



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 07:27 pm BST

PDB ID : 6U0S
Title : Crystal structure of the flavin-dependent monooxygenase PieE in complex with FAD and substrate
Authors : Shi, R.; Manenda, M.
Deposited on : 2019-08-14
Resolution : 2.52 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

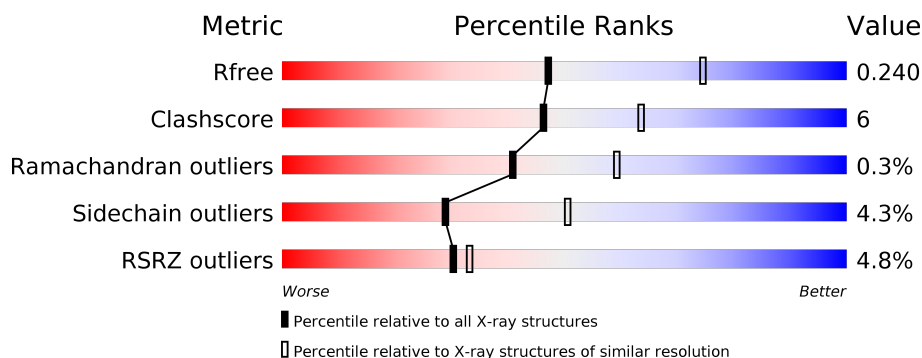
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 on 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	601	<div> <div>83%</div> <div>13%</div> <div>•</div> </div>
1	B	601	<div> <div>2%</div> <div>79%</div> <div>17%</div> <div>• •</div> </div>
1	C	601	<div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
1	D	601	<div> <div>9%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	E	601	<div> <div>3%</div> <div>82%</div> <div>14%</div> <div>•</div> </div>
1	F	601	<div> <div>13%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>

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	CL	D	603	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27918 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 2,4-dichlorophenol 6-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	B	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	C	580	Total	C	N	O	S	0	0	0
			4430	2768	829	823	10			
1	D	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	E	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	F	580	Total	C	N	O	S	0	0	0
			4427	2765	829	823	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP W0C4C9
A	-1	SER	-	expression tag	UNP W0C4C9
A	0	HIS	-	expression tag	UNP W0C4C9
B	-2	GLY	-	expression tag	UNP W0C4C9
B	-1	SER	-	expression tag	UNP W0C4C9
B	0	HIS	-	expression tag	UNP W0C4C9
C	-2	GLY	-	expression tag	UNP W0C4C9
C	-1	SER	-	expression tag	UNP W0C4C9
C	0	HIS	-	expression tag	UNP W0C4C9
D	-2	GLY	-	expression tag	UNP W0C4C9
D	-1	SER	-	expression tag	UNP W0C4C9
D	0	HIS	-	expression tag	UNP W0C4C9
E	-2	GLY	-	expression tag	UNP W0C4C9
E	-1	SER	-	expression tag	UNP W0C4C9
E	0	HIS	-	expression tag	UNP W0C4C9
F	-2	GLY	-	expression tag	UNP W0C4C9
F	-1	SER	-	expression tag	UNP W0C4C9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP W0C4C9

-
- The chemical structure of FAD (Flavin Adenine Dinucleotide) is shown. It consists of a flavin isoalloxazine ring system (top) connected via a ribitol chain (middle) to an adenine ring system (bottom). The flavin ring is labeled with N1A, N3A, C2A, C4A, C6A, C8A, N7A, and C8A. The ribitol chain is labeled with C1B, C2B, C3B, C4B, C5B, and C6B. The adenine ring is labeled with N1B, N3B, C2B, C4B, C6B, C8B, N7B, and C8B. The structure is color-coded: blue for nitrogen atoms, red for oxygen atoms, and green for carbon atoms. The ribitol chain is shown in a zig-zag conformation, and the adenine ring is shown in a planar conformation.

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | D | 2 | Total Cl
2 2 | 0 | 0 |
| 3 | E | 2 | Total Cl
2 2 | 0 | 0 |

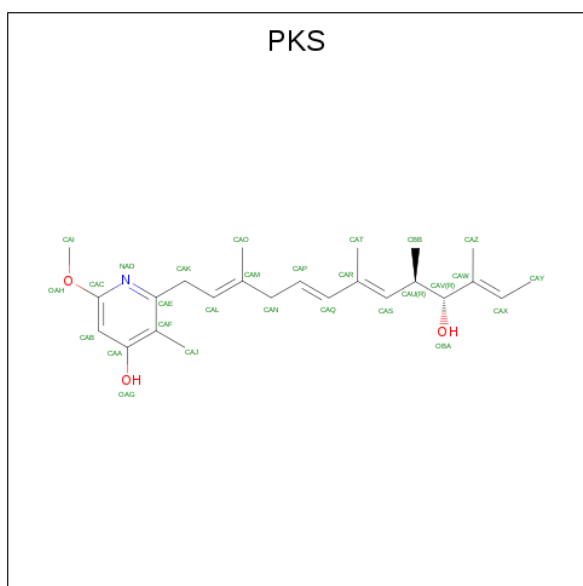


WORLD WIDE
PDB
PROTEIN DATA BANK

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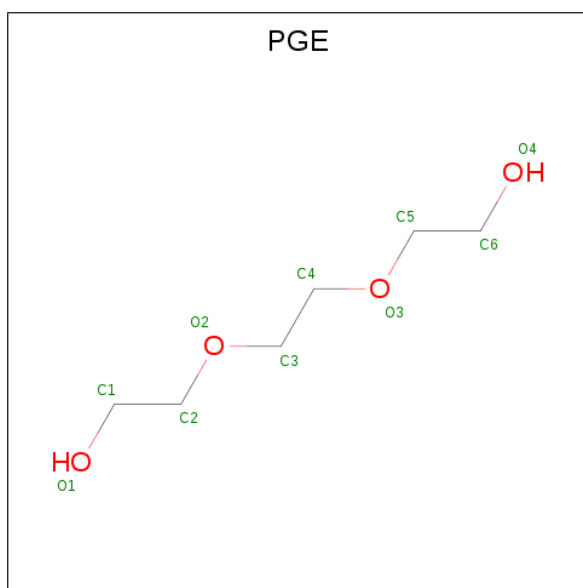
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		
3	A	2	Total	Cl	0	0
			2	2		
3	F	2	Total	Cl	0	0
			2	2		

- Molecule 4 is 2-[(2E,5E,7E,9R,10R,11E)-10-hydroxy-3,7,9,11-tetramethyltrideca-2,5,7,11-tetraen-1-yl]-6-methoxy-3-methylpyridin-4-ol (three-letter code: PKS) (formula: C₂₄H₃₅NO₃) (labeled as "Ligand of Interest" by author).



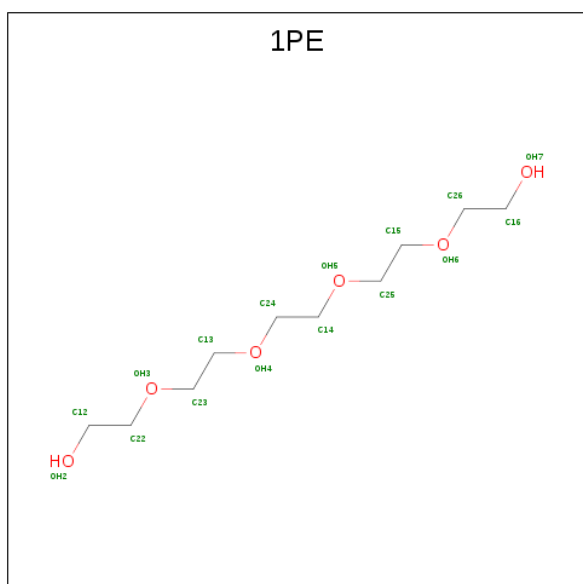
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	24	1	3		
4	B	1	Total	C	N	O	0	0
			28	24	1	3		
4	C	1	Total	C	N	O	0	0
			28	24	1	3		
4	D	1	Total	C	N	O	0	0
			28	24	1	3		
4	E	1	Total	C	N	O	0	0
			28	24	1	3		
4	F	1	Total	C	N	O	0	0
			28	24	1	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



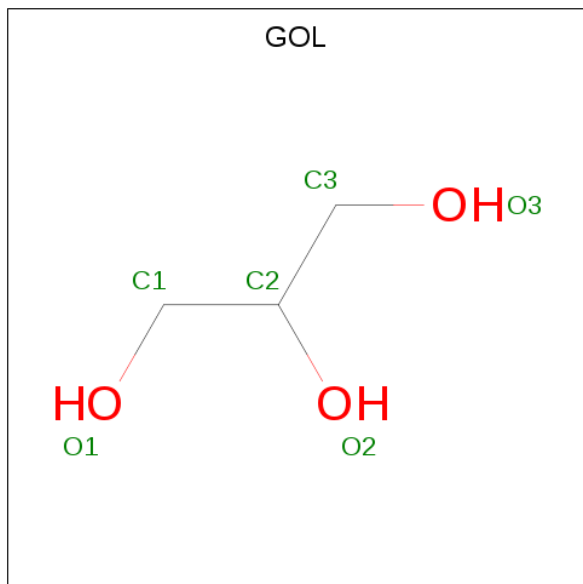
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	B	1	Total	C	O	0	0
			16	10	6		
6	C	1	Total	C	O	0	0
			16	10	6		
6	D	1	Total	C	O	0	0
			16	10	6		
6	E	1	Total	C	O	0	0
			16	10	6		
6	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

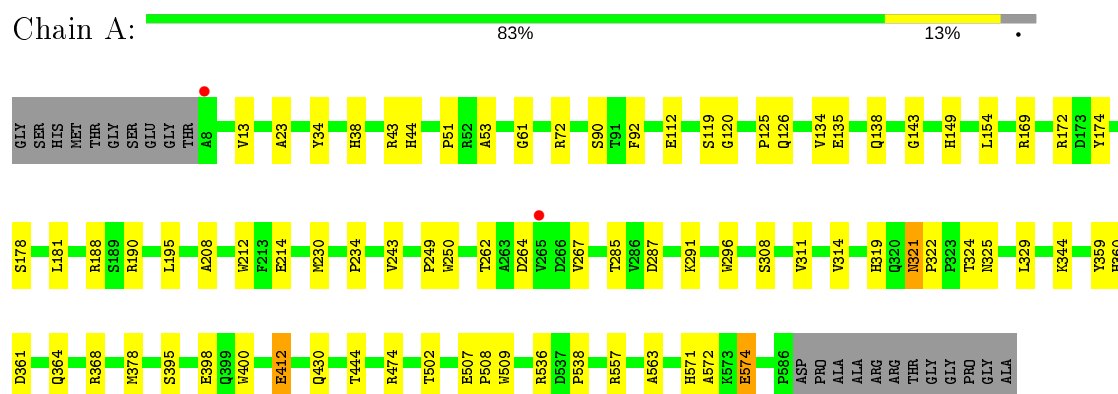
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	177	Total 177	O 177	0	0
8	B	113	Total 113	O 113	0	0
8	C	205	Total 205	O 205	0	0
8	D	88	Total 88	O 88	0	0
8	E	56	Total 56	O 56	0	0
8	F	61	Total 61	O 61	0	0

