



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:20 PM UTC

PDB ID : 4F07 / pdb_00004f07
Title : Structure of the Styrene Monooxygenase Flavin Reductase (SMOB) from *Pseudomonas putida* S12
Authors : Sazinsky, M.H.; Morrison, E.; Kantz, A.; Gassner, G.
Deposited on : 2012-05-03
Resolution : 2.30 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

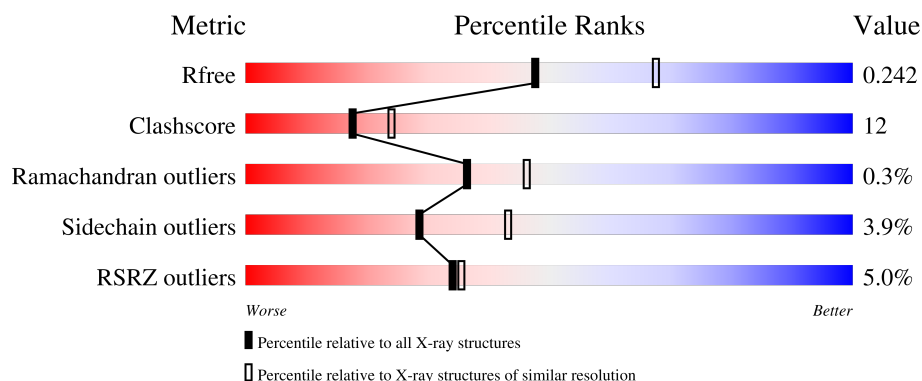
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	190	4% 54% 24% .. 20%
1	B	190	2% 63% 15% .. 19%
1	C	190	5% 56% 21% . 20%
1	D	190	6% 59% 19% . 19%
1	E	190	6% 56% 22% . 22%

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Mol	Chain	Length	Quality of chain
1	F	190	
1	G	190	
1	H	190	
1	I	190	
1	J	190	
1	K	190	
1	L	190	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO3	H	202	-	-	X	-
3	NO3	J	202	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15130 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 Styrene monooxygenase component 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1149	735	194	213	7			
1	B	154	Total	C	N	O	S	0	1	0
			1168	746	198	217	7			
1	C	152	Total	C	N	O	S	0	0	0
			1144	732	194	211	7			
1	D	153	Total	C	N	O	S	0	0	0
			1152	737	195	213	7			
1	E	149	Total	C	N	O	S	0	0	0
			1124	721	191	205	7			
1	F	155	Total	C	N	O	S	0	0	0
			1167	745	198	217	7			
1	G	153	Total	C	N	O	S	0	1	0
			1159	741	196	215	7			
1	H	154	Total	C	N	O	S	0	0	0
			1158	740	196	215	7			
1	I	155	Total	C	N	O	S	0	0	0
			1166	744	198	217	7			
1	J	155	Total	C	N	O	S	0	0	0
			1167	745	198	217	7			
1	K	155	Total	C	N	O	S	0	1	0
			1163	746	198	212	7			
1	L	151	Total	C	N	O	S	0	0	0
			1138	729	193	209	7			

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O33495
A	-18	GLY	-	expression tag	UNP O33495
A	-17	SER	-	expression tag	UNP O33495
A	-16	SER	-	expression tag	UNP O33495
A	-15	HIS	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP O33495
A	-13	HIS	-	expression tag	UNP O33495
A	-12	HIS	-	expression tag	UNP O33495
A	-11	HIS	-	expression tag	UNP O33495
A	-10	HIS	-	expression tag	UNP O33495
A	-9	SER	-	expression tag	UNP O33495
A	-8	SER	-	expression tag	UNP O33495
A	-7	GLY	-	expression tag	UNP O33495
A	-6	LEU	-	expression tag	UNP O33495
A	-5	VAL	-	expression tag	UNP O33495
A	-4	PRO	-	expression tag	UNP O33495
A	-3	ARG	-	expression tag	UNP O33495
A	-2	GLY	-	expression tag	UNP O33495
A	-1	SER	-	expression tag	UNP O33495
A	0	HIS	-	expression tag	UNP O33495
A	151	THR	ALA	engineered mutation	UNP O33495
A	164	GLY	SER	engineered mutation	UNP O33495
B	-19	MET	-	expression tag	UNP O33495
B	-18	GLY	-	expression tag	UNP O33495
B	-17	SER	-	expression tag	UNP O33495
B	-16	SER	-	expression tag	UNP O33495
B	-15	HIS	-	expression tag	UNP O33495
B	-14	HIS	-	expression tag	UNP O33495
B	-13	HIS	-	expression tag	UNP O33495
B	-12	HIS	-	expression tag	UNP O33495
B	-11	HIS	-	expression tag	UNP O33495
B	-10	HIS	-	expression tag	UNP O33495
B	-9	SER	-	expression tag	UNP O33495
B	-8	SER	-	expression tag	UNP O33495
B	-7	GLY	-	expression tag	UNP O33495
B	-6	LEU	-	expression tag	UNP O33495
B	-5	VAL	-	expression tag	UNP O33495
B	-4	PRO	-	expression tag	UNP O33495
B	-3	ARG	-	expression tag	UNP O33495
B	-2	GLY	-	expression tag	UNP O33495
B	-1	SER	-	expression tag	UNP O33495
B	0	HIS	-	expression tag	UNP O33495
B	151	THR	ALA	engineered mutation	UNP O33495
B	164	GLY	SER	engineered mutation	UNP O33495
C	-19	MET	-	expression tag	UNP O33495
C	-18	GLY	-	expression tag	UNP O33495
C	-17	SER	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	SER	-	expression tag	UNP O33495
C	-15	HIS	-	expression tag	UNP O33495
C	-14	HIS	-	expression tag	UNP O33495
C	-13	HIS	-	expression tag	UNP O33495
C	-12	HIS	-	expression tag	UNP O33495
C	-11	HIS	-	expression tag	UNP O33495
C	-10	HIS	-	expression tag	UNP O33495
C	-9	SER	-	expression tag	UNP O33495
C	-8	SER	-	expression tag	UNP O33495
C	-7	GLY	-	expression tag	UNP O33495
C	-6	LEU	-	expression tag	UNP O33495
C	-5	VAL	-	expression tag	UNP O33495
C	-4	PRO	-	expression tag	UNP O33495
C	-3	ARG	-	expression tag	UNP O33495
C	-2	GLY	-	expression tag	UNP O33495
C	-1	SER	-	expression tag	UNP O33495
C	0	HIS	-	expression tag	UNP O33495
C	151	THR	ALA	engineered mutation	UNP O33495
C	164	GLY	SER	engineered mutation	UNP O33495
D	-19	MET	-	expression tag	UNP O33495
D	-18	GLY	-	expression tag	UNP O33495
D	-17	SER	-	expression tag	UNP O33495
D	-16	SER	-	expression tag	UNP O33495
D	-15	HIS	-	expression tag	UNP O33495
D	-14	HIS	-	expression tag	UNP O33495
D	-13	HIS	-	expression tag	UNP O33495
D	-12	HIS	-	expression tag	UNP O33495
D	-11	HIS	-	expression tag	UNP O33495
D	-10	HIS	-	expression tag	UNP O33495
D	-9	SER	-	expression tag	UNP O33495
D	-8	SER	-	expression tag	UNP O33495
D	-7	GLY	-	expression tag	UNP O33495
D	-6	LEU	-	expression tag	UNP O33495
D	-5	VAL	-	expression tag	UNP O33495
D	-4	PRO	-	expression tag	UNP O33495
D	-3	ARG	-	expression tag	UNP O33495
D	-2	GLY	-	expression tag	UNP O33495
D	-1	SER	-	expression tag	UNP O33495
D	0	HIS	-	expression tag	UNP O33495
D	151	THR	ALA	engineered mutation	UNP O33495
D	164	GLY	SER	engineered mutation	UNP O33495
E	-19	MET	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	GLY	-	expression tag	UNP O33495
E	-17	SER	-	expression tag	UNP O33495
E	-16	SER	-	expression tag	UNP O33495
E	-15	HIS	-	expression tag	UNP O33495
E	-14	HIS	-	expression tag	UNP O33495
E	-13	HIS	-	expression tag	UNP O33495
E	-12	HIS	-	expression tag	UNP O33495
E	-11	HIS	-	expression tag	UNP O33495
E	-10	HIS	-	expression tag	UNP O33495
E	-9	SER	-	expression tag	UNP O33495
E	-8	SER	-	expression tag	UNP O33495
E	-7	GLY	-	expression tag	UNP O33495
E	-6	LEU	-	expression tag	UNP O33495
E	-5	VAL	-	expression tag	UNP O33495
E	-4	PRO	-	expression tag	UNP O33495
E	-3	ARG	-	expression tag	UNP O33495
E	-2	GLY	-	expression tag	UNP O33495
E	-1	SER	-	expression tag	UNP O33495
E	0	HIS	-	expression tag	UNP O33495
E	151	THR	ALA	engineered mutation	UNP O33495
E	164	GLY	SER	engineered mutation	UNP O33495
F	-19	MET	-	expression tag	UNP O33495
F	-18	GLY	-	expression tag	UNP O33495
F	-17	SER	-	expression tag	UNP O33495
F	-16	SER	-	expression tag	UNP O33495
F	-15	HIS	-	expression tag	UNP O33495
F	-14	HIS	-	expression tag	UNP O33495
F	-13	HIS	-	expression tag	UNP O33495
F	-12	HIS	-	expression tag	UNP O33495
F	-11	HIS	-	expression tag	UNP O33495
F	-10	HIS	-	expression tag	UNP O33495
F	-9	SER	-	expression tag	UNP O33495
F	-8	SER	-	expression tag	UNP O33495
F	-7	GLY	-	expression tag	UNP O33495
F	-6	LEU	-	expression tag	UNP O33495
F	-5	VAL	-	expression tag	UNP O33495
F	-4	PRO	-	expression tag	UNP O33495
F	-3	ARG	-	expression tag	UNP O33495
F	-2	GLY	-	expression tag	UNP O33495
F	-1	SER	-	expression tag	UNP O33495
F	0	HIS	-	expression tag	UNP O33495
F	151	THR	ALA	engineered mutation	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
F	164	GLY	SER	engineered mutation	UNP O33495
G	-19	MET	-	expression tag	UNP O33495
G	-18	GLY	-	expression tag	UNP O33495
G	-17	SER	-	expression tag	UNP O33495
G	-16	SER	-	expression tag	UNP O33495
G	-15	HIS	-	expression tag	UNP O33495
G	-14	HIS	-	expression tag	UNP O33495
G	-13	HIS	-	expression tag	UNP O33495
G	-12	HIS	-	expression tag	UNP O33495
G	-11	HIS	-	expression tag	UNP O33495
G	-10	HIS	-	expression tag	UNP O33495
G	-9	SER	-	expression tag	UNP O33495
G	-8	SER	-	expression tag	UNP O33495
G	-7	GLY	-	expression tag	UNP O33495
G	-6	LEU	-	expression tag	UNP O33495
G	-5	VAL	-	expression tag	UNP O33495
G	-4	PRO	-	expression tag	UNP O33495
G	-3	ARG	-	expression tag	UNP O33495
G	-2	GLY	-	expression tag	UNP O33495
G	-1	SER	-	expression tag	UNP O33495
G	0	HIS	-	expression tag	UNP O33495
G	151	THR	ALA	engineered mutation	UNP O33495
G	164	GLY	SER	engineered mutation	UNP O33495
H	-19	MET	-	expression tag	UNP O33495
H	-18	GLY	-	expression tag	UNP O33495
H	-17	SER	-	expression tag	UNP O33495
H	-16	SER	-	expression tag	UNP O33495
H	-15	HIS	-	expression tag	UNP O33495
H	-14	HIS	-	expression tag	UNP O33495
H	-13	HIS	-	expression tag	UNP O33495
H	-12	HIS	-	expression tag	UNP O33495
H	-11	HIS	-	expression tag	UNP O33495
H	-10	HIS	-	expression tag	UNP O33495
H	-9	SER	-	expression tag	UNP O33495
H	-8	SER	-	expression tag	UNP O33495
H	-7	GLY	-	expression tag	UNP O33495
H	-6	LEU	-	expression tag	UNP O33495
H	-5	VAL	-	expression tag	UNP O33495
H	-4	PRO	-	expression tag	UNP O33495
H	-3	ARG	-	expression tag	UNP O33495
H	-2	GLY	-	expression tag	UNP O33495
H	-1	SER	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	HIS	-	expression tag	UNP O33495
H	151	THR	ALA	engineered mutation	UNP O33495
H	164	GLY	SER	engineered mutation	UNP O33495
I	-19	MET	-	expression tag	UNP O33495
I	-18	GLY	-	expression tag	UNP O33495
I	-17	SER	-	expression tag	UNP O33495
I	-16	SER	-	expression tag	UNP O33495
I	-15	HIS	-	expression tag	UNP O33495
I	-14	HIS	-	expression tag	UNP O33495
I	-13	HIS	-	expression tag	UNP O33495
I	-12	HIS	-	expression tag	UNP O33495
I	-11	HIS	-	expression tag	UNP O33495
I	-10	HIS	-	expression tag	UNP O33495
I	-9	SER	-	expression tag	UNP O33495
I	-8	SER	-	expression tag	UNP O33495
I	-7	GLY	-	expression tag	UNP O33495
I	-6	LEU	-	expression tag	UNP O33495
I	-5	VAL	-	expression tag	UNP O33495
I	-4	PRO	-	expression tag	UNP O33495
I	-3	ARG	-	expression tag	UNP O33495
I	-2	GLY	-	expression tag	UNP O33495
I	-1	SER	-	expression tag	UNP O33495
I	0	HIS	-	expression tag	UNP O33495
I	151	THR	ALA	engineered mutation	UNP O33495
I	164	GLY	SER	engineered mutation	UNP O33495
J	-19	MET	-	expression tag	UNP O33495
J	-18	GLY	-	expression tag	UNP O33495
J	-17	SER	-	expression tag	UNP O33495
J	-16	SER	-	expression tag	UNP O33495
J	-15	HIS	-	expression tag	UNP O33495
J	-14	HIS	-	expression tag	UNP O33495
J	-13	HIS	-	expression tag	UNP O33495
J	-12	HIS	-	expression tag	UNP O33495
J	-11	HIS	-	expression tag	UNP O33495
J	-10	HIS	-	expression tag	UNP O33495
J	-9	SER	-	expression tag	UNP O33495
J	-8	SER	-	expression tag	UNP O33495
J	-7	GLY	-	expression tag	UNP O33495
J	-6	LEU	-	expression tag	UNP O33495
J	-5	VAL	-	expression tag	UNP O33495
J	-4	PRO	-	expression tag	UNP O33495
J	-3	ARG	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	expression tag	UNP O33495
J	-1	SER	-	expression tag	UNP O33495
J	0	HIS	-	expression tag	UNP O33495
J	151	THR	ALA	engineered mutation	UNP O33495
J	164	GLY	SER	engineered mutation	UNP O33495
K	-19	MET	-	expression tag	UNP O33495
K	-18	GLY	-	expression tag	UNP O33495
K	-17	SER	-	expression tag	UNP O33495
K	-16	SER	-	expression tag	UNP O33495
K	-15	HIS	-	expression tag	UNP O33495
K	-14	HIS	-	expression tag	UNP O33495
K	-13	HIS	-	expression tag	UNP O33495
K	-12	HIS	-	expression tag	UNP O33495
K	-11	HIS	-	expression tag	UNP O33495
K	-10	HIS	-	expression tag	UNP O33495
K	-9	SER	-	expression tag	UNP O33495
K	-8	SER	-	expression tag	UNP O33495
K	-7	GLY	-	expression tag	UNP O33495
K	-6	LEU	-	expression tag	UNP O33495
K	-5	VAL	-	expression tag	UNP O33495
K	-4	PRO	-	expression tag	UNP O33495
K	-3	ARG	-	expression tag	UNP O33495
K	-2	GLY	-	expression tag	UNP O33495
K	-1	SER	-	expression tag	UNP O33495
K	0	HIS	-	expression tag	UNP O33495
K	151	THR	ALA	engineered mutation	UNP O33495
K	164	GLY	SER	engineered mutation	UNP O33495
L	-19	MET	-	expression tag	UNP O33495
L	-18	GLY	-	expression tag	UNP O33495
L	-17	SER	-	expression tag	UNP O33495
L	-16	SER	-	expression tag	UNP O33495
L	-15	HIS	-	expression tag	UNP O33495
L	-14	HIS	-	expression tag	UNP O33495
L	-13	HIS	-	expression tag	UNP O33495
L	-12	HIS	-	expression tag	UNP O33495
L	-11	HIS	-	expression tag	UNP O33495
L	-10	HIS	-	expression tag	UNP O33495
L	-9	SER	-	expression tag	UNP O33495
L	-8	SER	-	expression tag	UNP O33495
L	-7	GLY	-	expression tag	UNP O33495
L	-6	LEU	-	expression tag	UNP O33495
L	-5	VAL	-	expression tag	UNP O33495

