



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:54 AM UTC

PDB ID : 6TW5 / pdb_00006tw5
Title : Plasmodium vivax N-myristoyltransferase with bound indazole inhibitor IMP-917
Authors : Brannigan, J.A.
Deposited on : 2020-01-12
Resolution : 1.55 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	:	4-5-2 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

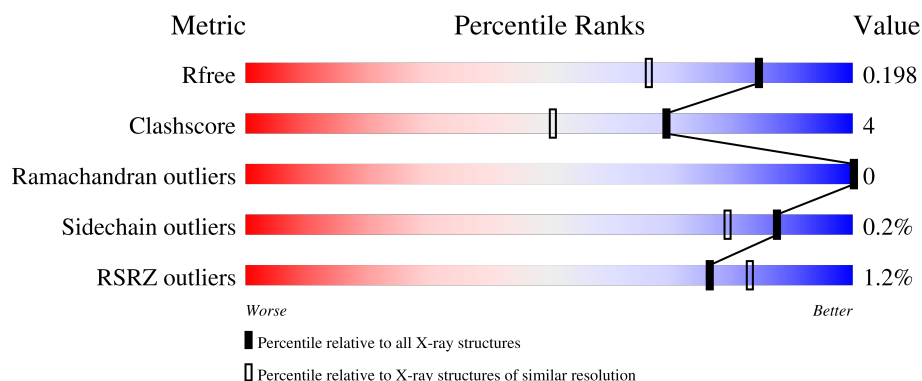
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

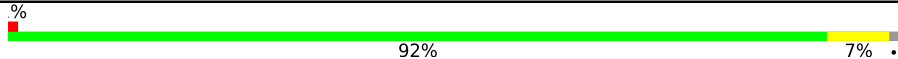
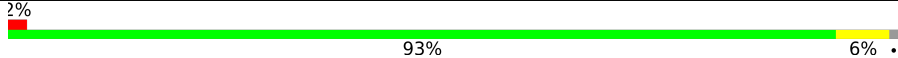
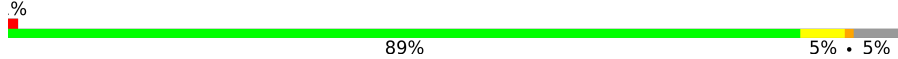
The reported resolution of this entry is 1.55 Å.

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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	AAA	388	
1	BBB	388	
1	CCC	388	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	BBB	504	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12014 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

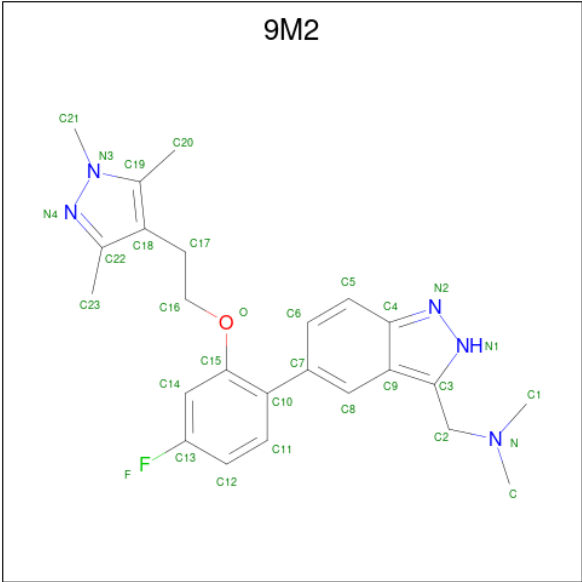
- Molecule 1 is a protein called Glycylpeptide N-tetradecanoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	384	Total	C	N	O	S	0	35	0
			3384	2212	544	616	12			
1	BBB	384	Total	C	N	O	S	0	39	0
			3396	2228	544	612	12			
1	CCC	369	Total	C	N	O	S	0	36	0
			3253	2134	516	592	11			

There are 12 discrepancies between the modelled and reference sequences:

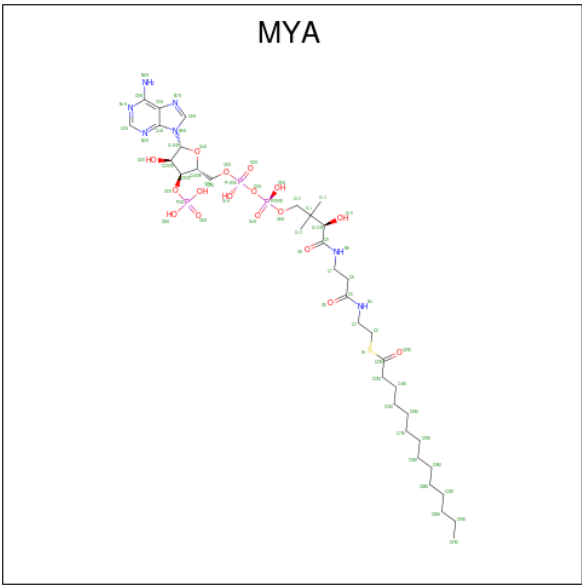
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	23	GLY	-	expression tag	UNP A5K1A2
AAA	24	PRO	-	expression tag	UNP A5K1A2
AAA	25	HIS	-	expression tag	UNP A5K1A2
AAA	26	MET	-	expression tag	UNP A5K1A2
BBB	23	GLY	-	expression tag	UNP A5K1A2
BBB	24	PRO	-	expression tag	UNP A5K1A2
BBB	25	HIS	-	expression tag	UNP A5K1A2
BBB	26	MET	-	expression tag	UNP A5K1A2
CCC	23	GLY	-	expression tag	UNP A5K1A2
CCC	24	PRO	-	expression tag	UNP A5K1A2
CCC	25	HIS	-	expression tag	UNP A5K1A2
CCC	26	MET	-	expression tag	UNP A5K1A2

- Molecule 2 is 1-[5-[4-fluoranyl-2-[2-(1,3,5-trimethylpyrazol-4-yl)ethoxy]phenyl]-2 {H}-indazo l-3-yl]- {N}, {N}-dimethyl-methanamine (CCD ID: 9M2) (formula: C₂₄H₂₈FN₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	0	0
			31	24	1	5	1		
2	BBB	1	Total	C	F	N	O	0	0
			31	24	1	5	1		
2	CCC	1	Total	C	F	N	O	0	0
			31	24	1	5	1		

- Molecule 3 is TETRADECANOYL-COA (CCD ID: MYA) (formula: $C_{35}H_{62}N_7O_{17}P_3S$).



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

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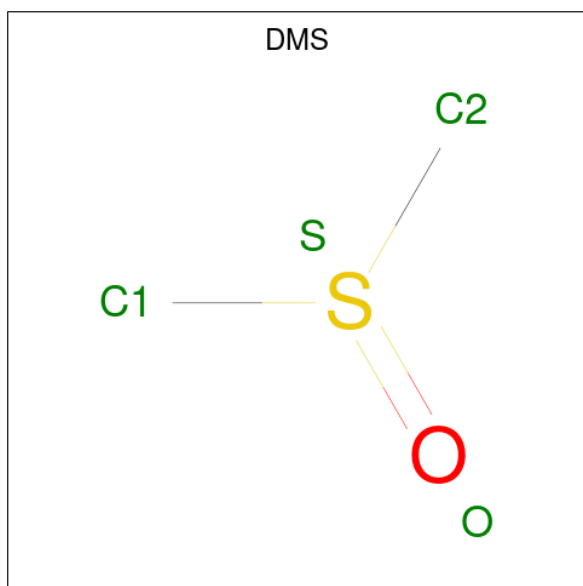
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	BBB	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		
3	CCC	1	Total	C	N	O	P	S	0	0
			63	35	7	17	3	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Mg	0	0
			1	1		
4	BBB	1	Total	Mg	0	0
			1	1		
4	CCC	1	Total	Mg	0	0
			1	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).