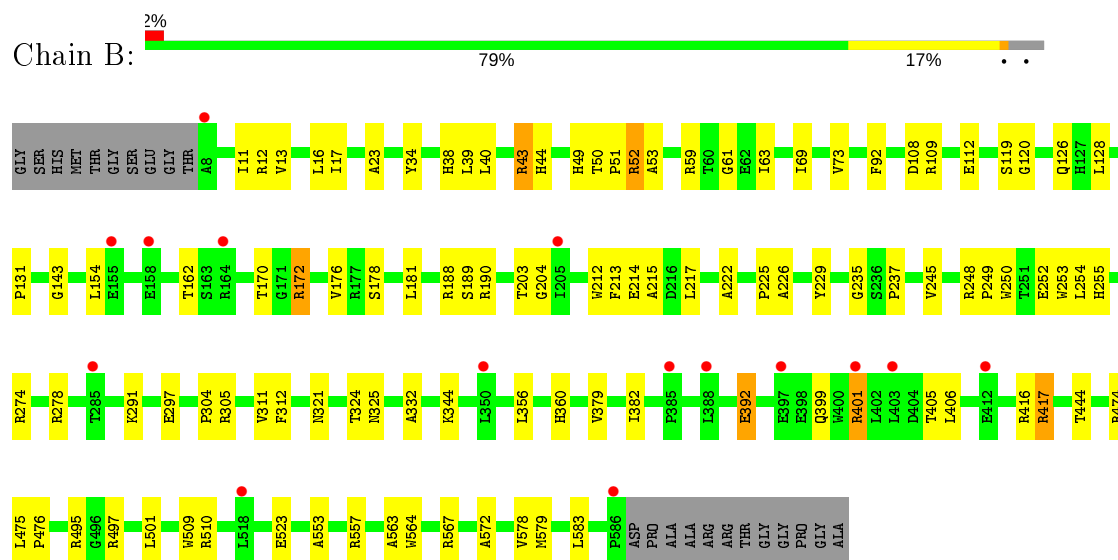
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

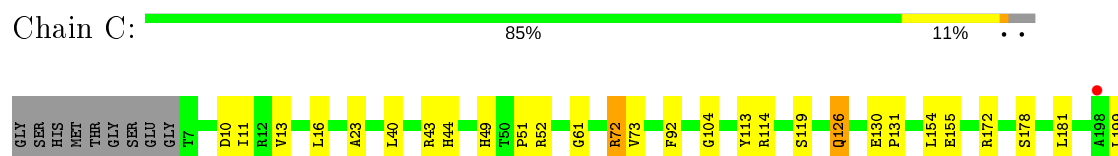
- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

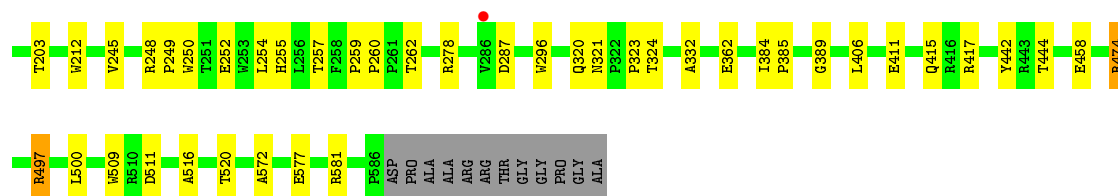


- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

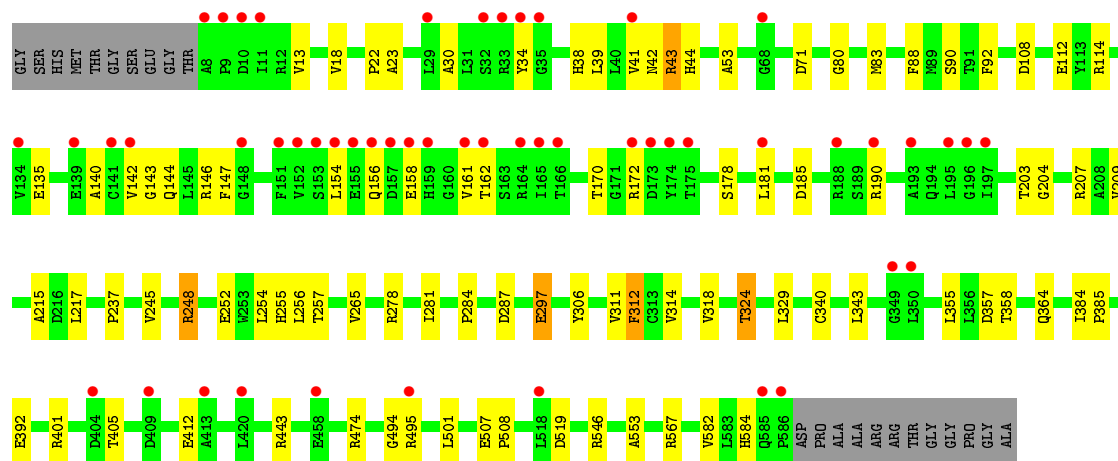
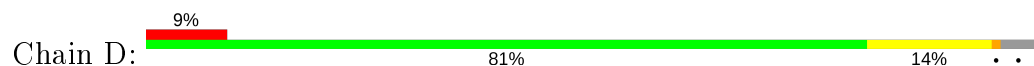


- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

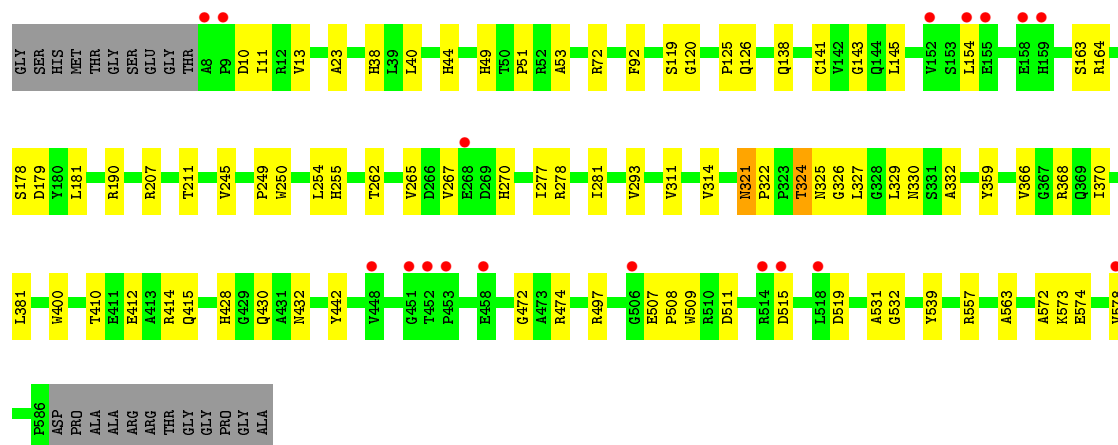
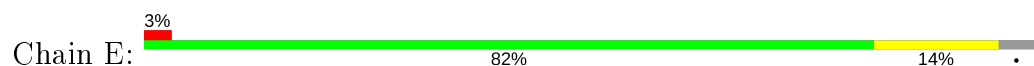




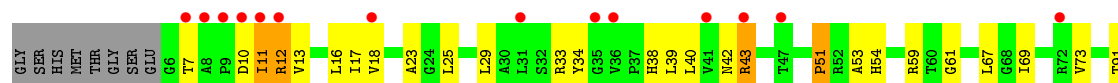
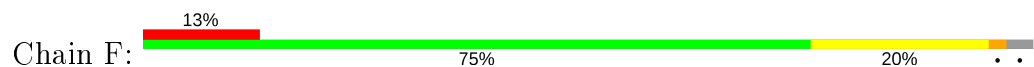
• Molecule 1: 2,4-dichlorophenol 6-monooxygenase

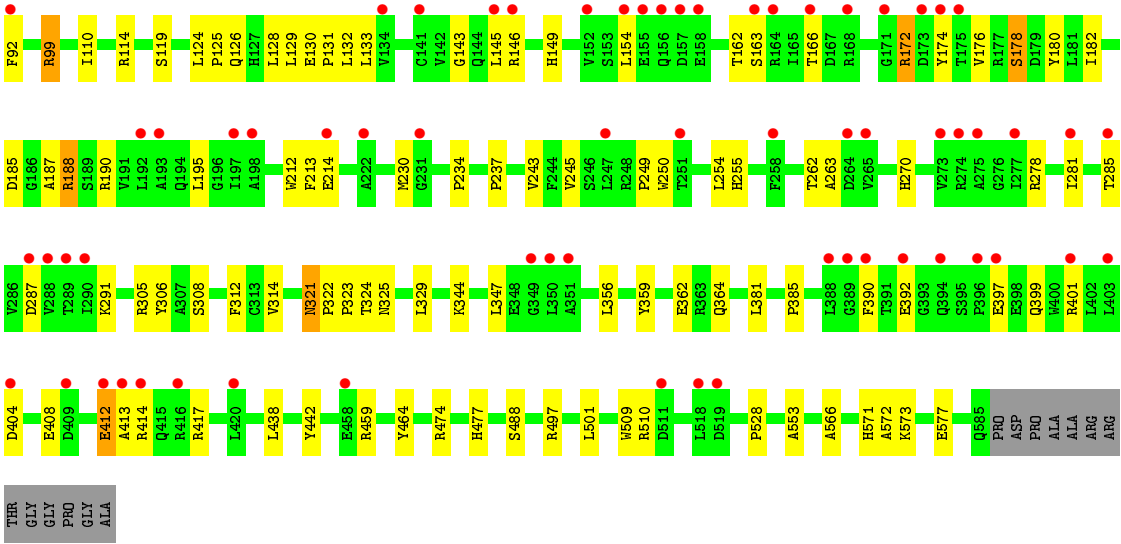


• Molecule 1: 2,4-dichlorophenol 6-monooxygenase



• Molecule 1: 2,4-dichlorophenol 6-monooxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.34Å 187.13Å 239.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.52 49.12 – 2.52	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.12-2.52) 100.0 (49.12-2.52)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.239 0.187 , 0.240	Depositor DCC
R_{free} test set	6860 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27918	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, CL, 1PE, PKS, FAD

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	0.38	0/4537	0.78	0/6194
1	B	0.38	0/4537	0.74	0/6194
1	C	0.41	0/4544	0.77	0/6204
1	D	0.38	0/4537	0.74	0/6194
1	E	0.35	0/4537	0.71	0/6194
1	F	0.34	0/4540	0.72	0/6197
All	All	0.37	0/27232	0.74	0/37177

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4423	0	4297	47	0
1	B	4423	0	4297	63	0
1	C	4430	0	4304	39	0
1	D	4423	0	4297	63	0
1	E	4423	0	4297	42	0
1	F	4427	0	4300	81	0
2	A	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	5	0
2	C	53	0	31	5	0
2	D	53	0	31	14	0
2	E	53	0	31	5	0
2	F	53	0	31	8	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	3	0
3	E	2	0	0	0	0
3	F	2	0	0	1	0
4	A	28	0	0	1	0
4	B	28	0	0	0	0
4	C	28	0	0	0	0
4	D	28	0	0	1	0
4	E	28	0	0	0	0
4	F	28	0	0	1	0
5	A	10	0	14	0	0
5	C	20	0	28	0	0
5	E	10	0	14	0	0
6	A	16	0	22	2	0
6	B	16	0	22	2	0
6	C	16	0	22	2	0
6	D	16	0	22	0	0
6	E	16	0	22	3	0
6	F	16	0	22	0	0
7	A	12	0	16	1	0
7	D	12	0	16	1	0
7	E	12	0	16	0	0
8	A	177	0	0	5	0
8	B	113	0	0	3	0
8	C	205	0	0	4	0
8	D	88	0	0	4	0
8	E	56	0	0	2	0
8	F	61	0	0	3	0
All	All	27918	0	26214	338	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 6.

