



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:57 pm BST

PDB ID : 6BDO  
Title : Structure of bacterial type II NADH dehydrogenase from *Caldalkalibacillus thermarum* complexed with a quinone inhibitor HQNO at 2.8Å resolution  
Authors : Cook, G.M.; Aragao, D.; Nakatani, Y.  
Deposited on : 2017-10-23  
Resolution : 2.80 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

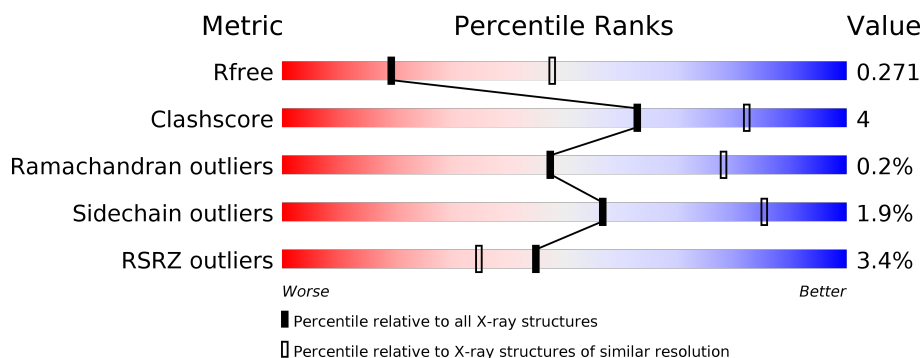
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	405	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	B	405	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	C	405	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	D	405	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11896 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 FAD-dependent pyridine nucleotide-disulfide oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	394	Total	C	N	O	S	0	0	0
			2931	1866	508	548	9			
1	A	394	Total	C	N	O	S	0	0	0
			2921	1864	505	544	8			
1	D	395	Total	C	N	O	S	0	0	0
			2870	1831	500	532	7			
1	C	394	Total	C	N	O	S	0	0	0
			2881	1837	494	542	8			

There are 24 discrepancies between the modelled and reference sequences:

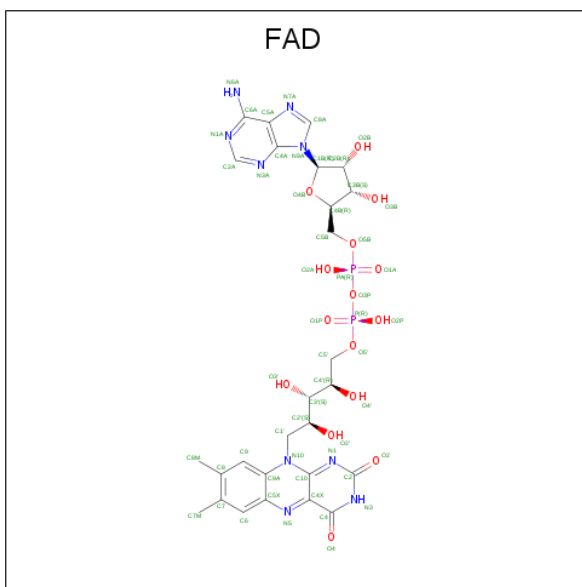
Chain	Residue	Modelled	Actual	Comment	Reference
B	400	HIS	-	expression tag	UNP F5L3B8
B	401	HIS	-	expression tag	UNP F5L3B8
B	402	HIS	-	expression tag	UNP F5L3B8
B	403	HIS	-	expression tag	UNP F5L3B8
B	404	HIS	-	expression tag	UNP F5L3B8
B	405	HIS	-	expression tag	UNP F5L3B8
A	400	HIS	-	expression tag	UNP F5L3B8
A	401	HIS	-	expression tag	UNP F5L3B8
A	402	HIS	-	expression tag	UNP F5L3B8
A	403	HIS	-	expression tag	UNP F5L3B8
A	404	HIS	-	expression tag	UNP F5L3B8
A	405	HIS	-	expression tag	UNP F5L3B8
D	400	HIS	-	expression tag	UNP F5L3B8
D	401	HIS	-	expression tag	UNP F5L3B8
D	402	HIS	-	expression tag	UNP F5L3B8
D	403	HIS	-	expression tag	UNP F5L3B8
D	404	HIS	-	expression tag	UNP F5L3B8
D	405	HIS	-	expression tag	UNP F5L3B8
C	400	HIS	-	expression tag	UNP F5L3B8
C	401	HIS	-	expression tag	UNP F5L3B8
C	402	HIS	-	expression tag	UNP F5L3B8

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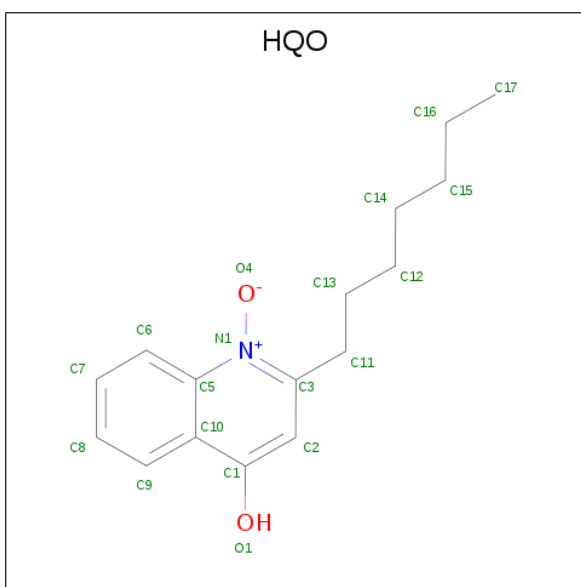
Chain	Residue	Modelled	Actual	Comment	Reference
C	403	HIS	-	expression tag	UNP F5L3B8
C	404	HIS	-	expression tag	UNP F5L3B8
C	405	HIS	-	expression tag	UNP F5L3B8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



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

- Molecule 3 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: C<sub>16</sub>H<sub>21</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			19	16	1	2		
3	C	1	Total	C	N	O	0	0
			19	16	1	2		

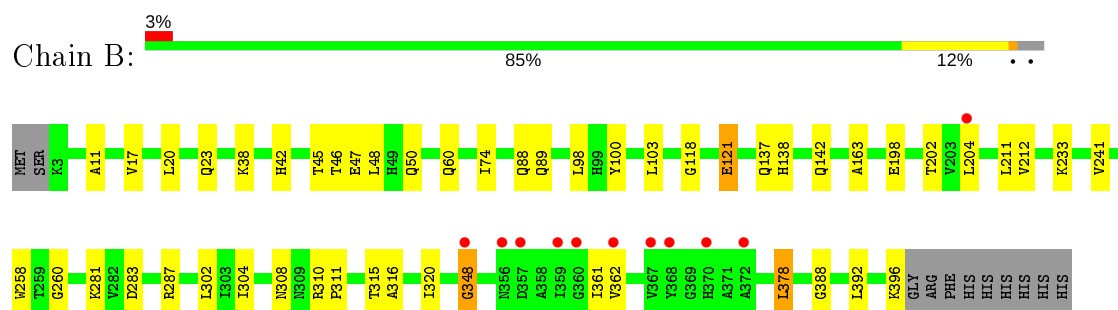
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	14	Total	O	0	0
			14	14		
4	A	14	Total	O	0	0
			14	14		
4	D	3	Total	O	0	0
			3	3		
4	C	12	Total	O	0	0
			12	12		

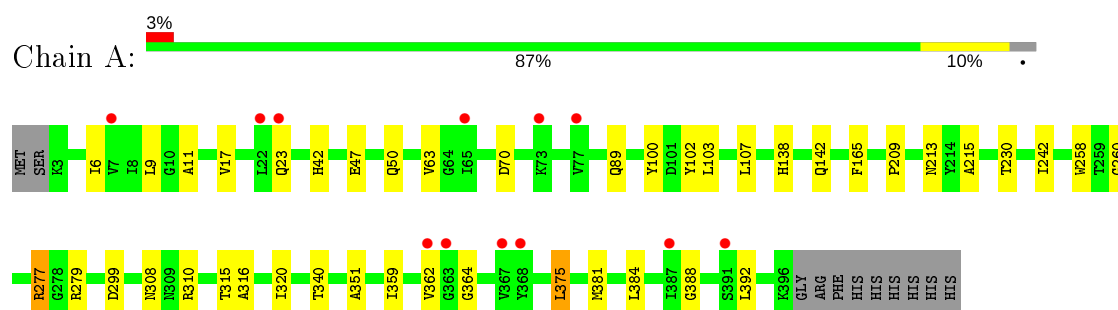
### 3 Residue-property plots [i](#)

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.