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-4	PRO	-	expression tag	UNP O33495
L	-3	ARG	-	expression tag	UNP O33495
L	-2	GLY	-	expression tag	UNP O33495
L	-1	SER	-	expression tag	UNP O33495
L	0	HIS	-	expression tag	UNP O33495
L	151	THR	ALA	engineered mutation	UNP O33495
L	164	GLY	SER	engineered mutation	UNP O33495

- # FAD

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

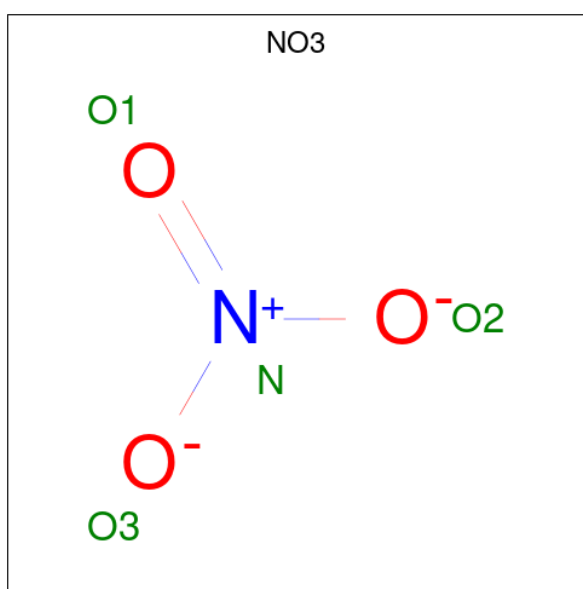


WORLD WIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	L	1	Total	C	N	O	P	0	0
			52	27	9	14	2		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



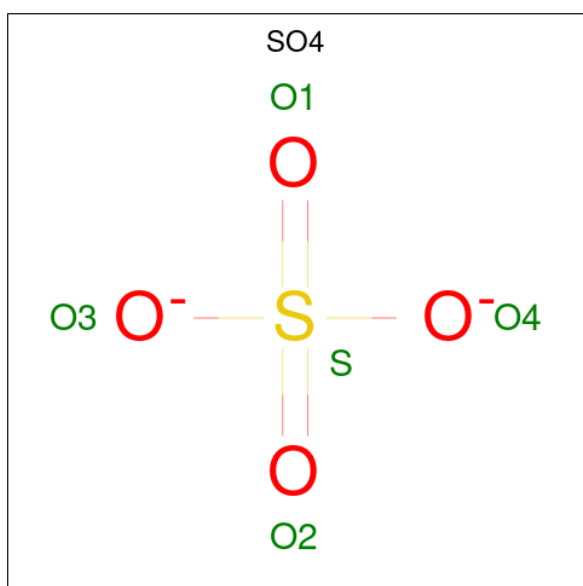
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		
3	A	1	Total	N	O	0	0
			4	1	3		
3	B	1	Total	N	O	0	0
			4	1	3		
3	C	1	Total	N	O	0	0
			4	1	3		
3	D	1	Total	N	O	0	0
			4	1	3		
3	E	1	Total	N	O	0	0
			4	1	3		
3	G	1	Total	N	O	0	0
			4	1	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	N	O	0	0
			4	1	3		
3	I	1	Total	N	O	0	0
			4	1	3		
3	J	1	Total	N	O	0	0
			4	1	3		
3	J	1	Total	N	O	0	0
			4	1	3		
3	L	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		

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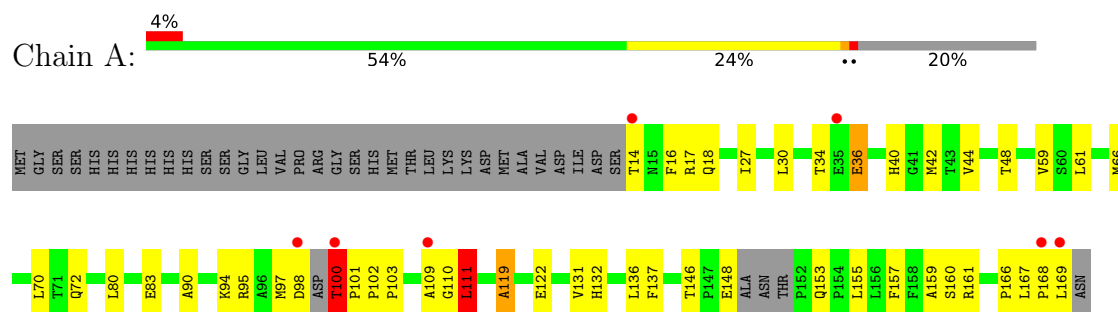
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	61	Total 61	O 61	0	0
5	C	45	Total 45	O 45	0	0
5	D	33	Total 33	O 33	0	0
5	E	40	Total 40	O 40	0	0
5	F	45	Total 45	O 45	0	0
5	G	42	Total 42	O 42	0	0
5	H	35	Total 35	O 35	0	0
5	I	52	Total 52	O 52	0	0
5	J	66	Total 66	O 66	0	0
5	K	54	Total 54	O 54	0	0
5	L	64	Total 64	O 64	0	0

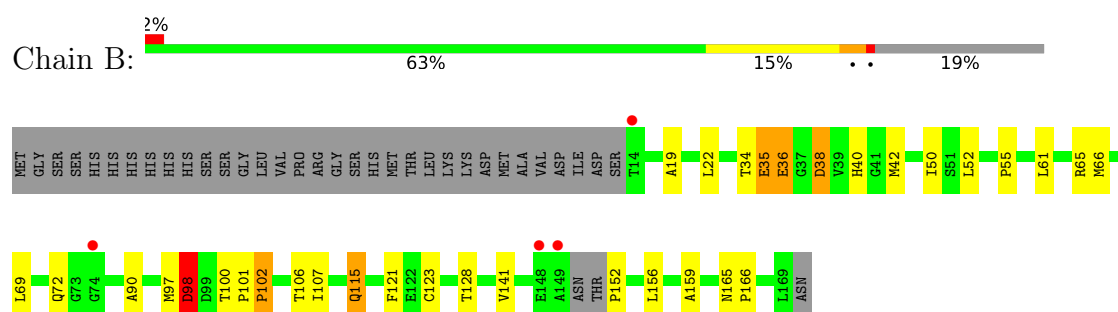
3 Residue-property plots [i](#)

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

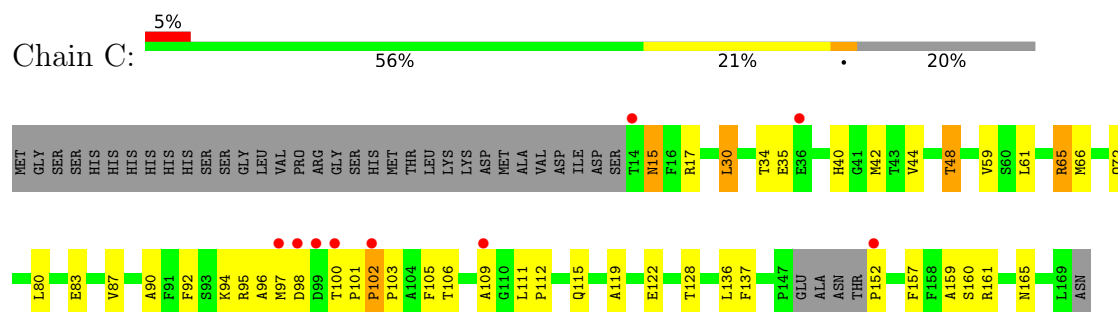
- Molecule 1: Styrene monooxygenase component 2



- Molecule 1: Styrene monooxygenase component 2

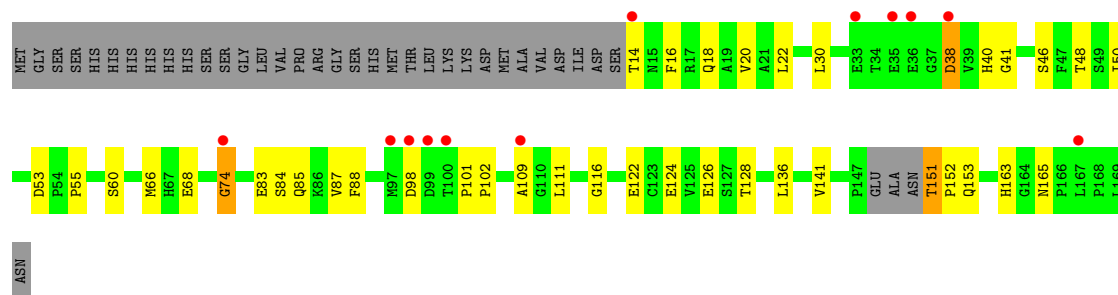


- Molecule 1: Styrene monooxygenase component 2

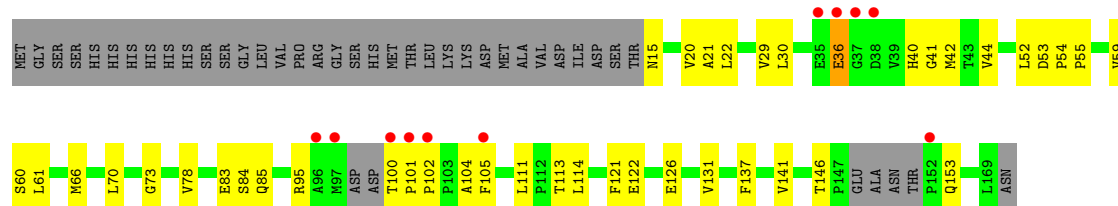


- Molecule 1: Styrene monooxygenase component 2

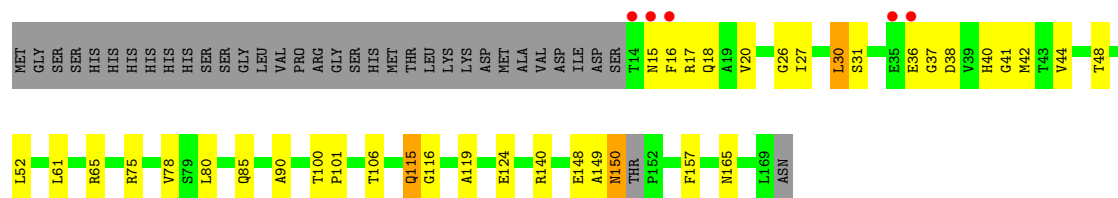




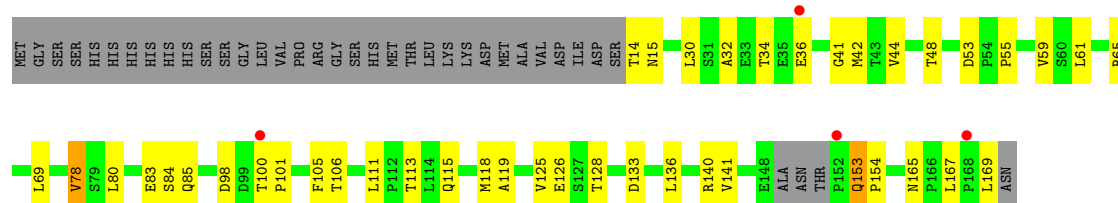
• Molecule 1: Styrene monooxygenase component 2



