



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 16, 2026 – 04:34 PM UTC

PDB ID : 9H8P / pdb_00009h8p
Title : Eugenol Oxidase (EUGO) from *Rhodococcus jostii* RHA1, mutant DTT
Authors : Rozeboom, H.J.; Fraaije, M.W.
Deposited on : 2024-10-29
Resolution : 1.47 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

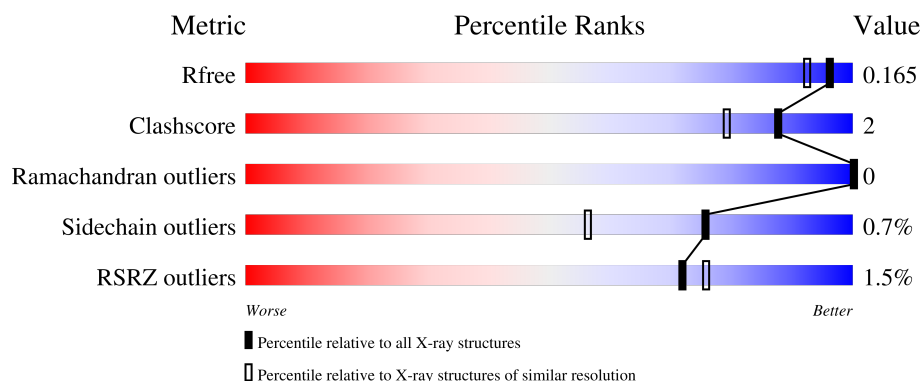
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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.



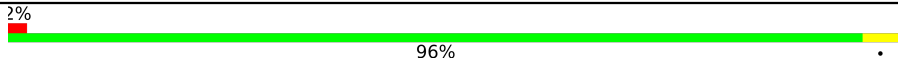
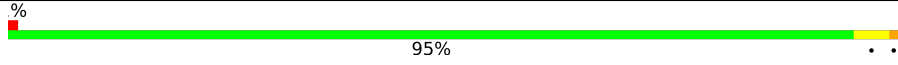
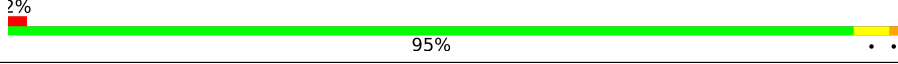
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	526	2% 94% 5%
1	B	526	2% 95% 2%
1	C	526	2% 95% 2%
1	D	526	2% 96% 2%
1	E	526	2% 93% 6%

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Mol	Chain	Length	Quality of chain
1	F	526	
1	G	526	
1	H	526	

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
6	CL	E	604	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 36894 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 Probable vanillyl-alcohol oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4133	2634	700	775	24			
1	B	525	Total	C	N	O	S	0	1	0
			4141	2639	701	776	25			
1	C	525	Total	C	N	O	S	0	1	0
			4141	2638	701	778	24			
1	D	525	Total	C	N	O	S	0	1	0
			4141	2639	701	776	25			
1	E	525	Total	C	N	O	S	0	1	0
			4141	2639	701	776	25			
1	F	525	Total	C	N	O	S	0	1	0
			4141	2639	701	776	25			
1	G	525	Total	C	N	O	S	0	1	0
			4141	2640	701	776	24			
1	H	525	Total	C	N	O	S	0	1	0
			4141	2638	701	778	24			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	HIS	SER	engineered mutation	UNP Q0SBK1
A	394	VAL	SER	engineered mutation	UNP Q0SBK1
A	423	MET	ALA	engineered mutation	UNP Q0SBK1
A	425	THR	GLN	engineered mutation	UNP Q0SBK1
A	427	THR	ILE	engineered mutation	UNP Q0SBK1
A	434	TYR	HIS	engineered mutation	UNP Q0SBK1
A	445	ASP	ILE	engineered mutation	UNP Q0SBK1
A	518	PRO	SER	engineered mutation	UNP Q0SBK1
B	81	HIS	SER	engineered mutation	UNP Q0SBK1
B	394	VAL	SER	engineered mutation	UNP Q0SBK1
B	423	MET	ALA	engineered mutation	UNP Q0SBK1
B	425	THR	GLN	engineered mutation	UNP Q0SBK1
B	427	THR	ILE	engineered mutation	UNP Q0SBK1

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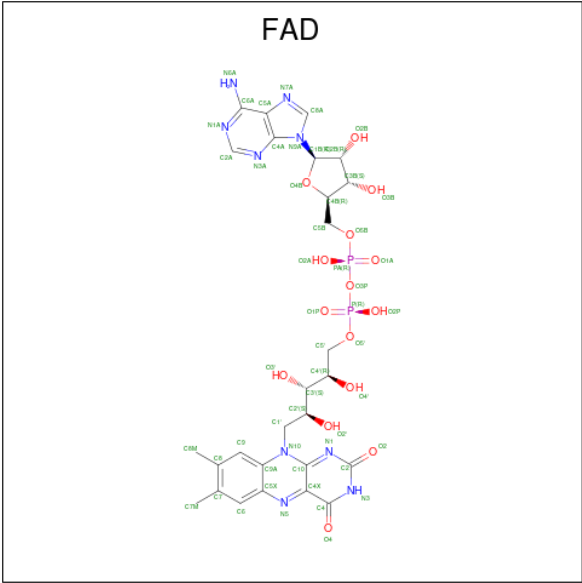
Chain	Residue	Modelled	Actual	Comment	Reference
B	434	TYR	HIS	engineered mutation	UNP Q0SBK1
B	445	ASP	ILE	engineered mutation	UNP Q0SBK1
B	518	PRO	SER	engineered mutation	UNP Q0SBK1
C	81	HIS	SER	engineered mutation	UNP Q0SBK1
C	394	VAL	SER	engineered mutation	UNP Q0SBK1
C	423	MET	ALA	engineered mutation	UNP Q0SBK1
C	425	THR	GLN	engineered mutation	UNP Q0SBK1
C	427	THR	ILE	engineered mutation	UNP Q0SBK1
C	434	TYR	HIS	engineered mutation	UNP Q0SBK1
C	445	ASP	ILE	engineered mutation	UNP Q0SBK1
C	518	PRO	SER	engineered mutation	UNP Q0SBK1
D	81	HIS	SER	engineered mutation	UNP Q0SBK1
D	394	VAL	SER	engineered mutation	UNP Q0SBK1
D	423	MET	ALA	engineered mutation	UNP Q0SBK1
D	425	THR	GLN	engineered mutation	UNP Q0SBK1
D	427	THR	ILE	engineered mutation	UNP Q0SBK1
D	434	TYR	HIS	engineered mutation	UNP Q0SBK1
D	445	ASP	ILE	engineered mutation	UNP Q0SBK1
D	518	PRO	SER	engineered mutation	UNP Q0SBK1
E	81	HIS	SER	engineered mutation	UNP Q0SBK1
E	394	VAL	SER	engineered mutation	UNP Q0SBK1
E	423	MET	ALA	engineered mutation	UNP Q0SBK1
E	425	THR	GLN	engineered mutation	UNP Q0SBK1
E	427	THR	ILE	engineered mutation	UNP Q0SBK1
E	434	TYR	HIS	engineered mutation	UNP Q0SBK1
E	445	ASP	ILE	engineered mutation	UNP Q0SBK1
E	518	PRO	SER	engineered mutation	UNP Q0SBK1
F	81	HIS	SER	engineered mutation	UNP Q0SBK1
F	394	VAL	SER	engineered mutation	UNP Q0SBK1
F	423	MET	ALA	engineered mutation	UNP Q0SBK1
F	425	THR	GLN	engineered mutation	UNP Q0SBK1
F	427	THR	ILE	engineered mutation	UNP Q0SBK1
F	434	TYR	HIS	engineered mutation	UNP Q0SBK1
F	445	ASP	ILE	engineered mutation	UNP Q0SBK1
F	518	PRO	SER	engineered mutation	UNP Q0SBK1
G	81	HIS	SER	engineered mutation	UNP Q0SBK1
G	394	VAL	SER	engineered mutation	UNP Q0SBK1
G	423	MET	ALA	engineered mutation	UNP Q0SBK1
G	425	THR	GLN	engineered mutation	UNP Q0SBK1
G	427	THR	ILE	engineered mutation	UNP Q0SBK1
G	434	TYR	HIS	engineered mutation	UNP Q0SBK1
G	445	ASP	ILE	engineered mutation	UNP Q0SBK1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	518	PRO	SER	engineered mutation	UNP Q0SBK1
H	81	HIS	SER	engineered mutation	UNP Q0SBK1
H	394	VAL	SER	engineered mutation	UNP Q0SBK1
H	423	MET	ALA	engineered mutation	UNP Q0SBK1
H	425	THR	GLN	engineered mutation	UNP Q0SBK1
H	427	THR	ILE	engineered mutation	UNP Q0SBK1
H	434	TYR	HIS	engineered mutation	UNP Q0SBK1
H	445	ASP	ILE	engineered mutation	UNP Q0SBK1
H	518	PRO	SER	engineered mutation	UNP Q0SBK1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



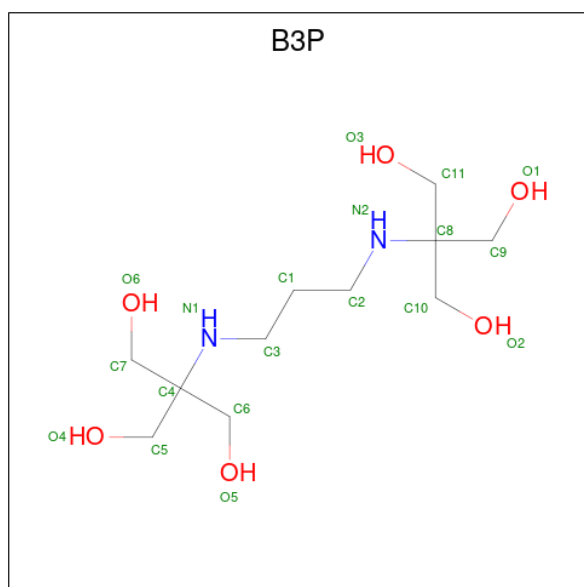
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G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

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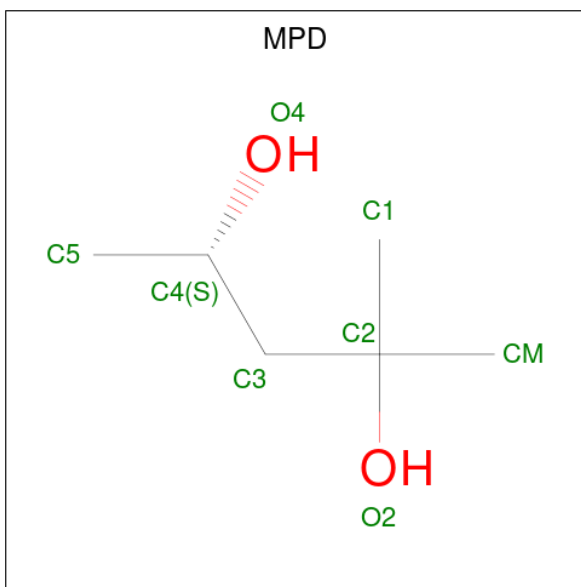
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



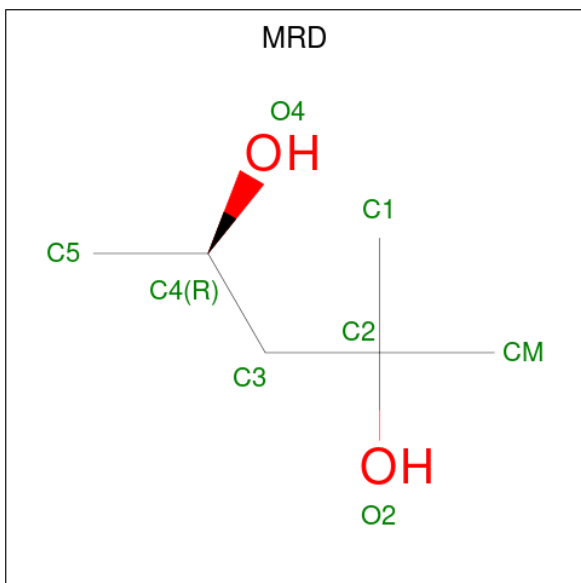
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			19	11	2	6			
3	A	1	Total	C	N	O		0	0
			19	11	2	6			
3	B	1	Total	C	N	O		0	0
			19	11	2	6			
3	C	1	Total	C	N	O		0	0
			19	11	2	6			
3	D	1	Total	C	N	O		0	0
			19	11	2	6			
3	E	1	Total	C	N	O		0	0
			19	11	2	6			
3	F	1	Total	C	N	O		0	0
			19	11	2	6			
3	H	1	Total	C	N	O		0	0
			19	11	2	6			

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		
6	D	2	Total	Cl	0	0
			2	2		
6	E	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		
6	G	1	Total	Cl	0	0
			1	1		
6	H	1	Total	Cl	0	0
			1	1		

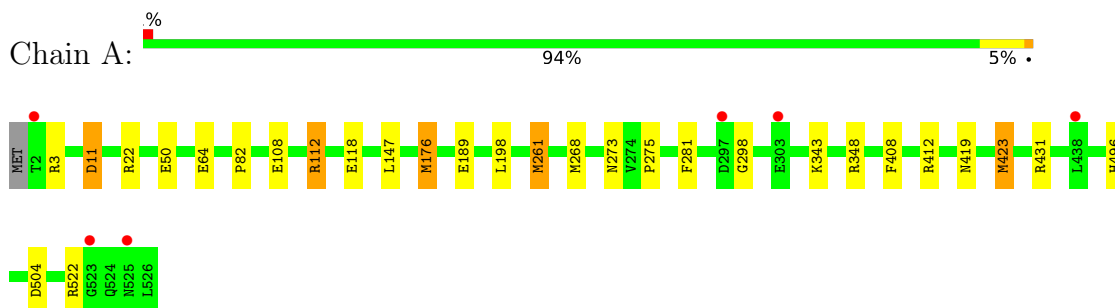
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	443	Total	O	0	0
			443	443		
7	B	392	Total	O	0	0
			392	392		
7	C	373	Total	O	0	0
			373	373		
7	D	410	Total	O	0	0
			410	410		
7	E	441	Total	O	0	0
			441	441		
7	F	407	Total	O	0	0
			407	407		
7	G	320	Total	O	0	0
			320	320		
7	H	363	Total	O	0	0
			363	363		

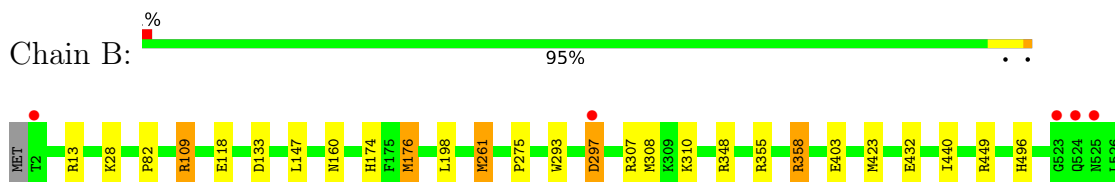
3 Residue-property plots [i](#)

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.

