



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 20, 2025 – 09:50 pm GMT

PDB ID : 9H8Q  
Title : Eugenol Oxidase (EUGO) from *Rhodococcus jostii* RHA1, mutant DTT-T425G  
Authors : Rozeboom, H.J.; Fraaije, M.W.  
Deposited on : 2024-10-29  
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

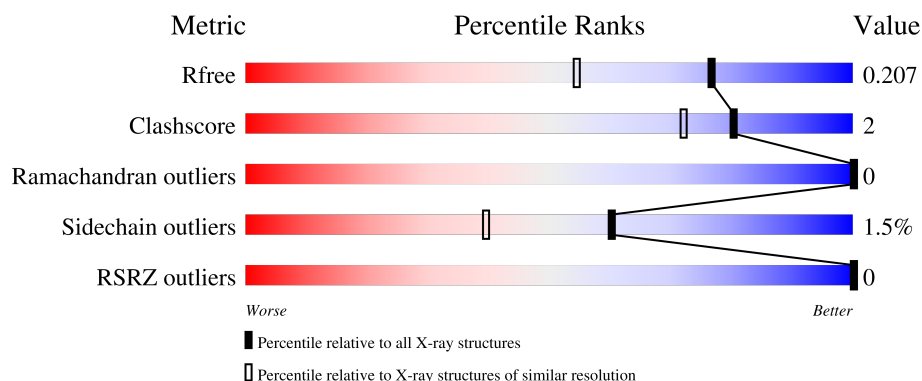
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

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



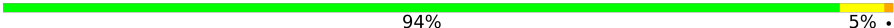

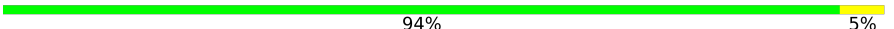
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	526	<div> <div>92%</div> <div>7%</div> </div>
1	B	526	<div> <div>94%</div> <div>6%</div> </div>
1	C	526	<div> <div>94%</div> <div>5%</div> </div>
1	D	526	<div> <div>94%</div> <div>5%</div> </div>
1	E	526	<div> <div>92%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	526	 94% 5% •
1	G	526	 93% 6% •
1	H	526	 94% 5% •

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36661 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	2	0
			4146	2642	702	776	26			
1	B	525	Total	C	N	O	S	0	1	0
			4138	2637	701	775	25			
1	C	525	Total	C	N	O	S	0	3	0
			4154	2646	703	779	26			
1	D	525	Total	C	N	O	S	0	0	0
			4130	2632	700	774	24			
1	E	525	Total	C	N	O	S	0	2	0
			4146	2642	702	776	26			
1	F	525	Total	C	N	O	S	0	0	0
			4130	2632	700	774	24			
1	G	525	Total	C	N	O	S	0	1	0
			4138	2638	701	775	24			
1	H	525	Total	C	N	O	S	0	0	0
			4130	2632	700	774	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	GLY	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	GLY	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	GLY	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	GLY	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	GLY	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	GLY	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	GLY	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	GLY	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

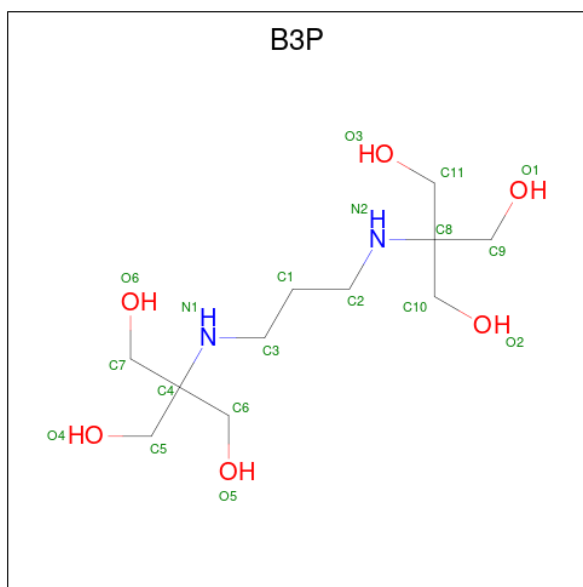
- # FAD

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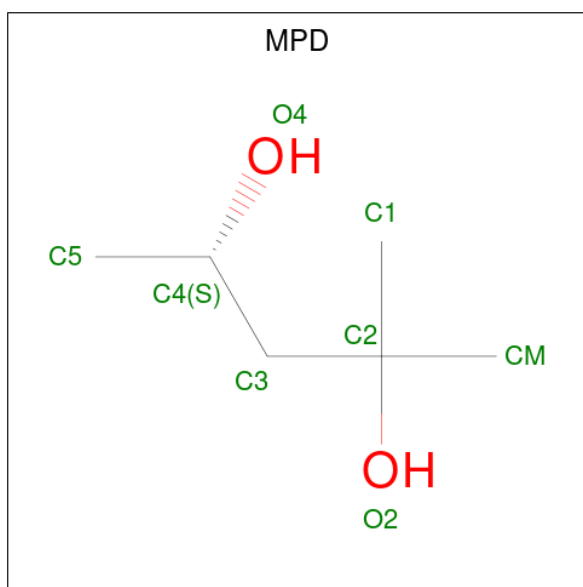
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			53	27	9	15		
2	H	1	Total	C	N	O	0	0
			53	27	9	15		

- Molecule 3 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: 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	F	1	Total	C	N	O	0	0
			19	11	2	6		
3	F	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: 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	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	392	Total	O	0	0
			392	392		

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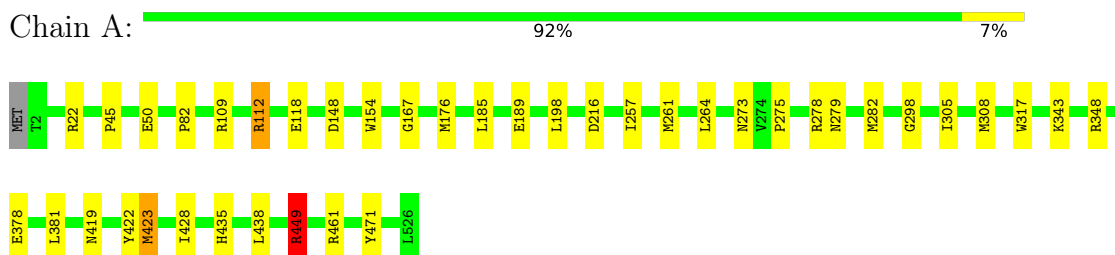
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	371	Total 371	O 371	0	0
6	C	374	Total 374	O 374	0	0
6	D	389	Total 389	O 389	0	0
6	E	420	Total 420	O 420	0	0
6	F	385	Total 385	O 385	0	0
6	G	329	Total 329	O 329	0	0
6	H	339	Total 339	O 339	0	0

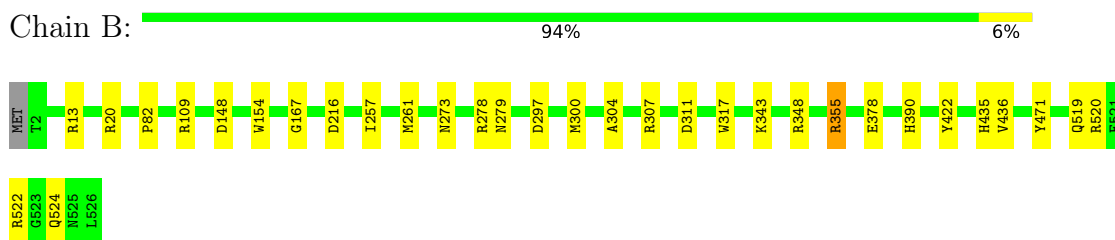
### 3 Residue-property plots

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

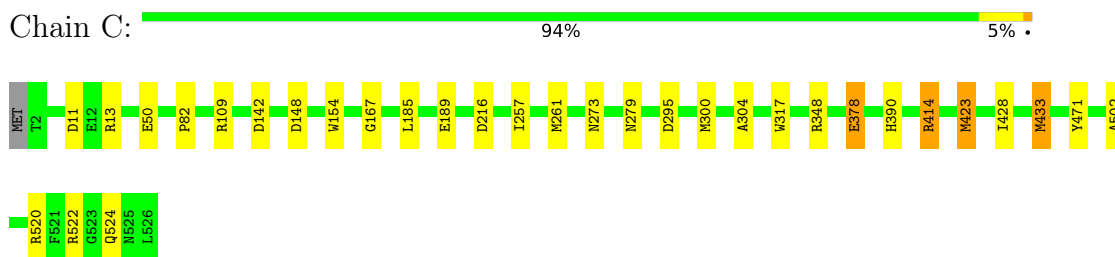
- Molecule 1: Probable vanillyl-alcohol oxidase



