



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:22 pm BST

PDB ID : 1LCA  
Title : LACTOBACILLUS CASEI THYMIDYLATE SYNTHASE TERNARY COM-  
PLEX WITH DUMP AND CB3717  
Authors : Birdsall, D.L.; Finer-Moore, J.; Stroud, R.M.  
Deposited on : 1995-06-22  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

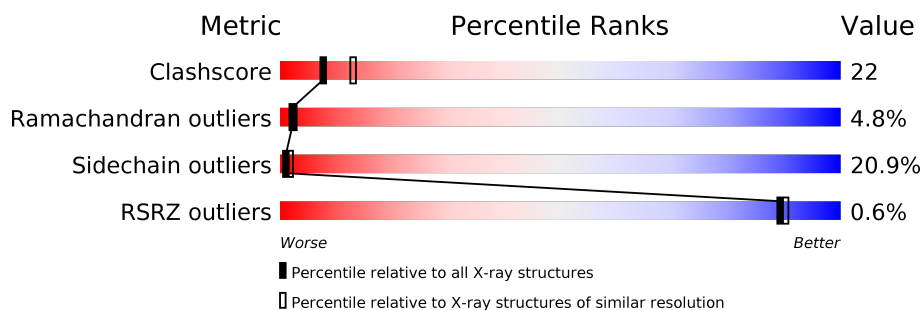
# 1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div></div> <div>37%</div> <div>44%</div> <div>15%</div> <div>.</div> </div>

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	317	X	-	-	-
3	CB3	A	318	-	-	X	-

## 2 Entry composition [i](#)

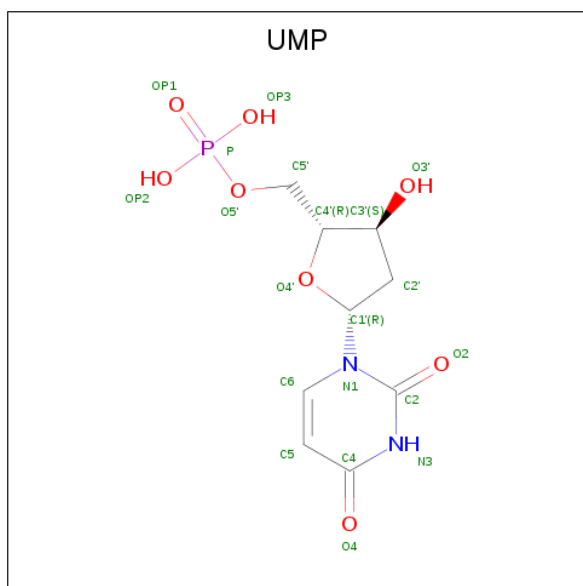
There are 4 unique types of molecules in this entry. The entry contains 3574 atoms, of which 804 are hydrogens and 0 are deuteriums.

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.

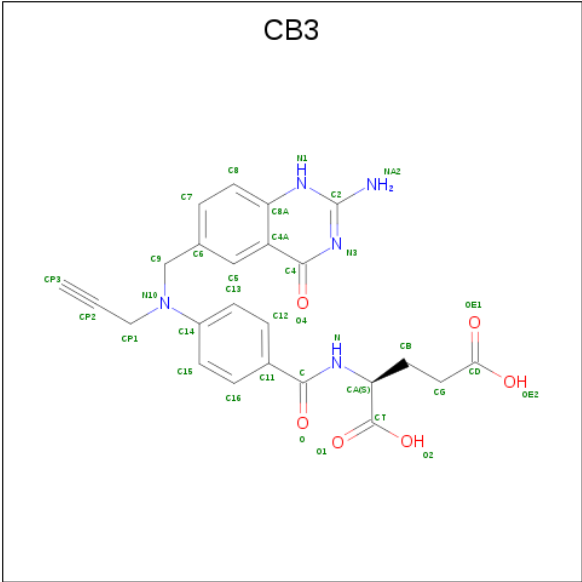
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	H	N	O	S	0	0	0
			3139	1677	549	438	467	8			

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



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

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula:  $C_{24}H_{23}N_5O_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			39	24	4	5	6		

