



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2021 – 04:11 PM EDT

PDB ID : 7MYB  
Title : Structure of proline utilization A with tetrahydrothiophene-2-carboxylate bound in the proline dehydrogenase active site  
Authors : Tanner, J.J.; Campbell, A.C.  
Deposited on : 2021-05-20  
Resolution : 1.52 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 : 2.23.1  
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) : 2.23.1

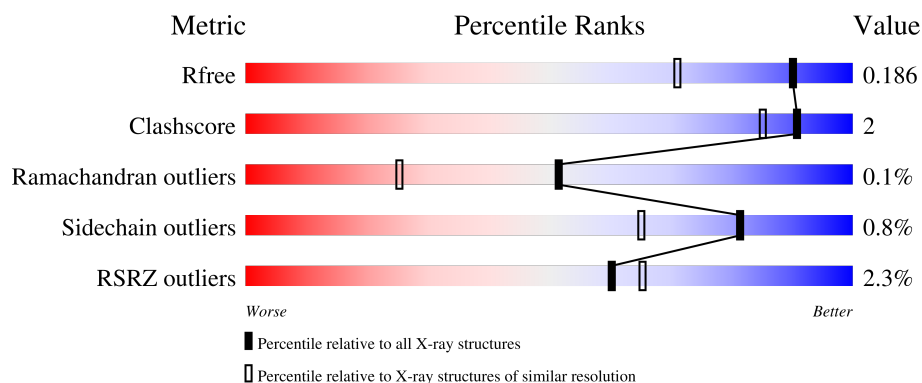
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.52 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	1235	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>
1	B	1235	<div> <div>2%</div> <div>94%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 20936 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.

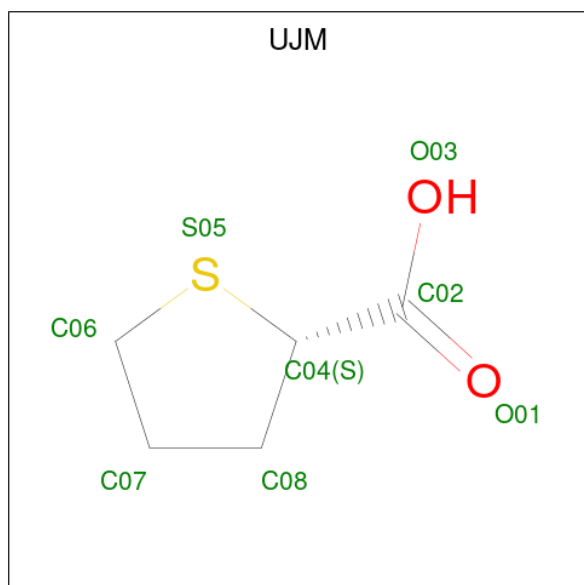
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1217	Total	C	N	O	S	0	16	0
			9108	5735	1635	1704	34			
1	B	1216	Total	C	N	O	S	0	18	0
			9114	5744	1627	1709	34			

There are 4 discrepancies between the modelled and reference sequences:

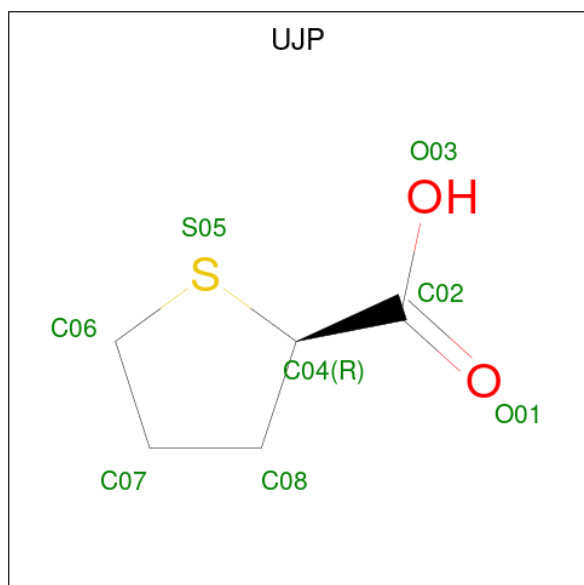
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is (2S)-thiolane-2-carboxylic acid (three-letter code: UJM) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



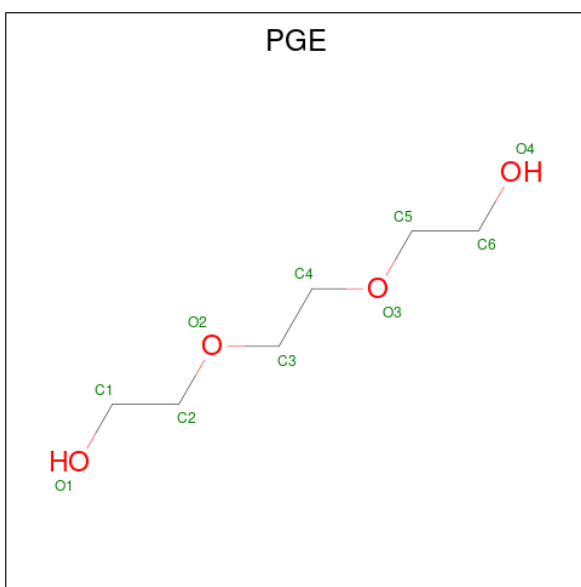
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	1
			8	5	2	1		
2	B	1	Total	C	O	S	0	1
			8	5	2	1		

- Molecule 3 is (2R)-thiolane-2-carboxylic acid (three-letter code: UJP) (formula: C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



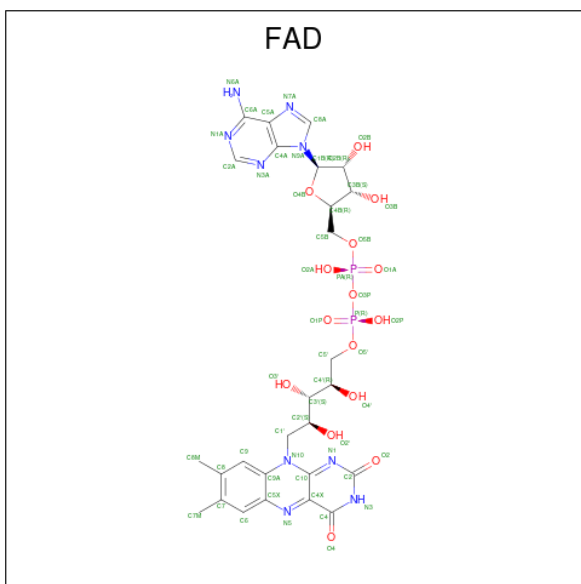
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	1
			8	5	2	1		
3	B	1	Total	C	O	S	0	1
			8	5	2	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



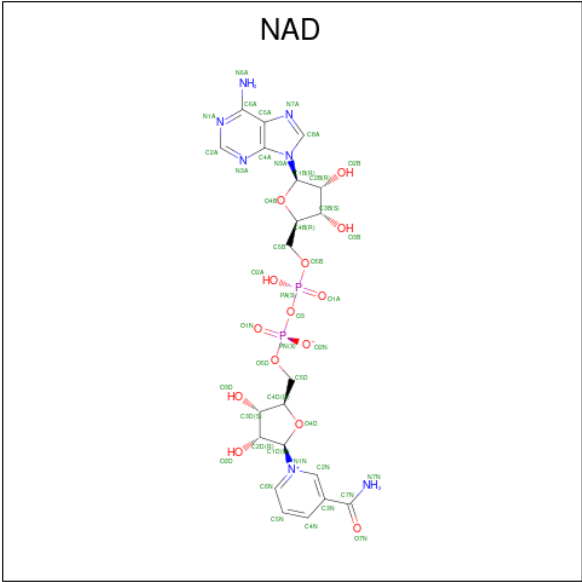
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	44	21	7	14	2	0	0
6	B	1	44	21	7	14	2	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

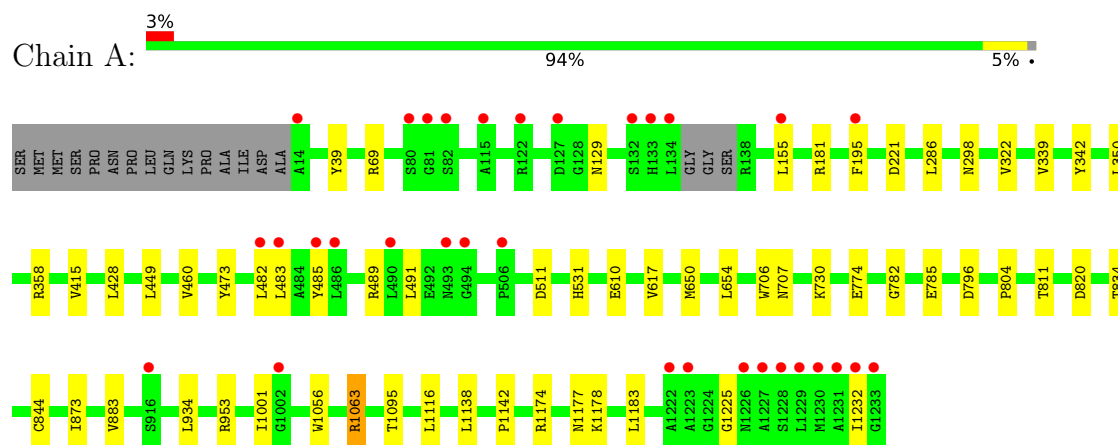
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1168	Total	O	0	0
			1168	1168		
10	B	1271	Total	O	0	0
			1271	1271		