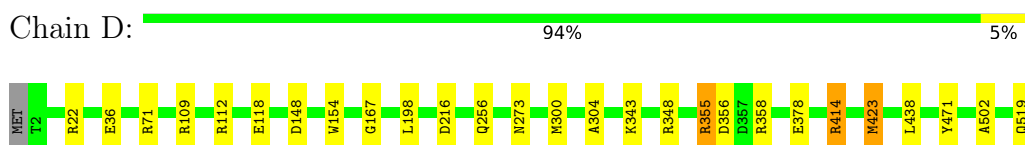
- Molecule 1: Probable vanillyl-alcohol oxidase



- Molecule 1: Probable vanillyl-alcohol oxidase

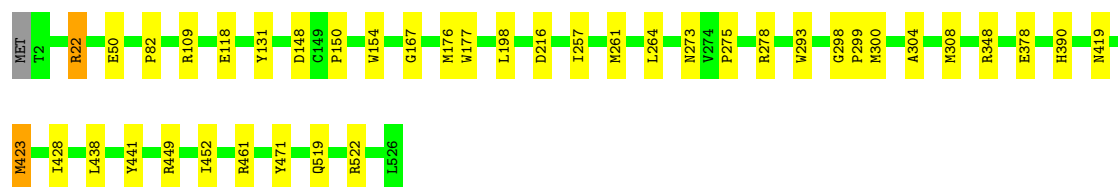


- Molecule 1: Probable vanillyl-alcohol oxidase



- Molecule 1: Probable vanillyl-alcohol oxidase

Chain E:  92% 7%



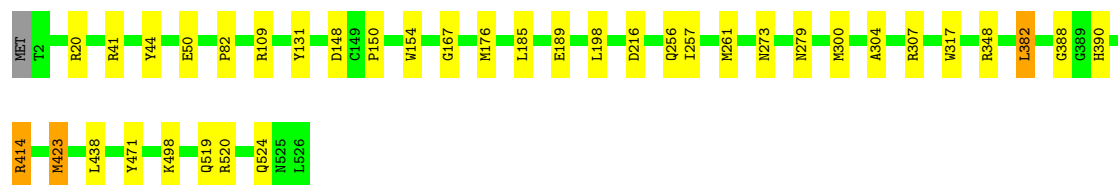
- Molecule 1: Probable vanillyl-alcohol oxidase

Chain F:  94% 5%



- Molecule 1: Probable vanillyl-alcohol oxidase

Chain G:  93% 6%



- Molecule 1: Probable vanillyl-alcohol oxidase

Chain H:  94% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.44Å 110.20Å 117.54Å 89.87° 89.34° 68.51°	Depositor
Resolution (Å)	102.75 – 1.60 102.75 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.2 (102.75-1.60) 93.2 (102.75-1.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.177 , 0.198 0.188 , 0.207	Depositor DCC
$R_{free}$ test set	25315 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 24.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for h,h-k,-l 0.137 for -h,-k,l 0.019 for -h,-h+k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	36661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B3P, FAD, MPD, CL

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	0.48	0/4255	0.85	12/5772 (0.2%)
1	B	0.47	0/4247	0.80	5/5762 (0.1%)
1	C	0.46	0/4263	0.82	8/5783 (0.1%)
1	D	0.51	0/4239	0.85	12/5752 (0.2%)
1	E	0.51	0/4255	0.86	13/5772 (0.2%)
1	F	0.48	0/4239	0.84	9/5752 (0.2%)
1	G	0.43	0/4247	0.79	6/5763 (0.1%)
1	H	0.46	0/4239	0.81	10/5752 (0.2%)
All	All	0.48	0/33984	0.83	75/46108 (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	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	3
1	H	0	1
All	All	0	16

There are no bond length outliers.

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	433	MET	CG-SD-CE	-12.34	80.46	100.20
1	G	176	MET	CG-SD-CE	10.52	117.03	100.20
1	A	423	MET	CG-SD-CE	-10.51	83.39	100.20
1	H	109	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	G	109	ARG	NE-CZ-NH2	-9.39	115.61	120.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
1	A	348	ARG	Sidechain
1	B	20	ARG	Sidechain
1	B	348	ARG	Sidechain
1	C	13	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	4146	0	4012	22	0
1	B	4138	0	4004	20	0
1	C	4154	0	4015	22	0
1	D	4130	0	3996	12	0
1	E	4146	0	4012	24	0
1	F	4130	0	3996	16	0
1	G	4138	0	4006	28	0
1	H	4130	0	3996	13	0
2	A	53	0	30	1	0
2	B	53	0	30	6	0
2	C	53	0	31	7	0
2	D	53	0	30	1	0
2	E	53	0	30	6	0
2	F	53	0	30	1	0
2	G	53	0	31	7	0
2	H	53	0	30	1	0
3	A	38	0	52	0	0
3	F	38	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	8	0	14	1	0
4	B	8	0	14	2	0
4	C	8	0	14	0	0
4	D	8	0	14	0	0
4	F	8	0	14	0	0
4	H	8	0	14	0	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
6	A	392	0	0	5	0
6	B	371	0	0	6	0
6	C	374	0	0	2	0
6	D	389	0	0	6	0
6	E	420	0	0	6	0
6	F	385	0	0	9	0
6	G	329	0	0	4	0
6	H	339	0	0	4	0
All	All	36661	0	32467	164	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 164 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:E:390:HIS:NE2	2:E:600:FAD:C8M	1.68	1.56
1:B:390:HIS:NE2	2:B:601:FAD:C8M	1.69	1.56
1:C:390:HIS:NE2	2:C:600:FAD:C8M	1.74	1.47
1:G:390:HIS:NE2	2:G:600:FAD:C8M	1.79	1.41
1:G:390:HIS:NE2	2:G:600:FAD:HM82	1.02	1.34

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	525/526 (100%)	515 (98%)	10 (2%)	0	100	100
1	B	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
1	C	526/526 (100%)	514 (98%)	12 (2%)	0	100	100
1	D	523/526 (99%)	512 (98%)	11 (2%)	0	100	100
1	E	525/526 (100%)	514 (98%)	11 (2%)	0	100	100
1	F	523/526 (99%)	511 (98%)	12 (2%)	0	100	100
1	G	524/526 (100%)	512 (98%)	12 (2%)	0	100	100
1	H	523/526 (99%)	513 (98%)	10 (2%)	0	100	100
All	All	4193/4208 (100%)	4103 (98%)	90 (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	435/434 (100%)	429 (99%)	6 (1%)	62	43
1	B	434/434 (100%)	427 (98%)	7 (2%)	58	37
1	C	436/434 (100%)	428 (98%)	8 (2%)	54	31
1	D	433/434 (100%)	426 (98%)	7 (2%)	58	37
1	E	435/434 (100%)	430 (99%)	5 (1%)	70	53
1	F	433/434 (100%)	426 (98%)	7 (2%)	58	37
1	G	434/434 (100%)	427 (98%)	7 (2%)	58	37
1	H	433/434 (100%)	427 (99%)	6 (1%)	62	43
All	All	3473/3472 (100%)	3420 (98%)	53 (2%)	60	39

5 of 53 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	E	154	TRP
1	F	273	ASN
1	H	216	ASP
1	E	198	LEU
1	E	471	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	256	GLN
1	H	205	GLN
1	F	67	GLN
1	H	419	ASN
1	G	419	ASN

