



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:23 AM UTC

PDB ID : 1VZB / pdb_00001vzb
Title : L. CASEI THYMIDYLATE SYNTHASE MUTANT E60Q BINARY COMPLEX WITH 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

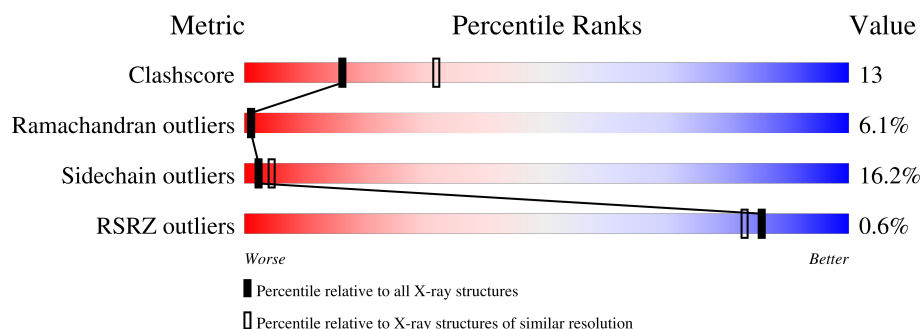
1 Overall quality at a glance

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	36% 39% 19% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3275 atoms, of which 621 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.

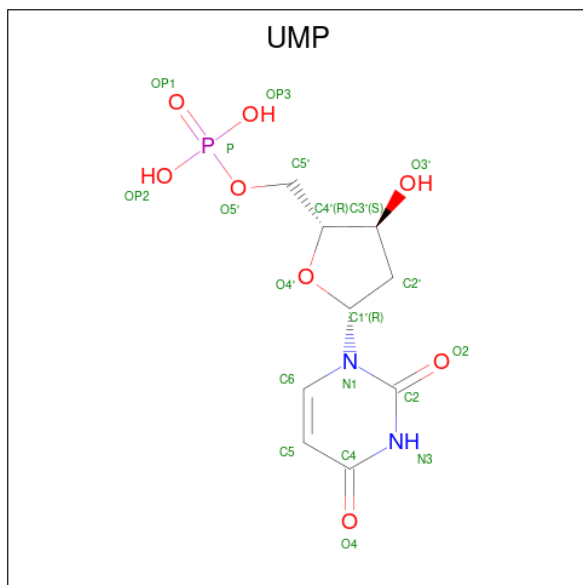
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	316	3122	1677	532	439	466	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	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

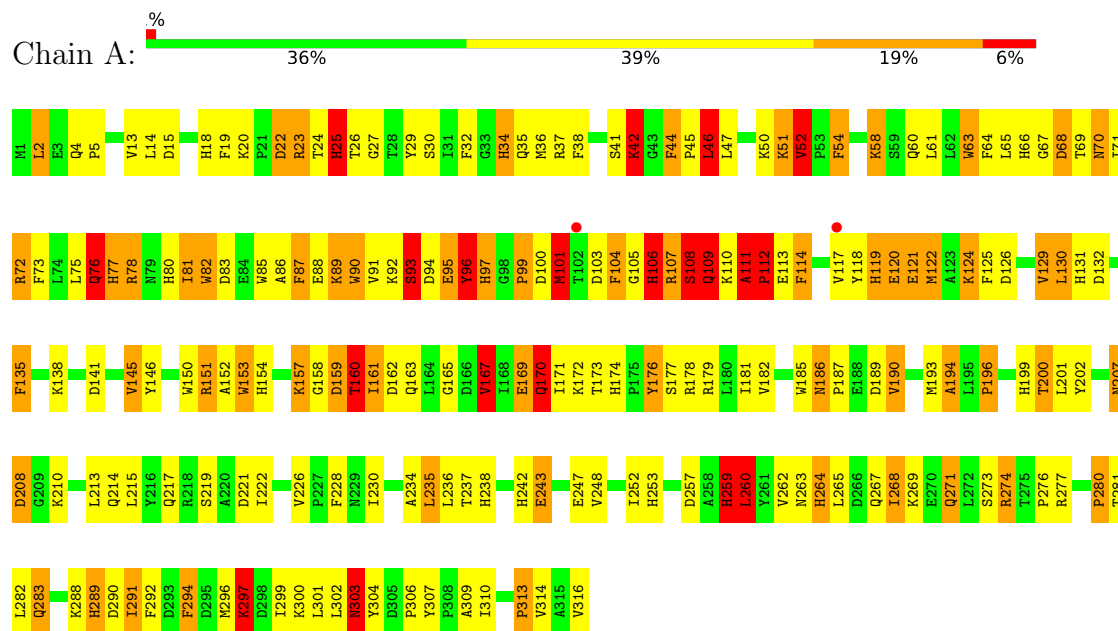
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	44	Total	H	O	0	0
			132	88	44		

