



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:12 PM UTC

PDB ID : 1ZPR / pdb_00001zpr
Title : E. COLI THYMIDYLATE SYNTHASE MUTANT E58Q IN COMPLEX
WITH CB3717 AND 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (DUMP)
Authors : Sage, C.R.; Stout, T.J.; Rutenber, E.E.; Stroud, R.M.
Deposited on : 1996-10-15
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

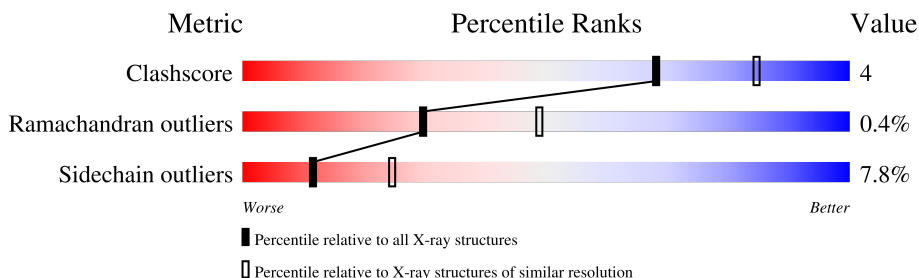
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4594 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

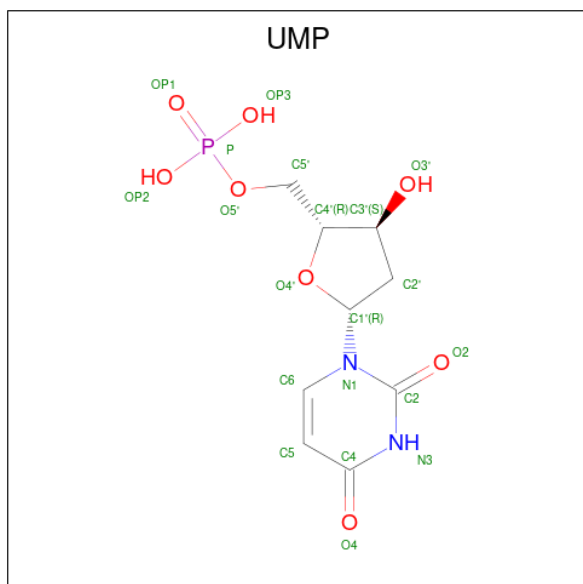
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2153	1375	372	394	12			
1	B	264	Total	C	N	O	S	0	0	0
			2153	1375	372	394	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	GLN	GLU	engineered mutation	UNP P0A884
B	58	GLN	GLU	engineered mutation	UNP P0A884

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



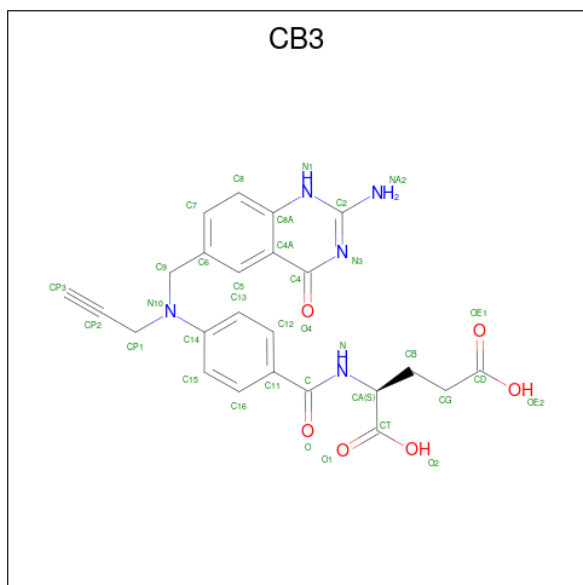
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is water.

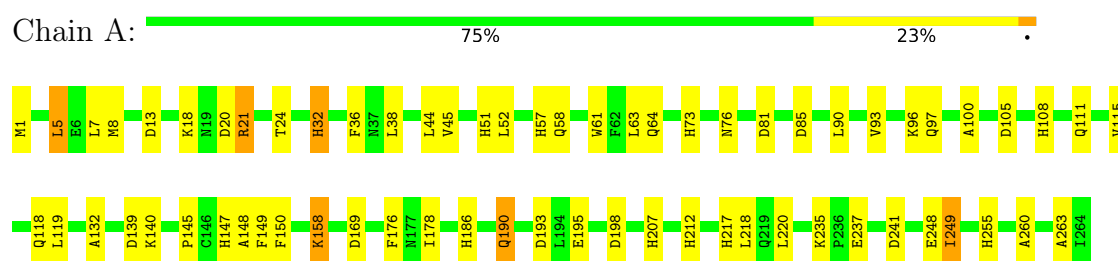
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	65	Total	O	0	0
			65	65		