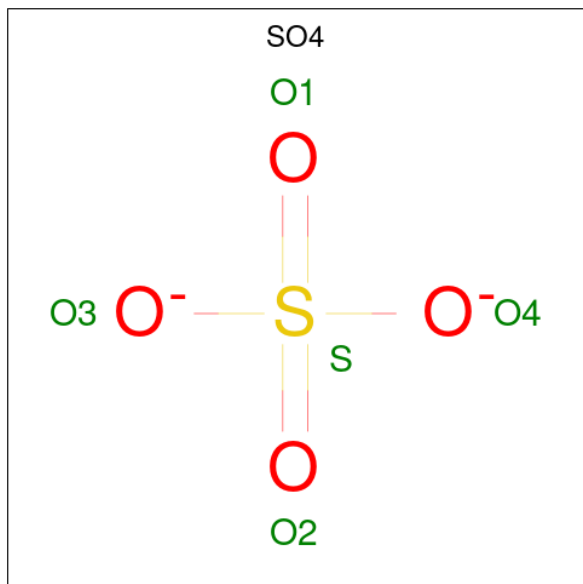


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	O	S	0	0
			4	2	1	1		
5	BBB	1	Total	C	O	S	0	0
			4	2	1	1		
5	CCC	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Cl 1 1	0	0
6	BBB	1	Total Cl 1 1	0	0
6	CCC	1	Total Cl 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total O S 5 4 1	0	0
7	AAA	1	Total O S 5 4 1	0	0
7	CCC	1	Total O S 5 4 1	0	0

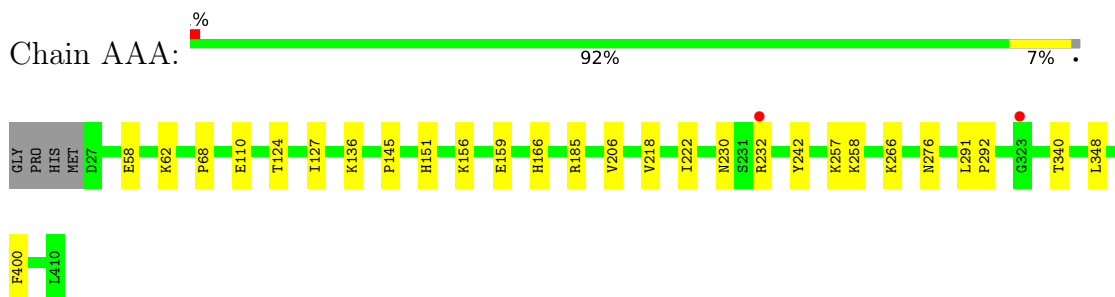
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	589	Total O 589 589	0	0
8	BBB	558	Total O 558 558	0	0
8	CCC	519	Total O 519 519	0	0

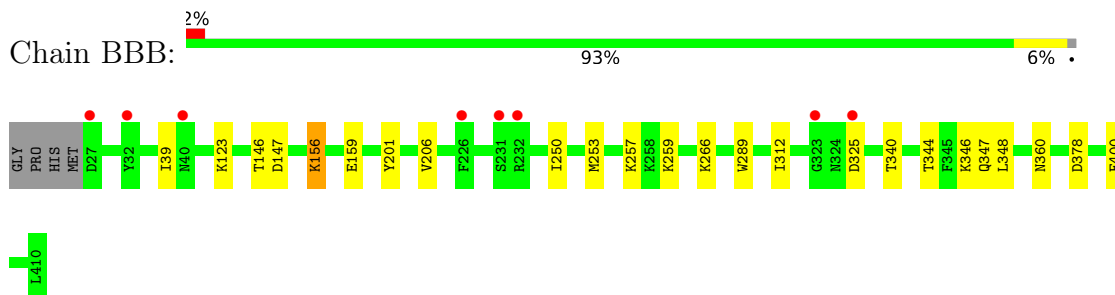
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

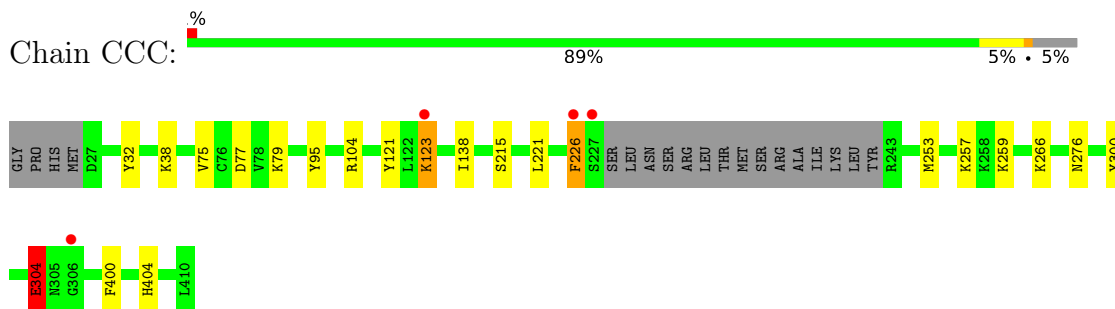
- Molecule 1: Glycylpeptide N-tetradecanoyltransferase



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase



- Molecule 1: Glycylpeptide N-tetradecanoyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.47Å 121.66Å 178.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 1.55 49.00 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-1.55) 99.9 (49.00-1.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.165 , 0.198 0.165 , 0.198	Depositor DCC
R_{free} test set	9126 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12014	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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, 9M2, SO4, DMS, 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	AAA	0.65	1/3553 (0.0%)	0.99	3/4806 (0.1%)
1	BBB	0.67	2/3592 (0.1%)	0.98	0/4850
1	CCC	0.71	3/3434 (0.1%)	0.98	5/4637 (0.1%)
All	All	0.68	6/10579 (0.1%)	0.98	8/14293 (0.1%)

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	CCC	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	304[A]	GLU	C-O	8.91	1.34	1.24
1	CCC	304[B]	GLU	C-O	8.91	1.34	1.24
1	BBB	156[A]	LYS	C-O	5.70	1.30	1.24
1	BBB	156[B]	LYS	C-O	5.70	1.30	1.24
1	CCC	404	HIS	CE1-NE2	5.68	1.38	1.32
1	AAA	166	HIS	CE1-NE2	5.63	1.38	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	123[A]	LYS	CA-C-O	7.20	128.23	120.10
1	CCC	123[B]	LYS	CA-C-O	7.20	128.23	120.10
1	AAA	110	GLU	CB-CG-CD	6.04	122.86	112.60
1	CCC	104	ARG	NE-CZ-NH2	5.85	124.47	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	68	PRO	CB-CA-C	5.70	116.75	111.39
1	AAA	68	PRO	O-C-N	-5.29	118.88	121.31
1	CCC	95	TYR	CA-C-N	5.21	127.56	120.63
1	CCC	95	TYR	C-N-CA	5.21	127.56	120.63

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	304[A]	GLU	Mainchain
1	CCC	304[B]	GLU	Mainchain

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	AAA	3384	0	3446	25	0
1	BBB	3396	0	3507	28	0
1	CCC	3253	0	3334	18	0
2	AAA	31	0	0	0	0
2	BBB	31	0	0	0	0
2	CCC	31	0	0	0	0
3	AAA	63	0	58	0	0
3	BBB	63	0	58	0	0
3	CCC	63	0	58	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
4	CCC	1	0	0	0	0
5	AAA	4	0	6	3	0
5	BBB	4	0	6	4	0
5	CCC	4	0	6	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
7	AAA	10	0	0	0	0
7	CCC	5	0	0	0	0
8	AAA	589	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	BBB	558	0	0	8	0
8	CCC	519	0	0	5	0
All	All	12014	0	10479	73	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 4.

