



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:26 AM UTC

PDB ID : 8VKB / pdb_00008vkb
Title : Crystal structure of Plasmodium vivax glycylpeptide N-tetradecanoyltransferase (N-myristoyltransferase, NMT) bound to myristoyl-CoA and inhibitor 10b
Authors : Fenwick, M.K.; Staker, B.L.; Phan, I.Q.; Early, J.; Myler, P.J.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-01-08
Resolution : 2.43 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (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

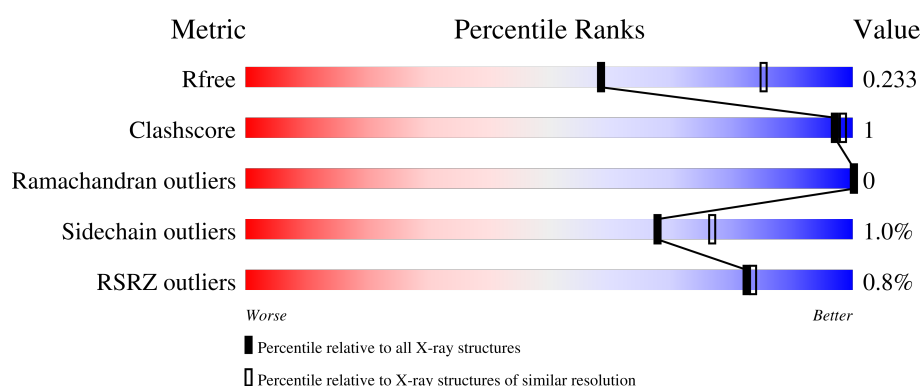
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

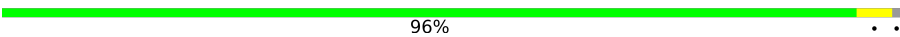
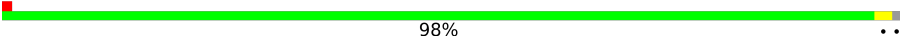
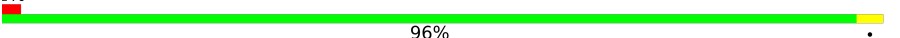
The reported resolution of this entry is 2.43 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	386	 96%
1	B	386	 98%
1	C	386	 96%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20693 atoms, of which 9986 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.

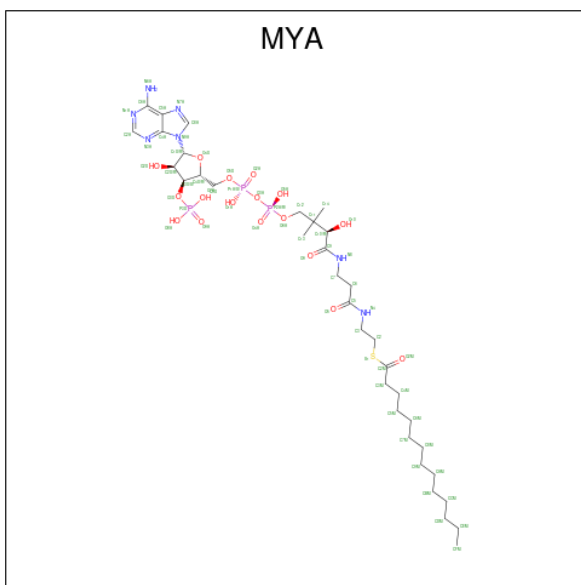
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	H	N	O	S	0	12	0
			6493	2113	3233	535	601	11			
1	B	384	Total	C	H	N	O	S	0	10	0
			6502	2114	3245	538	594	11			
1	C	385	Total	C	H	N	O	S	0	6	0
			6334	2069	3151	519	584	11			

There are 6 discrepancies between the modelled and reference sequences:

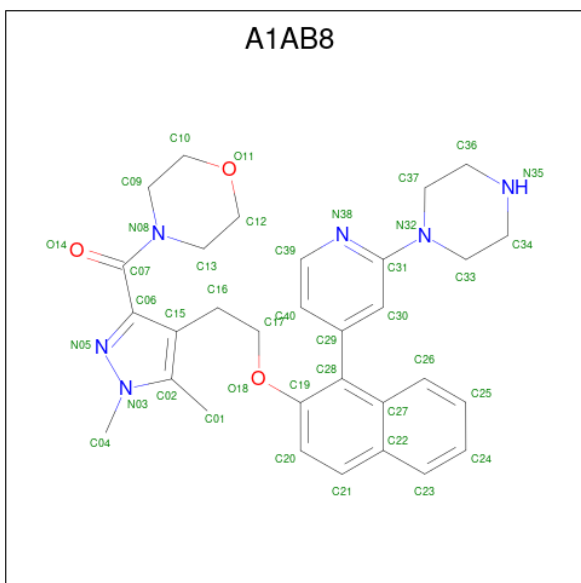
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP A5K1A2
A	26	PRO	-	expression tag	UNP A5K1A2
B	25	GLY	-	expression tag	UNP A5K1A2
B	26	PRO	-	expression tag	UNP A5K1A2
C	25	GLY	-	expression tag	UNP A5K1A2
C	26	PRO	-	expression tag	UNP A5K1A2

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



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			121	35	58	7	17	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			121	35	58	7	17	3	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			121	35	58	7	17	3	1		

- Molecule 3 is {1,5-dimethyl-4-[2-((1P)-1-[2-(piperazin-1-yl)pyridin-4-yl]naphthalen-2-yl}oxy)ethyl]-1H-pyrazol-3-yl}(morpholin-4-yl)methanone (CCD ID: A1AB8) (formula: $C_{31}H_{36}N_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			77	31	37	6	3		
3	B	1	Total	C	H	N	O	0	0
			77	31	37	6	3		
3	C	1	Total	C	H	N	O	0	0
			77	31	37	6	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

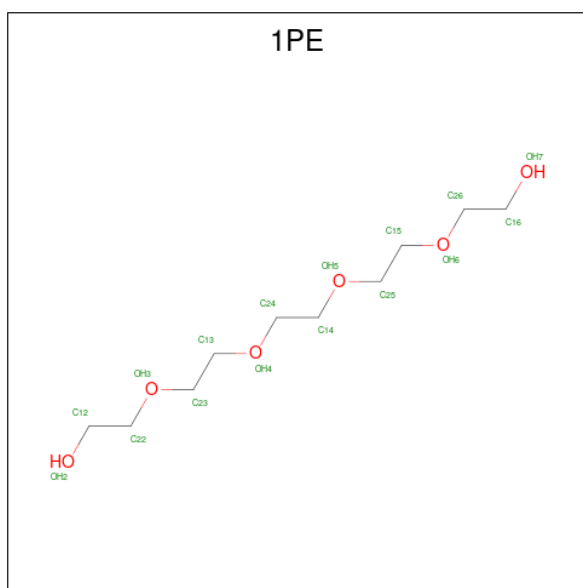
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Cl	0	0
			5	5		
4	B	5	Total	Cl	0	0
			5	5		
4	C	8	Total	Cl	0	0
			8	8		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



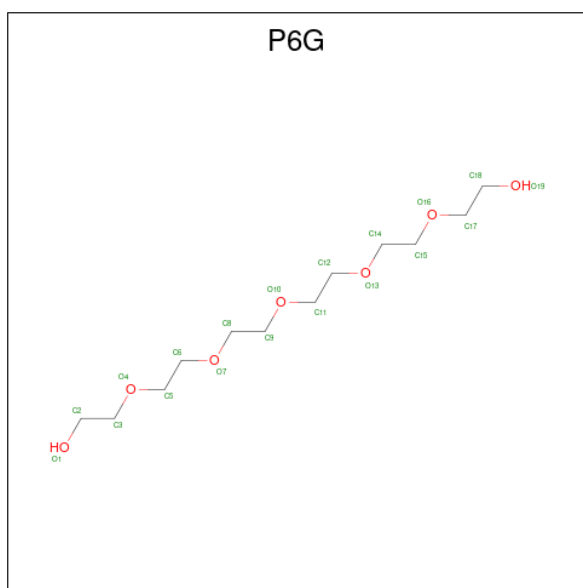
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 7 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			45	12	26	7		

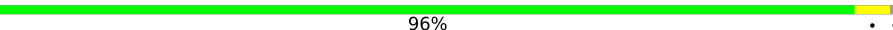
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	215	Total 219	O 219	0	7
8	B	222	Total 223	O 223	0	7
8	C	183	Total 185	O 185	0	3

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

Chain A:  96% . .



