



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2020 – 11:30 PM EST

PDB ID : 6X9B  
Title : Structure of proline utilization A with cis-4-hydroxy-D-proline bound in the L-glutamate-gamma-semialdehyde dehydrogenase active site  
Authors : Tanner, J.J.; Campbell, A.C.  
Deposited on : 2020-06-02  
Resolution : 1.46 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 : 2.16  
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) : 2.16

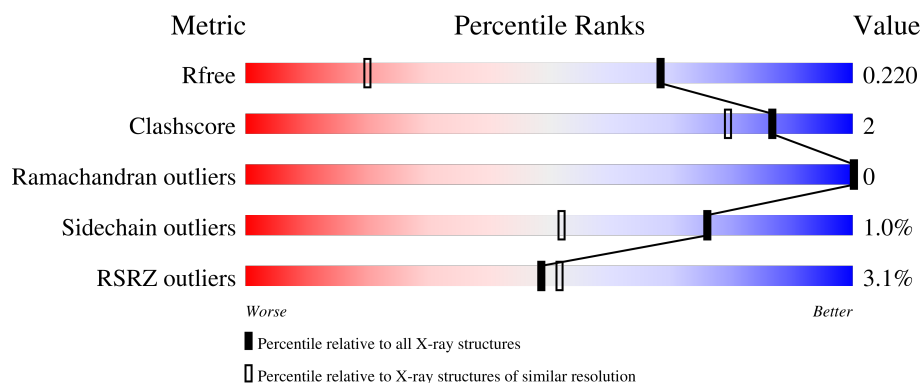
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.46 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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>• •</div> </div>
1	B	1235	<div> <div>4%</div> <div>92%</div> <div>6% •</div> </div>

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 20244 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	1214	Total	C	N	O	S	0	8	0
			9025	5686	1614	1691	34			
1	B	1214	Total	C	N	O	S	0	9	0
			8981	5662	1599	1686	34			

There are 4 discrepancies between the modelled and reference sequences:

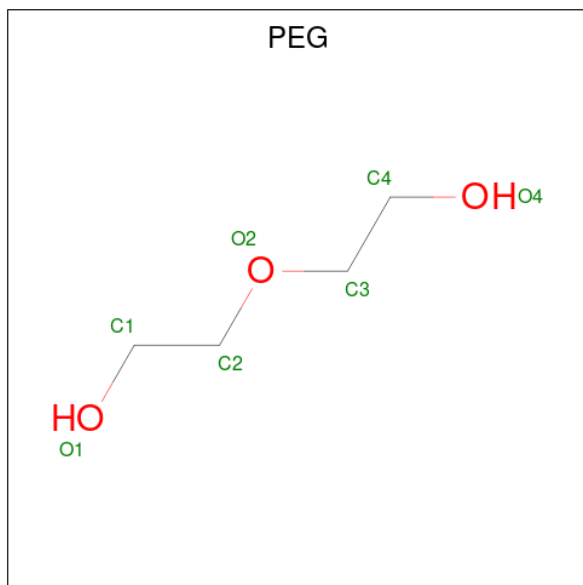
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



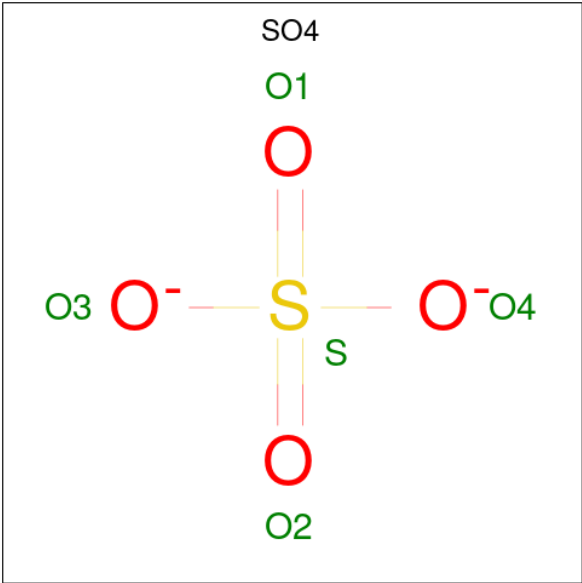
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

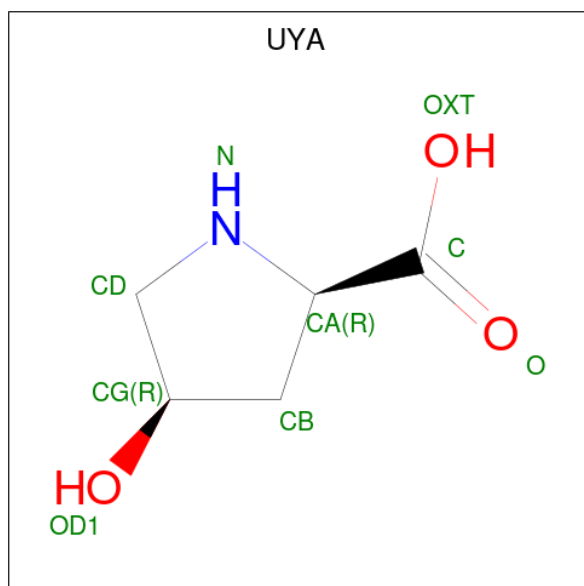


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

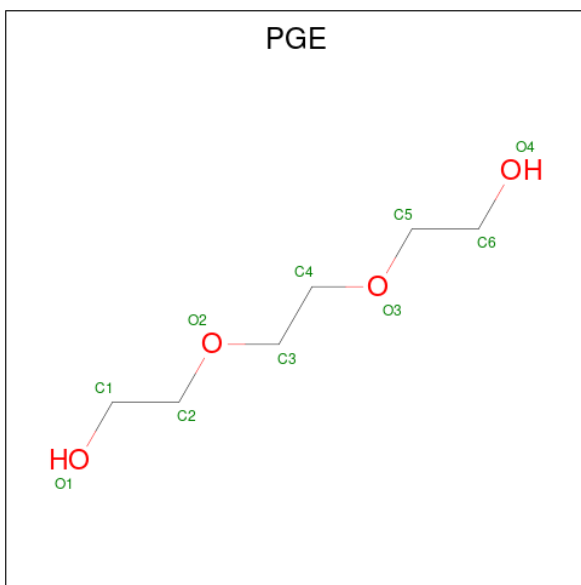
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is (4R)-4-hydroxy-D-proline (three-letter code: UYA) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			9	5	1	3		
7	B	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 8 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
8	B	1	Total	C	O	0	0
			10	6	4		

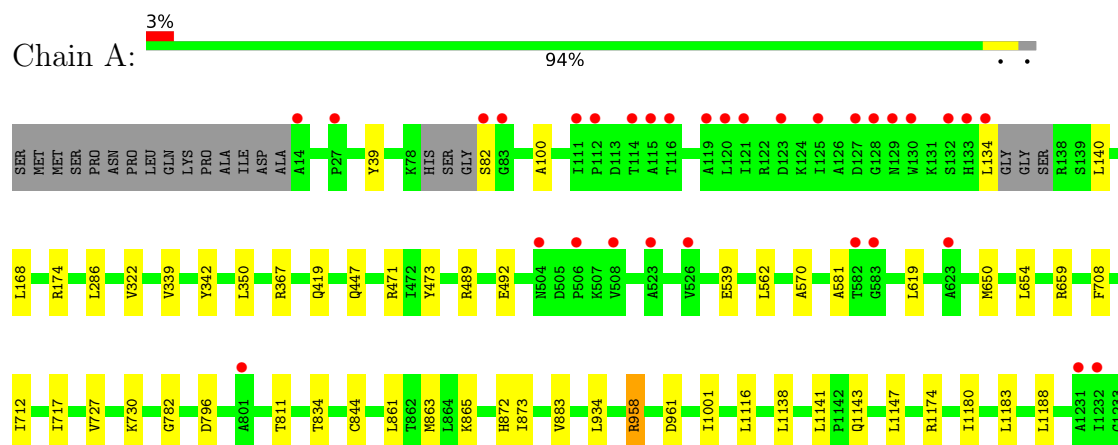
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1007	Total O 1007 1007	0	0
9	B	991	Total O 991 991	0	0

