



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2021 – 12:16 PM EST

PDB ID : 7KMY
Title : Structure of Mtb Lpd bound to 010705
Authors : Lima, C.D.
Deposited on : 2020-11-03
Resolution : 2.21 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 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 : 2.16
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) : 2.16

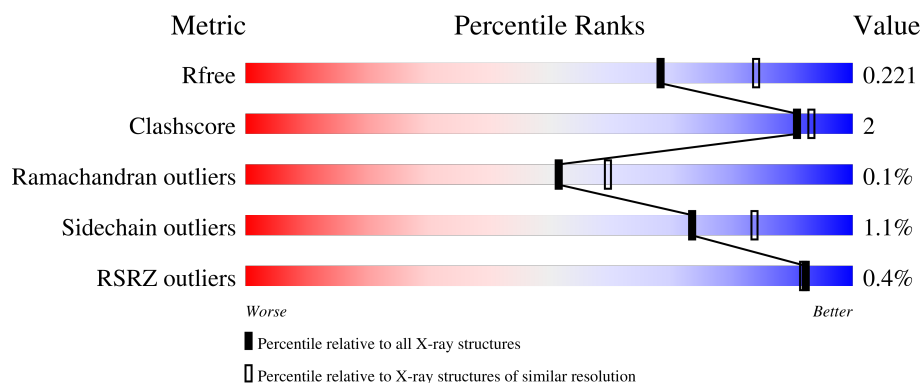
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	466	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 94% 5% </div> </div>
1	B	466	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 95% 5% </div> </div>
1	C	466	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 95% . </div> </div>
1	D	466	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 97% . </div> </div>
1	I	466	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 95% 5% </div> </div>

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Mol	Chain	Length	Quality of chain
1	J	466	<div><div>%</div><div><div></div><div>95%</div><div></div></div><div></div></div>
1	M	466	<div><div></div><div><div></div><div>95%</div><div></div></div><div></div></div>
1	N	466	<div><div></div><div><div></div><div>96%</div><div></div></div><div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30231 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 Dihydrolipoyl dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3475	2202	596	666	11			
1	B	465	Total	C	N	O	S	0	0	0
			3475	2202	596	666	11			
1	C	465	Total	C	N	O	S	0	1	0
			3484	2208	598	667	11			
1	D	465	Total	C	N	O	S	0	0	0
			3475	2202	596	666	11			
1	I	465	Total	C	N	O	S	0	0	0
			3475	2202	596	666	11			
1	J	465	Total	C	N	O	S	0	0	0
			3475	2202	596	666	11			
1	M	465	Total	C	N	O	S	0	0	0
			3475	2202	596	666	11			
1	N	465	Total	C	N	O	S	0	0	0
			3475	2202	596	666	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P9WHH9
A	0	SER	-	expression tag	UNP P9WHH9
B	-1	GLY	-	expression tag	UNP P9WHH9
B	0	SER	-	expression tag	UNP P9WHH9
C	-1	GLY	-	expression tag	UNP P9WHH9
C	0	SER	-	expression tag	UNP P9WHH9
D	-1	GLY	-	expression tag	UNP P9WHH9
D	0	SER	-	expression tag	UNP P9WHH9
I	-1	GLY	-	expression tag	UNP P9WHH9
I	0	SER	-	expression tag	UNP P9WHH9
J	-1	GLY	-	expression tag	UNP P9WHH9
J	0	SER	-	expression tag	UNP P9WHH9
M	-1	GLY	-	expression tag	UNP P9WHH9

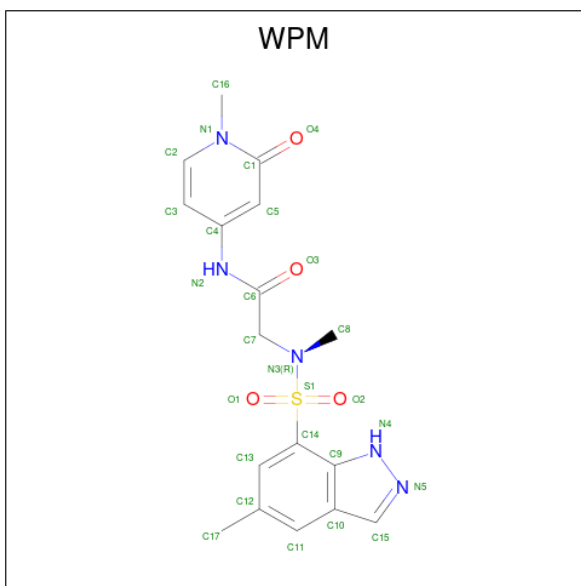
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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	SER	-	expression tag	UNP P9WHH9
N	-1	GLY	-	expression tag	UNP P9WHH9
N	0	SER	-	expression tag	UNP P9WHH9

- # FAD

- Molecule 3 is N 2 -methyl-N 2 -[(5-methyl-1H-indazol-7-yl)sulfonyl]-N-(1-methyl-2-oxo-1,2-dihydropyridin-4-yl)glycinamide (three-letter code: WPM) (formula: C₁₇H₁₉N₅O₄S) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	17	5	4	1		
3	A	1	Total	C	N	O	S	0	0
			27	17	5	4	1		
3	C	1	Total	C	N	O	S	0	0
			27	17	5	4	1		
3	D	1	Total	C	N	O	S	0	0
			27	17	5	4	1		
3	J	1	Total	C	N	O	S	0	0
			27	17	5	4	1		
3	J	1	Total	C	N	O	S	0	0
			27	17	5	4	1		
3	M	1	Total	C	N	O	S	0	0
			27	17	5	4	1		
3	M	1	Total	C	N	O	S	0	0
			27	17	5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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

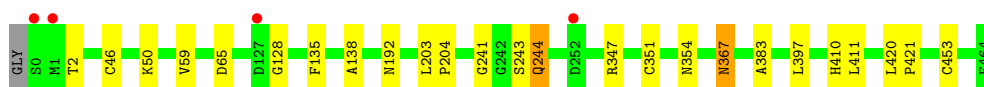
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	195	Total	O	0	0
			195	195		
5	B	187	Total	O	0	0
			187	187		
5	C	201	Total	O	0	0
			201	201		
5	D	201	Total	O	0	0
			201	201		
5	I	192	Total	O	0	0
			192	192		
5	J	180	Total	O	0	0
			180	180		
5	M	215	Total	O	0	0
			215	215		
5	N	189	Total	O	0	0
			189	189		

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: Dihydrolipoyl dehydrogenase



- Molecule 1: Dihydrolipoyl dehydrogenase



- Molecule 1: Dihydrolipoyl dehydrogenase



- Molecule 1: Dihydrolipoyl dehydrogenase

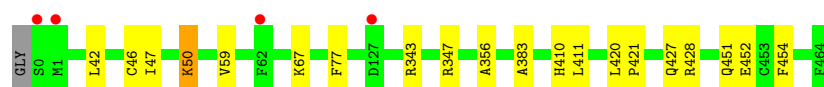


- Molecule 1: Dihydrolipoyl dehydrogenase



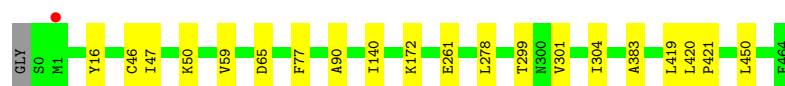
- Molecule 1: Dihydrolipoyl dehydrogenase

Chain J:  95%



• Molecule 1: Dihydrolipoyl dehydrogenase

Chain M:  95%



• Molecule 1: Dihydrolipoyl dehydrogenase

Chain N:  96%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.51Å 178.52Å 226.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.22 – 2.21 113.22 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.5 (113.22-2.21) 96.5 (113.22-2.21)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.181 , 0.218 0.186 , 0.221	Depositor DCC
R_{free} test set	10578 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30231	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: GOL, FAD, WPM

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	0.26	0/3537	0.44	0/4801
1	B	0.25	0/3537	0.44	0/4801
1	C	0.25	0/3546	0.44	0/4812
1	D	0.24	0/3537	0.44	0/4801
1	I	0.25	0/3537	0.44	0/4801
1	J	0.25	0/3537	0.44	0/4801
1	M	0.24	0/3537	0.44	0/4801
1	N	0.25	0/3537	0.44	0/4801
All	All	0.25	0/28305	0.44	0/38419

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	3475	0	3478	15	0
1	B	3475	0	3478	14	0
1	C	3484	0	3490	14	0
1	D	3475	0	3478	8	0
1	I	3475	0	3478	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3475	0	3478	14	0
1	M	3475	0	3478	11	0
1	N	3475	0	3478	12	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
2	I	53	0	31	1	0
2	J	53	0	31	0	0
2	M	53	0	31	0	0
2	N	53	0	31	1	0
3	A	54	0	0	0	0
3	C	27	0	0	0	0
3	D	27	0	0	0	0
3	J	54	0	0	0	0
3	M	54	0	0	0	0
4	A	30	0	40	1	0
4	B	42	0	56	2	0
4	C	42	0	56	1	0
4	D	12	0	16	0	0
4	I	24	0	32	0	0
4	J	36	0	48	3	0
4	M	24	0	32	1	0
4	N	12	0	16	0	0
5	A	195	0	0	2	1
5	B	187	0	0	3	2
5	C	201	0	0	3	0
5	D	201	0	0	2	2
5	I	192	0	0	4	2
5	J	180	0	0	2	0
5	M	215	0	0	1	1
5	N	189	0	0	1	0
All	All	30231	0	28380	98	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (98) 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:A:367:ASN:OD1	4:A:508:GOL:O3	1.85	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:505:GOL:O3	5:J:601:HOH:O	2.00	0.78
1:I:47:ILE:HD12	1:J:383:ALA:HB1	1.69	0.73
1:I:383:ALA:HB1	1:J:47:ILE:HD12	1.69	0.73
1:A:383:ALA:HB1	1:B:47:ILE:HD12	1.74	0.70
1:B:185:GLU:OE1	4:B:506:GOL:O3	2.08	0.70
1:M:299:THR:HG23	1:M:301:VAL:H	1.58	0.68
1:I:219:GLU:OE1	5:I:601:HOH:O	2.11	0.68
1:M:383:ALA:HB1	1:N:47:ILE:HD12	1.76	0.67
1:M:299:THR:HG22	1:M:304:ILE:O	1.96	0.66
1:M:65:ASP:OD2	4:M:507:GOL:O3	2.13	0.65
1:B:464:PHE:O	5:B:601:HOH:O	2.15	0.64
1:C:127:ASP:OD1	5:C:601:HOH:O	2.15	0.63
1:A:244:GLN:OE1	5:A:601:HOH:O	2.16	0.62
1:C:47:ILE:HD12	1:D:383:ALA:HB1	1.81	0.61
1:M:261:GLU:OE2	5:M:601:HOH:O	2.16	0.61
1:I:430:ASP:OD2	5:I:602:HOH:O	2.16	0.61
1:J:59:VAL:HG22	1:J:77:PHE:CD2	2.37	0.60
1:M:59:VAL:HG22	1:M:77:PHE:CD1	2.37	0.59
1:B:298:ARG:NH2	5:B:602:HOH:O	2.27	0.58
1:B:59:VAL:HG22	1:B:77:PHE:CG	2.39	0.57
1:I:428:ARG:NH2	5:I:605:HOH:O	2.36	0.57
1:C:362:GLU:OE2	1:C:366:ARG:NH1	2.39	0.56
1:J:428:ARG:NH1	5:J:604:HOH:O	2.41	0.53
1:N:148:LEU:HD21	1:N:154:LEU:HD21	1.91	0.53
1:J:427:GLN:O	4:J:507:GOL:O3	2.27	0.52
1:C:428:ARG:NH1	5:C:604:HOH:O	2.43	0.50
1:I:59:VAL:HG22	1:I:77:PHE:CD1	2.47	0.50
1:D:354:ASN:HB2	1:D:416:VAL:HG22	1.93	0.49
1:B:103:LYS:NZ	5:B:608:HOH:O	2.45	0.49
1:M:420:LEU:N	1:M:421:PRO:CD	2.75	0.49
1:D:50:LYS:NZ	2:D:501:FAD:O4	2.36	0.49
1:N:9:LEU:HD22	2:N:501:FAD:N1A	2.26	0.49
1:I:411:LEU:HD12	1:I:411:LEU:N	2.28	0.48
1:D:428:ARG:NH2	5:D:606:HOH:O	2.46	0.48
1:J:420:LEU:N	1:J:421:PRO:CD	2.76	0.48
1:C:420:LEU:N	1:C:421:PRO:CD	2.77	0.48
1:C:9:LEU:HD22	2:C:501:FAD:N1A	2.29	0.48
1:B:420:LEU:N	1:B:421:PRO:CD	2.76	0.48
1:B:348:ALA:O	4:B:506:GOL:H32	2.14	0.47
1:N:420:LEU:N	1:N:421:PRO:CD	2.77	0.47
1:B:411:LEU:HD12	1:B:411:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:LEU:N	1:D:421:PRO:CD	2.76	0.47
1:D:78:ASP:OD2	5:D:601:HOH:O	2.20	0.47
1:A:420:LEU:N	1:A:421:PRO:CD	2.77	0.47
1:B:170:LEU:HD22	1:B:190:LEU:HD22	1.97	0.47
1:J:343:ARG:O	1:J:347:ARG:NH2	2.48	0.47
1:A:411:LEU:HD12	1:A:411:LEU:N	2.30	0.46
1:I:420:LEU:N	1:I:421:PRO:CD	2.77	0.46
1:J:356:ALA:HB1	1:J:420:LEU:HD11	1.97	0.46
1:N:411:LEU:N	1:N:411:LEU:HD12	2.30	0.46
1:M:50:LYS:HD2	1:M:50:LYS:N	2.31	0.46
1:N:395:VAL:HG11	1:N:450:LEU:HD23	1.98	0.46
1:B:9:LEU:HD13	1:B:121:LEU:HD21	1.97	0.46
1:A:65:ASP:OD1	5:A:602:HOH:O	2.21	0.45
1:I:9:LEU:HD22	2:I:501:FAD:N1A	2.31	0.45
1:B:50:LYS:N	1:B:50:LYS:HD2	2.32	0.45
1:J:410:HIS:C	1:J:411:LEU:HD12	2.37	0.45
1:I:47:ILE:HD12	1:J:383:ALA:CB	2.43	0.44
1:C:59:VAL:HG22	1:C:77:PHE:CD2	2.52	0.44
1:A:397:LEU:HD12	1:A:453:CYS:HB3	1.99	0.44
1:J:452:GLU:OE1	4:J:504:GOL:O3	2.19	0.44
1:M:140:ILE:HD13	1:M:278:LEU:HD21	1.99	0.44
1:J:42:LEU:HA	1:J:47:ILE:HG12	1.99	0.44
1:N:64:LYS:N	5:N:605:HOH:O	2.49	0.44
1:N:410:HIS:C	1:N:411:LEU:HD12	2.38	0.44
1:C:59:VAL:O	1:C:63:THR:HG23	2.17	0.43
1:A:135:PHE:CE1	1:A:138:ALA:HB2	2.54	0.43
1:C:430:ASP:HB2	5:C:779:HOH:O	2.19	0.43
1:M:47:ILE:HG21	1:M:90:ALA:HA	1.99	0.43
1:I:426:ALA:HB2	1:I:436:LEU:HD21	2.00	0.43
1:N:42:LEU:HA	1:N:47:ILE:HG12	2.00	0.43
1:N:50:LYS:HD2	1:N:50:LYS:N	2.34	0.43
1:D:50:LYS:HD2	1:D:50:LYS:N	2.34	0.43
1:A:383:ALA:HB1	1:B:47:ILE:CD1	2.45	0.43
1:C:272:ASN:HA	4:C:506:GOL:H32	2.02	0.42
1:A:351:CYS:O	1:A:354:ASN:ND2	2.48	0.42
1:I:405:GLU:OE1	5:I:602:HOH:O	2.21	0.42
1:C:59:VAL:HG22	1:C:77:PHE:CG	2.54	0.42
1:N:287:ASP:N	1:N:287:ASP:OD1	2.51	0.42
1:D:411:LEU:N	1:D:411:LEU:HD12	2.35	0.42
1:I:241:GLY:O	1:I:243:SER:N	2.53	0.42
1:I:59:VAL:HG22	1:I:77:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:451:GLN:HA	1:J:454:PHE:CD1	2.55	0.42
1:A:50:LYS:HD2	1:A:50:LYS:N	2.35	0.41
1:A:59:VAL:HG11	1:A:192:ASN:O	2.21	0.41
1:B:410:HIS:C	1:B:411:LEU:HD12	2.40	0.41
1:C:62:PHE:O	1:C:66:ALA:HB2	2.20	0.41
1:J:50:LYS:N	1:J:50:LYS:HD2	2.35	0.41
1:A:203:LEU:HB3	1:A:204:PRO:HD2	2.03	0.41
1:A:410:HIS:C	1:A:411:LEU:HD12	2.41	0.41
1:I:42:LEU:HA	1:I:47:ILE:HG12	2.03	0.41
1:N:343:ARG:O	1:N:347:ARG:NH2	2.54	0.41
1:C:411:LEU:N	1:C:411:LEU:HD12	2.36	0.40
1:C:451:GLN:HA	1:C:454:PHE:CD1	2.56	0.40
1:A:241:GLY:O	1:A:243:SER:N	2.52	0.40
1:I:11:ALA:HA	1:I:31:ILE:HD11	2.03	0.40
1:M:419:LEU:HB3	1:M:450:LEU:HD11	2.02	0.40

