



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 02:16 AM EDT

PDB ID : 5G21
Title : Leishmania major N-myristoyltransferase in complex with a quinoline inhibitor (compound 26).
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Deposited on : 2016-04-06
Resolution : 1.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

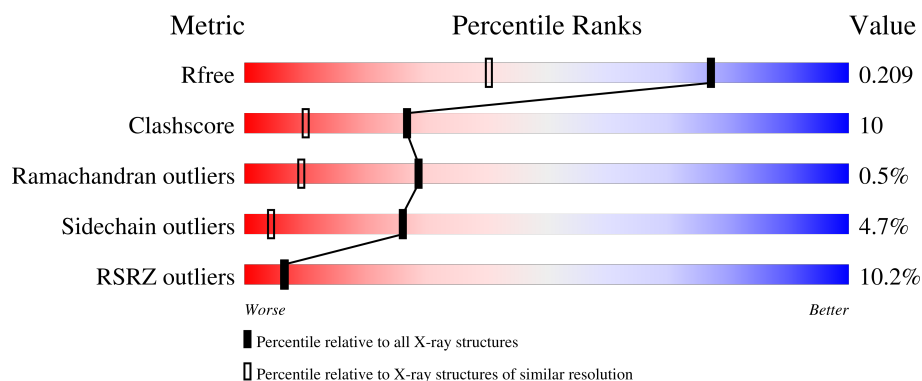
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	411	<div> <div>10%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4073 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.

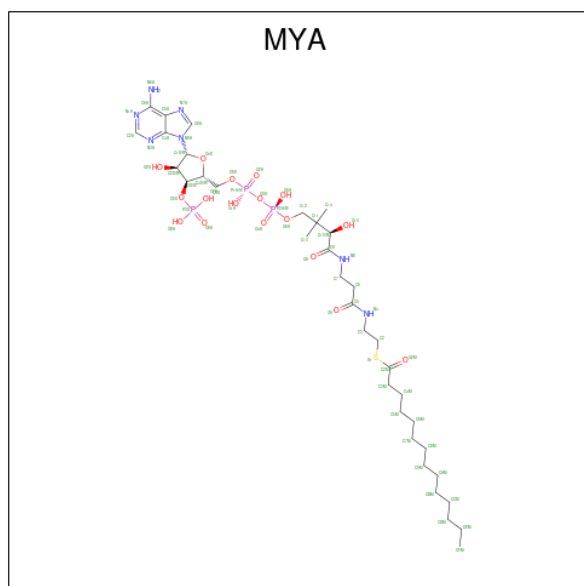
- Molecule 1 is a protein called GLYCYLPEPTIDE N-TETRADECANOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	37	0
			3565	2318	594	636	17			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

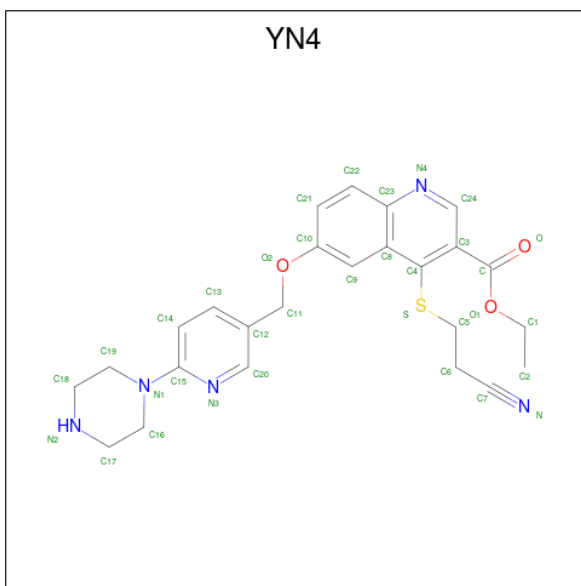
- Molecule 3 is TETRADECANOYL-COA (three-letter code: MYA) (formula: C₃₅H₆₂N₇O₁₇P₃S).



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

- Molecule 4 is ETHYL 4-[(2-CYANOETHYL)SULFANYL]-6-[[6-(PIPERAZIN-1-YL)

(three-letter code: YN4) (formula: C₂₅H₂₇N₅O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			68	50	10	6	2		