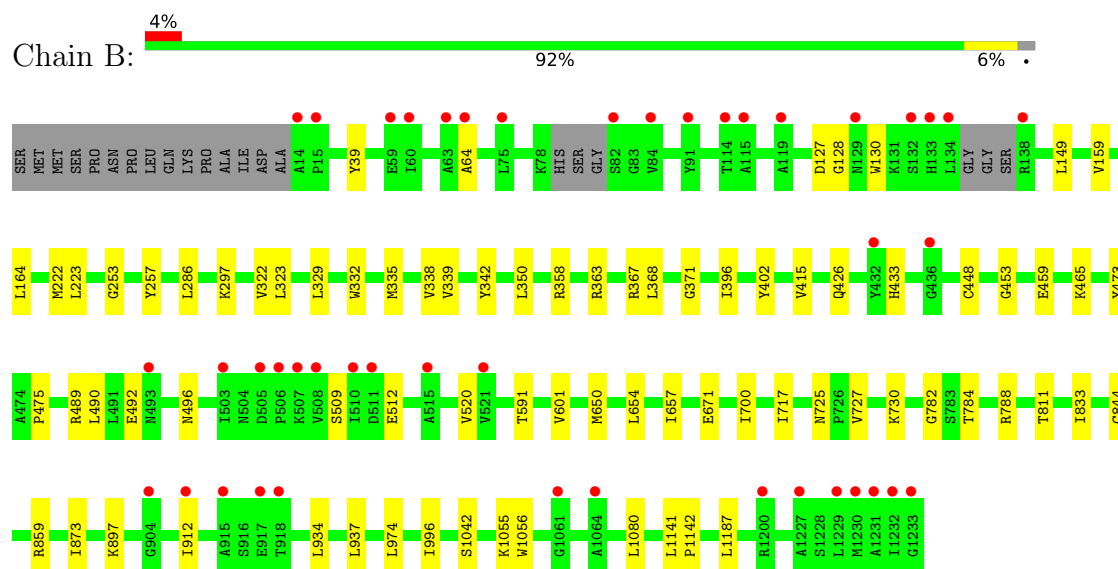
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	100.89Å 101.92Å 126.20Å 90.00° 106.44° 90.00°	Depositor
Resolution (Å)	48.38 – 1.46 48.38 – 1.46	Depositor EDS
% Data completeness (in resolution range)	90.8 (48.38-1.46) 90.9 (48.38-1.46)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 1.46Å)	Xtriage
Refinement program	PHENIX 1.14	Depositor
R, $R_{free}$	0.194 , 0.220 0.194 , 0.220	Depositor DCC
$R_{free}$ test set	19058 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% 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: MG, PGE, NAD, UYA, SO4, PEG, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/9207	0.55	1/12527 (0.0%)
1	B	0.33	0/9165	0.55	0/12481
All	All	0.33	0/18372	0.55	1/25008 (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	174	ARG	NE-CZ-NH1	5.23	122.92	120.30

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	9025	0	9071	31	0
1	B	8981	0	8999	45	0
2	A	53	0	31	3	0
2	B	53	0	31	4	0
3	A	7	0	10	0	0
4	A	44	0	26	2	0
4	B	44	0	26	2	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	5	0	0	0	0
6	A	1	0	0	0	0
7	A	9	0	0	0	0
7	B	9	0	0	0	0
8	B	10	0	14	0	0
9	A	1007	0	0	2	0
9	B	991	0	0	5	0
All	All	20244	0	18208	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (75) 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:473:TYR:HB2	2:B:2001:FAD:HM72	1.64	0.79
1:A:473:TYR:HB2	2:A:2001:FAD:HM72	1.63	0.79
1:B:788:ARG:HD2	1:B:1187:LEU:HD11	1.68	0.74
1:B:844:CYS:SG	4:B:2003:NAD:C4N	2.79	0.70
1:A:844:CYS:SG	4:A:2003:NAD:C4N	2.80	0.69
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.76	0.67
1:A:1183:LEU:O	9:A:2101:HOH:O	2.14	0.66
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.81	0.63
1:A:539:GLU:OE2	9:A:2102:HOH:O	2.16	0.60
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.84	0.59
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.85	0.59
1:B:788:ARG:NH2	9:B:2105:HOH:O	2.37	0.57
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.39	0.57
1:A:650:MET:O	1:A:654:LEU:HG	2.04	0.56
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.88	0.55
1:B:339:VAL:HG21	1:B:350:LEU:HD21	1.88	0.54
1:B:323:LEU:HD13	1:B:335:MET:HE3	1.90	0.53
1:A:717:ILE:HG12	1:A:727:VAL:HG11	1.92	0.52
1:B:371:GLY:N	2:B:2001:FAD:O2'	2.43	0.50
1:B:844:CYS:SG	4:B:2003:NAD:C3N	3.00	0.50
1:A:134:LEU:HB3	1:A:140:LEU:HD11	1.93	0.50
1:A:1116[B]:LEU:HD11	1:A:1138:LEU:HD11	1.93	0.49
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.94	0.49
1:B:974:LEU:HB3	1:B:996:ILE:HD13	1.95	0.49
1:A:861:LEU:HD22	1:A:865:LYS:HE3	1.95	0.49
1:B:650:MET:O	1:B:654:LEU:HG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ARG:HG3	1:B:415:VAL:HG21	1.95	0.48
1:A:844:CYS:SG	4:A:2003:NAD:C3N	3.02	0.47
1:A:473:TYR:CB	2:A:2001:FAD:HM72	2.40	0.47
1:B:253:GLY:HA2	9:B:2915:HOH:O	2.15	0.47
1:A:581:ALA:HB3	1:A:619:LEU:HD13	1.96	0.47
1:A:492:GLU:HB3	2:A:2001:FAD:H4'	1.96	0.47
1:B:782:GLY:O	1:B:811:THR:HA	2.15	0.47
1:B:859:ARG:NH1	9:B:2123:HOH:O	2.47	0.46
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.40	0.46
1:B:492:GLU:HB3	2:B:2001:FAD:H4'	1.98	0.46
1:A:958:ARG:O	1:A:961:ASP:HB2	2.16	0.46
1:B:159:VAL:HG13	1:B:164:LEU:HD12	1.99	0.45
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	1.98	0.45
1:B:338:VAL:HG22	1:B:367:ARG:HD2	1.98	0.45
1:A:1143:GLN:O	1:A:1147:LEU:HG	2.17	0.45
1:A:570:ALA:HA	1:A:659:ARG:NH1	2.32	0.45
1:B:784:THR:O	1:B:788:ARG:HG2	2.16	0.45
1:B:448:CYS:HB2	1:B:453:GLY:HA3	2.00	0.44
1:B:222:MET:HG2	9:B:2179:HOH:O	2.18	0.44
1:B:509:SER:OG	1:B:512:GLU:HG3	2.17	0.44
1:B:657:ILE:HD13	1:B:671:GLU:HG2	1.99	0.44
1:B:897:LYS:NZ	9:B:2130:HOH:O	2.49	0.44
1:A:834:THR:HG22	1:A:1001:ILE:HD11	1.99	0.44
1:B:128:GLY:O	1:B:130:TRP:N	2.46	0.44
1:A:100:ALA:HB1	1:A:168:LEU:HB2	1.99	0.44
1:A:367:ARG:HA	1:A:419:GLN:HB2	2.00	0.43
1:A:796:ASP:HA	1:A:1174:ARG:HG2	2.00	0.43
1:B:396:ILE:HD11	1:B:520:VAL:HB	2.00	0.43
1:A:708:PHE:HB2	1:A:712:ILE:HD12	2.01	0.43
1:A:863:MET:HB2	1:A:863:MET:HE2	1.86	0.43
1:B:1042:SER:O	1:B:1080[A]:LEU:HD13	2.18	0.43
1:B:873:ILE:HD11	1:B:912:ILE:HD11	2.01	0.42
1:B:475:PRO:HG2	1:B:489:ARG:HH12	1.85	0.42
1:B:591[A]:THR:OG1	1:B:601:VAL:HG13	2.19	0.42
1:B:700[B]:ILE:HG12	1:B:725:ASN:HB3	2.01	0.42
1:B:257:TYR:OH	1:B:363:ARG:NH1	2.52	0.42
1:B:149:LEU:HA	1:B:149:LEU:HD23	1.92	0.42
1:B:149:LEU:HD13	1:B:490:LEU:HB2	2.03	0.41
1:A:1138:LEU:HD13	1:A:1141:LEU:HD11	2.01	0.41
1:B:368:LEU:HG	1:B:402:TYR:CE2	2.55	0.41
1:A:447:GLN:HG2	1:A:471:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LEU:HD11	1:A:654:LEU:HD12	2.02	0.41
1:B:149:LEU:HB3	1:B:490:LEU:HD13	2.02	0.41
1:B:473:TYR:CB	2:B:2001:FAD:HM72	2.44	0.41
1:B:459:GLU:HA	1:B:465:LYS:HD2	2.02	0.40
1:A:782:GLY:O	1:A:811:THR:HA	2.21	0.40
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.96	0.40
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.04	0.40
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1216/1235 (98%)	1195 (98%)	21 (2%)	0	100	100
1	B	1217/1235 (98%)	1195 (98%)	22 (2%)	0	100	100
All	All	2433/2470 (98%)	2390 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	909/951 (96%)	901 (99%)	8 (1%)	78	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	901/951 (95%)	891 (99%)	10 (1%)	73	48
All	All	1810/1902 (95%)	1792 (99%)	18 (1%)	76	52

