



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 6, 2022 – 04:36 pm BST

PDB ID : 7P9X  
Title : Structure of cyclohex-1-ene-1-carboxyl-CoA dehydrogenase complexed with c  
yclohex-1-ene-1-carboxyl-CoA  
Authors : Ermler, U.; Weidenweber, S.; Boll, M.  
Deposited on : 2021-07-28  
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.29  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

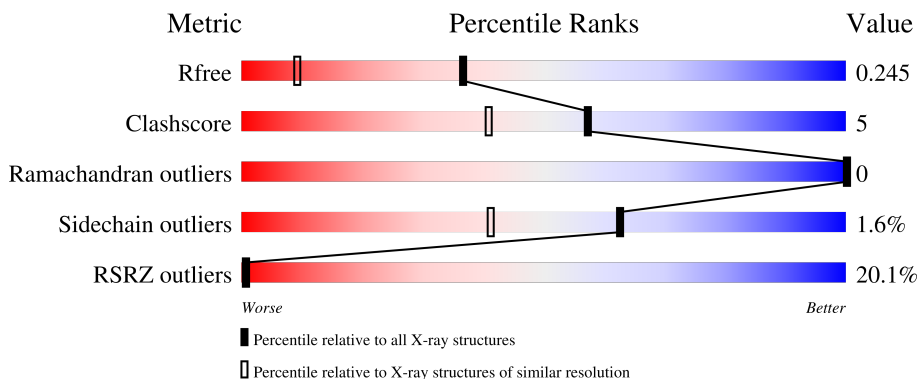
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




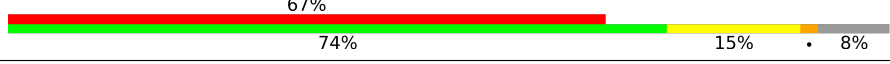
The reported resolution of this entry is 1.65 Å.

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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	412	
1	B	412	
1	C	412	
1	D	412	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	GOL	D	503	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 13151 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 Short-chain acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	2899	1819	503	556	21	0	6	0
1	B	378	2889	1814	501	552	22	0	5	0
1	C	378	2904	1826	502	554	22	0	7	0
1	D	377	2892	1814	506	551	21	0	6	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	LYS	-	expression tag	UNP Q39QF5
A	382	GLY	-	expression tag	UNP Q39QF5
A	383	GLU	-	expression tag	UNP Q39QF5
A	384	LEU	-	expression tag	UNP Q39QF5
A	385	ASN	-	expression tag	UNP Q39QF5
A	386	SER	-	expression tag	UNP Q39QF5
A	387	LYS	-	expression tag	UNP Q39QF5
A	388	LEU	-	expression tag	UNP Q39QF5
A	389	GLU	-	expression tag	UNP Q39QF5
A	390	GLY	-	expression tag	UNP Q39QF5
A	391	LYS	-	expression tag	UNP Q39QF5
A	392	PRO	-	expression tag	UNP Q39QF5
A	393	ILE	-	expression tag	UNP Q39QF5
A	394	PRO	-	expression tag	UNP Q39QF5
A	395	ASN	-	expression tag	UNP Q39QF5
A	396	PRO	-	expression tag	UNP Q39QF5
A	397	LEU	-	expression tag	UNP Q39QF5
A	398	LEU	-	expression tag	UNP Q39QF5
A	399	GLY	-	expression tag	UNP Q39QF5
A	400	LEU	-	expression tag	UNP Q39QF5
A	401	ASP	-	expression tag	UNP Q39QF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	402	SER	-	expression tag	UNP Q39QF5
A	403	THR	-	expression tag	UNP Q39QF5
A	404	ARG	-	expression tag	UNP Q39QF5
A	405	THR	-	expression tag	UNP Q39QF5
A	406	GLY	-	expression tag	UNP Q39QF5
A	407	HIS	-	expression tag	UNP Q39QF5
A	408	HIS	-	expression tag	UNP Q39QF5
A	409	HIS	-	expression tag	UNP Q39QF5
A	410	HIS	-	expression tag	UNP Q39QF5
A	411	HIS	-	expression tag	UNP Q39QF5
A	412	HIS	-	expression tag	UNP Q39QF5
B	381	LYS	-	expression tag	UNP Q39QF5
B	382	GLY	-	expression tag	UNP Q39QF5
B	383	GLU	-	expression tag	UNP Q39QF5
B	384	LEU	-	expression tag	UNP Q39QF5
B	385	ASN	-	expression tag	UNP Q39QF5
B	386	SER	-	expression tag	UNP Q39QF5
B	387	LYS	-	expression tag	UNP Q39QF5
B	388	LEU	-	expression tag	UNP Q39QF5
B	389	GLU	-	expression tag	UNP Q39QF5
B	390	GLY	-	expression tag	UNP Q39QF5
B	391	LYS	-	expression tag	UNP Q39QF5
B	392	PRO	-	expression tag	UNP Q39QF5
B	393	ILE	-	expression tag	UNP Q39QF5
B	394	PRO	-	expression tag	UNP Q39QF5
B	395	ASN	-	expression tag	UNP Q39QF5
B	396	PRO	-	expression tag	UNP Q39QF5
B	397	LEU	-	expression tag	UNP Q39QF5
B	398	LEU	-	expression tag	UNP Q39QF5
B	399	GLY	-	expression tag	UNP Q39QF5
B	400	LEU	-	expression tag	UNP Q39QF5
B	401	ASP	-	expression tag	UNP Q39QF5
B	402	SER	-	expression tag	UNP Q39QF5
B	403	THR	-	expression tag	UNP Q39QF5
B	404	ARG	-	expression tag	UNP Q39QF5
B	405	THR	-	expression tag	UNP Q39QF5
B	406	GLY	-	expression tag	UNP Q39QF5
B	407	HIS	-	expression tag	UNP Q39QF5
B	408	HIS	-	expression tag	UNP Q39QF5
B	409	HIS	-	expression tag	UNP Q39QF5
B	410	HIS	-	expression tag	UNP Q39QF5
B	411	HIS	-	expression tag	UNP Q39QF5

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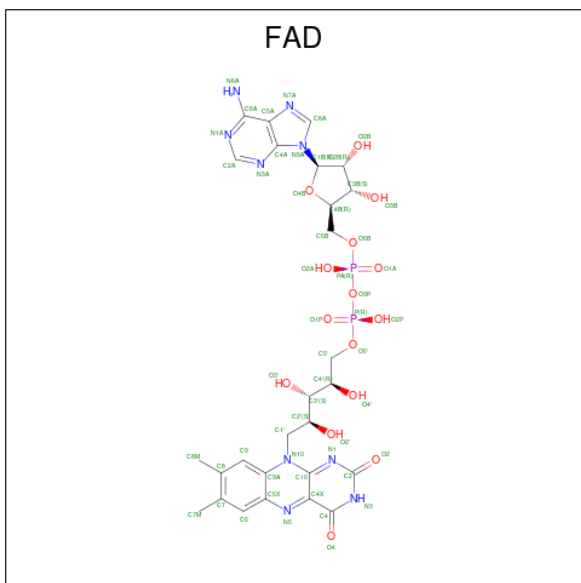
Chain	Residue	Modelled	Actual	Comment	Reference
B	412	HIS	-	expression tag	UNP Q39QF5
C	381	LYS	-	expression tag	UNP Q39QF5
C	382	GLY	-	expression tag	UNP Q39QF5
C	383	GLU	-	expression tag	UNP Q39QF5
C	384	LEU	-	expression tag	UNP Q39QF5
C	385	ASN	-	expression tag	UNP Q39QF5
C	386	SER	-	expression tag	UNP Q39QF5
C	387	LYS	-	expression tag	UNP Q39QF5
C	388	LEU	-	expression tag	UNP Q39QF5
C	389	GLU	-	expression tag	UNP Q39QF5
C	390	GLY	-	expression tag	UNP Q39QF5
C	391	LYS	-	expression tag	UNP Q39QF5
C	392	PRO	-	expression tag	UNP Q39QF5
C	393	ILE	-	expression tag	UNP Q39QF5
C	394	PRO	-	expression tag	UNP Q39QF5
C	395	ASN	-	expression tag	UNP Q39QF5
C	396	PRO	-	expression tag	UNP Q39QF5
C	397	LEU	-	expression tag	UNP Q39QF5
C	398	LEU	-	expression tag	UNP Q39QF5
C	399	GLY	-	expression tag	UNP Q39QF5
C	400	LEU	-	expression tag	UNP Q39QF5
C	401	ASP	-	expression tag	UNP Q39QF5
C	402	SER	-	expression tag	UNP Q39QF5
C	403	THR	-	expression tag	UNP Q39QF5
C	404	ARG	-	expression tag	UNP Q39QF5
C	405	THR	-	expression tag	UNP Q39QF5
C	406	GLY	-	expression tag	UNP Q39QF5
C	407	HIS	-	expression tag	UNP Q39QF5
C	408	HIS	-	expression tag	UNP Q39QF5
C	409	HIS	-	expression tag	UNP Q39QF5
C	410	HIS	-	expression tag	UNP Q39QF5
C	411	HIS	-	expression tag	UNP Q39QF5
C	412	HIS	-	expression tag	UNP Q39QF5
D	381	LYS	-	expression tag	UNP Q39QF5
D	382	GLY	-	expression tag	UNP Q39QF5
D	383	GLU	-	expression tag	UNP Q39QF5
D	384	LEU	-	expression tag	UNP Q39QF5
D	385	ASN	-	expression tag	UNP Q39QF5
D	386	SER	-	expression tag	UNP Q39QF5
D	387	LYS	-	expression tag	UNP Q39QF5
D	388	LEU	-	expression tag	UNP Q39QF5
D	389	GLU	-	expression tag	UNP Q39QF5

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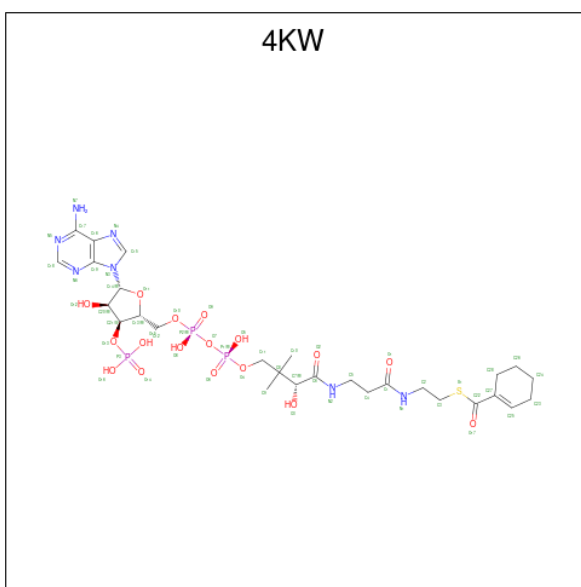
Chain	Residue	Modelled	Actual	Comment	Reference
D	390	GLY	-	expression tag	UNP Q39QF5
D	391	LYS	-	expression tag	UNP Q39QF5
D	392	PRO	-	expression tag	UNP Q39QF5
D	393	ILE	-	expression tag	UNP Q39QF5
D	394	PRO	-	expression tag	UNP Q39QF5
D	395	ASN	-	expression tag	UNP Q39QF5
D	396	PRO	-	expression tag	UNP Q39QF5
D	397	LEU	-	expression tag	UNP Q39QF5
D	398	LEU	-	expression tag	UNP Q39QF5
D	399	GLY	-	expression tag	UNP Q39QF5
D	400	LEU	-	expression tag	UNP Q39QF5
D	401	ASP	-	expression tag	UNP Q39QF5
D	402	SER	-	expression tag	UNP Q39QF5
D	403	THR	-	expression tag	UNP Q39QF5
D	404	ARG	-	expression tag	UNP Q39QF5
D	405	THR	-	expression tag	UNP Q39QF5
D	406	GLY	-	expression tag	UNP Q39QF5
D	407	HIS	-	expression tag	UNP Q39QF5
D	408	HIS	-	expression tag	UNP Q39QF5
D	409	HIS	-	expression tag	UNP Q39QF5
D	410	HIS	-	expression tag	UNP Q39QF5
D	411	HIS	-	expression tag	UNP Q39QF5
D	412	HIS	-	expression tag	UNP Q39QF5

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0
2	B	1	53	27	9	15	2	0	0
2	C	1	53	27	9	15	2	0	0
2	D	1	53	27	9	15	2	0	0

- Molecule 3 is 1-monoenoyl-CoA (three-letter code: 4KW) (formula:  $C_{28}H_{44}N_7O_{17}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	56	28	7	17	3	1	0	0
3	B	1	56	28	7	17	3	1	0	0
3	C	1	56	28	7	17	3	1	0	0
3	D	1	56	28	7	17	3	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	307	Total O 307 307	0	0
5	B	328	Total O 329 329	0	1
5	C	336	Total O 336 336	0	0
5	D	117	Total O 117 117	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.91Å 333.85Å 76.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 1.65 47.19 – 1.65	Depositor EDS
% Data completeness (in resolution range)	93.0 (48.25-1.65) 93.0 (47.19-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 1.65Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.222 , 0.236 0.232 , 0.245	Depositor DCC
$R_{free}$ test set	12200 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13151	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1094e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FAD, 4KW

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	0.47	0/2937	0.59	0/3967
1	B	0.48	0/2927	0.58	0/3953
1	C	0.49	0/2942	0.59	0/3973
1	D	0.53	0/2929	0.72	4/3954 (0.1%)
All	All	0.49	0/11735	0.62	4/15847 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	6	GLU	CB-CA-C	9.06	128.53	110.40
1	D	196	ARG	CB-CA-C	-5.94	98.53	110.40
1	D	236	GLN	CB-CA-C	5.62	121.64	110.40
1	D	274	ILE	CB-CA-C	5.42	122.45	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	196	ARG	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	A	2899	0	2947	8	0
1	B	2889	0	2943	12	0
1	C	2904	0	2964	11	0
1	D	2892	0	2946	88	0
2	A	53	0	27	1	0
2	B	53	0	27	3	0
2	C	53	0	27	2	0
2	D	53	0	27	0	0
3	A	56	0	0	0	0
3	B	56	0	0	0	0
3	C	56	0	0	0	0
3	D	56	0	0	0	0
4	A	6	0	8	0	0
4	B	12	0	16	0	0
4	C	12	0	16	0	0
4	D	12	0	16	1	0
5	A	307	0	0	1	0
5	B	329	0	0	1	0
5	C	336	0	0	1	0
5	D	117	0	0	12	0
All	All	13151	0	11964	118	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 5.