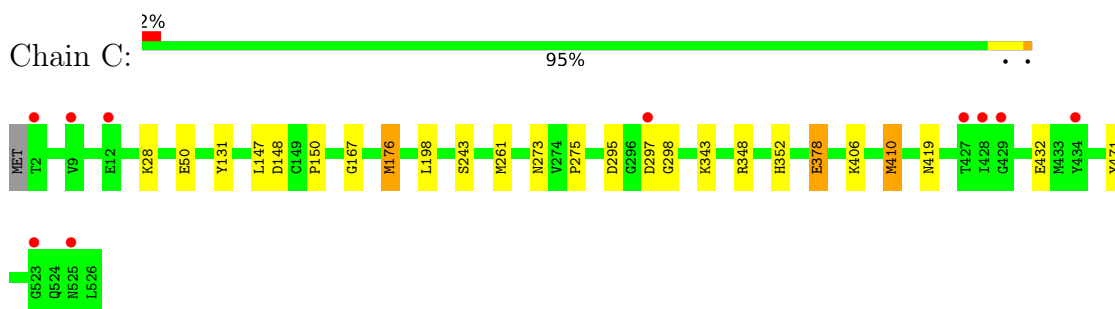
- Molecule 1: Probable vanillyl-alcohol oxidase



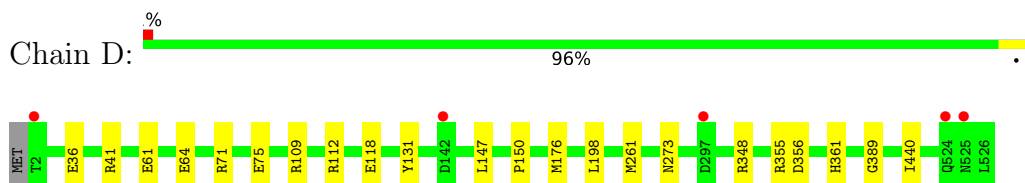
- Molecule 1: Probable vanillyl-alcohol oxidase



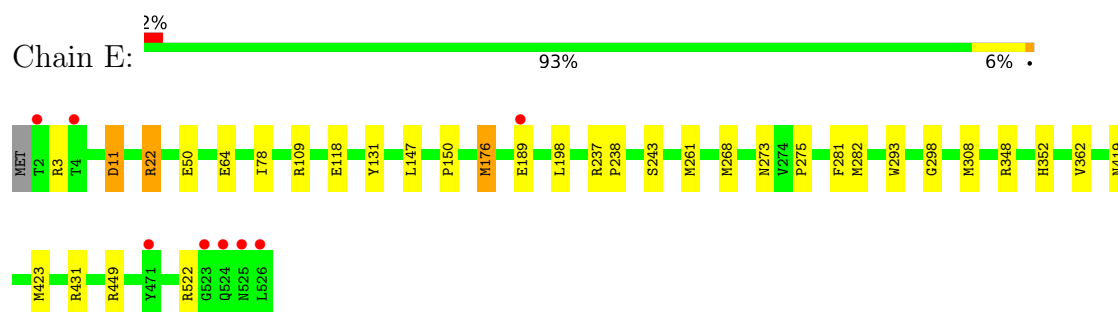
- Molecule 1: Probable vanillyl-alcohol oxidase



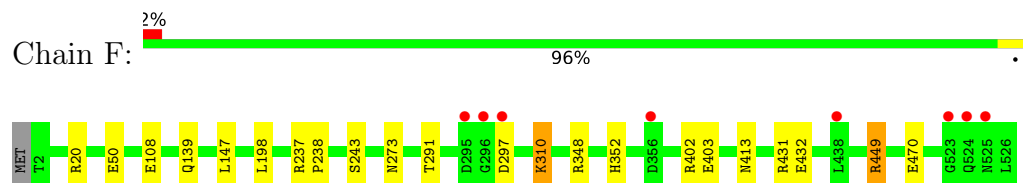
- Molecule 1: Probable vanillyl-alcohol oxidase



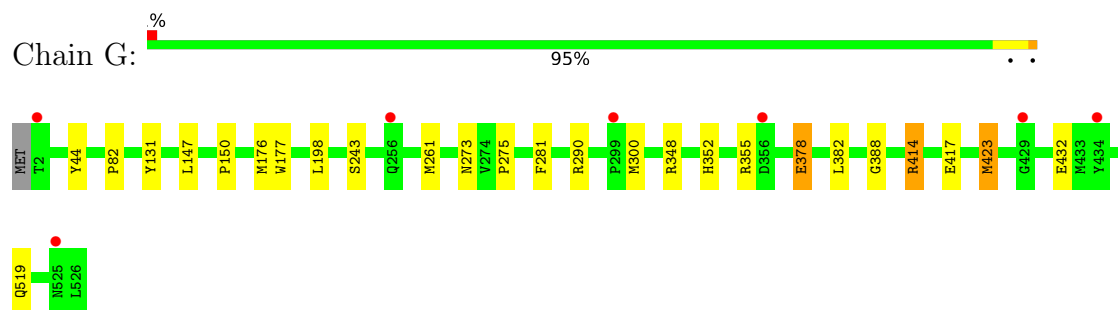
- Molecule 1: Probable vanillyl-alcohol oxidase



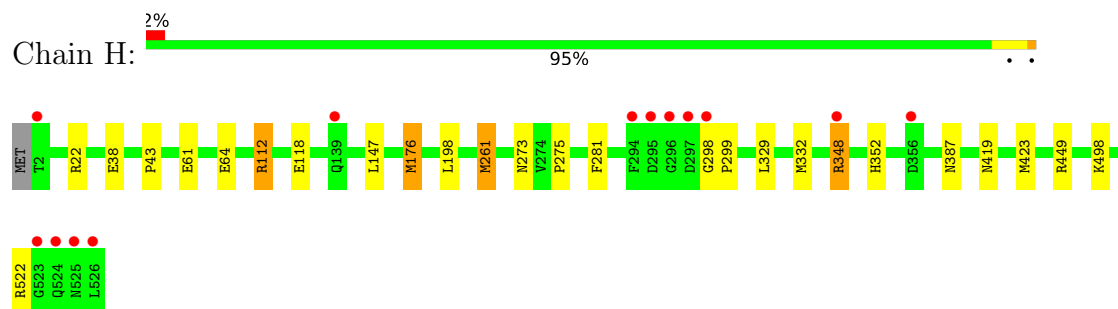
- Molecule 1: Probable vanillyl-alcohol oxidase



- Molecule 1: Probable vanillyl-alcohol oxidase



- Molecule 1: Probable vanillyl-alcohol oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.35Å 110.23Å 117.26Å 89.75° 89.50° 68.43°	Depositor
Resolution (Å)	102.72 – 1.47 102.72 – 1.47	Depositor EDS
% Data completeness (in resolution range)	92.2 (102.72-1.47) 92.5 (102.72-1.47)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.149 , 0.165 0.149 , 0.165	Depositor DCC
R_{free} test set	32662 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for h,h-k,-l 0.056 for -h,-k,l 0.011 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36894	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: MRD, FAD, B3P, CL, MPD

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	0.76	0/4242	1.06	15/5757 (0.3%)
1	B	0.72	0/4250	1.05	16/5767 (0.3%)
1	C	0.72	0/4250	1.00	5/5768 (0.1%)
1	D	0.74	0/4250	1.04	8/5767 (0.1%)
1	E	0.78	0/4250	1.04	11/5767 (0.2%)
1	F	0.74	0/4250	1.02	6/5767 (0.1%)
1	G	0.66	0/4250	0.96	4/5768 (0.1%)
1	H	0.69	0/4250	1.01	12/5768 (0.2%)
All	All	0.73	0/33992	1.02	77/46129 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	3
1	G	0	4
1	H	0	3
All	All	0	18

There are no bond length outliers.

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	176	MET	CG-SD-CE	-11.45	75.70	100.90
1	C	176	MET	CG-SD-CE	-10.42	77.97	100.90
1	B	176	MET	CG-SD-CE	-9.81	79.31	100.90
1	E	176	MET	CG-SD-CE	-9.01	81.08	100.90
1	H	118	GLU	CG-CD-OE2	-8.58	98.67	118.40

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
1	A	348	ARG	Sidechain
1	B	109	ARG	Sidechain
1	B	348	ARG	Sidechain
1	C	348	ARG	Sidechain

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	4133	0	4000	24	0
1	B	4141	0	4008	15	0
1	C	4141	0	4003	17	0
1	D	4141	0	4008	13	0
1	E	4141	0	4008	18	0
1	F	4141	0	4008	10	0
1	G	4141	0	4010	19	0
1	H	4141	0	4003	15	0
2	A	53	0	30	1	0
2	B	53	0	30	1	0
2	C	53	0	30	1	0
2	D	53	0	30	1	0
2	E	53	0	30	1	0
2	F	53	0	30	1	0
2	G	53	0	30	1	0
2	H	53	0	30	1	0
3	A	38	0	52	0	0
3	B	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	19	0	26	0	0
3	D	19	0	26	3	0
3	E	19	0	26	0	0
3	F	19	0	26	0	0
3	H	19	0	26	4	0
4	A	8	0	14	1	0
4	B	8	0	14	1	0
4	E	8	0	14	1	0
4	F	8	0	14	0	0
5	A	8	0	14	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	E	1	0	0	2	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	443	0	0	10	0
7	B	392	0	0	5	0
7	C	373	0	0	4	0
7	D	410	0	0	4	0
7	E	441	0	0	3	0
7	F	407	0	0	4	0
7	G	320	0	0	2	0
7	H	363	0	0	8	0
All	All	36894	0	32566	134	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 2.

The worst 5 of 134 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:G:44:TYR:CZ	1:G:382[A]:LEU:HD11	2.00	0.96
3:H:602:B3P:H92	7:H:816:HOH:O	1.72	0.89
1:A:343:LYS:CE	7:A:3409:HOH:O	2.24	0.83
1:A:176:MET:HE2	1:B:176:MET:HE2	1.61	0.82
1:C:343:LYS:CE	7:C:800:HOH:O	2.27	0.82

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	523/526 (99%)	512 (98%)	11 (2%)	0	100	100
1	B	524/526 (100%)	513 (98%)	11 (2%)	0	100	100
1	C	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
1	D	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
1	E	524/526 (100%)	511 (98%)	13 (2%)	0	100	100
1	F	524/526 (100%)	513 (98%)	11 (2%)	0	100	100
1	G	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
1	H	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
All	All	4191/4208 (100%)	4097 (98%)	94 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	434/435 (100%)	432 (100%)	2 (0%)	81	65
1	B	435/435 (100%)	433 (100%)	2 (0%)	81	65
1	C	435/435 (100%)	429 (99%)	6 (1%)	59	31
1	D	435/435 (100%)	432 (99%)	3 (1%)	76	56
1	E	435/435 (100%)	433 (100%)	2 (0%)	81	65
1	F	435/435 (100%)	431 (99%)	4 (1%)	70	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	435/435 (100%)	432 (99%)	3 (1%)	76	56
1	H	435/435 (100%)	433 (100%)	2 (0%)	81	65
All	All	3479/3480 (100%)	3455 (99%)	24 (1%)	76	56

