



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2024 – 12:30 PM JST

PDB ID : 8WVT  
Title : Crystal structure of Lsd18 in complex with ligands  
Authors : Deng, Y.M.; Hu, Y.L.; Chen, X.  
Deposited on : 2023-10-24  
Resolution : 1.75 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](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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

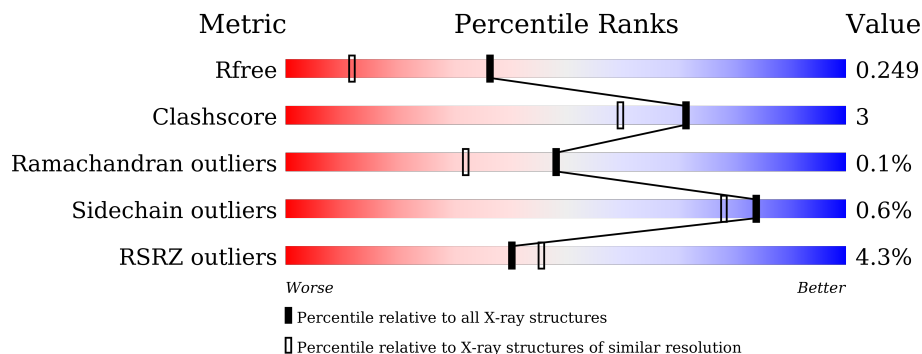
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

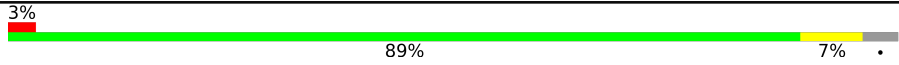
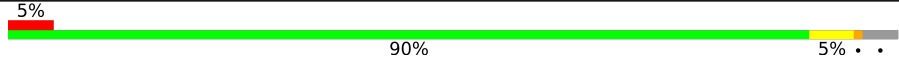
The reported resolution of this entry is 1.75 Å.

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))
$R_{free}$	164625	2888 (1.76-1.76)
Clashscore	180529	3097 (1.76-1.76)
Ramachandran outliers	177936	3072 (1.76-1.76)
Sidechain outliers	177891	3072 (1.76-1.76)
RSRZ outliers	164620	2887 (1.76-1.76)

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	488	 3% 89% 7% .
1	B	488	 5% 90% 5% . .

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7861 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 Putative epoxidase LasC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3451	2153	644	642	12	0	1	0
1	B	468	3451	2151	647	641	12	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

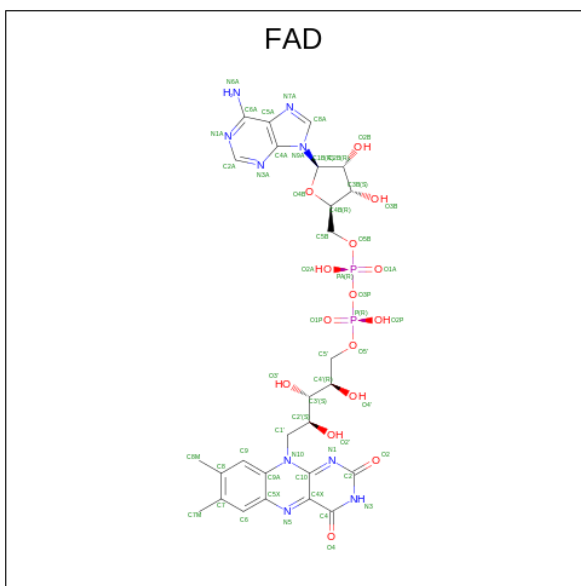
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP B5M9L6
A	2	ASN	-	expression tag	UNP B5M9L6
A	3	HIS	-	expression tag	UNP B5M9L6
A	4	LYS	-	expression tag	UNP B5M9L6
A	5	VAL	-	expression tag	UNP B5M9L6
A	6	HIS	-	expression tag	UNP B5M9L6
A	7	HIS	-	expression tag	UNP B5M9L6
A	8	HIS	-	expression tag	UNP B5M9L6
A	9	HIS	-	expression tag	UNP B5M9L6
A	10	HIS	-	expression tag	UNP B5M9L6
A	11	HIS	-	expression tag	UNP B5M9L6
A	12	ILE	-	expression tag	UNP B5M9L6
A	13	GLU	-	expression tag	UNP B5M9L6
A	14	GLY	-	expression tag	UNP B5M9L6
A	15	ARG	-	expression tag	UNP B5M9L6
A	16	HIS	-	expression tag	UNP B5M9L6
B	1	MET	-	initiating methionine	UNP B5M9L6
B	2	ASN	-	expression tag	UNP B5M9L6
B	3	HIS	-	expression tag	UNP B5M9L6
B	4	LYS	-	expression tag	UNP B5M9L6
B	5	VAL	-	expression tag	UNP B5M9L6
B	6	HIS	-	expression tag	UNP B5M9L6
B	7	HIS	-	expression tag	UNP B5M9L6
B	8	HIS	-	expression tag	UNP B5M9L6
B	9	HIS	-	expression tag	UNP B5M9L6

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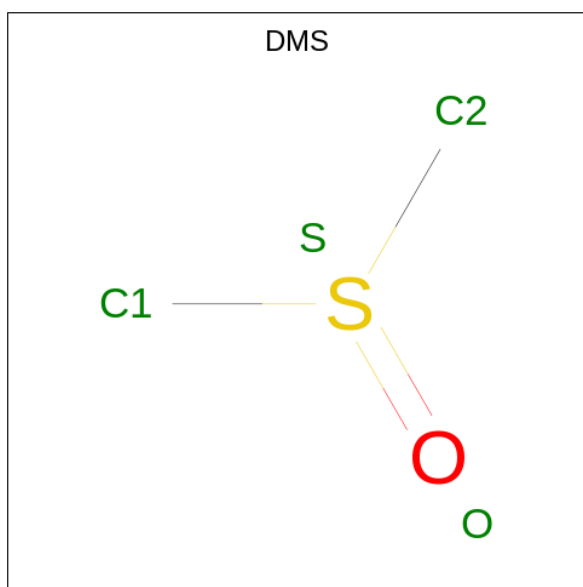
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	HIS	-	expression tag	UNP B5M9L6
B	11	HIS	-	expression tag	UNP B5M9L6
B	12	ILE	-	expression tag	UNP B5M9L6
B	13	GLU	-	expression tag	UNP B5M9L6
B	14	GLY	-	expression tag	UNP B5M9L6
B	15	ARG	-	expression tag	UNP B5M9L6
B	16	HIS	-	expression tag	UNP B5M9L6

- 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).



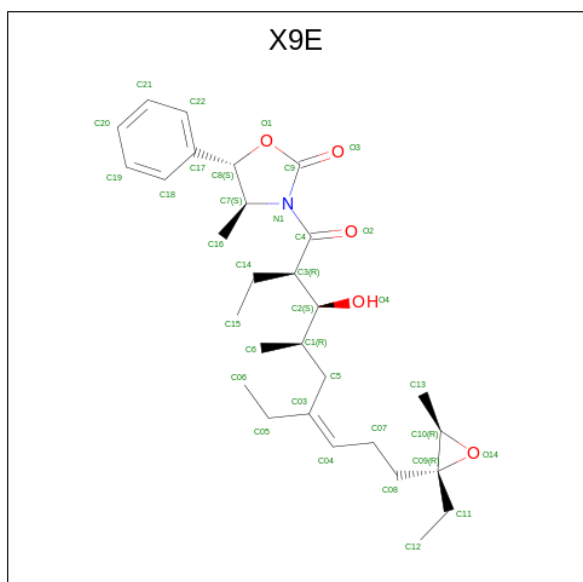
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is (4R,5S)-3-((2R,3S,4S,E)-2,6-diethyl-9-((2R,3R)-2-ethyl-3-methyloxiran-2-yl)-3-hydroxy-4-methylnon-6-enoyl)-4-methyl-5-phenyloxazolidin-2-one (three-letter code: X9E) (formula: C<sub>29</sub>H<sub>43</sub>NO<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

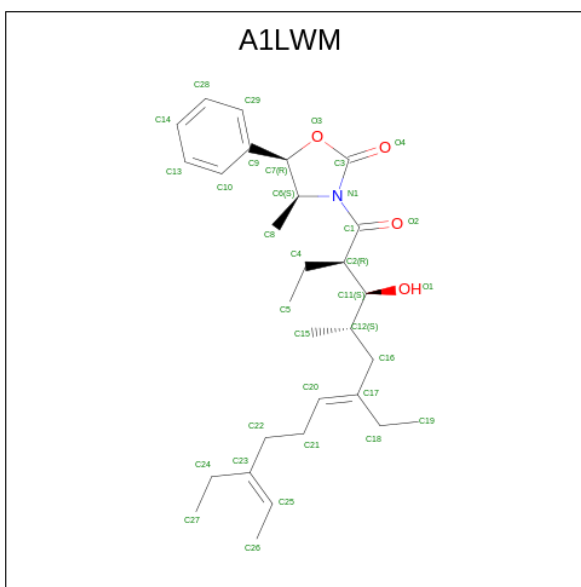


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	A	1	Total	C	O	0	0
			13	12	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is (4R,5S)-4-methyl-5-phenyl-3-((2R,3S,4S,6E,10E)-2,6,10-triethyl-3-hydroxy-4-methyldodeca-6,10-dienoyl)oxazolidin-2-one (three-letter code: A1LWM) (formula: C<sub>29</sub>H<sub>43</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	B	1	Total	C	O	0	0
			16	15	1		

