



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2026 – 05:28 PM JST

PDB ID : 9UU6 / pdb\_00009uu6  
Title : Structure of cyclohexanone monooxygenase mutant from *Acinetobacter calcoaceticus*  
Authors : Geng, Q.; Yu, H.  
Deposited on : 2025-05-06  
Resolution : 1.84 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.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

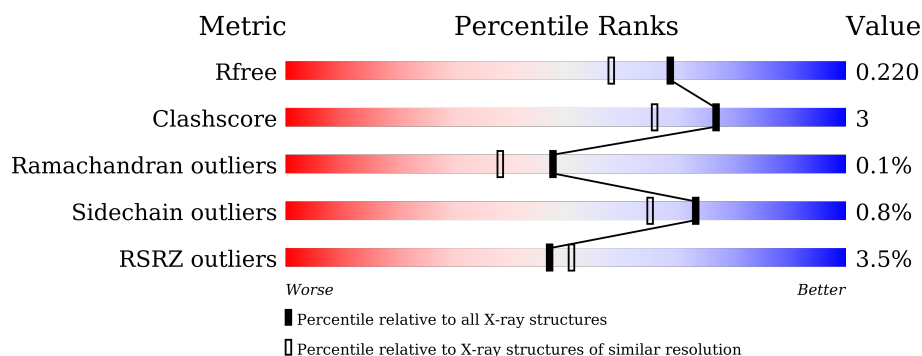
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	548	
1	B	548	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9630 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 Putative flavin-binding monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4189	2673	700	798	18			
1	B	522	Total	C	N	O	S	0	0	0
			4144	2643	691	793	17			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	TYR	LEU	conflict	UNP A0A0A8XFY0
A	70	GLY	GLU	engineered mutation	UNP A0A0A8XFY0
A	123	LYS	ASN	engineered mutation	UNP A0A0A8XFY0
A	128	LYS	ASN	engineered mutation	UNP A0A0A8XFY0
A	133	LEU	THR	engineered mutation	UNP A0A0A8XFY0
A	143	PRO	LEU	engineered mutation	UNP A0A0A8XFY0
A	145	SER	ALA	engineered mutation	UNP A0A0A8XFY0
A	146	SER	ALA	engineered mutation	UNP A0A0A8XFY0
A	149	TRP	LEU	engineered mutation	UNP A0A0A8XFY0
A	151	ILE	LYS	engineered mutation	UNP A0A0A8XFY0
A	246	TYR	PHE	engineered mutation	UNP A0A0A8XFY0
A	277	LEU	PHE	conflict	UNP A0A0A8XFY0
A	326	CYS	LYS	engineered mutation	UNP A0A0A8XFY0
A	337	VAL	ILE	conflict	UNP A0A0A8XFY0
A	386	SER	ASN	engineered mutation	UNP A0A0A8XFY0
A	388	LYS	ILE	engineered mutation	UNP A0A0A8XFY0
A	390	ILE	MET	engineered mutation	UNP A0A0A8XFY0
A	403	TYR	HIS	conflict	UNP A0A0A8XFY0
A	426	PHE	LEU	engineered mutation	UNP A0A0A8XFY0
A	432	LEU	PHE	engineered mutation	UNP A0A0A8XFY0
A	433	ALA	THR	engineered mutation	UNP A0A0A8XFY0
A	435	SER	LEU	engineered mutation	UNP A0A0A8XFY0
A	438	ILE	SER	engineered mutation	UNP A0A0A8XFY0
A	488	LYS	GLU	engineered mutation	UNP A0A0A8XFY0
A	489	CYS	SER	engineered mutation	UNP A0A0A8XFY0

