Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2024 – 04:05 PM EDT

PDB ID	:	8VKA
Title	:	Crystal structure of Plasmodium vivax glycylpeptide N-tetradecanoyltransferase (N-myristoyltransferase, NMT) bound to myristoyl-CoA and inhibitor 9c
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	:	1.97 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:

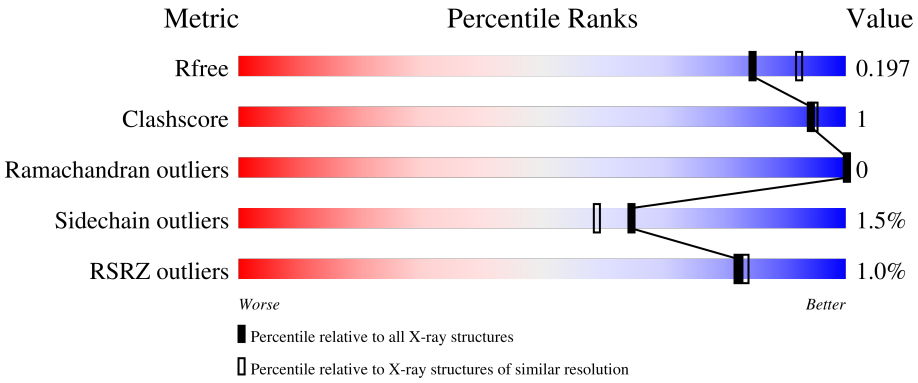
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	95%
1	B	386	97%
1	C	386	96%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 22204 atoms, of which 10606 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.

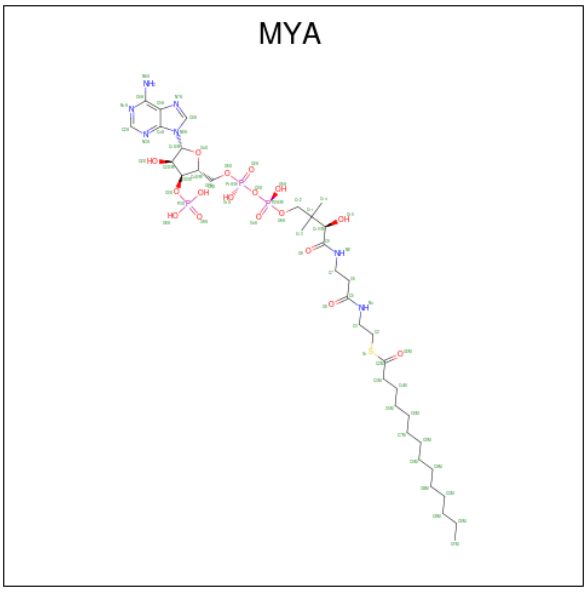
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	H	N	O	S	0	40	0
			6954	2240	3488	581	632	13			
1	B	385	Total	C	H	N	O	S	0	23	0
			6637	2155	3324	545	601	12			
1	C	385	Total	C	H	N	O	S	0	24	0
			6698	2174	3348	550	614	12			

There are 6 discrepancies between the modelled and reference sequences:

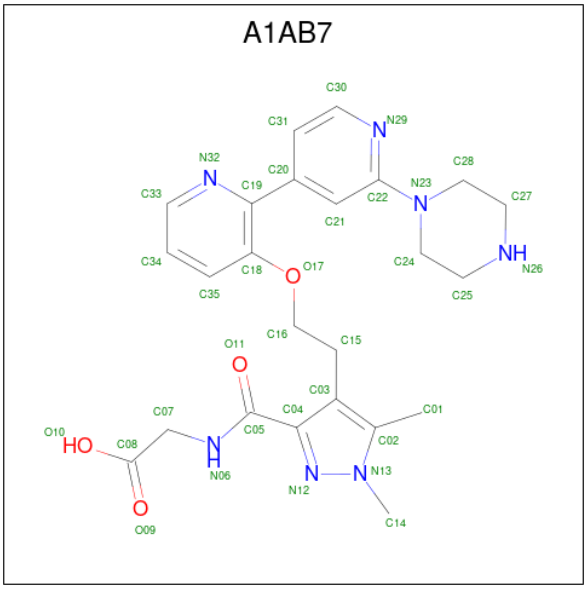
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP A5K1A2
A	26	PRO	-	expression tag	UNP A5K1A2
B	25	GLY	-	expression tag	UNP A5K1A2
B	26	PRO	-	expression tag	UNP A5K1A2
C	25	GLY	-	expression tag	UNP A5K1A2
C	26	PRO	-	expression tag	UNP A5K1A2

- Molecule 2 is TETRADECANOYL-COA (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
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 N-[1,5-dimethyl-4-(2-{[(2M)-2'-(piperazin-1-yl)[2,4'-bipyridin]-3-yl]oxy}ethyl)-1H-pyrazole-3-carbonyl]glycine (three-letter code: A1AB7) (formula: $C_{24}H_{29}N_7O_4$) (labeled as "Ligand of Interest" by depositor).

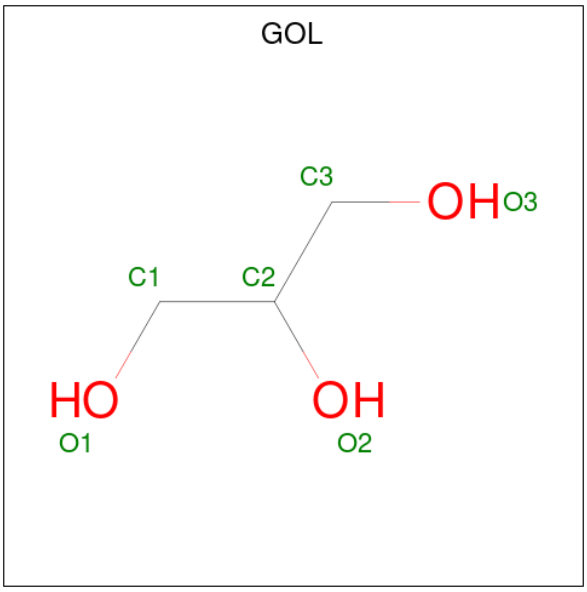


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	1
			128	48	58	14	8		
3	B	1	Total	C	H	N	O	0	1
			128	48	58	14	8		
3	C	1	Total	C	H	N	O	0	1
			128	48	58	14	8		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

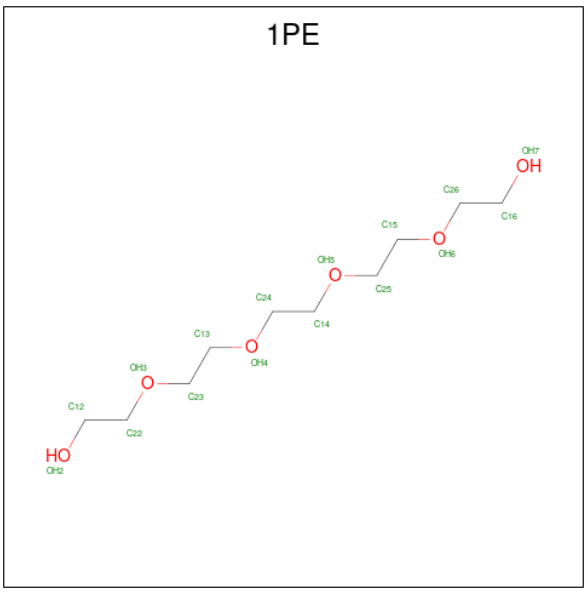
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	Cl	0	1
			13	13		
4	B	4	Total	Cl	0	1
			4	4		
4	C	7	Total	Cl	0	0
			7	7		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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 (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

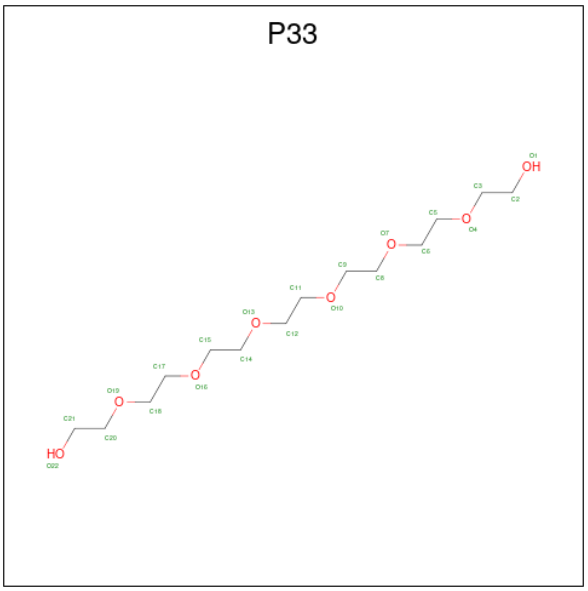


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 38 10 22 6	0	0
6	C	1	Total C H O 38 10 22 6	0	1

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Mg 1 1	0	0

- Molecule 8 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	H	O	0	0
			52	14	30	8		

- Molecule 9 is water.

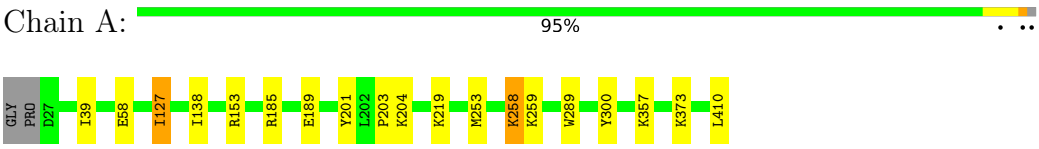
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	353	Total	O	0	28
			360	360		
9	B	309	Total	O	0	18
			316	316		
9	C	289	Total	O	0	16
			297	297		

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.

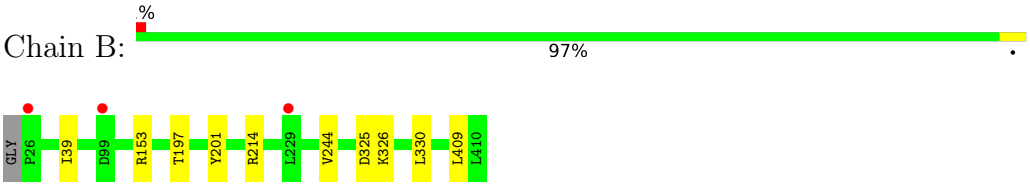
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain A:



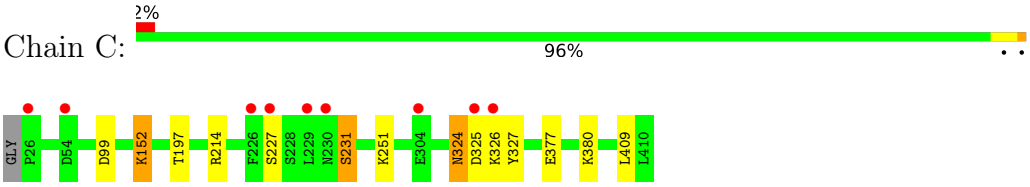
• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain B:



• Molecule 1: Glycylpeptide N-tetradecanoyltransferase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.34Å 119.28Å 173.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.87 – 1.97 44.87 – 1.97	Depositor EDS
% Data completeness (in resolution range)	94.3 (44.87-1.97) 94.3 (44.87-1.97)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.157 , 0.198 0.157 , 0.197	Depositor DCC
R_{free} test set	4044 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 59.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22204	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, A1AB7, P33, CL, MYA, MG, 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	0.50	0/3571	0.57	0/4822
1	B	0.50	0/3407	0.57	0/4611
1	C	0.51	0/3445	0.56	0/4661
All	All	0.50	0/10423	0.57	0/14094