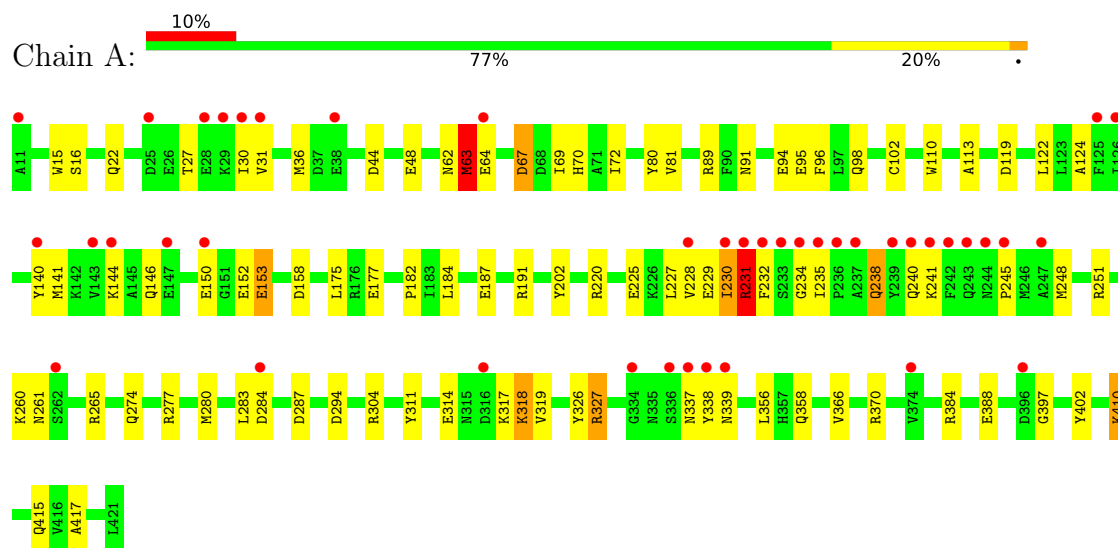
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	376	Total	O	0	0
			376	376		

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.68Å 91.07Å 53.57Å 90.00° 114.55° 90.00°	Depositor
Resolution (Å)	48.73 – 1.50 24.36 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.73-1.50) 99.7 (24.36-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.174 , 0.209 0.174 , 0.209	Depositor DCC
R_{free} test set	3355 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4073	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYA, MG, YN4

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	1.38	10/3777 (0.3%)	1.38	26/5128 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	397	GLY	N-CA	-9.96	1.31	1.46
1	A	67[A]	ASP	CB-CG	8.01	1.68	1.51
1	A	67[B]	ASP	CB-CG	8.01	1.68	1.51
1	A	110	TRP	CG-CD1	7.49	1.47	1.36
1	A	15	TRP	CG-CD1	6.65	1.46	1.36
1	A	94	GLU	CD-OE2	-5.98	1.19	1.25
1	A	110	TRP	CZ3-CH2	5.92	1.49	1.40
1	A	384	ARG	CZ-NH2	5.72	1.40	1.33
1	A	265	ARG	CZ-NH1	5.38	1.40	1.33
1	A	388	GLU	CD-OE1	5.01	1.31	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	MET	CG-SD-CE	13.42	121.67	100.20
1	A	370	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	384	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	89	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	A	326	TYR	CB-CG-CD2	-8.42	115.95	121.00
1	A	96	PHE	CB-CG-CD2	-8.24	115.03	120.80
1	A	294	ASP	CB-CG-OD1	7.42	124.98	118.30
1	A	80	TYR	CB-CG-CD2	-7.36	116.59	121.00
1	A	327	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	326	TYR	CB-CG-CD1	7.15	125.29	121.00
1	A	158	ASP	CB-CG-OD1	7.10	124.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	67[A]	ASP	N-CA-CB	-6.13	99.57	110.60
1	A	67[B]	ASP	N-CA-CB	-6.13	99.57	110.60
1	A	202	TYR	CD1-CE1-CZ	5.95	125.15	119.80
1	A	304	ARG	CG-CD-NE	-5.78	99.65	111.80
1	A	44	ASP	CB-CA-C	-5.63	99.14	110.40
1	A	177	GLU	CA-CB-CG	-5.46	101.39	113.40
1	A	89	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	220	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	95	GLU	CG-CD-OE1	5.22	128.74	118.30
1	A	119	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	175	LEU	CB-CG-CD1	5.21	119.85	111.00
1	A	227	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	A	356	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	A	402	TYR	CZ-CE2-CD2	-5.01	115.29	119.80

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	3565	0	3605	75	0
2	A	1	0	0	0	0
3	A	63	0	58	0	0
4	A	68	0	0	2	0
5	A	376	0	0	11	0
All	All	4073	0	3663	75	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 10.

