



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 11:18 PM EDT

PDB ID : 6B1L  
Title : Crystal structure of glycolpeptide N-tetradecanoyltransferase from Plasmodium vivax in complex with inhibitor IMP-0001173  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2017-09-18  
Resolution : 2.30 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

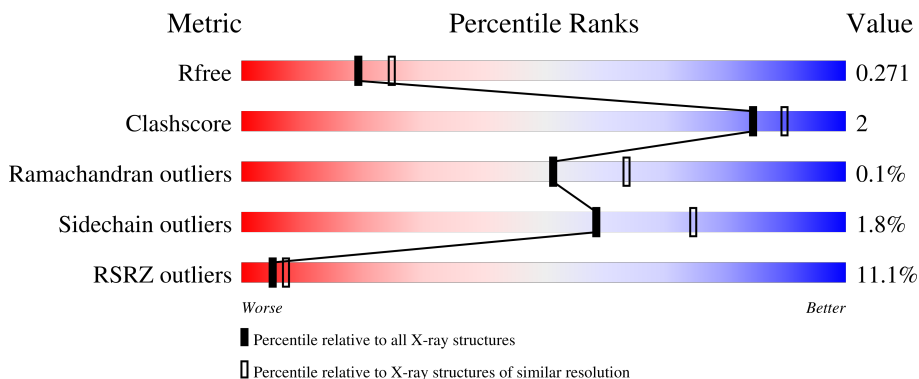
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	405	
1	B	405	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5563 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
			Total	C	N	O	S			
1	A	378	3031	1972	490	558	11	0	1	0
1	B	315	2250	1447	375	421	7	0	1	0

There are 42 discrepancies between the modelled and reference sequences:

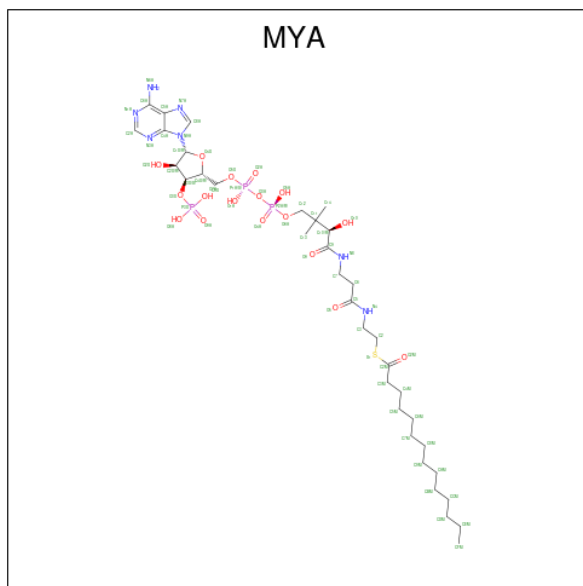
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	expression tag	UNP A5K1A2
A	7	GLY	-	expression tag	UNP A5K1A2
A	8	SER	-	expression tag	UNP A5K1A2
A	9	SER	-	expression tag	UNP A5K1A2
A	10	HIS	-	expression tag	UNP A5K1A2
A	11	HIS	-	expression tag	UNP A5K1A2
A	12	HIS	-	expression tag	UNP A5K1A2
A	13	HIS	-	expression tag	UNP A5K1A2
A	14	HIS	-	expression tag	UNP A5K1A2
A	15	HIS	-	expression tag	UNP A5K1A2
A	16	SER	-	expression tag	UNP A5K1A2
A	17	ALA	-	expression tag	UNP A5K1A2
A	18	ALA	-	expression tag	UNP A5K1A2
A	19	LEU	-	expression tag	UNP A5K1A2
A	20	GLU	-	expression tag	UNP A5K1A2
A	21	VAL	-	expression tag	UNP A5K1A2
A	22	LEU	-	expression tag	UNP A5K1A2
A	23	PHE	-	expression tag	UNP A5K1A2
A	24	GLN	-	expression tag	UNP A5K1A2
A	25	GLY	-	expression tag	UNP A5K1A2
A	26	PRO	-	expression tag	UNP A5K1A2
B	6	MET	-	expression tag	UNP A5K1A2
B	7	GLY	-	expression tag	UNP A5K1A2
B	8	SER	-	expression tag	UNP A5K1A2
B	9	SER	-	expression tag	UNP A5K1A2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	HIS	-	expression tag	UNP A5K1A2
B	11	HIS	-	expression tag	UNP A5K1A2
B	12	HIS	-	expression tag	UNP A5K1A2
B	13	HIS	-	expression tag	UNP A5K1A2
B	14	HIS	-	expression tag	UNP A5K1A2
B	15	HIS	-	expression tag	UNP A5K1A2
B	16	SER	-	expression tag	UNP A5K1A2
B	17	ALA	-	expression tag	UNP A5K1A2
B	18	ALA	-	expression tag	UNP A5K1A2
B	19	LEU	-	expression tag	UNP A5K1A2
B	20	GLU	-	expression tag	UNP A5K1A2
B	21	VAL	-	expression tag	UNP A5K1A2
B	22	LEU	-	expression tag	UNP A5K1A2
B	23	PHE	-	expression tag	UNP A5K1A2
B	24	GLN	-	expression tag	UNP A5K1A2
B	25	GLY	-	expression tag	UNP A5K1A2
B	26	PRO	-	expression tag	UNP A5K1A2