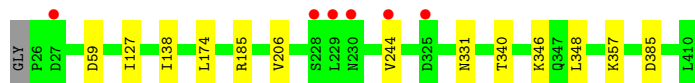
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain B:  98% . .



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain C:  96% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.37Å 119.78Å 176.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 2.43 48.13 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.13-2.43) 98.4 (48.13-2.43)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.233 0.185 , 0.233	Depositor DCC
R_{free} test set	2347 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20693	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 1PE, MYA, A1AB8, P6G, GOL

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	0.09	0/3352	0.24	0/4539
1	B	0.08	0/3338	0.25	0/4517
1	C	0.08	0/3280	0.24	0/4445
All	All	0.08	0/9970	0.24	0/13501

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	3260	3233	3209	9	0
1	B	3257	3245	3235	2	0
1	C	3183	3151	3122	7	0
2	A	63	58	58	0	0
2	B	63	58	58	0	0
2	C	63	58	58	0	0
3	A	40	37	0	0	0
3	B	40	37	0	0	0
3	C	40	37	0	0	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
4	C	8	0	0	0	0
5	A	6	8	8	0	0
5	B	6	8	8	0	0
5	C	6	8	8	0	0
6	A	16	22	22	0	0
7	B	19	26	26	0	0
8	A	219	0	0	3	0
8	B	223	0	0	0	0
8	C	185	0	0	3	0
All	All	10707	9986	9812	18	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 1.

All (18) 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:197:THR:HG23	1:B:409:LEU:HD22	1.75	0.69
1:A:141:ILE:HD12	1:A:163:LEU:HD13	1.90	0.53
1:C:385:ASP:O	8:C:601:HOH:O	2.19	0.50
1:C:340:THR:HB	1:C:348:LEU:HD22	1.93	0.50
1:A:61:ARG:NH2	8:A:609:HOH:O	2.39	0.50
1:A:174:LEU:HD23	1:A:174:LEU:O	2.15	0.47
1:A:245:GLU:OE1	8:A:601:HOH:O	2.20	0.47
1:A:131:TYR:CE2	1:A:133:ALA:HB3	2.51	0.46
1:A:138:ILE:HD12	1:A:138:ILE:C	2.40	0.46
1:C:59:ASP:OD1	8:C:602:HOH:O	2.20	0.45
1:A:185:ARG:NH1	8:A:623:HOH:O	2.50	0.45
1:A:211:TYR:HB3	1:A:367:LEU:HD23	1.99	0.43
1:C:127:ILE:HD11	1:C:185:ARG:HD2	2.01	0.43
1:C:206:VAL:HG13	8:C:605:HOH:O	2.19	0.42
1:C:138:ILE:C	1:C:138:ILE:HD12	2.44	0.42
1:C:244:VAL:HG11	1:C:357:LYS:HD2	2.02	0.42
1:B:138:ILE:C	1:B:138:ILE:HD12	2.45	0.42
1:A:197:THR:HG23	1:A:409:LEU:HD22	2.01	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	394/386 (102%)	382 (97%)	12 (3%)	0	100	100
1	B	392/386 (102%)	378 (96%)	14 (4%)	0	100	100
1	C	389/386 (101%)	374 (96%)	15 (4%)	0	100	100
All	All	1175/1158 (102%)	1134 (96%)	41 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	360/351 (103%)	358 (99%)	2 (1%)	78	85
1	B	357/351 (102%)	352 (99%)	5 (1%)	59	70
1	C	349/351 (99%)	346 (99%)	3 (1%)	70	80
All	All	1066/1053 (101%)	1056 (99%)	10 (1%)	68	80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	VAL
1	A	329	THR
1	B	150	ILE
1	B	172	LYS
1	B	244	VAL

