



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:49 pm BST

PDB ID : 2VF0  
Title : CRYSTAL STRUCTURE OF THE THYMIDYLATE SYNTHASE K48Q  
COMPLEXED WITH 5NO2DUMP AND BW1843U89  
Authors : Sotelo-Mundo, R.R.; Arreola, R.; Maley, F.; Montfort, W.R.  
Deposited on : 2007-10-27  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

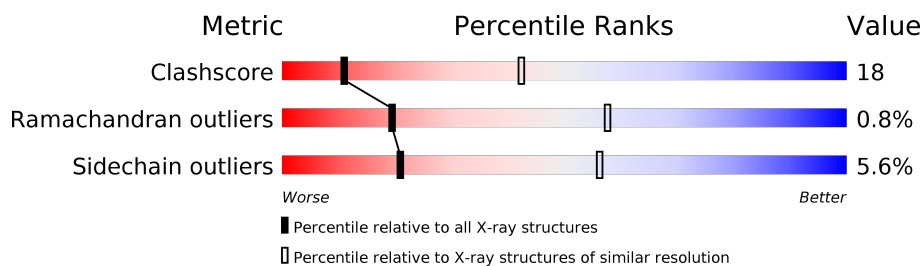
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

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

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	NDU	A	1265	X	-	-	-
2	NDU	B	1265	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4474 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.

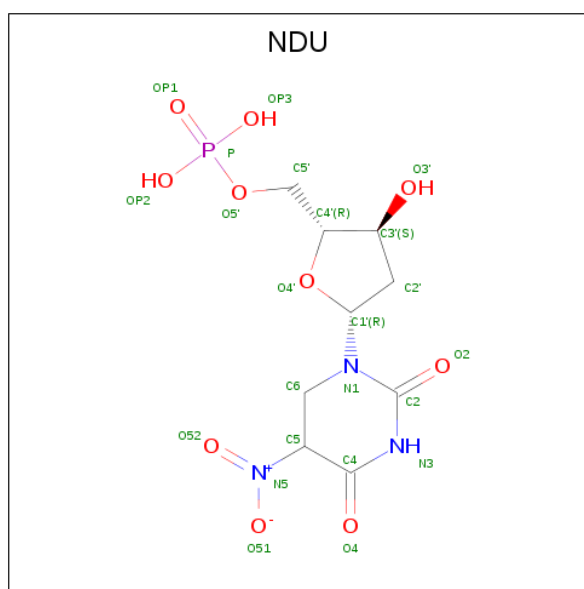
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2153	1374	371	396	12			
1	B	264	Total	C	N	O	S	0	1	0
			2167	1385	373	397	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLN	LYS	engineered mutation	UNP P0A884
B	48	GLN	LYS	engineered mutation	UNP P0A884

- Molecule 2 is 2'-DEOXY-5-NITROURIDINE 5'-MONOPHOSPHATE (three-letter code: NDU) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>3</sub>O<sub>10</sub>P).



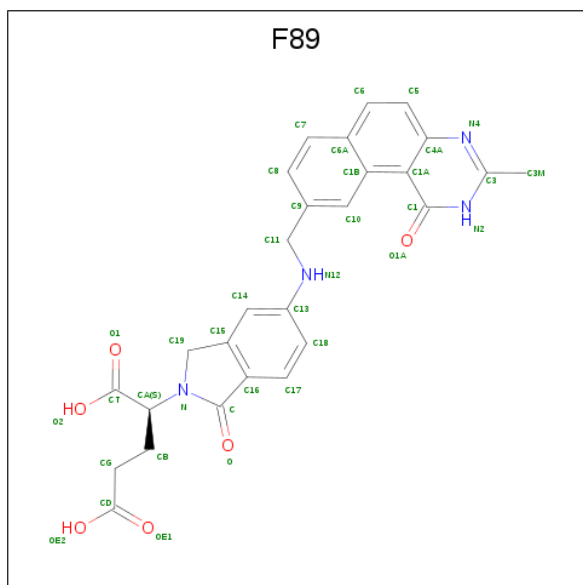
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	9	3	10	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			23	9	3	10	1		

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

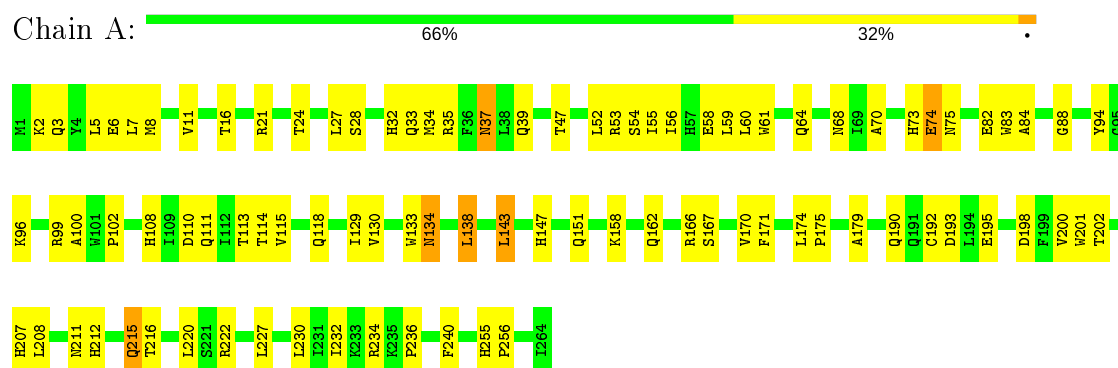
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total	O	0	0
			13	13		
5	B	16	Total	O	0	0
			16	16		