3 Residue-property plots [i](#)

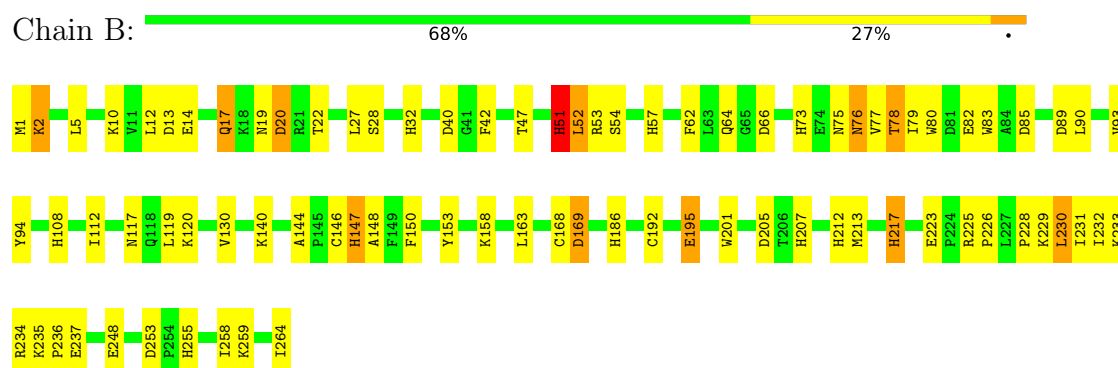
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: THYMIDYLATE SYNTHASE



• Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	127.22Å 127.22Å 68.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	86.3 (7.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.152 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4594	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, CB3, CXM

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	1.08	13/2202 (0.6%)	1.83	42/2990 (1.4%)
1	B	1.06	11/2202 (0.5%)	1.84	55/2990 (1.8%)
All	All	1.07	24/4404 (0.5%)	1.83	97/5980 (1.6%)

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	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	45	VAL	CA-CB	7.06	1.61	1.54
1	B	57	HIS	CD2-NE2	-6.97	1.30	1.37
1	B	255	HIS	CD2-NE2	-6.86	1.30	1.37
1	B	73	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	57	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	51	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	212	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	108	HIS	CG-ND1	-6.55	1.31	1.38
1	A	73	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	255	HIS	CD2-NE2	-6.50	1.30	1.37
1	B	147	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	217	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	217	HIS	CD2-NE2	-6.12	1.31	1.37
1	A	207	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	186	HIS	CD2-NE2	-5.87	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	32	HIS	CD2-NE2	-5.84	1.31	1.37
1	A	51	HIS	CD2-NE2	-5.72	1.31	1.37
1	B	212	HIS	CD2-NE2	-5.70	1.31	1.37
1	B	186	HIS	CD2-NE2	-5.55	1.31	1.37
1	B	108	HIS	CD2-NE2	-5.52	1.31	1.37
1	B	207	HIS	CD2-NE2	-5.50	1.31	1.37
1	B	32	HIS	CD2-NE2	-5.46	1.31	1.37