All (4) 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)
5:A:752:HOH:O	5:B:768:HOH:O[4_455]	1.89	0.31
5:D:766:HOH:O	5:I:743:HOH:O[2_555]	2.06	0.14
5:B:771:HOH:O	5:M:787:HOH:O[2_454]	2.09	0.11
5:D:625:HOH:O	5:I:612:HOH:O[2_555]	2.13	0.07

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	463/466 (99%)	448 (97%)	14 (3%)	1 (0%)	47 54
1	B	463/466 (99%)	445 (96%)	18 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	464/466 (100%)	448 (97%)	16 (3%)	0	100	100
1	D	463/466 (99%)	448 (97%)	14 (3%)	1 (0%)	47	54
1	I	463/466 (99%)	444 (96%)	19 (4%)	0	100	100
1	J	463/466 (99%)	449 (97%)	14 (3%)	0	100	100
1	M	463/466 (99%)	443 (96%)	20 (4%)	0	100	100
1	N	463/466 (99%)	450 (97%)	13 (3%)	0	100	100
All	All	3705/3728 (99%)	3575 (96%)	128 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	D	459	GLY

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	361/361 (100%)	356 (99%)	5 (1%)	67	78
1	B	361/361 (100%)	355 (98%)	6 (2%)	60	73
1	C	362/361 (100%)	360 (99%)	2 (1%)	86	92
1	D	361/361 (100%)	358 (99%)	3 (1%)	81	89
1	I	361/361 (100%)	356 (99%)	5 (1%)	67	78
1	J	361/361 (100%)	358 (99%)	3 (1%)	81	89
1	M	361/361 (100%)	358 (99%)	3 (1%)	81	89
1	N	361/361 (100%)	357 (99%)	4 (1%)	73	84
All	All	2889/2888 (100%)	2858 (99%)	31 (1%)	73	84

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	46	CYS
1	A	244	GLN
1	A	347	ARG
1	A	367	ASN
1	B	16	TYR
1	B	46	CYS
1	B	50	LYS
1	B	288	ARG
1	B	347	ARG
1	B	460	HIS
1	C	46	CYS
1	C	288	ARG
1	D	46	CYS
1	D	196	ASP
1	D	347	ARG
1	I	16	TYR
1	I	46	CYS
1	I	50	LYS
1	I	67	LYS
1	I	347	ARG
1	J	46	CYS
1	J	50	LYS
1	J	67	LYS
1	M	16	TYR
1	M	46	CYS
1	M	172	LYS
1	N	46	CYS
1	N	50	LYS
1	N	67	LYS
1	N	162	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	N	414	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

53 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	C	504	-	5,5,5	0.92	0	5,5,5	0.96	0
4	GOL	N	503	-	5,5,5	1.05	0	5,5,5	0.65	0
4	GOL	D	503	-	5,5,5	0.88	0	5,5,5	0.97	0
4	GOL	M	506	-	5,5,5	0.92	0	5,5,5	0.96	0
3	WPM	D	502	-	27,29,29	2.06	6 (22%)	30,43,43	1.49	4 (13%)
4	GOL	J	505	-	5,5,5	0.91	0	5,5,5	0.93	0
4	GOL	A	504	-	5,5,5	0.96	0	5,5,5	0.97	0
2	FAD	A	501	-	51,58,58	1.21	5 (9%)	60,89,89	2.19	7 (11%)
3	WPM	M	502	-	27,29,29	2.03	6 (22%)	30,43,43	1.46	4 (13%)
4	GOL	M	504	-	5,5,5	0.84	0	5,5,5	1.02	0
2	FAD	N	501	-	51,58,58	1.23	5 (9%)	60,89,89	2.19	7 (11%)
4	GOL	J	507	-	5,5,5	0.97	0	5,5,5	0.91	0
4	GOL	B	502	-	5,5,5	0.90	0	5,5,5	0.99	0
3	WPM	A	502	-	27,29,29	2.08	6 (22%)	30,43,43	1.50	5 (16%)
4	GOL	A	507	-	5,5,5	0.92	0	5,5,5	0.98	0
3	WPM	C	502	-	27,29,29	2.05	6 (22%)	30,43,43	1.50	4 (13%)
4	GOL	I	502	-	5,5,5	0.96	0	5,5,5	0.93	0
4	GOL	M	505	-	5,5,5	0.92	0	5,5,5	0.98	0
4	GOL	C	505	-	5,5,5	0.93	0	5,5,5	0.99	0
4	GOL	A	505	-	5,5,5	0.83	0	5,5,5	0.97	0
4	GOL	B	505	-	5,5,5	0.92	0	5,5,5	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	508	-	5,5,5	1.05	0	5,5,5	0.70	0
4	GOL	C	508	-	5,5,5	0.96	0	5,5,5	0.91	0
2	FAD	I	501	-	51,58,58	1.22	5 (9%)	60,89,89	2.17	7 (11%)
4	GOL	M	507	-	5,5,5	1.35	0	5,5,5	0.70	0
4	GOL	J	508	-	5,5,5	0.93	0	5,5,5	0.94	0
4	GOL	J	504	-	5,5,5	0.91	0	5,5,5	0.98	0
4	GOL	C	507	-	5,5,5	0.89	0	5,5,5	0.99	0
4	GOL	C	503	-	5,5,5	0.92	0	5,5,5	0.91	0
4	GOL	B	507	-	5,5,5	0.91	0	5,5,5	0.90	0
3	WPM	J	502	-	27,29,29	2.04	6 (22%)	30,43,43	1.48	3 (10%)
3	WPM	M	503	-	27,29,29	2.06	6 (22%)	30,43,43	1.51	4 (13%)
4	GOL	B	503	-	5,5,5	0.94	0	5,5,5	0.90	0
4	GOL	I	505	-	5,5,5	0.97	0	5,5,5	0.86	0
4	GOL	N	502	-	5,5,5	0.86	0	5,5,5	0.97	0
4	GOL	B	504	-	5,5,5	0.89	0	5,5,5	0.98	0
2	FAD	B	501	-	51,58,58	1.23	5 (9%)	60,89,89	2.20	7 (11%)
3	WPM	J	503	-	27,29,29	2.07	6 (22%)	30,43,43	1.48	4 (13%)
4	GOL	J	506	-	5,5,5	0.90	0	5,5,5	0.94	0
2	FAD	C	501	-	51,58,58	1.22	5 (9%)	60,89,89	2.18	7 (11%)
3	WPM	A	503	-	27,29,29	2.05	6 (22%)	30,43,43	1.53	5 (16%)
2	FAD	J	501	-	51,58,58	1.22	5 (9%)	60,89,89	2.20	7 (11%)
4	GOL	B	506	-	5,5,5	0.93	0	5,5,5	0.88	0
4	GOL	I	503	-	5,5,5	0.95	0	5,5,5	0.93	0
2	FAD	M	501	-	51,58,58	1.21	5 (9%)	60,89,89	2.19	7 (11%)
2	FAD	D	501	-	51,58,58	1.23	5 (9%)	60,89,89	2.18	7 (11%)
4	GOL	A	506	-	5,5,5	1.04	0	5,5,5	0.77	0
4	GOL	C	509	-	5,5,5	1.11	0	5,5,5	0.63	0
4	GOL	C	506	-	5,5,5	1.03	0	5,5,5	0.79	0
4	GOL	D	504	-	5,5,5	0.92	0	5,5,5	0.94	0
4	GOL	J	509	-	5,5,5	1.10	0	5,5,5	0.70	0
4	GOL	I	504	-	5,5,5	0.90	0	5,5,5	0.99	0
4	GOL	A	508	-	5,5,5	1.08	0	5,5,5	0.80	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
4	GOL	C	504	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	N	503	-	-	2/4/4/4	-
4	GOL	D	503	-	-	0/4/4/4	-
4	GOL	M	506	-	-	2/4/4/4	-
3	WPM	D	502	-	-	1/20/20/20	0/3/3/3
4	GOL	J	505	-	-	2/4/4/4	-
4	GOL	A	504	-	-	2/4/4/4	-
2	FAD	A	501	-	-	3/30/50/50	0/6/6/6
3	WPM	M	502	-	-	1/20/20/20	0/3/3/3
4	GOL	M	504	-	-	2/4/4/4	-
2	FAD	N	501	-	-	3/30/50/50	0/6/6/6
4	GOL	J	507	-	-	2/4/4/4	-
4	GOL	B	502	-	-	0/4/4/4	-
3	WPM	A	502	-	-	2/20/20/20	0/3/3/3
4	GOL	A	507	-	-	1/4/4/4	-
3	WPM	C	502	-	-	2/20/20/20	0/3/3/3
4	GOL	I	502	-	-	2/4/4/4	-
4	GOL	M	505	-	-	2/4/4/4	-
4	GOL	C	505	-	-	2/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-
4	GOL	B	505	-	-	2/4/4/4	-
4	GOL	B	508	-	-	2/4/4/4	-
4	GOL	C	508	-	-	2/4/4/4	-
2	FAD	I	501	-	-	3/30/50/50	0/6/6/6
4	GOL	M	507	-	-	4/4/4/4	-
4	GOL	J	508	-	-	2/4/4/4	-
4	GOL	J	504	-	-	0/4/4/4	-
4	GOL	C	507	-	-	3/4/4/4	-
4	GOL	C	503	-	-	2/4/4/4	-
4	GOL	B	507	-	-	2/4/4/4	-
3	WPM	J	502	-	-	1/20/20/20	0/3/3/3
3	WPM	M	503	-	-	1/20/20/20	0/3/3/3
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	I	505	-	-	2/4/4/4	-
4	GOL	N	502	-	-	2/4/4/4	-
4	GOL	B	504	-	-	0/4/4/4	-
2	FAD	B	501	-	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WPM	J	503	-	-	1/20/20/20	0/3/3/3
4	GOL	J	506	-	-	2/4/4/4	-
2	FAD	C	501	-	-	2/30/50/50	0/6/6/6
3	WPM	A	503	-	-	1/20/20/20	0/3/3/3
2	FAD	J	501	-	-	2/30/50/50	0/6/6/6
4	GOL	B	506	-	-	2/4/4/4	-
4	GOL	I	503	-	-	1/4/4/4	-
2	FAD	M	501	-	-	2/30/50/50	0/6/6/6
2	FAD	D	501	-	-	2/30/50/50	0/6/6/6
4	GOL	A	506	-	-	2/4/4/4	-
4	GOL	C	509	-	-	3/4/4/4	-
4	GOL	C	506	-	-	2/4/4/4	-
4	GOL	D	504	-	-	2/4/4/4	-
4	GOL	J	509	-	-	4/4/4/4	-
4	GOL	I	504	-	-	2/4/4/4	-
4	GOL	A	508	-	-	2/4/4/4	-

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	501	FAD	C4X-C10	5.59	1.44	1.38
2	N	501	FAD	C4X-C10	5.58	1.44	1.38
2	D	501	FAD	C4X-C10	5.53	1.44	1.38
2	B	501	FAD	C4X-C10	5.52	1.44	1.38
2	M	501	FAD	C4X-C10	5.50	1.44	1.38
2	J	501	FAD	C4X-C10	5.50	1.44	1.38
2	A	501	FAD	C4X-C10	5.46	1.44	1.38
2	C	501	FAD	C4X-C10	5.39	1.44	1.38
3	J	503	WPM	S1-N3	5.24	1.77	1.63
3	M	502	WPM	S1-N3	5.20	1.77	1.63
3	J	502	WPM	S1-N3	5.16	1.77	1.63
3	C	502	WPM	S1-N3	5.15	1.77	1.63
3	A	503	WPM	S1-N3	5.11	1.77	1.63
3	A	502	WPM	S1-N3	5.10	1.77	1.63
3	D	502	WPM	S1-N3	5.09	1.77	1.63
3	M	503	WPM	S1-N3	5.08	1.77	1.63
3	J	503	WPM	C3-C4	4.37	1.46	1.39
3	A	502	WPM	C3-C4	4.35	1.46	1.39
3	M	503	WPM	C3-C4	4.34	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	WPM	C3-C4	4.33	1.46	1.39
3	C	502	WPM	C3-C4	4.33	1.46	1.39
3	J	502	WPM	C3-C4	4.31	1.46	1.39
3	D	502	WPM	C3-C4	4.26	1.46	1.39
3	M	502	WPM	C3-C4	4.24	1.46	1.39
3	A	502	WPM	C14-C9	-3.88	1.40	1.42
3	D	502	WPM	O1-S1	3.70	1.47	1.43
3	J	503	WPM	C5-C4	-3.69	1.36	1.40
3	A	502	WPM	C5-C4	-3.68	1.36	1.40
3	A	503	WPM	C14-C9	-3.65	1.40	1.42
3	D	502	WPM	C5-C4	-3.63	1.36	1.40
3	C	502	WPM	C14-C9	-3.61	1.40	1.42
3	M	502	WPM	C5-C4	-3.60	1.36	1.40
3	M	503	WPM	C5-C4	-3.60	1.36	1.40
3	M	503	WPM	O2-S1	3.58	1.47	1.43
3	A	503	WPM	C5-C4	-3.55	1.36	1.40
3	M	503	WPM	O1-S1	3.54	1.47	1.43
3	J	503	WPM	O2-S1	3.50	1.47	1.43
3	J	502	WPM	C5-C4	-3.49	1.36	1.40
3	D	502	WPM	O2-S1	3.48	1.47	1.43
3	C	502	WPM	C5-C4	-3.47	1.36	1.40
3	A	502	WPM	O1-S1	3.44	1.47	1.43
3	A	503	WPM	O1-S1	3.44	1.47	1.43
3	C	502	WPM	O1-S1	3.43	1.47	1.43
3	A	502	WPM	O2-S1	3.43	1.47	1.43
3	J	503	WPM	O1-S1	3.42	1.47	1.43
3	M	502	WPM	O2-S1	3.42	1.47	1.43
3	A	503	WPM	O2-S1	3.40	1.47	1.43
3	J	502	WPM	O1-S1	3.39	1.47	1.43
3	M	502	WPM	O1-S1	3.39	1.47	1.43
3	J	502	WPM	O2-S1	3.39	1.47	1.43
3	C	502	WPM	O2-S1	3.38	1.47	1.43
3	D	502	WPM	C14-C9	-3.35	1.40	1.42
3	J	502	WPM	C14-C9	-3.34	1.40	1.42
3	M	503	WPM	C14-C9	-3.33	1.40	1.42
2	C	501	FAD	C4-N3	3.28	1.38	1.33
2	N	501	FAD	C4-N3	3.24	1.38	1.33
3	J	503	WPM	C14-C9	-3.24	1.40	1.42
2	A	501	FAD	C4-N3	3.24	1.38	1.33
2	J	501	FAD	C4-N3	3.17	1.38	1.33
2	I	501	FAD	C4-N3	3.16	1.38	1.33
2	B	501	FAD	C4-N3	3.16	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C4-N3	3.15	1.38	1.33
2	M	501	FAD	C4-N3	3.14	1.38	1.33
3	M	502	WPM	C14-C9	-3.04	1.40	1.42
2	C	501	FAD	C4-C4X	2.49	1.45	1.41
2	M	501	FAD	C4-C4X	2.48	1.45	1.41
2	J	501	FAD	C4-C4X	2.45	1.45	1.41
2	I	501	FAD	C4-C4X	2.41	1.45	1.41
2	D	501	FAD	C5X-N5	2.39	1.39	1.35
2	C	501	FAD	C5X-N5	2.37	1.39	1.35
2	N	501	FAD	C5X-N5	2.35	1.39	1.35
2	B	501	FAD	C4-C4X	2.33	1.45	1.41
2	N	501	FAD	C4-C4X	2.33	1.45	1.41
2	A	501	FAD	C4-C4X	2.32	1.45	1.41
2	I	501	FAD	C5X-N5	2.31	1.39	1.35
2	D	501	FAD	C4-C4X	2.30	1.45	1.41
2	M	501	FAD	C5X-N5	2.29	1.39	1.35
2	N	501	FAD	C9A-N10	2.29	1.41	1.38
2	J	501	FAD	C5X-N5	2.29	1.39	1.35
2	I	501	FAD	C9A-N10	2.28	1.41	1.38
2	B	501	FAD	C9A-N10	2.27	1.41	1.38
2	B	501	FAD	C5X-N5	2.26	1.39	1.35
2	D	501	FAD	C9A-N10	2.25	1.41	1.38
2	A	501	FAD	C9A-N10	2.24	1.41	1.38
2	J	501	FAD	C9A-N10	2.23	1.41	1.38
2	M	501	FAD	C9A-N10	2.22	1.41	1.38
2	C	501	FAD	C9A-N10	2.20	1.41	1.38
2	A	501	FAD	C5X-N5	2.19	1.39	1.35

