



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 08:43 PM UTC

PDB ID : 6F56 / pdb\_00006f56  
Title : Mutant of Human N-myristoyltransferase with bound myristoyl-CoA  
Authors : Brenk, R.; Kehrein, J.; Kersten, C.  
Deposited on : 2017-11-30  
Resolution : 1.94 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

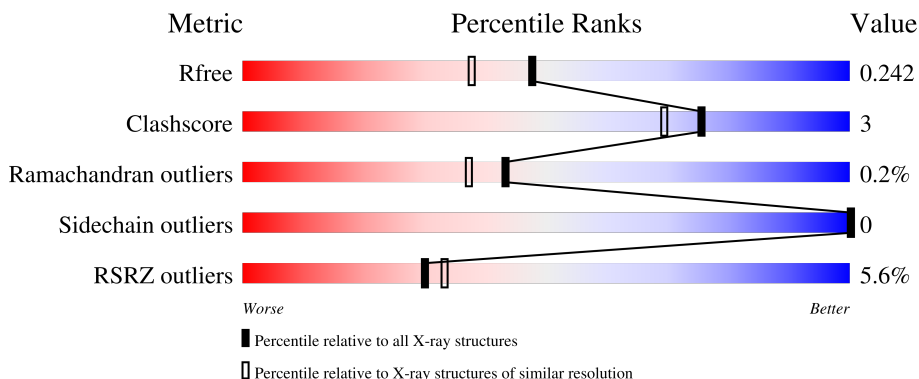
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
$R_{free}$	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	410	 4% 87% 6% 7%
1	B	410	 5% 86% 6% 7%
1	C	410	 7% 85% 8% 7%
1	D	410	 5% 85% 8% 7%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13363 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	3168	2053	535	562	18	152	7	0
1	B	382	3142	2036	531	557	18	155	2	0
1	C	382	3139	2034	530	557	18	177	2	0
1	D	382	3141	2035	531	557	18	338	2	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	MET	-	initiating methionine	UNP P30419
A	88	GLY	-	expression tag	UNP P30419
A	89	SER	-	expression tag	UNP P30419
A	90	SER	-	expression tag	UNP P30419
A	91	HIS	-	expression tag	UNP P30419
A	92	HIS	-	expression tag	UNP P30419
A	93	HIS	-	expression tag	UNP P30419
A	94	HIS	-	expression tag	UNP P30419
A	95	HIS	-	expression tag	UNP P30419
A	96	HIS	-	expression tag	UNP P30419
A	97	SER	-	expression tag	UNP P30419
A	98	SER	-	expression tag	UNP P30419
A	99	GLY	-	expression tag	UNP P30419
A	100	LEU	-	expression tag	UNP P30419
A	101	GLU	-	expression tag	UNP P30419
A	102	VAL	-	expression tag	UNP P30419
A	103	LEU	-	expression tag	UNP P30419
A	104	PHE	-	expression tag	UNP P30419
A	105	GLN	-	expression tag	UNP P30419
A	106	GLY	-	expression tag	UNP P30419
A	107	PRO	-	expression tag	UNP P30419

