



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:01 am BST

PDB ID : 5X1Y  
Title : Structure of mercuric reductase from Lysinibacillus sphaericus  
Authors : Khan, F.; Suguna, K.  
Deposited on : 2017-01-28  
Resolution : 3.48 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 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

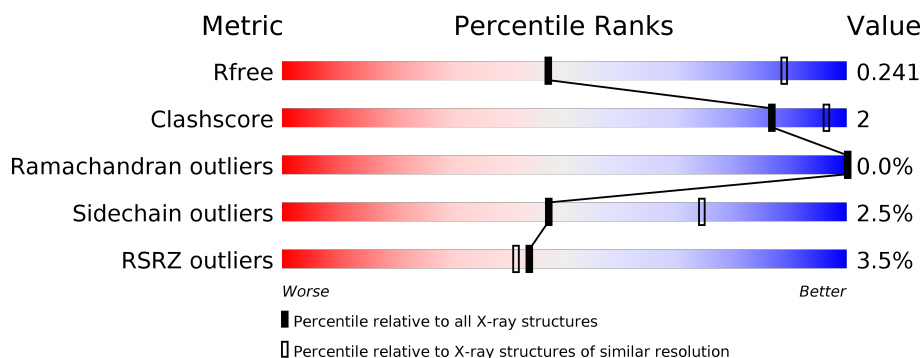
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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  $\geq 3$ , 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	554	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>5%</div> <div>18%</div> </div> </div>
1	B	554	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>6%</div> <div>18%</div> </div> </div>
1	C	554	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>6%</div> <div>18%</div> </div> </div>
1	D	554	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>5%</div> <div>18%</div> </div> </div>
1	E	554	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>6%</div> <div>18%</div> </div> </div>
1	F	554	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>•</div> <div>18%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40020 atoms, of which 19925 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 Mercuric reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	454	Total	C	H	N	O	S	0	0	0
			6464	2070	3199	537	650	8			
1	A	453	Total	C	H	N	O	S	0	0	0
			6603	2096	3305	546	649	7			
1	C	453	Total	C	H	N	O	S	0	0	0
			6612	2098	3310	546	651	7			
1	D	453	Total	C	H	N	O	S	0	0	0
			6609	2097	3307	546	651	8			
1	E	453	Total	C	H	N	O	S	0	0	0
			6592	2094	3297	543	651	7			
1	F	453	Total	C	H	N	O	S	0	0	0
			6641	2107	3326	546	654	8			

There are 48 discrepancies between the modelled and reference sequences:

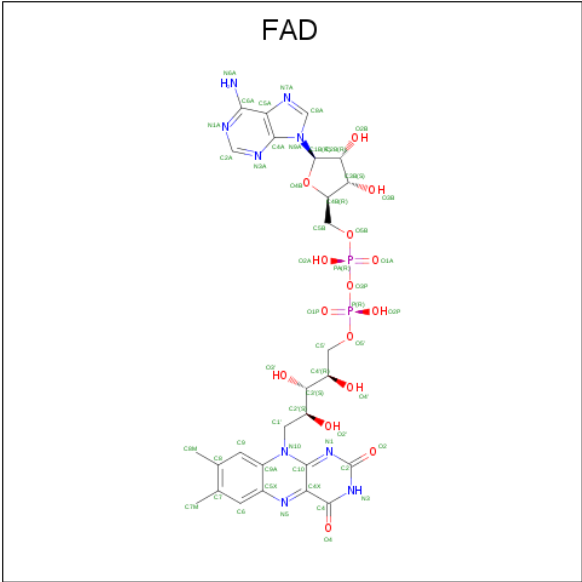
Chain	Residue	Modelled	Actual	Comment	Reference
B	547	LEU	-	expression tag	UNP D9J041
B	548	GLU	-	expression tag	UNP D9J041
B	549	HIS	-	expression tag	UNP D9J041
B	550	HIS	-	expression tag	UNP D9J041
B	551	HIS	-	expression tag	UNP D9J041
B	552	HIS	-	expression tag	UNP D9J041
B	553	HIS	-	expression tag	UNP D9J041
B	554	HIS	-	expression tag	UNP D9J041
A	547	LEU	-	expression tag	UNP D9J041
A	548	GLU	-	expression tag	UNP D9J041
A	549	HIS	-	expression tag	UNP D9J041
A	550	HIS	-	expression tag	UNP D9J041
A	551	HIS	-	expression tag	UNP D9J041
A	552	HIS	-	expression tag	UNP D9J041
A	553	HIS	-	expression tag	UNP D9J041
A	554	HIS	-	expression tag	UNP D9J041
C	547	LEU	-	expression tag	UNP D9J041

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Chain	Residue	Modelled	Actual	Comment	Reference
C	548	GLU	-	expression tag	UNP D9J041
C	549	HIS	-	expression tag	UNP D9J041
C	550	HIS	-	expression tag	UNP D9J041
C	551	HIS	-	expression tag	UNP D9J041
C	552	HIS	-	expression tag	UNP D9J041
C	553	HIS	-	expression tag	UNP D9J041
C	554	HIS	-	expression tag	UNP D9J041
D	547	LEU	-	expression tag	UNP D9J041
D	548	GLU	-	expression tag	UNP D9J041
D	549	HIS	-	expression tag	UNP D9J041
D	550	HIS	-	expression tag	UNP D9J041
D	551	HIS	-	expression tag	UNP D9J041
D	552	HIS	-	expression tag	UNP D9J041
D	553	HIS	-	expression tag	UNP D9J041
D	554	HIS	-	expression tag	UNP D9J041
E	547	LEU	-	expression tag	UNP D9J041
E	548	GLU	-	expression tag	UNP D9J041
E	549	HIS	-	expression tag	UNP D9J041
E	550	HIS	-	expression tag	UNP D9J041
E	551	HIS	-	expression tag	UNP D9J041
E	552	HIS	-	expression tag	UNP D9J041
E	553	HIS	-	expression tag	UNP D9J041
E	554	HIS	-	expression tag	UNP D9J041
F	547	LEU	-	expression tag	UNP D9J041
F	548	GLU	-	expression tag	UNP D9J041
F	549	HIS	-	expression tag	UNP D9J041
F	550	HIS	-	expression tag	UNP D9J041
F	551	HIS	-	expression tag	UNP D9J041
F	552	HIS	-	expression tag	UNP D9J041
F	553	HIS	-	expression tag	UNP D9J041
F	554	HIS	-	expression tag	UNP D9J041

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

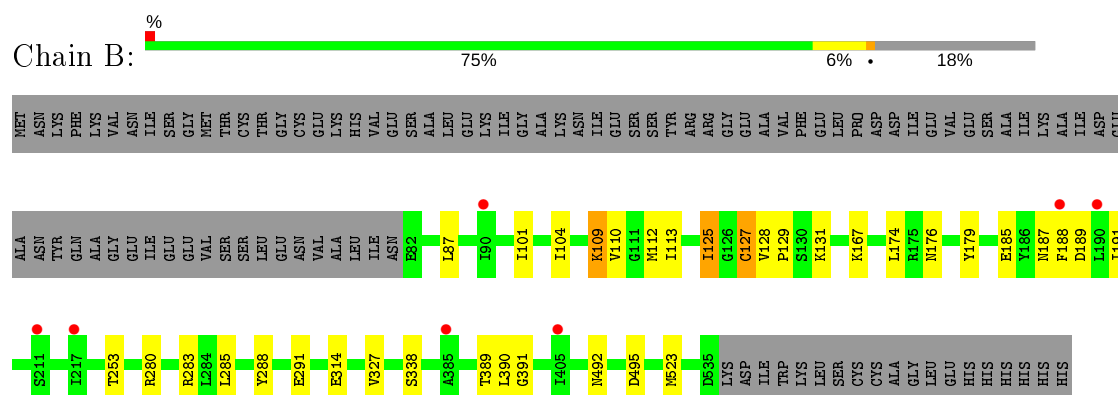


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	A	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	E	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		
2	F	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

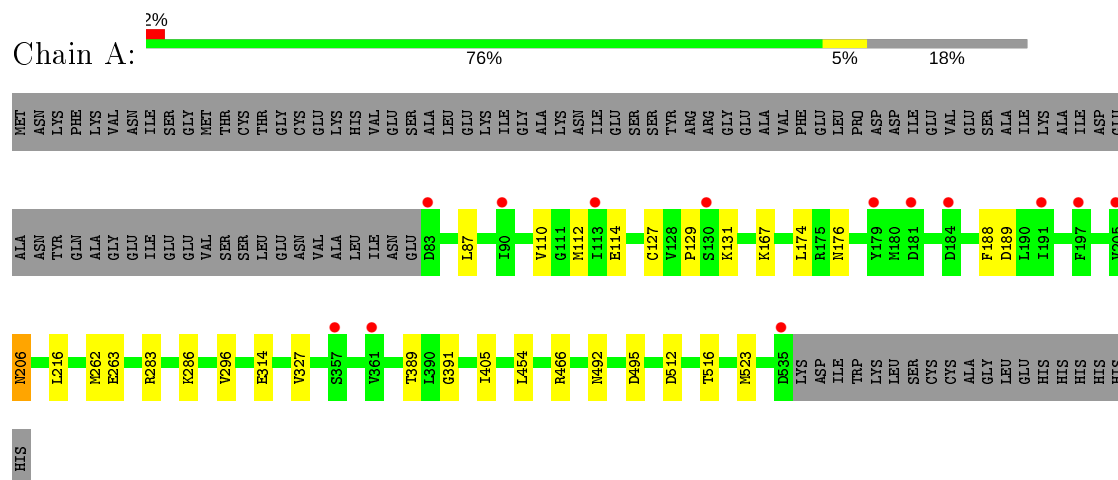
### 3 Residue-property plots [i](#)

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.