The worst 5 of 118 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:D:269:GLN:HB2	1:D:274:ILE:CD1	1.93	0.99
1:D:269:GLN:HB2	1:D:274:ILE:HD12	1.49	0.92
1:D:4:LEU:HD21	1:D:9:LYS:CD	2.03	0.89
1:B:208:ASN:HB2	5:B:605[B]:HOH:O	1.75	0.86
1:D:29:GLU:HG3	5:D:619:HOH:O	1.77	0.83

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/412 (93%)	377 (99%)	5 (1%)	0	100	100
1	B	381/412 (92%)	376 (99%)	5 (1%)	0	100	100
1	C	383/412 (93%)	378 (99%)	5 (1%)	0	100	100
1	D	379/412 (92%)	374 (99%)	5 (1%)	0	100	100
All	All	1525/1648 (92%)	1505 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/328 (93%)	301 (99%)	3 (1%)	76	62
1	B	303/328 (92%)	301 (99%)	2 (1%)	84	73
1	C	305/328 (93%)	300 (98%)	5 (2%)	62	41
1	D	303/328 (92%)	292 (96%)	11 (4%)	35	11
All	All	1215/1312 (93%)	1194 (98%)	21 (2%)	62	39

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	236	GLN
1	D	303	GLU
1	D	362	TYR

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Mol	Chain	Res	Type
1	D	311	LYS
1	D	276	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3	HIS
1	D	276	HIS
1	D	367	GLN
1	B	152	GLN
1	A	367	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

15 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	$\# Z  > 2$
3	4KW	A	502	-	51,59,59	1.72	10 (19%)	61,87,87	1.92	17 (27%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	4KW	D	502	-	51,59,59	1.69	10 (19%)	61,87,87	1.96	17 (27%)
2	FAD	A	501	-	53,58,58	2.28	9 (16%)	68,89,89	2.17	22 (32%)
3	4KW	B	502	-	51,59,59	1.68	10 (19%)	61,87,87	1.95	14 (22%)
4	GOL	D	504	-	5,5,5	0.27	0	5,5,5	0.39	0
2	FAD	C	501	-	53,58,58	2.33	10 (18%)	68,89,89	2.06	22 (32%)
3	4KW	C	502	-	51,59,59	1.70	10 (19%)	61,87,87	1.99	17 (27%)
4	GOL	B	503	-	5,5,5	0.20	0	5,5,5	0.36	0
4	GOL	B	504	-	5,5,5	0.13	0	5,5,5	0.28	0
4	GOL	A	503	-	5,5,5	0.09	0	5,5,5	0.78	0
2	FAD	B	501	-	53,58,58	2.32	10 (18%)	68,89,89	2.11	22 (32%)
4	GOL	C	503	-	5,5,5	0.17	0	5,5,5	0.22	0
4	GOL	C	504	-	5,5,5	0.12	0	5,5,5	0.20	0
4	GOL	D	503	-	5,5,5	0.21	0	5,5,5	0.57	0
2	FAD	D	501	-	53,58,58	2.38	12 (22%)	68,89,89	2.09	22 (32%)

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
3	4KW	A	502	-	-	5/48/79/79	0/4/4/4
3	4KW	D	502	-	-	6/48/79/79	0/4/4/4
2	FAD	A	501	-	-	6/30/50/50	0/6/6/6
3	4KW	B	502	-	-	5/48/79/79	0/4/4/4
4	GOL	D	504	-	-	0/4/4/4	-
2	FAD	C	501	-	-	6/30/50/50	0/6/6/6
3	4KW	C	502	-	-	4/48/79/79	0/4/4/4
4	GOL	B	503	-	-	0/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	A	503	-	-	3/4/4/4	-
2	FAD	B	501	-	-	6/30/50/50	0/6/6/6
4	GOL	C	503	-	-	0/4/4/4	-
4	GOL	C	504	-	-	1/4/4/4	-
4	GOL	D	503	-	-	2/4/4/4	-
2	FAD	D	501	-	-	6/30/50/50	0/6/6/6

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	FAD	C4X-N5	10.07	1.50	1.30
2	B	501	FAD	C4X-N5	9.67	1.49	1.30
2	C	501	FAD	C4X-N5	9.66	1.49	1.30
2	A	501	FAD	C4X-N5	9.50	1.49	1.30
2	D	501	FAD	C2'-C3'	-8.91	1.36	1.53

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FAD	C9A-C5X-N5	-8.35	113.35	122.43
2	B	501	FAD	C9A-C5X-N5	-7.69	114.08	122.43
2	C	501	FAD	C9A-C5X-N5	-7.48	114.30	122.43
2	D	501	FAD	C9A-C5X-N5	-6.91	114.92	122.43
3	D	502	4KW	C3-S1-C22	6.78	108.31	99.80

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	FAD	C2'-C1'-N10-C10
2	A	501	FAD	N10-C1'-C2'-C3'
2	A	501	FAD	C1'-C2'-C3'-C4'
2	A	501	FAD	O2'-C2'-C3'-C4'
2	A	501	FAD	O3'-C3'-C4'-C5'

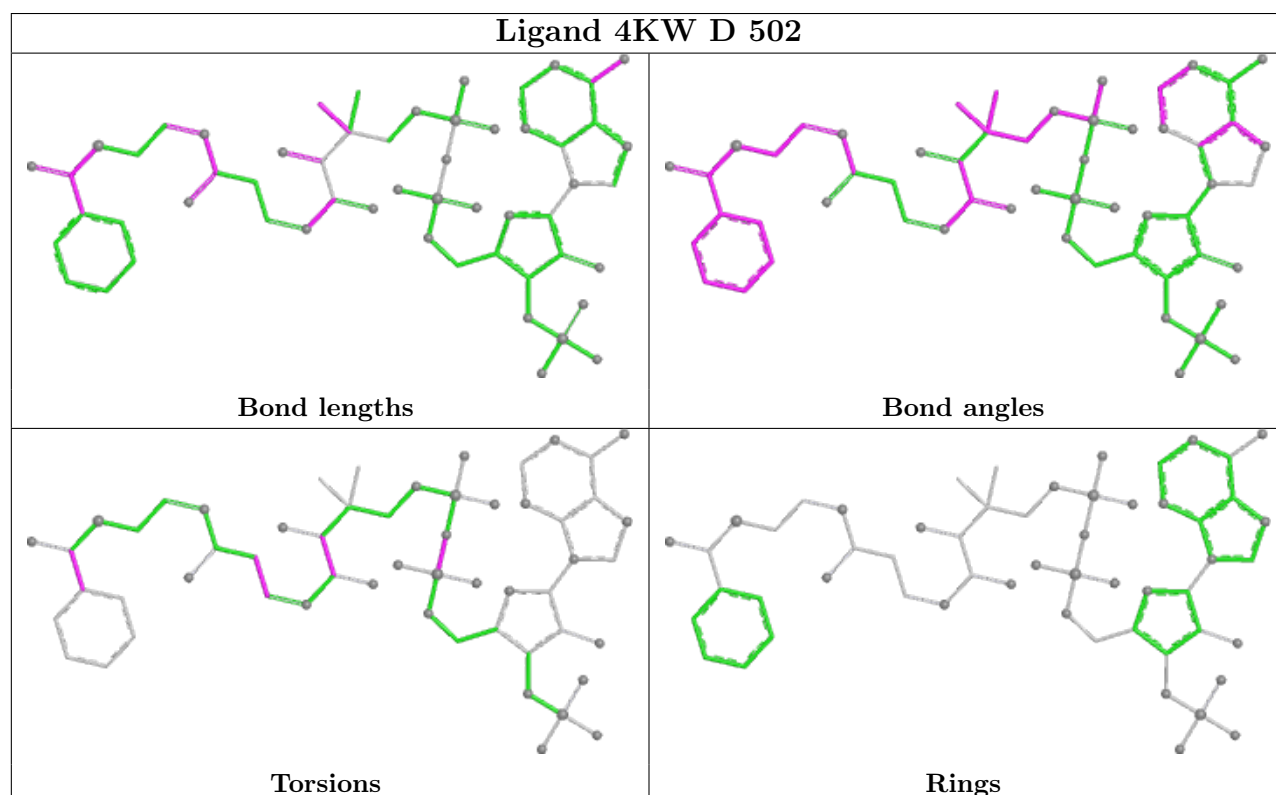
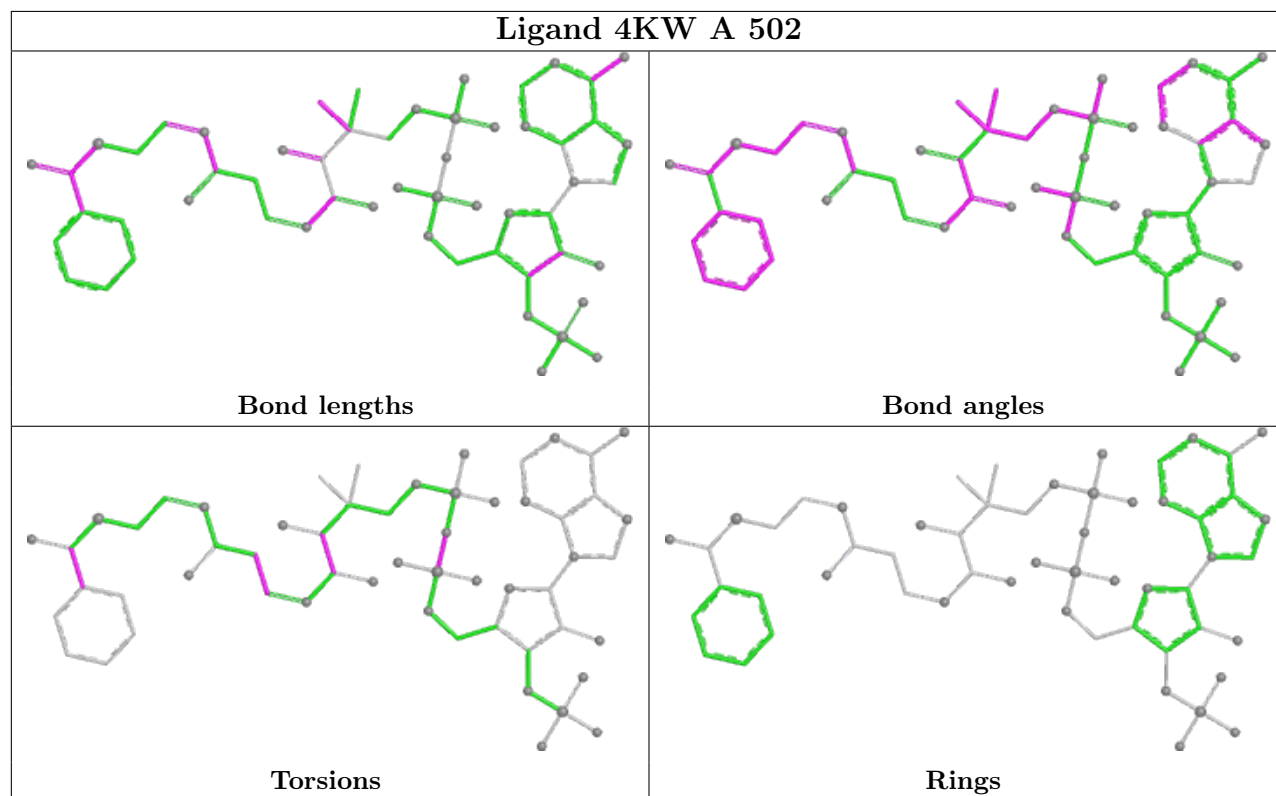
There are no ring outliers.