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	HIS	-	expression tag	UNP P30419
A	295	GLN	ARG	engineered mutation	UNP P30419
A	297	PHE	TRP	engineered mutation	UNP P30419
A	452	MET	ALA	engineered mutation	UNP P30419
A	453	VAL	LEU	engineered mutation	UNP P30419
A	462	VAL	LEU	engineered mutation	UNP P30419
A	473	HIS	ASN	engineered mutation	UNP P30419
A	495	MET	LEU	engineered mutation	UNP P30419
A	496	LEU	GLN	engineered mutation	UNP P30419
B	87	MET	-	initiating methionine	UNP P30419
B	88	GLY	-	expression tag	UNP P30419
B	89	SER	-	expression tag	UNP P30419
B	90	SER	-	expression tag	UNP P30419
B	91	HIS	-	expression tag	UNP P30419
B	92	HIS	-	expression tag	UNP P30419
B	93	HIS	-	expression tag	UNP P30419
B	94	HIS	-	expression tag	UNP P30419
B	95	HIS	-	expression tag	UNP P30419
B	96	HIS	-	expression tag	UNP P30419
B	97	SER	-	expression tag	UNP P30419
B	98	SER	-	expression tag	UNP P30419
B	99	GLY	-	expression tag	UNP P30419
B	100	LEU	-	expression tag	UNP P30419
B	101	GLU	-	expression tag	UNP P30419
B	102	VAL	-	expression tag	UNP P30419
B	103	LEU	-	expression tag	UNP P30419
B	104	PHE	-	expression tag	UNP P30419
B	105	GLN	-	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
B	295	GLN	ARG	engineered mutation	UNP P30419
B	297	PHE	TRP	engineered mutation	UNP P30419
B	452	MET	ALA	engineered mutation	UNP P30419
B	453	VAL	LEU	engineered mutation	UNP P30419
B	462	VAL	LEU	engineered mutation	UNP P30419
B	473	HIS	ASN	engineered mutation	UNP P30419
B	495	MET	LEU	engineered mutation	UNP P30419
B	496	LEU	GLN	engineered mutation	UNP P30419
C	87	MET	-	initiating methionine	UNP P30419
C	88	GLY	-	expression tag	UNP P30419
C	89	SER	-	expression tag	UNP P30419

*Continued on next page...*

*Continued from previous page...*

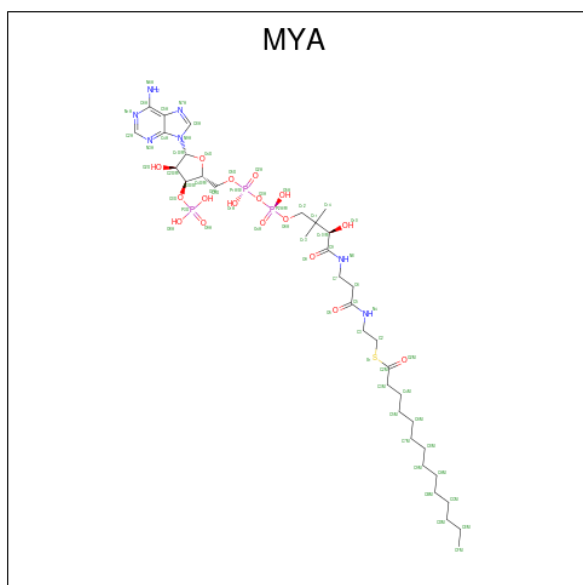
Chain	Residue	Modelled	Actual	Comment	Reference
C	90	SER	-	expression tag	UNP P30419
C	91	HIS	-	expression tag	UNP P30419
C	92	HIS	-	expression tag	UNP P30419
C	93	HIS	-	expression tag	UNP P30419
C	94	HIS	-	expression tag	UNP P30419
C	95	HIS	-	expression tag	UNP P30419
C	96	HIS	-	expression tag	UNP P30419
C	97	SER	-	expression tag	UNP P30419
C	98	SER	-	expression tag	UNP P30419
C	99	GLY	-	expression tag	UNP P30419
C	100	LEU	-	expression tag	UNP P30419
C	101	GLU	-	expression tag	UNP P30419
C	102	VAL	-	expression tag	UNP P30419
C	103	LEU	-	expression tag	UNP P30419
C	104	PHE	-	expression tag	UNP P30419
C	105	GLN	-	expression tag	UNP P30419
C	106	GLY	-	expression tag	UNP P30419
C	107	PRO	-	expression tag	UNP P30419
C	108	HIS	-	expression tag	UNP P30419
C	295	GLN	ARG	engineered mutation	UNP P30419
C	297	PHE	TRP	engineered mutation	UNP P30419
C	452	MET	ALA	engineered mutation	UNP P30419
C	453	VAL	LEU	engineered mutation	UNP P30419
C	462	VAL	LEU	engineered mutation	UNP P30419
C	473	HIS	ASN	engineered mutation	UNP P30419
C	495	MET	LEU	engineered mutation	UNP P30419
C	496	LEU	GLN	engineered mutation	UNP P30419
D	87	MET	-	initiating methionine	UNP P30419
D	88	GLY	-	expression tag	UNP P30419
D	89	SER	-	expression tag	UNP P30419
D	90	SER	-	expression tag	UNP P30419
D	91	HIS	-	expression tag	UNP P30419
D	92	HIS	-	expression tag	UNP P30419
D	93	HIS	-	expression tag	UNP P30419
D	94	HIS	-	expression tag	UNP P30419
D	95	HIS	-	expression tag	UNP P30419
D	96	HIS	-	expression tag	UNP P30419
D	97	SER	-	expression tag	UNP P30419
D	98	SER	-	expression tag	UNP P30419
D	99	GLY	-	expression tag	UNP P30419
D	100	LEU	-	expression tag	UNP P30419
D	101	GLU	-	expression tag	UNP P30419