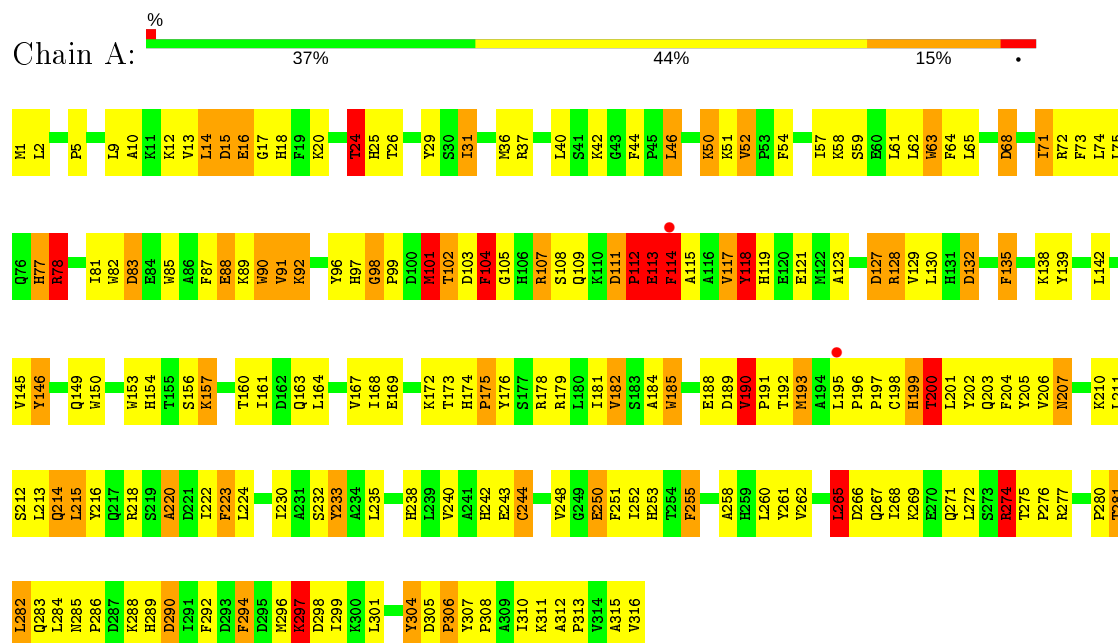
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	125	Total	H	O	0	0
			375	250	125		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	78.70 Å 78.70 Å 230.10 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 65.35 – 2.51	Depositor EDS
% Data completeness (in resolution range)	59.2 (15.00-2.50) 59.5 (65.35-2.51)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.51 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.187 , (Not available) 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 954.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3574	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CB3, 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	1.20	2/2674 (0.1%)	2.09	84/3634 (2.3%)

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	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	113	GLU	CB-CG	6.85	1.65	1.52
1	A	85	TRP	CD1-NE1	-5.16	1.29	1.38