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 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	78.30Å 78.30Å 242.30Å 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) 70.9 (15.00-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.215 , (Not available) 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 44.4	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	0.95	EDS
Total number of atoms	3275	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.66	42/2674 (1.6%)	2.58	210/3634 (5.8%)

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	4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	HIS	CG-ND1	-8.05	1.29	1.38
1	A	281	THR	CA-CB	-7.47	1.41	1.53
1	A	219	SER	CA-CB	-7.47	1.40	1.53
1	A	253	HIS	CD2-NE2	-7.37	1.29	1.37
1	A	52	VAL	CA-CB	-7.27	1.49	1.54
1	A	77	HIS	CG-ND1	-7.18	1.30	1.38
1	A	80	HIS	CD2-NE2	-6.72	1.30	1.37
1	A	81	ILE	CA-CB	6.71	1.63	1.54
1	A	182	VAL	CA-CB	-6.65	1.46	1.54
1	A	63	TRP	CA-CB	-6.41	1.43	1.53
1	A	13	VAL	CA-CB	-6.38	1.45	1.54
1	A	248	VAL	CA-CB	-6.38	1.46	1.54
1	A	259	HIS	CG-ND1	-6.28	1.31	1.38
1	A	199	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	242	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	131	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	82	TRP	NE1-CE2	-6.06	1.30	1.37
1	A	176	TYR	CA-C	-6.03	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	HIS	CG-ND1	-5.93	1.31	1.38
1	A	2	LEU	CA-C	-5.84	1.45	1.52
1	A	77	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	106	HIS	CG-ND1	-5.74	1.31	1.38
1	A	162	ASP	CA-C	-5.74	1.47	1.53
1	A	259	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	75	LEU	CA-CB	-5.63	1.44	1.53
1	A	238	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	66	HIS	CD2-NE2	-5.47	1.31	1.37
1	A	264	HIS	CG-ND1	-5.46	1.32	1.38
1	A	131	HIS	CG-ND1	-5.34	1.32	1.38
1	A	264	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	66	HIS	CG-ND1	-5.26	1.32	1.38
1	A	95	GLU	CA-CB	5.25	1.62	1.53
1	A	106	HIS	CG-CD2	5.16	1.41	1.35
1	A	80	HIS	CG-ND1	-5.15	1.32	1.38
1	A	119	HIS	CD2-NE2	-5.15	1.32	1.37
1	A	154	HIS	CB-CG	5.13	1.57	1.50
1	A	119	HIS	CG-ND1	-5.12	1.32	1.38
1	A	280	PRO	CA-CB	-5.12	1.46	1.53
1	A	34	HIS	CD2-NE2	-5.12	1.32	1.37
1	A	259	HIS	CA-CB	-5.10	1.44	1.53
1	A	34	HIS	CG-ND1	-5.04	1.32	1.38
1	A	314	VAL	CA-C	5.01	1.59	1.52