*Continued on next page...*

*Continued from previous page...*

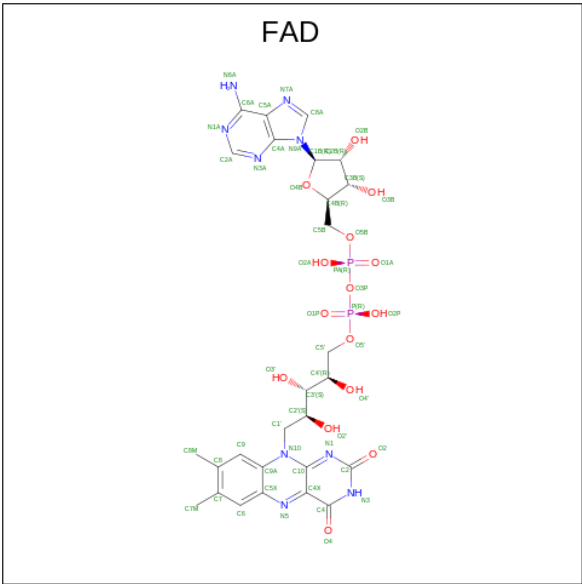
Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ARG	TRP	engineered mutation	UNP A0A0A8XFY0
A	497	SER	PRO	conflict	UNP A0A0A8XFY0
A	505	LEU	PHE	engineered mutation	UNP A0A0A8XFY0
A	526	ARG	LYS	engineered mutation	UNP A0A0A8XFY0
A	534	PHE	-	insertion	UNP A0A0A8XFY0
A	535	ALA	-	insertion	UNP A0A0A8XFY0
A	536	ASP	-	insertion	UNP A0A0A8XFY0
A	537	ASN	-	insertion	UNP A0A0A8XFY0
A	538	ALA	-	insertion	UNP A0A0A8XFY0
A	539	PRO	-	insertion	UNP A0A0A8XFY0
B	55	TYR	LEU	conflict	UNP A0A0A8XFY0
B	70	GLY	GLU	engineered mutation	UNP A0A0A8XFY0
B	123	LYS	ASN	engineered mutation	UNP A0A0A8XFY0
B	128	LYS	ASN	engineered mutation	UNP A0A0A8XFY0
B	133	LEU	THR	engineered mutation	UNP A0A0A8XFY0
B	143	PRO	LEU	engineered mutation	UNP A0A0A8XFY0
B	145	SER	ALA	engineered mutation	UNP A0A0A8XFY0
B	146	SER	ALA	engineered mutation	UNP A0A0A8XFY0
B	149	TRP	LEU	engineered mutation	UNP A0A0A8XFY0
B	151	ILE	LYS	engineered mutation	UNP A0A0A8XFY0
B	246	TYR	PHE	engineered mutation	UNP A0A0A8XFY0
B	277	LEU	PHE	conflict	UNP A0A0A8XFY0
B	326	CYS	LYS	engineered mutation	UNP A0A0A8XFY0
B	337	VAL	ILE	conflict	UNP A0A0A8XFY0
B	386	SER	ASN	engineered mutation	UNP A0A0A8XFY0
B	388	LYS	ILE	engineered mutation	UNP A0A0A8XFY0
B	390	ILE	MET	engineered mutation	UNP A0A0A8XFY0
B	403	TYR	HIS	conflict	UNP A0A0A8XFY0
B	426	PHE	LEU	engineered mutation	UNP A0A0A8XFY0
B	432	LEU	PHE	engineered mutation	UNP A0A0A8XFY0
B	433	ALA	THR	engineered mutation	UNP A0A0A8XFY0
B	435	SER	LEU	engineered mutation	UNP A0A0A8XFY0
B	438	ILE	SER	engineered mutation	UNP A0A0A8XFY0
B	488	LYS	GLU	engineered mutation	UNP A0A0A8XFY0
B	489	CYS	SER	engineered mutation	UNP A0A0A8XFY0
B	490	ARG	TRP	engineered mutation	UNP A0A0A8XFY0
B	497	SER	PRO	conflict	UNP A0A0A8XFY0
B	505	LEU	PHE	engineered mutation	UNP A0A0A8XFY0
B	526	ARG	LYS	engineered mutation	UNP A0A0A8XFY0
B	534	PHE	-	insertion	UNP A0A0A8XFY0
B	535	ALA	-	insertion	UNP A0A0A8XFY0
B	536	ASP	-	insertion	UNP A0A0A8XFY0

*Continued on next page...*

Continued from previous page...

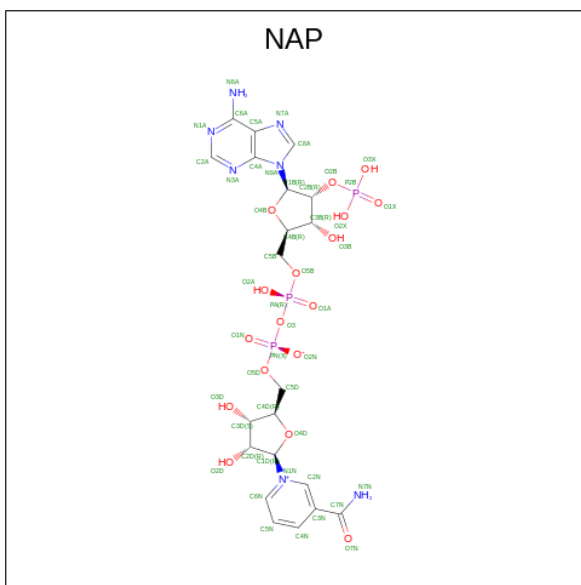
Chain	Residue	Modelled	Actual	Comment	Reference
B	537	ASN	-	insertion	UNP A0A0A8XFY0
B	538	ALA	-	insertion	UNP A0A0A8XFY0
B	539	PRO	-	insertion	UNP A0A0A8XFY0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

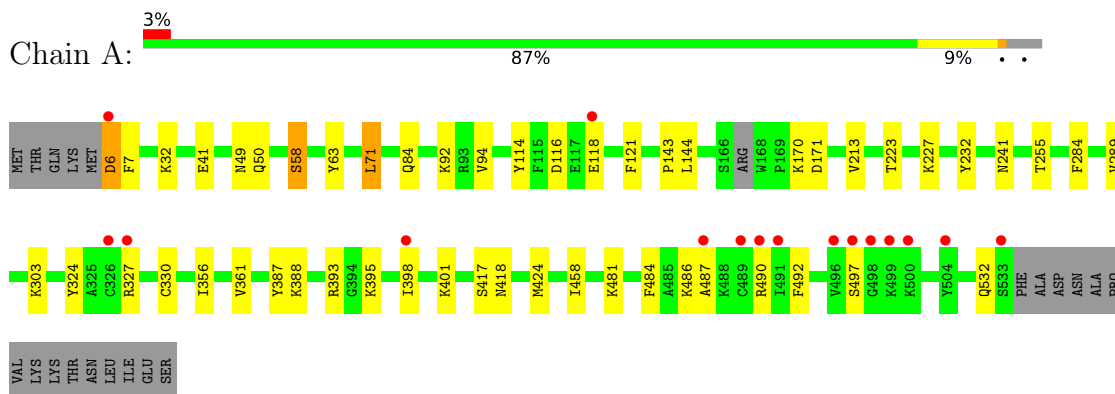
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	570	Total O 570 570	0	0
4	B	525	Total O 525 525	0	0

