



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 09:27 am GMT

PDB ID : 5O6J  
Title : Human NMT1 in complex with myristoyl-CoA and inhibitor IMP-1031  
Authors : Brannigan, J.A.; Wilkinson, A.J.  
Deposited on : 2017-06-06  
Resolution : 1.45 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

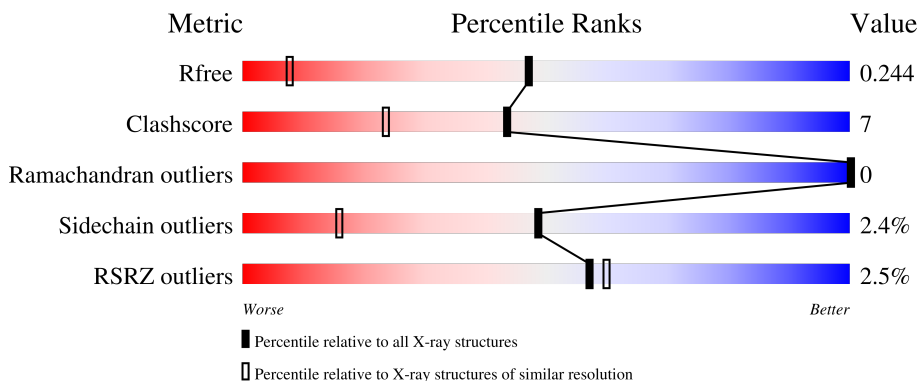
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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))
$R_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	391	 2% 87% 9% ..
1	B	391	 3% 83% 13% ..

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7681 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.

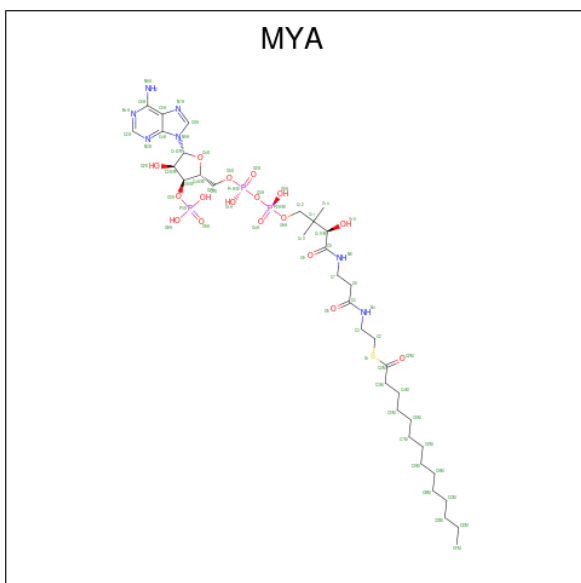
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	3331	2171	556	584	20	0	34	0
1	B	383	3308	2152	554	584	18	0	28	0

There are 6 discrepancies between the modelled and reference sequences:

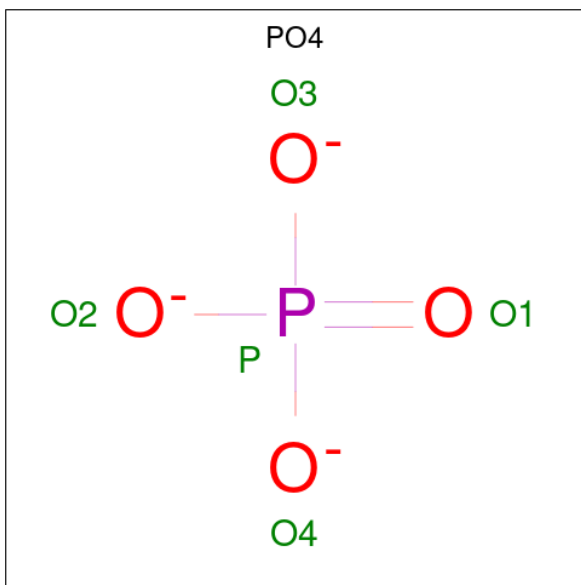
Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	expression tag	UNP P30419
A	107	PRO	-	expression tag	UNP P30419
A	108	HIS	-	expression tag	UNP P30419
B	106	GLY	-	expression tag	UNP P30419
B	107	PRO	-	expression tag	UNP P30419
B	108	HIS	-	expression tag	UNP P30419

- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula:  $C_{35}H_{62}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

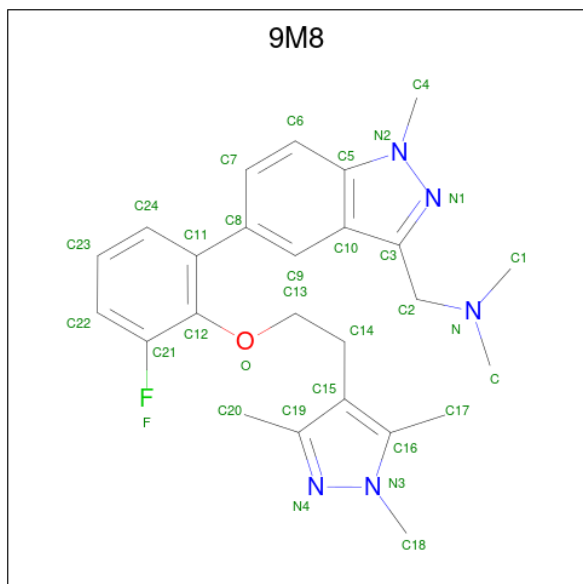


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O P	0	0
			5	4 1		
3	A	1	Total	O P	0	0
			5	4 1		
3	A	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		
3	B	1	Total	O P	0	0
			5	4 1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg	0	0
			1 1		
4	B	1	Total Mg	0	0
			1 1		

- Molecule 5 is 1-[5-[3-fluoranyl-2-[2-(1,3,5-trimethylpyrazol-4-yl)ethoxy]phenyl]-1-methyl-indazol-3-yl]-{N}, {N}-dimethyl-methanamine (three-letter code: 9M8) (formula: C<sub>25</sub>H<sub>30</sub>FN<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			32	25	1	5	1		
5	B	1	Total	C	F	N	O	0	0
			32	25	1	5	1		