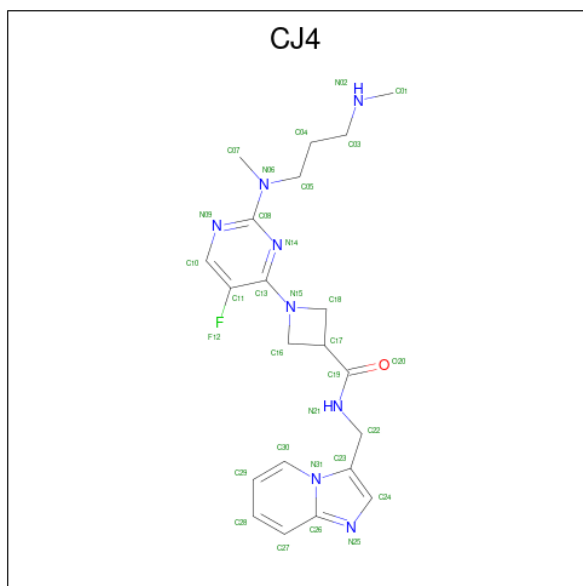
- Molecule 2 is TETRADECANOYL-COA (three-letter code: MYA) (formula:  $C_{35}H_{62}N_7O_{17}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1-(5-fluoro-2-{methyl[3-(methylamino)propyl]amino}pyrimidin-4-yl)-N-[(imidazo[1,2-a]pyridin-3-yl)methyl]azetidine-3-carboxamide (three-letter code: CJ4) (formula:

C<sub>21</sub>H<sub>27</sub>FN<sub>8</sub>O (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	31	21	1	8	1	0	0

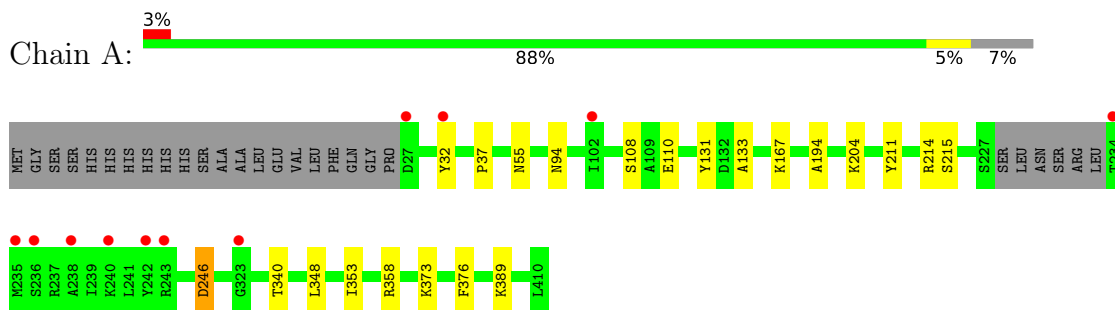
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	150	152	152	0	2
4	B	36	36	36	0	0