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	273	ASN
1	F	297	ASP
1	F	273	ASN
1	F	310	LYS
1	C	273	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	205	GLN
1	H	387	ASN
1	E	419	ASN
1	G	352	HIS
1	E	352	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 9 are monoatomic - leaving 21 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$
4	MPD	A	604	-	7,7,7	0.43	0	9,10,10	1.10	1 (11%)
3	B3P	C	602	-	18,18,18	0.40	0	23,23,23	1.14	2 (8%)
2	FAD	H	601	1	58,58,58	0.77	1 (1%)	85,89,89	0.82	1 (1%)
2	FAD	F	601	1	58,58,58	0.88	2 (3%)	85,89,89	0.84	3 (3%)
3	B3P	B	602	-	18,18,18	0.27	0	23,23,23	1.04	2 (8%)
5	MRD	A	605	-	7,7,7	0.21	0	9,10,10	0.83	0
2	FAD	D	601	1	58,58,58	1.02	2 (3%)	85,89,89	0.89	2 (2%)
3	B3P	F	602	-	18,18,18	0.30	0	23,23,23	0.92	1 (4%)
3	B3P	D	604	-	18,18,18	0.34	0	23,23,23	1.03	1 (4%)
3	B3P	A	602	-	18,18,18	0.57	0	23,23,23	0.81	1 (4%)
4	MPD	E	603	-	7,7,7	0.57	0	9,10,10	1.31	2 (22%)
4	MPD	B	603	-	7,7,7	0.85	0	9,10,10	1.05	1 (11%)
3	B3P	A	603	-	18,18,18	0.38	0	23,23,23	1.23	3 (13%)
3	B3P	E	602	-	18,18,18	0.46	0	23,23,23	0.93	1 (4%)
3	B3P	H	602	-	18,18,18	0.30	0	23,23,23	1.64	6 (26%)
4	MPD	F	603	-	7,7,7	0.64	0	9,10,10	1.04	1 (11%)
2	FAD	B	601	1	58,58,58	1.00	5 (8%)	85,89,89	0.89	4 (4%)
2	FAD	A	601	1	58,58,58	1.03	2 (3%)	85,89,89	1.03	4 (4%)
2	FAD	C	601	-	58,58,58	0.85	1 (1%)	85,89,89	0.83	4 (4%)
2	FAD	G	601	-	58,58,58	1.10	2 (3%)	85,89,89	0.85	2 (2%)
2	FAD	E	601	1	58,58,58	1.18	3 (5%)	85,89,89	0.82	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	A	604	-	-	3/5/5/5	-
3	B3P	C	602	-	-	7/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	H	601	1	-	4/34/50/50	0/6/6/6
2	FAD	F	601	1	-	5/34/50/50	0/6/6/6
3	B3P	B	602	-	-	8/28/28/28	-
5	MRD	A	605	-	-	0/5/5/5	-
2	FAD	D	601	1	-	7/34/50/50	0/6/6/6
3	B3P	F	602	-	-	1/28/28/28	-
3	B3P	D	604	-	-	5/28/28/28	-
3	B3P	A	602	-	-	0/28/28/28	-
4	MPD	E	603	-	-	2/5/5/5	-
4	MPD	B	603	-	-	3/5/5/5	-
3	B3P	A	603	-	-	2/28/28/28	-
3	B3P	E	602	-	-	3/28/28/28	-
3	B3P	H	602	-	-	8/28/28/28	-
4	MPD	F	603	-	-	2/5/5/5	-
2	FAD	B	601	1	-	6/34/50/50	0/6/6/6
2	FAD	A	601	1	-	4/34/50/50	0/6/6/6
2	FAD	C	601	-	-	5/34/50/50	0/6/6/6
2	FAD	G	601	-	-	4/34/50/50	0/6/6/6
2	FAD	E	601	1	-	6/34/50/50	0/6/6/6

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FAD	PA-O3P	-5.85	1.53	1.59
2	E	601	FAD	P-O3P	5.05	1.65	1.59
2	D	601	FAD	P-O3P	4.61	1.64	1.59
2	E	601	FAD	PA-O3P	-4.37	1.54	1.59
2	A	601	FAD	P-O3P	4.25	1.64	1.59

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	B3P	C9-C8-N2	3.82	120.43	109.02
3	D	604	B3P	C3-N1-C4	3.48	121.25	116.17
2	A	601	FAD	O2'-C2'-C3'	-3.44	101.19	109.25
2	D	601	FAD	O2'-C2'-C3'	-3.37	101.36	109.25
2	A	601	FAD	N3A-C2A-N1A	3.23	133.47	128.58

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

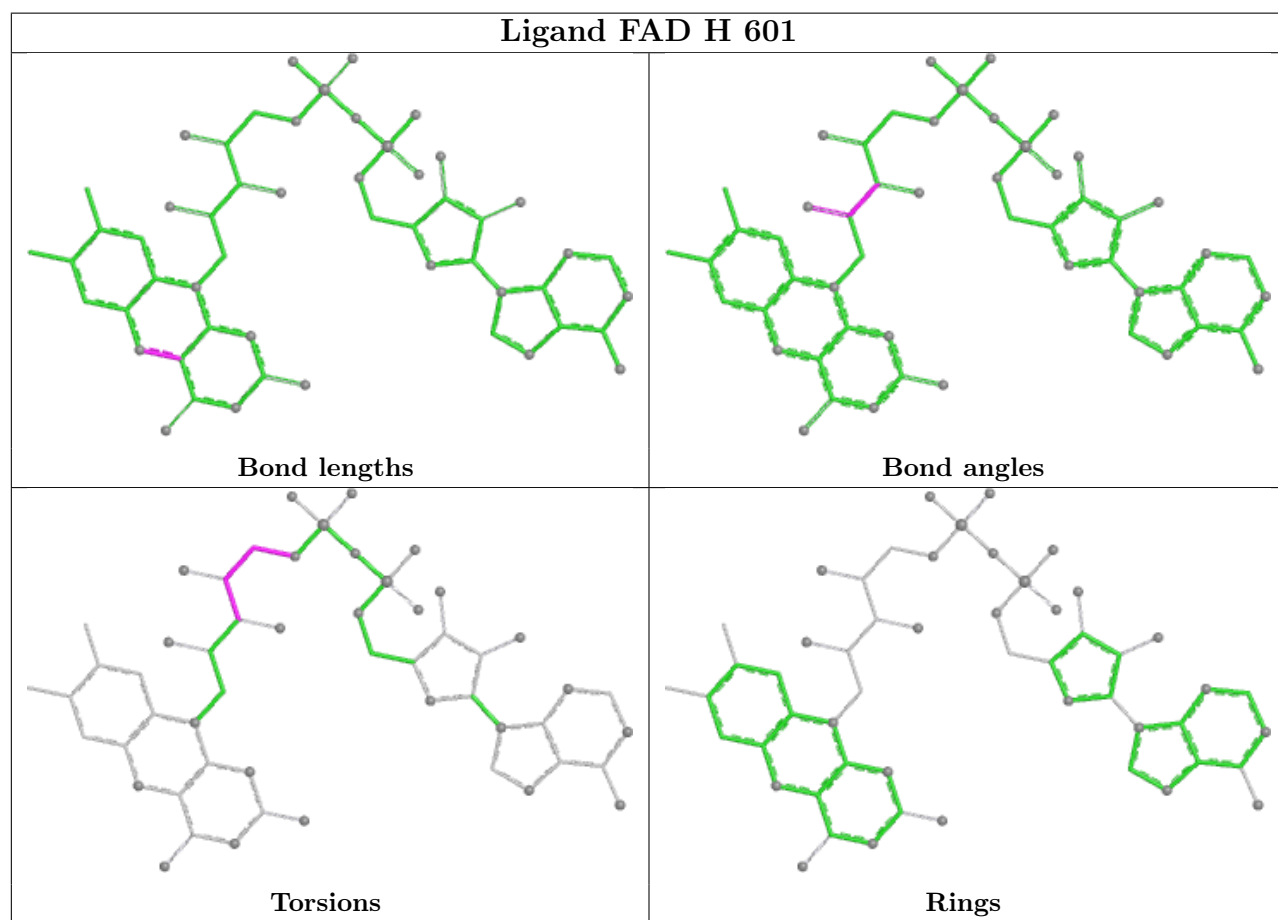
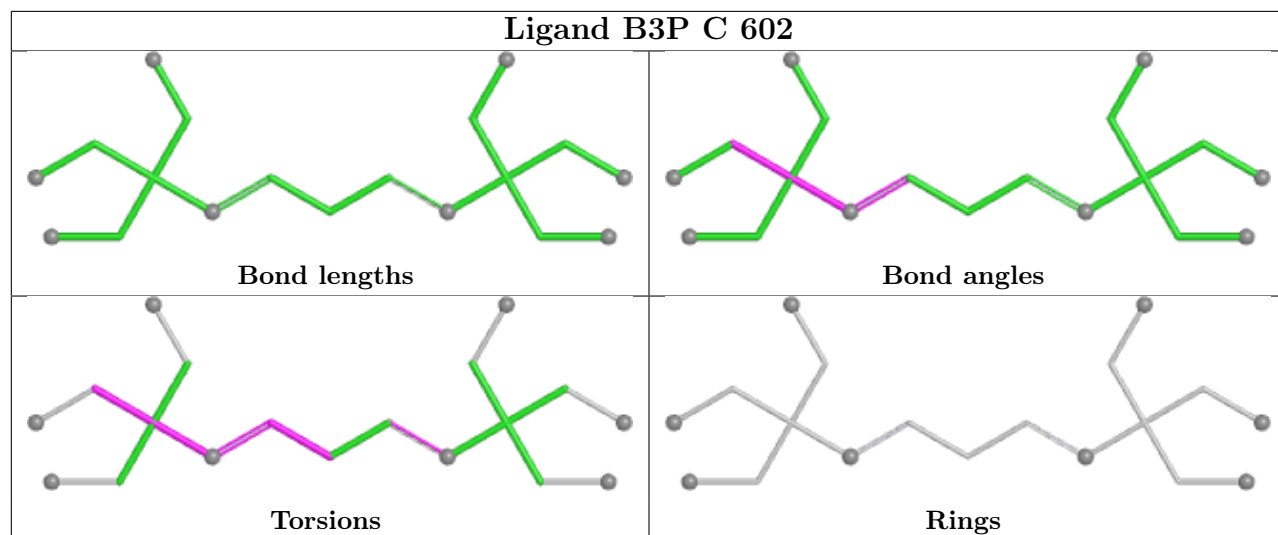
Mol	Chain	Res	Type	Atoms
3	B	602	B3P	N1-C4-C6-O5
3	B	602	B3P	C5-C4-C6-O5
3	B	602	B3P	C7-C4-C6-O5
3	B	602	B3P	C10-C8-C9-O1
3	B	602	B3P	C11-C8-C9-O1

There are no ring outliers.

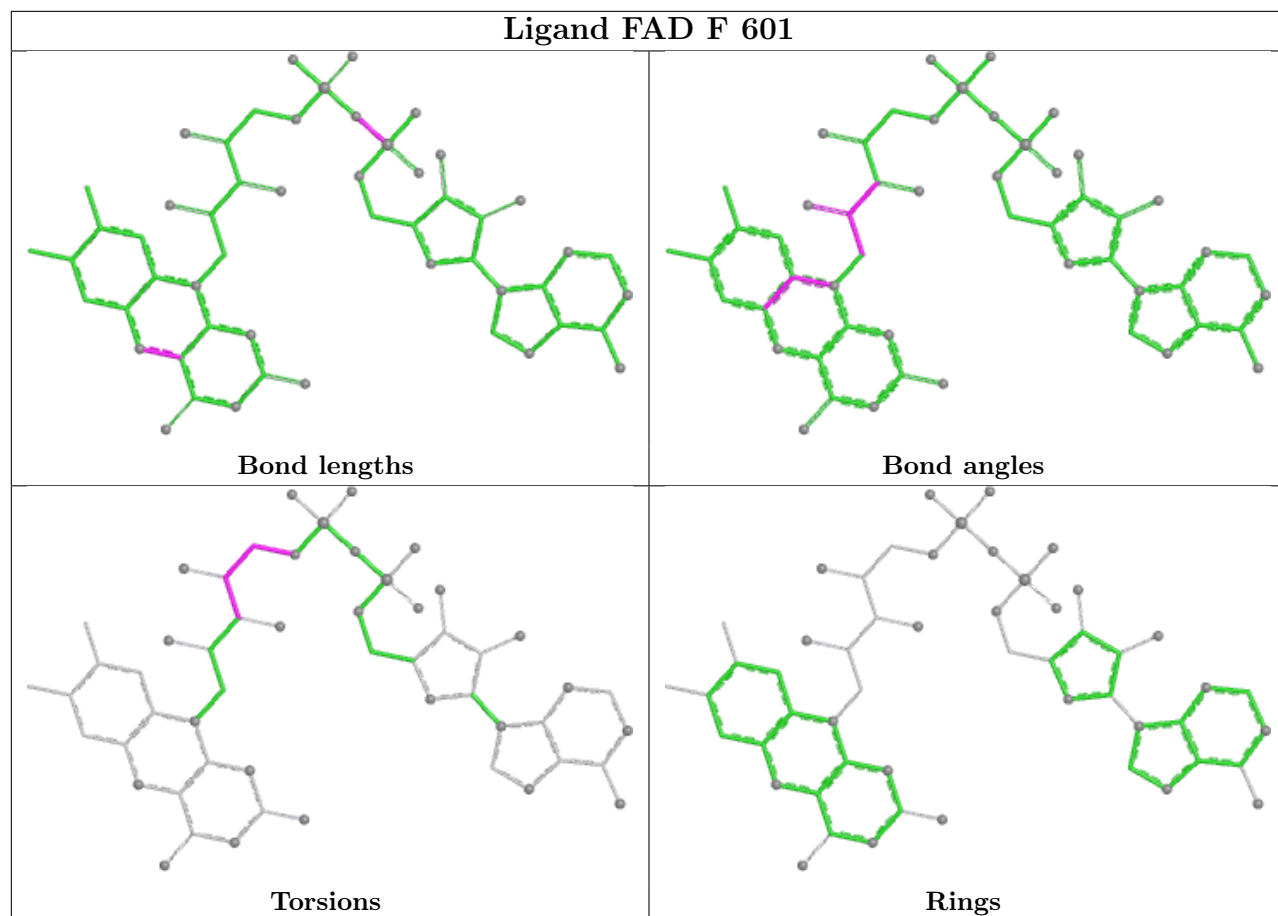
13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	MPD	1	0
2	H	601	FAD	1	0
2	F	601	FAD	1	0
2	D	601	FAD	1	0
3	D	604	B3P	3	0
4	E	603	MPD	1	0
4	B	603	MPD	1	0
3	H	602	B3P	4	0
2	B	601	FAD	1	0
2	A	601	FAD	1	0
2	C	601	FAD	1	0
2	G	601	FAD	1	0
2	E	601	FAD	1	0

