



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:16 AM UTC

PDB ID : 1TSD / pdb\_00001tsd  
Title : THYMIDYLATE SYNTHASE COMPLEX WITH 2'-DEOXYURIDINE 5'-  
MONOPHOSPHATE (DUMP) AND FOLATE ANALOG 1843U89  
Authors : Weichsel, A.; Montfort, W.R.  
Deposited on : 1995-08-15  
Resolution : 1.95 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.

The types of validation reports are described at

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

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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)  
Xtrriage (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

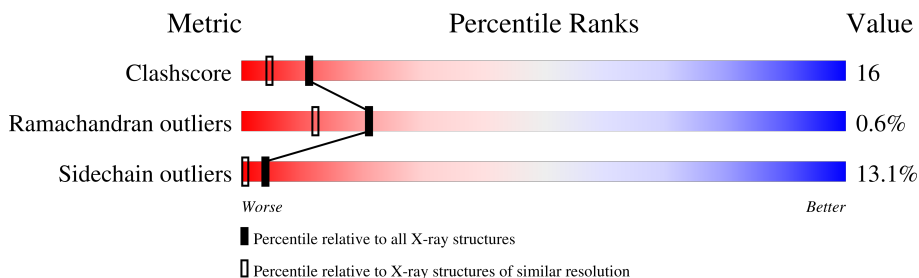
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	265	51% (green), 33% (yellow), 12% (orange/red)
1	B	265	42% (green), 42% (yellow), 12% (orange/red)

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	BME	A	265	-	-	X	-
2	BME	A	266	-	-	X	-

## 2 Entry composition [i](#)

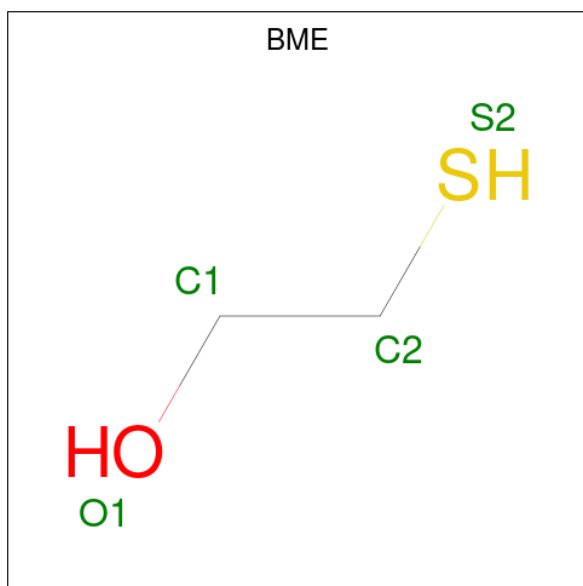
There are 5 unique types of molecules in this entry. The entry contains 4616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

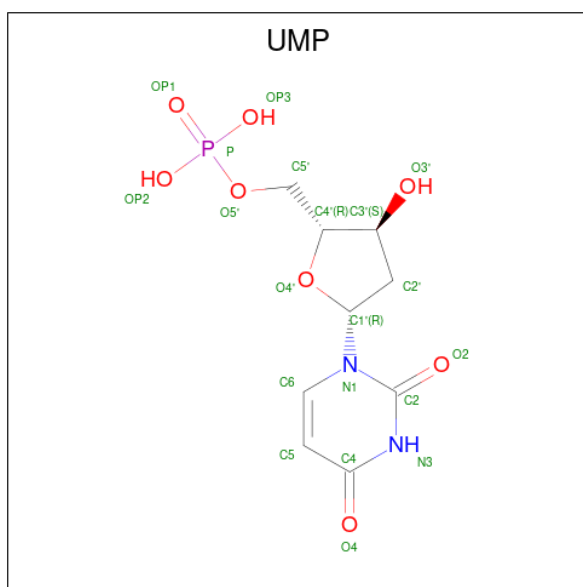
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2153	1375	371	395	12	0	0	0
1	B	265	2153	1375	371	395	12	0	0	0

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



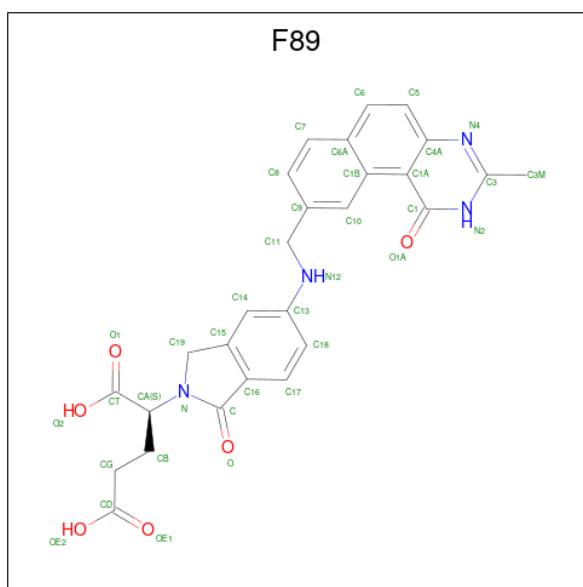
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
2	A	1	4	2	1	1	0	0
2	A	1	4	2	1	1	0	0

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>8</sub>P).



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

- Molecule 4 is *S*-2-(5(((1,2-DIHYDRO-3-METHYL-1-OXOBENZO(F)QUINAZOLIN-9-YL)METHYL)AMINO)1-OXO-2-ISOINDOLINYL)GLUTARIC ACID (CCD ID: F89) (formula: C<sub>27</sub>H<sub>24</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	37	27	4	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	37	27	4	6	0	0

- Molecule 5 is water.

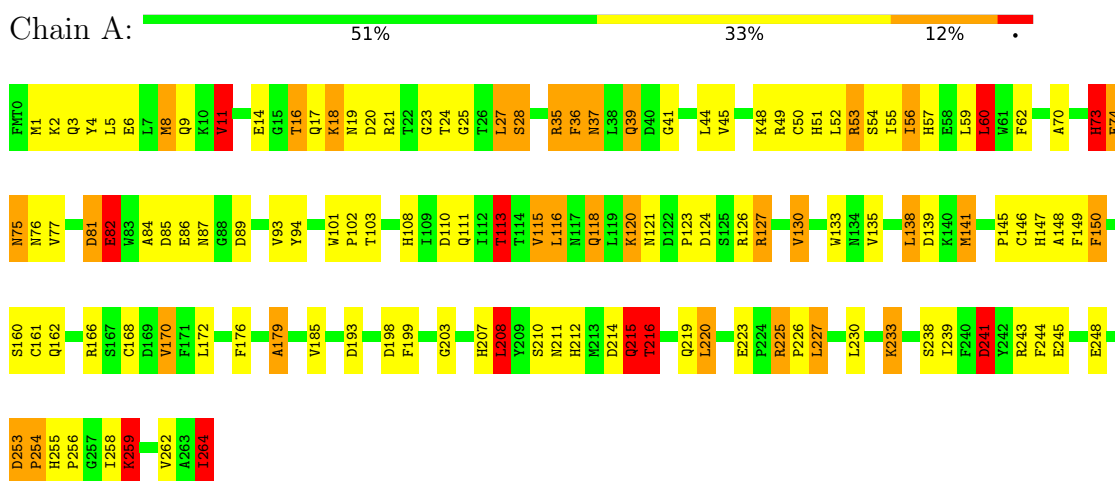
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	80	Total	O	0	0
			80	80		