### 3 Residue-property plots

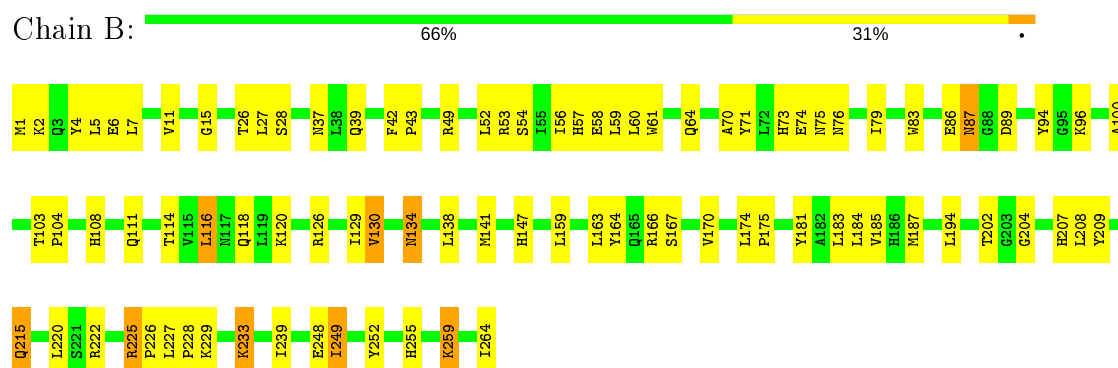
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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, $\alpha$ , $\beta$ , $\gamma$	127.16 Å 127.16 Å 67.95 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.98 – 3.00	Depositor
% Data completeness (in resolution range)	95.1 (33.98-3.00)	Depositor
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.180 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4474	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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: F89, NDU, SO4, 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	0.37	0/2202	0.65	0/2991
1	B	0.37	0/2218	0.64	0/3014
All	All	0.37	0/4420	0.65	0/6005

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2074	71	0
1	B	2167	0	2083	89	0
2	A	23	0	10	0	0
2	B	23	0	10	0	0
3	A	37	0	23	1	0
3	B	37	0	23	2	0
4	B	5	0	0	0	0
5	A	13	0	0	0	0
5	B	16	0	0	0	0
All	All	4474	0	4223	157	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 18.