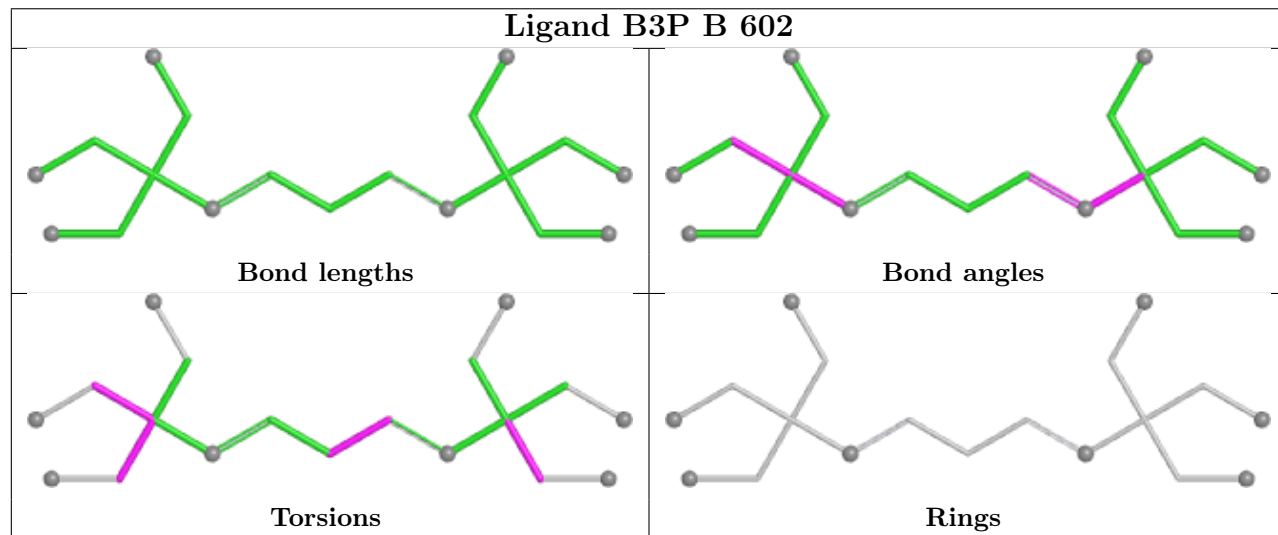
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



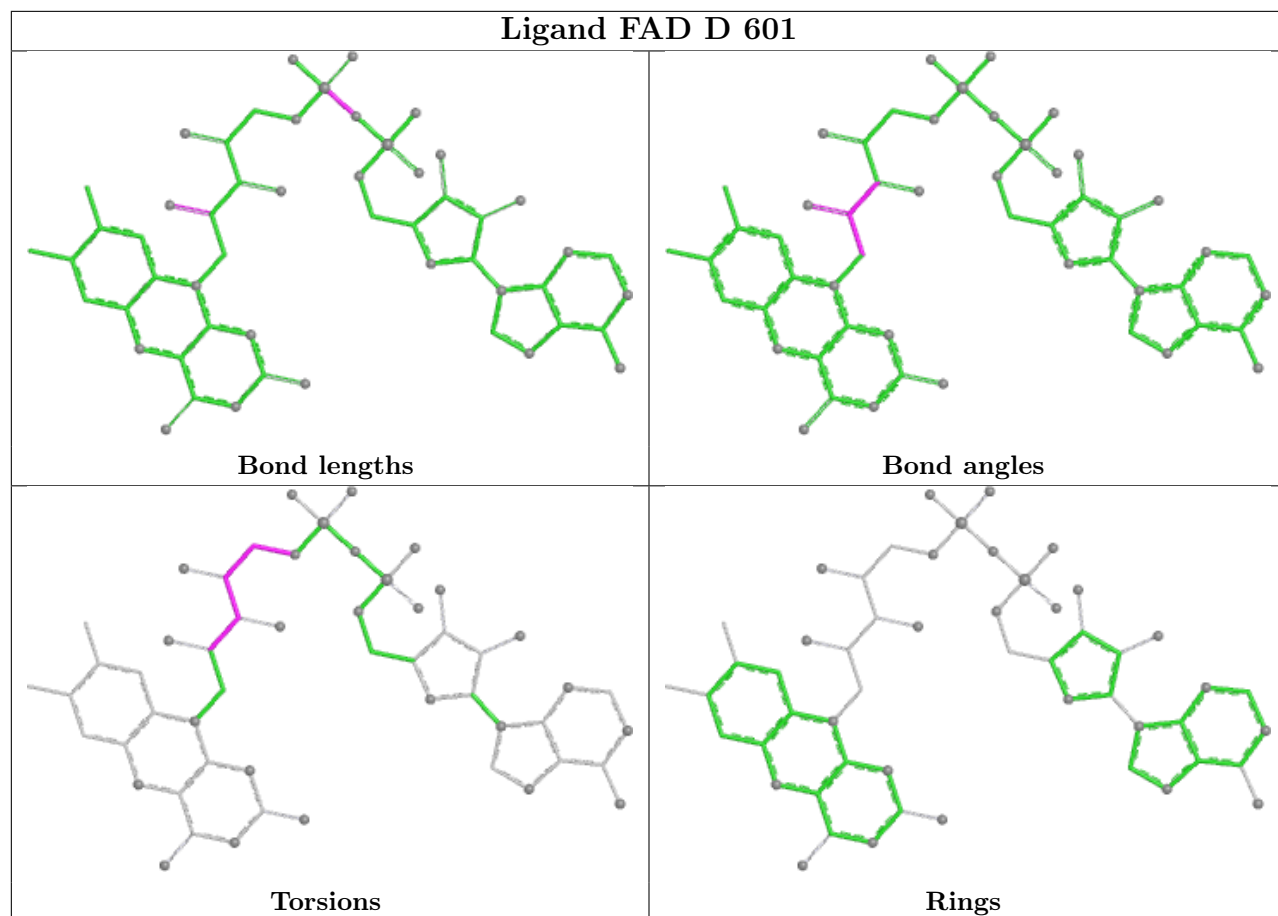
Ligand FAD F 601



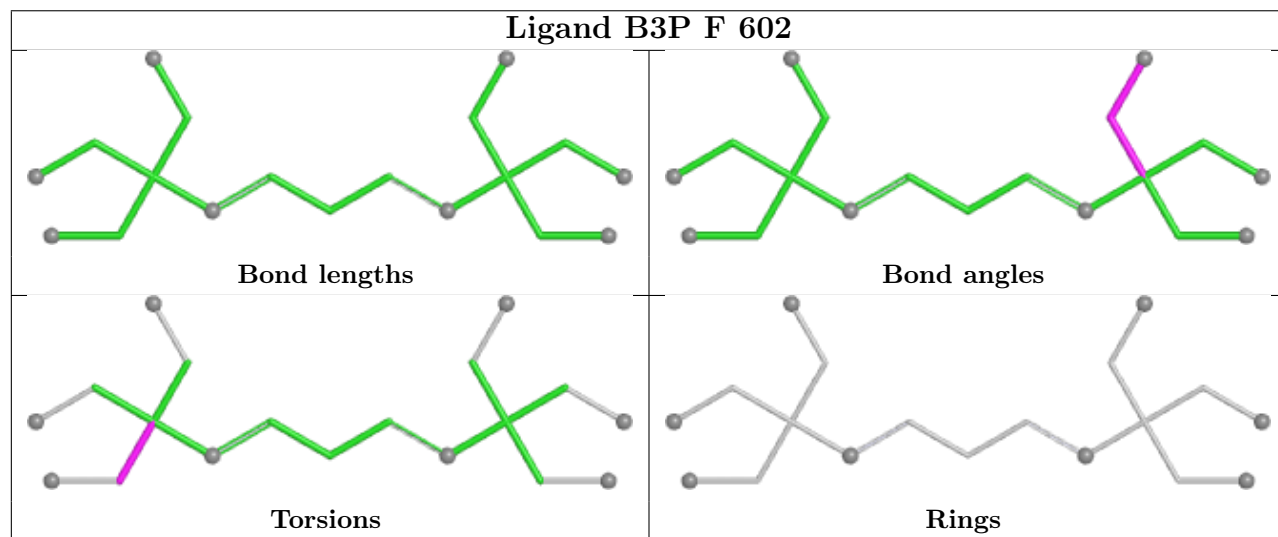
Ligand B3P B 602

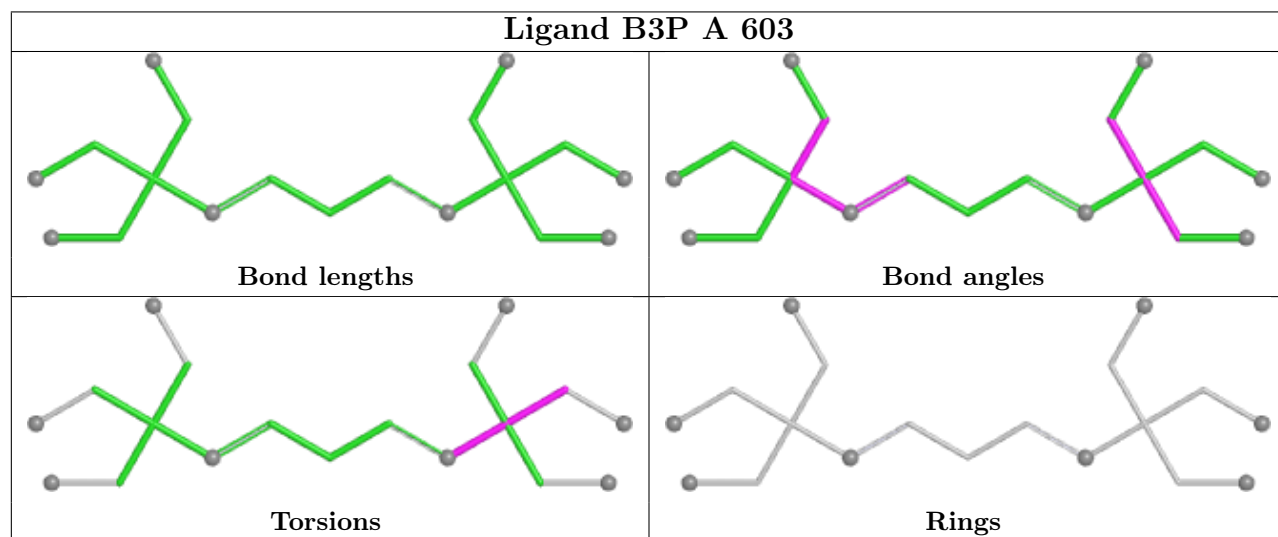
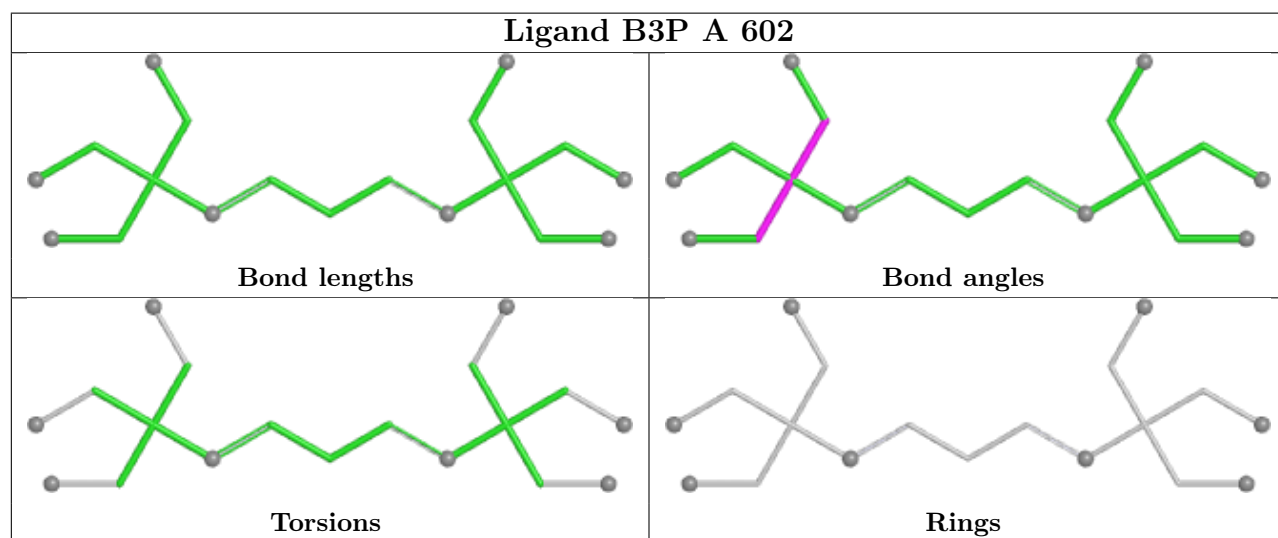
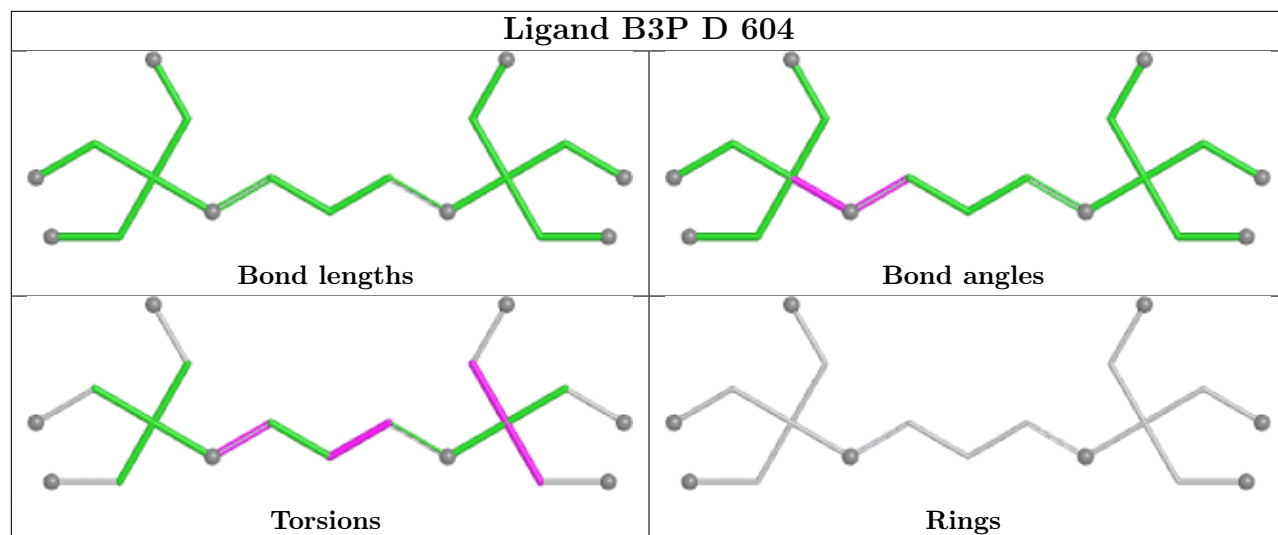