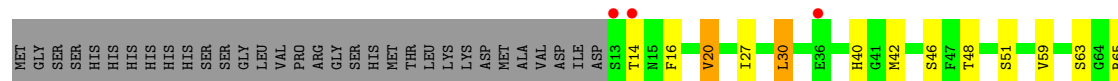
• Molecule 1: Styrene monooxygenase component 2

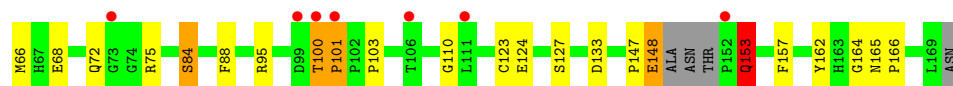


• Molecule 1: Styrene monooxygenase component 2

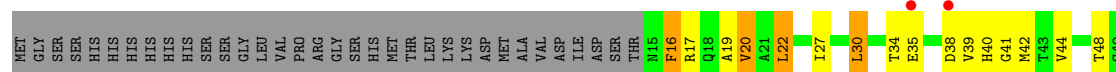


• Molecule 1: Styrene monooxygenase component 2

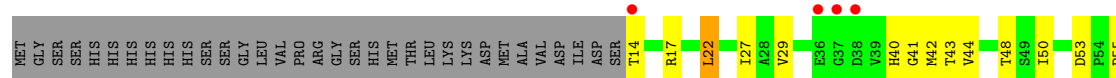




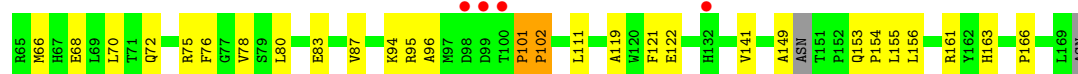
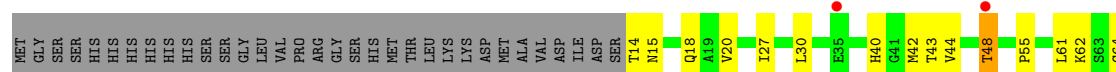
- Molecule 1: Styrene monooxygenase component 2



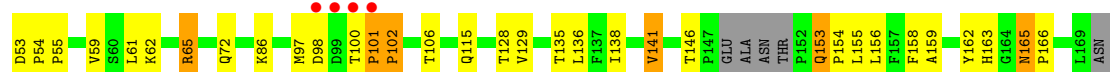
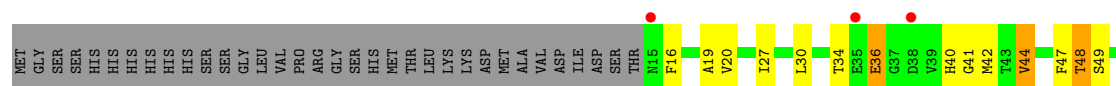
- Molecule 1: Styrene monooxygenase component 2



- Molecule 1: Styrene monooxygenase component 2



- Molecule 1: Styrene monooxygenase component 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	130.03Å 130.03Å 95.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.47 – 2.30 48.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.47-2.30) 99.9 (48.47-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.185 , 0.248 0.198 , 0.242	Depositor DCC
R_{free} test set	4078 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.198 for -h,-k,l 0.008 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.884 for H, K, L 0.116 for -h,-k,l	Depositor
Outliers	0 of 79988 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15130	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.97 % 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 1.6803e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: FAD, NO3, SO4

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	1.37	3/1177 (0.3%)	1.17	3/1598 (0.2%)
1	B	1.34	6/1197 (0.5%)	1.24	7/1627 (0.4%)
1	C	1.19	2/1173 (0.2%)	1.15	5/1594 (0.3%)
1	D	1.30	3/1181 (0.3%)	1.12	4/1607 (0.2%)
1	E	1.37	8/1152 (0.7%)	1.20	5/1563 (0.3%)
1	F	1.29	2/1196 (0.2%)	1.13	3/1626 (0.2%)
1	G	1.36	6/1191 (0.5%)	1.21	2/1619 (0.1%)
1	H	1.32	3/1187 (0.3%)	1.17	4/1614 (0.2%)
1	I	1.55	8/1196 (0.7%)	1.26	6/1629 (0.4%)
1	J	1.44	6/1196 (0.5%)	1.22	3/1626 (0.2%)
1	K	1.42	4/1195 (0.3%)	1.28	4/1625 (0.2%)
1	L	1.50	11/1167 (0.9%)	1.30	6/1586 (0.4%)
All	All	1.37	62/14208 (0.4%)	1.21	52/19314 (0.3%)

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	151	THR	CA-C	-11.50	1.41	1.53
1	J	59	VAL	CA-C	8.76	1.63	1.52
1	I	39	VAL	C-O	-7.97	1.15	1.24
1	L	44	VAL	C-O	-7.54	1.16	1.23
1	I	151	THR	CA-CB	-7.32	1.42	1.53

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	101	PRO	CA-C-N	11.18	127.82	119.66
1	K	101	PRO	C-N-CA	11.18	127.82	119.66
1	C	165	ASN	CA-C-N	-7.81	111.96	119.85
1	C	165	ASN	C-N-CA	-7.81	111.96	119.85
1	I	50	ILE	CB-CA-C	-7.63	105.22	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1149	0	1128	43	0
1	B	1168	0	1143	19	0
1	C	1144	0	1121	35	0
1	D	1152	0	1131	28	0
1	E	1124	0	1107	25	0
1	F	1167	0	1142	30	0
1	G	1159	0	1137	24	0
1	H	1158	0	1131	32	0
1	I	1166	0	1140	35	0
1	J	1167	0	1142	42	0
1	K	1163	0	1144	34	0
1	L	1138	0	1118	33	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	3	0
2	D	53	0	31	2	0
2	E	53	0	31	2	0
2	F	53	0	31	4	0
2	G	53	0	31	2	0
2	H	53	0	31	6	0
2	I	53	0	31	4	0
2	J	53	0	31	2	0
2	K	53	0	31	4	0
2	L	52	0	31	2	0
3	A	8	0	0	1	0
3	B	4	0	0	0	0
3	C	4	0	0	1	0
3	D	4	0	0	1	0
3	E	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	2	0
3	I	4	0	0	0	0
3	J	8	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	4	0	0	1	0
4	D	10	0	0	0	0
4	J	5	0	0	1	0
5	A	40	0	0	0	0
5	B	61	0	0	2	0
5	C	45	0	0	3	0
5	D	33	0	0	0	0
5	E	40	0	0	0	0
5	F	45	0	0	2	0
5	G	42	0	0	0	0
5	H	35	0	0	0	0
5	I	52	0	0	2	0
5	J	66	0	0	2	0
5	K	54	0	0	4	0
5	L	64	0	0	1	0
All	All	15130	0	13956	353	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 12.

The worst 5 of 353 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:83:GLU:OE1	1:H:84:SER:HB3	1.43	1.18
1:A:110:GLY:C	1:A:111:LEU:HD13	1.76	1.10
1:I:34:THR:CG2	1:I:35:GLU:H	1.65	1.10
1:I:34:THR:HG22	1:I:35:GLU:H	1.11	1.03
1:I:34:THR:HG22	1:I:35:GLU:N	1.65	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	146/190 (77%)	138 (94%)	8 (6%)	0	100	100
1	B	151/190 (80%)	142 (94%)	9 (6%)	0	100	100
1	C	148/190 (78%)	140 (95%)	8 (5%)	0	100	100
1	D	149/190 (78%)	140 (94%)	8 (5%)	1 (1%)	18	23
1	E	143/190 (75%)	134 (94%)	7 (5%)	2 (1%)	9	9
1	F	151/190 (80%)	142 (94%)	7 (5%)	2 (1%)	9	10
1	G	150/190 (79%)	144 (96%)	6 (4%)	0	100	100
1	H	150/190 (79%)	139 (93%)	11 (7%)	0	100	100
1	I	153/190 (80%)	145 (95%)	8 (5%)	0	100	100
1	J	151/190 (80%)	144 (95%)	7 (5%)	0	100	100
1	K	152/190 (80%)	143 (94%)	9 (6%)	0	100	100
1	L	147/190 (77%)	140 (95%)	7 (5%)	0	100	100
All	All	1791/2280 (79%)	1691 (94%)	95 (5%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	37	GLY
1	E	84	SER
1	F	101	PRO
1	E	102	PRO
1	D	74	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	125/159 (79%)	119 (95%)	6 (5%)	23	35
1	B	126/159 (79%)	121 (96%)	5 (4%)	28	42
1	C	124/159 (78%)	118 (95%)	6 (5%)	23	35
1	D	125/159 (79%)	124 (99%)	1 (1%)	73	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	122/159 (77%)	119 (98%)	3 (2%)	42	60
1	F	126/159 (79%)	122 (97%)	4 (3%)	34	51
1	G	126/159 (79%)	123 (98%)	3 (2%)	43	62
1	H	125/159 (79%)	117 (94%)	8 (6%)	16	23
1	I	126/159 (79%)	120 (95%)	6 (5%)	23	35
1	J	126/159 (79%)	118 (94%)	8 (6%)	16	23
1	K	124/159 (78%)	121 (98%)	3 (2%)	43	62
1	L	123/159 (77%)	118 (96%)	5 (4%)	27	41
All	All	1498/1908 (78%)	1440 (96%)	58 (4%)	28	43

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	30	LEU
1	L	72	GLN
1	H	153	GLN
1	L	36	GLU
1	J	148	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	115	GLN
1	L	40	HIS
1	L	153	GLN
1	K	72	GLN
1	G	132	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 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	SO4	D	204	-	4,4,4	0.23	0	6,6,6	0.18	0
2	FAD	C	201	-	58,58,58	1.17	5 (8%)	85,89,89	1.76	20 (23%)
3	NO3	A	202	-	1,3,3	3.06	1 (100%)	0,3,3	-	-
3	NO3	A	203	-	1,3,3	3.04	1 (100%)	0,3,3	-	-
2	FAD	I	201	-	58,58,58	1.28	6 (10%)	85,89,89	1.85	22 (25%)
3	NO3	J	202	-	1,3,3	3.36	1 (100%)	0,3,3	-	-
4	SO4	D	203	-	4,4,4	0.16	0	6,6,6	0.58	0
3	NO3	J	203	-	1,3,3	2.96	1 (100%)	0,3,3	-	-
3	NO3	I	202	-	1,3,3	4.06	1 (100%)	0,3,3	-	-
2	FAD	A	201	-	58,58,58	1.33	5 (8%)	85,89,89	1.82	25 (29%)
2	FAD	L	201	-	54,57,58	1.18	6 (11%)	78,86,89	1.97	22 (28%)
3	NO3	C	202	-	1,3,3	3.27	1 (100%)	0,3,3	-	-
3	NO3	H	202	-	1,3,3	3.80	1 (100%)	0,3,3	-	-
2	FAD	F	500	-	58,58,58	1.25	9 (15%)	85,89,89	1.87	22 (25%)
3	NO3	G	202	-	1,3,3	3.25	1 (100%)	0,3,3	-	-
4	SO4	J	204	-	4,4,4	0.28	0	6,6,6	0.50	0
2	FAD	B	201	-	58,58,58	1.71	10 (17%)	85,89,89	1.92	22 (25%)
3	NO3	E	202	-	1,3,3	3.75	1 (100%)	0,3,3	-	-
3	NO3	L	202	-	1,3,3	2.62	1 (100%)	0,3,3	-	-
2	FAD	E	201	-	58,58,58	1.22	6 (10%)	85,89,89	1.73	19 (22%)
2	FAD	G	201	-	58,58,58	1.24	6 (10%)	85,89,89	1.79	15 (17%)
2	FAD	K	500	-	58,58,58	1.36	9 (15%)	85,89,89	2.12	29 (34%)
3	NO3	D	202	-	1,3,3	3.54	1 (100%)	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	D	201	-	58,58,58	1.29	7 (12%)	85,89,89	1.75	20 (23%)
2	FAD	H	201	-	58,58,58	1.24	8 (13%)	85,89,89	1.79	19 (22%)
3	NO3	B	202	-	1,3,3	3.46	1 (100%)	0,3,3	-	-
2	FAD	J	201	-	58,58,58	1.43	7 (12%)	85,89,89	1.76	21 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	F	500	-	-	12/34/50/50	0/6/6/6
2	FAD	G	201	-	-	6/34/50/50	0/6/6/6
2	FAD	C	201	-	-	7/34/50/50	0/6/6/6
2	FAD	K	500	-	-	9/34/50/50	0/6/6/6
2	FAD	B	201	-	-	9/34/50/50	0/6/6/6
2	FAD	A	201	-	-	3/34/50/50	0/6/6/6
2	FAD	L	201	-	-	10/28/48/50	0/6/6/6
2	FAD	I	201	-	-	2/34/50/50	0/6/6/6
2	FAD	D	201	-	-	11/34/50/50	0/6/6/6
2	FAD	H	201	-	-	1/34/50/50	0/6/6/6
2	FAD	J	201	-	-	9/34/50/50	0/6/6/6
2	FAD	E	201	-	-	10/34/50/50	0/6/6/6

