



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 09:33 AM EDT

PDB ID : 1VZE
Title : L. CASEI THYMIDYLATE SYNTHASE MUTANT E60Q TERNARY COMPLEX WITH DUMP AND CB3717
Authors : Birdsall, D.L.; Finer-Moore, J.; Stroud, R.M.
Deposited on : 1996-09-18
Resolution : 2.30 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 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 : 2.23.2
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) : 2.23.2

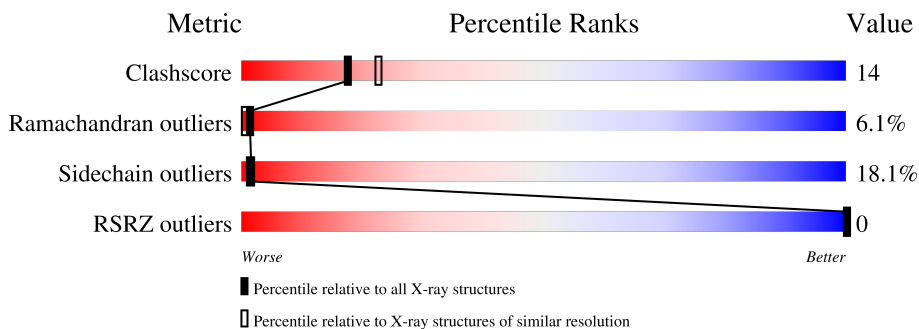
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3896 atoms, of which 1013 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.

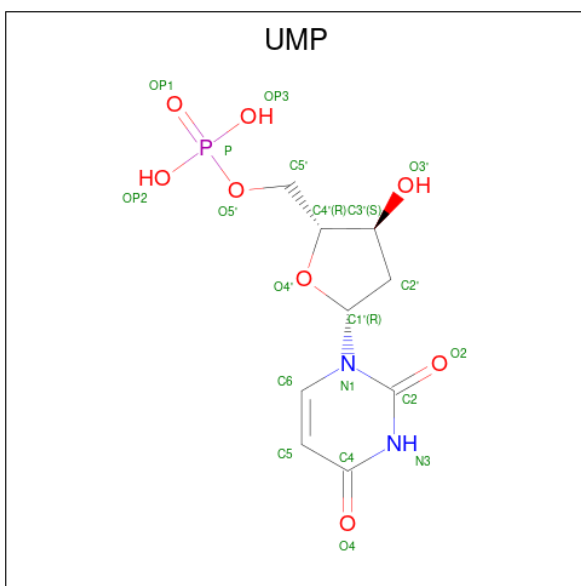
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

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

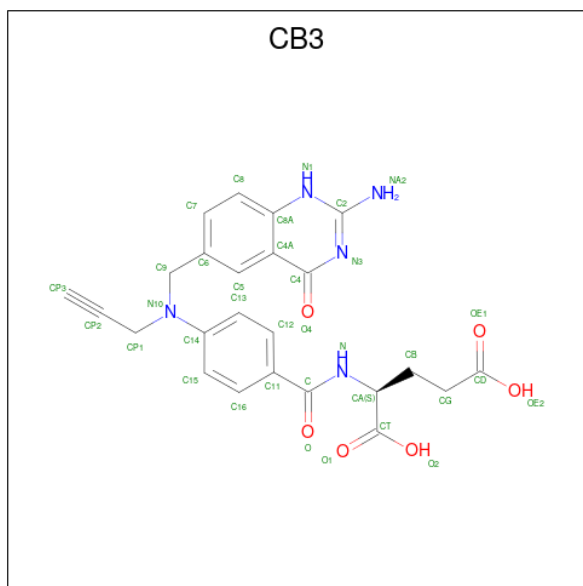
- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



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 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3)

(formula: C₂₄H₂₃N₅O₆).