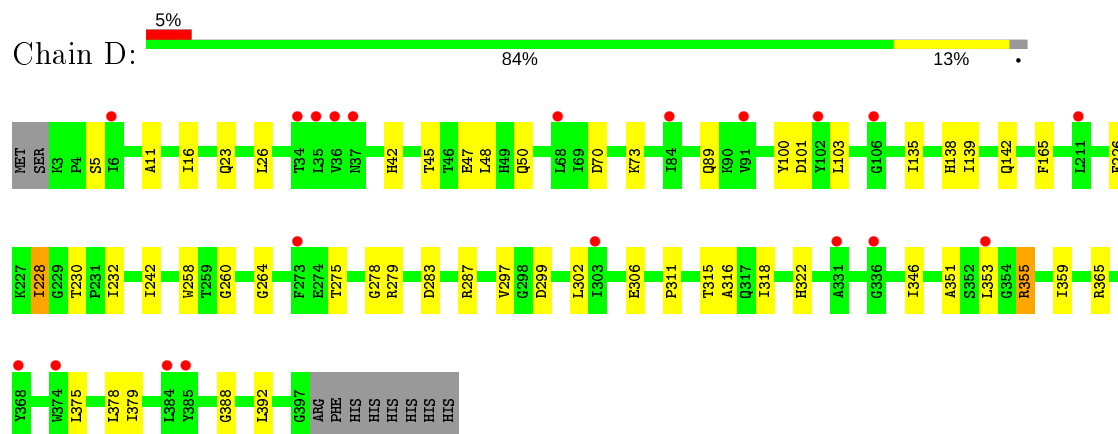
- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



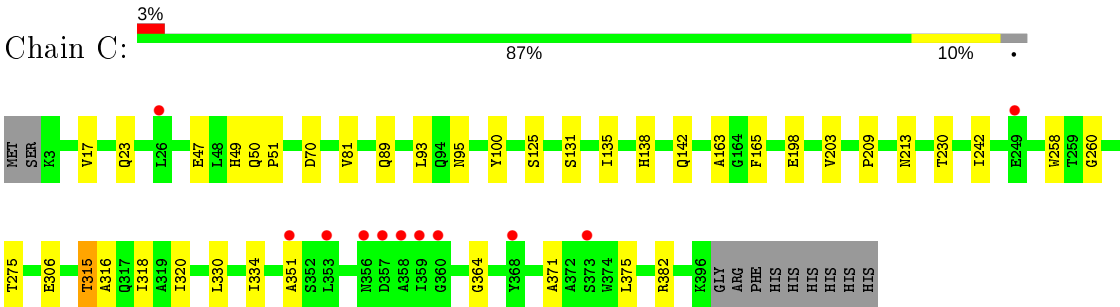
- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.85Å 114.34Å 130.06Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	43.34 – 2.80 44.27 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.34-2.80) 99.7 (44.27-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.227 , 0.268 0.234 , 0.271	Depositor DCC
$R_{free}$ test set	2595 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, HQO

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	0/2980	0.47	0/4062
1	B	0.27	0/2988	0.48	0/4068
1	C	0.26	0/2938	0.45	0/4010
1	D	0.26	0/2928	0.45	0/3997
All	All	0.27	0/11834	0.46	0/16137

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	2921	0	2836	22	1
1	B	2931	0	2861	28	0
1	C	2881	0	2760	21	1
1	D	2870	0	2746	29	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
3	B	19	0	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	19	0	21	0	0
4	A	14	0	0	0	0
4	B	14	0	0	0	0
4	C	12	0	0	0	0
4	D	3	0	0	0	0
All	All	11896	0	11369	100	1

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 4.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:GLU:OE2	1:D:50:GLN:NE2	2.23	0.71
1:C:125:SER:O	1:C:131:SER:OG	2.08	0.70
1:D:50:GLN:OE1	1:D:355:ARG:NH1	2.22	0.68
1:B:163:ALA:N	1:B:198:GLU:OE1	2.23	0.67
1:C:163:ALA:H	1:C:198:GLU:HG2	1.61	0.66
1:C:315:THR:OG1	2:C:601:FAD:O2	2.13	0.66
1:D:26:LEU:O	1:D:73:LYS:NZ	2.29	0.65
1:A:258:TRP:CZ2	1:A:260:GLY:HA3	2.34	0.63
1:D:89:GLN:NE2	1:D:100:TYR:O	2.31	0.63
1:A:63:VAL:HG21	1:A:392:LEU:HD11	1.82	0.61
1:A:89:GLN:NE2	1:A:100:TYR:O	2.34	0.61
1:A:23:GLN:OE1	1:A:70:ASP:N	2.33	0.60
1:C:330:LEU:O	1:C:334:ILE:HG12	2.05	0.57
1:C:23:GLN:OE1	1:C:70:ASP:N	2.30	0.56
1:B:302:LEU:HD11	1:B:311:PRO:HB3	1.88	0.55
1:D:23:GLN:OE1	1:D:70:ASP:N	2.38	0.55
1:B:281:LYS:HE2	1:B:304:ILE:HG13	1.89	0.55
1:D:5:SER:N	1:D:101:ASP:OD2	2.35	0.55
1:A:47:GLU:OE1	1:A:50:GLN:NE2	2.40	0.54
1:A:215:ALA:HB2	1:A:359:ILE:HD13	1.89	0.54
1:B:211:LEU:HD11	1:B:361:ILE:HG12	1.88	0.54
1:C:165:PHE:CE2	1:C:351:ALA:HB2	2.43	0.54
1:C:316:ALA:HB2	2:C:601:FAD:H2'	1.90	0.54
1:C:209:PRO:O	1:C:213:ASN:ND2	2.27	0.54
1:A:308:ASN:OD1	1:A:310:ARG:HG2	2.08	0.53
1:A:17:VAL:HG21	1:A:320:ILE:HG23	1.89	0.53
1:D:299:ASP:OD1	2:D:601:FAD:H5'2	2.08	0.53
1:A:277:ARG:HA	1:A:277:ARG:HH11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:GLY:HA3	1:D:392:LEU:HD22	1.90	0.51
1:B:258:TRP:CZ2	1:B:260:GLY:HA3	2.46	0.51
1:D:11:ALA:O	1:D:42:HIS:ND1	2.40	0.51
1:D:258:TRP:CZ2	1:D:260:GLY:HA3	2.46	0.50
1:D:315:THR:HB	2:D:601:FAD:O2	2.11	0.50
1:D:45:THR:HA	1:D:48:LEU:HG	1.94	0.50
1:B:138:HIS:O	1:B:142:GLN:HG2	2.12	0.50
1:A:230:THR:HG21	1:A:242:ILE:HD12	1.94	0.50
1:B:204:LEU:HB2	1:B:212:VAL:HG22	1.93	0.49
1:D:138:HIS:O	1:D:142:GLN:HG2	2.13	0.48
1:B:316:ALA:HB2	2:B:601:FAD:H2'	1.95	0.48
1:B:17:VAL:HG21	1:B:320:ILE:HG23	1.94	0.48
1:D:297:VAL:HG12	1:D:322:HIS:HB3	1.94	0.48
1:C:371:ALA:O	1:C:375:LEU:HD13	2.14	0.48
1:B:308:ASN:HB2	1:B:310:ARG:HD3	1.95	0.47
1:D:230:THR:HG21	1:D:242:ILE:HD12	1.96	0.47
1:C:230:THR:HG21	1:C:242:ILE:HD12	1.96	0.47
1:B:45:THR:HA	1:B:48:LEU:HG	1.95	0.47
1:C:138:HIS:O	1:C:142:GLN:HG2	2.14	0.47
1:B:11:ALA:O	1:B:42:HIS:ND1	2.44	0.47
1:D:375:LEU:O	1:D:379:ILE:HG13	2.15	0.47
1:A:315:THR:HB	2:A:601:FAD:O2	2.15	0.47
1:B:388:GLY:HA3	1:B:392:LEU:HD22	1.97	0.47
1:D:355:ARG:HE	1:D:355:ARG:HA	1.80	0.46
1:C:81:VAL:HA	1:C:93:LEU:HD23	1.97	0.46
1:B:46:THR:HG21	3:B:602:HQO:HC8	1.98	0.46
1:D:302:LEU:HD11	1:D:311:PRO:HB3	1.98	0.46
1:B:60:GLN:OE1	1:B:396:LYS:HG3	2.16	0.46
1:C:315:THR:HG23	1:C:318:ILE:HG22	1.99	0.45
1:C:163:ALA:HB1	1:C:203:VAL:HG13	1.99	0.45
1:A:316:ALA:HB2	2:A:601:FAD:H2'	1.99	0.45
1:C:306:GLU:HG2	1:C:306:GLU:H	1.59	0.44
1:A:138:HIS:O	1:A:142:GLN:HG2	2.18	0.44
1:B:118:GLY:HA2	1:B:121:GLU:HG2	1.98	0.44
1:B:233:LYS:N	1:B:241:VAL:O	2.51	0.44
1:D:100:TYR:CD2	1:D:103:LEU:HB2	2.52	0.44
1:D:135:ILE:O	1:D:139:ILE:HG13	2.17	0.44
1:B:23:GLN:HB3	1:B:74:ILE:HD11	2.00	0.44
1:B:47:GLU:OE2	1:B:50:GLN:NE2	2.50	0.44
1:D:316:ALA:HB2	2:D:601:FAD:H2'	1.98	0.44
1:A:165:PHE:CE2	1:A:351:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLY:HA3	1:A:392:LEU:HD22	2.00	0.43
1:A:209:PRO:O	1:A:213:ASN:ND2	2.29	0.43
1:A:100:TYR:CD1	1:A:103:LEU:HB2	2.54	0.43
1:D:264:GLY:HA3	1:D:278:GLY:O	2.19	0.43
1:D:353:LEU:HD11	1:D:359:ILE:HG23	1.99	0.43
1:A:362:VAL:HG21	1:A:375:LEU:HD12	2.00	0.42
1:C:131:SER:O	1:C:135:ILE:HG13	2.19	0.42
1:D:318:ILE:HD13	1:D:346:ILE:HD11	2.01	0.42
1:D:165:PHE:CE2	1:D:351:ALA:HB2	2.53	0.42
1:A:279:ARG:HD3	1:A:299:ASP:O	2.19	0.42
1:C:258:TRP:CZ2	1:C:260:GLY:HA3	2.54	0.42
1:A:11:ALA:O	1:A:42:HIS:ND1	2.44	0.42
1:B:348:GLY:HA3	1:B:362:VAL:HG22	2.00	0.42
1:C:50:GLN:HB2	1:C:51:PRO:HD3	2.01	0.42
1:B:283:ASP:OD2	1:B:287:ARG:HB2	2.20	0.42
1:B:348:GLY:HA2	1:B:361:ILE:O	2.20	0.42
1:A:6:ILE:HG12	1:A:102:TYR:HB2	2.02	0.42
1:C:47:GLU:HA	1:C:49:HIS:CE1	2.55	0.42
1:B:89:GLN:NE2	1:B:100:TYR:O	2.52	0.41
1:C:17:VAL:HG21	1:C:320:ILE:HG23	2.03	0.41
1:D:226:PHE:HB3	1:D:228:ILE:HD11	2.01	0.41
1:B:315:THR:HB	2:B:601:FAD:O2	2.20	0.41
1:B:100:TYR:CD2	1:B:103:LEU:HB2	2.55	0.41
1:D:283:ASP:OD1	1:D:287:ARG:N	2.53	0.41
1:A:9:LEU:HB3	1:A:107:LEU:HD21	2.03	0.41
1:D:232:ILE:HA	1:D:242:ILE:HG22	2.02	0.41
1:B:98:LEU:HA	1:B:98:LEU:HD23	1.95	0.40
1:C:89:GLN:NE2	1:C:100:TYR:O	2.50	0.40
1:D:279:ARG:HB3	1:D:302:LEU:HB2	2.02	0.40
1:B:20:LEU:O	1:B:23:GLN:HG2	2.21	0.40
1:B:378:LEU:HD22	1:B:378:LEU:HA	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:NH1	1:C:95:ASN:O[2_545]	2.12	0.08

