Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 12:44 pm GMT

PDB ID	:	5O6H
Title	:	Human NMT1 in complex with myristoyl-CoA and inhibitor IMP-917
Authors	:	Brannigan, J.A.; Wilkinson, A.J.
Deposited on	:	2017-06-06
Resolution	:	1.29 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

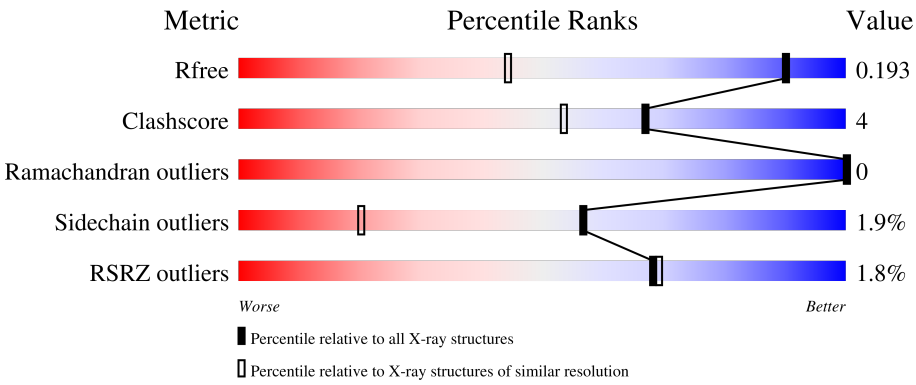
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.29 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 84% 13% ••
1	B	391	2% 84% 13% ••

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
3	PO4	A	2003	-	X	-	-
3	PO4	B	2002	-	X	-	-
6	GOL	B	2010	-	X	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7829 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.

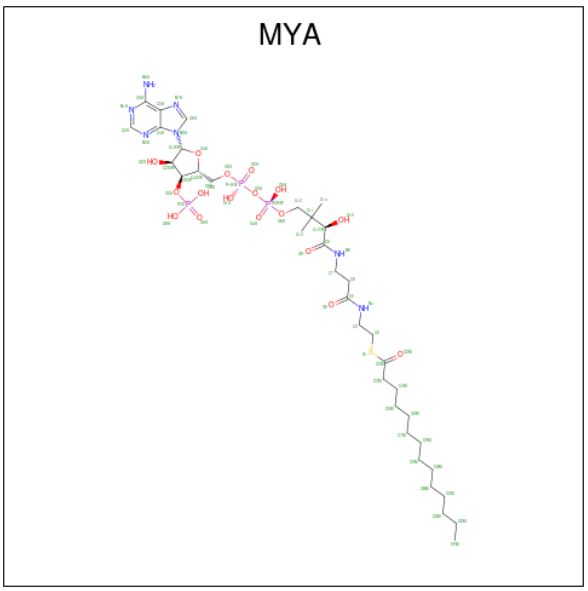
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	3298	2145	553	583	17	0	28	0
1	B	382	3261	2122	545	577	17	0	23	0

There are 6 discrepancies between the modelled and reference sequences:

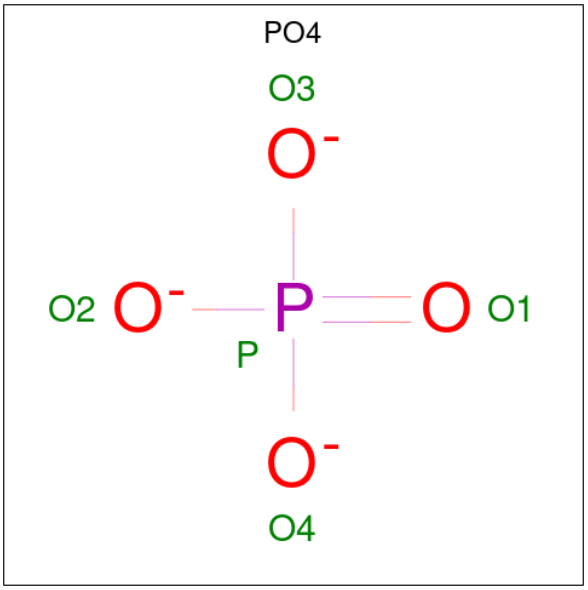
Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLY	-	expression tag	UNP P30419
A	107	PRO	-	expression tag	UNP P30419
A	108	HIS	-	expression tag	UNP P30419
B	106	GLY	-	expression tag	UNP P30419
B	107	PRO	-	expression tag	UNP P30419
B	108	HIS	-	expression tag	UNP P30419

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



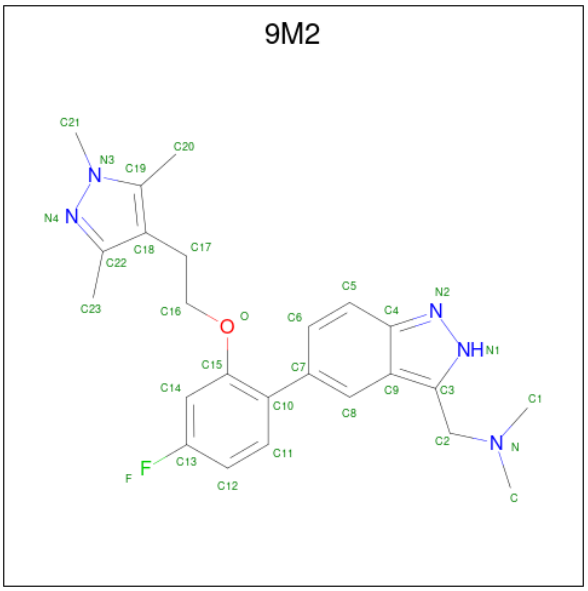
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	63	35	7	17	3	1	0	0
2	B	1	63	35	7	17	3	1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is 1-[5-[4-fluoranyl-2-[2-(1,3,5-trimethylpyrazol-4-yl)ethoxy]phenyl]-2 {H}-indazol-3-yl]- {N}, {N}-dimethyl-methanamine (three-letter code: 9M2) (formula: $C_{24}H_{28}FN_5O$).