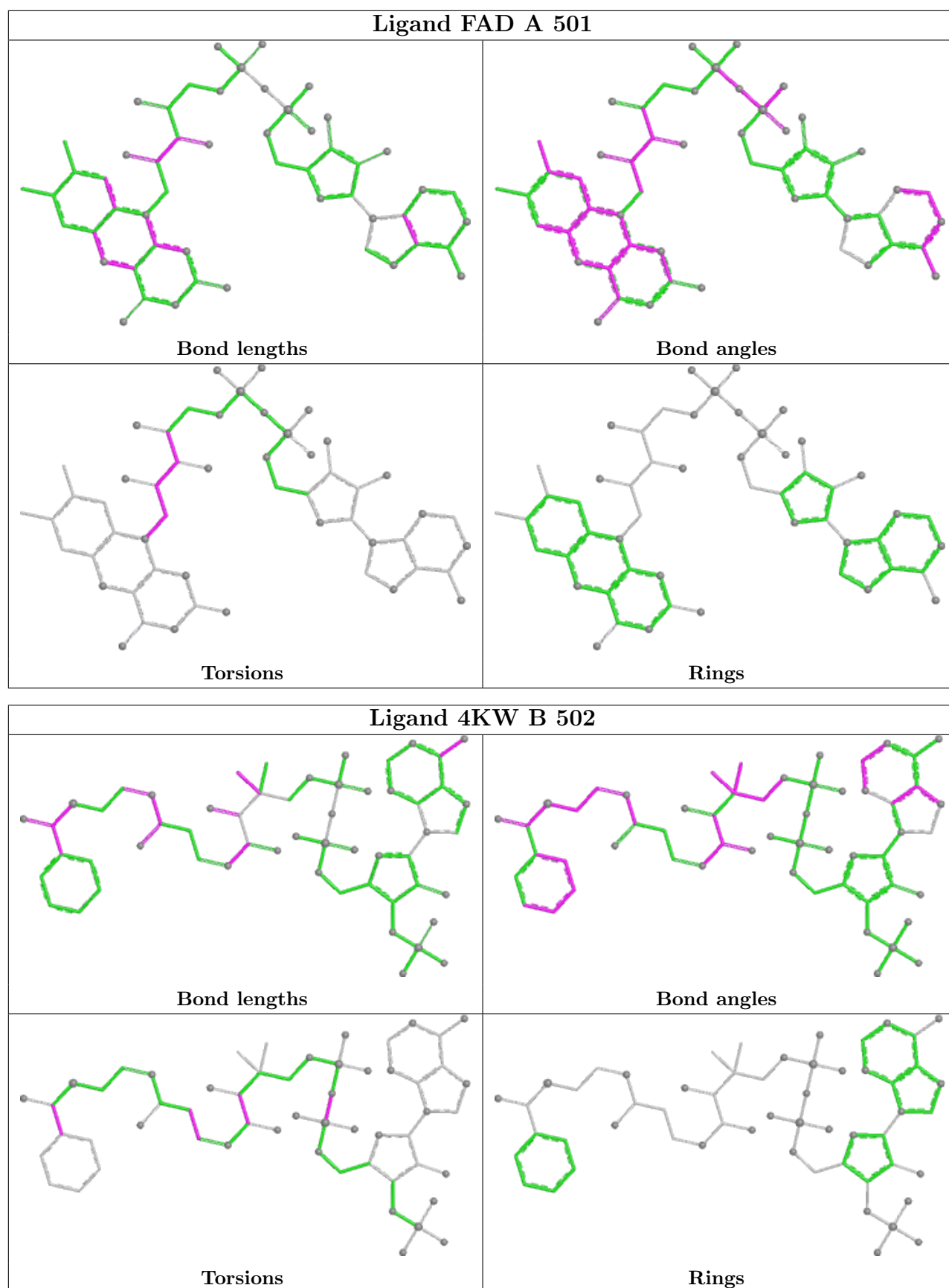
4 monomers are involved in 7 short contacts:

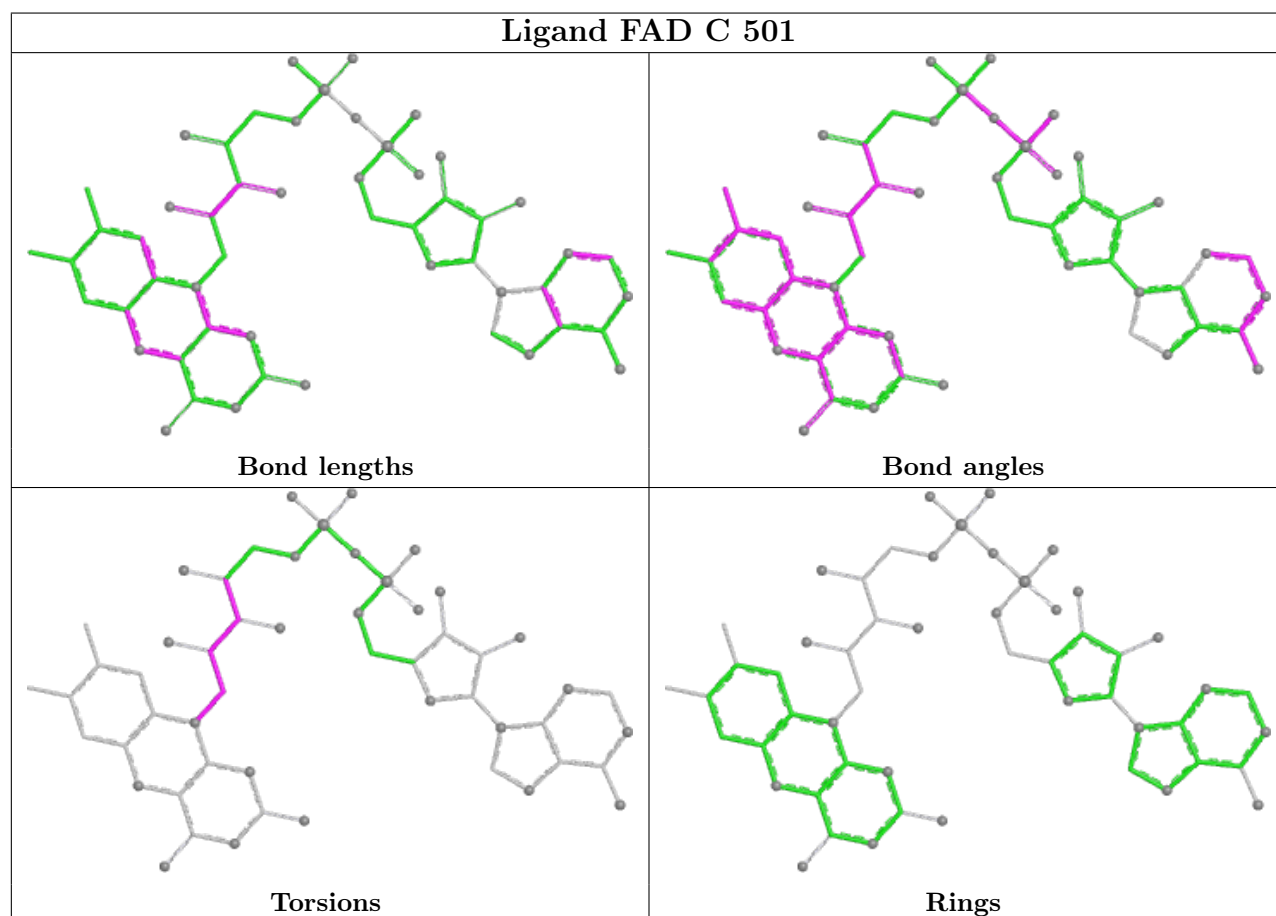
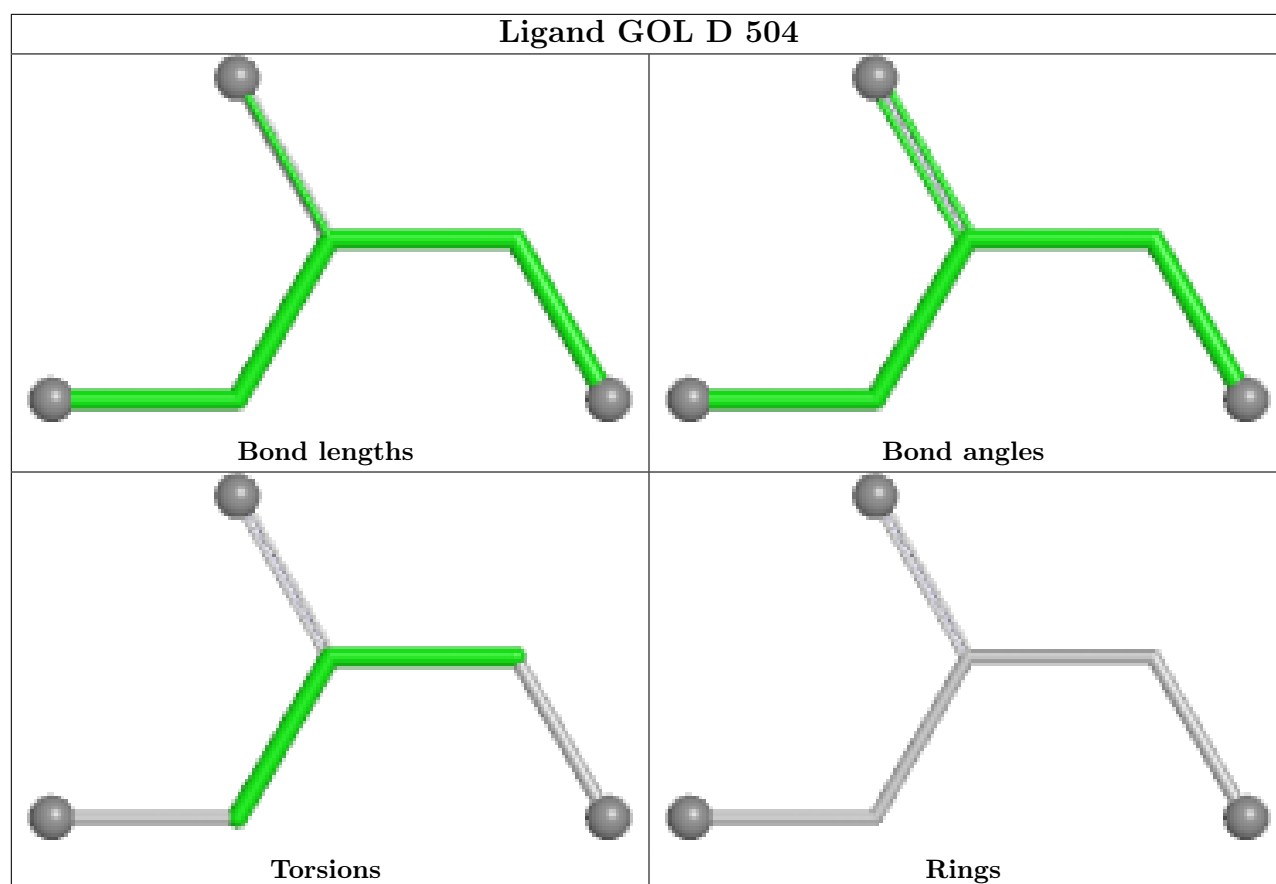
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FAD	1	0
4	D	504	GOL	1	0
2	C	501	FAD	2	0
2	B	501	FAD	3	0