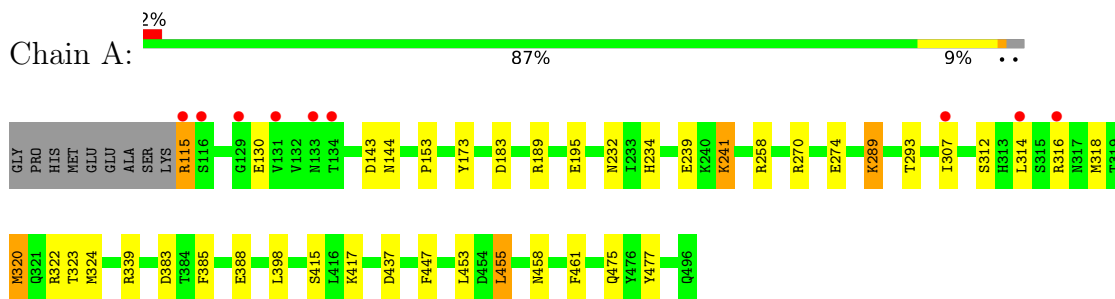
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	405	Total	O	0	0
			405	405		
6	B	415	Total	O	0	0
			415	415		

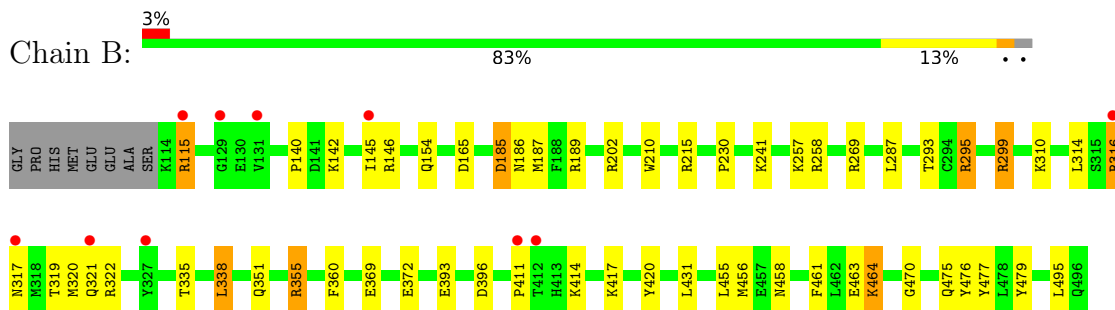
### 3 Residue-property plots [i](#)

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

- Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.92Å 177.28Å 58.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 1.45 59.36 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.8 (80.00-1.45) 97.9 (59.36-1.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.45Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.213 , 0.244 0.213 , 0.244	Depositor DCC
$R_{free}$ test set	7227 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtrriage
Anisotropy	0.800	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PO4, 9M8, MYA

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	1.15	1/3520 (0.0%)	1.16	10/4769 (0.2%)
1	B	1.20	4/3476 (0.1%)	1.21	21/4714 (0.4%)
All	All	1.17	5/6996 (0.1%)	1.19	31/9483 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	479	TYR	CE1-CZ	6.21	1.46	1.38
1	B	420	TYR	CZ-OH	6.19	1.48	1.37
1	B	476	TYR	CE1-CZ	6.17	1.46	1.38
1	A	477	TYR	CE1-CZ	5.84	1.46	1.38
1	B	210	TRP	CG-CD1	5.30	1.44	1.36

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ARG	NE-CZ-NH1	-15.47	112.57	120.30
1	A	289	LYS	CD-CE-NZ	-8.68	91.74	111.70
1	A	189	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	B	185	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	189	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	B	338[A]	LEU	CB-CG-CD2	-8.08	97.27	111.00
1	B	338[B]	LEU	CB-CG-CD2	-8.08	97.27	111.00
1	B	189	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	B	495	LEU	CB-CG-CD2	7.26	123.34	111.00
1	B	215	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	B	299	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	269	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	A	183	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	165	ASP	CB-CG-OD1	6.43	124.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	B	287	LEU	CB-CG-CD1	-6.32	100.26	111.00
1	B	258	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	383	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	258	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	146	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	270	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	215	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	431	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	B	464	LYS	CD-CE-NZ	5.51	124.38	111.70
1	A	339	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	202	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	A	173	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
1	B	477	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	396	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	258	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	388	GLU	OE1-CD-OE2	-5.02	117.28	123.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3331	0	3420	41	0
1	B	3308	0	3370	49	0
2	A	63	0	58	1	0
2	B	63	0	58	1	0
3	A	15	0	0	0	0
3	B	15	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	32	0	0	0	0
5	B	32	0	0	0	0
6	A	405	0	0	8	0
6	B	415	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7681	0	6906	92	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 7.