All (157) 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:215:GLN:HE21	1:B:215:GLN:H	1.11	0.99
1:B:215:GLN:NE2	1:B:215:GLN:H	1.67	0.91
1:B:166:ARG:NH1	1:B:167:SER:HB2	1.93	0.83
1:A:215:GLN:NE2	1:A:215:GLN:H	1.78	0.81
1:B:87:ASN:N	1:B:87:ASN:HD22	1.80	0.80
1:B:228:PRO:HB2	1:B:249:ILE:HD11	1.69	0.74
1:A:166:ARG:NH1	1:A:167:SER:HB2	2.05	0.71
1:B:170:VAL:HG23	1:B:207:HIS:O	1.90	0.71
1:B:215:GLN:HE21	1:B:215:GLN:N	1.88	0.70
1:B:228:PRO:CB	1:B:249:ILE:HD11	2.22	0.70
1:A:215:GLN:HE21	1:A:215:GLN:H	1.39	0.70
1:B:184:LEU:HA	1:B:187:MET:HE2	1.74	0.68
1:A:222:ARG:HD3	1:A:255:HIS:ND1	2.08	0.68
1:A:212:HIS:O	1:A:216:THR:HG23	1.94	0.67
1:B:54:SER:HB3	3:B:1266:F89:H17	1.74	0.67
1:B:52:LEU:HG	1:B:56:ILE:CD1	2.26	0.66
1:B:49:ARG:HH11	1:B:49:ARG:HB2	1.61	0.66
1:B:181:TYR:O	1:B:185:VAL:HG23	1.97	0.64
1:B:58:GLU:O	1:B:61:TRP:HB3	1.97	0.64
1:B:129:ILE:HG22	1:B:130:VAL:N	2.13	0.63
1:B:87:ASN:ND2	1:B:87:ASN:N	2.43	0.62
1:B:138:LEU:HD23	1:B:141:MET:HE1	1.80	0.62
1:A:110:ASP:OD2	1:A:113:THR:HG23	1.99	0.62
1:A:7:LEU:HD13	1:A:32:HIS:CD2	2.34	0.62
1:B:166:ARG:HH12	1:B:167:SER:HB2	1.62	0.62
1:B:249:ILE:CD1	1:B:252:TYR:HB2	2.30	0.62
1:A:53:ARG:CZ	1:A:53:ARG:HB2	2.29	0.61
1:B:86:GLU:C	1:B:87:ASN:HD22	2.03	0.61
1:B:174:LEU:HB3	1:B:175:PRO:HD3	1.81	0.61
1:A:54:SER:HB3	3:A:1266:F89:H17	1.83	0.61
1:B:52:LEU:HG	1:B:56:ILE:HD13	1.82	0.61
1:B:264:ILE:O	1:B:264:ILE:HD12	2.01	0.60
1:A:73:HIS:C	1:A:75:ASN:H	2.03	0.60
1:A:28:SER:HB3	1:A:207:HIS:HB3	1.84	0.60
1:A:216:THR:O	1:A:220:LEU:HB2	2.02	0.60
1:B:233:LYS:NZ	1:B:233:LYS:HB2	2.17	0.60
1:A:114:THR:O	1:A:118:GLN:HG3	2.03	0.59
1:A:133:TRP:CZ2	1:A:138:LEU:HD21	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD22	1:B:249:ILE:HG21	1.85	0.58
1:A:24:THR:HG21	1:A:211:ASN:HD21	1.69	0.58
1:B:100:ALA:HB1	1:B:108:HIS:HD2	1.68	0.57
1:B:114:THR:O	1:B:118:GLN:HG3	2.03	0.57
1:A:158:LYS:HA	1:A:195:GLU:O	2.05	0.57
1:A:58:GLU:O	1:A:61:TRP:HB3	2.04	0.56
1:A:34:MET:HG3	1:A:201:TRP:HB3	1.87	0.56
1:B:52:LEU:O	1:B:56:ILE:HD13	2.05	0.56
1:A:5:LEU:HD11	1:A:47:THR:HG21	1.88	0.55
1:A:60:LEU:O	1:A:64:GLN:HG2	2.06	0.55
1:B:76:ASN:HD22	1:B:76:ASN:N	2.02	0.55
1:A:5:LEU:HD23	1:A:8:MET:CE	2.37	0.55
1:A:232:ILE:N	1:A:232:ILE:HD12	2.21	0.55
1:A:35:ARG:HD3	1:A:198:ASP:OD2	2.07	0.55
1:A:37:ASN:ND2	1:A:39:GLN:H	2.03	0.55
1:B:49:ARG:NH1	1:B:49:ARG:HB2	2.22	0.55
1:B:59:LEU:HD23	1:B:183:LEU:HD12	1.89	0.55
1:A:170:VAL:HB	1:A:208:LEU:CD1	2.37	0.54
1:A:32:HIS:HE2	1:A:34:MET:HE3	1.72	0.54
1:B:73:HIS:C	1:B:75:ASN:H	2.10	0.54
1:A:73:HIS:C	1:A:75:ASN:N	2.61	0.54
1:B:170:VAL:HB	1:B:208:LEU:HD13	1.88	0.54
1:A:114:THR:HG22	1:A:118:GLN:NE2	2.23	0.54
1:A:255:HIS:HB3	1:A:256:PRO:CD	2.38	0.54
1:A:134:ASN:C	1:A:134:ASN:HD22	2.11	0.54
1:A:171:PHE:CD1	1:A:216:THR:HG22	2.42	0.54
1:A:84:ALA:HB1	1:A:88:GLY:HA2	1.90	0.54
1:B:166:ARG:HG3	1:B:167:SER:N	2.23	0.53
1:A:64:GLN:NE2	1:A:64:GLN:HA	2.24	0.52
1:A:82:GLU:HB2	1:A:83:TRP:CE3	2.45	0.52
1:B:129:ILE:CG2	1:B:130:VAL:N	2.72	0.52
1:B:54:SER:HB3	3:B:1266:F89:C17	2.40	0.52
1:B:15:GLY:HA2	1:B:28:SER:O	2.10	0.52
1:B:147:HIS:HB2	1:B:163:LEU:HD21	1.92	0.51
1:A:37:ASN:C	1:A:37:ASN:HD22	2.14	0.51
1:B:249:ILE:HD13	1:B:249:ILE:C	2.31	0.51
1:A:222:ARG:HB3	1:A:255:HIS:CE1	2.45	0.51
1:B:100:ALA:HB1	1:B:108:HIS:CD2	2.47	0.50
1:A:151:GLN:HE22	1:B:204:GLY:HA3	1.76	0.50
1:A:52:LEU:O	1:A:56:ILE:HG13	2.11	0.50
1:B:70:ALA:O	1:B:73:HIS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:HIS:O	1:A:75:ASN:N	2.44	0.49