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

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	3466	3488	3433	11	1
1	B	3313	3324	3301	5	0
1	C	3350	3348	3331	6	0
2	A	63	58	58	0	0
2	B	63	58	58	0	0
2	C	63	58	57	0	0
3	A	70	58	0	0	0
3	B	70	58	0	1	0
3	C	70	58	0	0	0
4	A	13	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	4	0	0	1	0
4	C	7	0	0	2	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	1	0
6	C	16	22	22	0	0
7	B	1	0	0	0	0
8	C	22	30	30	0	0
9	A	360	0	0	4	0
9	B	316	0	0	1	0
9	C	297	0	0	3	0
All	All	11598	10606	10336	28	1

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 (28) 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)
9:A:891:HOH:O	4:B:504:CL:CL	2.48	0.67
4:C:509:CL:CL	9:C:734:HOH:O	2.49	0.66
4:A:513:CL:CL	9:B:844:HOH:O	2.51	0.66
1:B:325:ASP:OD1	1:B:326:LYS:N	2.35	0.59
4:A:508[A]:CL:CL	9:A:887:HOH:O	2.51	0.57
1:C:380:LYS:NZ	9:C:609:HOH:O	2.38	0.57
1:A:39:ILE:HD11	1:A:201:TYR:HE1	1.70	0.56
1:A:127[B]:ILE:HD11	1:A:185[B]:ARG:HD2	1.91	0.52
1:B:197:THR:HG23	1:B:409:LEU:HD22	1.92	0.51
1:B:39[B]:ILE:HD12	1:B:201:TYR:HE2	1.75	0.51
1:C:324:ASN:HB3	1:C:327:TYR:O	2.12	0.50
1:A:39:ILE:HD11	1:A:201:TYR:CE1	2.47	0.49
1:A:253[B]:MET:HG3	1:A:300:TYR:HB3	1.95	0.47
1:B:39[B]:ILE:HD12	1:B:201:TYR:CE2	2.49	0.47
1:C:325[B]:ASP:O	1:C:326[B]:LYS:HB3	2.14	0.47
1:A:259:LYS:NZ	9:A:611:HOH:O	2.48	0.46
6:A:517:1PE:H122	6:A:517:1PE:H131	1.99	0.45
1:A:58[B]:GLU:OE1	1:A:58[B]:GLU:N	2.45	0.43
1:C:152:LYS:HA	1:C:152:LYS:HD2	1.86	0.42
1:A:373[A]:LYS:NZ	9:A:614:HOH:O	2.53	0.42
4:C:507:CL:CL	9:C:860:HOH:O	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:TRP:CZ3	1:A:410:LEU:HD11	2.56	0.41
1:A:203:PRO:HA	1:A:204[B]:LYS:HA	1.89	0.41
1:C:197:THR:HG23	1:C:409:LEU:HD22	2.02	0.41
1:C:231:SER:O	1:C:231:SER:OG	2.32	0.41
1:B:330:LEU:HD23	3:B:502[B]:A1AB7:C07	2.51	0.41
1:A:138:ILE:C	1:A:138:ILE:HD12	2.41	0.41
1:A:203:PRO:HA	1:A:204[A]:LYS:HA	1.90	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:OE2	1:A:258[A]:LYS:NZ[4_555]	2.16	0.04

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	422/386 (109%)	413 (98%)	9 (2%)	0	100	100
1	B	404/386 (105%)	391 (97%)	13 (3%)	0	100	100
1	C	407/386 (105%)	389 (96%)	18 (4%)	0	100	100
All	All	1233/1158 (106%)	1193 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	385/351 (110%)	375 (97%)	10 (3%)	46	37
1	B	366/351 (104%)	362 (99%)	4 (1%)	73	70
1	C	371/351 (106%)	362 (98%)	9 (2%)	49	41
All	All	1122/1053 (107%)	1099 (98%)	23 (2%)	65	48

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

Mol	Chain	Res	Type
1	A	127[A]	ILE
1	A	127[B]	ILE
1	A	153	ARG
1	A	219[A]	LYS
1	A	219[B]	LYS
1	A	219[C]	LYS
1	A	258[A]	LYS
1	A	258[B]	LYS
1	A	357[A]	LYS
1	A	357[B]	LYS
1	B	153	ARG
1	B	214	ARG
1	B	244[A]	VAL
1	B	244[B]	VAL
1	C	99	ASP
1	C	152	LYS
1	C	214	ARG
1	C	227[A]	SER
1	C	227[B]	SER
1	C	231	SER
1	C	251	LYS
1	C	324	ASN
1	C	377	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	GLN
1	B	106	ASN
1	B	320	GLN

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Mol	Chain	Res	Type
1	C	106	ASN
1	C	320	GLN

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 40 ligands modelled in this entry, 25 are monoatomic - leaving 15 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	-	57,65,65	1.54	10 (17%)	68,91,91	1.50	10 (14%)
5	GOL	A	516	-	5,5,5	0.28	0	5,5,5	0.14	0
5	GOL	B	508	-	5,5,5	0.39	0	5,5,5	0.26	0
6	1PE	C	511[B]	-	15,15,15	0.14	0	14,14,14	0.11	0
3	A1AB7	A	502[A]	-	37,38,38	1.69	4 (10%)	44,52,52	1.73	9 (20%)
6	1PE	A	517	-	15,15,15	0.18	0	14,14,14	0.23	0
3	A1AB7	B	502[B]	-	37,38,38	1.81	5 (13%)	44,52,52	1.48	6 (13%)
2	MYA	C	501	-	57,65,65	1.61	12 (21%)	68,91,91	1.60	9 (13%)
3	A1AB7	C	502[B]	-	37,38,38	1.72	5 (13%)	44,52,52	1.58	9 (20%)
8	P33	C	512	-	21,21,21	0.29	0	20,20,20	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	A1AB7	C	502[A]	-	37,38,38	1.74	5 (13%)	44,52,52	1.54	8 (18%)
5	GOL	C	510	-	5,5,5	0.29	0	5,5,5	0.16	0
3	A1AB7	B	502[A]	-	37,38,38	1.78	5 (13%)	44,52,52	1.66	8 (18%)
2	MYA	A	501	-	57,65,65	1.51	10 (17%)	68,91,91	1.61	10 (14%)
3	A1AB7	A	502[B]	-	37,38,38	1.70	6 (16%)	44,52,52	1.72	9 (20%)

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	-	-	5/60/80/80	0/3/3/3
5	GOL	A	516	-	-	0/4/4/4	-
5	GOL	B	508	-	-	2/4/4/4	-
6	1PE	C	511[B]	-	-	6/13/13/13	-
3	A1AB7	A	502[A]	-	-	1/19/31/31	0/4/4/4
6	1PE	A	517	-	-	10/13/13/13	-
3	A1AB7	B	502[B]	-	-	1/19/31/31	0/4/4/4
2	MYA	C	501	-	-	4/60/80/80	0/3/3/3
3	A1AB7	C	502[B]	-	-	4/19/31/31	0/4/4/4
8	P33	C	512	-	-	11/19/19/19	-
3	A1AB7	C	502[A]	-	-	4/19/31/31	0/4/4/4
5	GOL	C	510	-	-	0/4/4/4	-
3	A1AB7	B	502[A]	-	-	1/19/31/31	0/4/4/4
2	MYA	A	501	-	-	1/60/80/80	0/3/3/3
3	A1AB7	A	502[B]	-	-	1/19/31/31	0/4/4/4

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MYA	C2M-S1	5.76	1.90	1.76
3	B	502[B]	A1AB7	C05-N06	5.65	1.46	1.33
3	C	502[A]	A1AB7	C05-N06	5.45	1.45	1.33
3	C	502[B]	A1AB7	C05-N06	5.36	1.45	1.33
3	B	502[A]	A1AB7	C05-N06	5.34	1.45	1.33
3	A	502[B]	A1AB7	C05-N06	5.24	1.45	1.33
3	A	502[A]	A1AB7	C05-N06	5.22	1.45	1.33
2	C	501	MYA	C2M-S1	4.81	1.87	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502[A]	A1AB7	C02-N13	-4.57	1.30	1.37
3	B	502[B]	A1AB7	C22-N23	4.51	1.46	1.37
3	B	502[A]	A1AB7	C22-N23	4.42	1.46	1.37
3	A	502[B]	A1AB7	C22-N23	4.33	1.46	1.37
3	B	502[B]	A1AB7	C02-N13	-4.32	1.31	1.37
3	A	502[A]	A1AB7	C22-N23	4.25	1.46	1.37
3	C	502[A]	A1AB7	C22-N23	4.23	1.46	1.37
3	C	502[B]	A1AB7	C22-N23	4.16	1.46	1.37
3	A	502[A]	A1AB7	C02-N13	-4.12	1.31	1.37
2	C	501	MYA	P3X-O3X	4.03	1.66	1.59
2	A	501	MYA	C4A-N3A	4.00	1.41	1.35
3	C	502[B]	A1AB7	C02-N13	-3.86	1.31	1.37
3	C	502[A]	A1AB7	C02-N13	-3.82	1.31	1.37
2	A	501	MYA	C2M-S1	3.64	1.84	1.76
3	A	502[B]	A1AB7	C02-N13	-3.51	1.32	1.37
2	B	501	MYA	C2A-N1A	3.39	1.40	1.33
3	B	502[B]	A1AB7	C20-C19	3.34	1.52	1.49
2	C	501	MYA	C9-N8	3.27	1.40	1.33
3	C	502[B]	A1AB7	C20-C19	3.26	1.52	1.49
3	B	502[A]	A1AB7	C20-C19	3.24	1.52	1.49
2	A	501	MYA	C3M-C2M	3.22	1.54	1.50
2	C	501	MYA	C3X-C4X	3.22	1.61	1.52
3	C	502[A]	A1AB7	C20-C19	3.20	1.52	1.49
2	B	501	MYA	C3M-C2M	3.06	1.54	1.50
3	A	502[A]	A1AB7	C20-C19	3.04	1.52	1.49
2	B	501	MYA	C2X-C3X	3.02	1.59	1.52
2	B	501	MYA	C3X-C4X	2.99	1.60	1.52
2	C	501	MYA	C4A-N3A	2.94	1.39	1.35
2	A	501	MYA	C2X-C3X	2.92	1.59	1.52
3	A	502[B]	A1AB7	C20-C19	2.91	1.52	1.49
2	A	501	MYA	C3X-C4X	2.85	1.60	1.52
2	A	501	MYA	C2A-N1A	2.84	1.39	1.33
2	A	501	MYA	O3X-C3X	-2.79	1.33	1.44
2	C	501	MYA	O3X-C3X	-2.78	1.34	1.44
2	C	501	MYA	C2A-N1A	2.74	1.39	1.33
2	B	501	MYA	C4A-N3A	2.74	1.39	1.35
2	B	501	MYA	C5-N4	2.73	1.39	1.33
2	C	501	MYA	O2X-C2X	-2.71	1.36	1.43
3	C	502[A]	A1AB7	C04-N12	-2.61	1.33	1.35
2	B	501	MYA	O6A-C12	-2.59	1.35	1.43
3	B	502[A]	A1AB7	C04-N12	-2.45	1.33	1.35
2	A	501	MYA	C6-C5	2.40	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MYA	O3X-C3X	-2.33	1.35	1.44
2	C	501	MYA	O6A-C12	-2.28	1.36	1.43
3	A	502[B]	A1AB7	O11-C05	-2.25	1.18	1.23
3	C	502[B]	A1AB7	O11-C05	-2.23	1.18	1.23
3	B	502[B]	A1AB7	C04-N12	-2.22	1.33	1.35
2	A	501	MYA	C9-N8	2.21	1.38	1.33
2	A	501	MYA	O2X-C2X	-2.19	1.37	1.43
2	C	501	MYA	C6-C5	2.13	1.55	1.51
2	C	501	MYA	C5-N4	2.13	1.38	1.33
2	C	501	MYA	C2-S1	2.11	1.90	1.81
2	B	501	MYA	C2A-N3A	2.01	1.35	1.32
3	A	502[B]	A1AB7	C04-C05	2.00	1.53	1.50