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

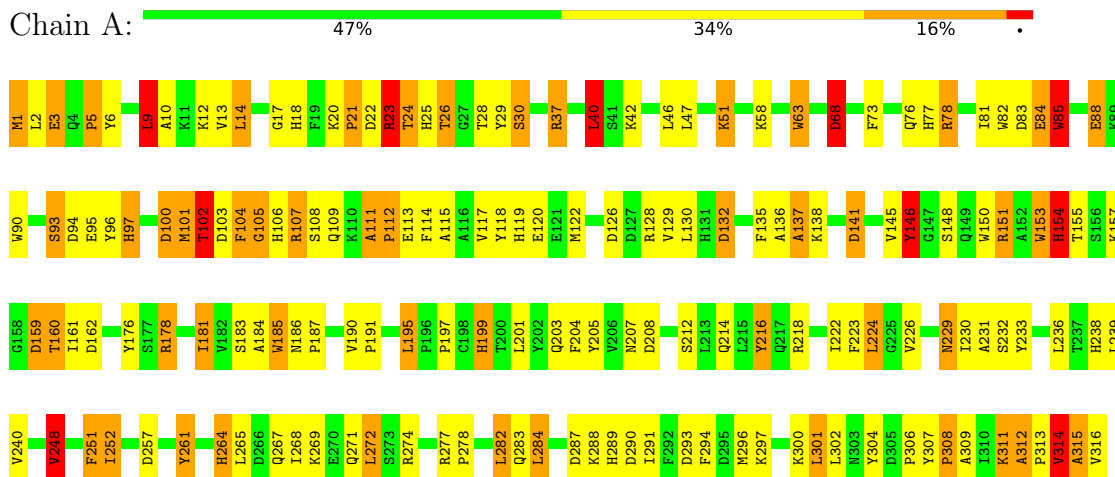
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
4	A	238	714	476	238	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 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	78.90Å 78.90Å 230.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.30 65.52 – 2.18	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.30) 54.9 (65.52-2.18)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.18Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , (Not available) 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 902.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3896	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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, CB3