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	102	VAL	-	expression tag	UNP P30419
D	103	LEU	-	expression tag	UNP P30419
D	104	PHE	-	expression tag	UNP P30419
D	105	GLN	-	expression tag	UNP P30419
D	106	GLY	-	expression tag	UNP P30419
D	107	PRO	-	expression tag	UNP P30419
D	108	HIS	-	expression tag	UNP P30419
D	295	GLN	ARG	engineered mutation	UNP P30419
D	297	PHE	TRP	engineered mutation	UNP P30419
D	452	MET	ALA	engineered mutation	UNP P30419
D	453	VAL	LEU	engineered mutation	UNP P30419
D	462	VAL	LEU	engineered mutation	UNP P30419
D	473	HIS	ASN	engineered mutation	UNP P30419
D	495	MET	LEU	engineered mutation	UNP P30419
D	496	LEU	GLN	engineered mutation	UNP P30419

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

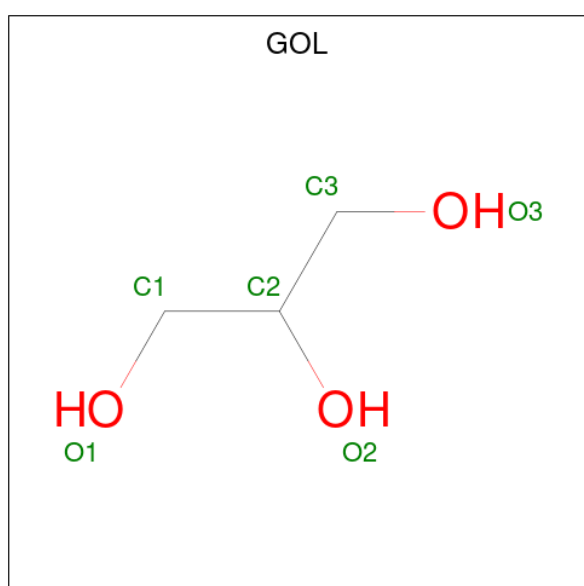


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0
2	B	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0
2	C	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0
2	D	1	Total 63	C 35	N 7	O 17	P 3	S 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

*Continued on next page...*

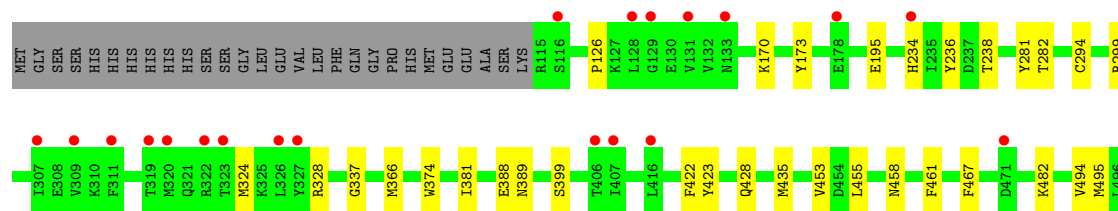
*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total	O	0	0
			135	135		
5	B	139	Total	O	0	0
			139	139		
5	C	92	Total	O	0	0
			92	92		
5	D	97	Total	O	0	0
			97	97		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.19Å 159.13Å 174.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.50 – 1.94 87.50 – 1.94	Depositor EDS
% Data completeness (in resolution range)	92.7 (87.50-1.94) 88.1 (87.50-1.94)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.94Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.200 , 0.239 0.202 , 0.242	Depositor DCC
$R_{free}$ test set	5517 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtrriage
Anisotropy	0.844	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13363	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.74% 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: GOL, MG, 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	0.15	0/3278	0.37	0/4449
1	B	0.16	0/3237	0.49	5/4395 (0.1%)
1	C	0.15	0/3234	0.37	0/4391
1	D	0.15	0/3236	0.37	0/4394
All	All	0.15	0/12985	0.40	5/17629 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	414	LYS	N-CA-C	10.66	125.39	111.75
1	B	413	HIS	N-CA-C	9.54	131.12	110.80
1	B	413	HIS	CB-CA-C	-6.87	96.75	110.42
1	B	411	PRO	CA-C-N	5.04	131.17	121.54
1	B	411	PRO	C-N-CA	5.04	131.17	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	411	PRO	Peptide