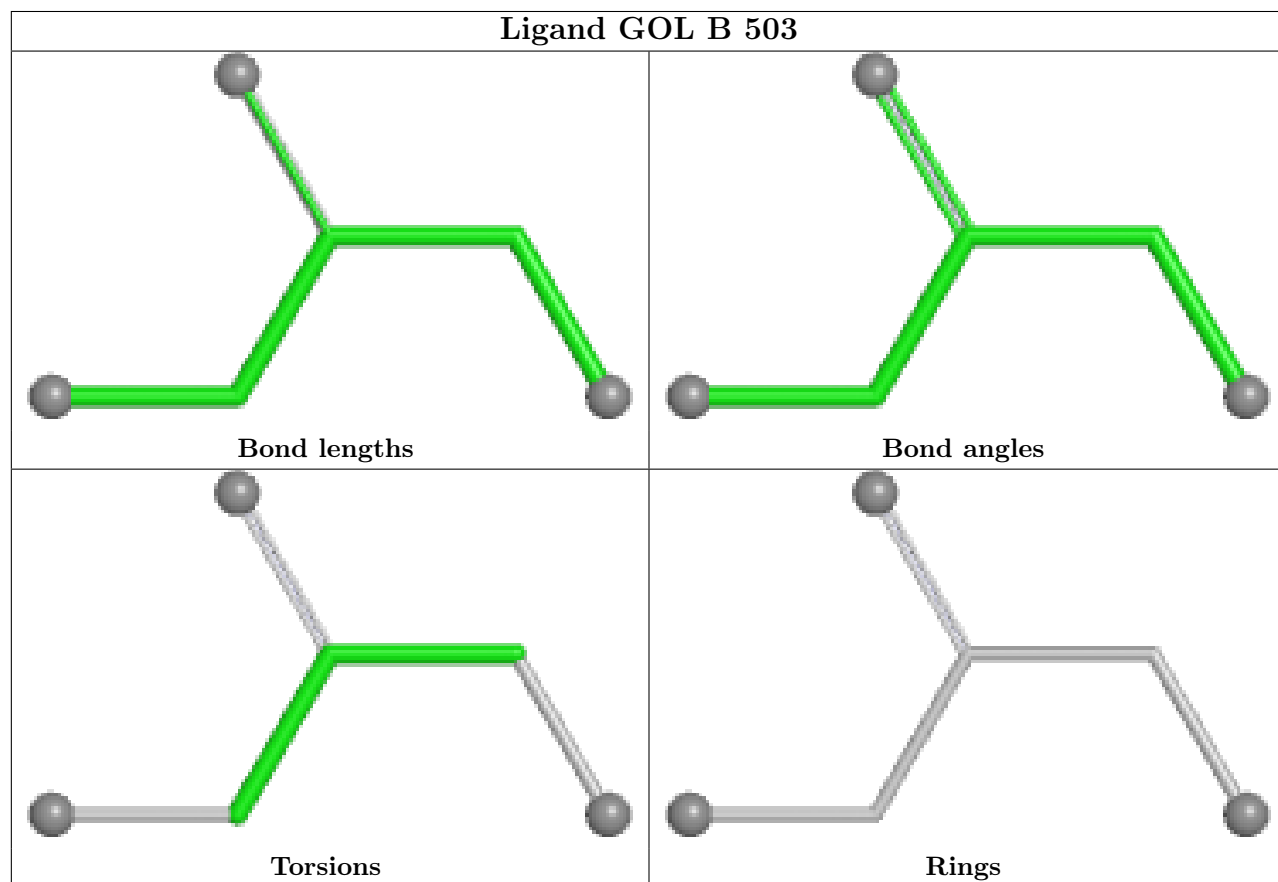
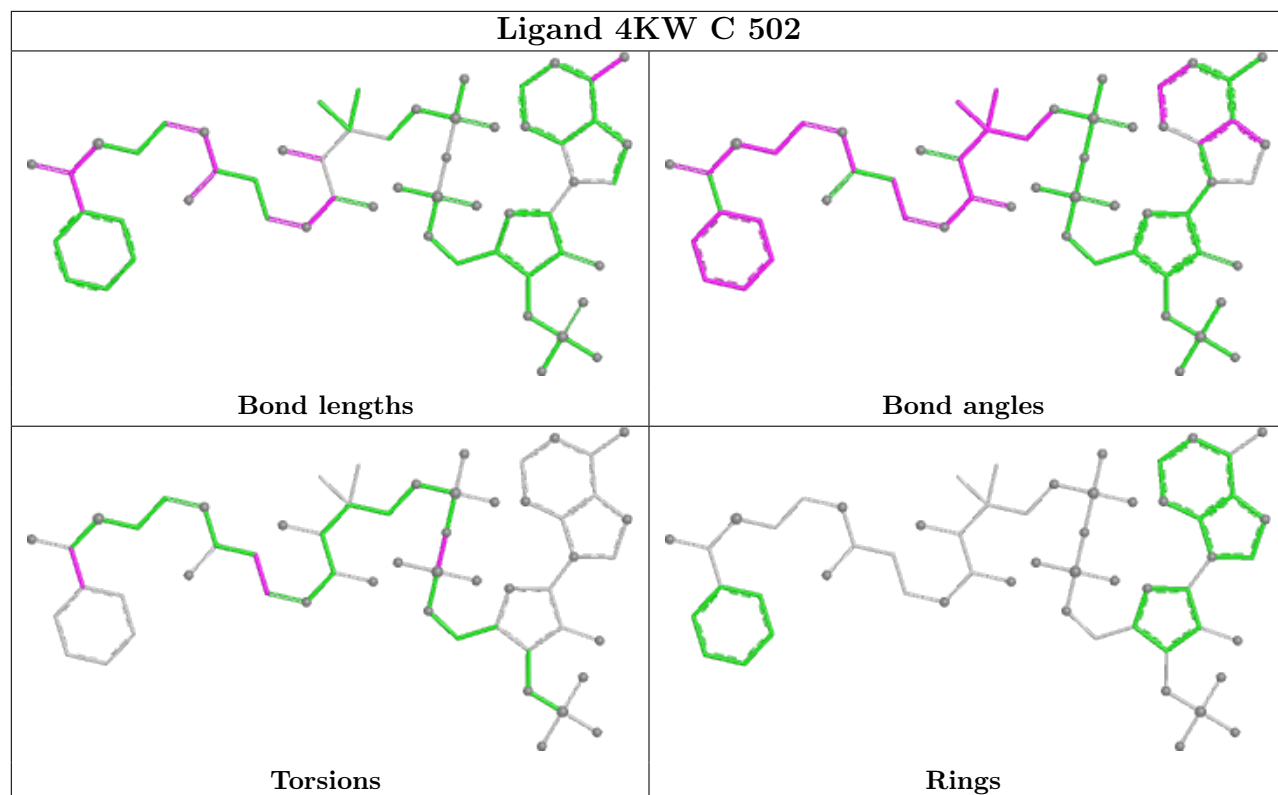
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

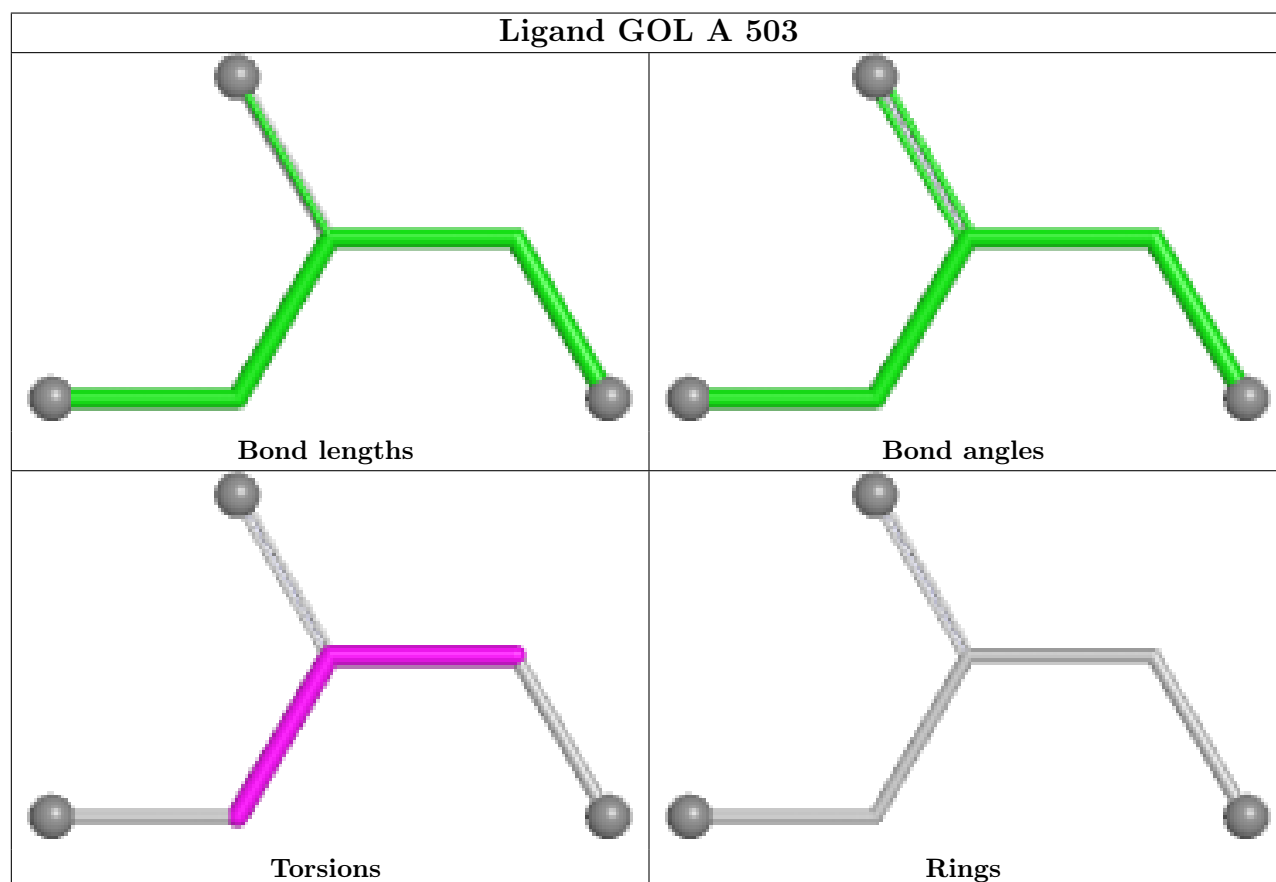
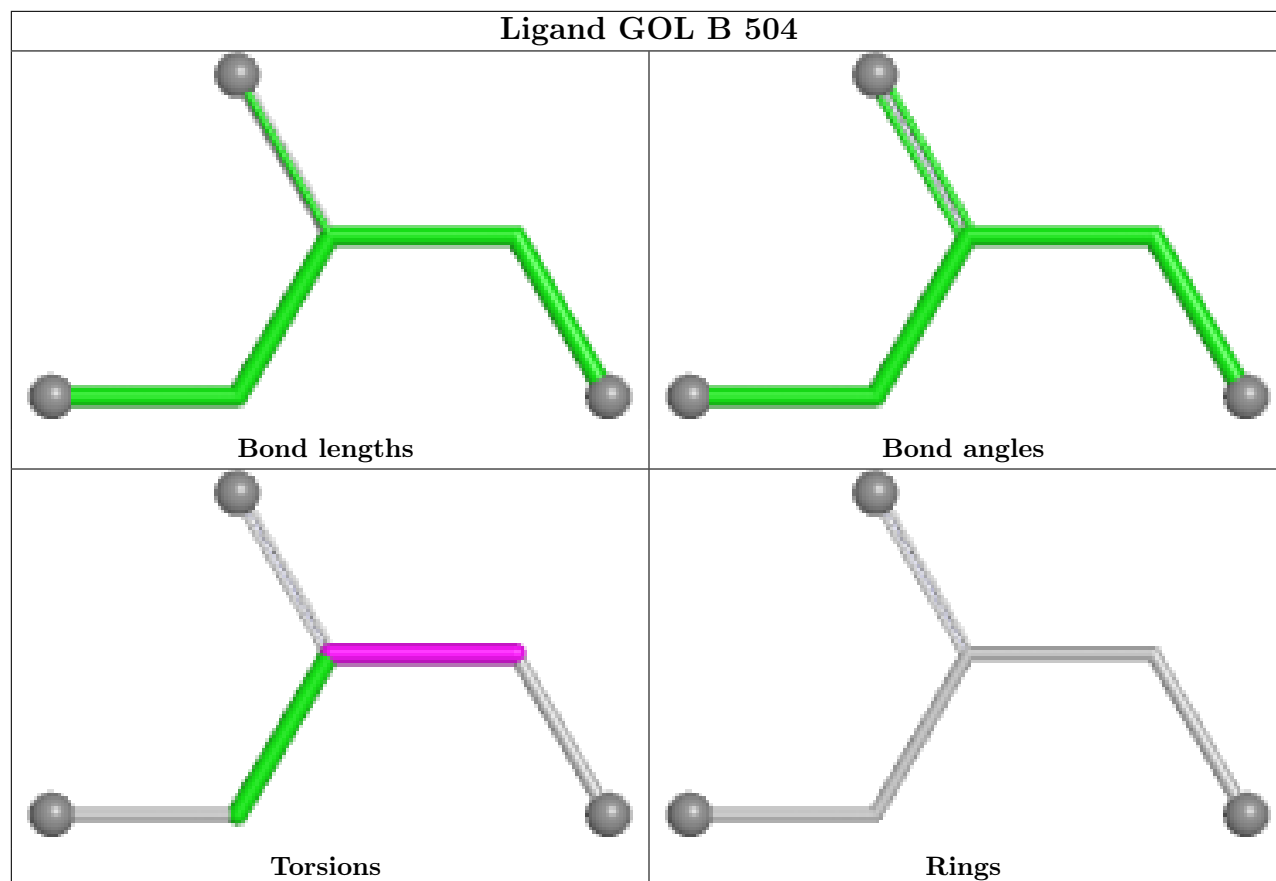
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