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ASP	CA-CB-CG	16.41	129.01	112.60
1	A	113	GLU	N-CA-C	-12.87	96.75	111.03
1	A	207	ASN	CA-CB-CG	12.15	124.75	112.60
1	A	52	VAL	CA-C-O	11.94	126.15	119.94
1	A	124	LYS	N-CA-C	-10.82	99.17	110.97
1	A	68	ASP	CA-CB-CG	10.52	123.12	112.60
1	A	242	HIS	CA-CB-CG	10.39	124.19	113.80
1	A	170	GLN	OE1-CD-NE2	-10.23	112.36	122.60
1	A	303	ASN	OD1-CG-ND2	-10.19	112.42	122.60
1	A	242	HIS	N-CA-C	-10.11	100.27	111.28
1	A	90	TRP	N-CA-C	-10.02	96.23	111.56
1	A	23	ARG	CA-C-N	-9.56	111.06	122.44
1	A	23	ARG	C-N-CA	-9.56	111.06	122.44
1	A	95	GLU	N-CA-C	-9.38	98.54	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASP	CA-CB-CG	9.31	121.91	112.60
1	A	161	ILE	N-CA-CB	-9.17	98.78	111.25
1	A	173	THR	O-C-N	-9.13	111.12	122.35
1	A	95	GLU	CB-CG-CD	9.10	128.06	112.60
1	A	176	TYR	N-CA-C	-8.99	96.34	109.11
1	A	119	HIS	ND1-CG-CD2	8.95	115.05	106.10
1	A	268	ILE	N-CA-C	-8.84	101.61	110.62
1	A	273	SER	CA-C-O	8.83	128.76	119.05
1	A	200	THR	N-CA-C	8.62	121.45	111.11
1	A	207	ASN	OD1-CG-ND2	-8.61	113.99	122.60
1	A	108	SER	N-CA-C	-8.60	92.49	110.80
1	A	314	VAL	N-CA-C	8.44	126.90	109.34
1	A	100	ASP	CA-CB-CG	8.41	121.01	112.60
1	A	264	HIS	CA-CB-CG	8.39	122.19	113.80
1	A	112	PRO	N-CA-C	8.36	129.69	112.47
1	A	303	ASN	CB-CG-ND2	8.25	128.77	116.40
1	A	299	ILE	O-C-N	-7.99	115.78	122.97
1	A	257	ASP	O-C-N	-7.99	112.90	122.96
1	A	189	ASP	N-CA-C	-7.96	103.57	113.28
1	A	159	ASP	CA-CB-CG	7.85	120.45	112.60
1	A	87	PHE	CA-CB-CG	7.74	121.54	113.80
1	A	13	VAL	CA-CB-CG2	-7.72	97.27	110.40
1	A	96	TYR	CA-C-N	-7.70	111.18	122.65
1	A	96	TYR	C-N-CA	-7.70	111.18	122.65
1	A	29	TYR	N-CA-C	-7.61	96.49	108.90
1	A	111	ALA	CA-C-N	7.60	129.34	119.84
1	A	111	ALA	C-N-CA	7.60	129.34	119.84
1	A	80	HIS	ND1-CG-CD2	7.59	113.69	106.10
1	A	146	TYR	CA-C-O	-7.59	112.42	120.92
1	A	94	ASP	N-CA-C	7.51	122.09	113.15
1	A	119	HIS	N-CA-C	7.46	119.05	111.07
1	A	135	PHE	CA-CB-CG	7.45	121.25	113.80
1	A	158	GLY	CA-C-N	7.43	135.72	121.54
1	A	158	GLY	C-N-CA	7.43	135.72	121.54
1	A	66	HIS	ND1-CG-CD2	7.39	113.49	106.10
1	A	291	ILE	CA-CB-CG2	-7.35	98.00	110.50
1	A	37	ARG	N-CA-CB	-7.33	99.05	110.57
1	A	289	HIS	CA-C-N	-7.25	111.97	122.19
1	A	289	HIS	C-N-CA	-7.25	111.97	122.19
1	A	112	PRO	CA-N-CD	-7.23	101.88	112.00
1	A	61	LEU	CA-C-O	-7.20	113.48	120.90
1	A	182	VAL	N-CA-C	-7.20	97.75	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	MET	N-CA-C	7.16	126.04	110.80
1	A	199	HIS	CA-C-N	7.12	130.15	120.54
1	A	199	HIS	C-N-CA	7.12	130.15	120.54
1	A	289	HIS	ND1-CG-CD2	7.08	113.18	106.10
1	A	170	GLN	N-CA-C	-7.08	104.52	113.01
1	A	70	ASN	CA-CB-CG	-7.06	105.54	112.60
1	A	18	HIS	CA-CB-CG	7.06	120.86	113.80
1	A	274	ARG	N-CA-C	-6.96	99.97	110.28
1	A	196	PRO	N-CA-C	-6.93	102.25	110.70
1	A	109	GLN	N-CA-C	6.91	125.53	110.80
1	A	76	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	A	97	HIS	N-CA-C	-6.90	98.45	109.76
1	A	288	LYS	CA-CB-CG	-6.85	100.41	114.10
1	A	25	HIS	ND1-CG-CD2	6.82	112.92	106.10
1	A	25	HIS	CB-CG-CD2	-6.81	122.35	131.20
1	A	165	GLY	N-CA-C	-6.76	104.12	112.77