1:B:138:LEU:HA	1:B:141:MET:HE3	1.94	0.49
1:A:96:LYS:HE2	1:A:100:ALA:O	2.13	0.49
1:B:53:ARG:HH22	1:B:75:ASN:HD22	1.60	0.49
1:B:228:PRO:HB2	1:B:249:ILE:CD1	2.41	0.49
1:B:76:ASN:ND2	1:B:76:ASN:N	2.60	0.49
1:A:37:ASN:ND2	1:A:39:GLN:HB2	2.28	0.48
1:B:233:LYS:HZ2	1:B:233:LYS:HB2	1.78	0.48
1:B:53:ARG:NH2	1:B:75:ASN:HD22	2.11	0.48
1:A:151:GLN:NE2	1:B:164:TYR:OH	2.46	0.47
1:A:174:LEU:HB3	1:A:175:PRO:HD3	1.96	0.47
1:A:24:THR:CG2	1:A:211:ASN:HD21	2.27	0.47
1:A:102:PRO:HB3	1:A:108:HIS:CE1	2.49	0.47
1:B:249:ILE:HD11	1:B:252:TYR:HB2	1.96	0.47
1:B:222:ARG:HB3	1:B:255:HIS:CE1	2.50	0.47
1:A:111:GLN:O	1:A:115:VAL:HG23	2.14	0.47
1:B:134:ASN:C	1:B:134:ASN:HD22	2.17	0.47
1:B:259:LYS:HE3	1:B:259:LYS:H	1.80	0.47
1:B:79:ILE:O	1:B:83[A]:TRP:HZ3	1.97	0.47
1:A:83:TRP:CD1	1:A:143:LEU:HD13	2.49	0.47
1:A:190:GLN:HE22	1:A:232:ILE:HG21	1.80	0.47
1:B:116:LEU:CD1	1:B:120:LYS:HE3	2.45	0.47
1:A:234:ARG:O	1:A:236:PRO:HD3	2.15	0.46
1:B:56:ILE:O	1:B:60:LEU:HG	2.15	0.46
1:B:103:THR:HB	1:B:104:PRO:HD2	1.98	0.46
1:A:55:ILE:HD13	1:A:179:ALA:HB3	1.97	0.46
1:B:184:LEU:HA	1:B:187:MET:CE	2.42	0.46
1:B:225:ARG:O	1:B:226:PRO:C	2.54	0.46
1:A:70:ALA:O	1:A:74:GLU:HG3	2.16	0.46
1:B:166:ARG:NH1	1:B:167:SER:CB	2.75	0.45
1:A:129:ILE:HG22	1:A:130:VAL:N	2.32	0.45
1:B:183:LEU:O	1:B:187:MET:HG3	2.16	0.45
1:B:53:ARG:HG3	1:B:53:ARG:HH11	1.82	0.45
1:A:113:THR:HG22	1:A:240:PHE:HE2	1.81	0.45
1:B:2:LYS:O	1:B:6:GLU:HG3	2.17	0.45
1:B:73:HIS:C	1:B:75:ASN:N	2.70	0.45
1:B:215:GLN:NE2	1:B:215:GLN:N	2.50	0.45
1:A:147:HIS:CD2	1:A:147:HIS:H	2.36	0.44
1:B:57:HIS:NE2	1:B:75:ASN:ND2	2.66	0.44
1:A:115:VAL:HG21	1:A:130:VAL:HG23	2.00	0.44
1:A:99:ARG:HG3	1:A:99:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HH11	1:A:21:ARG:HG3	1.83	0.44
1:A:68:ASN:HA	1:A:88:GLY:O	2.18	0.44
1:A:37:ASN:HD21	1:A:39:GLN:HB2	1.83	0.43
1:B:11:VAL:HG11	1:B:208:LEU:HB2	2.00	0.43
1:B:228:PRO:O	1:B:229:LYS:HD2	2.18	0.43
1:B:71:TYR:C	1:B:71:TYR:CD1	2.91	0.43
1:B:166:ARG:HG3	1:B:166:ARG:NH1	2.34	0.43
1:B:26:THR:HG22	1:B:209:TYR:CD1	2.53	0.43
1:B:37:ASN:OD1	1:B:39:GLN:HB2	2.17	0.43
1:B:52:LEU:HG	1:B:56:ILE:HD11	1.97	0.43
1:A:202:THR:HG21	1:B:202:THR:HG21	2.01	0.43
1:A:37:ASN:HD22	1:A:39:GLN:H	1.67	0.43
1:B:138:LEU:HD23	1:B:141:MET:CE	2.49	0.43
1:A:8:MET:O	1:A:11:VAL:HG12	2.18	0.43
1:A:2:LYS:O	1:A:6:GLU:HG3	2.19	0.43
1:B:7:LEU:O	1:B:11:VAL:HG23	2.19	0.43
1:B:59:LEU:CD2	1:B:187:MET:HE1	2.49	0.42
1:B:159:LEU:HB2	1:B:194:LEU:HD13	2.01	0.42
1:A:162:GLN:HG3	1:A:200:VAL:HB	2.01	0.42
1:B:233:LYS:HE3	1:B:248:GLU:HB2	2.02	0.42
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.85	0.42
1:B:111:GLN:OE1	1:B:130:VAL:HA	2.20	0.41
1:A:215:GLN:HE21	1:A:215:GLN:N	2.14	0.41
1:B:208:LEU:HA	1:B:208:LEU:HD12	1.91	0.41
1:B:27:LEU:HD23	1:B:27:LEU:HA	1.80	0.41
1:B:1:CXM:HG3	1:B:227:LEU:HD11	2.03	0.41
1:B:4:TYR:CZ	1:B:175:PRO:HG3	2.55	0.41
1:A:115:VAL:HG21	1:A:130:VAL:CG2	2.51	0.41
1:B:166:ARG:HG3	1:B:166:ARG:HH11	1.85	0.41
1:B:225:ARG:NH1	1:B:255:HIS:NE2	2.69	0.40
1:B:42:PHE:HA	1:B:43:PRO:HD3	1.84	0.40
1:A:3:GLN:O	1:A:34:MET:HE1	2.21	0.40
1:B:79:ILE:O	1:B:79:ILE:HG13	2.21	0.40
1:A:192:CYS:O	1:A:193:ASP:HB2	2.22	0.40
1:B:73:HIS:O	1:B:75:ASN:N	2.55	0.40
1:A:33:GLN:HA	1:A:201:TRP:O	2.21	0.40
1:A:24:THR:CG2	1:A:211:ASN:ND2	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	234 (89%)	26 (10%)	2 (1%)	19	57
1	B	263/264 (100%)	240 (91%)	21 (8%)	2 (1%)	19	57
All	All	525/528 (99%)	474 (90%)	47 (9%)	4 (1%)	19	57