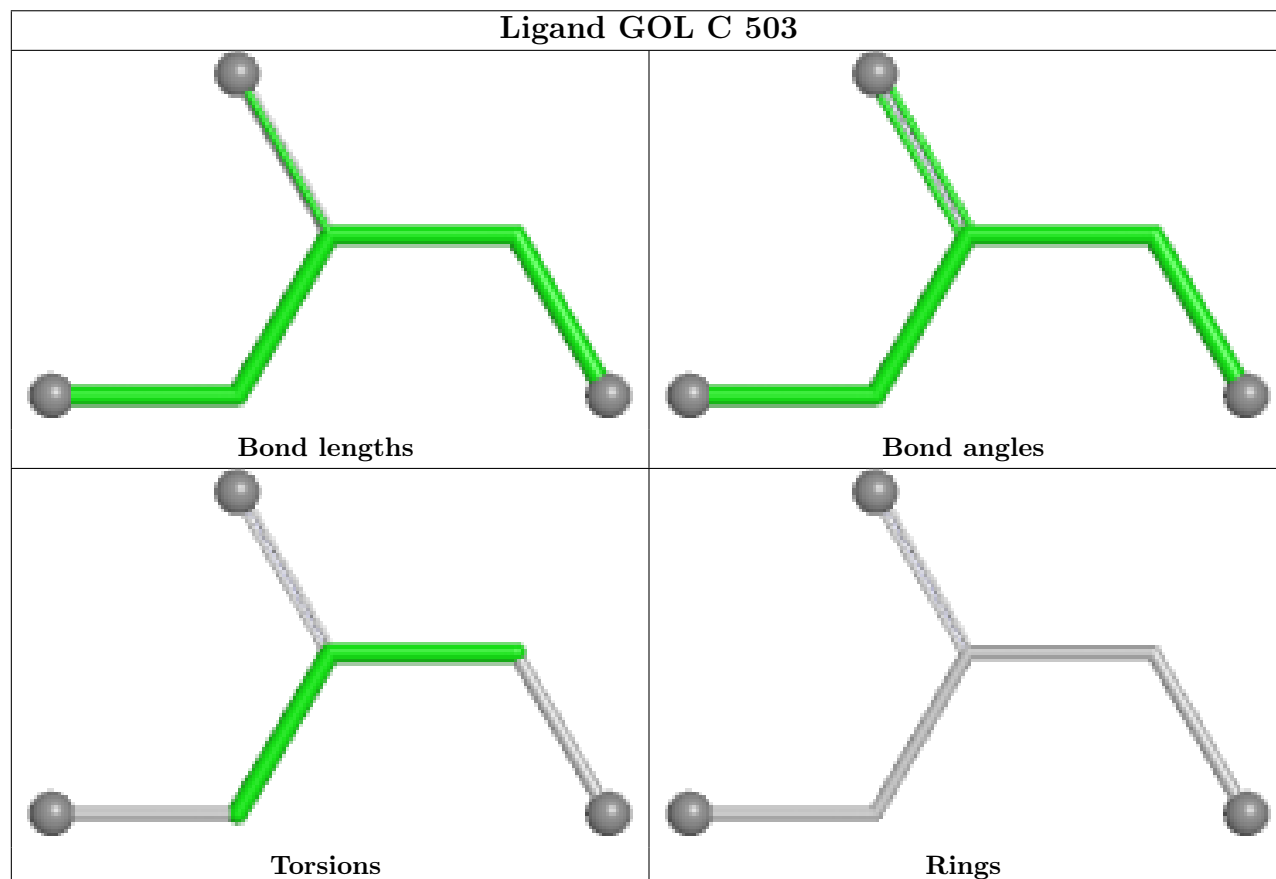
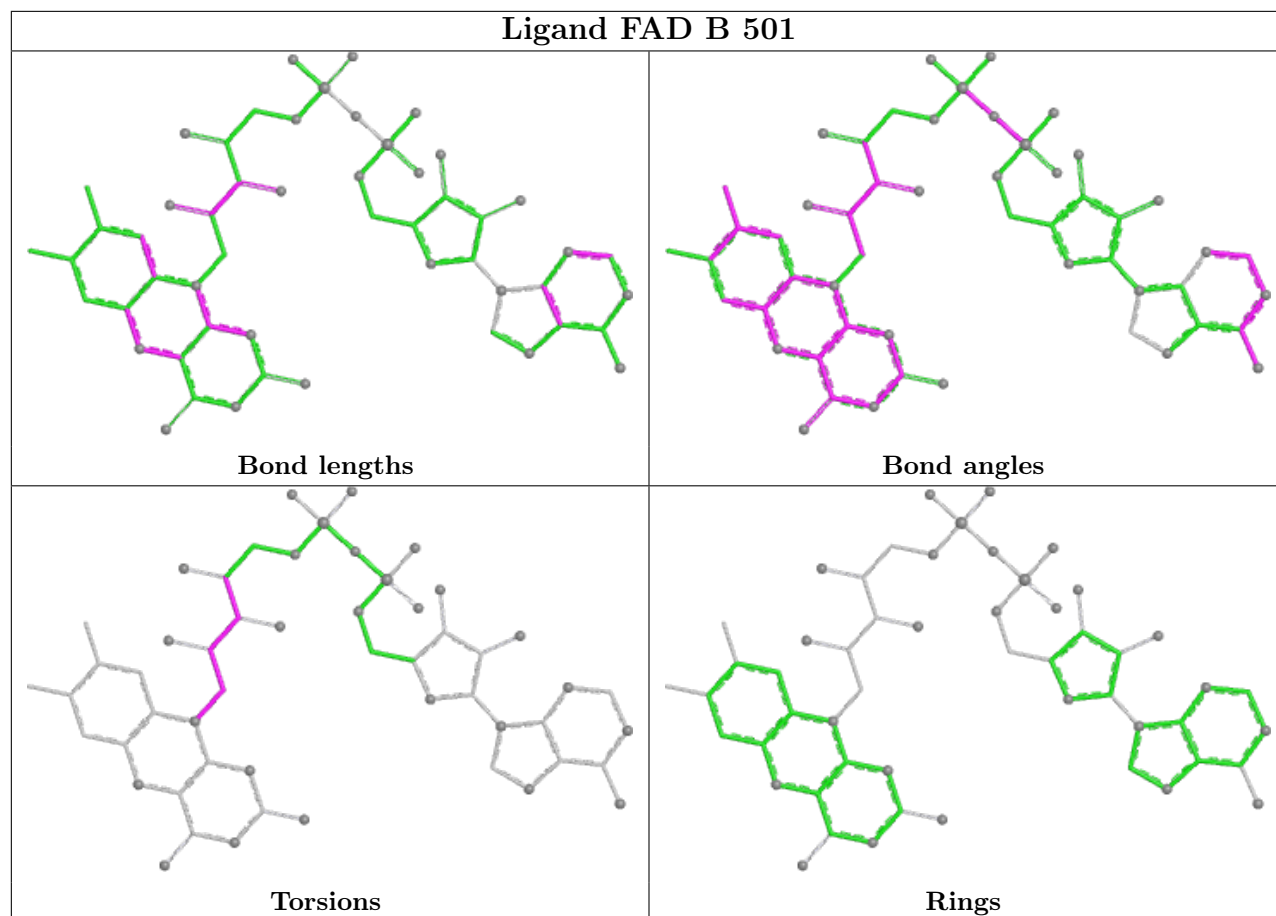




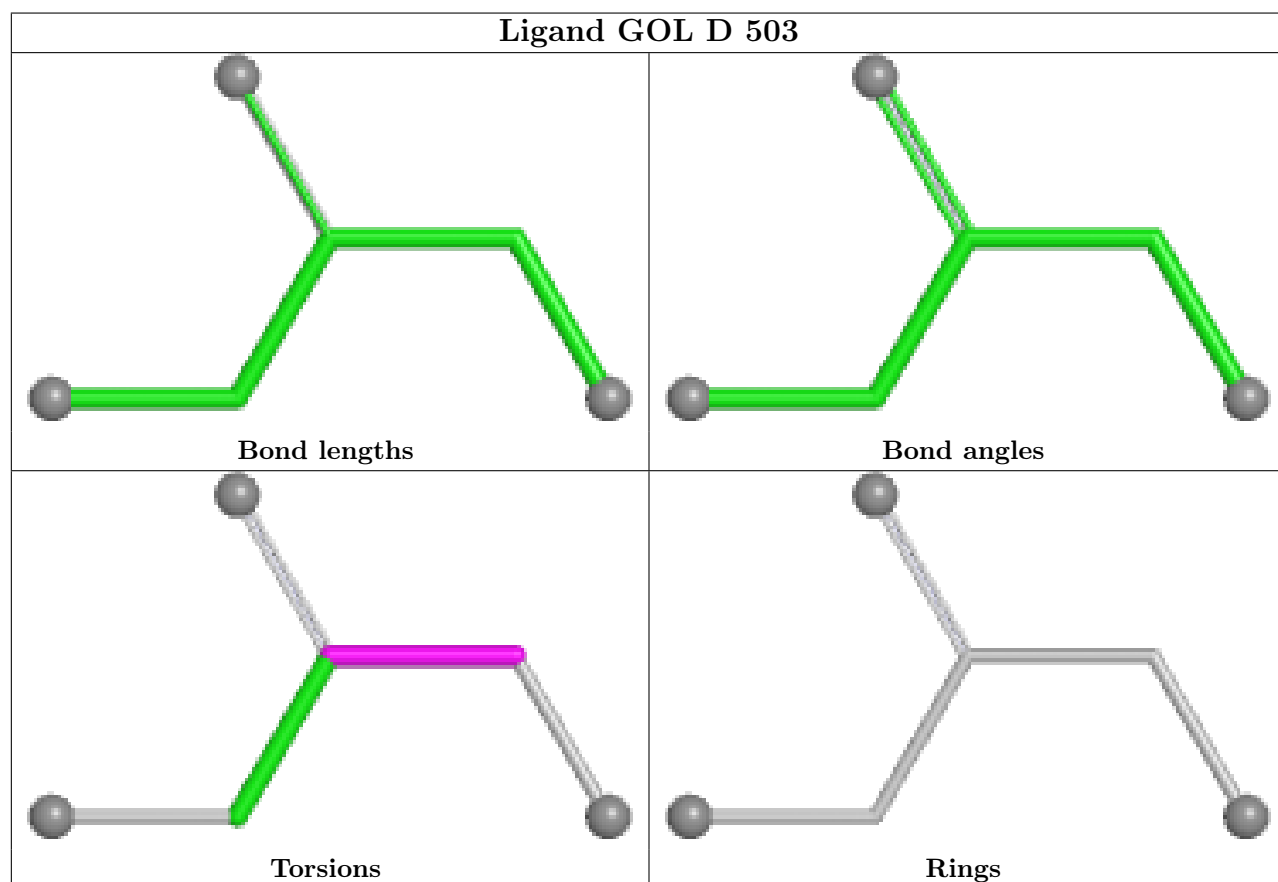
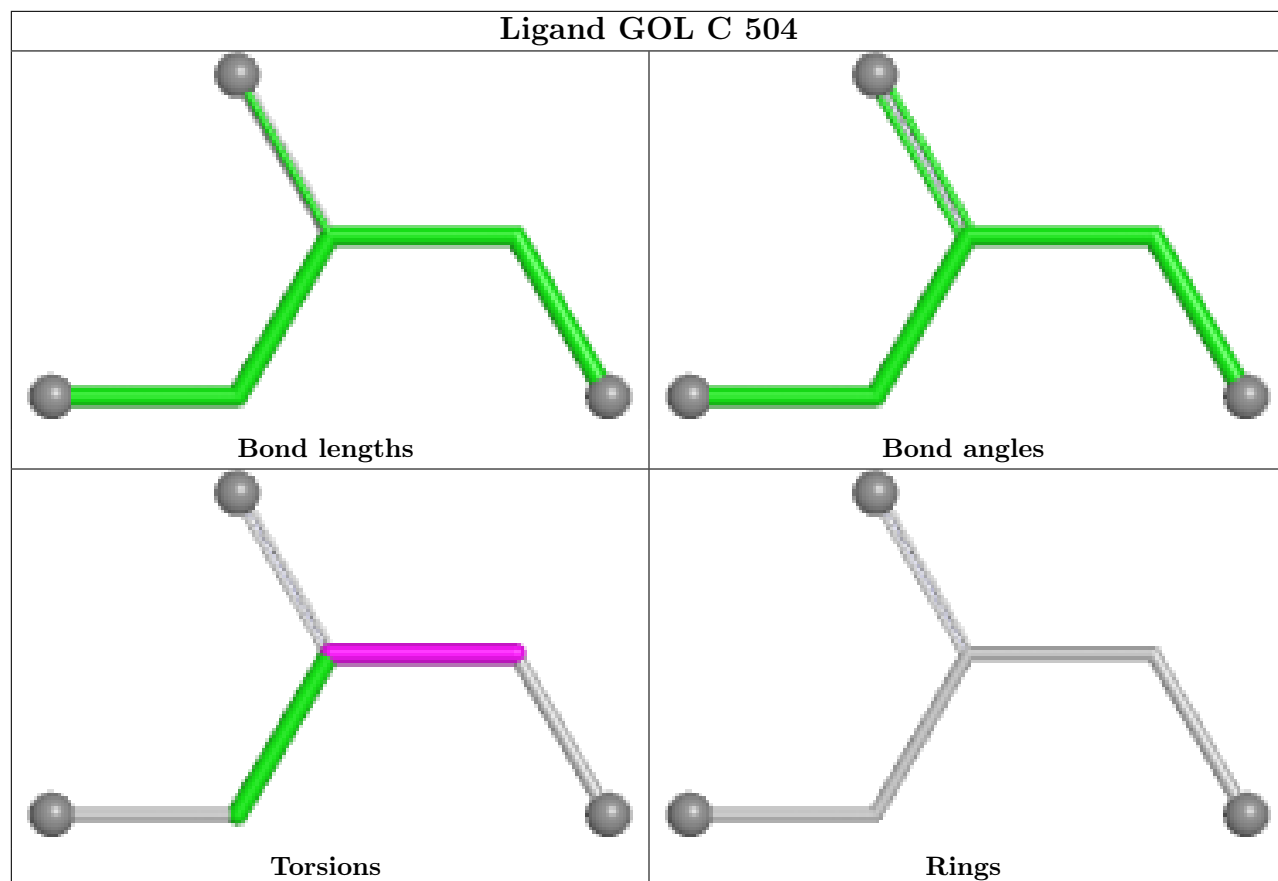