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	82	SER
1	A	342	TYR
1	A	489	ARG
1	A	730	LYS
1	A	872	HIS
1	A	934	LEU
1	A	958	ARG
1	B	39	TYR
1	B	127	ASP
1	B	342	TYR
1	B	426	GLN
1	B	496	ASN
1	B	730	LYS
1	B	833	ILE
1	B	934	LEU
1	B	937	LEU
1	B	1141	LEU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
7	UYA	A	2006	-	6,9,9	0.67	0	5,12,12	0.70	0
3	PEG	A	2002	-	6,6,6	0.45	0	5,5,5	0.21	0
4	NAD	A	2003	6	42,48,48	3.56	16 (38%)	50,73,73	1.63	6 (12%)
5	SO4	B	2004	-	4,4,4	0.20	0	6,6,6	0.20	0
7	UYA	B	2005	-	6,9,9	0.91	0	5,12,12	0.64	0
5	SO4	A	2004	-	4,4,4	0.15	0	6,6,6	0.25	0
2	FAD	A	2001	-	51,58,58	2.13	17 (33%)	60,89,89	1.83	10 (16%)
4	NAD	B	2003	-	42,48,48	3.40	17 (40%)	50,73,73	1.73	5 (10%)
8	PGE	B	2002	-	9,9,9	0.52	0	8,8,8	0.16	0
2	FAD	B	2001	-	51,58,58	2.19	18 (35%)	60,89,89	1.82	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
7	UYA	A	2006	-	-	0/0/13/13	0/1/1/1
3	PEG	A	2002	-	-	2/4/4/4	-
4	NAD	A	2003	6	-	2/26/62/62	0/5/5/5
7	UYA	B	2005	-	-	0/0/13/13	0/1/1/1
2	FAD	A	2001	-	-	7/30/50/50	0/6/6/6
4	NAD	B	2003	-	-	2/26/62/62	0/5/5/5
8	PGE	B	2002	-	-	2/7/7/7	-
2	FAD	B	2001	-	-	7/30/50/50	0/6/6/6

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2003	NAD	O4D-C1D	-9.10	1.28	1.41
4	B	2003	NAD	O4D-C1D	-8.76	1.28	1.41
4	A	2003	NAD	C7N-N7N	8.23	1.48	1.33
4	B	2003	NAD	C3B-C4B	-8.18	1.32	1.53
4	A	2003	NAD	C3B-C4B	-8.15	1.32	1.53
4	B	2003	NAD	C7N-N7N	7.90	1.48	1.33
4	A	2003	NAD	C3D-C4D	-7.54	1.33	1.53
4	A	2003	NAD	O4B-C4B	7.45	1.61	1.45
4	A	2003	NAD	O4D-C4D	7.03	1.60	1.45
4	B	2003	NAD	C3D-C4D	-6.97	1.35	1.53
4	B	2003	NAD	O4B-C4B	6.79	1.60	1.45
4	B	2003	NAD	O4D-C4D	6.74	1.60	1.45
2	B	2001	FAD	C4X-C10	6.29	1.45	1.38
2	A	2001	FAD	C4X-C10	5.53	1.44	1.38
4	A	2003	NAD	O4B-C1B	-5.41	1.33	1.41
2	A	2001	FAD	C4-C4X	5.32	1.50	1.41
2	A	2001	FAD	O4-C4	4.89	1.36	1.24
2	B	2001	FAD	O4-C4	4.88	1.36	1.24
2	B	2001	FAD	C4-C4X	4.74	1.49	1.41
4	B	2003	NAD	O4B-C1B	-4.62	1.34	1.41
4	A	2003	NAD	C3N-C7N	4.53	1.57	1.50
2	B	2001	FAD	C10-N1	4.40	1.38	1.33
4	B	2003	NAD	O3D-C3D	4.35	1.53	1.43
4	A	2003	NAD	O3D-C3D	4.27	1.53	1.43
2	A	2001	FAD	C4X-N5	4.23	1.39	1.33
2	B	2001	FAD	C4X-N5	4.22	1.39	1.33
4	B	2003	NAD	C6A-N6A	4.21	1.49	1.34
4	A	2003	NAD	C6A-N6A	4.18	1.49	1.34
2	A	2001	FAD	C10-N1	3.80	1.38	1.33
4	B	2003	NAD	C3N-C7N	3.72	1.56	1.50
2	B	2001	FAD	C9A-N10	3.32	1.43	1.38
2	B	2001	FAD	C2B-C1B	-3.30	1.48	1.53
2	A	2001	FAD	C5X-N5	3.29	1.40	1.35
2	B	2001	FAD	C2-N1	3.26	1.44	1.38
4	A	2003	NAD	O3B-C3B	3.04	1.50	1.43
2	A	2001	FAD	O2'-C2'	-3.03	1.36	1.43
4	B	2003	NAD	O3B-C3B	2.95	1.49	1.43
2	A	2001	FAD	C6A-N6A	2.90	1.44	1.34
2	A	2001	FAD	C9A-N10	2.88	1.42	1.38
2	B	2001	FAD	C2A-N3A	2.85	1.36	1.32
4	B	2003	NAD	C2A-N1A	2.85	1.39	1.33
2	A	2001	FAD	C2-N1	2.79	1.43	1.38
2	B	2001	FAD	C6A-N6A	2.79	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	FAD	O2'-C2'	-2.78	1.37	1.43
2	A	2001	FAD	PA-O5B	-2.72	1.48	1.59
4	A	2003	NAD	C2A-N1A	2.71	1.38	1.33
4	A	2003	NAD	C2N-N1N	2.67	1.38	1.35
2	A	2001	FAD	C4-N3	2.63	1.37	1.33
4	B	2003	NAD	C2N-N1N	2.58	1.38	1.35
4	B	2003	NAD	C2A-N3A	2.56	1.36	1.32
2	B	2001	FAD	O4B-C4B	-2.49	1.39	1.45
2	B	2001	FAD	C4-N3	2.48	1.37	1.33
2	A	2001	FAD	C2A-N3A	2.48	1.36	1.32
2	B	2001	FAD	O4'-C4'	-2.39	1.38	1.43
2	B	2001	FAD	C5X-N5	2.38	1.39	1.35
2	A	2001	FAD	O4B-C4B	-2.35	1.39	1.45
2	A	2001	FAD	C2B-C1B	-2.33	1.50	1.53
4	A	2003	NAD	C2A-N3A	2.33	1.35	1.32
4	A	2003	NAD	C5A-C4A	-2.32	1.34	1.40
2	B	2001	FAD	PA-O5B	-2.32	1.49	1.59
2	A	2001	FAD	O4'-C4'	-2.19	1.38	1.43
2	A	2001	FAD	PA-O2A	-2.16	1.45	1.55
4	B	2003	NAD	C5A-C4A	-2.13	1.35	1.40
4	B	2003	NAD	O7N-C7N	-2.11	1.20	1.24
4	A	2003	NAD	O7N-C7N	-2.10	1.20	1.24
4	B	2003	NAD	O2B-C2B	-2.08	1.38	1.43
2	B	2001	FAD	O2B-C2B	-2.05	1.38	1.43
2	B	2001	FAD	PA-O2A	-2.04	1.45	1.55