All (92) 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:463[B]:GLU:OE2	6:B:2105:HOH:O	1.58	1.18
1:B:295[A]:ARG:HD3	6:B:2109:HOH:O	1.44	1.16
1:A:115:ARG:N	1:A:115:ARG:HD3	1.55	1.15
1:A:144[B]:ASN:OD1	6:A:2103:HOH:O	1.62	1.15
1:B:115:ARG:HG2	1:B:115:ARG:HH11	0.94	1.09
1:A:115:ARG:HG2	1:A:115:ARG:HH11	0.93	1.05
1:B:115:ARG:HH11	1:B:115:ARG:CG	1.75	0.98
1:A:385:PHE:HB2	1:A:398[B]:LEU:HD21	1.43	0.98
1:B:187[A]:MET:HA	1:B:187[A]:MET:HE2	1.46	0.95
1:A:115:ARG:HG2	1:A:115:ARG:NH1	1.68	0.93
1:B:115:ARG:HG2	1:B:115:ARG:NH1	1.76	0.92
1:A:115:ARG:HH11	1:A:115:ARG:CG	1.83	0.91
1:B:187[A]:MET:HA	1:B:187[A]:MET:CE	2.05	0.86
1:B:295[B]:ARG:NH2	1:B:470:GLY:O	2.15	0.80
1:B:320[B]:MET:CE	1:B:320[B]:MET:HA	2.12	0.80
1:B:316:ARG:HE	1:B:316:ARG:H	1.30	0.78
1:A:320[A]:MET:HA	1:A:320[A]:MET:HE2	1.66	0.78
1:A:115:ARG:N	1:A:115:ARG:CD	2.36	0.78
1:B:317:ASN:HB3	6:B:2185:HOH:O	1.85	0.76
1:A:234[B]:HIS:ND1	1:A:239[B]:GLU:HG2	2.01	0.76
1:B:355[A]:ARG:HG2	1:B:355[A]:ARG:NH1	2.03	0.74
1:A:318[B]:MET:HG2	1:A:322[B]:ARG:HD2	1.69	0.73
1:B:372[B]:GLU:OE2	6:B:2106:HOH:O	2.10	0.69
1:A:320[A]:MET:HA	1:A:320[A]:MET:CE	2.25	0.67
1:B:320[B]:MET:HA	1:B:320[B]:MET:HE3	1.76	0.67
1:B:355[A]:ARG:HG2	1:B:355[A]:ARG:HH11	1.60	0.67
1:A:437[B]:ASP:OD1	6:A:2104:HOH:O	2.11	0.66
3:B:2003:PO4:O3	6:B:2107:HOH:O	2.13	0.66
1:A:195[A]:GLU:HG2	6:A:2101:HOH:O	1.96	0.65
1:B:355[A]:ARG:HH11	1:B:355[A]:ARG:CG	2.10	0.64
1:B:115:ARG:CG	1:B:115:ARG:NH1	2.41	0.63
1:A:115:ARG:NH1	1:A:115:ARG:CG	2.49	0.63
1:B:464:LYS:NZ	6:B:2108:HOH:O	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:O	1:A:289:LYS:NZ	2.27	0.62
1:B:186:ASN:O	1:B:187[A]:MET:HE3	1.98	0.62
1:A:314:LEU:HD13	1:A:320[A]:MET:HE3	1.82	0.62
1:B:351:GLN:O	1:B:355[A]:ARG:HD3	2.00	0.61
1:A:385:PHE:HB2	1:A:398[B]:LEU:CD2	2.27	0.60
1:A:234[B]:HIS:ND1	1:A:239[B]:GLU:OE2	2.36	0.59
1:B:316:ARG:O	1:B:317:ASN:HB2	2.04	0.56
1:B:295[A]:ARG:CD	6:B:2109:HOH:O	2.24	0.55
1:B:230:PRO:CB	1:B:241:LYS:HE3	2.37	0.55
1:A:144[B]:ASN:CG	6:A:2103:HOH:O	2.29	0.55
1:A:274:GLU:OE2	1:B:369:GLU:HG3	2.06	0.55
1:A:318[B]:MET:CG	1:A:322[B]:ARG:HD2	2.36	0.54
1:B:320[B]:MET:HA	1:B:320[B]:MET:HE2	1.87	0.54
1:B:142:LYS:HB2	1:B:145[A]:ILE:HD11	1.89	0.54
1:B:185:ASP:HB3	1:B:187[B]:MET:HG3	1.89	0.54
1:A:458:ASN:HA	1:A:461:PHE:CE2	2.42	0.53
1:A:232[A]:ASN:HD21	1:A:241[A]:LYS:HD2	1.72	0.53
1:B:230:PRO:HB2	1:B:241:LYS:HE3	1.89	0.53
1:A:320[A]:MET:HE2	1:A:323:THR:HB	1.91	0.53
1:B:458:ASN:HA	1:B:461:PHE:CE2	2.44	0.52
1:A:398[B]:LEU:H	1:A:398[B]:LEU:HD23	1.73	0.52
1:B:321[B]:GLN:H	1:B:321[B]:GLN:CD	2.13	0.52
1:A:318[B]:MET:HG2	1:A:322[B]:ARG:CD	2.37	0.52
1:B:257:LYS:HE2	6:B:2173:HOH:O	2.11	0.51
1:A:234[B]:HIS:ND1	1:A:239[B]:GLU:CG	2.72	0.51
1:A:415:SER:OG	1:A:417[B]:LYS:HE3	2.10	0.51
1:B:185:ASP:CB	1:B:187[B]:MET:HG3	2.41	0.50
1:A:320[A]:MET:HE2	1:A:320[A]:MET:CA	2.40	0.50
1:B:417[A]:LYS:NZ	6:B:2101:HOH:O	0.65	0.50
1:A:293:THR:OG1	1:A:475[A]:GLN:NE2	2.40	0.49
1:B:187[A]:MET:CE	1:B:187[A]:MET:CA	2.87	0.49
1:B:316:ARG:H	1:B:316:ARG:NE	2.04	0.49
1:B:393[B]:GLU:HG3	6:B:2411:HOH:O	2.12	0.49
1:B:321[B]:GLN:H	1:B:321[B]:GLN:NE2	2.11	0.48
1:B:335:THR:HB	1:B:338[B]:LEU:HD13	1.95	0.48
2:B:2001:MYA:H8A	6:B:2425:HOH:O	2.13	0.48
1:A:307[B]:ILE:HD12	1:A:312:SER:HB2	1.95	0.47
1:A:417[A]:LYS:HG3	6:A:2370:HOH:O	2.15	0.46
1:B:319:THR:HB	1:B:321[B]:GLN:HE21	1.80	0.46
1:B:335:THR:HB	1:B:338[B]:LEU:CD1	2.45	0.46
1:A:232[A]:ASN:ND2	1:A:241[A]:LYS:HE3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PRO:HG3	6:A:2106:HOH:O	2.15	0.45
1:A:453:LEU:HB2	1:A:455:LEU:HG	1.98	0.45
1:A:417[A]:LYS:HG2	1:A:447:PHE:CD1	2.52	0.44
1:B:314:LEU:HD21	1:B:320[B]:MET:HE3	2.00	0.43
1:A:316:ARG:H	1:A:316:ARG:HG3	1.62	0.43
1:A:232[A]:ASN:ND2	1:A:241[A]:LYS:HD2	2.33	0.43
1:B:293:THR:OG1	1:B:475[A]:GLN:NE2	2.49	0.43
1:B:355[A]:ARG:NH1	6:B:2123:HOH:O	2.51	0.43
1:A:144[B]:ASN:ND2	6:A:2103:HOH:O	2.48	0.43
1:B:417[B]:LYS:HB2	6:B:2399:HOH:O	2.18	0.43
1:B:295[A]:ARG:HH11	1:B:295[A]:ARG:HG3	1.84	0.42
1:B:360:PHE:CE1	1:B:456:MET:HA	2.55	0.42
1:B:316:ARG:HE	1:B:316:ARG:N	2.09	0.41
1:B:417[B]:LYS:HB2	1:B:417[B]:LYS:HE2	1.71	0.41
2:A:2001:MYA:H8A	6:A:2367:HOH:O	2.20	0.41
1:B:115:ARG:NH1	1:B:115:ARG:CB	2.82	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	414/391 (106%)	402 (97%)	12 (3%)	0	100	100
1	B	409/391 (105%)	395 (97%)	14 (3%)	0	100	100
All	All	823/782 (105%)	797 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	382/355 (108%)	374 (98%)	8 (2%)	53	19
1	B	377/355 (106%)	362 (96%)	15 (4%)	31	4
All	All	759/710 (107%)	736 (97%)	23 (3%)	49	9