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	FAD	C4-N3-C2	12.77	125.92	115.14
2	C	501	FAD	C4-N3-C2	12.69	125.86	115.14
2	A	501	FAD	C4-N3-C2	12.69	125.85	115.14
2	M	501	FAD	C4-N3-C2	12.67	125.84	115.14
2	B	501	FAD	C4-N3-C2	12.67	125.84	115.14
2	N	501	FAD	C4-N3-C2	12.67	125.83	115.14
2	D	501	FAD	C4-N3-C2	12.63	125.80	115.14
2	I	501	FAD	C4-N3-C2	12.61	125.79	115.14
2	C	501	FAD	C4X-C4-N3	-6.99	113.87	123.43
2	J	501	FAD	C4X-C4-N3	-6.98	113.89	123.43
2	I	501	FAD	C4X-C4-N3	-6.96	113.91	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C4X-C4-N3	-6.94	113.94	123.43
2	N	501	FAD	C4X-C4-N3	-6.92	113.96	123.43
2	M	501	FAD	C4X-C4-N3	-6.92	113.97	123.43
2	B	501	FAD	C4X-C4-N3	-6.91	113.98	123.43
2	D	501	FAD	C4X-C4-N3	-6.85	114.06	123.43
3	J	503	WPM	C13-C14-C9	-5.52	116.67	121.04
3	M	503	WPM	C13-C14-C9	-5.41	116.76	121.04
3	J	502	WPM	C13-C14-C9	-5.40	116.77	121.04
3	C	502	WPM	C13-C14-C9	-5.35	116.81	121.04
3	M	502	WPM	C13-C14-C9	-5.34	116.82	121.04
3	D	502	WPM	C13-C14-C9	-5.32	116.83	121.04
3	A	503	WPM	C13-C14-C9	-5.16	116.95	121.04
3	A	502	WPM	C13-C14-C9	-5.04	117.05	121.04
2	B	501	FAD	C10-C4X-N5	4.75	124.54	121.26
2	N	501	FAD	C10-C4X-N5	4.74	124.53	121.26
2	D	501	FAD	C10-C4X-N5	4.72	124.52	121.26
2	J	501	FAD	C10-C4X-N5	4.72	124.52	121.26
2	A	501	FAD	C10-C4X-N5	4.63	124.46	121.26
2	M	501	FAD	C10-C4X-N5	4.58	124.42	121.26
2	C	501	FAD	C10-C4X-N5	4.56	124.41	121.26
2	I	501	FAD	C10-C4X-N5	4.55	124.41	121.26
2	M	501	FAD	C4-C4X-C10	-3.90	117.37	119.95
2	B	501	FAD	C4-C4X-C10	-3.89	117.37	119.95
2	D	501	FAD	C4-C4X-C10	-3.85	117.40	119.95
2	J	501	FAD	C4-C4X-C10	-3.83	117.41	119.95
2	C	501	FAD	C4-C4X-C10	-3.82	117.42	119.95
2	A	501	FAD	C4-C4X-C10	-3.78	117.45	119.95
2	N	501	FAD	C4-C4X-C10	-3.75	117.47	119.95
2	I	501	FAD	C4-C4X-C10	-3.73	117.48	119.95
2	B	501	FAD	C4X-C10-N10	-3.45	116.76	120.30
2	J	501	FAD	C4X-C10-N10	-3.45	116.76	120.30
2	N	501	FAD	C4X-C10-N10	-3.45	116.76	120.30
2	D	501	FAD	C1'-N10-C9A	3.43	120.99	118.29
2	M	501	FAD	C4X-C10-N10	-3.42	116.78	120.30
2	A	501	FAD	C4X-C10-N10	-3.42	116.79	120.30
2	D	501	FAD	C4X-C10-N10	-3.41	116.80	120.30
2	C	501	FAD	C4X-C10-N10	-3.41	116.80	120.30
2	I	501	FAD	C4X-C10-N10	-3.39	116.82	120.30
3	A	502	WPM	C13-C14-S1	3.39	122.02	117.33
2	I	501	FAD	C1'-N10-C9A	3.37	120.94	118.29
2	B	501	FAD	C1'-N10-C9A	3.35	120.93	118.29
2	J	501	FAD	C1'-N10-C9A	3.30	120.89	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C1'-N10-C9A	3.30	120.89	118.29
2	C	501	FAD	C1'-N10-C9A	3.28	120.87	118.29
2	N	501	FAD	C1'-N10-C9A	3.23	120.83	118.29
2	M	501	FAD	C1'-N10-C9A	3.20	120.81	118.29
3	A	503	WPM	C13-C14-S1	3.18	121.73	117.33
3	M	503	WPM	C13-C14-S1	3.02	121.51	117.33
3	C	502	WPM	C13-C14-S1	3.02	121.51	117.33
3	J	502	WPM	C13-C14-S1	2.96	121.42	117.33
3	D	502	WPM	C13-C14-S1	2.94	121.40	117.33
3	J	503	WPM	C13-C14-S1	2.70	121.07	117.33
3	J	503	WPM	C12-C11-C10	-2.48	118.78	121.84
3	M	502	WPM	C13-C14-S1	2.48	120.76	117.33
3	C	502	WPM	C12-C11-C10	-2.44	118.84	121.84
3	D	502	WPM	C12-C11-C10	-2.41	118.87	121.84
3	A	502	WPM	C12-C11-C10	-2.40	118.88	121.84
3	M	502	WPM	C12-C11-C10	-2.39	118.89	121.84
3	A	503	WPM	C8-N3-C7	2.37	121.18	114.75
3	J	502	WPM	C12-C11-C10	-2.37	118.92	121.84
3	A	503	WPM	C12-C11-C10	-2.37	118.92	121.84
2	D	501	FAD	C5A-C6A-N6A	2.34	123.91	120.35
3	M	503	WPM	C12-C11-C10	-2.34	118.96	121.84
2	M	501	FAD	C5A-C6A-N6A	2.34	123.91	120.35
2	C	501	FAD	C5A-C6A-N6A	2.34	123.90	120.35
3	C	502	WPM	C8-N3-C7	2.33	121.07	114.75
2	N	501	FAD	C5A-C6A-N6A	2.32	123.88	120.35
2	B	501	FAD	C5A-C6A-N6A	2.32	123.88	120.35
3	D	502	WPM	C8-N3-C7	2.32	121.02	114.75
2	I	501	FAD	C5A-C6A-N6A	2.31	123.86	120.35
2	A	501	FAD	C5A-C6A-N6A	2.31	123.86	120.35
3	M	502	WPM	C8-N3-C7	2.31	121.00	114.75
2	J	501	FAD	C5A-C6A-N6A	2.30	123.85	120.35
3	M	503	WPM	C8-N3-C7	2.19	120.68	114.75
3	A	502	WPM	C8-N3-C7	2.14	120.54	114.75
3	J	503	WPM	C4-N2-C6	-2.10	123.81	127.50
3	A	502	WPM	C4-N2-C6	-2.06	123.88	127.50
3	A	503	WPM	C4-N2-C6	-2.01	123.98	127.50

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	504	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	504	GOL	O1-C1-C2-C3
4	J	506	GOL	O1-C1-C2-C3
4	J	507	GOL	O1-C1-C2-C3
3	A	502	WPM	C9-C14-S1-O1
3	C	502	WPM	C9-C14-S1-O1
4	N	503	GOL	C1-C2-C3-O3
4	I	502	GOL	C1-C2-C3-O3
4	M	505	GOL	O1-C1-C2-C3
4	C	505	GOL	O1-C1-C2-C3
4	B	505	GOL	O1-C1-C2-C3
4	B	508	GOL	O1-C1-C2-C3
4	C	508	GOL	O1-C1-C2-C3
4	M	507	GOL	O1-C1-C2-C3
4	M	507	GOL	C1-C2-C3-O3
4	M	507	GOL	O2-C2-C3-O3
4	J	508	GOL	O1-C1-C2-C3
4	C	507	GOL	O1-C1-C2-C3
4	C	503	GOL	O1-C1-C2-C3
4	B	503	GOL	O1-C1-C2-C3
4	I	505	GOL	O1-C1-C2-C3
4	N	502	GOL	C1-C2-C3-O3
2	D	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	PA-O3P-P-O5'
2	J	501	FAD	O4B-C4B-C5B-O5B
4	B	506	GOL	O1-C1-C2-C3
4	A	506	GOL	C1-C2-C3-O3
2	N	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	C3B-C4B-C5B-O5B
2	M	501	FAD	O4B-C4B-C5B-O5B
4	B	508	GOL	O1-C1-C2-O2
4	C	503	GOL	O1-C1-C2-O2
4	I	505	GOL	O1-C1-C2-O2
2	I	501	FAD	O4B-C4B-C5B-O5B
2	J	501	FAD	C3B-C4B-C5B-O5B
4	C	504	GOL	C1-C2-C3-O3
4	M	506	GOL	C1-C2-C3-O3
4	J	505	GOL	O1-C1-C2-C3
4	C	506	GOL	O1-C1-C2-C3
4	M	504	GOL	O1-C1-C2-C3
4	A	505	GOL	O1-C1-C2-C3
4	B	507	GOL	O1-C1-C2-C3
4	I	503	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	509	GOL	C1-C2-C3-O3
4	D	504	GOL	O1-C1-C2-C3
4	J	509	GOL	C1-C2-C3-O3
4	A	504	GOL	O1-C1-C2-O2
4	J	506	GOL	O1-C1-C2-O2
4	J	505	GOL	O1-C1-C2-O2
4	J	507	GOL	O1-C1-C2-O2
4	N	503	GOL	O2-C2-C3-O3
4	C	505	GOL	O1-C1-C2-O2
4	A	505	GOL	O1-C1-C2-O2
4	B	505	GOL	O1-C1-C2-O2
4	C	508	GOL	O1-C1-C2-O2
4	M	507	GOL	O1-C1-C2-O2
4	J	508	GOL	O1-C1-C2-O2
4	B	507	GOL	O1-C1-C2-O2
4	B	503	GOL	O1-C1-C2-O2
4	N	502	GOL	O2-C2-C3-O3
4	A	506	GOL	O2-C2-C3-O3
2	B	501	FAD	O4B-C4B-C5B-O5B
2	M	501	FAD	C3B-C4B-C5B-O5B
4	M	506	GOL	O2-C2-C3-O3
4	M	504	GOL	O1-C1-C2-O2
4	I	502	GOL	O2-C2-C3-O3
4	M	505	GOL	O1-C1-C2-O2
4	B	506	GOL	O1-C1-C2-O2
4	A	508	GOL	O1-C1-C2-O2
4	C	504	GOL	O1-C1-C2-O2
4	A	507	GOL	O1-C1-C2-O2
4	D	504	GOL	O1-C1-C2-O2
4	J	509	GOL	O1-C1-C2-O2
3	D	502	WPM	C9-C14-S1-O1
3	M	502	WPM	C9-C14-S1-O1
3	A	502	WPM	C9-C14-S1-O2
3	J	502	WPM	C9-C14-S1-O1
3	M	503	WPM	C9-C14-S1-O1
3	J	503	WPM	C9-C14-S1-O1
3	A	503	WPM	C9-C14-S1-O1
2	A	501	FAD	PA-O3P-P-O5'
2	N	501	FAD	PA-O3P-P-O5'
2	I	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
4	C	504	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	506	GOL	O1-C1-C2-O2
4	C	507	GOL	O1-C1-C2-O2
4	J	509	GOL	O2-C2-C3-O3
4	I	504	GOL	O1-C1-C2-O2
2	A	501	FAD	O4B-C4B-C5B-O5B
2	C	501	FAD	O4B-C4B-C5B-O5B
4	J	509	GOL	O1-C1-C2-C3
4	I	504	GOL	O1-C1-C2-C3
4	A	508	GOL	O1-C1-C2-C3
2	N	501	FAD	C3B-C4B-C5B-O5B
4	C	509	GOL	O1-C1-C2-C3
2	I	501	FAD	C3B-C4B-C5B-O5B
3	C	502	WPM	C9-C14-S1-O2
2	B	501	FAD	C3B-C4B-C5B-O5B
4	C	509	GOL	O2-C2-C3-O3
4	C	507	GOL	O2-C2-C3-O3
2	A	501	FAD	C3B-C4B-C5B-O5B