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	NAD	C1B-N9A-C4A	-7.49	113.49	126.64
2	B	2001	FAD	C4-N3-C2	7.23	121.25	115.14
4	B	2003	NAD	C1B-N9A-C4A	-6.93	114.47	126.64
2	A	2001	FAD	N3A-C2A-N1A	-6.10	119.14	128.68
2	A	2001	FAD	C4-C4X-C10	-5.97	116.00	119.95
4	B	2003	NAD	N3A-C2A-N1A	-5.23	120.50	128.68
2	B	2001	FAD	N3A-C2A-N1A	-5.11	120.70	128.68
2	A	2001	FAD	C4-C4X-N5	5.09	124.42	118.60
4	A	2003	NAD	N3A-C2A-N1A	-4.91	121.00	128.68
2	A	2001	FAD	C4-N3-C2	4.75	119.16	115.14
4	B	2003	NAD	C3N-C2N-N1N	-4.26	116.27	120.43
2	B	2001	FAD	C5X-C9A-N10	3.74	120.43	117.72
2	B	2001	FAD	C4X-C4-N3	-3.70	118.38	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2003	NAD	O4D-C1D-C2D	-3.45	101.88	106.93
2	B	2001	FAD	C4X-N5-C5X	3.12	119.89	116.77
4	A	2003	NAD	C3N-C2N-N1N	-3.07	117.43	120.43
2	B	2001	FAD	O5'-P-O1P	2.76	119.86	109.07
2	A	2001	FAD	C4X-N5-C5X	2.76	119.53	116.77
4	B	2003	NAD	C2N-C3N-C4N	2.71	121.33	118.26
2	B	2001	FAD	C1'-N10-C9A	2.70	120.42	118.29
2	B	2001	FAD	C4-C4X-C10	-2.69	118.17	119.95
4	A	2003	NAD	O4B-C1B-C2B	-2.64	103.07	106.93
2	A	2001	FAD	C10-C4X-N5	-2.47	119.55	121.26
2	B	2001	FAD	C4-C4X-N5	2.46	121.41	118.60
2	A	2001	FAD	C1'-N10-C9A	2.31	120.11	118.29
2	A	2001	FAD	C2A-N1A-C6A	2.30	122.69	118.75
4	A	2003	NAD	PN-O3-PA	-2.29	124.97	132.83
2	A	2001	FAD	C4A-C5A-N7A	-2.22	107.09	109.40
2	B	2001	FAD	O2P-P-O5'	-2.16	97.71	107.75
2	A	2001	FAD	O5'-P-O1P	2.13	117.40	109.07
2	B	2001	FAD	C1'-N10-C10	2.09	120.28	118.41
4	A	2003	NAD	O4D-C1D-C2D	-2.08	103.89	106.93
2	B	2001	FAD	C4A-C5A-N7A	-2.07	107.24	109.40
2	B	2001	FAD	C9A-N10-C10	-2.07	119.20	121.91
2	B	2001	FAD	C1B-N9A-C4A	-2.05	123.04	126.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	FAD	C2'-C3'-C4'-O4'
2	A	2001	FAD	C2'-C3'-C4'-C5'
2	A	2001	FAD	O3'-C3'-C4'-O4'
2	A	2001	FAD	O3'-C3'-C4'-C5'
2	B	2001	FAD	C2'-C3'-C4'-O4'
2	B	2001	FAD	C2'-C3'-C4'-C5'
2	B	2001	FAD	O3'-C3'-C4'-O4'
2	B	2001	FAD	O3'-C3'-C4'-C5'
8	B	2002	PGE	O3-C5-C6-O4
3	A	2002	PEG	O2-C3-C4-O4
2	A	2001	FAD	P-O3P-PA-O5B
2	B	2001	FAD	P-O3P-PA-O5B
3	A	2002	PEG	C1-C2-O2-C3
8	B	2002	PGE	C3-C4-O3-C5
2	B	2001	FAD	C5B-O5B-PA-O3P

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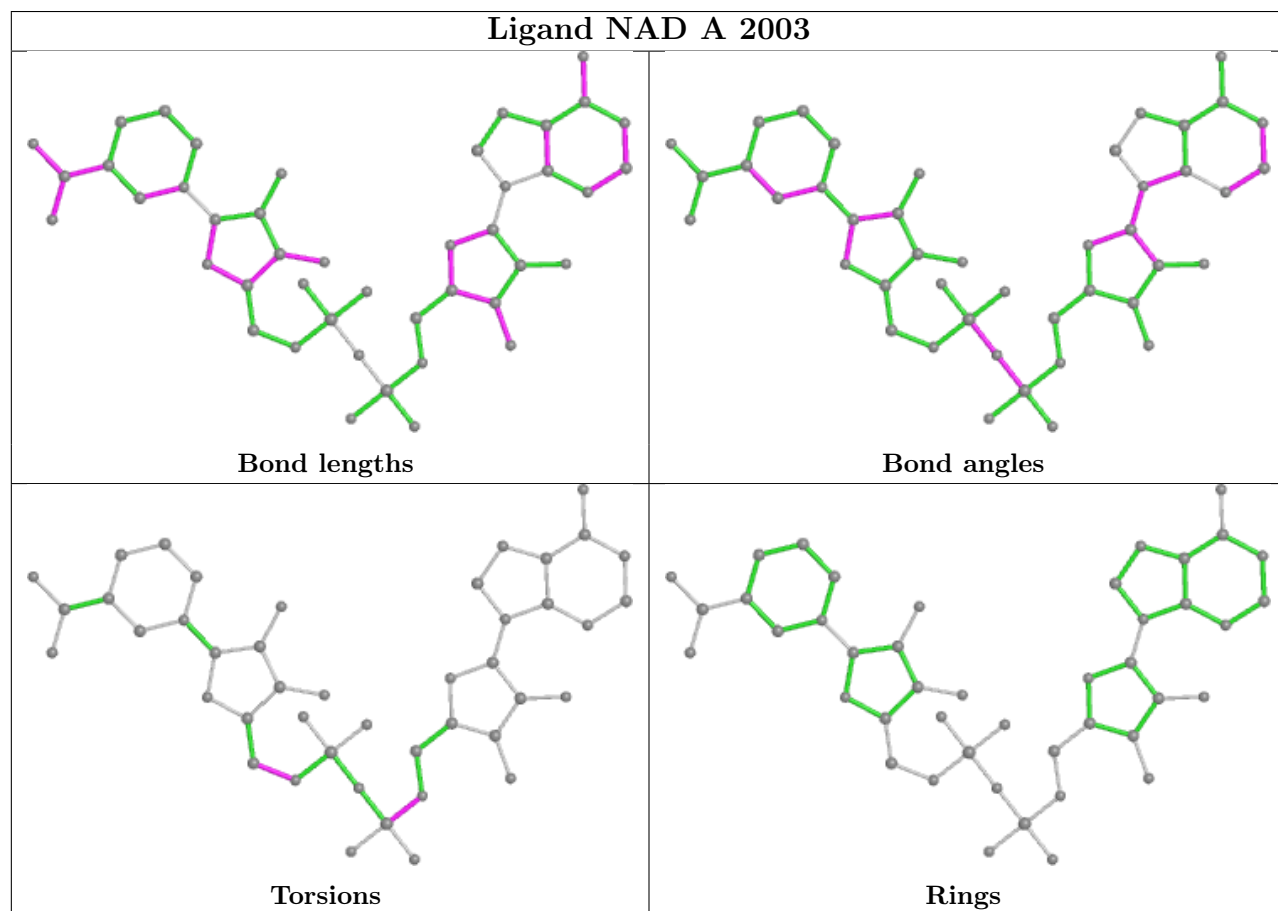
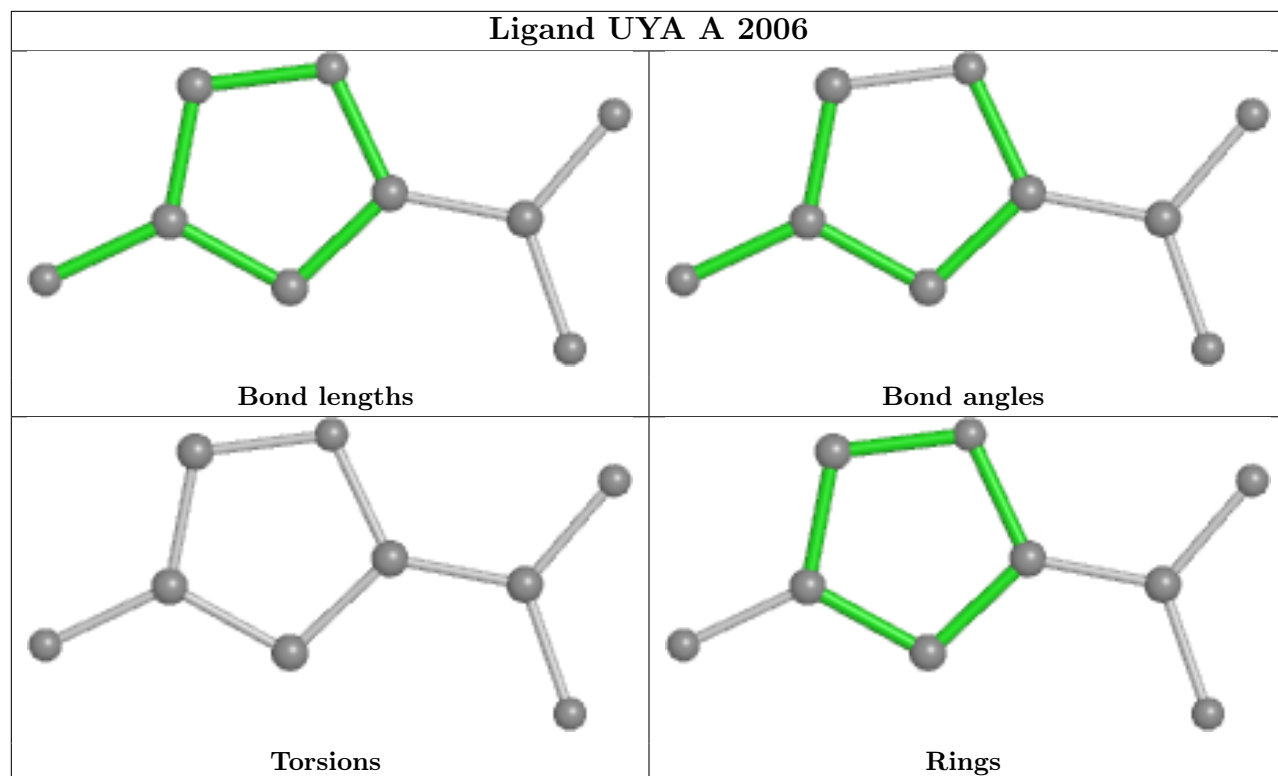
Mol	Chain	Res	Type	Atoms
4	A	2003	NAD	C4D-C5D-O5D-PN
4	B	2003	NAD	C4D-C5D-O5D-PN
2	A	2001	FAD	C3B-C4B-C5B-O5B
2	B	2001	FAD	C3B-C4B-C5B-O5B
2	A	2001	FAD	C5B-O5B-PA-O3P
4	A	2003	NAD	C5B-O5B-PA-O1A
4	B	2003	NAD	C5B-O5B-PA-O1A