All (4) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/232 (100%)	222 (96%)	10 (4%)	29	66
1	B	233/232 (100%)	217 (93%)	16 (7%)	15	48
All	All	465/464 (100%)	439 (94%)	26 (6%)	21	56

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	37	ASN
1	A	59	LEU
1	A	134	ASN
1	A	138	LEU
1	A	143	LEU
1	A	215	GLN
1	A	227	LEU
1	A	230	LEU
1	B	5	LEU
1	B	64	GLN
1	B	87	ASN
1	B	89	ASP
1	B	96	LYS
1	B	116	LEU
1	B	126	ARG
1	B	130	VAL
1	B	134	ASN
1	B	215	GLN
1	B	220	LEU
1	B	225	ARG
1	B	233	LYS
1	B	239	ILE
1	B	249	ILE
1	B	259	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	37	ASN
1	A	51	HIS
1	A	64	GLN
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	162	GLN
1	A	190	GLN

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Mol	Chain	Res	Type
1	A	211	ASN
1	A	215	GLN
1	A	217	HIS
1	B	33	GLN
1	B	57	HIS
1	B	73	HIS
1	B	75	ASN
1	B	76	ASN
1	B	87	ASN
1	B	117	ASN
1	B	134	ASN
1	B	151	GLN
1	B	162	GLN
1	B	215	GLN

### 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	6,10,11	0.57	0	5,11,13	0.87	0
1	CXM	B	1	1	6,10,11	0.46	0	5,11,13	0.84	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
1	CXM	A	1	1	-	0/7/10/12	-
1	CXM	B	1	1	-	0/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	CXM	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
3	F89	B	1266	-	34,41,41	3.47	18 (52%)	45,60,60	3.88	14 (31%)
4	SO4	B	1268	-	4,4,4	0.19	0	6,6,6	0.18	0
2	NDU	A	1265	1	22,24,24	3.81	6 (27%)	30,36,36	3.47	9 (30%)
2	NDU	B	1265	1	22,24,24	3.54	6 (27%)	30,36,36	3.11	8 (26%)
3	F89	A	1266	-	34,41,41	3.18	17 (50%)	45,60,60	4.02	14 (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
3	F89	B	1266	-	-	0/12/30/30	0/5/5/5
2	NDU	A	1265	1	1/1/9/10	1/11/42/42	0/2/2/2
2	NDU	B	1265	1	1/1/9/10	2/11/42/42	0/2/2/2
3	F89	A	1266	-	-	3/12/30/30	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1265	NDU	C6-N1	12.09	1.62	1.46
2	B	1265	NDU	C6-N1	11.77	1.61	1.46
3	B	1266	F89	C19-N	9.62	1.54	1.46
3	A	1266	F89	CB-CA	8.65	1.63	1.53
2	A	1265	NDU	C6-C5	8.49	1.64	1.52
3	B	1266	F89	CA-N	7.90	1.58	1.47
2	A	1265	NDU	C2-N1	7.07	1.45	1.35
3	B	1266	F89	C3-N2	7.05	1.46	1.34
3	A	1266	F89	C3-N2	6.89	1.46	1.34
3	A	1266	F89	C19-N	6.84	1.52	1.46
2	B	1265	NDU	C6-C5	6.66	1.61	1.52
3	B	1266	F89	CB-CA	6.38	1.60	1.53
3	A	1266	F89	CA-N	6.04	1.55	1.47
2	B	1265	NDU	C2-N1	5.68	1.43	1.35
3	B	1266	F89	C4A-N4	5.50	1.46	1.37
3	A	1266	F89	C4A-N4	5.45	1.46	1.37
3	B	1266	F89	C14-C13	4.73	1.47	1.39
2	B	1265	NDU	C1'-N1	4.70	1.52	1.45
2	B	1265	NDU	C5-C4	4.20	1.60	1.51
2	A	1265	NDU	C5-C4	3.69	1.59	1.51
3	B	1266	F89	C19-C15	3.68	1.55	1.50
3	A	1266	F89	C14-C13	3.60	1.45	1.39
2	A	1265	NDU	C1'-N1	3.32	1.50	1.45
3	B	1266	F89	C17-C16	3.25	1.45	1.39
3	A	1266	F89	C1B-C1A	3.21	1.47	1.41
3	B	1266	F89	C1B-C6A	3.12	1.48	1.42
3	B	1266	F89	C13-N12	3.09	1.47	1.38
2	A	1265	NDU	C4-N3	3.06	1.42	1.37
3	A	1266	F89	C1A-C4A	3.00	1.47	1.42
3	A	1266	F89	C1B-C6A	2.74	1.47	1.42
3	B	1266	F89	C16-C	2.74	1.53	1.48
3	A	1266	F89	C17-C16	2.71	1.44	1.39
3	A	1266	F89	C19-C15	2.60	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1266	F89	C13-N12	2.56	1.46	1.38
3	B	1266	F89	C1A-C4A	2.49	1.47	1.42
2	B	1265	NDU	C4-N3	2.45	1.41	1.37
3	B	1266	F89	C18-C13	2.35	1.43	1.39
3	A	1266	F89	CB-CG	2.34	1.63	1.52
3	A	1266	F89	C10-C9	2.32	1.42	1.37
3	B	1266	F89	C8-C9	2.31	1.43	1.38
3	A	1266	F89	C8-C9	2.31	1.43	1.38
3	B	1266	F89	C18-C17	2.25	1.42	1.38
3	B	1266	F89	C6-C5	2.24	1.41	1.35
3	B	1266	F89	C10-C9	2.21	1.42	1.37
3	A	1266	F89	C6-C5	2.15	1.41	1.35
3	B	1266	F89	C7-C8	2.12	1.41	1.36
3	A	1266	F89	C7-C8	2.01	1.40	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1266	F89	O-C-N	16.37	137.53	125.24
3	B	1266	F89	O-C-N	15.79	137.09	125.24
2	A	1265	NDU	O4'-C1'-N1	12.95	124.92	108.41
3	B	1266	F89	C3-N4-C4A	12.38	124.93	116.54
3	A	1266	F89	C3-N4-C4A	11.97	124.65	116.54
2	B	1265	NDU	O4'-C1'-N1	10.45	121.73	108.41
3	B	1266	F89	C19-C15-C16	-8.13	104.67	109.75
2	A	1265	NDU	C6-N1-C1'	-7.76	105.67	120.94
2	B	1265	NDU	C1'-N1-C2	7.68	128.69	118.50
3	A	1266	F89	C15-C19-N	-7.36	99.73	102.18
2	B	1265	NDU	C6-N1-C1'	-7.07	107.03	120.94
3	A	1266	F89	C19-C15-C16	-6.73	105.55	109.75
3	B	1266	F89	O-C-C16	-6.09	116.84	128.68
3	A	1266	F89	O-C-C16	-5.79	117.41	128.68
2	A	1265	NDU	C1'-N1-C2	5.68	126.05	118.50
3	B	1266	F89	C15-C19-N	-5.55	100.33	102.18
2	A	1265	NDU	P-O5'-C5'	5.49	133.41	118.30
3	A	1266	F89	C19-N-CA	-5.40	118.65	123.71
3	B	1266	F89	C1A-C1-N2	-5.37	119.32	124.09
3	A	1266	F89	CB-CA-N	-4.93	107.02	112.65
3	A	1266	F89	C1A-C1-N2	-4.91	119.73	124.09
2	A	1265	NDU	C2'-C1'-N1	-4.76	109.79	115.61
3	A	1266	F89	CA-N-C	4.43	128.69	121.82
3	B	1266	F89	CB-CA-N	-4.20	107.86	112.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1266	F89	C15-C16-C	-4.02	106.78	108.94
2	B	1265	NDU	P-O5'-C5'	4.00	129.32	118.30
3	A	1266	F89	C15-C16-C	-3.73	106.94	108.94
3	B	1266	F89	C11-C9-C10	-3.68	114.92	121.51
3	A	1266	F89	C11-C9-C10	-3.68	114.93	121.51
3	B	1266	F89	C19-N-C	-3.38	111.73	113.12
2	B	1265	NDU	C6-C5-C4	3.26	118.30	111.25
2	A	1265	NDU	OP2-P-O5'	-3.20	98.22	106.73
2	A	1265	NDU	OP3-P-OP2	2.97	119.00	107.64
3	A	1266	F89	N4-C3-N2	-2.91	120.36	125.72
2	B	1265	NDU	O5'-C5'-C4'	2.87	118.86	108.99
3	B	1266	F89	N4-C3-N2	-2.72	120.71	125.72
3	A	1266	F89	C16-C-N	-2.69	104.86	106.44
2	A	1265	NDU	C6-C5-C4	2.57	116.80	111.25
2	B	1265	NDU	C2'-C1'-N1	-2.51	112.54	115.61
3	A	1266	F89	C3M-C3-N2	2.41	120.91	117.15
2	B	1265	NDU	O5'-P-OP1	2.37	113.13	106.47
3	B	1266	F89	CA-N-C	2.27	125.33	121.82
2	A	1265	NDU	O5'-P-OP1	2.16	112.53	106.47
3	B	1266	F89	C14-C13-N12	-2.13	115.35	120.77
3	B	1266	F89	C18-C13-N12	2.10	125.32	120.97