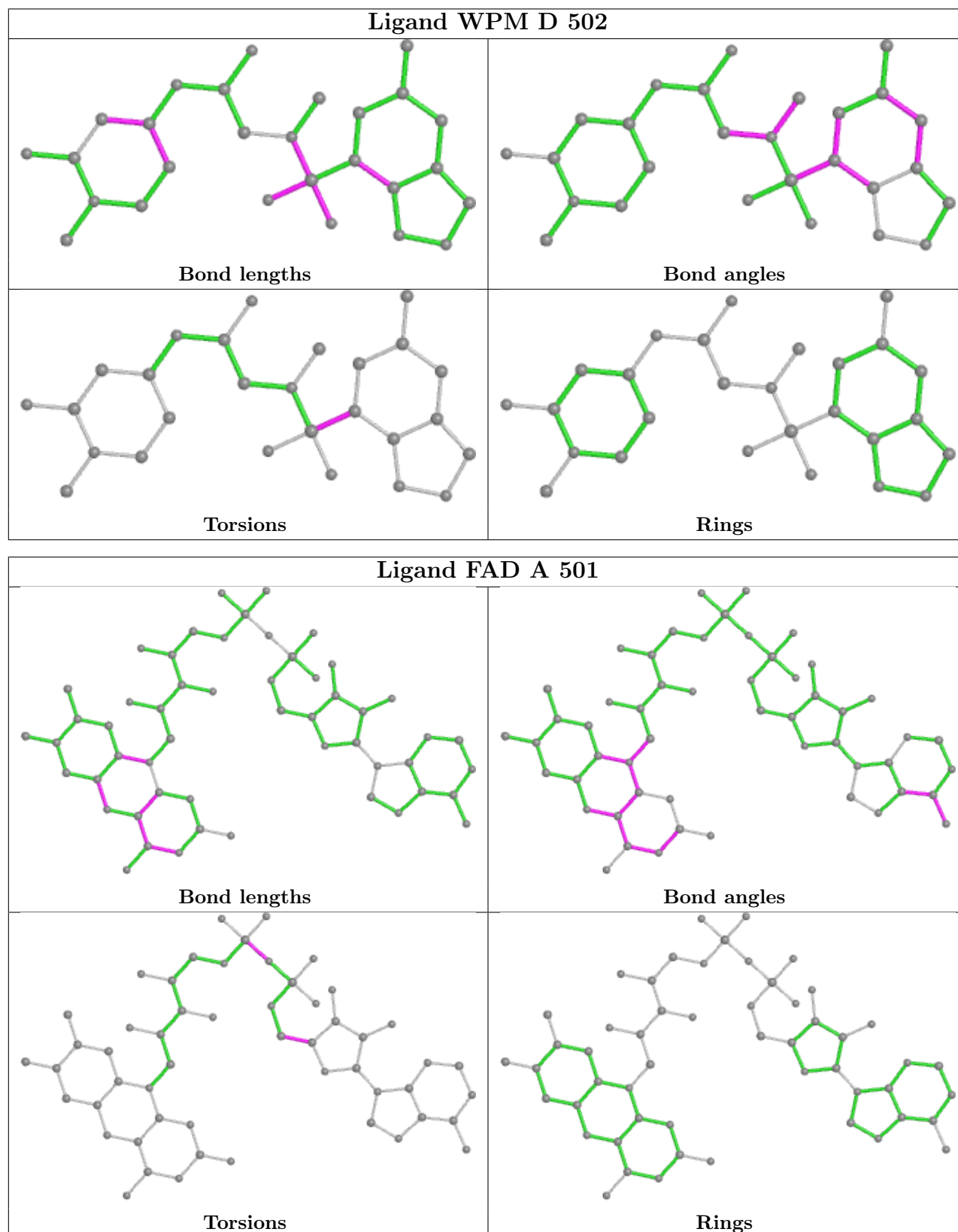
There are no ring outliers.

11 monomers are involved in 12 short contacts:

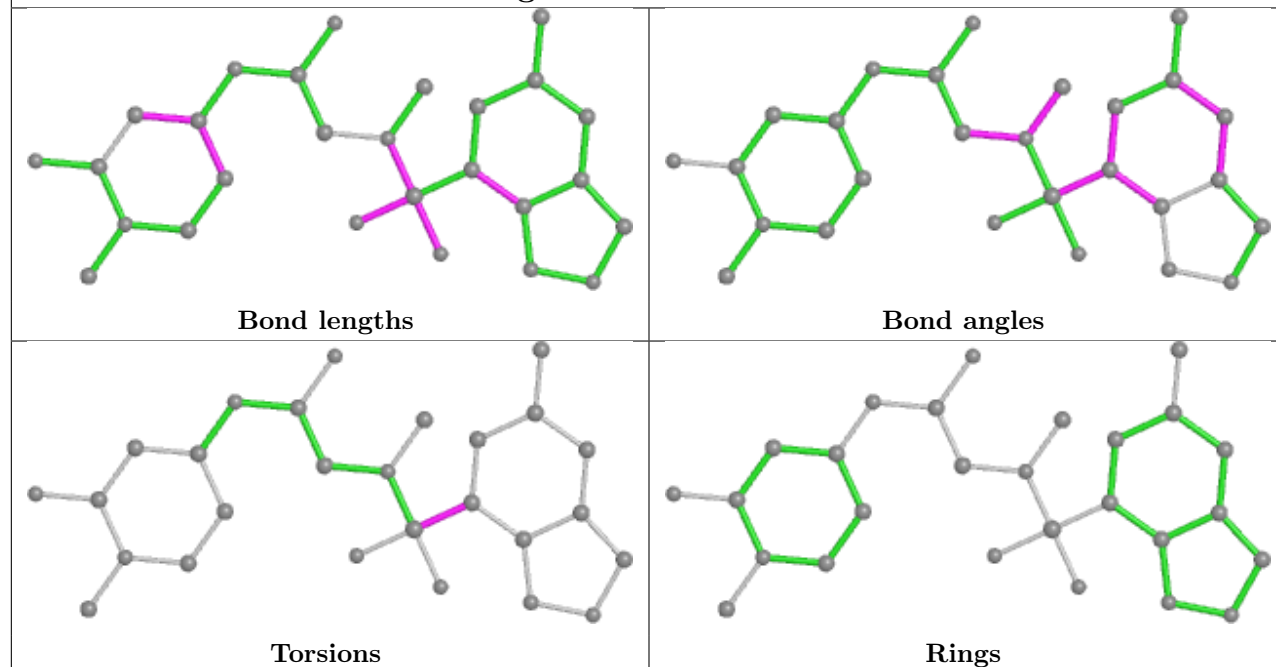
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	505	GOL	1	0
2	N	501	FAD	1	0
4	J	507	GOL	1	0
2	I	501	FAD	1	0
4	M	507	GOL	1	0
4	J	504	GOL	1	0
2	C	501	FAD	1	0
4	B	506	GOL	2	0
2	D	501	FAD	1	0
4	C	506	GOL	1	0
4	A	508	GOL	1	0

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

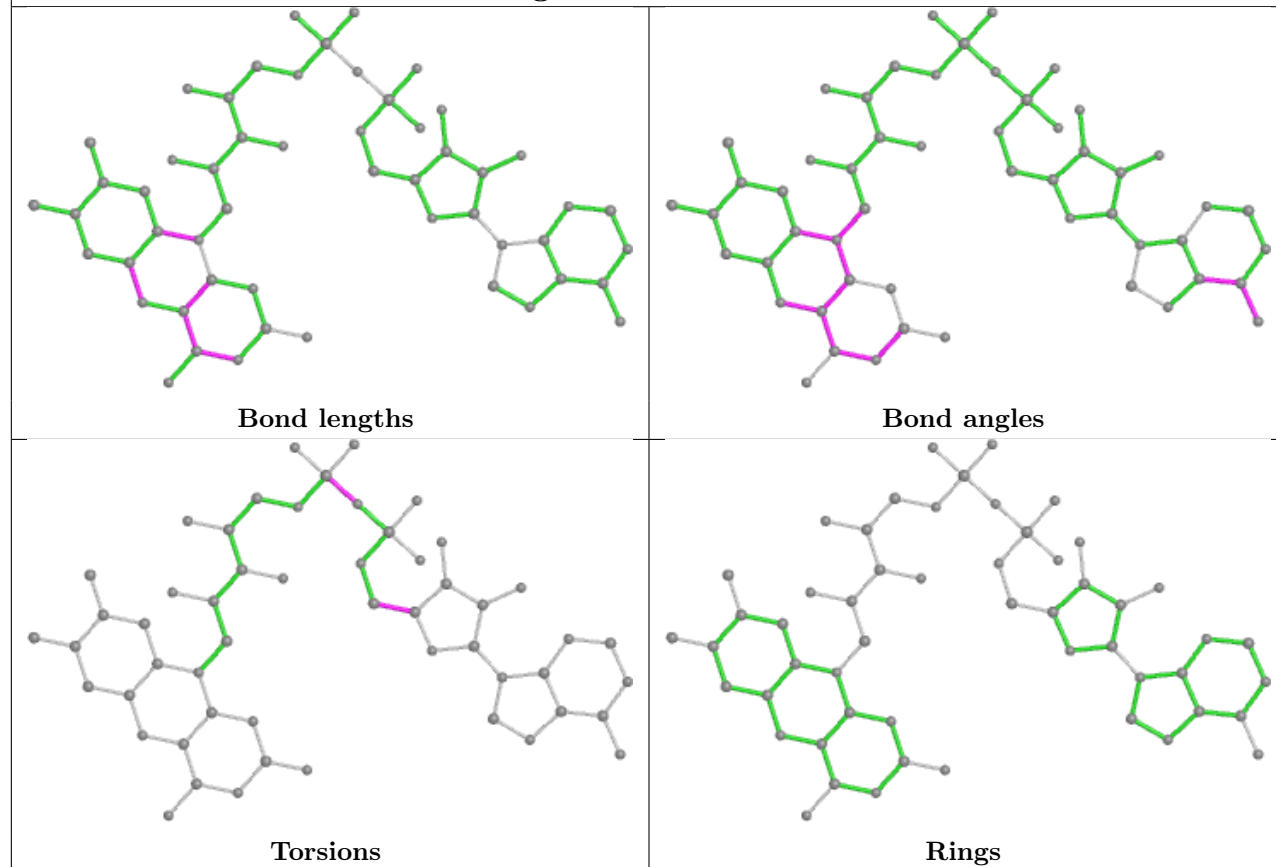
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

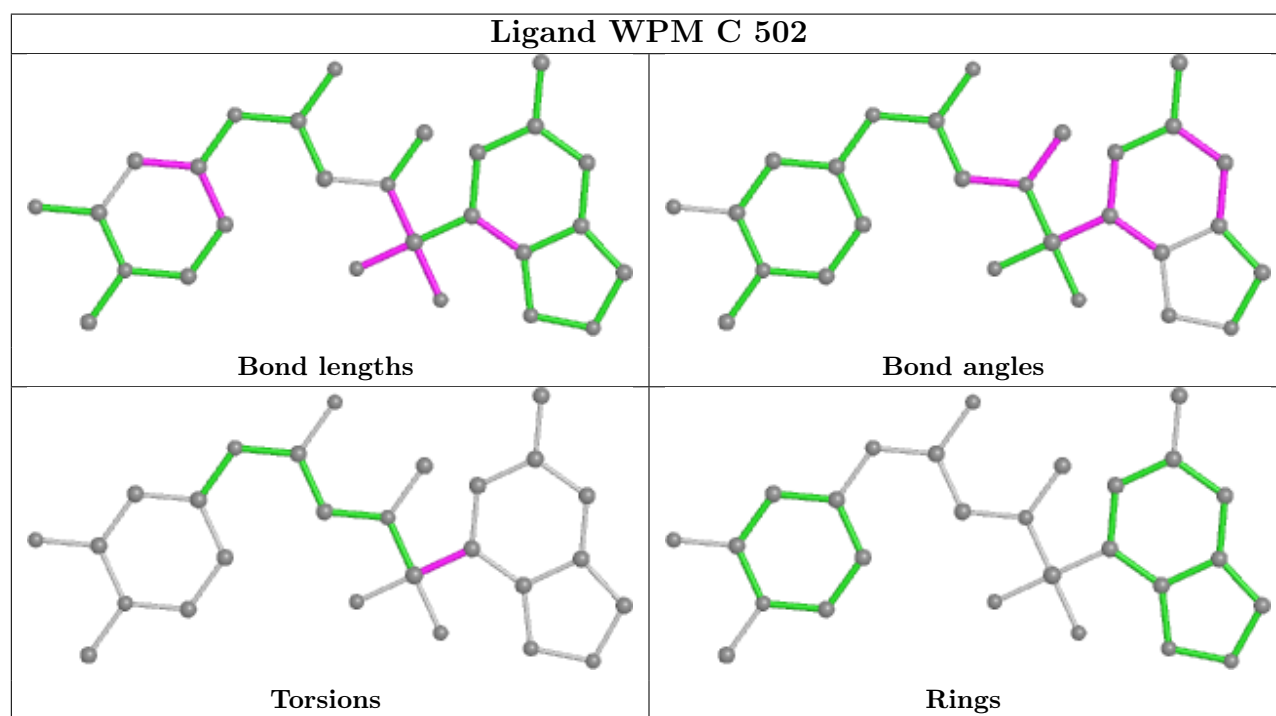
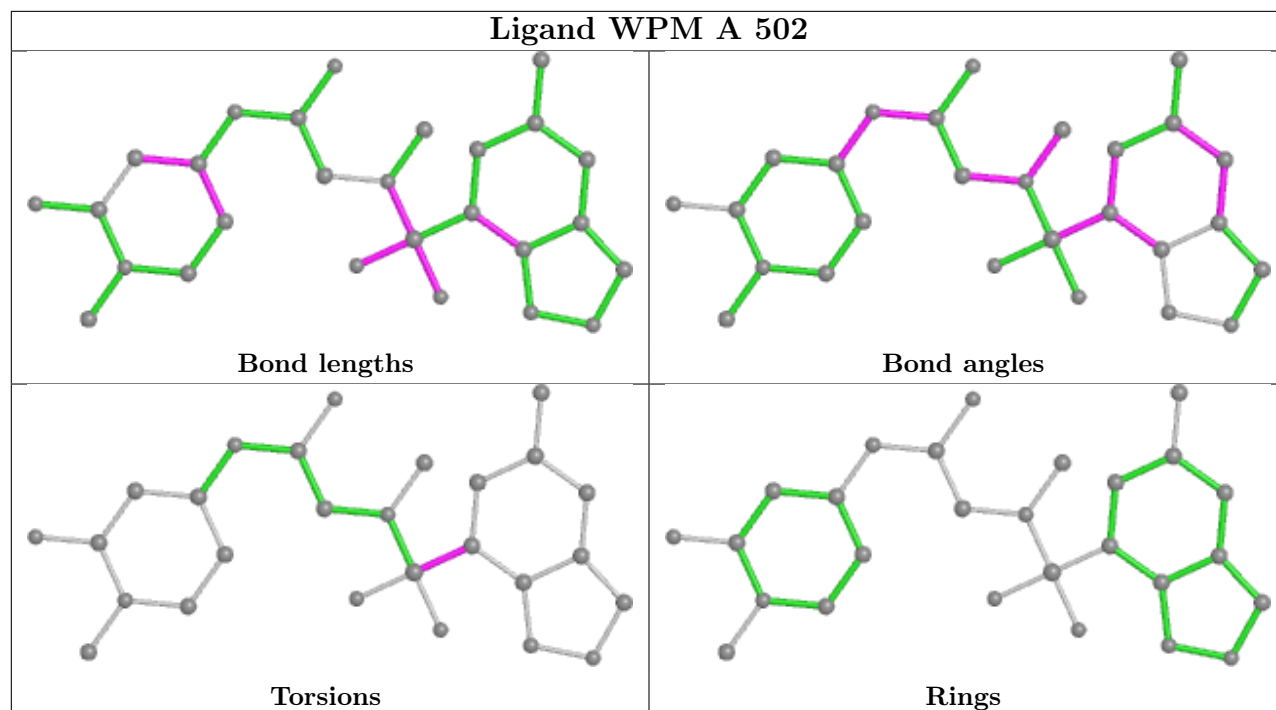