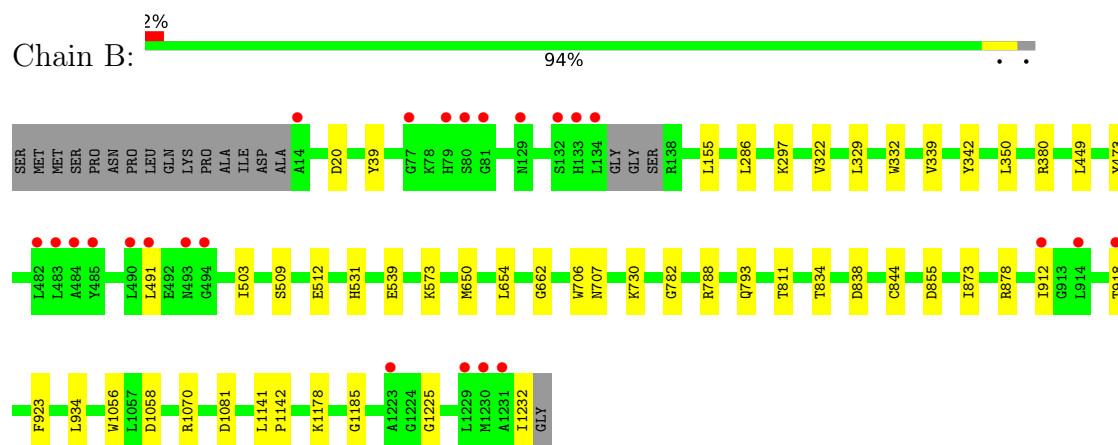
### 3 Residue-property plots [i](#)

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: Bifunctional protein PutA



#### • Molecule 1: Bifunctional protein PutA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.88Å 103.02Å 127.06Å 90.00° 106.44° 90.00°	Depositor
Resolution (Å)	97.72 – 1.52 97.72 – 1.52	Depositor EDS
% Data completeness (in resolution range)	99.0 (97.72-1.52) 99.0 (97.72-1.52)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.52Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, $R_{free}$	0.164 , 0.186 0.164 , 0.186	Depositor DCC
$R_{free}$ test set	19044 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20936	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 3.65% 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: PEG, PGE, UJP, MG, FAD, NAD, SO4, UJM

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	0.31	0/9300	0.54	1/12650 (0.0%)
1	B	0.33	0/9332	0.55	0/12698
All	All	0.32	0/18632	0.54	1/25348 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	820	ASP	CB-CG-OD1	5.33	123.10	118.30

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	9108	0	9176	33	0
1	B	9114	0	9184	29	0
2	A	8	0	0	1	0
2	B	8	0	0	0	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	10	0	14	0	0
4	B	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	31	3	0
5	B	53	0	31	2	0
6	A	44	0	26	1	0
6	B	44	0	26	2	0
7	A	15	0	0	0	0
7	B	5	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	7	0	10	0	0
10	A	1168	0	0	5	0
10	B	1271	0	0	6	1
All	All	20936	0	18512	63	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 2.

All (63) 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:B:491:LEU:HD21	1:B:1225:GLY:HA3	1.53	0.91
1:A:491:LEU:HD21	1:A:1225:GLY:HA3	1.51	0.90
1:A:804:PRO:HG3	1:A:1177[B]:ASN:HD21	1.54	0.73
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.73	0.71
1:B:844:CYS:SG	6:B:1305:NAD:C4N	2.79	0.69
1:B:1081:ASP:OD1	10:B:1401:HOH:O	2.10	0.68
1:B:539:GLU:OE1	10:B:1402:HOH:O	2.13	0.66
1:B:339[B]:VAL:HG21	1:B:350:LEU:HD21	1.79	0.63
1:A:1183:LEU:O	10:A:1401:HOH:O	2.16	0.62
1:B:155:LEU:HD22	1:B:491:LEU:HD11	1.80	0.62
1:A:155:LEU:HD22	1:A:491:LEU:HD11	1.82	0.61
1:A:69:ARG:NH2	1:A:511:ASP:OD1	2.35	0.60
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.84	0.59
1:B:473:TYR:HB2	5:B:1304:FAD:HM72	1.85	0.59
1:A:1174:ARG:HG2	1:A:1178[B]:LYS:HZ3	1.67	0.58
1:A:449:LEU:HG	5:A:1304:FAD:HM82	1.86	0.57
1:B:20:ASP:OD2	1:B:878:ARG:NH1	2.37	0.56
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.40	0.56
1:B:793:GLN:OE1	10:B:1403:HOH:O	2.18	0.56
1:A:844:CYS:SG	6:A:1305:NAD:C4N	2.94	0.55
1:A:298:ASN:ND2	10:A:1403:HOH:O	2.26	0.55
1:A:1095[B]:THR:HG22	10:A:2117:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.89	0.53
1:A:195:PHE:HB3	1:A:482:LEU:HD11	1.89	0.53
1:A:449:LEU:HD23	1:A:473:TYR:HB3	1.91	0.53
1:B:449[A]:LEU:HG	5:B:1304:FAD:HM82	1.90	0.52
1:B:650:MET:O	1:B:654:LEU:HG	2.09	0.52
1:A:834:THR:HG22	1:A:1001[B]:ILE:HD11	1.92	0.52
1:B:782:GLY:O	1:B:811:THR:HA	2.10	0.51
1:A:473:TYR:HB2	5:A:1304:FAD:HM72	1.93	0.50
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.94	0.50
1:B:834:THR:O	1:B:838[B]:ASP:HB2	2.11	0.50
1:B:380[A]:ARG:NH2	10:B:1418:HOH:O	2.45	0.49
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.93	0.49
1:B:573:LYS:NZ	10:B:1417:HOH:O	2.45	0.49
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.95	0.48
1:A:785:GLU:CD	1:A:785:GLU:H	2.17	0.48
1:A:953:ARG:HD3	10:A:1648:HOH:O	2.13	0.47
1:A:796:ASP:HA	1:A:1178[B]:LYS:NZ	2.29	0.47
1:A:650:MET:O	1:A:654:LEU:HG	2.15	0.47
1:B:788:ARG:NH1	1:B:1185:GLY:O	2.44	0.47
1:B:844:CYS:SG	6:B:1305:NAD:C3N	3.03	0.47
1:A:1116[B]:LEU:HD11	1:A:1138:LEU:HD11	1.97	0.46
1:A:782:GLY:O	1:A:811:THR:HA	2.16	0.46
1:B:1058:ASP:OD2	1:B:1070[B]:ARG:NH2	2.40	0.46
1:A:221:ASP:HB2	1:A:473:TYR:CZ	2.51	0.46
1:A:617:VAL:HG12	1:A:774:GLU:HB2	1.97	0.46
1:B:662:GLY:HA2	10:B:1528:HOH:O	2.15	0.45
1:B:531:HIS:NE2	1:B:1232:ILE:HG23	2.32	0.44
1:A:1063:ARG:HG2	10:A:1499:HOH:O	2.17	0.44
1:A:358:ARG:NH1	1:A:415:VAL:HG21	2.33	0.44
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.52	0.44
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.53	0.44
1:B:509:SER:OG	1:B:512:GLU:HG3	2.18	0.44
1:A:428:LEU:HD11	1:A:460:VAL:HG21	2.01	0.43
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.54	0.43
1:A:485:TYR:O	1:A:489:ARG:HG2	2.19	0.42
1:A:489:ARG:HH12	2:A:1301[A]:UJM:C02	2.29	0.42
1:A:531:HIS:CE1	1:A:1232:ILE:HG23	2.55	0.41
1:B:873:ILE:HD11	1:B:912:ILE:HD11	2.01	0.41
1:B:1178:LYS:HB3	1:B:1178:LYS:HE3	1.89	0.41
1:B:918:THR:HB	1:B:923:PHE:CD1	2.56	0.41
5:A:1304:FAD:H4'	5:A:1304:FAD:H1'1	1.90	0.41

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)
10:B:1426:HOH:O	10:B:2492:HOH:O[2_646]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1229/1235 (100%)	1200 (98%)	27 (2%)	2 (0%)	47	23
1	B	1231/1235 (100%)	1206 (98%)	25 (2%)	0	100	100
All	All	2460/2470 (100%)	2406 (98%)	52 (2%)	2 (0%)	51	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	LEU
1	A	129	ASN

### 5.3.2 Protein sidechains [i](#)

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	919/951 (97%)	912 (99%)	7 (1%)	81	65
1	B	926/951 (97%)	919 (99%)	7 (1%)	81	65
All	All	1845/1902 (97%)	1831 (99%)	14 (1%)	81	65

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	181	ARG
1	A	342	TYR
1	A	610	GLU
1	A	730	LYS
1	A	934	LEU
1	A	1063	ARG
1	B	39	TYR
1	B	342	TYR
1	B	503	ILE
1	B	730	LYS
1	B	855	ASP
1	B	934	LEU
1	B	1141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	PGE	A	1303	-	9,9,9	0.30	0	8,8,8	0.29	0
7	SO4	A	1306	-	4,4,4	0.19	0	6,6,6	0.12	0
7	SO4	A	1308	-	4,4,4	0.15	0	6,6,6	0.06	0
3	UJP	A	1302[B]	-	4,8,8	0.63	0	4,10,10	1.07	0
2	UJM	B	1301[A]	-	4,8,8	0.55	0	4,10,10	0.87	0
2	UJM	A	1301[A]	-	4,8,8	0.41	0	4,10,10	0.93	0
5	FAD	B	1304	-	51,58,58	1.96	15 (29%)	60,89,89	1.75	9 (15%)
7	SO4	B	1306	-	4,4,4	0.23	0	6,6,6	0.23	0
9	PEG	B	1308	-	6,6,6	0.30	0	5,5,5	0.33	0
6	NAD	A	1305	8	42,48,48	3.48	17 (40%)	50,73,73	1.60	4 (8%)
3	UJP	B	1302[B]	-	4,8,8	0.75	0	4,10,10	1.18	0
7	SO4	A	1307	-	4,4,4	0.15	0	6,6,6	0.07	0
6	NAD	B	1305	8	42,48,48	3.24	14 (33%)	50,73,73	1.53	5 (10%)
5	FAD	A	1304	-	51,58,58	2.08	17 (33%)	60,89,89	1.75	7 (11%)
4	PGE	B	1303	-	9,9,9	0.30	0	8,8,8	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	A	1303	-	-	5/7/7/7	-
3	UJP	A	1302[B]	-	-	0/0/11/11	0/1/1/1
2	UJM	B	1301[A]	-	-	0/0/11/11	0/1/1/1
2	UJM	A	1301[A]	-	-	0/0/11/11	0/1/1/1
5	FAD	B	1304	-	-	4/30/50/50	0/6/6/6
9	PEG	B	1308	-	-	1/4/4/4	-
6	NAD	A	1305	8	-	2/26/62/62	0/5/5/5
3	UJP	B	1302[B]	-	-	0/0/11/11	0/1/1/1
6	NAD	B	1305	8	-	2/26/62/62	0/5/5/5
5	FAD	A	1304	-	-	4/30/50/50	0/6/6/6
4	PGE	B	1303	-	-	4/7/7/7	-