All (75) 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:63:MET:HE3	1:A:69[B]:ILE:HD13	1.14	1.14
1:A:63:MET:HE1	1:A:72:ILE:HD12	1.42	0.99
1:A:63:MET:CE	1:A:72:ILE:HD12	1.97	0.93
1:A:63:MET:HE3	1:A:69[B]:ILE:CD1	2.01	0.89
1:A:153[B]:GLU:OE1	5:A:2197:HOH:O	1.91	0.88
1:A:63:MET:HE1	1:A:72:ILE:CD1	2.04	0.87
1:A:238:GLN:HE21	1:A:238:GLN:H	1.22	0.86
1:A:63:MET:CE	1:A:72:ILE:CD1	2.54	0.86
1:A:235:ILE:HD13	1:A:245:PRO:HB2	1.60	0.83
1:A:230:ILE:O	1:A:232:PHE:N	2.11	0.83
1:A:48[A]:GLU:OE2	5:A:2058:HOH:O	2.03	0.77
1:A:124:ALA:HB1	1:A:184[A]:LEU:HD11	1.66	0.76
1:A:63:MET:CE	1:A:69[B]:ILE:HD13	2.08	0.74
1:A:229:GLU:HB2	1:A:338:TYR:CE2	2.22	0.74
1:A:229:GLU:HB2	1:A:338:TYR:HE2	1.52	0.74
1:A:274:GLN:HG2	1:A:277[B]:ARG:HH22	1.53	0.72
1:A:69[A]:ILE:HD13	1:A:98[A]:GLN:HG2	1.70	0.71
1:A:260[B]:LYS:HE3	1:A:260[B]:LYS:HA	1.74	0.69
1:A:62[A]:ASN:OD1	1:A:64[A]:GLU:HG2	1.93	0.69
1:A:229:GLU:CB	1:A:338:TYR:HE2	2.06	0.69
1:A:63:MET:HE2	1:A:72:ILE:CD1	2.24	0.67
1:A:231[A]:ARG:HD3	1:A:231[A]:ARG:H	1.60	0.67
1:A:31:VAL:HA	1:A:141:MET:HE2	1.76	0.66
1:A:228:VAL:HA	1:A:234:GLY:H	1.60	0.66
1:A:146:GLN:NE2	1:A:146:GLN:HA	2.10	0.66
1:A:69[A]:ILE:HD13	1:A:98[A]:GLN:CG	2.28	0.63
1:A:261:ASN:ND2	1:A:358:GLN:HE21	1.96	0.62
1:A:63:MET:HB3	1:A:102:CYS:SG	2.40	0.61
1:A:229:GLU:CB	1:A:338:TYR:CE2	2.82	0.61
1:A:261:ASN:HD21	1:A:358:GLN:HE21	1.48	0.60
1:A:146:GLN:HA	1:A:146:GLN:HE21	1.68	0.59
1:A:69[A]:ILE:CD1	1:A:98[A]:GLN:HG2	2.34	0.58
1:A:238:GLN:HE21	1:A:238:GLN:N	1.99	0.57
1:A:228:VAL:HG22	1:A:235:ILE:H	1.71	0.56
1:A:314[A]:GLU:OE2	1:A:317:LYS:HA	2.07	0.55
1:A:274:GLN:HE22	1:A:319:VAL:H	1.55	0.55
1:A:274:GLN:NE2	1:A:319:VAL:H	2.04	0.54
1:A:62[A]:ASN:HD21	1:A:64[A]:GLU:HG2	1.72	0.53
1:A:311:TYR:CE1	1:A:366:VAL:HG11	2.44	0.53
1:A:27:THR:HA	1:A:30:ILE:HD12	1.91	0.53
1:A:62[A]:ASN:ND2	1:A:64[A]:GLU:HG2	2.24	0.53
1:A:287:ASP:OD2	1:A:415[B]:GLN:NE2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:MET:HE2	1:A:72:ILE:HD13	1.91	0.52
1:A:274:GLN:HG2	1:A:277[B]:ARG:NH2	2.24	0.52
1:A:153[B]:GLU:CD	5:A:2197:HOH:O	2.44	0.51
1:A:16:SER:HA	1:A:22:GLN:HE22	1.75	0.51
1:A:280[B]:MET:HE3	1:A:280[B]:MET:HA	1.93	0.51
1:A:62[A]:ASN:HD21	1:A:64[A]:GLU:CG	2.24	0.51
1:A:63:MET:HE2	1:A:72:ILE:HD12	1.87	0.49
1:A:31:VAL:HA	1:A:141:MET:CE	2.42	0.49
1:A:280[B]:MET:HA	1:A:280[B]:MET:CE	2.43	0.49
1:A:280[B]:MET:HE3	5:A:2287:HOH:O	2.12	0.48
1:A:283[A]:LEU:HD22	1:A:417:ALA:HB1	1.96	0.48
1:A:62[A]:ASN:CG	1:A:64[A]:GLU:HG2	2.35	0.47
1:A:274:GLN:HE22	1:A:318:LYS:HA	1.81	0.44
1:A:152:GLU:HB3	5:A:2197:HOH:O	2.16	0.44
1:A:187:GLU:OE2	1:A:191[B]:ARG:HD2	2.18	0.44
1:A:146:GLN:HE21	1:A:146:GLN:CA	2.27	0.43
1:A:81:VAL:HG11	4:A:1002[A]:YN4:C13	2.49	0.42
1:A:31:VAL:CA	1:A:141:MET:HE2	2.49	0.42
1:A:16:SER:HA	1:A:22:GLN:NE2	2.34	0.42
1:A:48[A]:GLU:HB2	5:A:2051:HOH:O	2.19	0.41
1:A:113:ALA:HB1	1:A:122:LEU:CD1	2.49	0.41
1:A:152:GLU:CB	5:A:2194:HOH:O	2.68	0.41
1:A:248:MET:HE3	1:A:251[A]:ARG:HD3	2.01	0.41
1:A:229:GLU:HA	1:A:231[A]:ARG:NH1	2.35	0.41
1:A:410[A]:LYS:HD3	5:A:2244:HOH:O	2.21	0.41
1:A:81:VAL:HG11	4:A:1002[B]:YN4:C13	2.50	0.41
1:A:70:HIS:HD2	5:A:2090:HOH:O	2.04	0.41
1:A:22:GLN:NE2	5:A:2022:HOH:O	2.54	0.41
1:A:63:MET:O	1:A:69[A]:ILE:HD11	2.21	0.41
1:A:240:GLN:HA	1:A:240:GLN:OE1	2.21	0.41
1:A:327:ARG:NH1	5:A:2135:HOH:O	2.50	0.41