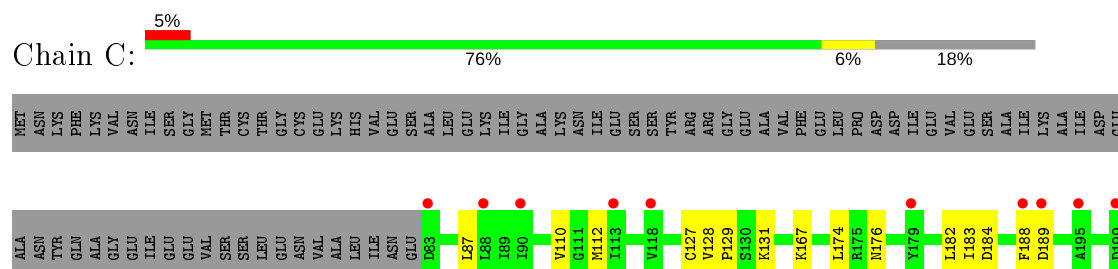
#### • Molecule 1: Mercuric reductase

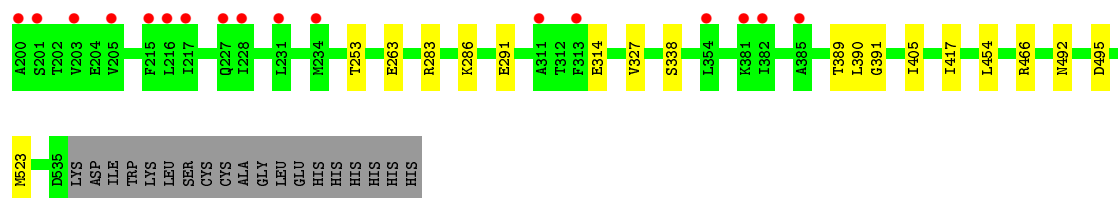


#### • Molecule 1: Mercuric reductase

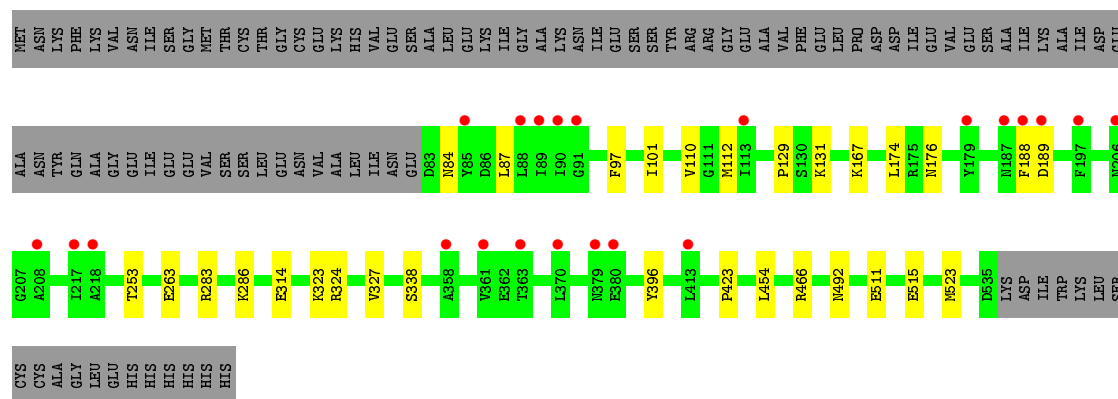
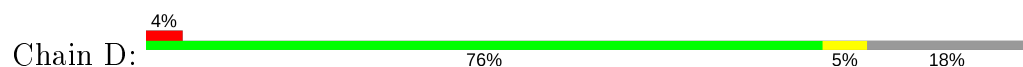


#### • Molecule 1: Mercuric reductase

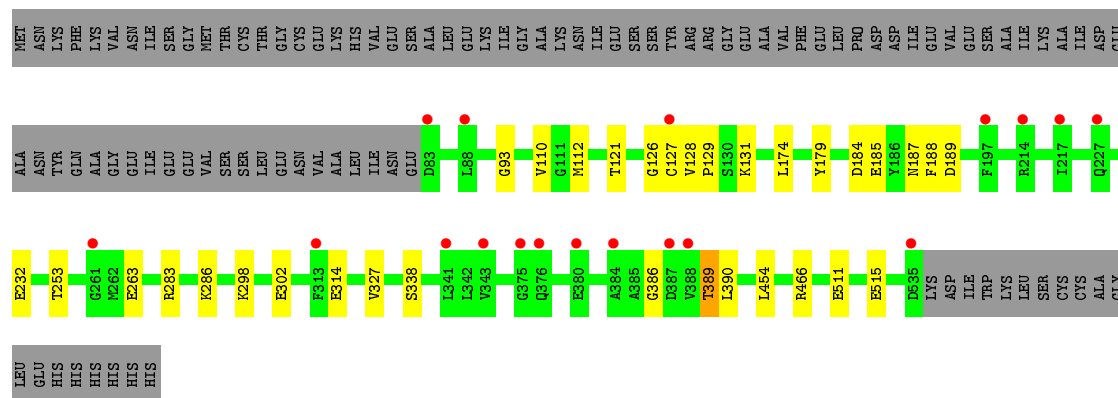
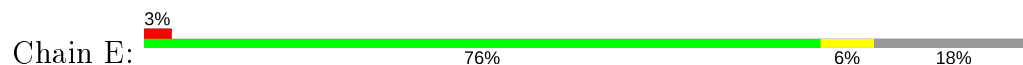




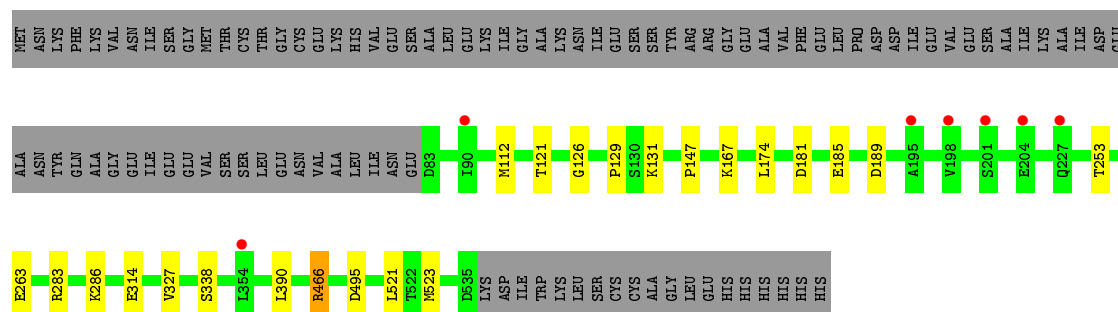
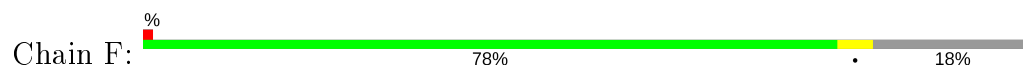
• Molecule 1: Mercuric reductase



• Molecule 1: Mercuric reductase



• Molecule 1: Mercuric reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	236.38Å 150.27Å 122.78Å 90.00° 92.62° 90.00°	Depositor
Resolution (Å)	87.07 – 3.48 87.07 – 3.48	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.07-3.48) 100.0 (87.07-3.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.191 , 0.240 0.192 , 0.241	Depositor DCC
$R_{free}$ test set	2763 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	40020	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/3339	0.45	0/4537
1	B	0.27	0/3306	0.45	0/4505
1	C	0.27	0/3343	0.45	0/4542
1	D	0.27	0/3343	0.46	0/4541
1	E	0.27	0/3336	0.45	0/4534
1	F	0.26	0/3357	0.45	0/4560
All	All	0.27	0/20024	0.45	0/27219

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	3298	3305	3305	14	0
1	B	3265	3199	3199	18	0
1	C	3302	3310	3309	18	0
1	D	3302	3307	3307	14	0
1	E	3295	3297	3296	14	0
1	F	3315	3326	3325	12	0
2	A	53	30	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	30	31	0	0
2	C	53	30	31	0	0
2	D	53	30	31	0	0
2	E	53	30	31	1	0
2	F	53	31	31	0	0
All	All	20095	19925	19927	83	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.