### 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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	B	602	-	7,7,7	0.35	0	9,10,10	0.44	0
2	FAD	H	602	-	53,58,58	0.69	0	68,89,89	0.95	4 (5%)
4	MPD	F	603	-	7,7,7	0.21	0	9,10,10	0.62	0
3	B3P	F	602	-	18,18,18	0.20	0	21,23,23	0.80	0
4	MPD	H	601	-	7,7,7	0.25	0	9,10,10	0.34	0
4	MPD	C	601	-	7,7,7	0.21	0	9,10,10	0.56	0
2	FAD	B	601	-	53,58,58	0.70	0	68,89,89	1.00	5 (7%)
2	FAD	G	600	-	53,58,58	0.67	0	68,89,89	0.82	1 (1%)
2	FAD	C	600	-	53,58,58	0.74	1 (1%)	68,89,89	0.75	0
2	FAD	F	601	-	53,58,58	0.83	1 (1%)	68,89,89	0.98	2 (2%)
2	FAD	A	600	-	53,58,58	0.81	1 (1%)	68,89,89	0.85	3 (4%)
4	MPD	A	603	-	7,7,7	0.30	0	9,10,10	0.42	0
3	B3P	A	601	-	18,18,18	0.36	0	21,23,23	0.80	1 (4%)
3	B3P	A	602	-	18,18,18	0.21	0	21,23,23	0.82	1 (4%)
4	MPD	D	601	-	7,7,7	0.20	0	9,10,10	0.40	0
2	FAD	D	600	-	53,58,58	0.77	1 (1%)	68,89,89	1.07	4 (5%)
3	B3P	F	604	-	18,18,18	0.23	0	21,23,23	1.04	1 (4%)
2	FAD	E	600	-	53,58,58	0.65	0	68,89,89	0.83	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	B	602	-	-	1/5/5/5	-
2	FAD	H	602	-	-	7/30/50/50	0/6/6/6
4	MPD	F	603	-	-	0/5/5/5	-
3	B3P	F	602	-	-	3/28/28/28	-
4	MPD	H	601	-	-	0/5/5/5	-
4	MPD	C	601	-	-	1/5/5/5	-
2	FAD	B	601	-	-	5/30/50/50	0/6/6/6
2	FAD	G	600	-	-	5/30/50/50	0/6/6/6
2	FAD	C	600	-	-	6/30/50/50	0/6/6/6
2	FAD	F	601	-	-	4/30/50/50	0/6/6/6
2	FAD	A	600	-	-	4/30/50/50	0/6/6/6
4	MPD	A	603	-	-	0/5/5/5	-
3	B3P	A	601	-	-	3/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B3P	A	602	-	-	0/28/28/28	-
4	MPD	D	601	-	-	0/5/5/5	-
2	FAD	D	600	-	-	3/30/50/50	0/6/6/6
3	B3P	F	604	-	-	9/28/28/28	-
2	FAD	E	600	-	-	5/30/50/50	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	C1'-C2'	2.49	1.56	1.52
2	C	600	FAD	C8A-N7A	-2.30	1.30	1.34
2	A	600	FAD	C8A-N7A	-2.22	1.30	1.34
2	F	601	FAD	O4B-C1B	2.13	1.44	1.41

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	O2'-C2'-C3'	-4.04	99.27	109.10
2	D	600	FAD	P-O3P-PA	-3.45	120.99	132.83
2	D	600	FAD	O2'-C2'-C3'	-3.42	100.79	109.10
2	F	601	FAD	P-O3P-PA	-3.15	122.02	132.83
2	E	600	FAD	P-O3P-PA	-3.00	122.52	132.83

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	602	B3P	N1-C4-C7-O6
3	F	602	B3P	C5-C4-C7-O6
3	F	602	B3P	C6-C4-C7-O6
3	F	604	B3P	C6-C4-C5-O4
3	F	604	B3P	N1-C4-C7-O6

There are no ring outliers.

11 monomers are involved in 34 short contacts:

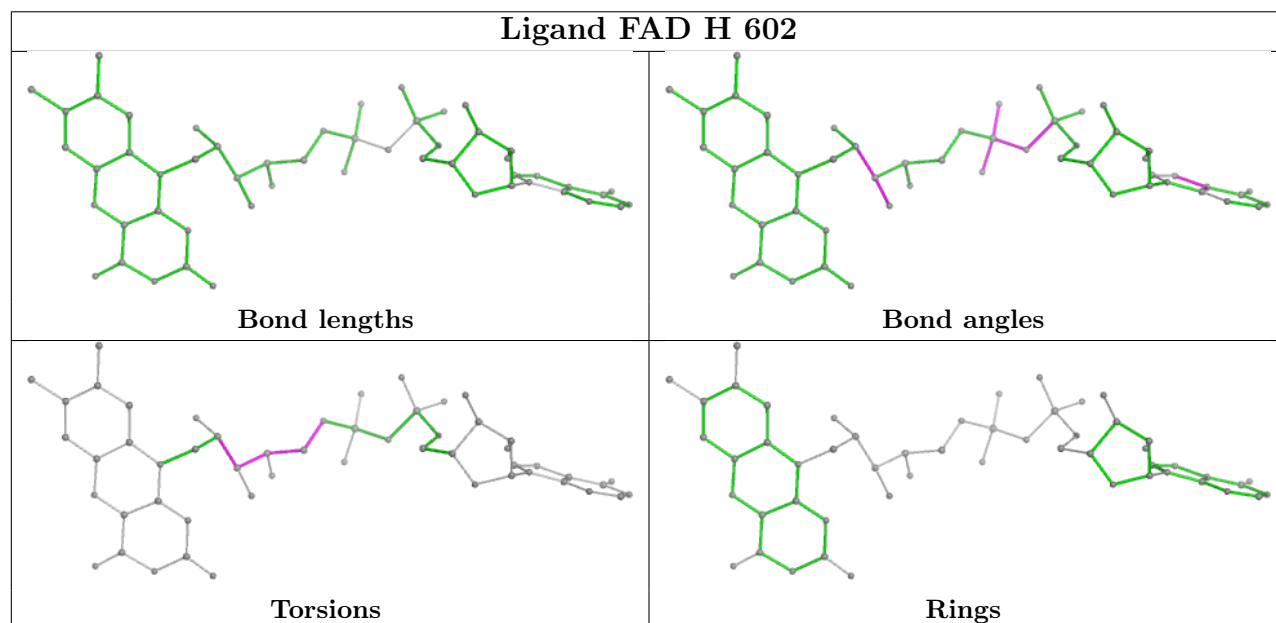
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	MPD	2	0
2	H	602	FAD	1	0
2	B	601	FAD	6	0

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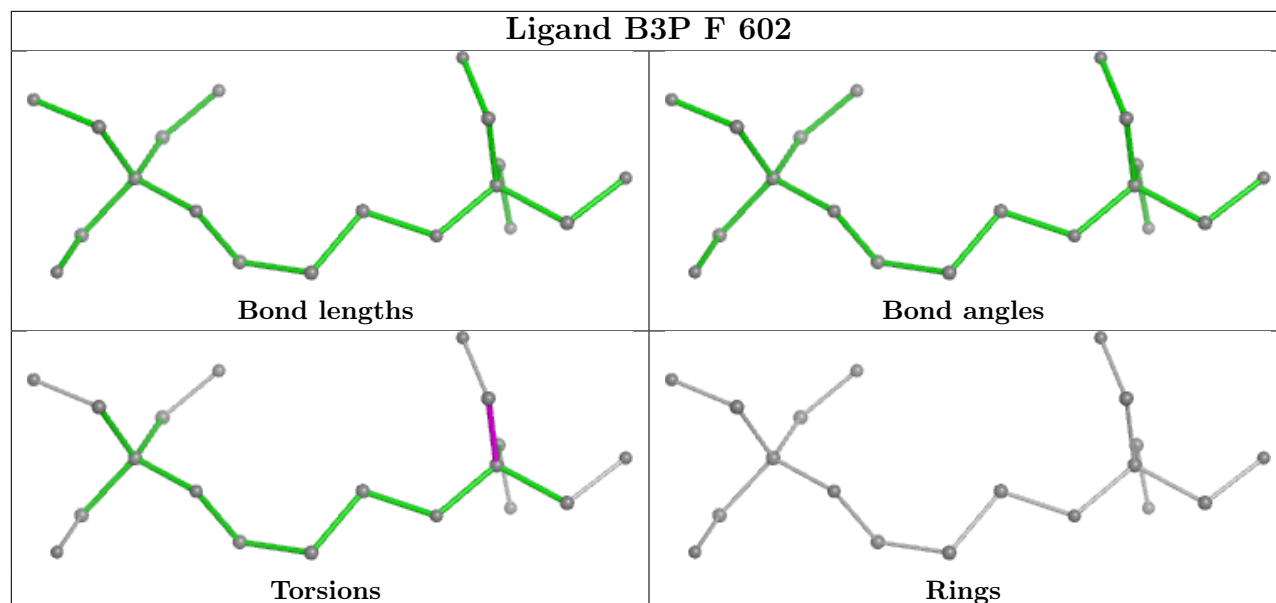
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	600	FAD	7	0
2	C	600	FAD	7	0
2	F	601	FAD	1	0
2	A	600	FAD	1	0
4	A	603	MPD	1	0
2	D	600	FAD	1	0
3	F	604	B3P	1	0
2	E	600	FAD	6	0