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	TYR	CB-CG-CD2	-12.61	113.43	121.00
1	A	178	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	A	85	TRP	CD1-CG-CD2	11.56	115.55	106.30
1	A	85	TRP	CE2-CD2-CG	-9.52	99.68	107.30
1	A	150	TRP	CD1-CG-CD2	9.18	113.64	106.30
1	A	154	HIS	CA-CB-CG	-9.07	98.17	113.60
1	A	90	TRP	CD1-CG-CD2	8.97	113.47	106.30
1	A	37	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	A	90	TRP	CE2-CD2-CG	-8.56	100.45	107.30
1	A	82	TRP	CD1-CG-CD2	8.42	113.03	106.30
1	A	146	TYR	CB-CG-CD1	8.00	125.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	TYR	CB-CG-CD2	-7.91	116.25	121.00
1	A	91	VAL	CG1-CB-CG2	-7.79	98.43	110.90
1	A	185	TRP	CE2-CD2-CG	-7.79	101.07	107.30
1	A	85	TRP	CG-CD1-NE1	-7.60	102.50	110.10
1	A	185	TRP	CD1-CG-CD2	7.53	112.32	106.30
1	A	36	MET	CA-CB-CG	7.48	126.01	113.30
1	A	179	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	114	PHE	CA-CB-CG	-7.38	96.19	113.90
1	A	176	TYR	N-CA-C	7.37	130.90	111.00
1	A	261	TYR	CB-CG-CD1	-7.34	116.60	121.00
1	A	262	VAL	CG1-CB-CG2	-7.32	99.19	110.90
1	A	243	GLU	CA-CB-CG	-7.31	97.33	113.40
1	A	153	TRP	CD1-CG-CD2	7.17	112.03	106.30
1	A	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A	153	TRP	CE2-CD2-CG	-6.93	101.76	107.30
1	A	63	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	A	118	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	A	289	HIS	N-CA-C	6.79	129.33	111.00
1	A	150	TRP	CE2-CD2-CG	-6.73	101.91	107.30
1	A	63	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	A	15	ASP	CA-C-N	6.68	131.90	117.20
1	A	101	MET	CA-CB-CG	-6.64	102.00	113.30
1	A	178	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	182	VAL	CA-CB-CG1	-6.37	101.35	110.90
1	A	288	LYS	CA-C-N	-6.34	103.26	117.20
1	A	132	ASP	CA-C-N	-6.30	103.33	117.20
1	A	284	LEU	CA-C-N	-6.28	103.39	117.20
1	A	107	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	255	PHE	CB-CA-C	-6.22	97.95	110.40
1	A	104	PHE	CA-C-N	6.22	128.64	116.20
1	A	85	TRP	CG-CD2-CE3	6.20	139.48	133.90
1	A	185	TRP	CB-CG-CD1	-6.18	118.97	127.00
1	A	83	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	265	LEU	CA-CB-CG	6.12	129.39	115.30
1	A	161	ILE	CA-CB-CG1	-6.07	99.46	111.00
1	A	92	LYS	CA-CB-CG	6.06	126.74	113.40
1	A	185	TRP	CG-CD2-CE3	6.05	139.35	133.90
1	A	15	ASP	O-C-N	-6.04	113.04	122.70
1	A	150	TRP	CG-CD1-NE1	-6.02	104.08	110.10
1	A	233	TYR	CA-CB-CG	-6.00	102.01	113.40
1	A	216	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	A	97	HIS	CA-CB-CG	-5.98	103.44	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	THR	OG1-CB-CG2	-5.86	96.52	110.00
1	A	242	HIS	CA-CB-CG	5.80	123.47	113.60
1	A	304	TYR	CB-CG-CD1	5.68	124.41	121.00
1	A	24	THR	CA-CB-CG2	-5.65	104.48	112.40
1	A	42	LYS	CA-C-N	5.65	127.50	116.20
1	A	118	TYR	CB-CG-CD1	5.60	124.36	121.00
1	A	188	GLU	CA-CB-CG	5.59	125.70	113.40
1	A	14	LEU	CA-C-N	-5.58	104.92	117.20
1	A	68	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	82	TRP	CG-CD1-NE1	-5.54	104.56	110.10
1	A	274	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	90	TRP	CG-CD1-NE1	-5.47	104.62	110.10
1	A	150	TRP	CB-CG-CD2	-5.47	119.49	126.60
1	A	85	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	A	112	PRO	N-CA-CB	-5.43	96.62	102.60
1	A	220	ALA	CA-C-N	5.42	129.12	117.20
1	A	46	LEU	N-CA-C	-5.36	96.52	111.00
1	A	193	MET	CA-CB-CG	-5.33	104.23	113.30
1	A	90	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	A	1	MET	CA-C-N	5.31	128.88	117.20
1	A	253	HIS	CA-CB-CG	5.27	122.56	113.60
1	A	173	THR	CA-CB-CG2	5.26	119.76	112.40
1	A	290	ASP	N-CA-C	-5.24	96.86	111.00
1	A	128	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	274	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	50	LYS	N-CA-C	-5.12	97.18	111.00
1	A	223	PHE	CA-CB-CG	-5.12	101.62	113.90
1	A	206	VAL	CA-CB-CG2	-5.08	103.28	110.90
1	A	82	TRP	CG-CD2-CE3	5.06	138.46	133.90
1	A	214	GLN	CA-CB-CG	-5.05	102.28	113.40
1	A	200	THR	CA-CB-CG2	-5.03	105.36	112.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ASP	Peptide
1	A	118	TYR	Sidechain
1	A	190	VAL	Peptide
1	A	233	TYR	Sidechain
1	A	312	ALA	Peptide
1	A	98	GLY	Peptide

## 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	549	2496	105	1
2	A	20	1	10	2	0
3	A	35	4	21	9	0
4	A	125	250	0	2	1
All	All	2770	804	2527	113	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 22.