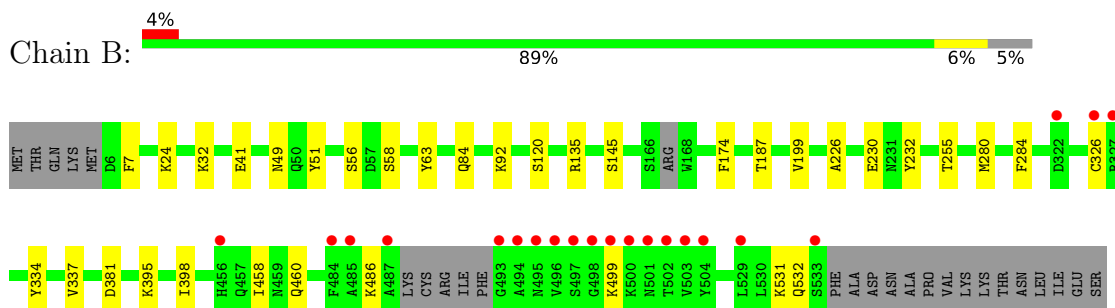
### 3 Residue-property plots [i](#)

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

- Molecule 1: Putative flavin-binding monooxygenase



- Molecule 1: Putative flavin-binding monooxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.11Å 53.31Å 107.73Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	49.89 – 1.84 49.89 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.89-1.84) 99.9 (49.89-1.84)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.177 , 0.218 0.179 , 0.220	Depositor DCC
$R_{free}$ test set	5277 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9630	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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, NAP

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	0.36	0/4284	0.56	0/5796
1	B	0.35	0/4237	0.56	2/5733 (0.0%)
All	All	0.36	0/8521	0.56	2/11529 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	SER	CA-C-N	5.44	131.53	121.52
1	B	56	SER	C-N-CA	5.44	131.53	121.52

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	4189	0	4101	31	0
1	B	4144	0	4051	17	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
4	A	570	0	0	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	525	0	0	1	0
All	All	9630	0	8264	49	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 3.

All (49) 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:A:41:GLU:HG2	1:A:92:LYS:HE2	1.64	0.78
1:A:50:GLN:NE2	4:A:701:HOH:O	2.23	0.72
1:B:145:SER:HB3	1:B:381:ASP:HB2	1.71	0.70
1:A:6:ASP:N	4:A:702:HOH:O	2.26	0.68
1:A:486:LYS:HG3	1:A:487:ALA:H	1.57	0.68
1:A:458:ILE:HD13	1:A:532:GLN:HG2	1.76	0.67
1:A:484:PHE:O	1:A:490:ARG:HA	1.98	0.62
1:B:395:LYS:O	1:B:398:ILE:HG22	1.99	0.62
1:B:41:GLU:HG2	1:B:92:LYS:HE2	1.82	0.59
1:A:41:GLU:CG	1:A:92:LYS:HE2	2.33	0.58
1:A:223:THR:O	1:A:227:LYS:HG2	2.02	0.58
1:B:280:MET:HE2	1:B:326:CYS:O	2.04	0.57
1:A:303:LYS:NZ	4:A:703:HOH:O	2.31	0.57
1:A:388:LYS:HG2	1:A:401:LYS:HA	1.86	0.57
1:A:170:LYS:HE3	1:A:171:ASP:OD2	2.07	0.55
1:B:226:ALA:O	1:B:230:GLU:HG3	2.07	0.54
1:A:417:SER:O	1:A:418:ASN:HB2	2.09	0.52
1:A:324:TYR:HE2	1:A:486:LYS:HG2	1.75	0.51
1:B:58:SER:HB2	1:B:63:TYR:HB2	1.93	0.50
1:A:241:ASN:ND2	4:A:711:HOH:O	2.44	0.50
1:A:387:TYR:OH	1:A:424:MET:HG2	2.12	0.50
1:B:49:ASN:O	1:B:84:GLN:HG3	2.13	0.49
1:A:71:LEU:HD21	1:A:94:VAL:HG22	1.94	0.49
1:B:334:TYR:O	1:B:337:VAL:HG22	2.13	0.48
1:B:460:GLN:HB3	1:B:531:LYS:HB2	1.95	0.48
1:B:458:ILE:CD1	1:B:532:GLN:HG2	2.43	0.48
1:A:49:ASN:O	1:A:84:GLN:HG3	2.12	0.48
1:A:58:SER:HB2	1:A:63:TYR:HB2	1.95	0.48
1:A:116:ASP:OD1	1:A:118:GLU:HG2	2.15	0.46
1:A:490:ARG:CZ	1:A:492:PHE:HB2	2.46	0.46
1:A:7:PHE:HD1	1:A:32:LYS:HG3	1.81	0.45
1:A:213:VAL:O	1:A:330:CYS:HA	2.17	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:O	1:A:144:LEU:HD23	2.17	0.44
1:A:395:LYS:O	1:A:398:ILE:HD12	2.17	0.44
1:B:255:THR:HA	1:B:284:PHE:CD1	2.52	0.44
1:A:324:TYR:CE2	1:A:486:LYS:HG2	2.53	0.44
1:A:486:LYS:CG	1:A:487:ALA:H	2.29	0.44
1:B:7:PHE:HD1	1:B:32:LYS:HG3	1.82	0.44
3:B:602:NAP:H5N	4:B:1092:HOH:O	2.17	0.44
1:B:51:TYR:CZ	1:B:187:THR:HG23	2.53	0.43
1:B:120:SER:O	1:B:135:ARG:NH1	2.52	0.43
1:A:255:THR:HA	1:A:284:PHE:CD1	2.54	0.43
1:A:121:PHE:CD1	1:A:121:PHE:C	2.98	0.42
1:B:486:LYS:N	1:B:486:LYS:HD2	2.34	0.41
1:B:174:PHE:HB3	1:B:199:VAL:HG12	2.01	0.41
1:A:289:VAL:HG13	1:A:481:LYS:O	2.21	0.41
1:A:114:TYR:CE1	1:A:393:ARG:HG3	2.56	0.40
1:A:356:ILE:HG12	1:A:361:VAL:HG22	2.02	0.40
1:B:24:LYS:HA	1:B:24:LYS:HD3	1.89	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	523/548 (95%)	512 (98%)	10 (2%)	1 (0%)	43	34
1	B	516/548 (94%)	506 (98%)	10 (2%)	0	100	100
All	All	1039/1096 (95%)	1018 (98%)	20 (2%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/471 (96%)	447 (99%)	5 (1%)	65	54
1	B	447/471 (95%)	445 (100%)	2 (0%)	84	78
All	All	899/942 (95%)	892 (99%)	7 (1%)	73	65