The worst 5 of 338 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:F:53:ALA:HB2	2:F:601:FAD:O2'	1.71	0.91
1:C:44:HIS:HD2	2:C:702:FAD:O2B	1.54	0.90
1:C:44:HIS:CD2	2:C:702:FAD:O2B	2.27	0.88
1:F:146:ARG:HD3	1:F:149:HIS:CE1	2.09	0.88
1:F:34:TYR:HB3	1:F:344:LYS:HD2	1.58	0.86

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	577/601 (96%)	559 (97%)	17 (3%)	1 (0%)	47	67
1	B	577/601 (96%)	551 (96%)	25 (4%)	1 (0%)	47	67
1	C	578/601 (96%)	563 (97%)	15 (3%)	0	100	100
1	D	577/601 (96%)	550 (95%)	25 (4%)	2 (0%)	41	59
1	E	577/601 (96%)	549 (95%)	25 (4%)	3 (0%)	29	47
1	F	578/601 (96%)	546 (94%)	28 (5%)	4 (1%)	22	37
All	All	3464/3606 (96%)	3318 (96%)	135 (4%)	11 (0%)	41	59

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	262	THR
1	F	263	ALA
1	E	532	GLY
1	F	7	THR
1	A	90	SER

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	447/460 (97%)	432 (97%)	15 (3%)	37	61
1	B	447/460 (97%)	426 (95%)	21 (5%)	26	46
1	C	448/460 (97%)	430 (96%)	18 (4%)	31	54
1	D	447/460 (97%)	432 (97%)	15 (3%)	37	61
1	E	447/460 (97%)	422 (94%)	25 (6%)	21	38
1	F	447/460 (97%)	425 (95%)	22 (5%)	25	45
All	All	2683/2760 (97%)	2567 (96%)	116 (4%)	29	50

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	500	LEU
1	D	324	THR
1	F	287	ASP
1	D	43	ARG
1	D	203	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	299	ASN
1	D	123	ASN
1	F	81	HIS
1	C	320	GLN
1	C	360	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 11 are monoatomic - leaving 28 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	$\# Z > 2$
6	1PE	D	605	-	15,15,15	0.60	0	14,14,14	0.30	0
7	GOL	D	601	-	5,5,5	0.18	0	5,5,5	0.46	0
4	PKS	B	603	-	28,28,28	1.99	8 (28%)	35,37,37	2.23	10 (28%)
6	1PE	A	605	-	15,15,15	0.52	0	14,14,14	0.48	0
2	FAD	B	601	-	51,58,58	2.37	9 (17%)	60,89,89	1.73	12 (20%)
2	FAD	F	601	-	51,58,58	2.28	10 (19%)	60,89,89	2.02	10 (16%)
6	1PE	C	705	-	15,15,15	0.67	0	14,14,14	0.61	0
4	PKS	D	604	-	28,28,28	2.34	9 (32%)	35,37,37	1.80	7 (20%)
4	PKS	F	603	-	28,28,28	2.07	5 (17%)	35,37,37	2.29	8 (22%)
6	1PE	B	604	-	15,15,15	0.58	0	14,14,14	0.42	0
5	PGE	C	704	-	9,9,9	0.28	0	8,8,8	0.16	0
7	GOL	A	608	-	5,5,5	0.11	0	5,5,5	0.25	0
4	PKS	C	703	-	28,28,28	2.29	8 (28%)	35,37,37	2.23	13 (37%)
5	PGE	A	604	-	9,9,9	0.27	0	8,8,8	0.18	0
7	GOL	A	607	-	5,5,5	0.13	0	5,5,5	0.33	0
5	PGE	C	701	-	9,9,9	0.31	0	8,8,8	0.16	0
4	PKS	E	603	-	28,28,28	2.05	8 (28%)	35,37,37	2.17	8 (22%)
2	FAD	A	601	-	51,58,58	2.72	10 (19%)	60,89,89	1.89	16 (26%)
7	GOL	E	608	-	5,5,5	0.15	0	5,5,5	0.50	0
6	1PE	E	605	-	15,15,15	0.59	0	14,14,14	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	E	601	-	51,58,58	2.30	8 (15%)	60,89,89	1.86	12 (20%)
2	FAD	D	602	-	51,58,58	2.29	9 (17%)	60,89,89	1.77	12 (20%)
5	PGE	E	604	-	9,9,9	0.34	0	8,8,8	0.18	0
6	1PE	F	604	-	15,15,15	0.65	0	14,14,14	0.39	0
7	GOL	D	607	-	5,5,5	0.12	0	5,5,5	0.39	0
4	PKS	A	603	-	28,28,28	2.48	9 (32%)	35,37,37	2.65	16 (45%)
7	GOL	E	607	-	5,5,5	0.16	0	5,5,5	0.53	0
2	FAD	C	702	-	51,58,58	2.50	11 (21%)	60,89,89	2.26	14 (23%)

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
6	1PE	D	605	-	-	9/13/13/13	-
7	GOL	D	601	-	-	4/4/4/4	-
4	PKS	B	603	-	-	4/27/27/27	0/1/1/1
6	1PE	A	605	-	-	7/13/13/13	-
2	FAD	B	601	-	-	13/30/50/50	0/6/6/6
2	FAD	F	601	-	-	4/30/50/50	0/6/6/6
6	1PE	C	705	-	-	7/13/13/13	-
4	PKS	D	604	-	-	10/27/27/27	0/1/1/1
4	PKS	F	603	-	-	9/27/27/27	0/1/1/1
6	1PE	B	604	-	-	10/13/13/13	-
5	PGE	C	704	-	-	3/7/7/7	-
7	GOL	A	608	-	-	4/4/4/4	-
4	PKS	C	703	-	-	11/27/27/27	0/1/1/1
5	PGE	A	604	-	-	5/7/7/7	-
7	GOL	A	607	-	-	4/4/4/4	-
5	PGE	C	701	-	-	4/7/7/7	-
4	PKS	E	603	-	-	10/27/27/27	0/1/1/1
2	FAD	A	601	-	-	7/30/50/50	0/6/6/6
7	GOL	E	608	-	-	4/4/4/4	-
6	1PE	E	605	-	-	12/13/13/13	-
2	FAD	E	601	-	-	4/30/50/50	0/6/6/6
2	FAD	D	602	-	-	9/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	E	604	-	-	3/7/7/7	-
6	1PE	F	604	-	-	10/13/13/13	-
7	GOL	D	607	-	-	4/4/4/4	-
4	PKS	A	603	-	-	9/27/27/27	0/1/1/1
7	GOL	E	607	-	-	0/4/4/4	-
2	FAD	C	702	-	-	9/30/50/50	0/6/6/6

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-C10	14.47	1.53	1.38
2	C	702	FAD	C4X-C10	12.51	1.51	1.38
2	B	601	FAD	C4X-C10	12.40	1.51	1.38
2	E	601	FAD	C4X-C10	12.29	1.51	1.38
2	F	601	FAD	C4X-C10	11.55	1.50	1.38

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	FAD	C4-N3-C2	9.60	123.25	115.14
4	A	603	PKS	CAN-CAP-CAQ	-8.90	110.35	124.18
2	F	601	FAD	C4-N3-C2	7.75	121.68	115.14
4	C	703	PKS	CAP-CAQ-CAR	-7.07	115.20	125.89
2	D	602	FAD	C4-N3-C2	6.74	120.83	115.14

There are no chirality outliers.

5 of 189 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	601	GOL	O1-C1-C2-C3
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	B	601	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 55 short contacts:

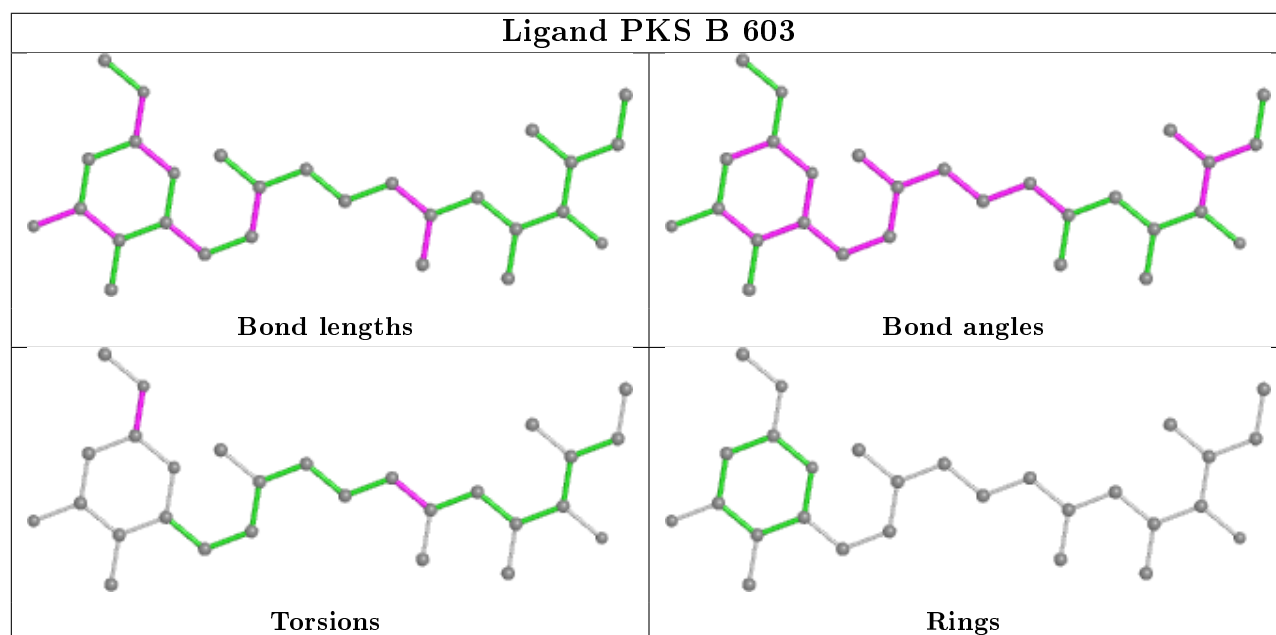
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	605	1PE	2	0