All (63) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1305	NAD	O4D-C1D	-8.64	1.29	1.41
6	A	1305	NAD	C3B-C4B	-8.24	1.31	1.53
6	B	1305	NAD	O4D-C1D	-8.06	1.29	1.41
6	A	1305	NAD	C7N-N7N	7.86	1.48	1.33
6	B	1305	NAD	C3B-C4B	-7.85	1.32	1.53
6	B	1305	NAD	C7N-N7N	7.53	1.47	1.33
6	A	1305	NAD	C3D-C4D	-7.44	1.34	1.53
6	A	1305	NAD	O4B-C4B	7.25	1.61	1.45
6	A	1305	NAD	O4D-C4D	6.92	1.60	1.45
6	B	1305	NAD	O4B-C4B	6.79	1.60	1.45
6	B	1305	NAD	C3D-C4D	-6.69	1.35	1.53
6	B	1305	NAD	O4D-C4D	6.33	1.59	1.45
5	A	1304	FAD	C4X-C10	5.70	1.44	1.38
6	A	1305	NAD	O4B-C1B	-5.11	1.33	1.41
5	B	1304	FAD	C4X-C10	4.91	1.43	1.38
5	A	1304	FAD	O4-C4	4.66	1.36	1.24
5	A	1304	FAD	C4-C4X	4.65	1.49	1.41
5	B	1304	FAD	O4-C4	4.57	1.36	1.24
5	A	1304	FAD	C4X-N5	4.46	1.39	1.33
5	B	1304	FAD	C4-C4X	4.41	1.49	1.41
6	A	1305	NAD	C3N-C7N	4.25	1.57	1.50
6	B	1305	NAD	C6A-N6A	4.25	1.49	1.34
6	B	1305	NAD	O3D-C3D	4.17	1.52	1.43
6	A	1305	NAD	O3D-C3D	4.11	1.52	1.43
5	B	1304	FAD	C4X-N5	4.11	1.39	1.33
6	A	1305	NAD	C6A-N6A	4.08	1.49	1.34
6	B	1305	NAD	O4B-C1B	-4.07	1.35	1.41
6	B	1305	NAD	C3N-C7N	3.66	1.56	1.50
5	A	1304	FAD	C10-N1	3.46	1.37	1.33
6	B	1305	NAD	C2N-N1N	3.31	1.39	1.35
5	B	1304	FAD	C9A-N10	3.31	1.43	1.38
5	B	1304	FAD	C10-N1	3.29	1.37	1.33
5	A	1304	FAD	C5X-N5	3.21	1.40	1.35
6	A	1305	NAD	O3B-C3B	3.18	1.50	1.43
5	A	1304	FAD	C9A-N10	3.04	1.42	1.38
5	A	1304	FAD	C4-N3	2.90	1.38	1.33
6	B	1305	NAD	O3B-C3B	2.88	1.49	1.43
5	B	1304	FAD	C6A-N6A	2.81	1.44	1.34
5	A	1304	FAD	O2'-C2'	-2.80	1.37	1.43
5	B	1304	FAD	C2B-C1B	-2.78	1.49	1.53
5	A	1304	FAD	C6A-N6A	2.75	1.44	1.34
5	A	1304	FAD	C2B-C1B	-2.71	1.49	1.53
6	A	1305	NAD	C2A-N1A	2.71	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1304	FAD	C5X-N5	2.60	1.39	1.35
6	A	1305	NAD	C2N-N1N	2.60	1.38	1.35
6	A	1305	NAD	C2A-N3A	2.56	1.36	1.32
5	B	1304	FAD	C2A-N3A	2.56	1.36	1.32
5	B	1304	FAD	O2'-C2'	-2.48	1.38	1.43
6	A	1305	NAD	C5A-C4A	-2.48	1.34	1.40
5	A	1304	FAD	PA-O5B	-2.45	1.49	1.59
5	B	1304	FAD	C4-N3	2.40	1.37	1.33
5	A	1304	FAD	C2A-N3A	2.39	1.35	1.32
6	B	1305	NAD	C2A-N1A	2.38	1.38	1.33
5	A	1304	FAD	O4'-C4'	-2.33	1.38	1.43
6	A	1305	NAD	O7N-C7N	-2.33	1.19	1.24
5	A	1304	FAD	O4B-C4B	-2.29	1.39	1.45
6	A	1305	NAD	O2B-C2B	-2.21	1.37	1.43
5	B	1304	FAD	PA-O2A	-2.16	1.45	1.55
5	B	1304	FAD	C2-N1	2.16	1.42	1.38
5	B	1304	FAD	O4B-C4B	-2.16	1.40	1.45
6	B	1305	NAD	C5A-C4A	-2.12	1.35	1.40
5	A	1304	FAD	C2-N1	2.09	1.42	1.38
5	A	1304	FAD	PA-O2A	-2.09	1.45	1.55

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1305	NAD	C1B-N9A-C4A	-7.05	114.25	126.64
5	B	1304	FAD	C4-N3-C2	6.64	120.75	115.14
5	A	1304	FAD	N3A-C2A-N1A	-6.07	119.20	128.68
6	B	1305	NAD	C1B-N9A-C4A	-5.94	116.20	126.64
5	A	1304	FAD	C4-N3-C2	5.82	120.06	115.14
6	A	1305	NAD	N3A-C2A-N1A	-5.75	119.68	128.68
5	A	1304	FAD	C4-C4X-C10	-5.74	116.15	119.95
6	B	1305	NAD	N3A-C2A-N1A	-5.59	119.94	128.68
5	B	1304	FAD	N3A-C2A-N1A	-5.25	120.47	128.68
5	A	1304	FAD	C4-C4X-N5	4.34	123.56	118.60
5	B	1304	FAD	C4-C4X-C10	-4.16	117.20	119.95
5	B	1304	FAD	C4-C4X-N5	3.79	122.93	118.60
5	B	1304	FAD	C4X-C4-N3	-2.99	119.34	123.43
5	B	1304	FAD	C1'-N10-C9A	2.82	120.51	118.29
6	B	1305	NAD	C3N-C2N-N1N	-2.81	117.68	120.43
6	A	1305	NAD	O4B-C1B-C2B	-2.81	102.82	106.93
6	B	1305	NAD	O4B-C1B-C2B	-2.75	102.91	106.93
5	A	1304	FAD	C1'-N10-C9A	2.68	120.40	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1304	FAD	C4X-N5-C5X	2.61	119.38	116.77
6	B	1305	NAD	O4D-C1D-C2D	-2.60	103.12	106.93
5	B	1304	FAD	C2A-N1A-C6A	2.46	122.97	118.75
6	A	1305	NAD	O4D-C1D-C2D	-2.33	103.53	106.93
5	A	1304	FAD	C5X-C9A-N10	2.24	119.34	117.72
5	A	1304	FAD	C4X-N5-C5X	2.13	118.91	116.77
5	B	1304	FAD	C10-C4X-N5	-2.02	119.86	121.26

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1304	FAD	P-O3P-PA-O5B
5	A	1304	FAD	N10-C1'-C2'-O2'
5	A	1304	FAD	N10-C1'-C2'-C3'
5	A	1304	FAD	C1'-C2'-C3'-C4'
5	B	1304	FAD	P-O3P-PA-O5B
5	B	1304	FAD	N10-C1'-C2'-O2'
5	B	1304	FAD	N10-C1'-C2'-C3'
4	A	1303	PGE	O1-C1-C2-O2
4	A	1303	PGE	O2-C3-C4-O3
4	B	1303	PGE	O3-C5-C6-O4
4	A	1303	PGE	C4-C3-O2-C2
6	A	1305	NAD	C4D-C5D-O5D-PN
6	B	1305	NAD	C4D-C5D-O5D-PN
5	B	1304	FAD	C1'-C2'-C3'-C4'
4	A	1303	PGE	C6-C5-O3-C4
4	B	1303	PGE	C3-C4-O3-C5
4	B	1303	PGE	C1-C2-O2-C3
9	B	1308	PEG	C1-C2-O2-C3
4	B	1303	PGE	O1-C1-C2-O2
4	A	1303	PGE	O3-C5-C6-O4
6	A	1305	NAD	C5B-O5B-PA-O1A
6	B	1305	NAD	C5B-O5B-PA-O1A

There are no ring outliers.