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	58	SER
1	A	71	LEU
1	A	232	TYR
1	A	327	ARG
1	B	232	TYR
1	B	499	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	163	HIS
1	A	206	GLN
1	A	459	ASN
1	A	470	ASN
1	A	532	GLN
1	B	49	ASN
1	B	163	HIS
1	B	272	GLN
1	B	418	ASN
1	B	515	ASN
1	B	523	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	$\# Z  > 2$
3	NAP	B	602	-	49,52,52	0.56	0	69,80,80	0.83	2 (2%)
2	FAD	A	601	-	56,58,58	1.51	10 (17%)	81,89,89	1.56	14 (17%)
3	NAP	A	602	-	49,52,52	0.52	0	69,80,80	0.91	3 (4%)
2	FAD	B	601	-	56,58,58	1.40	10 (17%)	81,89,89	1.66	19 (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
3	NAP	B	602	-	-	1/35/67/67	0/5/5/5
2	FAD	A	601	-	-	3/34/50/50	0/6/6/6
3	NAP	A	602	-	-	2/35/67/67	0/5/5/5
2	FAD	B	601	-	-	4/34/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C9A-C5X	5.20	1.49	1.41
2	B	601	FAD	C9A-C5X	4.65	1.49	1.41
2	A	601	FAD	C5A-C4A	4.32	1.47	1.39
2	B	601	FAD	C5A-C4A	3.80	1.46	1.39
2	B	601	FAD	C8-C7	3.21	1.48	1.40
2	A	601	FAD	C8-C7	3.12	1.48	1.40
2	A	601	FAD	C4A-N9A	-2.93	1.31	1.37
2	B	601	FAD	C4-N3	-2.90	1.33	1.38
2	A	601	FAD	C4-N3	-2.84	1.33	1.38
2	A	601	FAD	C4X-N5	2.64	1.35	1.30
2	A	601	FAD	C5A-N7A	-2.63	1.34	1.39
2	B	601	FAD	C5A-N7A	-2.59	1.34	1.39
2	A	601	FAD	C5X-N5	-2.44	1.34	1.39
2	B	601	FAD	C5A-C6A	2.39	1.47	1.41
2	B	601	FAD	C4X-N5	2.33	1.35	1.30
2	B	601	FAD	C8A-N7A	2.33	1.36	1.31
2	A	601	FAD	C5A-C6A	2.32	1.47	1.41
2	B	601	FAD	C4A-N9A	-2.27	1.32	1.37
2	A	601	FAD	C8A-N7A	2.16	1.35	1.31
2	B	601	FAD	C5X-N5	-2.09	1.35	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C5A-C4A-N3A	-4.81	120.47	126.75
2	A	601	FAD	N3A-C2A-N1A	-4.47	121.61	128.60
3	A	602	NAP	O4D-C1D-C2D	-4.44	100.44	106.93
3	B	602	NAP	O4D-C1D-C2D	-4.35	100.56	106.93
2	B	601	FAD	N3A-C4A-N9A	4.27	134.11	127.08
2	A	601	FAD	C5A-C4A-N3A	-3.84	121.74	126.75
2	B	601	FAD	C4A-N9A-C8A	3.76	109.80	105.73
2	A	601	FAD	C2A-N1A-C6A	3.56	124.88	118.77
2	A	601	FAD	C4A-N9A-C8A	3.39	109.40	105.73
2	A	601	FAD	N3A-C4A-N9A	3.36	132.62	127.08
2	B	601	FAD	C2A-N3A-C4A	3.26	119.46	111.75
2	B	601	FAD	N3A-C2A-N1A	-3.25	123.52	128.60
2	B	601	FAD	O2-C2-N1	-3.23	116.47	121.83
2	A	601	FAD	C2A-N3A-C4A	3.23	119.38	111.75
2	B	601	FAD	N9A-C8A-N7A	-2.98	109.83	113.91
2	B	601	FAD	C4-C4X-N5	2.80	122.21	118.23
2	B	601	FAD	C5A-N7A-C8A	2.71	107.36	103.51
2	B	601	FAD	N6A-C6A-N1A	2.62	124.10	118.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4-C4X-N5	2.58	121.91	118.23
2	A	601	FAD	C6A-C5A-N7A	2.58	136.83	132.02
2	B	601	FAD	O4-C4-C4X	-2.51	119.93	126.60
2	A	601	FAD	C4A-C5A-N7A	-2.49	107.58	110.62
2	B	601	FAD	C4A-C5A-N7A	-2.48	107.60	110.62
2	B	601	FAD	C5A-C6A-N6A	-2.46	118.07	123.43
2	A	601	FAD	O4-C4-C4X	-2.45	120.09	126.60
2	B	601	FAD	C4X-C10-N10	2.42	120.02	116.48
3	B	602	NAP	C6N-N1N-C2N	-2.42	119.77	121.97
2	A	601	FAD	C5X-C9A-N10	2.35	120.38	117.95
3	A	602	NAP	C4N-C3N-C7N	2.23	127.02	121.04
2	A	601	FAD	N9A-C8A-N7A	-2.22	110.88	113.91
2	B	601	FAD	C1'-N10-C9A	2.22	124.21	120.51
2	B	601	FAD	O2P-P-O1P	2.20	123.13	112.24
2	B	601	FAD	C4-N3-C2	-2.18	121.62	125.64
2	B	601	FAD	N3-C2-N1	2.13	123.56	119.38
2	B	601	FAD	C4X-C10-N1	-2.11	119.83	124.73
2	A	601	FAD	C5A-N7A-C8A	2.10	106.50	103.51
2	A	601	FAD	C4X-C4-N3	2.09	118.49	113.19
3	A	602	NAP	C6N-N1N-C2N	-2.01	120.14	121.97

There are no chirality outliers.