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	HIS	CA-CB-CG	12.90	126.70	113.80
1	A	85	ASP	CA-CB-CG	10.85	123.44	112.60
1	A	147	HIS	CA-CB-CG	10.06	123.86	113.80
1	B	51	HIS	CB-CG-CD2	-9.20	119.23	131.20
1	B	85	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	148	ALA	N-CA-C	8.46	123.38	112.89
1	A	105	ASP	CA-CB-CG	8.17	120.77	112.60
1	B	169	ASP	CA-CB-CG	8.09	120.69	112.60
1	B	40	ASP	CA-CB-CG	7.89	120.49	112.60
1	B	150	PHE	CA-CB-CG	7.88	121.68	113.80
1	A	13	ASP	CA-CB-CG	7.80	120.40	112.60
1	A	149	PHE	CA-CB-CG	7.75	121.55	113.80
1	A	150	PHE	CA-CB-CG	7.70	121.50	113.80
1	B	51	HIS	CB-CG-ND1	7.26	133.60	122.70
1	B	93	VAL	N-CA-CB	-6.99	99.70	111.23
1	A	97	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	B	76	ASN	CA-CB-CG	-6.77	105.83	112.60
1	B	27	LEU	N-CA-C	-6.77	97.38	108.41
1	A	158	LYS	CB-CG-CD	-6.71	95.86	111.30
1	B	147	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	B	75	ASN	CA-CB-CG	-6.58	106.02	112.60
1	B	78	THR	N-CA-CB	-6.57	101.53	110.67
1	B	66	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	260	ALA	CA-C-N	6.53	126.45	119.85
1	A	260	ALA	C-N-CA	6.53	126.45	119.85
1	A	57	HIS	CA-CB-CG	-6.52	107.28	113.80
1	A	64	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	B	147	HIS	CA-CB-CG	6.47	120.27	113.80
1	B	20	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	57	HIS	CA-CB-CG	-6.42	107.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ILE	N-CA-C	-6.37	98.95	108.12
1	A	198	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	52	LEU	N-CA-C	6.28	118.93	111.71
1	B	117	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	21	ARG	NE-CZ-NH2	-6.24	113.58	119.20
1	A	111	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	B	28	SER	N-CA-C	6.15	119.22	109.50
1	A	21	ARG	CB-CG-CD	-6.11	97.24	111.30
1	A	193	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	20	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	148	ALA	N-CA-C	5.97	119.75	112.23
1	B	255	HIS	CB-CG-CD2	-5.85	123.60	131.20
1	B	207	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	A	58	GLN	OE1-CD-NE2	-5.82	116.78	122.60
1	A	140	LYS	N-CA-C	-5.79	106.26	113.38
1	A	217	HIS	CB-CG-CD2	-5.75	123.73	131.20
1	B	253	ASP	CA-C-N	5.64	125.84	120.31
1	B	253	ASP	C-N-CA	5.64	125.84	120.31
1	B	140	LYS	N-CA-C	-5.64	106.17	113.16
1	A	21	ARG	CA-CB-CG	5.59	125.28	114.10
1	B	83	TRP	CG-CD2-CE3	5.59	139.49	133.90
1	A	51	HIS	CA-CB-CG	-5.57	108.23	113.80
1	B	13	ASP	N-CA-C	5.55	119.22	112.23
1	B	80	TRP	CE2-CD2-CG	-5.52	100.57	107.20
1	B	217	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	B	212	HIS	N-CA-C	-5.50	105.19	112.94
1	A	207	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	207	HIS	N-CA-C	5.47	117.39	109.07
1	B	205	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	132	ALA	N-CA-C	-5.43	106.70	113.38
1	B	93	VAL	CA-CB-CG2	-5.42	101.19	110.40
1	A	21	ARG	N-CA-CB	-5.41	101.60	110.14
1	B	2	LYS	CA-CB-CG	5.40	124.89	114.10
1	B	19	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	A	263	ALA	N-CA-C	-5.32	100.63	109.46
1	B	64	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	B	230	LEU	CD1-CG-CD2	-5.30	99.14	110.80
1	A	21	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	A	61	TRP	CG-CD2-CE3	5.30	139.20	133.90
1	B	147	HIS	CB-CG-ND1	5.30	130.64	122.70
1	A	235	LYS	CA-C-N	5.28	125.57	119.92
1	A	235	LYS	C-N-CA	5.28	125.57	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ILE	N-CA-C	-5.26	100.18	107.80
1	A	20	ASP	CA-C-N	5.24	128.04	120.38
1	A	20	ASP	C-N-CA	5.24	128.04	120.38
1	B	57	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	B	78	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	57	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	B	17	GLN	CB-CG-CD	5.20	121.44	112.60
1	B	62	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	83	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	B	112	ILE	O-C-N	-5.17	116.50	121.83
1	B	130	VAL	N-CA-C	-5.15	100.70	108.12
1	B	144	ALA	CA-C-N	5.14	125.38	119.83
1	B	144	ALA	C-N-CA	5.14	125.38	119.83
1	A	44	LEU	CA-C-O	-5.13	114.84	120.43
1	B	89	ASP	N-CA-C	5.13	118.11	110.52
1	A	51	HIS	CB-CG-CD2	-5.12	124.54	131.20
1	B	93	VAL	CA-CB-CG1	5.11	119.09	110.40
1	A	81	ASP	N-CA-C	5.10	116.84	111.28
1	A	169	ASP	N-CA-C	-5.05	100.28	108.41
1	B	235	LYS	CA-C-N	5.05	125.05	120.21
1	B	235	LYS	C-N-CA	5.05	125.05	120.21
1	A	139	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	190	GLN	CG-CD-NE2	5.03	123.94	116.40
1	B	201	TRP	CG-CD2-CE3	5.02	138.92	133.90
1	B	76	ASN	N-CA-C	5.01	118.69	112.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	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	2153	0	2081	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2153	0	2082	17	0
2	A	20	0	10	1	0
2	B	20	0	11	1	0
3	A	35	0	21	2	0
3	B	35	0	21	4	0
4	A	113	0	0	0	0
4	B	65	0	0	0	0
All	All	4594	0	4226	31	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 4.