### 3 Residue-property plots [i](#)

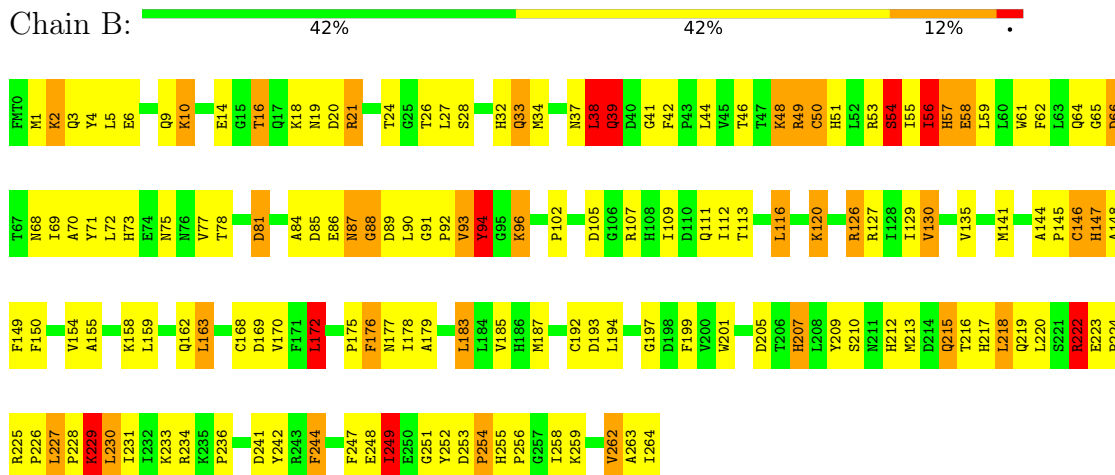
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.52Å 127.52Å 68.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 1.95	Depositor
% Data completeness (in resolution range)	98.9 (7.00-1.95)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, $R_{free}$	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 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: FMT, BME, F89, 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	1.40	1/2210 (0.0%)	2.37	133/3000 (4.4%)
1	B	1.35	1/2210 (0.0%)	2.42	156/3000 (5.2%)
All	All	1.37	2/4420 (0.0%)	2.39	289/6000 (4.8%)

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	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	TYR	N-CA	6.62	1.54	1.45
1	A	133	TRP	CA-C	-5.18	1.47	1.53