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	447/411 (109%)	427 (96%)	17 (4%)	3 (1%)	22	6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231[A]	ARG
1	A	231[B]	ARG
1	A	144	LYS

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	400/362 (110%)	377 (94%)	23 (6%)	20	2

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

Mol	Chain	Res	Type
1	A	36[A]	MET
1	A	36[B]	MET
1	A	63	MET
1	A	67[A]	ASP
1	A	67[B]	ASP
1	A	91	ASN
1	A	150	GLU
1	A	153[A]	GLU
1	A	153[B]	GLU
1	A	182	PRO
1	A	225	GLU
1	A	230	ILE
1	A	231[A]	ARG
1	A	231[B]	ARG
1	A	238	GLN
1	A	241	LYS

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Mol	Chain	Res	Type
1	A	284[A]	ASP
1	A	284[B]	ASP
1	A	318	LYS
1	A	337	ASN
1	A	339	ASN
1	A	410[A]	LYS
1	A	410[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	146	GLN
1	A	238	GLN
1	A	252	ASN
1	A	261	ASN
1	A	274	GLN
1	A	339	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	YN4	A	1002[A]	-	37,37,37	1.30	5 (13%)	46,49,49	2.38	21 (45%)
4	YN4	A	1002[B]	1	37,37,37	1.31	5 (13%)	46,49,49	2.12	18 (39%)
3	MYA	A	1001	2	57,65,65	1.30	7 (12%)	68,91,91	1.74	15 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	YN4	A	1002[A]	-	-	5/21/29/29	0/4/4/4
4	YN4	A	1002[B]	1	-	4/21/29/29	0/4/4/4
3	MYA	A	1001	2	-	3/60/80/80	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	MYA	C3M-C2M	4.24	1.55	1.50
4	A	1002[B]	YN4	C3-C4	3.52	1.46	1.40
4	A	1002[A]	YN4	C3-C4	3.50	1.46	1.40
4	A	1002[A]	YN4	C8-C23	2.74	1.47	1.42
4	A	1002[B]	YN4	C8-C23	2.59	1.46	1.42
3	A	1001	MYA	C2M-S1	-2.51	1.70	1.76
3	A	1001	MYA	C9-N8	-2.50	1.28	1.33
3	A	1001	MYA	P2A-O4A	-2.32	1.42	1.50
3	A	1001	MYA	C13-C11	2.29	1.58	1.53
4	A	1002[B]	YN4	C4-S	-2.17	1.75	1.77
4	A	1002[B]	YN4	C4-C8	2.12	1.46	1.43
3	A	1001	MYA	C2A-N1A	2.09	1.37	1.33
3	A	1001	MYA	C3X-C4X	-2.07	1.47	1.52
4	A	1002[A]	YN4	C24-N4	2.07	1.35	1.31
4	A	1002[A]	YN4	C4-S	-2.05	1.75	1.77
4	A	1002[B]	YN4	C24-N4	2.04	1.35	1.31
4	A	1002[A]	YN4	O1-C	2.03	1.38	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002[A]	YN4	C5-C6-C7	-6.21	94.44	111.97
4	A	1002[B]	YN4	C24-N4-C23	5.60	123.65	116.91
3	A	1001	MYA	O2M-C2M-C3M	-5.53	117.46	123.99
4	A	1002[A]	YN4	C24-N4-C23	5.34	123.33	116.91
3	A	1001	MYA	O6A-C12-C11	-5.28	102.06	110.55
4	A	1002[B]	YN4	C3-C24-N4	-4.82	118.61	125.14
4	A	1002[A]	YN4	C3-C24-N4	-4.77	118.67	125.14
4	A	1002[A]	YN4	C16-N1-C19	4.65	121.79	111.52
4	A	1002[B]	YN4	C16-N1-C19	4.65	121.79	111.52
3	A	1001	MYA	N3A-C2A-N1A	-4.05	122.34	128.68
4	A	1002[A]	YN4	C5-S-C4	3.64	113.19	101.88
4	A	1002[A]	YN4	C22-C21-C10	3.52	124.90	120.17
4	A	1002[B]	YN4	C22-C21-C10	3.50	124.87	120.17
4	A	1002[A]	YN4	C24-C3-C4	3.49	122.46	117.18
3	A	1001	MYA	C4A-C5A-N7A	-3.38	105.88	109.40
4	A	1002[B]	YN4	C24-C3-C4	3.30	122.17	117.18
4	A	1002[B]	YN4	C4-C8-C23	-3.18	114.03	117.57
3	A	1001	MYA	C2X-C3X-C4X	3.14	108.78	103.22
3	A	1001	MYA	C3-N4-C5	3.03	128.46	122.84
3	A	1001	MYA	C3M-C2M-S1	2.92	116.86	113.46
4	A	1002[A]	YN4	C4-C8-C23	-2.92	114.32	117.57
3	A	1001	MYA	O4X-C1X-C2X	-2.89	102.70	106.93
4	A	1002[B]	YN4	C20-N3-C15	2.87	122.53	117.30
4	A	1002[A]	YN4	C24-C3-C	-2.86	112.34	118.99
4	A	1002[B]	YN4	C17-N2-C18	2.84	118.50	110.34
4	A	1002[A]	YN4	C6-C5-S	-2.79	105.63	113.36
4	A	1002[A]	YN4	C17-N2-C18	2.75	118.23	110.34
4	A	1002[B]	YN4	C8-C4-S	-2.69	113.91	119.05
4	A	1002[B]	YN4	C24-C3-C	-2.65	112.82	118.99
3	A	1001	MYA	O4X-C4X-C5X	-2.65	100.67	109.37
4	A	1002[A]	YN4	C20-N3-C15	2.63	122.11	117.30
4	A	1002[B]	YN4	C12-C20-N3	-2.63	119.81	123.95
4	A	1002[A]	YN4	C9-C8-C23	2.63	122.17	118.94
4	A	1002[A]	YN4	O1-C-C3	2.56	117.27	112.21
4	A	1002[A]	YN4	N3-C15-N1	2.54	120.60	116.79
3	A	1001	MYA	O8A-P3X-O7A	2.53	117.31	107.64
4	A	1002[B]	YN4	N3-C15-N1	2.50	120.54	116.79
4	A	1002[A]	YN4	C12-C20-N3	-2.49	120.03	123.95
4	A	1002[B]	YN4	C9-C8-C23	2.46	121.96	118.94
4	A	1002[B]	YN4	O1-C-C3	2.45	117.05	112.21
4	A	1002[B]	YN4	C14-C15-N3	-2.43	118.95	123.41
4	A	1002[A]	YN4	C10-C9-C8	-2.38	116.89	120.05
3	A	1001	MYA	O2M-C2M-S1	2.34	125.65	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002[A]	YN4	C8-C4-S	-2.32	114.61	119.05
3	A	1001	MYA	C4M-C3M-C2M	-2.30	107.23	112.33
4	A	1002[A]	YN4	C14-C15-N3	-2.27	119.24	123.41
3	A	1001	MYA	O5-C5-N4	-2.27	118.72	123.01
4	A	1002[B]	YN4	C10-C9-C8	-2.24	117.08	120.05
4	A	1002[A]	YN4	C4-C3-C	2.20	125.17	120.59
4	A	1002[A]	YN4	C17-C16-N1	2.16	115.16	110.48
4	A	1002[B]	YN4	C4-C3-C	2.12	125.00	120.59
4	A	1002[B]	YN4	C17-C16-N1	2.11	115.06	110.48
3	A	1001	MYA	C2-C3-N4	-2.06	108.09	112.42
3	A	1001	MYA	O6A-P2A-O4A	-2.05	101.06	109.07