All (10) torsion outliers are listed below:

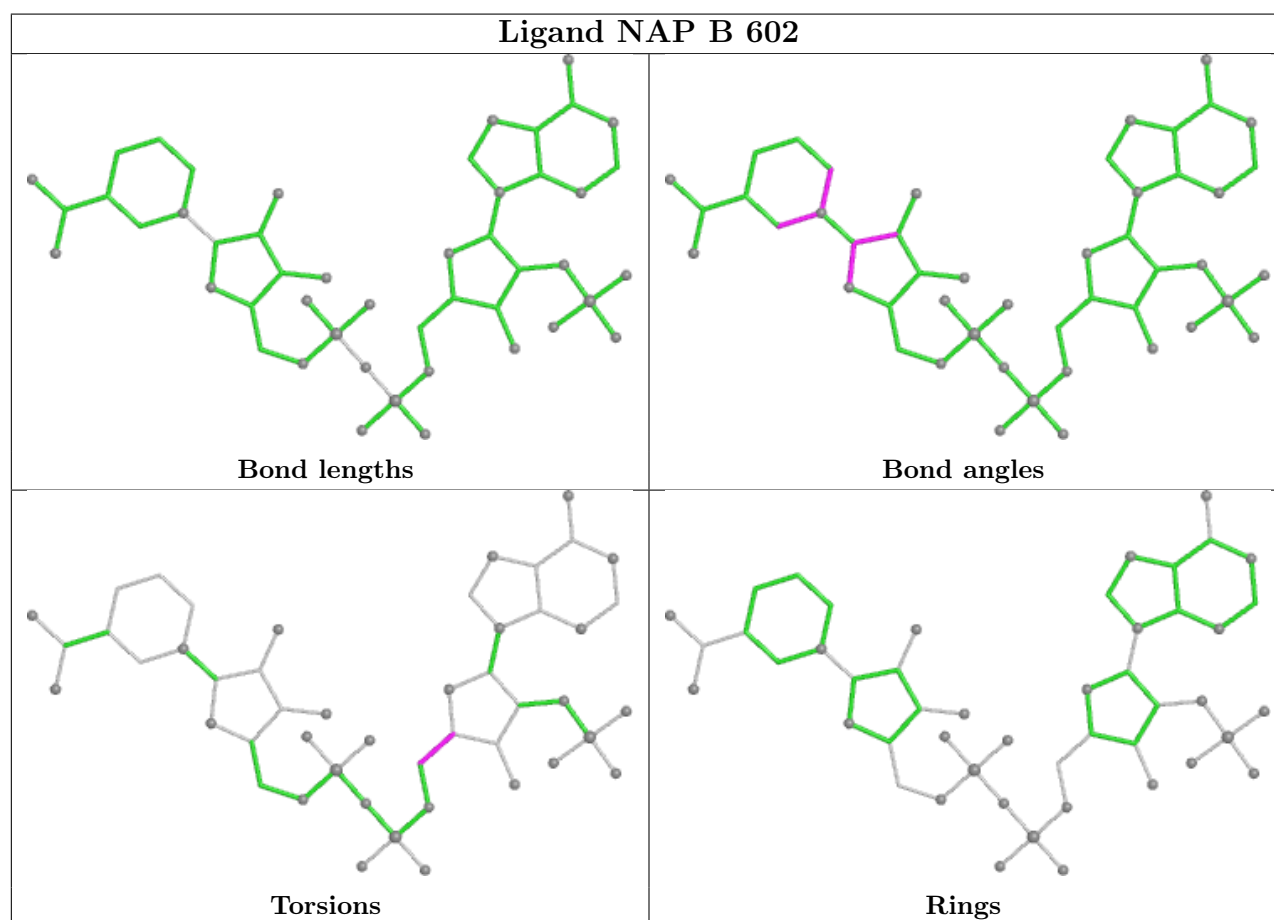
Mol	Chain	Res	Type	Atoms
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
3	A	602	NAP	C2B-O2B-P2B-O3X
2	B	601	FAD	PA-O3P-P-O5'
3	B	602	NAP	O4B-C4B-C5B-O5B
3	A	602	NAP	O4B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