All (113) 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)
3:A:318:CB3:CP2	3:A:318:CB3:C13	2.56	0.83
1:A:10:ALA:HB1	1:A:268:ILE:HD11	1.60	0.82
3:A:318:CB3:CP3	3:A:318:CB3:C13	2.58	0.81
3:A:318:CB3:CP3	4:A:406:HOH:O	2.29	0.81
1:A:51:LYS:HG3	1:A:306:PRO:HG3	1.64	0.81
1:A:222:ILE:HD11	1:A:258:ALA:HB1	1.65	0.78
1:A:71:ILE:O	1:A:75:LEU:HD23	1.85	0.77
3:A:318:CB3:CP3	3:A:318:CB3:H13	2.16	0.74
1:A:62:LEU:HD21	1:A:299:ILE:HD11	1.70	0.74
1:A:172:LYS:HG3	1:A:244:CYS:HB3	1.73	0.69
1:A:117:VAL:O	1:A:121:GLU:HB2	1.93	0.68
3:A:318:CB3:CP2	3:A:318:CB3:H13	2.22	0.67
1:A:18:HIS:O	1:A:29:TYR:HA	1.94	0.67
1:A:54:PHE:O	1:A:58:LYS:HG2	1.96	0.66
1:A:220:ALA:HB3	1:A:258:ALA:HA	1.77	0.66
1:A:75:LEU:HB3	1:A:130:LEU:HD13	1.79	0.65
1:A:88:GLU:HA	1:A:91:VAL:HG12	1.79	0.62
1:A:9:LEU:O	1:A:13:VAL:HG23	1.99	0.62
1:A:44:PHE:HB3	1:A:280:PRO:HG2	1.81	0.62
1:A:297:LYS:HE2	1:A:297:LYS:H	1.65	0.61
1:A:114:PHE:HD2	1:A:118:TYR:HB2	1.67	0.60
1:A:168:ILE:HG23	1:A:244:CYS:SG	2.43	0.58
1:A:17:GLY:HA3	1:A:29:TYR:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:CE2	1:A:101:MET:HG3	2.39	0.57
1:A:90:TRP:HA	1:A:139:TYR:CD2	2.40	0.57
1:A:184:ALA:O	1:A:197:PRO:HG2	2.05	0.56
1:A:54:PHE:CE2	1:A:301:LEU:HB2	2.40	0.56
1:A:105:GLY:HA2	1:A:108:SER:OG	2.06	0.56
1:A:274:ARG:HG2	1:A:307:TYR:CD2	2.41	0.55
1:A:202:TYR:HB2	1:A:213:LEU:HD21	1.87	0.55
1:A:58:LYS:HG3	1:A:296:MET:HE1	1.89	0.53
1:A:72:ARG:O	1:A:75:LEU:HB2	2.08	0.53
1:A:205:TYR:CE1	1:A:207:ASN:HB2	2.44	0.52
1:A:195:LEU:HG	1:A:196:PRO:O	2.09	0.52
1:A:54:PHE:HZ	1:A:282:LEU:HD11	1.75	0.52
1:A:181:ILE:HG12	1:A:203:GLN:HG3	1.91	0.52
1:A:274:ARG:HG2	1:A:307:TYR:CE2	2.45	0.52
1:A:54:PHE:CG	1:A:301:LEU:HD22	2.44	0.52
1:A:104:PHE:HB2	1:A:118:TYR:CG	2.45	0.52
1:A:138:LYS:HD2	1:A:139:TYR:CE1	2.45	0.51
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.45	0.51
1:A:132:ASP:HB3	1:A:135:PHE:HB2	1.93	0.51
1:A:71:ILE:HG22	1:A:129:VAL:HG11	1.93	0.50
1:A:197:PRO:O	1:A:218:ARG:HD3	2.11	0.50
1:A:81:ILE:O	3:A:318:CB3:H15	2.12	0.50
1:A:138:LYS:HB3	1:A:139:TYR:CD1	2.46	0.50
1:A:185:TRP:HB2	1:A:200:THR:HG22	1.94	0.50
1:A:204:PHE:CZ	1:A:240:VAL:HG11	2.47	0.49
1:A:112:PRO:HB3	1:A:113:GLU:OE1	2.12	0.49
1:A:13:VAL:HG21	1:A:222:ILE:CD1	2.43	0.49
1:A:91:VAL:HG23	1:A:96:TYR:CE2	2.48	0.49
1:A:223:PHE:HB2	1:A:260:LEU:HD11	1.94	0.49
1:A:61:LEU:O	1:A:64:PHE:HB2	2.13	0.48
1:A:204:PHE:HB3	1:A:211:LEU:HD11	1.94	0.48
1:A:212:SER:HA	1:A:250:GLU:O	2.12	0.48
3:A:318:CB3:CP2	4:A:406:HOH:O	2.56	0.48
1:A:198:CYS:SG	2:A:317:UMP:H5''	2.55	0.47