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Mol	Chain	Res	Type
1	B	373	LYS
1	B	409	LEU
1	C	174	LEU
1	C	331	ASN
1	C	346	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	320	GLN
1	B	187	ASN
1	B	331	ASN
1	C	151	HIS
1	C	187	ASN
1	C	295	ASN
1	C	371	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 29 ligands modelled in this entry, 18 are monoatomic - leaving 11 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	B	501	-	63,65,65	1.78	15 (23%)	85,91,91	1.63	13 (15%)
5	GOL	A	506	-	5,5,5	0.92	0	5,5,5	1.03	0
3	A1AB8	B	502	-	45,45,45	1.80	8 (17%)	59,63,63	1.43	8 (13%)
5	GOL	C	511	-	5,5,5	0.89	0	5,5,5	1.03	0
3	A1AB8	A	502	-	45,45,45	1.78	8 (17%)	59,63,63	1.57	9 (15%)
2	MYA	C	501	-	63,65,65	1.80	15 (23%)	85,91,91	1.66	14 (16%)
2	MYA	A	501	-	63,65,65	1.78	14 (22%)	85,91,91	1.63	15 (17%)
6	1PE	A	507	-	15,15,15	0.12	0	14,14,14	0.13	0
7	P6G	B	508	-	18,18,18	0.11	0	17,17,17	0.09	0
3	A1AB8	C	502	-	45,45,45	1.79	9 (20%)	59,63,63	1.43	8 (13%)
5	GOL	B	509	-	5,5,5	0.87	0	5,5,5	1.13	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	B	501	-	-	12/64/80/80	0/3/3/3
5	GOL	A	506	-	-	4/4/4/4	-
3	A1AB8	B	502	-	-	1/22/38/38	0/6/6/6
5	GOL	C	511	-	-	4/4/4/4	-
3	A1AB8	A	502	-	-	3/22/38/38	0/6/6/6
2	MYA	C	501	-	-	13/64/80/80	0/3/3/3
2	MYA	A	501	-	-	13/64/80/80	0/3/3/3
6	1PE	A	507	-	-	6/13/13/13	-
7	P6G	B	508	-	-	1/16/16/16	-
3	A1AB8	C	502	-	-	0/22/38/38	0/6/6/6
5	GOL	B	509	-	-	2/4/4/4	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	A1AB8	C07-N08	7.35	1.47	1.34
3	C	502	A1AB8	C07-N08	7.21	1.47	1.34
3	A	502	A1AB8	C07-N08	6.99	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	MYA	C12-C11	5.94	1.62	1.52
2	B	501	MYA	C12-C11	5.85	1.62	1.52
2	C	501	MYA	C12-C11	5.79	1.62	1.52
2	C	501	MYA	C2M-S1	4.59	1.87	1.76
2	A	501	MYA	C2M-S1	4.54	1.87	1.76
2	B	501	MYA	C2M-S1	4.54	1.86	1.76
3	C	502	A1AB8	C31-N32	3.93	1.46	1.37
3	A	502	A1AB8	C31-N32	3.91	1.46	1.37
3	B	502	A1AB8	C31-N32	3.87	1.46	1.37
2	C	501	MYA	C3M-C2M	3.70	1.54	1.50
2	A	501	MYA	C5-N4	3.67	1.42	1.33
2	C	501	MYA	C5-N4	3.60	1.41	1.33
2	B	501	MYA	C5-N4	3.60	1.41	1.33
2	A	501	MYA	C3M-C2M	3.50	1.54	1.50
2	B	501	MYA	C3M-C2M	3.37	1.54	1.50
3	B	502	A1AB8	C27-C22	-3.29	1.36	1.43
3	C	502	A1AB8	C27-C22	-3.29	1.36	1.43
2	C	501	MYA	C9-N8	3.28	1.41	1.33
3	A	502	A1AB8	C27-C22	-3.27	1.36	1.43
2	A	501	MYA	O3X-C3X	-3.26	1.32	1.44
2	C	501	MYA	C5A-C4A	3.23	1.44	1.39
2	B	501	MYA	O3X-C3X	-3.19	1.33	1.44
2	B	501	MYA	C5A-C4A	3.18	1.44	1.39
2	C	501	MYA	O3X-C3X	-3.17	1.33	1.44
2	B	501	MYA	C9-N8	3.16	1.41	1.33
2	A	501	MYA	C5A-C4A	3.15	1.44	1.39
2	A	501	MYA	C9-N8	3.03	1.40	1.33
2	C	501	MYA	C3X-C4X	3.00	1.60	1.52
2	A	501	MYA	C3X-C4X	2.98	1.60	1.52
3	B	502	A1AB8	C28-C29	2.95	1.53	1.49
2	A	501	MYA	C2A-N1A	2.95	1.39	1.33
2	B	501	MYA	C3X-C4X	2.93	1.60	1.52
2	B	501	MYA	C2A-N1A	2.90	1.39	1.33
2	C	501	MYA	C2A-N1A	2.88	1.39	1.33
3	A	502	A1AB8	C28-C29	2.85	1.53	1.49
3	C	502	A1AB8	C28-C29	2.83	1.53	1.49
2	A	501	MYA	O6A-C12	-2.70	1.35	1.43
2	C	501	MYA	O6A-C12	-2.68	1.35	1.43
2	C	501	MYA	C4A-N3A	2.68	1.39	1.34
2	B	501	MYA	O6A-C12	-2.63	1.35	1.43
2	B	501	MYA	C4A-N3A	2.60	1.39	1.34
2	A	501	MYA	C4A-N3A	2.60	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	A1AB8	C06-C15	-2.57	1.39	1.45
3	A	502	A1AB8	C01-C02	2.52	1.53	1.49
3	C	502	A1AB8	C01-C02	2.52	1.53	1.49
3	B	502	A1AB8	C01-C02	2.52	1.53	1.49
3	B	502	A1AB8	C06-C15	-2.51	1.39	1.45
2	B	501	MYA	C8A-N7A	2.40	1.36	1.31
2	C	501	MYA	C8A-N7A	2.38	1.36	1.31
3	C	502	A1AB8	C06-C15	-2.37	1.39	1.45
2	C	501	MYA	C2-S1	2.36	1.91	1.81
2	A	501	MYA	C8A-N7A	2.35	1.36	1.31
3	B	502	A1AB8	C06-C07	2.29	1.53	1.49
3	C	502	A1AB8	C06-C07	2.29	1.53	1.49
3	A	502	A1AB8	O14-C07	-2.27	1.18	1.23
3	A	502	A1AB8	C06-C07	2.22	1.53	1.49
2	C	501	MYA	C6A-N6A	2.22	1.39	1.34
3	C	502	A1AB8	O14-C07	-2.21	1.18	1.23
2	A	501	MYA	C2-S1	2.19	1.91	1.81
2	B	501	MYA	C2-S1	2.19	1.91	1.81
2	A	501	MYA	C6A-N6A	2.16	1.39	1.34
3	C	502	A1AB8	O18-C19	2.15	1.41	1.37
3	B	502	A1AB8	O14-C07	-2.14	1.18	1.23
2	B	501	MYA	C6A-N6A	2.14	1.39	1.34
2	C	501	MYA	C6-C5	2.12	1.55	1.51
2	B	501	MYA	C2X-C3X	2.01	1.57	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	MYA	C3M-C2M-S1	6.18	120.76	113.40
2	B	501	MYA	C3M-C2M-S1	5.97	120.51	113.40
2	A	501	MYA	C3M-C2M-S1	5.95	120.50	113.40
3	A	502	A1AB8	C12-C13-N08	4.78	119.88	109.82
2	A	501	MYA	C6-C5-N4	4.72	124.95	116.34
2	B	501	MYA	C6-C5-N4	4.61	124.75	116.34
2	C	501	MYA	C6-C5-N4	4.52	124.57	116.34
3	C	502	A1AB8	C15-C06-N05	-4.45	107.82	111.64
3	B	502	A1AB8	C15-C06-N05	-4.29	107.96	111.64
3	A	502	A1AB8	C15-C06-N05	-4.21	108.03	111.64
2	B	501	MYA	O5A-P2A-O3A	4.07	118.28	107.27
2	A	501	MYA	O5A-P2A-O3A	4.07	118.28	107.27
2	C	501	MYA	O5A-P2A-O3A	3.96	117.99	107.27
2	B	501	MYA	C2-S1-C2M	3.78	113.03	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1AB8	C04-N03-N05	3.78	124.94	119.29
2	A	501	MYA	C2-S1-C2M	3.72	112.85	101.84
2	C	501	MYA	C10-C9-N8	3.68	123.46	116.48
2	B	501	MYA	C10-C9-N8	3.67	123.44	116.48
2	C	501	MYA	C2-S1-C2M	3.66	112.65	101.84
3	C	502	A1AB8	C04-N03-N05	3.52	124.56	119.29
3	B	502	A1AB8	C29-C30-C31	3.44	119.38	118.17
3	A	502	A1AB8	C29-C30-C31	3.42	119.37	118.17
2	A	501	MYA	C10-C9-N8	3.42	122.97	116.48
3	B	502	A1AB8	C04-N03-N05	3.37	124.32	119.29
2	C	501	MYA	O2M-C2M-C3M	-3.18	120.31	123.98
2	A	501	MYA	O2M-C2M-C3M	-3.17	120.32	123.98
2	B	501	MYA	O2M-C2M-C3M	-3.11	120.39	123.98
2	C	501	MYA	O5-C5-N4	-3.06	117.03	123.03
2	C	501	MYA	C5A-C4A-N3A	-2.99	122.60	126.72
2	A	501	MYA	O5-C5-N4	-2.97	117.20	123.03
2	C	501	MYA	O2M-C2M-S1	-2.96	118.92	122.68
2	B	501	MYA	O5-C5-N4	-2.94	117.27	123.03
2	A	501	MYA	C5A-C4A-N3A	-2.90	122.73	126.72
3	C	502	A1AB8	C29-C30-C31	2.88	119.18	118.17
3	A	502	A1AB8	C04-N03-C02	-2.88	125.47	128.09
2	B	501	MYA	O2M-C2M-S1	-2.82	119.09	122.68
2	C	501	MYA	C7-C6-C5	2.80	117.06	112.39
2	B	501	MYA	C5A-C4A-N3A	-2.77	122.91	126.72
2	B	501	MYA	O3X-P3X-O9A	-2.76	99.51	109.33
2	C	501	MYA	O3X-P3X-O9A	-2.75	99.52	109.33
2	A	501	MYA	O2M-C2M-S1	-2.75	119.18	122.68
2	A	501	MYA	O3X-P3X-O9A	-2.59	100.09	109.33
3	C	502	A1AB8	C39-N38-C31	2.58	120.57	116.81
2	A	501	MYA	O9-C9-N8	-2.52	117.64	122.98
3	C	502	A1AB8	C04-N03-C02	-2.48	125.82	128.09
2	B	501	MYA	O9-C9-N8	-2.46	117.77	122.98
3	A	502	A1AB8	C39-N38-C31	2.45	120.37	116.81
2	C	501	MYA	O9-C9-N8	-2.39	117.93	122.98
3	B	502	A1AB8	C39-N38-C31	2.36	120.24	116.81
2	A	501	MYA	C7-C6-C5	2.35	116.31	112.39
2	B	501	MYA	C7-C6-C5	2.35	116.30	112.39
2	A	501	MYA	O5-C5-C6	-2.30	117.85	122.02
2	B	501	MYA	O5-C5-C6	-2.23	117.98	122.02
3	B	502	A1AB8	C01-C02-N03	2.23	126.49	122.97
3	C	502	A1AB8	C37-N32-C33	-2.22	106.57	111.57
3	C	502	A1AB8	C01-C02-N03	2.22	126.48	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	A1AB8	O11-C12-C13	2.19	116.49	111.77
3	C	502	A1AB8	C36-N35-C34	2.18	116.55	110.40
3	A	502	A1AB8	O14-C07-N08	-2.16	119.26	122.67
3	B	502	A1AB8	C30-C31-N32	-2.11	119.80	122.35
3	B	502	A1AB8	C04-N03-C02	-2.11	126.17	128.09
2	A	501	MYA	C4M-C3M-C2M	2.08	116.87	112.27
3	B	502	A1AB8	C36-N35-C34	2.08	116.27	110.40
2	C	501	MYA	N3A-C4A-N9A	2.07	130.69	127.17
3	A	502	A1AB8	C30-C31-N32	-2.06	119.86	122.35
2	C	501	MYA	C4M-C3M-C2M	2.05	116.79	112.27
2	A	501	MYA	N3A-C4A-N9A	2.02	130.59	127.17