All (83) 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:253:THR:HG1	1:F:338:SER:HG	1.05	0.83
1:C:283:ARG:NH2	1:C:286:LYS:O	2.20	0.74
1:E:253:THR:HG1	1:E:338:SER:HG	1.12	0.68
1:D:283:ARG:NH2	1:D:286:LYS:O	2.26	0.68
1:E:283:ARG:NH2	1:E:286:LYS:O	2.30	0.64
1:A:114:GLU:OE1	2:A:601:FAD:O2B	2.13	0.63
1:A:131:LYS:NZ	1:A:263:GLU:OE1	2.32	0.62
1:B:389:THR:O	1:B:391:GLY:N	2.33	0.62
1:C:131:LYS:NZ	1:C:263:GLU:OE1	2.35	0.59
1:F:283:ARG:NH2	1:F:286:LYS:O	2.36	0.58
1:A:492:ASN:ND2	1:A:495:ASP:OD2	2.37	0.58
1:E:121:THR:O	1:E:126:GLY:N	2.36	0.58
1:E:131:LYS:NZ	1:E:263:GLU:OE1	2.38	0.57
1:C:253:THR:OG1	1:C:338:SER:OG	2.08	0.53
1:D:131:LYS:NZ	1:D:263:GLU:OE1	2.42	0.53
1:B:314:GLU:H	1:B:327:VAL:CB	2.24	0.51
1:B:495:ASP:OD2	1:C:492:ASN:ND2	2.43	0.51
1:B:492:ASN:ND2	1:C:495:ASP:OD2	2.43	0.51
1:F:181:ASP:N	1:F:181:ASP:OD1	2.41	0.51
1:D:314:GLU:H	1:D:327:VAL:CB	2.23	0.51
1:F:131:LYS:NZ	1:F:263:GLU:OE1	2.45	0.49
1:C:389:THR:O	1:C:391:GLY:N	2.46	0.49
1:D:253:THR:OG1	1:D:338:SER:OG	1.90	0.49
1:F:185:GLU:N	1:F:185:GLU:OE1	2.46	0.49
1:C:129:PRO:HB3	1:C:167:LYS:HD2	1.95	0.48
1:A:283:ARG:NH2	1:A:286:LYS:O	2.46	0.48
1:F:121:THR:O	1:F:126:GLY:N	2.47	0.48
1:C:291:GLU:N	1:C:291:GLU:OE2	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:HB	1:B:129:PRO:HD3	1.96	0.48
1:C:253:THR:HG1	1:C:338:SER:HG	1.28	0.47
1:A:314:GLU:H	1:A:327:VAL:CB	2.27	0.47
1:A:389:THR:O	1:A:391:GLY:N	2.46	0.47
1:E:386:GLY:O	1:E:389:THR:HG22	2.15	0.47
1:A:216:LEU:HD13	1:A:405:ILE:HG21	1.98	0.46
1:D:323:LYS:O	1:D:324:ARG:HD2	2.15	0.46
1:C:128:VAL:HB	1:C:129:PRO:HD3	1.97	0.46
1:C:110:VAL:O	1:C:188:PHE:HA	2.15	0.46
1:E:314:GLU:H	1:E:327:VAL:CB	2.29	0.45
1:E:110:VAL:O	1:E:188:PHE:HA	2.15	0.45
1:A:129:PRO:HB3	1:A:167:LYS:HD2	1.97	0.45
1:D:129:PRO:HB3	1:D:167:LYS:HD2	1.99	0.45
1:B:104:ILE:HG12	1:B:187:ASN:CB	2.46	0.45
1:F:129:PRO:HB3	1:F:167:LYS:HD2	1.97	0.45
1:B:176:ASN:HB3	1:A:176:ASN:HB3	1.97	0.45
1:B:113:ILE:HA	1:B:191:ILE:O	2.16	0.45
1:B:109:LYS:NZ	1:A:206:ASN:O	2.46	0.45
1:E:128:VAL:HB	1:E:129:PRO:HD3	1.98	0.45
1:C:176:ASN:HB3	1:D:176:ASN:HB3	1.98	0.45
1:F:181:ASP:O	1:F:185:GLU:HB2	2.17	0.45
1:E:185:GLU:O	1:E:187:ASN:N	2.47	0.44
1:E:93:GLY:HA3	2:E:601:FAD:O1A	2.18	0.44
1:A:262:MET:HE1	1:A:296:VAL:HG21	1.99	0.44
1:B:127:CYS:O	1:B:131:LYS:HD3	2.18	0.44
1:E:511:GLU:O	1:E:515:GLU:HG2	2.17	0.44
1:B:125:ILE:O	1:B:125:ILE:HD12	2.18	0.43
1:D:110:VAL:HG23	1:D:188:PHE:HB2	2.01	0.42
1:F:314:GLU:H	1:F:327:VAL:CB	2.32	0.42
1:C:183:ILE:HG23	1:C:184:ASP:H	1.84	0.42
1:C:87:LEU:HB3	1:C:110:VAL:HG12	2.01	0.42
1:E:298:LYS:NZ	1:E:302:GLU:OE2	2.53	0.42
1:D:511:GLU:O	1:D:515:GLU:HG2	2.20	0.42
1:B:291:GLU:N	1:B:291:GLU:OE2	2.42	0.41
1:C:405:ILE:HD11	1:C:417:ILE:HD11	2.02	0.41
1:D:396:TYR:OH	1:D:423:PRO:O	2.27	0.41
1:A:512:ASP:O	1:A:516:THR:HG23	2.20	0.41
1:B:110:VAL:HG23	1:B:188:PHE:CB	2.50	0.41
1:C:314:GLU:H	1:C:327:VAL:CB	2.33	0.41
1:A:110:VAL:HG23	1:A:188:PHE:HB2	2.02	0.41
1:B:129:PRO:HB3	1:B:167:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:ASP:HB2	1:E:187:ASN:CB	2.51	0.41
1:E:110:VAL:HG23	1:E:188:PHE:CB	2.51	0.41
1:F:147:PRO:HB2	1:F:466:ARG:HD2	2.02	0.41
1:D:492:ASN:ND2	1:F:495:ASP:OD2	2.54	0.41
1:C:110:VAL:HG23	1:C:188:PHE:HB2	2.01	0.41
1:D:97:PHE:O	1:D:101:ILE:HG12	2.21	0.41
1:B:285:LEU:HB3	1:B:288:TYR:CD1	2.56	0.41
1:B:253:THR:OG1	1:B:338:SER:OG	2.01	0.41
1:C:87:LEU:O	1:C:110:VAL:HA	2.21	0.41
1:D:131:LYS:CG	1:F:521:LEU:HD13	2.50	0.41
1:B:176:ASN:HA	1:B:179:TYR:HD2	1.86	0.41
1:A:87:LEU:O	1:A:110:VAL:HA	2.20	0.40
1:B:101:ILE:CD1	1:B:185:GLU:HG3	2.52	0.40
1:D:110:VAL:HG23	1:D:188:PHE:CB	2.51	0.40

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	451/554 (81%)	427 (95%)	24 (5%)	0	100	100
1	B	452/554 (82%)	429 (95%)	22 (5%)	1 (0%)	47	80
1	C	451/554 (81%)	426 (94%)	25 (6%)	0	100	100
1	D	451/554 (81%)	424 (94%)	27 (6%)	0	100	100
1	E	451/554 (81%)	428 (95%)	23 (5%)	0	100	100
1	F	451/554 (81%)	430 (95%)	21 (5%)	0	100	100
All	All	2707/3324 (81%)	2564 (95%)	142 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	390	LEU

### 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	342/458 (75%)	334 (98%)	8 (2%)	50	76
1	B	332/458 (72%)	322 (97%)	10 (3%)	41	70
1	C	343/458 (75%)	334 (97%)	9 (3%)	46	73
1	D	343/458 (75%)	335 (98%)	8 (2%)	50	76
1	E	342/458 (75%)	332 (97%)	10 (3%)	42	71
1	F	346/458 (76%)	340 (98%)	6 (2%)	60	82
All	All	2048/2748 (74%)	1997 (98%)	51 (2%)	47	74

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	LEU
1	B	109	LYS
1	B	112	MET
1	B	125	ILE
1	B	127	CYS
1	B	174	LEU
1	B	189	ASP
1	B	280	ARG
1	B	283	ARG
1	B	523	MET
1	A	112	MET
1	A	127	CYS
1	A	174	LEU
1	A	189	ASP
1	A	206	ASN
1	A	454	LEU
1	A	466	ARG
1	A	523	MET