1:A:63:TRP:CD2	1:A:74:LEU:HD11	2.49	0.47
1:A:96:TYR:OH	1:A:101:MET:HG2	2.15	0.47
1:A:59:SER:CA	1:A:296:MET:HE3	2.45	0.47
1:A:275:THR:HA	1:A:276:PRO:HD2	1.62	0.46
1:A:65:LEU:O	1:A:292:PHE:HD1	1.98	0.46
1:A:63:TRP:HB2	1:A:73:PHE:CD1	2.51	0.46
1:A:199:HIS:HB3	1:A:215:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:HD2	1:A:296:MET:SD	2.39	0.46
1:A:101:MET:SD	1:A:104:PHE:HB3	2.56	0.45
1:A:91:VAL:HG23	1:A:96:TYR:CD2	2.51	0.45
1:A:59:SER:HA	1:A:296:MET:HE3	1.98	0.45
1:A:24:THR:HG21	1:A:316:VAL:HG11	1.99	0.45
1:A:114:PHE:CD2	1:A:118:TYR:HB2	2.48	0.44
1:A:78:ARG:HH12	1:A:130:LEU:HD22	1.82	0.44
1:A:146:TYR:HA	1:A:149:GLN:HB2	2.00	0.44
1:A:285:ASN:HA	1:A:286:PRO:HD3	1.62	0.44
1:A:112:PRO:HB2	1:A:114:PHE:HD1	1.82	0.44
1:A:58:LYS:O	1:A:62:LEU:HG	2.18	0.44
1:A:87:PHE:HE2	1:A:101:MET:HG3	1.82	0.44
1:A:163:GLN:OE1	1:A:182:VAL:HA	2.17	0.44
1:A:12:LYS:O	1:A:16:GLU:HG2	2.17	0.43
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.65	0.43
1:A:277:ARG:HD2	1:A:305:ASP:O	2.19	0.43
1:A:31:ILE:HA	1:A:31:ILE:HD13	1.91	0.43
1:A:74:LEU:N	1:A:74:LEU:HD12	2.33	0.43
1:A:172:LYS:CG	1:A:244:CYS:HB3	2.44	0.43
3:A:318:CB3:C13	3:A:318:CB3:H5	2.49	0.43
3:A:318:CB3:CT	3:A:318:CB3:H12	2.49	0.42
1:A:123:ALA:O	1:A:127:ASP:HB2	2.18	0.42
1:A:98:GLY:HA3	1:A:99:PRO:HD3	1.61	0.42
1:A:135:PHE:CE1	1:A:139:TYR:CD1	3.07	0.42
1:A:235:LEU:HD21	1:A:299:ILE:HD13	2.01	0.42
1:A:91:VAL:HG21	1:A:101:MET:HB3	2.02	0.42
1:A:190:VAL:HA	1:A:193:MET:HB2	2.02	0.42
1:A:214:GLN:HG3	1:A:252:ILE:HB	2.02	0.42
1:A:198:CYS:SG	2:A:317:UMP:C6	3.13	0.42
1:A:50:LYS:HD2	1:A:223:PHE:CZ	2.54	0.42
1:A:20:LYS:HE3	1:A:20:LYS:HB3	1.79	0.41
1:A:40:LEU:HB2	1:A:248:VAL:HG22	2.01	0.41
1:A:230:ILE:HG23	1:A:251:PHE:HE2	1.85	0.41
1:A:266:ASP:HB2	1:A:267:GLN:OE1	2.20	0.41
1:A:238:HIS:CD2	1:A:248:VAL:HG21	2.56	0.41
1:A:271:GLN:HA	1:A:274:ARG:HD3	2.02	0.41
1:A:265:LEU:O	1:A:269:LYS:HG3	2.21	0.41
1:A:46:LEU:HB3	1:A:304:TYR:CE1	2.56	0.41
1:A:46:LEU:HD22	1:A:52:VAL:HB	2.01	0.41
1:A:274:ARG:NH2	1:A:310:ILE:HD11	2.35	0.41
1:A:24:THR:HB	1:A:25:HIS:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:O	1:A:167:VAL:N	2.55	0.40
1:A:266:ASP:O	1:A:269:LYS:HB2	2.21	0.40
1:A:223:PHE:HB3	1:A:224:LEU:HD12	2.03	0.40
1:A:224:LEU:HD12	1:A:224:LEU:N	2.36	0.40
1:A:62:LEU:CD1	1:A:296:MET:HG2	2.51	0.40
1:A:115:ALA:O	1:A:119:HIS:HB2	2.21	0.40
1:A:294:PHE:CE2	1:A:298:ASP:HB3	2.57	0.40
1:A:58:LYS:HG3	1:A:296:MET:CE	2.50	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:157:LYS:HZ1	4:A:402:HOH:H2[5_564]	1.32	0.28