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	MYA	C3M-C2M-S1	6.30	120.79	113.46
3	A	502[A]	A1AB7	C04-C05-N06	6.20	121.72	115.67
2	C	501	MYA	C3M-C2M-S1	6.11	120.57	113.46
2	A	501	MYA	C3M-C2M-S1	6.08	120.53	113.46
3	A	502[B]	A1AB7	C04-C05-N06	5.31	120.85	115.67
3	B	502[B]	A1AB7	C20-C21-C22	4.76	119.93	118.25
3	B	502[A]	A1AB7	C04-C05-N06	4.71	120.26	115.67
3	A	502[B]	A1AB7	C20-C21-C22	4.70	119.91	118.25
2	C	501	MYA	O2M-C2M-C3M	-4.66	118.49	123.99
3	B	502[A]	A1AB7	C20-C21-C22	4.64	119.89	118.25
2	A	501	MYA	O5-C5-N4	-4.52	114.49	123.01
2	A	501	MYA	C6-C5-N4	4.50	124.00	116.42
3	C	502[A]	A1AB7	C20-C21-C22	4.46	119.83	118.25
2	C	501	MYA	C6-C5-N4	4.19	123.48	116.42
2	C	501	MYA	O5-C5-N4	-4.06	115.35	123.01
3	A	502[A]	A1AB7	C20-C21-C22	4.01	119.67	118.25
2	B	501	MYA	C6-C5-N4	3.80	122.82	116.42
3	C	502[B]	A1AB7	C04-C05-N06	3.76	119.33	115.67
3	C	502[B]	A1AB7	C20-C21-C22	3.63	119.53	118.25
2	B	501	MYA	O2M-C2M-C3M	-3.59	119.75	123.99
2	A	501	MYA	O2M-C2M-C3M	-3.37	120.01	123.99
2	C	501	MYA	C2-S1-C2M	3.29	112.12	101.87
2	B	501	MYA	O5-C5-N4	-3.23	116.92	123.01
3	A	502[A]	A1AB7	C14-N13-C02	-3.16	124.69	128.82
3	C	502[A]	A1AB7	C14-N13-C02	-3.15	124.71	128.82
3	A	502[B]	A1AB7	C15-C03-C02	-3.11	125.11	127.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502[A]	A1AB7	C30-N29-C22	3.03	120.86	116.86
3	C	502[B]	A1AB7	C30-N29-C22	3.00	120.82	116.86
3	C	502[A]	A1AB7	C04-C05-N06	2.98	118.58	115.67
2	A	501	MYA	C2-S1-C2M	2.94	111.03	101.87
2	A	501	MYA	C7-C6-C5	2.92	117.22	112.36
3	C	502[B]	A1AB7	C14-N13-C02	-2.80	125.17	128.82
2	C	501	MYA	C10-C9-N8	2.80	122.15	116.58
3	B	502[A]	A1AB7	C33-N32-C19	2.78	122.25	116.81
3	B	502[B]	A1AB7	C33-N32-C19	2.75	122.19	116.81
3	A	502[A]	A1AB7	C30-N29-C22	2.74	120.48	116.86
3	A	502[B]	A1AB7	C30-N29-C22	2.71	120.44	116.86
3	C	502[A]	A1AB7	C21-C22-N23	-2.70	119.09	122.29
3	B	502[A]	A1AB7	C14-N13-C02	-2.62	125.40	128.82
2	C	501	MYA	O3X-P3X-O9A	-2.57	99.45	109.39
3	B	502[B]	A1AB7	C04-C05-N06	2.55	118.15	115.67
2	A	501	MYA	O8A-P3X-O7A	2.54	117.36	107.64
2	A	501	MYA	O2M-C2M-S1	-2.53	119.32	122.61
3	B	502[B]	A1AB7	C30-N29-C22	2.50	120.17	116.86
2	B	501	MYA	O2M-C2M-S1	-2.49	119.38	122.61
3	A	502[A]	A1AB7	C33-N32-C19	2.45	121.61	116.81
2	A	501	MYA	O3X-P3X-O9A	-2.43	99.99	109.39
3	B	502[A]	A1AB7	C30-N29-C22	2.43	120.08	116.86
3	A	502[B]	A1AB7	C14-N13-C02	-2.42	125.66	128.82
2	B	501	MYA	C2-S1-C2M	2.39	109.31	101.87
3	C	502[B]	A1AB7	C21-C22-N23	-2.39	119.46	122.29
3	A	502[B]	A1AB7	C33-N32-C19	2.36	121.43	116.81
3	B	502[A]	A1AB7	C15-C03-C02	-2.33	125.66	127.30
3	C	502[A]	A1AB7	C33-N32-C19	2.32	121.35	116.81
3	A	502[B]	A1AB7	C21-C22-N23	-2.31	119.55	122.29
3	C	502[A]	A1AB7	N29-C22-N23	2.30	120.24	116.79
2	B	501	MYA	C1X-N9A-C4A	-2.30	122.60	126.64
3	A	502[A]	A1AB7	C15-C03-C02	-2.29	125.69	127.30
3	B	502[B]	A1AB7	C14-N13-C02	-2.28	125.85	128.82
3	C	502[B]	A1AB7	C33-N32-C19	2.27	121.26	116.81
3	C	502[B]	A1AB7	O10-C08-C07	2.22	120.44	112.74
2	B	501	MYA	C7-N8-C9	2.22	126.54	122.59
3	A	502[A]	A1AB7	C24-N23-C22	2.21	125.52	120.39
3	B	502[A]	A1AB7	C21-C22-N23	-2.20	119.67	122.29
3	C	502[B]	A1AB7	C27-C28-N23	2.19	115.23	110.48
3	A	502[B]	A1AB7	O10-C08-C07	2.18	120.31	112.74
3	A	502[A]	A1AB7	C21-C22-N23	-2.16	119.72	122.29
3	B	502[B]	A1AB7	C21-C22-N23	-2.11	119.78	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502[A]	A1AB7	O10-C08-C07	2.11	120.06	112.74
3	A	502[B]	A1AB7	C28-N23-C22	2.10	125.25	120.39
2	C	501	MYA	O8A-P3X-O7A	2.09	115.64	107.64
2	A	501	MYA	C10-C9-N8	2.09	120.74	116.58
2	B	501	MYA	O3X-P3X-O9A	-2.07	101.39	109.39
2	B	501	MYA	C10-C9-N8	2.07	120.70	116.58
3	C	502[B]	A1AB7	C28-C27-N26	2.02	116.36	111.12
3	C	502[A]	A1AB7	O10-C08-C07	2.02	119.75	112.74
2	C	501	MYA	C7-C6-C5	2.02	115.72	112.36
3	A	502[A]	A1AB7	O10-C08-C07	2.01	119.73	112.74

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502[A]	A1AB7	N06-C07-C08-O09
3	C	502[A]	A1AB7	N06-C07-C08-O10
3	C	502[A]	A1AB7	C08-C07-N06-C05
8	C	512	P33	C8-C9-O10-C11
2	B	501	MYA	C5M-C6M-C7M-C8M
6	C	511[B]	1PE	OH6-C15-C25-OH5
8	C	512	P33	O16-C17-C18-O19
8	C	512	P33	O4-C5-C6-O7
6	A	517	1PE	OH6-C15-C25-OH5
6	A	517	1PE	OH2-C12-C22-OH3
6	C	511[B]	1PE	OH7-C16-C26-OH6
8	C	512	P33	O10-C11-C12-O13
3	A	502[B]	A1AB7	C03-C15-C16-O17
3	B	502[B]	A1AB7	C03-C15-C16-O17
6	A	517	1PE	OH4-C13-C23-OH3
8	C	512	P33	C21-C20-O19-C18
5	B	508	GOL	O1-C1-C2-C3
5	B	508	GOL	O1-C1-C2-O2
8	C	512	P33	O7-C8-C9-O10
8	C	512	P33	O13-C14-C15-O16
3	B	502[A]	A1AB7	C03-C15-C16-O17
3	C	502[A]	A1AB7	C03-C15-C16-O17
6	A	517	1PE	OH7-C16-C26-OH6
2	B	501	MYA	C6M-C7M-C8M-C9M
6	A	517	1PE	C24-C14-OH5-C25
6	C	511[B]	1PE	C23-C13-OH4-C24
2	B	501	MYA	C8M-C9M-CAM-CBM

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Mol	Chain	Res	Type	Atoms
8	C	512	P33	C6-C5-O4-C3
3	C	502[B]	A1AB7	N06-C07-C08-O10
6	A	517	1PE	C13-C23-OH3-C22
2	B	501	MYA	C6-C7-N8-C9
8	C	512	P33	O1-C2-C3-O4
6	A	517	1PE	C14-C24-OH4-C13
8	C	512	P33	C17-C18-O19-C20
2	B	501	MYA	C4M-C5M-C6M-C7M
6	C	511[B]	1PE	C12-C22-OH3-C23
3	C	502[B]	A1AB7	N06-C07-C08-O09
6	C	511[B]	1PE	OH4-C13-C23-OH3
2	C	501	MYA	O2M-C2M-C3M-C4M
3	C	502[B]	A1AB7	C03-C15-C16-O17
6	C	511[B]	1PE	C24-C14-OH5-C25
2	C	501	MYA	C3M-C2M-S1-C2
6	A	517	1PE	C12-C22-OH3-C23
6	A	517	1PE	C16-C26-OH6-C15
2	A	501	MYA	CAM-CBM-CCM-CDM
3	A	502[A]	A1AB7	C03-C15-C16-O17
3	C	502[B]	A1AB7	C08-C07-N06-C05
8	C	512	P33	C5-C6-O7-C8
2	C	501	MYA	C6-C7-N8-C9
6	A	517	1PE	OH5-C14-C24-OH4
2	C	501	MYA	S1-C2-C3-N4

There are no ring outliers.