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Mol	Chain	Res	Type
1	C	112	MET
1	C	127	CYS
1	C	174	LEU
1	C	182	LEU
1	C	189	ASP
1	C	390	LEU
1	C	454	LEU
1	C	466	ARG
1	C	523	MET
1	D	84	ASN
1	D	87	LEU
1	D	112	MET
1	D	174	LEU
1	D	189	ASP
1	D	454	LEU
1	D	466	ARG
1	D	523	MET
1	E	112	MET
1	E	127	CYS
1	E	174	LEU
1	E	179	TYR
1	E	189	ASP
1	E	232	GLU
1	E	389	THR
1	E	390	LEU
1	E	454	LEU
1	E	466	ARG
1	F	112	MET
1	F	174	LEU
1	F	189	ASP
1	F	390	LEU
1	F	466	ARG
1	F	523	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	F	601	-	51,58,58	1.85	6 (11%)	60,89,89	1.99	10 (16%)
2	FAD	D	601	-	51,58,58	1.83	6 (11%)	60,89,89	1.92	10 (16%)
2	FAD	B	601	-	51,58,58	1.85	6 (11%)	60,89,89	1.98	10 (16%)
2	FAD	E	601	-	51,58,58	1.90	7 (13%)	60,89,89	2.05	10 (16%)
2	FAD	C	601	-	51,58,58	1.87	6 (11%)	60,89,89	2.07	9 (15%)
2	FAD	A	601	-	51,58,58	1.93	6 (11%)	60,89,89	2.04	10 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	F	601	-	-	5/30/50/50	0/6/6/6
2	FAD	D	601	-	-	3/30/50/50	0/6/6/6
2	FAD	B	601	-	-	2/30/50/50	0/6/6/6
2	FAD	E	601	-	-	5/30/50/50	0/6/6/6
2	FAD	C	601	-	-	3/30/50/50	0/6/6/6
2	FAD	A	601	-	-	4/30/50/50	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-C10	9.97	1.48	1.38
2	E	601	FAD	C4X-C10	9.79	1.48	1.38
2	C	601	FAD	C4X-C10	9.61	1.48	1.38
2	B	601	FAD	C4X-C10	9.44	1.48	1.38
2	D	601	FAD	C4X-C10	9.37	1.48	1.38
2	F	601	FAD	C4X-C10	9.37	1.48	1.38
2	F	601	FAD	C4-C4X	4.34	1.48	1.41
2	A	601	FAD	C4-C4X	4.24	1.48	1.41
2	B	601	FAD	C4-C4X	4.21	1.48	1.41
2	C	601	FAD	C4-C4X	4.20	1.48	1.41
2	E	601	FAD	C4-C4X	4.14	1.48	1.41
2	A	601	FAD	C9A-C5X	4.02	1.50	1.42
2	D	601	FAD	C4-C4X	3.87	1.48	1.41
2	C	601	FAD	C9A-C5X	3.79	1.50	1.42
2	B	601	FAD	C9A-C5X	3.76	1.50	1.42
2	E	601	FAD	C9A-C5X	3.75	1.50	1.42
2	F	601	FAD	C9A-C5X	3.71	1.50	1.42
2	D	601	FAD	C9A-C5X	3.69	1.50	1.42
2	E	601	FAD	C9A-N10	3.56	1.43	1.38
2	A	601	FAD	C9A-N10	3.38	1.43	1.38
2	B	601	FAD	C9A-N10	3.30	1.43	1.38
2	F	601	FAD	C8-C7	3.24	1.49	1.40
2	C	601	FAD	C8-C7	3.23	1.49	1.40
2	D	601	FAD	C8-C7	3.23	1.48	1.40
2	A	601	FAD	C8-C7	3.17	1.48	1.40
2	C	601	FAD	C9A-N10	3.16	1.42	1.38
2	B	601	FAD	C8-C7	3.13	1.48	1.40
2	E	601	FAD	C8-C7	3.09	1.48	1.40
2	F	601	FAD	C9A-N10	3.04	1.42	1.38
2	D	601	FAD	C9A-N10	2.91	1.42	1.38
2	F	601	FAD	C5A-C4A	2.35	1.47	1.40
2	D	601	FAD	C5A-C4A	2.32	1.47	1.40
2	E	601	FAD	C5A-C4A	2.32	1.47	1.40
2	A	601	FAD	C5A-C4A	2.28	1.47	1.40
2	C	601	FAD	C5A-C4A	2.24	1.46	1.40
2	B	601	FAD	C5A-C4A	2.23	1.46	1.40
2	E	601	FAD	O4B-C1B	2.08	1.44	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	FAD	C1'-N10-C9A	8.80	125.22	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C1'-N10-C9A	8.51	124.99	118.29
2	B	601	FAD	C1'-N10-C9A	8.18	124.73	118.29
2	C	601	FAD	C4-N3-C2	8.04	121.93	115.14
2	A	601	FAD	C1'-N10-C9A	8.00	124.59	118.29
2	F	601	FAD	C1'-N10-C9A	7.94	124.54	118.29
2	F	601	FAD	C4-N3-C2	7.73	121.67	115.14
2	E	601	FAD	C4-N3-C2	7.64	121.59	115.14
2	B	601	FAD	C4-N3-C2	7.60	121.56	115.14
2	D	601	FAD	C4-N3-C2	7.51	121.48	115.14
2	A	601	FAD	C4-N3-C2	7.48	121.46	115.14
2	D	601	FAD	C1'-N10-C9A	7.11	123.89	118.29
2	A	601	FAD	N3A-C2A-N1A	-4.10	122.27	128.68
2	F	601	FAD	C4X-N5-C5X	4.08	120.85	116.77
2	C	601	FAD	C4X-C4-N3	-4.03	117.92	123.43
2	D	601	FAD	C9A-N10-C10	-4.00	116.67	121.91
2	A	601	FAD	P-O3P-PA	-3.96	119.24	132.83
2	A	601	FAD	C9A-N10-C10	-3.93	116.77	121.91
2	E	601	FAD	C4X-C4-N3	-3.80	118.23	123.43
2	E	601	FAD	C9A-N10-C10	-3.80	116.94	121.91
2	C	601	FAD	P-O3P-PA	-3.77	119.89	132.83
2	B	601	FAD	C4X-N5-C5X	3.69	120.46	116.77
2	F	601	FAD	N3A-C2A-N1A	-3.67	122.94	128.68
2	D	601	FAD	C4X-C4-N3	-3.66	118.42	123.43
2	F	601	FAD	C4X-C4-N3	-3.66	118.43	123.43
2	C	601	FAD	C9A-N10-C10	-3.65	117.12	121.91
2	E	601	FAD	N3A-C2A-N1A	-3.65	122.97	128.68
2	B	601	FAD	C4X-C4-N3	-3.62	118.48	123.43
2	C	601	FAD	N3A-C2A-N1A	-3.62	123.03	128.68
2	B	601	FAD	N3A-C2A-N1A	-3.57	123.09	128.68
2	C	601	FAD	C4X-N5-C5X	3.52	120.29	116.77
2	A	601	FAD	C4X-N5-C5X	3.48	120.25	116.77
2	D	601	FAD	N3A-C2A-N1A	-3.47	123.26	128.68
2	E	601	FAD	C4X-N5-C5X	3.44	120.21	116.77
2	A	601	FAD	C4X-C4-N3	-3.42	118.76	123.43
2	F	601	FAD	C4-C4X-C10	-3.40	117.70	119.95
2	E	601	FAD	P-O3P-PA	-3.38	121.24	132.83
2	B	601	FAD	C4-C4X-C10	-3.36	117.73	119.95
2	B	601	FAD	C9A-N10-C10	-3.36	117.51	121.91
2	B	601	FAD	P-O3P-PA	-3.32	121.42	132.83
2	D	601	FAD	C4X-N5-C5X	3.26	120.03	116.77
2	F	601	FAD	P-O3P-PA	-3.22	121.77	132.83
2	A	601	FAD	C4-C4X-C10	-3.21	117.83	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C4-C4X-C10	-3.20	117.83	119.95
2	E	601	FAD	C4-C4X-C10	-3.16	117.86	119.95
2	F	601	FAD	C9A-N10-C10	-3.12	117.82	121.91
2	C	601	FAD	C4-C4X-C10	-3.02	117.95	119.95
2	C	601	FAD	C4A-C5A-N7A	-2.95	106.32	109.40
2	D	601	FAD	P-O3P-PA	-2.87	122.99	132.83
2	B	601	FAD	C4A-C5A-N7A	-2.80	106.48	109.40
2	A	601	FAD	C3B-C2B-C1B	2.73	105.08	100.98
2	F	601	FAD	C4A-C5A-N7A	-2.66	106.63	109.40
2	F	601	FAD	C4-C4X-N5	2.61	121.58	118.60
2	A	601	FAD	C4A-C5A-N7A	-2.57	106.72	109.40
2	D	601	FAD	C4A-C5A-N7A	-2.56	106.73	109.40
2	E	601	FAD	C4A-C5A-N7A	-2.48	106.82	109.40
2	D	601	FAD	C5X-C9A-N10	2.45	119.49	117.72
2	B	601	FAD	C4-C4X-N5	2.20	121.11	118.60
2	E	601	FAD	C3B-C2B-C1B	2.04	104.04	100.98

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	FAD	C5B-O5B-PA-O1A
2	F	601	FAD	C5B-O5B-PA-O2A
2	F	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
2	E	601	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	O4'-C4'-C5'-O5'
2	E	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
2	F	601	FAD	O4B-C4B-C5B-O5B
2	E	601	FAD	C4B-C5B-O5B-PA
2	A	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	PA-O3P-P-O5'
2	F	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	C5B-O5B-PA-O3P
2	E	601	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	601	FAD	O4'-C4'-C5'-O5'

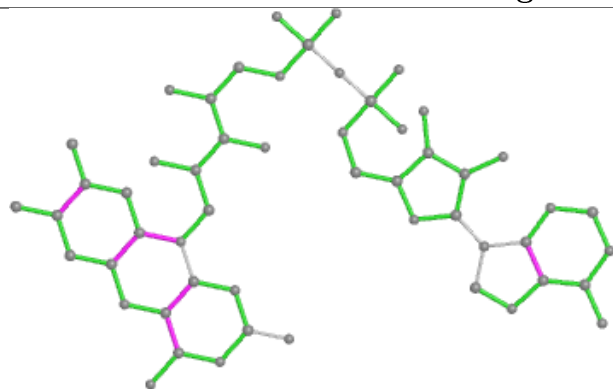
There are no ring outliers.