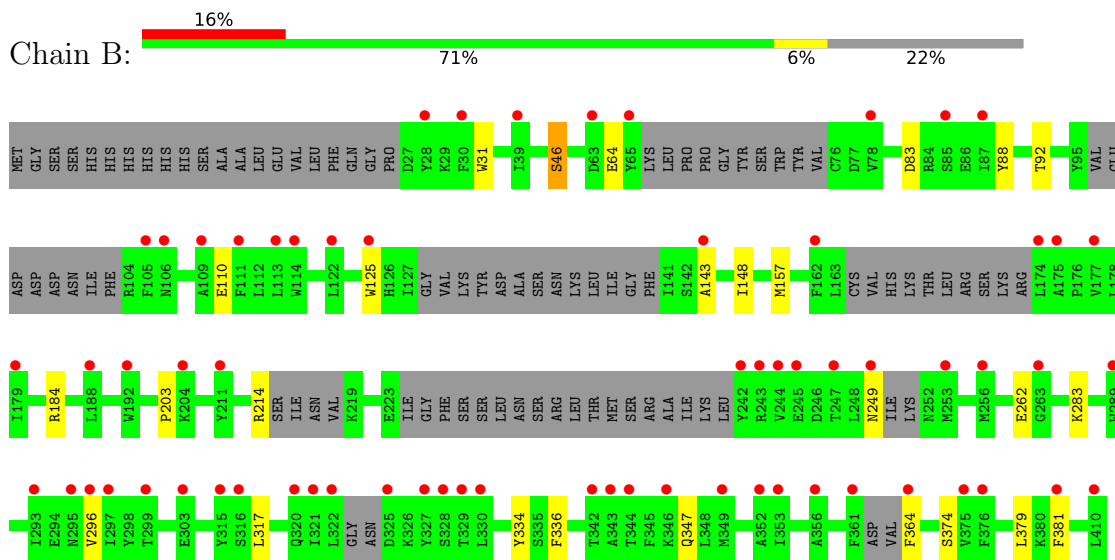
### 3 Residue-property plots [i](#)

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



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.03Å 81.49Å 119.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 2.30 48.17 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.17-2.30) 99.1 (48.17-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.232 , 0.271 0.232 , 0.271	Depositor DCC
$R_{free}$ test set	1884 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtrriage
Anisotropy	0.539	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: CJ4, 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	0.25	0/3112	0.42	0/4237
1	B	0.24	0/2303	0.41	0/3152
All	All	0.24	0/5415	0.42	0/7389

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3031	0	2893	13	0
1	B	2250	0	1827	13	0
2	A	63	0	58	1	0
3	A	31	0	0	0	0
4	A	152	0	0	1	0
4	B	36	0	0	0	0
All	All	5563	0	4778	23	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 2.