5 monomers are involved in 9 short contacts:

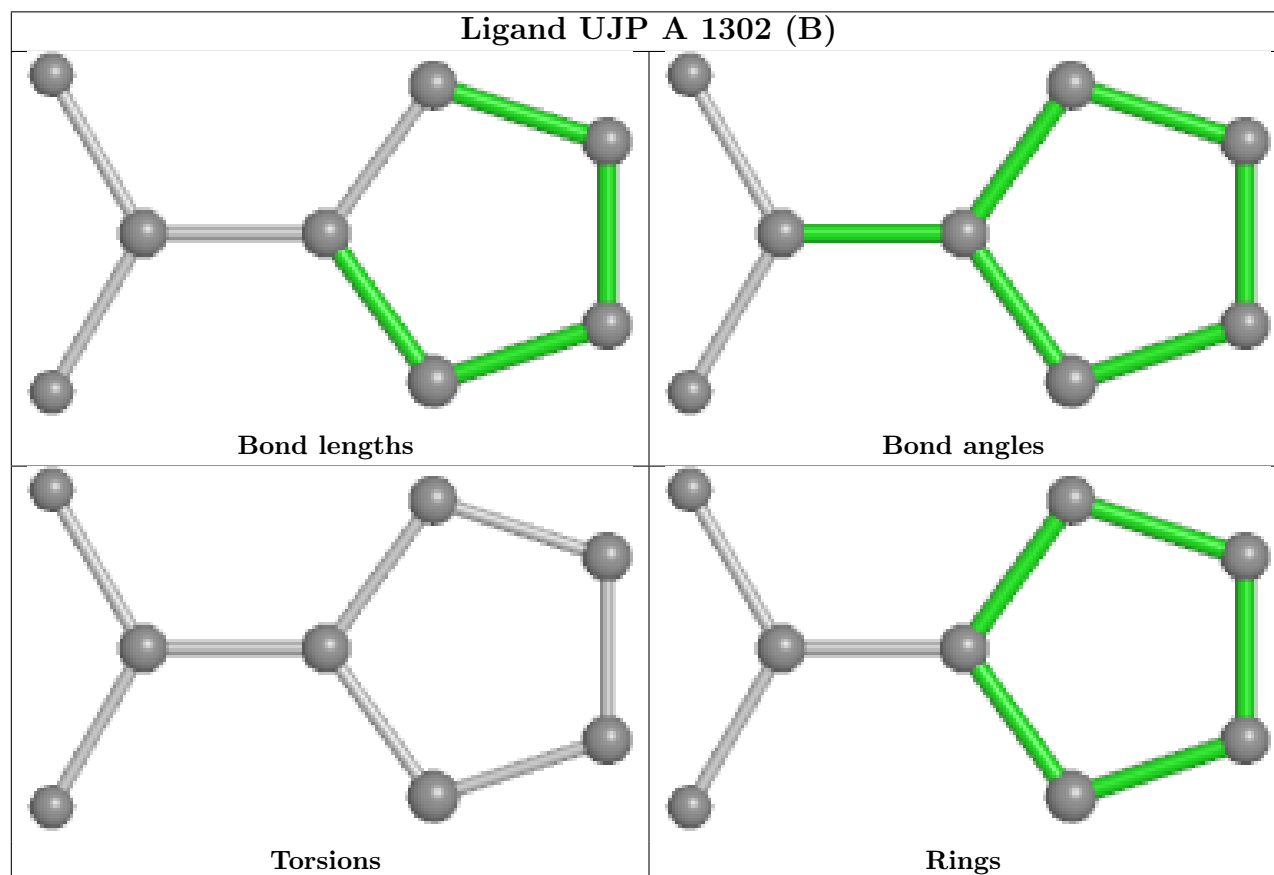
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301[A]	UJM	1	0
5	B	1304	FAD	2	0