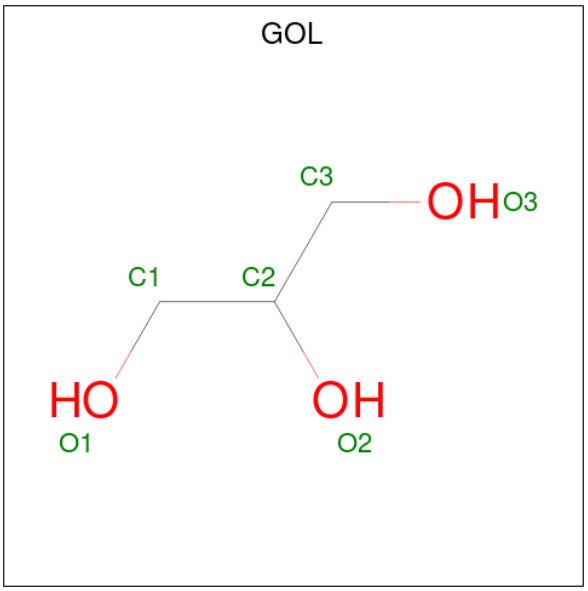


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			31	24	1	5	1		
4	B	1	Total	C	F	N	O	0	0
			31	24	1	5	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

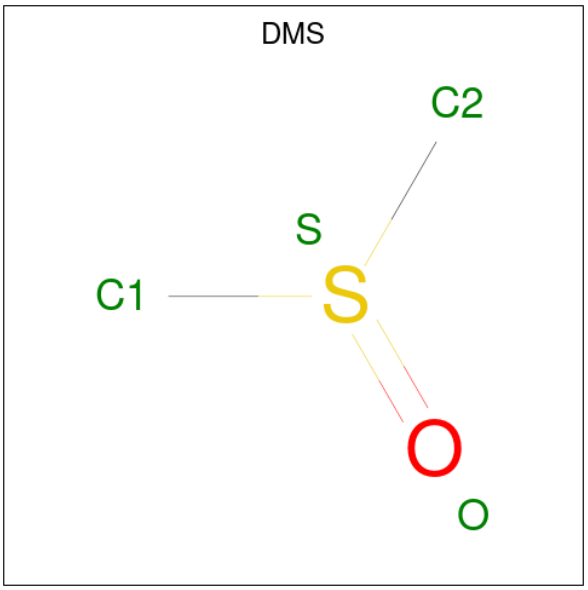
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
6	A	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0
			Total	C	O			
6	B	1	6	3	3		0	0

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 8 is water.

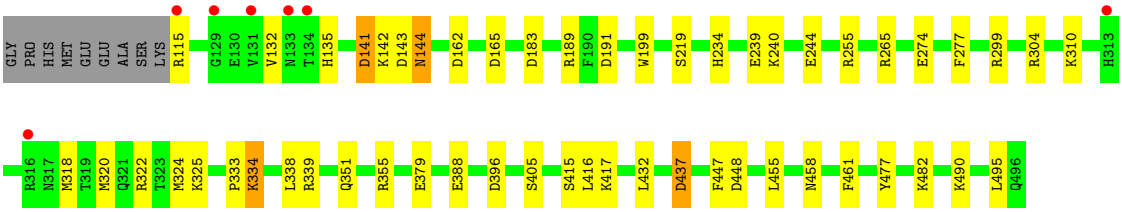
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	497	497	497	0	0
			Total	O		
8	B	521	521	521	0	0

3 Residue-property plots (i)

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

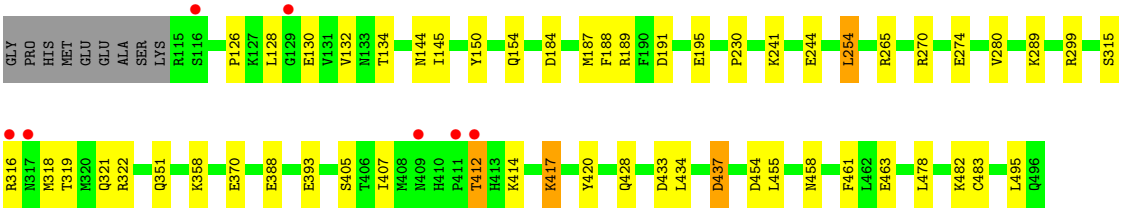
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1

Chain A:



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	79.14Å 178.85Å 58.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.00 – 1.29 55.57 – 1.29	Depositor EDS
% Data completeness (in resolution range)	98.7 (55.00-1.29) 98.7 (55.57-1.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.29Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.164 , 0.193 0.164 , 0.193	Depositor DCC
R_{free} test set	10300 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	11.1	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7829	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 9M2, MG, PO4, DMS, GOL, 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	1.37	8/3469 (0.2%)	1.33	31/4703 (0.7%)
1	B	1.37	10/3417 (0.3%)	1.53	24/4638 (0.5%)
All	All	1.37	18/6886 (0.3%)	1.43	55/9341 (0.6%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	GLU	CD-OE1	8.84	1.35	1.25
1	B	189	ARG	CD-NE	-8.02	1.32	1.46
1	B	388	GLU	CD-OE1	7.33	1.33	1.25
1	A	199	TRP	CG-CD1	7.14	1.46	1.36
1	A	415	SER	CB-OG	6.99	1.51	1.42
1	B	189	ARG	CZ-NH2	-6.81	1.24	1.33
1	B	195	GLU	CD-OE1	6.41	1.32	1.25
1	A	244	GLU	CD-OE2	6.34	1.32	1.25
1	B	270	ARG	NE-CZ	-6.20	1.25	1.33
1	B	244	GLU	CD-OE1	-6.07	1.19	1.25
1	A	219	SER	CB-OG	6.00	1.50	1.42
1	B	405	SER	CB-OG	5.57	1.49	1.42
1	A	379[C]	GLU	CD-OE1	5.42	1.31	1.25
1	A	379[D]	GLU	CD-OE1	5.42	1.31	1.25
1	B	370	GLU	CD-OE2	5.37	1.31	1.25
1	A	405	SER	CB-OG	5.34	1.49	1.42
1	B	463	GLU	CD-OE2	5.08	1.31	1.25
1	B	428	GLN	CG-CD	5.06	1.62	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	ARG	NE-CZ-NH1	41.87	141.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	ARG	NE-CZ-NH2	-41.66	99.47	120.30
1	B	189	ARG	CD-NE-CZ	14.14	143.39	123.60
1	A	299	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	A	189	ARG	NE-CZ-NH1	-12.22	114.19	120.30
1	B	274	GLU	OE1-CD-OE2	8.19	133.12	123.30
1	A	388	GLU	OE1-CD-OE2	-8.06	113.63	123.30
1	A	299	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	A	274	GLU	OE1-CD-OE2	7.60	132.42	123.30
1	A	141[A]	ASP	CB-CG-OD1	7.35	124.91	118.30
1	A	141[B]	ASP	CB-CG-OD1	7.35	124.91	118.30
1	B	270	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	165	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	339	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	A	162	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	448	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	388	GLU	CG-CD-OE2	6.39	131.07	118.30
1	B	420	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	A	396	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	A	191	ASP	CB-CG-OD1	6.23	123.90	118.30
1	B	270	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	388	GLU	OE1-CD-OE2	-6.10	115.97	123.30
1	A	244	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	B	299	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	183	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	143[A]	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	143[B]	ASP	CB-CG-OD2	5.85	123.56	118.30
1	B	358	LYS	CD-CE-NZ	5.79	125.03	111.70
1	B	463	GLU	OE1-CD-OE2	5.76	130.22	123.30
1	A	277	PHE	CB-CG-CD1	-5.72	116.79	120.80
1	B	433	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	A	477	TYR	CZ-CE2-CD2	-5.68	114.69	119.80
1	A	437[A]	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	437[B]	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	432	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	B	191	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	265	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	388	GLU	CG-CD-OE2	5.50	129.30	118.30
1	B	150	TYR	CB-CG-CD1	5.50	124.30	121.00
1	B	454	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	495	LEU	CB-CG-CD2	5.42	120.21	111.00
1	B	437[A]	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	437[B]	ASP	CB-CG-OD1	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	254[A]	LEU	CB-CG-CD1	-5.40	101.82	111.00
1	B	254[B]	LEU	CB-CG-CD1	-5.40	101.82	111.00
1	B	495	LEU	CB-CG-CD2	5.40	120.17	111.00
1	A	416	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	184	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	143[A]	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	143[B]	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	339	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	265	ARG	CG-CD-NE	5.26	122.85	111.80
1	A	142	LYS	C-N-CA	-5.12	108.91	121.70
1	B	128	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	255	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	3298	0	3362	31	0
1	B	3261	0	3313	25	0
2	A	63	0	58	0	0
2	B	63	0	58	0	0
3	A	15	0	0	0	0
3	B	25	0	0	0	0
4	A	31	0	0	0	0
4	B	31	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	6	0	8	0	0
6	B	12	0	16	0	0
7	A	4	0	6	0	0
8	A	497	0	0	8	0
8	B	521	0	0	5	0
All	All	7829	0	6821	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:MET:CE	1:A:322:ARG:HG3	1.71	1.20
1:A:318:MET:HE3	1:A:322:ARG:HG3	1.04	1.03
1:A:144[B]:ASN:HD21	1:B:351:GLN:NE2	1.60	0.99
1:A:318:MET:HE3	1:A:322:ARG:CG	1.95	0.97
1:B:280[B]:VAL:HG22	1:B:478:LEU:HD23	1.55	0.87
1:A:144[B]:ASN:ND2	1:B:351:GLN:NE2	2.23	0.85
1:B:280[B]:VAL:HG22	1:B:478:LEU:CD2	2.06	0.84
1:B:393[B]:GLU:HG3	8:B:2420:HOH:O	1.83	0.77
1:A:141[B]:ASP:OD1	8:A:2105:HOH:O	2.02	0.76
1:B:187[A]:MET:HE2	8:B:2211:HOH:O	1.92	0.70
1:A:437[B]:ASP:OD1	8:A:2106:HOH:O	2.09	0.69
1:A:351:GLN:HE21	1:A:355:ARG:NH2	1.90	0.69
1:A:234[B]:HIS:ND1	8:A:2102:HOH:O	2.26	0.69
1:A:144[A]:ASN:HD22	1:A:144[A]:ASN:H	1.41	0.67
1:B:130:GLU:O	1:B:289[B]:LYS:HE2	1.98	0.63
1:A:333:PRO:HB3	1:A:437[B]:ASP:CG	2.21	0.61
1:B:412:THR:HB	8:B:2485:HOH:O	2.00	0.60
1:A:135:HIS:HE1	8:A:2472:HOH:O	1.85	0.60
1:B:482:LYS:HB3	8:B:2207:HOH:O	2.01	0.59
1:A:318:MET:HE2	1:A:322:ARG:HG3	1.76	0.59
1:A:144[A]:ASN:ND2	8:A:2104:HOH:O	2.01	0.56
1:B:319:THR:HB	1:B:321[B]:GLN:HE21	1.72	0.54
1:A:144[B]:ASN:HD21	1:B:351:GLN:CD	2.12	0.52
1:B:132:VAL:CG1	1:B:482:LYS:HG2	2.41	0.50
1:B:458:ASN:HA	1:B:461:PHE:CE2	2.47	0.50
1:B:318:MET:HG3	1:B:322:ARG:HG2	1.93	0.50
1:B:315:SER:HB2	1:B:318:MET:HE3	1.94	0.49
1:A:417[A]:LYS:HG2	1:A:447:PHE:CD1	2.49	0.48
1:B:434:LEU:O	1:B:437[A]:ASP:HB2	2.14	0.48
1:A:458:ASN:HA	1:A:461:PHE:CE2	2.49	0.48
1:B:230:PRO:HB2	1:B:241[A]:LYS:HE3	1.96	0.47
1:B:132:VAL:HG11	1:B:482:LYS:HG2	1.96	0.47
1:B:126:PRO:HG3	1:B:482:LYS:HG3	1.97	0.47
1:B:417[A]:LYS:HA	1:B:417[A]:LYS:HD2	1.57	0.46
1:A:240:LYS:HE3	8:A:2480:HOH:O	2.16	0.45
1:A:490:LYS:NZ	8:A:2110:HOH:O	2.36	0.45
1:A:234[B]:HIS:ND1	1:A:239[B]:GLU:CG	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:MET:O	1:A:324[B]:MET:HG3	2.16	0.45
1:A:334:LYS:N	1:A:437[B]:ASP:OD1	2.49	0.45
1:A:132:VAL:CG1	1:A:482[A]:LYS:HG2	2.48	0.43
1:A:135:HIS:CE1	8:A:2472:HOH:O	2.67	0.43
1:B:437[B]:ASP:OD1	8:B:2102:HOH:O	2.21	0.43
1:B:134:THR:O	1:B:483:CYS:HA	2.20	0.42
1:B:254[A]:LEU:HD23	1:B:254[A]:LEU:HA	1.79	0.42
1:A:338[B]:LEU:HD11	1:A:437[B]:ASP:OD2	2.20	0.42
1:B:188:PHE:HE1	1:B:407[A]:ILE:HD12	1.86	0.41
1:A:320:MET:O	1:A:324[B]:MET:CG	2.70	0.40
1:B:144:ASN:C	1:B:145[A]:ILE:HD12	2.42	0.40
1:A:132:VAL:HG13	1:A:482[A]:LYS:HG2	2.03	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	408/391 (104%)	399 (98%)	9 (2%)	0	100	100
1	B	403/391 (103%)	394 (98%)	9 (2%)	0	100	100
All	All	811/782 (104%)	793 (98%)	18 (2%)	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	376/355 (106%)	367 (98%)	9 (2%)	49 12
1	B	371/355 (104%)	363 (98%)	8 (2%)	52 15
All	All	747/710 (105%)	730 (98%)	17 (2%)	57 13