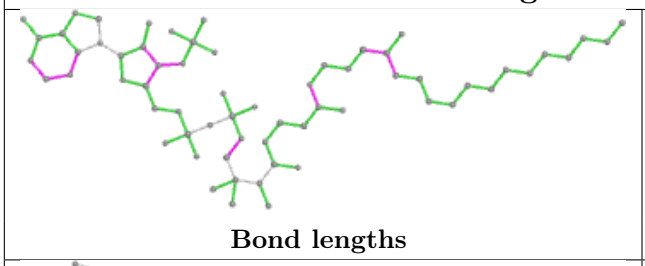
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	517	1PE	1	0
3	B	502[B]	A1AB7	1	0

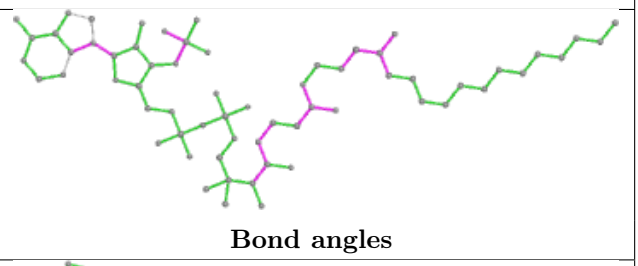
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

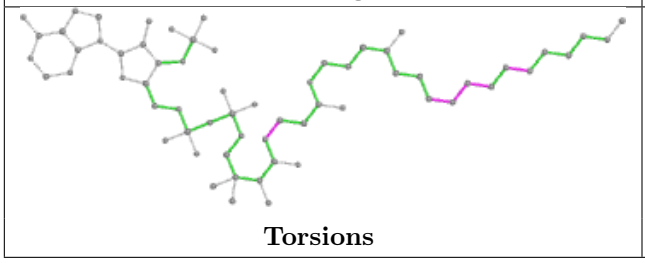
Ligand MYA B 501



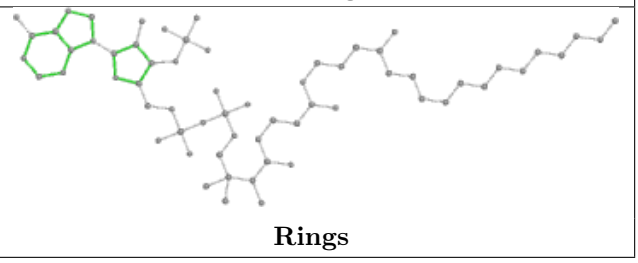
Bond lengths



Bond angles

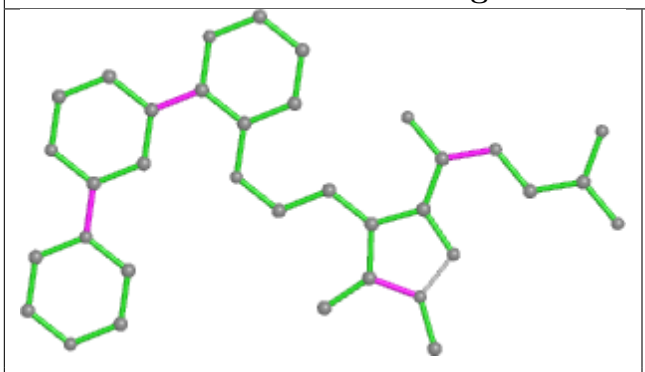


Torsions

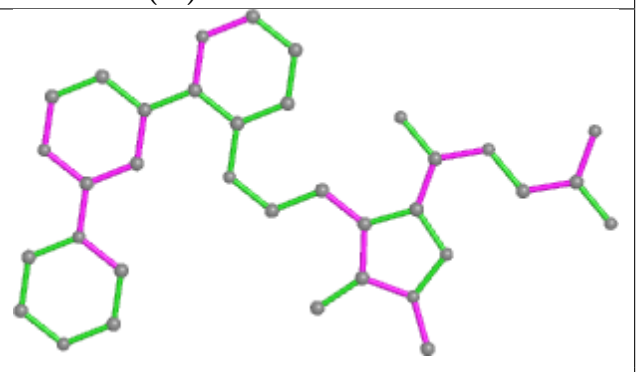


Rings

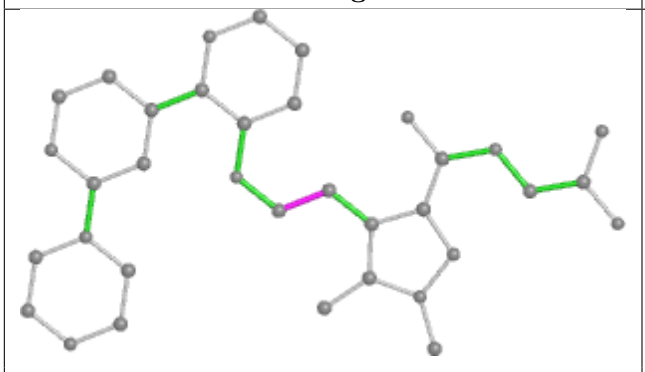
Ligand A1AB7 A 502 (A)



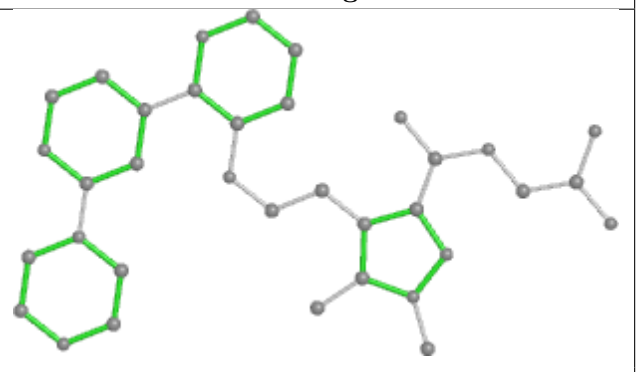
Bond lengths



Bond angles

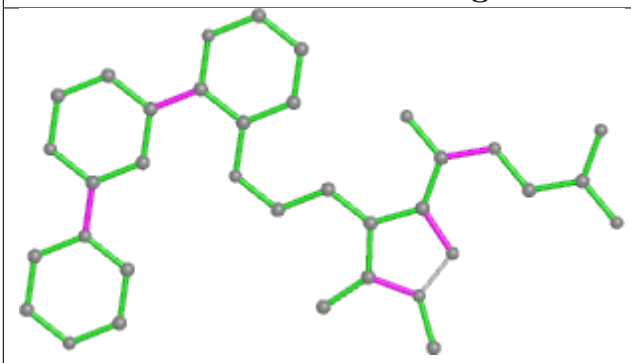


Torsions

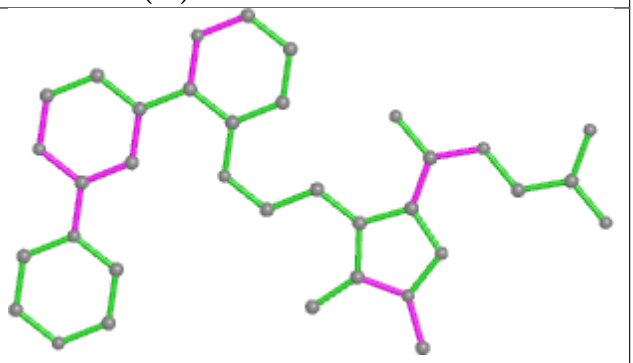


Rings

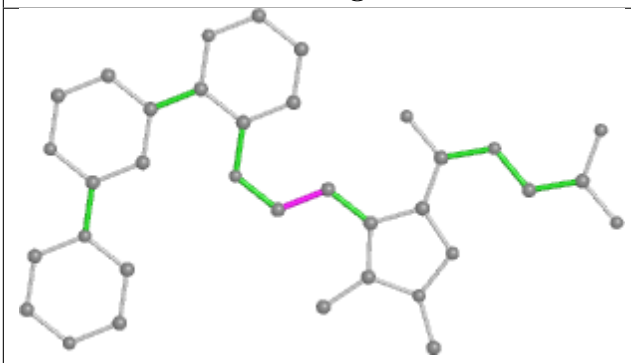
Ligand A1AB7 B 502 (B)



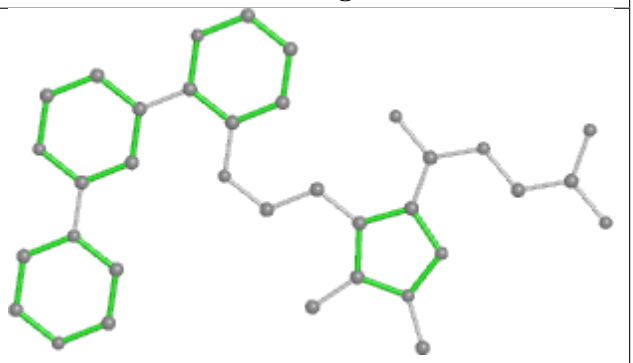
Bond lengths



Bond angles

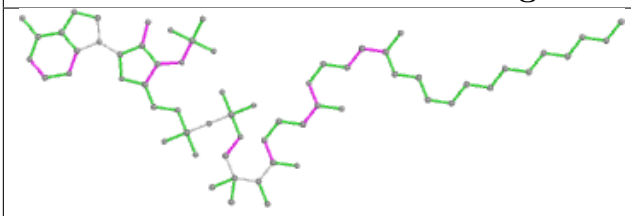


Torsions

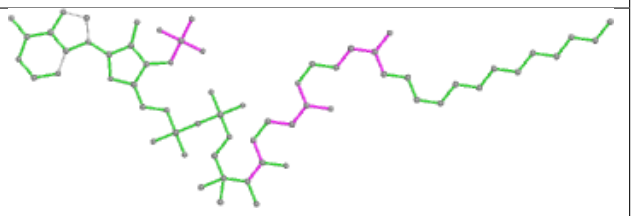


Rings

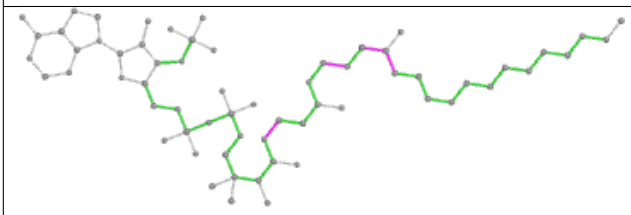
Ligand MYA C 501



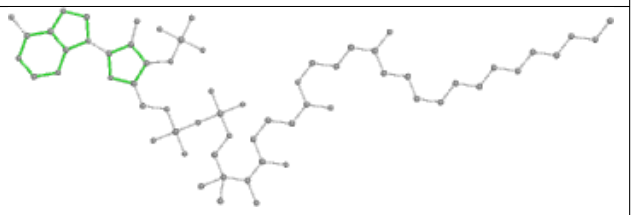
Bond lengths



Bond angles

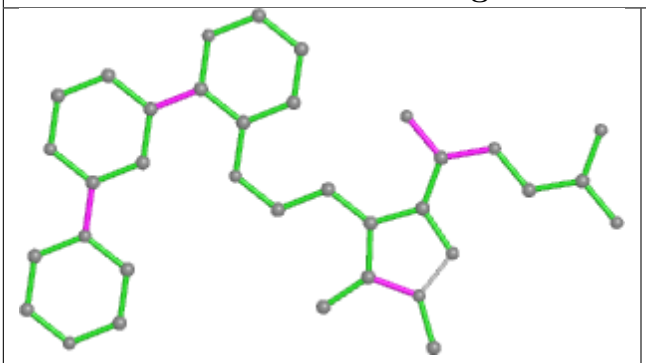


Torsions

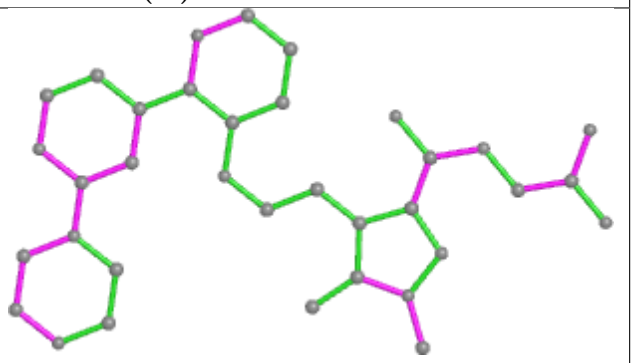


Rings

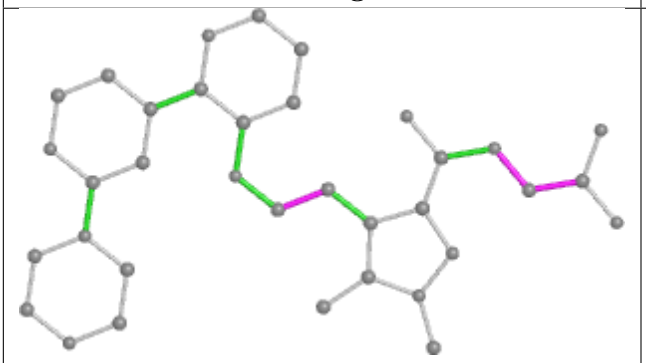
Ligand A1AB7 C 502 (B)