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASP	CA-CB-CG	11.68	124.28	112.60
1	B	147	HIS	CA-CB-CG	11.33	125.13	113.80
1	B	126	ARG	NE-CZ-NH2	-10.90	109.39	119.20
1	A	214	ASP	CA-CB-CG	10.62	123.22	112.60
1	B	68	ASN	CA-CB-CG	-10.28	102.32	112.60
1	A	73	HIS	CA-CB-CG	-9.91	103.89	113.80
1	B	94	TYR	CA-C-N	9.89	131.17	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	TYR	C-N-CA	9.89	131.17	119.99
1	B	130	VAL	N-CA-CB	9.87	125.02	111.41
1	A	76	ASN	OD1-CG-ND2	9.84	132.44	122.60
1	B	56	ILE	CA-CB-CG2	9.70	126.98	110.50
1	A	76	ASN	CA-CB-CG	-9.50	103.10	112.60
1	B	149	PHE	N-CA-CB	-9.36	94.20	111.13
1	B	116	LEU	CA-C-N	9.28	132.72	120.28
1	B	116	LEU	C-N-CA	9.28	132.72	120.28
1	B	44	LEU	CA-C-O	-8.98	110.44	120.32
1	B	41	GLY	CA-C-O	-8.95	115.45	122.52
1	B	20	ASP	CA-C-N	8.84	134.07	120.82
1	B	20	ASP	C-N-CA	8.84	134.07	120.82
1	A	262	VAL	CA-C-O	-8.78	110.66	121.11
1	A	48	LYS	CA-C-O	-8.76	111.25	120.89
1	A	141	MET	CA-C-O	-8.73	111.10	121.05
1	A	77	VAL	CB-CA-C	8.50	123.21	111.31
1	A	227	LEU	N-CA-CB	-8.45	96.71	109.98
1	B	254	PRO	CA-C-N	8.40	132.41	120.49
1	B	254	PRO	C-N-CA	8.40	132.41	120.49
1	B	168	CYS	CA-C-O	8.34	131.46	120.21
1	B	150	PHE	CA-CB-CG	8.32	122.12	113.80
1	B	241	ASP	CA-CB-CG	8.29	120.89	112.60
1	A	166	ARG	NE-CZ-NH1	-8.29	113.21	121.50
1	A	216	THR	CA-CB-CG2	8.29	124.59	110.50
1	A	259	LYS	N-CA-CB	8.25	123.86	110.41
1	A	207	HIS	CA-C-O	8.23	130.71	121.40
1	B	130	VAL	CA-CB-CG1	8.17	124.29	110.40
1	B	66	ASP	CA-CB-CG	8.16	120.76	112.60
1	A	149	PHE	N-CA-CB	-8.12	96.61	110.99
1	B	116	LEU	O-C-N	-8.03	113.74	122.09
1	B	105	ASP	N-CA-C	8.01	123.15	112.25
1	B	9	GLN	OE1-CD-NE2	7.88	130.48	122.60
1	B	81	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	20	ASP	CA-C-O	-7.77	113.13	121.45
1	B	159	LEU	CA-C-O	-7.77	112.46	120.54
1	A	258	ILE	CA-C-O	-7.72	112.47	120.27
1	B	56	ILE	CB-CA-C	7.69	121.81	111.97
1	A	111	GLN	CG-CD-NE2	7.68	127.91	116.40
1	B	27	LEU	N-CA-C	-7.65	96.75	109.07
1	B	68	ASN	OD1-CG-ND2	7.51	130.11	122.60
1	B	130	VAL	CB-CA-C	7.48	121.70	110.63
1	A	84	ALA	CA-C-O	-7.27	112.76	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ALA	N-CA-C	7.27	122.28	113.41
1	B	62	PHE	CA-CB-CG	7.24	121.03	113.80
1	B	49	ARG	CA-C-O	-7.21	112.70	120.92
1	B	213	MET	O-C-N	7.21	129.50	122.07
1	B	213	MET	N-CA-CB	7.17	120.41	110.01
1	A	74	GLU	CB-CG-CD	7.10	124.67	112.60
1	B	10	LYS	O-C-N	7.10	129.64	122.12
1	B	135	VAL	CA-C-N	7.09	132.93	120.74
1	B	135	VAL	C-N-CA	7.09	132.93	120.74
1	A	62	PHE	CA-CB-CG	7.04	120.84	113.80
1	B	24	THR	N-CA-CB	6.98	120.81	110.33
1	B	146	CYS	CA-C-N	6.97	133.50	122.34
1	B	146	CYS	C-N-CA	6.97	133.50	122.34
1	B	51	HIS	CA-CB-CG	-6.96	106.84	113.80
1	B	126	ARG	NH1-CZ-NH2	6.94	128.32	119.30
1	A	111	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	B	249	ILE	CA-C-O	6.91	127.25	120.27
1	A	216	THR	N-CA-CB	6.90	120.26	110.12
1	A	36	PHE	CA-C-O	-6.87	112.95	120.30
1	A	150	PHE	CA-CB-CG	6.85	120.65	113.80
1	A	216	THR	CA-C-O	-6.83	113.31	120.55
1	A	9	GLN	CA-C-O	6.82	128.00	120.63
1	A	76	ASN	N-CA-C	6.80	120.92	111.74
1	A	108	HIS	CA-C-O	-6.79	113.04	120.24
1	B	32	HIS	CA-CB-CG	-6.78	107.02	113.80
1	B	127	ARG	CA-C-O	-6.75	112.35	120.65
1	A	130	VAL	CA-CB-CG2	6.74	121.85	110.40
1	A	28	SER	N-CA-CB	-6.72	99.02	111.53
1	B	93	VAL	CA-C-O	6.71	129.17	120.78
1	A	108	HIS	CA-CB-CG	-6.71	107.09	113.80
1	B	32	HIS	CA-C-O	-6.71	113.48	120.99
1	B	91	GLY	O-C-N	6.64	128.41	121.77
1	A	126	ARG	CB-CG-CD	6.62	126.54	111.30
1	A	170	VAL	N-CA-C	6.61	117.36	110.62
1	A	113	THR	OG1-CB-CG2	6.59	122.49	109.30
1	B	207	HIS	CA-CB-CG	-6.59	107.21	113.80
1	A	207	HIS	N-CA-C	6.55	119.14	109.24
1	A	108	HIS	N-CA-CB	6.55	121.05	110.77
1	A	87	ASN	CA-CB-CG	-6.53	106.07	112.60
1	A	139	ASP	CA-CB-CG	-6.53	106.07	112.60
1	B	244	PHE	CB-CA-C	6.52	121.61	110.79
1	B	3	GLN	O-C-N	6.51	129.57	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	A	14	GLU	O-C-N	6.49	129.30	122.23
1	A	225	ARG	CB-CA-C	6.49	119.69	109.96
1	A	60	LEU	CA-C-N	6.46	129.23	120.44
1	A	60	LEU	C-N-CA	6.46	129.23	120.44
1	A	35	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	A	139	ASP	CB-CA-C	6.42	122.73	109.95
1	B	212	HIS	N-CA-C	-6.40	103.78	113.89
1	B	249	ILE	CA-CB-CG2	6.39	121.36	110.50
1	B	19	ASN	CA-C-O	-6.37	113.54	120.36
1	B	48	LYS	CA-CB-CG	6.36	126.81	114.10
1	B	148	ALA	N-CA-C	6.36	121.28	112.45
1	B	1	MET	CB-CA-C	6.34	122.14	110.10
1	A	199	PHE	N-CA-CB	6.32	120.97	110.47
1	B	50	CYS	CA-C-O	-6.32	113.97	121.11
1	A	102	PRO	CB-CA-C	6.32	117.15	111.40
1	B	216	THR	CA-CB-CG2	6.32	121.24	110.50
1	B	16	THR	CA-C-O	-6.28	113.83	120.80
1	A	25	GLY	O-C-N	6.28	130.86	122.70
1	B	225	ARG	CD-NE-CZ	-6.25	115.65	124.40
1	B	120	LYS	CA-C-O	-6.24	113.31	120.24
1	B	116	LEU	CA-C-O	6.24	127.57	120.90
1	A	11	VAL	N-CA-CB	6.22	119.91	110.58
1	A	264	ILE	CA-CB-CG2	6.22	121.07	110.50
1	B	224	PRO	N-CA-C	-6.21	101.34	111.21
1	A	210	SER	CA-CB-OG	-6.20	98.70	111.10
1	A	27	LEU	CA-C-N	-6.18	112.09	122.29
1	A	27	LEU	C-N-CA	-6.18	112.09	122.29
1	A	82	GLU	O-C-N	6.17	129.44	122.22
1	B	170	VAL	CA-C-O	-6.17	114.63	121.17
1	A	39	GLN	CA-CB-CG	-6.15	101.79	114.10
1	B	57	HIS	CA-CB-CG	-6.15	107.65	113.80
1	A	56	ILE	N-CA-CB	6.13	117.31	110.62
1	B	86	GLU	N-CA-CB	6.12	120.38	110.40
1	B	176	PHE	CA-C-N	6.12	128.80	120.54
1	B	176	PHE	C-N-CA	6.12	128.80	120.54
1	B	65	GLY	O-C-N	6.12	129.50	122.34
1	B	64	GLN	CB-CG-CD	6.11	122.98	112.60
1	B	38	LEU	CB-CA-C	6.09	122.60	110.17
1	A	81	ASP	N-CA-C	6.08	118.69	111.33
1	A	87	ASN	OD1-CG-ND2	6.08	128.68	122.60
1	B	227	LEU	CB-CA-C	6.07	119.05	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	SER	CB-CA-C	6.07	120.87	110.79
1	A	75	ASN	CA-CB-CG	-6.07	106.53	112.60
1	A	254	PRO	CA-C-O	-6.07	114.67	122.13
1	B	169	ASP	CB-CA-C	6.06	121.60	111.30
1	B	89	ASP	CA-CB-CG	-6.04	106.56	112.60
1	B	162	GLN	OE1-CD-NE2	-6.03	116.58	122.60
1	B	199	PHE	N-CA-CB	6.01	120.45	110.47
1	A	3	GLN	N-CA-C	6.00	117.83	111.28
1	A	253	ASP	N-CA-CB	-6.00	102.38	111.21
1	A	82	GLU	CA-C-O	-5.99	113.33	120.10