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	144[A]	ASN
1	A	144[B]	ASN
1	A	304[A]	ARG
1	A	304[B]	ARG
1	A	310	LYS
1	A	325	LYS
1	A	334	LYS
1	A	455	LEU
1	B	154[A]	GLN
1	B	154[B]	GLN
1	B	316	ARG
1	B	412	THR
1	B	414	LYS
1	B	417[A]	LYS
1	B	417[B]	LYS
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	351	GLN
1	A	380	ASN
1	B	351	GLN

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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
4	9M2	B	2007	-	31,34,34	1.84	8 (25%)	39,49,49	3.89	13 (33%)
6	GOL	B	2010	-	5,5,5	1.01	0	5,5,5	1.92	2 (40%)
2	MYA	B	2001	5	57,65,65	1.10	5 (8%)	68,91,91	1.24	7 (10%)
7	DMS	A	2008	-	3,3,3	0.61	0	3,3,3	1.07	0
2	MYA	A	2001	5	57,65,65	1.13	4 (7%)	68,91,91	1.25	7 (10%)
3	PO4	B	2004	-	4,4,4	0.77	0	6,6,6	1.87	2 (33%)
4	9M2	A	2005	-	31,34,34	2.01	10 (32%)	39,49,49	3.35	14 (35%)
6	GOL	B	2009	-	5,5,5	1.45	1 (20%)	5,5,5	1.03	0
3	PO4	B	2005	-	4,4,4	0.83	0	6,6,6	1.01	0
3	PO4	A	2002	-	4,4,4	1.98	1 (25%)	6,6,6	1.81	2 (33%)
3	PO4	B	2002	-	4,4,4	1.58	2 (50%)	6,6,6	1.68	2 (33%)
3	PO4	A	2003	-	4,4,4	2.58	3 (75%)	6,6,6	2.08	1 (16%)
3	PO4	A	2004	-	4,4,4	0.48	0	6,6,6	1.66	2 (33%)
3	PO4	B	2006	-	4,4,4	0.63	0	6,6,6	1.05	0
6	GOL	A	2007	-	5,5,5	1.06	0	5,5,5	0.56	0
3	PO4	B	2003	-	4,4,4	2.75	2 (50%)	6,6,6	1.78	1 (16%)

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
4	9M2	B	2007	-	-	0/13/14/14	0/4/4/4
6	GOL	B	2010	-	-	4/4/4/4	-
2	MYA	B	2001	5	-	1/60/80/80	0/3/3/3
2	MYA	A	2001	5	-	0/60/80/80	0/3/3/3
4	9M2	A	2005	-	-	0/13/14/14	0/4/4/4
6	GOL	B	2009	-	-	0/4/4/4	-
6	GOL	A	2007	-	-	0/4/4/4	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2005	9M2	C18-C22	5.92	1.49	1.39
4	B	2007	9M2	C18-C22	4.92	1.48	1.39
3	B	2003	PO4	P-O1	4.56	1.61	1.50
3	A	2003	PO4	P-O3	-3.87	1.43	1.54
4	A	2005	9M2	C19-C18	3.55	1.46	1.39
2	B	2001	MYA	C2A-N3A	3.50	1.37	1.32
2	A	2001	MYA	O10-C10	3.37	1.48	1.42
4	B	2007	9M2	C5-C6	3.29	1.43	1.36
2	A	2001	MYA	C2A-N3A	3.21	1.37	1.32
4	A	2005	9M2	C10-C15	3.14	1.47	1.40
2	B	2001	MYA	O5-C5	3.14	1.29	1.23
4	A	2005	9M2	C3-N1	-3.05	1.30	1.34
4	A	2005	9M2	C17-C18	-3.03	1.47	1.52
2	A	2001	MYA	C6-C5	-2.97	1.45	1.51
3	A	2002	PO4	P-O1	2.95	1.57	1.50
4	B	2007	9M2	C19-C18	2.91	1.45	1.39
4	B	2007	9M2	C8-C7	2.77	1.45	1.38
4	B	2007	9M2	C1-N	2.73	1.54	1.46
2	B	2001	MYA	O10-C10	2.73	1.47	1.42
4	A	2005	9M2	C14-C13	2.50	1.41	1.37
3	B	2003	PO4	P-O3	-2.48	1.47	1.54
4	A	2005	9M2	C5-C6	2.45	1.41	1.36
2	B	2001	MYA	C3M-C2M	2.39	1.53	1.50
4	A	2005	9M2	C1-N	2.32	1.53	1.46
4	B	2007	9M2	C11-C10	2.32	1.43	1.40
3	B	2002	PO4	P-O3	-2.31	1.47	1.54
6	B	2009	GOL	O1-C1	2.28	1.52	1.42
3	A	2003	PO4	P-O2	-2.27	1.47	1.54
3	A	2003	PO4	P-O4	2.22	1.61	1.54
2	B	2001	MYA	P2A-O5A	-2.22	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2007	9M2	C14-C13	2.21	1.41	1.37
4	A	2005	9M2	C11-C10	2.17	1.43	1.40
4	A	2005	9M2	C10-C7	-2.14	1.45	1.49
2	A	2001	MYA	P2A-O5A	-2.12	1.45	1.55
4	B	2007	9M2	C22-N4	2.05	1.37	1.33
3	B	2002	PO4	P-O1	-2.04	1.46	1.50