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	1.16	5/2674 (0.2%)	2.04	94/3634 (2.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	GLU	CG-CD	5.43	1.60	1.51
1	A	63	TRP	CD1-NE1	-5.30	1.28	1.38
1	A	153	TRP	CG-CD2	-5.22	1.34	1.43
1	A	82	TRP	CG-CD2	-5.08	1.35	1.43
1	A	183	SER	CA-CB	-5.03	1.45	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	A	23	ARG	CA-CB-CG	10.12	135.66	113.40
1	A	201	LEU	CA-CB-CG	9.42	136.96	115.30
1	A	115	ALA	N-CA-C	-9.28	85.95	111.00
1	A	226	VAL	CG1-CB-CG2	-9.09	96.36	110.90
1	A	63	TRP	CD1-CG-CD2	8.95	113.46	106.30
1	A	82	TRP	CD1-CG-CD2	8.82	113.36	106.30
1	A	63	TRP	CE2-CD2-CG	-8.38	100.60	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	A	6	TYR	CB-CG-CD1	-7.83	116.30	121.00
1	A	150	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	A	85	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	153	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	A	122	MET	CG-SD-CE	-7.14	88.78	100.20
1	A	216	TYR	CB-CG-CD2	-7.12	116.73	121.00
1	A	9	LEU	CA-CB-CG	7.11	131.66	115.30
1	A	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	24	THR	CA-C-N	-7.08	101.63	117.20
1	A	90	TRP	CD1-CG-CD2	7.06	111.95	106.30
1	A	93	SER	CA-C-N	-7.02	101.75	117.20
1	A	185	TRP	CD1-CG-CD2	7.00	111.90	106.30
1	A	37	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	261	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	107	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	129	VAL	CG1-CB-CG2	-6.67	100.23	110.90
1	A	185	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	A	101	MET	CG-SD-CE	-6.52	89.76	100.20
1	A	153	TRP	CD1-CG-CD2	6.44	111.45	106.30
1	A	282	LEU	CA-CB-CG	6.43	130.08	115.30
1	A	90	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	A	178	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	145	VAL	CA-CB-CG2	-6.20	101.60	110.90
1	A	26	THR	N-CA-C	-6.17	94.33	111.00
1	A	132	ASP	CA-C-N	-6.15	103.66	117.20
1	A	126	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	3	GLU	CA-CB-CG	6.12	126.87	113.40
1	A	29	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	150	TRP	CE2-CD2-CG	-6.04	102.47	107.30
1	A	201	LEU	CB-CA-C	-6.02	98.75	110.20
1	A	199	HIS	N-CA-C	-5.98	94.86	111.00
1	A	37	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	78	ARG	CB-CG-CD	-5.94	96.16	111.60
1	A	26	THR	N-CA-CB	5.93	121.58	110.30
1	A	304	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	264	HIS	CA-C-N	5.88	130.14	117.20
1	A	58	LYS	CA-CB-CG	5.87	126.31	113.40
1	A	63	TRP	CG-CD2-CE3	5.84	139.16	133.90
1	A	22	ASP	N-CA-CB	-5.84	100.09	110.60
1	A	190	VAL	CA-CB-CG2	-5.82	102.17	110.90
1	A	17	GLY	CA-C-N	-5.82	104.41	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	TYR	CB-CG-CD1	-5.74	117.55	121.00
1	A	252	ILE	CA-C-N	5.73	129.80	117.20
1	A	233	TYR	CA-CB-CG	-5.72	102.53	113.40
1	A	78	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	102	THR	N-CA-CB	-5.71	99.44	110.30
1	A	84	GLU	CA-CB-CG	5.69	125.92	113.40
1	A	154	HIS	CA-CB-CG	-5.68	103.95	113.60
1	A	23	ARG	CA-C-N	5.67	129.67	117.20
1	A	314	VAL	O-C-N	-5.67	113.63	122.70
1	A	201	LEU	CD1-CG-CD2	-5.67	93.50	110.50
1	A	78	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	248	VAL	CG1-CB-CG2	-5.56	102.01	110.90
1	A	288	LYS	CA-C-N	-5.54	105.02	117.20
1	A	181	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	A	302	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	137	ALA	CA-C-N	-5.46	105.18	117.20
1	A	271	GLN	CA-C-N	-5.40	105.31	117.20
1	A	301	LEU	CA-CB-CG	5.39	127.71	115.30
1	A	58	LYS	CB-CG-CD	-5.39	97.58	111.60
1	A	58	LYS	N-CA-CB	-5.39	100.89	110.60
1	A	23	ARG	O-C-N	-5.35	114.13	122.70
1	A	23	ARG	N-CA-CB	-5.34	101.00	110.60
1	A	229	ASN	CB-CG-ND2	5.33	129.49	116.70
1	A	141	ASP	N-CA-C	-5.31	96.67	111.00
1	A	18	HIS	CA-CB-CG	5.29	122.58	113.60
1	A	272	LEU	CA-C-N	5.28	128.81	117.20
1	A	97	HIS	O-C-N	-5.28	114.23	123.20
1	A	155	THR	CA-CB-CG2	-5.25	105.05	112.40
1	A	201	LEU	CB-CG-CD2	5.24	119.90	111.00
1	A	95	GLU	CA-C-N	5.21	128.66	117.20
1	A	176	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	A	251	PHE	N-CA-C	-5.21	96.93	111.00
1	A	24	THR	CA-C-O	5.20	131.02	120.10
1	A	150	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	111	ALA	N-CA-CB	-5.17	102.86	110.10
1	A	68	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	151	ARG	CD-NE-CZ	-5.14	116.41	123.60
1	A	315	ALA	N-CA-C	-5.13	97.16	111.00
1	A	160	THR	N-CA-CB	-5.09	100.63	110.30
1	A	47	LEU	CA-CB-CG	5.07	126.95	115.30
1	A	63	TRP	CB-CG-CD1	-5.05	120.43	127.00
1	A	159	ASP	CA-C-N	-5.04	106.11	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	THR	CA-CB-OG1	-5.04	98.42	109.00
1	A	40	LEU	CB-CG-CD1	-5.01	102.49	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	HIS	Sidechain
1	A	205	TYR	Sidechain
1	A	216	TYR	Sidechain
1	A	312	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2590	532	2500	71	0
2	A	20	1	10	1	0
3	A	35	4	21	0	0
4	A	238	476	0	1	0
All	All	2883	1013	2531	71	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 14.