All (31) 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:B:233:LYS:HD2	1:B:248:GLU:HB2	1.77	0.67
1:A:52:LEU:HD21	1:A:249:ILE:HD13	1.82	0.62
1:B:158:LYS:HG2	1:B:195:GLU:HG2	1.81	0.61
1:B:231:ILE:HB	1:B:248:GLU:HB3	1.85	0.57
1:B:146:CYS:SG	3:B:300:CB3:NA2	2.77	0.57
1:B:10:LYS:HG2	1:B:14:GLU:OE1	2.06	0.56
1:B:147:HIS:HB2	1:B:163:LEU:HD11	1.88	0.56
3:B:300:CB3:H13	3:B:300:CB3:CP2	2.37	0.53
1:A:18:LYS:HE2	1:B:153:TYR:CE1	2.44	0.52
1:A:5:LEU:HD12	1:A:8:MET:HE2	1.95	0.48
1:B:5:LEU:HD11	1:B:47:THR:HG21	1.95	0.47
1:B:234:ARG:O	1:B:236:PRO:HD3	2.14	0.47
1:A:7:LEU:HD13	1:A:32:HIS:CD2	2.50	0.46
1:B:77:VAL:HG12	1:B:79:ILE:HG12	1.97	0.45
1:A:96:LYS:HE2	1:A:100:ALA:O	2.17	0.45
1:B:120:LYS:HE2	1:B:192:CYS:SG	2.57	0.45
1:A:8:MET:HE3	1:A:220:LEU:HG	1.99	0.44
1:A:36:PHE:CZ	1:A:178:ILE:HD13	2.53	0.44
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.85	0.44
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.83	0.43
3:B:300:CB3:HP11	3:B:300:CB3:H5	2.00	0.43
1:B:51:HIS:HE1	1:B:54:SER:OG	2.01	0.43
1:B:229:LYS:HD3	1:B:229:LYS:HA	1.86	0.43
2:A:301:UMP:O4	3:A:300:CB3:CP3	2.67	0.42
3:B:300:CB3:CP2	3:B:300:CB3:C13	2.94	0.42
1:B:168:CYS:HA	2:B:301:UMP:O2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD21	1:A:249:ILE:CD1	2.49	0.41
1:B:42:PHE:HB3	1:B:228:PRO:HG2	2.02	0.41
1:A:158:LYS:HA	1:A:195:GLU:O	2.19	0.41
3:A:300:CB3:CP2	3:A:300:CB3:H15	2.50	0.41
1:B:213:MET:O	1:B:217:HIS:ND1	2.55	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	262/264 (99%)	255 (97%)	6 (2%)	1 (0%)	30	49
1	B	262/264 (99%)	250 (95%)	11 (4%)	1 (0%)	30	49
All	All	524/528 (99%)	505 (96%)	17 (3%)	2 (0%)	30	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	TYR
1	A	93	VAL

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	232/232 (100%)	217 (94%)	15 (6%)	15	32
1	B	232/232 (100%)	211 (91%)	21 (9%)	9	19
All	All	464/464 (100%)	428 (92%)	36 (8%)	11	24

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	24	THR
1	A	38	LEU
1	A	63	LEU
1	A	76	ASN
1	A	90	LEU
1	A	119	LEU
1	A	145	PRO
1	A	176	PHE
1	A	190	GLN
1	A	218	LEU
1	A	237	GLU
1	A	241	ASP
1	A	248	GLU
1	A	249	ILE
1	B	2	LYS
1	B	12	LEU
1	B	17	GLN
1	B	20	ASP
1	B	22	THR
1	B	51	HIS
1	B	52	LEU
1	B	53	ARG
1	B	76	ASN
1	B	78	THR
1	B	82	GLU
1	B	90	LEU
1	B	169	ASP
1	B	195	GLU
1	B	223	GLU
1	B	225	ARG
1	B	226	PRO
1	B	230	LEU
1	B	237	GLU
1	B	259	LYS

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Mol	Chain	Res	Type
1	B	264	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	51	HIS
1	A	118	GLN
1	A	162	GLN
1	A	191	GLN
1	B	51	HIS
1	B	64	GLN
1	B	108	HIS
1	B	177	ASN
1	B	190	GLN
1	B	207	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CXM	A	1	1	9,10,11	0.85	0	9,11,13	4.16	3 (33%)
1	CXM	B	1	1	9,10,11	0.73	0	9,11,13	3.95	2 (22%)