2 monomers are involved in 2 short contacts:

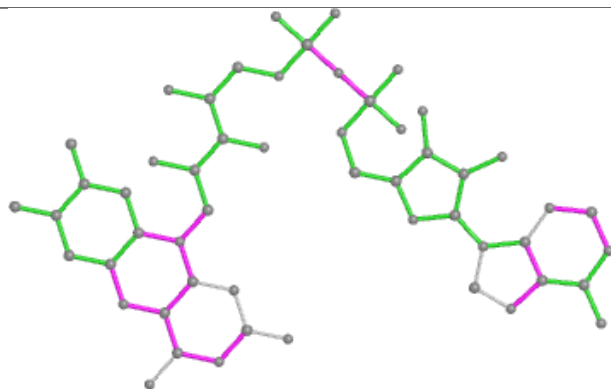
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	FAD	1	0
2	A	601	FAD	1	0

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.

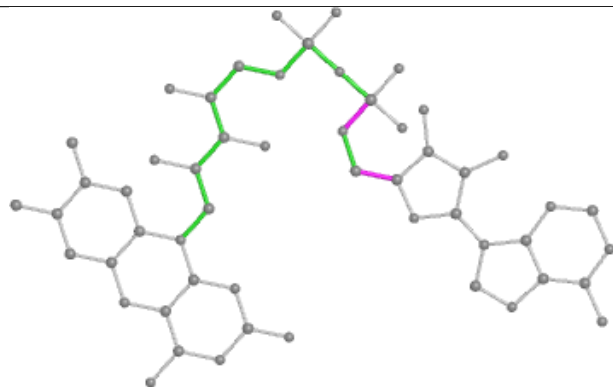
## Ligand FAD F 601



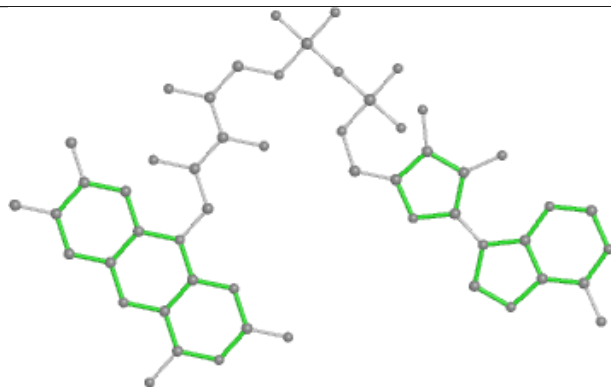
Bond lengths



Bond angles

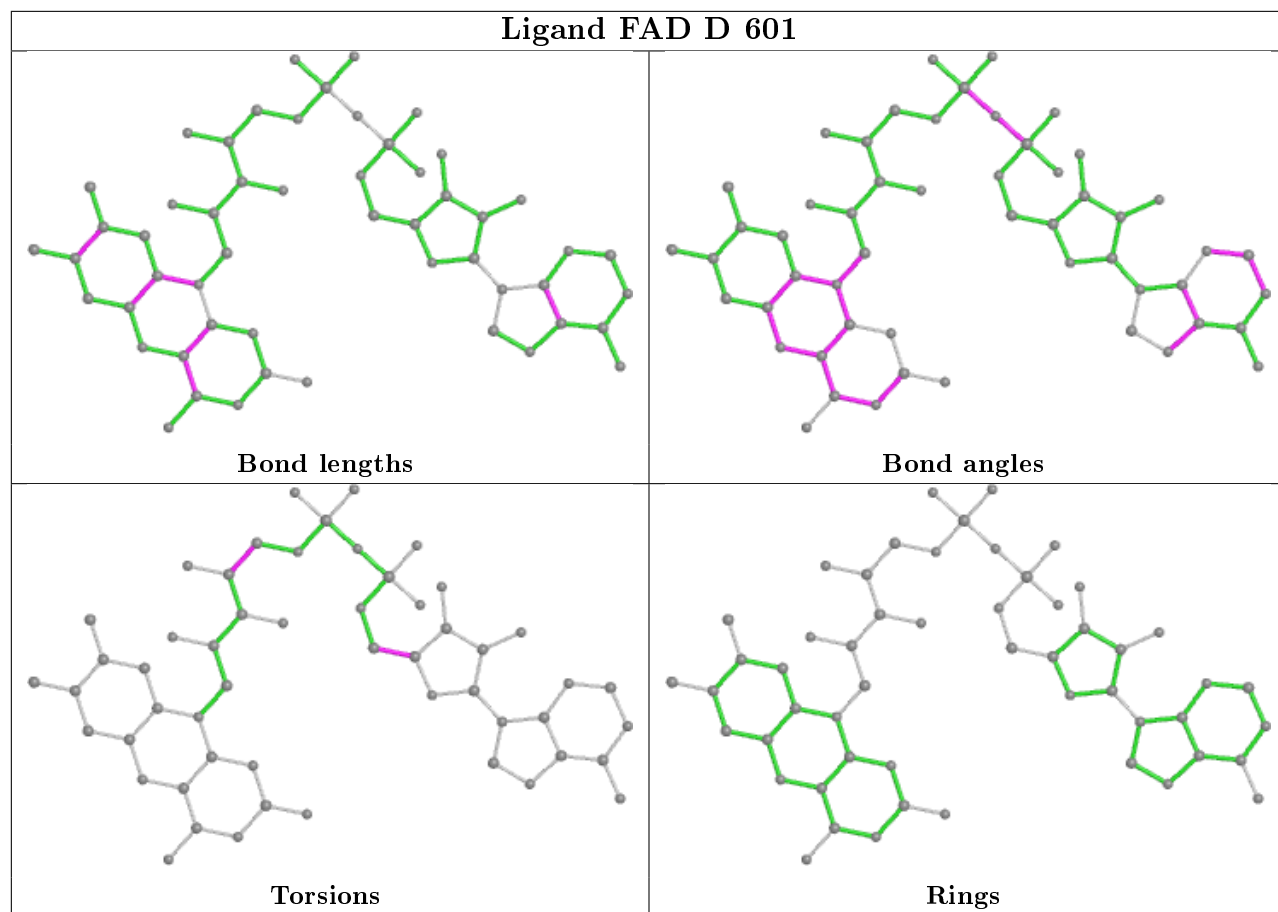


Torsions

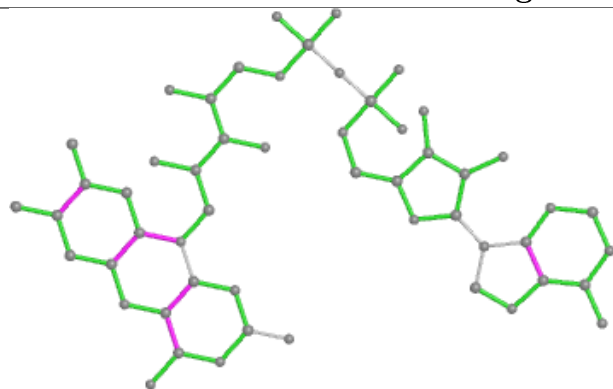


Rings

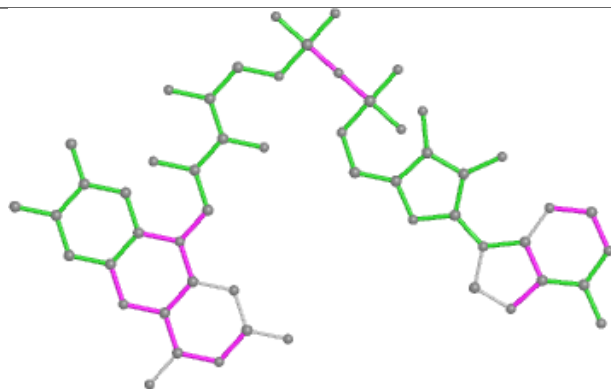
## Ligand FAD D 601



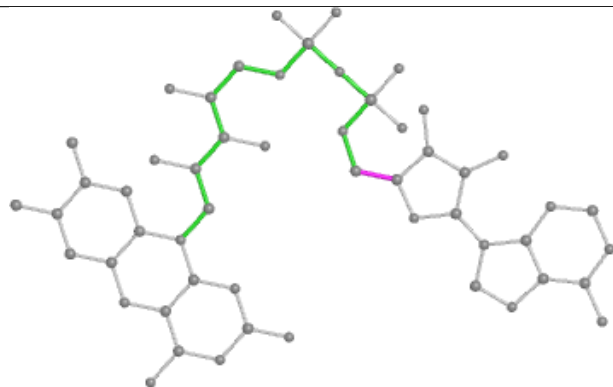
## Ligand FAD B 601



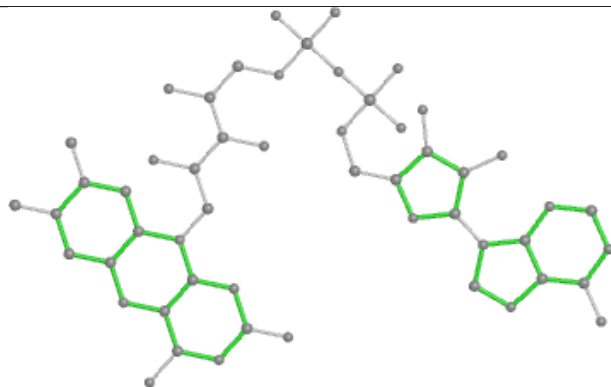
Bond lengths



Bond angles

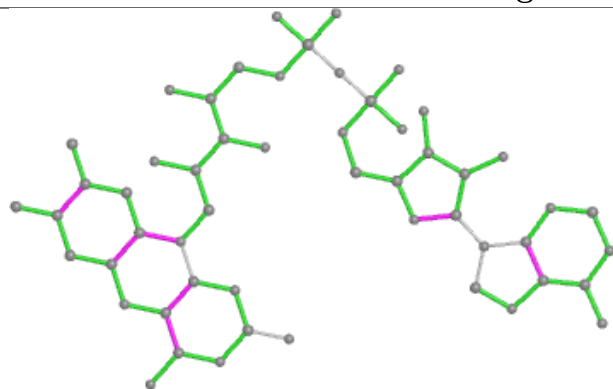


Torsions

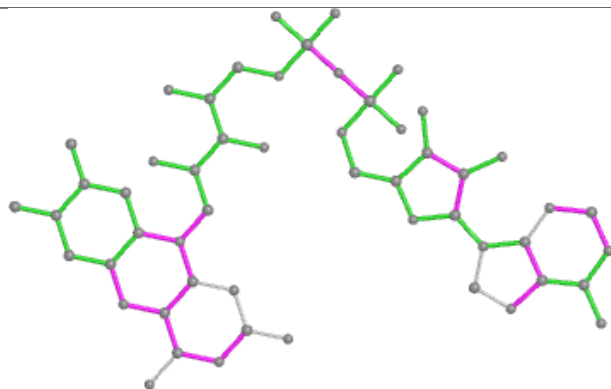


Rings

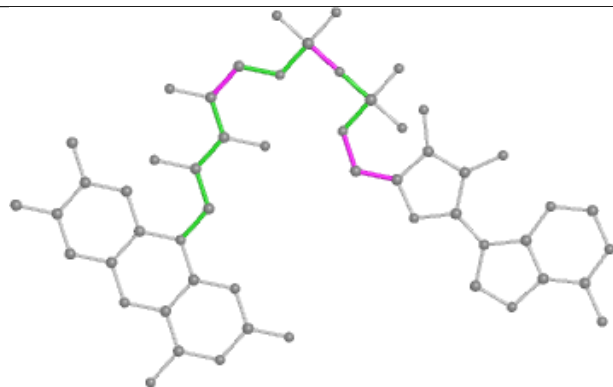
## Ligand FAD E 601



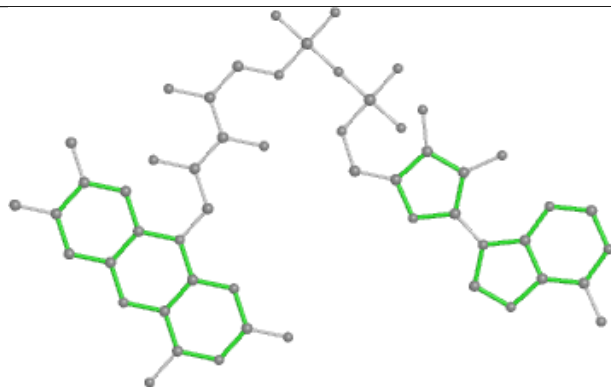
Bond lengths



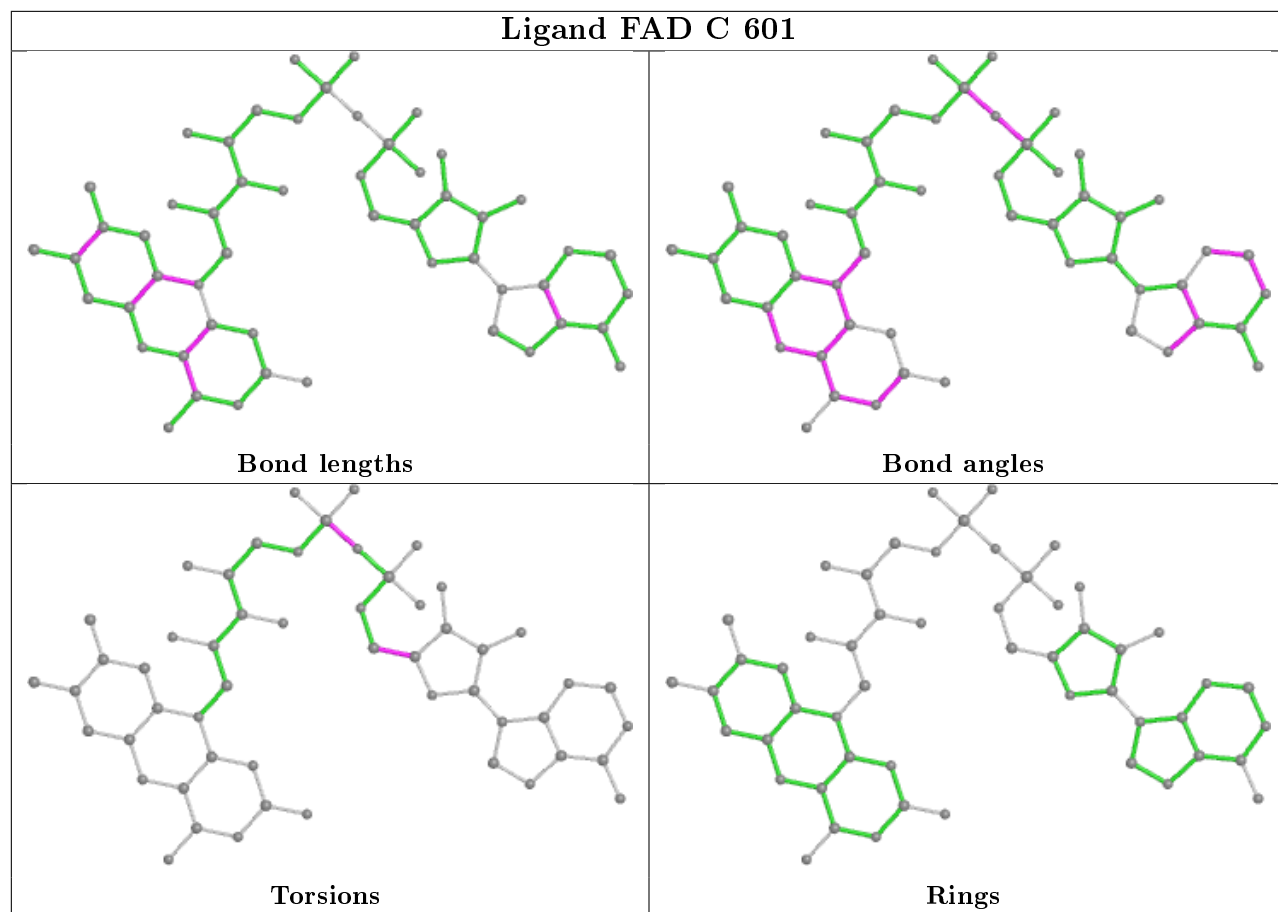
Bond angles

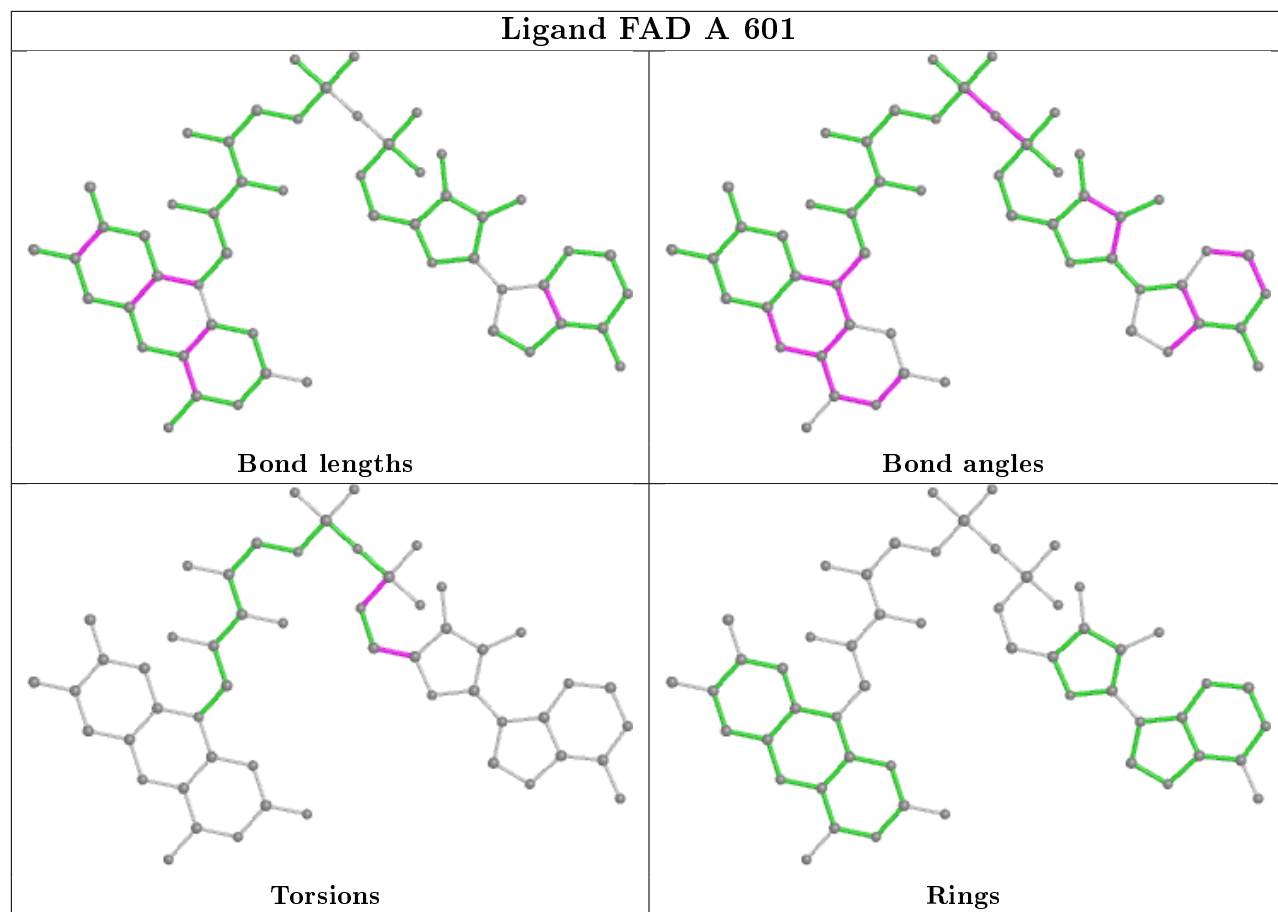


Torsions



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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	453/554 (81%)	0.44	13 (2%) 51 48	34, 55, 80, 113	0
1	B	454/554 (81%)	0.40	7 (1%) 73 70	29, 52, 74, 92	0