All (71) 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:108:SER:HA	1:A:114:PHE:HB3	1.52	0.91
1:A:51:LYS:HB2	1:A:309:ALA:HB2	1.52	0.91
1:A:101:MET:SD	1:A:118:TYR:HA	2.13	0.88
1:A:24:THR:HB	1:A:316:VAL:HB	1.63	0.79
1:A:85:TRP:HZ2	1:A:195:LEU:HB2	1.48	0.77
1:A:128:ARG:HB3	1:A:135:PHE:CD2	2.20	0.77
1:A:311:LYS:O	1:A:313:PRO:HD2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:HD2	1:A:224:LEU:HD22	1.57	0.70
1:A:132:ASP:HB3	1:A:135:PHE:HB2	1.74	0.68
1:A:111:ALA:HB1	1:A:112:PRO:HD3	1.78	0.65
1:A:107:ARG:O	1:A:111:ALA:HB3	1.96	0.65
1:A:42:LYS:N	1:A:42:LYS:HD2	2.17	0.60
1:A:106:HIS:HB2	1:A:316:VAL:HG13	1.87	0.57
1:A:85:TRP:CZ2	1:A:195:LEU:HB2	2.34	0.57
1:A:239:LEU:HD23	1:A:284:LEU:HD21	1.85	0.57
1:A:214:GLN:HG3	1:A:252:ILE:HB	1.87	0.56
1:A:284:LEU:HD23	1:A:294:PHE:HE2	1.70	0.55
1:A:20:LYS:HB2	1:A:30:SER:OG	2.07	0.54
1:A:118:TYR:HD2	1:A:119:HIS:ND1	2.05	0.54
1:A:314:VAL:HG22	1:A:315:ALA:H	1.73	0.54
1:A:85:TRP:CH2	1:A:195:LEU:HD23	2.43	0.53
1:A:10:ALA:O	1:A:14:LEU:HD22	2.08	0.53
1:A:13:VAL:HG21	1:A:222:ILE:HD11	1.90	0.53
1:A:274:ARG:HG2	1:A:307:TYR:CE1	2.44	0.53
1:A:297:LYS:HB2	1:A:297:LYS:NZ	2.24	0.53
1:A:287:ASP:O	1:A:289:HIS:CD2	2.62	0.52
1:A:230:ILE:HG23	1:A:251:PHE:CE2	2.44	0.52
1:A:101:MET:CE	1:A:117:VAL:HG12	2.40	0.52
1:A:224:LEU:HD23	1:A:264:HIS:CE1	2.45	0.51
1:A:230:ILE:HG23	1:A:251:PHE:HE2	1.76	0.51
1:A:101:MET:O	1:A:104:PHE:HD2	1.94	0.51
1:A:274:ARG:HG2	1:A:307:TYR:CD1	2.47	0.50
1:A:100:ASP:OD2	1:A:102:THR:HB	2.12	0.49
1:A:73:PHE:O	1:A:77:HIS:HB2	2.12	0.49
1:A:101:MET:SD	1:A:118:TYR:CA	2.95	0.49
1:A:223:PHE:CD2	1:A:224:LEU:HD22	2.41	0.49
1:A:101:MET:HE3	1:A:117:VAL:HG12	1.95	0.49
1:A:84:GLU:HG2	1:A:104:PHE:CE1	2.49	0.48
1:A:136:ALA:O	1:A:138:LYS:N	2.46	0.48
1:A:13:VAL:HG21	1:A:222:ILE:CD1	2.44	0.48
1:A:195:LEU:HD11	2:A:317:UMP:H5''	1.95	0.48
1:A:238:HIS:CD2	1:A:282:LEU:HD23	2.48	0.48
1:A:153:TRP:CH2	1:A:186:ASN:HB2	2.49	0.48
1:A:185:TRP:HE3	1:A:197:PRO:HG2	1.79	0.47
1:A:204:PHE:CE1	1:A:240:VAL:HG11	2.50	0.47
1:A:204:PHE:CZ	1:A:240:VAL:HG21	2.48	0.47
1:A:187:PRO:O	1:A:191:PRO:HD2	2.16	0.46
1:A:9:LEU:O	1:A:12:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PHE:HZ	1:A:240:VAL:HG21	1.80	0.46
1:A:1:MET:HB3	1:A:2:LEU:H	1.67	0.46
1:A:63:TRP:CD1	1:A:68:ASP:HB3	2.52	0.45
1:A:84:GLU:HG2	1:A:104:PHE:HE1	1.81	0.45
1:A:103:ASP:O	1:A:105:GLY:N	2.50	0.45
1:A:78:ARG:HG3	1:A:78:ARG:HH11	1.82	0.44
1:A:30:SER:HB3	1:A:257:ASP:OD1	2.17	0.44
1:A:85:TRP:O	1:A:88:GLU:HB3	2.17	0.44
1:A:267:GLN:OE1	1:A:267:GLN:N	2.50	0.44
1:A:51:LYS:HG2	1:A:306:PRO:HB2	2.01	0.42
1:A:40:LEU:HD12	1:A:248:VAL:HG12	2.02	0.42
1:A:268:ILE:O	1:A:272:LEU:HD13	2.19	0.42
1:A:28:THR:HG22	1:A:261:TYR:CD2	2.54	0.42
1:A:76:GLN:HB3	1:A:130:LEU:HD21	2.02	0.42
1:A:97:HIS:HE1	4:A:424:HOH:O	2.02	0.42
1:A:24:THR:CB	1:A:316:VAL:HB	2.40	0.41
1:A:146:TYR:HH	1:A:199:HIS:H	1.68	0.41
1:A:224:LEU:HA	1:A:224:LEU:HD13	1.85	0.41
1:A:151:ARG:O	1:A:162:ASP:HA	2.20	0.41
1:A:46:LEU:HD12	1:A:231:ALA:HB2	2.02	0.40
1:A:151:ARG:HH11	1:A:151:ARG:HD3	1.71	0.40
1:A:184:ALA:O	1:A:197:PRO:HG3	2.22	0.40
1:A:20:LYS:HA	1:A:21:PRO:HD2	1.85	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	314/316 (99%)	255 (81%)	40 (13%)	19 (6%)	1 0