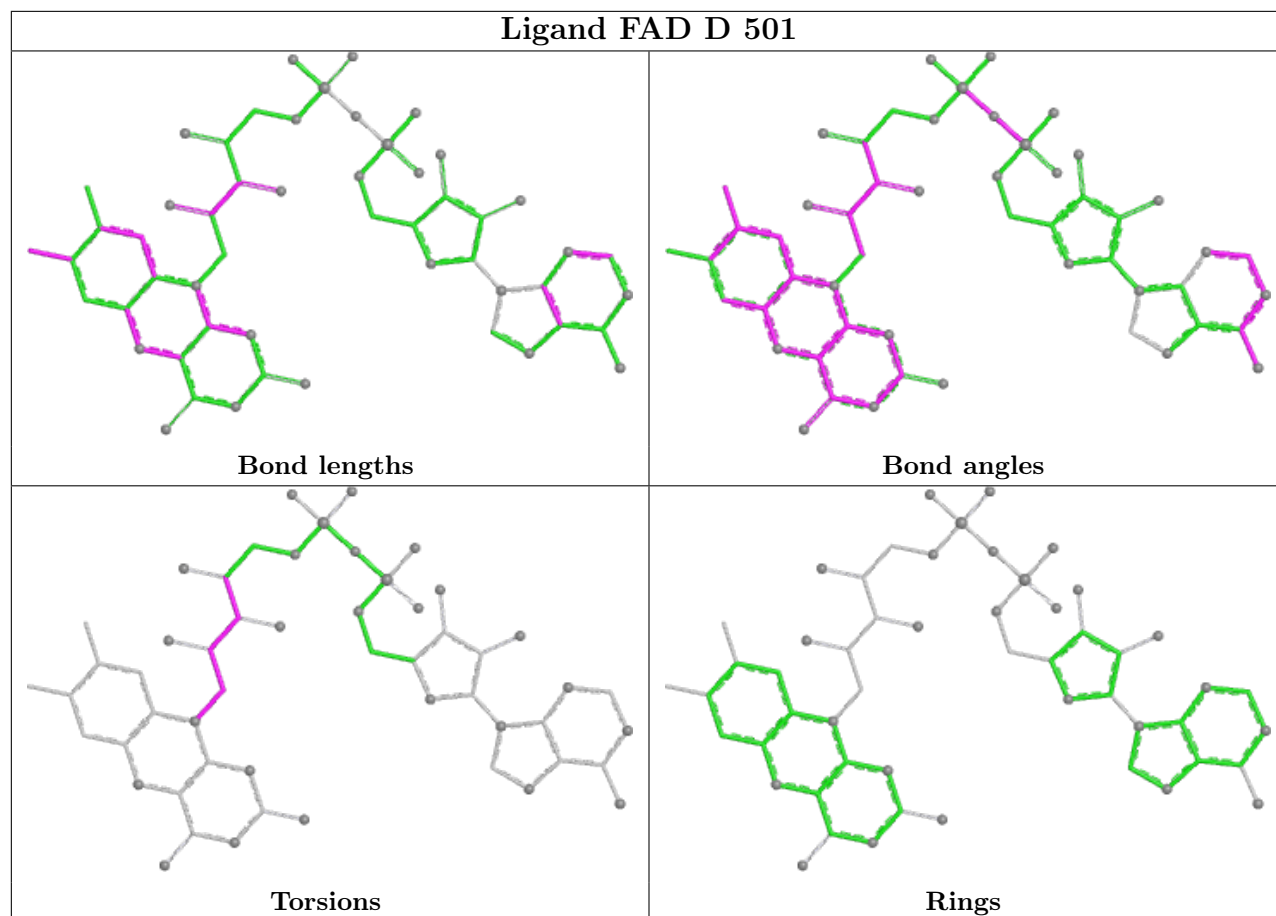












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	378/412 (91%)	0.18	5 (1%) 77 80	12, 23, 43, 70	0
1	B	378/412 (91%)	0.21	13 (3%) 45 45	12, 21, 39, 65	0
1	C	378/412 (91%)	0.26	11 (2%) 51 52	12, 22, 41, 65	0
1	D	377/412 (91%)	3.61	275 (72%) 0 0	22, 39, 63, 105	0
All	All	1511/1648 (91%)	1.06	304 (20%) 1 1	12, 25, 53, 105	0

The worst 5 of 304 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	LEU	16.4
1	D	11	THR	14.7
1	D	10	LEU	13.3
1	D	15	VAL	13.0
1	D	12	LEU	11.2

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

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

### 6.3 Carbohydrates [i](#)

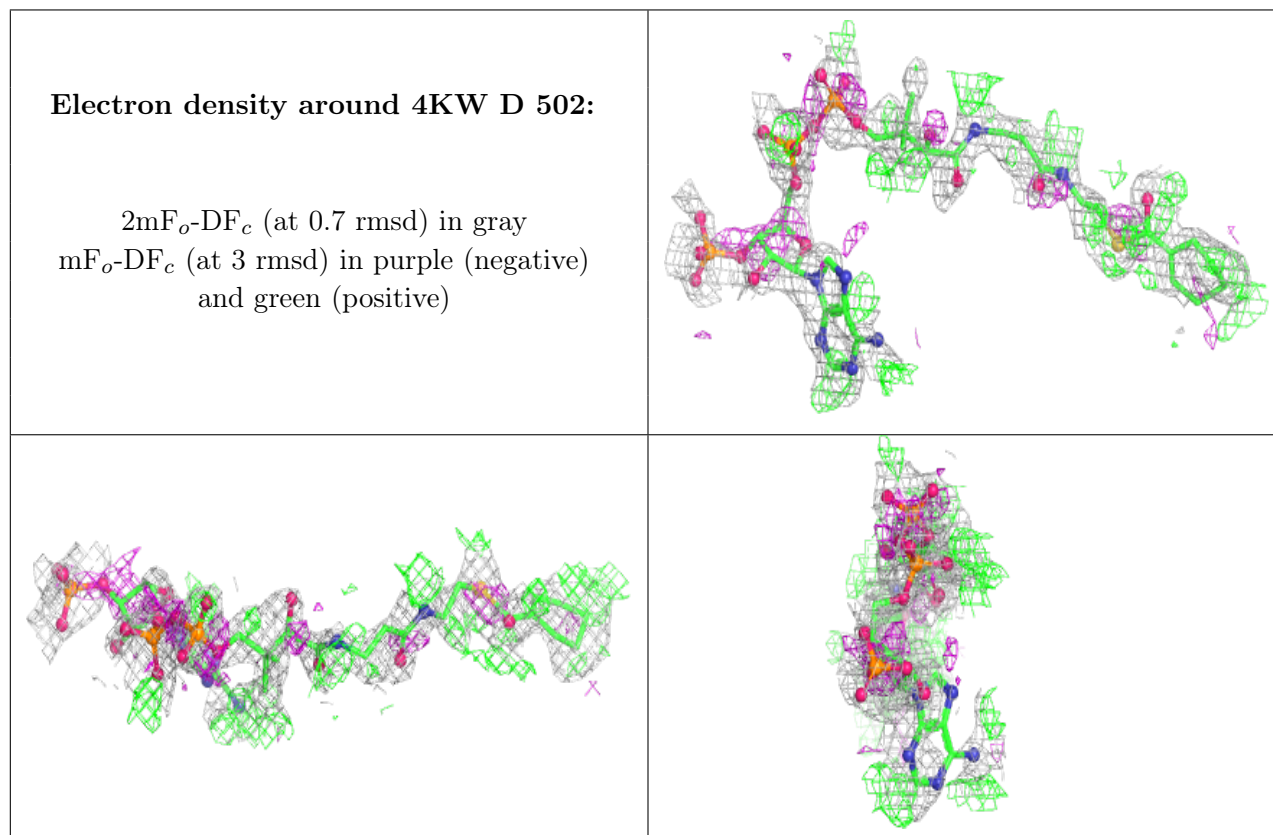
There are no monosaccharides in this entry.

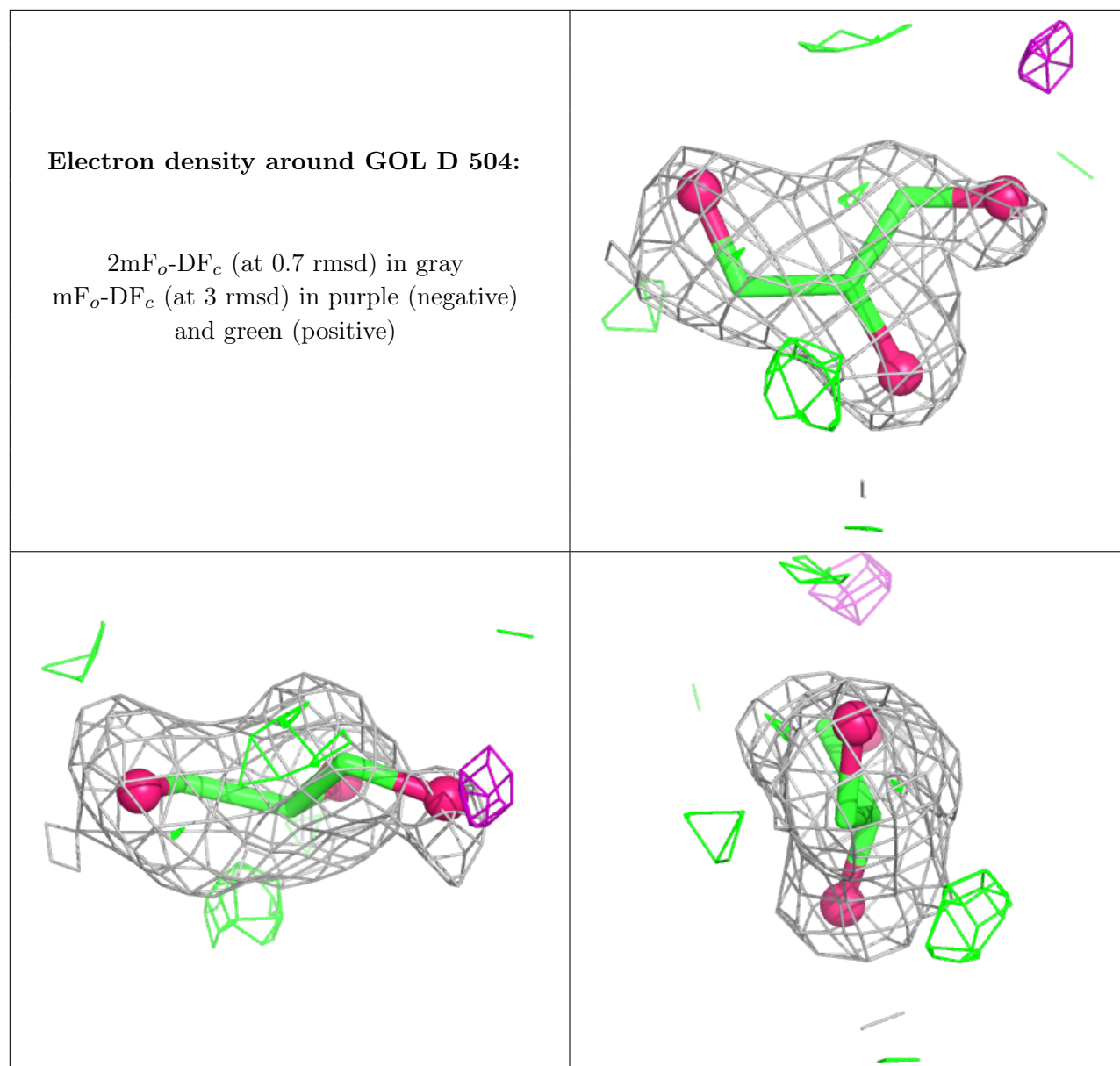
### 6.4 Ligands [i](#)