## 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%)	258 (82%)	41 (13%)	15 (5%)	<b>2</b> <b>2</b>

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	THR
1	A	104	PHE
1	A	112	PRO
1	A	142	LEU
1	A	175	PRO
1	A	78	ARG
1	A	103	ASP
1	A	2	LEU

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Mol	Chain	Res	Type
1	A	111	ASP
1	A	156	SER
1	A	297	LYS
1	A	308	PRO
1	A	191	PRO
1	A	190	VAL
1	A	315	ALA

### 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	277/278 (100%)	219 (79%)	58 (21%)	<b>1</b> <b>2</b>

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	A	14	LEU
1	A	15	ASP
1	A	16	GLU
1	A	24	THR
1	A	26	THR
1	A	31	ILE
1	A	52	VAL
1	A	57	ILE
1	A	71	ILE
1	A	77	HIS
1	A	78	ARG
1	A	83	ASP
1	A	88	GLU
1	A	89	LYS
1	A	92	LYS
1	A	101	MET
1	A	102	THR
1	A	107	ARG

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Mol	Chain	Res	Type
1	A	109	GLN
1	A	112	PRO
1	A	113	GLU
1	A	114	PHE
1	A	117	VAL
1	A	118	TYR
1	A	127	ASP
1	A	128	ARG
1	A	135	PHE
1	A	145	VAL
1	A	157	LYS
1	A	160	THR
1	A	169	GLU
1	A	174	HIS
1	A	175	PRO
1	A	189	ASP
1	A	192	THR
1	A	199	HIS
1	A	200	THR
1	A	201	LEU
1	A	207	ASN
1	A	210	LYS
1	A	215	LEU
1	A	232	SER
1	A	244	CYS
1	A	250	GLU
1	A	255	PHE
1	A	265	LEU
1	A	272	LEU
1	A	274	ARG
1	A	281	THR
1	A	282	LEU
1	A	283	GLN
1	A	290	ASP
1	A	294	PHE
1	A	297	LYS
1	A	306	PRO
1	A	311	LYS
1	A	313	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are 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	-	18,21,21	1.82	4 (22%)	21,31,31	1.89	3 (14%)
3	CB3	A	318	-	30,37,37	2.35	11 (36%)	38,51,51	2.89	12 (31%)

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	-	1/1/4/4	2/7/22/22	0/2/2/2
3	CB3	A	318	-	-	11/21/28/28	0/3/3/3



All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	318	CB3	O4-C4	6.24	1.40	1.24
2	A	317	UMP	C4-N3	5.56	1.42	1.33
3	A	318	CB3	CP1-N10	4.81	1.50	1.46
3	A	318	CB3	CB-CA	4.18	1.58	1.53
3	A	318	CB3	CA-N	3.97	1.51	1.46
3	A	318	CB3	C9-N10	3.83	1.51	1.46
3	A	318	CB3	C8-C7	3.00	1.42	1.36
3	A	318	CB3	CP1-CP2	2.75	1.50	1.47
2	A	317	UMP	O4'-C1'	2.71	1.48	1.42
2	A	317	UMP	C6-N1	-2.51	1.32	1.35
3	A	318	CB3	C5-C6	2.44	1.43	1.37
3	A	318	CB3	C4-N3	2.30	1.37	1.33
3	A	318	CB3	C9-C6	2.19	1.55	1.51
2	A	317	UMP	C2-N3	2.10	1.42	1.38
3	A	318	CB3	C7-C6	2.02	1.43	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	318	CB3	C4A-C4-N3	-8.26	118.64	124.40
3	A	318	CB3	CP1-N10-C9	7.85	124.57	117.10
3	A	318	CB3	CG-CB-CA	6.79	126.77	113.04
2	A	317	UMP	C2'-C1'-N1	5.72	127.47	114.27
3	A	318	CB3	C4A-C8A-N1	-5.22	120.77	123.60
3	A	318	CB3	CP1-CP2-CP3	-5.04	169.22	177.67
3	A	318	CB3	N1-C2-N3	-4.83	120.78	127.22
2	A	317	UMP	C5-C4-N3	-4.76	112.84	123.31
3	A	318	CB3	C4-N3-C2	3.78	121.93	115.93
2	A	317	UMP	OP2-P-O5'	2.99	114.69	106.73
3	A	318	CB3	CA-N-C	2.50	125.56	122.34
3	A	318	CB3	C6-C9-N10	2.33	117.92	114.18
3	A	318	CB3	C9-N10-C14	-2.23	116.94	120.78
3	A	318	CB3	C15-C14-N10	-2.06	118.54	121.38
3	A	318	CB3	O-C-N	-2.04	118.69	122.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	317	UMP	C1'

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	318	CB3	CP2-CP1-N10-C9
3	A	318	CB3	CP2-CP1-N10-C14
3	A	318	CB3	C11-C-N-CA
3	A	318	CB3	O-C-N-CA
3	A	318	CB3	N-CA-CB-CG
3	A	318	CB3	CT-CA-CB-CG
3	A	318	CB3	CA-CB-CG-CD
3	A	318	CB3	C13-C14-N10-C9
3	A	318	CB3	C15-C14-N10-C9
3	A	318	CB3	C15-C14-N10-CP1
3	A	318	CB3	C13-C14-N10-CP1
2	A	317	UMP	C4'-C5'-O5'-P
2	A	317	UMP	O4'-C4'-C5'-O5'