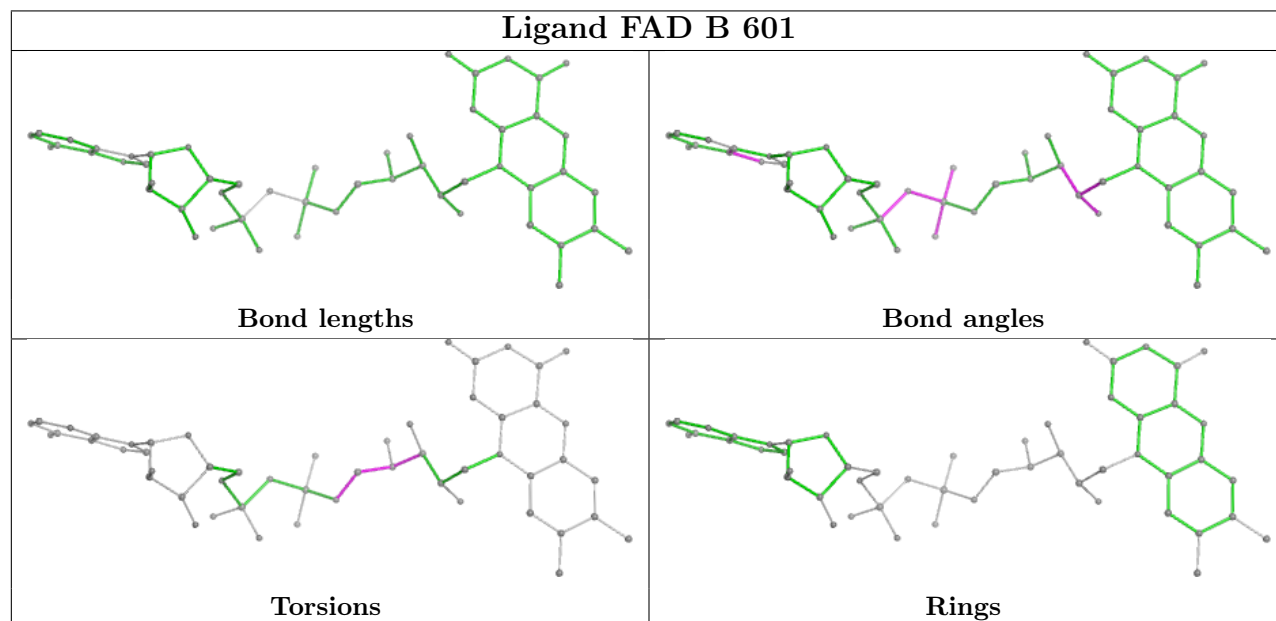
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