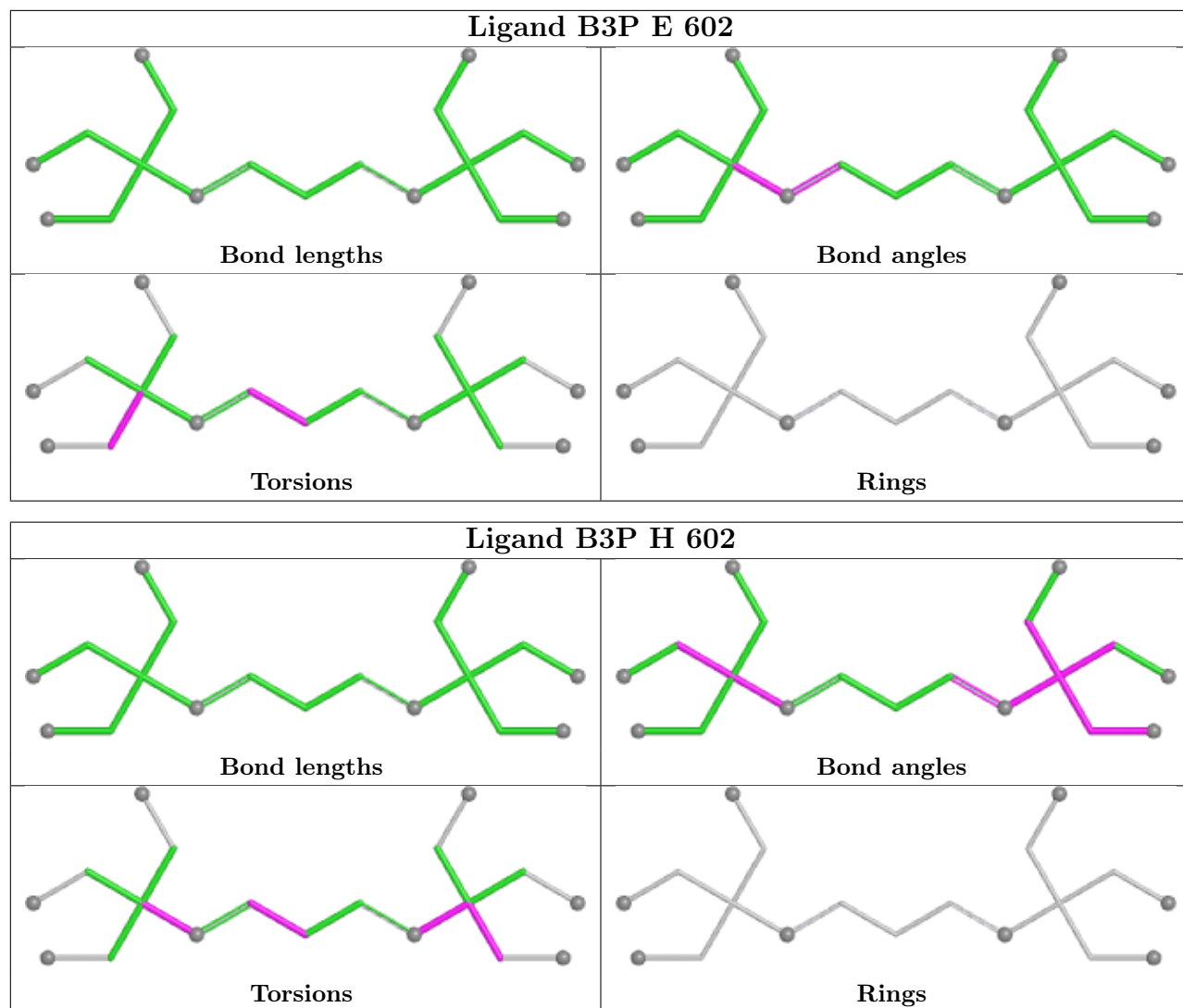
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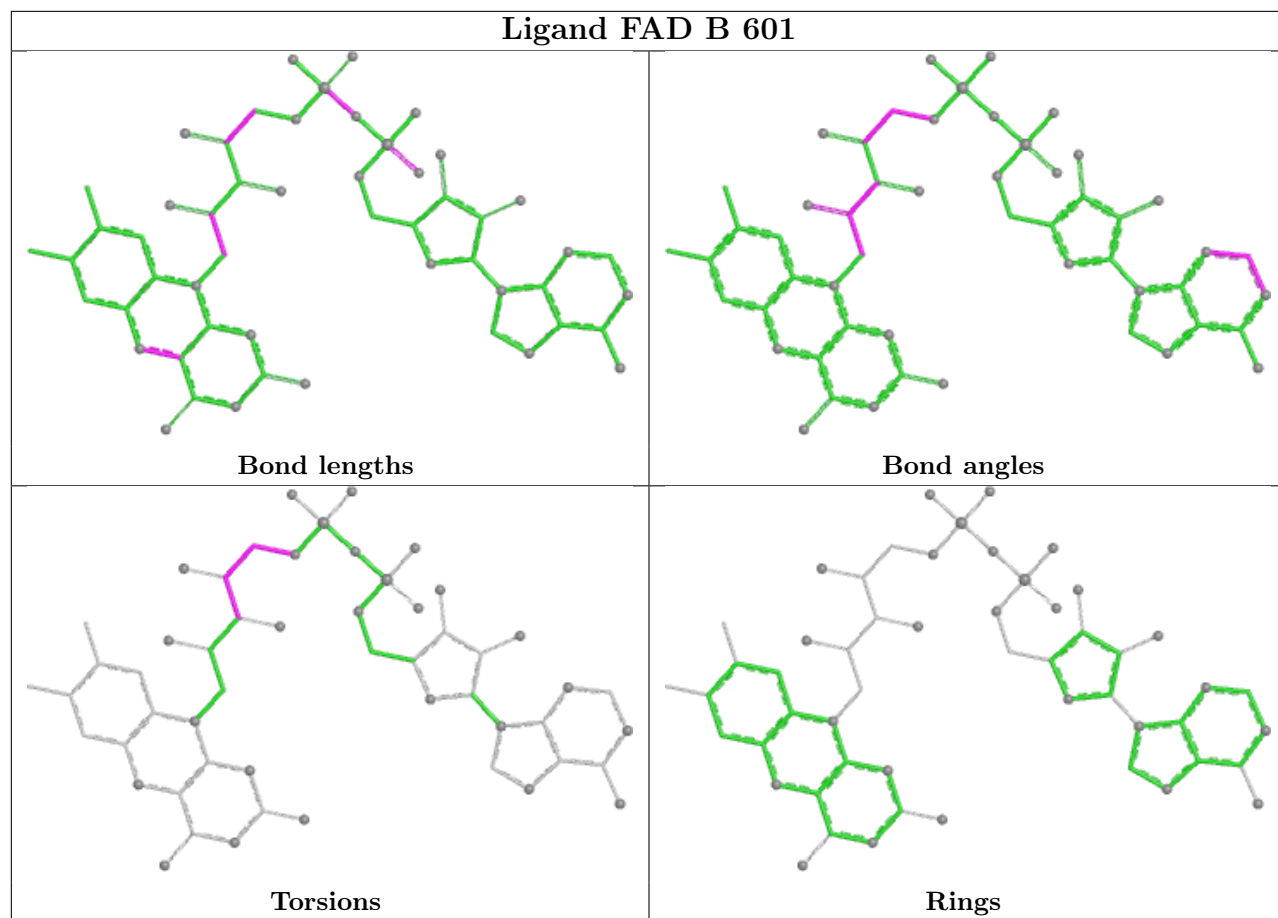