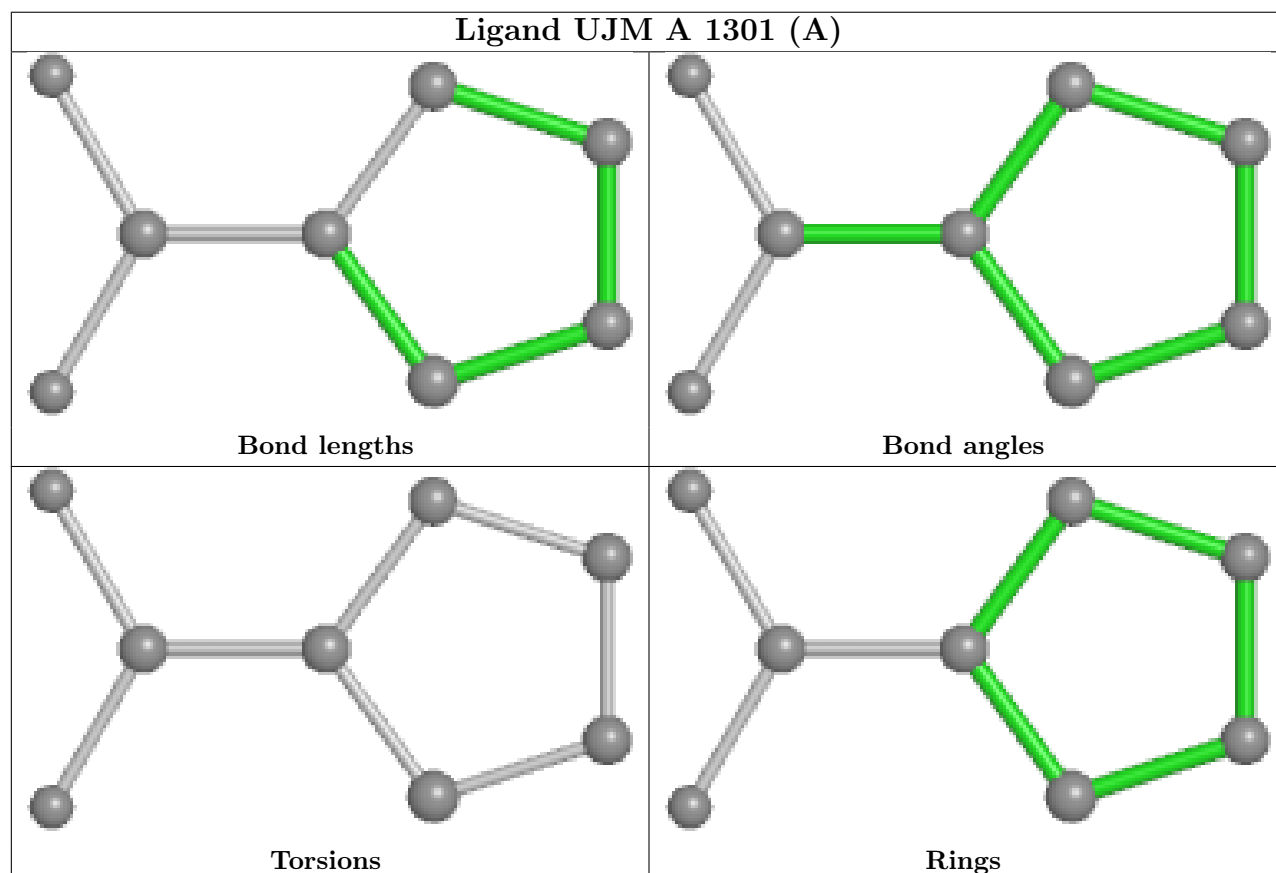
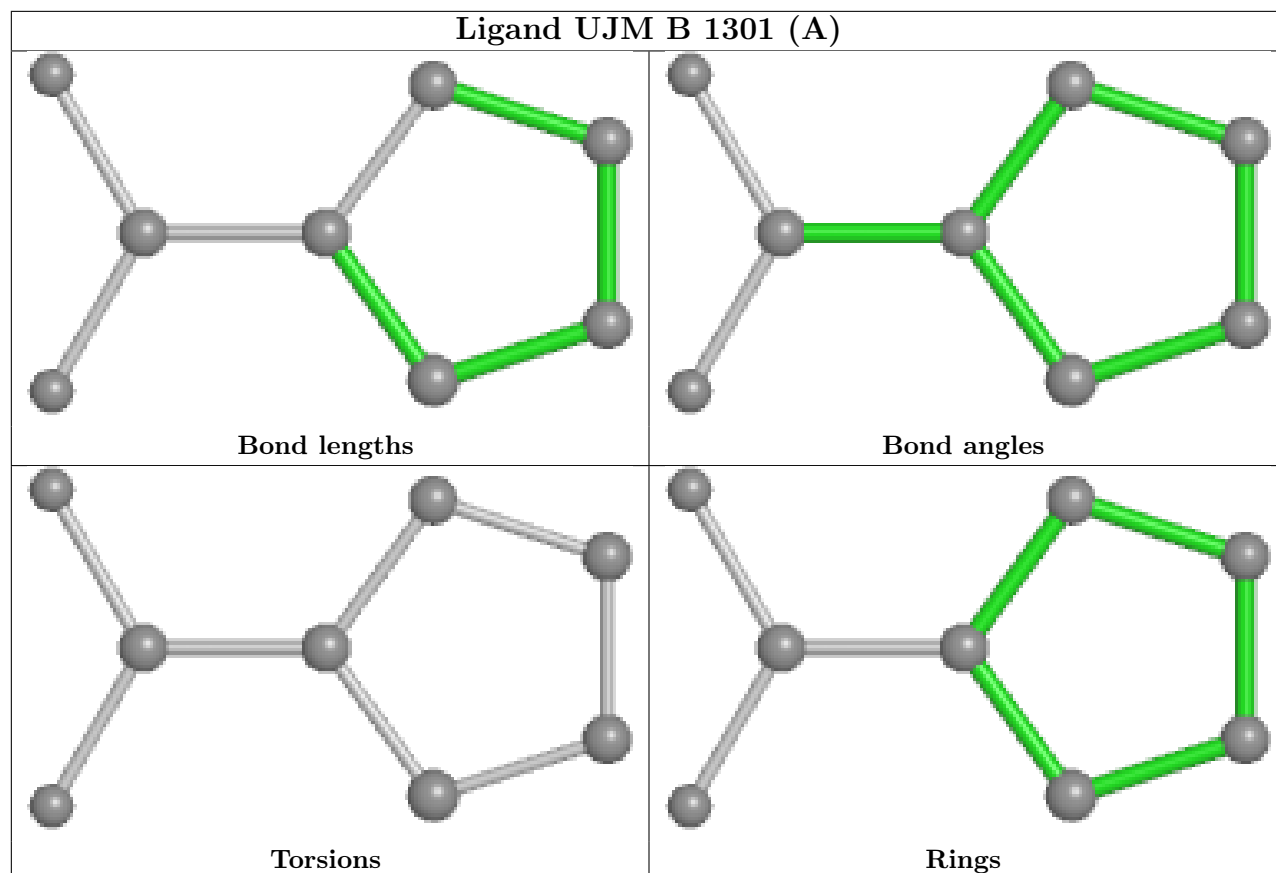
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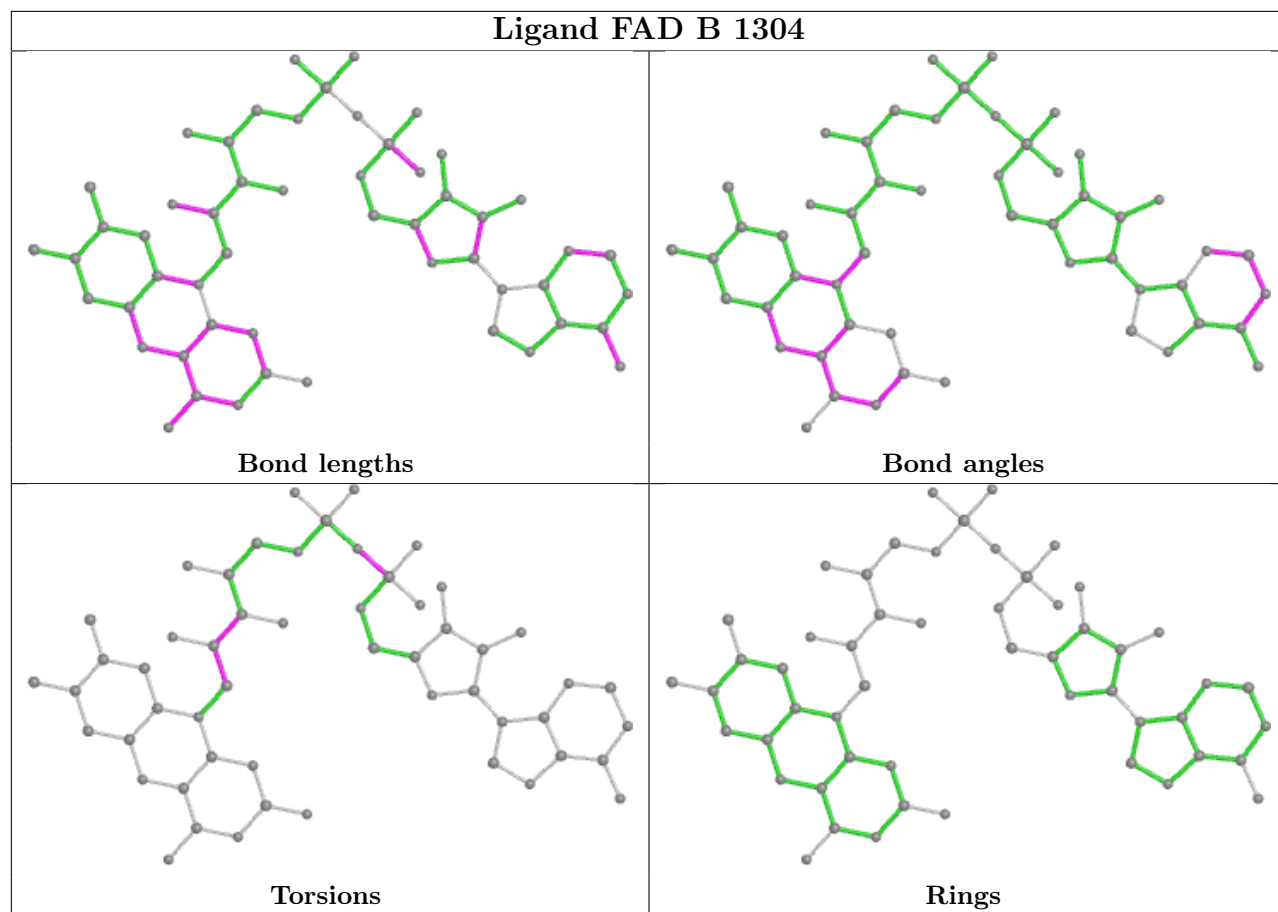
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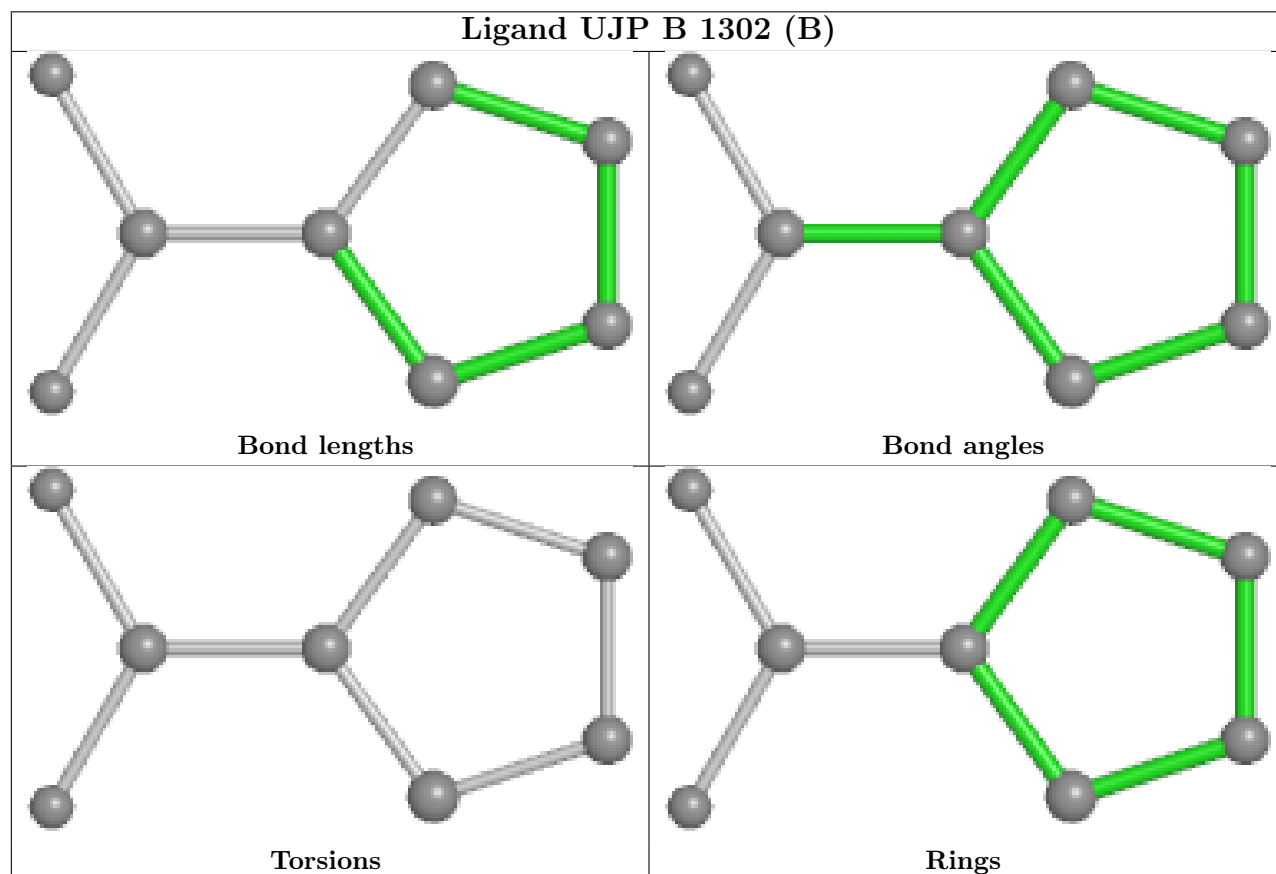
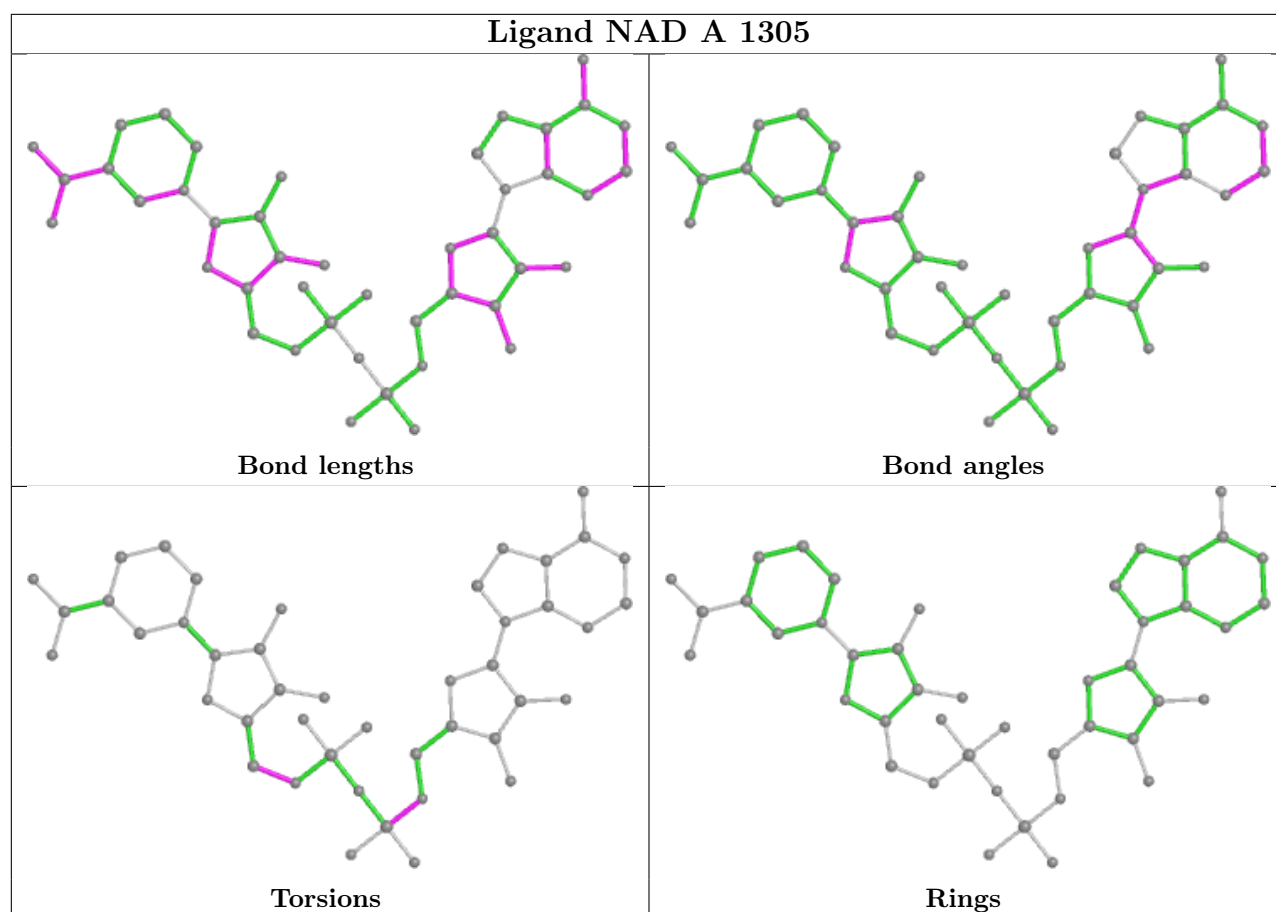
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1305	NAD	1	0
6	B	1305	NAD	2	0
5	A	1304	FAD	3	0