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	FAD	C4X-N5	5.61	1.42	1.30
2	J	201	FAD	C2A-N3A	4.54	1.42	1.33
2	A	201	FAD	P-O3P	4.38	1.64	1.59
2	A	201	FAD	C4X-N5	4.18	1.39	1.30
2	E	201	FAD	C4X-N5	4.07	1.39	1.30

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	FAD	N3A-C2A-N1A	-7.75	116.85	128.58
2	H	201	FAD	N3A-C2A-N1A	-6.98	118.01	128.58
2	E	201	FAD	N3A-C2A-N1A	-6.64	118.54	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	FAD	N3A-C2A-N1A	-6.47	118.78	128.58
2	B	201	FAD	N3A-C2A-N1A	-6.08	119.37	128.58

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	FAD	C5B-O5B-PA-O1A
2	B	201	FAD	C5B-O5B-PA-O2A
2	B	201	FAD	C5'-O5'-P-O2P
2	D	201	FAD	C5B-O5B-PA-O1A
2	D	201	FAD	C5B-O5B-PA-O3P

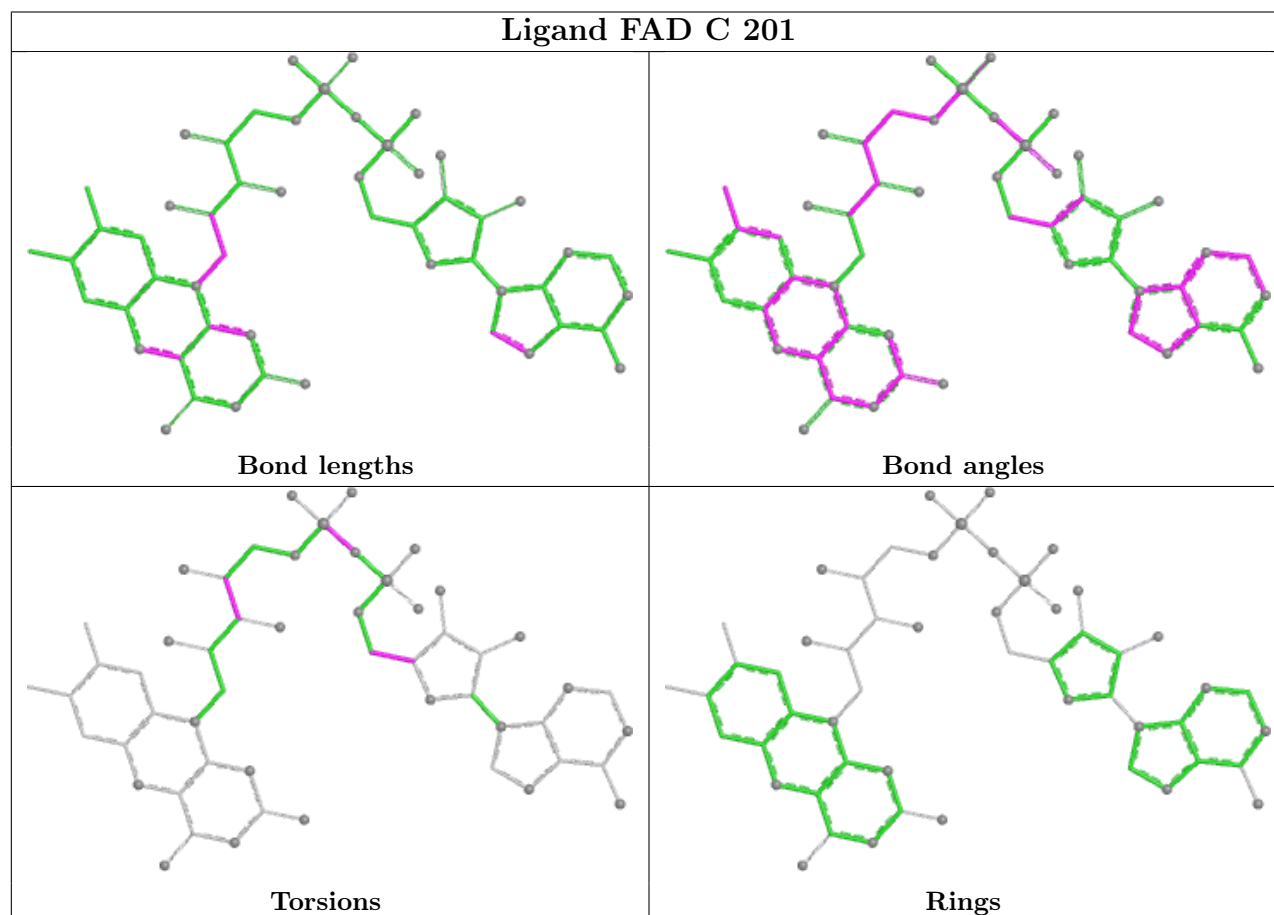
There are no ring outliers.

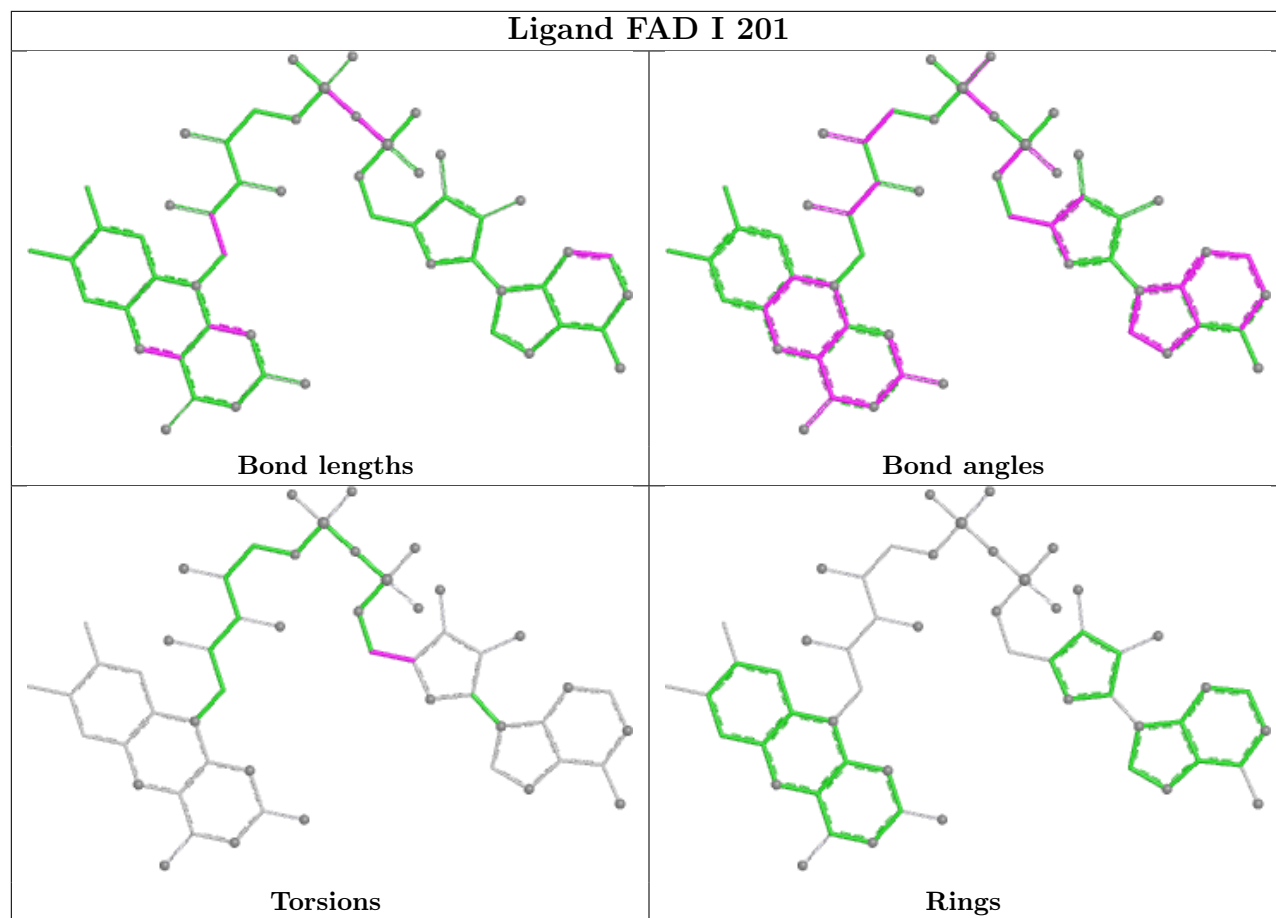
20 monomers are involved in 43 short contacts:

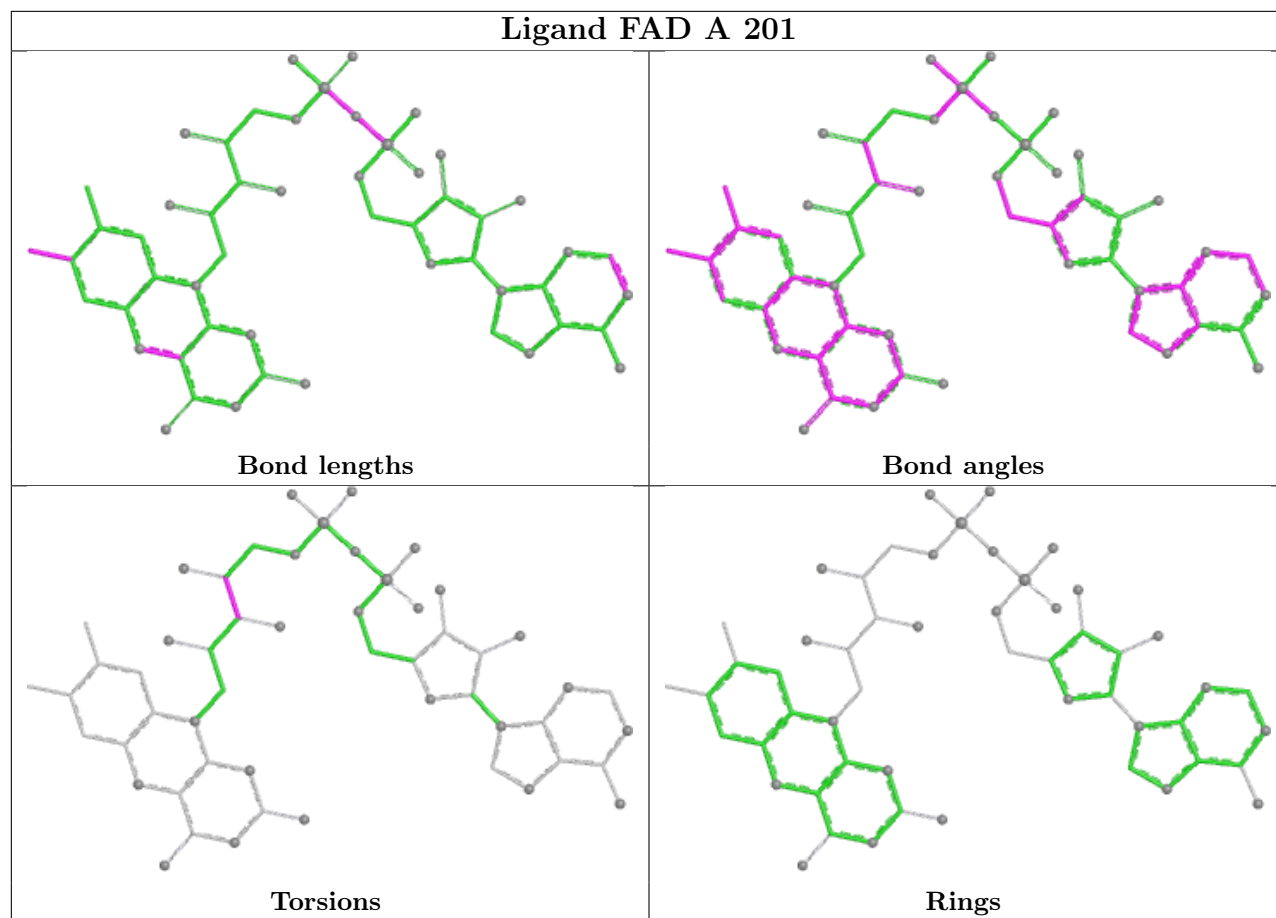
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	FAD	3	0
3	A	202	NO3	1	0
2	I	201	FAD	4	0
3	J	202	NO3	2	0
3	J	203	NO3	1	0
2	A	201	FAD	1	0
2	L	201	FAD	2	0
3	C	202	NO3	1	0
3	H	202	NO3	2	0
2	F	500	FAD	4	0
4	J	204	SO4	1	0
2	B	201	FAD	1	0
3	L	202	NO3	1	0
2	E	201	FAD	2	0
2	G	201	FAD	2	0
2	K	500	FAD	4	0
3	D	202	NO3	1	0
2	D	201	FAD	2	0
2	H	201	FAD	6	0
2	J	201	FAD	2	0