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	104	PHE
1	A	105	GLY
1	A	112	PRO
1	A	137	ALA
1	A	290	ASP
1	A	314	VAL
1	A	21	PRO
1	A	40	LEU
1	A	96	TYR
1	A	146	TYR
1	A	5	PRO
1	A	100	ASP
1	A	23	ARG
1	A	109	GLN
1	A	207	ASN
1	A	296	MET
1	A	312	ALA
1	A	308	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	277/277 (100%)	227 (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	3	GLU
1	A	5	PRO
1	A	9	LEU
1	A	14	LEU
1	A	23	ARG
1	A	26	THR
1	A	30	SER

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Mol	Chain	Res	Type
1	A	37	ARG
1	A	51	LYS
1	A	68	ASP
1	A	81	ILE
1	A	83	ASP
1	A	85	TRP
1	A	88	GLU
1	A	93	SER
1	A	94	ASP
1	A	102	THR
1	A	113	GLU
1	A	120	GLU
1	A	141	ASP
1	A	148	SER
1	A	154	HIS
1	A	157	LYS
1	A	159	ASP
1	A	160	THR
1	A	161	ILE
1	A	178	ARG
1	A	181	ILE
1	A	195	LEU
1	A	203	GLN
1	A	208	ASP
1	A	212	SER
1	A	218	ARG
1	A	224	LEU
1	A	229	ASN
1	A	232	SER
1	A	236	LEU
1	A	248	VAL
1	A	265	LEU
1	A	269	LYS
1	A	278	PRO
1	A	283	GLN
1	A	284	LEU
1	A	291	ILE
1	A	293	ASP
1	A	300	LYS
1	A	301	LEU
1	A	308	PRO
1	A	311	LYS

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	76	GLN
1	A	174	HIS
1	A	207	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](#)

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	1	18,21,21	3.69	6 (33%)	21,31,31	1.66	3 (14%)
3	CB3	A	318	-	30,37,37	2.18	10 (33%)	38,51,51	2.80	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	-	4/7/22/22	0/2/2/2
3	CB3	A	318	-	-	11/21/28/28	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	UMP	C6-N1	11.47	1.50	1.35
2	A	317	UMP	C6-C5	6.38	1.52	1.38
3	A	318	CB3	O4-C4	6.16	1.40	1.24
2	A	317	UMP	C4-N3	5.93	1.43	1.33
3	A	318	CB3	CP1-N10	4.63	1.50	1.46
3	A	318	CB3	C9-N10	3.80	1.51	1.46
2	A	317	UMP	O4'-C1'	3.52	1.50	1.42
3	A	318	CB3	C7-C6	2.94	1.45	1.38
3	A	318	CB3	C16-C15	2.82	1.43	1.38
2	A	317	UMP	C2-N3	2.75	1.43	1.38
3	A	318	CB3	C13-C14	2.47	1.44	1.39
3	A	318	CB3	C15-C14	2.47	1.44	1.39
3	A	318	CB3	C5-C6	2.36	1.42	1.37
3	A	318	CB3	C8-C7	2.33	1.41	1.36
3	A	318	CB3	C16-C11	2.31	1.43	1.39
2	A	317	UMP	P-OP3	-2.16	1.46	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	318	CB3	C4A-C8A-N1	-9.97	118.18	123.60
3	A	318	CB3	C4A-C4-N3	-8.22	118.67	124.40
3	A	318	CB3	N1-C2-N3	-5.21	120.28	127.22
2	A	317	UMP	C6-N1-C2	-4.45	114.12	121.20
3	A	318	CB3	C4-N3-C2	3.87	122.08	115.93
2	A	317	UMP	C5-C4-N3	-3.52	115.56	123.31
3	A	318	CB3	C6-C9-N10	3.50	119.82	114.18
3	A	318	CB3	O-C-C11	3.41	127.01	120.94
3	A	318	CB3	CP1-CP2-CP3	-2.87	172.86	177.67
3	A	318	CB3	CB-CG-CD	2.80	119.60	113.59
3	A	318	CB3	CP1-N10-C9	2.79	119.75	117.10
2	A	317	UMP	C5-C6-N1	-2.69	114.68	120.68
3	A	318	CB3	O-C-N	-2.66	117.55	122.45
3	A	318	CB3	CG-CB-CA	2.25	117.58	113.04
3	A	318	CB3	C7-C8-C8A	-2.22	118.04	120.84

There are no chirality outliers.