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	143[A]	ASP
1	A	143[B]	ASP
1	A	241[A]	LYS
1	A	241[B]	LYS
1	A	320[A]	MET
1	A	320[B]	MET
1	A	455	LEU
1	B	115	ARG
1	B	140	PRO
1	B	154[A]	GLN
1	B	154[B]	GLN
1	B	295[A]	ARG
1	B	295[B]	ARG
1	B	299	ARG
1	B	310	LYS
1	B	316	ARG
1	B	322	ARG
1	B	355[A]	ARG
1	B	355[B]	ARG
1	B	411	PRO
1	B	414	LYS
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	GLN
1	B	351	GLN
1	B	413	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 monosaccharides in this entry.

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

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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	MYA	A	2001	4	57,65,65	1.14	4 (7%)	68,91,91	1.71	13 (19%)
3	PO4	A	2004	-	4,4,4	0.66	0	6,6,6	0.99	0
3	PO4	A	2003	-	4,4,4	1.50	0	6,6,6	1.80	1 (16%)
2	MYA	B	2001	4	57,65,65	1.41	4 (7%)	68,91,91	1.71	11 (16%)
5	9M8	A	2006	-	30,35,35	1.49	5 (16%)	39,51,51	2.72	8 (20%)
3	PO4	B	2002	-	4,4,4	1.36	1 (25%)	6,6,6	1.46	1 (16%)
3	PO4	B	2004	-	4,4,4	1.10	0	6,6,6	0.68	0
5	9M8	B	2006	-	30,35,35	1.56	7 (23%)	39,51,51	3.73	13 (33%)
3	PO4	B	2003	-	4,4,4	1.46	1 (25%)	6,6,6	1.57	1 (16%)
3	PO4	A	2002	-	4,4,4	0.90	0	6,6,6	1.26	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	MYA	A	2001	4	-	2/60/80/80	0/3/3/3
5	9M8	B	2006	-	-	0/13/14/14	0/4/4/4
5	9M8	A	2006	-	-	0/13/14/14	0/4/4/4
2	MYA	B	2001	4	-	1/60/80/80	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	MYA	C3M-C2M	-5.11	1.45	1.50
2	B	2001	MYA	O4X-C1X	3.81	1.46	1.41
5	A	2006	9M8	C6-C7	3.74	1.44	1.36
2	A	2001	MYA	C2A-N3A	3.60	1.37	1.32
2	B	2001	MYA	C8A-N7A	3.41	1.40	1.34
5	B	2006	9M8	C19-N4	3.16	1.39	1.33
5	B	2006	9M8	C16-C15	3.09	1.45	1.39
5	B	2006	9M8	C17-C16	2.84	1.55	1.49
3	B	2002	PO4	P-O1	-2.67	1.44	1.50
5	A	2006	9M8	C2-C3	-2.65	1.50	1.51
2	A	2001	MYA	P3X-O3X	2.54	1.64	1.59
5	A	2006	9M8	C16-N3	-2.53	1.33	1.37
2	A	2001	MYA	P2A-O5A	-2.49	1.43	1.55
2	B	2001	MYA	C14-C11	2.45	1.59	1.53
5	B	2006	9M8	C12-C21	2.42	1.44	1.39
5	B	2006	9M8	C6-C7	2.37	1.41	1.36
5	B	2006	9M8	C15-C19	2.23	1.43	1.39
2	A	2001	MYA	O10-C10	2.17	1.46	1.42
3	B	2003	PO4	P-O1	2.14	1.55	1.50
5	B	2006	9M8	C22-C21	2.11	1.42	1.37
5	A	2006	9M8	O-C12	-2.09	1.34	1.39
5	A	2006	9M8	C20-C19	2.08	1.53	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2006	9M8	C14-C15-C16	-14.71	116.96	127.30
5	B	2006	9M8	C14-C15-C19	13.54	136.81	127.30
5	A	2006	9M8	C14-C15-C16	-10.35	120.03	127.30
5	A	2006	9M8	C14-C15-C19	8.83	133.50	127.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2006	9M8	C3-N1-N2	6.83	110.38	104.48
2	B	2001	MYA	C3M-C2M-S1	6.49	121.01	113.46
2	A	2001	MYA	C3M-C2M-S1	6.48	121.00	113.46
2	B	2001	MYA	O4X-C1X-C2X	-5.84	98.40	106.93
5	A	2006	9M8	C3-N1-N2	5.25	109.00	104.48
2	A	2001	MYA	C13-C11-C10	4.52	116.65	108.82
2	A	2001	MYA	O2M-C2M-S1	-3.93	117.51	122.61
5	B	2006	9M8	C20-C19-N4	3.73	127.85	119.78
2	B	2001	MYA	C7-N8-C9	3.61	129.03	122.59
5	A	2006	9M8	C15-C16-N3	-3.59	103.93	106.79
3	A	2003	PO4	O3-P-O2	3.58	119.45	107.97
2	B	2001	MYA	O2M-C2M-C3M	-3.51	119.84	123.99
2	A	2001	MYA	O5-C5-N4	-3.43	116.54	123.01
5	B	2006	9M8	C20-C19-C15	-3.36	122.13	129.47
2	B	2001	MYA	C13-C11-C10	3.33	114.59	108.82
2	A	2001	MYA	P2A-O3A-P1A	-3.27	121.59	132.83
2	A	2001	MYA	C3-N4-C5	3.10	128.60	122.84
5	B	2006	9M8	C10-C5-N2	-3.10	104.87	109.17
3	B	2003	PO4	O3-P-O2	3.07	117.82	107.97
2	B	2001	MYA	N3A-C2A-N1A	-2.92	124.12	128.68
2	B	2001	MYA	O2M-C2M-S1	-2.88	118.88	122.61
2	A	2001	MYA	O5-C5-C6	2.54	126.67	122.02
5	A	2006	9M8	C20-C19-C15	-2.51	123.99	129.47
5	B	2006	9M8	F-C21-C12	-2.44	114.23	117.58
2	A	2001	MYA	O9-C9-N8	-2.42	117.79	122.99
2	A	2001	MYA	N3A-C2A-N1A	-2.40	124.92	128.68
3	B	2002	PO4	O4-P-O2	-2.39	100.30	107.97
5	B	2006	9M8	C7-C8-C9	2.39	121.83	118.09
2	A	2001	MYA	C4M-C3M-C2M	-2.36	107.11	112.33
2	A	2001	MYA	O2M-C2M-C3M	-2.34	121.23	123.99
2	B	2001	MYA	C14-C11-C10	-2.34	104.77	108.82
2	B	2001	MYA	C2-S1-C2M	2.29	109.00	101.87
5	A	2006	9M8	C10-C5-N2	-2.26	106.04	109.17
5	B	2006	9M8	C1-N-C2	2.26	115.36	110.69
2	A	2001	MYA	C14-C11-C12	-2.24	104.58	108.23
5	B	2006	9M8	F-C21-C22	2.22	123.53	118.59
5	B	2006	9M8	C18-N3-C16	2.20	131.69	128.82
5	A	2006	9M8	C20-C19-N4	2.17	124.47	119.78
5	A	2006	9M8	C7-C6-C5	-2.15	116.40	119.70
5	B	2006	9M8	C15-C16-N3	-2.14	105.09	106.79
5	B	2006	9M8	C8-C9-C10	-2.11	117.68	122.30
2	B	2001	MYA	O3X-C3X-C2X	-2.10	104.07	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	MYA	C7-N8-C9	2.05	126.24	122.59
2	B	2001	MYA	C5A-C6A-N1A	-2.01	115.81	120.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