Ligand WPM M 502

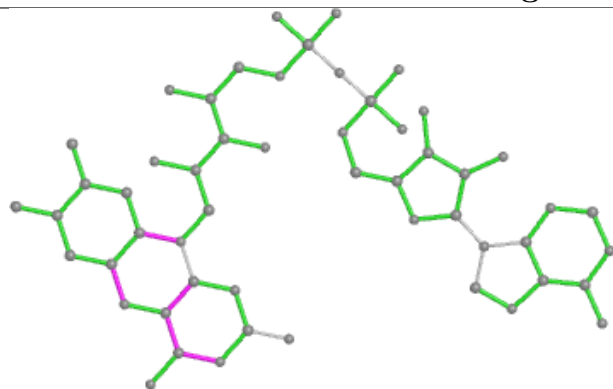


Ligand FAD N 501

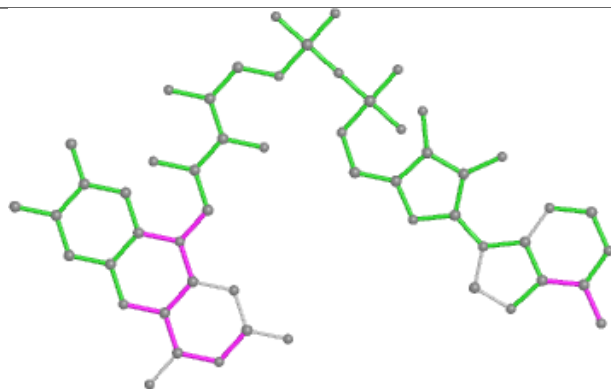




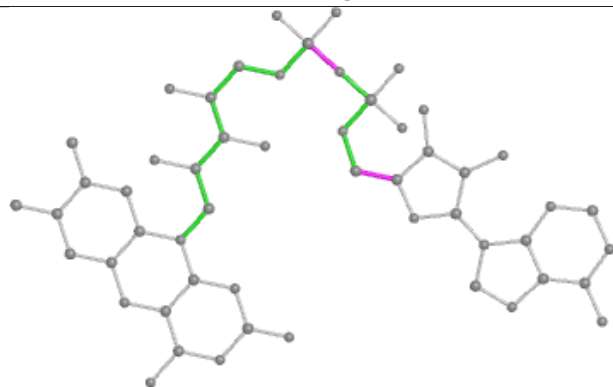
Ligand FAD I 501



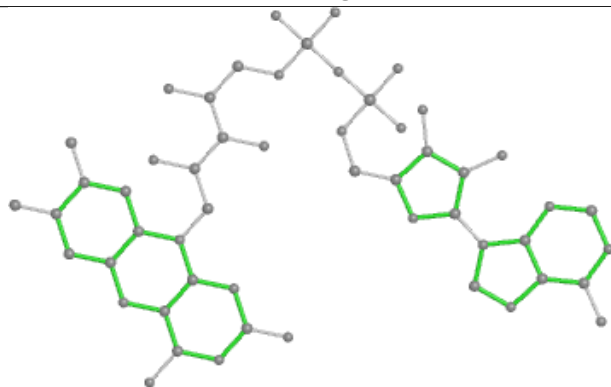
Bond lengths



Bond angles

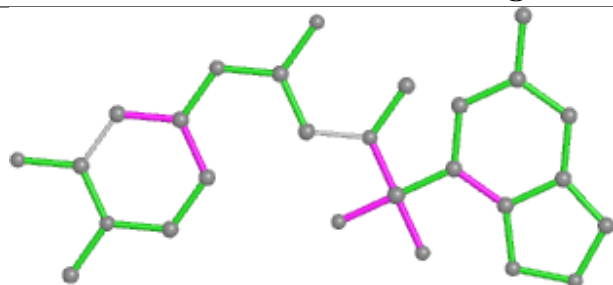


Torsions

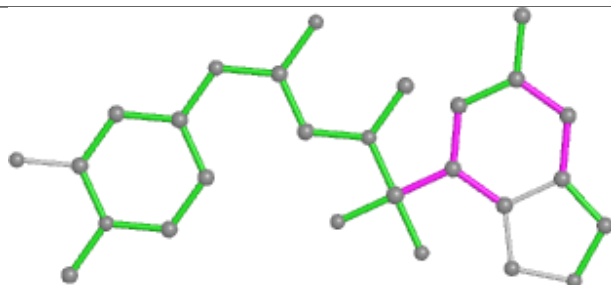


Rings

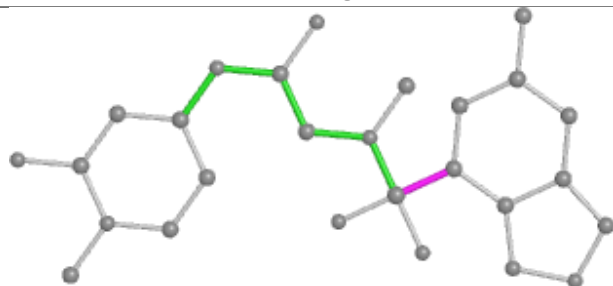
Ligand WPM J 502



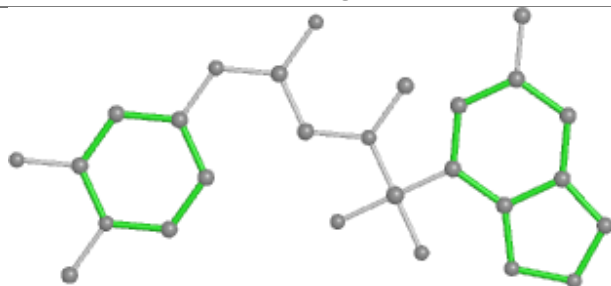
Bond lengths



Bond angles

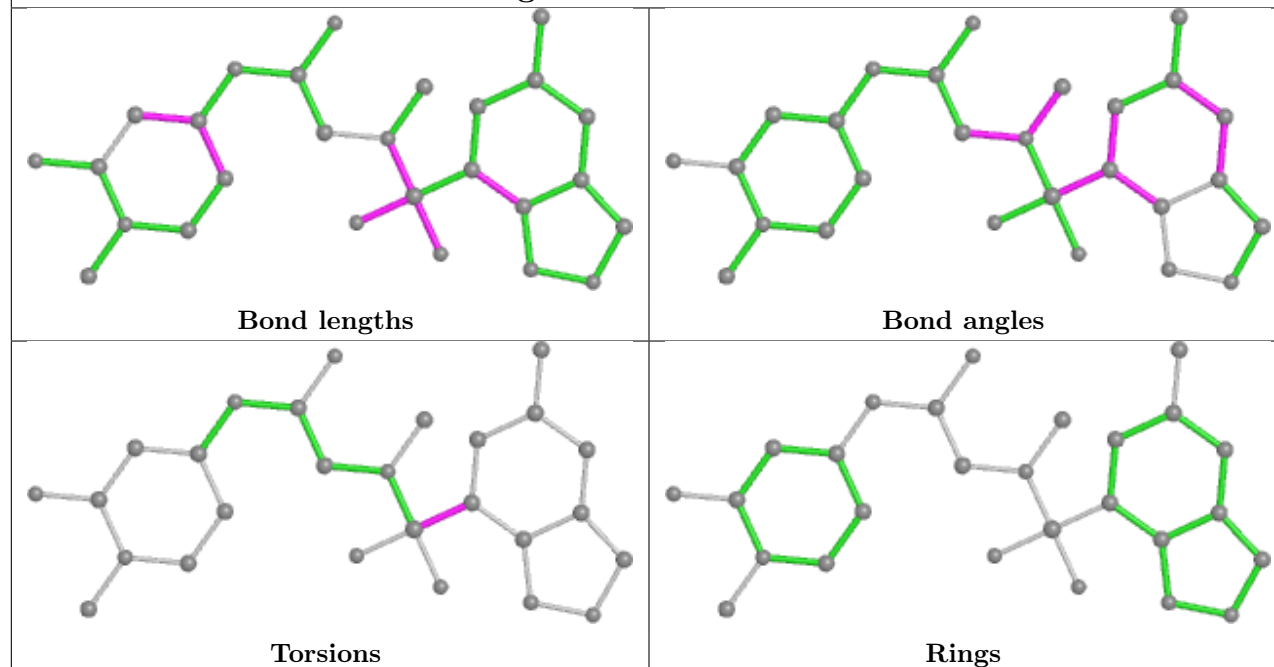


Torsions

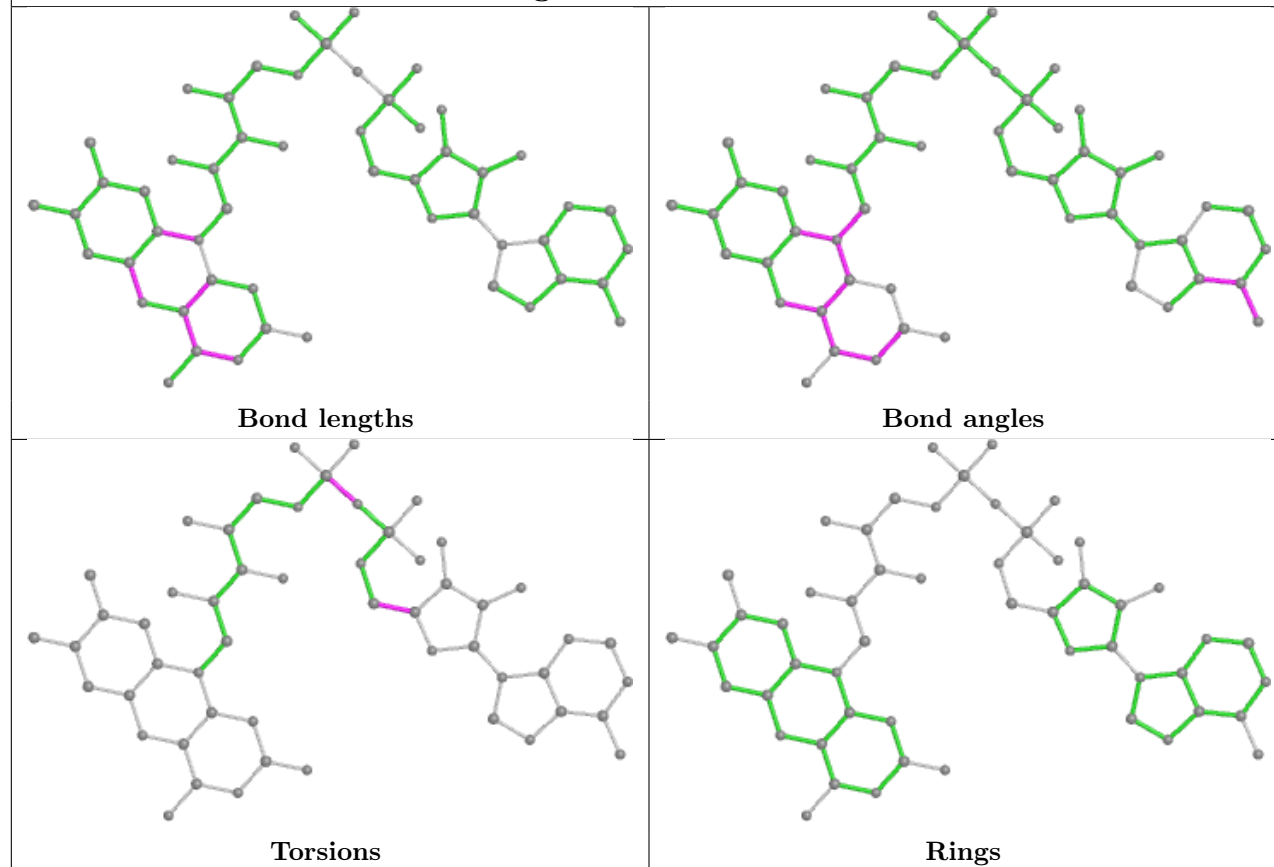


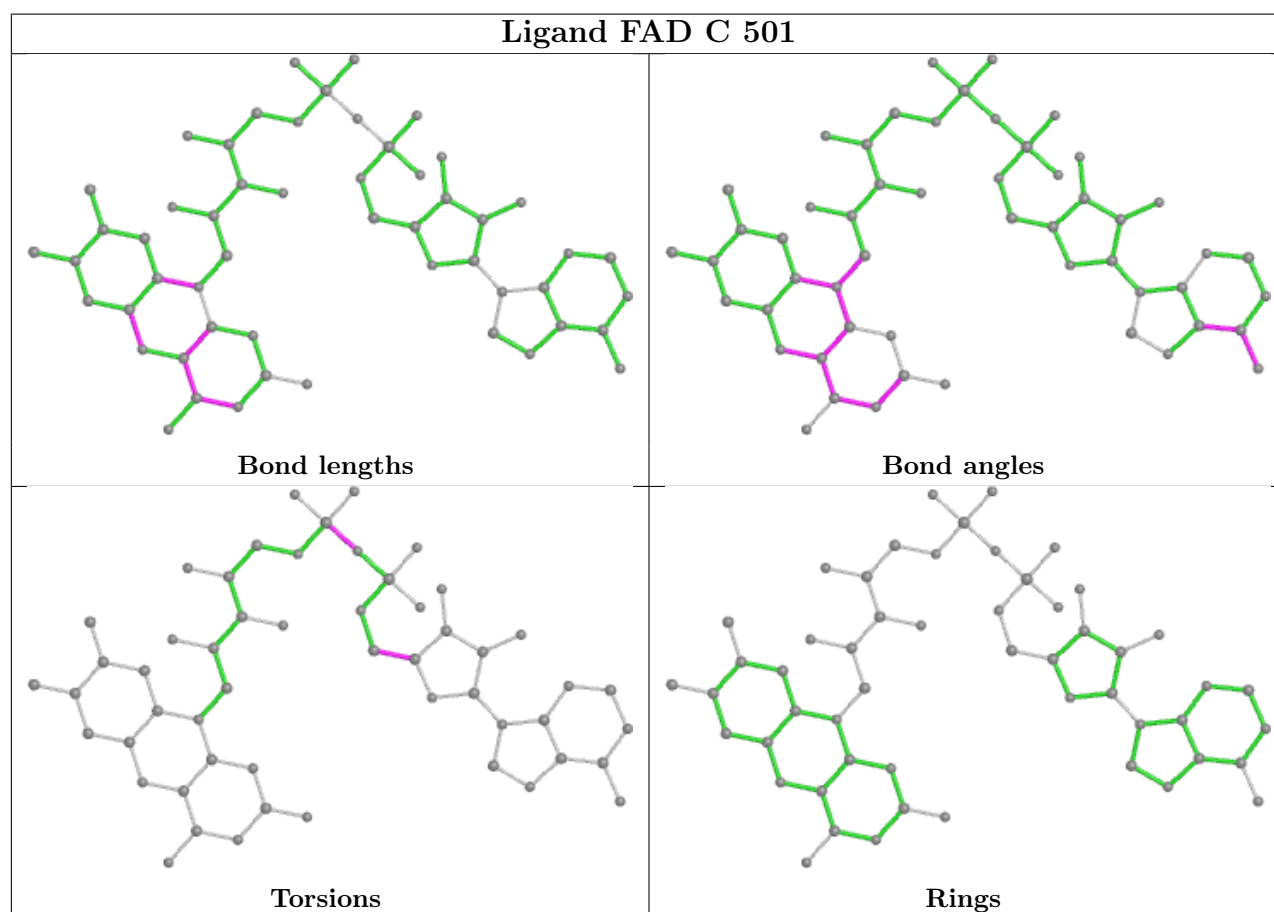
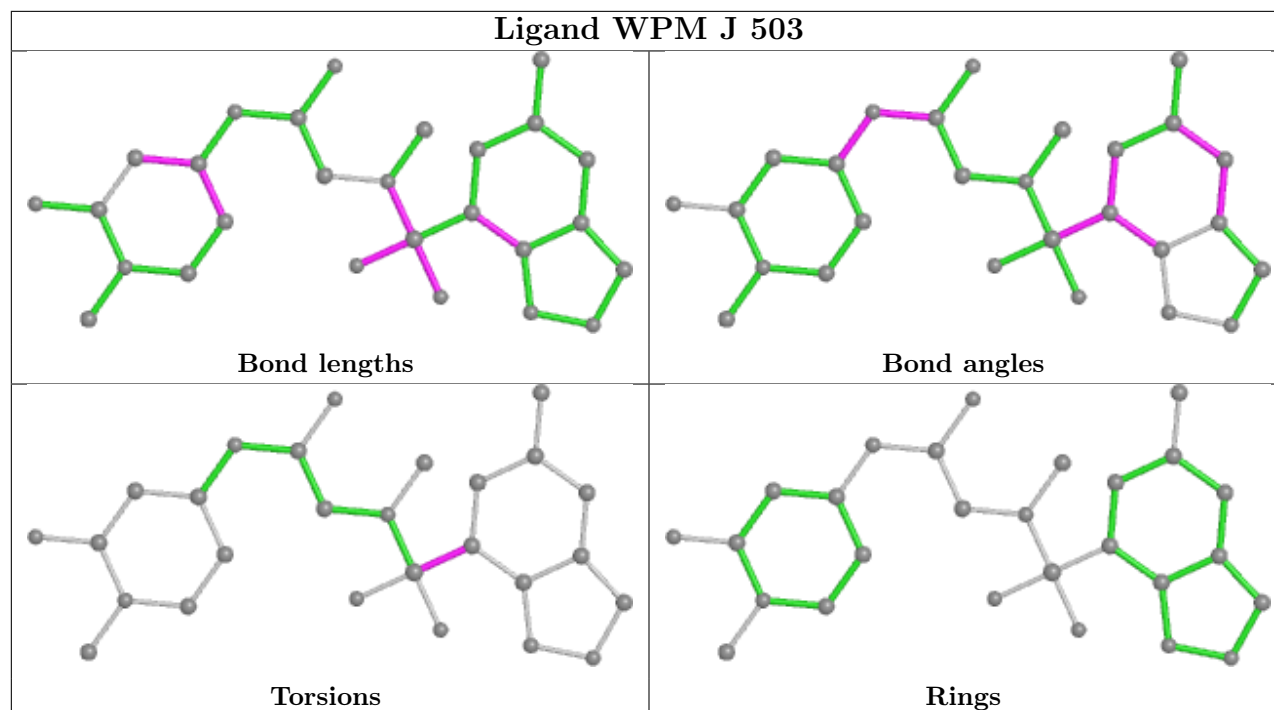
Rings