All (15) torsion outliers are listed below:

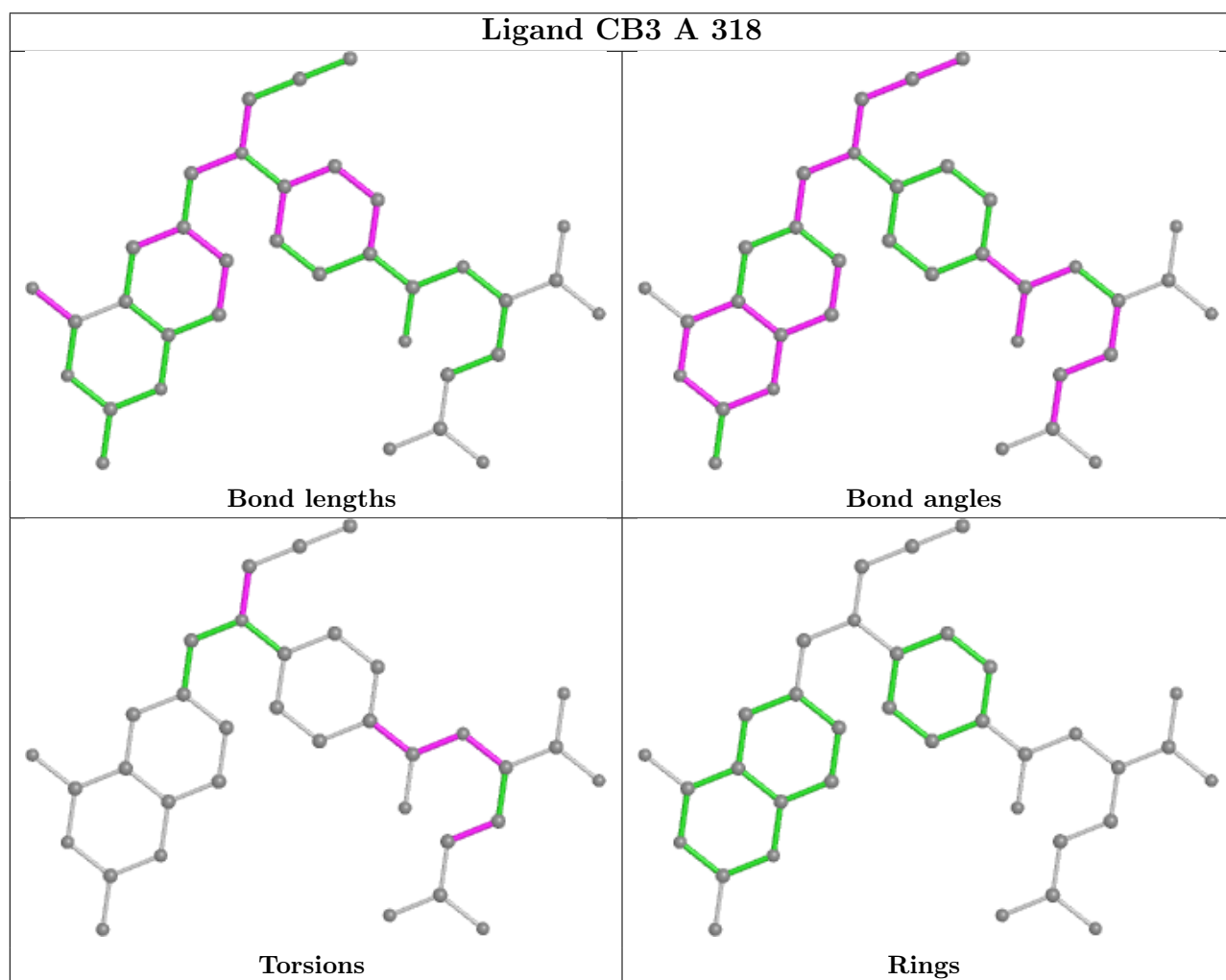
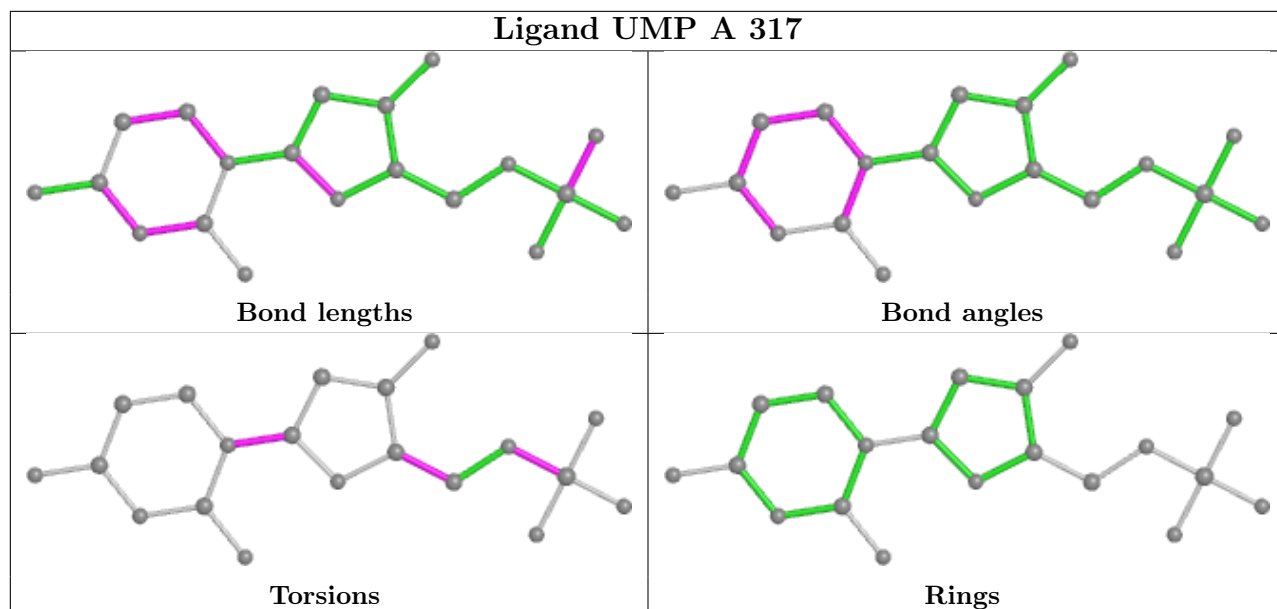
Mol	Chain	Res	Type	Atoms
2	A	317	UMP	O4'-C1'-N1-C6
3	A	318	CB3	CP2-CP1-N10-C9
3	A	318	CB3	C11-C-N-CA
3	A	318	CB3	CT-CA-N-C
3	A	318	CB3	O-C-C11-C12
3	A	318	CB3	N-C-C11-C12
3	A	318	CB3	O-C-C11-C16
3	A	318	CB3	N-C-C11-C16
3	A	318	CB3	O-C-N-CA
2	A	317	UMP	O4'-C4'-C5'-O5'
3	A	318	CB3	CA-CB-CG-CD
3	A	318	CB3	CB-CA-N-C
3	A	318	CB3	CP2-CP1-N10-C14
2	A	317	UMP	C3'-C4'-C5'-O5'
2	A	317	UMP	C5'-O5'-P-OP3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	317	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 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%)	-0.80	0 100 100	7, 15, 24, 30	0