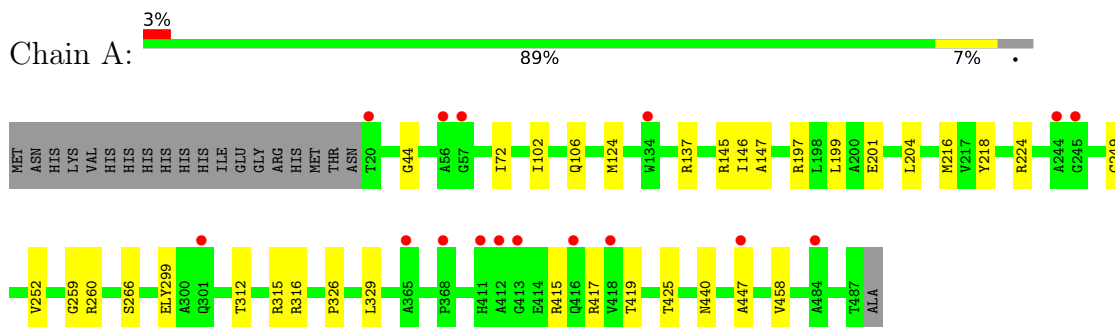
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	401	Total	O	0	0
			401	401		
7	B	405	Total	O	0	0
			405	405		

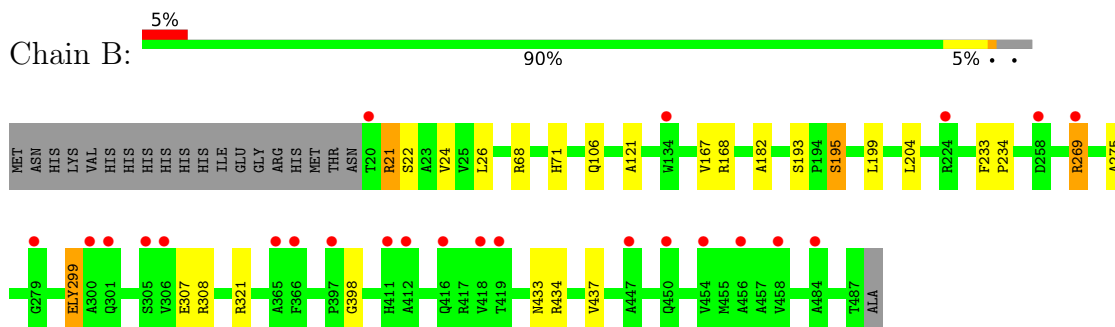
### 3 Residue-property plots

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: Putative epoxidase LasC



- Molecule 1: Putative epoxidase LasC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.92Å 61.80Å 75.63Å 74.61° 81.74° 76.79°	Depositor
Resolution (Å)	25.28 – 1.75 25.28 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.3 (25.28-1.75) 95.3 (25.28-1.75)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 1.75Å)	Xtrriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, $R_{free}$	0.208 , 0.249 0.208 , 0.249	Depositor DCC
$R_{free}$ test set	3950 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7861	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: DMS, CL, FAD, ELY, X9E, A1LWM

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	0.36	0/3509	0.54	0/4786
1	B	0.37	0/3506	0.54	0/4781
All	All	0.36	0/7015	0.54	0/9567

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	ELY	Mainchain
1	B	299	ELY	Mainchain

### 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	3451	0	3404	24	0
1	B	3451	0	3405	19	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
3	A	8	0	12	3	0
3	B	8	0	12	0	0
4	A	13	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	16	0	0	1	0
7	A	401	0	0	8	0
7	B	405	0	0	5	0
All	All	7861	0	6895	44	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 3.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:GLN:NE2	6:B:704:A1LWM:O1	2.21	0.74
1:A:137:ARG:NH1	7:A:801:HOH:O	2.22	0.72
1:A:147:ALA:N	7:A:802:HOH:O	2.23	0.70
1:B:168:ARG:NH1	7:B:807:HOH:O	2.29	0.64
1:A:252:VAL:HG21	4:A:704:X9E:C08	2.27	0.64
1:A:440:ASN:ND2	7:A:807:HOH:O	2.29	0.63
1:B:321:ARG:NH1	7:B:808:HOH:O	2.30	0.62
1:A:260:ARG:NH2	7:A:809:HOH:O	2.31	0.62
1:A:199:LEU:HD22	1:A:204:LEU:HD12	1.83	0.59
1:B:195:SER:O	1:B:199:LEU:HG	2.02	0.59
1:A:415:ARG:O	1:A:419:THR:HG23	2.04	0.57
1:A:199:LEU:HD21	1:A:329:LEU:HD21	1.88	0.56
1:A:197:ARG:O	1:A:201:GLU:HG3	2.06	0.55
1:A:315:ARG:HD3	3:A:703:DMS:H12	1.92	0.51
1:B:269:ARG:NH1	7:B:827:HOH:O	2.48	0.46
1:B:233:PHE:CG	1:B:234:PRO:HD2	2.51	0.45
1:A:216:MET:O	1:A:312:THR:OG1	2.29	0.45
1:B:106:GLN:HG2	7:B:927:HOH:O	2.16	0.45
1:B:26:LEU:HD21	1:B:167:VAL:HG11	1.98	0.45
1:A:72:ILE:HG12	1:A:124:MET:HE3	1.98	0.44
1:B:121:ALA:HB2	1:B:434:ARG:HG2	1.99	0.44
1:B:22:SER:OG	1:B:182:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HD2	1:B:307:GLU:HG3	1.98	0.44
1:A:417:ARG:NE	7:A:813:HOH:O	2.51	0.43
1:B:24:VAL:HG23	1:B:182:ALA:HB2	2.01	0.43
1:A:425:THR:HG21	1:A:458:VAL:HA	2.00	0.43
1:A:315:ARG:HH11	3:A:703:DMS:H12	1.84	0.43
1:A:447:ALA:HB1	7:A:1073:HOH:O	2.18	0.43
1:B:269:ARG:NH1	1:B:398:GLY:O	2.52	0.42
1:A:315:ARG:HH11	3:A:703:DMS:C1	2.32	0.42
1:B:299:ELY:HT1B	1:B:299:ELY:HH2	1.92	0.42
1:A:224:ARG:HD2	1:A:259:GLY:O	2.20	0.41
1:A:102:ILE:HG23	1:A:106:GLN:OE1	2.21	0.41
1:B:433:ASN:O	1:B:437:VAL:HG22	2.20	0.41
1:B:21:ARG:NH2	7:B:836:HOH:O	2.53	0.41
1:B:199:LEU:HB3	1:B:204:LEU:HD12	2.03	0.41
1:A:146:ILE:C	7:A:802:HOH:O	2.57	0.41
1:B:275:ALA:HB2	1:B:308:ARG:HD2	2.02	0.41
1:A:316:ARG:NH2	7:A:803:HOH:O	2.45	0.40
1:B:71:HIS:HA	2:B:701:FAD:O4	2.22	0.40
1:A:44:GLY:O	1:A:145:ARG:HD2	2.22	0.40
1:A:218:TYR:CD2	2:A:701:FAD:HM73	2.56	0.40
1:A:249:CYS:HA	1:A:266:SER:O	2.21	0.40
2:A:701:FAD:H9	2:A:701:FAD:H1'1	1.88	0.40

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	466/488 (96%)	456 (98%)	10 (2%)	0	100	100
1	B	465/488 (95%)	457 (98%)	7 (2%)	1 (0%)	44	28
All	All	931/976 (95%)	913 (98%)	17 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	ARG

### 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	341/376 (91%)	340 (100%)	1 (0%)	91	88
1	B	341/376 (91%)	338 (99%)	3 (1%)	75	65
All	All	682/752 (91%)	678 (99%)	4 (1%)	84	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	PRO
1	B	193	SER
1	B	195	SER
1	B	269	ARG

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

Mol	Chain	Res	Type
1	B	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](#)

2 non-standard protein/DNA/RNA residues 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
1	ELY	A	299	1	11,12,13	0.54	0	8,13,15	0.59	0
1	ELY	B	299	1	11,12,13	0.57	0	8,13,15	0.66	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
1	ELY	A	299	1	-	4/12/13/15	-
1	ELY	B	299	1	-	1/12/13/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	299	ELY	O-C-CA-CB
1	A	299	ELY	CA-CB-CG-CD
1	A	299	ELY	CT1-CH1-NZ-CH2
1	A	299	ELY	CT1-CH1-NZ-CE
1	B	299	ELY	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	299	ELY	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	DMS	A	702	-	3,3,3	0.65	0	3,3,3	0.67	0
2	FAD	A	701	-	53,58,58	0.55	0	68,89,89	0.59	1 (1%)
3	DMS	B	703	-	3,3,3	0.71	0	3,3,3	0.63	0
6	A1LWM	B	704	-	13,15,35	2.70	3 (23%)	12,17,47	2.04	5 (41%)
4	X9E	A	704	-	12,13,37	1.45	1 (8%)	10,18,53	2.71	4 (40%)
3	DMS	A	703	-	3,3,3	0.64	0	3,3,3	0.71	0
2	FAD	B	701	-	53,58,58	0.52	0	68,89,89	0.57	1 (1%)
3	DMS	B	702	-	3,3,3	0.61	0	3,3,3	0.64	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	X9E	A	704	-	-	8/12/20/62	0/1/1/3
2	FAD	B	701	-	-	1/30/50/50	0/6/6/6
6	A1LWM	B	704	-	-	5/18/18/54	-
2	FAD	A	701	-	-	1/30/50/50	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	704	A1LWM	C16-C17	8.61	1.60	1.51
4	A	704	X9E	O14-C09	4.42	1.60	1.46
6	B	704	A1LWM	C22-C23	3.16	1.56	1.51
6	B	704	A1LWM	C21-C20	2.09	1.57	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	X9E	C08-C09-C10	-5.70	109.01	119.09
6	B	704	A1LWM	C26-C25-C23	-4.74	118.19	127.19
4	A	704	X9E	O14-C10-C13	-3.75	109.78	117.33
4	A	704	X9E	C07-C08-C09	-3.12	105.03	114.05
6	B	704	A1LWM	C24-C23-C22	2.78	121.38	115.45
6	B	704	A1LWM	C18-C17-C16	2.48	120.83	115.50
6	B	704	A1LWM	C16-C12-C11	2.35	112.72	110.15
2	A	701	FAD	C5A-C6A-N6A	2.25	123.77	120.35
2	B	701	FAD	C5A-C6A-N6A	2.22	123.73	120.35
4	A	704	X9E	C07-C04-C03	-2.15	122.49	127.66
6	B	704	A1LWM	C18-C17-C20	-2.00	118.60	122.17