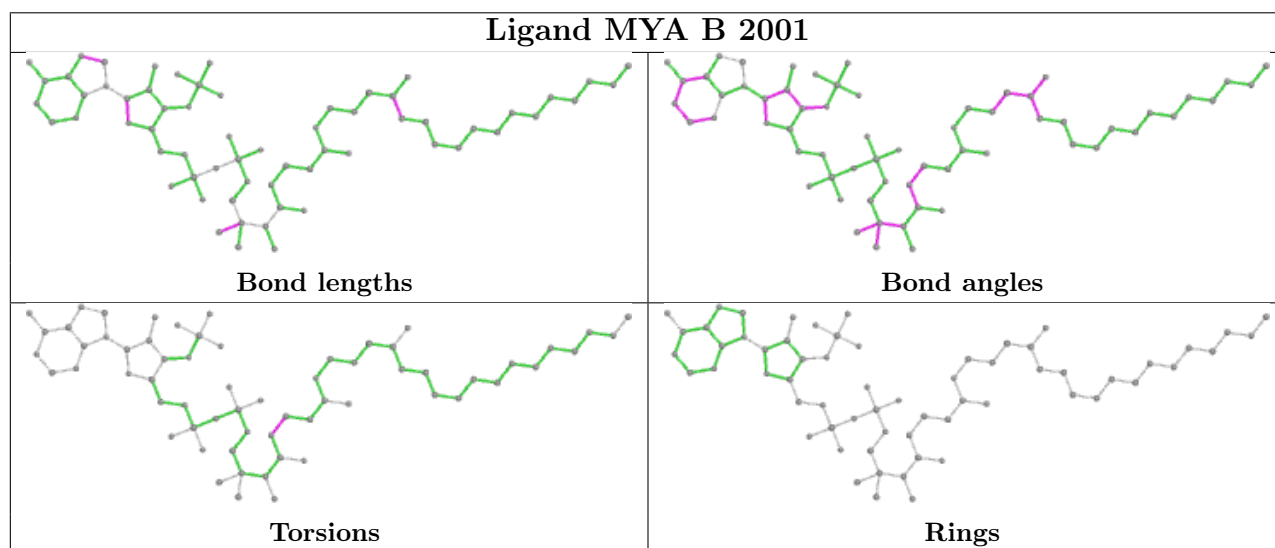
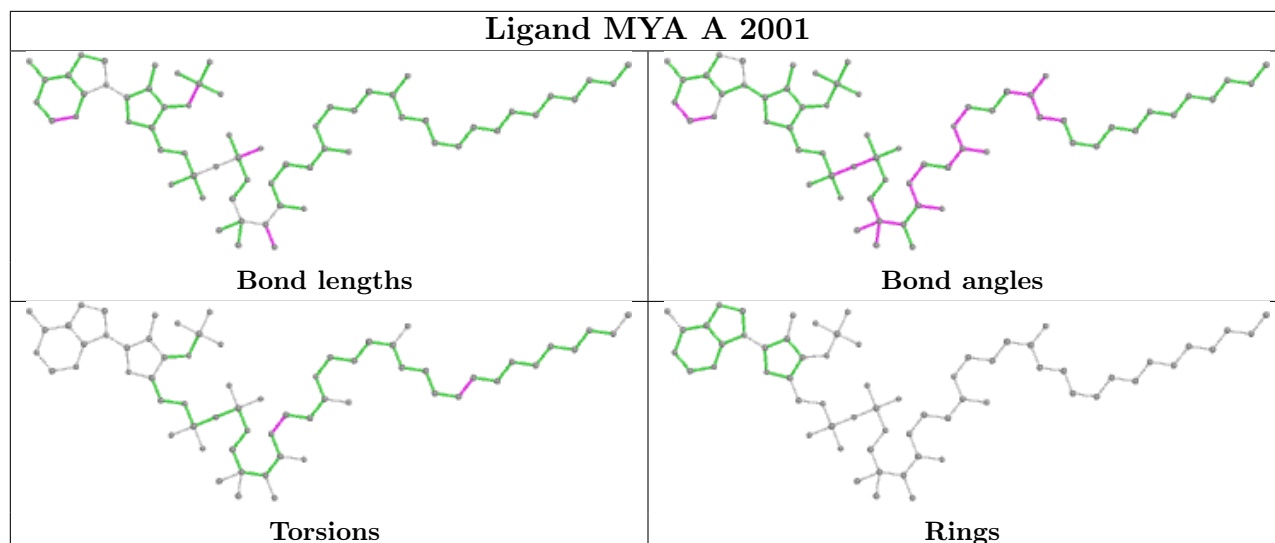
Mol	Chain	Res	Type	Atoms
2	A	2001	MYA	C6-C7-N8-C9
2	B	2001	MYA	C6-C7-N8-C9
2	A	2001	MYA	C5M-C6M-C7M-C8M