There are no RSRZ outliers to report.

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 monosaccharides in this entry.

6.4 Ligands [i](#)

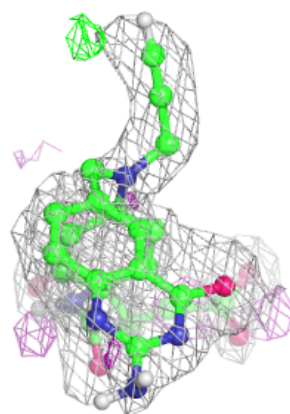
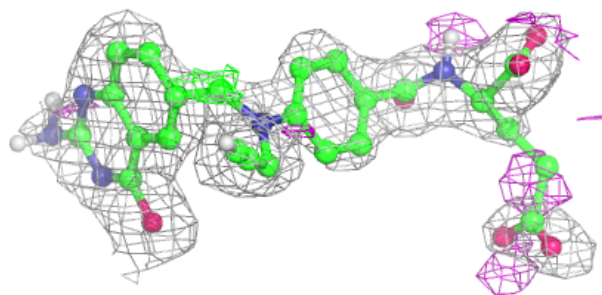
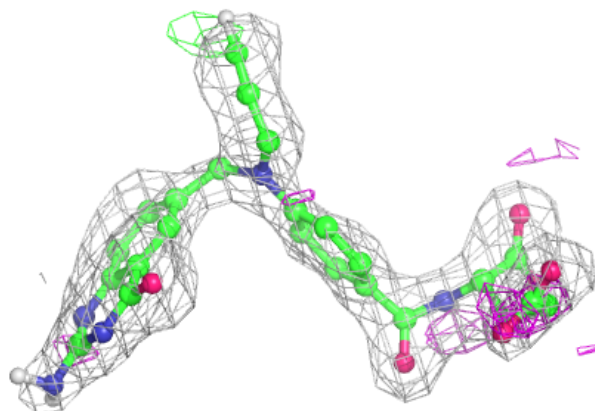
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