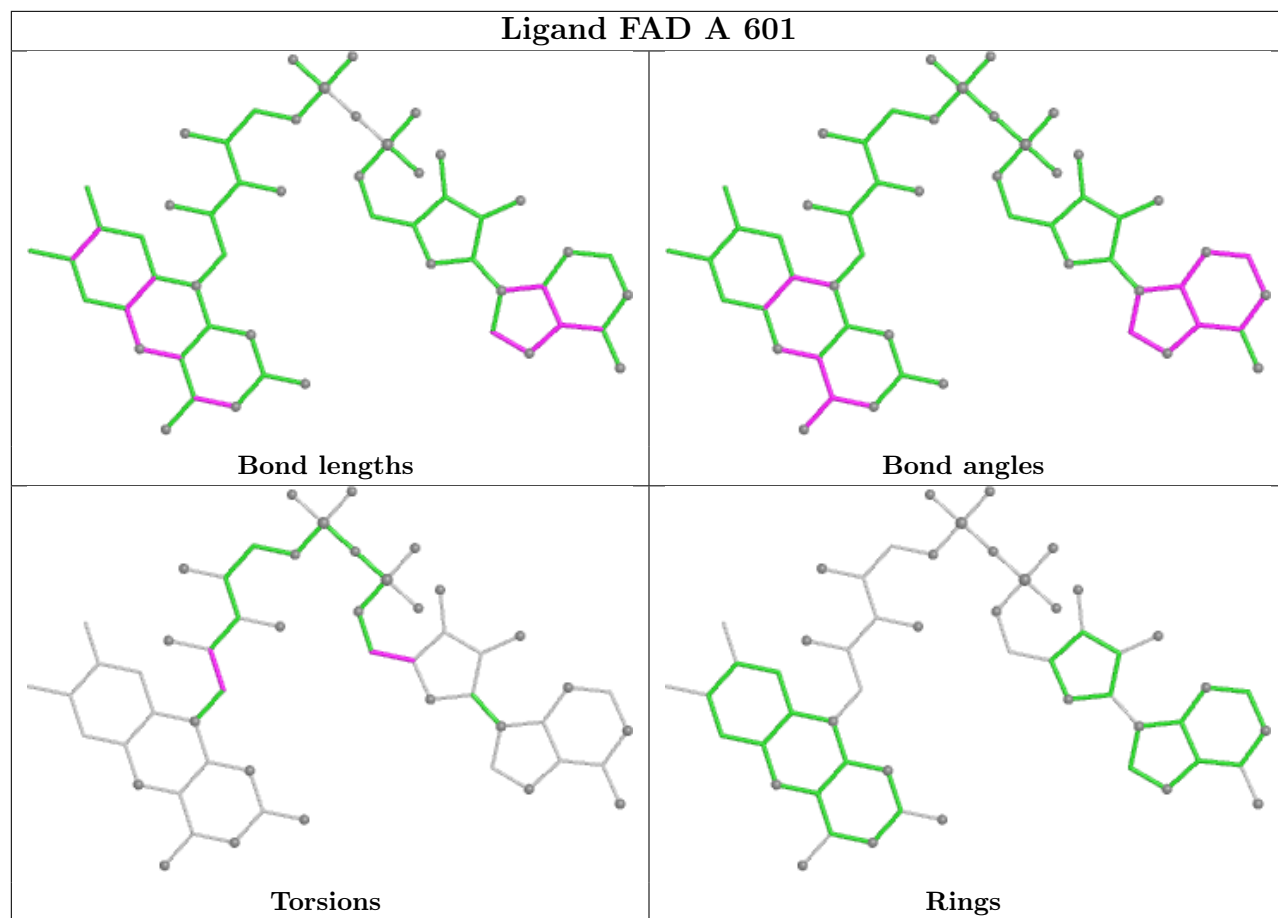
1 monomer is involved in 1 short contact:

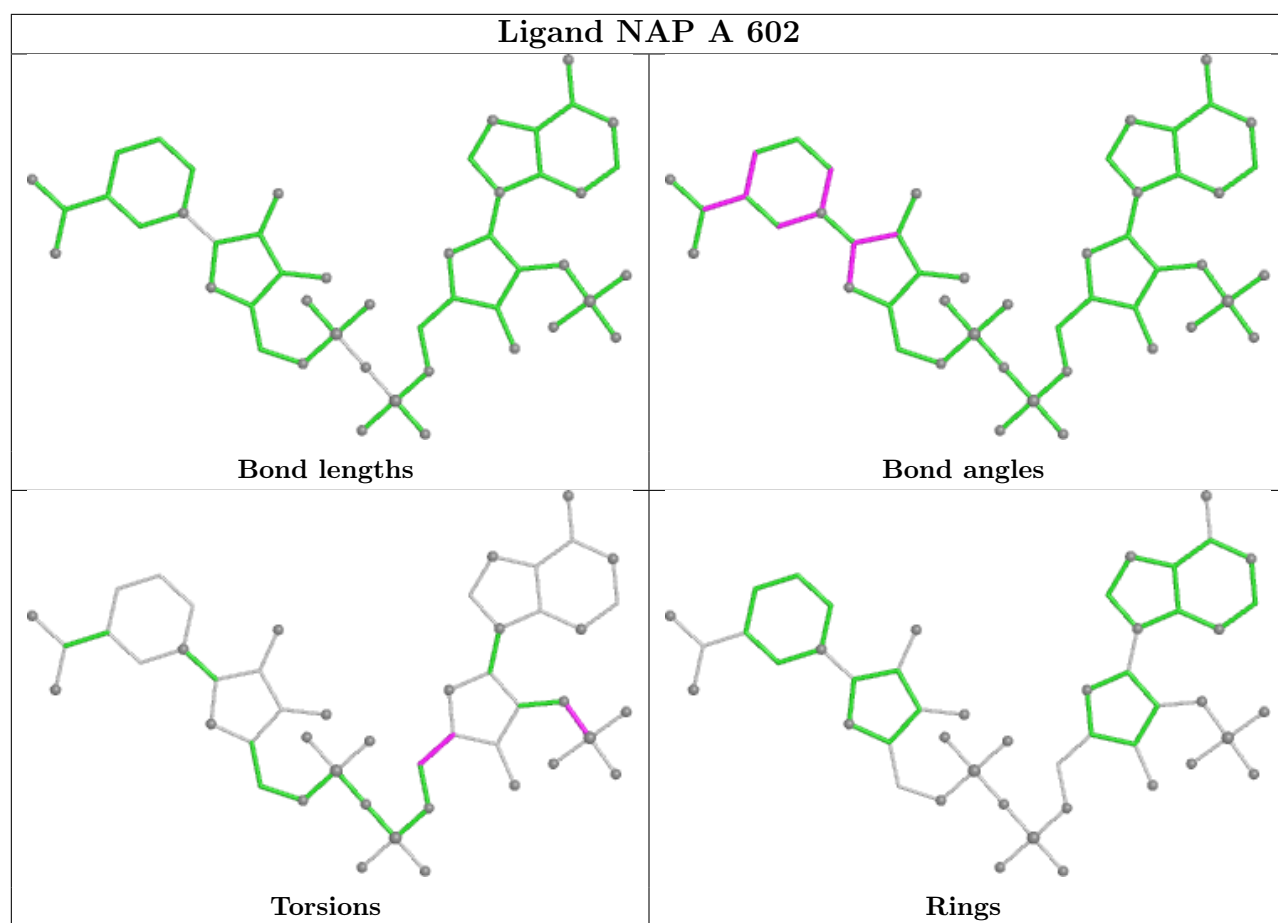
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	NAP	1	0