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	704	X9E	C10-C09-C11-C12
4	A	704	X9E	O14-C09-C11-C12
4	A	704	X9E	C08-C09-C11-C12
6	B	704	A1LWM	C15-C12-C16-C17
6	B	704	A1LWM	C11-C12-C16-C17
6	B	704	A1LWM	O1-C11-C12-C15
6	B	704	A1LWM	O1-C11-C12-C16
6	B	704	A1LWM	C20-C21-C22-C23
4	A	704	X9E	C07-C08-C09-O14
4	A	704	X9E	C04-C07-C08-C09
4	A	704	X9E	C5-C03-C05-C06
4	A	704	X9E	C07-C08-C09-C10
2	A	701	FAD	O4B-C4B-C5B-O5B
4	A	704	X9E	C03-C04-C07-C08
2	B	701	FAD	O4B-C4B-C5B-O5B

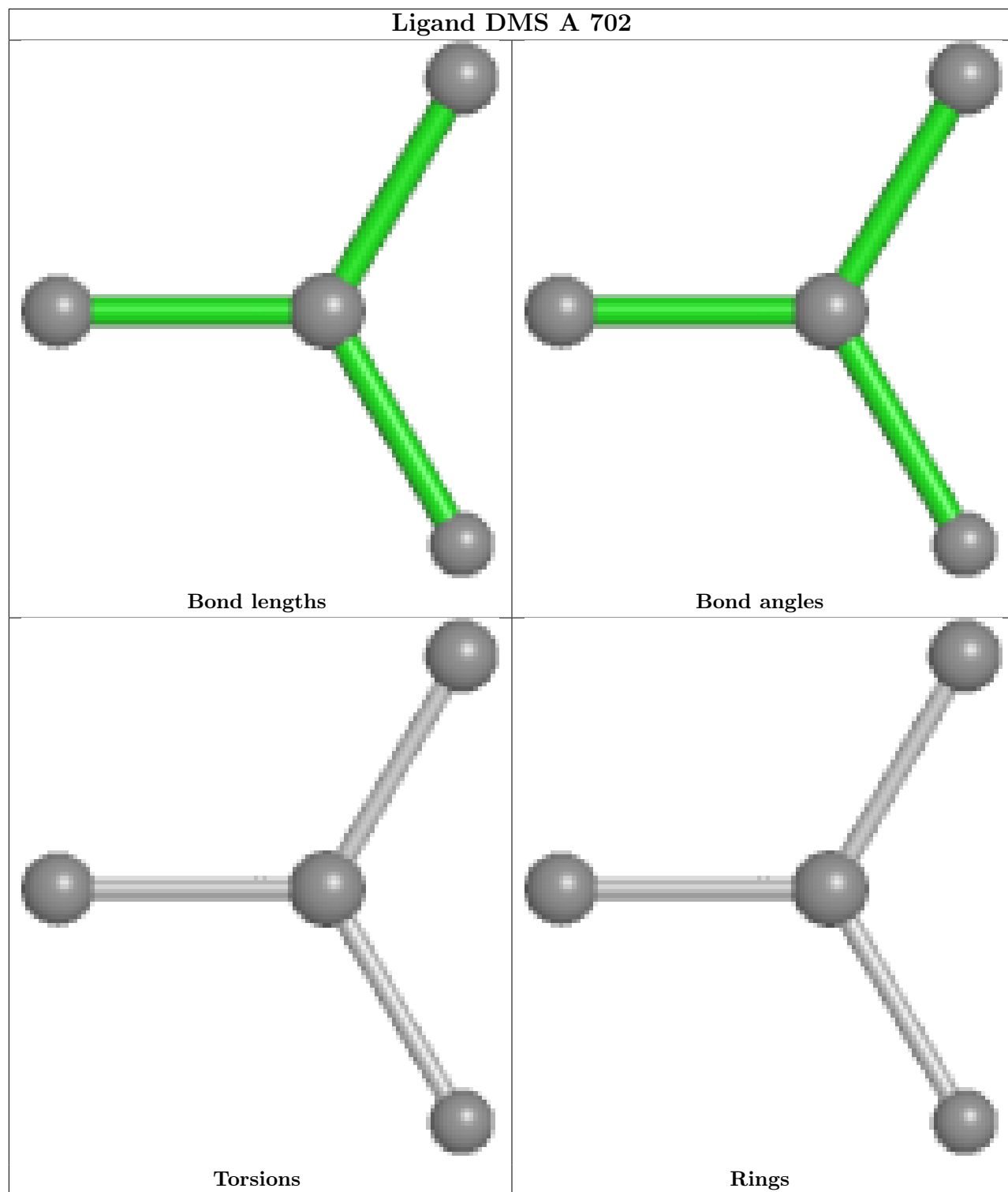
There are no ring outliers.

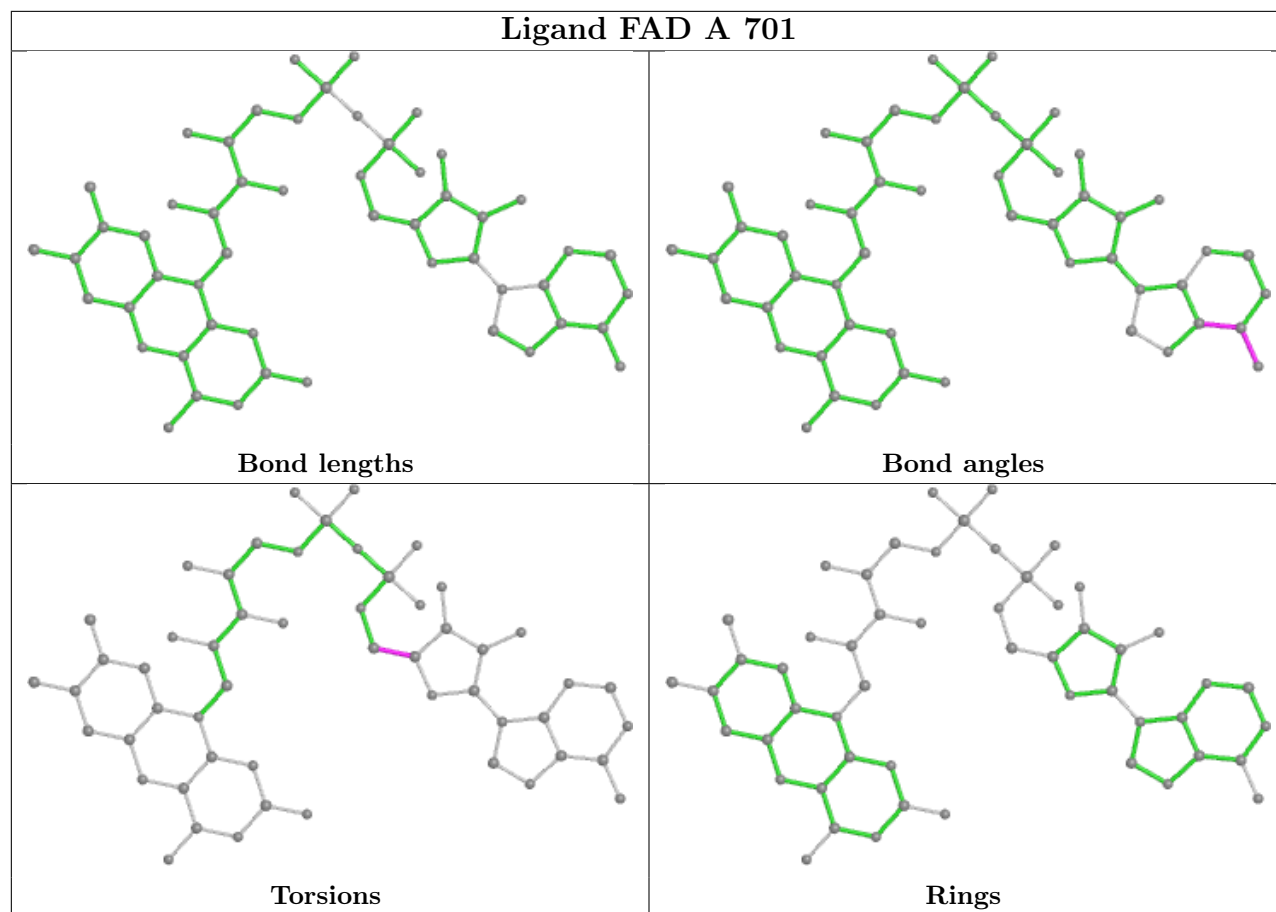
5 monomers are involved in 8 short contacts:

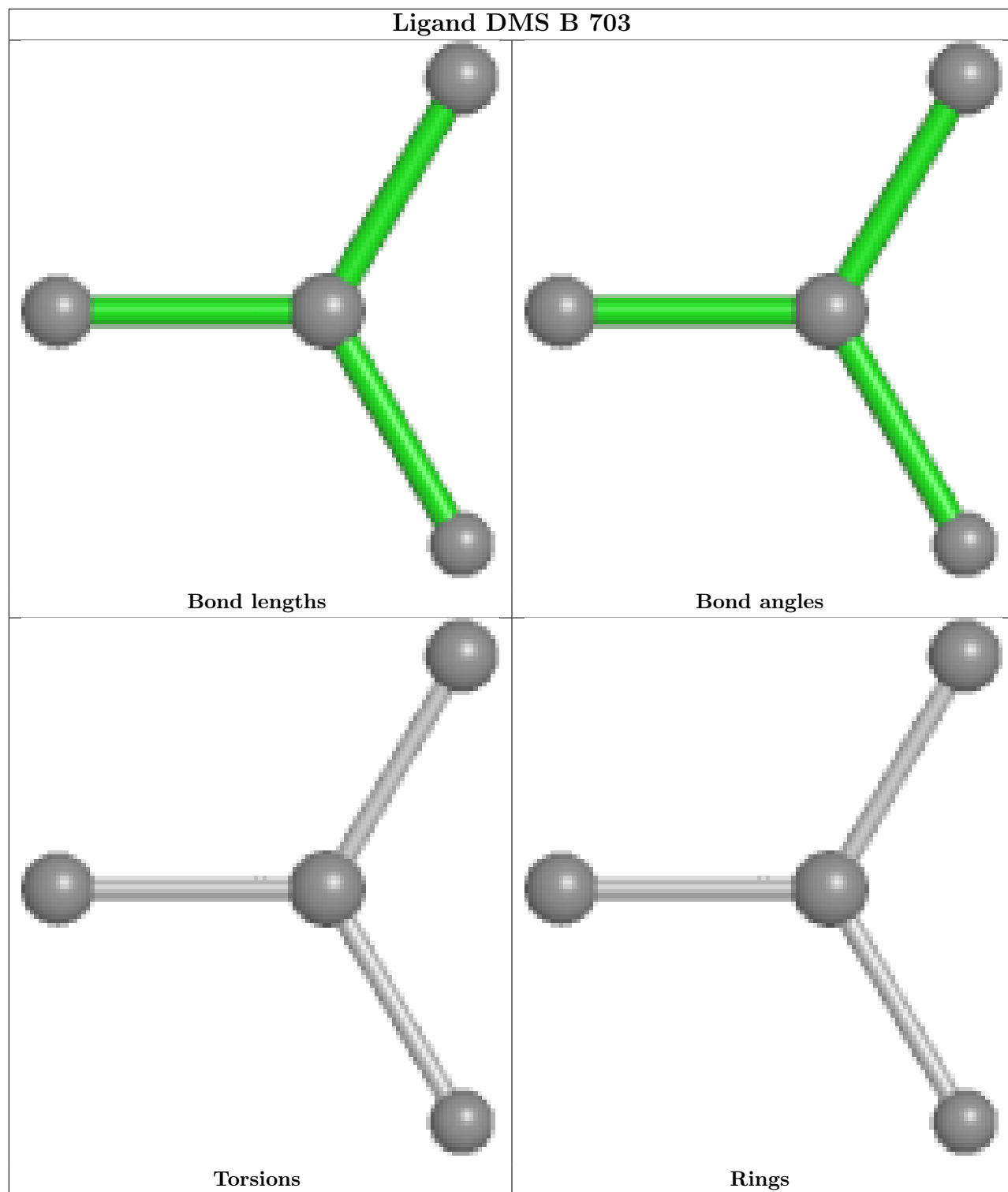
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	2	0
6	B	704	A1LWM	1	0
4	A	704	X9E	1	0
3	A	703	DMS	3	0
2	B	701	FAD	1	0

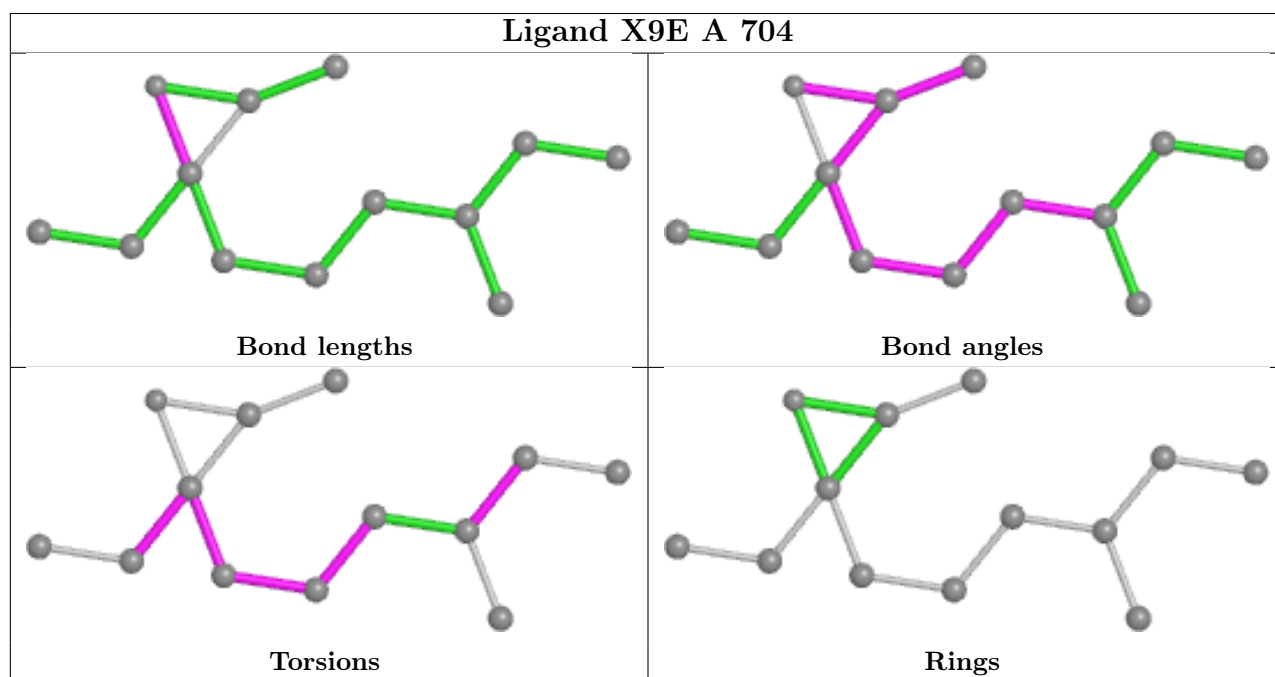
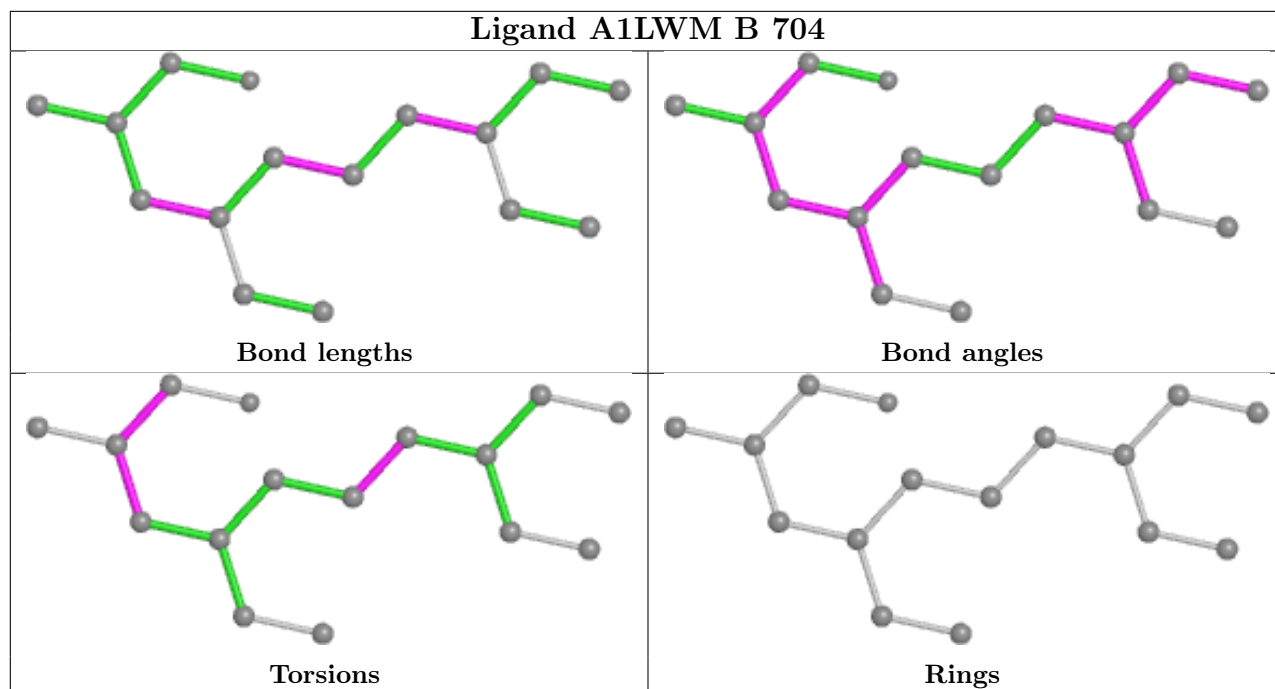
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