1	A	17	GLN	OE1-CD-NE2	5.98	128.58	122.60
1	B	249	ILE	O-C-N	-5.98	116.96	123.18
1	B	172	LEU	N-CA-CB	-5.98	100.92	110.19
1	B	175	PRO	CA-C-N	5.97	128.56	120.44
1	B	175	PRO	C-N-CA	5.97	128.56	120.44
1	A	149	PHE	CA-C-O	-5.93	113.43	120.43
1	A	214	ASP	N-CA-CB	5.91	118.64	110.07
1	A	123	PRO	CB-CA-C	5.91	120.31	111.68
1	B	4	TYR	CA-C-N	5.90	128.19	120.28
1	B	4	TYR	C-N-CA	5.90	128.19	120.28
1	B	28	SER	N-CA-CB	-5.88	100.35	111.00
1	A	185	VAL	CA-C-N	5.88	128.48	120.54
1	A	185	VAL	C-N-CA	5.88	128.48	120.54
1	B	33	GLN	CA-C-O	-5.84	114.28	121.06
1	B	194	LEU	CA-C-O	-5.84	114.81	121.58
1	B	42	PHE	CA-C-O	-5.82	113.98	119.80
1	B	230	LEU	CB-CA-C	5.81	119.12	109.53
1	B	87	ASN	CA-CB-CG	5.78	118.38	112.60
1	A	4	TYR	N-CA-CB	-5.76	101.71	110.07
1	A	121	ASN	N-CA-C	5.76	120.59	113.50
1	B	9	GLN	CA-C-N	5.76	128.00	120.28
1	B	9	GLN	C-N-CA	5.76	128.00	120.28
1	A	113	THR	CA-CB-CG2	5.75	120.28	110.50
1	A	113	THR	CB-CA-C	5.75	120.63	110.85
1	B	51	HIS	CB-CA-C	-5.75	101.42	110.79
1	B	126	ARG	CB-CG-CD	-5.69	98.21	111.30
1	B	56	ILE	CA-C-O	-5.68	115.14	121.17
1	B	54	SER	O-C-N	5.67	128.22	122.09
1	A	168	CYS	N-CA-C	5.67	117.68	108.26
1	B	56	ILE	N-CA-CB	5.67	117.18	110.55
1	A	24	THR	CA-C-O	-5.66	114.42	120.42
1	A	248	GLU	CA-CB-CG	5.65	125.41	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	VAL	CB-CA-C	5.65	120.55	111.29
1	B	216	THR	CA-CB-OG1	-5.64	101.14	109.60
1	A	219	GLN	CA-C-N	5.63	129.61	120.60
1	A	219	GLN	C-N-CA	5.63	129.61	120.60
1	A	215	GLN	CG-CD-NE2	5.62	124.83	116.40
1	A	211	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	241	ASP	CA-C-O	-5.60	112.80	119.35
1	A	193	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	161	CYS	CA-C-O	-5.59	113.66	120.54
1	B	205	ASP	CB-CG-OD2	5.59	131.26	118.40
1	B	111	GLN	N-CA-CB	5.59	118.44	110.16
1	A	41	GLY	O-C-N	5.59	129.97	122.70
1	A	203	GLY	CA-C-N	5.59	132.36	121.41
1	A	203	GLY	C-N-CA	5.59	132.36	121.41
1	B	222	ARG	CD-NE-CZ	-5.58	116.59	124.40
1	A	57	HIS	CA-C-O	-5.57	114.64	120.55
1	A	133	TRP	O-C-N	-5.57	115.27	122.56
1	A	227	LEU	CB-CA-C	5.56	118.31	109.52
1	A	28	SER	N-CA-C	5.56	117.85	109.23
1	A	51	HIS	CA-CB-CG	-5.55	108.25	113.80
1	B	48	LYS	CA-C-O	-5.55	112.58	120.51
1	B	251	GLY	CA-C-N	-5.54	115.05	122.42
1	B	251	GLY	C-N-CA	-5.54	115.05	122.42
1	A	233	LYS	CB-CG-CD	5.52	124.00	111.30
1	B	262	VAL	O-C-N	5.51	129.22	122.72
1	A	127	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	B	34	MET	CB-CA-C	5.50	121.78	109.56
1	A	133	TRP	CB-CA-C	5.50	120.86	112.00
1	A	57	HIS	CA-CB-CG	-5.50	108.30	113.80
1	A	118	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	A	85	ASP	CA-C-N	5.48	128.18	120.28
1	A	85	ASP	C-N-CA	5.48	128.18	120.28
1	B	217	HIS	CA-CB-CG	-5.48	108.32	113.80
1	B	112	ILE	CA-C-N	5.46	127.53	120.44
1	B	112	ILE	C-N-CA	5.46	127.53	120.44
1	A	160	SER	CA-CB-OG	-5.45	100.20	111.10
1	A	101	TRP	O-C-N	5.44	126.24	121.18
1	B	207	HIS	N-CA-C	5.44	117.45	109.24
1	A	262	VAL	CB-CA-C	-5.44	103.62	111.34
1	A	73	HIS	O-C-N	5.43	127.90	122.03
1	B	88	GLY	CA-C-N	5.43	130.13	122.09
1	B	88	GLY	C-N-CA	5.43	130.13	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	A	52	LEU	CB-CA-C	5.43	119.81	110.79
1	A	35	ARG	NE-CZ-NH1	5.43	126.93	121.50
1	B	168	CYS	O-C-N	-5.43	116.76	123.44
1	A	19	ASN	N-CA-C	-5.42	103.54	110.53
1	A	75	ASN	OD1-CG-ND2	5.39	127.99	122.60
1	B	251	GLY	O-C-N	5.35	128.59	122.33
1	B	111	GLN	CA-C-O	-5.35	114.75	120.42
1	B	10	LYS	CA-C-O	-5.32	114.91	120.55
1	A	239	ILE	CB-CG1-CD1	5.32	124.96	113.80
1	B	39	GLN	CA-CB-CG	5.32	124.73	114.10
1	A	23	GLY	CA-C-N	5.31	127.83	120.29
1	A	23	GLY	C-N-CA	5.31	127.83	120.29
1	B	219	GLN	O-C-N	5.31	127.75	122.12
1	B	144	ALA	N-CA-CB	-5.30	101.64	110.02
1	B	213	MET	CA-C-O	-5.29	115.26	120.82
1	B	91	GLY	N-CA-C	-5.29	101.55	112.34
1	B	248	GLU	CA-C-O	-5.27	115.09	120.99
1	A	208	LEU	CA-CB-CG	5.25	134.68	116.30
1	A	166	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	B	247	PHE	O-C-N	5.23	129.75	123.16
1	B	223	GLU	N-CA-CB	5.23	117.95	109.90
1	B	172	LEU	N-CA-C	5.22	119.56	112.04
1	A	89	ASP	O-C-N	5.22	129.21	123.16
1	B	27	LEU	O-C-N	5.21	129.44	123.29
1	A	8	MET	CA-C-N	5.21	127.51	120.38
1	A	8	MET	C-N-CA	5.21	127.51	120.38
1	B	159	LEU	O-C-N	5.21	129.25	123.05
1	A	11	VAL	CA-CB-CG1	5.19	119.23	110.40
1	A	147	HIS	N-CA-C	-5.19	98.85	107.99
1	A	44	LEU	CA-C-O	-5.18	114.81	120.36
1	B	175	PRO	N-CD-CG	-5.18	95.43	103.20
1	B	230	LEU	N-CA-CB	-5.18	101.84	110.23
1	B	14	GLU	CA-C-N	5.17	125.01	120.10
1	B	14	GLU	C-N-CA	5.17	125.01	120.10
1	B	229	LYS	N-CA-CB	5.17	120.36	111.00
1	B	177	ASN	O-C-N	5.16	127.46	122.09
1	B	178	ILE	CA-C-N	5.16	127.20	120.28
1	B	178	ILE	C-N-CA	5.16	127.20	120.28
1	B	116	LEU	N-CA-CB	-5.15	102.26	109.94
1	B	34	MET	CA-C-O	-5.15	115.08	121.06
1	B	185	VAL	CB-CA-C	5.15	118.29	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	SER	CA-C-O	-5.15	113.26	119.49
1	B	46	THR	N-CA-C	-5.15	107.03	113.72
1	B	77	VAL	N-CA-C	-5.14	100.36	108.23
1	B	258	ILE	CA-C-O	-5.14	115.08	120.27
1	B	34	MET	O-C-N	5.13	129.22	123.27
1	A	141	MET	CA-C-N	5.12	127.66	120.28
1	A	141	MET	C-N-CA	5.12	127.66	120.28
1	B	53	ARG	N-CA-C	5.12	116.94	111.36
1	A	225	ARG	CA-C-O	5.12	126.59	121.27
1	B	194	LEU	N-CA-C	-5.10	101.65	109.41
1	B	185	VAL	CA-CB-CG1	5.10	119.08	110.40
1	A	185	VAL	O-C-N	-5.09	116.92	121.91
1	B	58	GLU	N-CA-CB	5.08	117.37	110.01
1	A	179	ALA	CA-C-N	5.07	127.03	120.44
1	A	179	ALA	C-N-CA	5.07	127.03	120.44
1	B	129	ILE	N-CA-CB	-5.07	102.56	111.93
1	B	113	THR	N-CA-C	-5.06	105.65	111.07
1	B	129	ILE	CA-C-N	5.06	129.76	123.14
1	B	129	ILE	C-N-CA	5.06	129.76	123.14
1	B	249	ILE	CB-CA-C	5.06	117.25	110.42
1	B	145	PRO	CA-C-N	5.05	129.14	120.71
1	B	145	PRO	C-N-CA	5.05	129.14	120.71
1	A	124	ASP	N-CA-CB	5.04	118.88	110.41
1	A	210	SER	CB-CA-C	-5.04	100.69	110.46
1	A	6	GLU	CB-CG-CD	5.03	121.16	112.60
1	A	241	ASP	N-CA-C	5.03	119.51	113.17
1	B	57	HIS	N-CA-CB	5.03	117.61	110.16
1	A	76	ASN	CB-CG-ND2	-5.02	108.86	116.40
1	A	118	GLN	N-CA-CB	5.01	117.49	110.12
1	A	253	ASP	O-C-N	5.01	125.88	121.37