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2007	9M2	C17-C18-C22	16.34	138.78	127.30
4	B	2007	9M2	C17-C18-C19	-9.44	120.66	127.30
4	A	2005	9M2	C19-N3-N4	9.02	123.11	112.10
4	A	2005	9M2	C17-C18-C22	8.94	133.57	127.30
4	A	2005	9M2	C18-C19-N3	-8.43	100.07	106.79
4	B	2007	9M2	C22-N4-N3	-7.87	97.59	104.35
4	A	2005	9M2	C22-N4-N3	-7.59	97.83	104.35
4	A	2005	9M2	C17-C18-C19	-6.15	122.98	127.30
4	B	2007	9M2	C19-N3-N4	6.13	119.58	112.10
4	B	2007	9M2	C8-C9-C4	4.92	124.99	118.26
3	A	2003	PO4	O3-P-O2	4.56	122.61	107.97
4	A	2005	9M2	C8-C9-C4	4.26	124.09	118.26
4	A	2005	9M2	C6-C5-C4	-4.08	115.70	120.84
4	B	2007	9M2	C6-C7-C8	3.97	124.31	118.09
2	B	2001	MYA	C3M-C2M-S1	3.93	118.04	113.46
4	B	2007	9M2	C19-C18-C22	-3.87	100.17	106.62
4	B	2007	9M2	C7-C8-C9	-3.75	114.10	122.30
3	B	2003	PO4	O3-P-O2	3.72	119.90	107.97
4	B	2007	9M2	C8-C7-C10	-3.67	115.07	120.72
2	B	2001	MYA	C13-C11-C10	3.63	115.11	108.82
4	A	2005	9M2	C8-C7-C10	-3.60	115.17	120.72
2	A	2001	MYA	C3M-C2M-S1	3.52	117.55	113.46
2	A	2001	MYA	C13-C11-C10	3.47	114.84	108.82
3	A	2002	PO4	O4-P-O3	3.28	118.49	107.97
6	B	2010	GOL	C3-C2-C1	-3.17	99.38	111.70
3	B	2004	PO4	O4-P-O1	-3.03	99.82	110.89
2	B	2001	MYA	O2M-C2M-C3M	-2.99	120.45	123.99
4	A	2005	9M2	C6-C7-C10	2.94	125.68	120.91
4	B	2007	9M2	C5-C4-N2	2.93	134.96	130.19
4	B	2007	9M2	C3-N1-N2	2.90	112.59	106.98
2	A	2001	MYA	O2M-C2M-S1	-2.90	118.85	122.61
2	A	2001	MYA	C5A-C6A-N6A	2.89	124.75	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2005	9M2	C7-C8-C9	-2.88	115.99	122.30
2	B	2001	MYA	C5A-C6A-N6A	2.68	124.43	120.35
3	A	2004	PO4	O4-P-O3	2.64	116.44	107.97
2	A	2001	MYA	C4M-C3M-C2M	-2.57	106.64	112.33
3	A	2004	PO4	O4-P-O1	-2.50	101.74	110.89
3	A	2002	PO4	O2-P-O1	-2.46	101.88	110.89
3	B	2002	PO4	O4-P-O1	-2.43	102.02	110.89
2	A	2001	MYA	N3A-C2A-N1A	-2.39	124.94	128.68
3	B	2004	PO4	O4-P-O2	2.38	115.62	107.97
2	B	2001	MYA	C14-C11-C10	-2.38	104.69	108.82
2	B	2001	MYA	N3A-C2A-N1A	-2.35	125.01	128.68
4	A	2005	9M2	C-N-C2	2.31	115.47	110.69
6	B	2010	GOL	O3-C3-C2	2.31	121.26	110.20
4	A	2005	9M2	C5-C6-C7	2.31	124.74	121.00
2	A	2001	MYA	O2X-C2X-C3X	2.30	117.70	111.17
3	B	2002	PO4	O4-P-O3	2.19	114.99	107.97
4	A	2005	9M2	C3-N1-N2	2.10	111.05	106.98
2	B	2001	MYA	C6-C5-N4	2.06	119.89	116.42
4	B	2007	9M2	C12-C13-C14	2.05	125.95	123.29
4	B	2007	9M2	C5-C6-C7	-2.03	117.70	121.00
4	A	2005	9M2	C20-C19-C18	2.03	133.62	129.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	2010	GOL	O1-C1-C2-C3
6	B	2010	GOL	C1-C2-C3-O3
6	B	2010	GOL	O1-C1-C2-O2
6	B	2010	GOL	O2-C2-C3-O3
2	B	2001	MYA	C6-C7-N8-C9

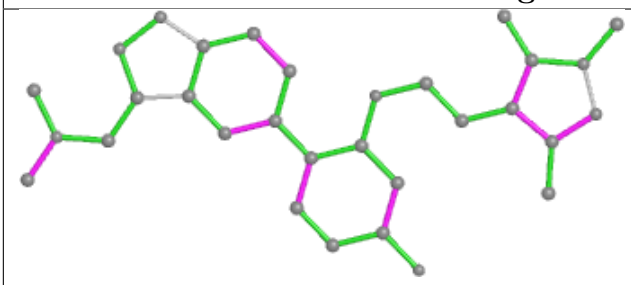
There are no ring outliers.

No monomer is involved in short contacts.

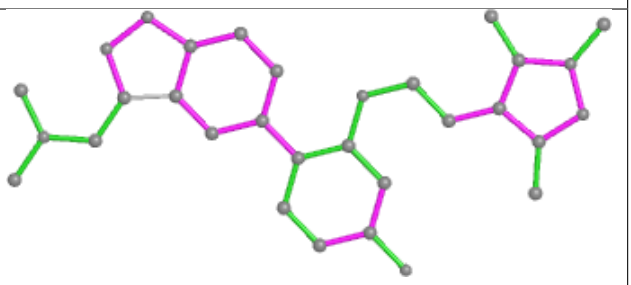
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