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002[A]	YN4	S-C5-C6-C7
4	A	1002[A]	YN4	C5-C6-C7-N
4	A	1002[B]	YN4	C5-C6-C7-N
3	A	1001	MYA	C8M-C9M-CAM-CBM
3	A	1001	MYA	C6-C7-N8-C9
4	A	1002[A]	YN4	C21-C10-O2-C11
4	A	1002[A]	YN4	C9-C10-O2-C11
4	A	1002[B]	YN4	C21-C10-O2-C11
4	A	1002[B]	YN4	C9-C10-O2-C11
4	A	1002[B]	YN4	O-C-C3-C4
3	A	1001	MYA	C5M-C6M-C7M-C8M
4	A	1002[A]	YN4	O-C-C3-C4

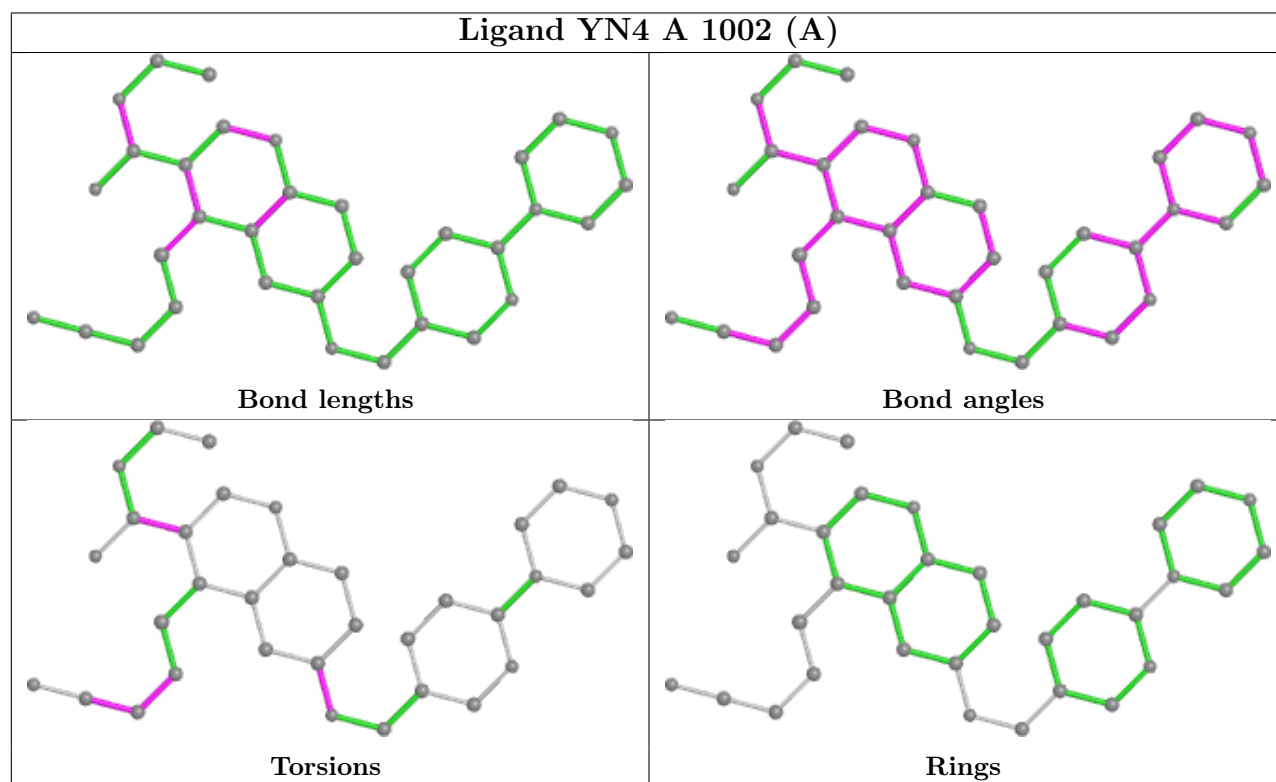
There are no ring outliers.

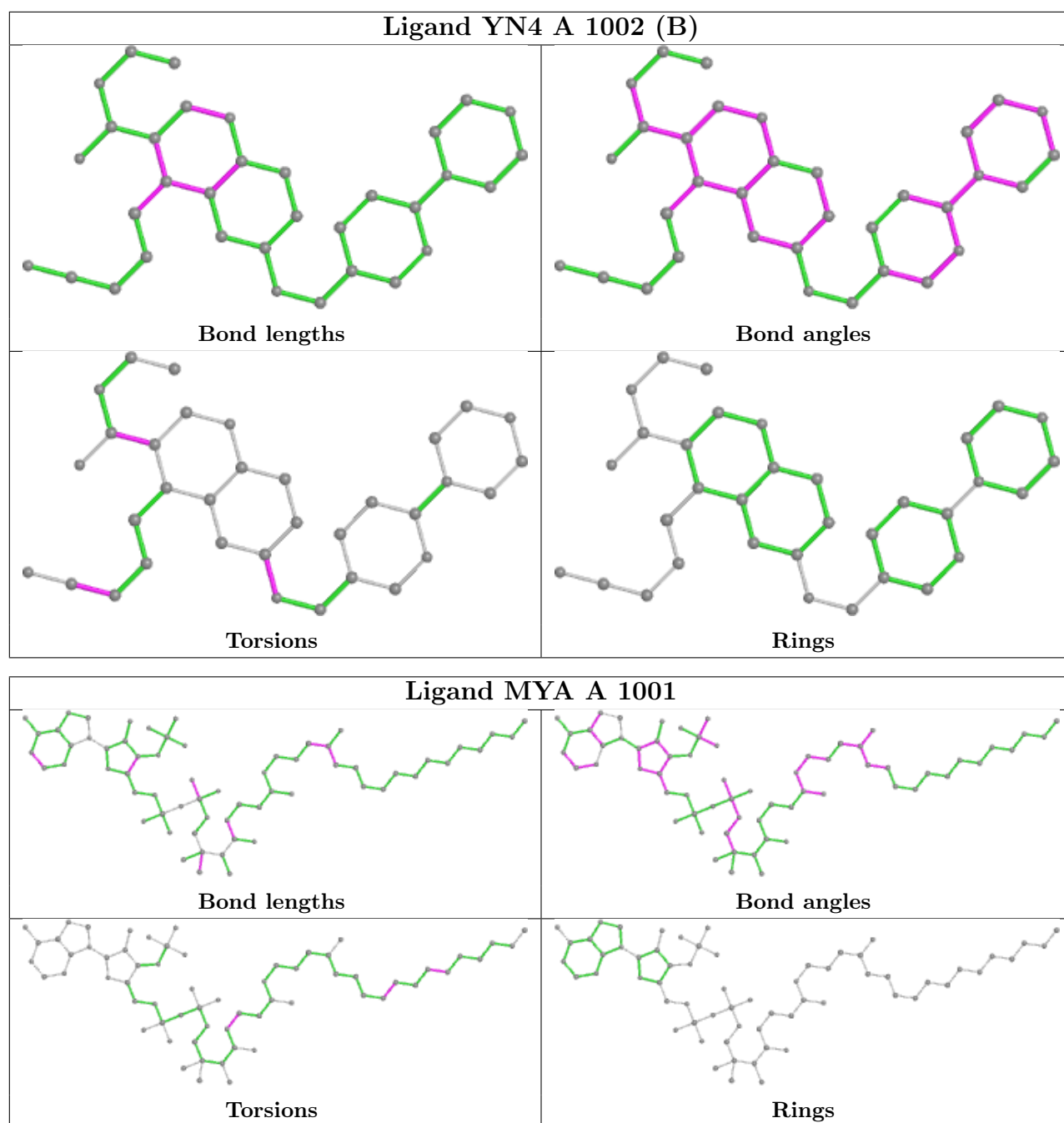
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002[A]	YN4	1	0
4	A	1002[B]	YN4	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	411/411 (100%)	0.51	42 (10%) 6 7	12, 21, 58, 134	9 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	GLY	11.2