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1265	NDU	C5
2	B	1265	NDU	C5

All (6) torsion outliers are listed below:

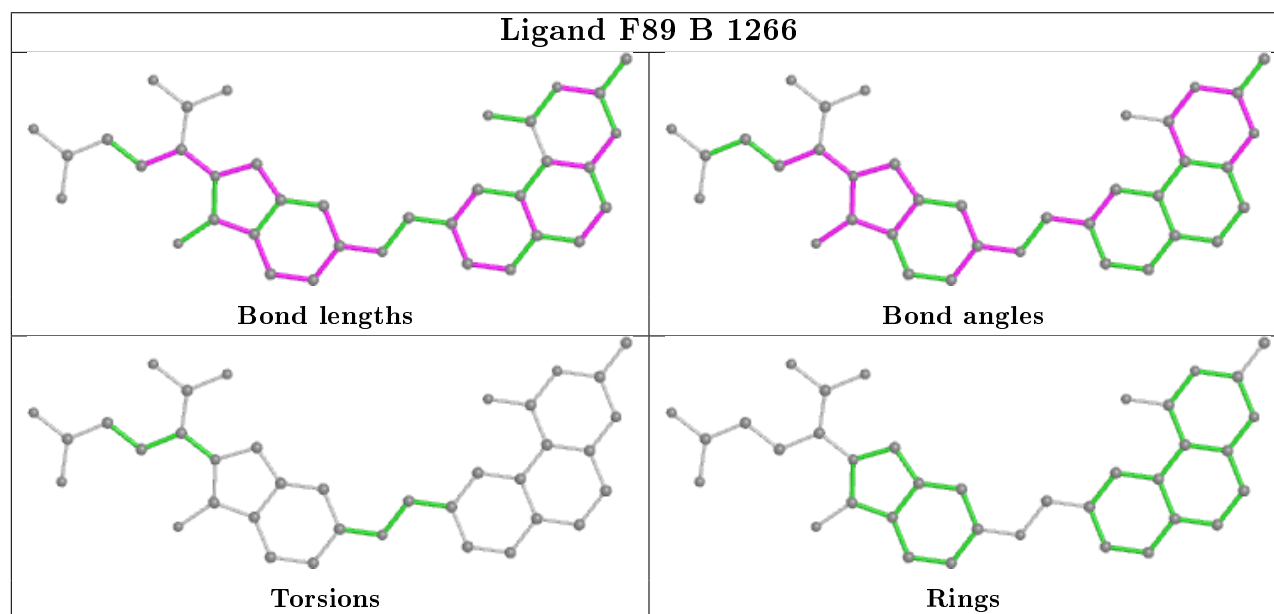
Mol	Chain	Res	Type	Atoms
3	A	1266	F89	CT-CA-N-C19
3	A	1266	F89	CB-CA-N-C
2	A	1265	NDU	O4'-C4'-C5'-O5'
2	B	1265	NDU	O4'-C4'-C5'-O5'
3	A	1266	F89	CB-CA-N-C19
2	B	1265	NDU	C5'-O5'-P-OP3