1	A	119	HIS	CB-CA-C	-6.75	100.27	110.88
1	A	36	MET	CA-CB-CG	6.75	127.60	114.10
1	A	228	PHE	CA-CB-CG	6.74	120.54	113.80
1	A	18	HIS	ND1-CG-CD2	6.72	112.82	106.10
1	A	77	HIS	ND1-CG-CD2	6.69	112.79	106.10
1	A	72	ARG	NE-CZ-NH2	-6.63	113.24	119.20
1	A	283	GLN	OE1-CD-NE2	-6.61	115.99	122.60
1	A	50	LYS	N-CA-C	-6.56	98.55	108.46
1	A	131	HIS	ND1-CG-CD2	6.54	112.64	106.10
1	A	259	HIS	N-CA-C	6.53	118.99	109.07
1	A	271	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	122	MET	N-CA-C	-6.49	103.90	110.97
1	A	119	HIS	CG-CD2-NE2	-6.48	100.72	107.20
1	A	114	PHE	O-C-N	-6.47	113.53	122.46
1	A	154	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	314	VAL	N-CA-CB	-6.43	100.61	111.23
1	A	151	ARG	CA-CB-CG	-6.41	101.27	114.10
1	A	158	GLY	O-C-N	6.40	131.02	122.70
1	A	253	HIS	ND1-CG-CD2	6.34	112.44	106.10
1	A	210	LYS	O-C-N	-6.32	115.92	123.31
1	A	243	GLU	CA-CB-CG	-6.31	101.49	114.10
1	A	163	GLN	CG-CD-NE2	6.31	125.86	116.40
1	A	97	HIS	ND1-CG-CD2	6.30	112.40	106.10
1	A	42	LYS	CA-CB-CG	6.25	126.61	114.10
1	A	63	TRP	N-CA-C	-6.25	104.09	111.03
1	A	259	HIS	ND1-CG-CD2	6.25	112.35	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	HIS	O-C-N	6.23	128.49	122.07
1	A	235	LEU	N-CA-C	-6.22	104.19	110.97
1	A	121	GLU	CA-C-O	6.21	127.88	120.92
1	A	171	ILE	CB-CA-C	-6.18	102.09	112.16
1	A	138	LYS	CB-CG-CD	6.16	125.47	111.30
1	A	66	HIS	N-CA-C	-6.16	105.41	113.17
1	A	199	HIS	ND1-CG-CD2	6.14	112.24	106.10
1	A	51	LYS	CA-C-O	-6.13	113.76	120.81
1	A	2	LEU	CB-CA-C	-6.12	101.54	110.96
1	A	310	ILE	N-CA-C	-6.11	99.36	108.46
1	A	178	ARG	CA-CB-CG	6.07	126.25	114.10
1	A	248	VAL	N-CA-CB	-6.05	97.52	111.81
1	A	50	LYS	CA-CB-CG	6.02	126.15	114.10
1	A	234	ALA	N-CA-C	-6.01	105.44	112.89
1	A	161	ILE	N-CA-C	6.01	116.58	108.17
1	A	208	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	46	LEU	O-C-N	-5.99	115.94	123.01
1	A	111	ALA	N-CA-C	5.97	123.01	109.81
1	A	78	ARG	CB-CG-CD	5.96	125.00	111.30
1	A	36	MET	CA-C-N	5.95	131.21	123.00
1	A	36	MET	C-N-CA	5.95	131.21	123.00
1	A	67	GLY	N-CA-C	-5.94	105.33	115.08
1	A	25	HIS	CA-CB-CG	5.94	119.74	113.80
1	A	193	MET	CA-CB-CG	5.93	125.97	114.10
1	A	13	VAL	CA-CB-CG1	5.92	120.47	110.40
1	A	186	ASN	CA-C-O	5.91	124.33	119.36
1	A	222	ILE	CB-CA-C	-5.91	103.43	112.05
1	A	97	HIS	CA-CB-CG	5.89	119.69	113.80
1	A	167	VAL	CG1-CB-CG2	-5.87	97.89	110.80
1	A	238	HIS	CA-C-O	-5.85	114.87	120.90
1	A	221	ASP	CA-C-O	-5.85	114.03	120.70
1	A	20	LYS	O-C-N	-5.83	116.20	121.39
1	A	86	ALA	CA-C-O	-5.81	113.80	120.24
1	A	129	VAL	N-CA-C	-5.80	106.06	111.45
1	A	167	VAL	CA-C-O	-5.79	115.03	121.17
1	A	202	TYR	CA-C-O	-5.78	114.87	121.58
1	A	283	GLN	CA-CB-CG	5.77	125.65	114.10
1	A	217	GLN	O-C-N	-5.76	116.59	123.27
1	A	120	GLU	N-CA-C	-5.75	104.38	111.40
1	A	26	THR	N-CA-C	-5.73	98.59	110.80
1	A	114	PHE	N-CA-C	5.73	119.89	113.01
1	A	294	PHE	O-C-N	5.72	129.31	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	A	93	SER	N-CA-C	5.69	118.34	109.52
1	A	297	LYS	CA-C-O	5.66	126.13	119.28
1	A	170	GLN	CG-CD-NE2	5.66	124.88	116.40
1	A	238	HIS	ND1-CG-CD2	5.65	111.75	106.10