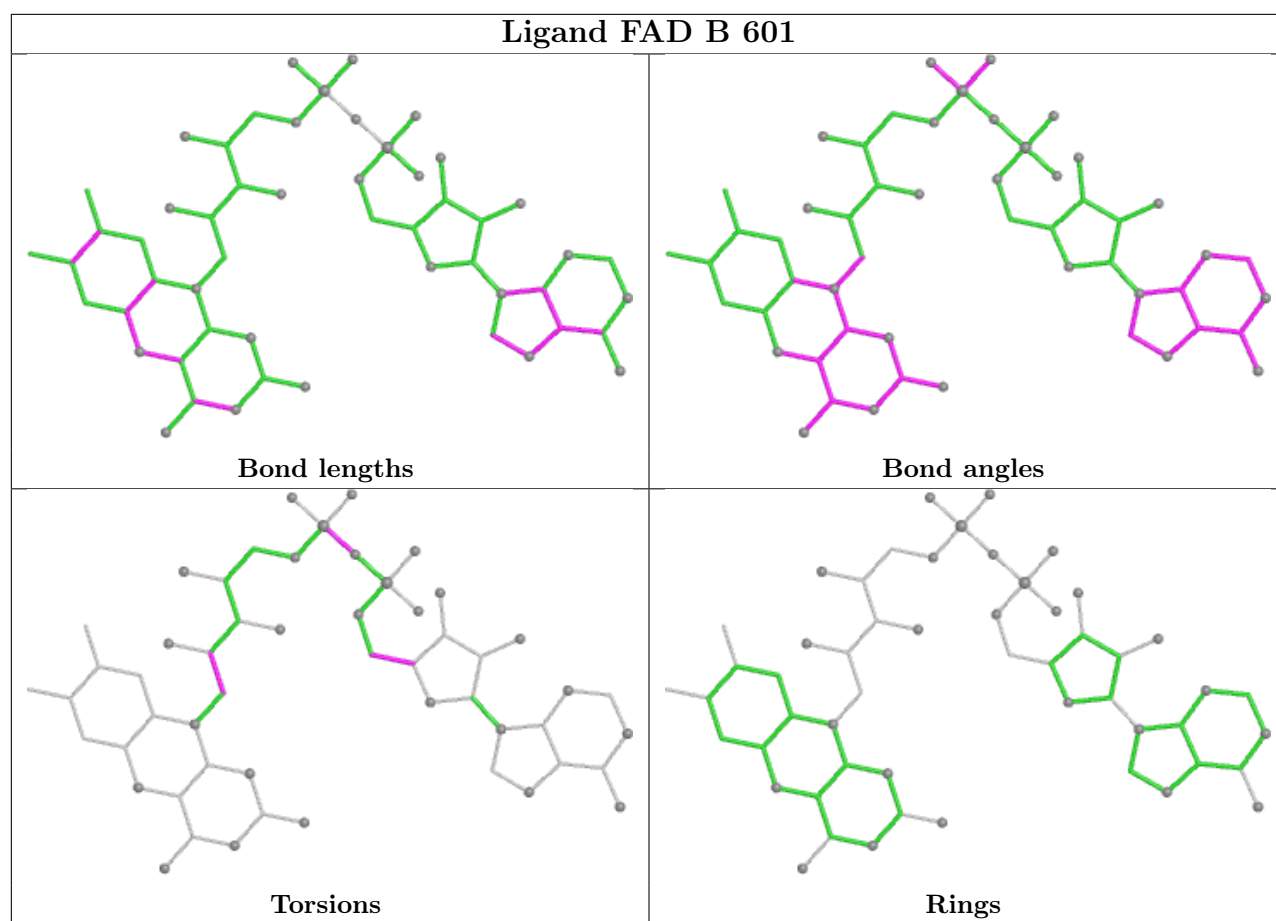
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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	527/548 (96%)	-0.15	16 (3%) 52 57	11, 19, 38, 79	0
1	B	522/548 (95%)	0.00	21 (4%) 42 45	12, 21, 48, 143	0
All	All	1049/1096 (95%)	-0.07	37 (3%) 47 51	11, 20, 42, 143	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	494	ALA	5.5
1	B	503	VAL	5.3
1	B	496	VAL	5.1
1	B	502	THR	4.7
1	B	493	GLY	4.6
1	B	326	CYS	4.6
1	B	487	ALA	4.5
1	B	504	TYR	4.3
1	B	501	ASN	3.9
1	A	496	VAL	3.6
1	A	327	ARG	3.6
1	B	499	LYS	3.5
1	B	500	LYS	3.5
1	A	533	SER	3.5
1	B	497	SER	3.4
1	B	498	GLY	3.3
1	B	484	PHE	3.2
1	B	533	SER	3.2
1	A	497	SER	3.1
1	B	529	LEU	2.9
1	A	498	GLY	2.7
1	A	487	ALA	2.7
1	A	499	LYS	2.4
1	B	322	ASP	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	485	ALA	2.3
1	A	490	ARG	2.3
1	A	326	CYS	2.3
1	B	327	ARG	2.2
1	A	491	ILE	2.2
1	A	6	ASP	2.2
1	B	456	HIS	2.2
1	A	504	TYR	2.2
1	A	500	LYS	2.2
1	B	495	ASN	2.2
1	A	118	GLU	2.1
1	A	489	CYS	2.0
1	A	398	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