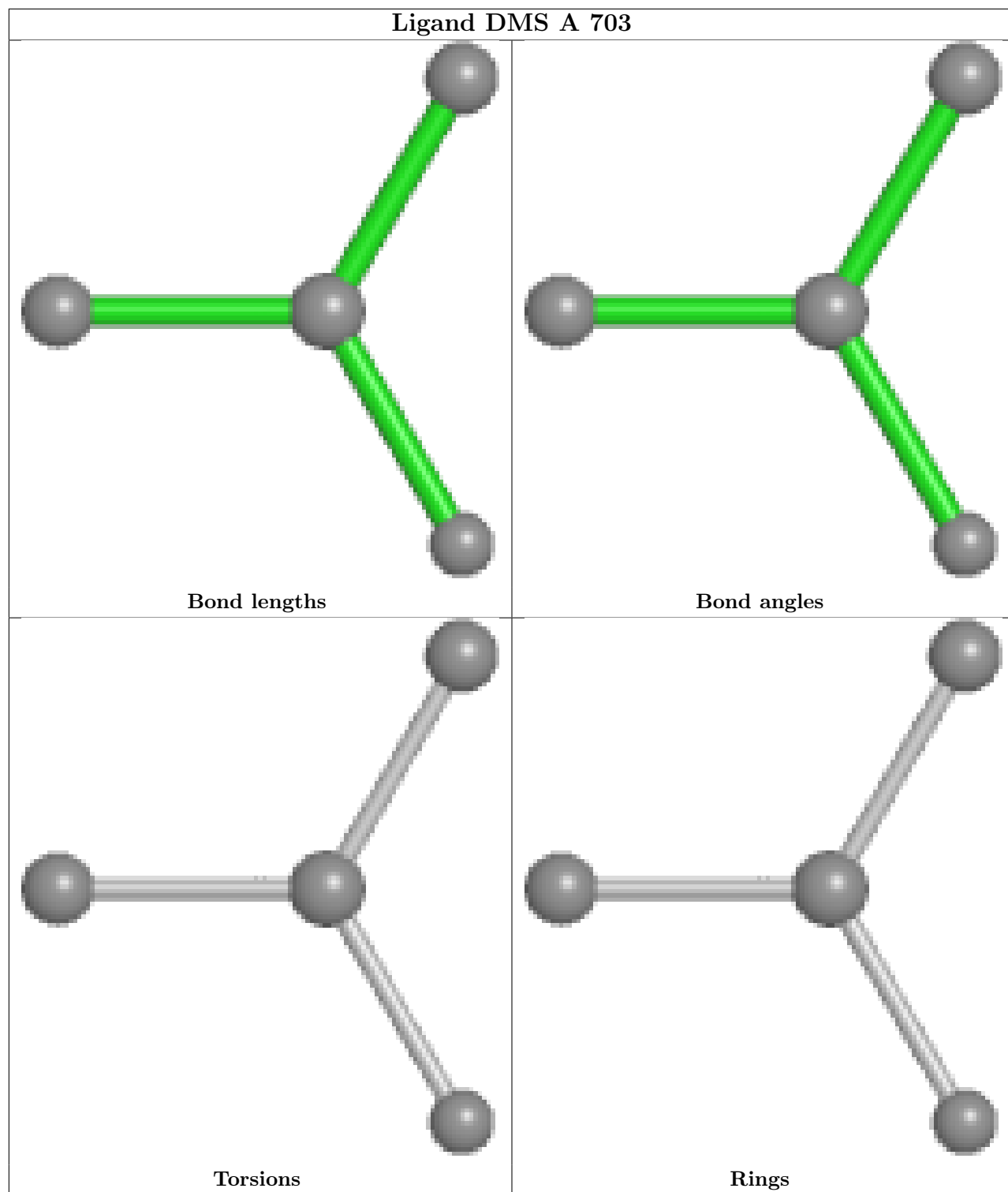


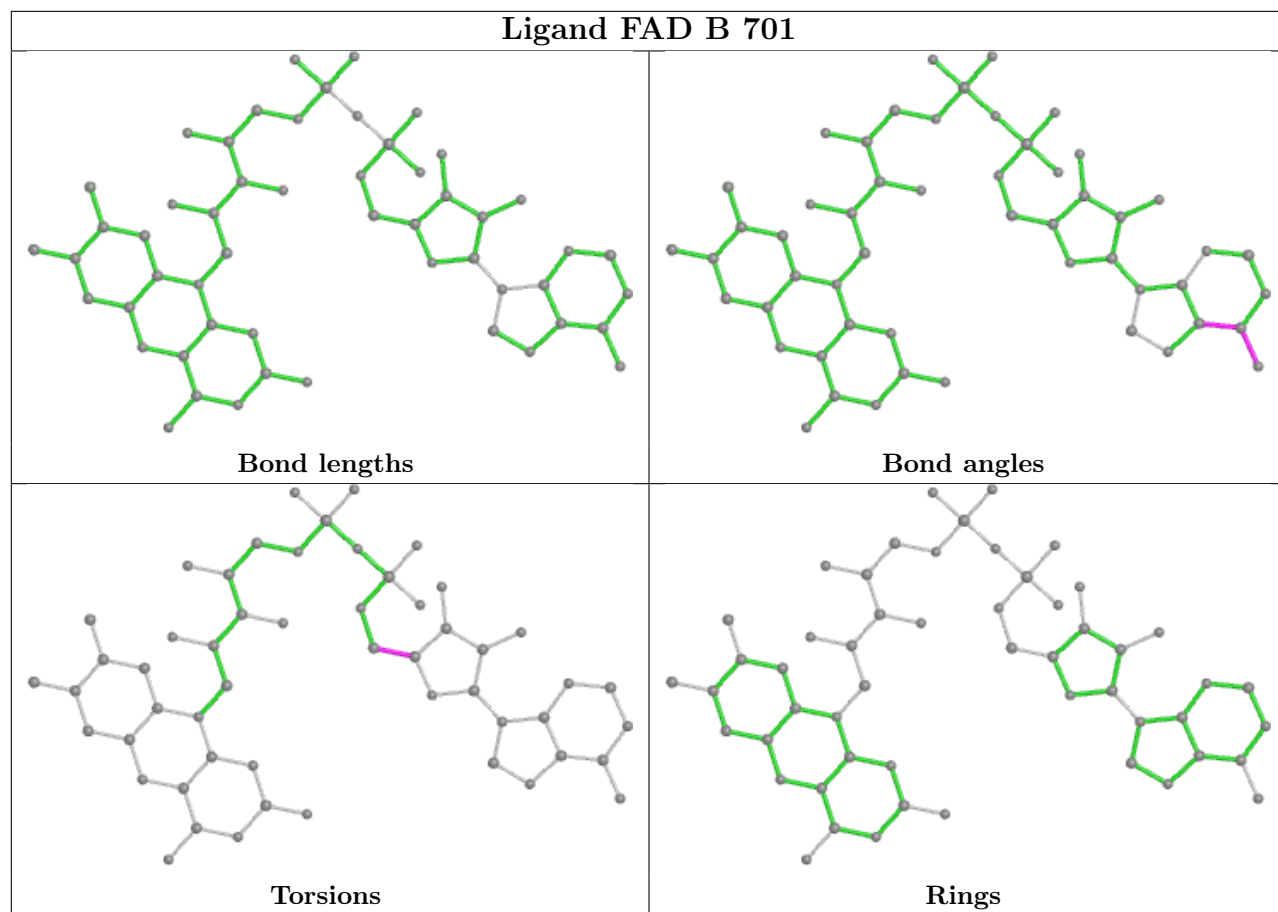


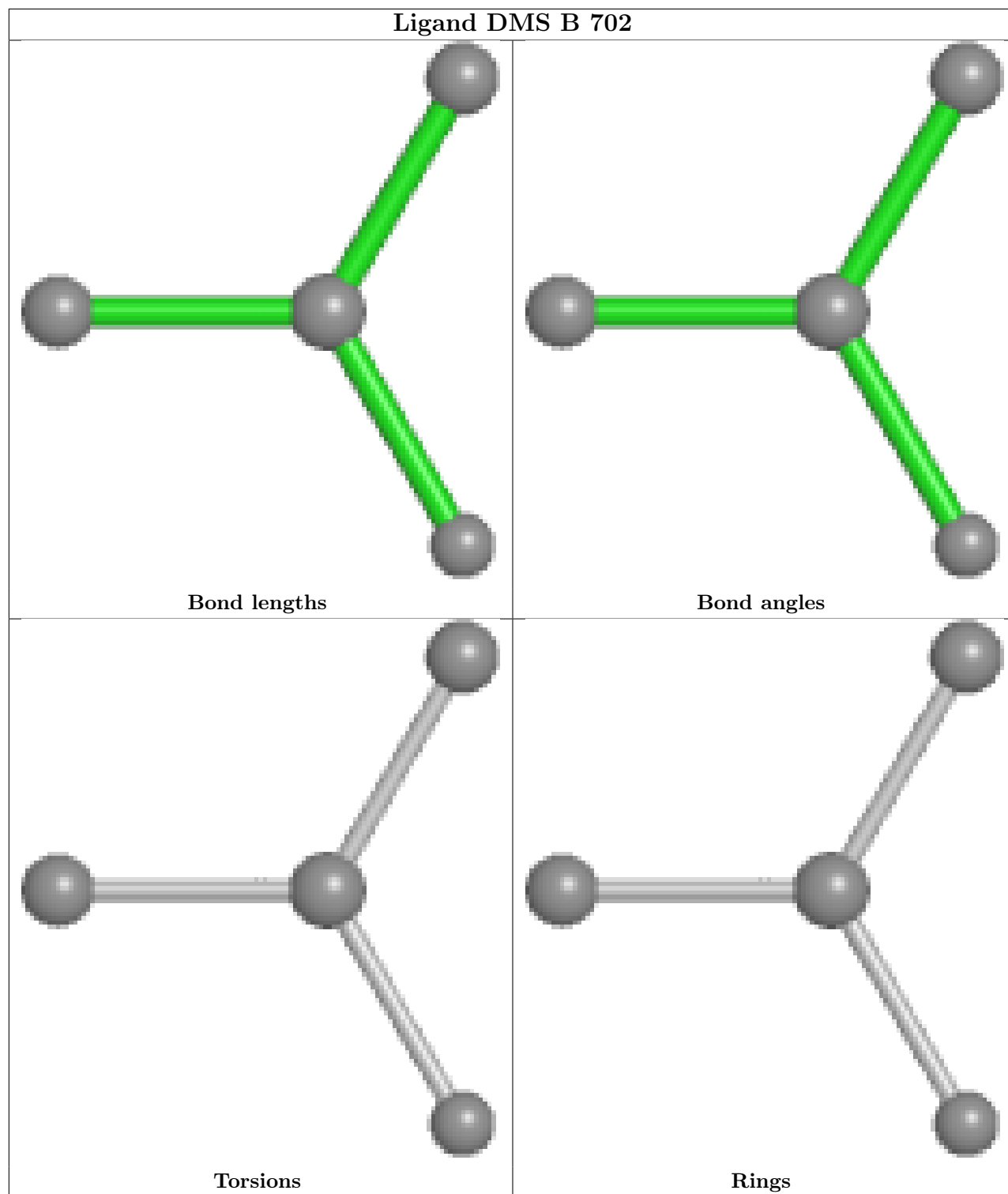












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	467/488 (95%)	0.32	16 (3%) 48 55	6, 13, 26, 42	1 (0%)
1	B	467/488 (95%)	0.43	24 (5%) 34 38	5, 14, 28, 34	0
All	All	934/976 (95%)	0.37	40 (4%) 40 45	5, 14, 27, 42	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	HIS	6.7
1	A	484	ALA	5.8
1	B	412	ALA	5.2
1	A	412	ALA	4.4
1	A	413	GLY	4.4
1	A	20	THR	4.3
1	B	484	ALA	4.2
1	A	56	ALA	3.6
1	B	454	VAL	3.4
1	B	418	VAL	3.3
1	B	258	ASP	3.3
1	B	411	HIS	3.2
1	A	418	VAL	3.2
1	B	365	ALA	3.2
1	B	20	THR	3.0
1	B	305	SER	2.7
1	B	447	ALA	2.7
1	B	269	ARG	2.7
1	B	416	GLN	2.7
1	B	456	ALA	2.6
1	B	134	TRP	2.6
1	B	419	THR	2.6
1	B	458	VAL	2.5
1	B	397	PRO	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	224	ARG	2.4
1	A	447	ALA	2.3
1	B	366	PHE	2.3
1	A	244	ALA	2.3
1	A	365	ALA	2.3
1	A	134	TRP	2.3
1	A	245	GLY	2.3
1	B	450	GLN	2.3
1	A	57	GLY	2.2
1	A	301	GLN	2.2
1	B	279	GLY	2.1
1	B	306	VAL	2.1
1	B	301	GLN	2.0
1	A	368	PRO	2.0
1	B	300	ALA	2.0
1	A	416	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	ELY	B	299	13/14	0.88	0.11	15,19,27,29	0
1	ELY	A	299	13/14	0.91	0.10	13,20,23,25	0