1	A	233	SER	9.0
1	A	235	ILE	8.5
1	A	242	PHE	7.9
1	A	338	TYR	7.8
1	A	241	LYS	6.0
1	A	337	ASN	5.9
1	A	336	SER	5.7
1	A	25	ASP	5.5
1	A	140[A]	TYR	5.2
1	A	11	ALA	5.2
1	A	240	GLN	5.0
1	A	28	GLU	4.5
1	A	237	ALA	4.2
1	A	143	VAL	4.0
1	A	244	ASN	3.9
1	A	30	ILE	3.8
1	A	147	GLU	3.4
1	A	38	GLU	3.4
1	A	243	GLN	3.3
1	A	232	PHE	3.2
1	A	245	PRO	3.1
1	A	64[A]	GLU	3.0
1	A	126	ILE	2.9
1	A	284[A]	ASP	2.8
1	A	150	GLU	2.7
1	A	396	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	247	ALA	2.7
1	A	144	LYS	2.7
1	A	29	LYS	2.5
1	A	236	PRO	2.5
1	A	125	PHE	2.4
1	A	239	TYR	2.4
1	A	228	VAL	2.3
1	A	262[A]	SER	2.3
1	A	334	GLY	2.3
1	A	31	VAL	2.2
1	A	339	ASN	2.2
1	A	231[A]	ARG	2.1
1	A	230	ILE	2.1
1	A	316	ASP	2.1
1	A	374	VAL	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](#)