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MYA	C5X-O5X-P1A-O2A
2	C	501	MYA	C2M-C3M-C4M-C5M
3	A	502	A1AB8	N05-C06-C07-O14
2	B	501	MYA	C3X-C4X-C5X-O5X
5	A	506	GOL	O2-C2-C3-O3
2	B	501	MYA	C6-C7-N8-C9
5	A	506	GOL	C1-C2-C3-O3
5	B	509	GOL	O1-C1-C2-C3
5	C	511	GOL	O1-C1-C2-C3
5	C	511	GOL	O1-C1-C2-O2
2	C	501	MYA	C4M-C5M-C6M-C7M
2	C	501	MYA	C3X-C4X-C5X-O5X
2	A	501	MYA	S1-C2-C3-N4
2	B	501	MYA	O4X-C4X-C5X-O5X
2	C	501	MYA	C6-C7-N8-C9
2	A	501	MYA	O2M-C2M-S1-C2
2	B	501	MYA	O2M-C2M-S1-C2
2	A	501	MYA	S1-C2M-C3M-C4M
2	A	501	MYA	O2M-C2M-C3M-C4M
2	B	501	MYA	S1-C2M-C3M-C4M
2	B	501	MYA	O2M-C2M-C3M-C4M
2	C	501	MYA	S1-C2M-C3M-C4M
2	C	501	MYA	O2M-C2M-C3M-C4M
2	A	501	MYA	C3M-C2M-S1-C2
2	B	501	MYA	C3M-C2M-S1-C2
6	A	507	1PE	C12-C22-OH3-C23

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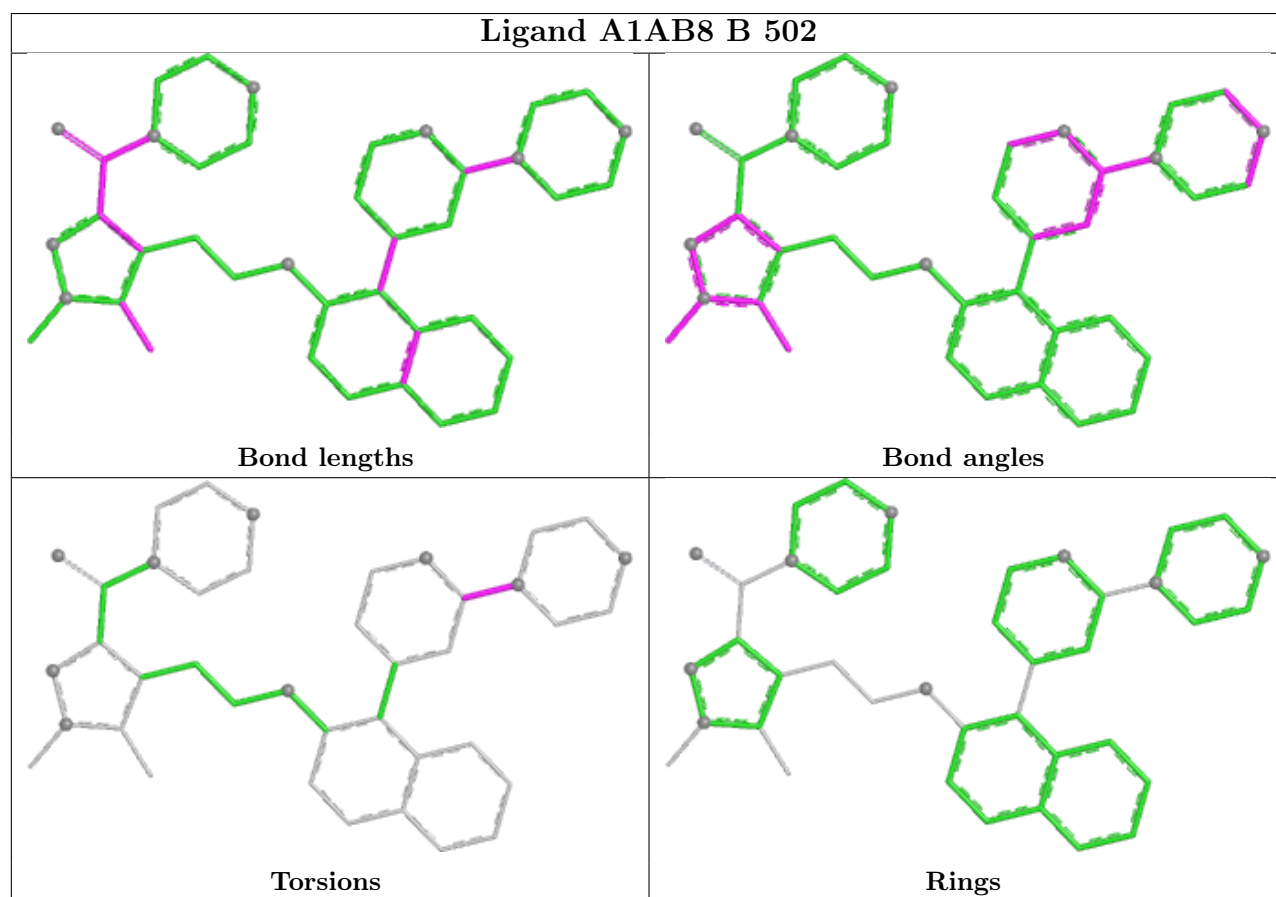
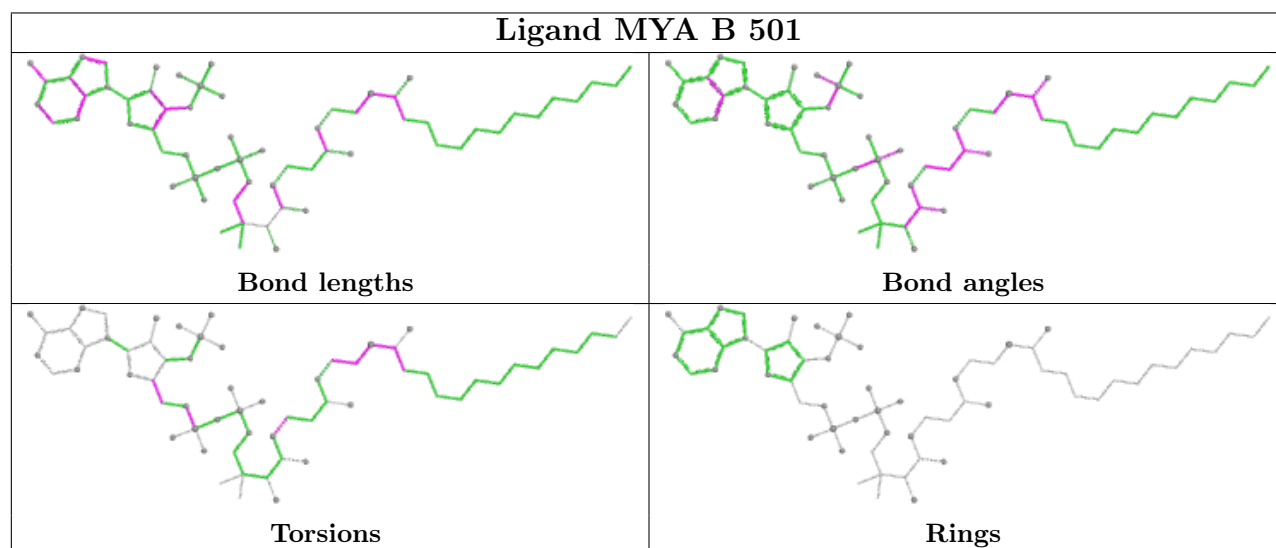
Mol	Chain	Res	Type	Atoms
5	A	506	GOL	O1-C1-C2-C3
3	A	502	A1AB8	C15-C06-C07-O14
6	A	507	1PE	OH2-C12-C22-OH3
2	A	501	MYA	C3X-C4X-C5X-O5X
2	B	501	MYA	S1-C2-C3-N4
2	A	501	MYA	C3-C2-S1-C2M
2	B	501	MYA	C3-C2-S1-C2M
2	C	501	MYA	C3-C2-S1-C2M
2	A	501	MYA	C5X-O5X-P1A-O1A
2	A	501	MYA	C5X-O5X-P1A-O3A
2	B	501	MYA	C5X-O5X-P1A-O1A
2	B	501	MYA	C5X-O5X-P1A-O2A
2	B	501	MYA	C5X-O5X-P1A-O3A
2	C	501	MYA	C5X-O5X-P1A-O1A
2	C	501	MYA	C5X-O5X-P1A-O2A
2	C	501	MYA	C5X-O5X-P1A-O3A
6	A	507	1PE	OH4-C13-C23-OH3
6	A	507	1PE	C16-C26-OH6-C15
7	B	508	P6G	C5-C6-O7-C8
5	B	509	GOL	O1-C1-C2-O2
2	C	501	MYA	O2M-C2M-S1-C2
3	A	502	A1AB8	C06-C15-C16-C17
2	C	501	MYA	C3M-C2M-S1-C2
2	A	501	MYA	C6-C7-N8-C9
3	B	502	A1AB8	N38-C31-N32-C37
6	A	507	1PE	OH7-C16-C26-OH6
5	C	511	GOL	C1-C2-C3-O3
5	A	506	GOL	O1-C1-C2-O2
5	C	511	GOL	O2-C2-C3-O3
2	A	501	MYA	C4M-C5M-C6M-C7M
2	A	501	MYA	C5M-C6M-C7M-C8M
6	A	507	1PE	C14-C24-OH4-C13
2	C	501	MYA	S1-C2-C3-N4