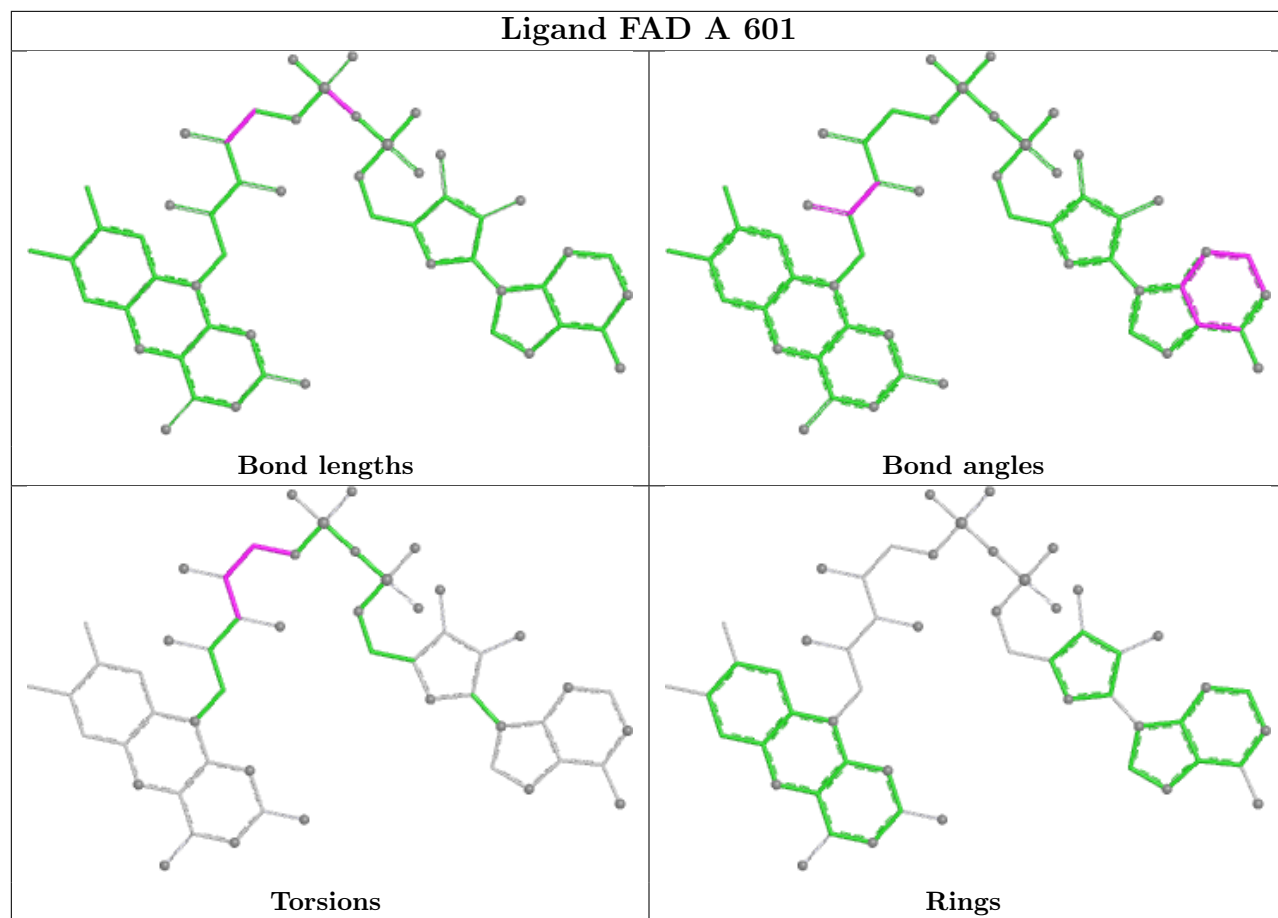
Ligand B3P F 602

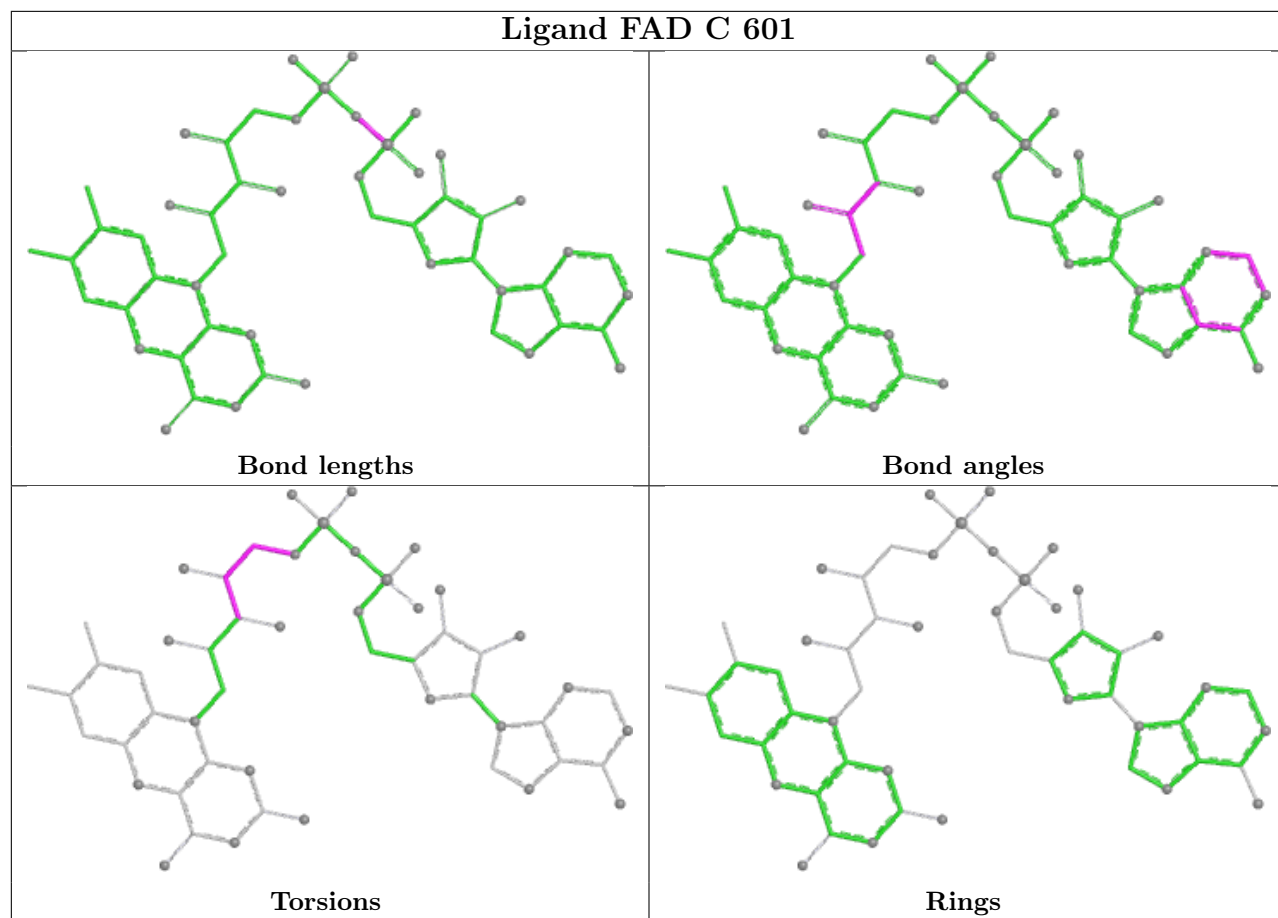




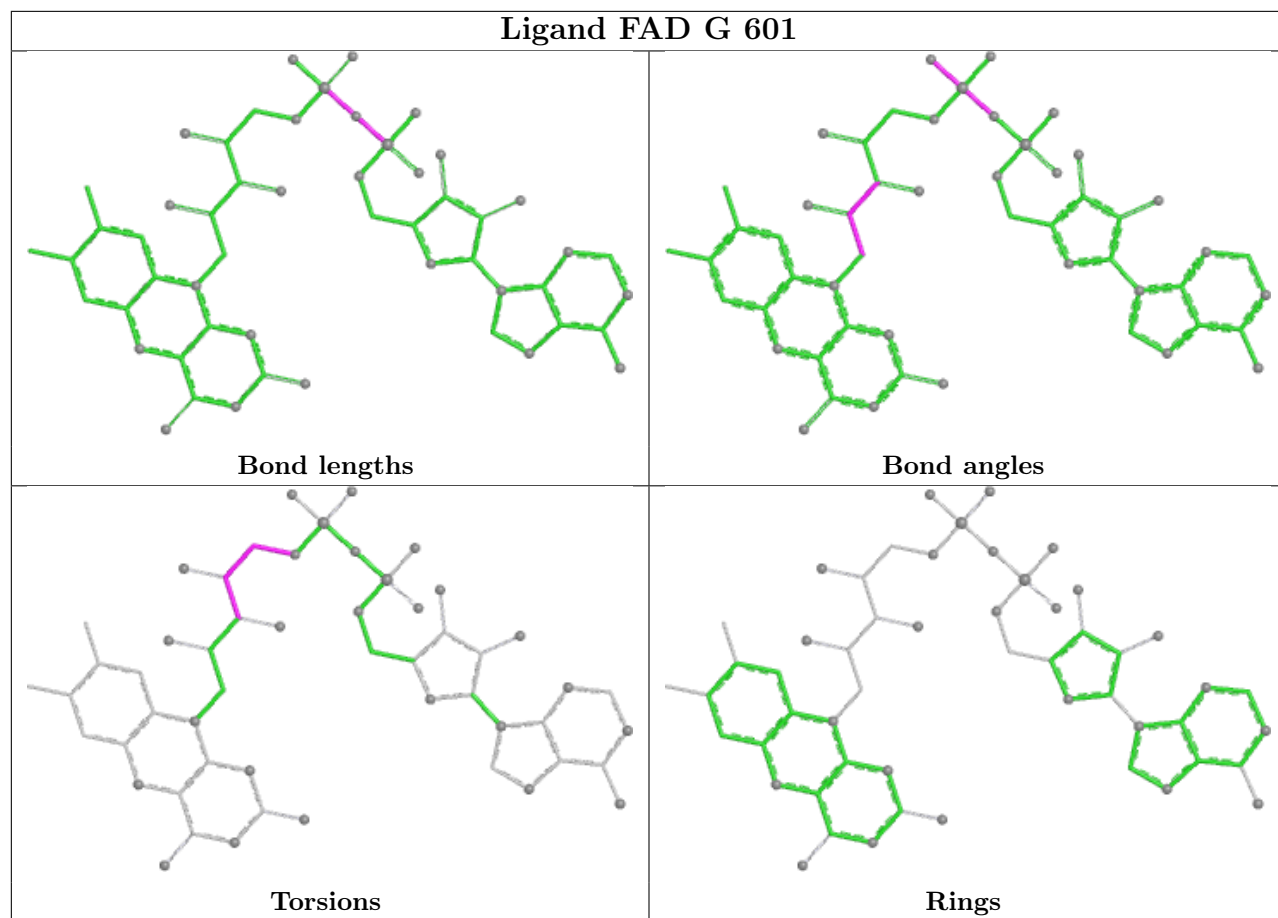


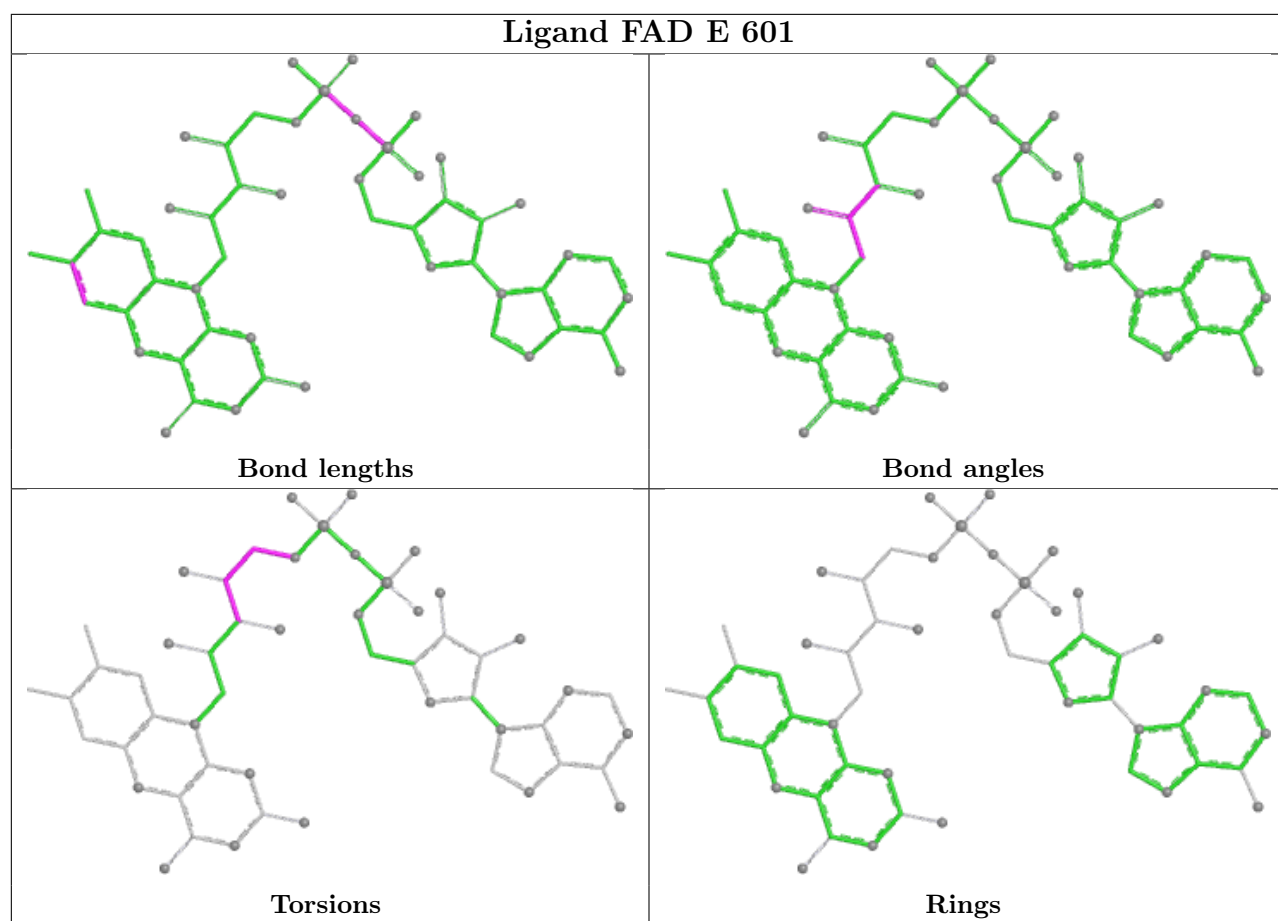






Ligand FAD G 601





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	525/526 (99%)	-0.34	6 (1%) 78 81	9, 13, 25, 61	0
1	B	525/526 (99%)	-0.20	5 (0%) 79 83	9, 15, 29, 56	1 (0%)
1	C	525/526 (99%)	-0.09	10 (1%) 66 70	9, 16, 31, 58	1 (0%)
1	D	525/526 (99%)	-0.25	5 (0%) 79 83	9, 14, 29, 53	1 (0%)
1	E	525/526 (99%)	-0.34	8 (1%) 72 76	8, 13, 25, 66	1 (0%)
1	F	525/526 (99%)	-0.24	8 (1%) 72 76	8, 14, 28, 66	1 (0%)
1	G	525/526 (99%)	0.06	7 (1%) 75 79	10, 20, 40, 60	1 (0%)
1	H	525/526 (99%)	-0.04	13 (2%) 58 62	11, 17, 34, 72	1 (0%)
All	All	4200/4208 (99%)	-0.18	62 (1%) 72 76	8, 15, 31, 72	7 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.2
1	E	2	THR	5.6
1	B	297	ASP	4.6
1	H	297	ASP	3.9
1	A	525	ASN	3.9

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

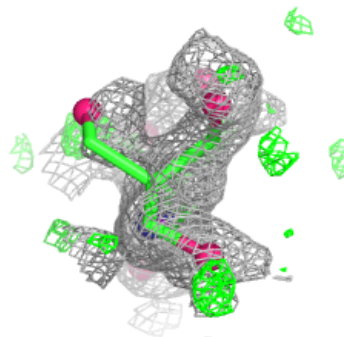
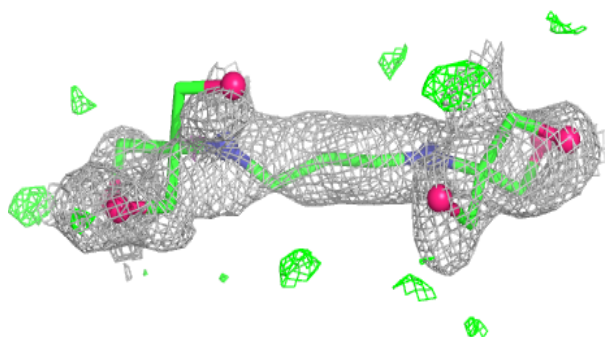
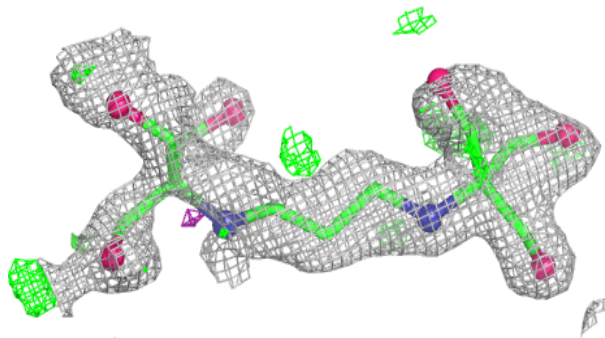
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B3P	H	602	19/19	0.72	0.19	35,50,64,68	0
3	B3P	B	602	19/19	0.75	0.17	33,42,63,69	0
3	B3P	E	602	19/19	0.77	0.15	30,38,44,47	0
3	B3P	C	602	19/19	0.79	0.15	34,42,49,50	0
5	MRD	A	605	8/8	0.79	0.19	32,37,44,48	0
4	MPD	B	603	8/8	0.80	0.17	25,29,34,35	0
4	MPD	A	604	8/8	0.81	0.17	24,30,36,41	0
3	B3P	A	603	19/19	0.85	0.13	24,30,36,37	0
3	B3P	F	602	19/19	0.85	0.12	23,29,32,35	0
4	MPD	E	603	8/8	0.87	0.15	20,27,35,45	0
3	B3P	D	604	19/19	0.88	0.15	20,33,70,73	0
4	MPD	F	603	8/8	0.91	0.13	23,27,38,44	0
3	B3P	A	602	19/19	0.91	0.09	17,23,25,26	0
6	CL	A	606	1/1	0.96	0.11	26,26,26,26	0
6	CL	C	603	1/1	0.97	0.07	27,27,27,27	0
6	CL	D	602	1/1	0.97	0.08	23,23,23,23	0
6	CL	E	604	1/1	0.97	0.09	24,24,24,24	0
2	FAD	G	601	53/53	0.98	0.05	11,13,17,18	0
2	FAD	A	601	53/53	0.98	0.04	7,9,12,13	0
6	CL	D	603	1/1	0.98	0.10	18,18,18,18	0
2	FAD	B	601	53/53	0.98	0.04	9,11,13,15	0
6	CL	H	603	1/1	0.98	0.05	24,24,24,24	0
6	CL	B	604	1/1	0.99	0.06	19,19,19,19	0
2	FAD	H	601	53/53	0.99	0.04	10,11,14,15	0
2	FAD	D	601	53/53	0.99	0.04	9,10,13,14	0
2	FAD	E	601	53/53	0.99	0.04	7,10,11,13	0
2	FAD	F	601	53/53	0.99	0.04	8,10,12,14	0
6	CL	F	604	1/1	0.99	0.04	19,19,19,19	0
6	CL	G	602	1/1	0.99	0.05	22,22,22,22	0
2	FAD	C	601	53/53	0.99	0.04	10,11,14,15	0