## 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	3168	0	3179	15	0
1	B	3142	0	3142	16	0
1	C	3139	0	3139	21	0
1	D	3141	0	3140	18	0
2	A	63	0	58	0	0
2	B	63	0	58	0	0
2	C	63	0	58	0	0
2	D	63	0	58	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
4	C	12	0	16	1	0
4	D	18	0	24	1	0
5	A	135	0	0	1	0
5	B	139	0	0	0	0
5	C	92	0	0	0	0
5	D	97	0	0	0	0
All	All	13363	0	12904	71	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 3.

The worst 5 of 71 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:C:187:MET:HE1	1:C:310:LYS:HB2	1.70	0.73
1:B:407:ILE:HD12	1:B:413:HIS:O	1.92	0.69
1:D:126:PRO:HG3	1:D:482:LYS:HG3	1.75	0.68
1:D:195:GLU:HB3	1:D:381:ILE:HD11	1.78	0.65
1:B:396:ASP:OD2	1:B:426:HIS:HA	1.97	0.65

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	387/410 (94%)	376 (97%)	11 (3%)	0	100	100
1	B	382/410 (93%)	369 (97%)	10 (3%)	3 (1%)	16	7
1	C	382/410 (93%)	374 (98%)	8 (2%)	0	100	100
1	D	382/410 (93%)	371 (97%)	11 (3%)	0	100	100
All	All	1533/1640 (94%)	1490 (97%)	40 (3%)	3 (0%)	43	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	412	THR
1	B	409	ASN
1	B	186	ASN

### 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	356/373 (95%)	356 (100%)	0	100	100
1	B	351/373 (94%)	351 (100%)	0	100	100
1	C	351/373 (94%)	351 (100%)	0	100	100
1	D	351/373 (94%)	351 (100%)	0	100	100
All	All	1409/1492 (94%)	1409 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	234	HIS
1	D	295	GLN
1	D	428	GLN
1	D	351	GLN
1	C	295	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 oligosaccharides in this entry.