All (73) 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:AAA:136[A]:LYS:HA	1:AAA:136[A]:LYS:HE2	1.33	1.09
1:CCC:75:VAL:HG12	1:CCC:123[A]:LYS:HE2	1.43	0.97
1:BBB:257[B]:LYS:HE3	8:BBB:708:HOH:O	1.78	0.83
1:AAA:159:GLU:OE1	5:AAA:504:DMS:H12	1.82	0.78
1:CCC:75:VAL:CG1	1:CCC:123[A]:LYS:HE2	2.15	0.77
1:AAA:136[A]:LYS:HE2	1:AAA:136[A]:LYS:CA	2.08	0.77
1:AAA:127[B]:ILE:HD12	1:AAA:185:ARG:NH1	1.99	0.76
1:AAA:258:LYS:HD2	1:AAA:291:LEU:HD11	1.68	0.75
1:AAA:230:ASN:OD1	1:AAA:232:ARG:HG3	1.87	0.74
1:BBB:146:THR:HG21	1:BBB:159[B]:GLU:CD	2.12	0.74
5:AAA:504:DMS:H13	8:AAA:648:HOH:O	1.88	0.74
1:BBB:257[A]:LYS:HD2	8:BBB:964:HOH:O	1.89	0.72
1:BBB:257[A]:LYS:CD	8:BBB:964:HOH:O	2.39	0.70
1:BBB:156[A]:LYS:HZ2	1:BBB:156[A]:LYS:HB3	1.60	0.66
1:AAA:124:THR:O	1:AAA:127[B]:ILE:HD11	1.95	0.65
1:BBB:253[B]:MET:HE2	1:BBB:312:ILE:HD12	1.77	0.65
1:BBB:344:THR:OG1	1:BBB:347[B]:GLN:HG3	1.97	0.65
1:AAA:258:LYS:HD2	1:AAA:291:LEU:CD1	2.27	0.64
1:BBB:156[A]:LYS:HB3	1:BBB:156[A]:LYS:NZ	2.12	0.64
1:AAA:127[B]:ILE:CD1	1:AAA:185:ARG:NH1	2.59	0.64
1:AAA:145:PRO:HB2	1:AAA:156[B]:LYS:HE3	1.81	0.63
1:BBB:206[B]:VAL:HG12	1:BBB:400:PHE:CE1	2.34	0.63
1:BBB:123:LYS:HB3	8:BBB:637:HOH:O	2.00	0.62
1:CCC:77:ASP:HA	1:CCC:123[A]:LYS:HE3	1.81	0.61
1:AAA:276[A]:ASN:ND2	1:AAA:400:PHE:CE2	2.69	0.60
1:BBB:146:THR:CG2	1:BBB:159[B]:GLU:CD	2.77	0.57
1:BBB:159[A]:GLU:OE2	5:BBB:504:DMS:H23	2.05	0.57
1:CCC:276[A]:ASN:ND2	1:CCC:400:PHE:CD1	2.72	0.56
1:AAA:230:ASN:OD1	1:AAA:232:ARG:CG	2.55	0.55
1:BBB:266[B]:LYS:HG3	8:BBB:942:HOH:O	2.05	0.54
1:CCC:32[A]:TYR:CE1	1:CCC:38:LYS:HE3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:62[B]:LYS:HD2	8:AAA:1179:HOH:O	2.07	0.54
1:CCC:257[A]:LYS:HD2	1:CCC:259[A]:LYS:NZ	2.23	0.54
1:CCC:266[B]:LYS:HG3	8:CCC:782:HOH:O	2.09	0.52
1:CCC:276[A]:ASN:ND2	1:CCC:400:PHE:CE1	2.76	0.52
1:CCC:215[B]:SER:OG	1:CCC:221:LEU:HD12	2.10	0.51
1:BBB:206[B]:VAL:CG1	1:BBB:400:PHE:CE1	2.93	0.51
1:BBB:360:ASN:ND2	8:BBB:606:HOH:O	2.44	0.51
1:CCC:77:ASP:CA	1:CCC:123[A]:LYS:HE3	2.41	0.49
5:AAA:504:DMS:H22	8:AAA:648:HOH:O	2.12	0.49
1:CCC:123[A]:LYS:HG2	8:CCC:663:HOH:O	2.11	0.49
1:BBB:346[A]:LYS:HE3	1:BBB:378:ASP:HB3	1.95	0.49
1:AAA:266[B]:LYS:HG3	8:AAA:789:HOH:O	2.13	0.48
1:CCC:253[A]:MET:HG3	1:CCC:300:TYR:HB3	1.96	0.47
1:CCC:276[B]:ASN:ND2	8:CCC:608:HOH:O	2.47	0.46
1:CCC:138:ILE:C	1:CCC:138:ILE:HD12	2.41	0.46
1:CCC:257[A]:LYS:HE3	8:CCC:735:HOH:O	2.15	0.46
1:BBB:289:TRP:CD2	5:BBB:504:DMS:H11	2.51	0.45
1:AAA:266[A]:LYS:HE2	8:AAA:1041:HOH:O	2.17	0.45
1:CCC:226:PHE:C	1:CCC:226:PHE:CD1	2.95	0.44
1:BBB:39:ILE:CD1	1:BBB:201:TYR:HE2	2.30	0.44
1:AAA:276[A]:ASN:ND2	1:AAA:400:PHE:CD2	2.79	0.44
1:BBB:289:TRP:CE2	5:BBB:504:DMS:H11	2.52	0.44
1:AAA:151[A]:HIS:HA	1:AAA:276[A]:ASN:OD1	2.17	0.44
1:AAA:340:THR:HB	1:AAA:348:LEU:HD22	1.98	0.44
1:BBB:250:ILE:O	1:BBB:253[B]:MET:HG2	2.18	0.44
1:BBB:259[A]:LYS:NZ	8:BBB:611:HOH:O	2.48	0.44
1:BBB:257[A]:LYS:HD3	8:BBB:964:HOH:O	2.11	0.43
1:AAA:206[B]:VAL:HG22	1:AAA:400:PHE:CE2	2.54	0.43
1:CCC:304[B]:GLU:HG2	8:CCC:747:HOH:O	2.18	0.43
1:AAA:257:LYS:HE3	8:AAA:806:HOH:O	2.18	0.43
1:AAA:291:LEU:HA	1:AAA:292:PRO:HD3	1.93	0.43
1:BBB:147:ASP:OD1	1:BBB:156[A]:LYS:HE2	2.19	0.43
1:BBB:340:THR:HB	1:BBB:348:LEU:HD22	2.01	0.43
1:AAA:218[B]:VAL:HG21	1:AAA:242:TYR:HB2	2.01	0.43
1:BBB:156[A]:LYS:NZ	1:BBB:156[A]:LYS:CB	2.78	0.42
1:AAA:127[A]:ILE:HD11	1:AAA:185:ARG:HD2	2.00	0.42
1:CCC:79:LYS:HE3	1:CCC:121:TYR:OH	2.20	0.41
1:BBB:159[B]:GLU:OE2	5:BBB:504:DMS:O	2.38	0.41
1:BBB:146:THR:CG2	1:BBB:159[B]:GLU:OE1	2.68	0.41
1:BBB:206[B]:VAL:HG12	1:BBB:400:PHE:CZ	2.56	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	AAA	417/388 (108%)	411 (99%)	6 (1%)	0	100	100
1	BBB	421/388 (108%)	411 (98%)	10 (2%)	0	100	100
1	CCC	401/388 (103%)	391 (98%)	10 (2%)	0	100	100
All	All	1239/1164 (106%)	1213 (98%)	26 (2%)	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	AAA	385/353 (109%)	385 (100%)	0	100	100
1	BBB	389/353 (110%)	388 (100%)	1 (0%)	86	77
1	CCC	372/353 (105%)	371 (100%)	1 (0%)	86	77
All	All	1146/1059 (108%)	1144 (100%)	2 (0%)	87	79