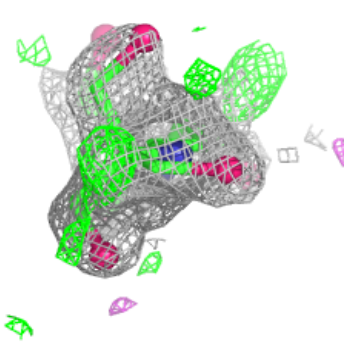
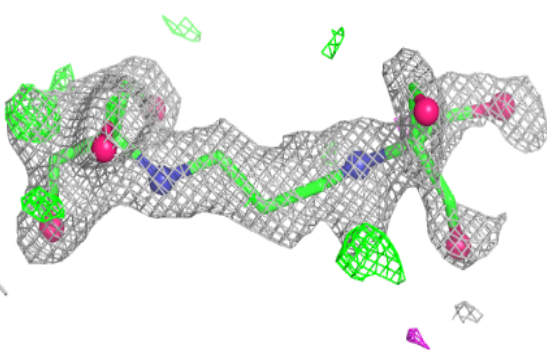
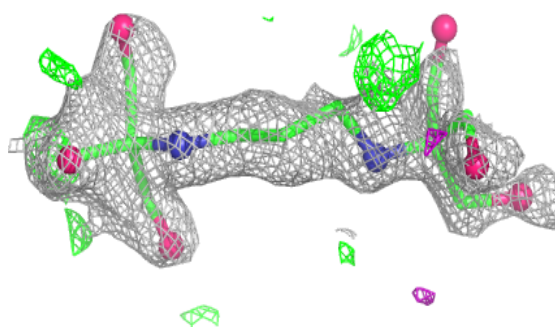
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3P H 602:

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

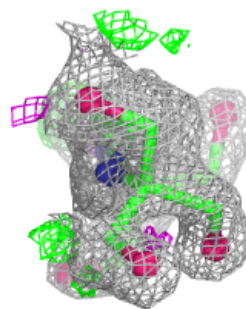
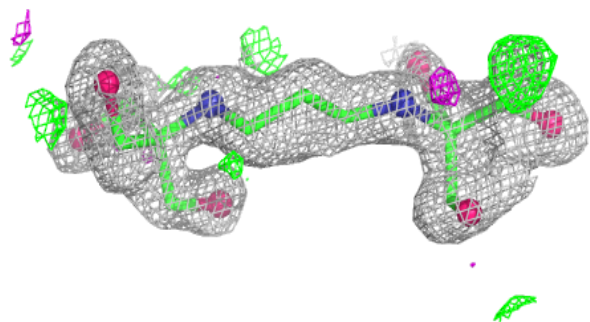
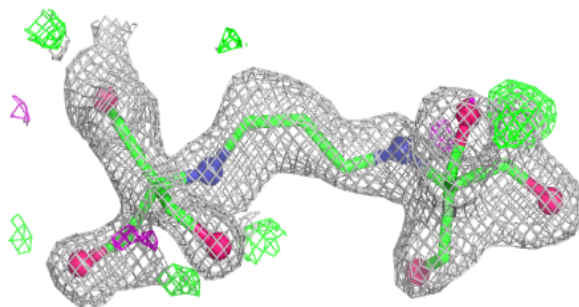
**Electron density around B3P B 602:**

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

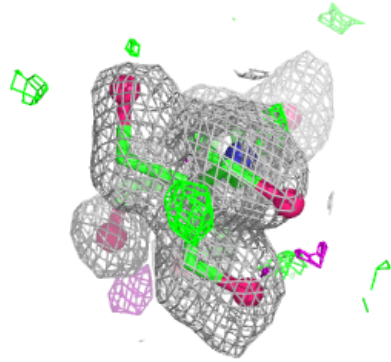
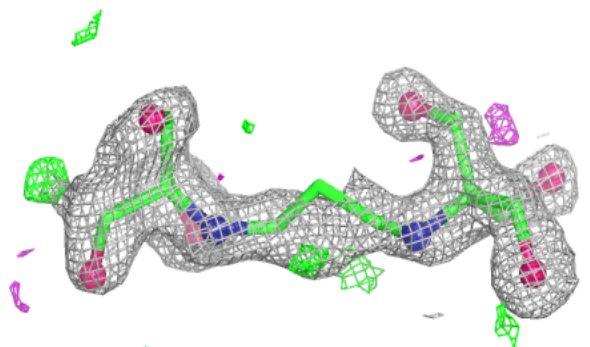
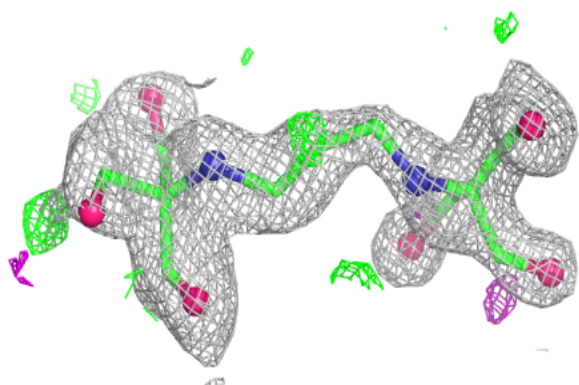


Electron density around B3P E 602:

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

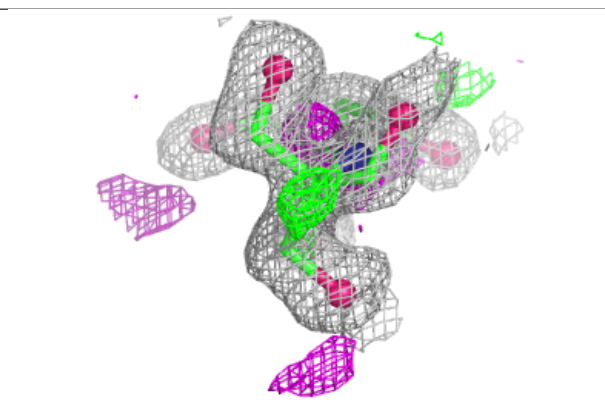
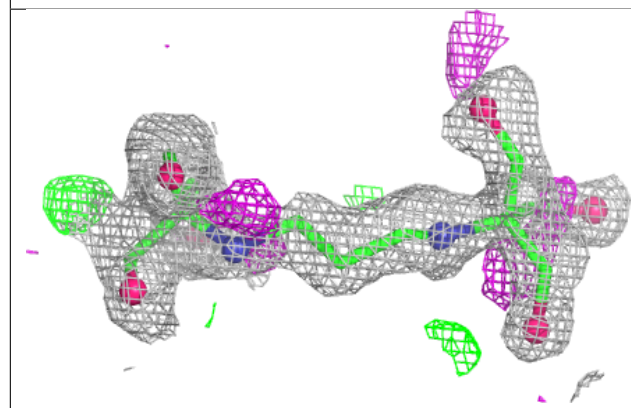
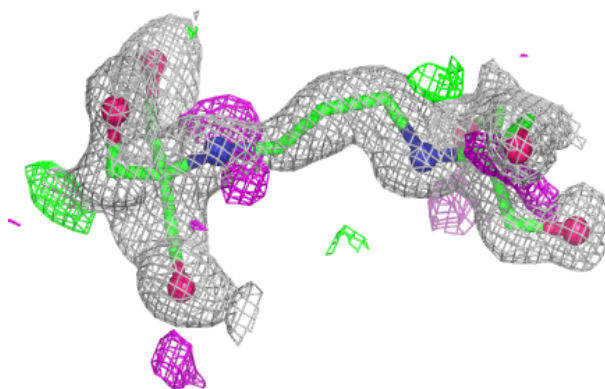
**Electron density around B3P C 602:**

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

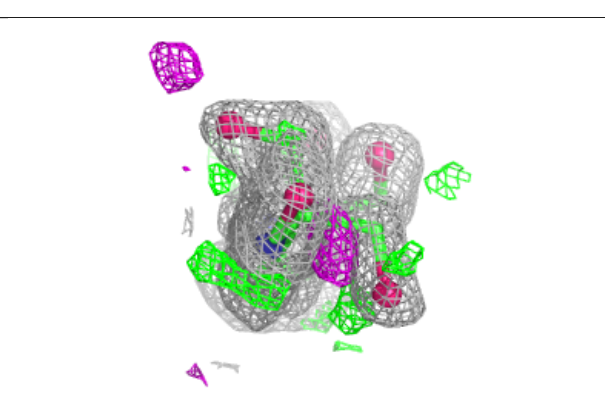
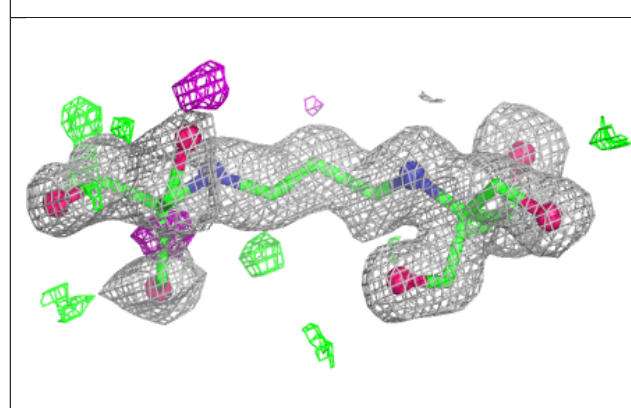
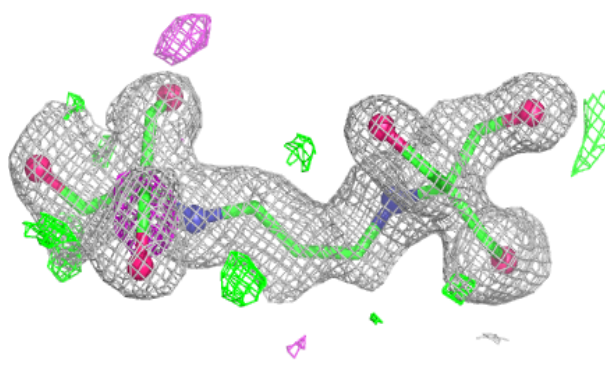


Electron density around B3P A 603:

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

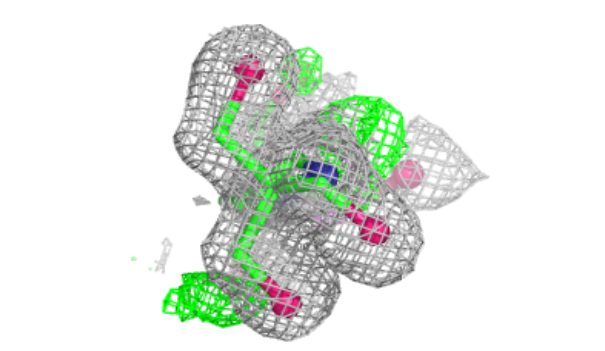
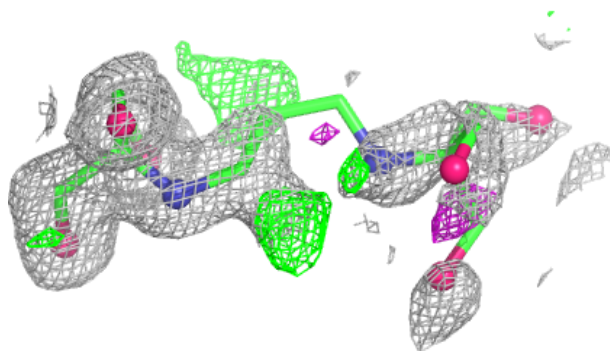
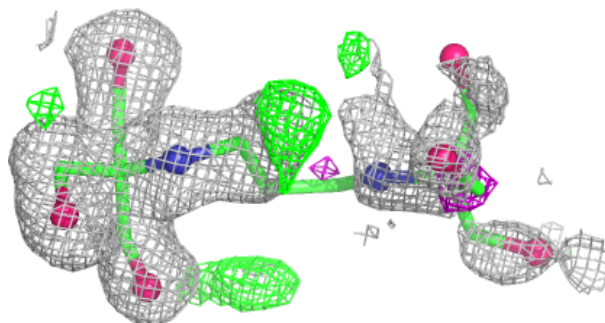
**Electron density around B3P F 602:**

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

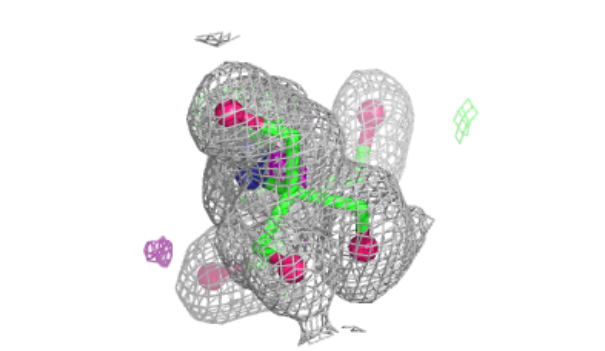
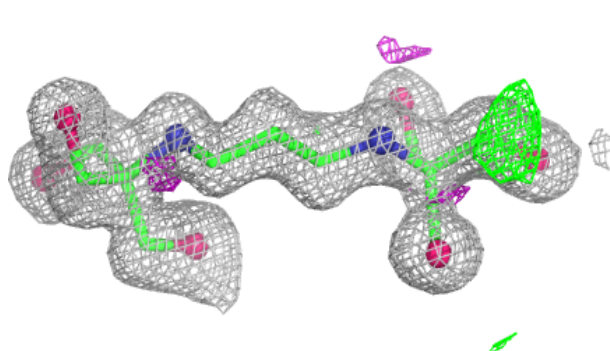
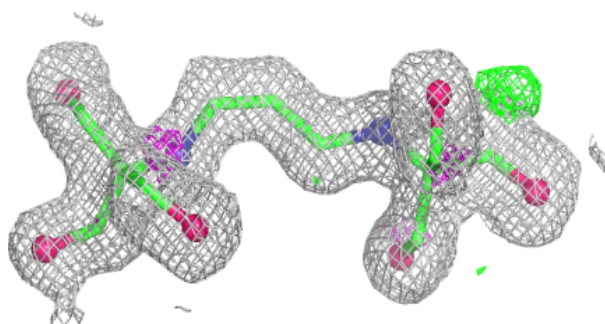