There are no ring outliers.

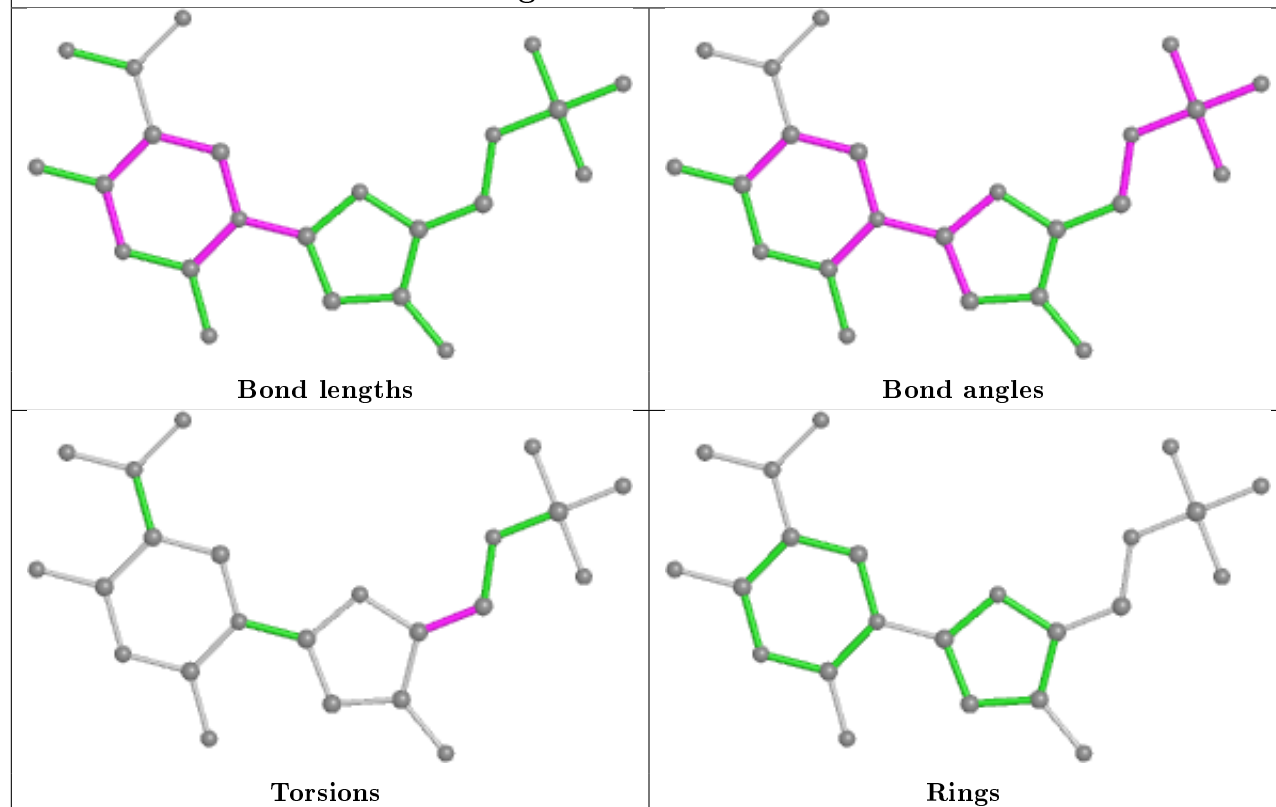
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1266	F89	2	0
3	A	1266	F89	1	0