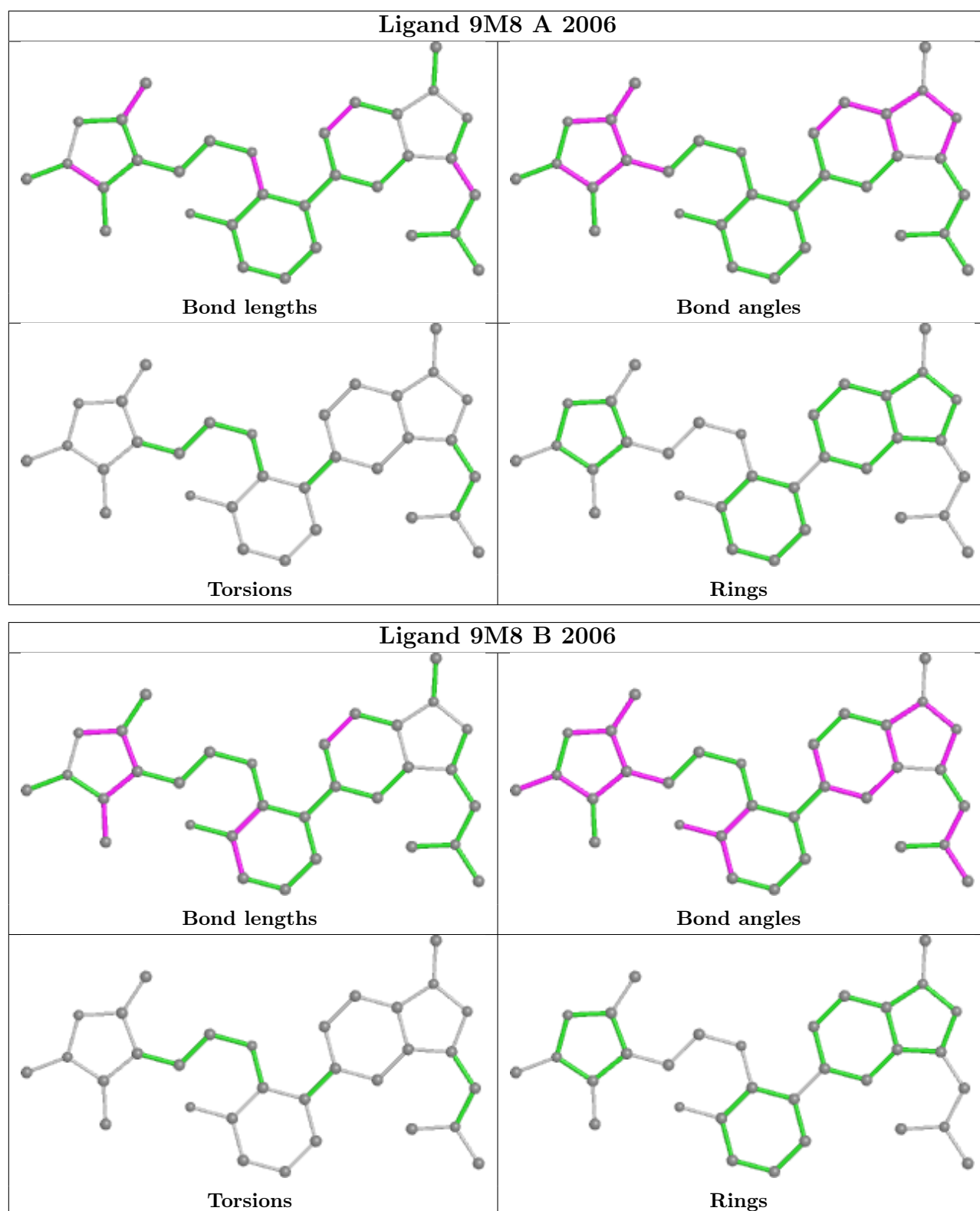
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	MYA	1	0
2	B	2001	MYA	1	0
3	B	2003	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	382/391 (97%)	0.16	9 (2%) 59 61	10, 17, 32, 58	9 (2%)
1	B	383/391 (97%)	0.26	10 (2%) 56 58	9, 17, 32, 57	10 (2%)
All	All	765/782 (97%)	0.21	19 (2%) 57 60	9, 17, 33, 58	19 (2%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	ARG	5.2
1	A	131[A]	VAL	4.8
1	A	316	ARG	4.4
1	B	412	THR	4.3
1	A	129	GLY	3.8
1	B	317	ASN	3.3
1	A	115	ARG	3.2
1	B	316	ARG	3.2
1	A	133	ASN	2.8
1	A	134	THR	2.5
1	A	314	LEU	2.4
1	A	116	SER	2.4
1	B	411	PRO	2.3
1	B	327	TYR	2.3
1	B	131	VAL	2.3
1	B	145[A]	ILE	2.3
1	A	307[A]	ILE	2.2
1	B	321[A]	GLN	2.0
1	B	129	GLY	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