All (23) 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:214:ARG:O	1:B:364:PHE:N	2.28	0.67
1:A:214:ARG:NH1	1:A:215:SER:O	2.35	0.59
1:A:214:ARG:HG2	1:A:353:ILE:HD13	1.83	0.58
1:B:148:ILE:HG13	1:B:157:MET:HE2	1.88	0.56
1:A:37:PRO:HG2	1:A:204:LYS:HB3	1.88	0.54
1:B:88:TYR:O	1:B:92:THR:OG1	2.20	0.53
1:B:31:TRP:HB3	1:B:203:PRO:HG2	1.92	0.51
1:B:262:GLU:OE2	1:B:283:LYS:NZ	2.42	0.50
1:A:108:SER:HB2	1:B:46:SER:HB2	1.94	0.48
1:A:340:THR:HB	1:A:348:LEU:HD22	1.98	0.45
1:A:110:GLU:HB3	1:B:46:SER:HB3	1.97	0.45
1:A:94:ASN:HA	1:A:167:LYS:HD2	1.98	0.45
1:B:125:TRP:HB3	1:B:143:ALA:HB3	1.97	0.45
1:A:389:LYS:NZ	4:A:612:HOH:O	2.50	0.44
1:A:194:ALA:HB2	2:A:501:MYA:HEM	1.99	0.43
1:A:131:TYR:CE2	1:A:133:ALA:HB3	2.54	0.43
1:A:110:GLU:CB	1:B:46:SER:HB3	2.50	0.42
1:B:317:LEU:HB3	1:B:334:TYR:CE1	2.55	0.42
1:B:379:LEU:O	1:B:381:PHE:N	2.53	0.42
1:B:64:GLU:HA	1:B:184:ARG:NH1	2.35	0.41
1:A:246:ASP:O	1:A:358[B]:ARG:NH2	2.53	0.41
1:A:373:LYS:HA	1:A:376:PHE:CD2	2.56	0.40
1:B:249:ASN:CG	1:B:347:GLN:HB2	2.42	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	375/405 (93%)	367 (98%)	8 (2%)	0	<a href="#">100</a> <a href="#">100</a>
1	B	296/405 (73%)	277 (94%)	18 (6%)	1 (0%)	<a href="#">41</a> <a href="#">50</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	671/810 (83%)	644 (96%)	26 (4%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	296	VAL

### 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	317/367 (86%)	313 (99%)	4 (1%)	69 82
1	B	182/367 (50%)	177 (97%)	5 (3%)	44 61
All	All	499/734 (68%)	490 (98%)	9 (2%)	59 75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	55	ASN
1	A	211	TYR
1	A	246	ASP
1	B	46	SER
1	B	83	ASP
1	B	110	GLU
1	B	336	PHE
1	B	374	SER

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

Mol	Chain	Res	Type
1	A	106	ASN
1	A	187	ASN
1	B	187	ASN

### 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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CJ4	A	502	-	29,34,34	0.84	1 (3%)	32,47,47	1.13	4 (12%)
2	MYA	A	501	-	57,65,65	0.88	2 (3%)	68,91,91	1.37	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CJ4	A	502	-	-	1/16/30/30	0/4/4/4
2	MYA	A	501	-	-	3/60/80/80	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MYA	C2M-S1	-3.76	1.67	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MYA	C5A-C4A	2.47	1.47	1.40
3	A	502	CJ4	C29-C28	2.17	1.43	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MYA	C3M-C2M-S1	6.08	120.53	113.46
2	A	501	MYA	N3A-C2A-N1A	-3.27	123.56	128.68
2	A	501	MYA	O2M-C2M-C3M	-3.15	120.27	123.99
2	A	501	MYA	C4A-C5A-N7A	-2.81	106.47	109.40
2	A	501	MYA	P2A-O3A-P1A	-2.81	123.17	132.83
2	A	501	MYA	O2M-C2M-S1	-2.64	119.19	122.61
3	A	502	CJ4	C18-N15-C13	2.57	133.87	125.64
3	A	502	CJ4	N09-C08-N14	-2.47	123.53	126.00
3	A	502	CJ4	C08-N14-C13	2.41	119.43	114.97
3	A	502	CJ4	F12-C11-C10	2.10	122.04	118.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MYA	C14-C11-C12-O6A
2	A	501	MYA	C3-C2-S1-C2M
2	A	501	MYA	P1A-O3A-P2A-O5A
3	A	502	CJ4	C18-C17-C19-O20