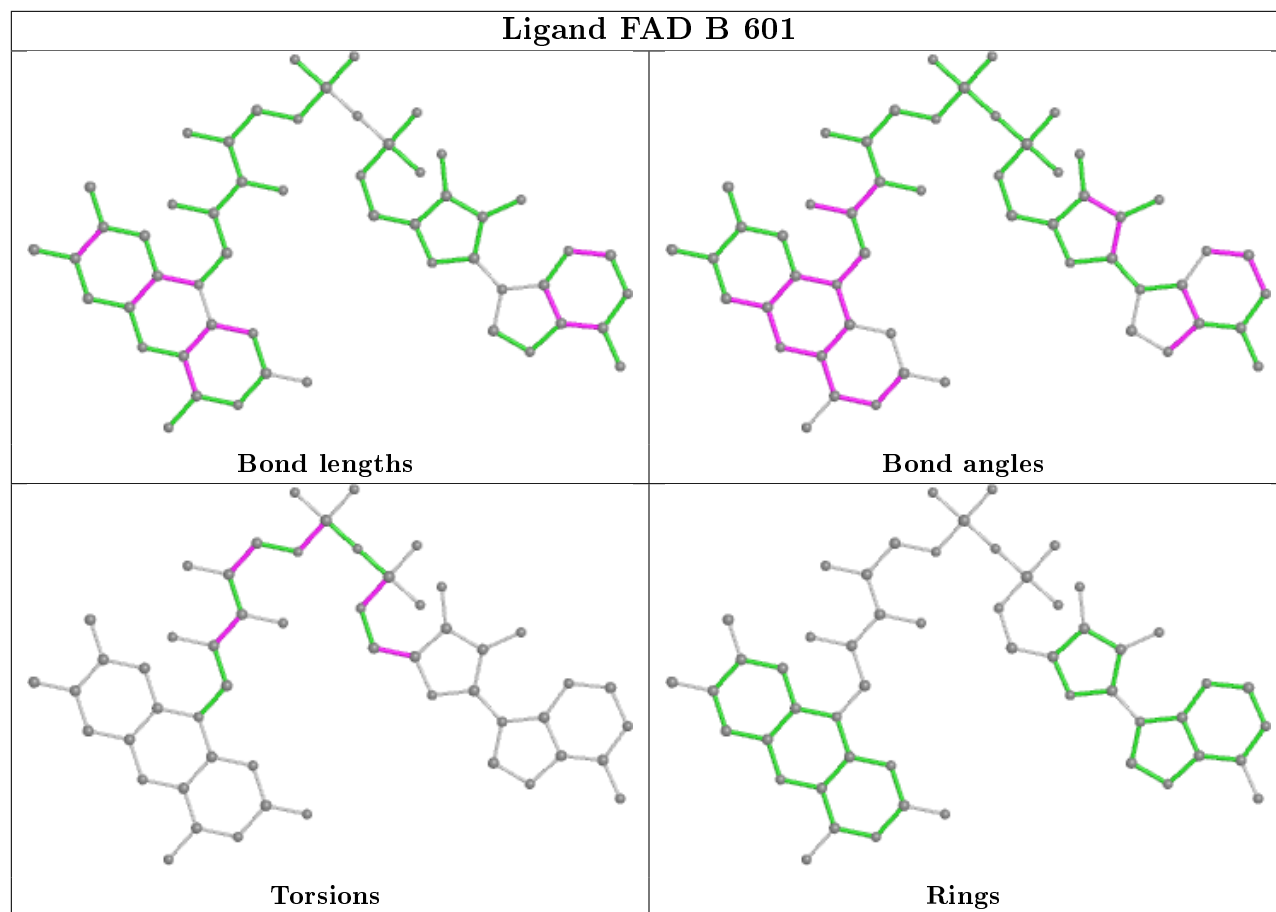
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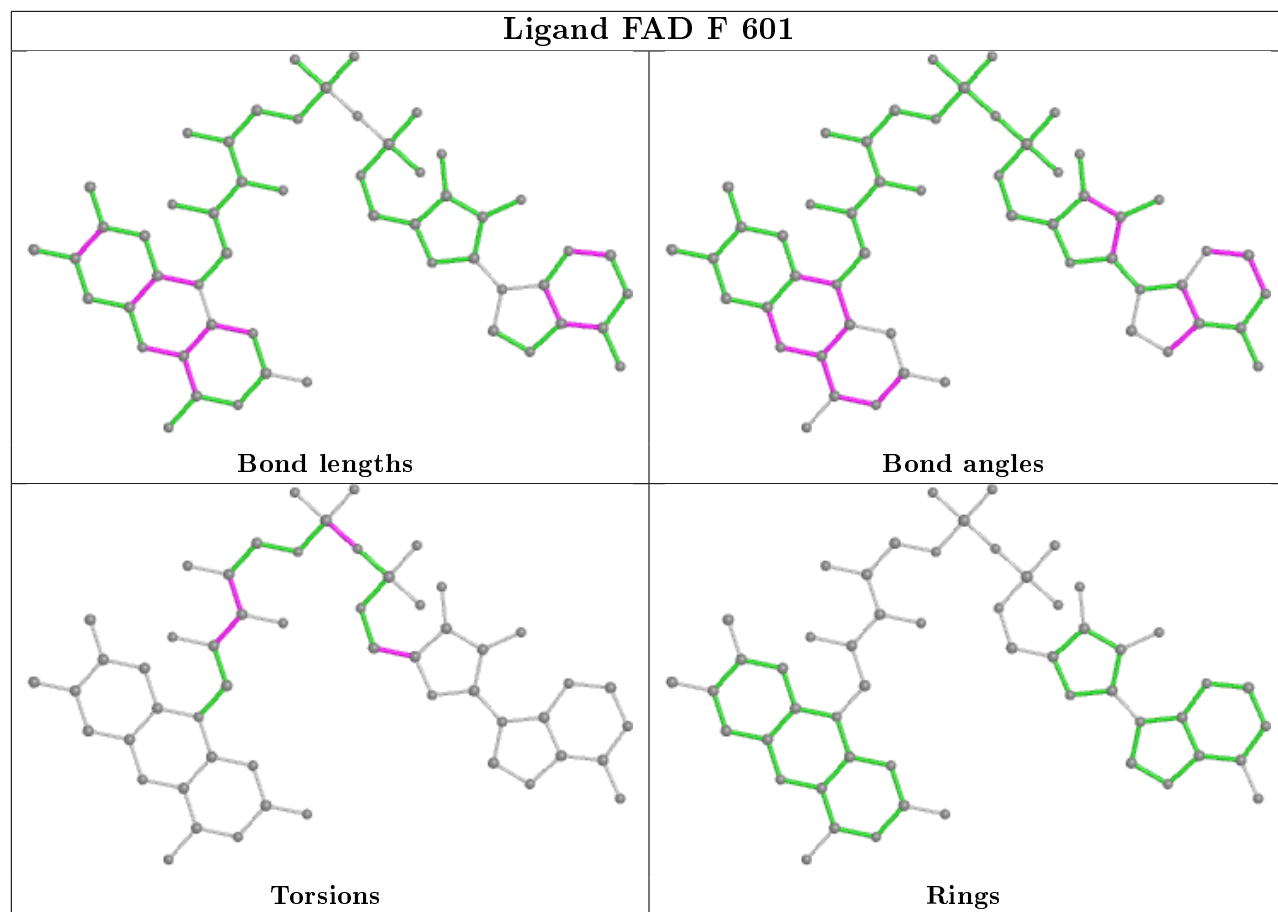
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	5	0
2	F	601	FAD	8	0
6	C	705	1PE	2	0
4	D	604	PKS	1	0
4	F	603	PKS	1	0
6	B	604	1PE	2	0
7	A	608	GOL	1	0
2	A	601	FAD	4	0
6	E	605	1PE	3	0
2	E	601	FAD	5	0
2	D	602	FAD	14	0
7	D	607	GOL	1	0
4	A	603	PKS	1	0
2	C	702	FAD	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

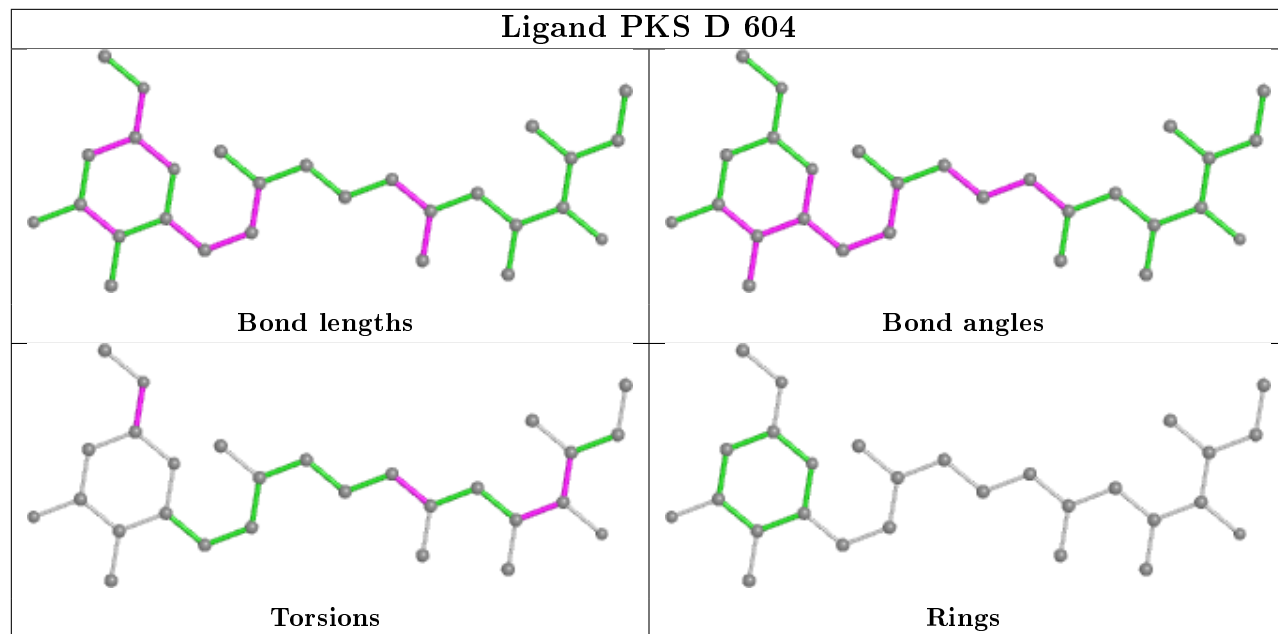


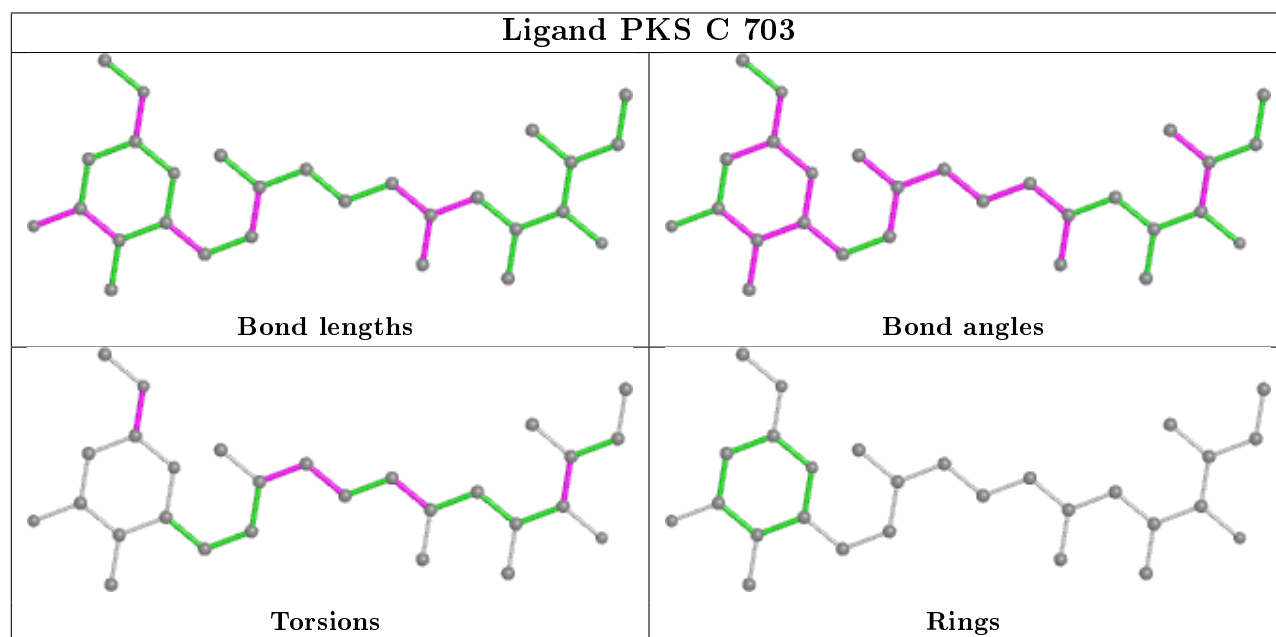
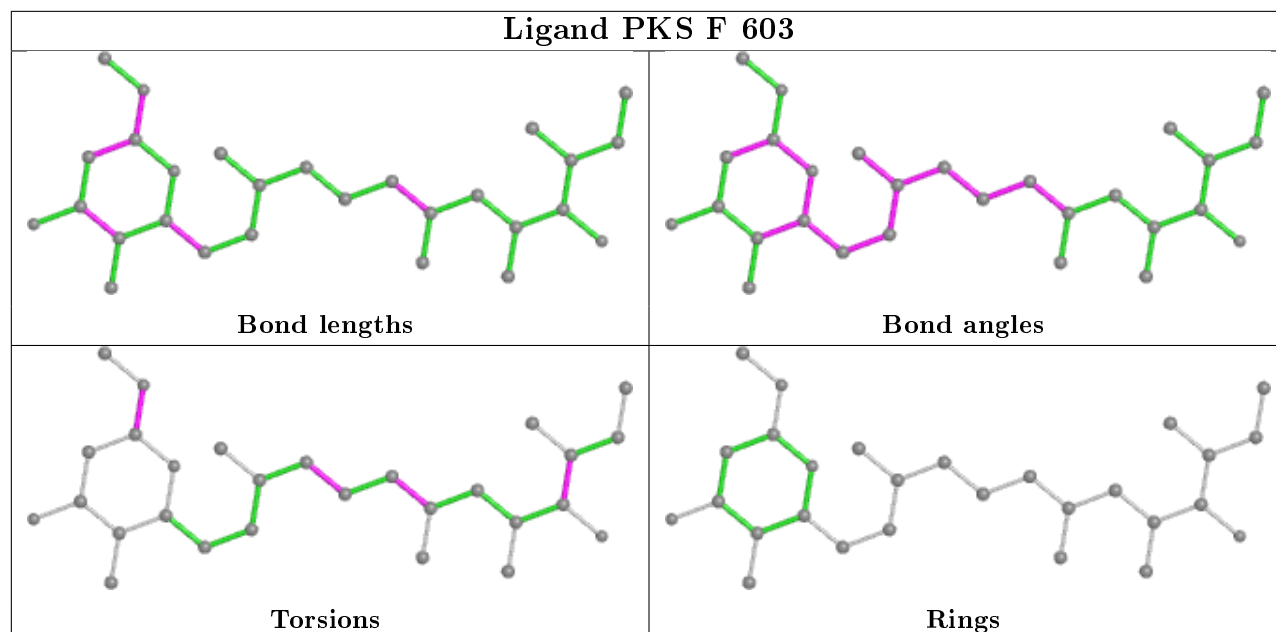