There are no ring outliers.

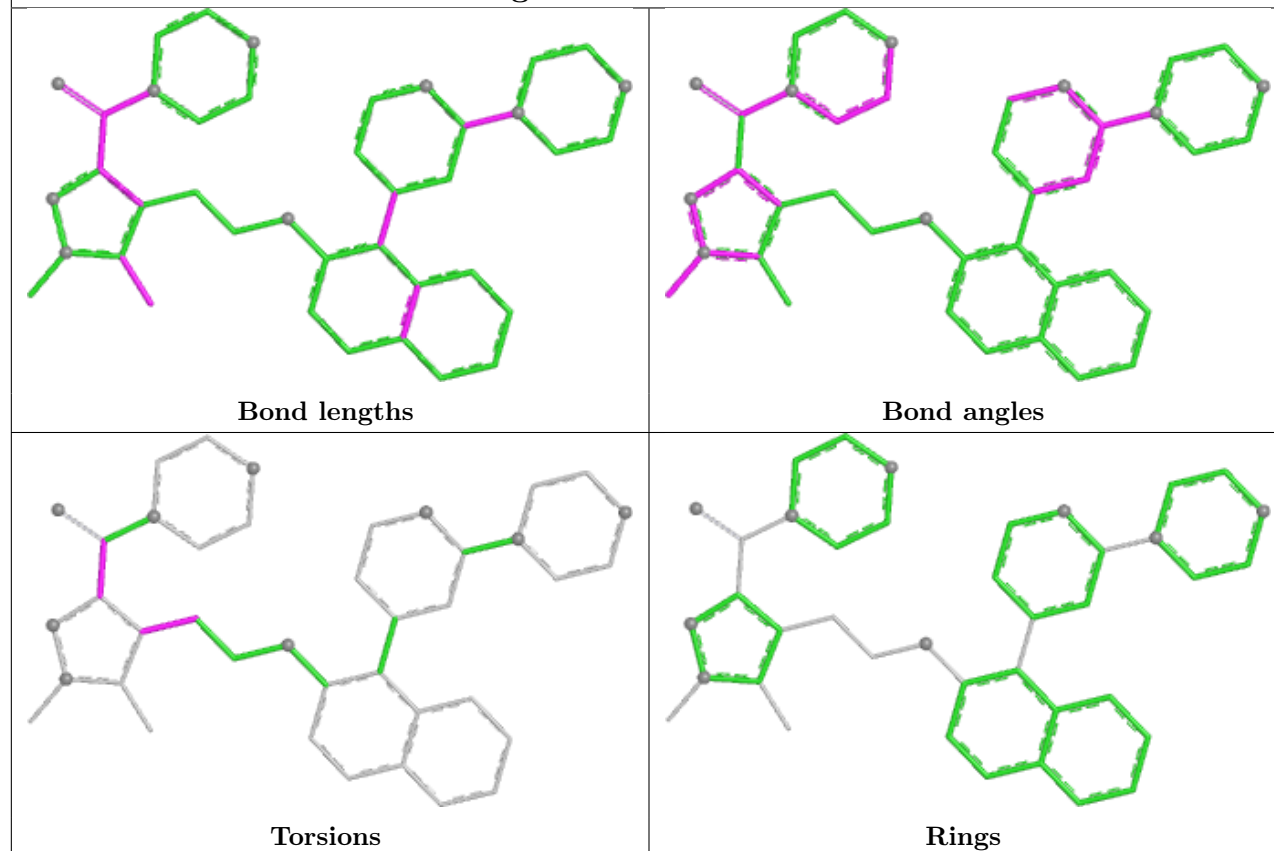
No monomer is involved in short contacts.

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 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

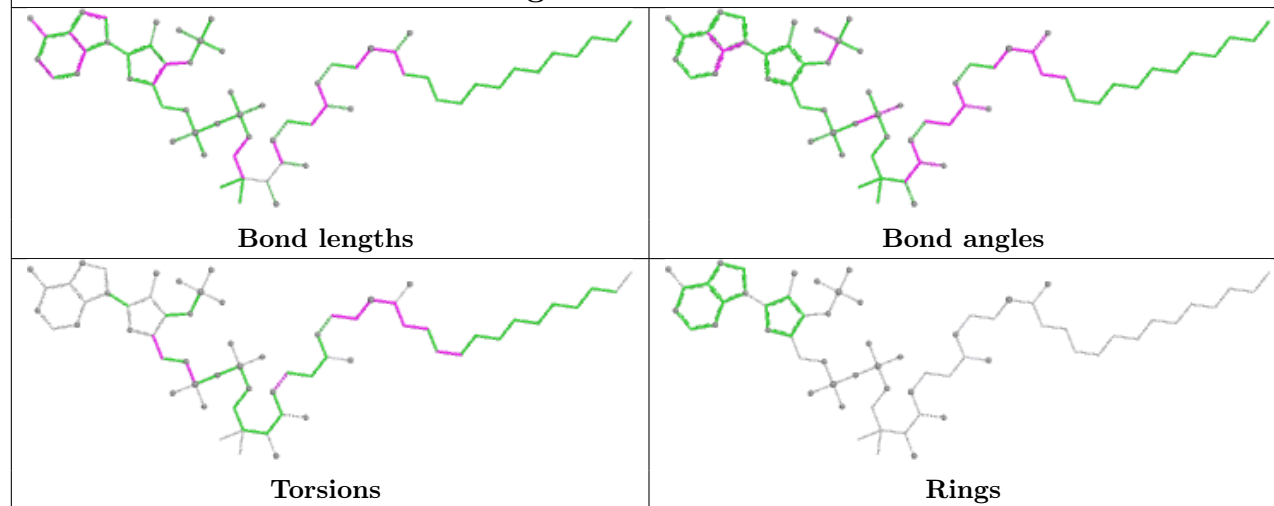
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