## 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	392/405 (97%)	380 (97%)	11 (3%)	1 (0%)	41	72
1	B	392/405 (97%)	380 (97%)	11 (3%)	1 (0%)	41	72
1	C	392/405 (97%)	381 (97%)	10 (3%)	1 (0%)	41	72
1	D	393/405 (97%)	381 (97%)	12 (3%)	0	100	100
All	All	1569/1620 (97%)	1522 (97%)	44 (3%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	348	GLY
1	A	364	GLY
1	C	364	GLY

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/329 (88%)	284 (98%)	5 (2%)	60	87
1	B	292/329 (89%)	286 (98%)	6 (2%)	53	84
1	C	280/329 (85%)	277 (99%)	3 (1%)	73	92
1	D	274/329 (83%)	267 (97%)	7 (3%)	46	79
All	All	1135/1316 (86%)	1114 (98%)	21 (2%)	57	85

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	LYS
1	B	88	GLN
1	B	121	GLU
1	B	137	GLN
1	B	202	THR
1	B	378	LEU
1	A	277	ARG
1	A	340	THR
1	A	375	LEU
1	A	381	MET
1	A	384	LEU
1	D	16	ILE
1	D	228	ILE
1	D	275	THR
1	D	306	GLU
1	D	355	ARG
1	D	365	ARG
1	D	378	LEU
1	C	275	THR
1	C	315	THR
1	C	382	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	GLN
1	A	89	GLN
1	D	89	GLN

### 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 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	D	601	-	51,58,58	4.31	20 (39%)	60,89,89	2.45	13 (21%)
2	FAD	C	601	-	51,58,58	4.30	21 (41%)	60,89,89	2.49	12 (20%)
3	HQO	C	602	-	20,20,20	1.01	1 (5%)	18,26,26	2.90	2 (11%)
3	HQO	B	602	-	20,20,20	1.01	1 (5%)	18,26,26	2.86	3 (16%)
2	FAD	B	601	-	51,58,58	4.29	19 (37%)	60,89,89	2.44	12 (20%)
2	FAD	A	601	-	51,58,58	4.28	20 (39%)	60,89,89	2.46	14 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	601	-	-	8/30/50/50	0/6/6/6
2	FAD	C	601	-	-	9/30/50/50	0/6/6/6
3	HQO	C	602	-	-	0/7/7/7	0/2/2/2
3	HQO	B	602	-	-	4/7/7/7	0/2/2/2
2	FAD	B	601	-	-	11/30/50/50	0/6/6/6
2	FAD	A	601	-	-	16/30/50/50	0/6/6/6