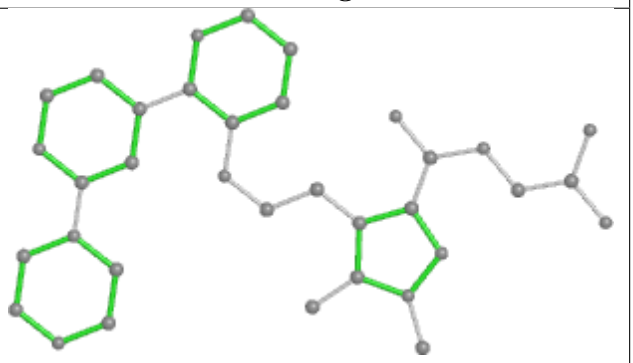
Bond lengths



Bond angles

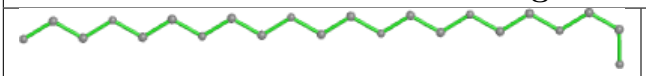


Torsions

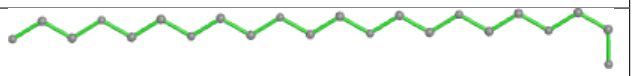


Rings

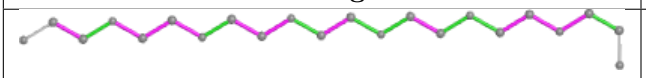
Ligand P33 C 512



Bond lengths



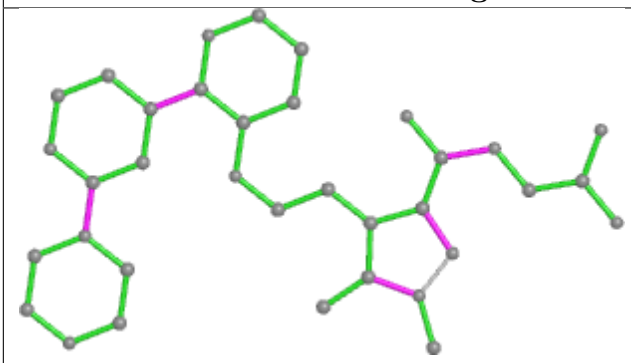
Bond angles



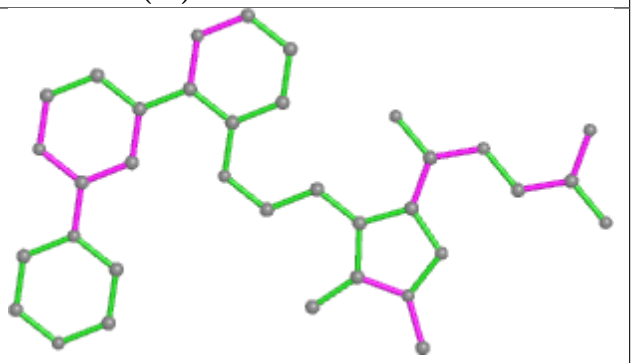
Torsions

Rings

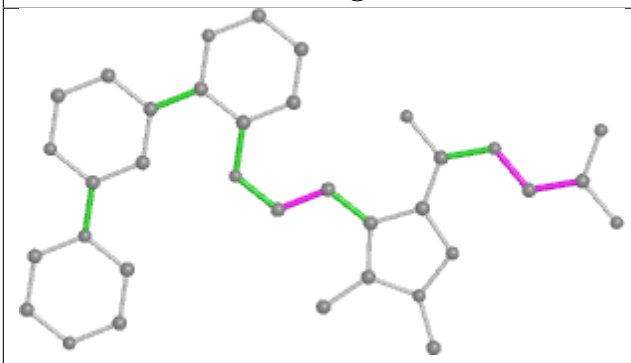
Ligand A1AB7 C 502 (A)



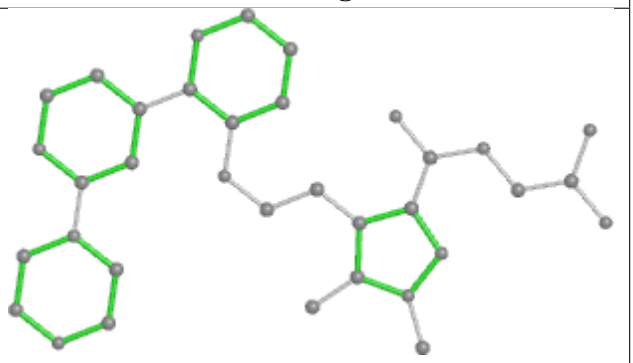
Bond lengths



Bond angles

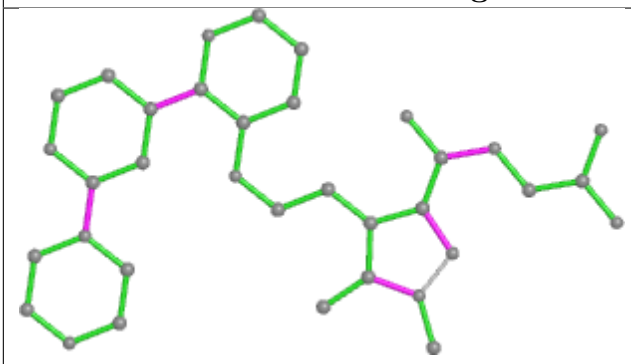


Torsions

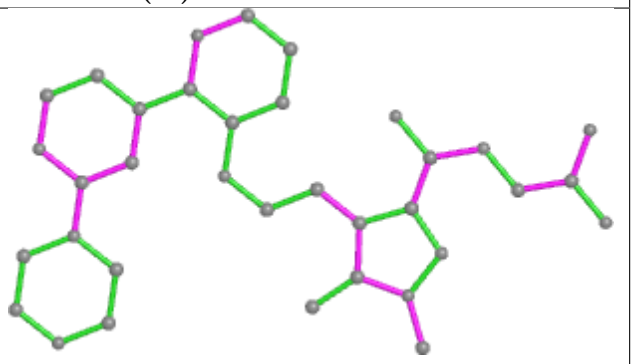


Rings

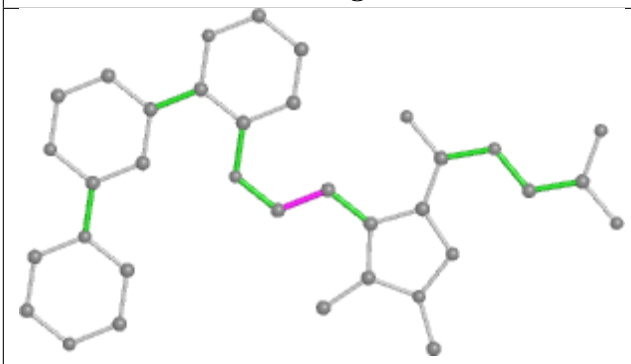
Ligand A1AB7 B 502 (A)