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
1	CXM	A	1	1	-	2/9/10/12	-
1	CXM	B	1	1	-	1/9/10/12	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	CXM	ON1-CN-N	-11.80	105.50	124.86
1	B	1	CXM	ON1-CN-N	-11.45	106.08	124.86
1	A	1	CXM	O-C-CA	-3.08	116.84	124.77
1	B	1	CXM	O-C-CA	-2.84	117.47	124.77
1	A	1	CXM	C-CA-N	-2.23	105.19	109.50

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	ON1-CN-N-CA
1	A	1	CXM	C-CA-N-CN
1	B	1	CXM	ON1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	B	301	-	21,21,21	1.37	2 (9%)	30,31,31	1.77	7 (23%)
2	UMP	A	301	1	21,21,21	2.74	5 (23%)	30,31,31	2.10	11 (36%)
3	CB3	B	300	-	37,37,37	2.03	6 (16%)	50,51,51	2.73	11 (22%)
3	CB3	A	300	-	37,37,37	2.01	6 (16%)	50,51,51	1.39	6 (12%)

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	B	301	-	-	4/10/22/22	0/2/2/2
2	UMP	A	301	1	-	0/10/22/22	0/2/2/2
3	CB3	B	300	-	-	7/27/28/28	0/3/3/3
3	CB3	A	300	-	-	7/27/28/28	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	UMP	C6-C5	9.39	1.56	1.35
3	B	300	CB3	O4-C4	8.83	1.38	1.23
3	A	300	CB3	O4-C4	8.53	1.37	1.23
2	A	301	UMP	C6-N1	5.50	1.51	1.38
3	A	300	CB3	C4A-C4	-4.06	1.41	1.48
2	A	301	UMP	C5-C4	3.90	1.52	1.43
3	B	300	CB3	C4A-C4	-3.66	1.41	1.48
2	B	301	UMP	O4'-C1'	3.02	1.49	1.42
3	B	300	CB3	C8A-N1	-2.89	1.35	1.39
2	B	301	UMP	C6-N1	-2.63	1.31	1.38
2	A	301	UMP	O4'-C1'	2.36	1.47	1.42
3	A	300	CB3	C9-N10	2.35	1.49	1.46
3	B	300	CB3	C9-N10	2.23	1.49	1.46
3	A	300	CB3	C8A-N1	-2.19	1.36	1.39
2	A	301	UMP	C2-N1	2.18	1.41	1.38
3	B	300	CB3	OE2-CD	-2.09	1.23	1.30
3	A	300	CB3	O2-CT	-2.09	1.24	1.30
3	A	300	CB3	OE2-CD	-2.05	1.24	1.30
3	B	300	CB3	O2-CT	-2.04	1.24	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	300	CB3	CP2-CP1-N10	-9.37	104.80	113.45
3	B	300	CB3	C6-C9-N10	8.49	127.88	114.13
3	B	300	CB3	CP1-N10-C9	7.05	124.29	117.19
2	B	301	UMP	O4'-C1'-N1	5.83	118.21	107.86
2	A	301	UMP	O4'-C1'-N1	5.62	117.83	107.86
3	B	300	CB3	CP1-CP2-CP3	-5.26	169.11	177.63
3	B	300	CB3	CG-CB-CA	4.98	122.34	113.16
3	B	300	CB3	C9-C6-C7	-4.86	111.80	120.75
2	A	301	UMP	C5-C6-N1	-4.76	114.10	121.84
3	B	300	CB3	C9-C6-C5	4.32	128.42	120.27
3	A	300	CB3	CP1-N10-C9	-4.09	113.07	117.19
2	B	301	UMP	C1'-N1-C6	-3.91	113.83	121.53
3	A	300	CB3	C9-N10-C14	3.67	127.07	120.72
3	B	300	CB3	C9-N10-C14	-3.65	114.40	120.72
3	B	300	CB3	C8A-C4A-C4	-3.24	116.61	120.11
3	A	300	CB3	CG-CB-CA	3.20	119.06	113.16
2	A	301	UMP	N3-C2-N1	3.08	118.90	114.89
3	A	300	CB3	C8A-C4A-C4	-2.89	116.99	120.11
2	B	301	UMP	C1'-N1-C2	2.78	123.10	117.66
2	B	301	UMP	OP2-P-O5'	2.69	113.68	106.67
2	A	301	UMP	O4-C4-C5	-2.58	120.72	125.16
2	A	301	UMP	OP3-P-O5'	2.54	113.30	106.67
2	A	301	UMP	O4'-C1'-C2'	-2.54	101.50	106.25
2	A	301	UMP	C1'-N1-C6	-2.50	116.61	121.53
2	A	301	UMP	O5'-P-OP1	2.47	113.11	106.44
2	B	301	UMP	O4'-C1'-C2'	-2.41	101.74	106.25
2	A	301	UMP	C2'-C3'-C4'	-2.31	98.11	102.80
2	A	301	UMP	O4-C4-N3	2.29	122.59	119.27
2	B	301	UMP	C2'-C3'-C4'	-2.24	98.26	102.80
3	A	300	CB3	CP2-CP1-N10	-2.21	111.41	113.45
2	B	301	UMP	O2-C2-N1	2.20	125.66	122.80
3	B	300	CB3	O-C-N	-2.11	118.46	122.47
3	B	300	CB3	C5-C4A-C4	2.09	124.24	119.51
3	A	300	CB3	CB-CG-CD	2.07	118.02	112.49
2	A	301	UMP	O2-C2-N3	-2.02	117.77	121.49