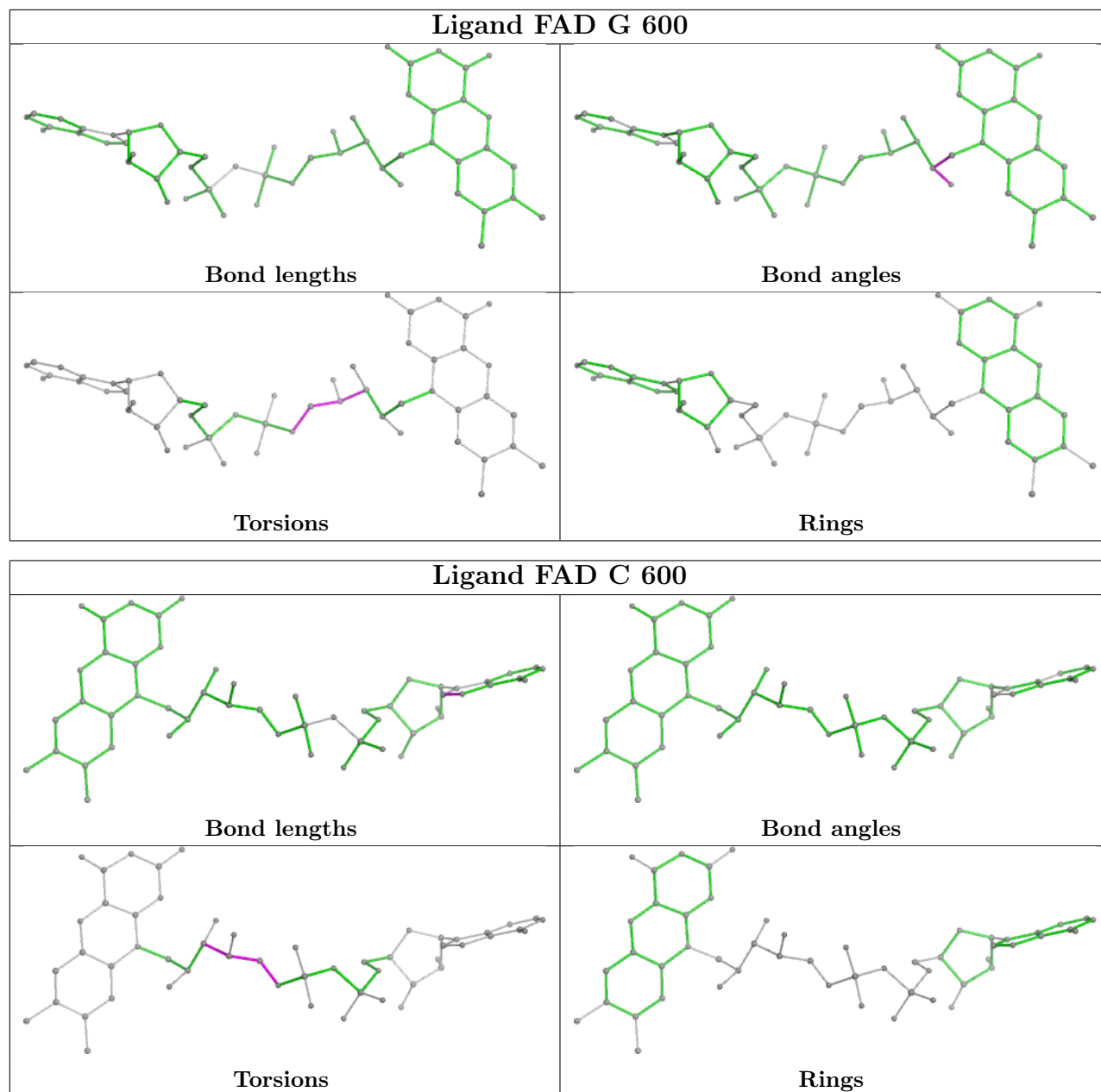


## Ligand B3P F 602

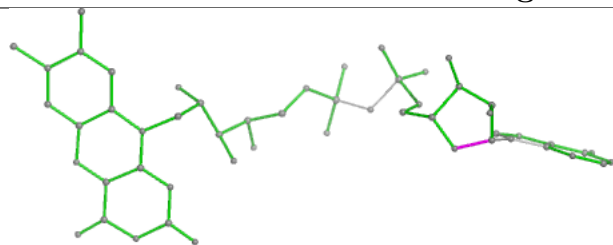


## Ligand FAD B 601

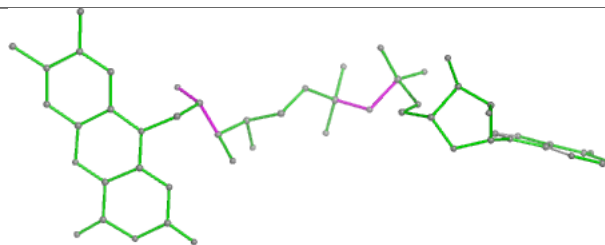




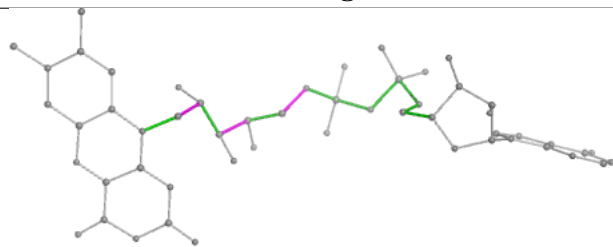
## Ligand FAD F 601



Bond lengths



Bond angles

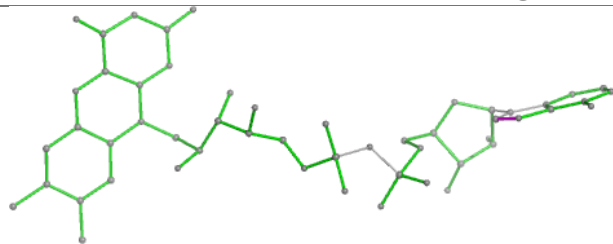


Torsions

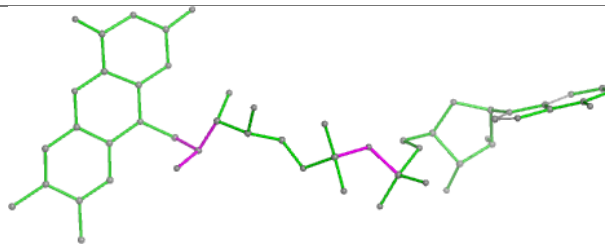


Rings

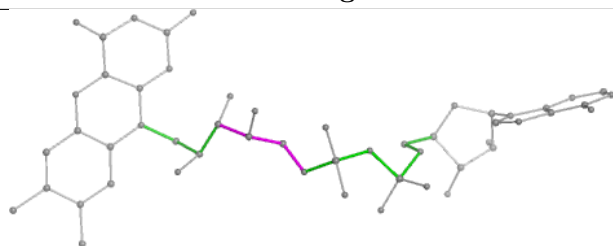
## Ligand FAD A 600



Bond lengths



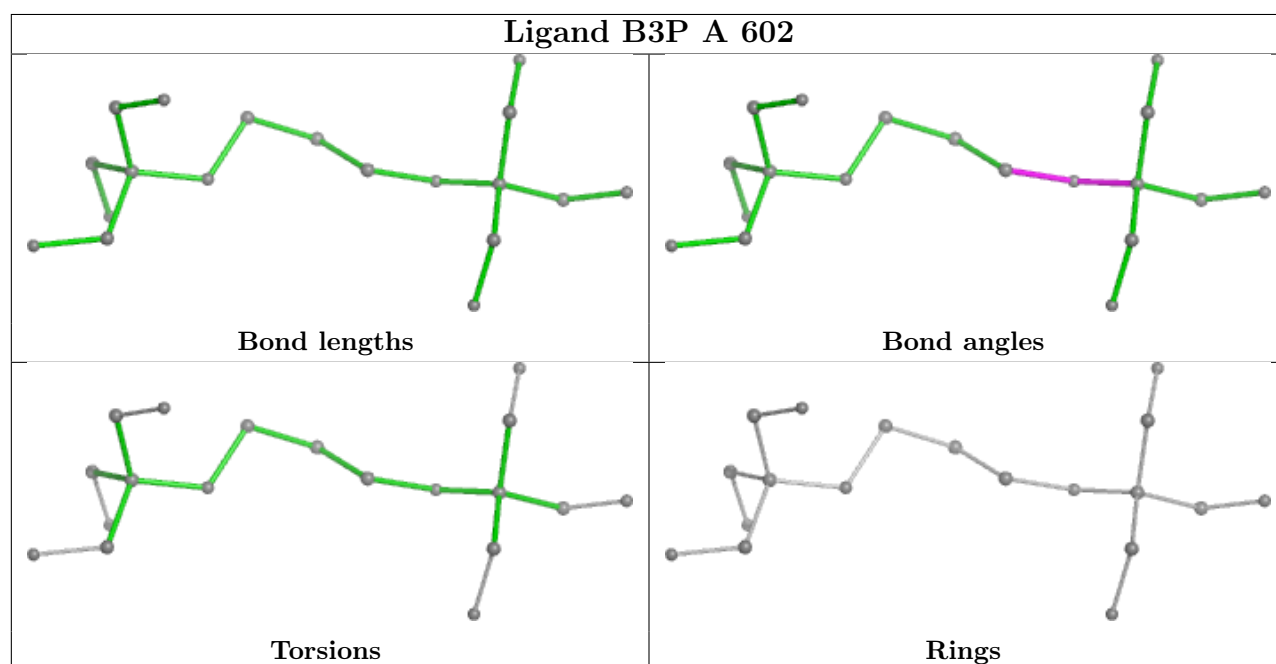
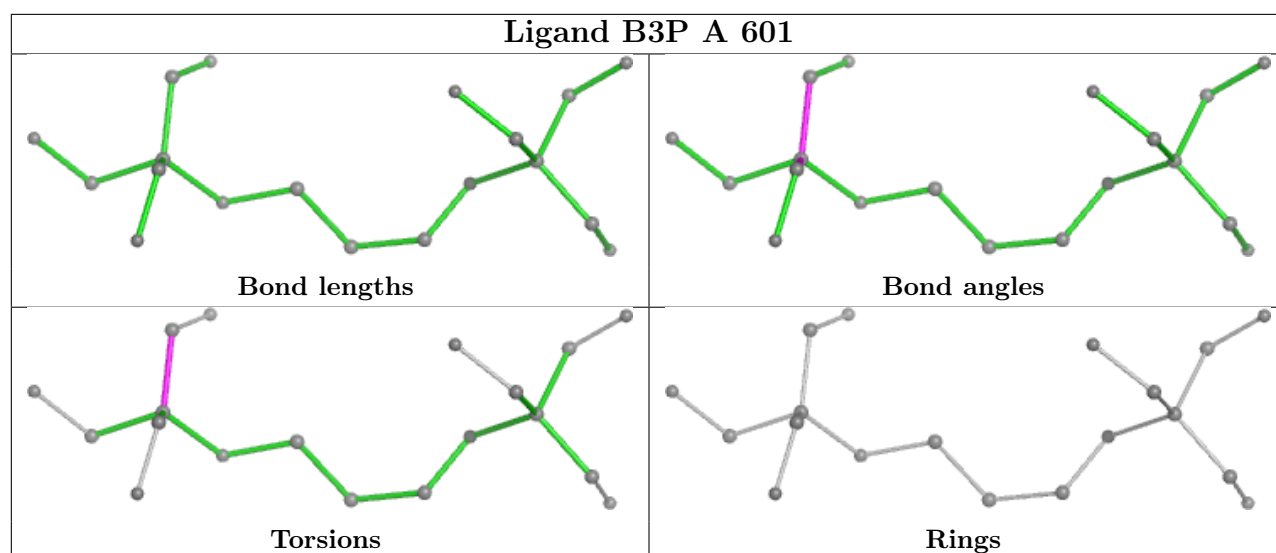
Bond angles