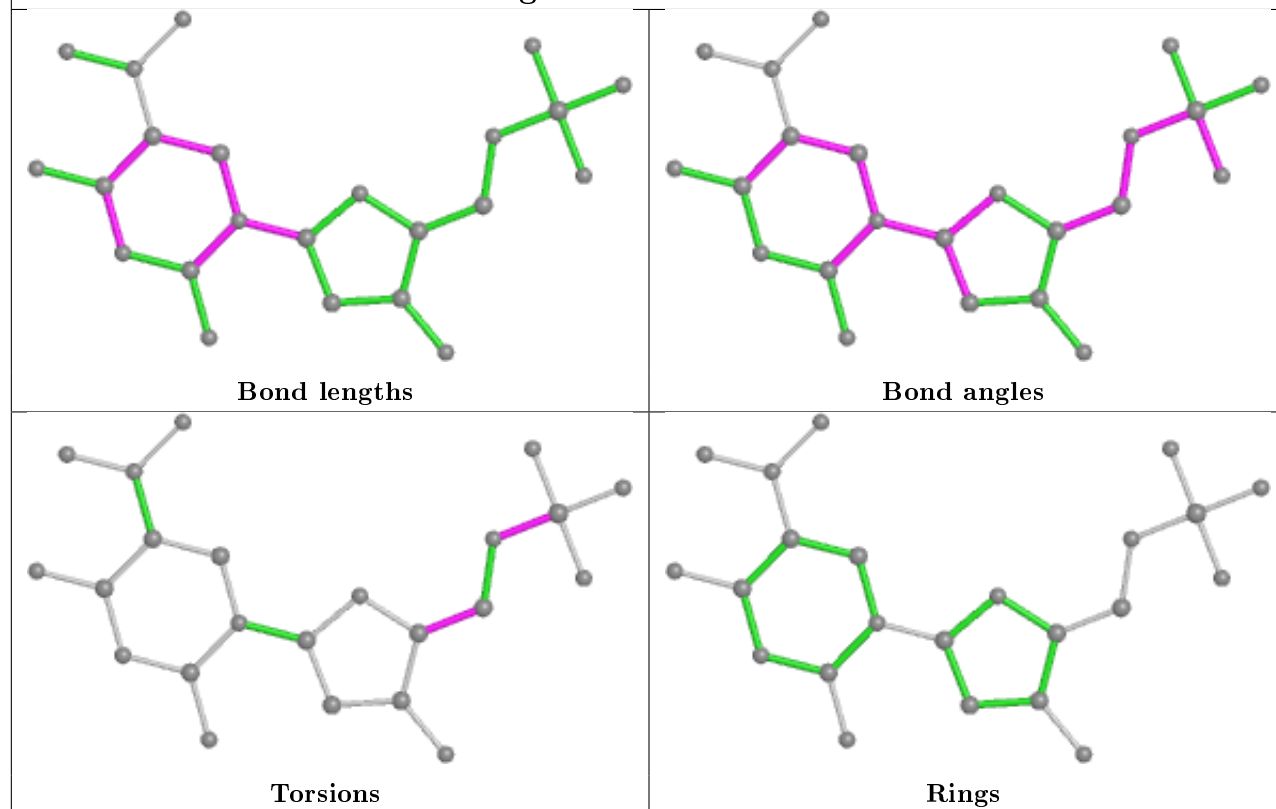
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

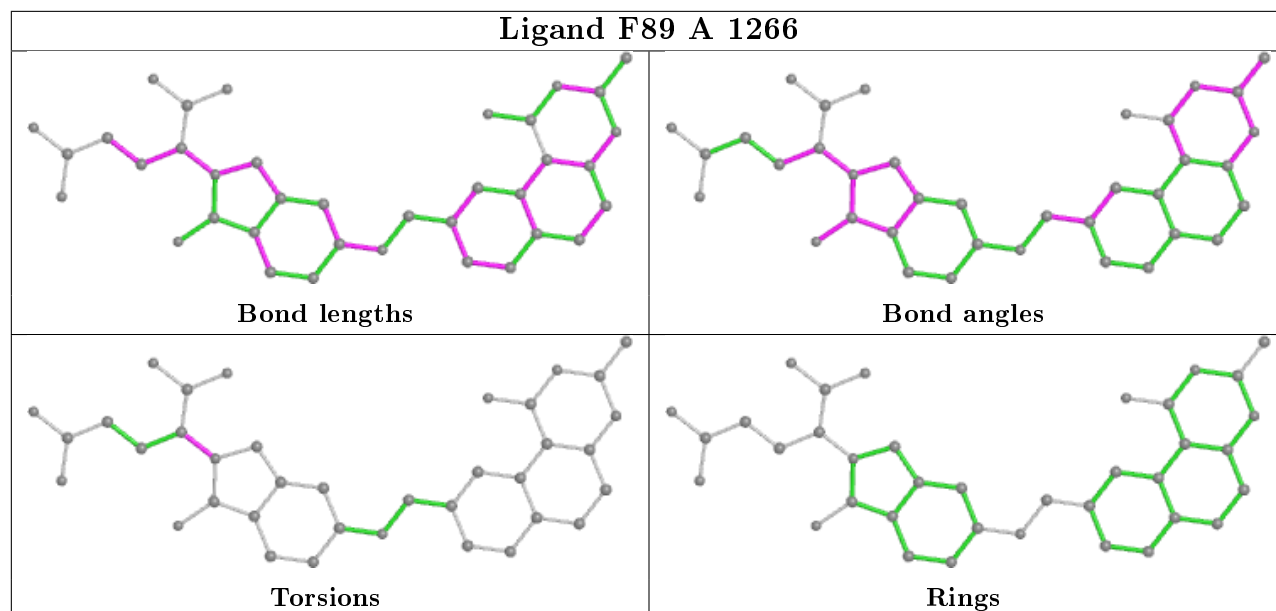


## Ligand NDU A 1265



## Ligand NDU B 1265





## 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.