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	300	CB3	N-CA-CB-CG
3	B	300	CB3	C6-C9-N10-CP1
3	A	300	CB3	CT-CA-CB-CG

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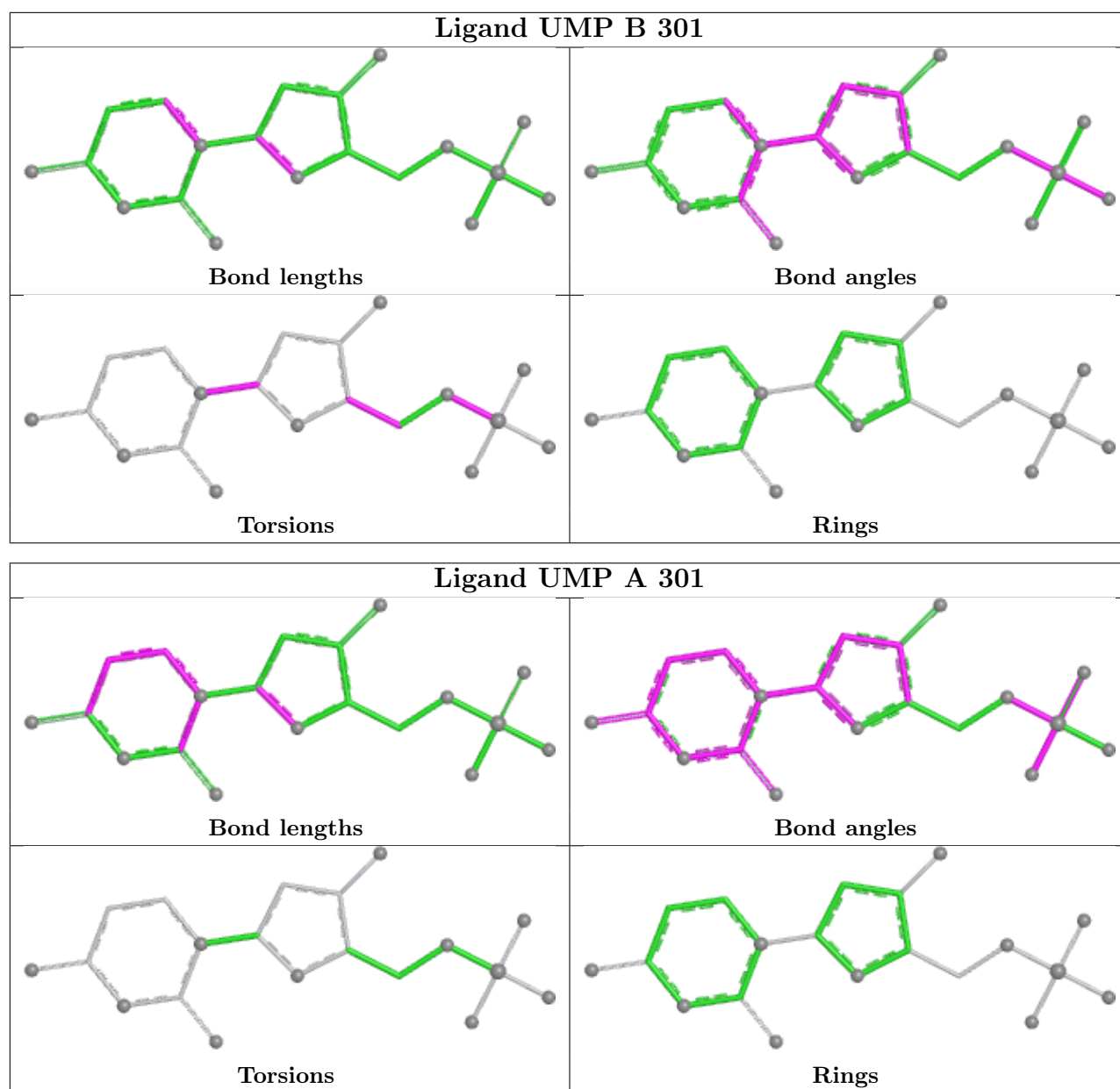
Mol	Chain	Res	Type	Atoms
2	B	301	UMP	O4'-C4'-C5'-O5'
2	B	301	UMP	C3'-C4'-C5'-O5'
2	B	301	UMP	C2'-C1'-N1-C2
3	A	300	CB3	N-CA-CB-CG
3	B	300	CB3	CT-CA-CB-CG
3	A	300	CB3	C15-C14-N10-C9
3	A	300	CB3	OE1-CD-CG-CB
3	A	300	CB3	OE2-CD-CG-CB
3	A	300	CB3	C13-C14-N10-C9
3	B	300	CB3	CA-CB-CG-CD
2	B	301	UMP	C5'-O5'-P-OP3
3	B	300	CB3	C6-C9-N10-C14
3	B	300	CB3	C13-C14-N10-C9
3	A	300	CB3	C5-C6-C9-N10
3	B	300	CB3	C15-C14-N10-C9