Ligand FAD F 601

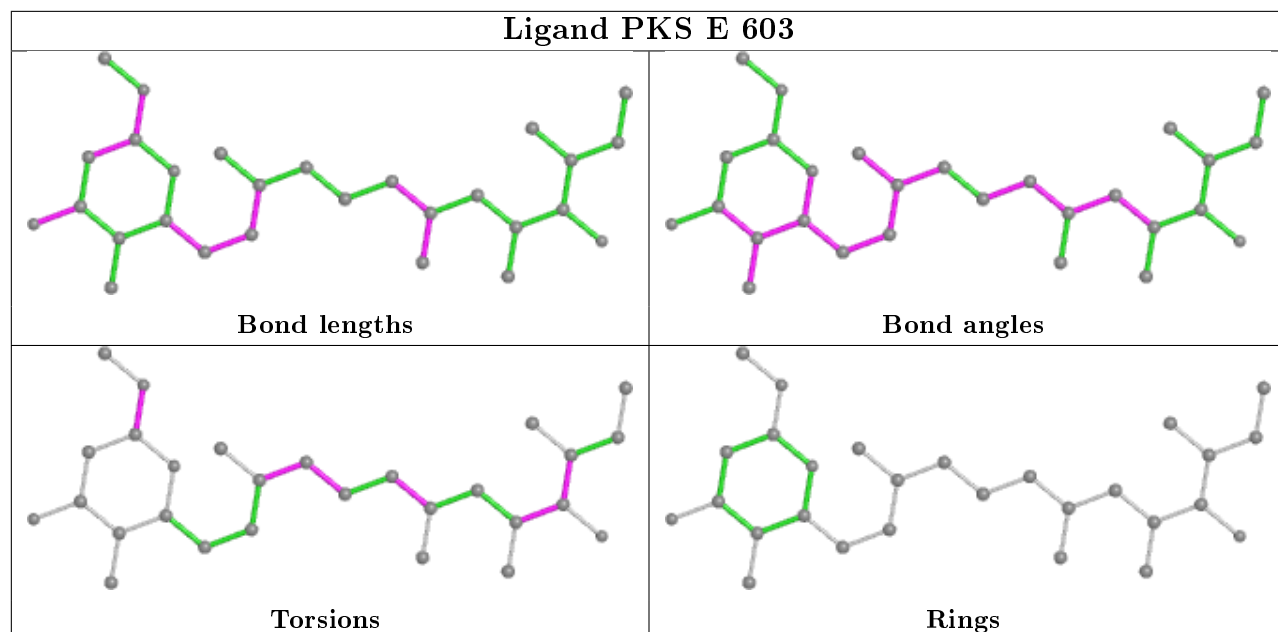


Ligand PKS D 604

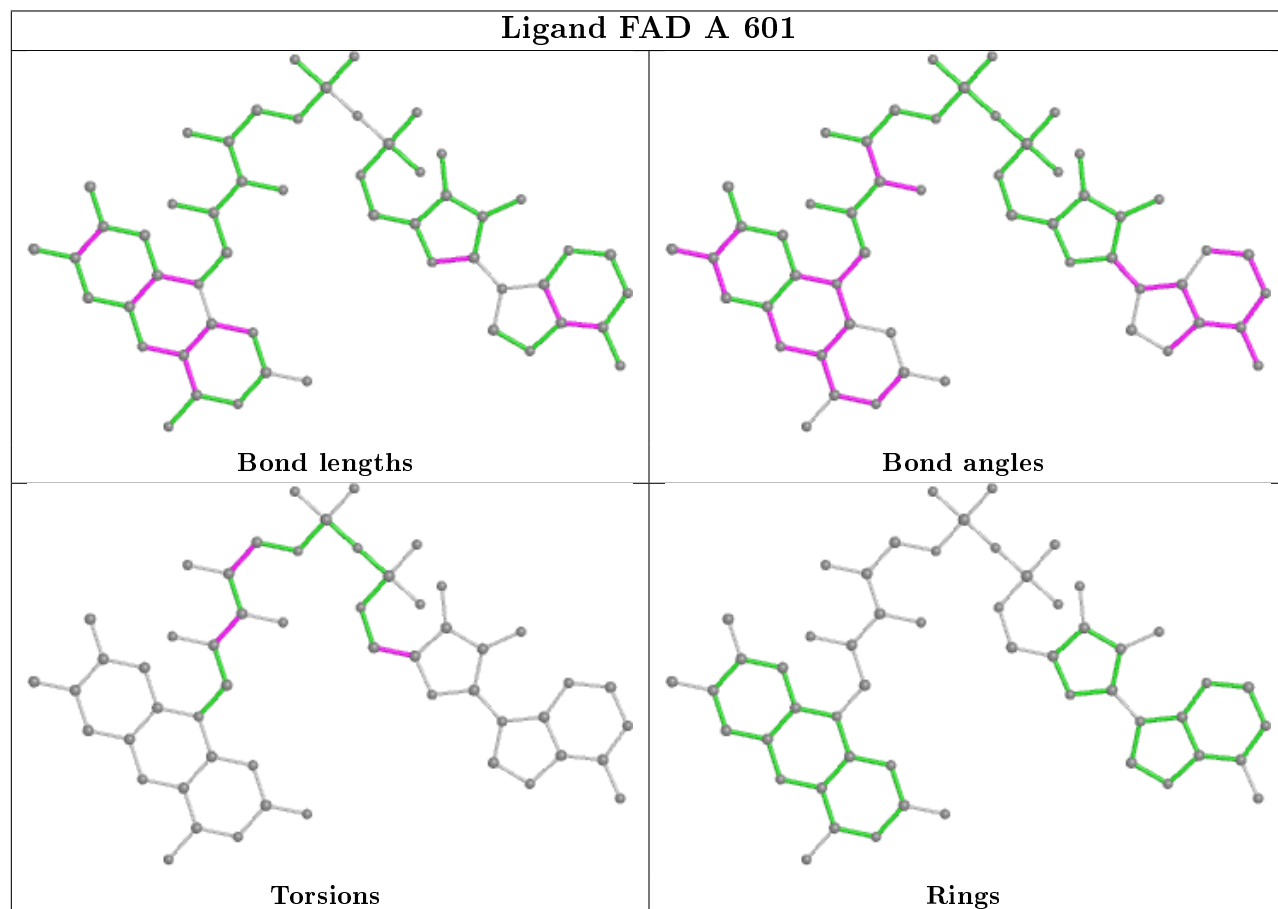




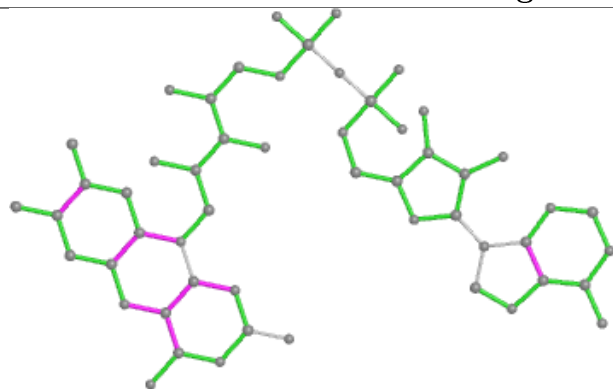
Ligand PKS E 603



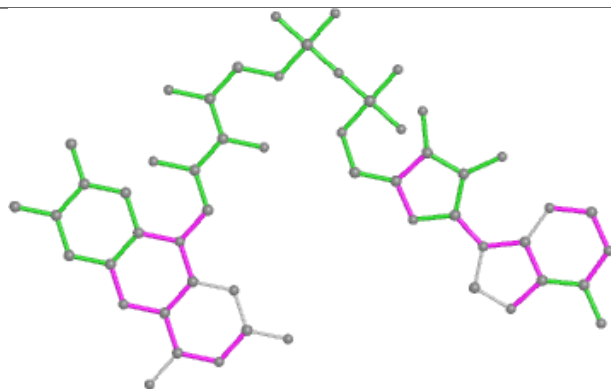
Ligand FAD A 601



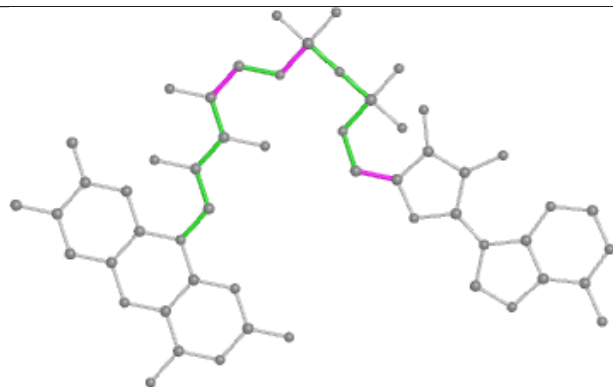
Ligand FAD E 601



Bond lengths



Bond angles

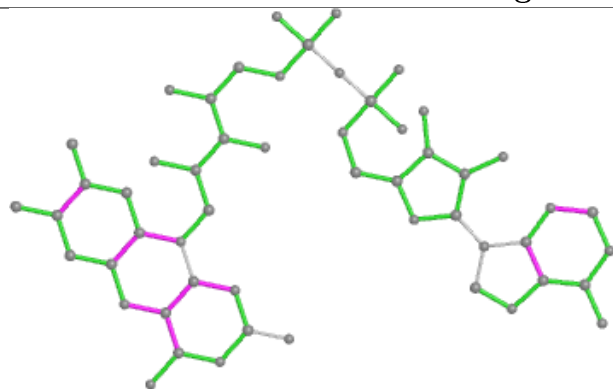


Torsions

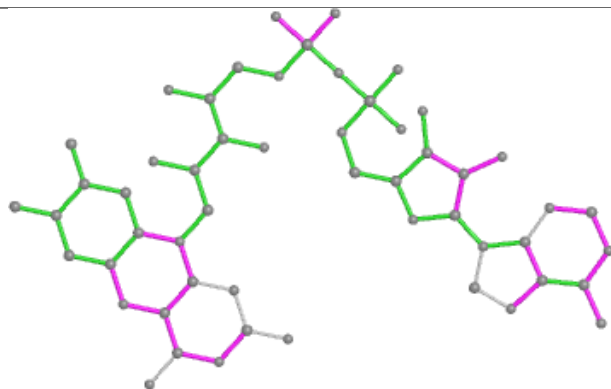


Rings

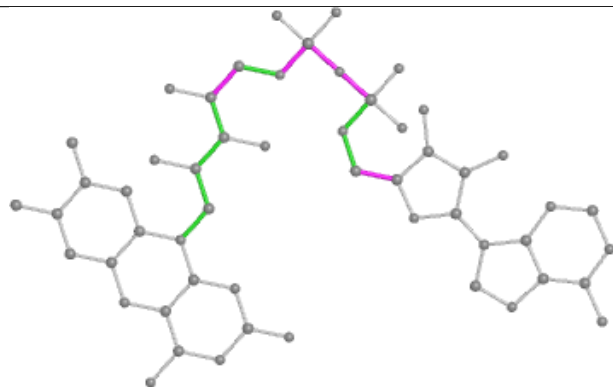
Ligand FAD D 602



Bond lengths



Bond angles

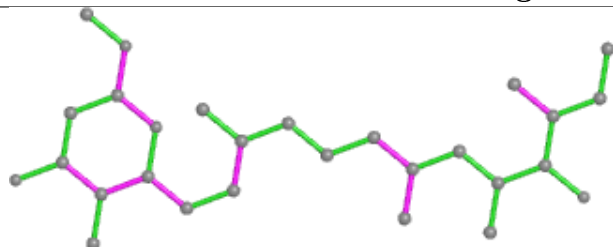


Torsions

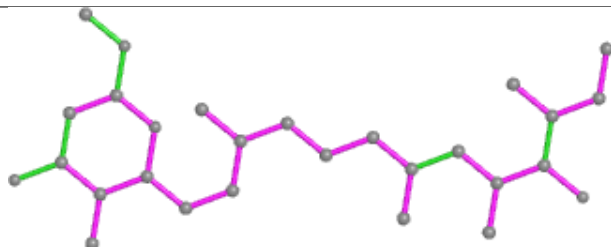


Rings

Ligand PKS A 603



Bond lengths



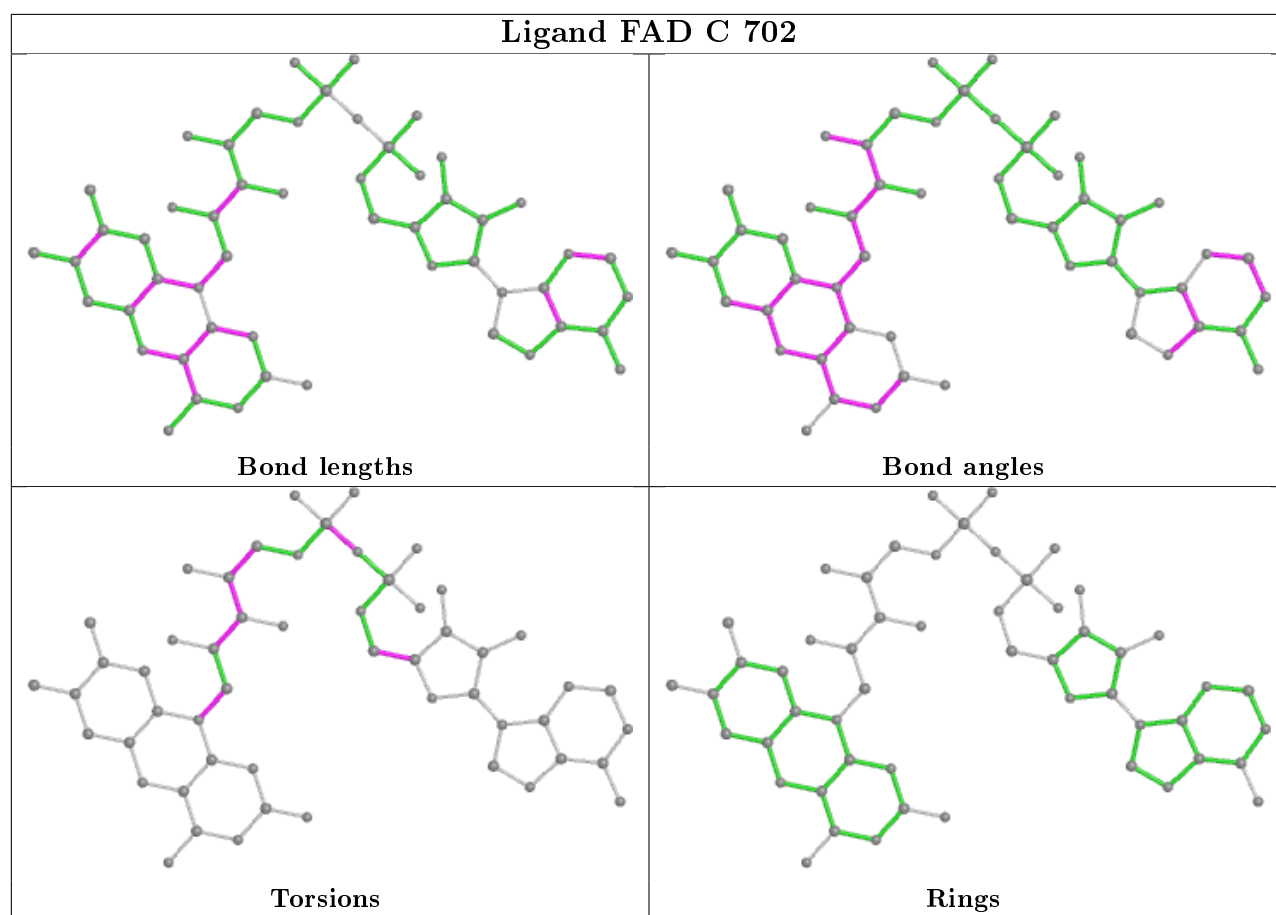
Bond angles



Torsions



Rings



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	579/601 (96%)	-0.25	2 (0%) 94 94	22, 40, 69, 104	0
1	B	579/601 (96%)	0.01	15 (2%) 56 59	24, 51, 87, 115	0
1	C	580/601 (96%)	-0.20	2 (0%) 94 94	24, 39, 70, 107	0
1	D	579/601 (96%)	0.43	52 (8%) 9 9	27, 61, 97, 137	0
1	E	579/601 (96%)	0.06	18 (3%) 49 53	33, 55, 93, 116	0
1	F	580/601 (96%)	0.66	78 (13%) 3 3	31, 71, 111, 142	0
All	All	3476/3606 (96%)	0.12	167 (4%) 30 33	22, 50, 95, 142	0

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	403	LEU	8.3
1	F	158	GLU	5.8
1	F	388	LEU	5.6
1	F	171	GLY	5.6
1	F	134	VAL	5.4

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 carbohydrates 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.

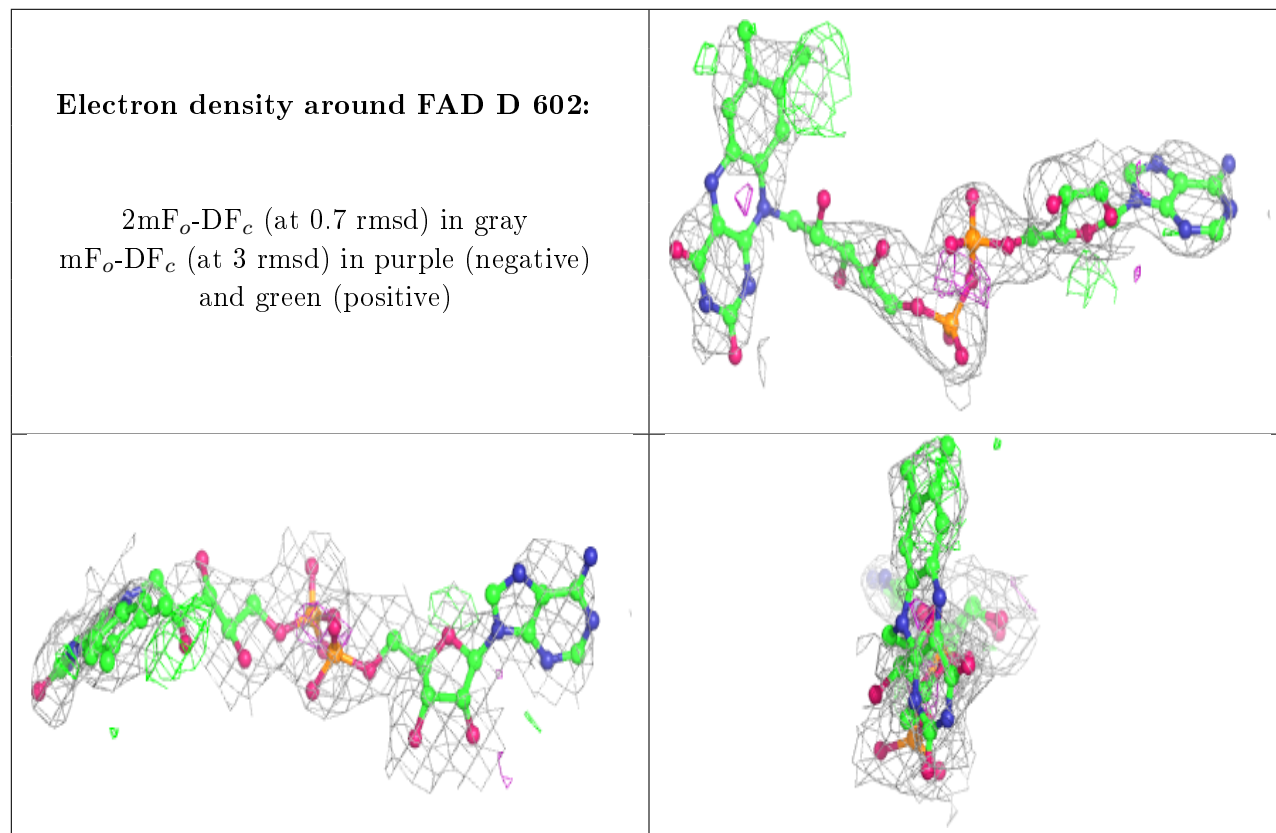
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	D	607	6/6	0.77	0.25	61,77,81,83	0