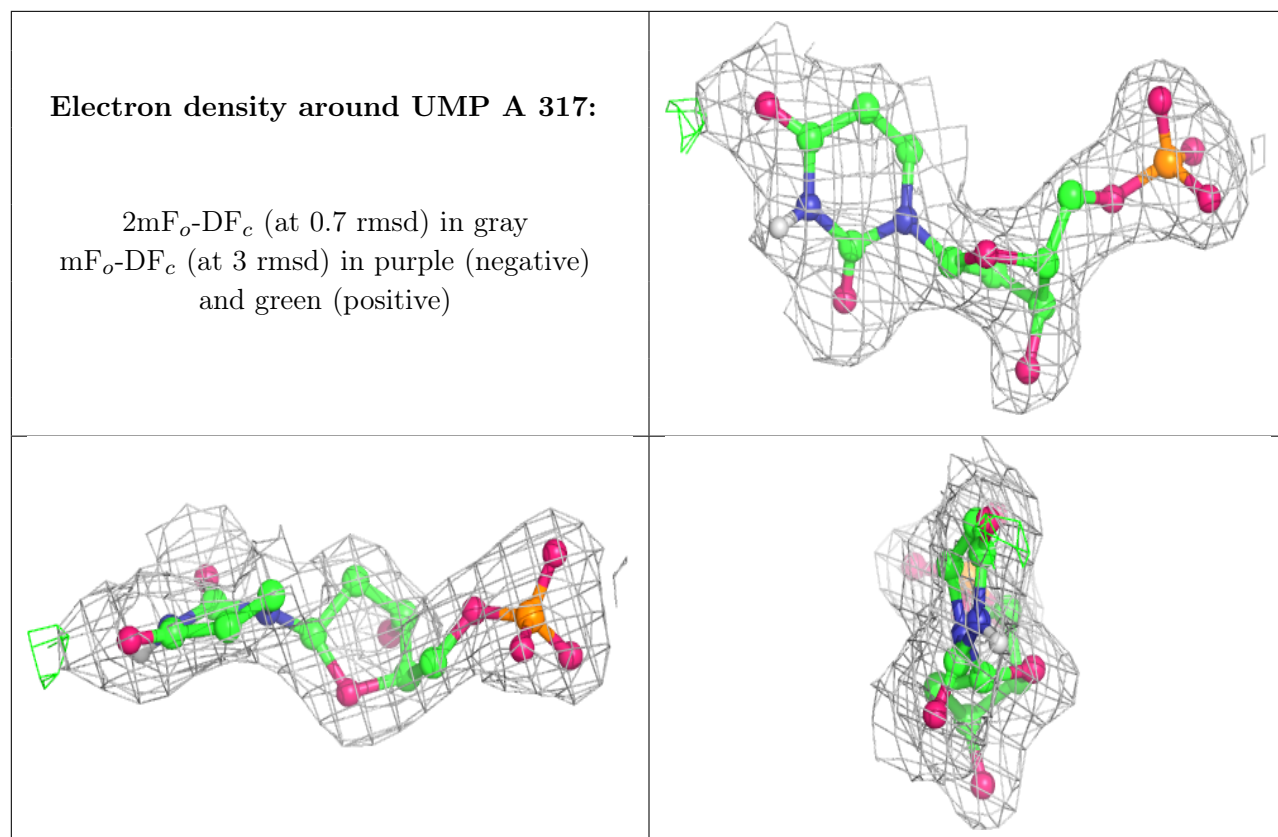
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CB3	A	318	35/35	0.87	0.18	15,29,34,34	0
2	UMP	A	317	20/20	0.96	0.09	15,19,21,22	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.