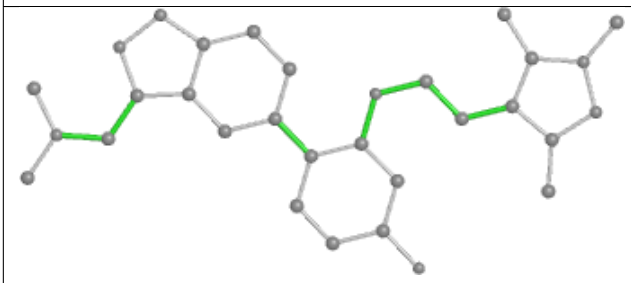
Ligand 9M2 B 2007



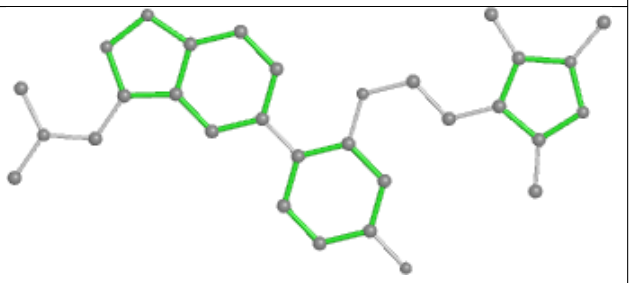
Bond lengths



Bond angles

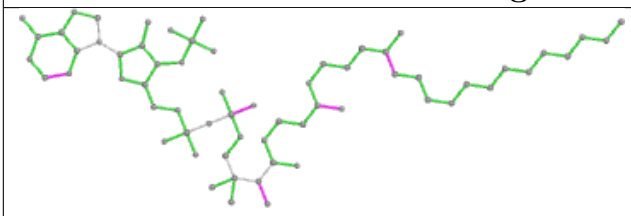


Torsions

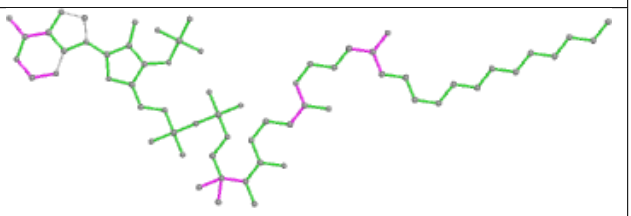


Rings

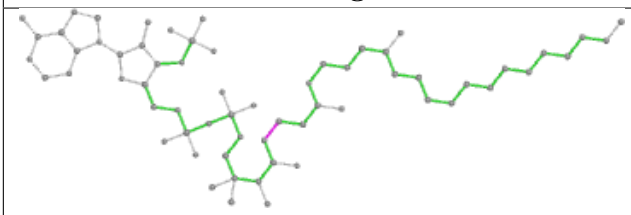
Ligand MYA B 2001



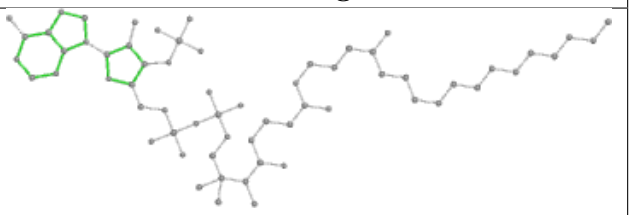
Bond lengths



Bond angles

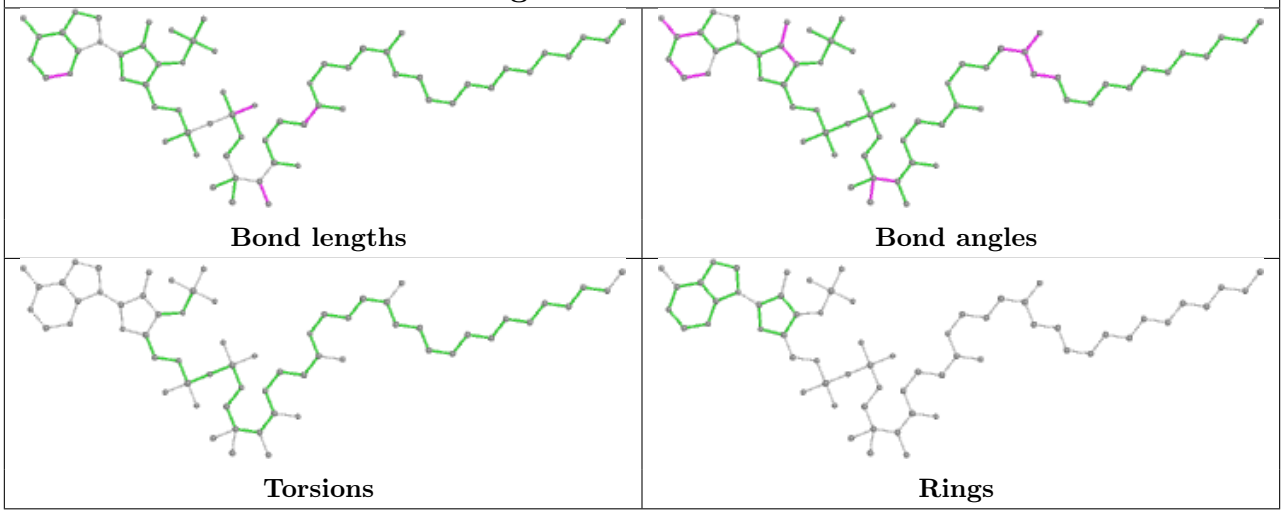


Torsions

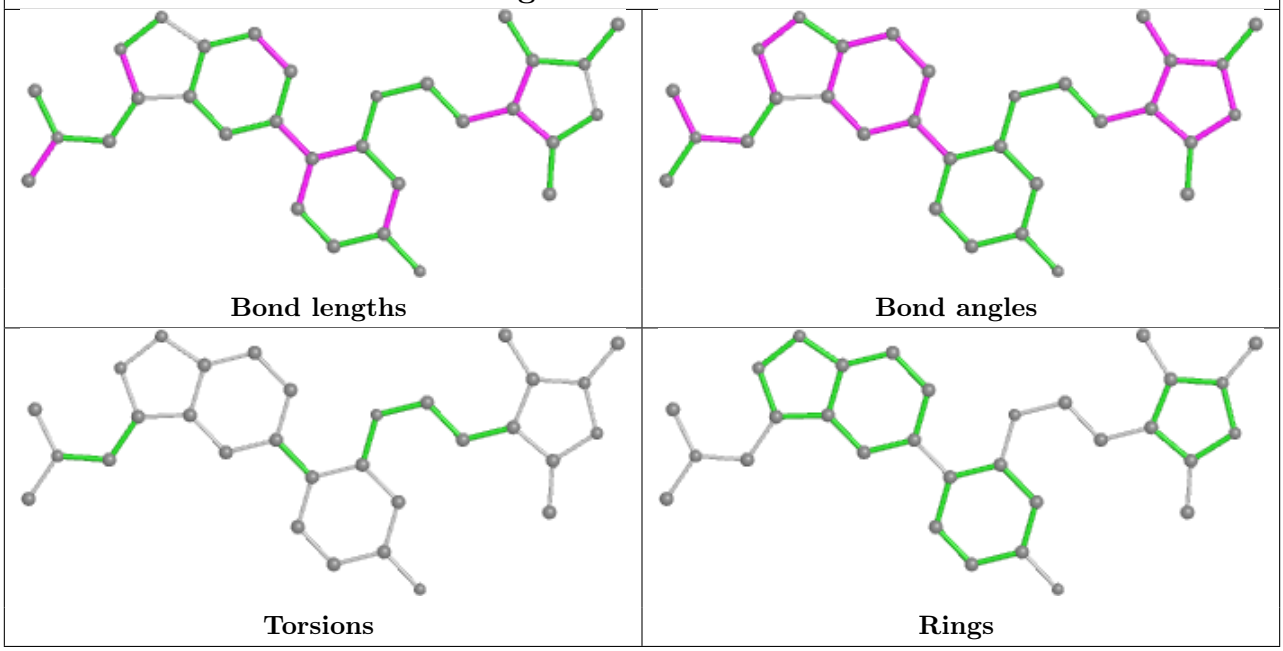


Rings

Ligand MYA A 2001



Ligand 9M2 A 2005



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	382/391 (97%)	-0.36	7 (1%)	68	69	8, 14, 29, 72	0
1	B	382/391 (97%)	-0.36	7 (1%)	68	69	8, 13, 30, 66	4 (1%)
All	All	764/782 (97%)	-0.36	14 (1%)	68	69	8, 13, 29, 72	4 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	ARG	3.6
1	B	412	THR	3.4
1	A	133	ASN	3.0
1	A	129	GLY	2.7
1	B	316	ARG	2.6
1	A	131[A]	VAL	2.5
1	A	134	THR	2.3
1	B	317	ASN	2.3
1	B	411	PRO	2.3
1	B	116	SER	2.2
1	B	129	GLY	2.1
1	A	313	HIS	2.1
1	A	316	ARG	2.1
1	B	409	ASN	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)