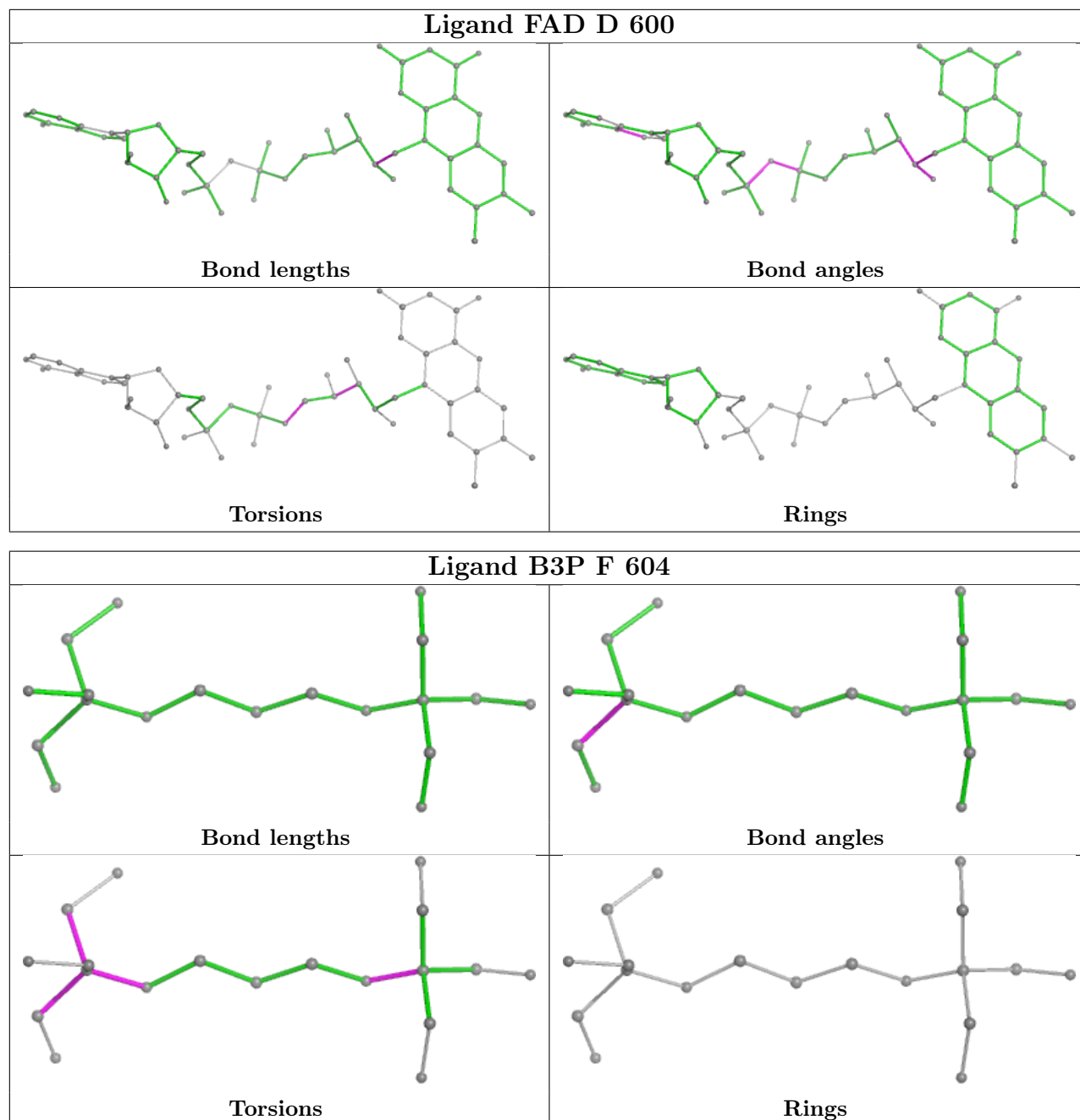
Torsions

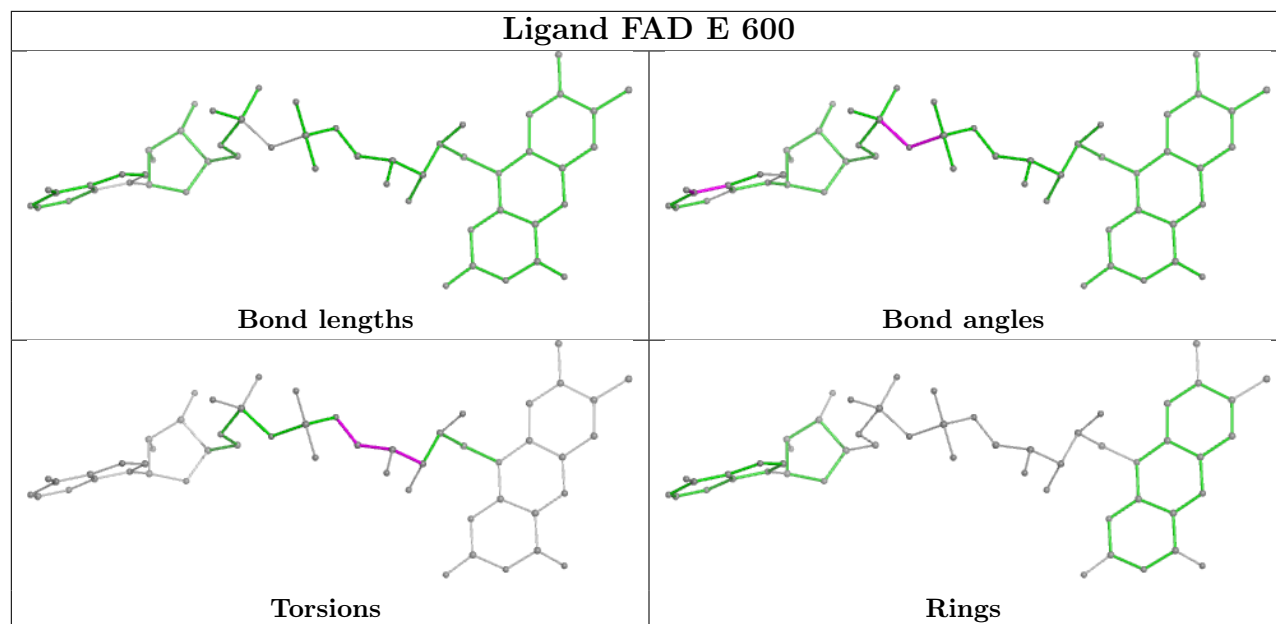


Rings









## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	525/526 (99%)	-1.30	0 100 100	10, 18, 31, 56	2 (0%)
1	B	525/526 (99%)	-1.28	0 100 100	11, 18, 33, 63	1 (0%)
1	C	525/526 (99%)	-1.25	0 100 100	10, 19, 34, 59	3 (0%)
1	D	525/526 (99%)	-1.31	0 100 100	10, 16, 32, 60	0
1	E	525/526 (99%)	-1.32	0 100 100	10, 17, 29, 66	2 (0%)
1	F	525/526 (99%)	-1.28	0 100 100	10, 17, 31, 71	0
1	G	525/526 (99%)	-1.20	0 100 100	11, 22, 40, 61	1 (0%)
1	H	525/526 (99%)	-1.26	0 100 100	12, 18, 34, 73	0
All	All	4200/4208 (99%)	-1.27	0 100 100	10, 18, 34, 73	9 (0%)

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

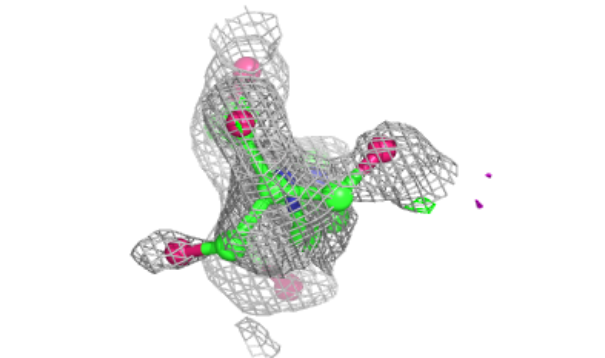
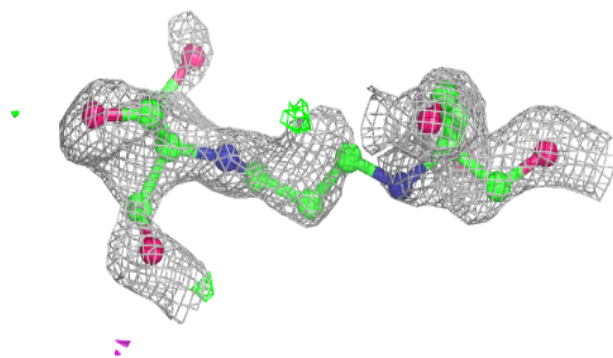
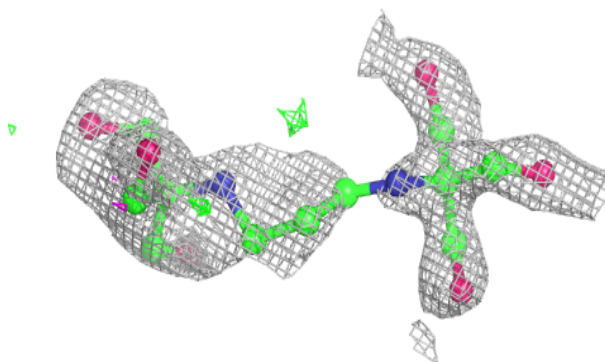
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	B3P	A	602	19/19	0.97	0.05	37,47,52,53	0
3	B3P	F	602	19/19	0.97	0.06	30,35,43,51	0
3	B3P	A	601	19/19	0.98	0.04	26,31,37,38	0
3	B3P	F	604	19/19	0.98	0.05	22,27,39,42	0
4	MPD	A	603	8/8	0.98	0.06	31,33,35,40	0
4	MPD	C	601	8/8	0.98	0.05	31,32,34,35	0
4	MPD	H	601	8/8	0.98	0.05	27,29,32,33	0
4	MPD	B	602	8/8	0.99	0.04	29,30,32,33	0
2	FAD	E	600	53/53	0.99	0.02	11,13,16,20	0
4	MPD	D	601	8/8	0.99	0.04	25,28,31,32	0
4	MPD	F	603	8/8	0.99	0.05	27,29,32,33	0
2	FAD	C	600	53/53	0.99	0.02	12,14,17,18	0
2	FAD	G	600	53/53	1.00	0.02	12,16,19,22	0
2	FAD	H	602	53/53	1.00	0.02	9,11,14,18	0
2	FAD	A	600	53/53	1.00	0.02	11,13,16,20	0
2	FAD	D	600	53/53	1.00	0.02	11,13,15,17	0
2	FAD	B	601	53/53	1.00	0.02	12,14,16,21	0
2	FAD	F	601	53/53	1.00	0.02	11,13,15,20	0
5	CL	B	603	1/1	1.00	0.04	25,25,25,25	0
5	CL	F	605	1/1	1.00	0.04	22,22,22,22	0

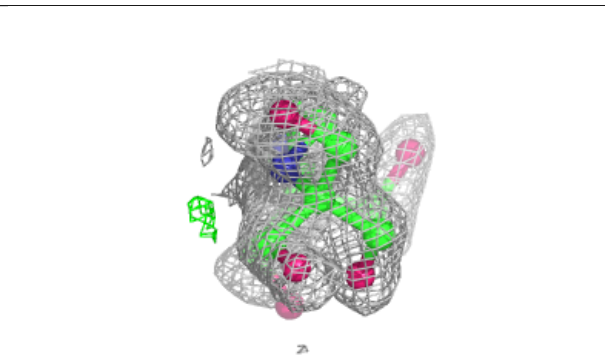
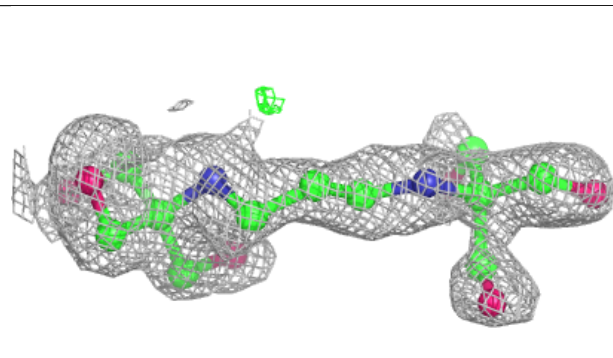
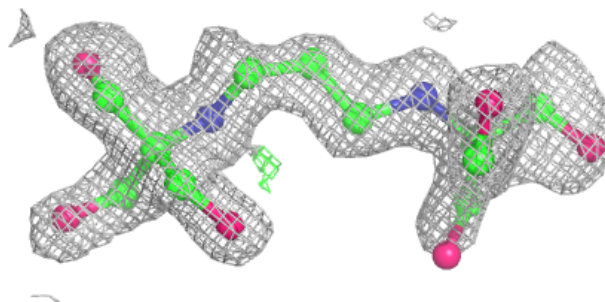
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around B3P 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)