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C2B-C1B	-16.58	1.28	1.53
2	C	601	FAD	C2B-C1B	-16.54	1.28	1.53
2	A	601	FAD	C2B-C1B	-16.50	1.28	1.53
2	D	601	FAD	C2B-C1B	-16.48	1.28	1.53
2	C	601	FAD	O4B-C1B	14.30	1.61	1.41
2	B	601	FAD	O4B-C1B	14.12	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	O4B-C1B	13.97	1.60	1.41
2	A	601	FAD	O4B-C1B	13.94	1.60	1.41
2	D	601	FAD	C5X-N5	8.14	1.48	1.35
2	A	601	FAD	C10-N1	8.01	1.43	1.33
2	C	601	FAD	C5X-N5	8.00	1.48	1.35
2	D	601	FAD	C10-N1	7.94	1.43	1.33
2	B	601	FAD	C5X-N5	7.93	1.48	1.35
2	A	601	FAD	C5X-N5	7.85	1.48	1.35
2	B	601	FAD	C10-N1	7.80	1.43	1.33
2	C	601	FAD	C10-N1	7.71	1.43	1.33
2	B	601	FAD	O4B-C4B	-7.22	1.28	1.45
2	D	601	FAD	O4B-C4B	-7.09	1.29	1.45
2	A	601	FAD	O4B-C4B	-7.06	1.29	1.45
2	D	601	FAD	C4X-N5	6.80	1.43	1.33
2	C	601	FAD	O4B-C4B	-6.78	1.29	1.45
2	C	601	FAD	C4X-N5	6.47	1.42	1.33
2	A	601	FAD	C4X-N5	6.31	1.42	1.33
2	B	601	FAD	C4X-N5	6.24	1.42	1.33
2	A	601	FAD	C4-N3	5.77	1.43	1.33
2	B	601	FAD	C4-N3	5.62	1.42	1.33
2	C	601	FAD	C4-N3	5.53	1.42	1.33
2	D	601	FAD	C4-N3	5.52	1.42	1.33
2	D	601	FAD	C9A-N10	5.49	1.45	1.38
2	B	601	FAD	C9A-N10	5.42	1.45	1.38
2	C	601	FAD	C9A-N10	5.31	1.45	1.38
2	A	601	FAD	C9A-N10	5.21	1.45	1.38
2	D	601	FAD	C4-C4X	4.81	1.49	1.41
2	A	601	FAD	C4X-C10	4.75	1.43	1.38
2	D	601	FAD	C4X-C10	4.75	1.43	1.38
2	C	601	FAD	C4-C4X	4.70	1.49	1.41
2	C	601	FAD	C4X-C10	4.60	1.43	1.38
2	C	601	FAD	O2B-C2B	4.45	1.53	1.43
2	B	601	FAD	O2B-C2B	4.43	1.53	1.43
2	D	601	FAD	O2B-C2B	4.40	1.53	1.43
2	D	601	FAD	C2-N1	4.34	1.46	1.38
2	A	601	FAD	O2B-C2B	4.34	1.53	1.43
2	B	601	FAD	C4X-C10	4.34	1.43	1.38
2	A	601	FAD	C2-N1	4.33	1.46	1.38
2	B	601	FAD	C2-N3	4.31	1.46	1.38
2	B	601	FAD	C4-C4X	4.31	1.48	1.41
2	A	601	FAD	C2-N3	4.30	1.46	1.38
2	B	601	FAD	C2-N1	4.24	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4-C4X	4.24	1.48	1.41
2	C	601	FAD	C2-N3	4.19	1.46	1.38
2	C	601	FAD	C2-N1	4.12	1.46	1.38
2	D	601	FAD	C2-N3	4.00	1.46	1.38
2	B	601	FAD	O4-C4	-3.77	1.15	1.24
2	A	601	FAD	O4-C4	-3.70	1.15	1.24
2	C	601	FAD	O4-C4	-3.67	1.15	1.24
2	D	601	FAD	O4-C4	-3.63	1.15	1.24
2	A	601	FAD	C6A-N6A	3.28	1.46	1.34
2	C	601	FAD	C6A-N6A	3.24	1.45	1.34
2	D	601	FAD	C6A-N6A	3.23	1.45	1.34
2	D	601	FAD	C2A-N3A	3.22	1.37	1.32
2	B	601	FAD	C6A-N6A	3.17	1.45	1.34
2	A	601	FAD	C2A-N3A	3.16	1.37	1.32
2	C	601	FAD	C2A-N3A	3.15	1.37	1.32
2	D	601	FAD	C8M-C8	3.07	1.57	1.51
2	B	601	FAD	C2A-N3A	3.06	1.37	1.32
2	C	601	FAD	C8M-C8	3.03	1.57	1.51
3	C	602	HQO	C10-C5	-3.01	1.37	1.42
3	B	602	HQO	C10-C5	-3.00	1.37	1.42
2	B	601	FAD	C8M-C8	2.92	1.56	1.51
2	B	601	FAD	O4'-C4'	-2.84	1.37	1.43
2	A	601	FAD	C8M-C8	2.81	1.56	1.51
2	D	601	FAD	O4'-C4'	-2.78	1.37	1.43
2	C	601	FAD	O4'-C4'	-2.74	1.37	1.43
2	B	601	FAD	C7M-C7	2.73	1.56	1.51
2	A	601	FAD	O4'-C4'	-2.73	1.37	1.43
2	D	601	FAD	C7M-C7	2.68	1.56	1.51
2	A	601	FAD	C7M-C7	2.67	1.56	1.51
2	C	601	FAD	C7M-C7	2.65	1.56	1.51
2	C	601	FAD	C5'-C4'	2.50	1.55	1.51
2	A	601	FAD	C5'-C4'	2.31	1.55	1.51
2	C	601	FAD	C2A-N1A	2.04	1.37	1.33
2	D	601	FAD	C2A-N1A	2.03	1.37	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	HQO	O1-C1-C10	11.09	130.17	116.31
3	B	602	HQO	O1-C1-C10	10.85	129.87	116.31
2	C	601	FAD	C5A-C6A-N6A	8.70	133.58	120.35
2	D	601	FAD	C5A-C6A-N6A	8.61	133.43	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C5A-C6A-N6A	8.38	133.09	120.35
2	B	601	FAD	C5A-C6A-N6A	8.22	132.84	120.35
2	C	601	FAD	C7M-C7-C8	7.86	136.85	120.74
2	B	601	FAD	C7M-C7-C8	7.81	136.74	120.74
2	D	601	FAD	C7M-C7-C8	7.46	136.02	120.74
2	A	601	FAD	C7M-C7-C8	7.34	135.79	120.74
2	C	601	FAD	C7M-C7-C6	-7.21	103.09	120.34
2	B	601	FAD	C7M-C7-C6	-7.08	103.40	120.34
2	D	601	FAD	C7M-C7-C6	-6.92	103.79	120.34
2	A	601	FAD	C7M-C7-C6	-6.69	104.33	120.34
2	C	601	FAD	N6A-C6A-N1A	-5.88	106.36	118.57
2	B	601	FAD	N3A-C2A-N1A	-5.76	119.67	128.68
2	D	601	FAD	N6A-C6A-N1A	-5.74	106.66	118.57
2	C	601	FAD	N3A-C2A-N1A	-5.62	119.89	128.68
2	B	601	FAD	C4-N3-C2	5.61	119.88	115.14
2	A	601	FAD	N6A-C6A-N1A	-5.58	106.98	118.57
2	D	601	FAD	N3A-C2A-N1A	-5.50	120.09	128.68
2	B	601	FAD	N6A-C6A-N1A	-5.49	107.18	118.57
2	A	601	FAD	C4-N3-C2	5.47	119.76	115.14
2	A	601	FAD	N3A-C2A-N1A	-5.45	120.16	128.68
2	C	601	FAD	C4-N3-C2	5.39	119.70	115.14
2	D	601	FAD	C4-N3-C2	5.22	119.55	115.14
2	A	601	FAD	C5X-C9A-N10	5.02	121.35	117.72
3	C	602	HQO	O1-C1-C2	-3.92	109.70	121.17
2	C	601	FAD	C5X-C9A-N10	3.90	120.54	117.72
3	B	602	HQO	O1-C1-C2	-3.76	110.17	121.17
2	A	601	FAD	C1'-N10-C10	3.71	121.73	118.41
2	B	601	FAD	C5X-C9A-N10	3.33	120.12	117.72
2	D	601	FAD	C4X-N5-C5X	3.28	120.05	116.77
2	D	601	FAD	C8M-C8-C7	-3.26	114.06	120.74
2	D	601	FAD	C5X-C9A-N10	3.17	120.02	117.72
2	C	601	FAD	C4X-C4-N3	-3.03	119.29	123.43
2	B	601	FAD	C8M-C8-C7	-3.01	114.56	120.74
2	A	601	FAD	C4X-C4-N3	-2.89	119.47	123.43
2	A	601	FAD	C8M-C8-C7	-2.83	114.93	120.74
2	B	601	FAD	C4X-C4-N3	-2.83	119.56	123.43
2	D	601	FAD	C4X-C4-N3	-2.82	119.58	123.43
2	B	601	FAD	C4X-N5-C5X	2.80	119.57	116.77
2	A	601	FAD	C4'-C3'-C2'	-2.73	107.69	113.36
2	C	601	FAD	C4X-N5-C5X	2.70	119.47	116.77
2	C	601	FAD	C8M-C8-C7	-2.70	115.21	120.74
2	C	601	FAD	C1'-N10-C9A	2.60	120.34	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C1'-N10-C9A	2.56	120.30	118.29
2	D	601	FAD	C1'-N10-C10	2.44	120.60	118.41
2	D	601	FAD	C8M-C8-C9	2.36	126.00	120.34
2	A	601	FAD	C4X-N5-C5X	2.36	119.13	116.77
3	B	602	HQO	C13-C11-C3	-2.29	107.78	113.82
2	D	601	FAD	C3B-C2B-C1B	2.28	104.41	100.98
2	A	601	FAD	C9A-N10-C10	-2.23	118.99	121.91
2	B	601	FAD	C4'-C3'-C2'	-2.22	108.74	113.36
2	A	601	FAD	C3B-C2B-C1B	2.18	104.26	100.98
2	C	601	FAD	C1'-N10-C10	2.05	120.24	118.41

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	FAD	C5B-O5B-PA-O3P
2	C	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	C5B-O5B-PA-O2A
3	B	602	HQO	C3-C11-C13-C12
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	B	601	FAD	C5'-O5'-P-O1P
2	B	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	PA-O3P-P-O5'
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O2A
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	D	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	C	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C2'-C3'-C4'-C5'
3	B	602	HQO	C13-C12-C14-C15
2	A	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	C4'-C5'-O5'-P
3	B	602	HQO	C14-C15-C16-C17
2	C	601	FAD	P-O3P-PA-O5B
2	A	601	FAD	PA-O3P-P-O5'
2	C	601	FAD	C4'-C5'-O5'-P
2	D	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5'-O5'-P-O3P
2	D	601	FAD	PA-O3P-P-O2P
2	D	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C4'-C5'-O5'-P
3	B	602	HQO	C14-C12-C13-C11
2	B	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C5B-O5B-PA-O3P
2	C	601	FAD	C5'-O5'-P-O3P
2	C	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	C5'-O5'-P-O2P