1	A	290	ASP	N-CA-C	-5.65	100.09	109.46
1	A	159	ASP	N-CA-CB	-5.64	100.95	110.49
1	A	174	HIS	ND1-CG-CD2	5.63	111.73	106.10
1	A	177	SER	CA-C-O	5.62	126.20	120.24
1	A	257	ASP	CA-C-O	-5.62	114.06	120.58
1	A	41	SER	N-CA-C	-5.57	101.27	109.62
1	A	154	HIS	ND1-CG-CD2	5.55	111.65	106.10
1	A	90	TRP	CB-CG-CD1	-5.52	118.62	126.90
1	A	163	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	A	77	HIS	CG-CD2-NE2	-5.50	101.70	107.20
1	A	248	VAL	CB-CA-C	5.48	119.77	110.95
1	A	242	HIS	ND1-CG-CD2	5.46	111.56	106.10
1	A	4	GLN	CA-C-O	-5.45	112.69	120.16
1	A	181	ILE	O-C-N	-5.45	117.17	123.00
1	A	90	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	A	160	THR	N-CA-CB	-5.44	101.30	110.49
1	A	78	ARG	CA-CB-CG	-5.43	103.23	114.10
1	A	77	HIS	N-CA-C	-5.43	103.83	110.61
1	A	4	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	20	LYS	CA-C-O	5.42	125.22	119.69
1	A	150	TRP	CG-CD1-NE1	-5.41	103.17	110.20
1	A	161	ILE	CB-CA-C	5.40	118.87	110.83
1	A	157	LYS	N-CA-CB	-5.38	102.53	110.49
1	A	260	LEU	N-CA-C	-5.38	99.64	108.41
1	A	68	ASP	CA-C-O	5.37	127.62	121.28
1	A	170	GLN	CB-CG-CD	5.36	121.71	112.60
1	A	37	ARG	O-C-N	-5.35	116.97	123.29
1	A	153	TRP	O-C-N	-5.35	116.78	123.04
1	A	34	HIS	ND1-CG-CD2	5.32	111.42	106.10
1	A	78	ARG	CA-C-N	-5.26	115.36	123.14
1	A	78	ARG	C-N-CA	-5.26	115.36	123.14
1	A	107	ARG	CA-C-O	5.26	126.09	120.20
1	A	190	VAL	N-CA-C	5.26	120.24	108.88
1	A	45	PRO	CA-C-N	-5.25	113.92	121.42
1	A	45	PRO	C-N-CA	-5.25	113.92	121.42
1	A	58	LYS	CB-CG-CD	-5.25	99.23	111.30
1	A	200	THR	N-CA-CB	-5.24	102.13	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	CA-C-O	-5.24	114.97	120.63
1	A	36	MET	N-CA-C	-5.23	100.17	109.06
1	A	90	TRP	CG-CD2-CE3	5.23	139.13	133.90
1	A	80	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	A	277	ARG	CB-CG-CD	-5.20	99.35	111.30
1	A	35	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	35	GLN	N-CA-CB	5.17	119.92	111.08
1	A	304	TYR	CA-C-O	5.16	126.43	120.60
1	A	292	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	44	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	90	TRP	CD1-CG-CD2	5.14	114.53	106.30
1	A	262	VAL	O-C-N	-5.13	117.07	122.20
1	A	306	PRO	O-C-N	5.12	129.39	123.14
1	A	235	LEU	CB-CA-C	-5.11	103.09	110.96
1	A	310	ILE	O-C-N	5.11	128.57	123.10
1	A	141	ASP	O-C-N	5.11	129.67	122.77
1	A	90	TRP	CG-CD1-NE1	-5.10	103.57	110.20
1	A	106	HIS	CA-C-O	-5.09	113.54	119.14
1	A	238	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	2	LEU	N-CA-CB	5.08	117.33	109.91
1	A	22	ASP	N-CA-C	5.08	115.04	107.88
1	A	186	ASN	CB-CA-C	-5.07	105.15	110.17
1	A	64	PHE	N-CA-C	5.05	119.70	111.37
1	A	32	PHE	N-CA-C	-5.04	100.95	109.07
1	A	242	HIS	CA-C-O	-5.03	115.22	120.55
1	A	38	PHE	O-C-N	-5.03	116.48	123.12
1	A	34	HIS	CA-C-O	-5.01	113.34	120.51
1	A	190	VAL	CA-CB-CG2	-5.01	101.88	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	176	TYR	Sidechain
1	A	25	HIS	Sidechain
1	A	259	HIS	Sidechain
1	A	34	HIS	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	2590	532	2501	67	1
2	A	20	1	11	0	0
3	A	44	88	0	0	0
All	All	2654	621	2512	67	1