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	B	21	ARG	Sidechain
1	B	222	ARG	Sidechain

## 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	2153	0	2078	67	0
1	B	2153	0	2080	71	0
2	A	8	0	10	11	0
3	A	20	0	9	2	0
3	B	20	0	11	4	0
4	A	37	0	23	5	0
4	B	37	0	22	3	0
5	A	108	0	0	0	0
5	B	80	0	0	3	0
All	All	4616	0	4233	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (141) 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:183:LEU:HD22	1:B:187:MET:HE2	1.39	1.03
1:A:215:GLN:H	1:A:215:GLN:NE2	1.66	0.91
1:A:215:GLN:H	1:A:215:GLN:HE21	0.93	0.91
1:A:120:LYS:HD2	2:A:266:BME:H11	1.57	0.87
1:B:215:GLN:HE21	1:B:215:GLN:H	1.22	0.85
1:B:234:ARG:O	1:B:236:PRO:HD3	1.77	0.84
1:B:218:LEU:HD11	1:B:222:ARG:HH21	1.42	0.84
1:A:8:MET:HE3	1:A:220:LEU:HD13	1.59	0.82
1:A:50:CYS:HB3	2:A:265:BME:H11	1.62	0.81
1:A:5:LEU:HD23	1:A:8:MET:HE2	1.62	0.80
1:B:10:LYS:HE2	5:B:454:HOH:O	1.83	0.79
1:B:183:LEU:HD22	1:B:187:MET:CE	2.12	0.79
1:A:215:GLN:HE21	1:A:215:GLN:N	1.78	0.76
1:A:110:ASP:OD2	1:A:113:THR:HG23	1.85	0.76
1:A:127:ARG:NH2	3:B:265:UMP:OP2	2.20	0.75
1:A:146:CYS:SG	3:A:267:UMP:C6	2.85	0.69
1:B:49:ARG:HH12	1:B:256:PRO:HA	1.57	0.68
1:A:176:PHE:CE1	2:A:265:BME:H21	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:CD2	1:B:187:MET:HE1	2.24	0.67
1:B:146:CYS:SG	3:B:265:UMP:C6	2.88	0.66
4:B:266:F89:CT	4:B:266:F89:O	2.44	0.66
1:A:243:ARG:NH1	1:A:245:GLU:HB2	2.12	0.64
1:B:37:ASN:OD1	1:B:39:GLN:HB2	1.98	0.64
1:A:255:HIS:HB3	1:A:256:PRO:HD2	1.78	0.64
1:B:228:PRO:O	1:B:229:LYS:HD2	1.98	0.64
1:A:243:ARG:HH12	1:A:245:GLU:HB2	1.63	0.64
1:B:49:ARG:NH1	1:B:256:PRO:HA	2.11	0.64
1:A:255:HIS:HB3	1:A:256:PRO:CD	2.29	0.62
1:A:120:LYS:HB2	2:A:266:BME:H11	1.81	0.62
1:A:176:PHE:CZ	2:A:265:BME:H21	2.34	0.61
1:A:120:LYS:HB2	2:A:266:BME:S2	2.40	0.61
1:B:59:LEU:HD23	1:B:187:MET:HE1	1.82	0.61
1:A:176:PHE:HZ	4:A:268:F89:O1	1.83	0.61
1:B:55:ILE:HD13	1:B:179:ALA:HB3	1.84	0.60
1:B:39:GLN:OE1	1:B:39:GLN:HA	2.02	0.59
1:A:50:CYS:CB	2:A:265:BME:H11	2.32	0.59
1:A:35:ARG:HD3	1:A:198:ASP:OD2	2.03	0.59
1:A:120:LYS:CD	2:A:266:BME:H11	2.32	0.58
1:B:228:PRO:C	1:B:229:LYS:HD2	2.29	0.57
1:A:73:HIS:CE1	1:A:81:ASP:OD1	2.56	0.57
1:B:93:VAL:O	1:B:94:TYR:C	2.47	0.57
1:A:238:SER:O	1:A:241:ASP:HB2	2.04	0.57
1:B:61:TRP:CE3	1:B:72:LEU:HD11	2.40	0.57
1:A:5:LEU:CD2	1:A:8:MET:HE2	2.34	0.56
1:B:56:ILE:C	1:B:56:ILE:HD13	2.30	0.56
1:B:69:ILE:HG23	1:B:90:LEU:HD11	1.87	0.56
1:B:61:TRP:CD2	1:B:72:LEU:HD11	2.41	0.55
1:A:212:HIS:O	1:A:216:THR:HG23	2.06	0.55
1:A:49:ARG:HH21	1:A:254:PRO:HG2	1.70	0.55
1:B:2:LYS:H	1:B:2:LYS:HE2	1.69	0.55
1:B:56:ILE:HD12	1:B:244:PHE:CD1	2.42	0.55
1:B:222:ARG:HB3	1:B:255:HIS:CE1	2.42	0.54
1:A:11:VAL:HG22	1:A:208:LEU:HD22	1.90	0.54
1:B:215:GLN:H	1:B:215:GLN:NE2	2.00	0.54
1:A:55:ILE:HD13	1:A:179:ALA:HB3	1.91	0.53
1:B:263:ALA:HB2	5:B:305:HOH:O	2.07	0.53
1:B:69:ILE:HD13	1:B:81:ASP:OD2	2.08	0.53
1:A:53:ARG:HA	1:A:244:PHE:HE1	1.73	0.53
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLU:O	1:B:61:TRP:HB3	2.09	0.52
1:A:56:ILE:HG22	1:A:60:LEU:HD22	1.92	0.52
1:A:53:ARG:HG3	1:A:53:ARG:HH11	1.75	0.52
1:A:70:ALA:O	1:A:73:HIS:HB2	2.10	0.51
4:A:268:F89:C9	4:A:268:F89:H14	2.40	0.51
1:B:2:LYS:H	1:B:2:LYS:CD	2.23	0.51
1:B:59:LEU:HD21	1:B:187:MET:HE1	1.91	0.51
4:B:266:F89:O1A	4:B:266:F89:H10	2.11	0.51
1:A:73:HIS:HE1	1:A:81:ASP:OD1	1.93	0.50
1:B:48:LYS:HG3	5:B:306:HOH:O	2.11	0.50
1:A:225:ARG:HD2	1:A:253:ASP:O	2.12	0.49
1:B:73:HIS:C	1:B:75:ASN:H	2.21	0.49
1:B:57:HIS:CD2	1:B:75:ASN:ND2	2.81	0.49
1:B:147:HIS:HB2	1:B:163:LEU:HD21	1.95	0.49
1:B:228:PRO:HG2	1:B:249:ILE:HD11	1.94	0.48
1:B:96:LYS:NZ	1:B:102:PRO:HG3	2.28	0.48
1:A:120:LYS:HB2	2:A:266:BME:C1	2.44	0.48
1:A:8:MET:CE	1:A:220:LEU:HD13	2.37	0.48
1:B:172:LEU:HD21	1:B:262:VAL:HG22	1.96	0.48
1:B:215:GLN:HE21	1:B:215:GLN:N	2.02	0.48
1:A:37:ASN:HD21	1:A:39:GLN:HB2	1.79	0.48
1:B:26:THR:HB	1:B:207:HIS:HB2	1.96	0.48
1:B:84:ALA:HB1	1:B:88:GLY:C	2.39	0.48
1:A:49:ARG:HE	1:A:49:ARG:HB2	1.37	0.47
1:B:2:LYS:H	1:B:2:LYS:CE	2.27	0.47
1:A:45:VAL:HG22	1:A:50:CYS:SG	2.54	0.47
1:B:33:GLN:HA	1:B:201:TRP:O	2.14	0.47
1:A:170:VAL:HB	1:A:208:LEU:HD13	1.97	0.47
1:B:78:THR:HA	1:B:81:ASP:OD1	2.16	0.46
1:A:53:ARG:HA	1:A:244:PHE:CE1	2.49	0.46
1:A:86:GLU:H	1:A:86:GLU:CD	2.24	0.46
1:A:141:MET:SD	1:A:145:PRO:HD3	2.56	0.46
1:A:176:PHE:CE2	2:A:265:BME:H12	2.51	0.46
1:A:127:ARG:HH21	3:B:265:UMP:P	2.38	0.46
1:A:212:HIS:O	1:A:216:THR:CG2	2.64	0.45
1:A:18:LYS:HE3	1:B:154:VAL:O	2.16	0.45
1:A:150:PHE:HA	1:A:162:GLN:O	2.16	0.45
1:B:179:ALA:O	1:B:183:LEU:HB2	2.16	0.45
1:A:176:PHE:CE1	4:A:268:F89:H192	2.52	0.45
1:A:259:LYS:HB3	1:A:259:LYS:HE2	1.63	0.44
1:A:135:VAL:HA	1:A:138:LEU:HD22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:O	1:B:6:GLU:HG3	2.18	0.44
1:B:92:PRO:O	1:B:141:MET:HE2	2.18	0.44
1:B:56:ILE:HD12	1:B:244:PHE:HD1	1.81	0.44
1:B:39:GLN:HE21	1:B:158:LYS:CE	2.30	0.44
1:B:187:MET:HG2	1:B:242:TYR:CE2	2.52	0.44
1:A:16:THR:HG21	1:B:155:ALA:HB1	1.99	0.44
1:B:49:ARG:NH1	1:B:49:ARG:HB2	2.33	0.43
1:B:55:ILE:HG12	1:B:176:PHE:HD2	1.82	0.43
1:A:215:GLN:NE2	1:A:215:GLN:N	2.50	0.43
1:B:39:GLN:HE21	1:B:158:LYS:HE3	1.82	0.43
1:A:82:GLU:HG3	1:A:264:ILE:HD11	1.99	0.43
3:A:267:UMP:OP2	1:B:126:ARG:HD3	2.18	0.43
1:B:57:HIS:NE2	1:B:75:ASN:ND2	2.64	0.43
1:A:49:ARG:NH2	1:A:254:PRO:HG2	2.34	0.43
1:A:116:LEU:O	2:A:266:BME:H22	2.19	0.42
1:A:82:GLU:CG	1:A:264:ILE:HD11	2.47	0.42
1:B:228:PRO:HB2	1:B:249:ILE:HG13	2.00	0.42
4:B:266:F89:H191	4:B:266:F89:HG2	2.01	0.42
1:A:56:ILE:HD12	1:A:244:PHE:CE1	2.54	0.42
1:A:73:HIS:C	1:A:75:ASN:N	2.77	0.42
1:B:192:CYS:O	1:B:193:ASP:C	2.62	0.42
1:B:85:ASP:OD1	1:B:87:ASN:HB2	2.19	0.42
1:A:49:ARG:NH2	1:A:254:PRO:HD2	2.34	0.41
1:B:54:SER:HB2	1:B:176:PHE:HE2	1.85	0.41
1:B:55:ILE:HG12	1:B:176:PHE:CD2	2.55	0.41
1:B:252:TYR:CE2	1:B:254:PRO:HG3	2.55	0.41
1:A:1:MET:HE1	1:A:36:PHE:CD1	2.54	0.41
1:B:146:CYS:SG	3:B:265:UMP:C5	3.13	0.41
1:B:70:ALA:O	1:B:73:HIS:N	2.51	0.41
1:B:71:TYR:CD1	1:B:71:TYR:C	2.98	0.41
1:B:38:LEU:HB2	1:B:197:GLY:O	2.21	0.41
1:B:252:TYR:CZ	1:B:254:PRO:HG3	2.56	0.41
1:A:37:ASN:ND2	1:A:39:GLN:H	2.19	0.41
1:A:176:PHE:CZ	4:A:268:F89:H192	2.55	0.41
1:B:228:PRO:HB2	1:B:249:ILE:CG1	2.51	0.40
1:A:115:VAL:HG21	1:A:130:VAL:HG23	2.02	0.40
1:A:225:ARG:HB3	1:A:226:PRO:CD	2.51	0.40
1:B:61:TRP:CD1	1:B:66:ASP:HB3	2.57	0.40
4:A:268:F89:O1A	4:A:268:F89:H10	2.21	0.40
1:B:228:PRO:HB2	1:B:249:ILE:HD11	2.03	0.40
1:B:102:PRO:HA	1:B:107:ARG:O	2.21	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	263/265 (99%)	256 (97%)	5 (2%)	2 (1%)	16	8
1	B	263/265 (99%)	250 (95%)	12 (5%)	1 (0%)	30	21
All	All	526/530 (99%)	506 (96%)	17 (3%)	3 (1%)	21	12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	TYR
1	A	74	GLU
1	A	94	TYR