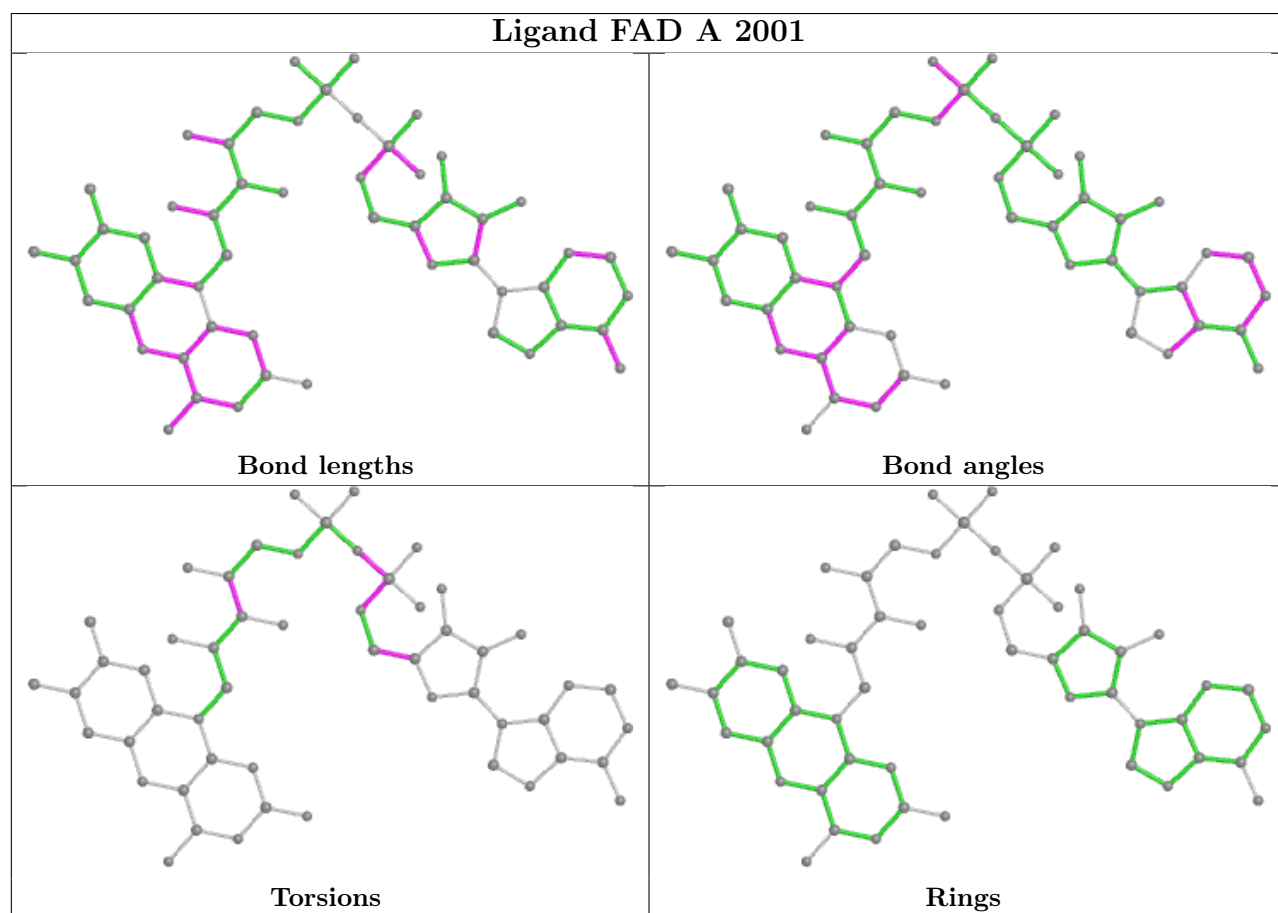
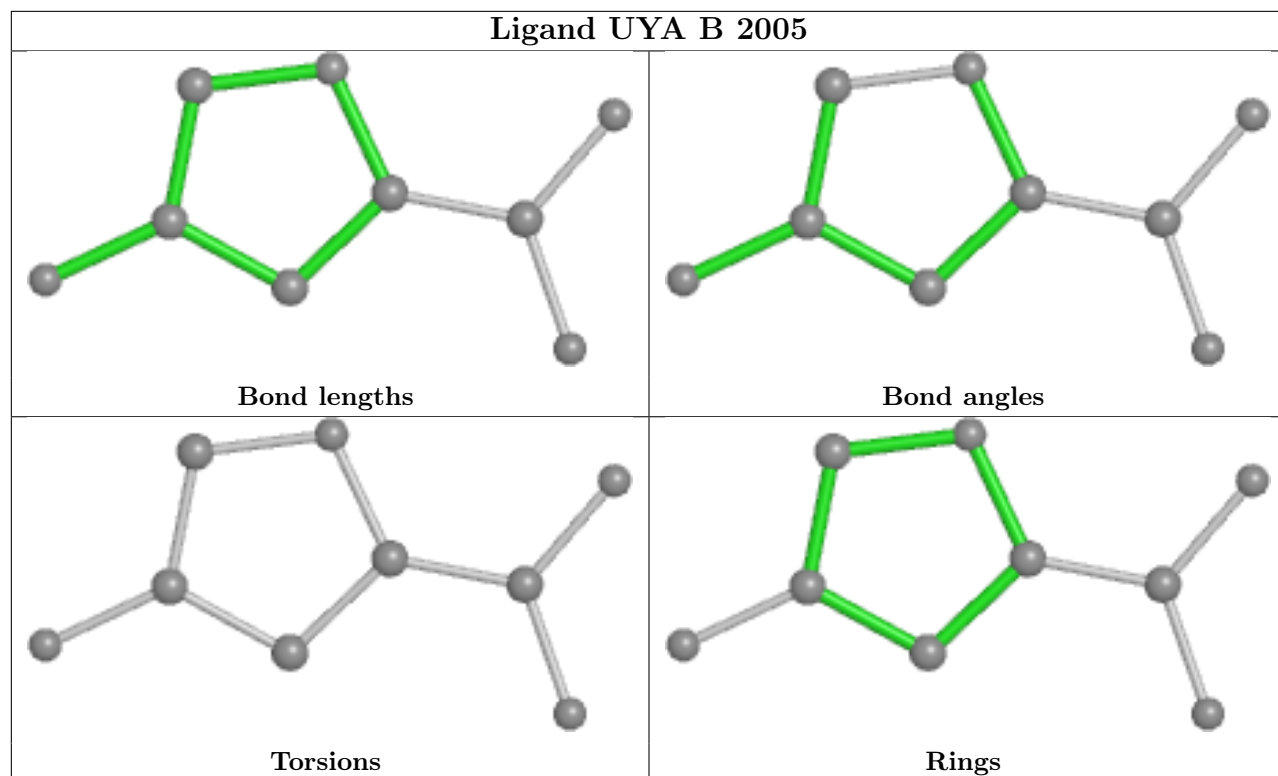
There are no ring outliers.