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

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	C	501	3	63,65,65	1.18	7 (11%)	85,91,91	1.75	16 (18%)
2	MYA	D	501	-	63,65,65	1.19	7 (11%)	85,91,91	1.73	16 (18%)
4	GOL	B	504	-	5,5,5	0.55	0	5,5,5	0.71	0
4	GOL	D	504	-	5,5,5	0.55	0	5,5,5	0.26	0
4	GOL	D	505	-	5,5,5	0.54	0	5,5,5	0.28	0
2	MYA	B	501	3	63,65,65	1.19	6 (9%)	85,91,91	1.73	16 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	503	-	5,5,5	0.57	0	5,5,5	0.17	0
2	MYA	A	501	3	63,65,65	1.18	8 (12%)	85,91,91	1.76	14 (16%)
4	GOL	A	504	-	5,5,5	0.52	0	5,5,5	0.26	0
4	GOL	B	503	-	5,5,5	0.56	0	5,5,5	0.35	0
4	GOL	D	503	-	5,5,5	0.55	0	5,5,5	0.55	0
4	GOL	C	503	-	5,5,5	0.56	0	5,5,5	0.63	0
4	GOL	C	504	-	5,5,5	0.55	0	5,5,5	0.28	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	C	501	3	-	1/64/80/80	0/3/3/3
2	MYA	D	501	-	-	0/64/80/80	0/3/3/3
4	GOL	B	504	-	-	0/4/4/4	-
4	GOL	D	504	-	-	0/4/4/4	-
4	GOL	D	505	-	-	0/4/4/4	-
2	MYA	B	501	3	-	2/64/80/80	0/3/3/3
4	GOL	A	503	-	-	0/4/4/4	-
2	MYA	A	501	3	-	1/64/80/80	0/3/3/3
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	B	503	-	-	0/4/4/4	-
4	GOL	D	503	-	-	0/4/4/4	-
4	GOL	C	503	-	-	2/4/4/4	-
4	GOL	C	504	-	-	0/4/4/4	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MYA	P1A-O3A	3.17	1.62	1.59
2	A	501	MYA	P1A-O3A	3.14	1.62	1.59
2	D	501	MYA	P1A-O3A	3.02	1.62	1.59
2	C	501	MYA	C8A-N7A	2.95	1.37	1.31
2	B	501	MYA	C8A-N7A	2.91	1.37	1.31

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	MYA	C3M-C2M-S1	6.81	121.51	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	MYA	C3M-C2M-S1	6.79	121.49	113.40
2	D	501	MYA	C3M-C2M-S1	6.69	121.38	113.40
2	A	501	MYA	C3M-C2M-S1	6.63	121.31	113.40
2	B	501	MYA	N3A-C2A-N1A	-6.17	119.24	128.58

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

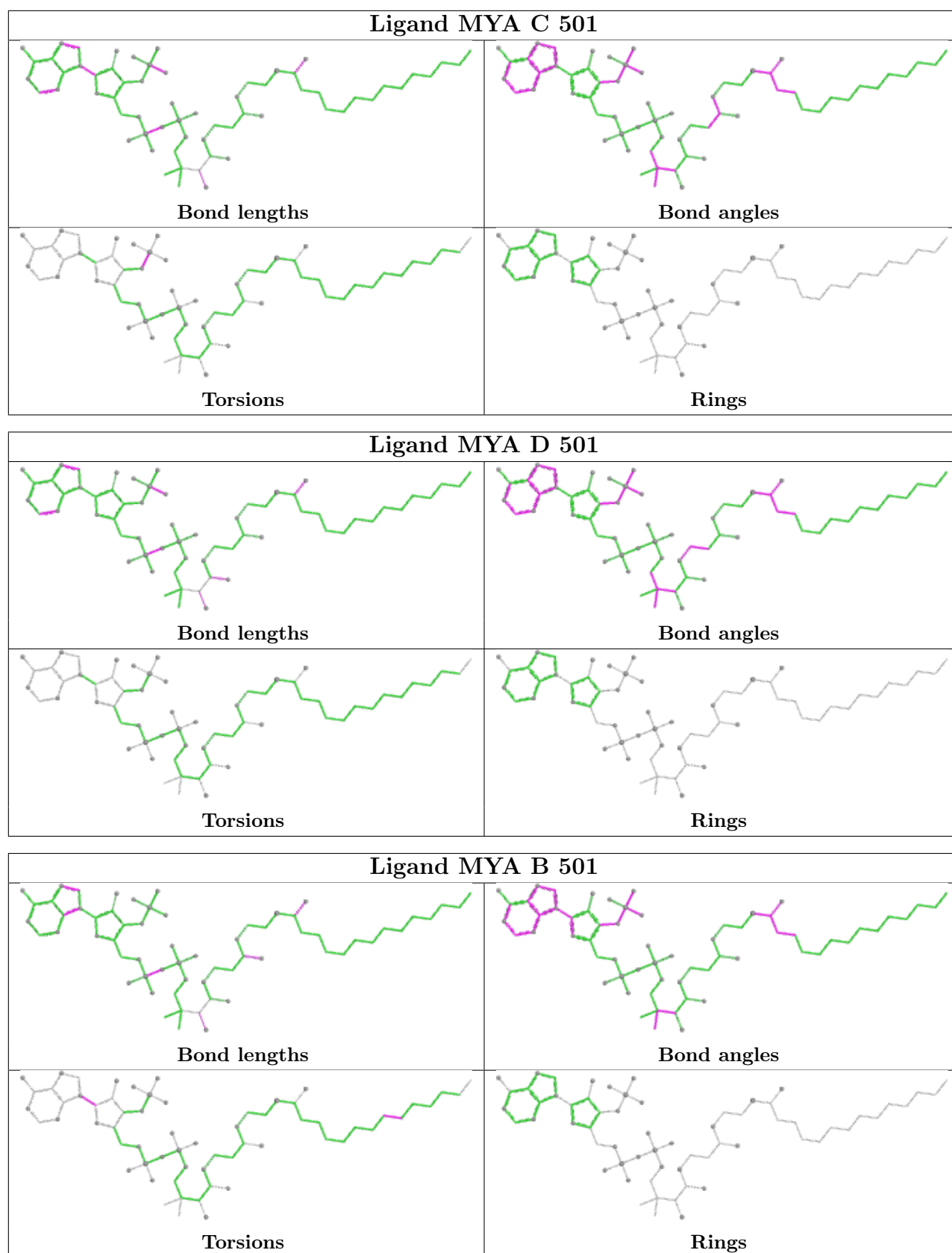
Mol	Chain	Res	Type	Atoms
4	C	503	GOL	C1-C2-C3-O3
4	C	503	GOL	O2-C2-C3-O3
2	A	501	MYA	C3X-O3X-P3X-O8A
2	B	501	MYA	C8M-C9M-CAM-CBM
2	C	501	MYA	C3X-O3X-P3X-O8A