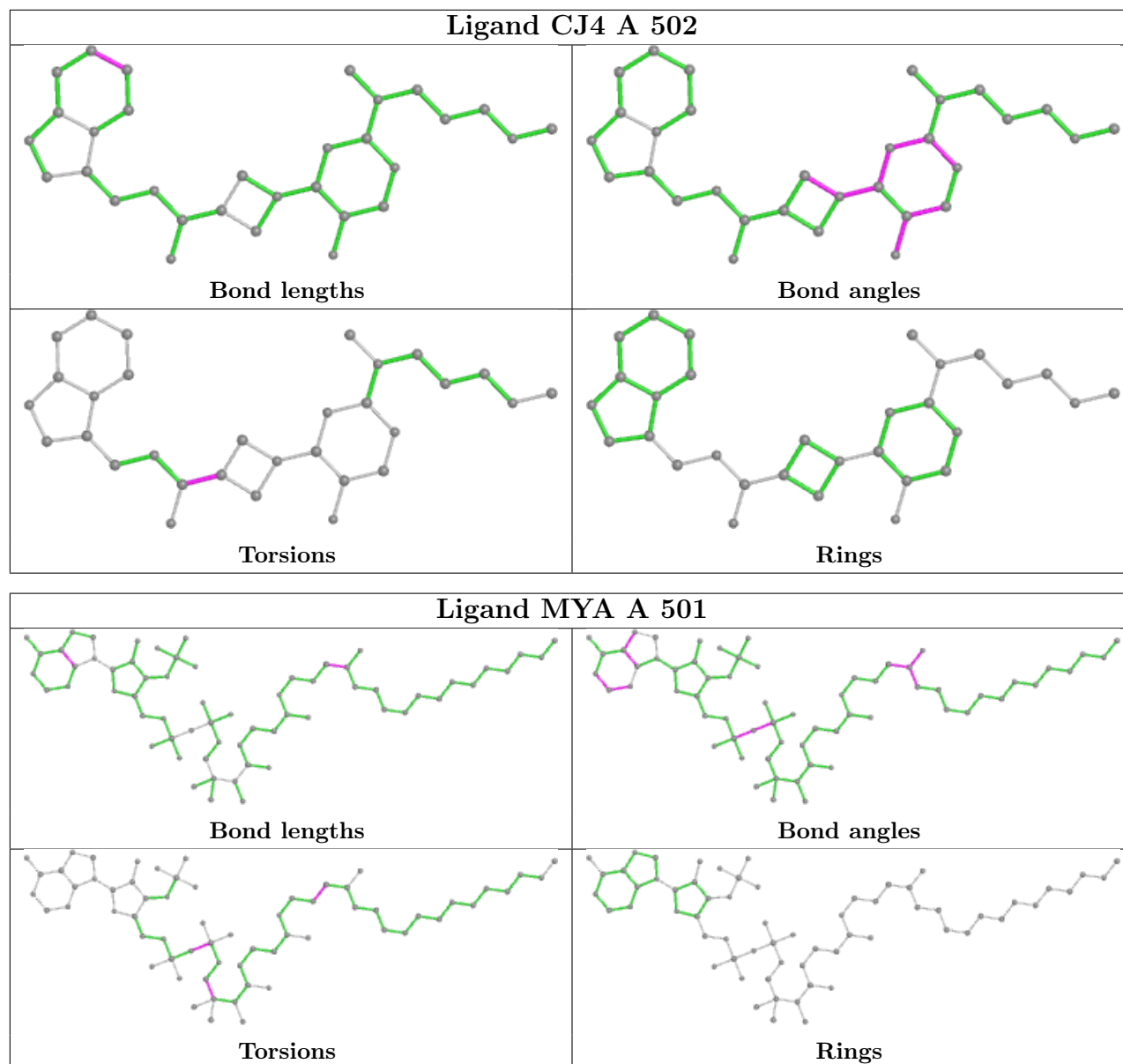
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MYA	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 [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	378/405 (93%)	0.01	11 (2%) 51 58	25, 40, 77, 99	0
1	B	315/405 (77%)	0.99	66 (20%) 1 1	39, 78, 114, 132	0
All	All	693/810 (85%)	0.45	77 (11%) 5 7	25, 54, 105, 132	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	MET	6.1
1	B	296	VAL	5.7
1	B	109	ALA	5.6
1	B	353	ILE	5.4
1	B	125	TRP	4.9
1	A	323	GLY	4.8
1	B	321	ILE	4.7
1	B	188	LEU	4.4
1	A	234	THR	4.3
1	B	344	THR	4.2
1	B	293	ILE	4.1
1	B	63	ASP	4.1
1	B	346	LYS	4.0
1	B	111	PHE	3.6
1	A	242	TYR	3.4
1	B	211	TYR	3.4
1	B	85	SER	3.4
1	B	295	ASN	3.3
1	B	78	VAL	3.3
1	B	243	ARG	3.2
1	B	256	MET	3.2
1	B	343	ALA	3.1
1	B	177	VAL	2.9
1	A	235	MET	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	263	GLY	2.9
1	B	175	ALA	2.8
1	A	102	ILE	2.8
1	B	376	PHE	2.8
1	B	410	LEU	2.8
1	B	192	TRP	2.8
1	B	143	ALA	2.7
1	B	65	TYR	2.7
1	A	27	ASP	2.7
1	B	28	TYR	2.7
1	B	315	TYR	2.6
1	B	253	MET	2.6
1	B	245	GLU	2.6
1	B	329	THR	2.6
1	B	381	PHE	2.6
1	B	356	ALA	2.6
1	B	289	TRP	2.6
1	A	236	SER	2.6
1	B	330	LEU	2.5
1	B	364	PHE	2.5
1	B	320	GLN	2.5
1	B	327	TYR	2.5
1	B	106	ASN	2.5
1	B	244	VAL	2.4
1	B	361	PHE	2.4
1	B	87	ILE	2.4
1	B	105	PHE	2.4
1	B	179	ILE	2.4
1	B	174	LEU	2.4
1	B	204	LYS	2.3
1	B	352	ALA	2.3
1	B	242	TYR	2.3
1	B	299	THR	2.3
1	B	297	ILE	2.3
1	B	122	LEU	2.3
1	B	316	SER	2.2
1	A	238	ALA	2.2
1	B	113	LEU	2.2
1	A	32	TYR	2.2
1	B	328	SER	2.2
1	B	303	GLU	2.2
1	B	162	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	375	VAL	2.1
1	B	322	LEU	2.1
1	B	247	THR	2.1
1	B	30	PHE	2.1
1	A	240	LYS	2.0
1	B	114	TRP	2.0
1	B	342	THR	2.0
1	B	249	ASN	2.0
1	B	39	ILE	2.0
1	A	243	ARG	2.0
1	B	325	ASP	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.