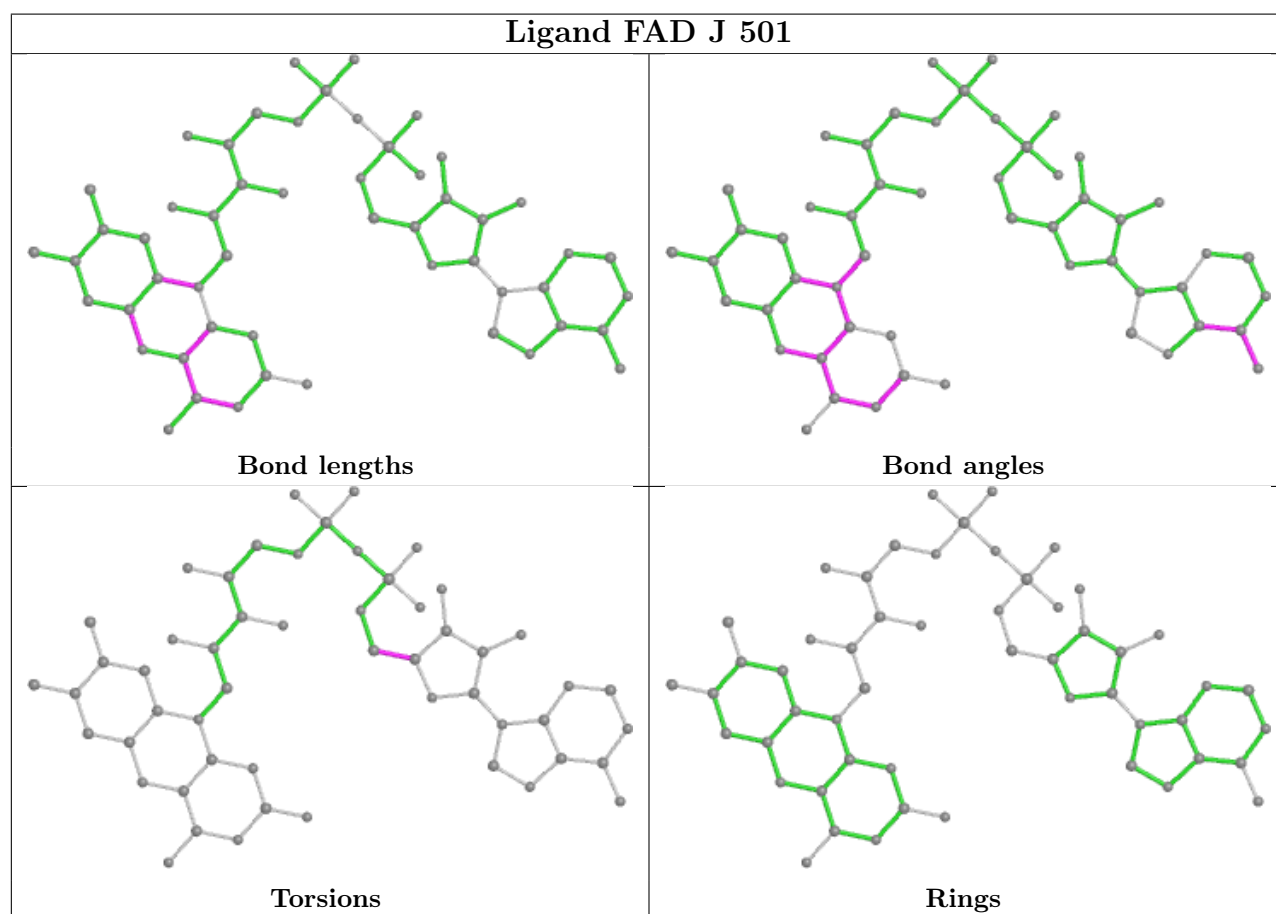
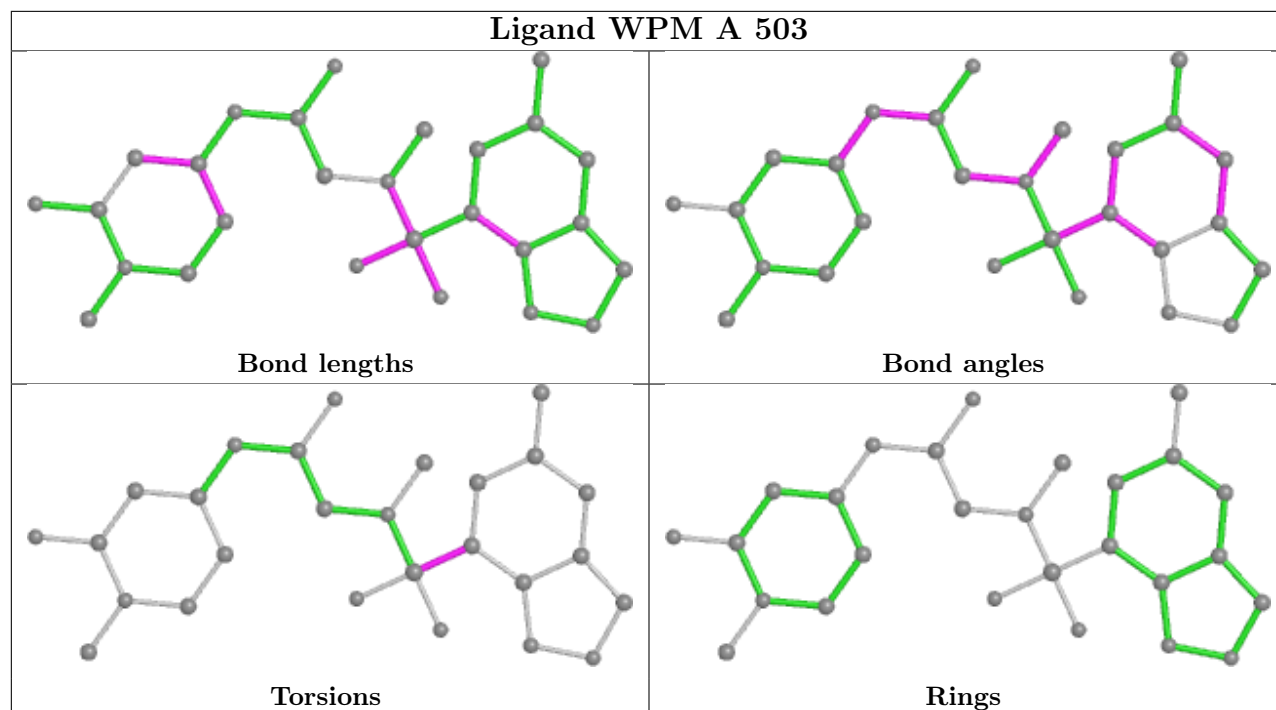
Ligand WPM M 503

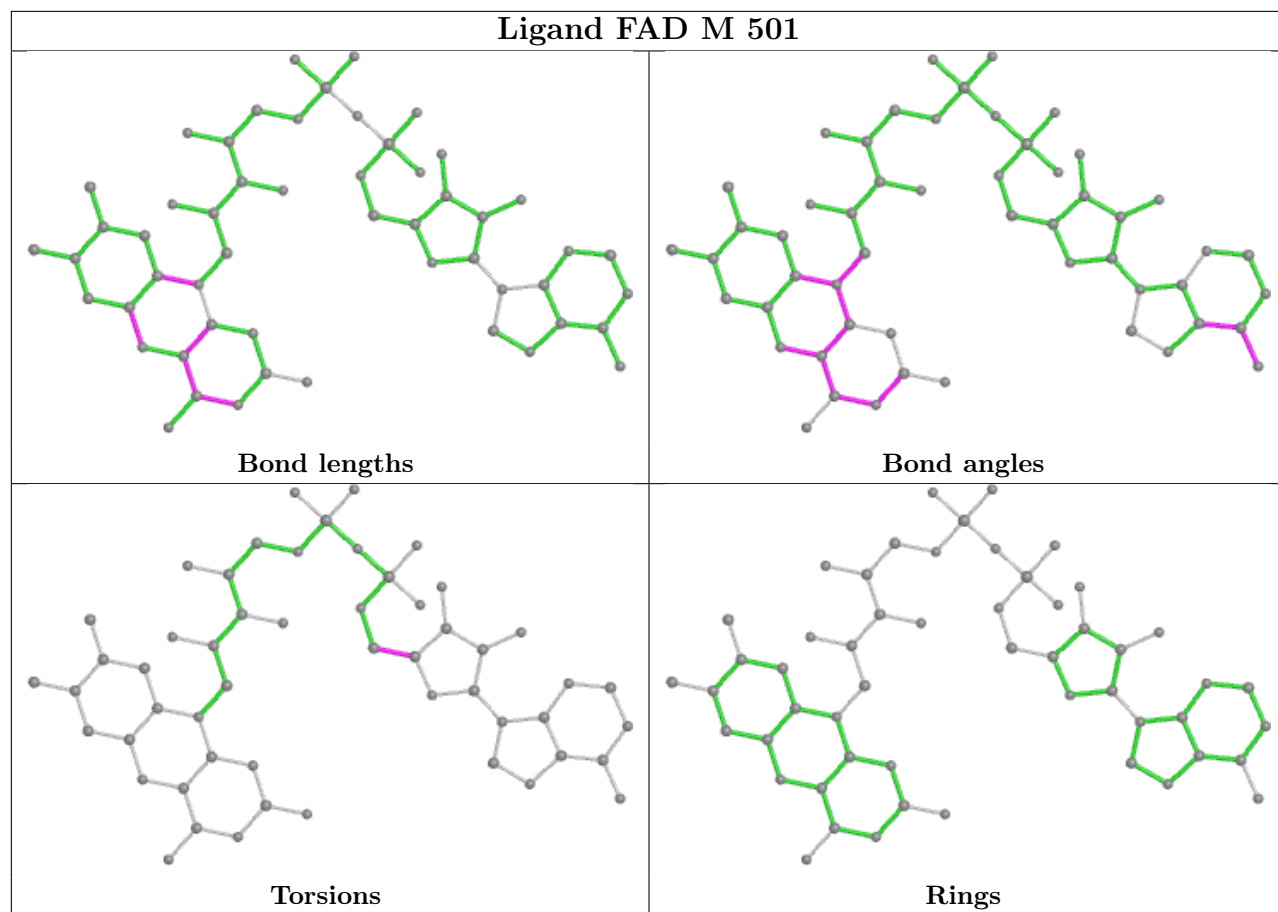


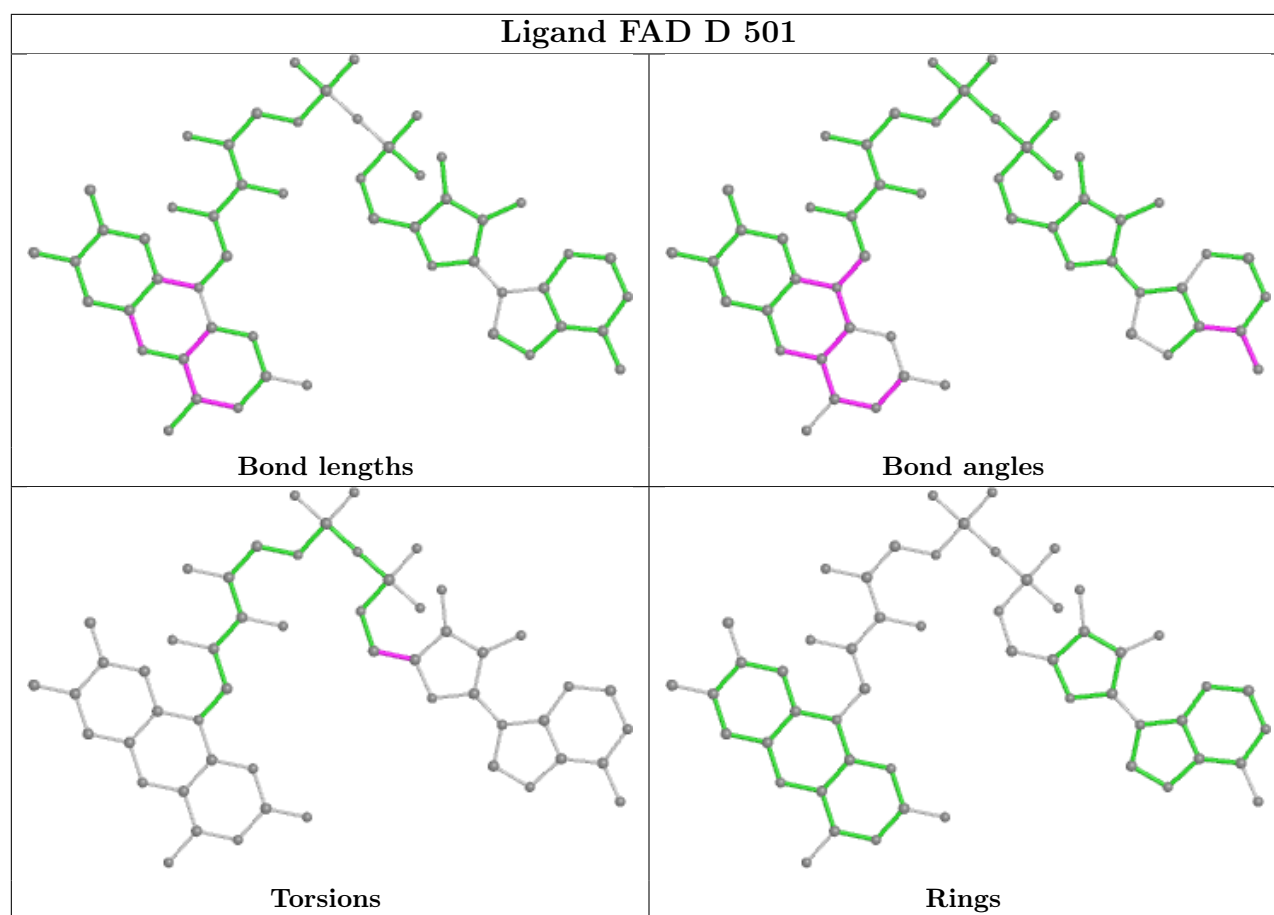
Ligand FAD B 501











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, 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	465/466 (99%)	-0.35	4 (0%) 84 83	14, 24, 40, 78	0
1	B	465/466 (99%)	-0.37	4 (0%) 84 83	13, 23, 40, 65	0
1	C	465/466 (99%)	-0.41	1 (0%) 95 95	14, 23, 38, 65	0
1	D	465/466 (99%)	-0.40	1 (0%) 95 95	16, 25, 43, 61	0
1	I	465/466 (99%)	-0.44	0 100 100	17, 24, 42, 66	0
1	J	465/466 (99%)	-0.35	4 (0%) 84 83	18, 26, 45, 67	0
1	M	465/466 (99%)	-0.43	1 (0%) 95 95	16, 25, 39, 67	0
1	N	465/466 (99%)	-0.35	1 (0%) 95 95	16, 25, 43, 64	0
All	All	3720/3728 (99%)	-0.39	16 (0%) 92 92	13, 24, 42, 78	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	7.0
1	B	1	MET	3.7
1	A	127	ASP	3.5
1	J	0	SER	3.4
1	J	62	PHE	3.1
1	C	1	MET	3.0
1	B	0	SER	2.8
1	D	0	SER	2.6
1	N	1	MET	2.6
1	J	1	MET	2.4
1	B	253	GLY	2.4
1	J	127	ASP	2.3
1	B	127	ASP	2.3
1	A	252	ASP	2.2
1	M	1	MET	2.1
1	A	0	SER	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 ⓘ