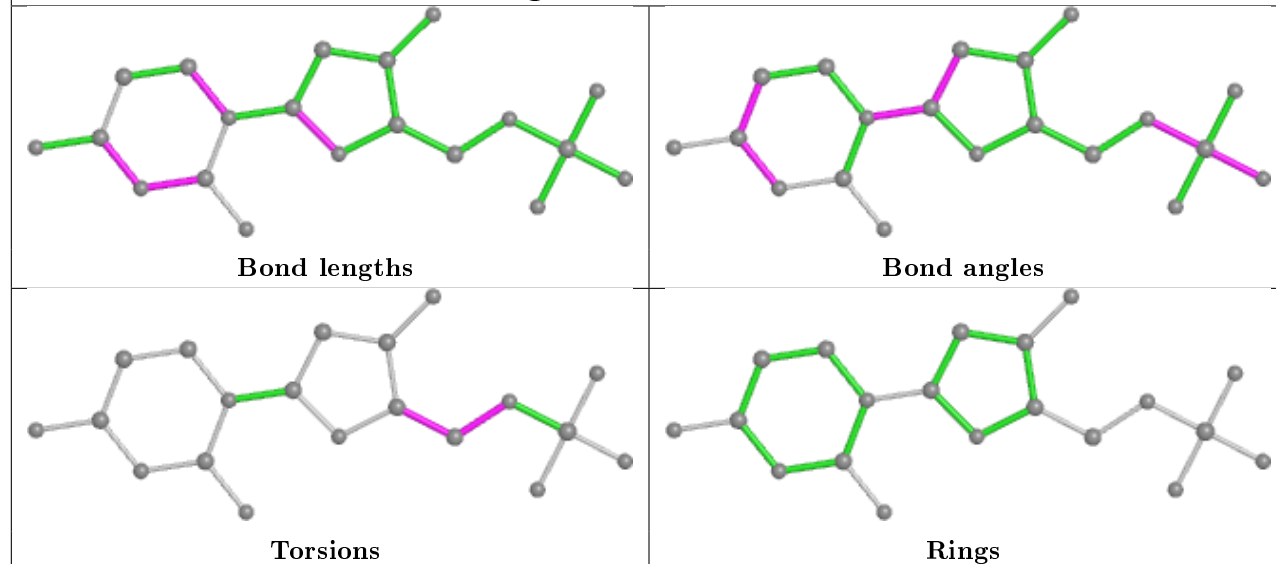
There are no ring outliers.

2 monomers are involved in 11 short contacts:

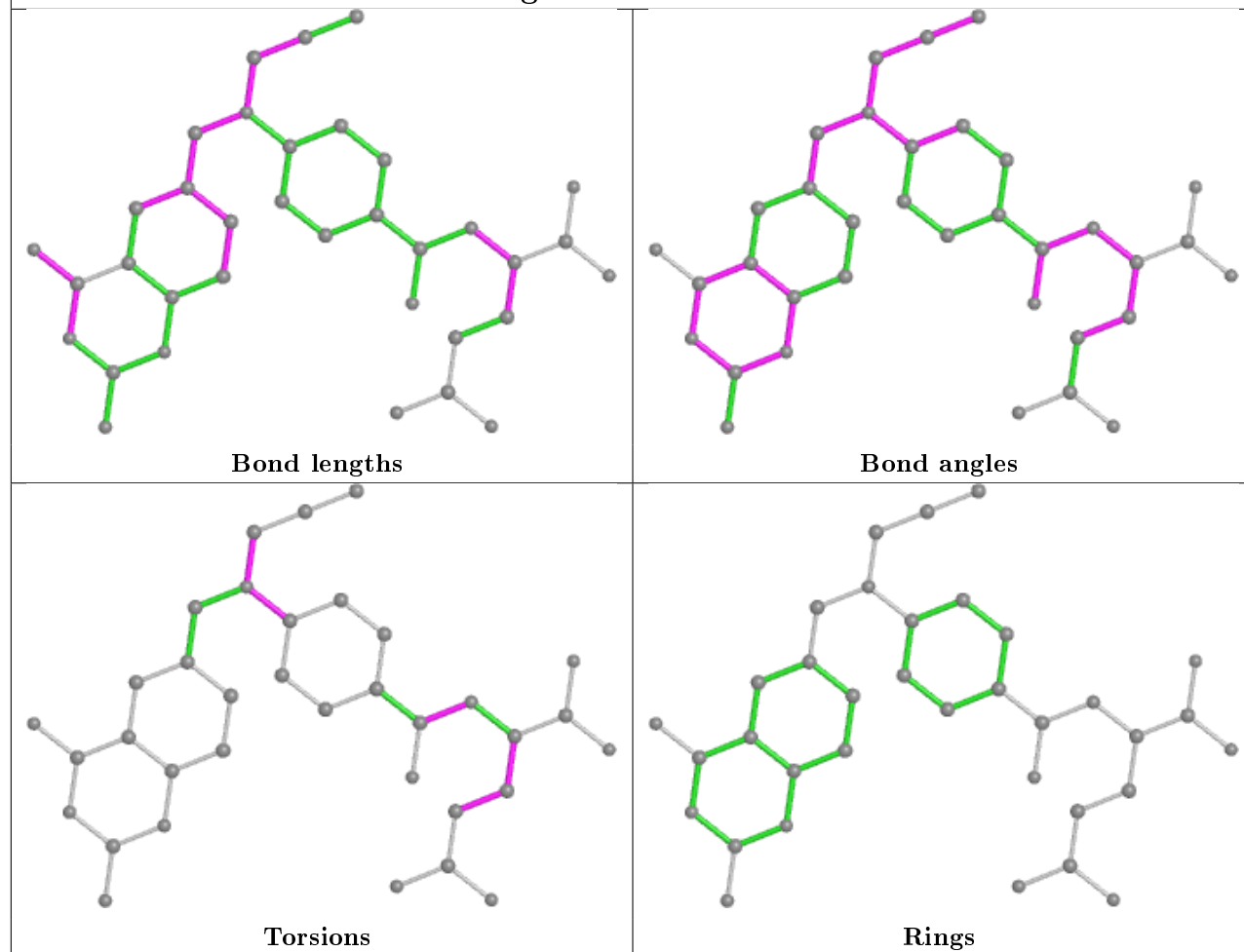
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	317	UMP	2	0
3	A	318	CB3	9	0

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.