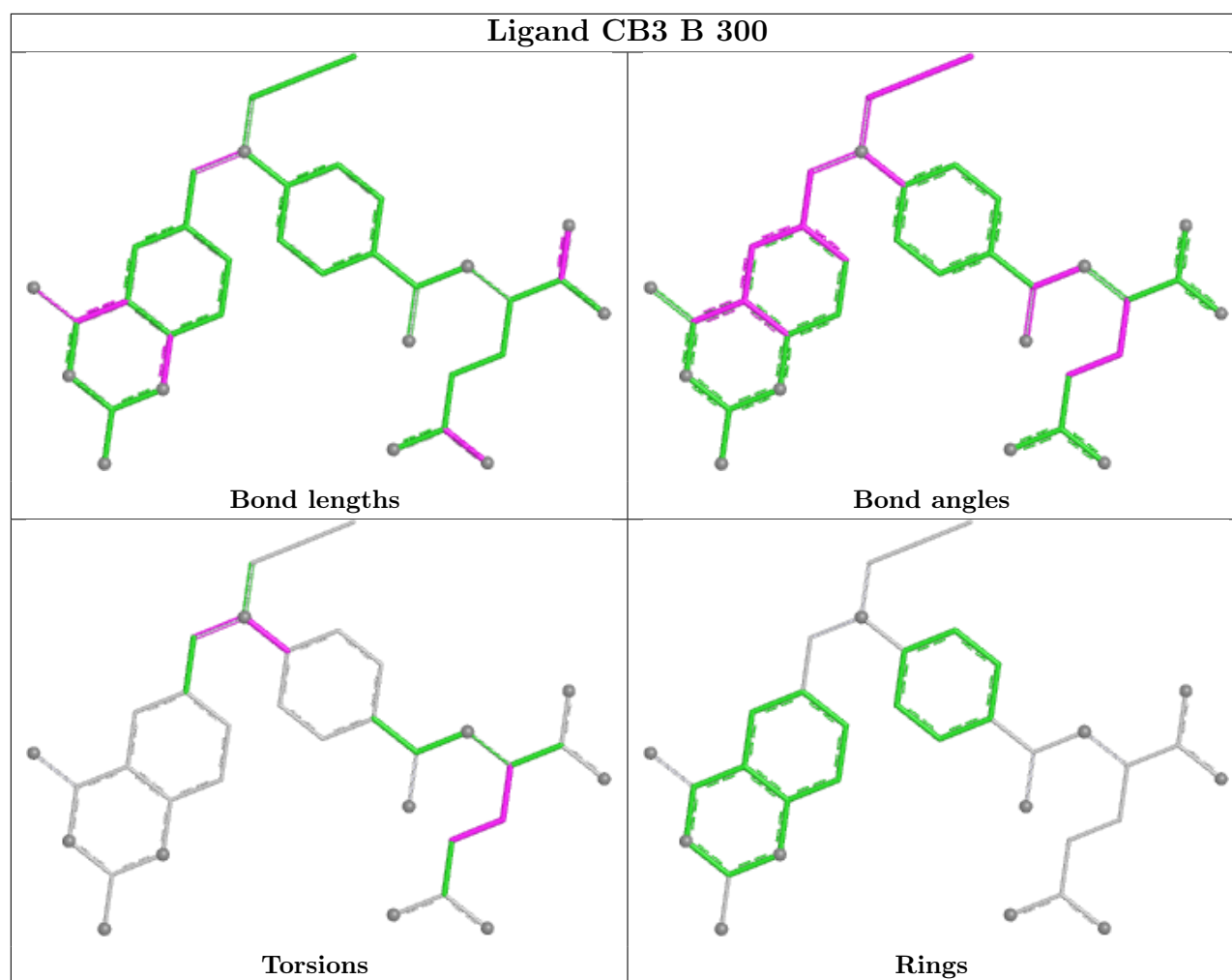
There are no ring outliers.