## 6.3 Carbohydrates [i](#)

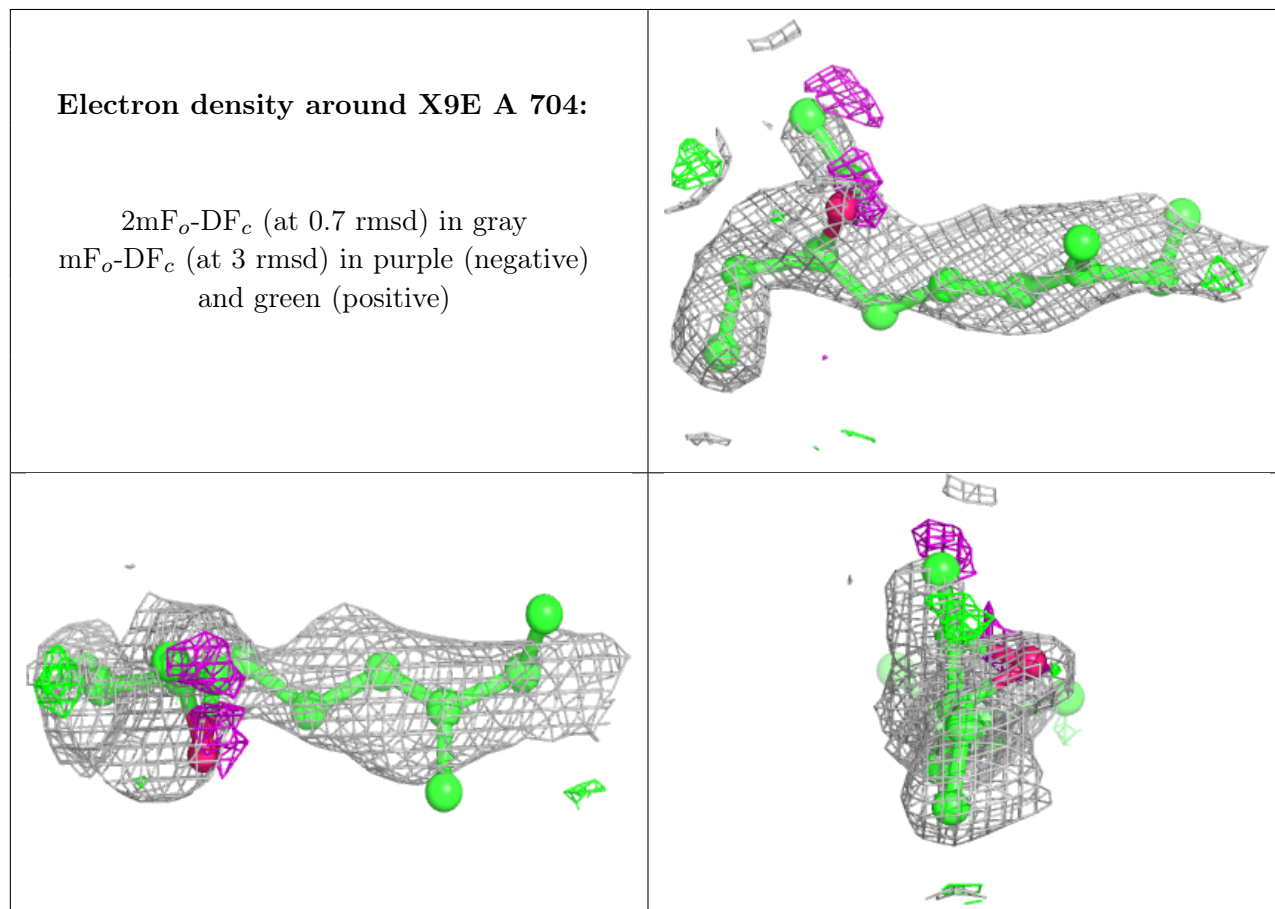
There are no monosaccharides in this entry.

## 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.

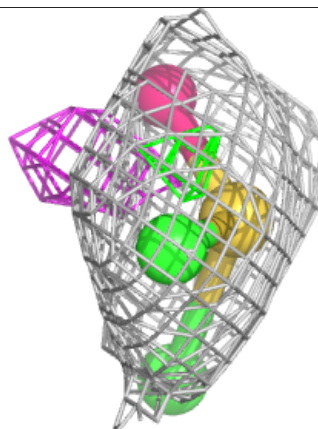
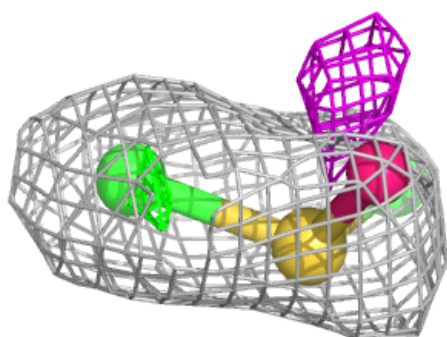
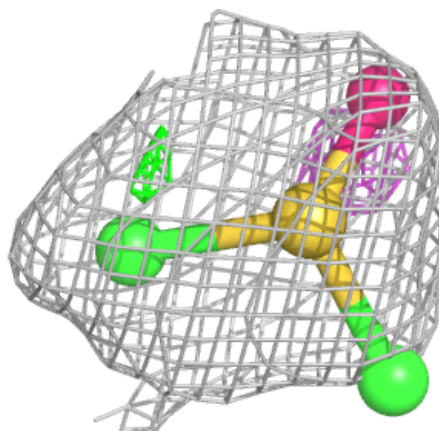
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	X9E	A	704	13/35	0.73	0.20	13,26,32,34	0
3	DMS	B	702	4/4	0.75	0.20	22,32,39,45	0
6	A1LWM	B	704	16/34	0.78	0.17	8,25,31,33	0
3	DMS	A	702	4/4	0.79	0.16	35,36,43,54	0
3	DMS	A	703	4/4	0.93	0.10	14,15,15,20	0
3	DMS	B	703	4/4	0.95	0.08	7,13,17,20	0
2	FAD	B	701	53/53	0.95	0.07	4,8,13,18	0
2	FAD	A	701	53/53	0.95	0.07	5,9,15,20	0
5	CL	A	705	1/1	0.97	0.04	20,20,20,20	0
5	CL	B	705	1/1	0.98	0.06	18,18,18,18	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.

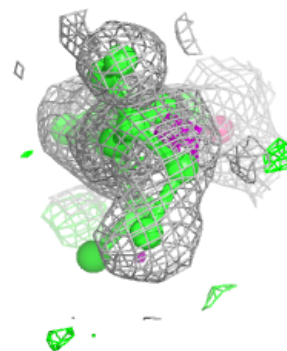
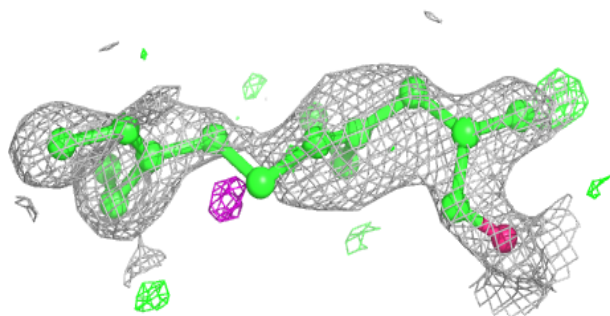
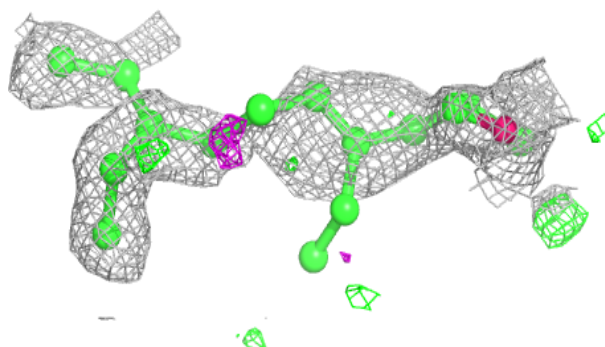