1	C	453/554 (81%)	0.55	27 (5%) 21 21	32, 57, 87, 114	0
1	D	453/554 (81%)	0.51	22 (4%) 29 28	34, 54, 80, 98	0
1	E	453/554 (81%)	0.65	18 (3%) 38 35	36, 54, 77, 101	0
1	F	453/554 (81%)	0.22	7 (1%) 73 70	38, 60, 91, 128	0
All	All	2719/3324 (81%)	0.46	94 (3%) 44 41	29, 55, 84, 128	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	83	ASP	6.0
1	C	83	ASP	5.2
1	D	179	TYR	3.8
1	C	231	LEU	3.3
1	C	201	SER	3.2
1	C	179	TYR	3.1
1	C	118	VAL	3.0
1	C	90	ILE	3.0
1	C	217	ILE	3.0
1	D	363	THR	3.0
1	A	83	ASP	2.9
1	C	227	GLN	2.8
1	D	113	ILE	2.8
1	A	205	VAL	2.8
1	C	313	PHE	2.8
1	F	201	SER	2.7
1	D	90	ILE	2.7
1	A	535	ASP	2.7
1	D	91	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	388	VAL	2.7
1	F	204	GLU	2.7
1	C	189	ASP	2.7
1	C	205	VAL	2.6
1	A	191	ILE	2.6
1	D	89	ILE	2.6
1	A	179	TYR	2.6
1	F	198	VAL	2.6
1	C	234	MET	2.6
1	F	227	GLN	2.6
1	E	127	CYS	2.6
1	C	195	ALA	2.5
1	A	361	VAL	2.5
1	D	197	PHE	2.5
1	C	382	ILE	2.5
1	C	216	LEU	2.5
1	B	188	PHE	2.5
1	D	206	ASN	2.5
1	A	184	ASP	2.4
1	B	405	ILE	2.4
1	A	113	ILE	2.4
1	D	188	PHE	2.4
1	E	376	GLN	2.4
1	D	361	VAL	2.4
1	A	197	PHE	2.3
1	E	535	ASP	2.3
1	E	227	GLN	2.3
1	E	387	ASP	2.3
1	C	188	PHE	2.3
1	A	181	ASP	2.3
1	B	385	ALA	2.3
1	D	88	LEU	2.3
1	A	357	SER	2.3
1	C	215	PHE	2.3
1	D	189	ASP	2.3