### 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	233/233 (100%)	203 (87%)	30 (13%)	4	1
1	B	233/233 (100%)	202 (87%)	31 (13%)	4	0
All	All	466/466 (100%)	405 (87%)	61 (13%)	4	0

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	11	VAL
1	A	16	THR
1	A	18	LYS
1	A	27	LEU
1	A	28	SER
1	A	37	ASN
1	A	53	ARG
1	A	59	LEU
1	A	60	LEU
1	A	73	HIS
1	A	82	GLU
1	A	103	THR
1	A	113	THR
1	A	115	VAL
1	A	116	LEU
1	A	120	LYS
1	A	138	LEU
1	A	172	LEU
1	A	208	LEU
1	A	215	GLN
1	A	216	THR
1	A	220	LEU
1	A	223	GLU
1	A	227	LEU
1	A	230	LEU
1	A	233	LYS
1	A	241	ASP
1	A	259	LYS
1	A	264	ILE
1	B	2	LYS
1	B	5	LEU
1	B	16	THR
1	B	18	LYS
1	B	21	ARG
1	B	38	LEU
1	B	39	GLN
1	B	50	CYS
1	B	54	SER
1	B	56	ILE
1	B	96	LYS
1	B	109	ILE
1	B	116	LEU

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Mol	Chain	Res	Type
1	B	120	LYS
1	B	130	VAL
1	B	163	LEU
1	B	172	LEU
1	B	183	LEU
1	B	215	GLN
1	B	218	LEU
1	B	220	LEU
1	B	226	PRO
1	B	227	LEU
1	B	229	LYS
1	B	230	LEU
1	B	231	ILE
1	B	233	LYS
1	B	249	ILE
1	B	253	ASP
1	B	259	LYS
1	B	264	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	39	GLN
1	A	51	HIS
1	A	64	GLN
1	A	73	HIS
1	A	75	ASN
1	A	87	ASN
1	A	97	GLN
1	A	108	HIS
1	A	117	ASN
1	A	118	GLN
1	A	134	ASN
1	A	151	GLN
1	A	191	GLN
1	A	215	GLN
1	A	217	HIS
1	B	87	ASN
1	B	117	ASN
1	B	121	ASN
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	151	GLN
1	B	190	GLN
1	B	215	GLN
1	B	217	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 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	BME	A	266	-	3,3,3	0.42	0	2,2,2	1.13	0
3	UMP	B	265	-	21,21,21	2.45	7 (33%)	30,31,31	2.48	11 (36%)
4	F89	B	266	-	41,41,41	2.40	11 (26%)	56,60,60	4.10	26 (46%)
3	UMP	A	267	-	21,21,21	2.31	7 (33%)	30,31,31	2.48	10 (33%)
4	F89	A	268	-	41,41,41	2.33	12 (29%)	56,60,60	3.03	20 (35%)
2	BME	A	265	-	3,3,3	0.47	0	2,2,2	1.09	0