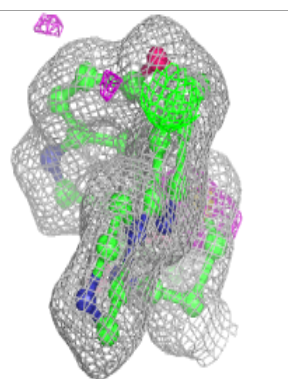
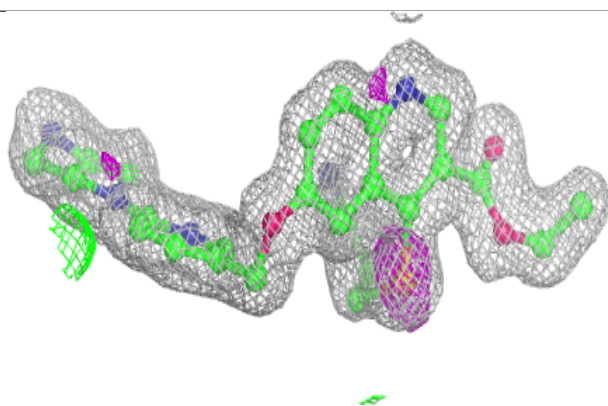
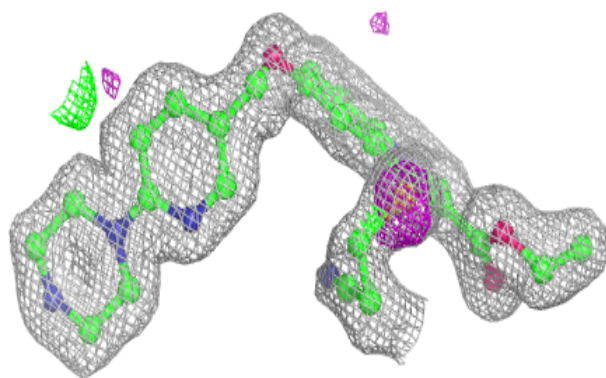
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	YN4	A	1002[A]	34/34	0.93	0.09	16,20,28,28	34
4	YN4	A	1002[B]	34/34	0.93	0.09	16,20,27,28	34
3	MYA	A	1001	63/63	0.96	0.08	11,17,22,23	0
2	MG	A	1000	1/1	0.98	0.06	29,29,29,29	0