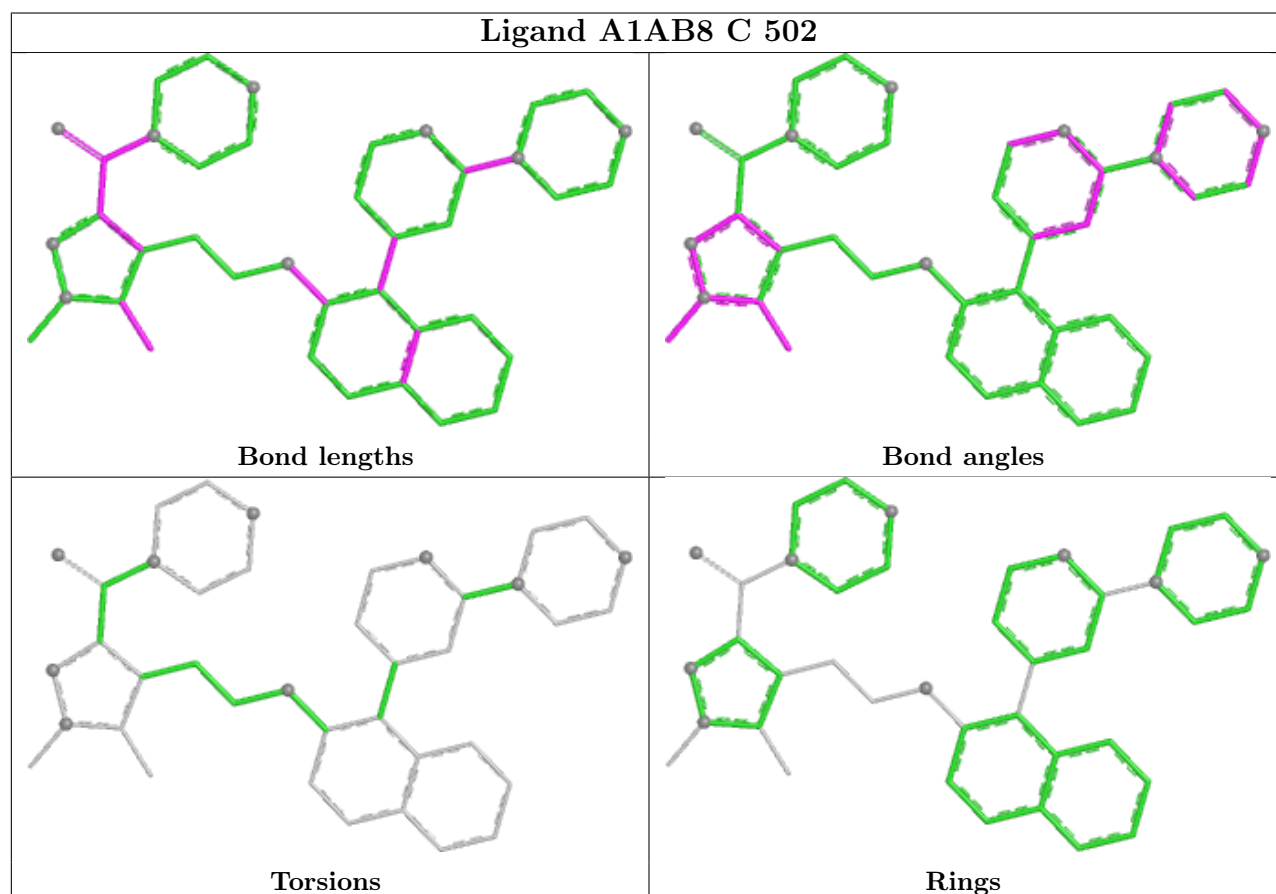
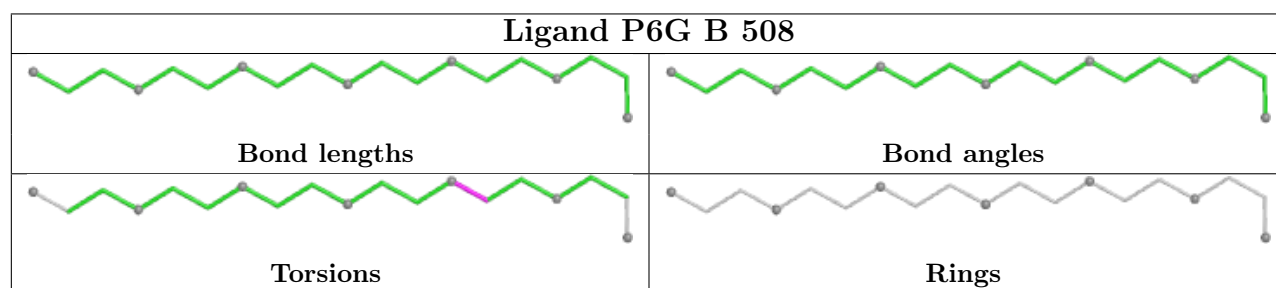
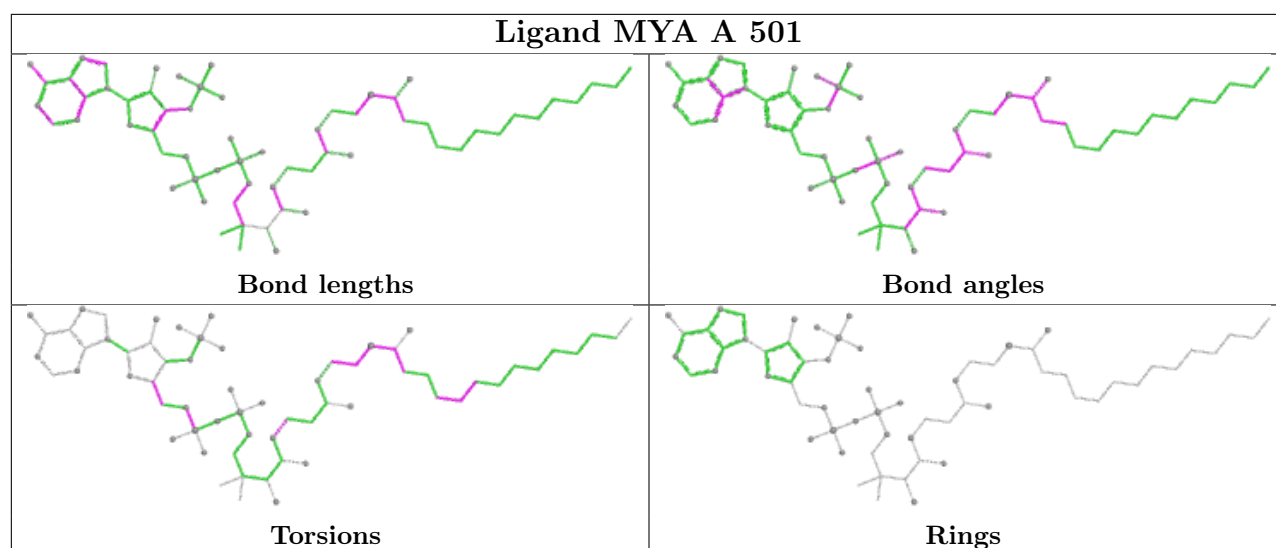


Ligand A1AB8 A 502



Ligand MYA C 501





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	384/386 (99%)	-0.35	1 (0%) 90 91	14, 30, 46, 78	11 (2%)
1	B	384/386 (99%)	-0.35	2 (0%) 87 89	13, 30, 52, 89	10 (2%)
1	C	385/386 (99%)	-0.17	6 (1%) 70 72	15, 34, 64, 102	4 (1%)
All	All	1153/1158 (99%)	-0.29	9 (0%) 82 83	13, 32, 55, 102	25 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	230	ASN	4.9
1	A	27	ASP	4.3
1	C	27	ASP	3.7
1	C	229	LEU	3.6
1	C	325	ASP	2.8
1	B	27	ASP	2.4
1	B	323	GLY	2.3
1	C	244	VAL	2.1
1	C	228	SER	2.1