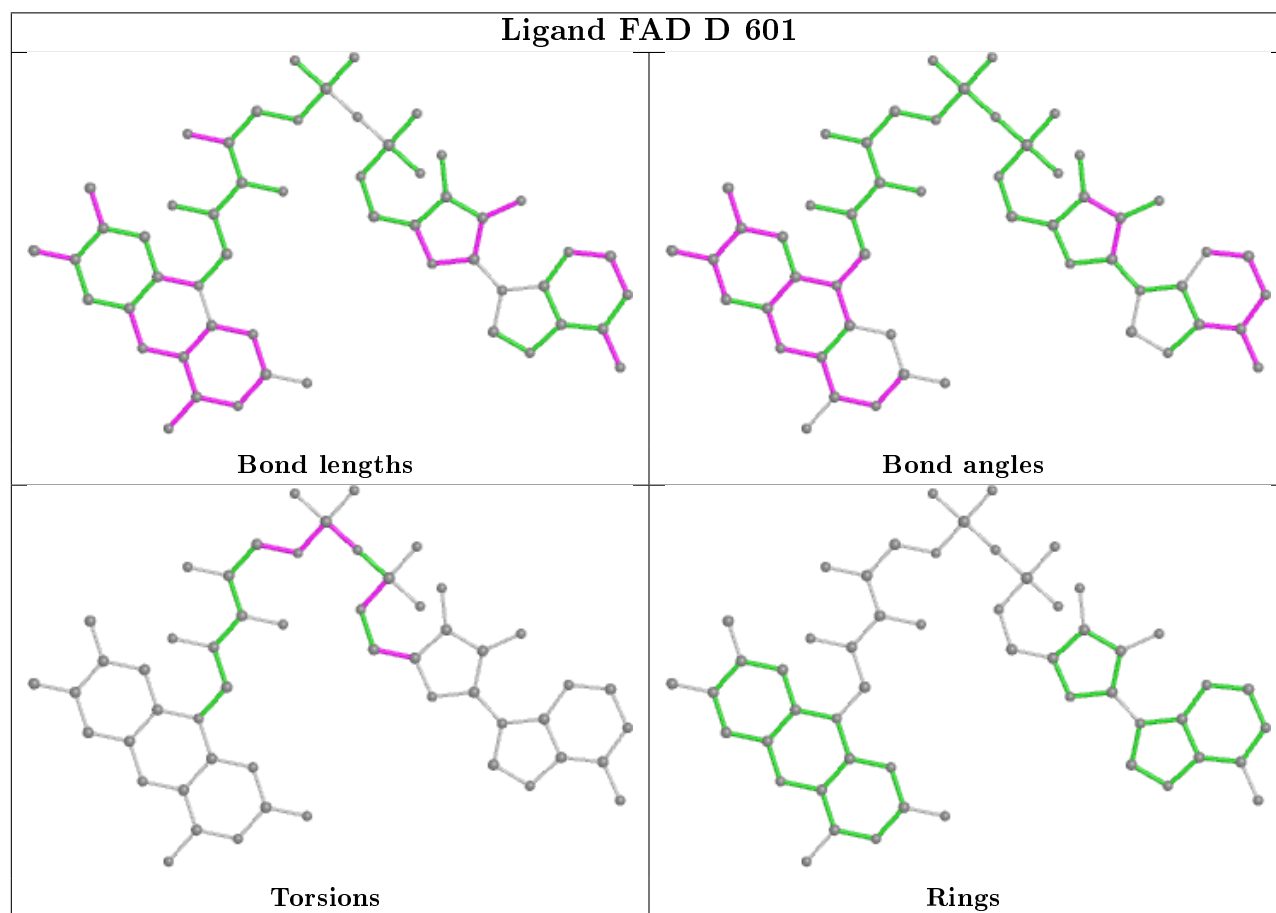
There are no ring outliers.

5 monomers are involved in 10 short contacts:

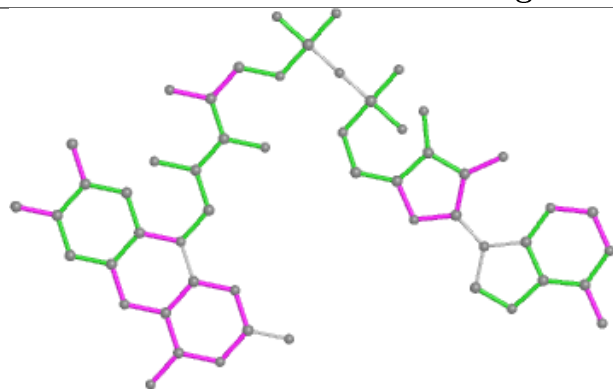
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	FAD	3	0
2	C	601	FAD	2	0
3	B	602	HQO	1	0
2	B	601	FAD	2	0
2	A	601	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

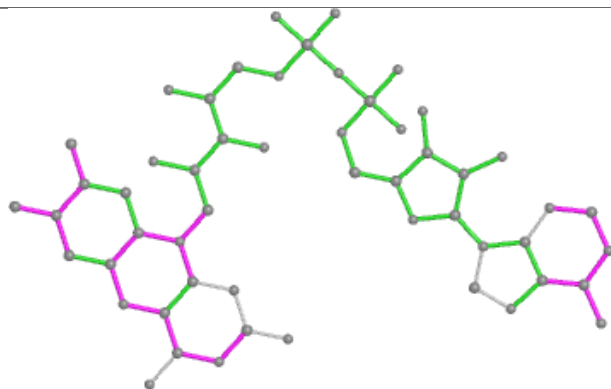
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