Electron density around B3P D 604:

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

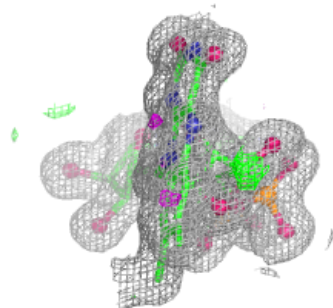
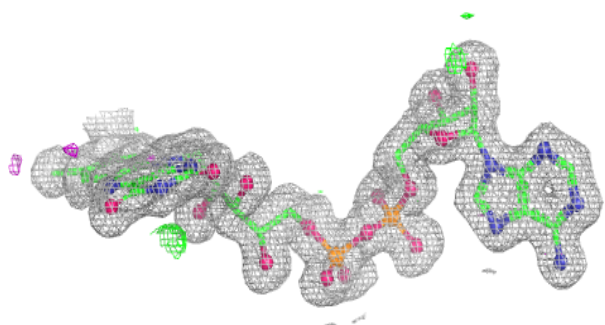
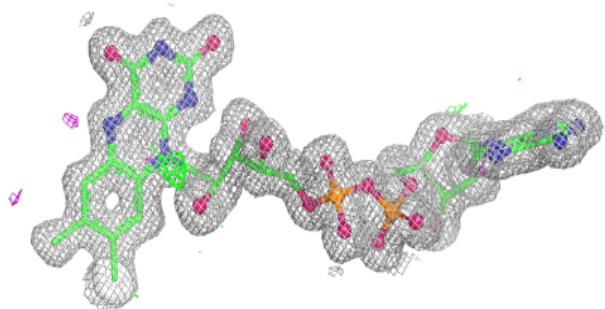
**Electron density around B3P A 602:**

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

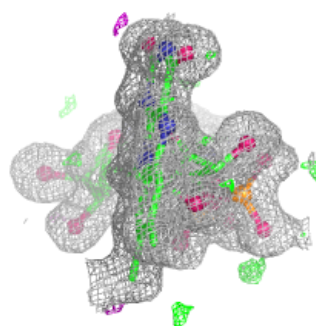
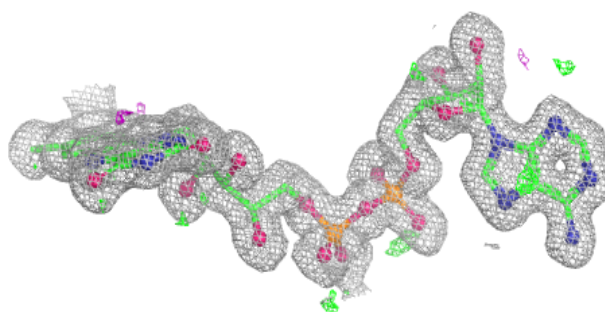
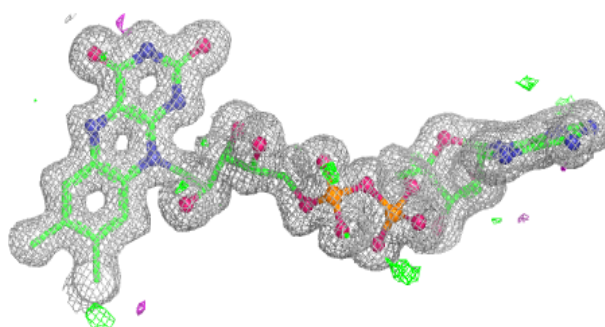


Electron density around FAD G 601:

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

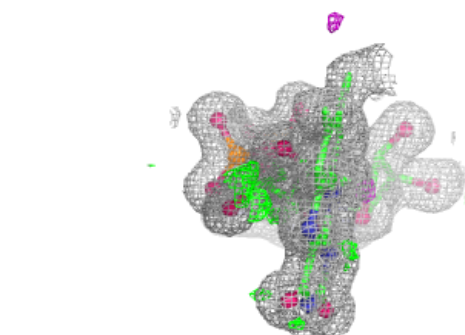
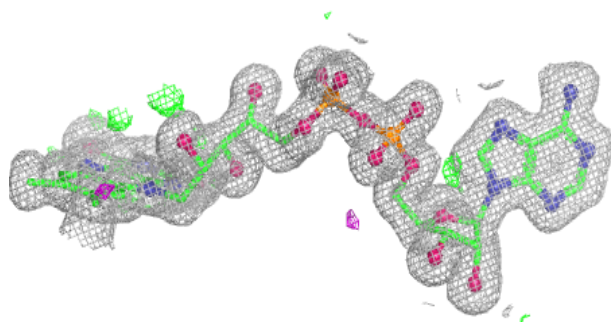
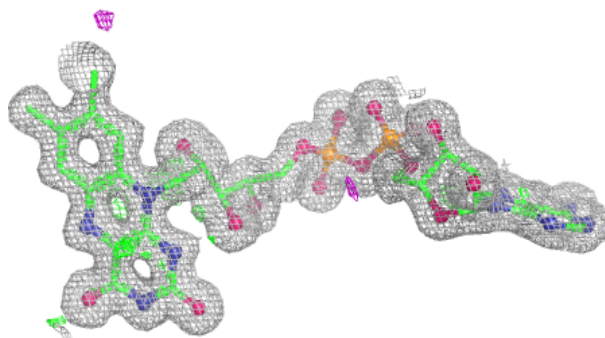
**Electron density around FAD A 601:**

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

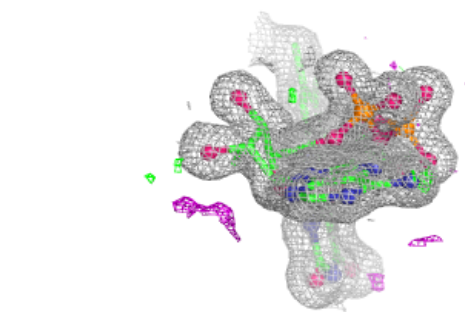
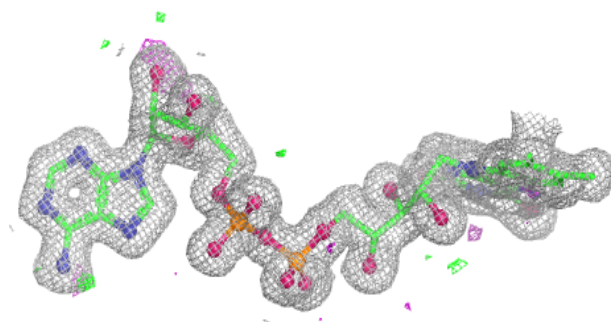
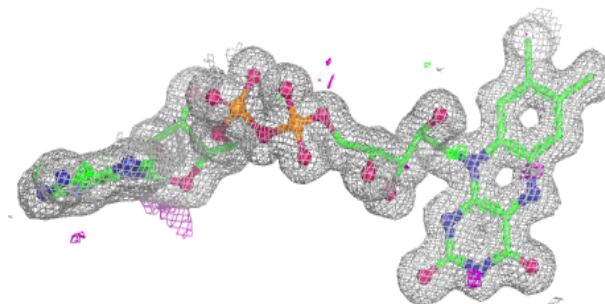


Electron density around FAD B 601:

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

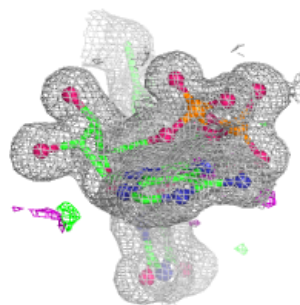
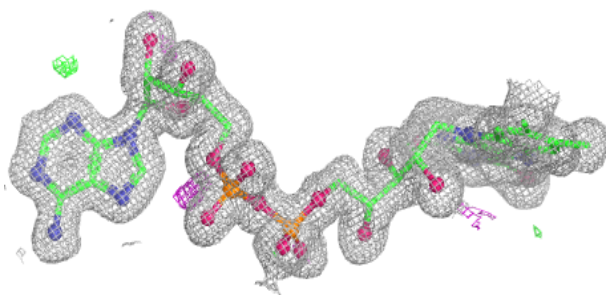
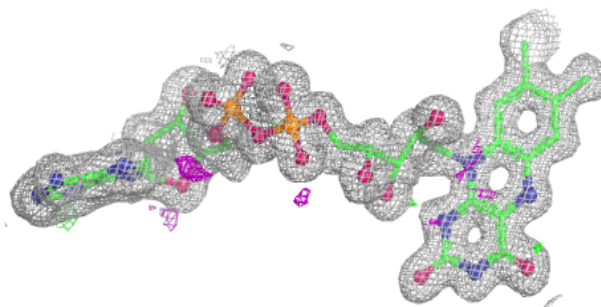
**Electron density around FAD H 601:**

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

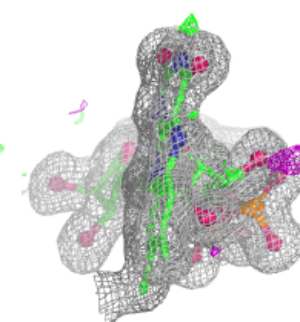
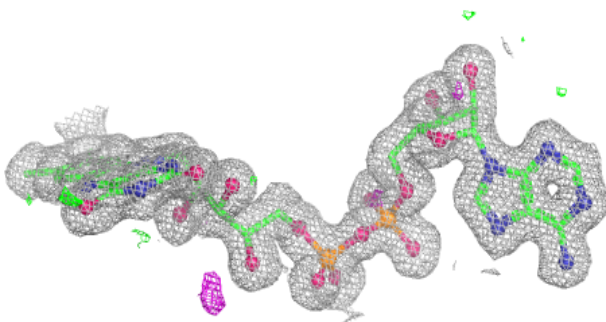
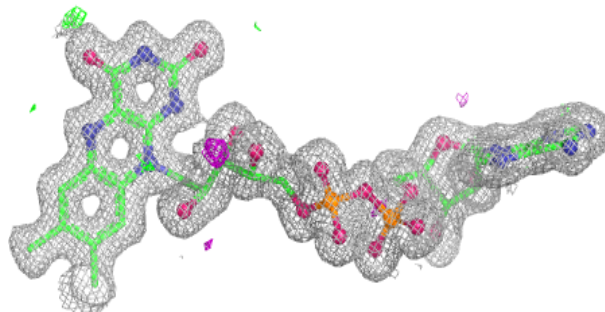


Electron density around FAD D 601:

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

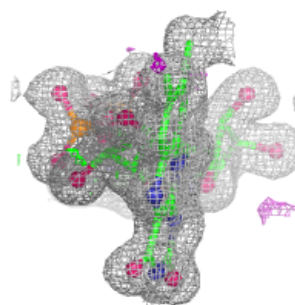
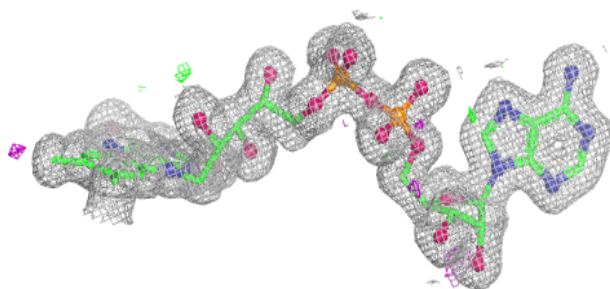
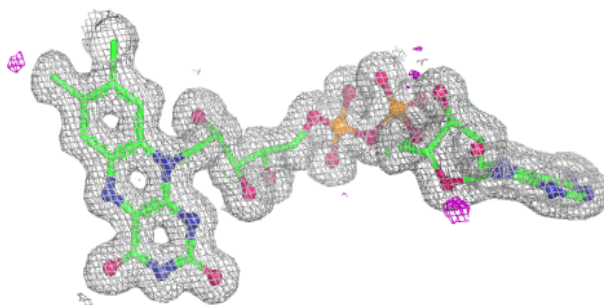
**Electron density around FAD E 601:**

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

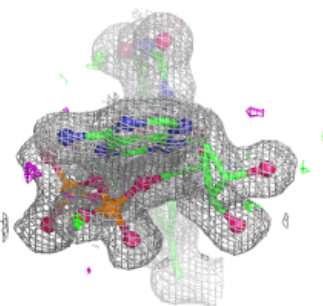
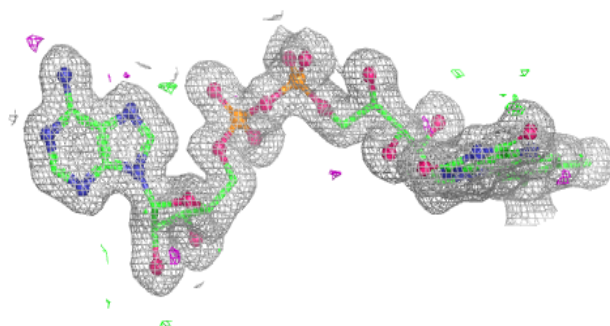
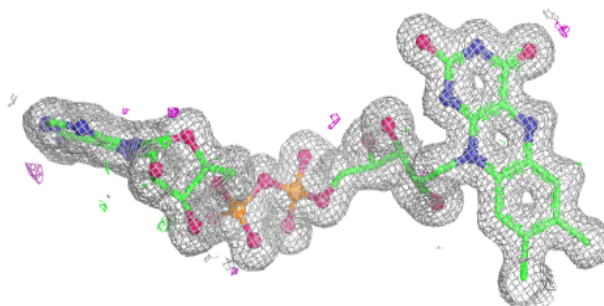


Electron density around FAD F 601:

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

**Electron density around FAD C 601:**

$2mF_o-DF_c$ (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.