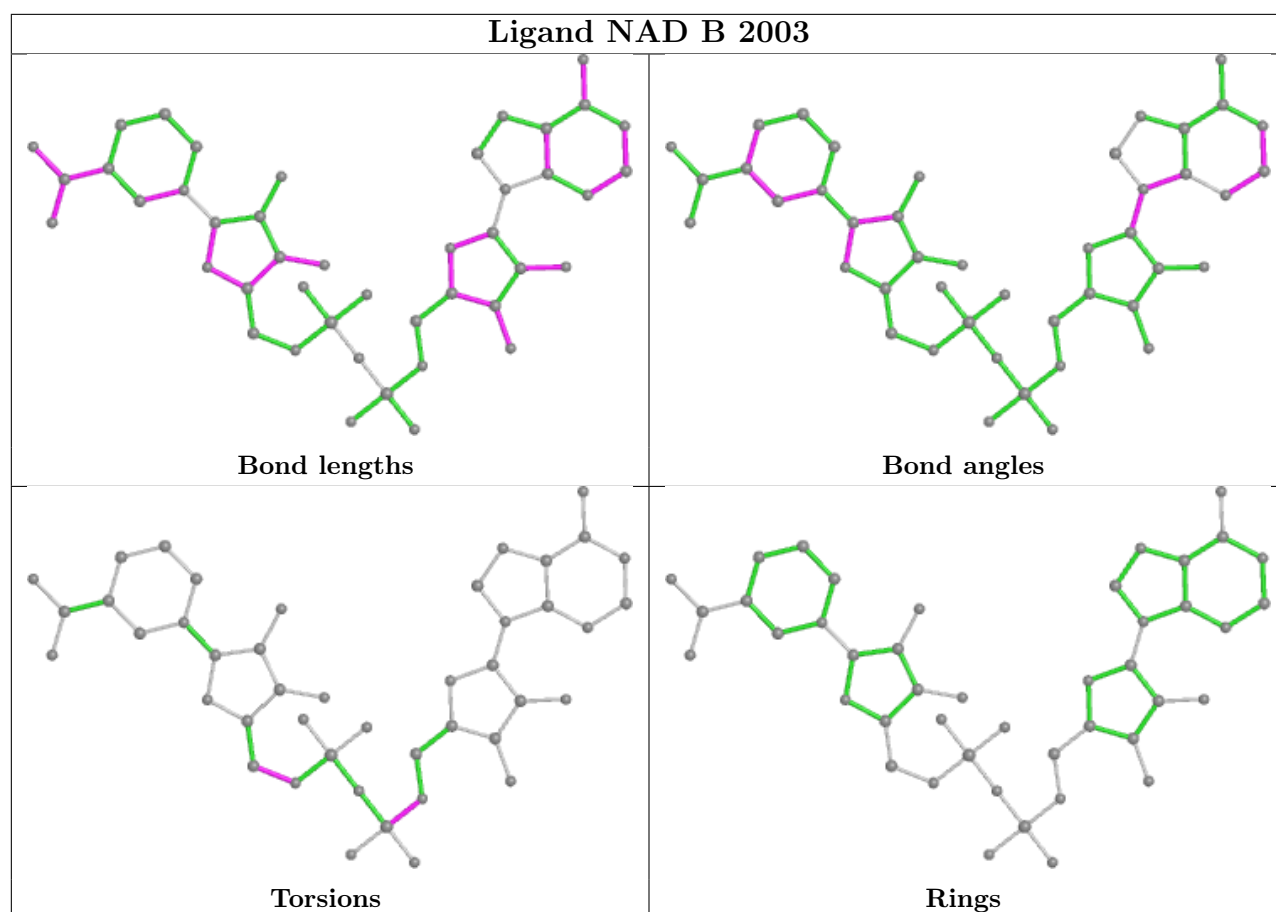
4 monomers are involved in 11 short contacts:

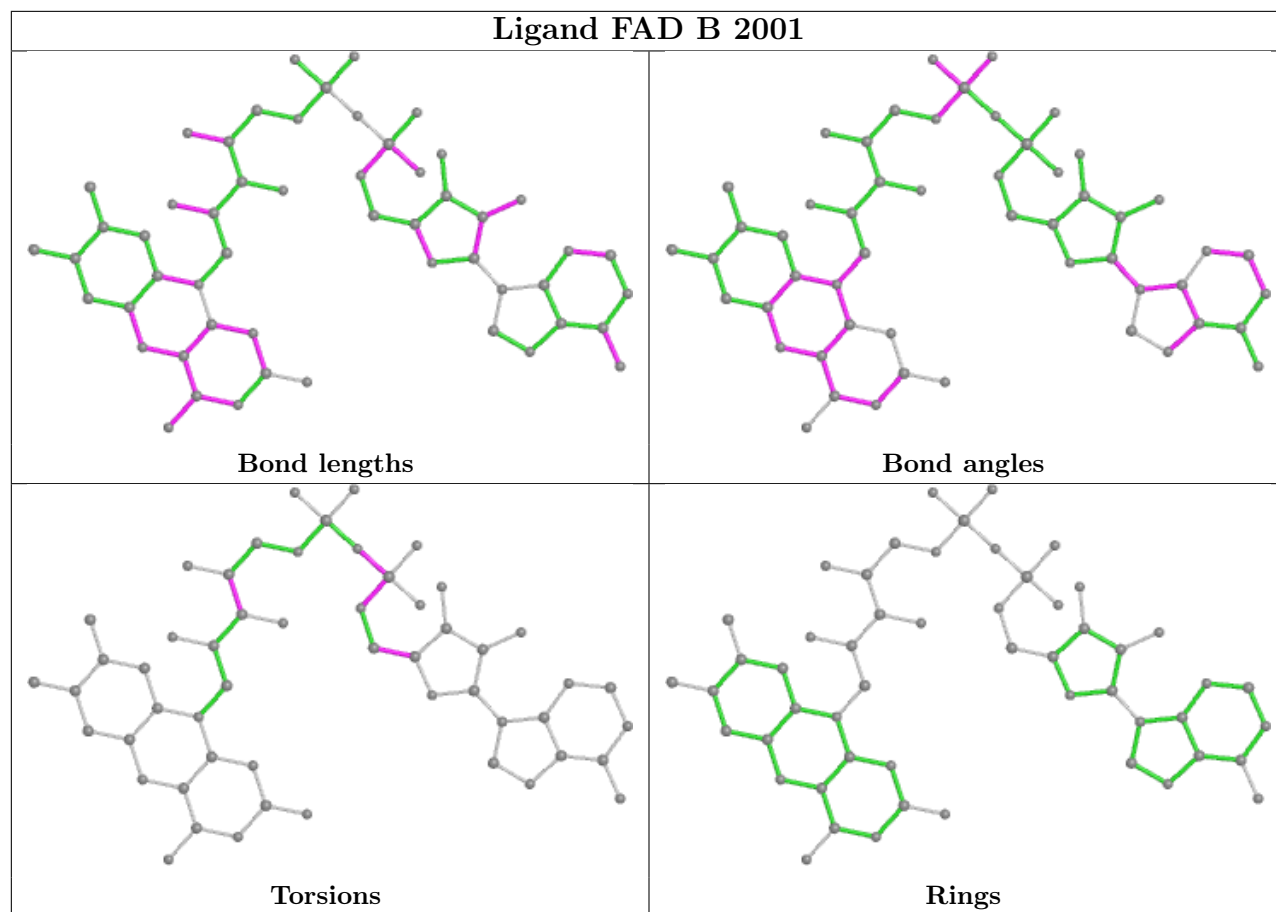
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2003	NAD	2	0
2	A	2001	FAD	3	0
4	B	2003	NAD	2	0
2	B	2001	FAD	4	0