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	BME	A	266	-	-	1/1/1/1	-
3	UMP	B	265	-	-	1/10/22/22	0/2/2/2
4	F89	B	266	-	-	10/18/30/30	0/5/5/5
3	UMP	A	267	-	-	1/10/22/22	0/2/2/2
4	F89	A	268	-	-	5/18/30/30	0/5/5/5
2	BME	A	265	-	-	0/1/1/1	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	266	F89	CA-N	7.54	1.55	1.46
4	A	268	F89	CA-N	6.84	1.54	1.46
4	B	266	F89	O1-CT	6.32	1.40	1.22
3	A	267	UMP	C1'-N1	-6.22	1.32	1.48
3	B	265	UMP	C1'-N1	-6.07	1.32	1.48
4	A	268	F89	C1A-C1	5.86	1.60	1.47
3	B	265	UMP	O2-C2	-5.49	1.13	1.23
4	A	268	F89	O1-CT	5.30	1.37	1.22
4	B	266	F89	C1A-C1	4.56	1.57	1.47
3	A	267	UMP	O2-C2	-4.33	1.15	1.23
4	A	268	F89	C19-N	4.26	1.51	1.47
4	B	266	F89	CB-CA	3.83	1.59	1.53
3	B	265	UMP	O5'-C5'	-3.79	1.30	1.44
4	A	268	F89	CB-CA	3.48	1.59	1.53
4	B	266	F89	C17-C16	3.42	1.45	1.39
4	B	266	F89	C19-N	3.37	1.50	1.47
4	B	266	F89	C3-N2	3.33	1.46	1.36
4	A	268	F89	C4A-N4	3.14	1.45	1.39
3	B	265	UMP	O4'-C1'	3.07	1.49	1.42
4	A	268	F89	C3-N2	3.06	1.45	1.36
4	A	268	F89	C-N	-3.03	1.33	1.36
3	A	267	UMP	C5'-C4'	-2.93	1.42	1.51
3	B	265	UMP	C2'-C1'	2.90	1.60	1.52
3	A	267	UMP	O4'-C1'	2.85	1.48	1.42
4	B	266	F89	C7-C8	2.83	1.42	1.36
3	A	267	UMP	O5'-C5'	-2.78	1.34	1.44
3	B	265	UMP	C5'-C4'	-2.73	1.43	1.51
3	A	267	UMP	C2'-C1'	2.69	1.59	1.52
4	A	268	F89	CA-CT	2.68	1.57	1.52
3	A	267	UMP	P-OP2	2.64	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	266	F89	C13-N12	2.58	1.46	1.38
4	A	268	F89	C13-N12	2.50	1.45	1.38
4	A	268	F89	CB-CG	2.46	1.60	1.52
4	A	268	F89	OE2-CD	2.35	1.38	1.30
4	B	266	F89	C4A-N4	2.25	1.43	1.39
4	B	266	F89	CG-CD	2.10	1.55	1.50
3	B	265	UMP	C2-N3	-2.05	1.34	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	268	F89	O-C-N	14.25	136.66	125.34
4	B	266	F89	C19-N-CA	13.91	136.93	123.68
4	B	266	F89	C19-C15-C16	-10.19	103.32	109.73
4	B	266	F89	O-C-N	9.63	132.98	125.34
4	B	266	F89	C19-N-C	-9.46	109.16	113.15
4	B	266	F89	C15-C19-N	8.43	106.79	102.31
4	B	266	F89	C4A-N4-C3	7.49	125.62	118.16
4	A	268	F89	C4A-N4-C3	6.62	124.76	118.16
4	A	268	F89	O-C-C16	-6.05	116.94	128.66
4	B	266	F89	C15-C16-C	6.04	112.22	108.94
3	A	267	UMP	C6-N1-C2	-5.90	113.82	121.00
4	B	266	F89	CA-N-C	-5.89	112.86	121.86
3	B	265	UMP	C1'-N1-C2	5.70	128.81	117.66
4	A	268	F89	C19-N-CA	-5.58	118.37	123.68
3	A	267	UMP	C1'-N1-C2	5.14	127.71	117.66
3	B	265	UMP	C6-N1-C2	-4.95	114.97	121.00
4	B	266	F89	C17-C16-C	-4.93	121.32	129.59
4	B	266	F89	C11-C9-C10	-4.93	112.70	121.46
4	A	268	F89	C1-N2-C3	-4.91	121.20	123.87
3	B	265	UMP	O4-C4-N3	4.82	126.27	119.27
3	B	265	UMP	N3-C2-N1	4.80	121.14	114.89
4	A	268	F89	C1B-C1A-C1	4.56	126.20	121.28
4	B	266	F89	O-C-C16	-4.50	119.94	128.66
4	B	266	F89	CB-CG-CD	-4.46	100.61	112.49
4	B	266	F89	C17-C16-C15	4.45	126.42	120.88
4	A	268	F89	O1-CT-CA	-4.41	108.90	122.44
4	B	266	F89	C18-C17-C16	-4.40	113.60	120.86
4	B	266	F89	C18-C13-C14	4.27	124.81	119.66
3	A	267	UMP	O4'-C1'-N1	4.16	115.25	107.86
3	A	267	UMP	N3-C2-N1	4.11	120.25	114.89
3	A	267	UMP	C2'-C1'-N1	4.10	124.08	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	268	F89	C19-C15-C16	-4.05	107.19	109.73
4	B	266	F89	C19-C15-C14	3.92	137.94	128.32
3	B	265	UMP	C2'-C1'-N1	3.91	123.60	113.81
3	A	267	UMP	C5-C6-N1	3.75	127.94	121.84
4	A	268	F89	C1A-C1-N2	3.54	119.17	115.17
4	B	266	F89	C13-C14-C15	-3.35	116.28	120.88
3	A	267	UMP	O5'-C5'-C4'	3.25	120.08	108.99
3	A	267	UMP	O4-C4-N3	3.09	123.76	119.27
3	A	267	UMP	OP2-P-O5'	-3.03	98.77	106.67
3	B	265	UMP	O4-C4-C5	-3.00	119.99	125.16
4	A	268	F89	C11-C9-C10	-2.95	116.21	121.46
3	B	265	UMP	C5-C6-N1	2.92	126.59	121.84
4	A	268	F89	C14-C13-N12	-2.86	113.08	120.78
3	B	265	UMP	O4'-C1'-N1	2.84	112.90	107.86
3	B	265	UMP	O2-C2-N3	-2.83	116.28	121.49
4	A	268	F89	O2-CT-O1	2.81	130.46	124.08
3	B	265	UMP	C1'-N1-C6	-2.76	116.11	121.53
4	B	266	F89	C1-N2-C3	-2.74	122.38	123.87
4	B	266	F89	C5-C4A-N4	2.67	122.01	118.61
4	B	266	F89	C11-C9-C8	2.66	126.36	120.94
3	B	265	UMP	O5'-C5'-C4'	2.66	118.04	108.99
4	B	266	F89	C14-C15-C16	-2.63	117.80	120.65
4	A	268	F89	C18-C13-N12	2.63	126.91	120.96
4	A	268	F89	C15-C19-N	-2.62	100.91	102.31
4	B	266	F89	C11-N12-C13	-2.60	113.55	121.87
4	A	268	F89	C15-C16-C	-2.59	107.53	108.94
4	B	266	F89	C1B-C1A-C1	2.58	124.06	121.28
3	A	267	UMP	O2-C2-N3	-2.52	116.84	121.49
4	A	268	F89	CG-CB-CA	-2.52	107.83	112.83
4	A	268	F89	CA-N-C	2.37	125.48	121.86
4	A	268	F89	C5-C4A-N4	2.34	121.58	118.61
4	B	266	F89	O1A-C1-N2	-2.25	117.95	120.62
4	B	266	F89	N2-C3-N4	-2.21	119.66	123.15
4	B	266	F89	O2-CT-CA	2.20	120.53	113.34
4	A	268	F89	O2-CT-CA	2.20	120.53	113.34
4	A	268	F89	C18-C17-C16	-2.14	117.33	120.86