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 13.

All (67) 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:44:PHE:HB3	1:A:280:PRO:HG2	1.70	0.73
1:A:153:TRP:HB3	1:A:161:ILE:HG22	1.70	0.73
1:A:194:ALA:O	1:A:196:PRO:HD3	1.88	0.72
1:A:153:TRP:HB3	1:A:161:ILE:CG2	2.23	0.68
1:A:104:PHE:HD1	1:A:105:GLY:H	1.46	0.64
1:A:260:LEU:HD12	1:A:265:LEU:HD23	1.80	0.64
1:A:106:HIS:HA	1:A:109:GLN:HB2	1.80	0.63
1:A:108:SER:O	1:A:110:LYS:N	2.33	0.62
1:A:274:ARG:NH1	1:A:307:TYR:HB3	2.16	0.61
1:A:226:VAL:O	1:A:230:ILE:HG13	2.02	0.59
1:A:71:ILE:HG22	1:A:129:VAL:HG11	1.86	0.57
1:A:152:ALA:HB1	1:A:160:THR:HG23	1.87	0.55
1:A:106:HIS:HD1	1:A:316:VAL:C	2.13	0.55
1:A:111:ALA:N	1:A:112:PRO:HD2	2.22	0.55
1:A:121:GLU:O	1:A:124:LYS:HB3	2.08	0.54
1:A:213:LEU:HD13	1:A:237:THR:OG1	2.07	0.54
1:A:19:PHE:CZ	1:A:27:GLY:HA3	2.43	0.53
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.73	0.53
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.44	0.52
1:A:132:ASP:HB3	1:A:135:PHE:HB3	1.92	0.52
1:A:169:GLU:HG2	1:A:172:LYS:HE3	1.91	0.52
1:A:167:VAL:HA	1:A:170:GLN:HE21	1.76	0.51
1:A:2:LEU:O	1:A:5:PRO:HD2	2.10	0.51
1:A:71:ILE:CG2	1:A:129:VAL:HG11	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ASN:N	1:A:303:ASN:OD1	2.43	0.49
1:A:72:ARG:O	1:A:76:GLN:HG3	2.13	0.49
1:A:126:ASP:O	1:A:130:LEU:HD22	2.13	0.49
1:A:69:THR:HG22	1:A:145:VAL:HG13	1.94	0.49
1:A:85:TRP:O	1:A:88:GLU:HB3	2.13	0.49
1:A:263:ASN:O	1:A:264:HIS:HD2	1.95	0.48
1:A:291:ILE:HA	1:A:294:PHE:CD1	2.49	0.48
1:A:89:LYS:O	1:A:93:SER:HB2	2.14	0.47
1:A:51:LYS:H	1:A:309:ALA:HA	1.80	0.47
1:A:265:LEU:O	1:A:268:ILE:HG22	2.14	0.47
1:A:120:GLU:O	1:A:124:LYS:N	2.45	0.47
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.64	0.47
1:A:104:PHE:O	1:A:106:HIS:N	2.48	0.46
1:A:87:PHE:CD2	1:A:122:MET:SD	3.09	0.45
1:A:301:LEU:C	1:A:302:LEU:HD12	2.42	0.45
1:A:93:SER:O	1:A:96:TYR:HB3	2.16	0.45
1:A:297:LYS:HD3	1:A:297:LYS:H	1.82	0.45
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.32	0.44
1:A:104:PHE:O	1:A:107:ARG:N	2.49	0.44
1:A:243:GLU:HG3	1:A:289:HIS:O	2.18	0.44
1:A:30:SER:HB3	1:A:259:HIS:HB3	1.99	0.44
1:A:267:GLN:OE1	1:A:267:GLN:N	2.51	0.44
1:A:95:GLU:O	1:A:97:HIS:N	2.49	0.44
1:A:90:TRP:O	1:A:93:SER:N	2.51	0.43
1:A:70:ASN:ND2	1:A:72:ARG:H	2.17	0.43
1:A:124:LYS:HE3	1:A:124:LYS:HB2	1.83	0.43
1:A:87:PHE:HZ	1:A:121:GLU:HB3	1.83	0.42
1:A:73:PHE:CE1	1:A:77:HIS:HE1	2.38	0.42
1:A:186:ASN:HA	1:A:187:PRO:HD3	1.79	0.42
1:A:271:GLN:HA	1:A:274:ARG:HD2	2.01	0.42
1:A:58:LYS:HG3	1:A:296:MET:HE1	2.01	0.42
1:A:72:ARG:HD3	1:A:76:GLN:HE21	1.85	0.42
1:A:214:GLN:HG3	1:A:252:ILE:HB	2.00	0.42
1:A:46:LEU:HD22	1:A:52:VAL:HB	2.02	0.41
1:A:72:ARG:HD3	1:A:76:GLN:NE2	2.35	0.41
1:A:82:TRP:O	1:A:83:ASP:C	2.63	0.41
1:A:87:PHE:HB2	1:A:122:MET:SD	2.61	0.41
1:A:107:ARG:O	1:A:111:ALA:HB3	2.19	0.41
1:A:122:MET:O	1:A:125:PHE:HB3	2.21	0.41
1:A:268:ILE:HA	1:A:268:ILE:HD12	1.78	0.40
1:A:101:MET:HE2	1:A:114:PHE:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TRP:O	1:A:187:PRO:HD3	2.22	0.40
1:A:260:LEU:HD12	1:A:265:LEU:CD2	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HH11	1:A:179:ARG:HH21[11_554]	1.12	0.48