2	FAD	D	602	53/53	0.83	0.22	60,88,110,115	21
3	CL	F	605	1/1	0.84	0.21	83,83,83,83	0
6	1PE	E	605	16/16	0.84	0.19	70,80,84,88	0
6	1PE	F	604	16/16	0.86	0.18	68,85,93,100	0
5	PGE	E	604	10/10	0.87	0.28	56,61,68,70	0
7	GOL	D	601	6/6	0.88	0.21	51,56,60,68	0
6	1PE	A	605	16/16	0.88	0.23	63,75,83,88	0
2	FAD	F	601	53/53	0.88	0.22	77,104,114,118	21
5	PGE	A	604	10/10	0.88	0.22	54,57,74,81	0
7	GOL	E	608	6/6	0.88	0.21	60,74,80,80	0
7	GOL	E	607	6/6	0.88	0.19	70,78,82,86	0
3	CL	F	602	1/1	0.89	0.14	70,70,70,70	1
5	PGE	C	704	10/10	0.89	0.19	48,56,59,64	0
6	1PE	B	604	16/16	0.89	0.18	63,71,78,80	0
7	GOL	A	608	6/6	0.89	0.23	60,66,70,70	0
3	CL	D	606	1/1	0.89	0.25	78,78,78,78	0
6	1PE	D	605	16/16	0.91	0.16	59,66,86,87	0
5	PGE	C	701	10/10	0.91	0.18	55,73,83,86	0
2	FAD	E	601	53/53	0.92	0.18	52,71,84,90	21
2	FAD	B	601	53/53	0.92	0.18	48,67,84,86	21
7	GOL	A	607	6/6	0.92	0.24	59,72,73,75	0
6	1PE	C	705	16/16	0.92	0.18	57,66,82,85	0
2	FAD	A	601	53/53	0.93	0.16	37,52,66,67	21
3	CL	D	603	1/1	0.94	0.16	68,68,68,68	1
3	CL	B	605	1/1	0.94	0.29	65,65,65,65	0
2	FAD	C	702	53/53	0.94	0.17	46,65,94,96	0
3	CL	A	602	1/1	0.95	0.11	59,59,59,59	1
4	PKS	F	603	28/28	0.95	0.27	53,68,94,105	0
3	CL	E	602	1/1	0.95	0.12	59,59,59,59	1
3	CL	E	606	1/1	0.95	0.33	71,71,71,71	0
3	CL	C	706	1/1	0.95	0.22	72,72,72,72	0
3	CL	B	602	1/1	0.96	0.15	63,63,63,63	1
4	PKS	A	603	28/28	0.96	0.19	24,41,52,64	0
4	PKS	B	603	28/28	0.97	0.24	40,47,71,77	0
4	PKS	D	604	28/28	0.97	0.20	37,54,69,70	0
4	PKS	E	603	28/28	0.97	0.16	31,41,68,70	0