1	D	208	ALA	2.3
1	E	384	ALA	2.3
1	E	380	GLU	2.3
1	D	370	LEU	2.3
1	E	341	LEU	2.3
1	F	354	LEU	2.3
1	C	354	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	217	ILE	2.3
1	C	113	ILE	2.2
1	C	88	LEU	2.2
1	C	203	VAL	2.2
1	C	200	ALA	2.2
1	C	228	ILE	2.2
1	E	217	ILE	2.2
1	C	381	LYS	2.2
1	E	375	GLY	2.2
1	A	130	SER	2.1
1	D	187	ASN	2.1
1	E	197	PHE	2.1
1	D	413	LEU	2.1
1	D	358	ALA	2.1
1	E	214	ARG	2.1
1	C	311	ALA	2.1
1	E	261	GLY	2.1
1	F	195	ALA	2.1
1	C	199	ASP	2.1
1	B	190	LEU	2.1
1	D	380	GLU	2.1
1	B	90	ILE	2.1
1	C	385	ALA	2.1
1	D	85	TYR	2.1
1	D	379	ASN	2.1
1	D	218	ALA	2.1
1	A	90	ILE	2.1
1	F	90	ILE	2.1
1	E	313	PHE	2.0
1	B	217	ILE	2.0
1	B	211	SER	2.0
1	E	88	LEU	2.0
1	E	343	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

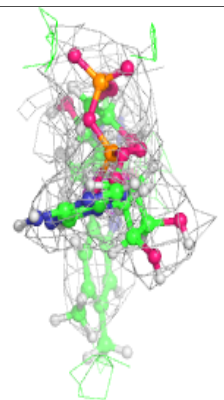
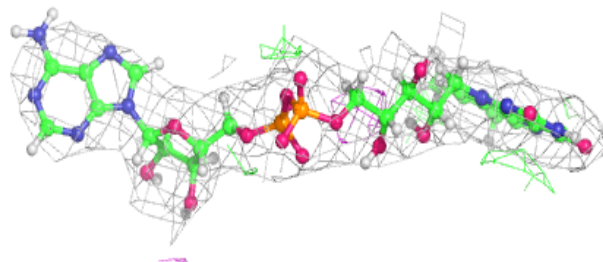
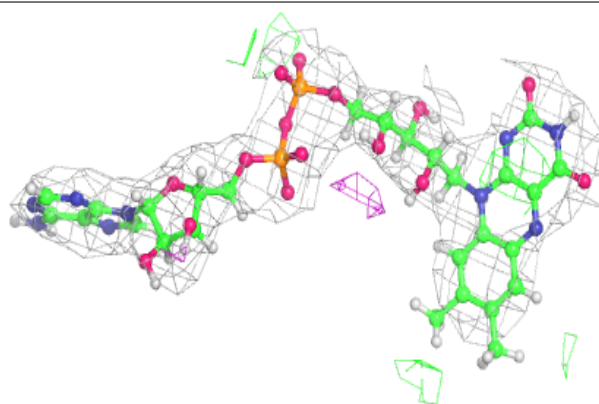
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FAD	F	601	53/53	0.95	0.26	40,56,78,85	0
2	FAD	D	601	53/53	0.95	0.29	28,49,72,83	0
2	FAD	E	601	53/53	0.95	0.35	32,56,83,85	0
2	FAD	C	601	53/53	0.96	0.27	33,50,69,88	0
2	FAD	B	601	53/53	0.97	0.26	33,50,67,79	0
2	FAD	A	601	53/53	0.97	0.26	36,51,70,79	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.