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	314/316 (99%)	246 (78%)	49 (16%)	19 (6%)	1 1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	101	MET
1	A	104	PHE
1	A	109	GLN
1	A	112	PRO
1	A	159	ASP
1	A	194	ALA
1	A	96	TYR
1	A	103	ASP
1	A	111	ALA
1	A	81	ILE
1	A	42	LYS
1	A	76	GLN
1	A	118	TYR

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Mol	Chain	Res	Type
1	A	313	PRO
1	A	54	PHE
1	A	99	PRO
1	A	276	PRO
1	A	117	VAL

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%)	232 (84%)	45 (16%)	2 4

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	24	THR
1	A	42	LYS
1	A	46	LEU
1	A	47	LEU
1	A	52	VAL
1	A	54	PHE
1	A	60	GLN
1	A	65	LEU
1	A	78	ARG
1	A	89	LYS
1	A	91	VAL
1	A	92	LYS
1	A	93	SER
1	A	99	PRO
1	A	101	MET
1	A	106	HIS
1	A	108	SER
1	A	109	GLN
1	A	112	PRO
1	A	119	HIS

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Mol	Chain	Res	Type
1	A	130	LEU
1	A	145	VAL
1	A	157	LYS
1	A	160	THR
1	A	167	VAL
1	A	169	GLU
1	A	170	GLN
1	A	190	VAL
1	A	200	THR
1	A	201	LEU
1	A	207	ASN
1	A	208	ASP
1	A	215	LEU
1	A	235	LEU
1	A	236	LEU
1	A	247	GLU
1	A	260	LEU
1	A	269	LYS
1	A	282	LEU
1	A	283	GLN
1	A	297	LYS
1	A	300	LYS
1	A	303	ASN
1	A	313	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	76	GLN
1	A	119	HIS
1	A	170	GLN

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 [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	1.45	3 (14%)	30,31,31	2.17	7 (23%)

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-N1	-3.55	1.29	1.38
2	A	317	UMP	C5'-C4'	2.52	1.59	1.51
2	A	317	UMP	C6-C5	2.01	1.39	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	UMP	O4'-C1'-N1	6.25	118.95	107.86
2	A	317	UMP	C1'-N1-C6	-4.24	113.19	121.53
2	A	317	UMP	O4-C4-N3	4.00	125.08	119.27
2	A	317	UMP	O4'-C1'-C2'	-3.96	98.84	106.25
2	A	317	UMP	C2'-C3'-C4'	-3.37	95.98	102.80
2	A	317	UMP	C1'-N1-C2	3.02	123.56	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	UMP	O4-C4-C5	-2.28	121.24	125.16

There are no chirality outliers.

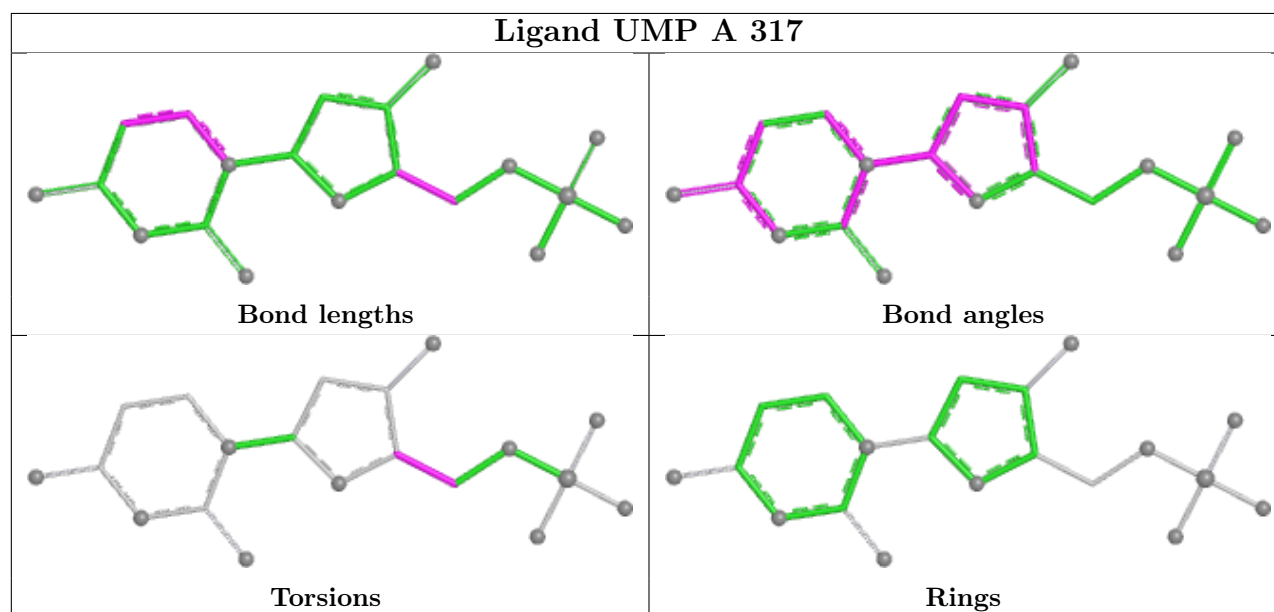
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	317	UMP	C3'-C4'-C5'-O5'
2	A	317	UMP	O4'-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%)	-0.05	2 (0%) 85 83	11, 21, 34, 40	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	VAL	2.6
1	A	102	THR	2.1