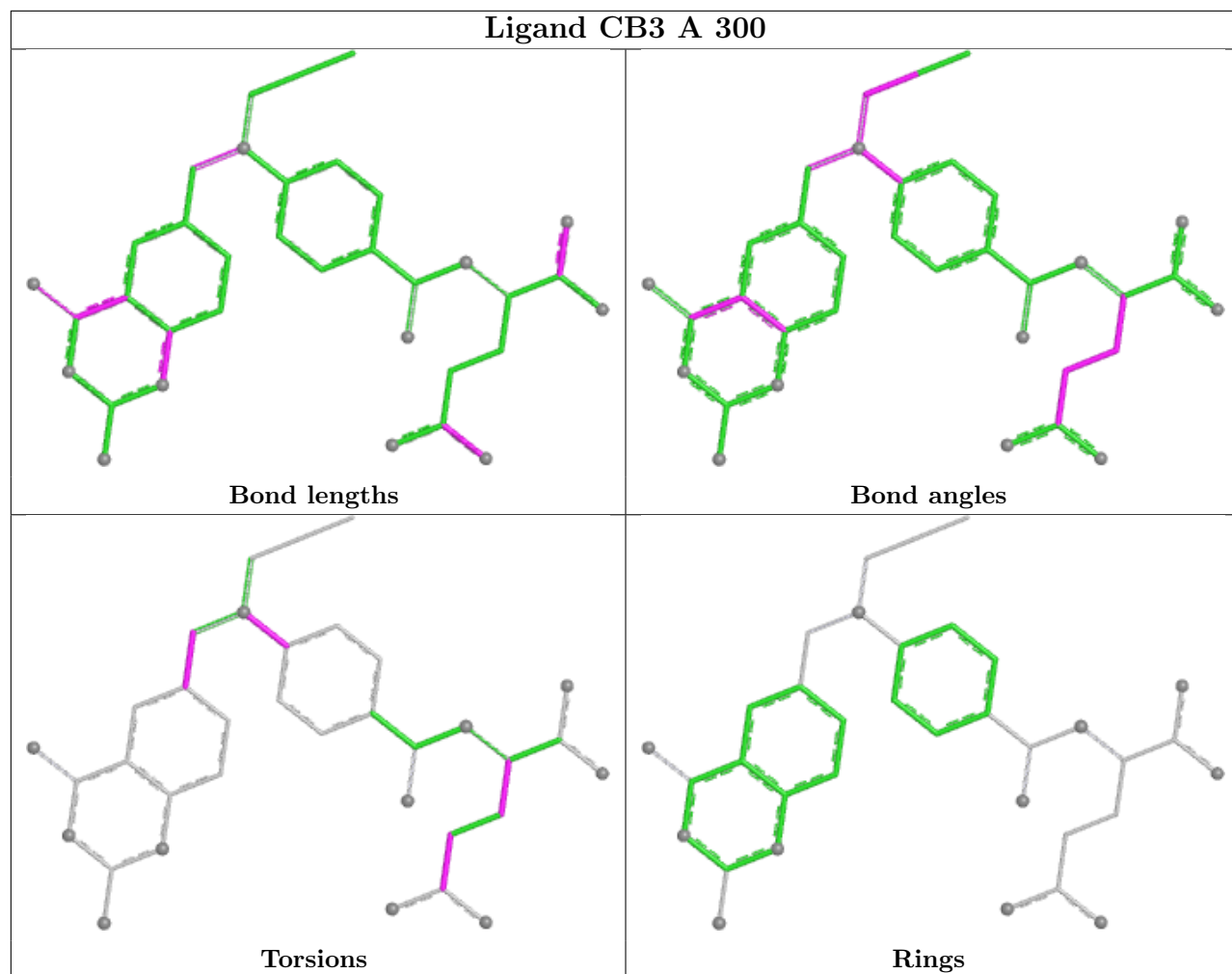
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	UMP	1	0
2	A	301	UMP	1	0
3	B	300	CB3	4	0
3	A	300	CB3	2	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.