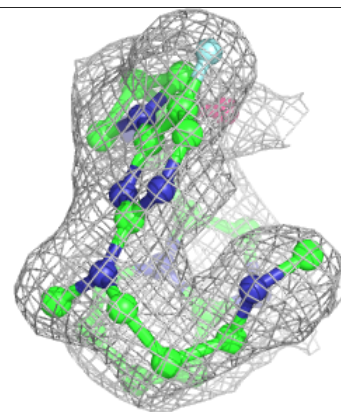
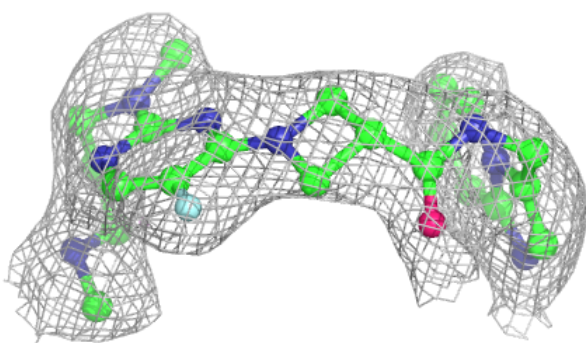
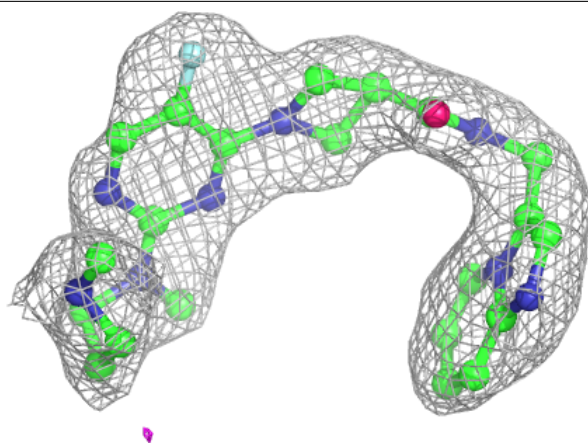
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CJ4	A	502	31/31	0.90	0.14	42,47,52,53	0
2	MYA	A	501	63/63	0.92	0.13	23,41,47,53	0