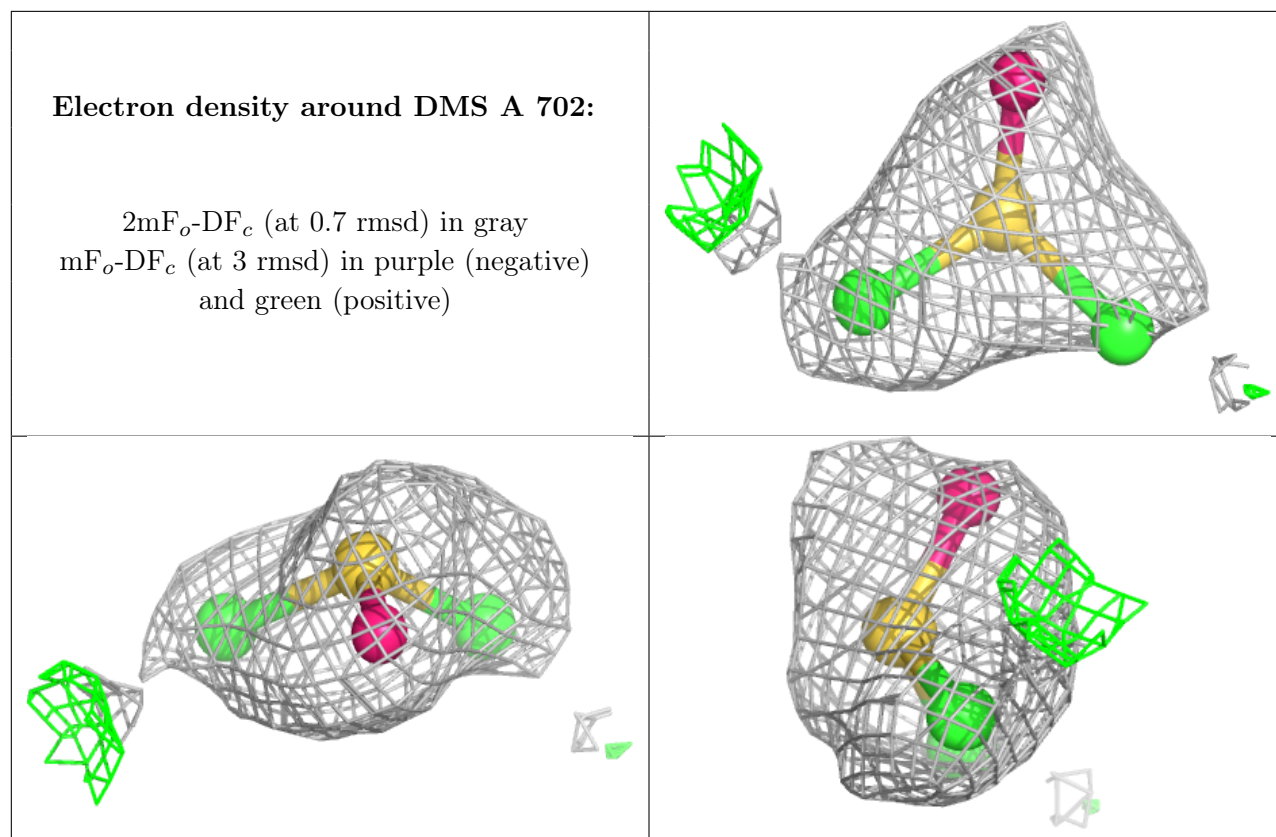
**Electron density around DMS B 702:**

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

**Electron density around A1LWM B 704:**

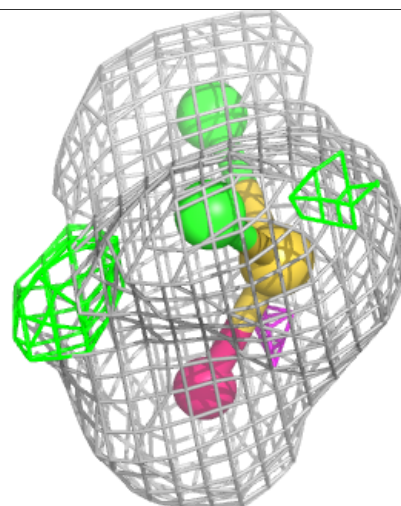
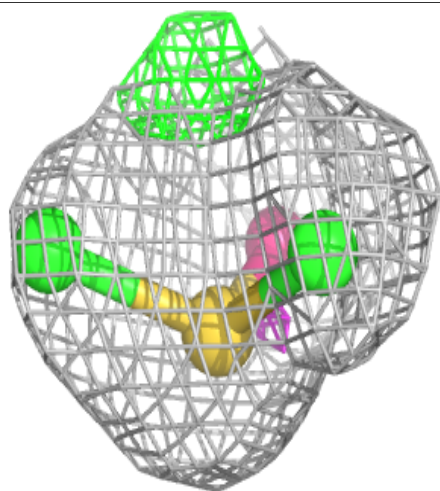
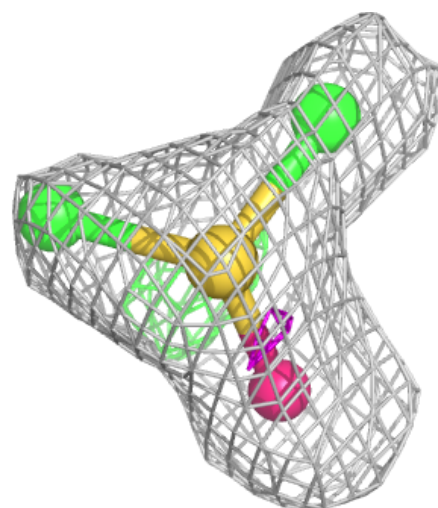
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





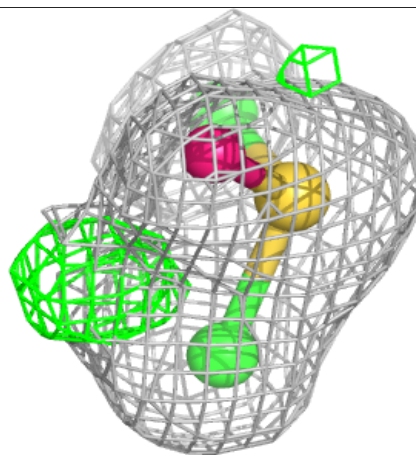
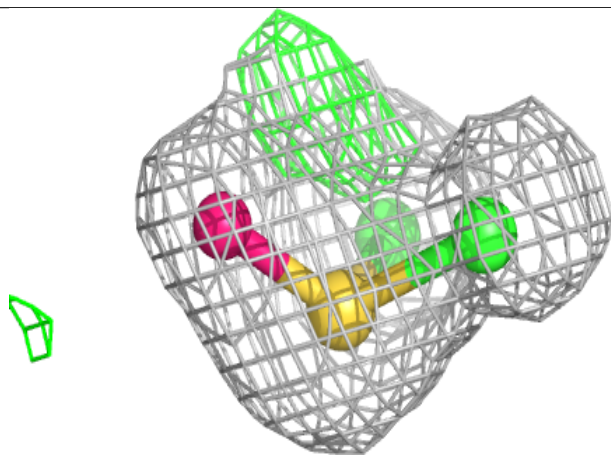
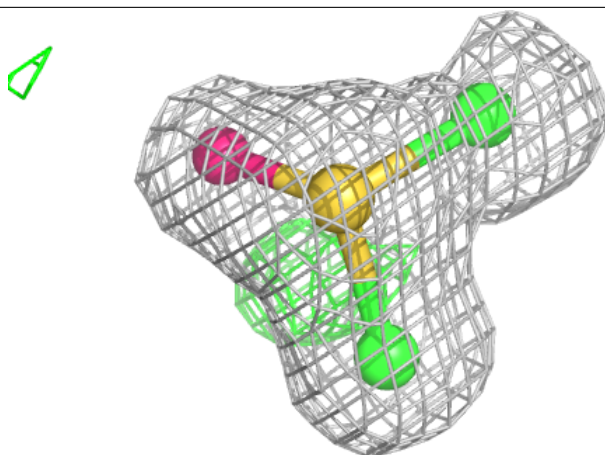
**Electron density around DMS A 703:**

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

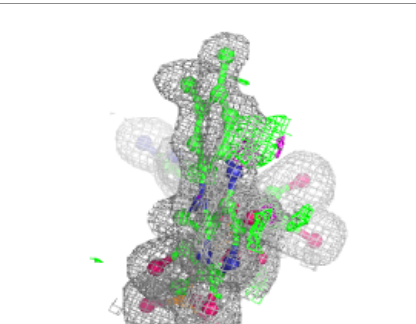
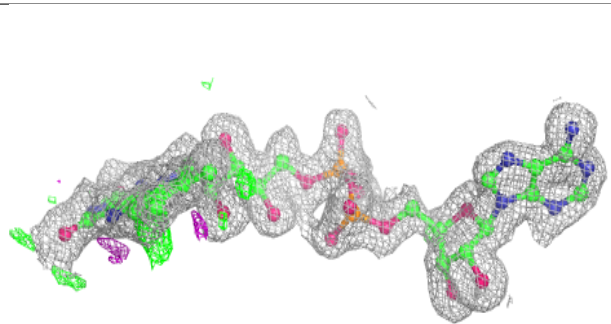
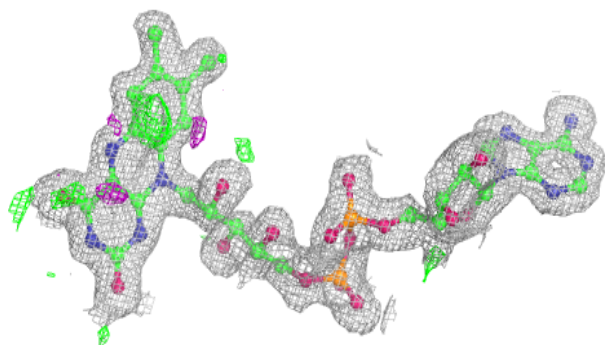