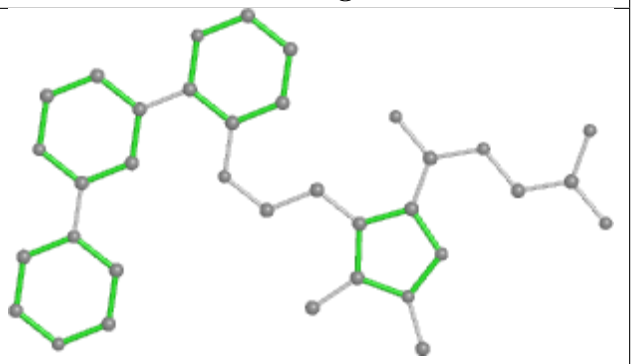
Bond lengths



Bond angles

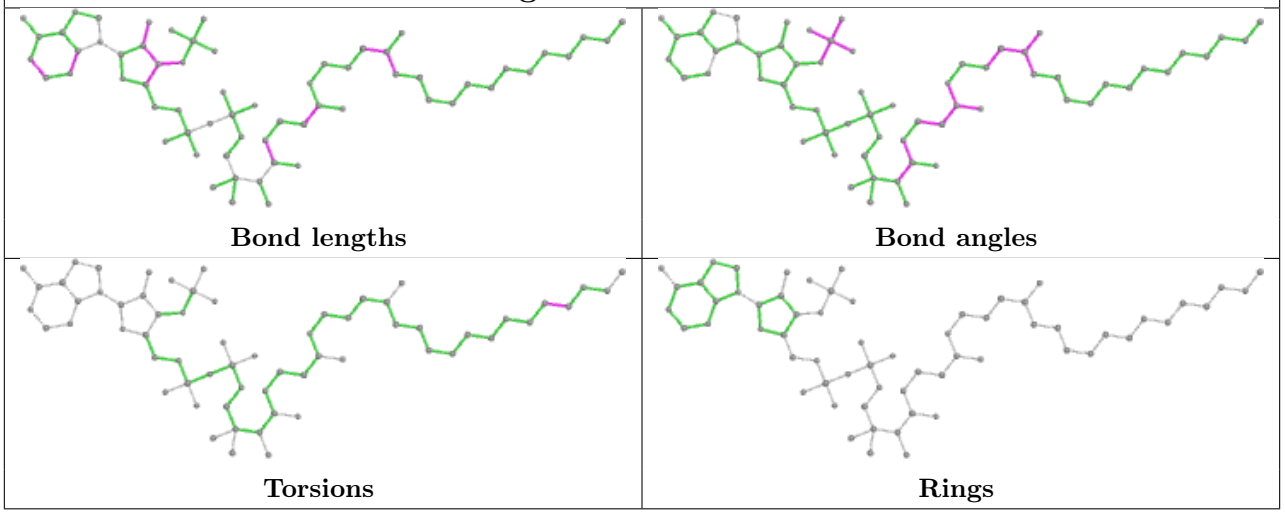


Torsions

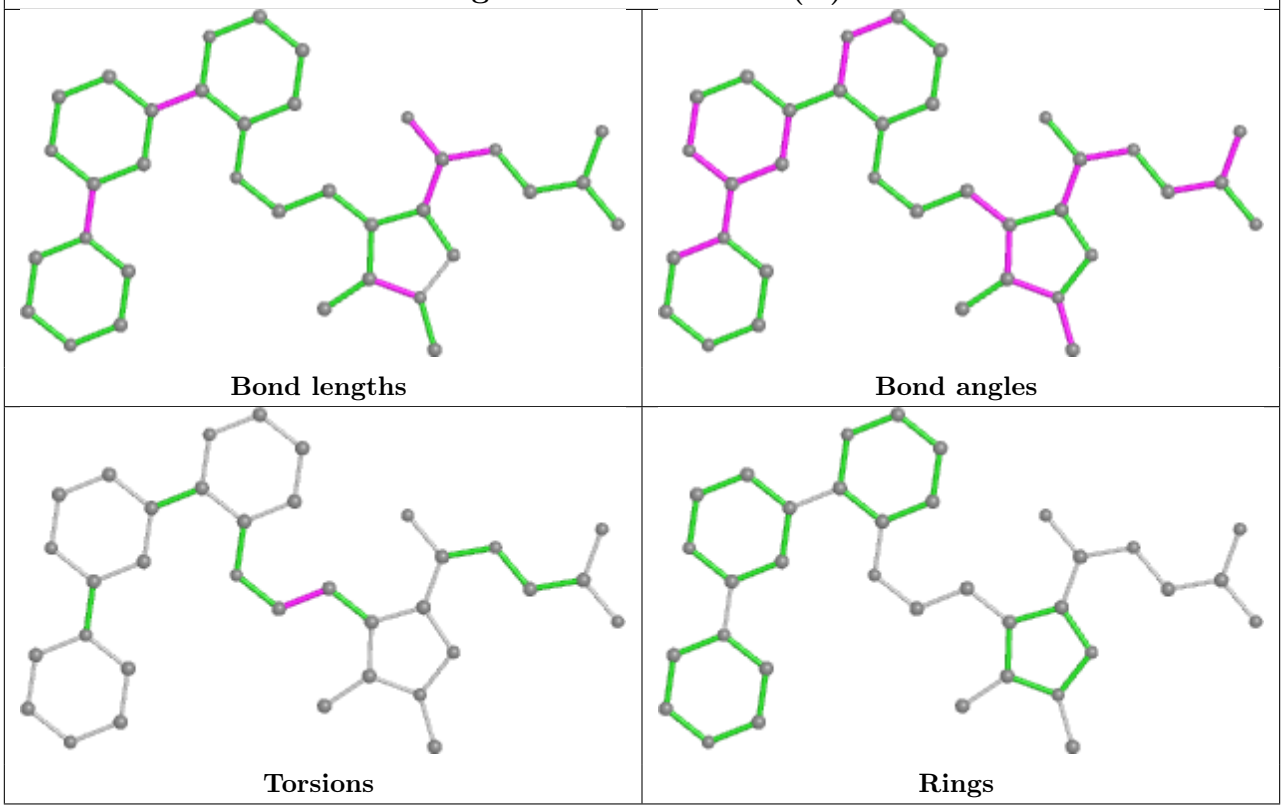


Rings

Ligand MYA A 501



Ligand A1AB7 A 502 (B)



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, 95^{th} 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%)	-0.26	0 100 100	15, 23, 40, 67	1 (0%)
1	B	385/386 (99%)	-0.18	3 (0%) 86 87	15, 24, 44, 79	1 (0%)
1	C	385/386 (99%)	-0.08	9 (2%) 60 62	15, 25, 54, 86	0
All	All	1154/1158 (99%)	-0.17	12 (1%) 82 83	15, 24, 47, 86	2 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	PRO	4.6
1	C	325[A]	ASP	4.4
1	C	227[A]	SER	3.9
1	B	26	PRO	3.5
1	C	226[A]	PHE	3.3
1	C	326[A]	LYS	2.9
1	C	54	ASP	2.7
1	C	229	LEU	2.4
1	C	230	ASN	2.2
1	C	304[A]	GLU	2.2
1	B	99[A]	ASP	2.0
1	B	229	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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^{th} 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	517	16/16	0.84	0.23	53,91,113,121	0
8	P33	C	512	22/22	0.84	0.21	48,90,132,137	0
5	GOL	C	510	6/6	0.86	0.15	39,47,56,59	0
6	1PE	C	511[B]	16/16	0.88	0.15	36,46,54,57	38
4	CL	A	511	1/1	0.89	0.09	65,65,65,65	0
4	CL	A	509	1/1	0.90	0.07	49,49,49,49	0
4	CL	C	508	1/1	0.90	0.23	51,51,51,51	0
3	A1AB7	C	502[A]	35/35	0.92	0.18	26,36,47,52	64
5	GOL	B	508	6/6	0.92	0.14	32,48,55,59	0
3	A1AB7	C	502[B]	35/35	0.92	0.18	26,36,55,68	64
5	GOL	A	516	6/6	0.94	0.12	28,41,48,57	0
3	A1AB7	B	502[A]	35/35	0.94	0.13	26,33,41,44	64
3	A1AB7	B	502[B]	35/35	0.94	0.13	26,33,40,44	64
4	CL	A	512	1/1	0.94	0.24	67,67,67,67	0
4	CL	A	513	1/1	0.94	0.10	41,41,41,41	0
4	CL	A	508[A]	1/1	0.94	0.15	34,34,34,34	1
3	A1AB7	A	502[B]	35/35	0.95	0.13	23,29,38,43	64
4	CL	C	509	1/1	0.95	0.20	46,46,46,46	0
3	A1AB7	A	502[A]	35/35	0.95	0.13	22,29,38,43	64
7	MG	B	507	1/1	0.95	0.14	67,67,67,67	0
4	CL	B	505[B]	1/1	0.95	0.28	40,40,40,40	1
4	CL	B	506	1/1	0.96	0.07	47,47,47,47	0
4	CL	A	510	1/1	0.96	0.06	43,43,43,43	0
4	CL	C	505	1/1	0.97	0.09	42,42,42,42	0
2	MYA	C	501	63/63	0.97	0.11	16,22,31,35	0
2	MYA	A	501	63/63	0.98	0.09	13,22,29,30	0
4	CL	C	504	1/1	0.98	0.07	37,37,37,37	0
4	CL	A	505	1/1	0.98	0.09	41,41,41,41	0
4	CL	C	506	1/1	0.98	0.17	35,35,35,35	0
4	CL	C	507	1/1	0.98	0.19	38,38,38,38	0
4	CL	A	514	1/1	0.98	0.06	44,44,44,44	0
2	MYA	B	501	63/63	0.98	0.09	13,21,28,30	0
4	CL	A	504	1/1	0.99	0.04	22,22,22,22	0
4	CL	A	503	1/1	0.99	0.04	29,29,29,29	0
4	CL	A	506	1/1	0.99	0.04	28,28,28,28	0
4	CL	A	515	1/1	0.99	0.20	43,43,43,43	0
4	CL	B	503	1/1	0.99	0.06	23,23,23,23	0

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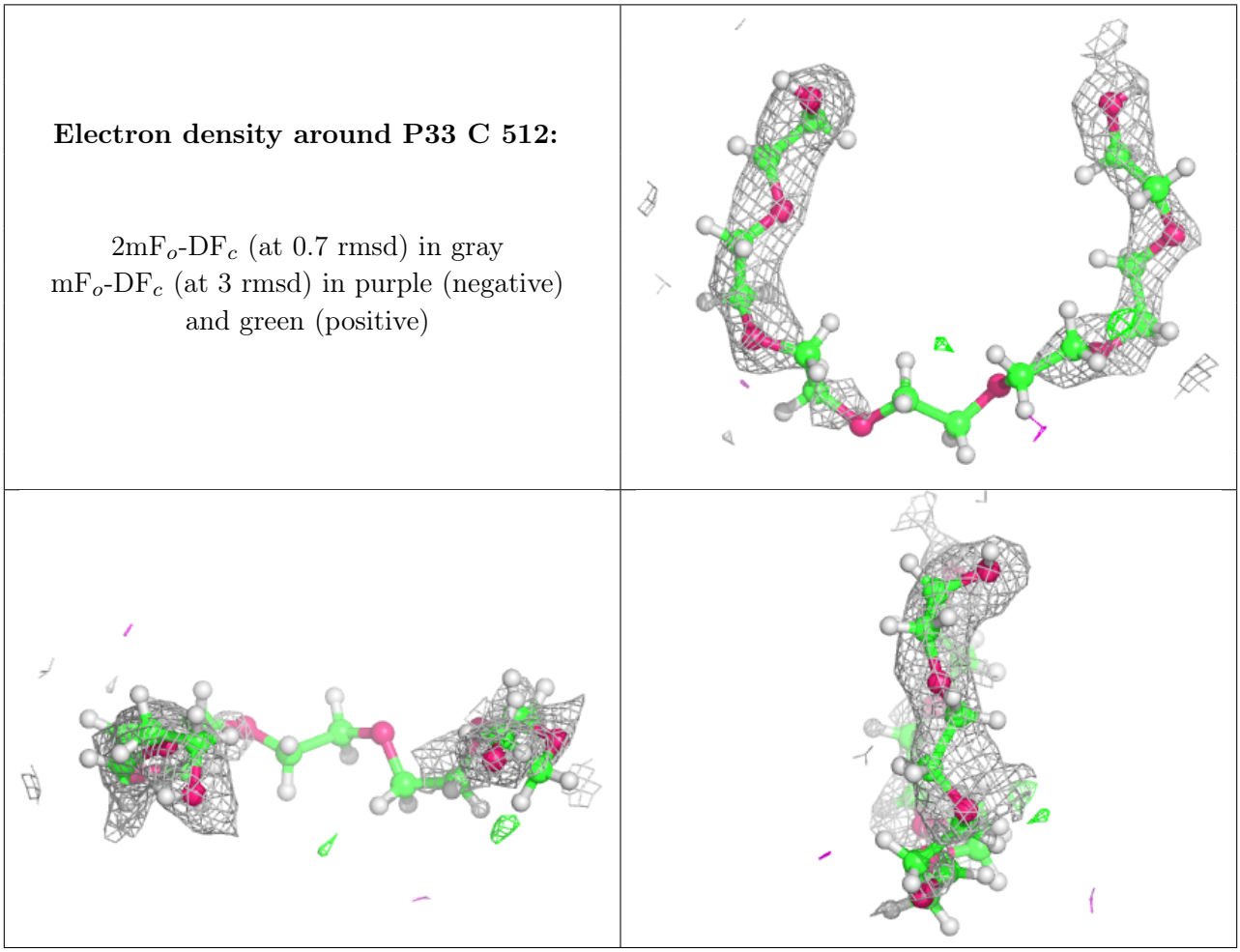
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	B	504	1/1	0.99	0.07	30,30,30,30	1
4	CL	A	507	1/1	0.99	0.09	33,33,33,33	0
4	CL	C	503	1/1	1.00	0.05	23,23,23,23	0

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.