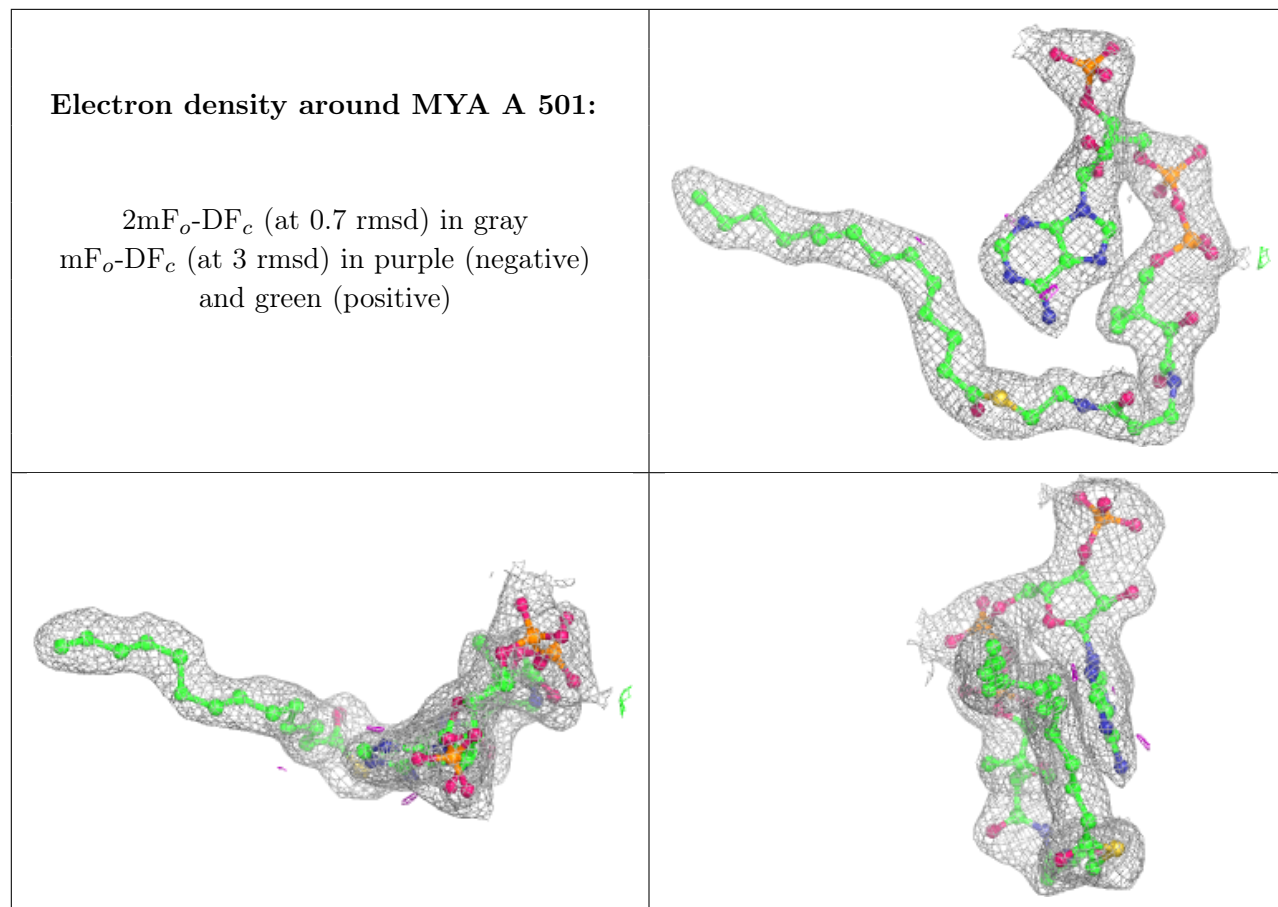
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around CJ4 A 502:**

$2mF_o-DF_c$  (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.