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](#)

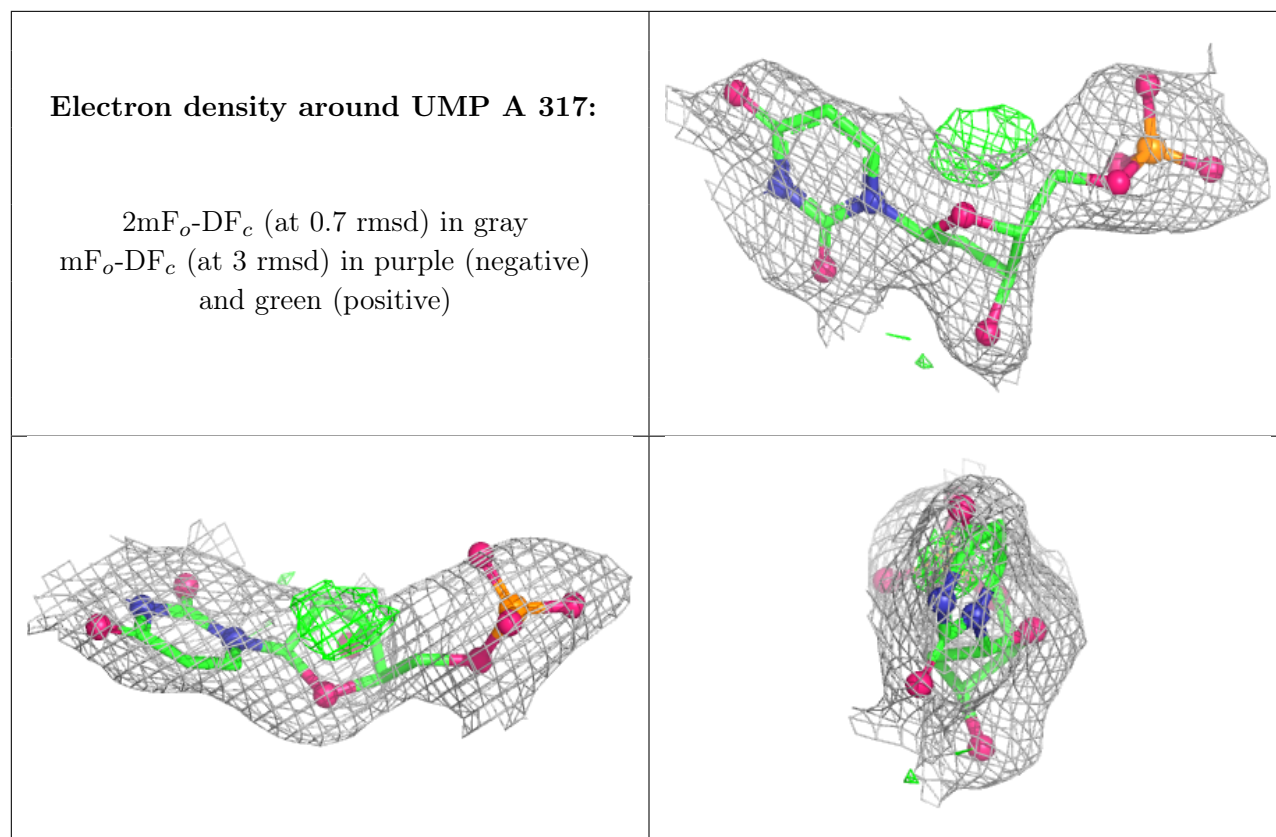
There are no oligosaccharides in this entry.

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	0.07	15,26,28,28	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.