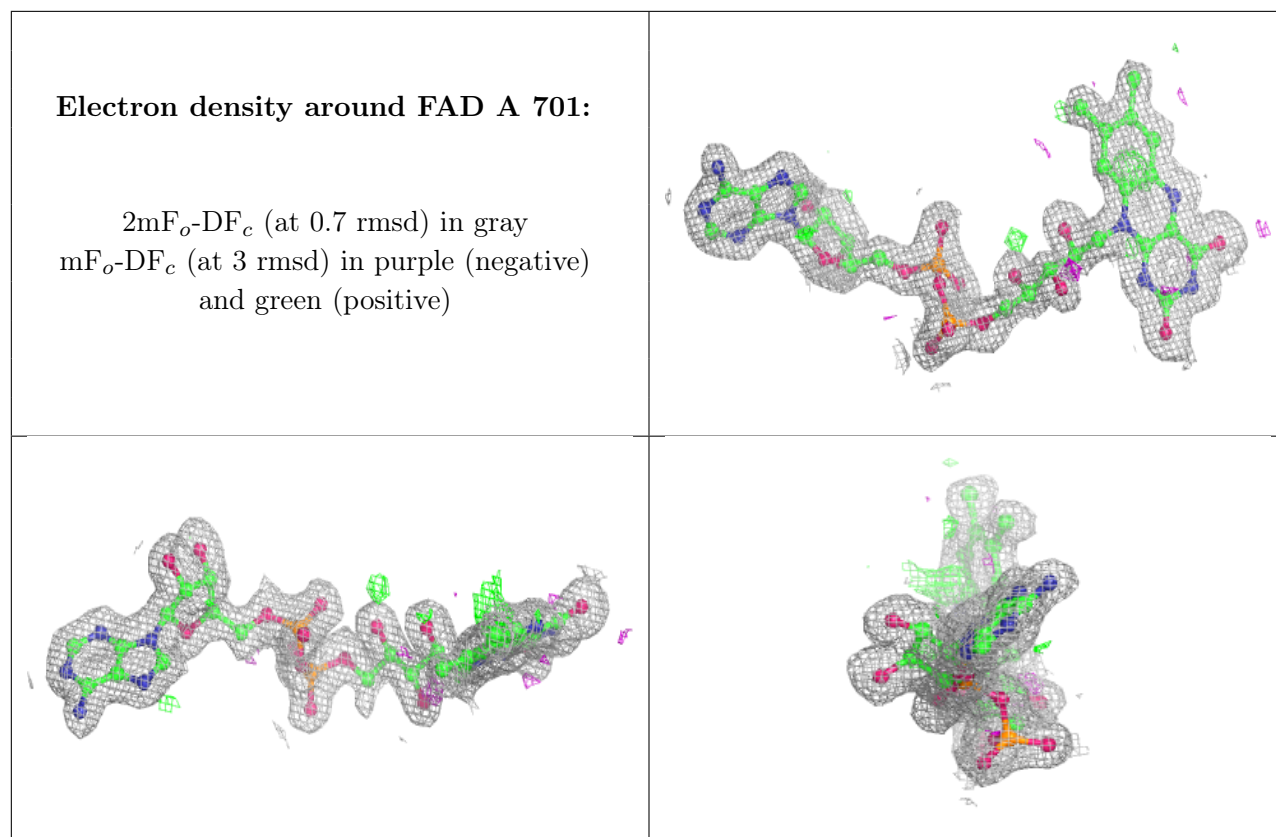
**Electron density around DMS B 703:**

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

**Electron density around FAD B 701:**

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

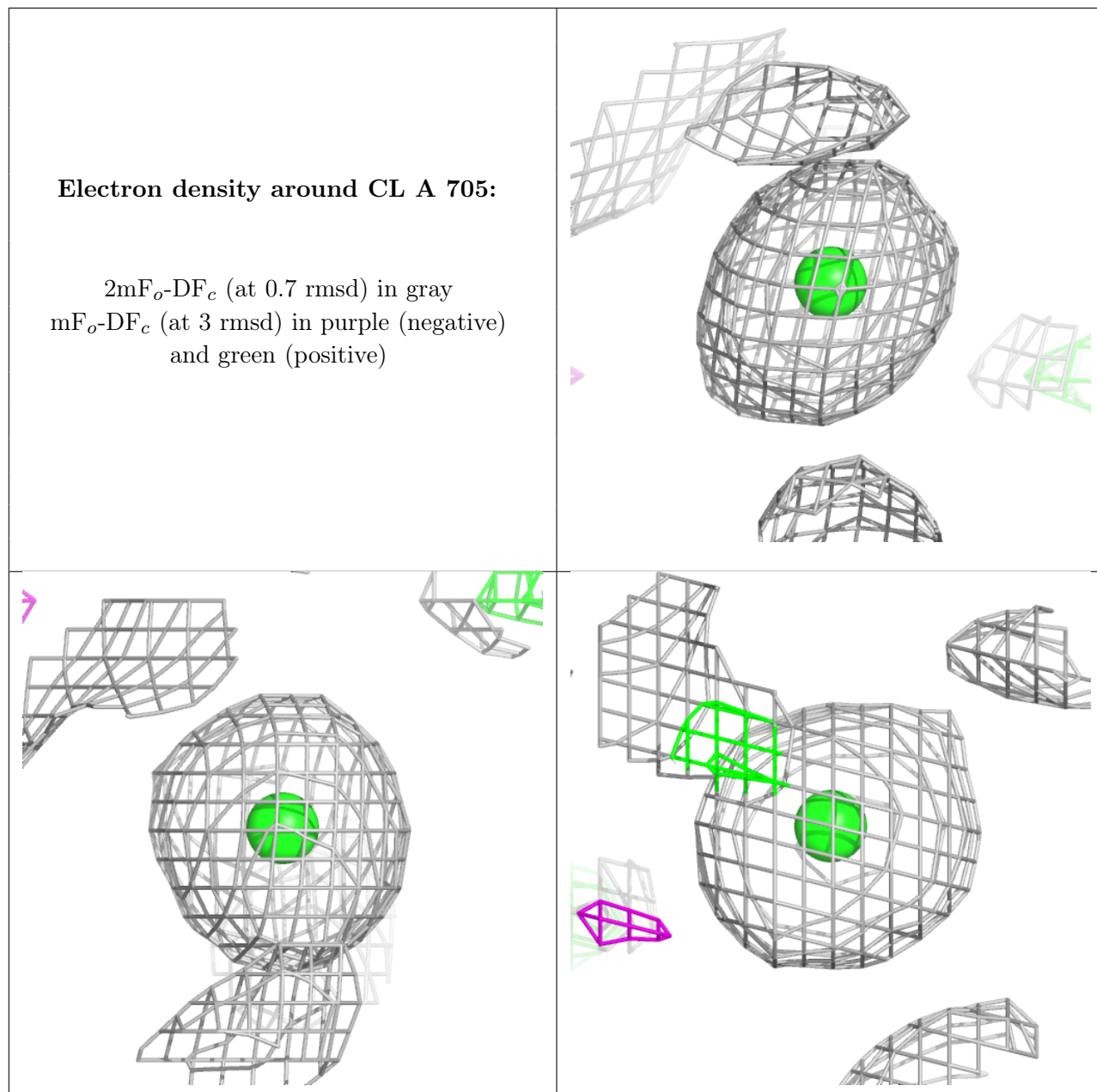


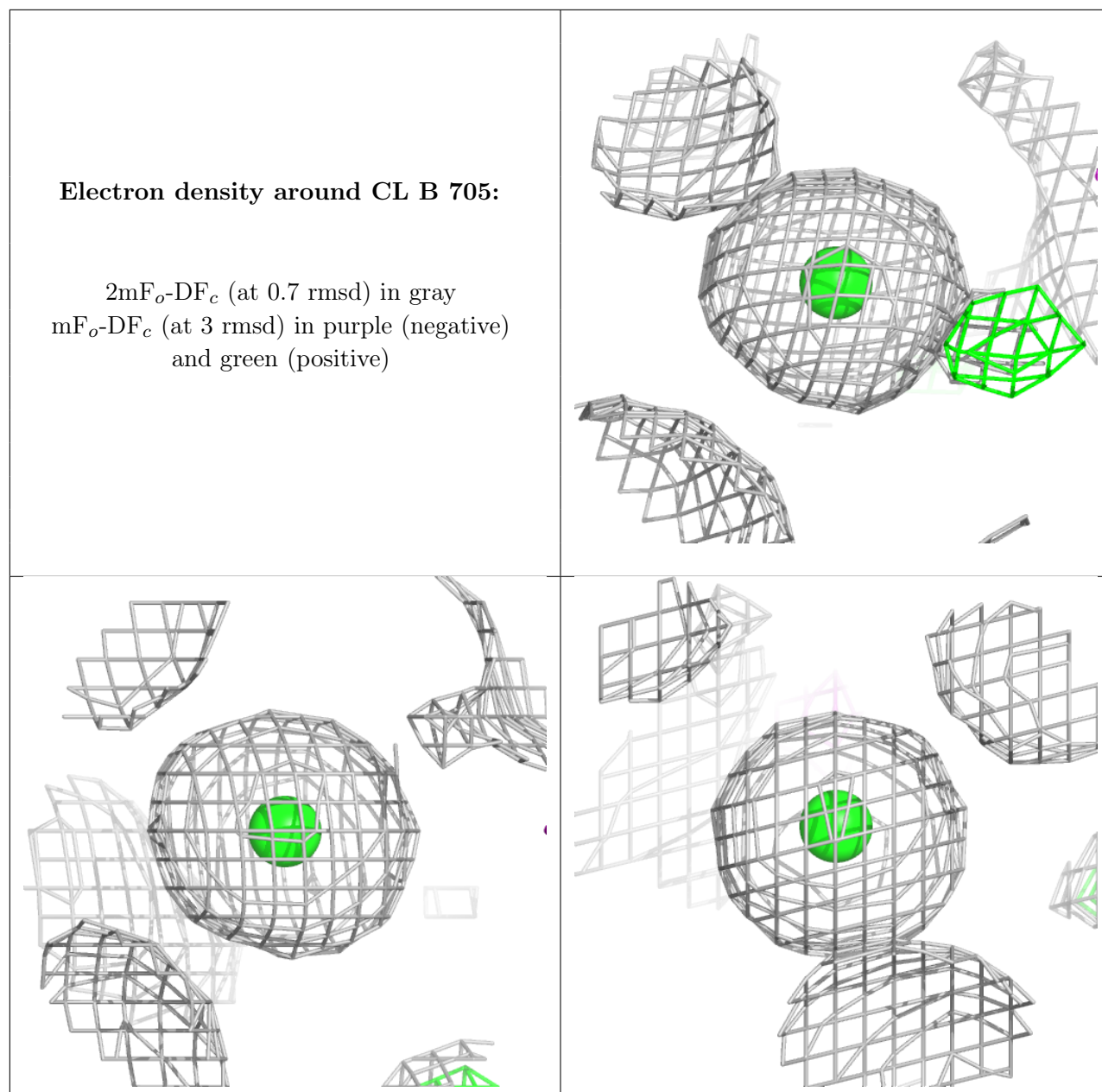




**Electron density around CL A 705:**

$2mF_o-DF_c$  (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.