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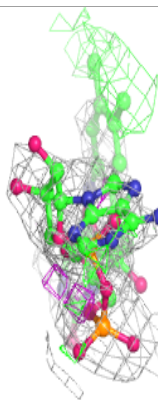
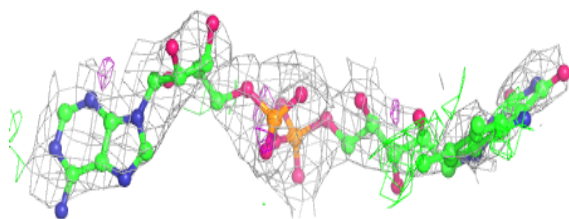
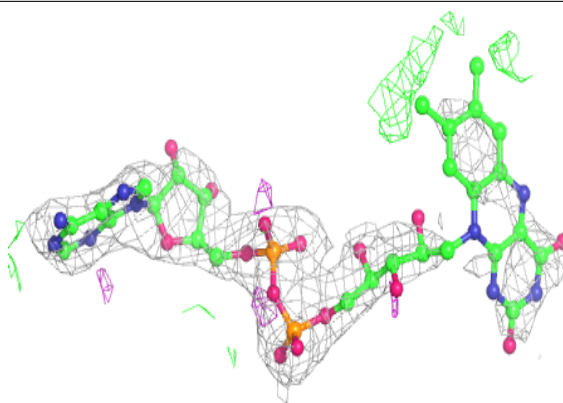
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PKS	C	703	28/28	0.98	0.18	23,32,60,61	0
3	CL	A	606	1/1	0.99	0.25	64,64,64,64	0

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.

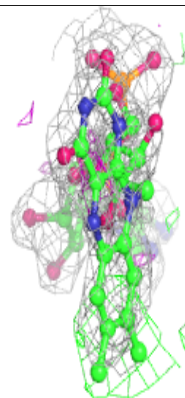
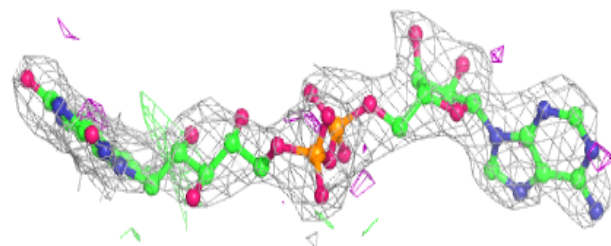
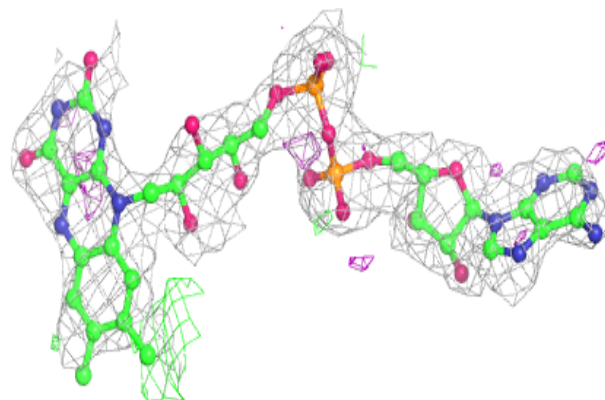


Electron density around FAD F 601:

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

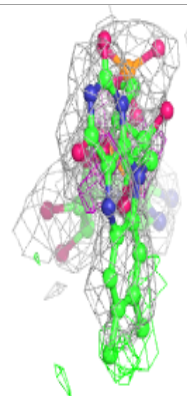
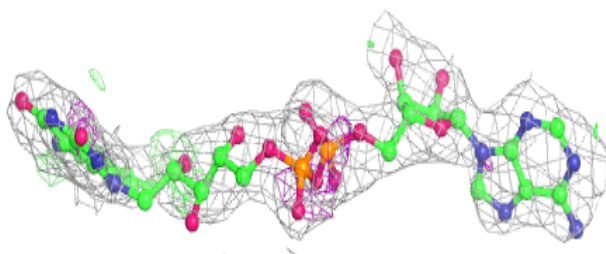
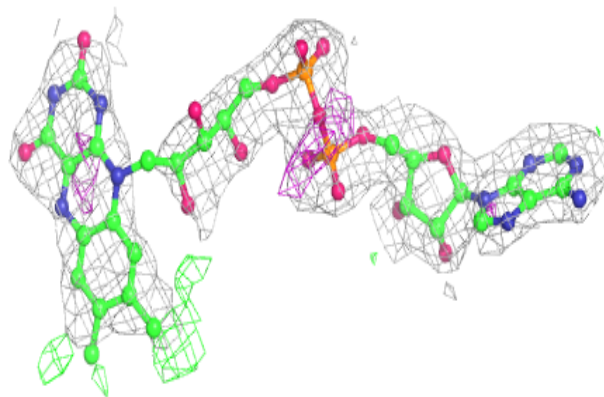
**Electron density around FAD E 601:**

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

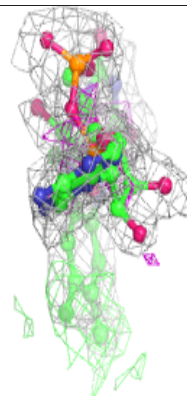
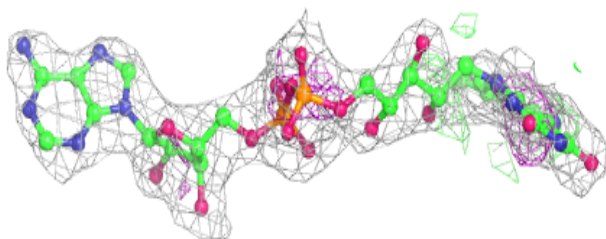
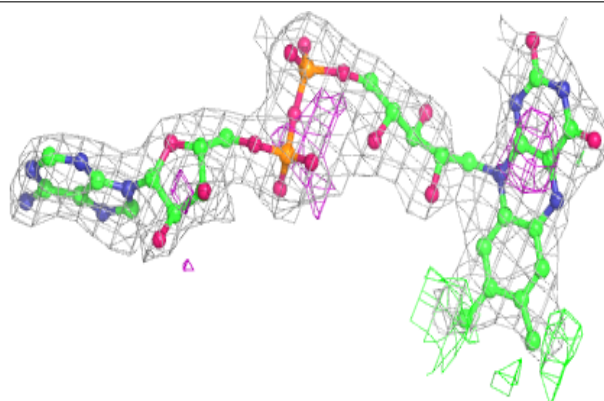


Electron density around FAD B 601:

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

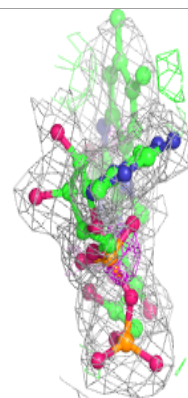
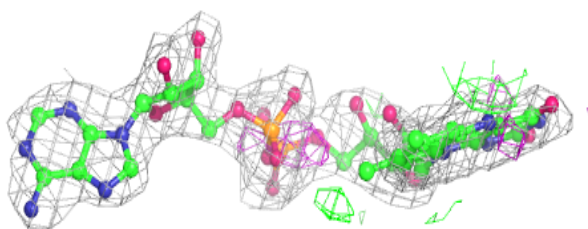
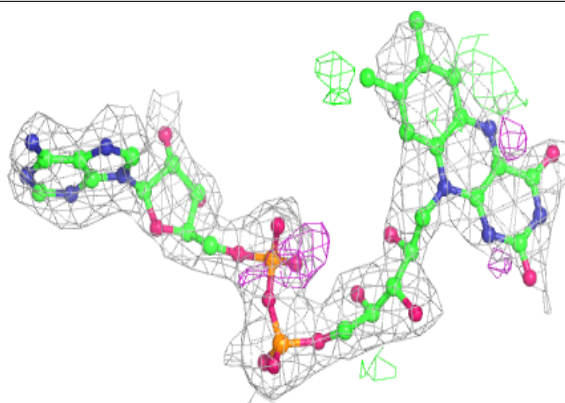
**Electron density around FAD A 601:**

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

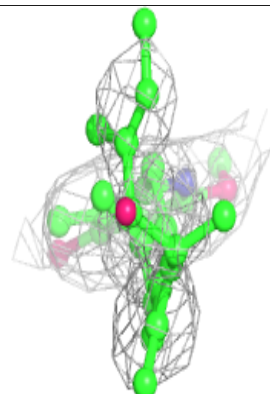
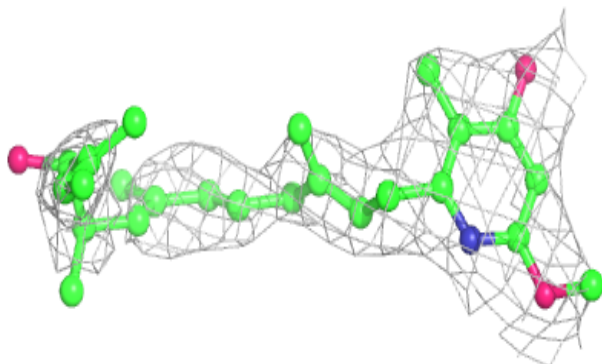
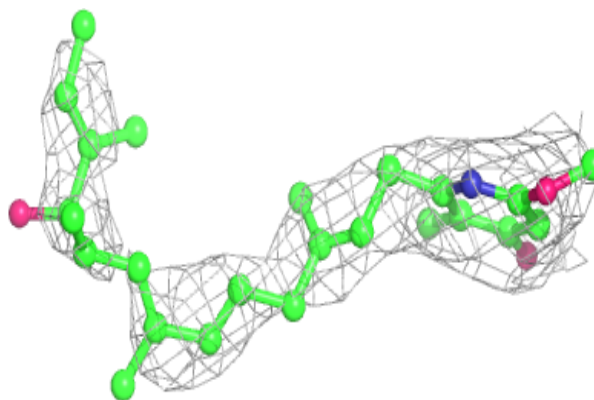