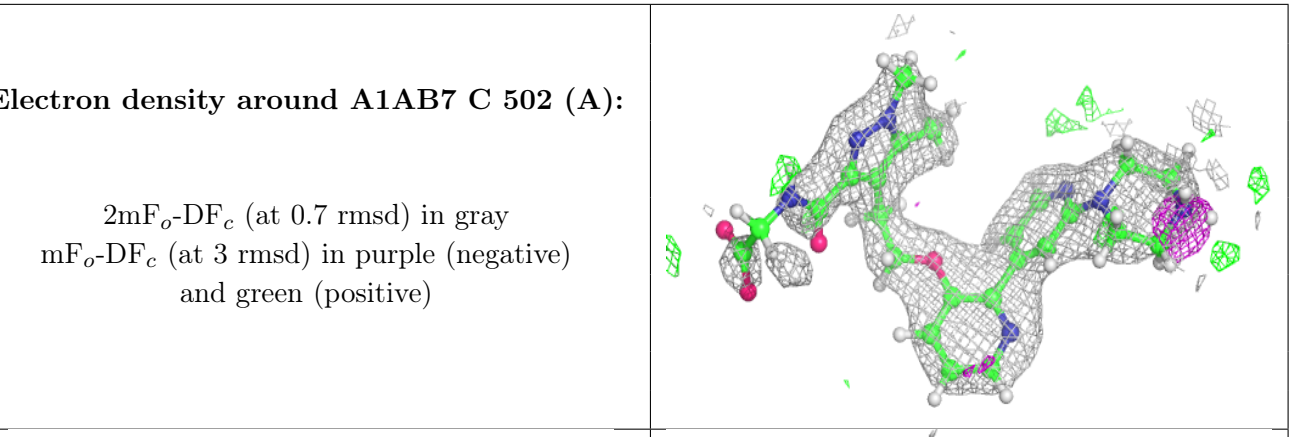
Electron density around P33 C 512:

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



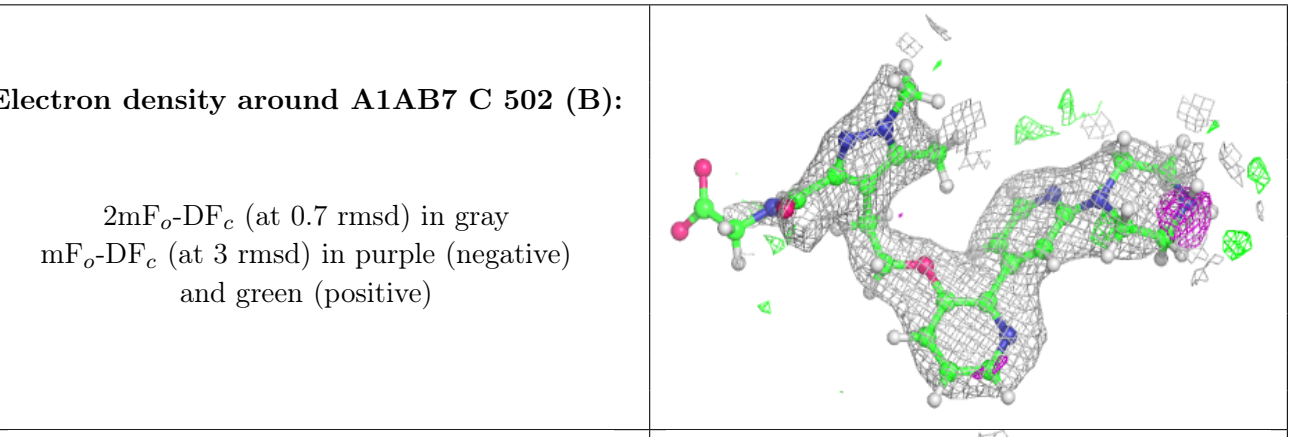
Electron density around A1AB7 C 502 (A):

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



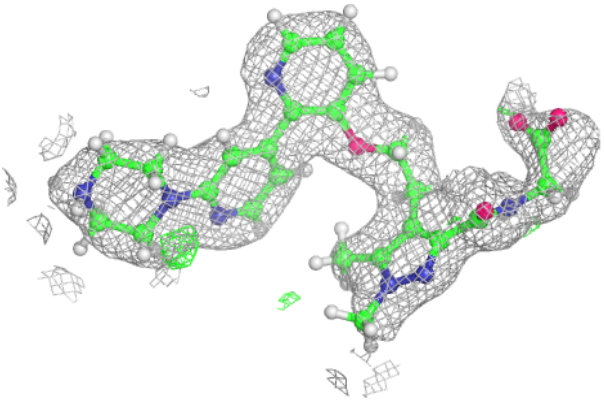
Electron density around A1AB7 C 502 (B):

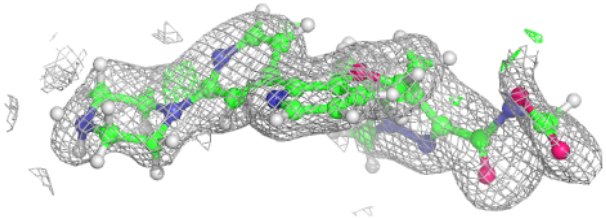
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

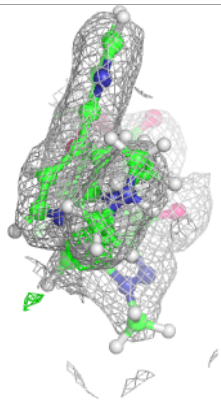


Electron density around A1AB7 B 502 (A):

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

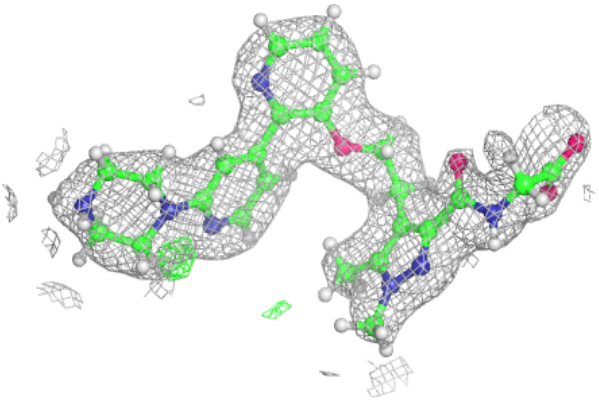


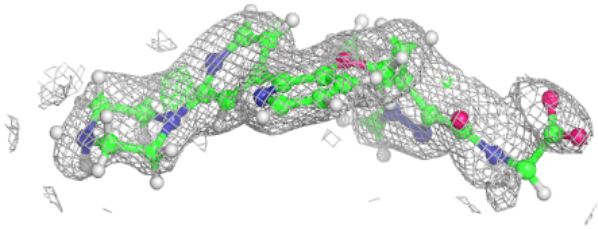


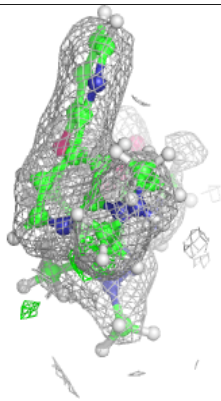


Electron density around A1AB7 B 502 (B):