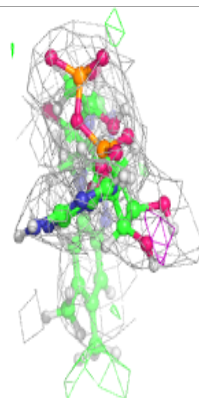
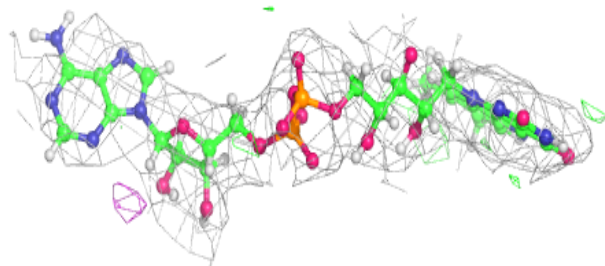
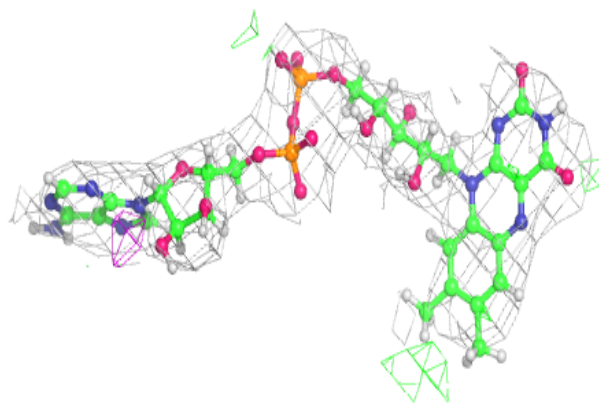
### Electron density around FAD F 601:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

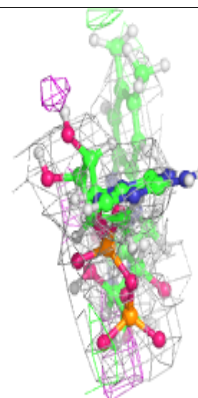
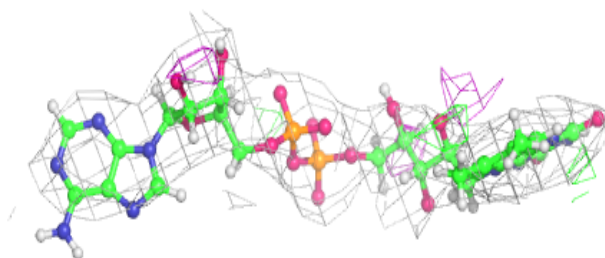
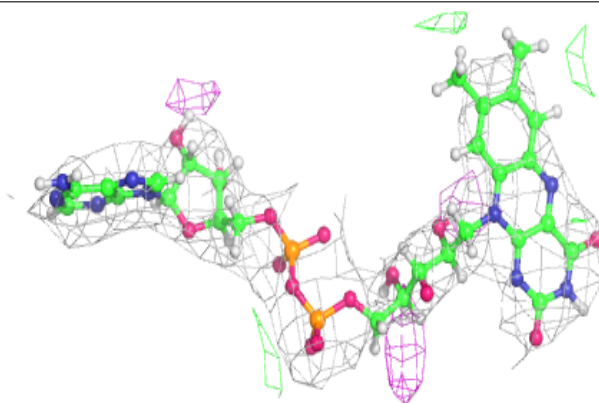


**Electron density around FAD D 601:**

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

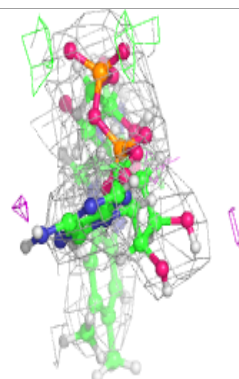
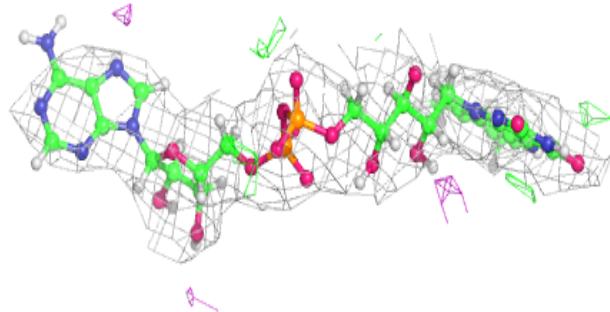
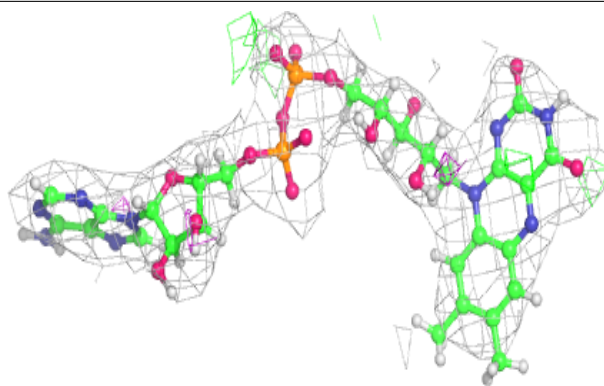
**Electron density around FAD E 601:**

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

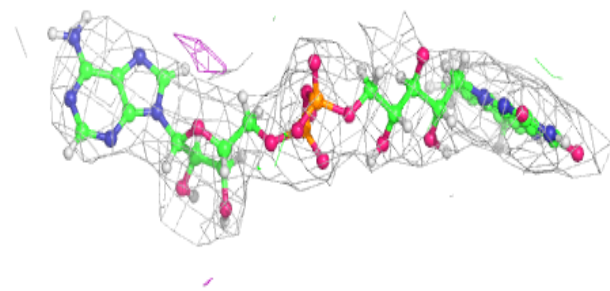
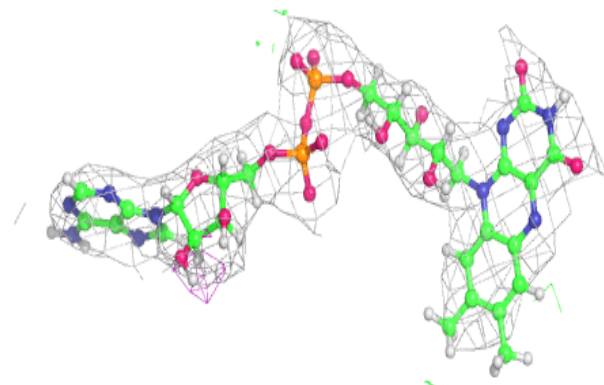


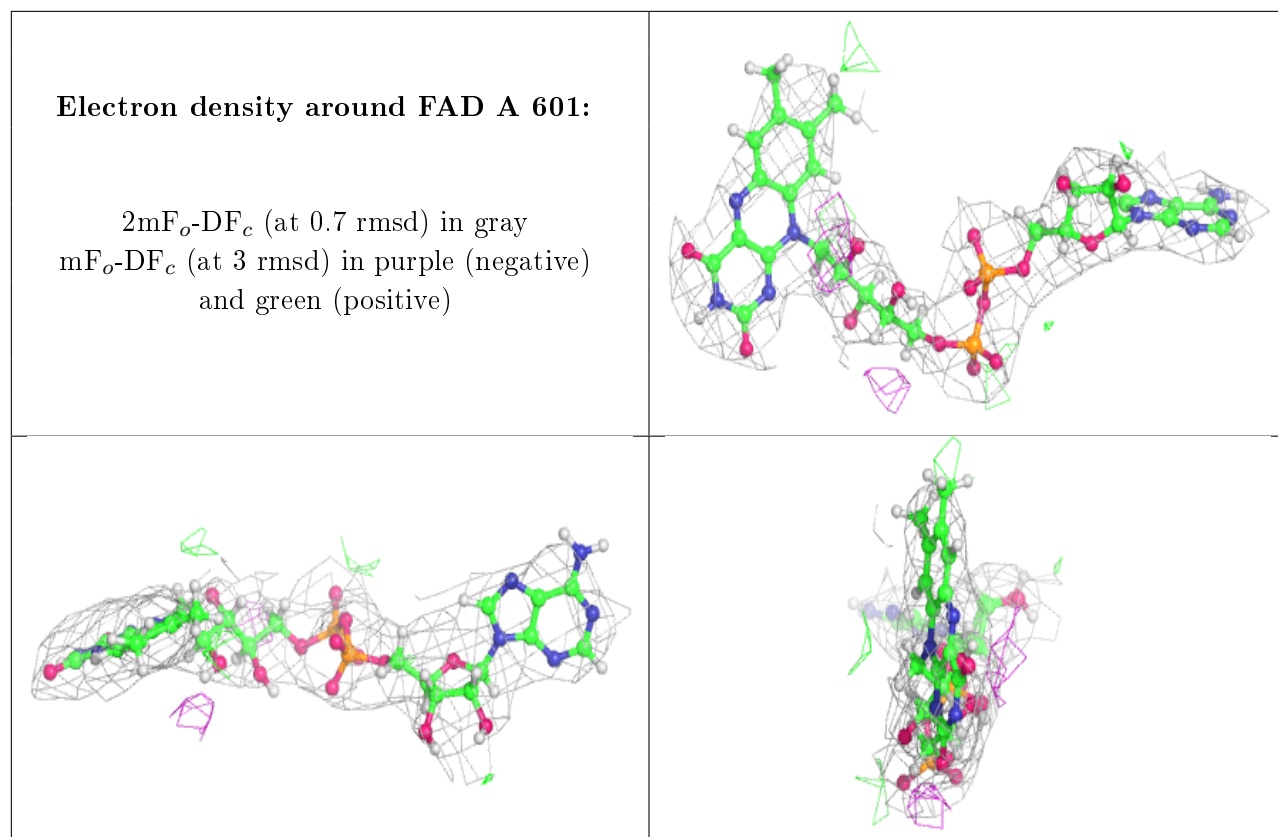
**Electron density around FAD C 601:**

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

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.