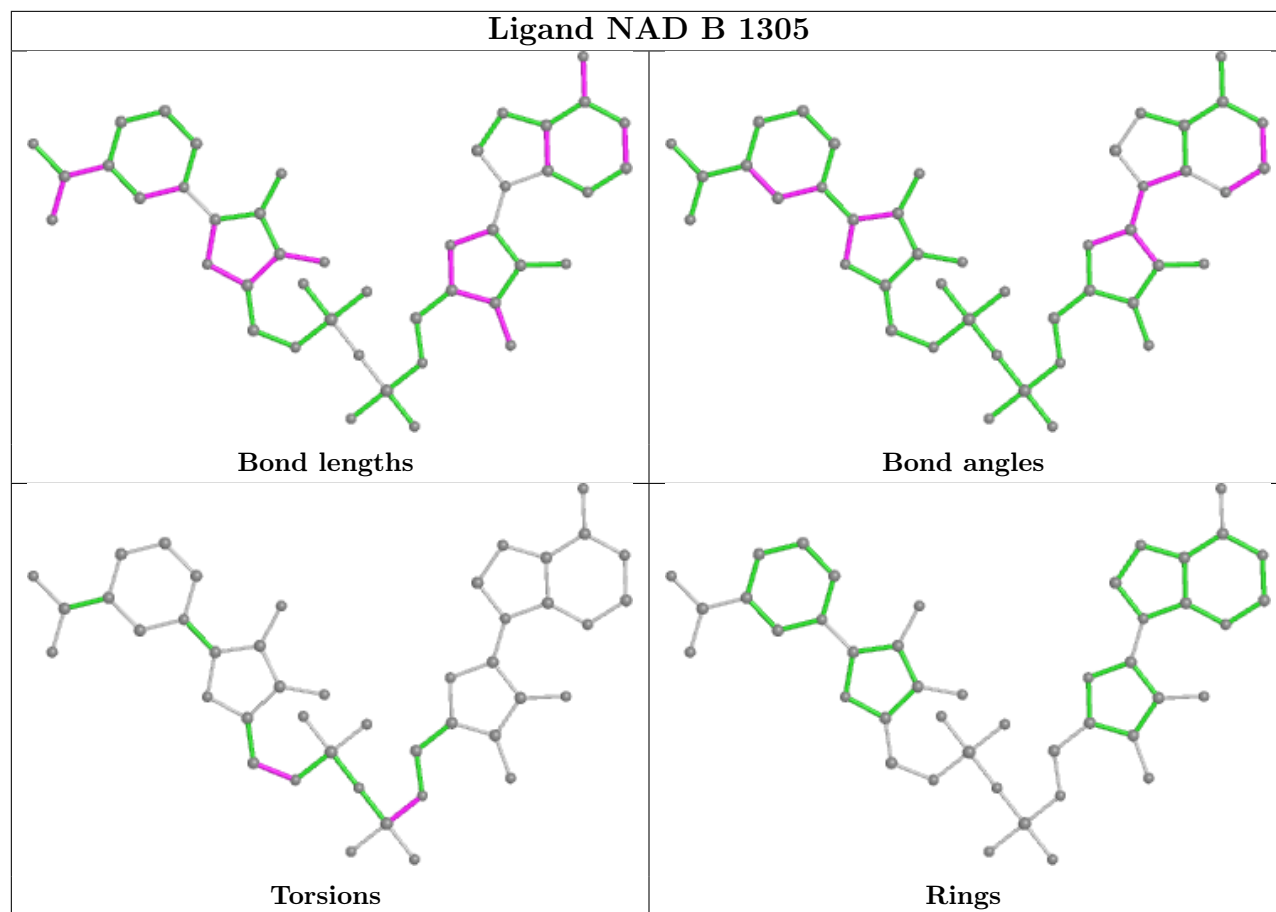
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



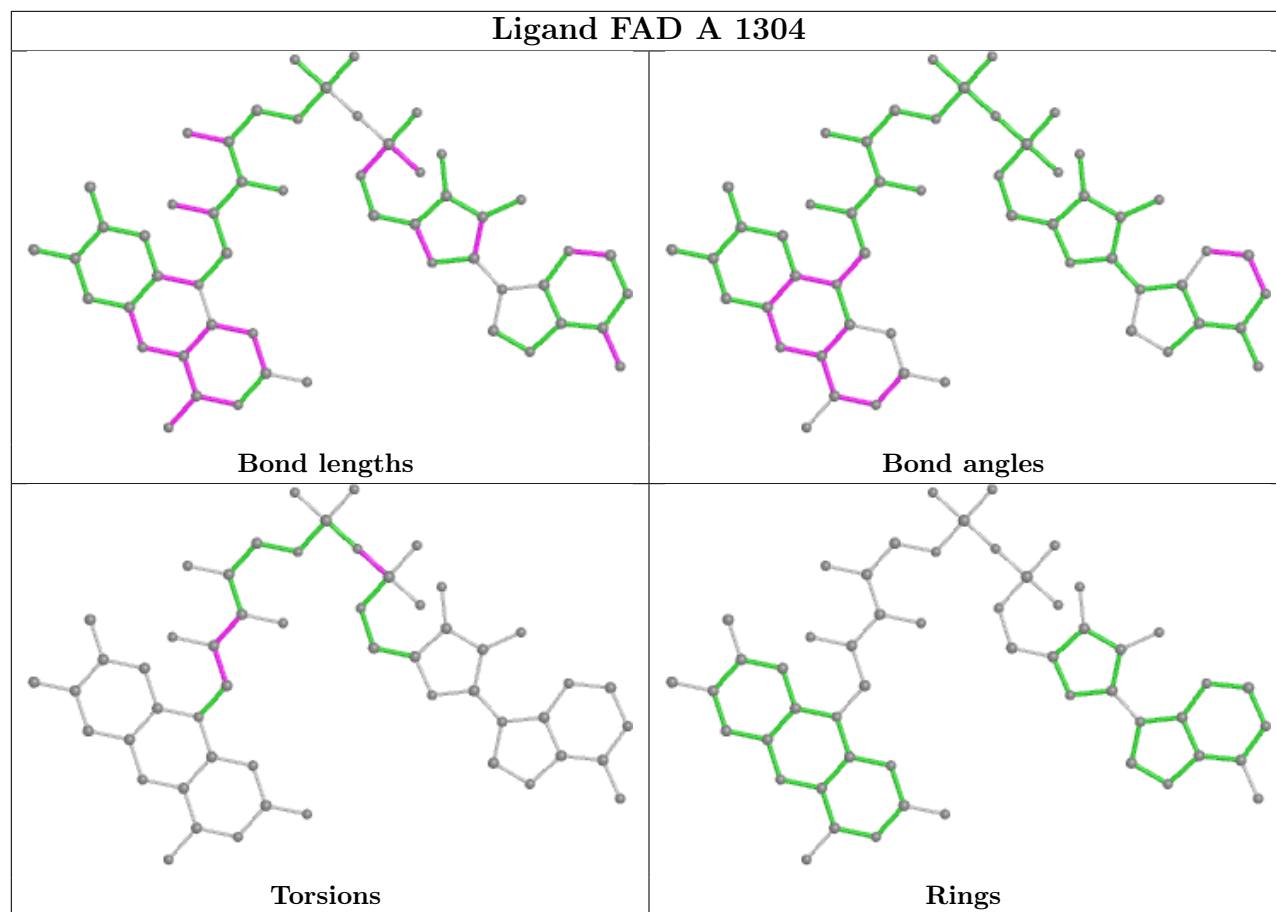












## 5.7 Other polymers [i](#)

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	1217/1235 (98%)	-0.05	32 (2%) 56 61	13, 22, 44, 75	0
1	B	1216/1235 (98%)	-0.13	24 (1%) 65 70	12, 19, 41, 79	0
All	All	2433/2470 (98%)	-0.09	56 (2%) 60 65	12, 20, 42, 79	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1231	ALA	6.9
1	A	81	GLY	6.3
1	B	1231	ALA	5.4
1	A	483	LEU	4.9
1	B	80	SER	4.8
1	A	490	LEU	4.8
1	A	1227	ALA	4.6
1	A	1232	ILE	4.4
1	B	1230	MET	4.3
1	A	14	ALA	4.3
1	A	482	LEU	4.2
1	A	1230	MET	4.1
1	B	81	GLY	4.0
1	A	134	LEU	3.8
1	B	912	ILE	3.7
1	B	132	SER	3.7
1	A	1223	ALA	3.6
1	A	485	TYR	3.6
1	B	491	LEU	3.6
1	A	127	ASP	3.6
1	B	1223	ALA	3.5
1	B	485	TYR	3.5
1	A	82	SER	3.5
1	A	1228	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	132	SER	3.3
1	A	506	PRO	3.2
1	B	14	ALA	3.1
1	A	1229	LEU	3.0
1	B	133	HIS	3.0
1	B	482	LEU	3.0
1	B	1229	LEU	3.0
1	A	493	ASN	2.9
1	A	1222	ALA	2.9
1	B	493	ASN	2.8
1	B	79	HIS	2.8
1	B	129	ASN	2.8
1	B	77	GLY	2.7
1	A	80	SER	2.7
1	A	1233	GLY	2.6
1	B	483	LEU	2.6
1	A	486	LEU	2.6
1	A	1002[A]	GLY	2.5
1	A	115	ALA	2.5
1	B	914	LEU	2.5
1	A	133	HIS	2.5
1	A	916	SER	2.4
1	A	195	PHE	2.3
1	B	918	THR	2.3
1	B	490	LEU	2.3
1	B	494	GLY	2.3
1	A	122	ARG	2.2
1	B	134	LEU	2.1
1	A	1226	ASN	2.1
1	B	484	ALA	2.1
1	A	494	GLY	2.1
1	A	155	LEU	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 monosaccharides in this entry.