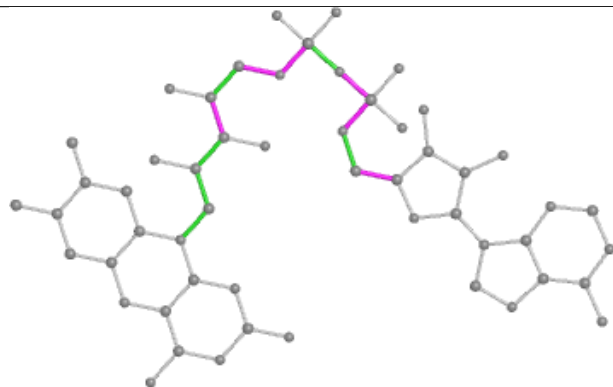
## Ligand FAD C 601



Bond lengths



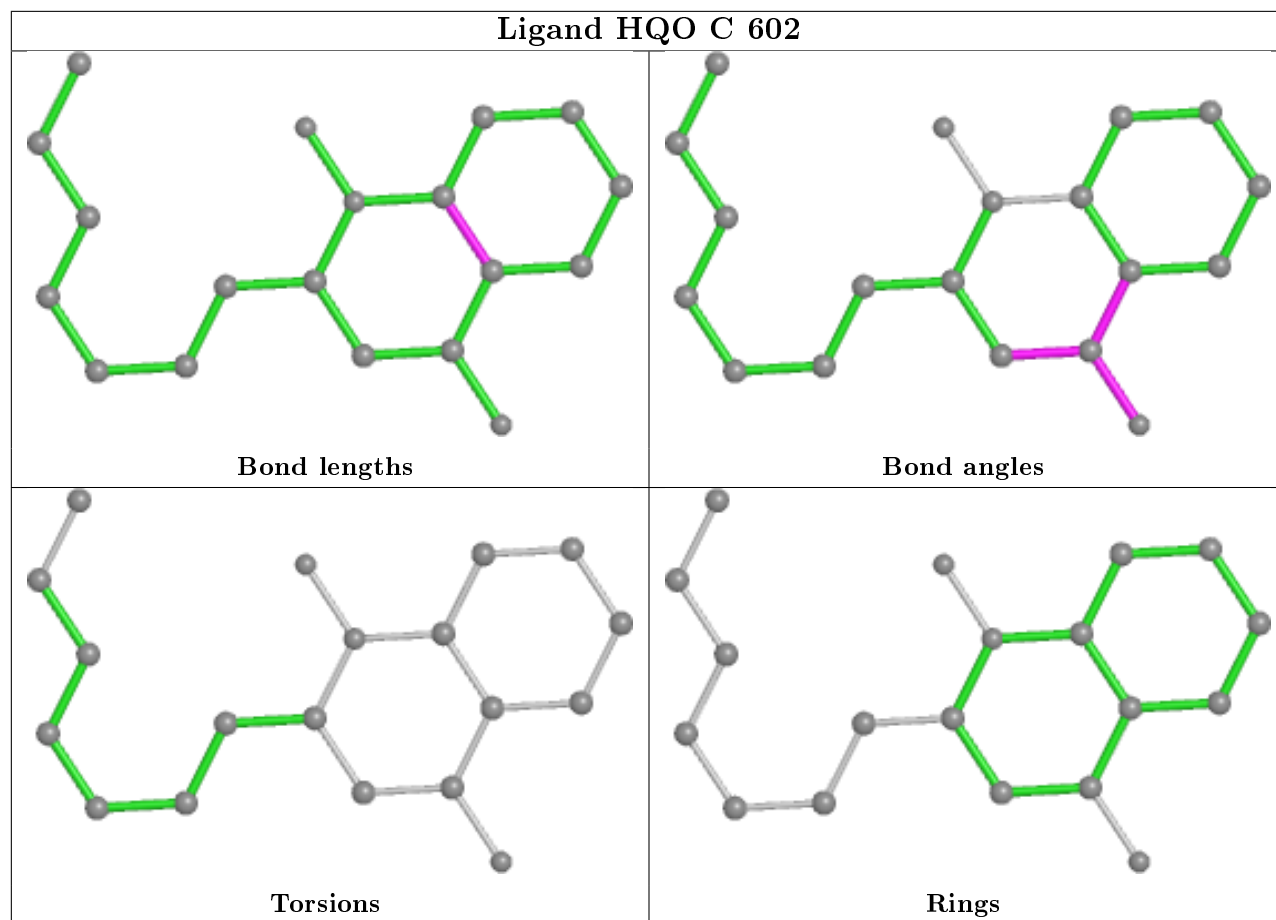
Bond angles

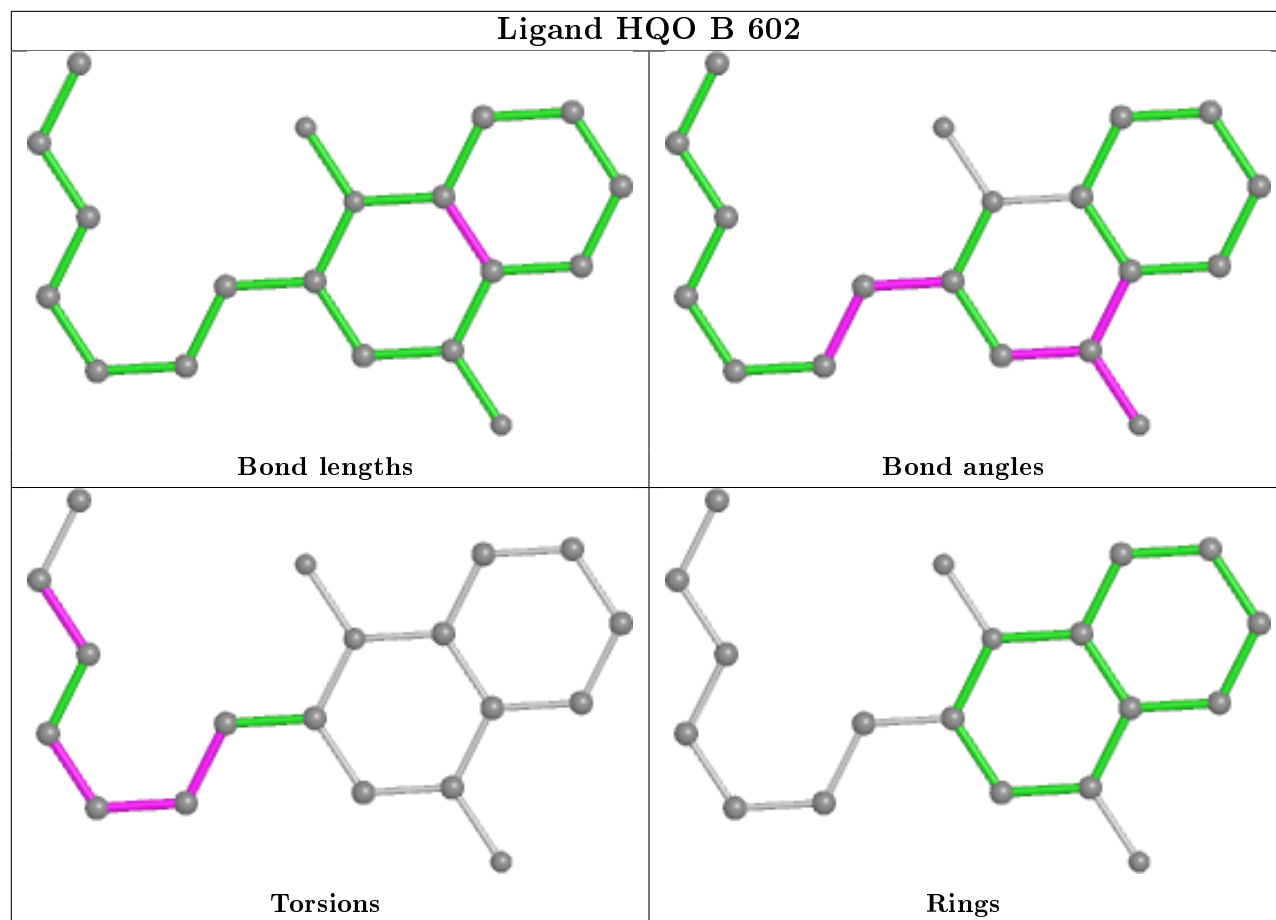


Torsions



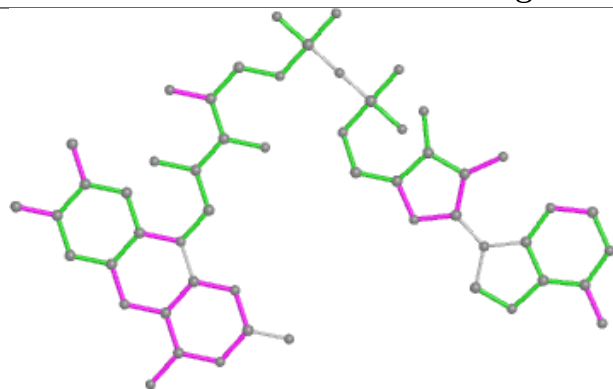
Rings



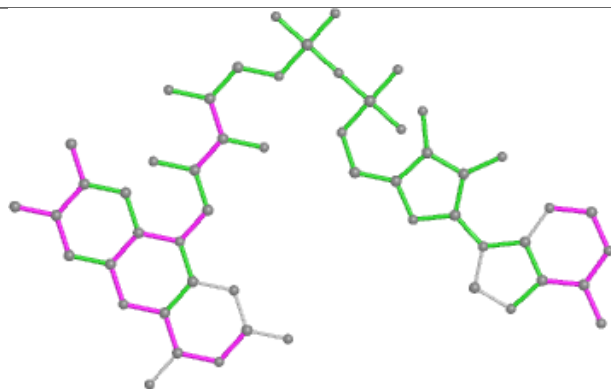




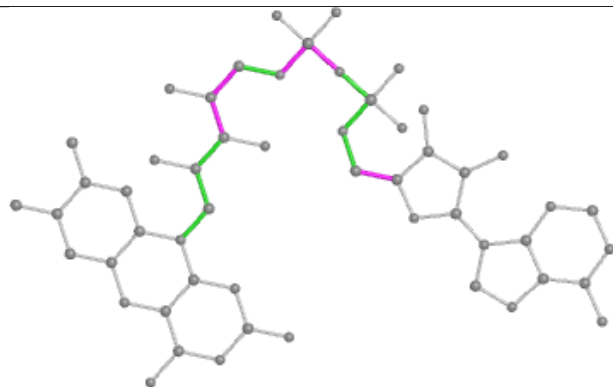
## Ligand FAD B 601



Bond lengths



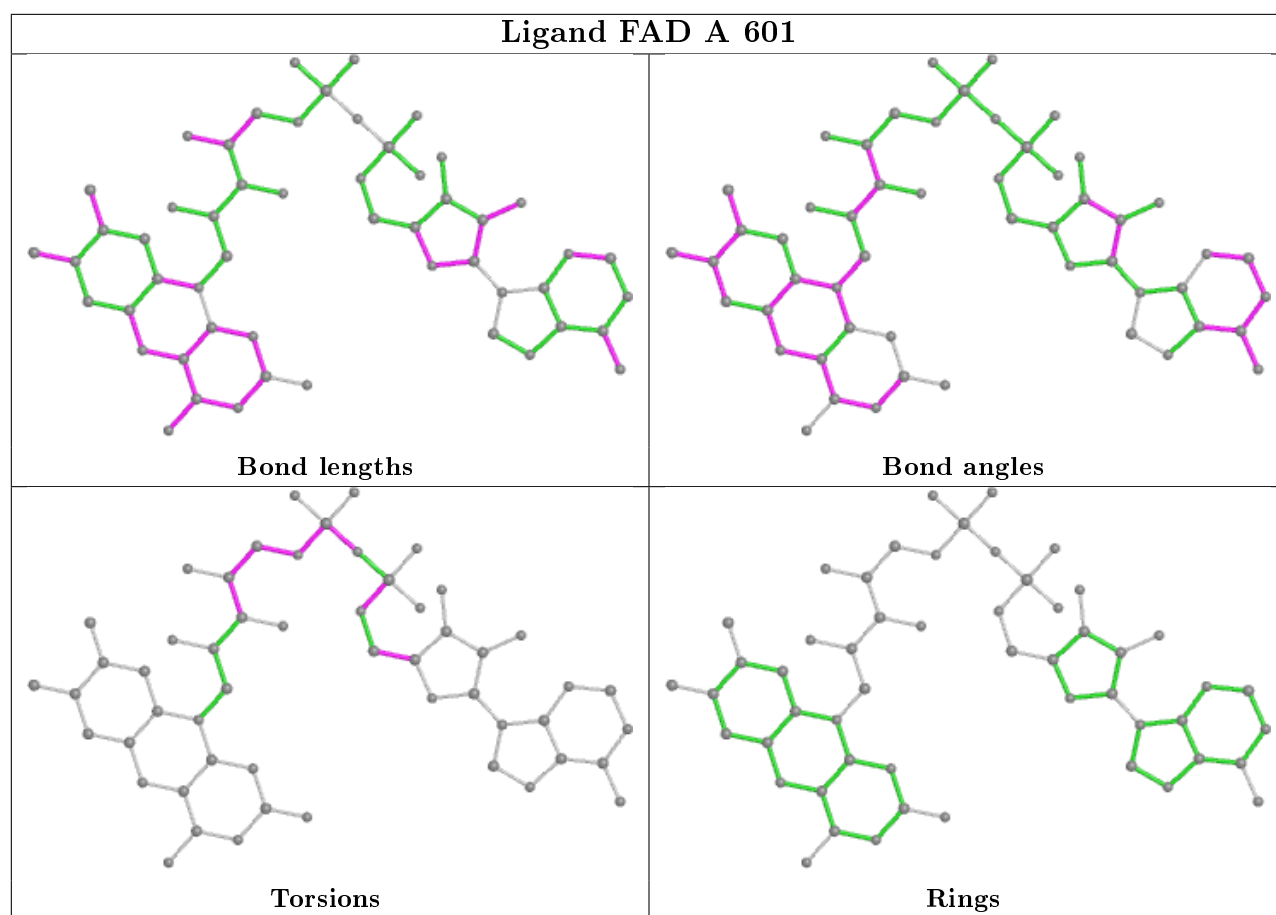
Bond angles



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	394/405 (97%)	0.11	12 (3%)	50 40	34, 66, 97, 120	0
1	B	394/405 (97%)	0.02	11 (2%)	53 43	34, 60, 92, 109	0
1	C	394/405 (97%)	0.03	11 (2%)	53 43	40, 62, 96, 117	0
1	D	395/405 (97%)	0.25	20 (5%)	28 19	41, 79, 104, 111	0
All	All	1577/1620 (97%)	0.10	54 (3%)	45 35	34, 67, 99, 120	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	356	ASN	4.2
1	D	34	THR	4.1
1	A	363	GLY	3.6
1	A	77	VAL	3.5
1	D	374	TRP	3.5
1	D	84	ILE	3.4
1	B	367	VAL	3.4
1	C	358	ALA	3.4
1	D	102	TYR	3.3
1	D	211	LEU	3.3
1	D	273	PHE	3.3
1	D	35	LEU	3.3
1	D	6	ILE	3.1
1	D	353	LEU	3.0
1	A	23	GLN	3.0
1	D	368	TYR	2.9
1	C	359	ILE	2.9
1	C	368	TYR	2.8
1	B	359	ILE	2.8
1	C	26	LEU	2.8
1	A	362	VAL	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	204	LEU	2.7