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
4	GOL	A	508	6/6	0.73	0.33	43,46,49,57	0
4	GOL	J	507	6/6	0.74	0.33	46,48,59,61	0
4	GOL	A	504	6/6	0.74	0.20	31,32,34,35	0
4	GOL	J	508	6/6	0.75	0.28	47,52,57,59	0
4	GOL	M	504	6/6	0.76	0.22	38,42,44,45	0
4	GOL	B	503	6/6	0.76	0.21	35,39,41,41	0
4	GOL	C	508	6/6	0.76	0.22	34,38,40,42	0
4	GOL	I	502	6/6	0.77	0.23	27,29,34,34	0
4	GOL	C	506	6/6	0.78	0.34	31,42,48,56	0
4	GOL	D	504	6/6	0.79	0.38	47,53,57,57	0
4	GOL	J	509	6/6	0.79	0.19	40,43,46,50	0
4	GOL	C	509	6/6	0.79	0.23	42,43,52,58	0
4	GOL	C	505	6/6	0.80	0.25	45,47,51,63	0
4	GOL	M	506	6/6	0.80	0.32	38,39,41,45	0
4	GOL	N	503	6/6	0.81	0.28	35,39,42,46	0
4	GOL	B	505	6/6	0.81	0.27	33,34,35,40	0
4	GOL	M	505	6/6	0.81	0.27	33,34,41,51	0
4	GOL	J	505	6/6	0.82	0.24	37,39,43,47	0
4	GOL	B	508	6/6	0.82	0.34	37,41,49,55	0
4	GOL	J	506	6/6	0.82	0.23	37,39,40,46	0
4	GOL	B	507	6/6	0.83	0.22	30,40,43,53	0
4	GOL	M	507	6/6	0.83	0.34	47,52,57,59	0
4	GOL	A	507	6/6	0.83	0.21	40,45,51,59	0
4	GOL	N	502	6/6	0.84	0.21	31,35,37,42	0
4	GOL	A	506	6/6	0.84	0.33	36,38,43,54	0
4	GOL	B	506	6/6	0.85	0.32	29,33,35,44	0
4	GOL	I	505	6/6	0.85	0.30	31,35,38,46	0

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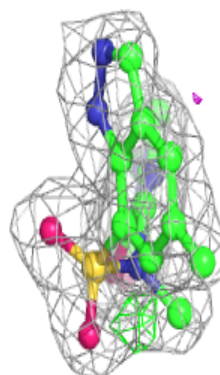
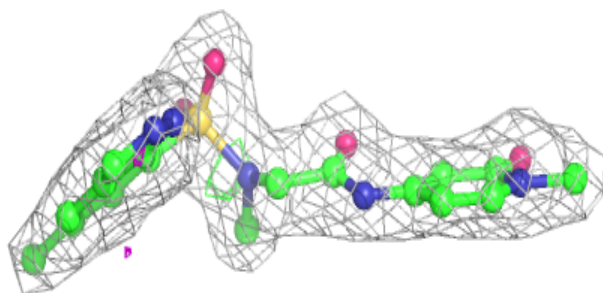
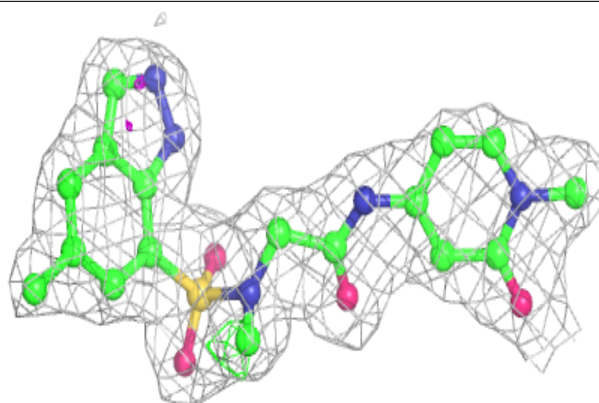
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	C	504	6/6	0.90	0.21	30,31,31,37	0
4	GOL	C	503	6/6	0.90	0.16	21,32,34,38	0
4	GOL	A	505	6/6	0.90	0.17	30,31,32,36	0
4	GOL	B	502	6/6	0.90	0.18	31,32,33,34	0
4	GOL	C	507	6/6	0.91	0.21	27,29,34,38	0
4	GOL	I	504	6/6	0.91	0.20	26,28,34,45	0
4	GOL	D	503	6/6	0.91	0.18	27,29,31,31	0
4	GOL	B	504	6/6	0.92	0.17	26,27,29,30	0
4	GOL	I	503	6/6	0.92	0.14	30,33,36,36	0
4	GOL	J	504	6/6	0.93	0.18	28,29,32,33	0
3	WPM	J	502	27/27	0.96	0.11	20,22,25,26	0
2	FAD	J	501	53/53	0.96	0.10	19,22,26,26	0
2	FAD	D	501	53/53	0.97	0.11	16,20,22,23	0
2	FAD	C	501	53/53	0.97	0.10	14,18,20,20	0
3	WPM	A	503	27/27	0.97	0.12	16,18,25,30	0
2	FAD	N	501	53/53	0.97	0.11	15,19,21,23	0
2	FAD	A	501	53/53	0.97	0.11	18,21,27,28	0
2	FAD	I	501	53/53	0.97	0.10	16,21,25,25	0
2	FAD	M	501	53/53	0.97	0.09	19,21,23,24	0
3	WPM	M	503	27/27	0.97	0.10	16,18,24,26	0
3	WPM	M	502	27/27	0.97	0.11	21,23,29,35	0
3	WPM	A	502	27/27	0.97	0.12	17,19,27,28	0
3	WPM	D	502	27/27	0.97	0.12	20,21,28,29	0
3	WPM	C	502	27/27	0.97	0.11	18,19,26,30	0
2	FAD	B	501	53/53	0.97	0.11	17,20,24,25	0
3	WPM	J	503	27/27	0.98	0.11	18,20,24,25	0

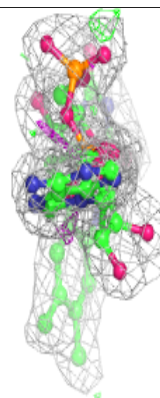
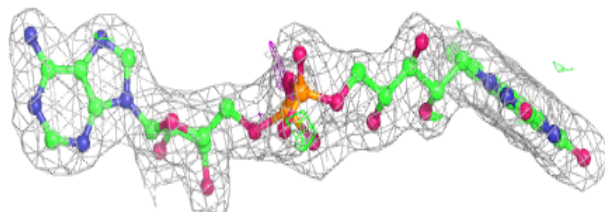
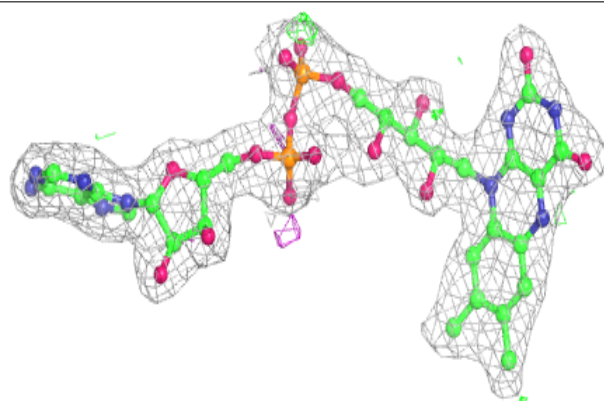
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WPM J 502:

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

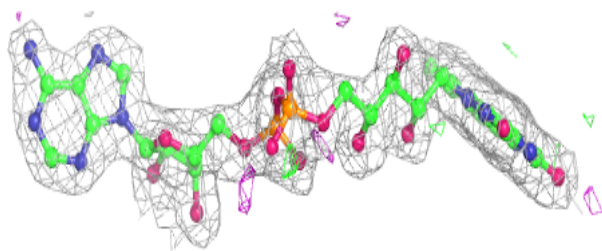
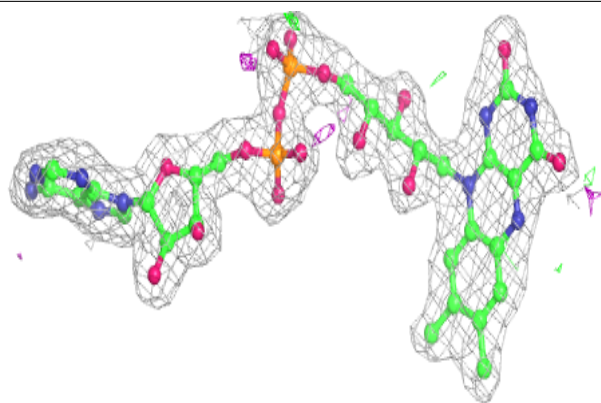
**Electron density around FAD J 501:**

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

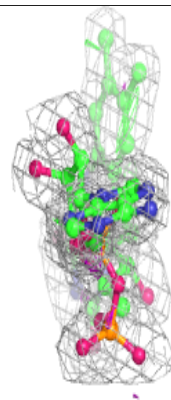
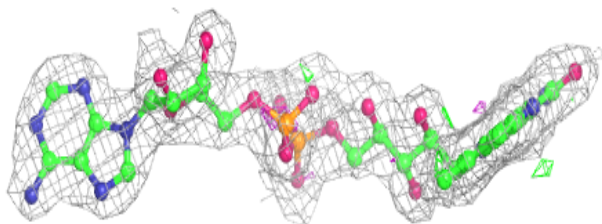
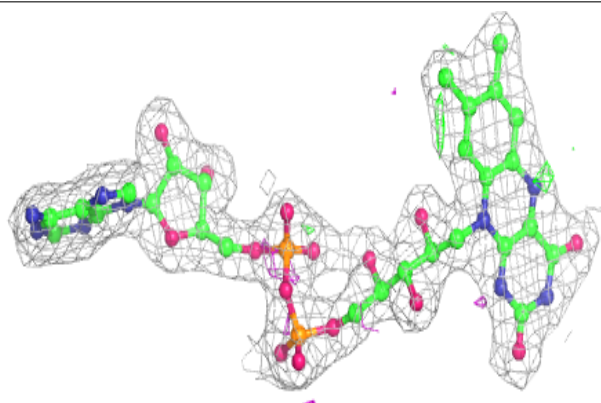


Electron density around FAD D 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

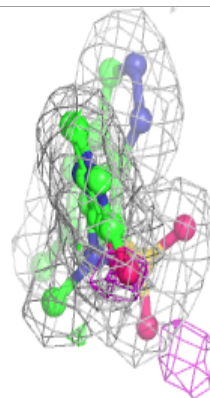
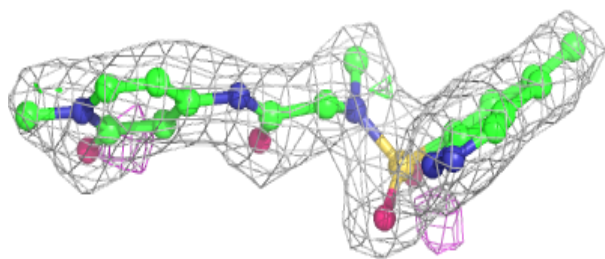
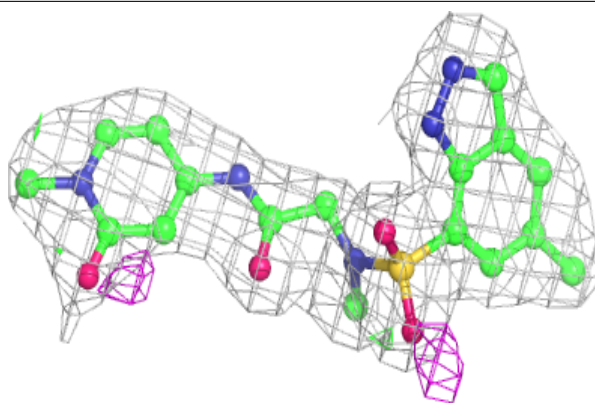
**Electron density around FAD C 501:**

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

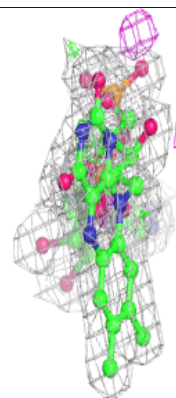
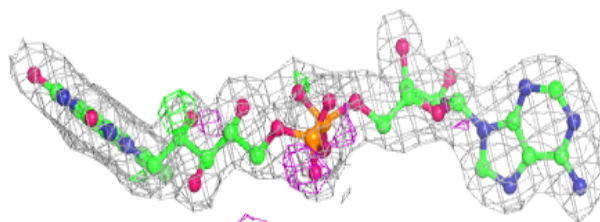
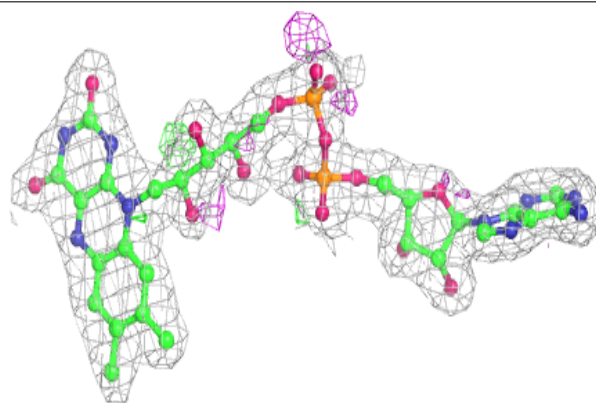


Electron density around WPM A 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

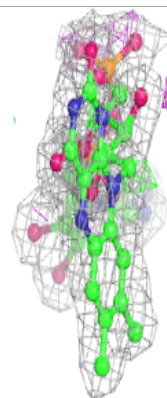
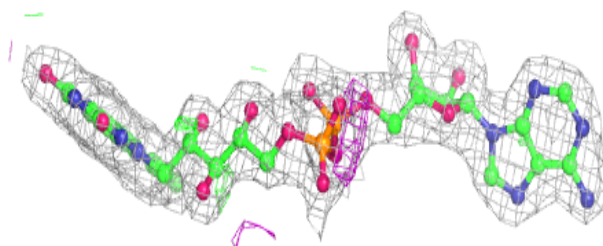
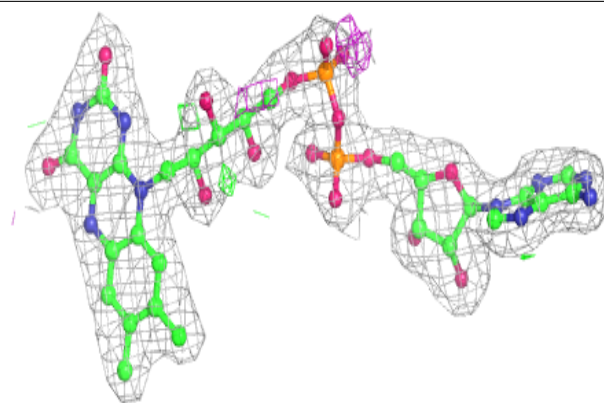
**Electron density around FAD N 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