## 6.4 Ligands

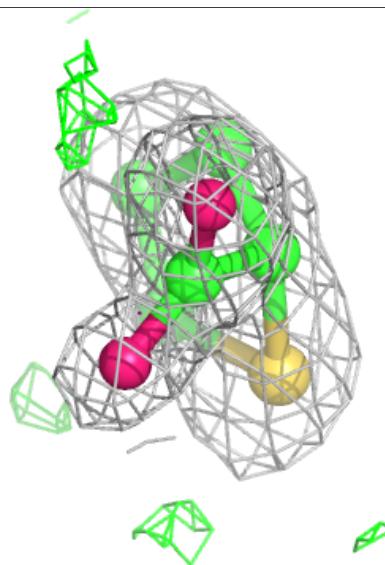
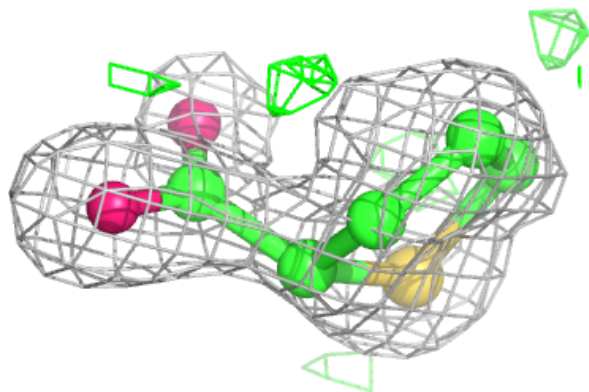
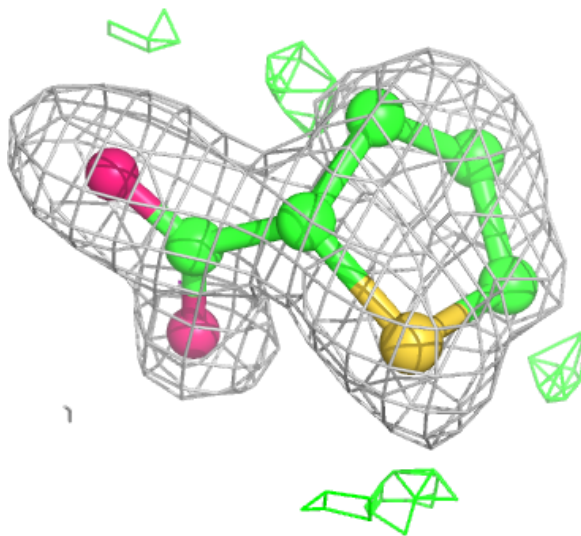
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	PGE	B	1303	10/10	0.81	0.17	41,50,57,58	0
9	PEG	B	1308	7/7	0.86	0.12	28,39,43,45	0
4	PGE	A	1303	10/10	0.87	0.16	37,48,59,63	0
2	UJM	B	1301[A]	8/8	0.89	0.14	29,32,34,35	8
7	SO4	A	1307	5/5	0.91	0.16	48,57,63,66	0
3	UJP	B	1302[B]	8/8	0.91	0.15	30,32,34,35	8
3	UJP	A	1302[B]	8/8	0.92	0.17	33,34,35,38	8
2	UJM	A	1301[A]	8/8	0.92	0.15	29,33,34,38	8
7	SO4	A	1308	5/5	0.93	0.19	78,82,85,85	0
6	NAD	A	1305	44/44	0.94	0.08	17,21,24,27	0
5	FAD	A	1304	53/53	0.95	0.09	16,21,25,27	0
5	FAD	B	1304	53/53	0.95	0.08	14,18,23,24	0
8	MG	A	1309	1/1	0.97	0.12	26,26,26,26	0
8	MG	B	1307	1/1	0.97	0.14	22,22,22,22	0
6	NAD	B	1305	44/44	0.97	0.08	12,14,17,29	0
7	SO4	B	1306	5/5	0.99	0.07	15,16,22,23	0
7	SO4	A	1306	5/5	0.99	0.05	17,18,21,23	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.

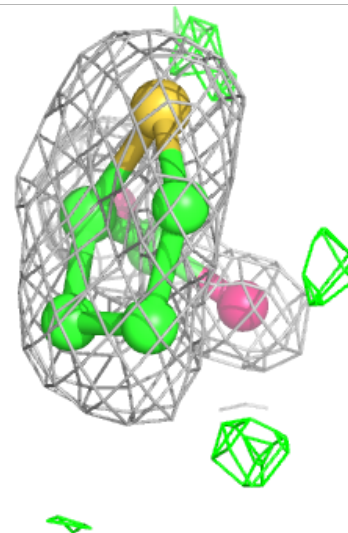
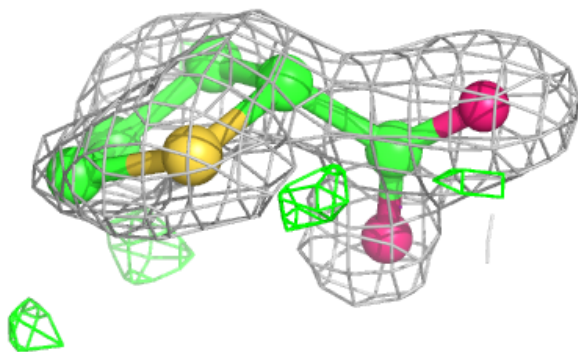
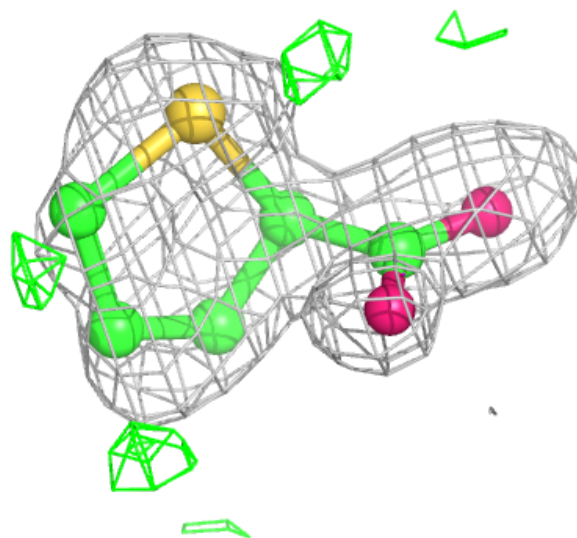
**Electron density around UJM B 1301 (A):**

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



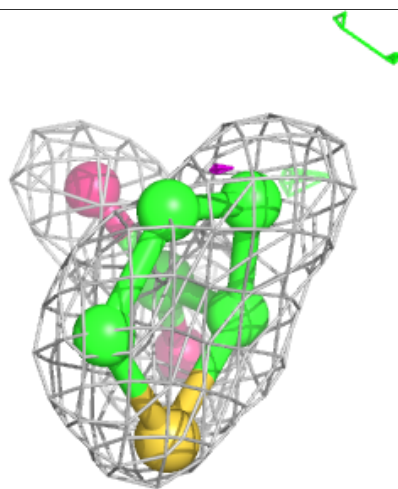
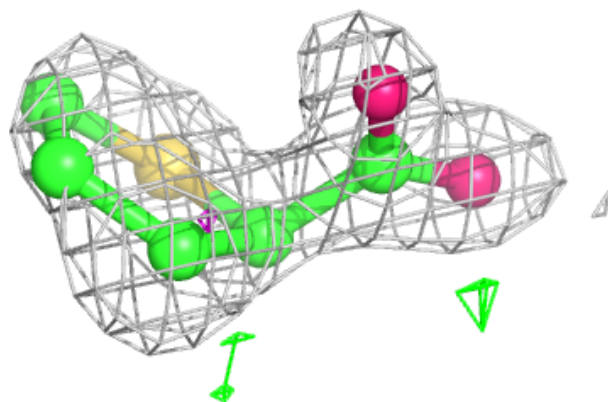
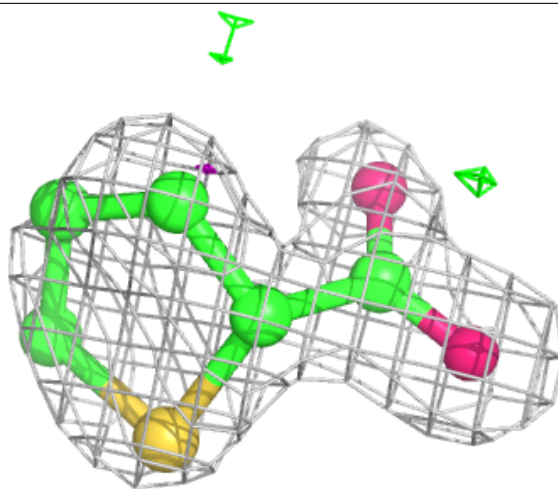
**Electron density around UJP B 1302 (B):**