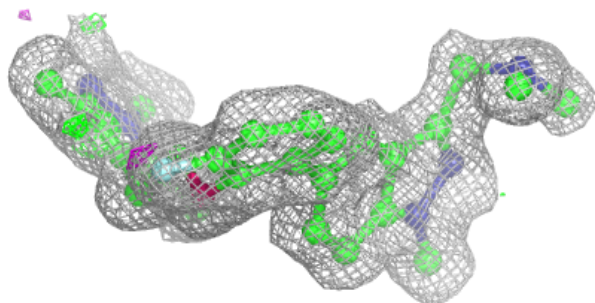
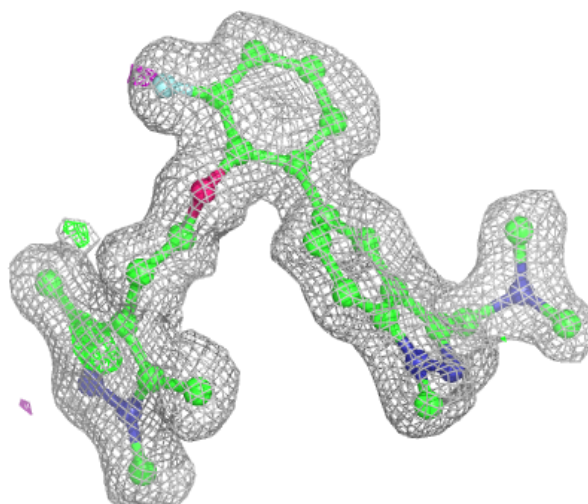
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	2004	5/5	0.42	0.37	89,93,104,106	0
3	PO4	B	2004	5/5	0.75	0.26	88,94,99,102	0
3	PO4	B	2003	5/5	0.90	0.17	17,18,19,22	5
5	9M8	A	2006	32/32	0.91	0.10	11,18,21,25	0
5	9M8	B	2006	32/32	0.92	0.09	13,17,22,23	0
4	MG	A	2005	1/1	0.94	0.08	29,29,29,29	0
2	MYA	A	2001	63/63	0.95	0.09	11,15,20,24	0
2	MYA	B	2001	63/63	0.96	0.08	9,14,17,21	0
3	PO4	A	2002	5/5	0.96	0.09	24,26,28,29	0
3	PO4	A	2003	5/5	0.96	0.10	24,26,29,31	0
3	PO4	B	2002	5/5	0.97	0.10	24,25,30,30	0
4	MG	B	2005	1/1	0.98	0.07	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

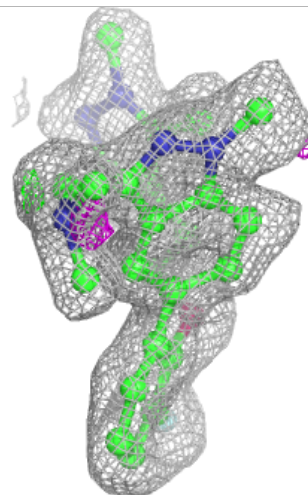
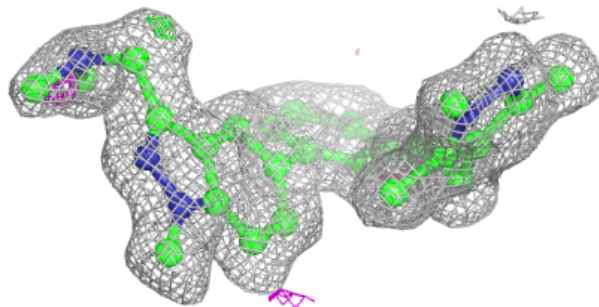
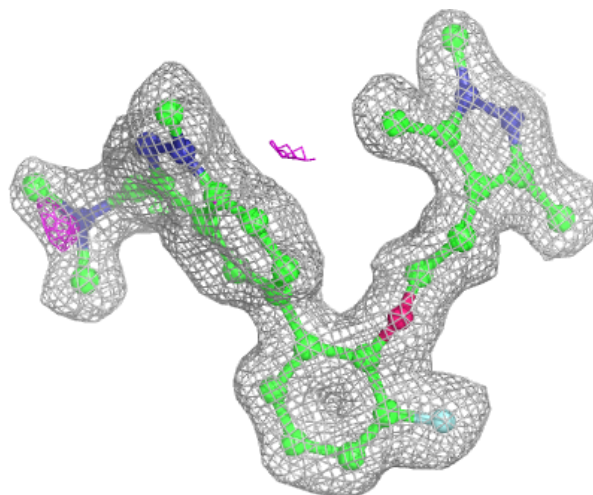
**Electron density around 9M8 A 2006:**