## Ligand UMP A 317



## Ligand CB3 A 318



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	316/316 (100%)	-0.78	2 (0%) 89 90	4, 14, 24, 31	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	LEU	2.2
1	A	114	PHE	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 carbohydrates 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, 95<sup>th</sup> 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.

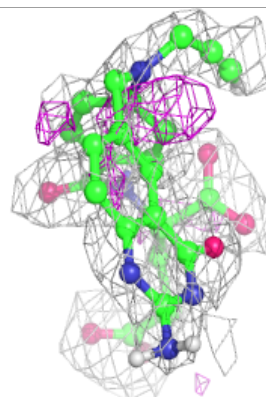
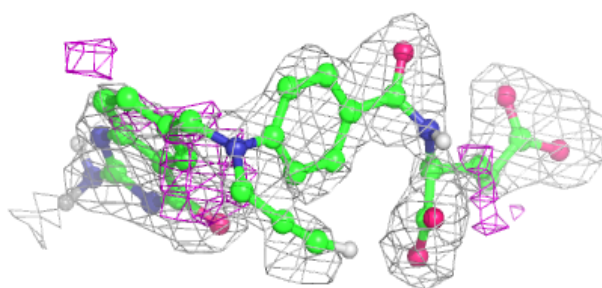
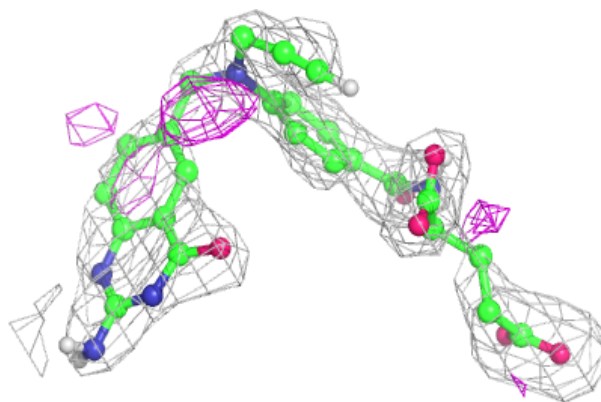
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CB3	A	318	35/35	0.91	0.32	15,25,38,38	0
2	UMP	A	317	20/20	0.94	0.17	15,21,21,21	0

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.

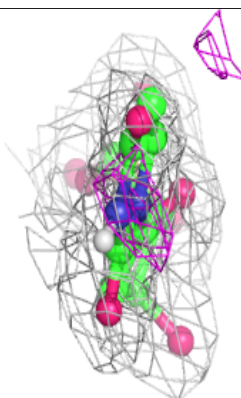
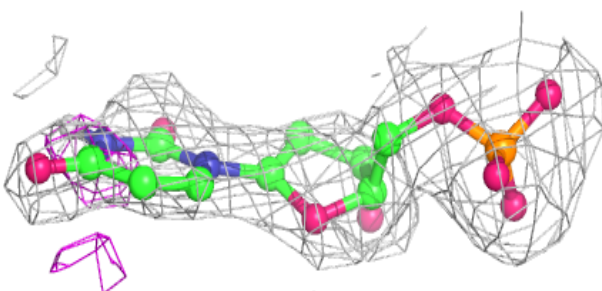
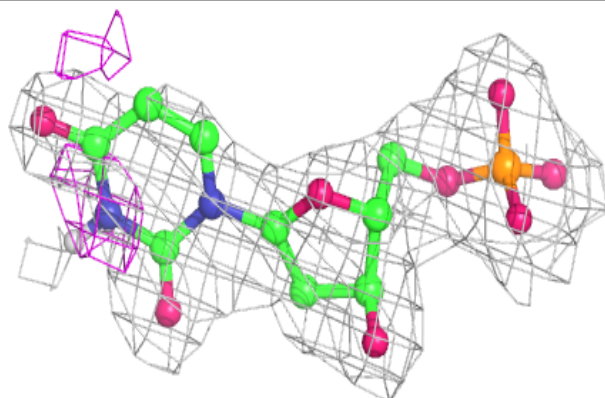
**Electron density around CB3 A 318:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around UMP A 317:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.