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	325	ASP
1	CCC	226	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	9M2	AAA	501	-	32,34,34	1.69	9 (28%)	38,49,49	1.69	8 (21%)
2	9M2	BBB	501	-	32,34,34	1.73	6 (18%)	38,49,49	1.76	7 (18%)
5	DMS	CCC	504	-	3,3,3	0.38	0	3,3,3	0.52	0
7	SO4	CCC	506	-	4,4,4	0.32	0	6,6,6	0.10	0
2	9M2	CCC	501	-	32,34,34	1.98	7 (21%)	38,49,49	1.45	2 (5%)
5	DMS	AAA	504	-	3,3,3	0.34	0	3,3,3	0.35	0
3	MYA	BBB	502	4	63,65,65	1.21	7 (11%)	85,91,91	1.56	10 (11%)
7	SO4	AAA	506	-	4,4,4	0.50	0	6,6,6	0.36	0
3	MYA	CCC	502	4	63,65,65	1.37	9 (14%)	85,91,91	1.65	18 (21%)
7	SO4	AAA	507	-	4,4,4	0.28	0	6,6,6	0.23	0
3	MYA	AAA	502	4	63,65,65	1.19	8 (12%)	85,91,91	1.61	16 (18%)
5	DMS	BBB	504	-	3,3,3	0.92	0	3,3,3	0.35	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	9M2	AAA	501	-	-	0/14/14/14	0/4/4/4
2	9M2	BBB	501	-	-	0/14/14/14	0/4/4/4
2	9M2	CCC	501	-	-	0/14/14/14	0/4/4/4
3	MYA	BBB	502	4	-	3/64/80/80	0/3/3/3
3	MYA	CCC	502	4	-	1/64/80/80	0/3/3/3
3	MYA	AAA	502	4	-	0/64/80/80	0/3/3/3

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	502	MYA	P1A-O3A	4.58	1.64	1.59
2	BBB	501	9M2	C4-N2	4.55	1.39	1.33
2	CCC	501	9M2	C19-C18	4.51	1.50	1.40
2	CCC	501	9M2	C18-C22	4.50	1.50	1.40
2	CCC	501	9M2	C4-N2	4.30	1.38	1.33
2	AAA	501	9M2	C19-C18	3.76	1.48	1.40
2	BBB	501	9M2	C18-C22	3.63	1.48	1.40
2	CCC	501	9M2	C10-C15	3.56	1.47	1.40
2	BBB	501	9M2	C10-C15	3.52	1.47	1.40
2	CCC	501	9M2	C2-C3	3.45	1.55	1.50
3	BBB	502	MYA	P3X-O3X	3.40	1.65	1.59
2	CCC	501	9M2	N3-N4	3.39	1.43	1.36
3	CCC	502	MYA	P3X-O3X	3.31	1.65	1.59
3	AAA	502	MYA	P3X-O3X	3.28	1.65	1.59
2	AAA	501	9M2	C3-N1	-3.27	1.32	1.35
3	BBB	502	MYA	P2A-O3A	-3.26	1.56	1.59
3	CCC	502	MYA	C3M-C2M	3.18	1.54	1.50
3	CCC	502	MYA	C8A-N7A	3.15	1.37	1.31
3	BBB	502	MYA	C3M-C2M	2.95	1.53	1.50
3	AAA	502	MYA	O2M-C2M	2.86	1.25	1.21
2	BBB	501	9M2	C6-C5	2.86	1.43	1.38
3	BBB	502	MYA	C8A-N7A	2.84	1.37	1.31
2	BBB	501	9M2	C19-C18	2.84	1.46	1.40
3	CCC	502	MYA	C5A-N7A	-2.83	1.33	1.39
3	AAA	502	MYA	C8A-N7A	2.81	1.37	1.31
2	AAA	501	9M2	C11-C10	2.73	1.44	1.40
2	AAA	501	9M2	C18-C22	2.69	1.46	1.40
3	AAA	502	MYA	C9-N8	-2.68	1.27	1.33
3	CCC	502	MYA	O2M-C2M	2.65	1.25	1.21
3	CCC	502	MYA	C2M-S1	-2.58	1.70	1.76
2	AAA	501	9M2	O-C15	-2.53	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	501	9M2	C21-N3	2.53	1.50	1.46
2	AAA	501	9M2	C19-N3	-2.34	1.29	1.35
3	AAA	502	MYA	P2A-O5A	-2.34	1.44	1.55
3	CCC	502	MYA	C4A-N3A	2.33	1.38	1.34
3	BBB	502	MYA	C2M-S1	-2.30	1.70	1.76
2	CCC	501	9M2	N1-N2	2.26	1.41	1.36
3	CCC	502	MYA	P2A-O5A	-2.26	1.44	1.55
3	BBB	502	MYA	O2M-C2M	2.22	1.24	1.21
3	AAA	502	MYA	C2M-S1	-2.21	1.71	1.76
2	AAA	501	9M2	C4-N2	2.13	1.36	1.33
3	AAA	502	MYA	C4A-N9A	-2.12	1.33	1.37
3	BBB	502	MYA	P1A-O3A	2.12	1.61	1.59
3	AAA	502	MYA	O10-C10	2.08	1.46	1.42
2	AAA	501	9M2	C6-C5	2.04	1.42	1.38
2	AAA	501	9M2	C2-C3	2.00	1.53	1.50

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	502	MYA	C3M-C2M-S1	6.58	121.25	113.40
3	CCC	502	MYA	C3M-C2M-S1	6.07	120.64	113.40
3	AAA	502	MYA	C3M-C2M-S1	5.96	120.51	113.40
3	BBB	502	MYA	O2M-C2M-C3M	-5.68	117.42	123.98
2	BBB	501	9M2	C6-C7-C8	4.77	124.80	118.23
3	AAA	502	MYA	C5A-C4A-N3A	-4.58	120.41	126.72
3	BBB	502	MYA	N3A-C2A-N1A	-4.54	121.70	128.58
3	CCC	502	MYA	N3A-C2A-N1A	-4.52	121.74	128.58
3	AAA	502	MYA	N9A-C8A-N7A	-4.48	107.58	113.94
3	CCC	502	MYA	C5A-C4A-N3A	-4.38	120.69	126.72
2	AAA	501	9M2	C6-C5-C4	-4.37	115.58	120.80
2	CCC	501	9M2	C21-N3-C19	4.36	132.07	128.09
2	BBB	501	9M2	C6-C5-C4	-4.14	115.85	120.80
2	AAA	501	9M2	C21-N3-N4	-3.89	113.46	119.29
2	BBB	501	9M2	C3-C2-N	3.76	120.08	112.81
3	AAA	502	MYA	O2M-C2M-C3M	-3.55	119.89	123.98
2	AAA	501	9M2	C1-N-C2	3.52	116.13	110.38
3	CCC	502	MYA	O3A-P2A-O4A	-3.31	100.74	110.70
3	BBB	502	MYA	C5A-C4A-N3A	-3.31	122.16	126.72
3	AAA	502	MYA	C4A-C5A-N7A	-3.24	106.87	110.58
3	CCC	502	MYA	N9A-C8A-N7A	-3.21	109.38	113.94
3	AAA	502	MYA	C4A-N9A-C8A	3.20	109.10	105.74
2	CCC	501	9M2	C21-N3-N4	-3.17	114.54	119.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	502	MYA	N3A-C4A-N9A	3.13	132.49	127.17
3	AAA	502	MYA	C4M-C3M-C2M	-3.07	105.49	112.27
2	BBB	501	9M2	C21-N3-N4	-3.05	114.72	119.29
3	CCC	502	MYA	O2M-C2M-C3M	-3.04	120.47	123.98
3	CCC	502	MYA	O2M-C2M-S1	-2.98	118.89	122.68
2	AAA	501	9M2	C3-C2-N	2.95	118.50	112.81
3	CCC	502	MYA	C7-N8-C9	2.90	127.75	122.55
3	CCC	502	MYA	C13-C11-C10	2.89	113.70	108.77
3	AAA	502	MYA	C5A-N7A-C8A	2.85	107.93	103.45
2	AAA	501	9M2	C8-C7-C10	-2.80	115.92	120.61
3	CCC	502	MYA	P3X-O3X-C3X	-2.74	116.10	123.43
3	BBB	502	MYA	P3X-O3X-C3X	-2.65	116.36	123.43
3	AAA	502	MYA	O3A-P2A-O4A	-2.61	102.84	110.70
3	BBB	502	MYA	C5A-C4A-N9A	2.54	108.58	105.81
2	AAA	501	9M2	C4-N2-N1	2.52	108.94	106.29
3	CCC	502	MYA	C2A-N3A-C4A	2.52	117.99	111.83
3	AAA	502	MYA	O2M-C2M-S1	-2.46	119.55	122.68
2	BBB	501	9M2	C23-C22-N4	2.46	124.17	119.39
3	BBB	502	MYA	C2A-N3A-C4A	2.42	117.73	111.83
3	AAA	502	MYA	C6A-C5A-C4A	2.36	120.41	117.18
2	AAA	501	9M2	C19-N3-N4	2.35	116.78	112.75
3	AAA	502	MYA	C5A-C4A-N9A	2.34	108.36	105.81
3	AAA	502	MYA	N3A-C4A-N9A	2.32	131.12	127.17
2	BBB	501	9M2	C4-N2-N1	2.30	108.70	106.29
3	CCC	502	MYA	C2A-N1A-C6A	2.28	122.48	118.73
3	CCC	502	MYA	O6A-C12-C11	-2.26	106.92	110.55
3	AAA	502	MYA	O5A-P2A-O3A	2.25	113.35	107.27
3	BBB	502	MYA	O6A-C12-C11	-2.24	106.94	110.55
3	BBB	502	MYA	C2A-N1A-C6A	2.24	122.41	118.73
3	CCC	502	MYA	C4A-N9A-C8A	2.22	108.06	105.74
3	CCC	502	MYA	C6-C7-N8	-2.18	107.37	112.00
3	AAA	502	MYA	C6-C7-N8	-2.13	107.47	112.00
3	CCC	502	MYA	C4M-C3M-C2M	-2.12	107.59	112.27
3	CCC	502	MYA	C5A-N7A-C8A	2.12	106.78	103.45
2	BBB	501	9M2	C8-C7-C10	-2.11	117.06	120.61
3	AAA	502	MYA	C13-C11-C10	2.09	112.34	108.77
3	BBB	502	MYA	C4A-C5A-N7A	-2.07	108.21	110.58
2	AAA	501	9M2	C6-C7-C8	2.02	121.01	118.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