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	266	BME	O1-C1-C2-S2

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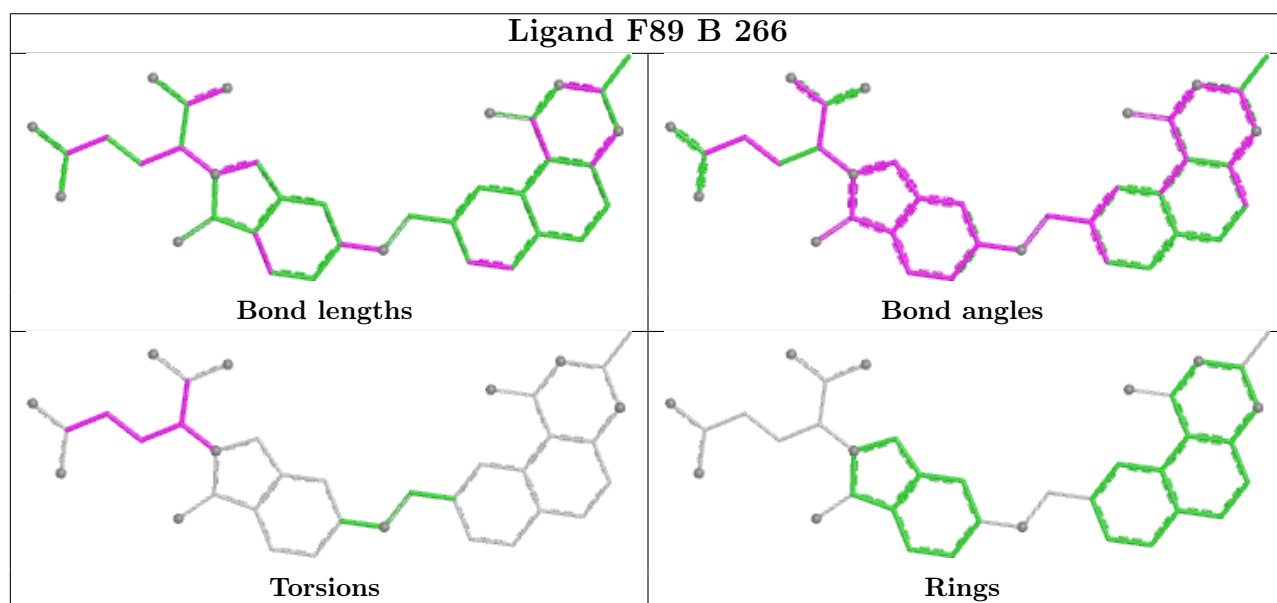
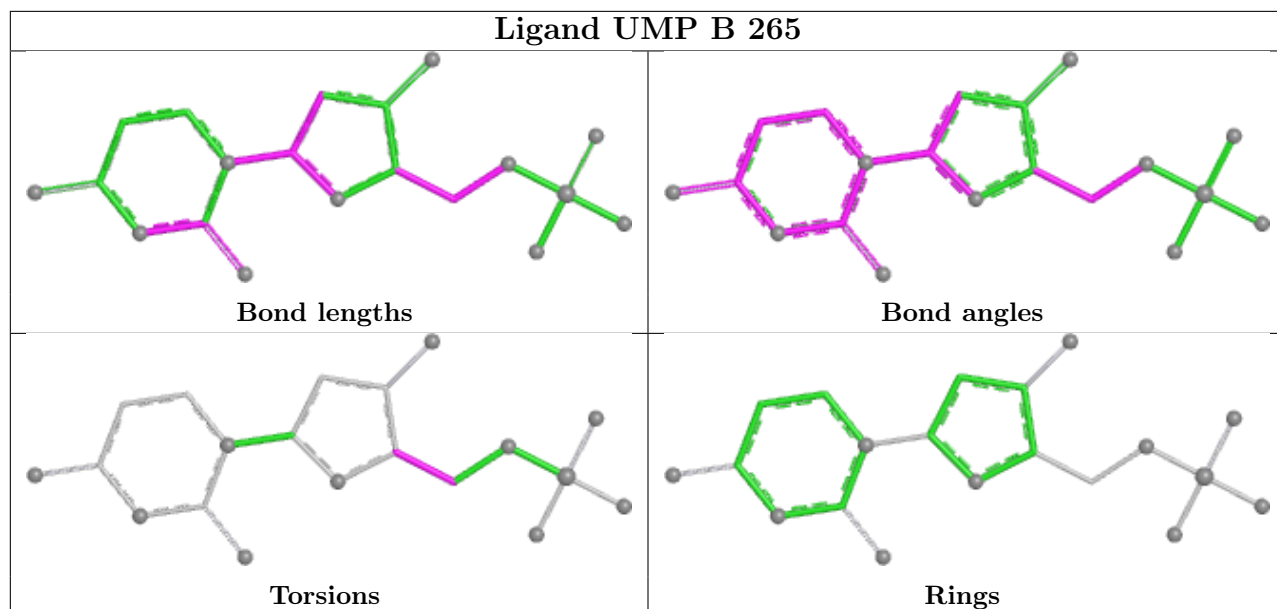
Mol	Chain	Res	Type	Atoms
4	A	268	F89	CB-CA-N-C
4	B	266	F89	CT-CA-N-C19
4	B	266	F89	CT-CA-N-C
4	B	266	F89	CB-CA-N-C
4	B	266	F89	CB-CA-N-C19
4	B	266	F89	CA-CB-CG-CD
4	A	268	F89	N-CA-CT-O1
4	A	268	F89	N-CA-CT-O2
4	A	268	F89	CT-CA-N-C19
4	B	266	F89	N-CA-CT-O1
4	B	266	F89	N-CA-CT-O2
4	B	266	F89	N-CA-CB-CG
3	B	265	UMP	O4'-C4'-C5'-O5'
4	B	266	F89	OE1-CD-CG-CB
4	B	266	F89	OE2-CD-CG-CB
3	A	267	UMP	O4'-C4'-C5'-O5'
4	A	268	F89	CB-CA-N-C19

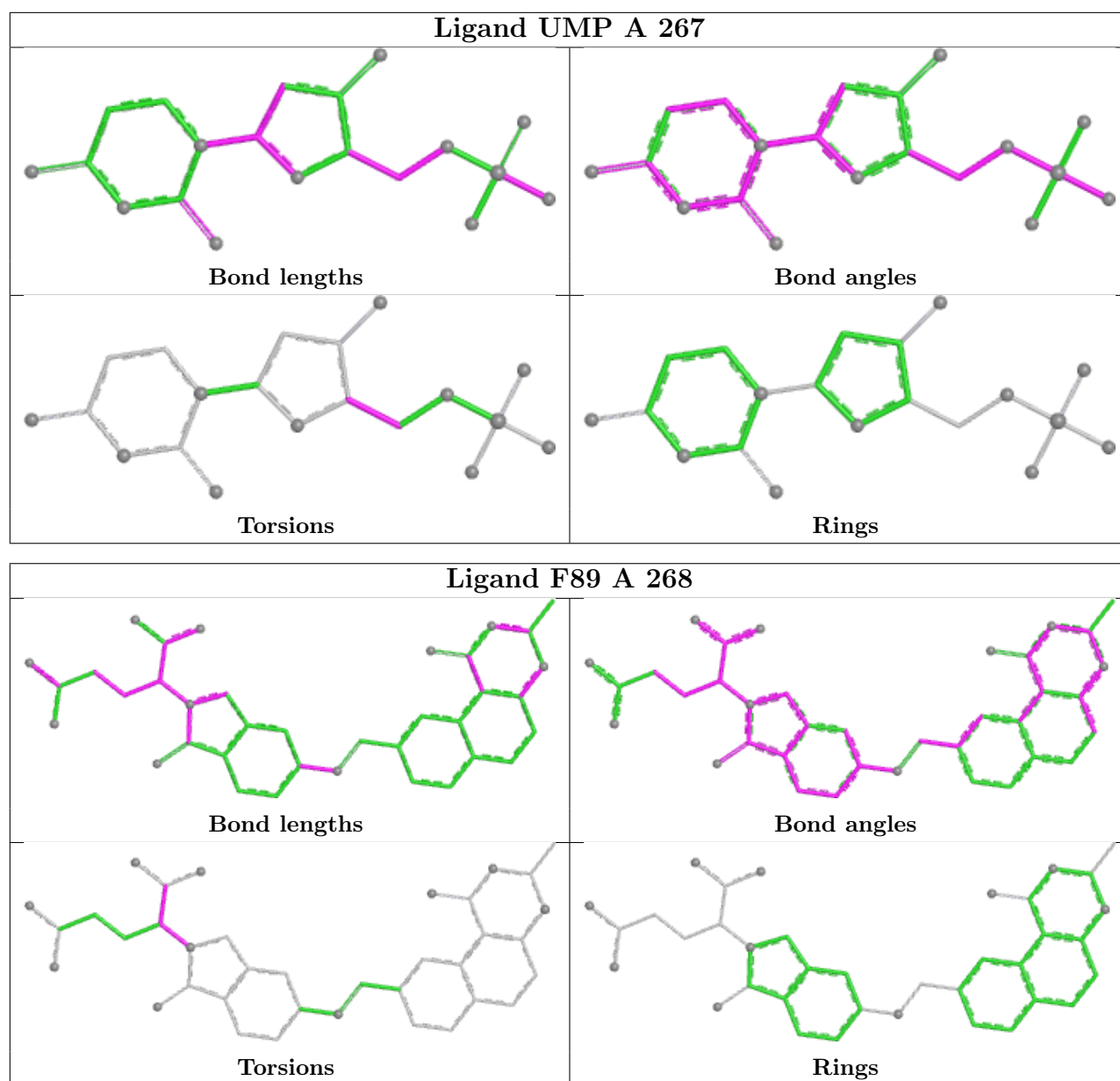
There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	266	BME	6	0
3	B	265	UMP	4	0
4	B	266	F89	3	0
3	A	267	UMP	2	0
4	A	268	F89	5	0
2	A	265	BME	5	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.