317	UMP	OP2-P-O5'	-2.94	99.00	106.67
2	A	317	UMP	O2-C2-N3	-2.67	116.56	121.49
2	A	317	UMP	O2-C2-N1	2.51	126.06	122.80
2	A	317	UMP	O4'-C1'-C2'	-2.49	101.60	106.25
2	A	317	UMP	C1'-N1-C2	2.38	122.31	117.66
2	A	317	UMP	O5'-P-OP1	2.22	112.45	106.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

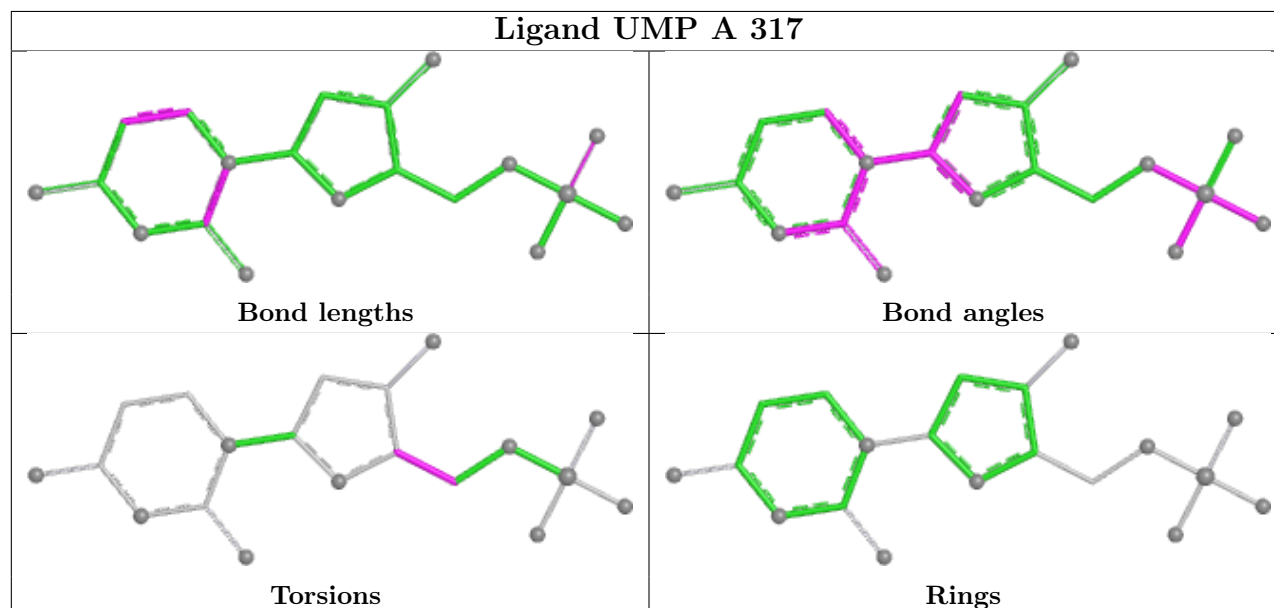
Mol	Chain	Res	Type	Atoms
2	A	317	UMP	O4'-C4'-C5'-O5'
2	A	317	UMP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	316/316 (100%)	-0.41	3 (0%) 81 78	11, 20, 34, 39	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	ALA	2.9
1	A	101	MET	2.2
1	A	93	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

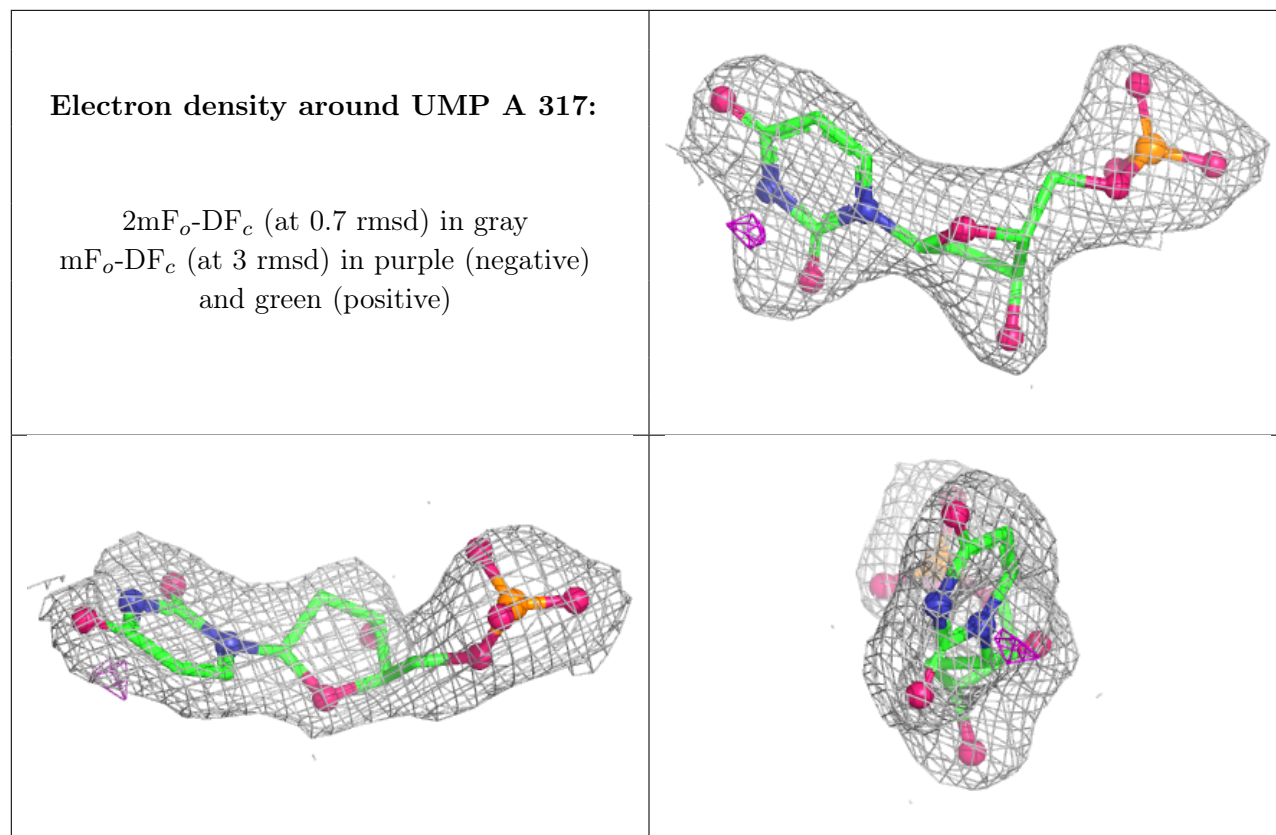
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UMP	A	317	20/20	0.96	0.06	15,28,32,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.