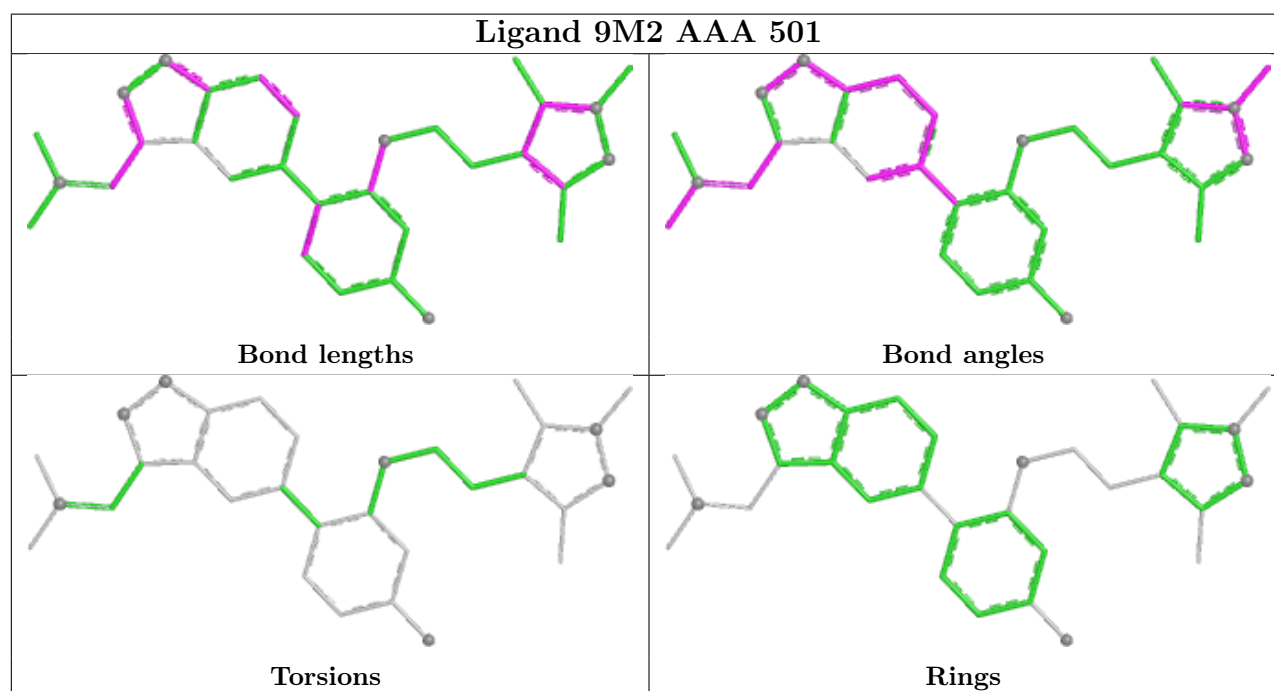
Mol	Chain	Res	Type	Atoms
3	BBB	502	MYA	C6-C7-N8-C9
3	BBB	502	MYA	C5M-C6M-C7M-C8M
3	CCC	502	MYA	C6-C7-N8-C9
3	BBB	502	MYA	C8M-C9M-CAM-CBM