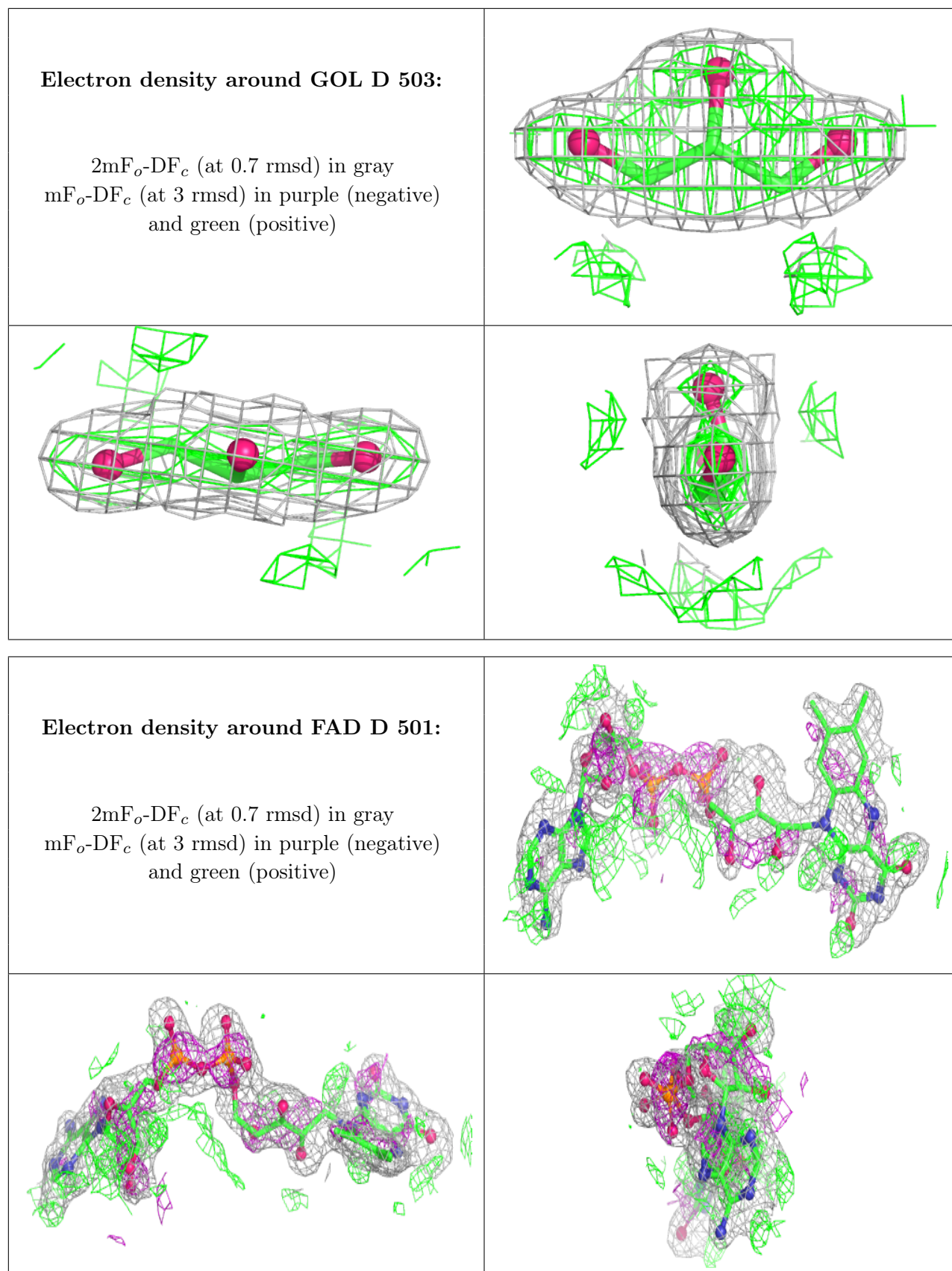
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	4KW	D	502	56/56	0.49	0.34	39,55,86,86	0
4	GOL	D	504	6/6	0.72	0.21	45,47,50,51	0
4	GOL	D	503	6/6	0.76	0.42	78,83,83,85	6
2	FAD	D	501	53/53	0.76	0.23	31,35,39,41	0
4	GOL	C	504	6/6	0.80	0.21	40,44,46,48	0
4	GOL	B	504	6/6	0.87	0.11	31,38,41,42	0
3	4KW	C	502	56/56	0.88	0.14	18,31,55,58	0
3	4KW	A	502	56/56	0.88	0.13	19,28,56,58	0
3	4KW	B	502	56/56	0.88	0.14	20,28,60,61	0
4	GOL	A	503	6/6	0.92	0.18	21,28,29,30	0
4	GOL	C	503	6/6	0.95	0.11	20,22,24,25	0
2	FAD	B	501	53/53	0.96	0.08	17,20,23,24	0
2	FAD	C	501	53/53	0.96	0.08	14,18,20,23	0
4	GOL	B	503	6/6	0.96	0.14	22,22,23,25	0
2	FAD	A	501	53/53	0.96	0.09	15,20,23,24	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.

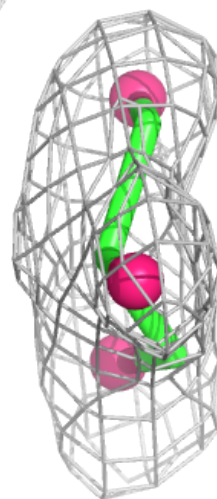
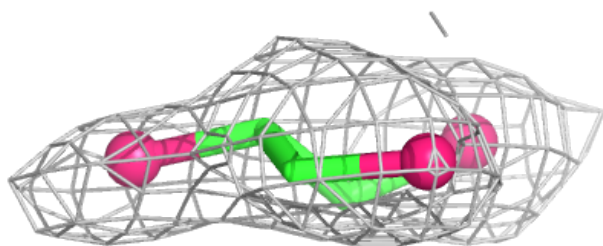
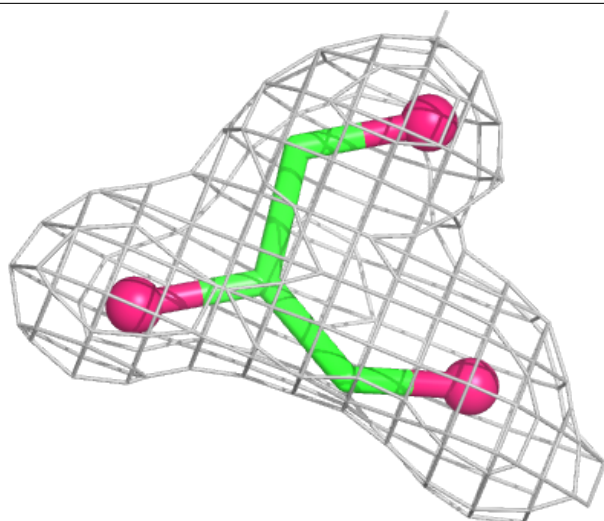




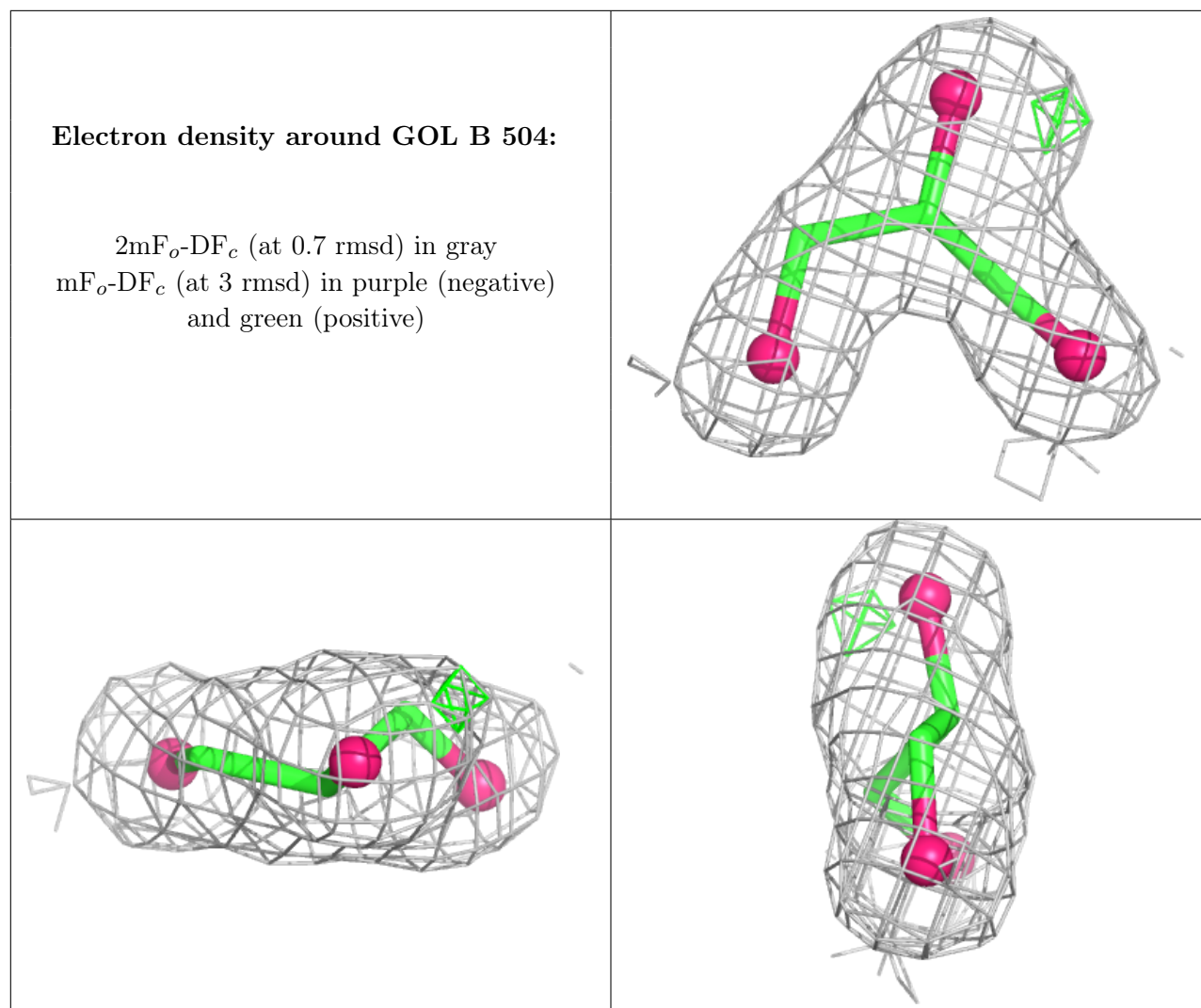


**Electron density around GOL C 504:**

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



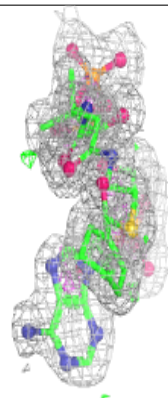
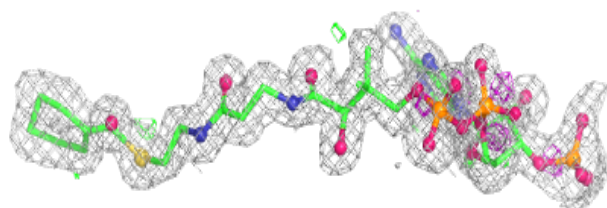
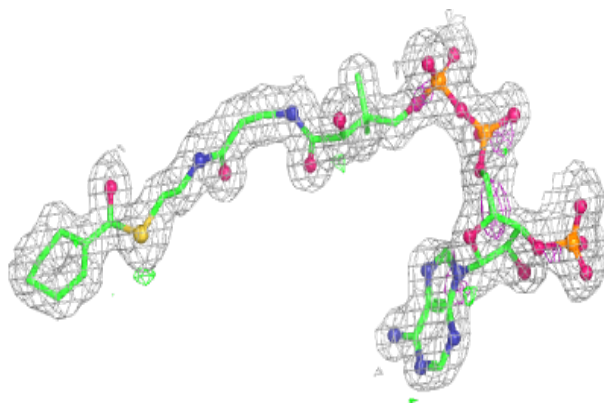




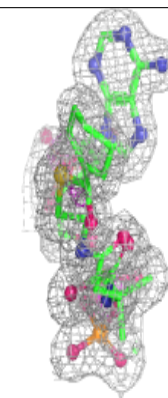
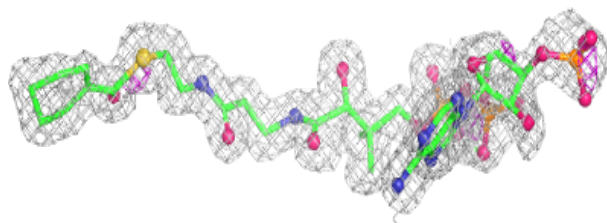
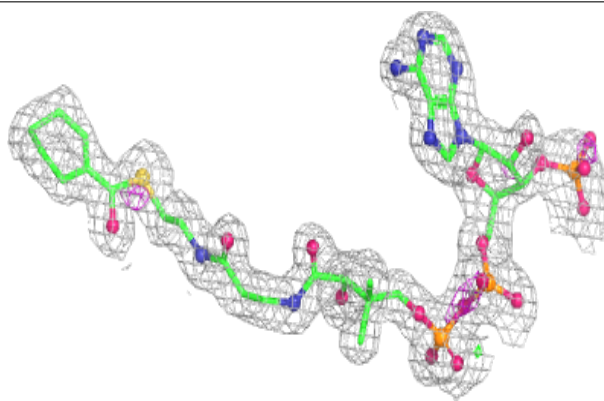


**Electron density around 4KW C 502:**

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

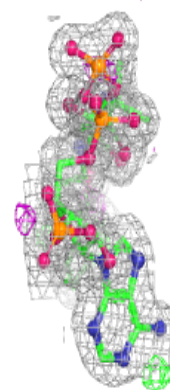
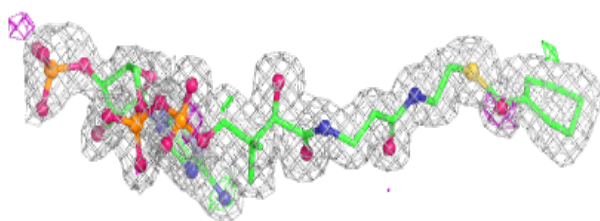
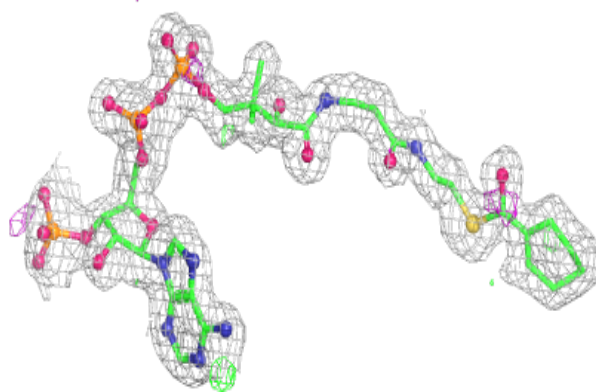
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