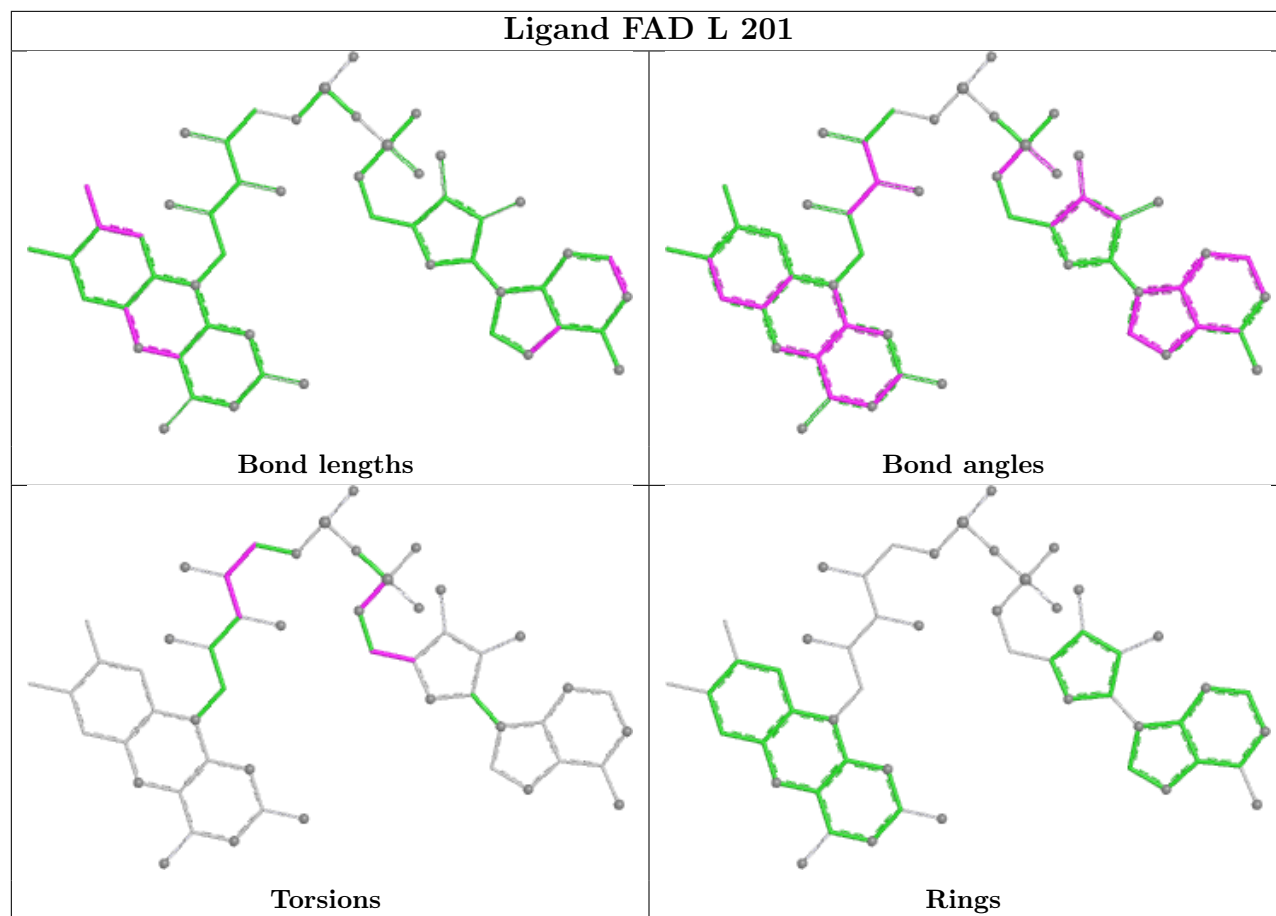
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

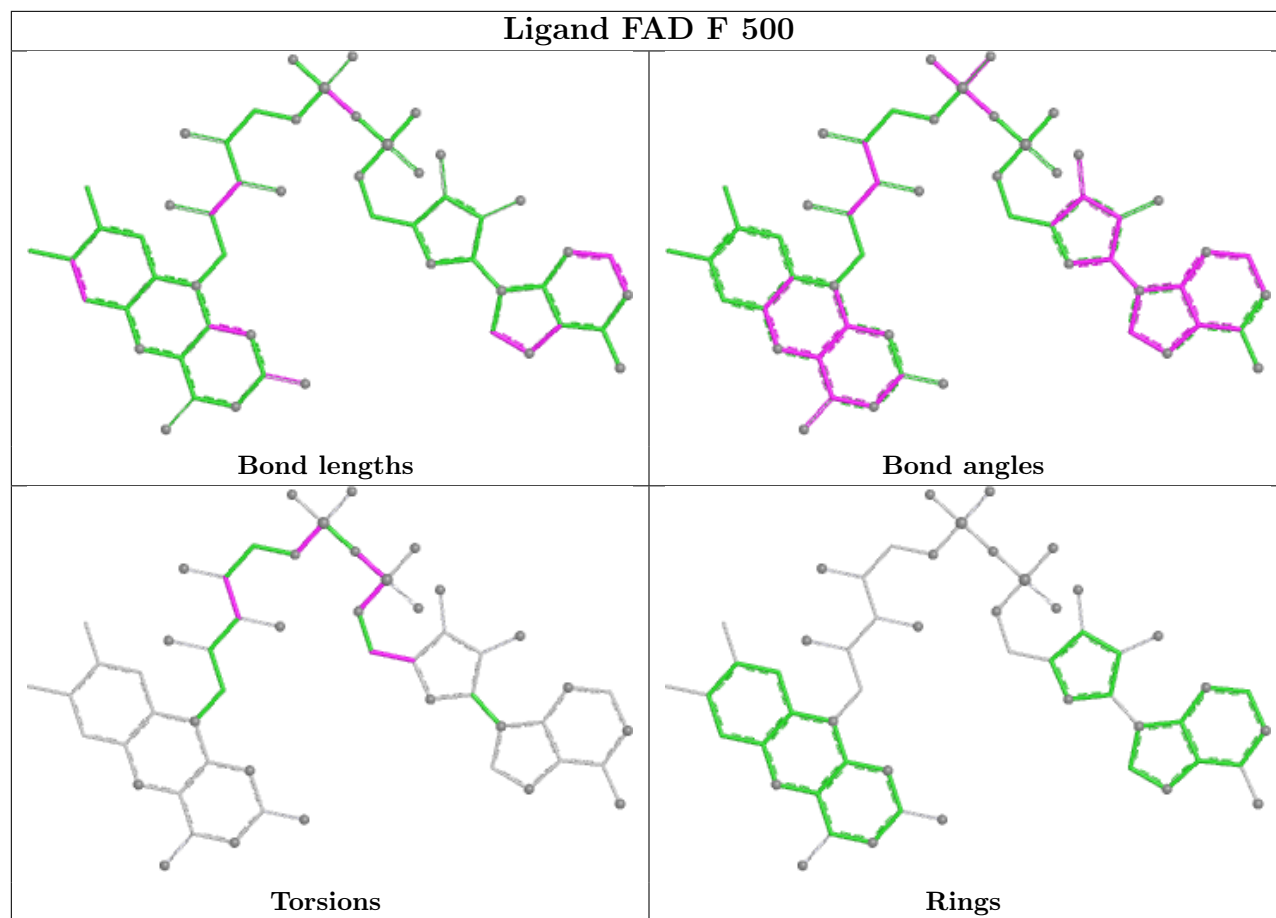
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