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

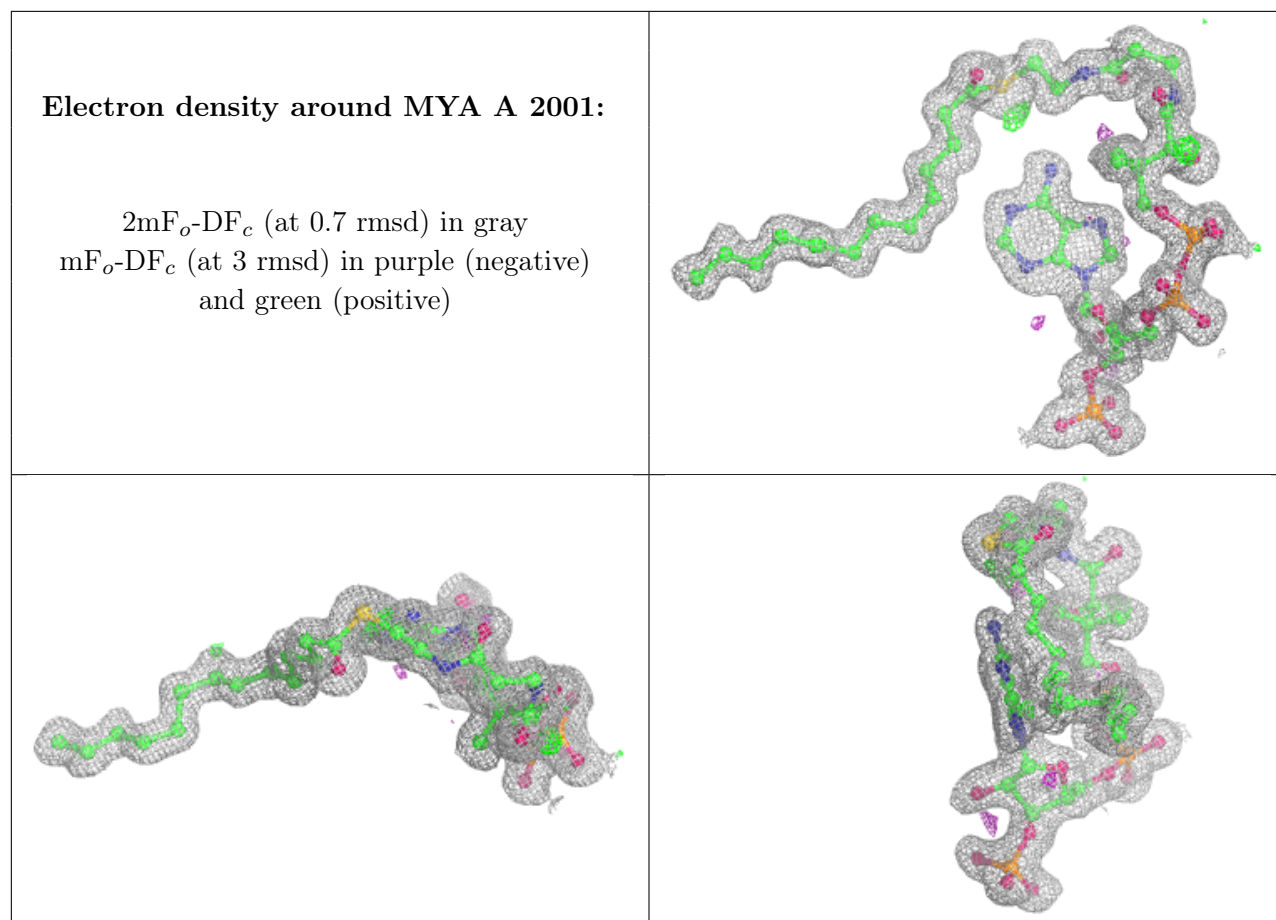


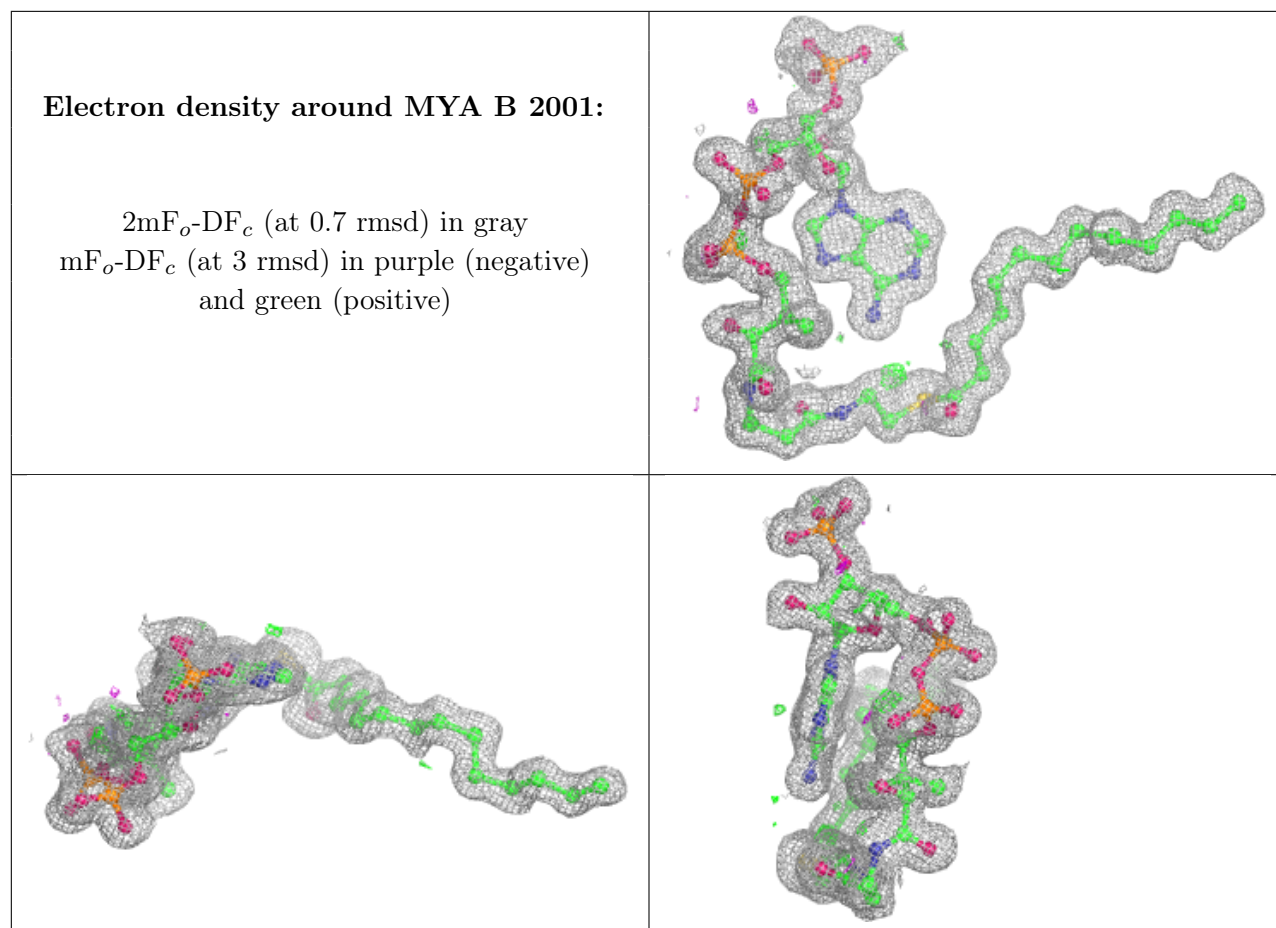
**Electron density around 9M8 B 2006:**

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









## 6.5 Other polymers [i](#)

There are no such residues in this entry.