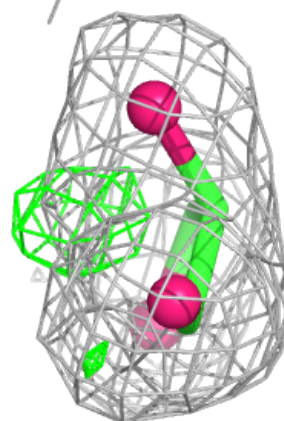
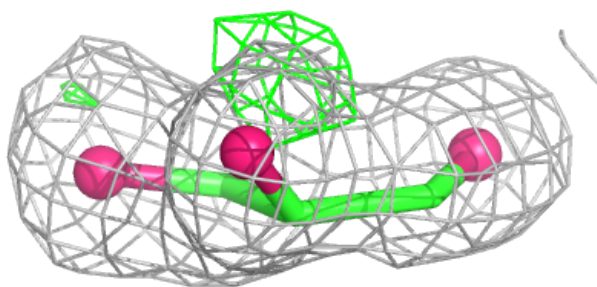
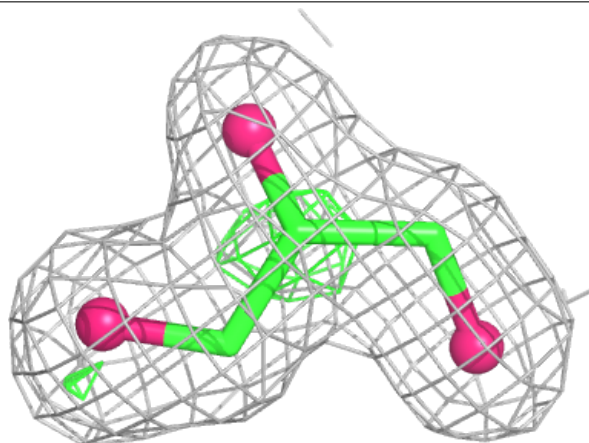


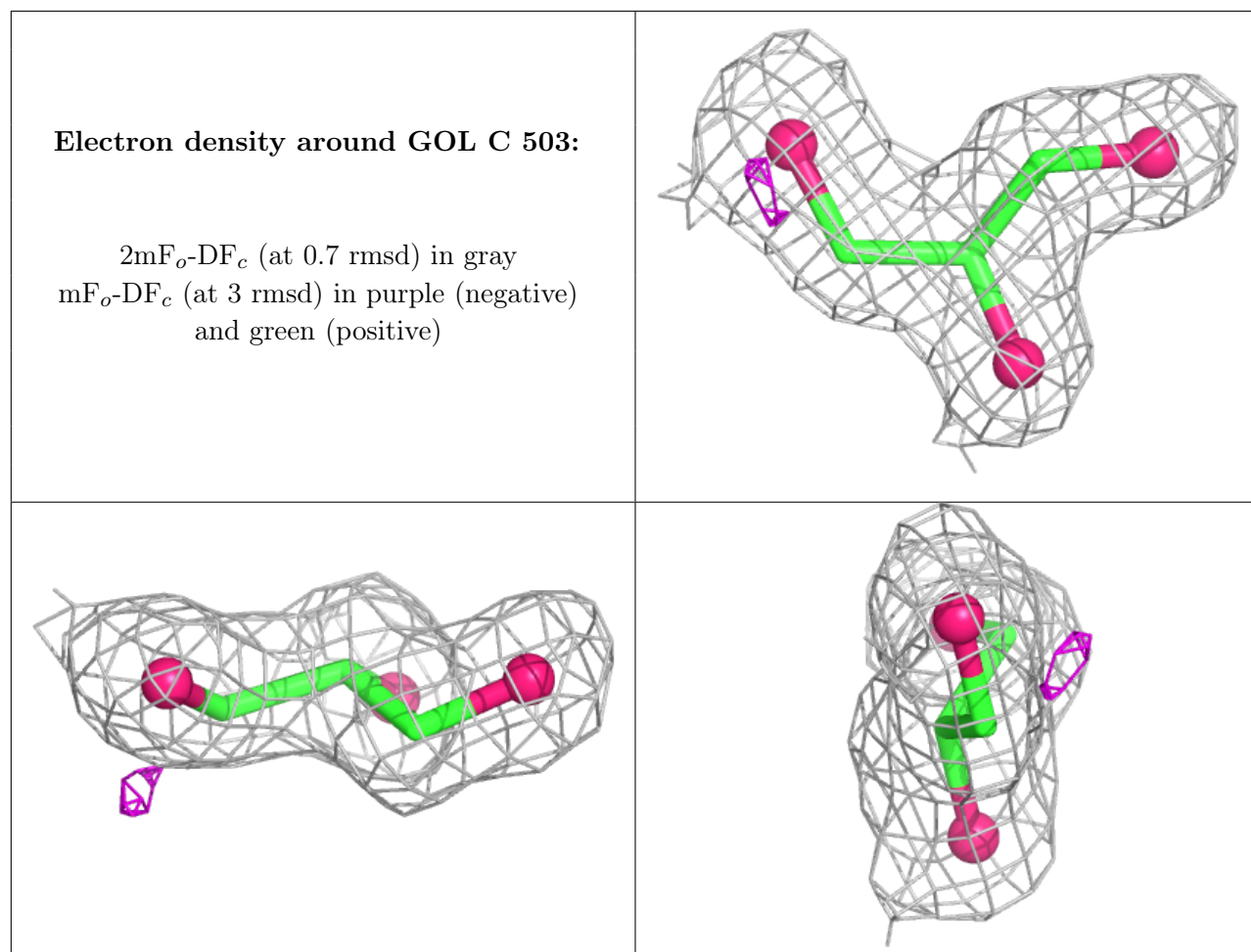
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and green (positive)

**Electron density around GOL A 503:**

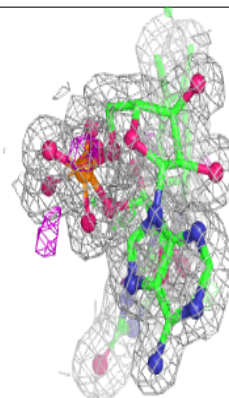
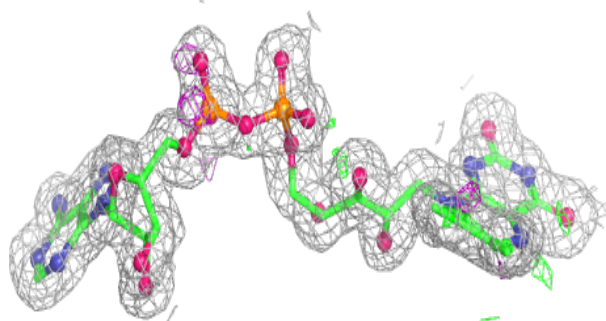
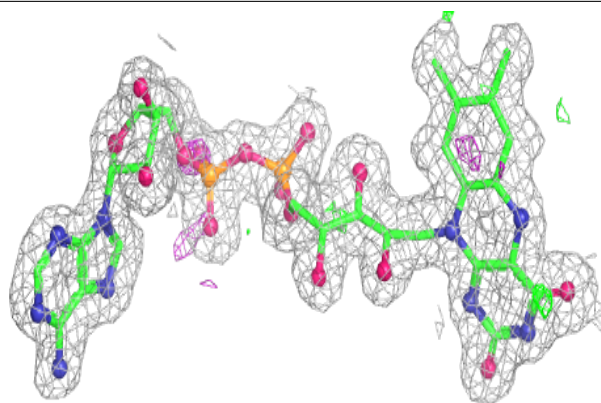
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



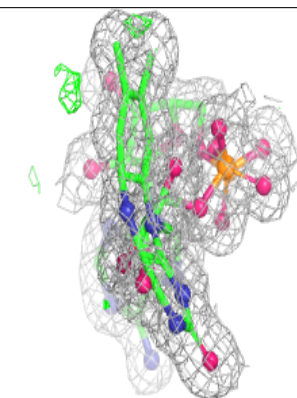
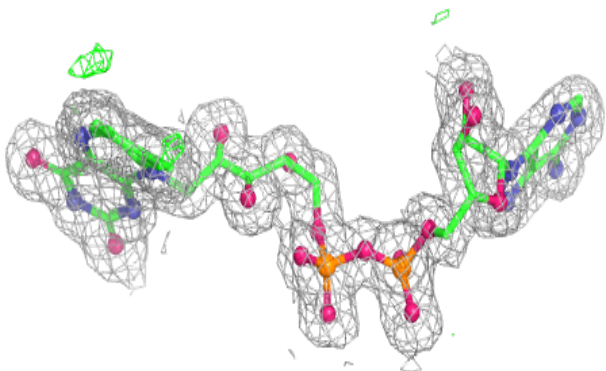
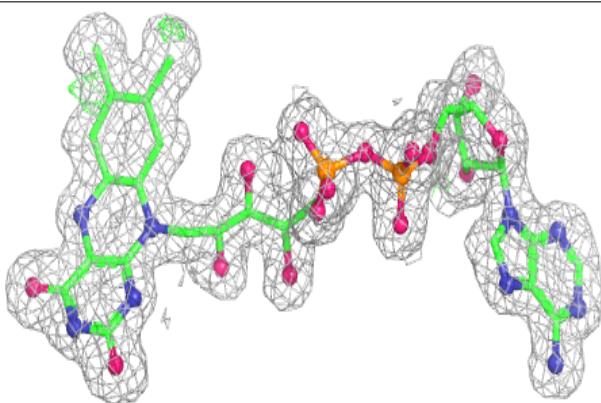


**Electron density around FAD B 501:**

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

**Electron density around FAD C 501:**

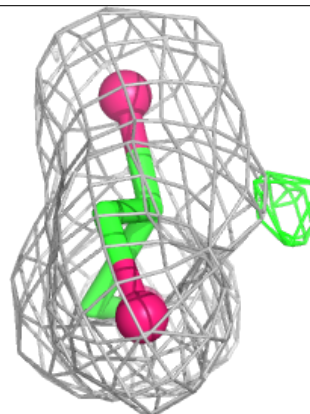
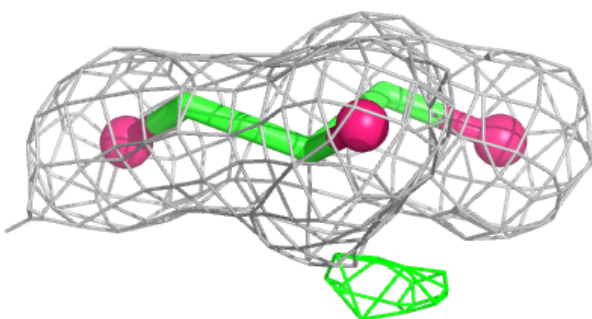
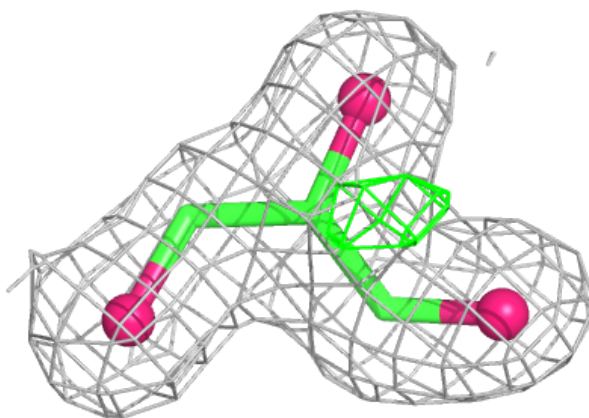
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



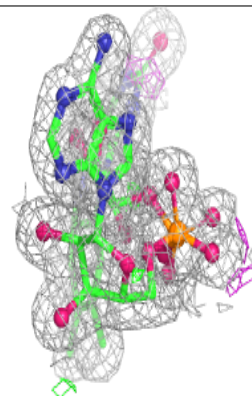
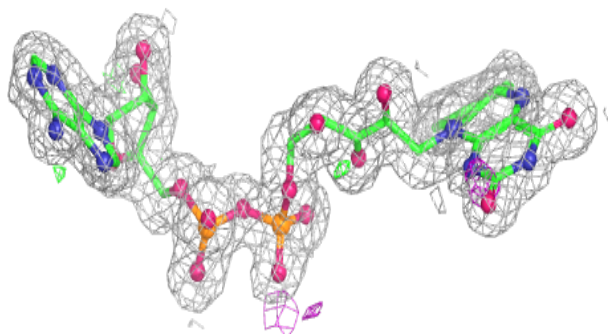
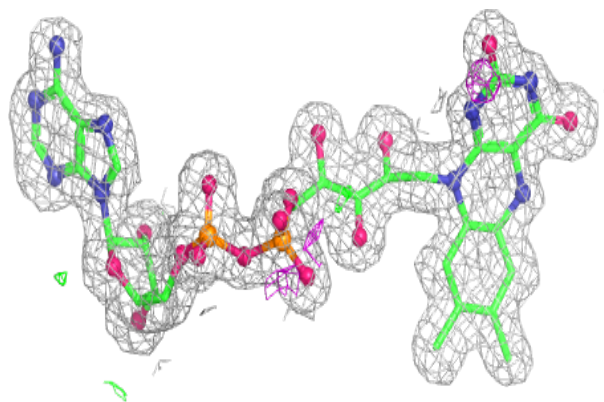


**Electron density around GOL B 503:**

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

**Electron density around FAD 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.