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	1214/1235 (98%)	0.15	32 (2%) 56 58	13, 21, 37, 66	0
1	B	1214/1235 (98%)	0.22	44 (3%) 42 46	12, 20, 40, 60	0
All	All	2428/2470 (98%)	0.18	76 (3%) 49 52	12, 20, 39, 66	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1231	ALA	7.9
1	A	82	SER	5.5
1	A	132	SER	5.4
1	B	14	ALA	4.5
1	A	127	ASP	4.4
1	B	503	ILE	4.2
1	A	506	PRO	4.2
1	B	508	VAL	4.1
1	A	14	ALA	4.0
1	B	436	GLY	4.0
1	A	134	LEU	3.9
1	B	506	PRO	3.6
1	B	1227	ALA	3.5
1	B	1232	ILE	3.5
1	B	60	ILE	3.5
1	A	130	TRP	3.3
1	B	1233	GLY	3.3
1	A	125	ILE	3.2
1	B	1229	LEU	3.1
1	B	918	THR	3.0
1	B	515	ALA	3.0
1	A	123	ASP	2.9
1	B	1230	MET	2.9
1	A	129	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	116	THR	2.8
1	A	120	LEU	2.8
1	B	912	ILE	2.8
1	B	75	LEU	2.8
1	A	128	GLY	2.8
1	A	523	ALA	2.7
1	A	115	ALA	2.7
1	B	15	PRO	2.6
1	A	133	HIS	2.6
1	A	583	GLY	2.6
1	B	115	ALA	2.6
1	A	526	VAL	2.6
1	B	510	ILE	2.6
1	B	129	ASN	2.6
1	B	132	SER	2.6
1	B	917	GLU	2.6
1	A	508	VAL	2.6
1	B	511	ASP	2.5
1	A	83	GLY	2.5
1	B	114	THR	2.5
1	B	63	ALA	2.5
1	A	1231	ALA	2.4
1	B	91	TYR	2.4
1	B	1061	GLY	2.4
1	A	1232	ILE	2.4
1	B	134	LEU	2.3
1	A	121	ILE	2.3
1	A	582	THR	2.3
1	B	64	ALA	2.3
1	B	915	ALA	2.3
1	B	505	ASP	2.3
1	B	507	LYS	2.3
1	B	84	VAL	2.3
1	A	623	ALA	2.2
1	A	114	THR	2.2
1	B	521	VAL	2.2
1	A	504	ASN	2.2
1	B	133	HIS	2.2
1	B	1200	ARG	2.2
1	A	27	PRO	2.2
1	A	111	ILE	2.1
1	B	432	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	904	GLY	2.1
1	B	59	GLU	2.1
1	B	119	ALA	2.1
1	B	1064	ALA	2.1
1	B	82	SER	2.1
1	A	112	PRO	2.0
1	B	493	ASN	2.0
1	B	138	ARG	2.0
1	A	119	ALA	2.0
1	A	801	ALA	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.

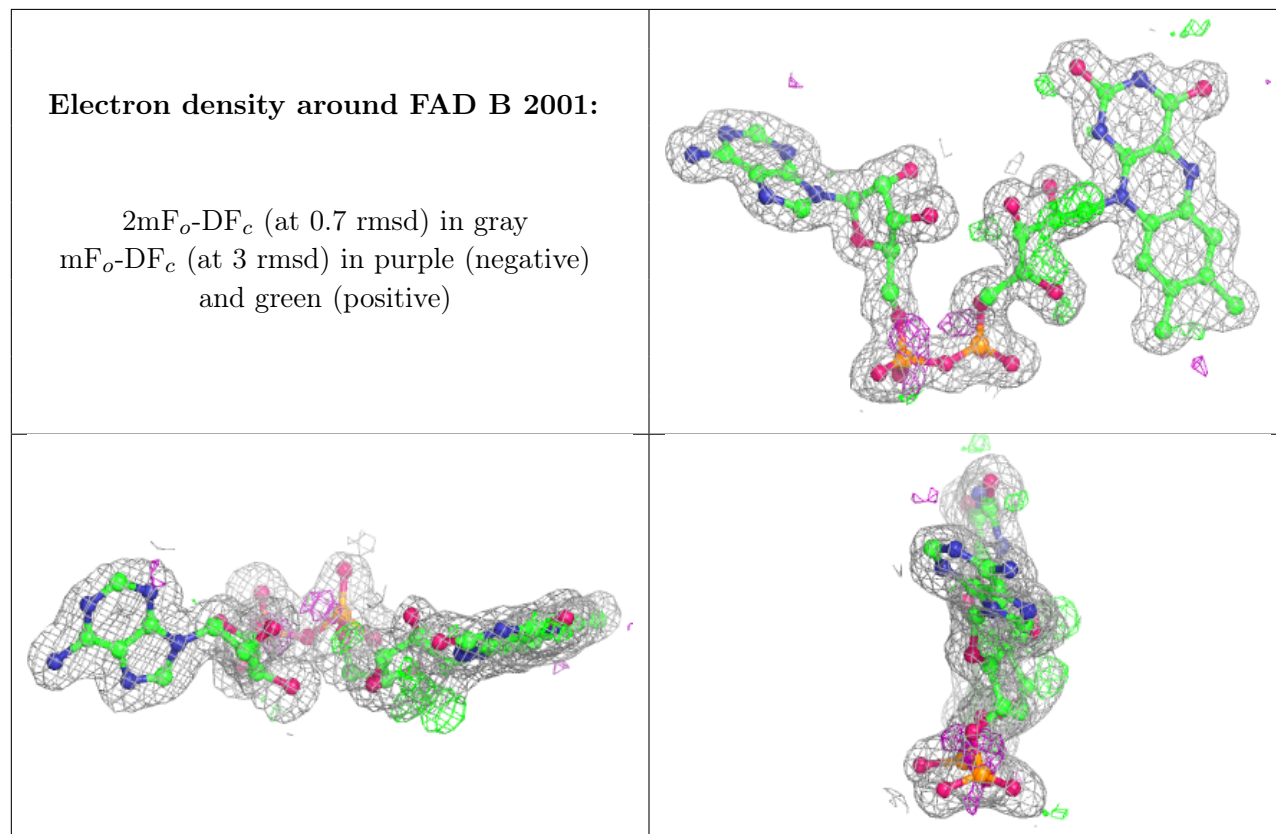
## 6.4 Ligands [i](#)

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	PEG	A	2002	7/7	0.83	0.13	27,32,43,45	0
2	FAD	B	2001	53/53	0.92	0.10	13,19,37,41	0
8	PGE	B	2002	10/10	0.93	0.10	39,45,49,50	0
6	MG	A	2005	1/1	0.93	0.15	30,30,30,30	0
4	NAD	A	2003	44/44	0.94	0.10	16,21,25,31	0
7	UYA	B	2005	9/9	0.94	0.10	16,18,22,24	0
2	FAD	A	2001	53/53	0.95	0.09	15,19,26,29	0
7	UYA	A	2006	9/9	0.96	0.08	15,17,23,23	0
4	NAD	B	2003	44/44	0.96	0.10	11,15,20,29	0
5	SO4	B	2004	5/5	0.99	0.07	15,15,19,19	0
5	SO4	A	2004	5/5	0.99	0.06	17,17,20,21	0

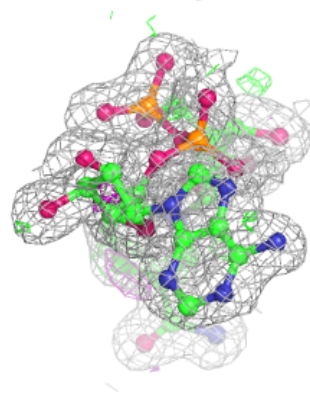
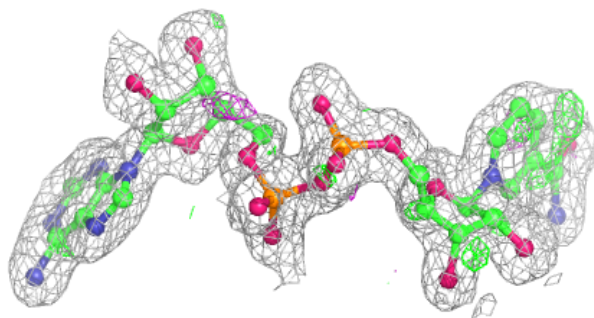
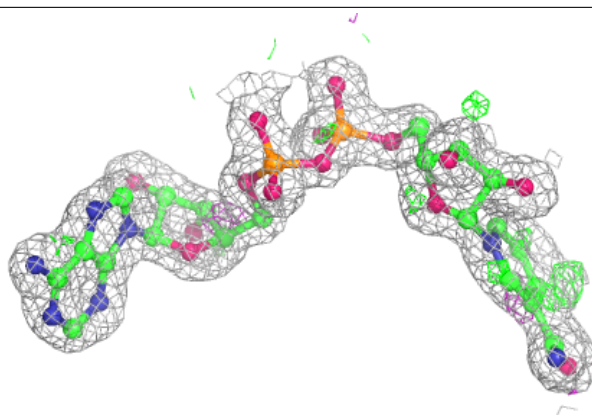
The following is a graphical depiction of the model fit to experimental electron density of all

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.