1	B	362	VAL	2.7
1	C	360	GLY	2.7
1	D	106	GLY	2.6
1	A	22	LEU	2.6
1	B	368	TYR	2.6
1	B	372	ALA	2.6
1	D	37	ASN	2.5
1	B	348	GLY	2.5
1	C	353	LEU	2.5
1	C	351	ALA	2.5
1	D	303	ILE	2.5
1	C	357	ASP	2.5
1	A	368	TYR	2.5
1	A	367	VAL	2.4
1	D	91	VAL	2.4
1	D	385	TYR	2.4
1	D	68	LEU	2.4
1	A	73	LYS	2.4
1	A	7	VAL	2.3
1	A	391	SER	2.3
1	C	373	SER	2.3
1	D	36	VAL	2.3
1	D	331	ALA	2.3
1	C	356	ASN	2.3
1	A	387	ILE	2.3
1	D	336	GLY	2.2
1	C	249	GLU	2.2
1	D	384	LEU	2.2
1	B	370	HIS	2.1
1	B	360	GLY	2.1
1	B	357	ASP	2.0
1	A	65	ILE	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 ⓘ

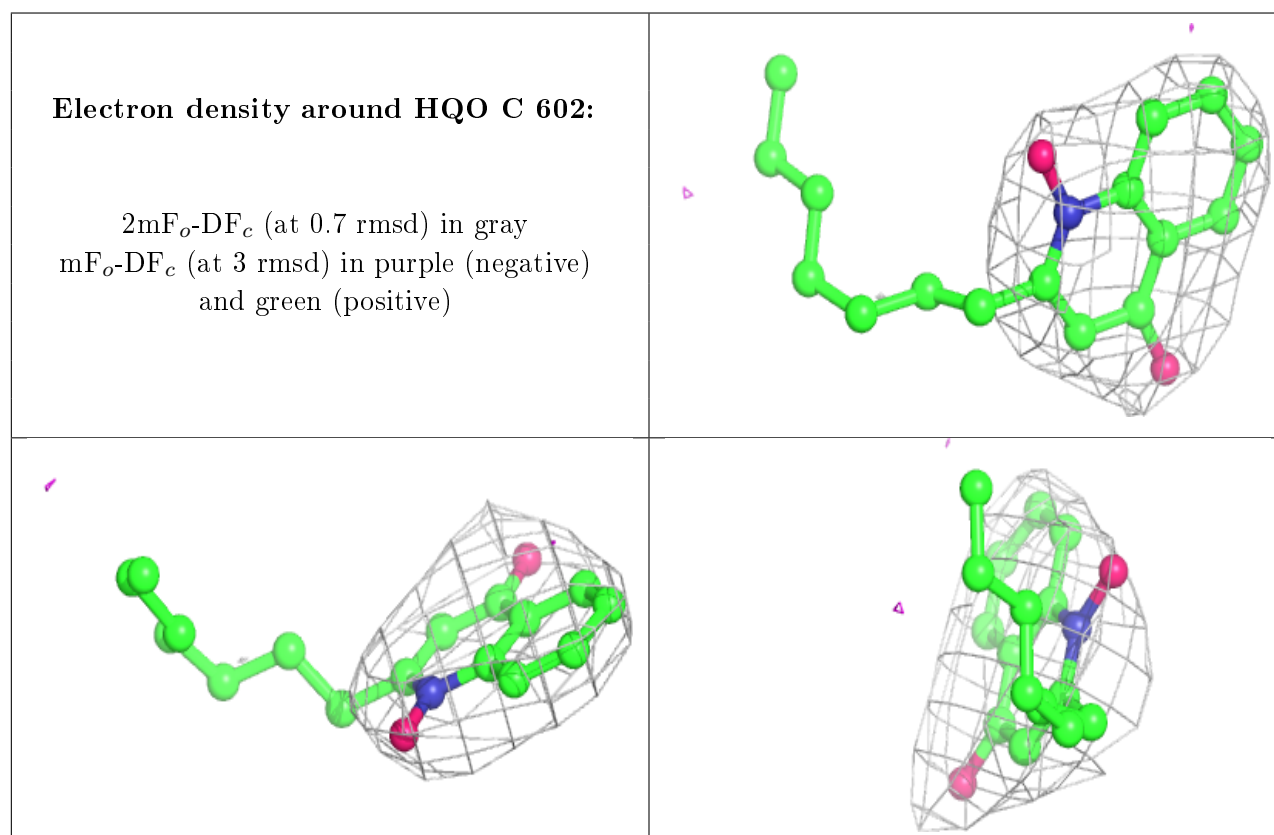
There are no carbohydrates in this entry.

## 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.

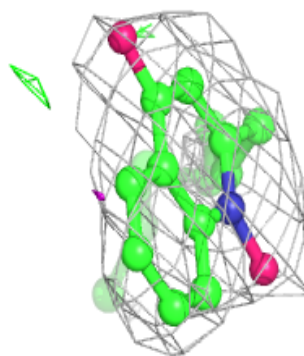
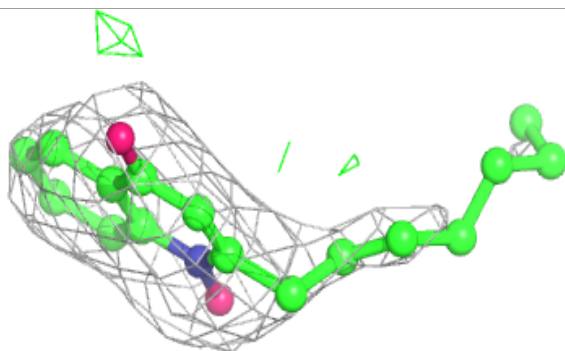
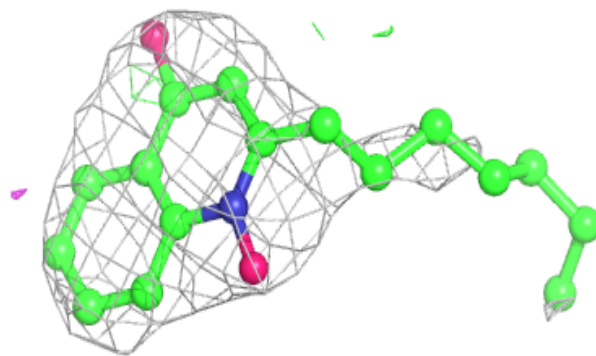
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	HQO	C	602	19/19	0.91	0.39	64,80,92,93	0
3	HQO	B	602	19/19	0.92	0.41	48,57,78,78	0
2	FAD	D	601	53/53	0.95	0.17	44,66,74,77	0
2	FAD	A	601	53/53	0.95	0.20	40,48,59,70	0
2	FAD	B	601	53/53	0.96	0.19	35,42,53,65	0
2	FAD	C	601	53/53	0.97	0.18	41,50,66,75	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.