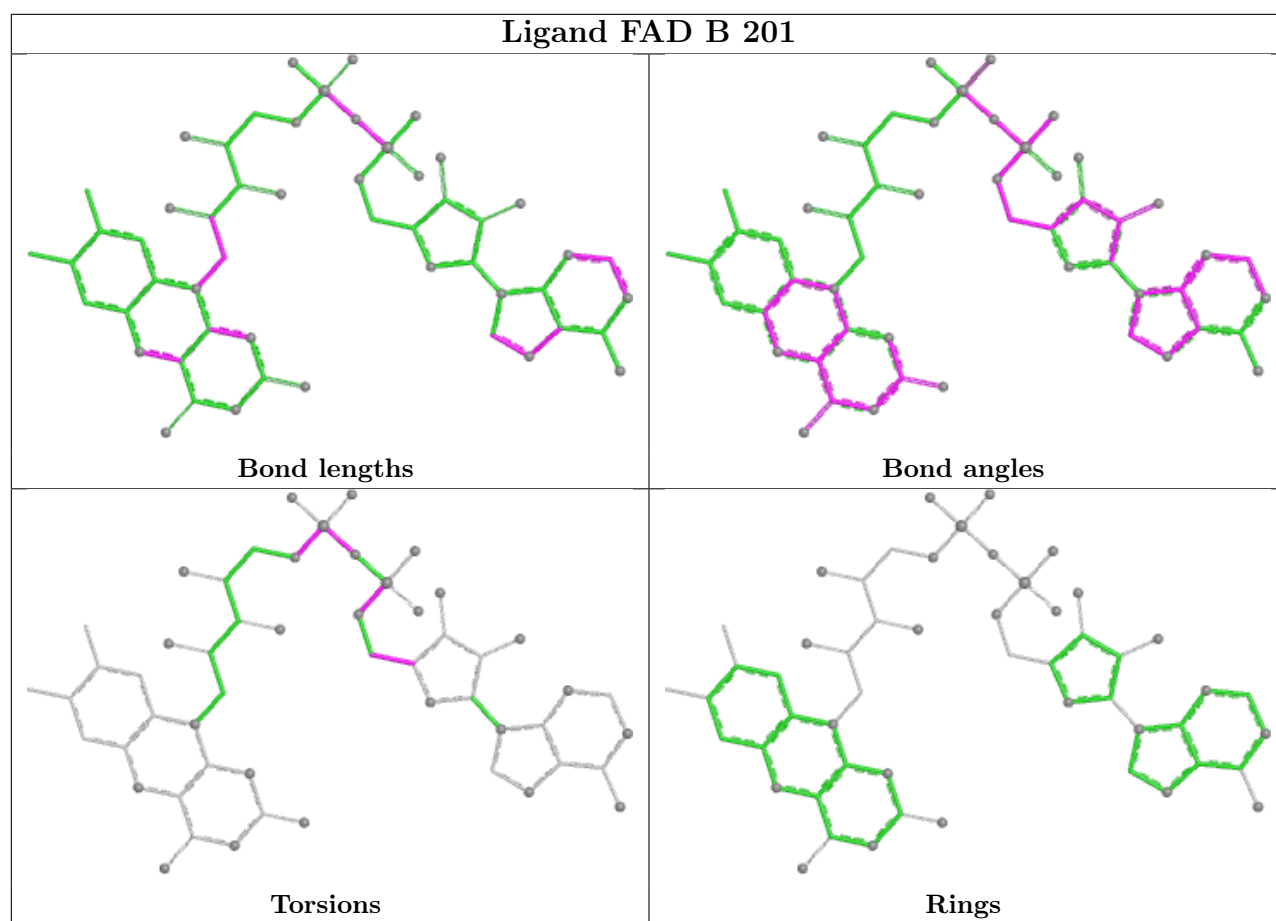


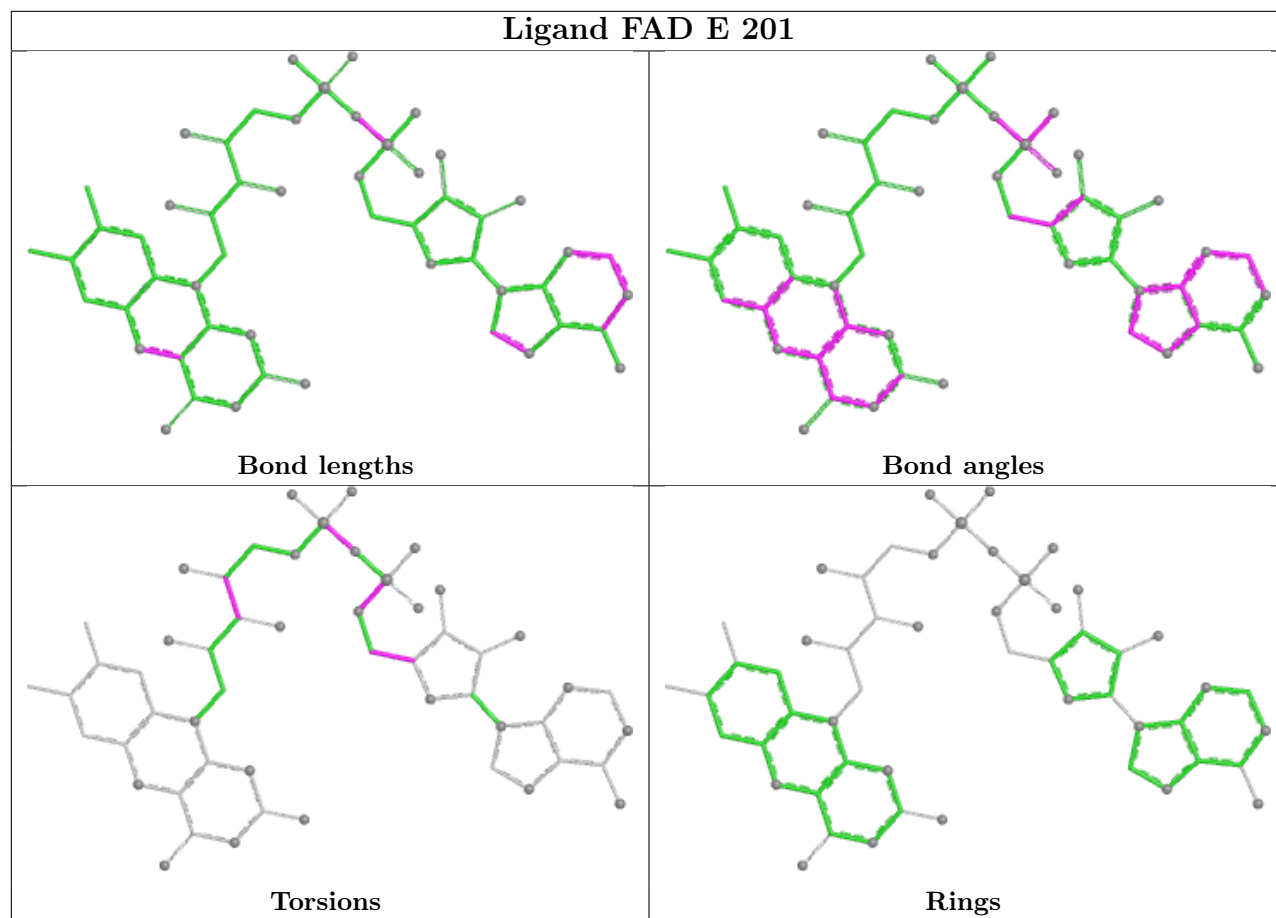


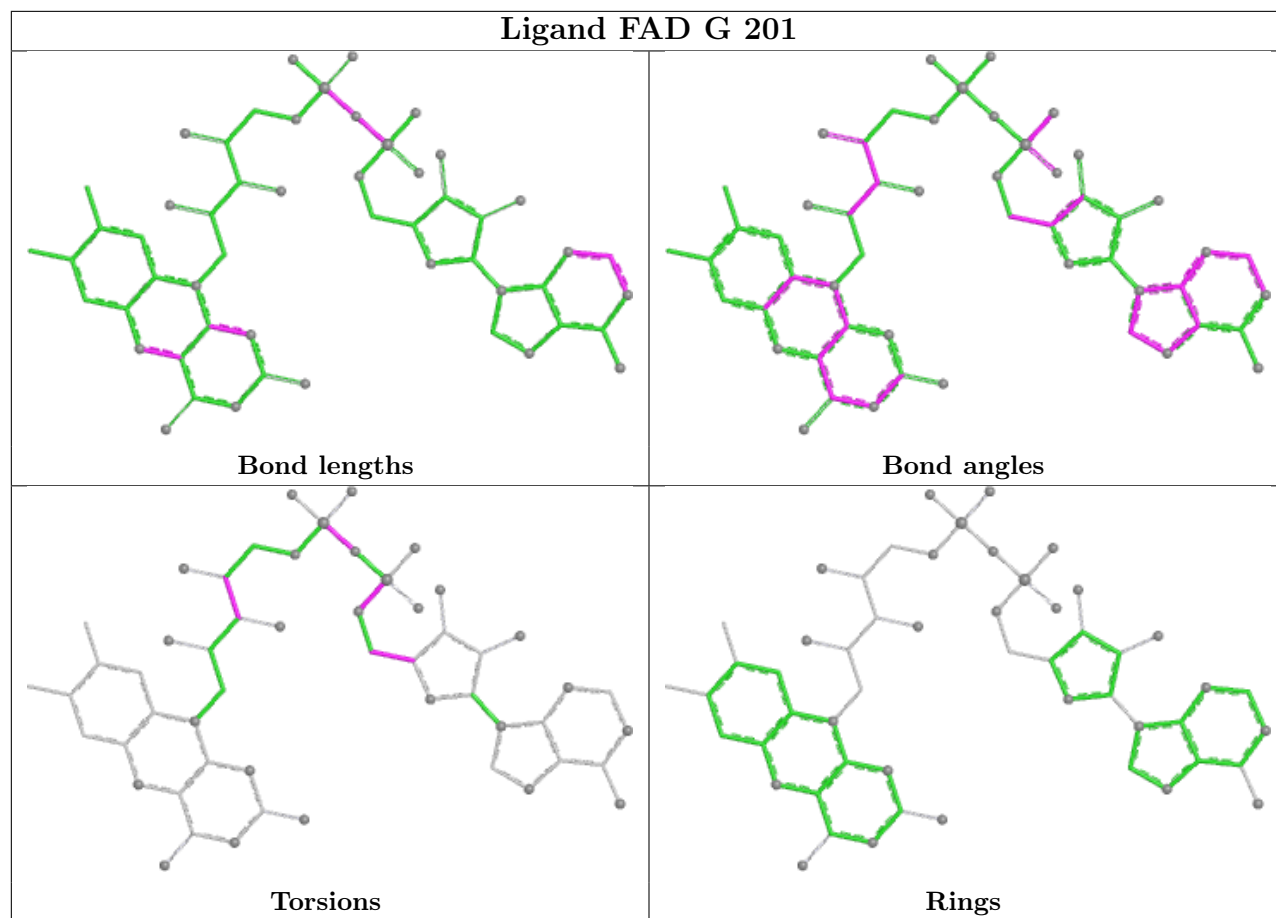


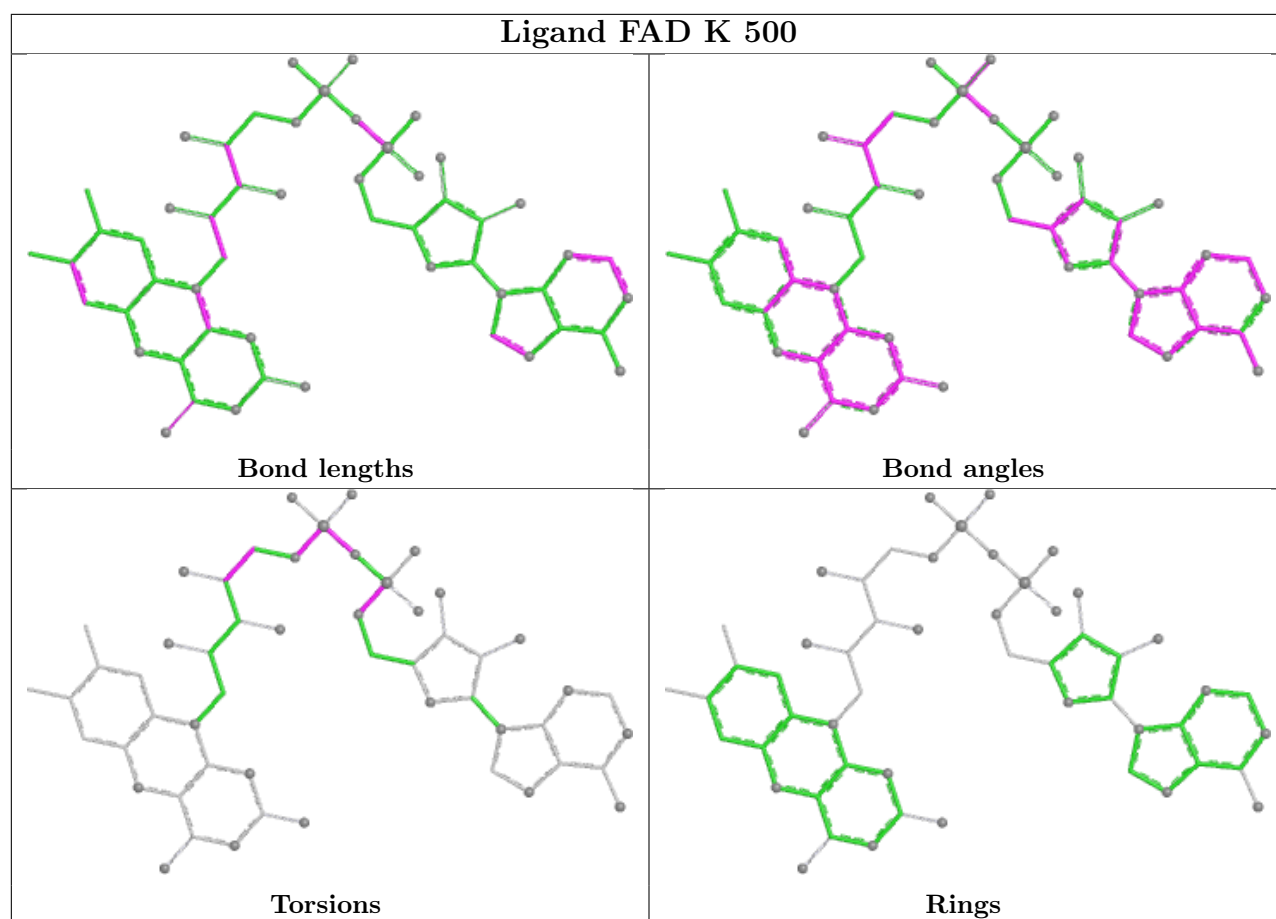


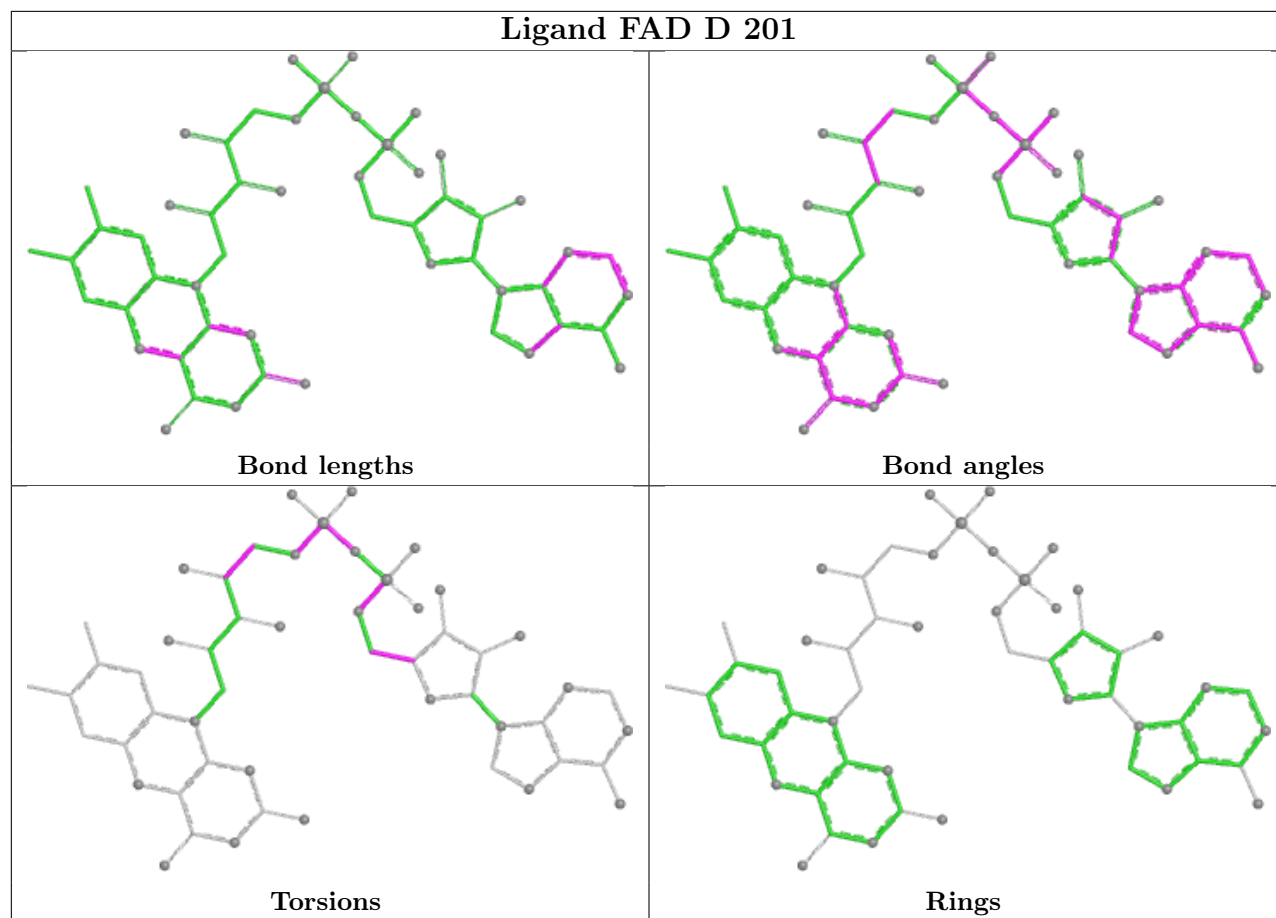


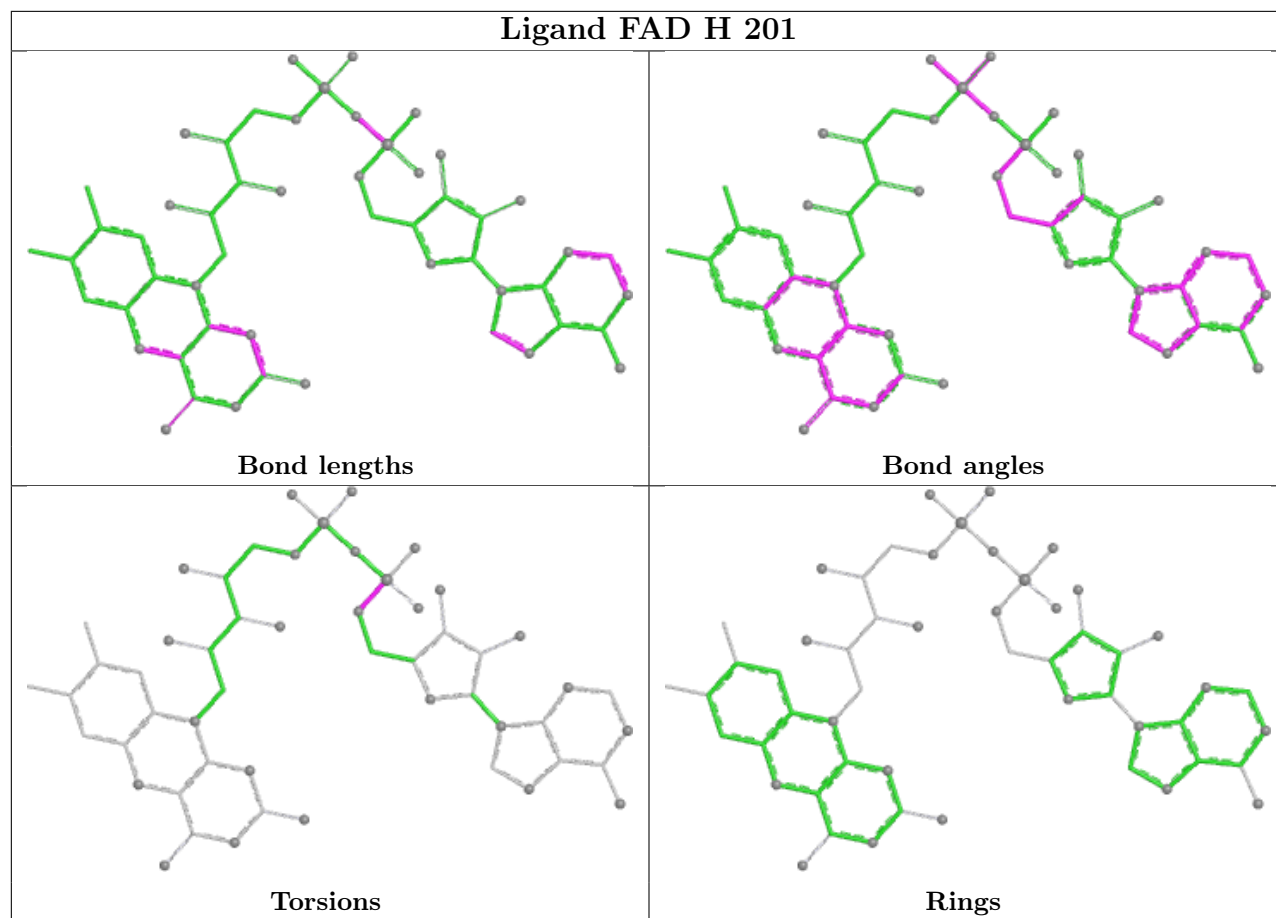


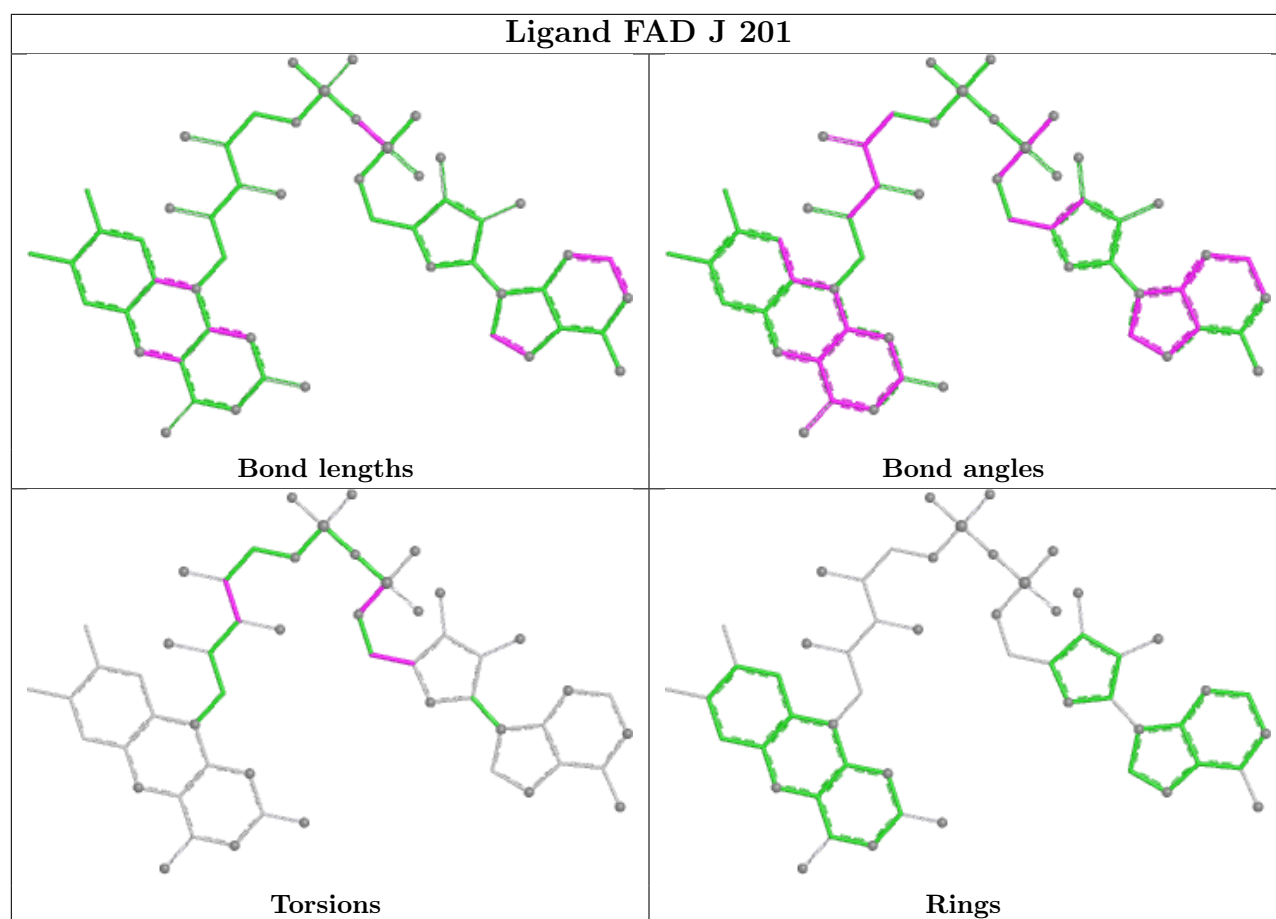












5.7 Other polymers [i](#)

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, 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	152/190 (80%)	0.37	7 (4%) 37 39	2, 14, 32, 42	0
1	B	154/190 (81%)	0.12	4 (2%) 57 59	2, 12, 31, 39	1 (0%)
1	C	152/190 (80%)	0.31	9 (5%) 28 30	5, 15, 38, 43	0
1	D	153/190 (80%)	0.47	12 (7%) 19 21	3, 17, 35, 45	0
1	E	149/190 (78%)	0.37	11 (7%) 20 22	2, 15, 34, 43	0
1	F	155/190 (81%)	0.20	5 (3%) 50 52	2, 13, 32, 37	0
1	G	153/190 (80%)	0.28	4 (2%) 57 59	2, 14, 30, 39	1 (0%)
1	H	154/190 (81%)	0.40	10 (6%) 25 27	3, 16, 35, 45	0
1	I	155/190 (81%)	0.16	3 (1%) 66 68	2, 11, 30, 44	0
1	J	155/190 (81%)	0.26	13 (8%) 17 18	2, 11, 35, 42	0
1	K	155/190 (81%)	0.26	6 (3%) 43 45	2, 11, 28, 35	1 (0%)
1	L	151/190 (79%)	0.08	7 (4%) 37 39	2, 10, 30, 44	0
All	All	1838/2280 (80%)	0.27	91 (4%) 34 35	2, 14, 33, 45	3 (0%)

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	36	GLU	6.2
1	K	98	ASP	5.8
1	D	38	ASP	5.3
1	C	100	THR	4.8
1	L	15	ASN	4.8

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

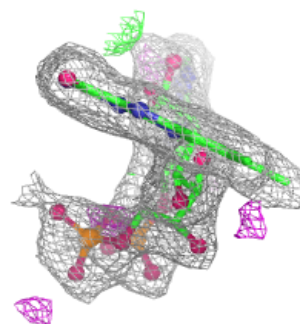
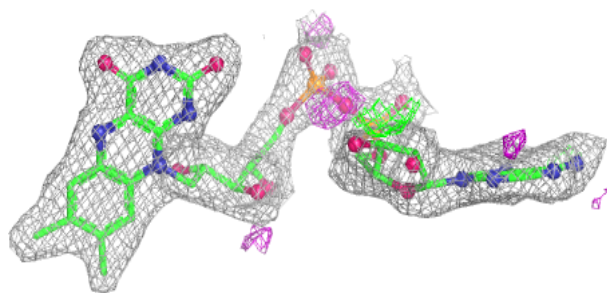
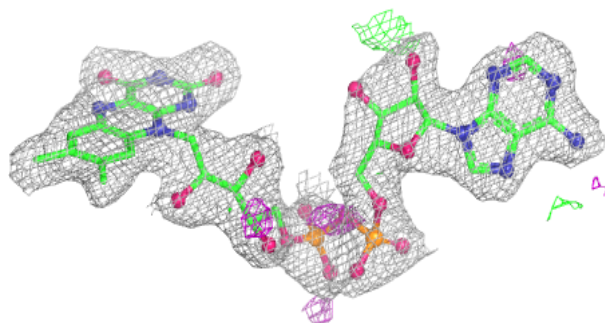
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NO3	I	202	4/4	0.77	0.16	13,17,18,20	0