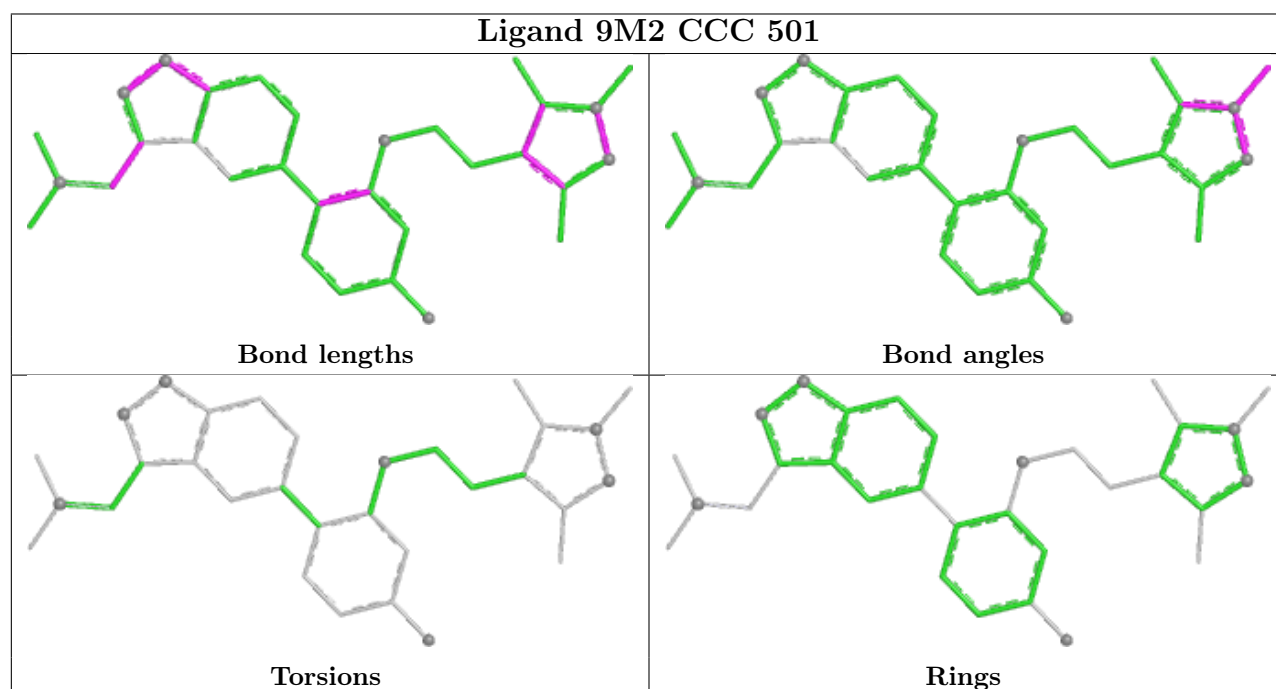
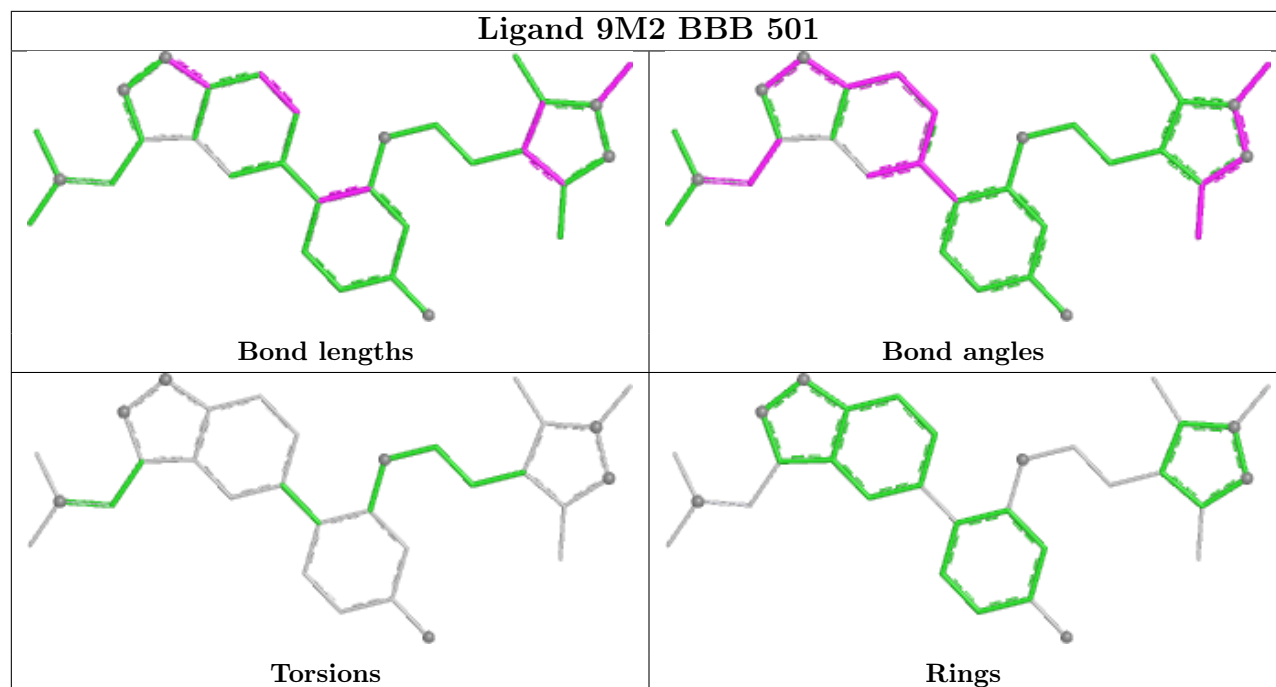
There are no ring outliers.

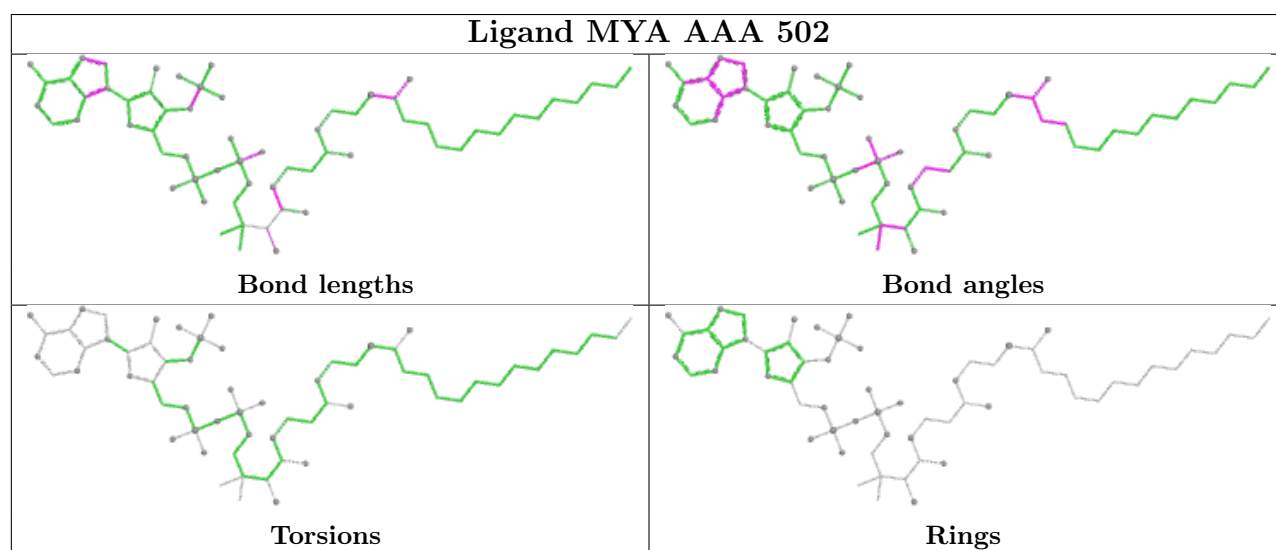
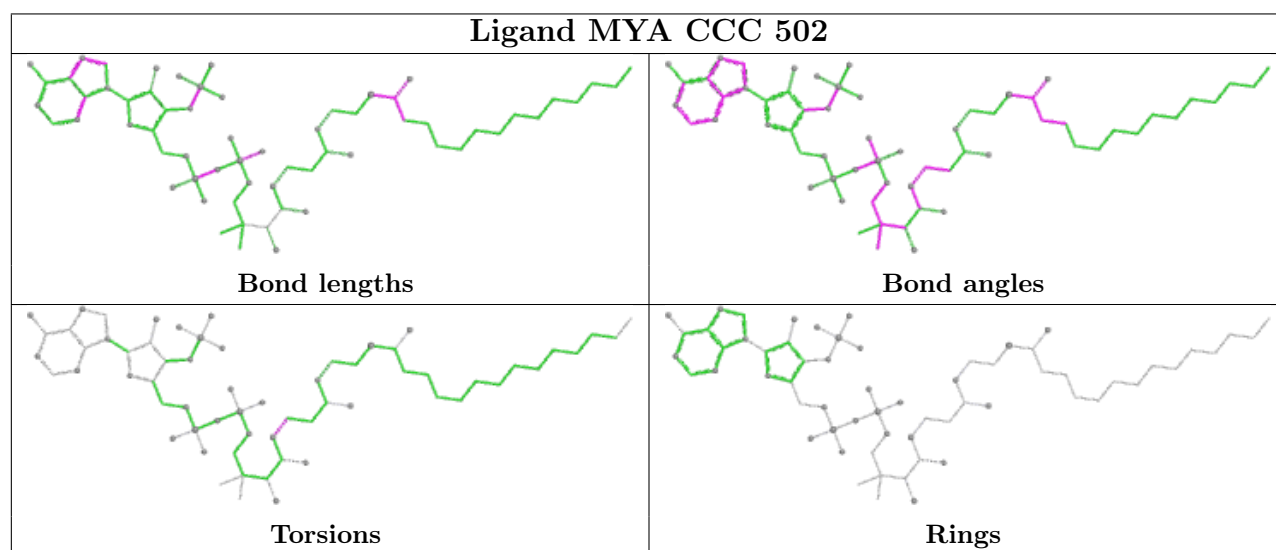
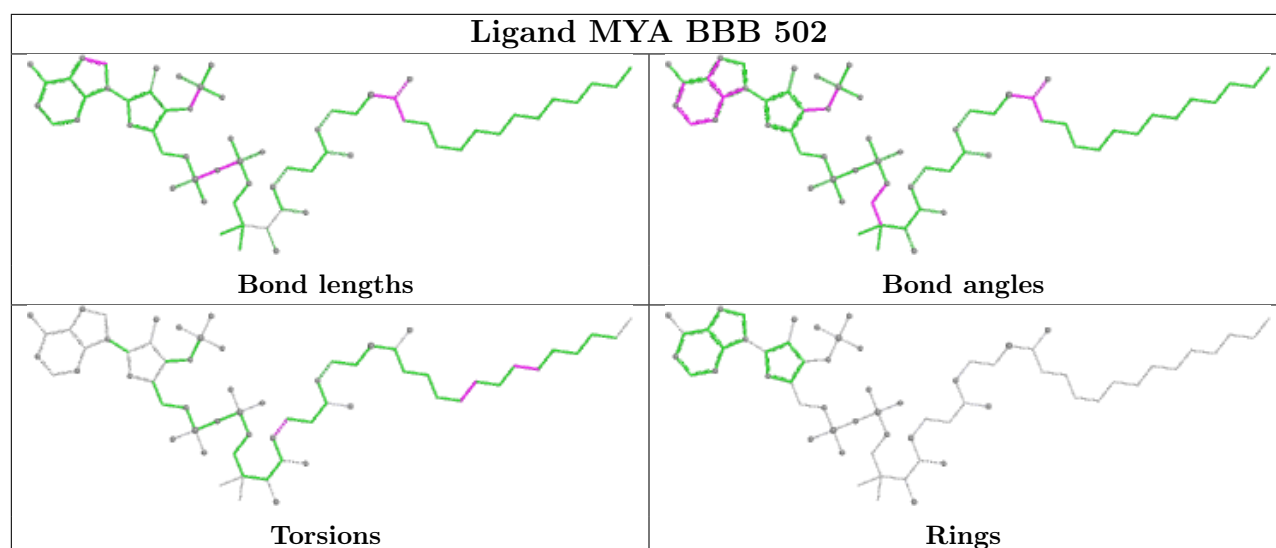
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	504	DMS	3	0
5	BBB	504	DMS	4	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