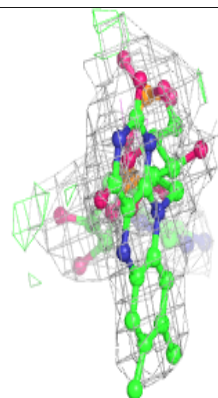
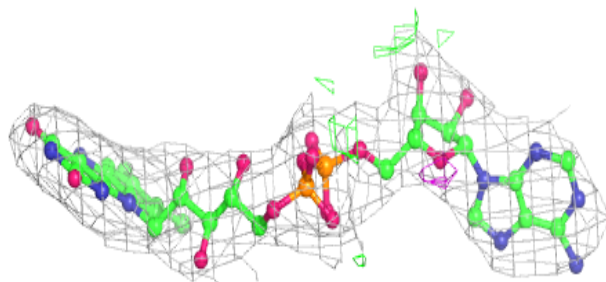
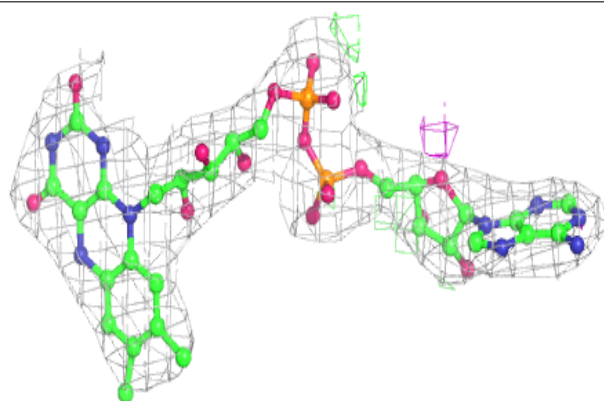


**Electron density around HQO B 602:**

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

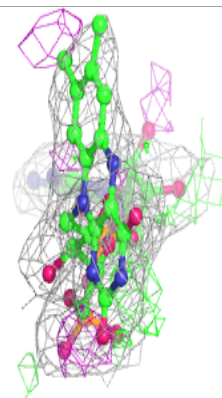
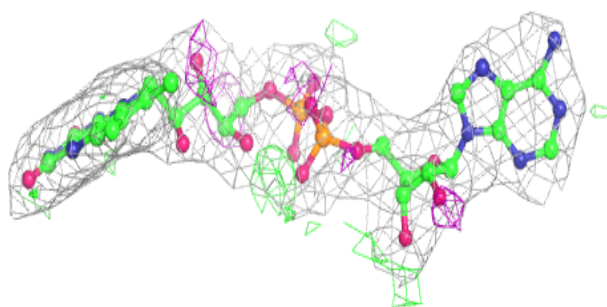
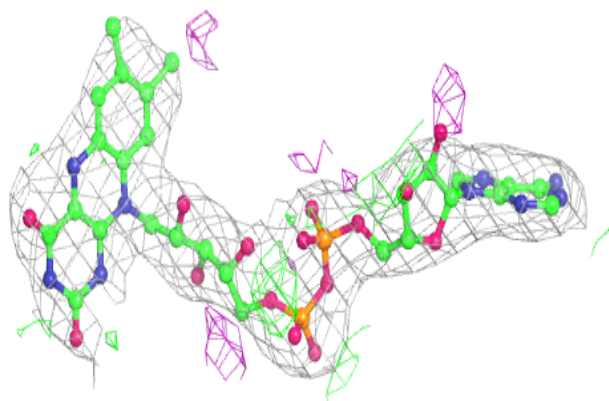
**Electron density around FAD D 601:**

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

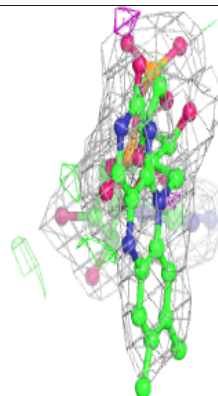
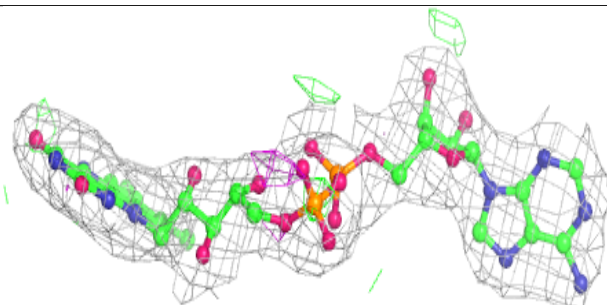
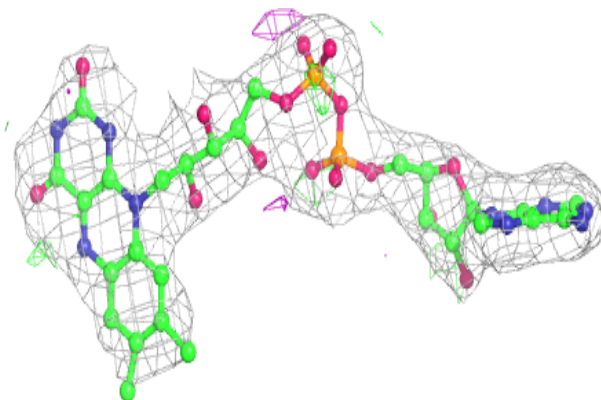


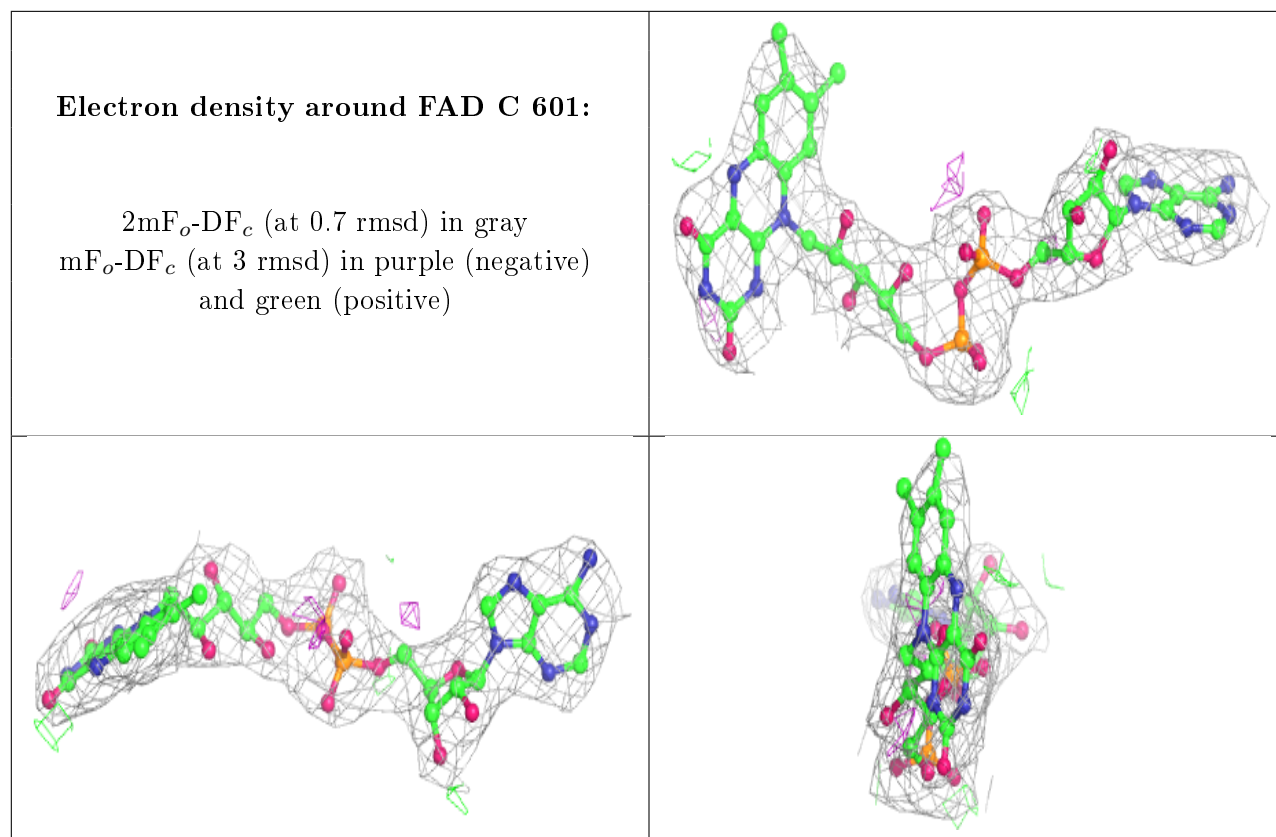
**Electron density around FAD A 601:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.