3	NO3	E	202	4/4	0.82	0.16	33,34,35,35	0
3	NO3	J	203	4/4	0.86	0.18	32,35,35,35	0
3	NO3	C	202	4/4	0.87	0.13	26,27,27,27	0
3	NO3	H	202	4/4	0.88	0.11	22,23,23,25	0
4	SO4	D	203	5/5	0.88	0.16	43,46,48,49	0
3	NO3	A	203	4/4	0.89	0.22	35,35,36,39	0
3	NO3	J	202	4/4	0.89	0.14	22,24,24,27	0
4	SO4	D	204	5/5	0.91	0.12	48,48,51,51	0
2	FAD	J	201	53/53	0.92	0.09	2,13,28,30	0
3	NO3	L	202	4/4	0.92	0.12	23,24,25,25	0
2	FAD	D	201	53/53	0.92	0.09	10,17,28,33	0
3	NO3	G	202	4/4	0.92	0.13	27,28,28,28	0
2	FAD	C	201	53/53	0.93	0.08	9,15,27,35	0
2	FAD	L	201	52/53	0.93	0.09	2,10,22,26	0
2	FAD	B	201	53/53	0.93	0.09	2,14,31,36	0
2	FAD	F	500	53/53	0.93	0.09	2,20,35,41	0
3	NO3	D	202	4/4	0.93	0.16	31,32,32,33	0
2	FAD	G	201	53/53	0.93	0.09	4,15,26,34	0
2	FAD	H	201	53/53	0.93	0.09	5,18,32,38	0
3	NO3	B	202	4/4	0.94	0.15	21,23,24,25	0
2	FAD	E	201	53/53	0.94	0.09	2,13,24,27	0
2	FAD	K	500	53/53	0.94	0.08	2,8,22,24	0
2	FAD	A	201	53/53	0.95	0.08	2,12,26,36	0
3	NO3	A	202	4/4	0.95	0.07	24,25,26,29	0
2	FAD	I	201	53/53	0.95	0.09	2,20,30,33	0
4	SO4	J	204	5/5	0.95	0.09	28,31,32,33	0

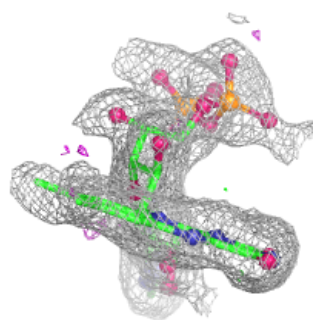
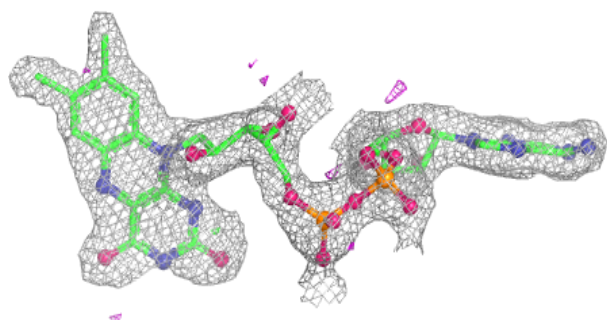
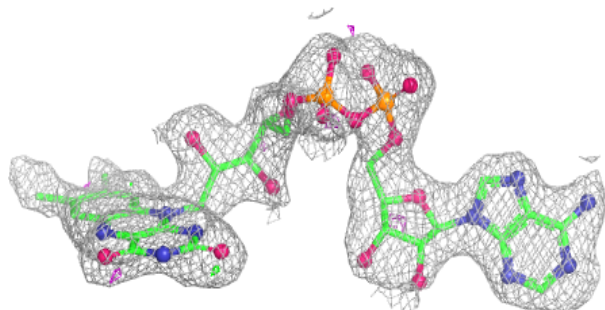
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD J 201:

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

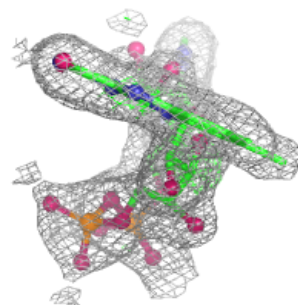
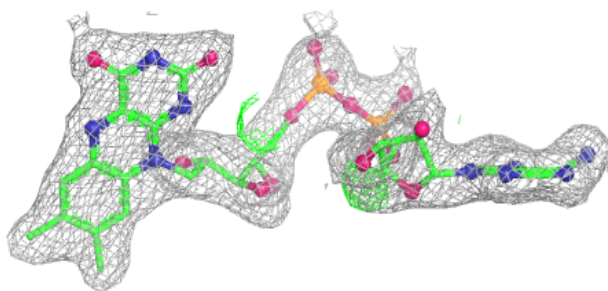
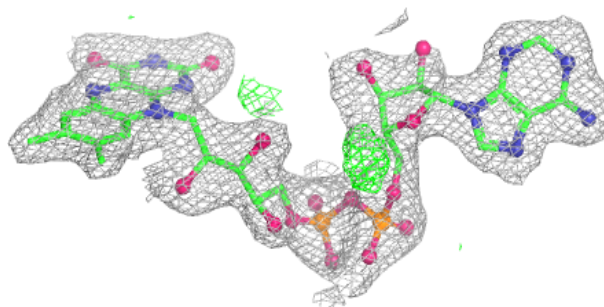
**Electron density around FAD D 201:**