Electron density around FAD C 702:

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

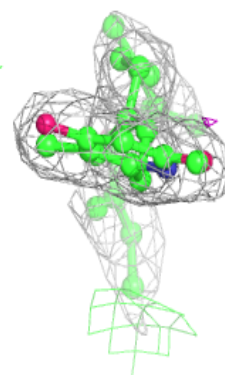
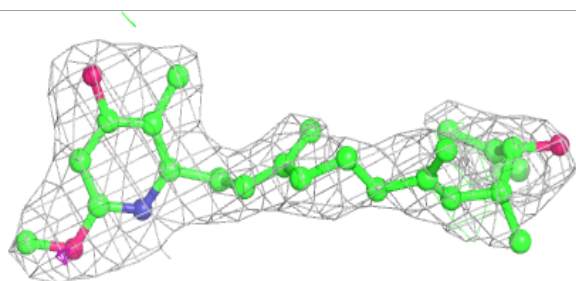
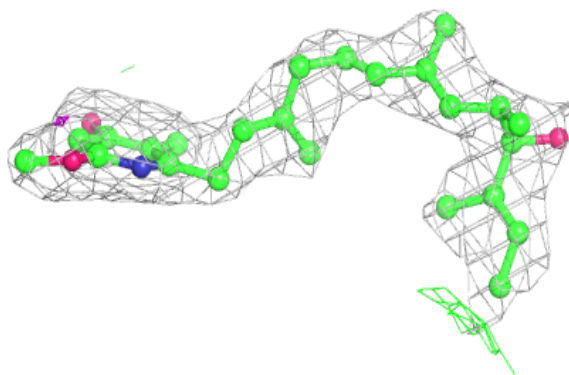
**Electron density around PKS F 603:**

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

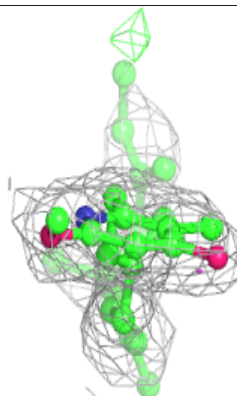
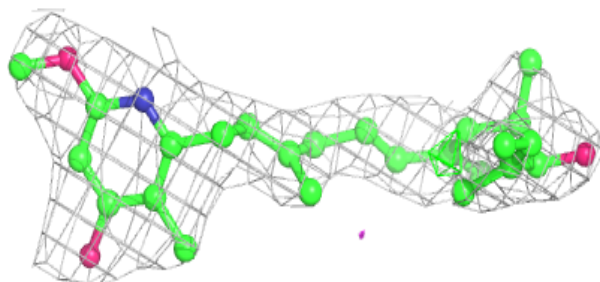
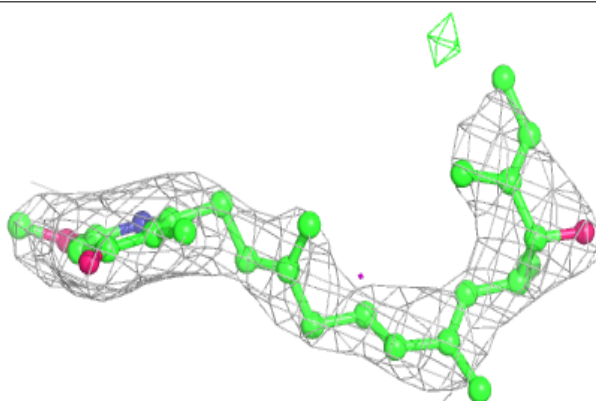


Electron density around PKS A 603:

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

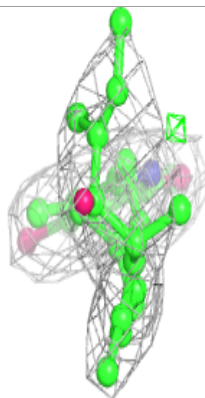
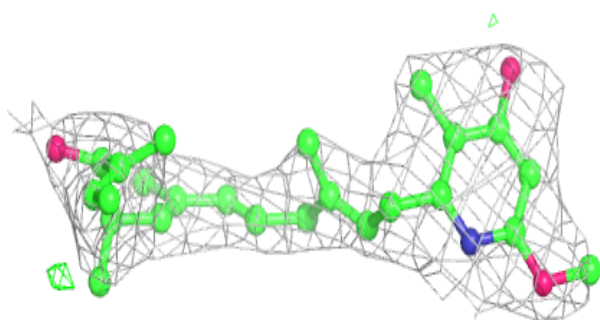
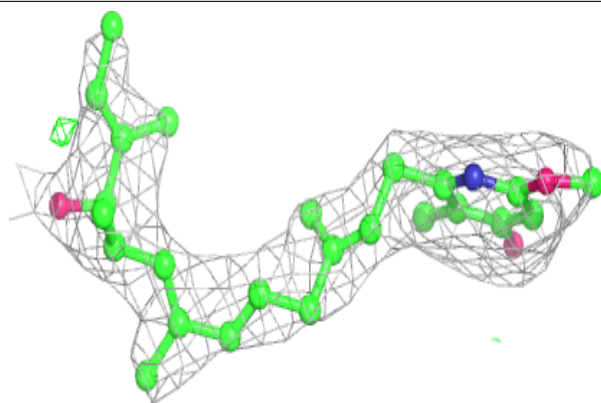
**Electron density around PKS B 603:**

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

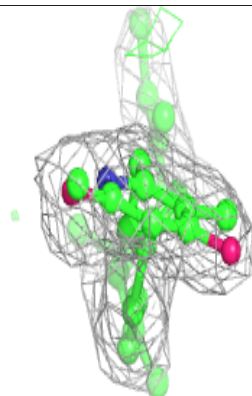
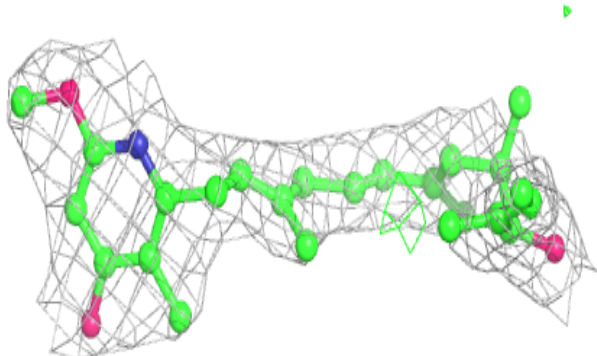
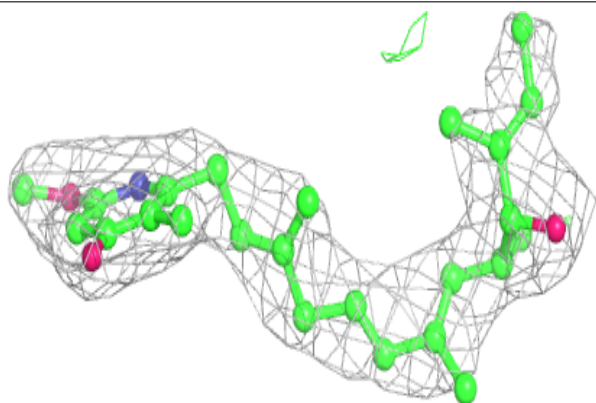


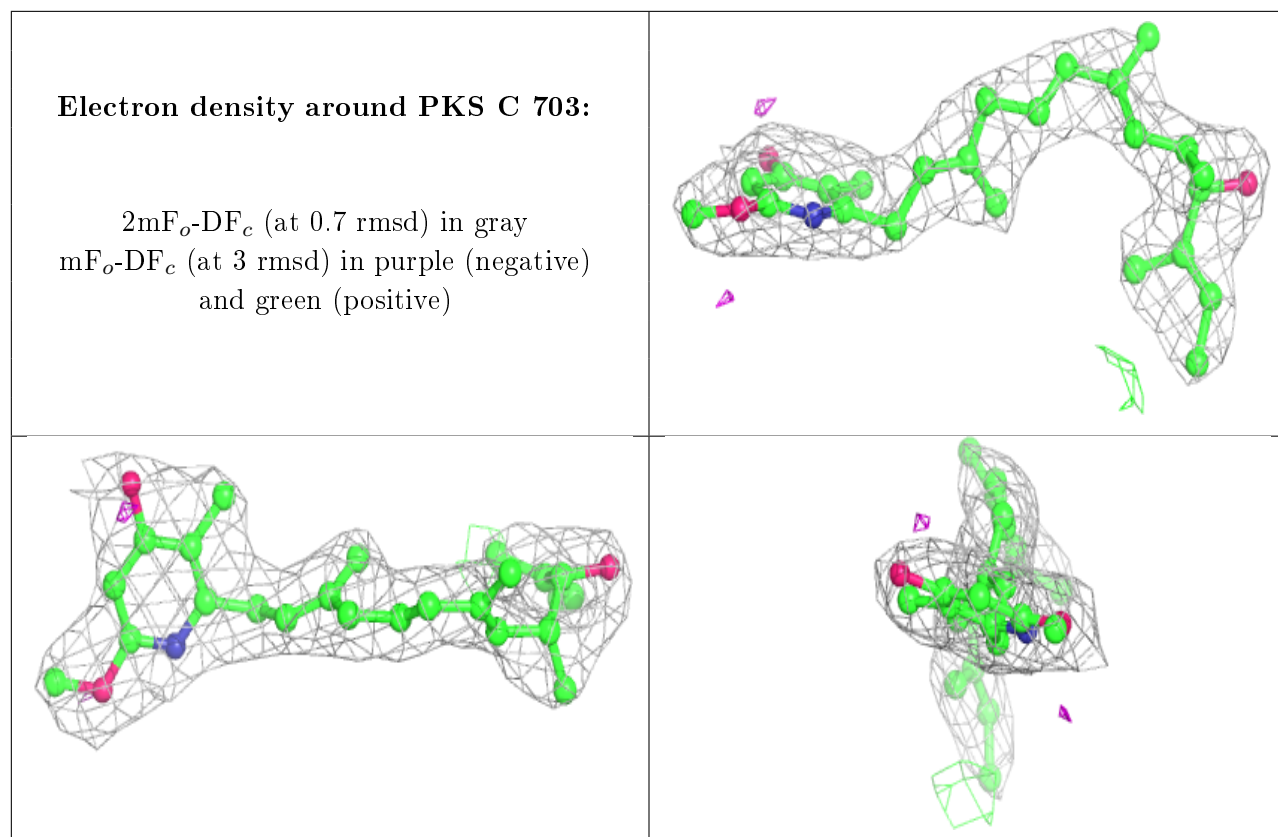
Electron density around PKS D 604:

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

**Electron density around PKS E 603:**

$2mF_o-DF_c$ (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.