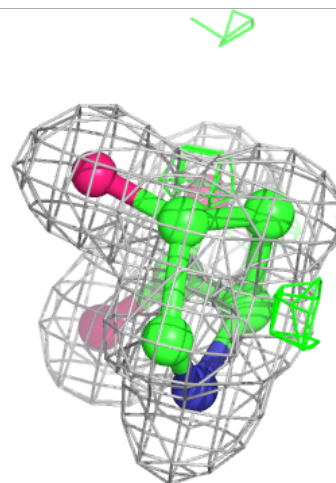
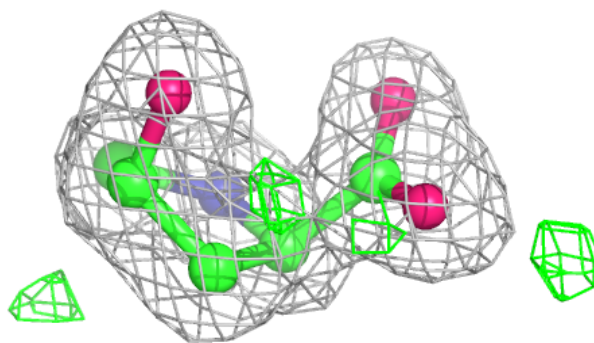
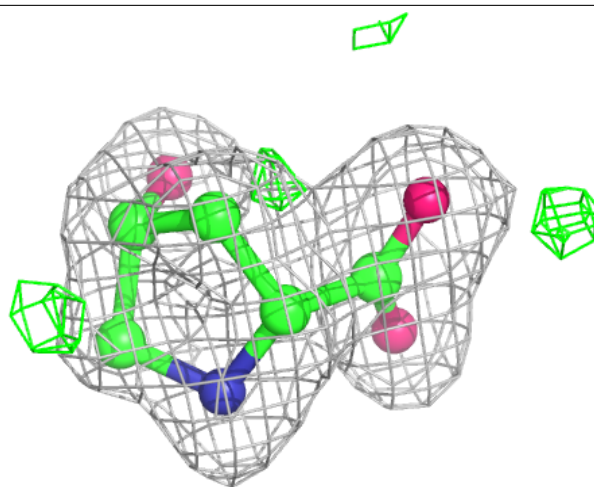
**Electron density around NAD A 2003:**

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



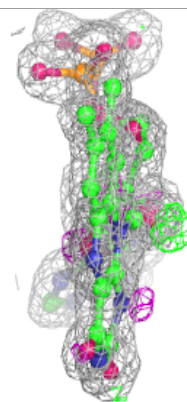
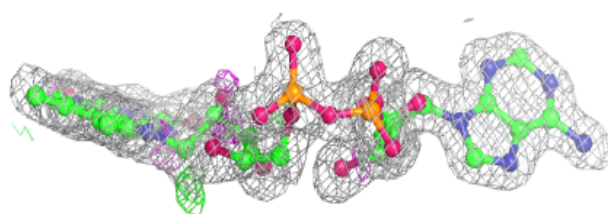
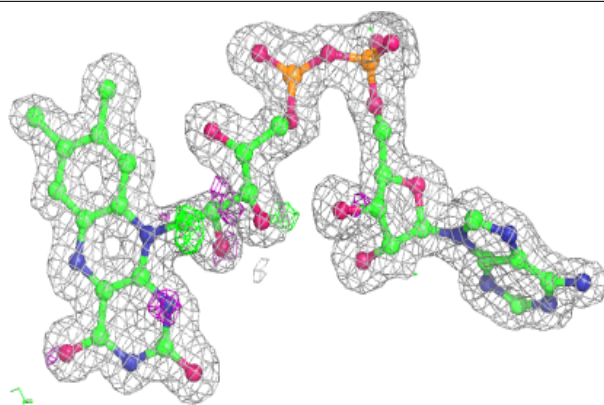
**Electron density around UYA B 2005:**

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



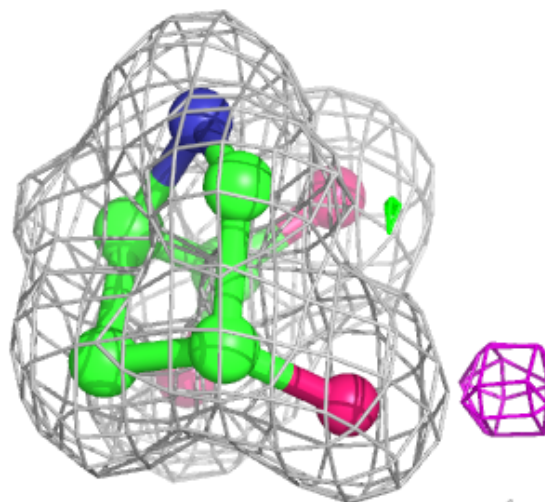
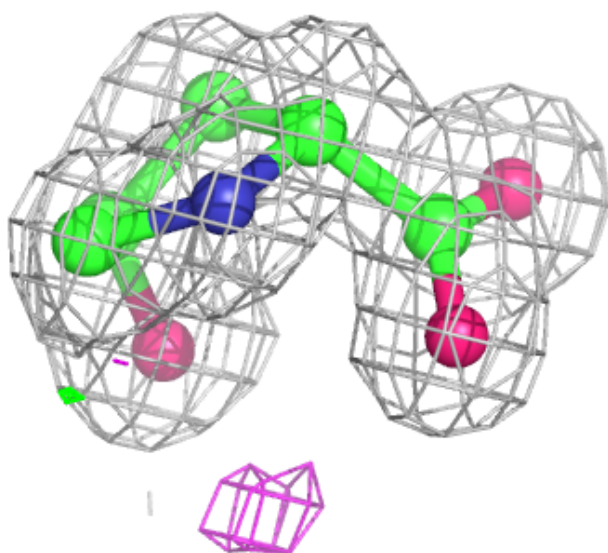
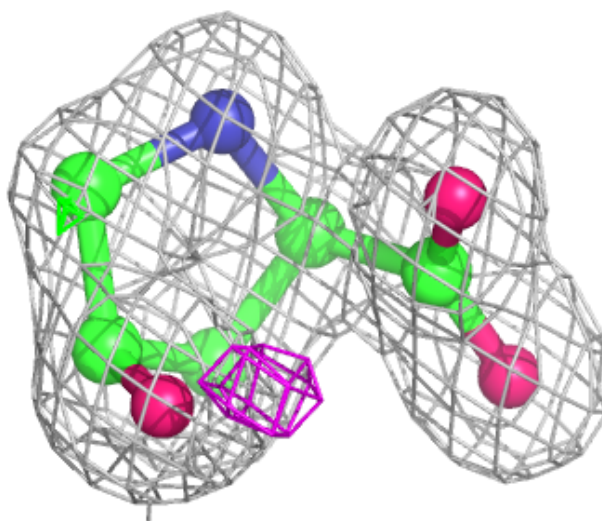
**Electron density around FAD A 2001:**

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



**Electron density around UYA A 2006:**

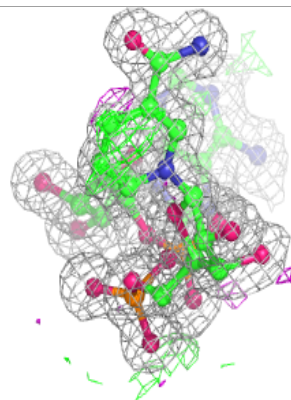
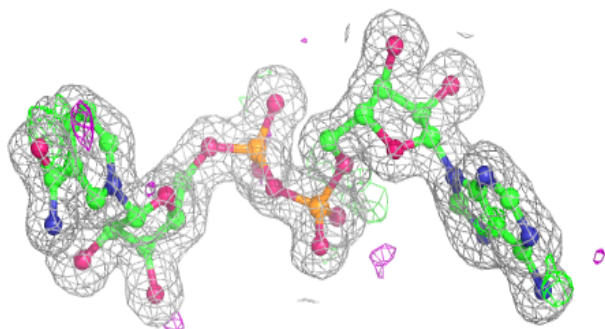
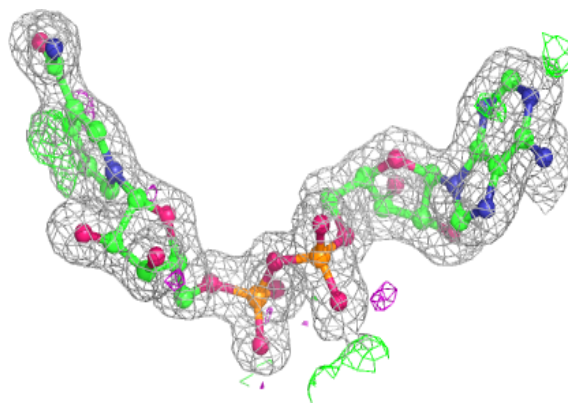
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around NAD B 2003:**

$2mF_o - DF_c$  (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.