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



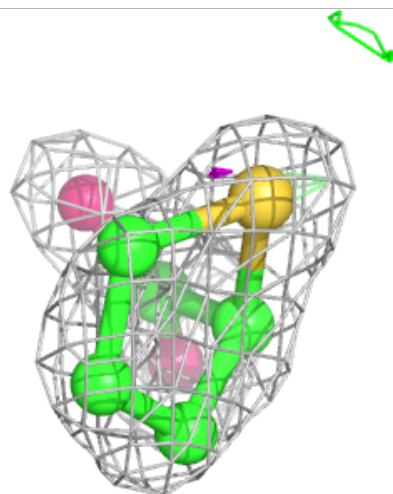
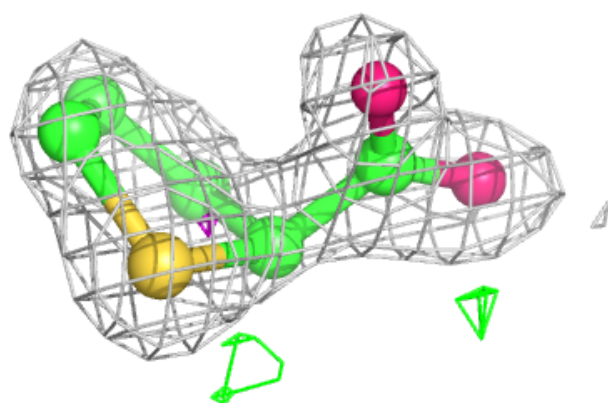
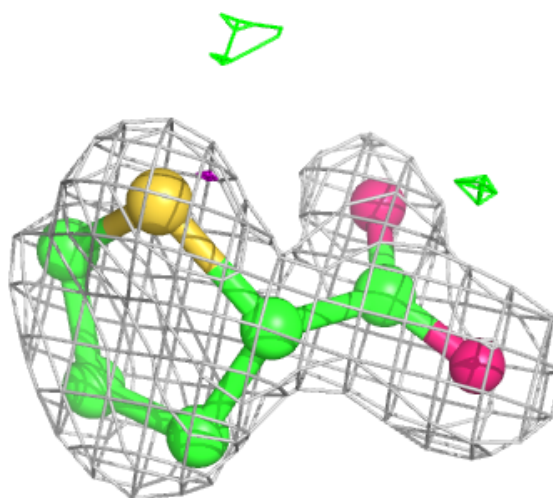
**Electron density around UJP A 1302 (B):**

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



**Electron density around UJM A 1301 (A):**

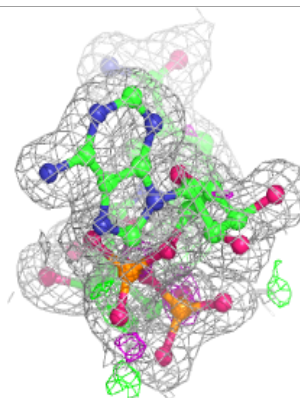
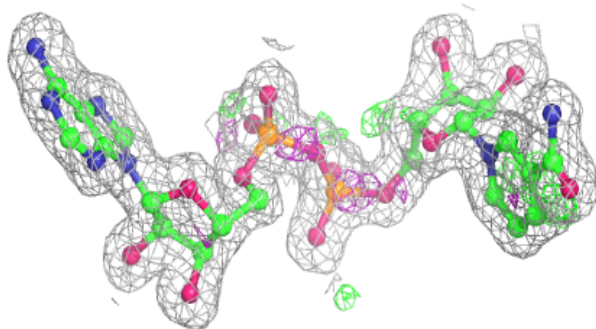
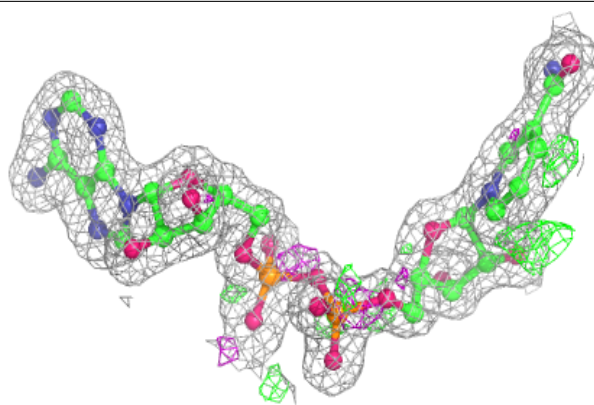
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



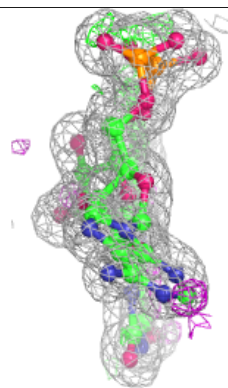
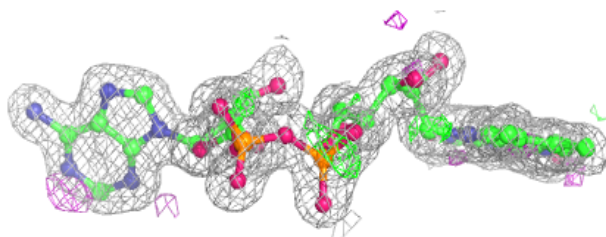
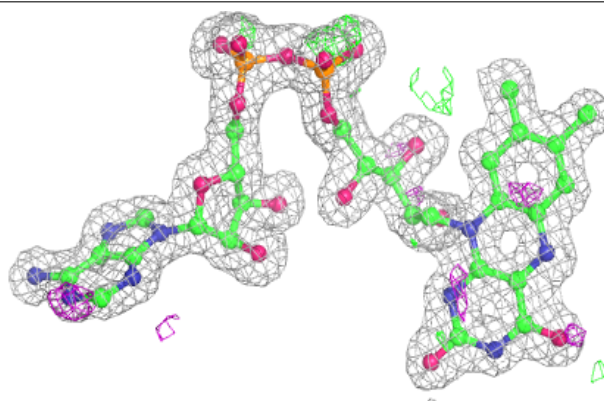


**Electron density around NAD A 1305:**

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

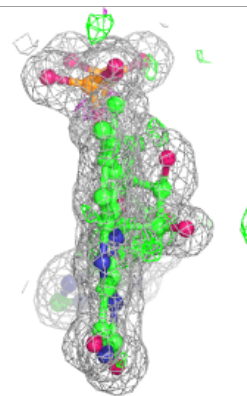
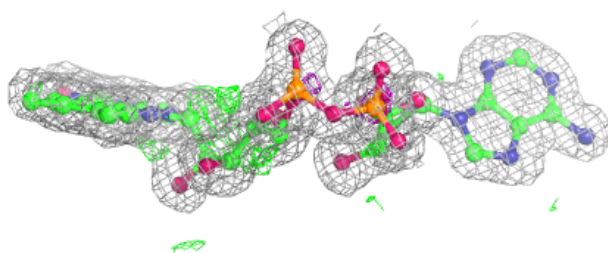
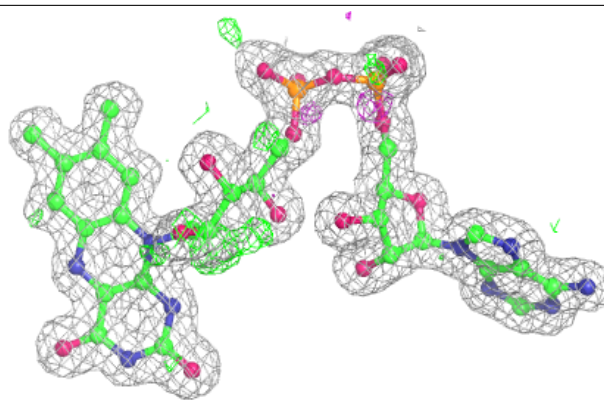
**Electron density around FAD A 1304:**

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

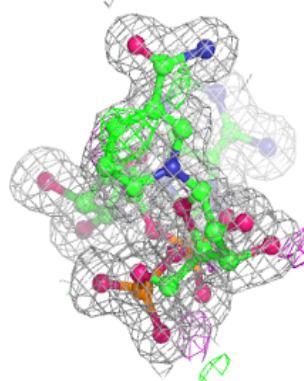
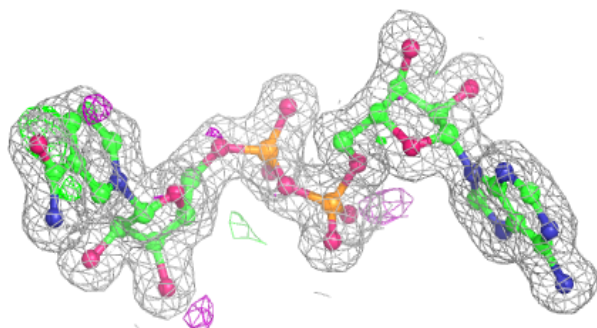
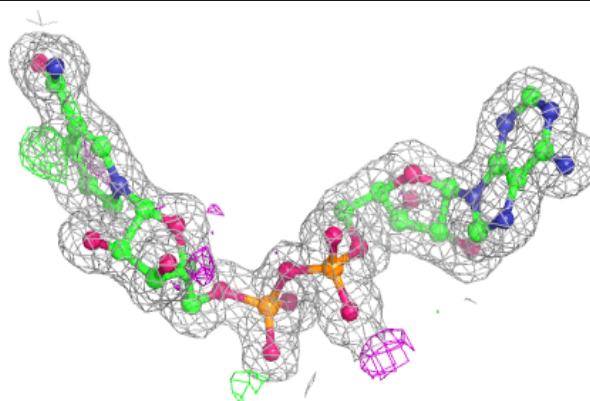


**Electron density around FAD B 1304:**

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

**Electron density around NAD B 1305:**

$2mF_o - DF_c$  (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.