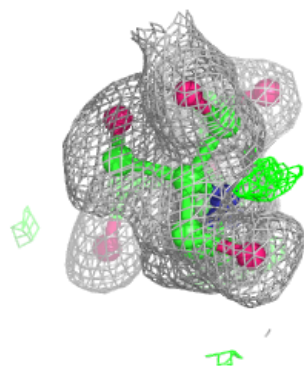
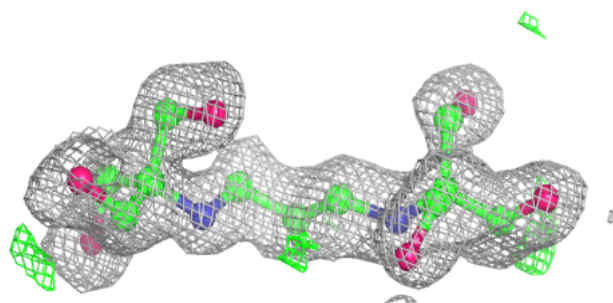
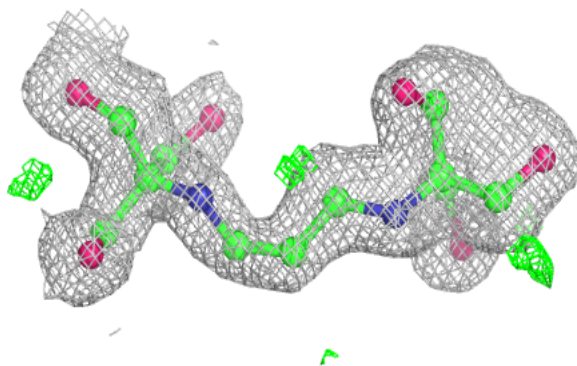
**Electron density around B3P F 602:**

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and green (positive)

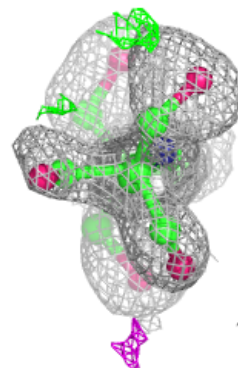
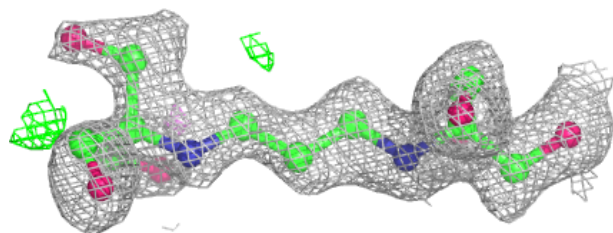
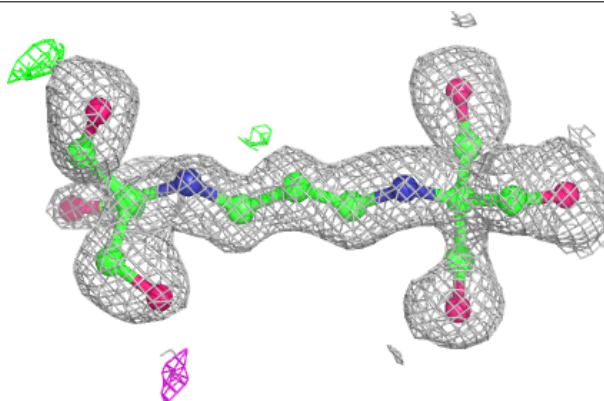


**Electron density around B3P A 601:**

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

**Electron density around B3P F 604:**

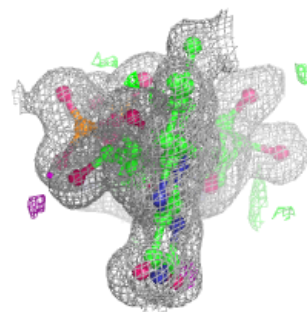
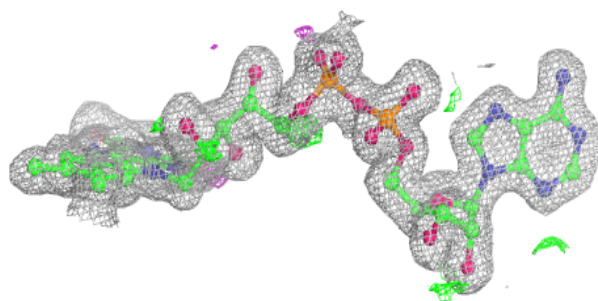
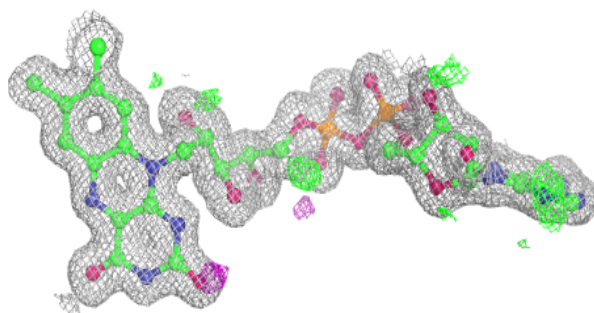
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



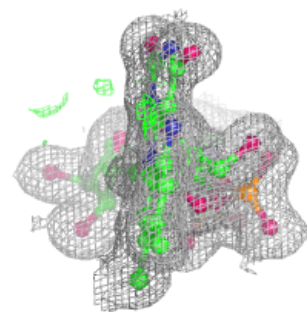
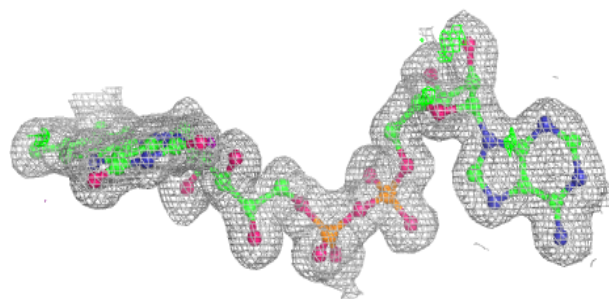
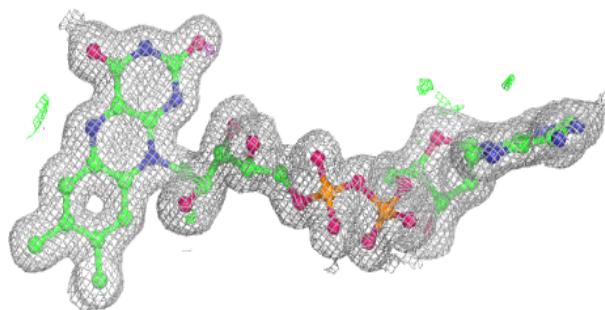


**Electron density around FAD E 600:**

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and green (positive)

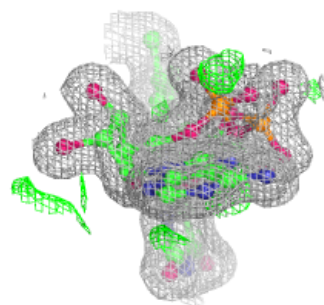
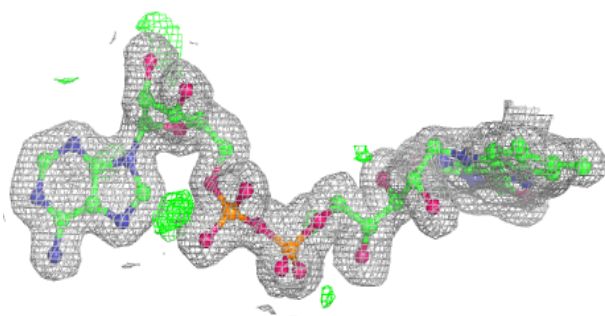
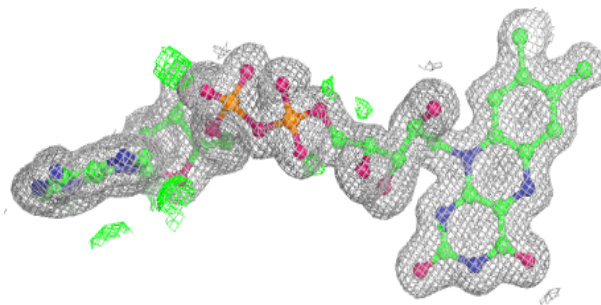
**Electron density around FAD C 600:**