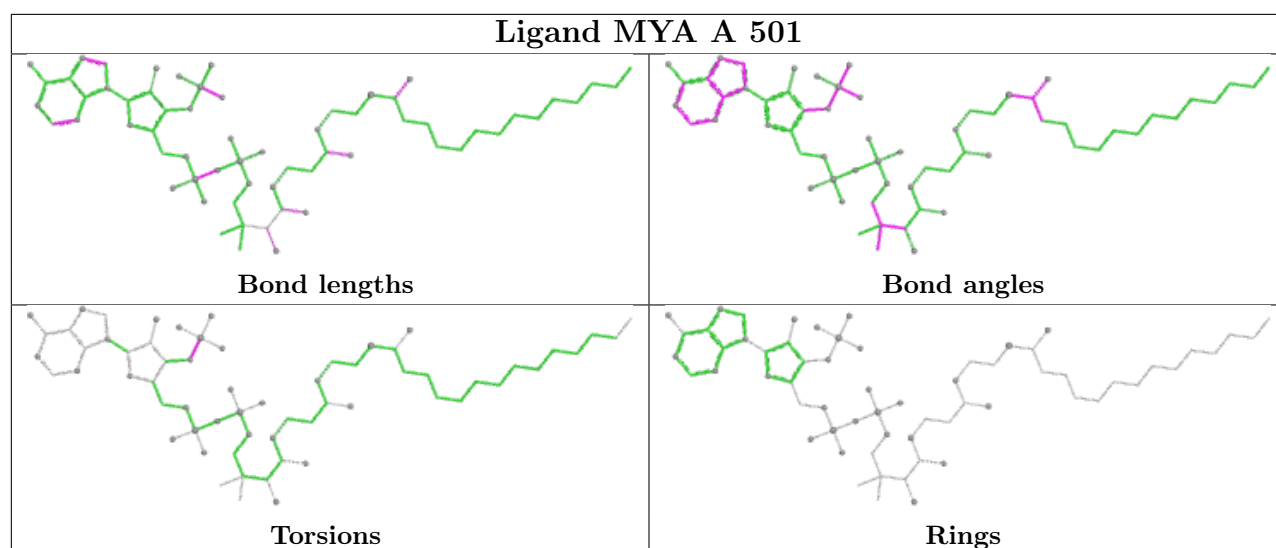
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	GOL	1	0
4	C	503	GOL	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	379/410 (92%)	0.29	15 (3%) 42 47	14, 29, 45, 56	48 (12%)
1	B	376/410 (91%)	0.25	22 (5%) 28 31	10, 27, 43, 86	31 (8%)
1	C	377/410 (91%)	0.61	27 (7%) 21 24	12, 34, 52, 69	40 (10%)
1	D	358/410 (87%)	0.53	20 (5%) 30 33	6, 33, 49, 61	35 (9%)
All	All	1490/1640 (90%)	0.42	84 (5%) 30 33	6, 31, 49, 86	154 (10%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	411	PRO	8.4
1	D	323	THR	5.1
1	D	311	PHE	4.8
1	D	407	ILE	4.6
1	B	410	HIS	4.5