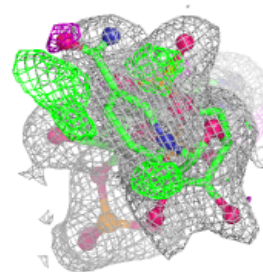
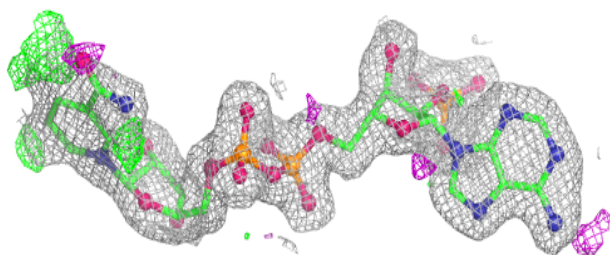
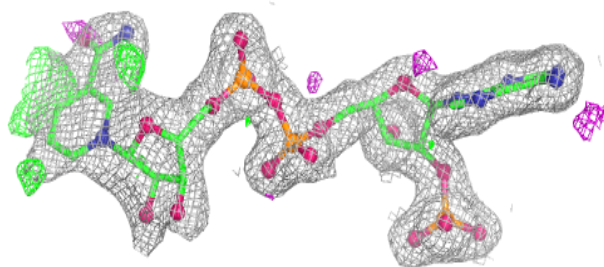
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	NAP	B	602	48/48	0.96	0.07	13,19,42,45	0
3	NAP	A	602	48/48	0.97	0.07	11,17,37,48	0
2	FAD	A	601	53/53	0.98	0.05	12,15,20,26	0
2	FAD	B	601	53/53	0.98	0.05	10,16,21,23	0

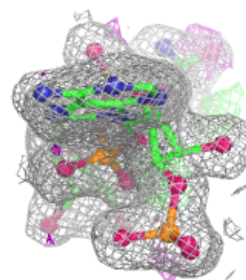
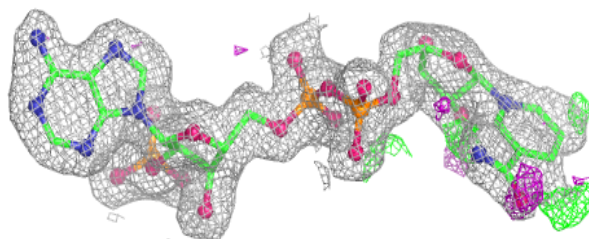
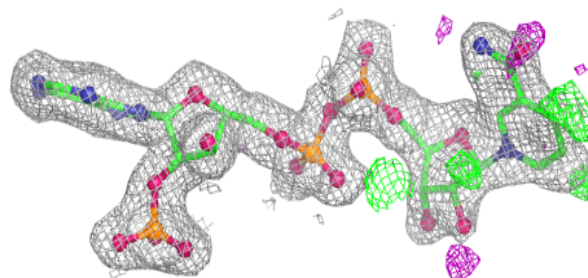
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP 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)

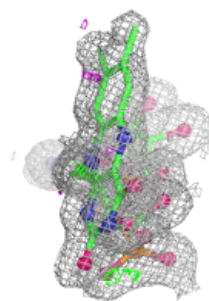
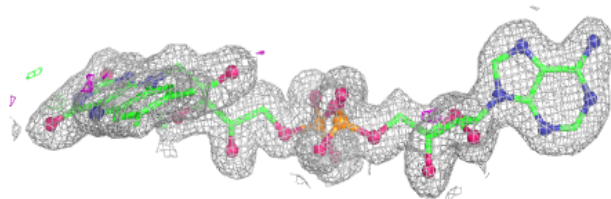
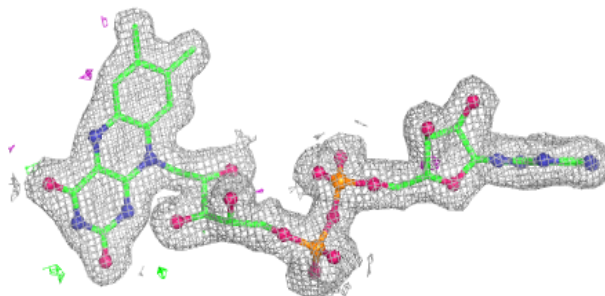
**Electron density around NAP A 602:**

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

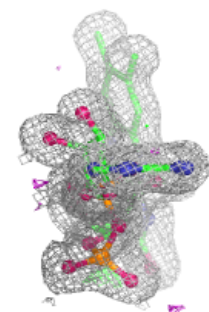
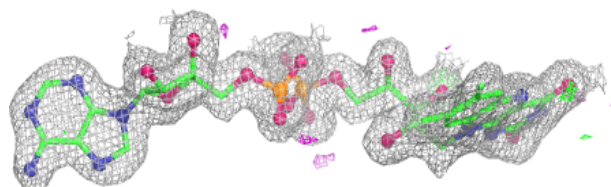
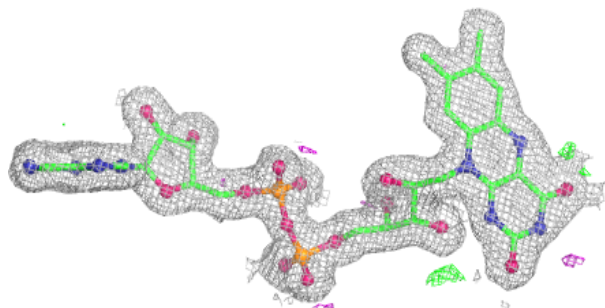


**Electron density around FAD A 601:**

$2mF_o-DF_c$  (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.