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and green (positive)

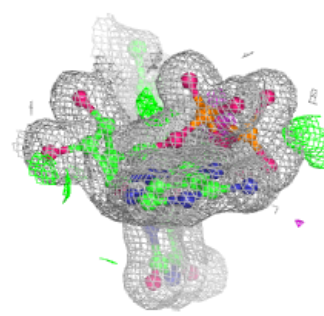
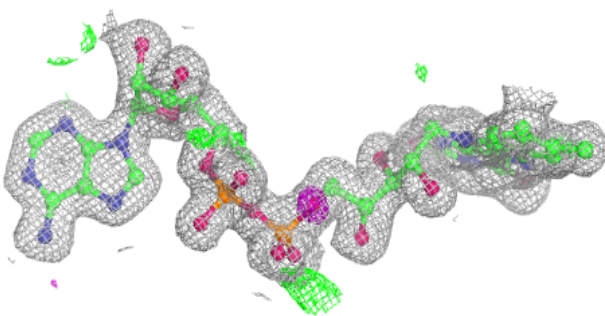
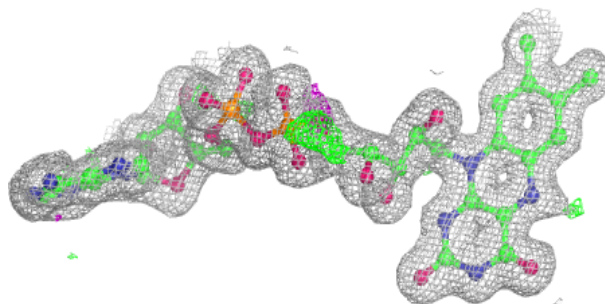


**Electron density around FAD G 600:**

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

**Electron density around FAD H 602:**

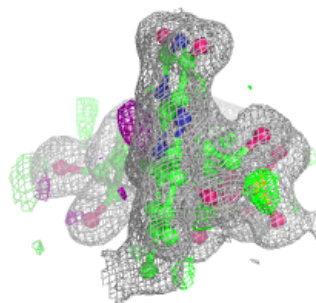
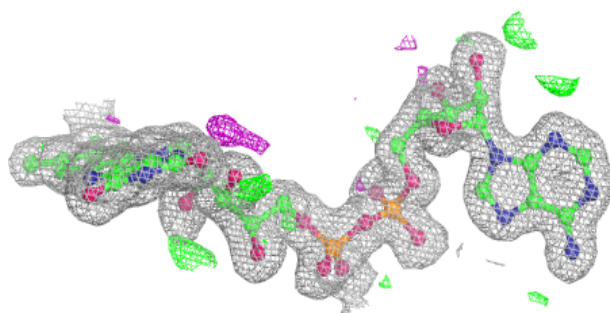
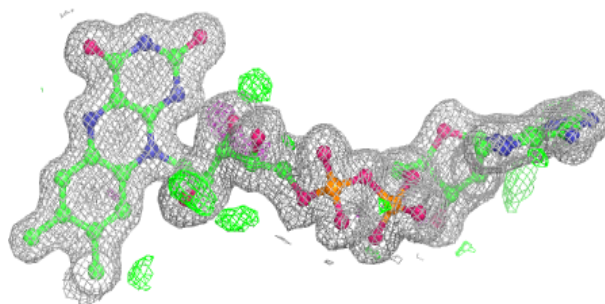
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



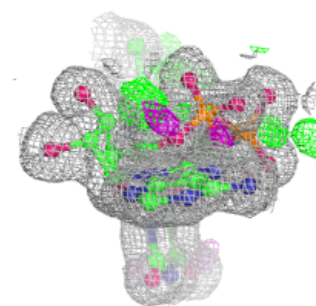
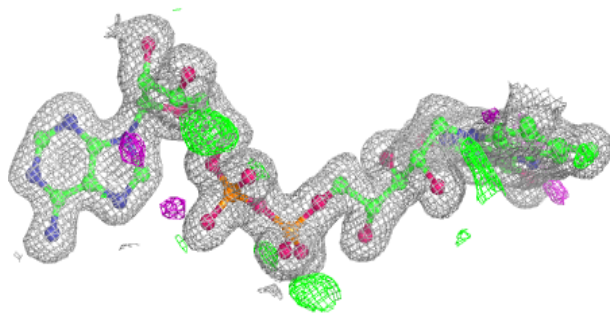
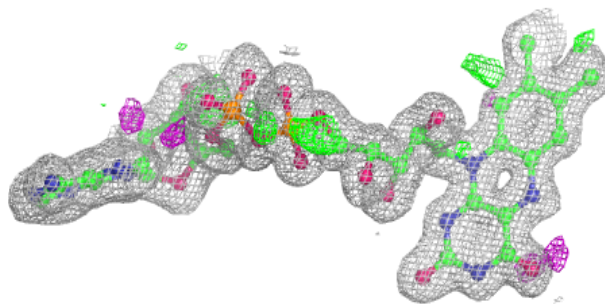


**Electron density around FAD A 600:**

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

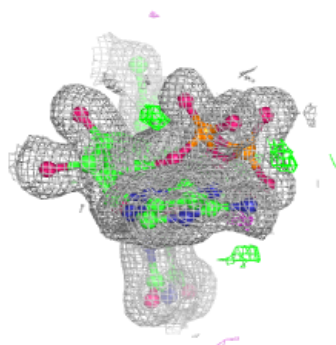
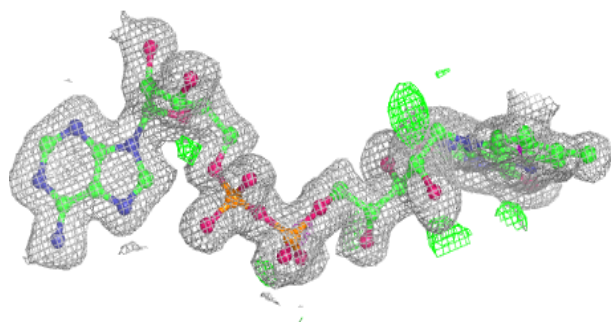
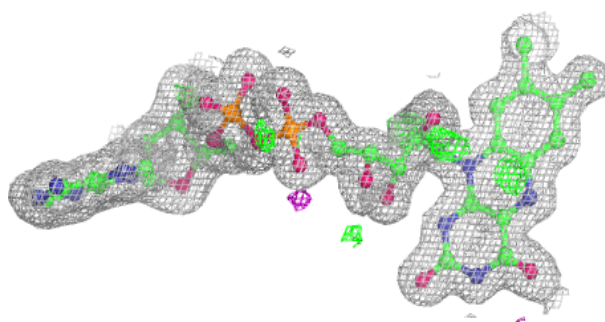
**Electron density around FAD D 600:**

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

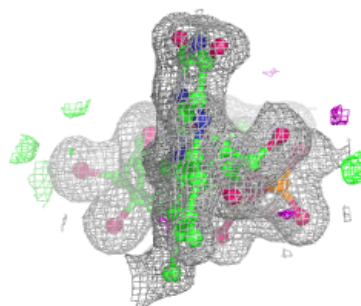
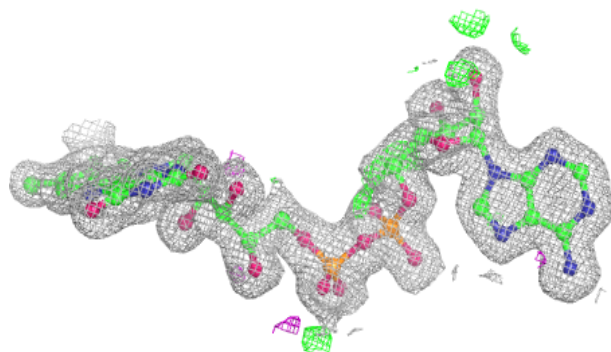
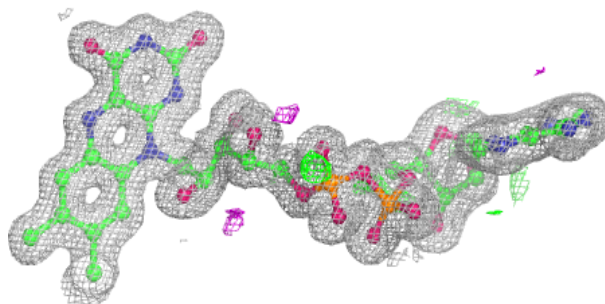


**Electron density around FAD B 601:**

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

**Electron density around FAD 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.