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

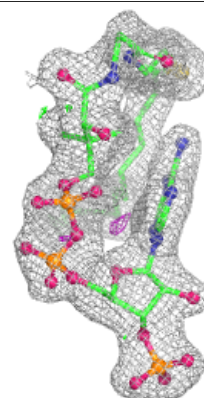
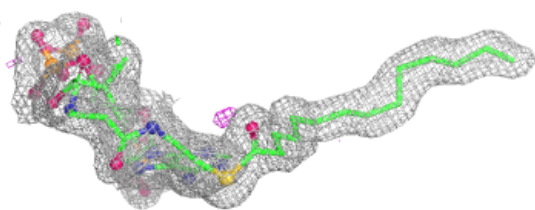
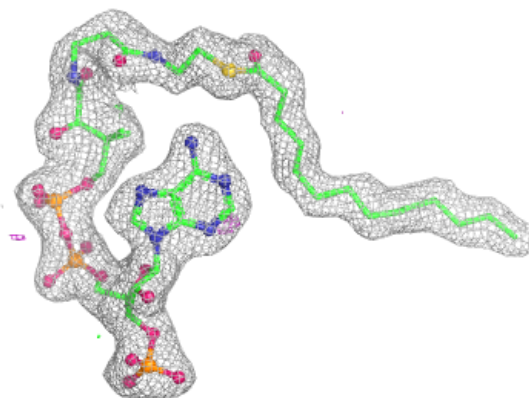
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 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
4	GOL	D	505	6/6	0.75	0.17	47,52,55,58	0
4	GOL	D	503	6/6	0.82	0.14	35,39,44,47	0
4	GOL	C	503	6/6	0.86	0.13	38,39,42,43	0
4	GOL	A	504	6/6	0.87	0.12	33,39,42,45	0
4	GOL	B	504	6/6	0.89	0.11	30,36,39,41	0
3	MG	C	502	1/1	0.91	0.17	50,50,50,50	0
3	MG	B	502	1/1	0.92	0.12	40,40,40,40	0
2	MYA	C	501	63/63	0.93	0.08	23,35,44,50	0
4	GOL	D	504	6/6	0.93	0.10	30,32,36,38	0
4	GOL	C	504	6/6	0.93	0.09	32,39,40,43	0
2	MYA	D	501	63/63	0.94	0.08	20,34,40,43	0
3	MG	A	502	1/1	0.95	0.14	42,42,42,42	0
2	MYA	A	501	63/63	0.95	0.08	14,30,37,41	0
2	MYA	B	501	63/63	0.96	0.07	15,28,34,36	0
4	GOL	B	503	6/6	0.96	0.08	28,30,33,36	0
3	MG	D	502	1/1	0.96	0.12	47,47,47,47	0
4	GOL	A	503	6/6	0.96	0.06	25,28,33,33	0