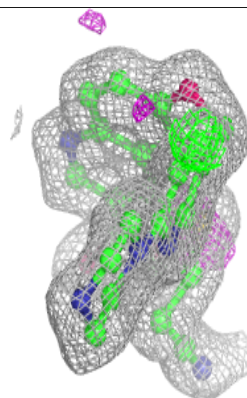
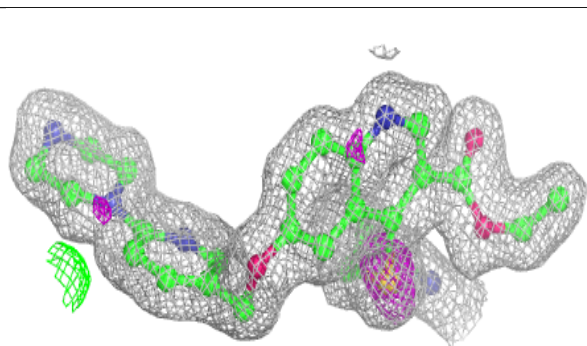
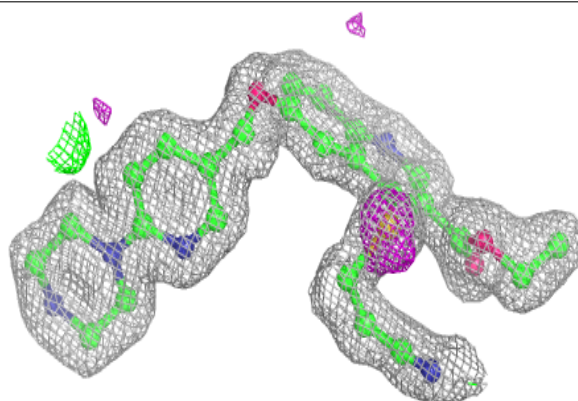
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

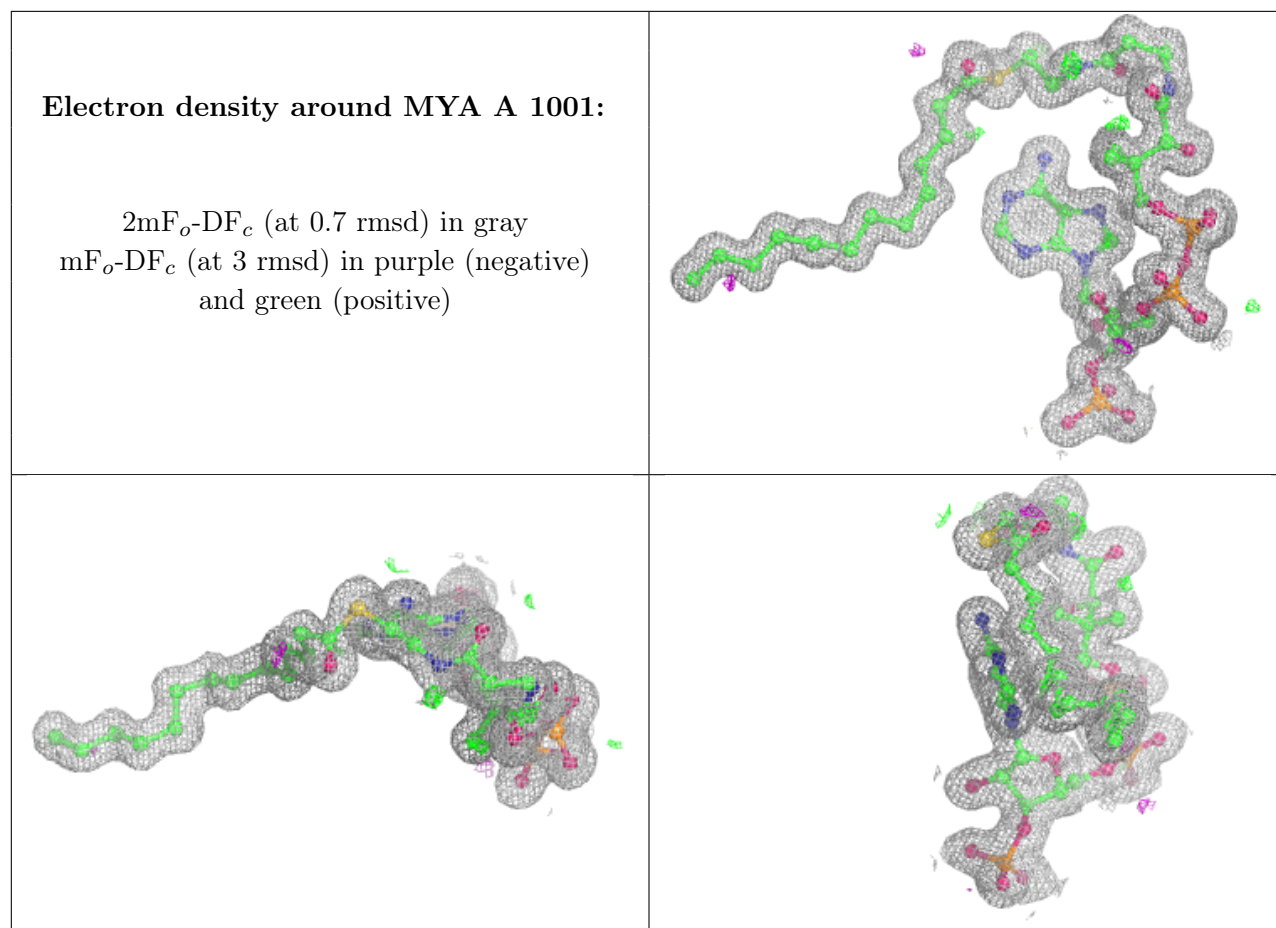
Electron density around YN4 A 1002 (A):

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

**Electron density around YN4 A 1002 (B):**

$2mF_o-DF_c$ (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.