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	384/388 (98%)	-0.46	2 (0%) 87 90	5, 13, 24, 40	52 (13%)
1	BBB	384/388 (98%)	-0.40	8 (2%) 63 72	7, 13, 28, 42	49 (12%)
1	CCC	369/388 (95%)	-0.40	4 (1%) 78 84	7, 14, 25, 53	44 (11%)
All	All	1137/1164 (97%)	-0.42	14 (1%) 76 83	5, 13, 25, 53	145 (12%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	226	PHE	3.9
1	BBB	232	ARG	3.3
1	AAA	232	ARG	3.2
1	CCC	306	GLY	2.9
1	CCC	227	SER	2.8
1	AAA	323	GLY	2.7
1	BBB	325	ASP	2.6
1	BBB	27	ASP	2.5
1	BBB	226	PHE	2.4
1	BBB	323	GLY	2.3
1	BBB	231	SER	2.2
1	BBB	40	ASN	2.1
1	CCC	123[A]	LYS	2.1
1	BBB	32[A]	TYR	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

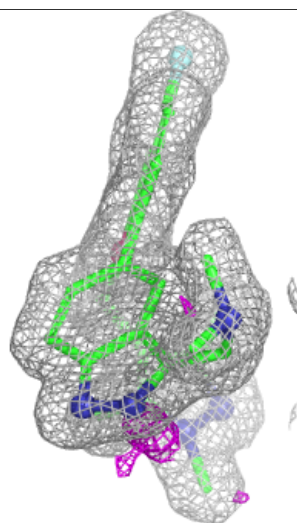
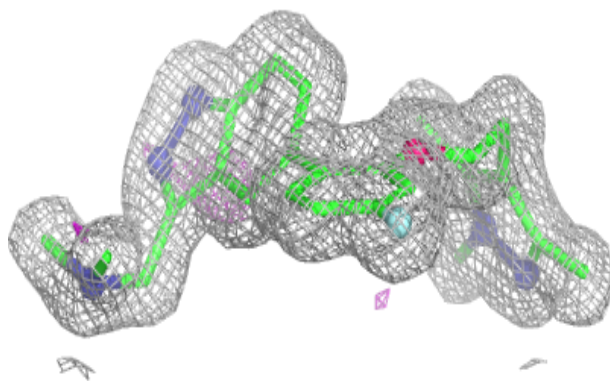
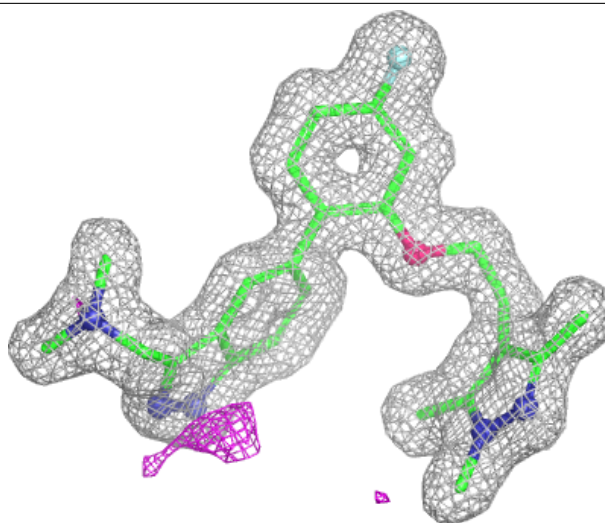
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	AAA	507	5/5	0.55	0.19	54,65,68,81	0
7	SO4	CCC	506	5/5	0.75	0.14	41,52,59,61	0
5	DMS	BBB	504	4/4	0.82	0.22	26,29,31,34	0
5	DMS	AAA	504	4/4	0.86	0.17	14,16,17,20	4
5	DMS	CCC	504	4/4	0.87	0.17	15,18,18,19	4
7	SO4	AAA	506	5/5	0.91	0.12	36,38,45,52	0
2	9M2	BBB	501	31/31	0.97	0.05	11,13,15,16	0
2	9M2	CCC	501	31/31	0.97	0.06	13,16,19,20	0
2	9M2	AAA	501	31/31	0.98	0.05	11,12,15,18	0
4	MG	BBB	503	1/1	0.98	0.05	23,23,23,23	0
3	MYA	CCC	502	63/63	0.99	0.03	9,12,15,18	0
4	MG	AAA	503	1/1	0.99	0.04	20,20,20,20	0
3	MYA	AAA	502	63/63	0.99	0.03	8,11,14,16	0
4	MG	CCC	503	1/1	0.99	0.04	21,21,21,21	0
3	MYA	BBB	502	63/63	0.99	0.04	9,12,15,17	0
6	CL	AAA	505	1/1	1.00	0.01	13,13,13,13	0
6	CL	BBB	505	1/1	1.00	0.01	13,13,13,13	0
6	CL	CCC	505	1/1	1.00	0.04	15,15,15,15	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.

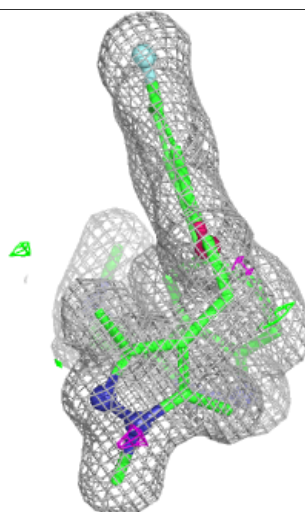
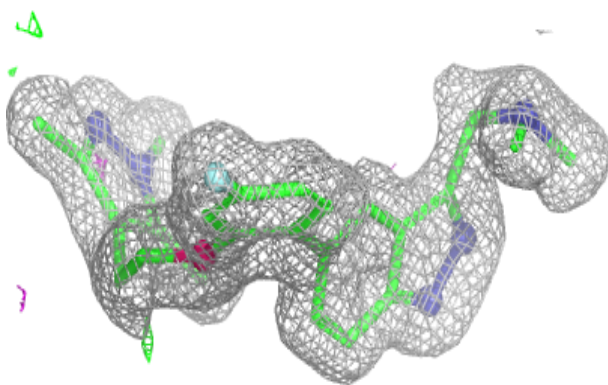
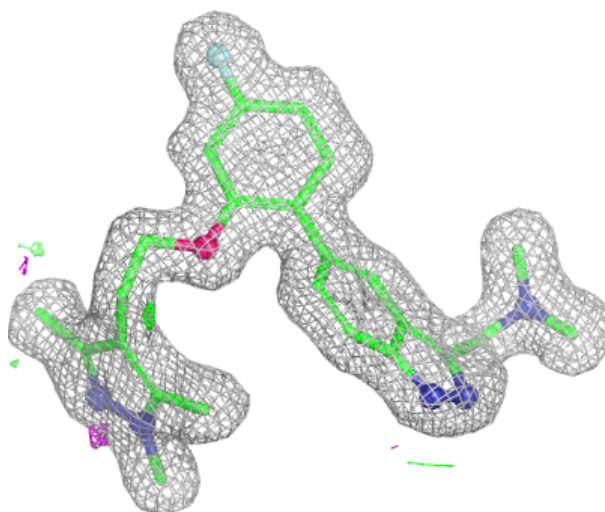
Electron density around 9M2 BBB 501:

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



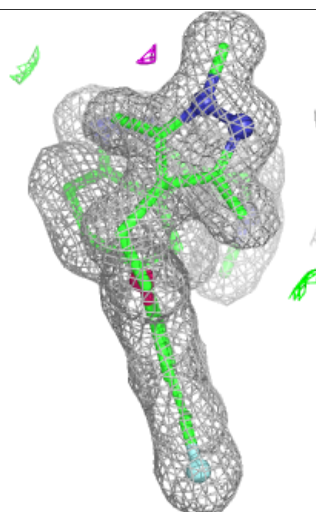
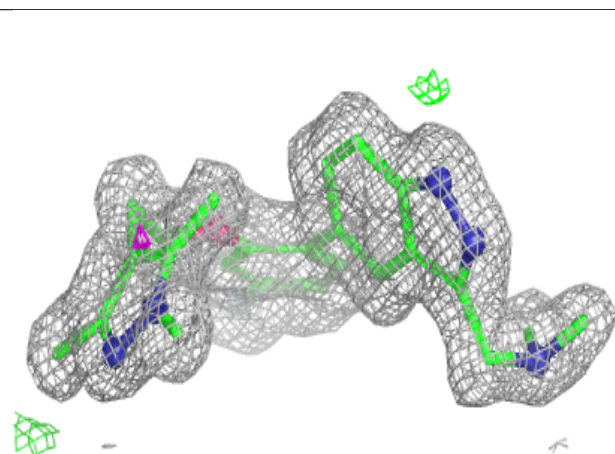
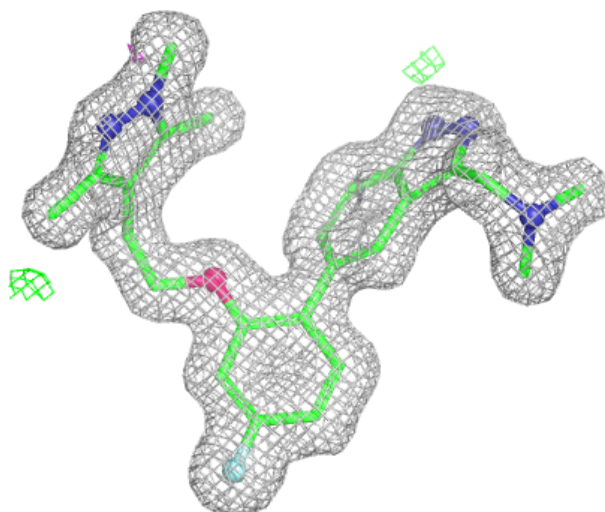
Electron density around 9M2 CCC 501:

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



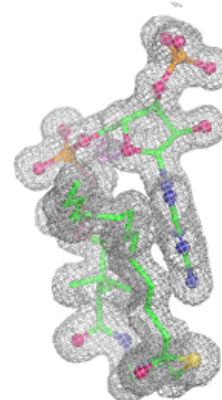
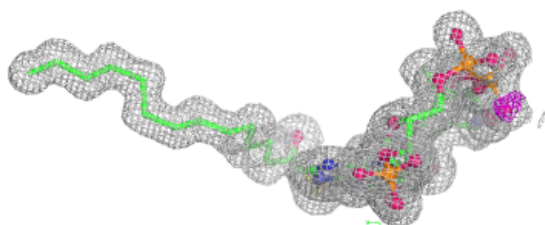
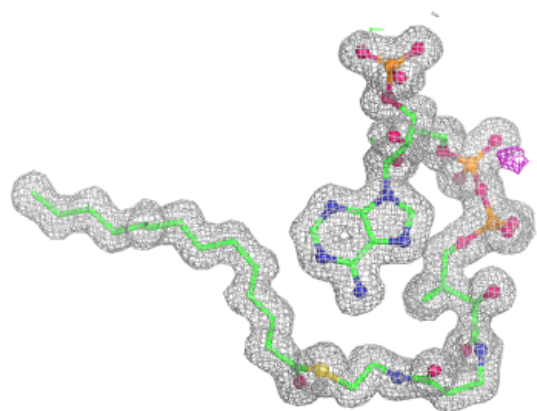
Electron density around 9M2 AAA 501:

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

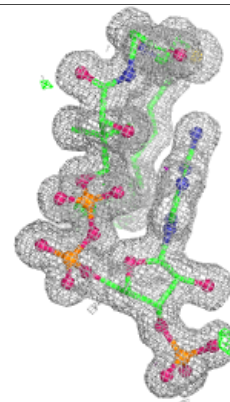
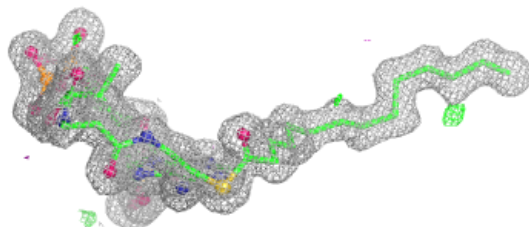
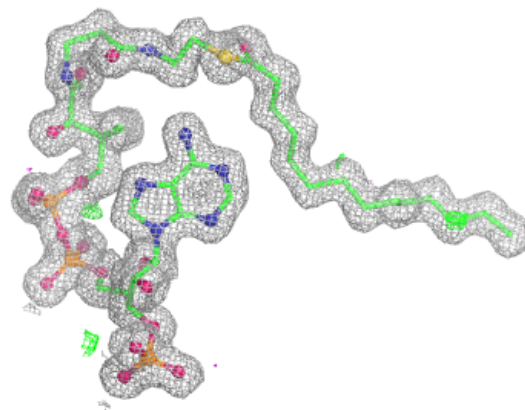


Electron density around MYA CCC 502:

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

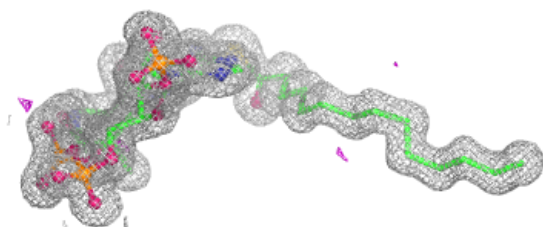
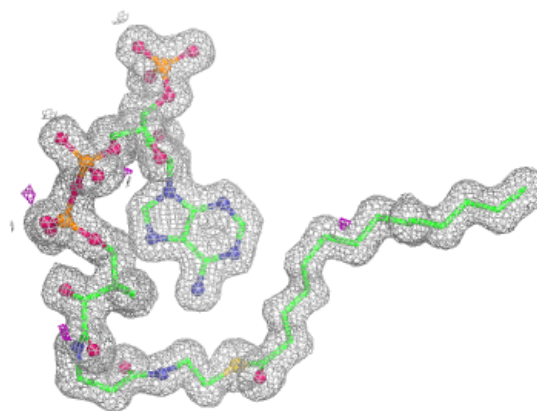
**Electron density around MYA AAA 502:**

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



Electron density around MYA BBB 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.