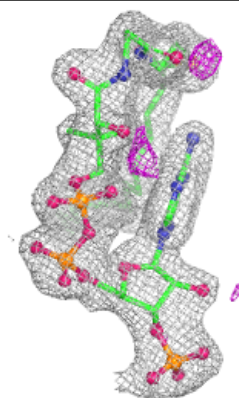
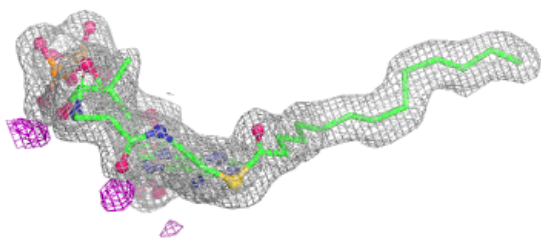
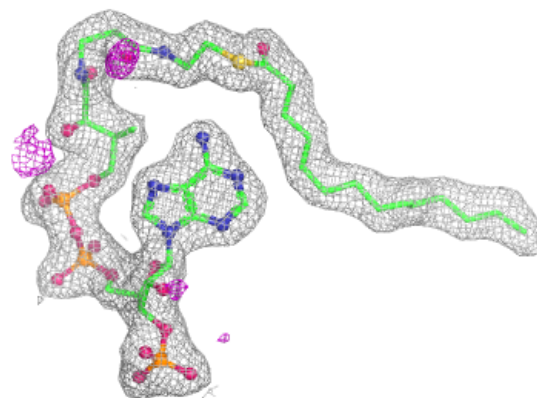
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around MYA C 501:**

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

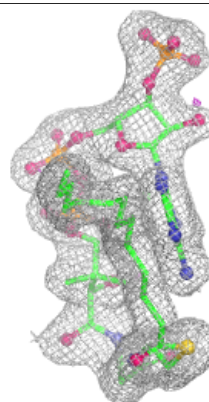
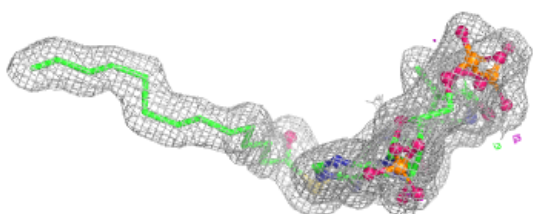
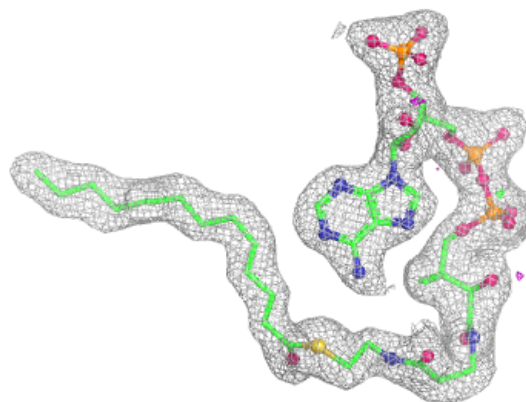
**Electron density around MYA D 501:**

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

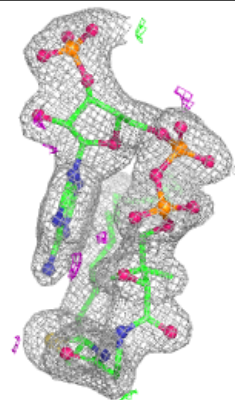
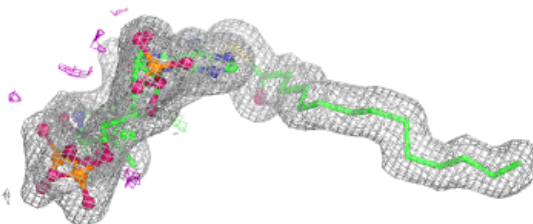
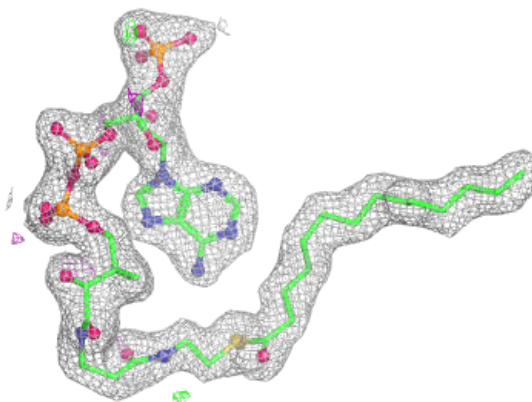


**Electron density around MYA A 501:**

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

**Electron density around MYA B 501:**

$2mF_o-DF_c$  (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.