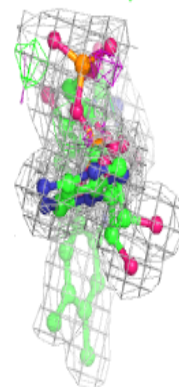
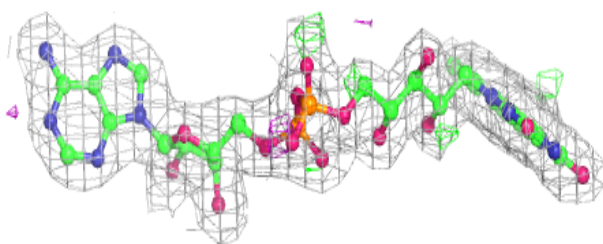
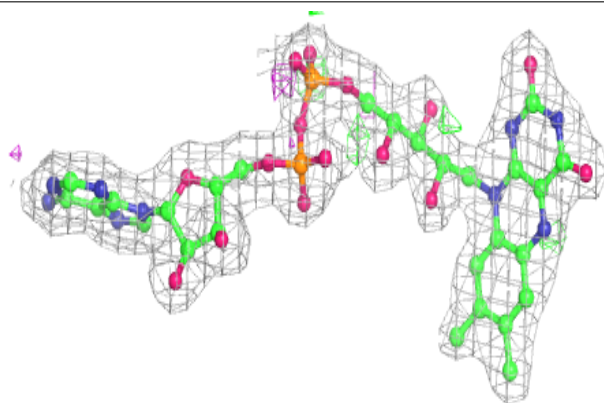


Electron density around FAD A 501:

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

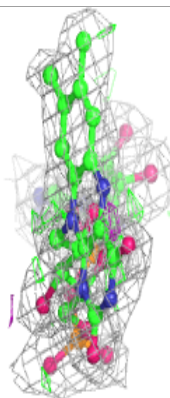
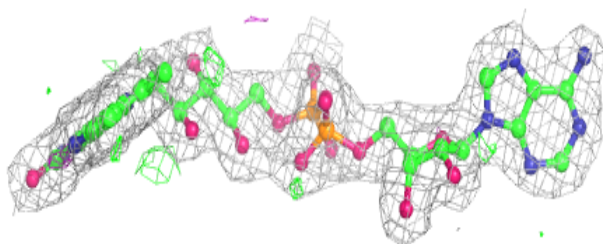
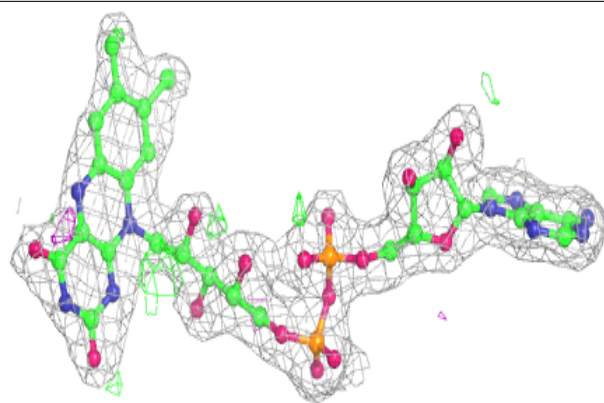
**Electron density around FAD I 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

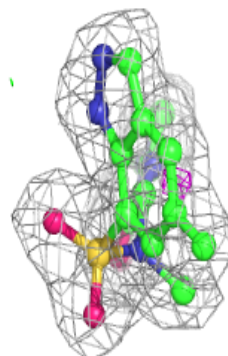
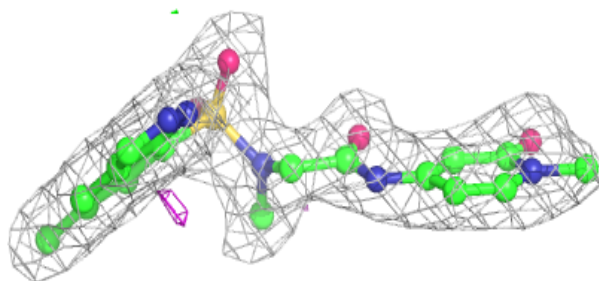
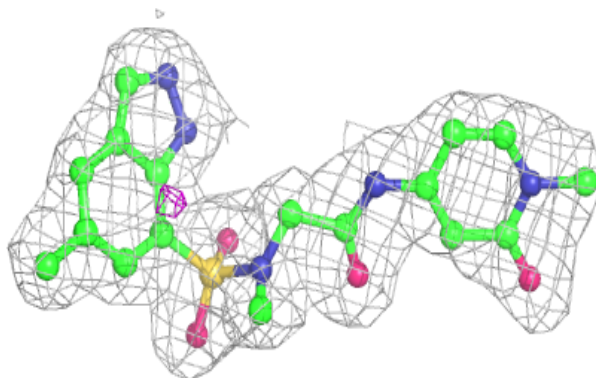


Electron density around FAD M 501:

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

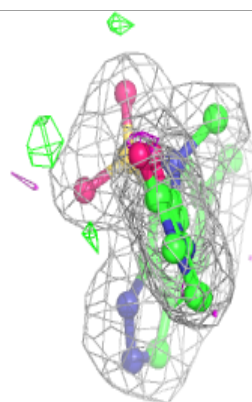
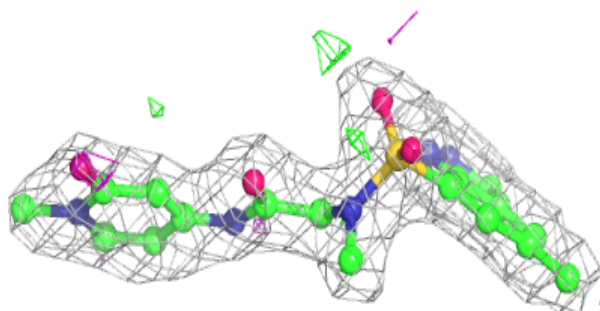
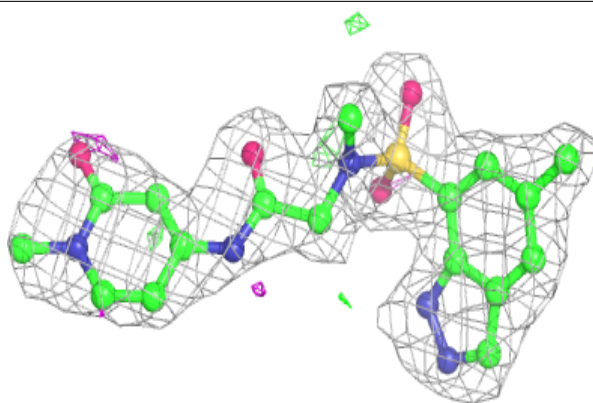
**Electron density around WPM M 503:**

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and green (positive)

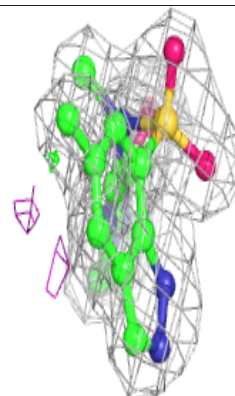
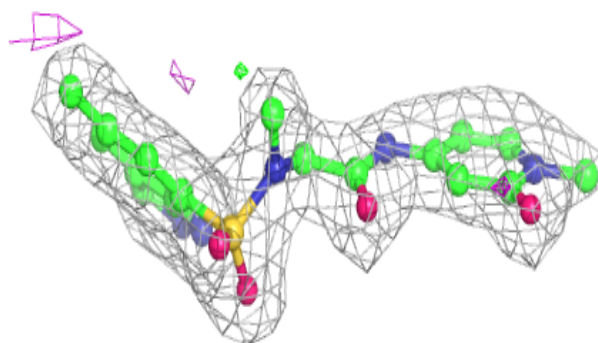
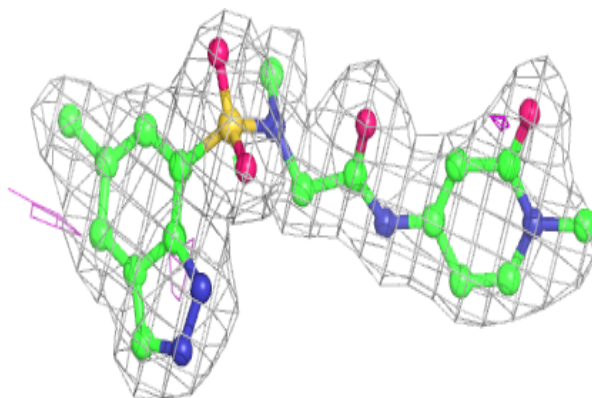


Electron density around WPM M 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

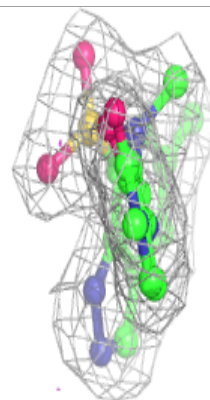
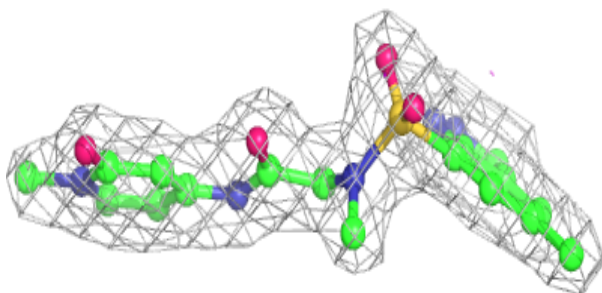
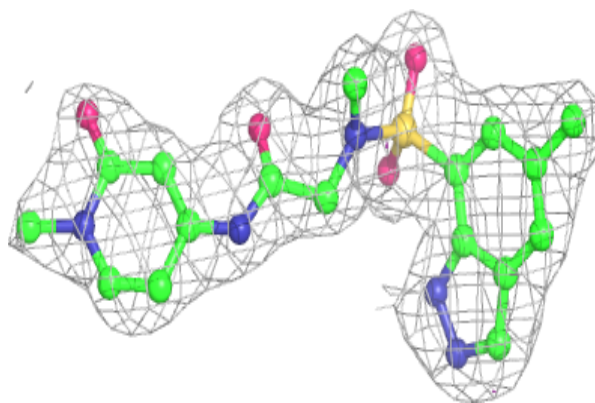
**Electron density around WPM A 502:**

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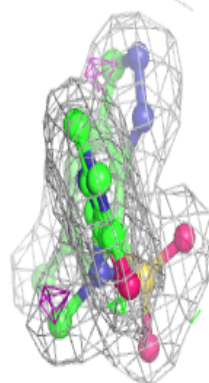
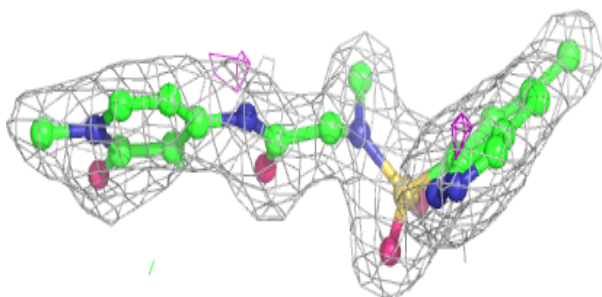
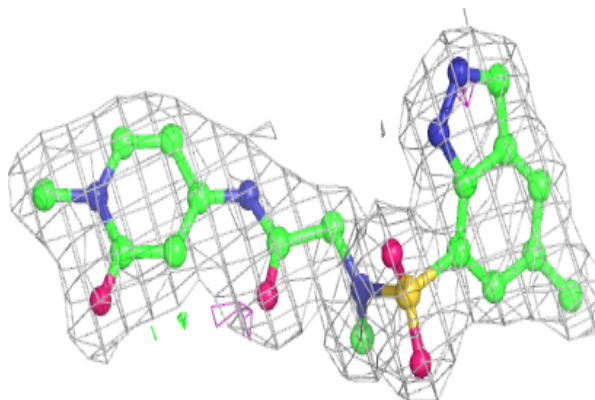


Electron density around WPM D 502:

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and green (positive)

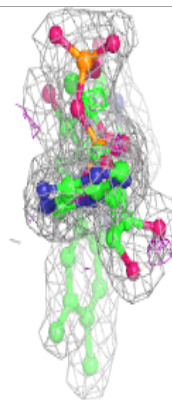
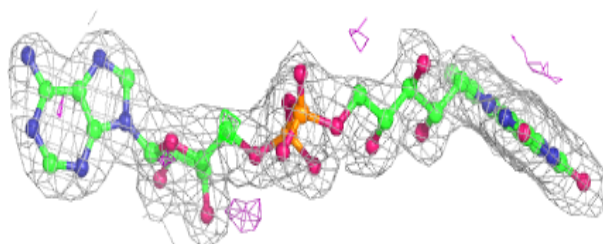
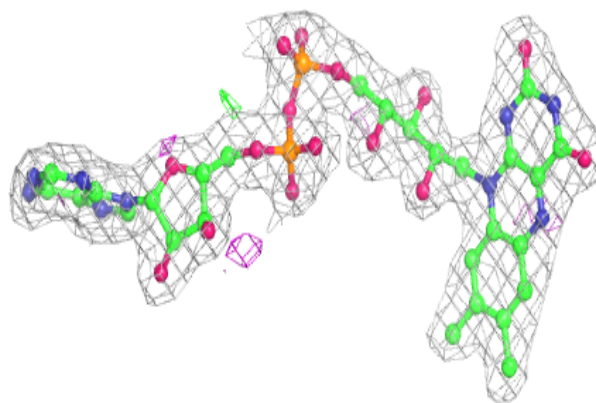
**Electron density around WPM C 502:**

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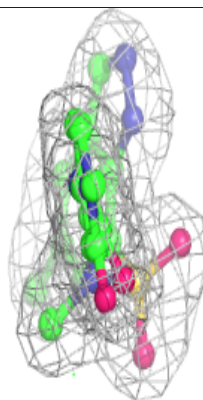
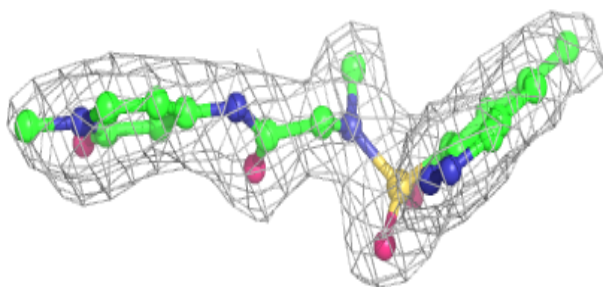
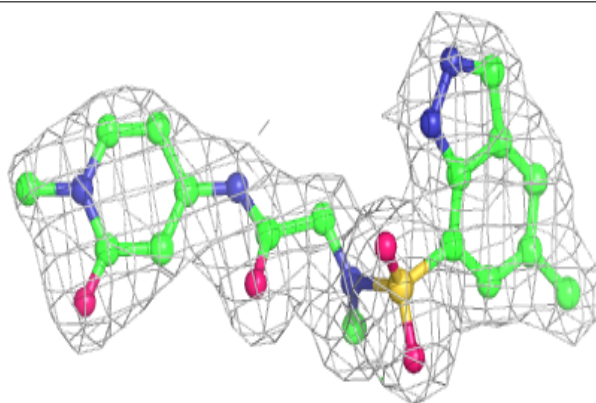


Electron density around FAD B 501:

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

**Electron density around WPM J 503:**

$2mF_o-DF_c$ (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.