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

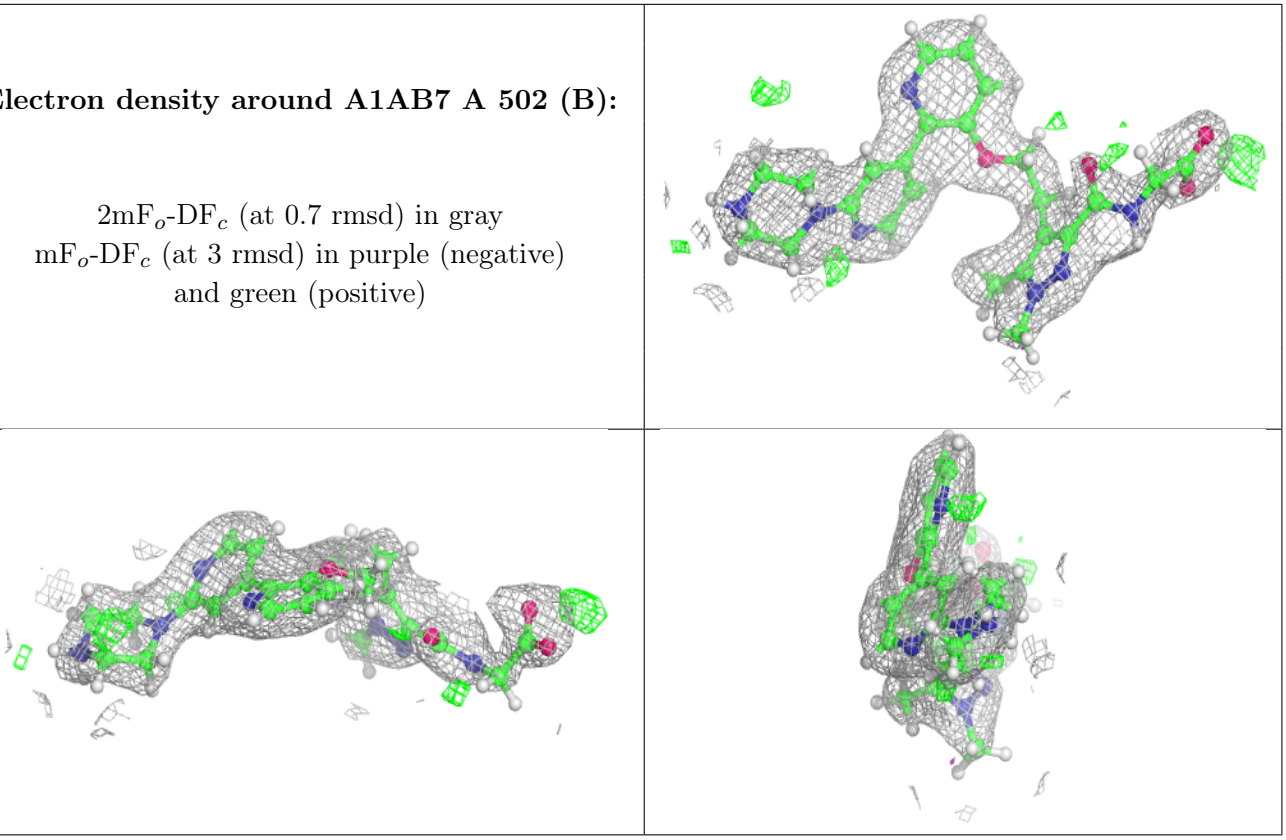






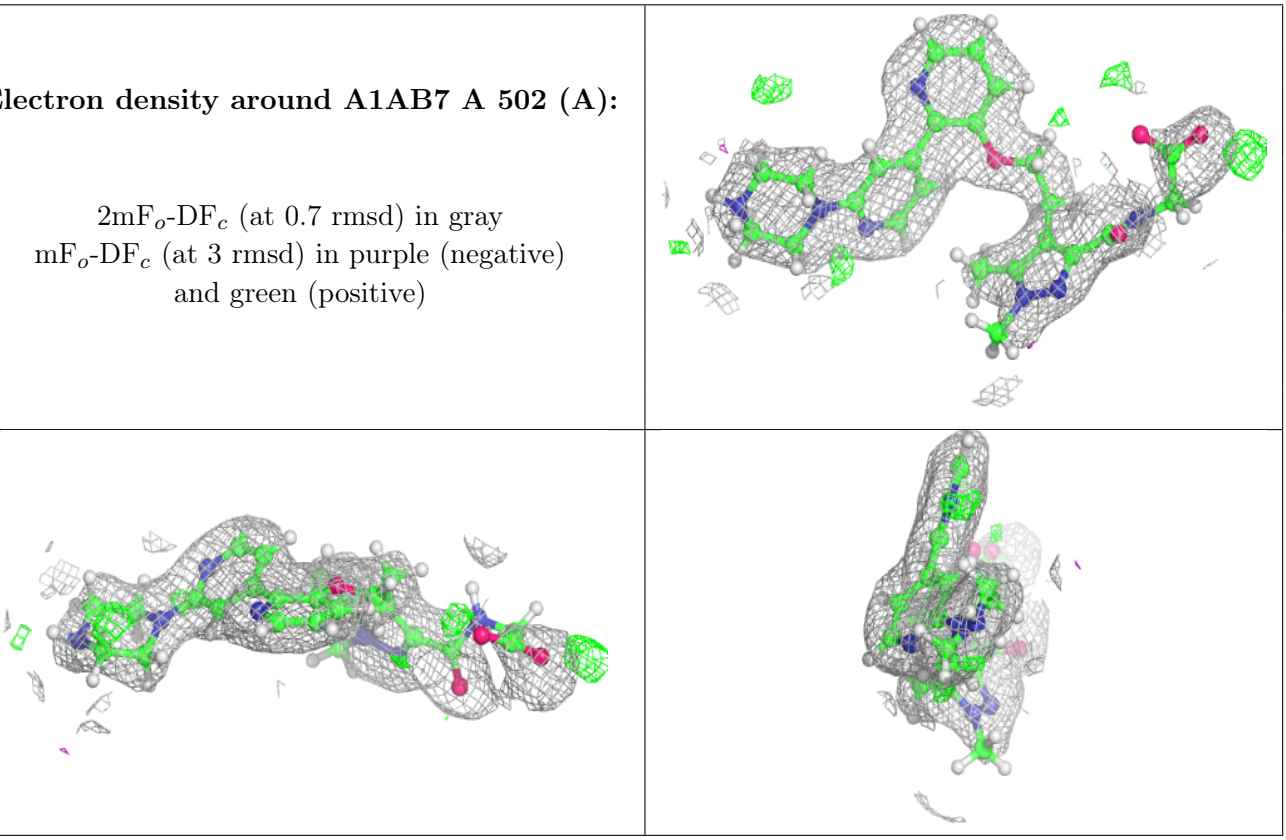
Electron density around A1AB7 A 502 (B):

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



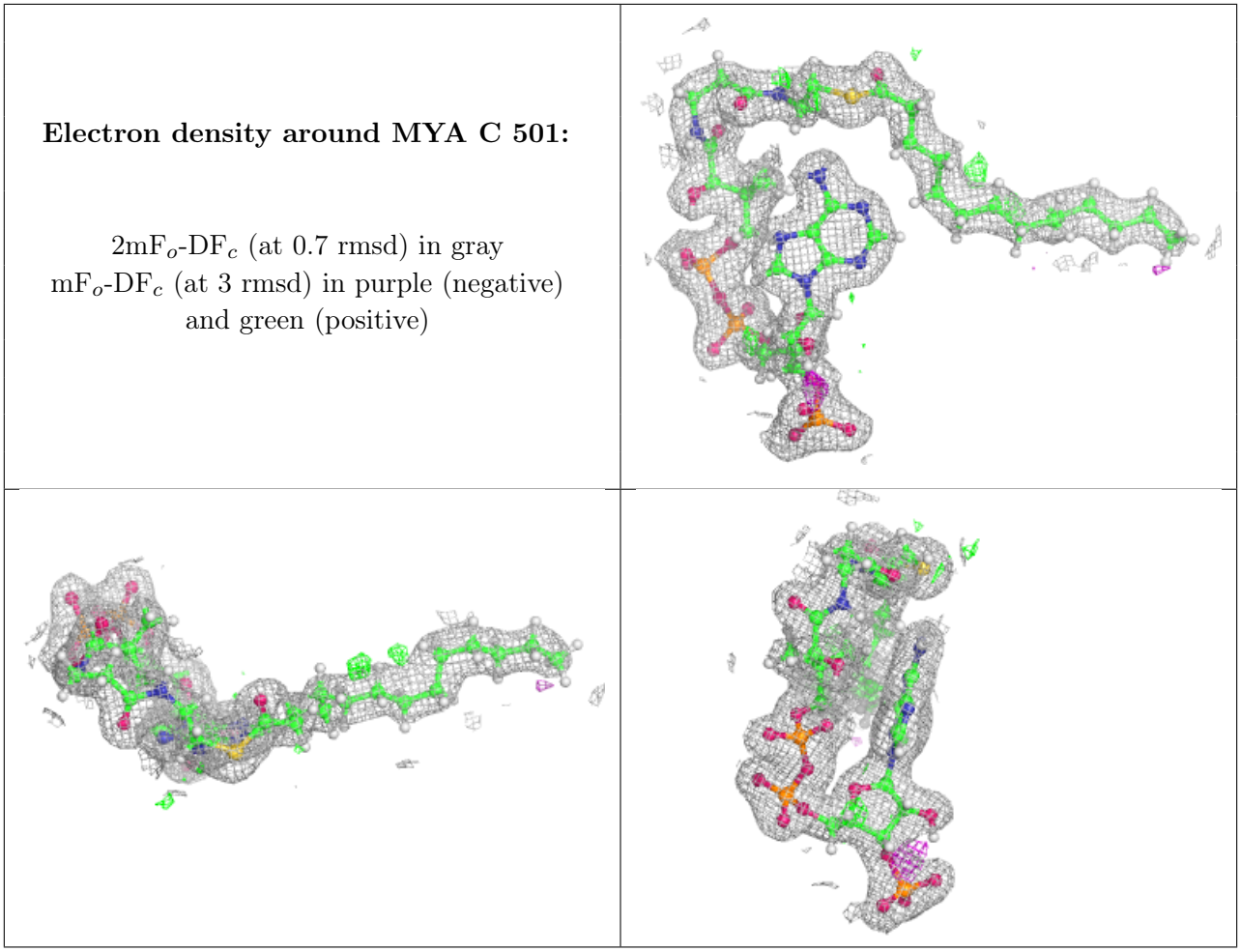
Electron density around A1AB7 A 502 (A):

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



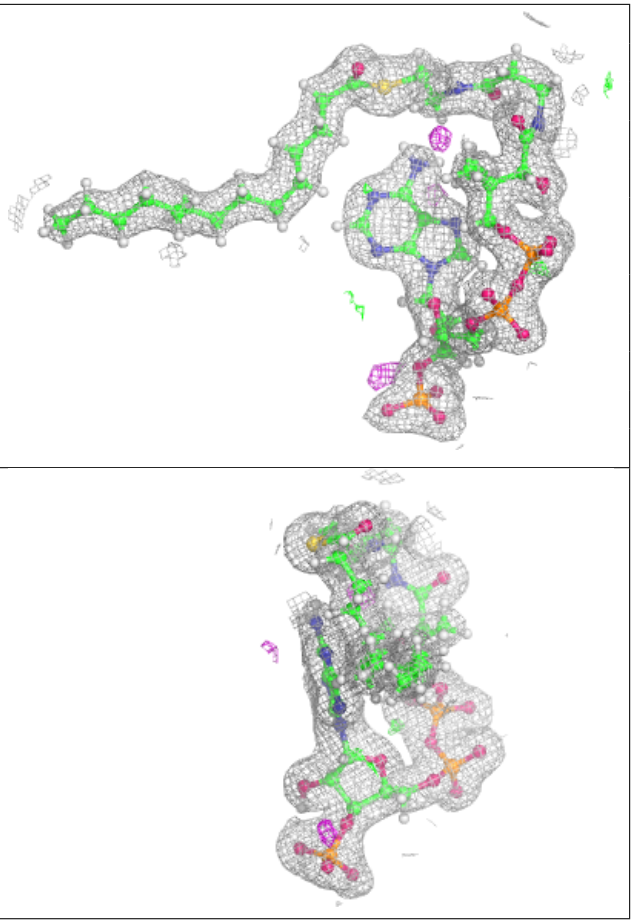
Electron density around MYA C 501:

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



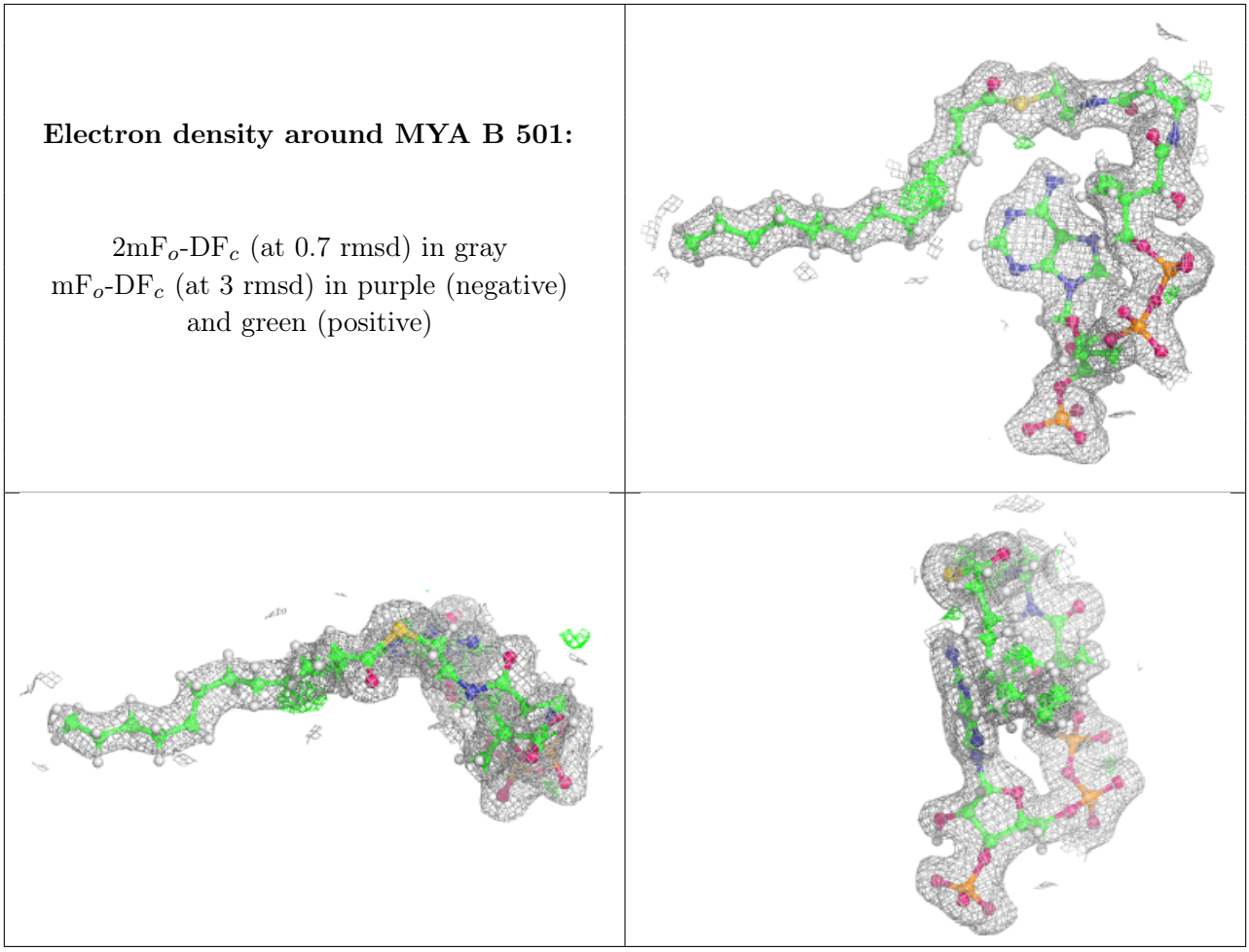
Electron density around MYA A 501:

$2mF_o$-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.