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 ⓘ

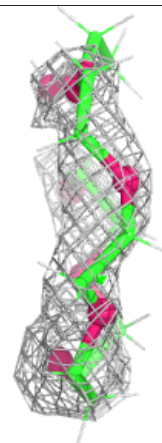
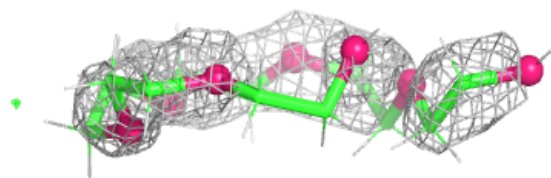
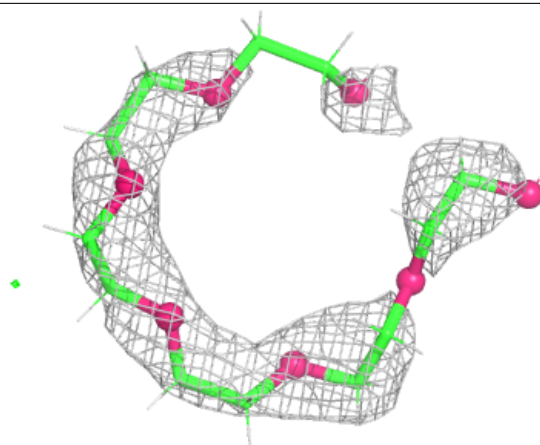
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	1PE	A	507	16/16	0.77	0.14	45,58,67,70	0
5	GOL	C	511	6/6	0.84	0.12	31,37,44,44	0
5	GOL	A	506	6/6	0.84	0.12	27,39,46,51	0
7	P6G	B	508	19/19	0.84	0.13	31,40,48,48	45
4	CL	A	505	1/1	0.87	0.14	56,56,56,56	0
3	A1AB8	B	502	40/40	0.89	0.09	25,34,42,45	0
3	A1AB8	C	502	40/40	0.89	0.09	29,41,50,50	0
5	GOL	B	509	6/6	0.89	0.09	30,36,43,52	0
4	CL	C	509	1/1	0.93	0.09	50,50,50,50	0
4	CL	B	505	1/1	0.94	0.14	47,47,47,47	0
3	A1AB8	A	502	40/40	0.94	0.07	25,31,44,48	0
4	CL	C	510	1/1	0.94	0.10	53,53,53,53	0
2	MYA	C	501	63/63	0.94	0.08	21,32,46,50	0
4	CL	B	504	1/1	0.95	0.11	38,38,38,38	0
2	MYA	B	501	63/63	0.95	0.08	19,26,32,36	0
2	MYA	A	501	63/63	0.95	0.07	18,26,35,40	0
4	CL	C	506	1/1	0.96	0.10	43,43,43,43	0
4	CL	A	504	1/1	0.97	0.04	24,24,24,24	0
4	CL	C	508	1/1	0.97	0.16	38,38,38,38	0
4	CL	A	509	1/1	0.97	0.06	35,35,35,35	0
4	CL	C	507	1/1	0.98	0.08	39,39,39,39	0
4	CL	C	505	1/1	0.98	0.04	39,39,39,39	0
4	CL	C	503	1/1	0.98	0.06	38,38,38,38	0
4	CL	C	504	1/1	0.99	0.02	26,26,26,26	0
4	CL	A	508	1/1	0.99	0.05	33,33,33,33	0
4	CL	A	503	1/1	0.99	0.02	21,21,21,21	0
4	CL	B	506	1/1	0.99	0.04	50,50,50,50	0
4	CL	B	507	1/1	0.99	0.05	28,28,28,28	0
4	CL	B	503	1/1	0.99	0.04	21,21,21,21	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.

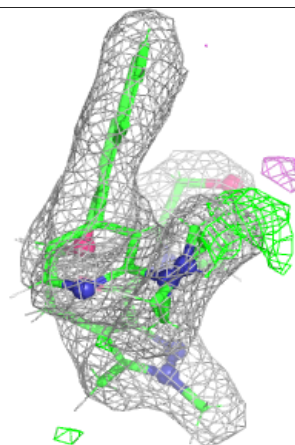
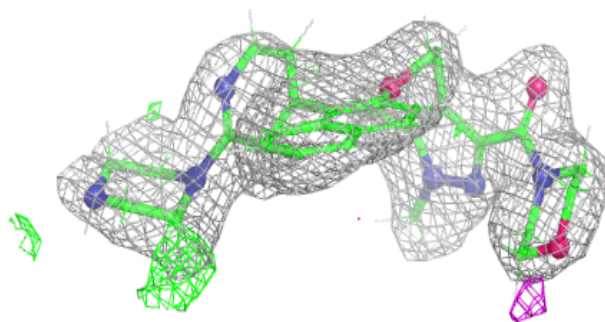
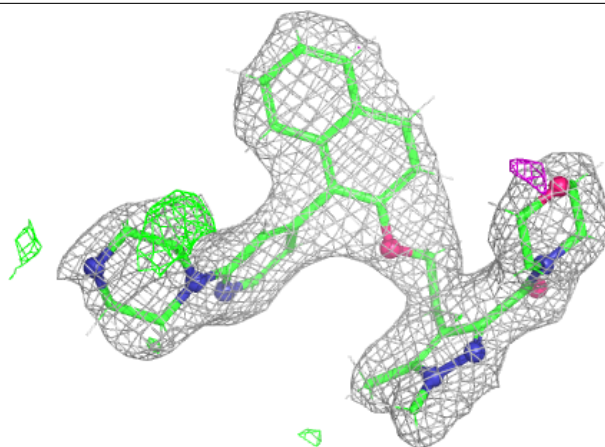
Electron density around P6G B 508:

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



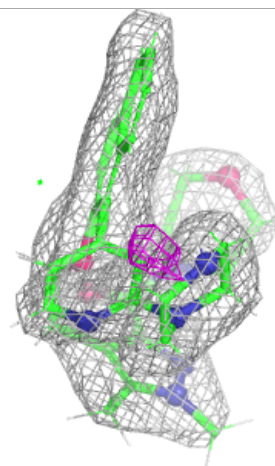
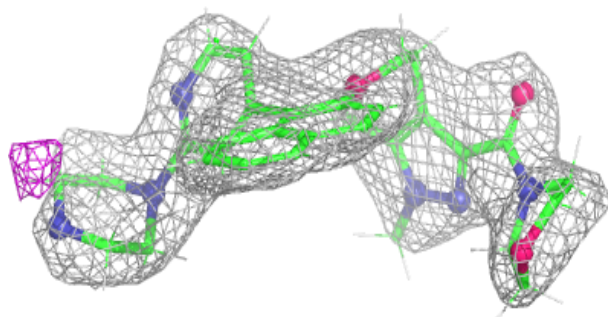
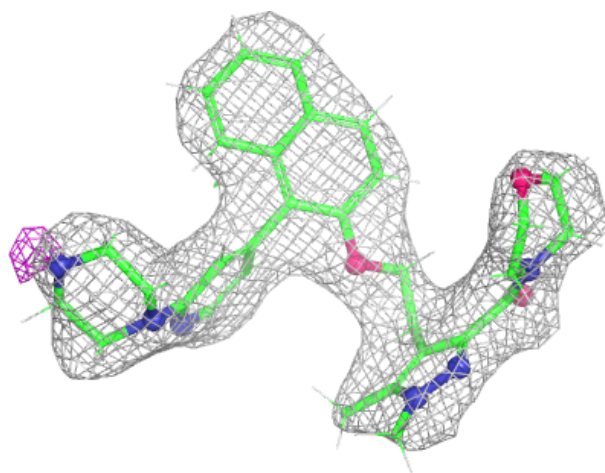
Electron density around A1AB8 B 502:

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



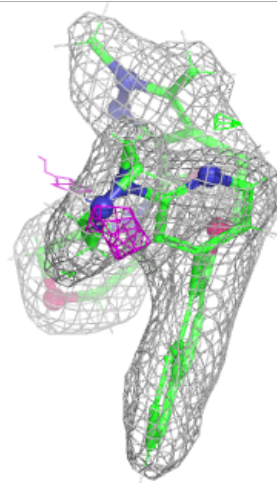
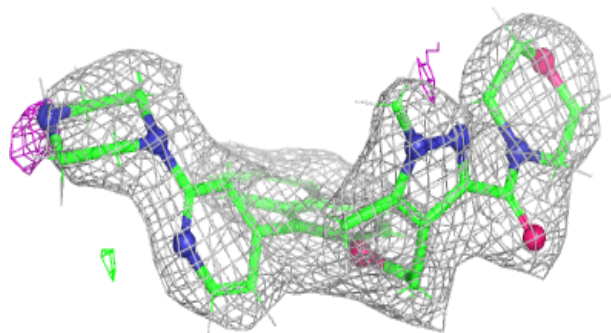
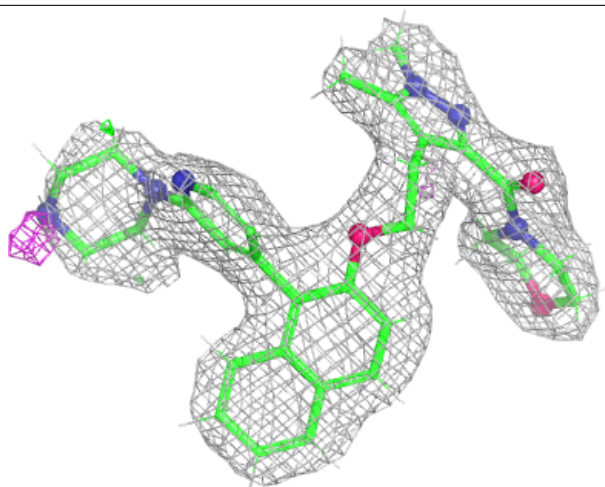
Electron density around A1AB8 C 502:

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



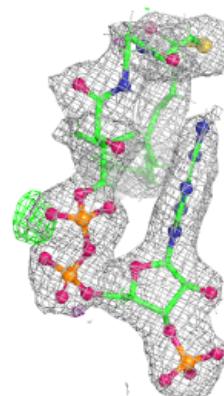
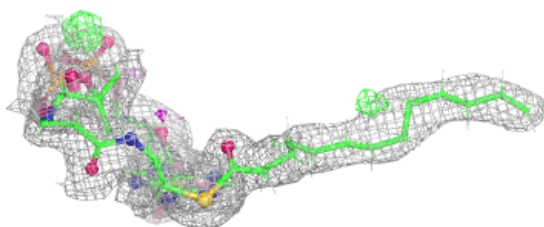
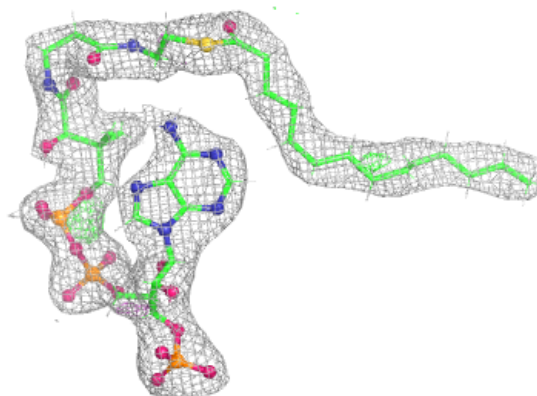
Electron density around A1AB8 A 502:

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

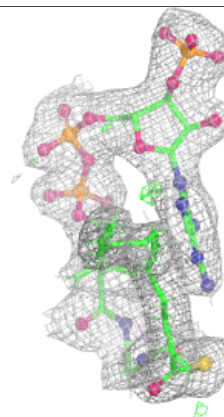
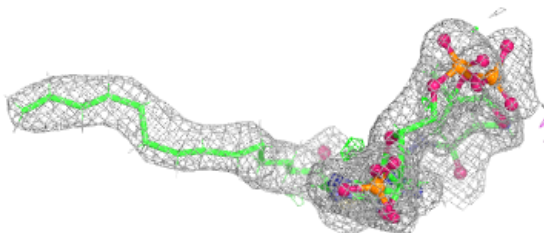
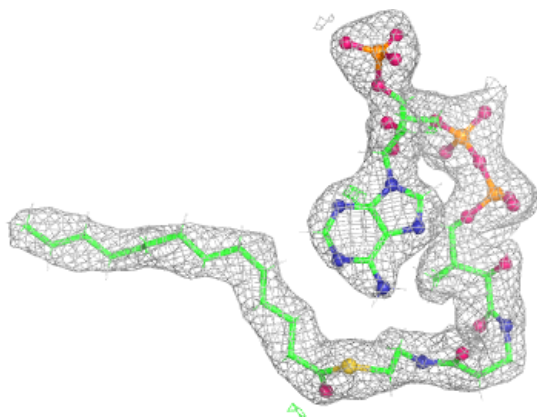


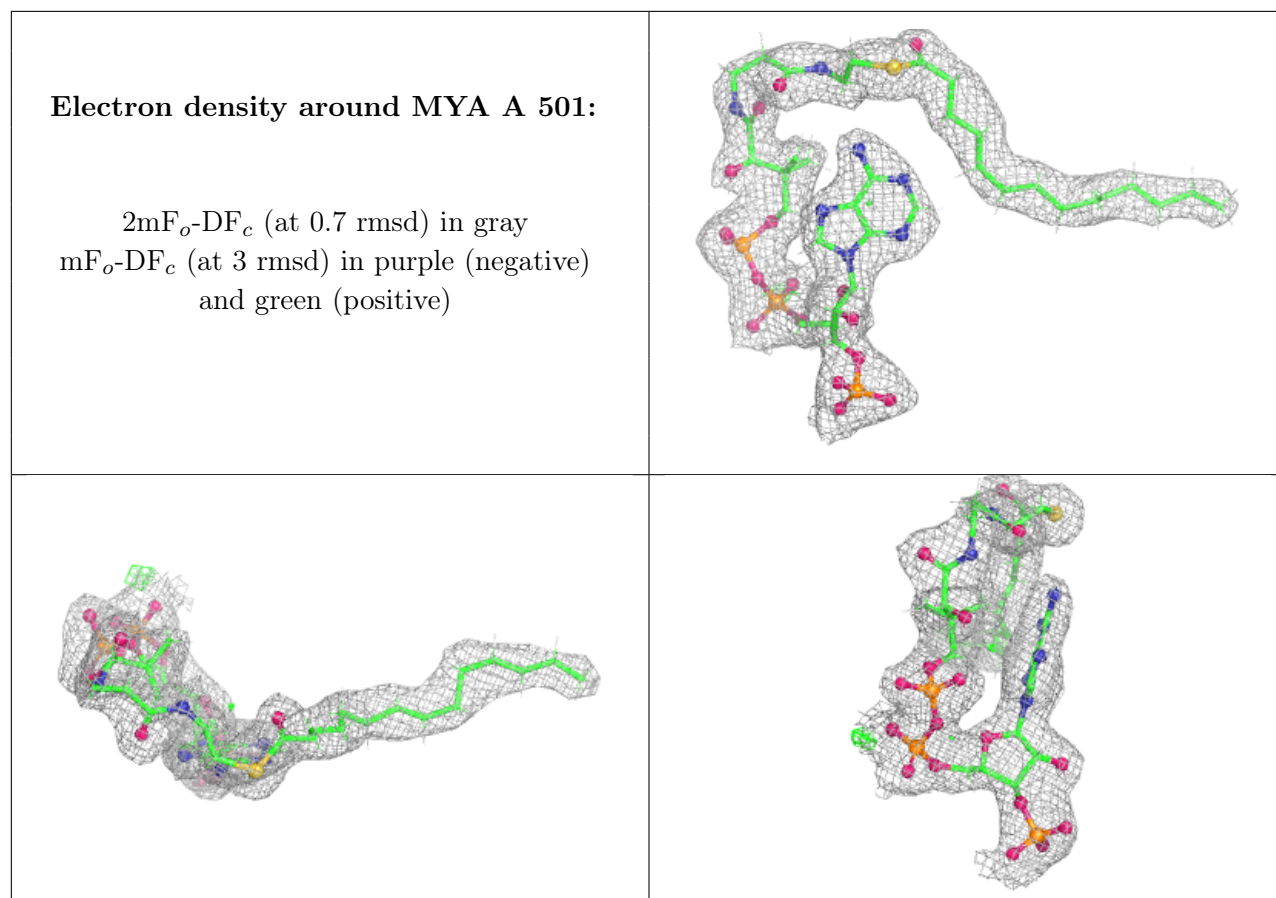
Electron density around MYA C 501:

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

**Electron density around MYA 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 ⓘ

There are no such residues in this entry.