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

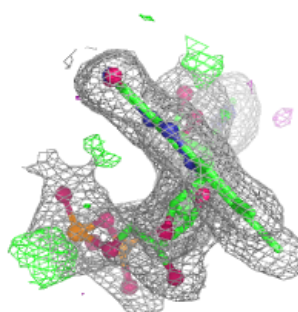
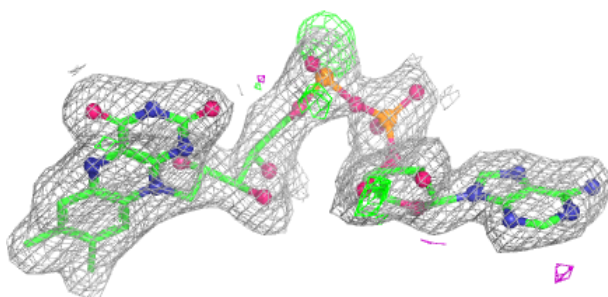
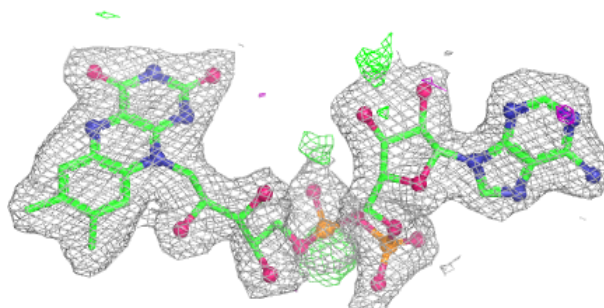


Electron density around FAD C 201:

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

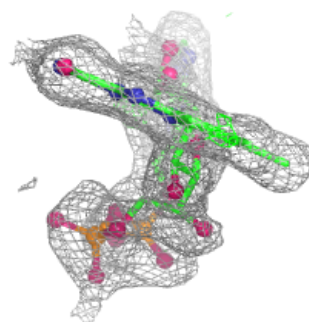
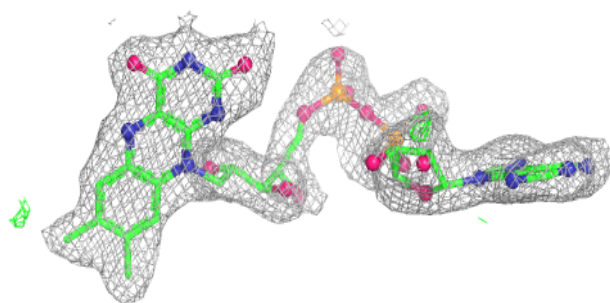
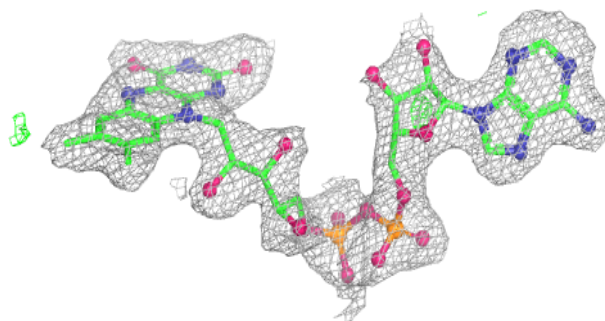
**Electron density around FAD L 201:**

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

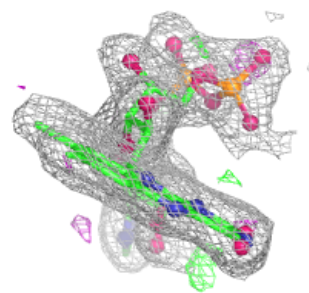
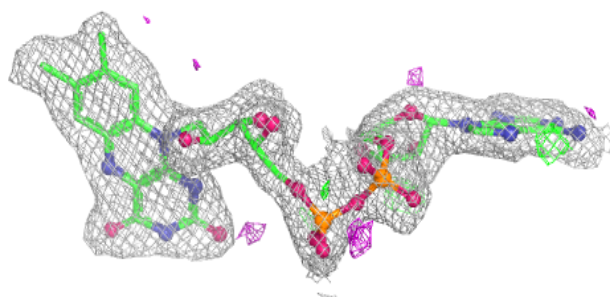
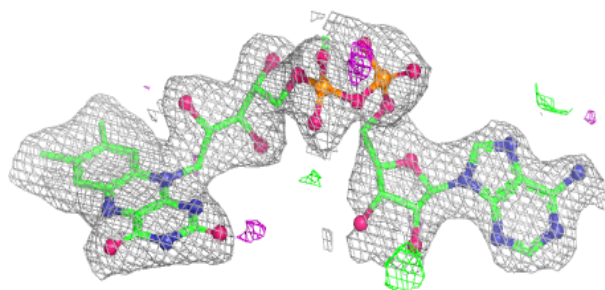


Electron density around FAD B 201:

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

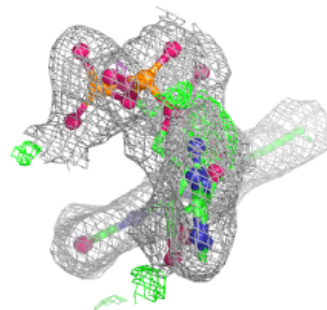
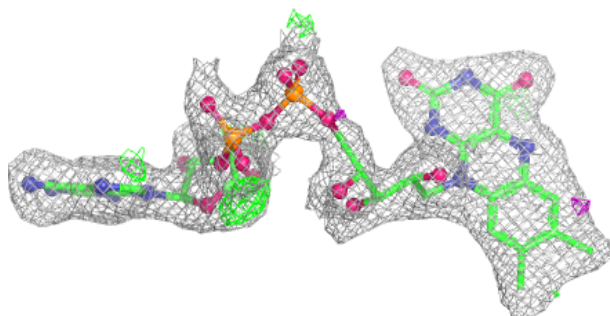
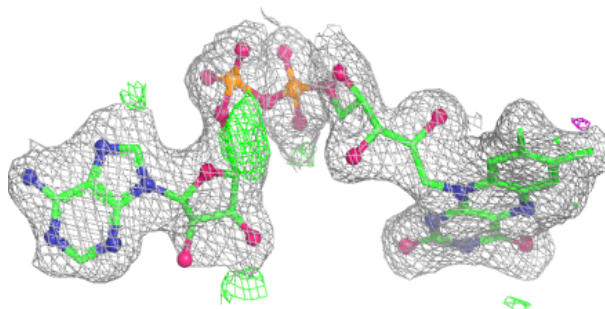
**Electron density around FAD F 500:**

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

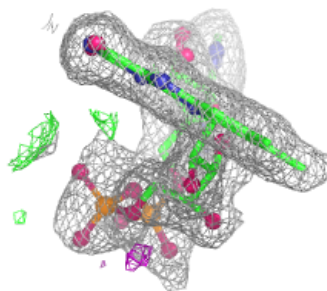
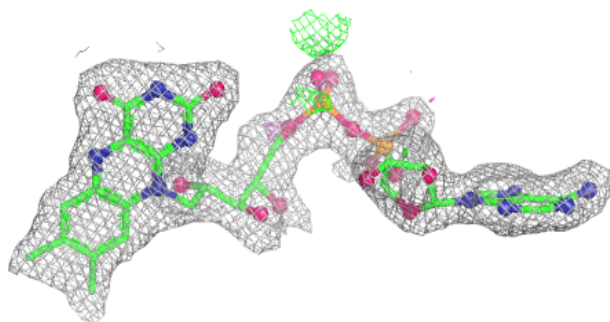
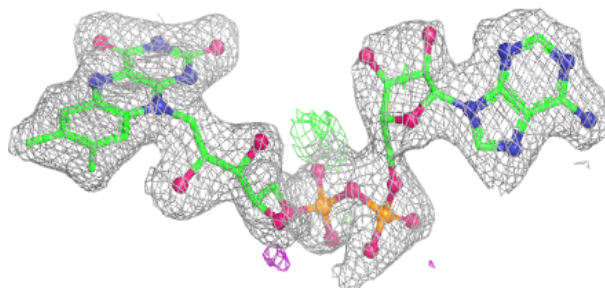


Electron density around FAD G 201:

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

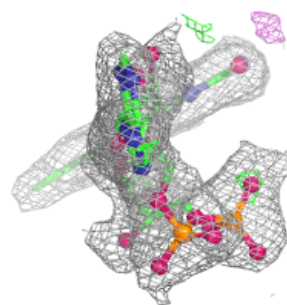
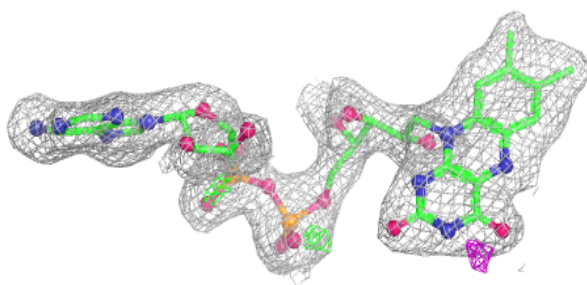
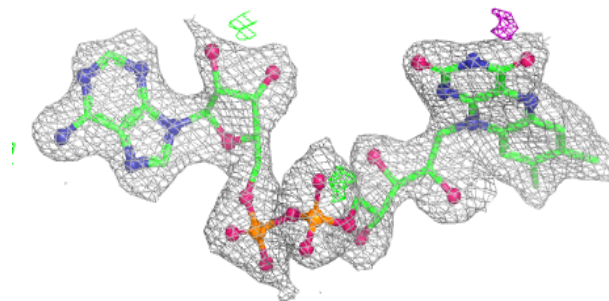
**Electron density around FAD H 201:**

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

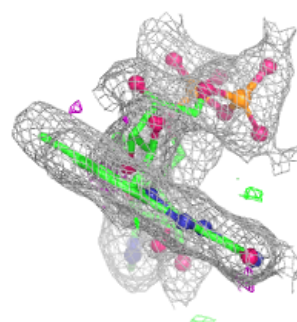
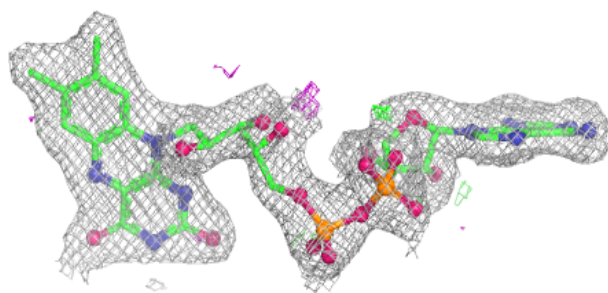
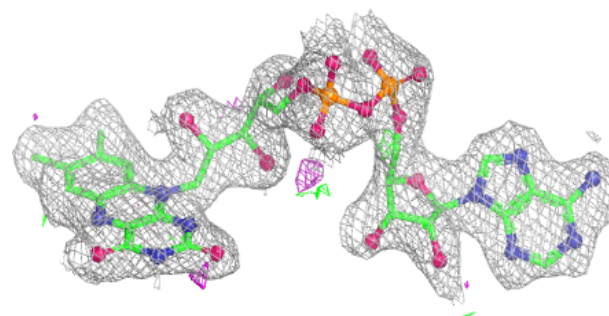


Electron density around FAD E 201:

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

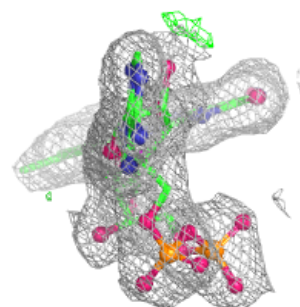
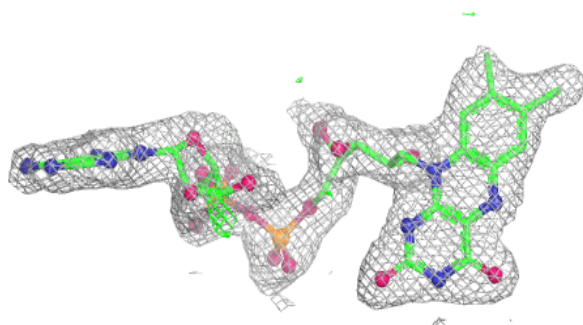
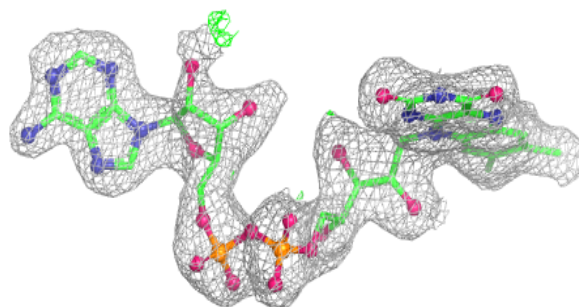
**Electron density around FAD K 500:**

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

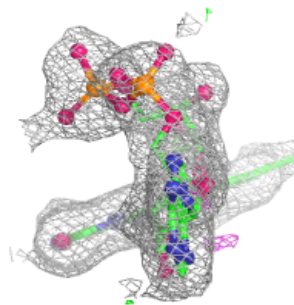
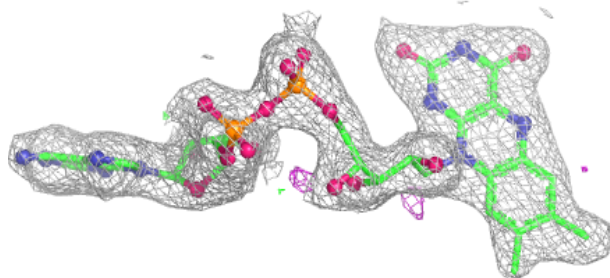
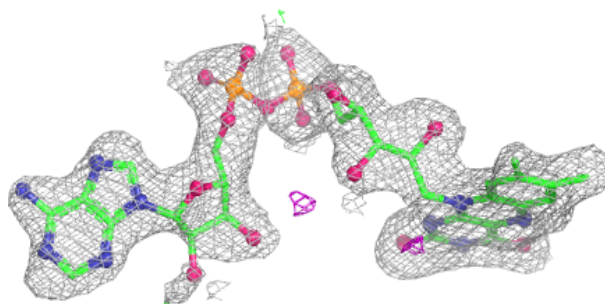


Electron density around FAD A 201:

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

**Electron density around FAD I 201:**

$2mF_o-DF_c$ (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.