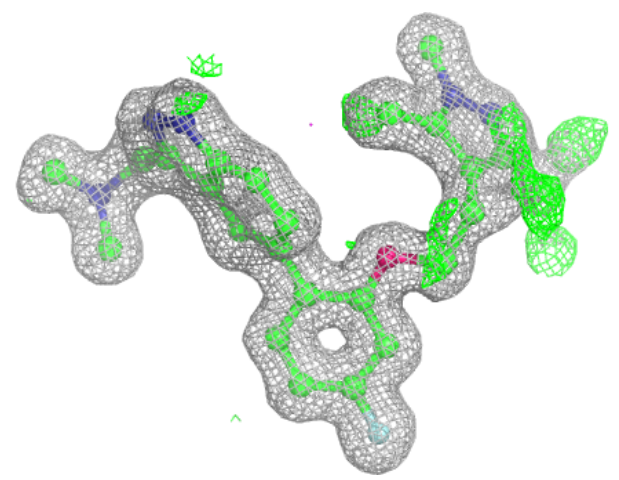
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

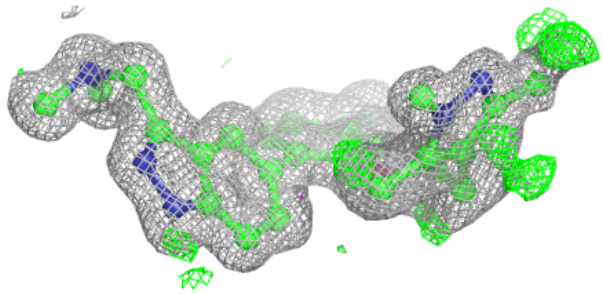
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	A	2004	5/5	0.83	0.26	46,54,62,64	0
3	PO4	B	2005	5/5	0.85	0.23	42,44,61,61	0
6	GOL	B	2010	6/6	0.85	0.24	23,33,38,49	0
3	PO4	B	2006	5/5	0.87	0.16	44,56,58,62	0
7	DMS	A	2008	4/4	0.88	0.18	36,37,39,40	0
6	GOL	B	2009	6/6	0.90	0.13	16,17,18,20	0
3	PO4	B	2004	5/5	0.92	0.33	48,48,64,64	0
6	GOL	A	2007	6/6	0.95	0.11	17,18,20,20	0
4	9M2	A	2005	31/31	0.96	0.06	12,14,20,24	0
4	9M2	B	2007	31/31	0.96	0.06	11,13,17,18	0
3	PO4	A	2003	5/5	0.98	0.06	16,16,19,19	0
2	MYA	A	2001	63/63	0.98	0.05	8,12,16,23	0
3	PO4	B	2003	5/5	0.98	0.10	16,16,18,20	0
2	MYA	B	2001	63/63	0.98	0.05	8,11,14,17	0
3	PO4	A	2002	5/5	0.99	0.05	17,18,20,21	0
3	PO4	B	2002	5/5	0.99	0.06	16,18,23,23	0
5	MG	A	2006	1/1	0.99	0.07	21,21,21,21	0
5	MG	B	2008	1/1	0.99	0.09	20,20,20,20	0

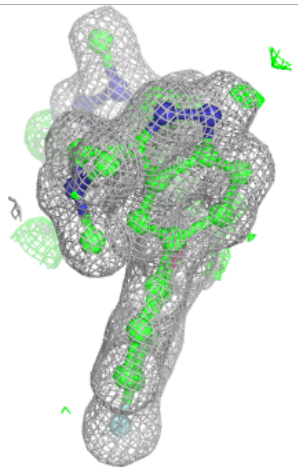
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 9M2 A 2005:

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

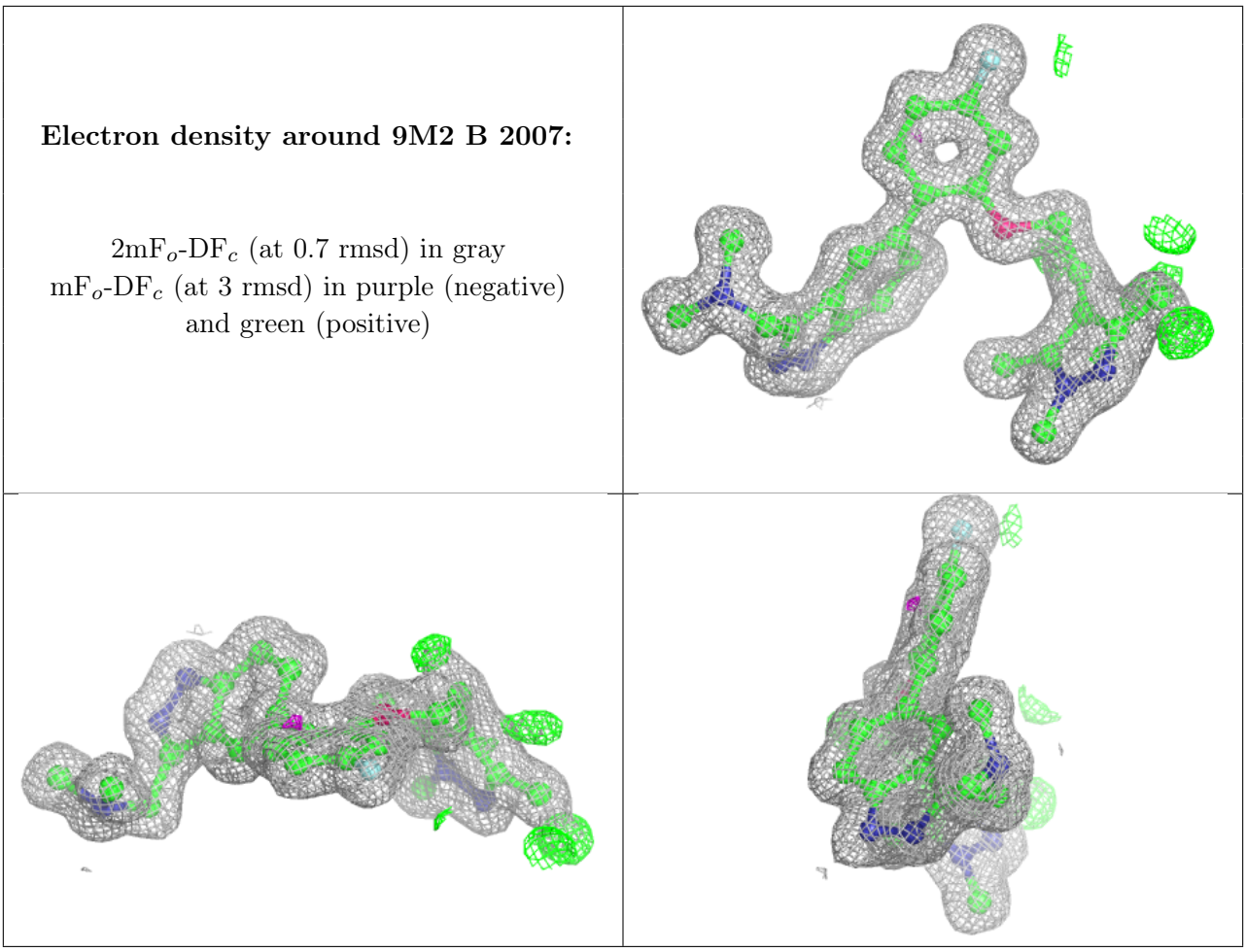






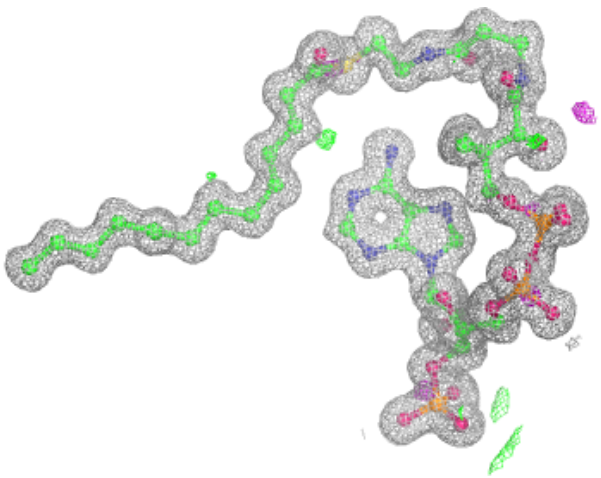
Electron density around 9M2 B 2007:

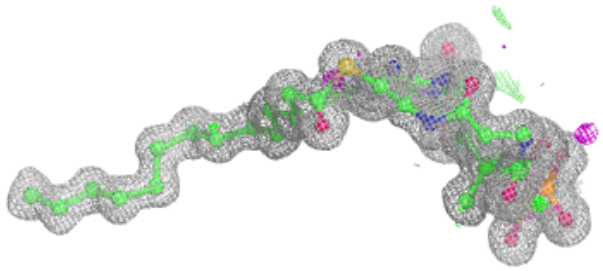
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

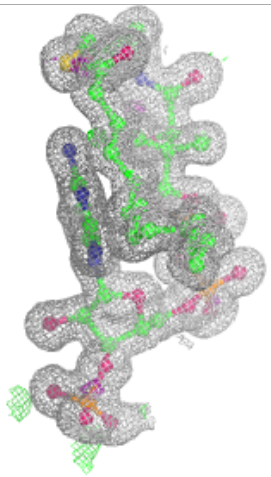


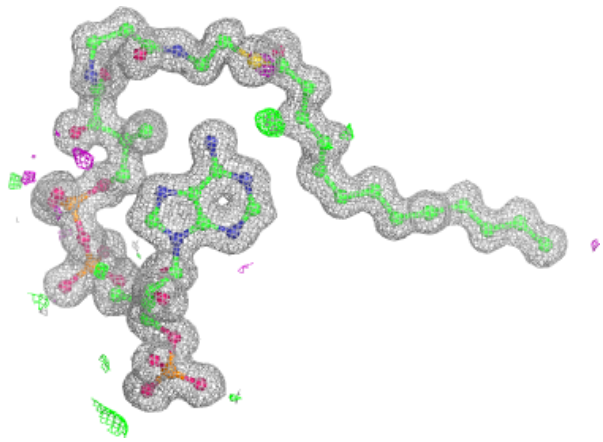
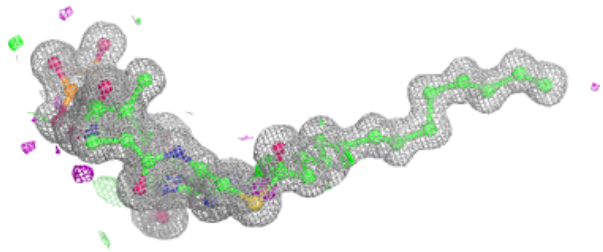
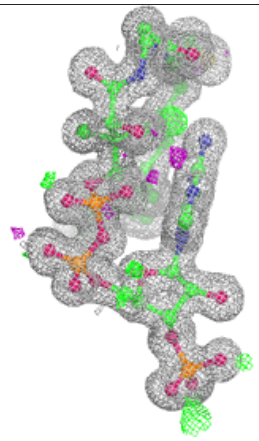
Electron density around MYA A 2001:

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







Electron density around MYA B 2001: 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.