



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:46 AM UTC

PDB ID : 5KF6 / pdb_00005kf6
Title : Structure of proline utilization A from Sinorhizobium meliloti complexed with L-tetrahydrofuroic acid and NAD⁺ in space group P21
Authors : Tanner, J.J.
Deposited on : 2016-06-12
Resolution : 1.70 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

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	:	2022.3.0, CSD as543be (2022)
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

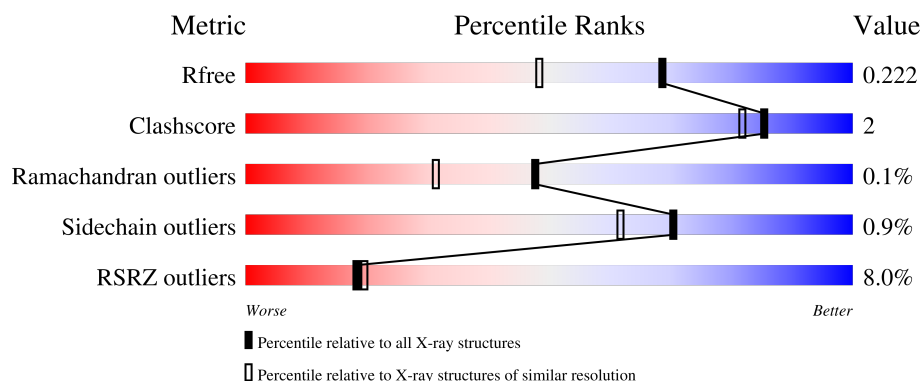
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 ≥ 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	6% 93% 5%
1	B	1235	10% 91% 6%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19406 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	1207	Total	C	N	O	S	0	3	0
			8948	5632	1605	1677	34			
1	B	1200	Total	C	N	O	S	0	8	0
			8879	5595	1582	1670	32			

There are 4 discrepancies between the modelled and reference sequences:

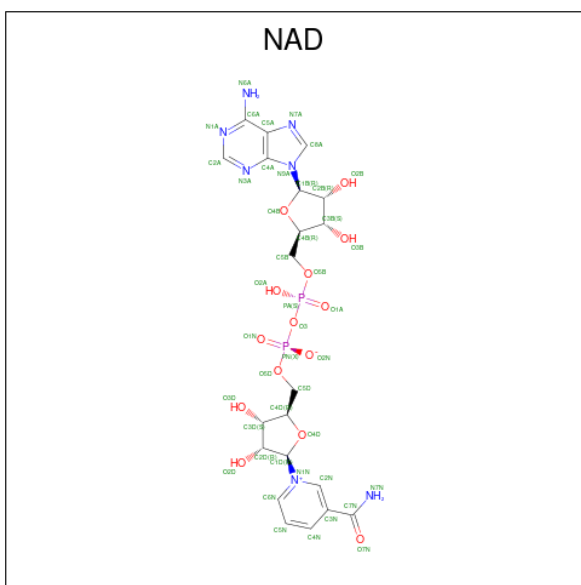
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



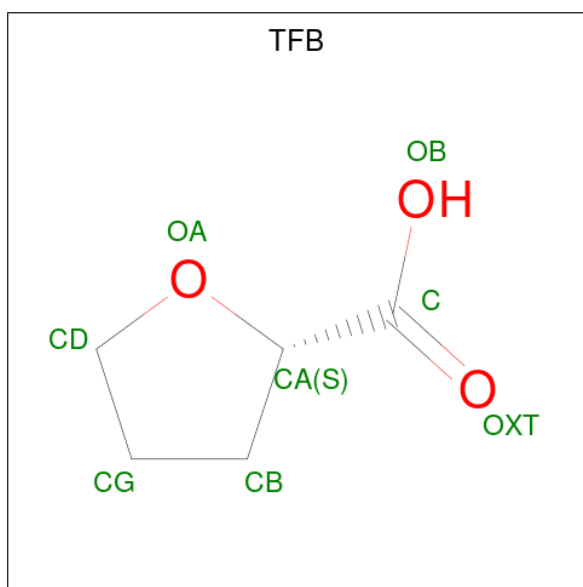
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

- Molecule 4 is TETRAHYDROFURAN-2-CARBOXYLIC ACID (CCD ID: TFB) (formula: $C_5H_8O_3$).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

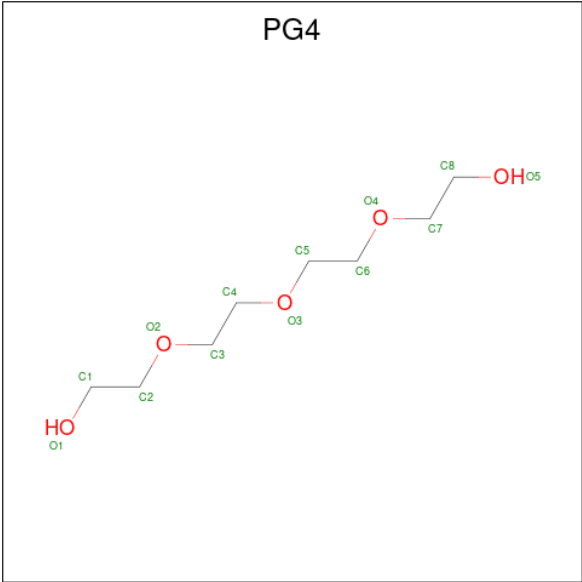
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		

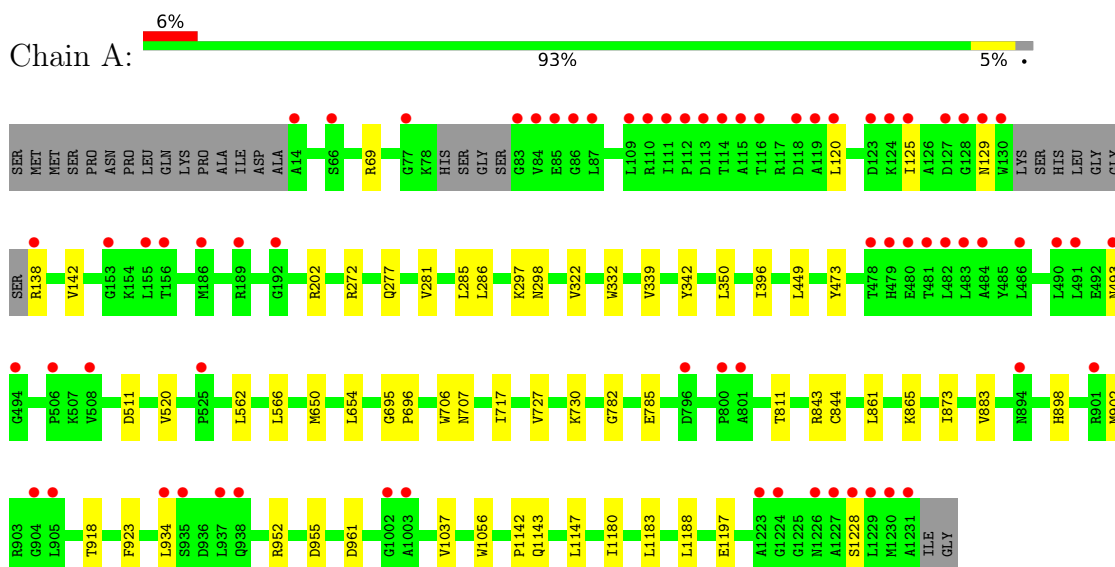
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	626	Total	O	0	0
			626	626		
8	B	660	Total	O	0	0
			660	660		

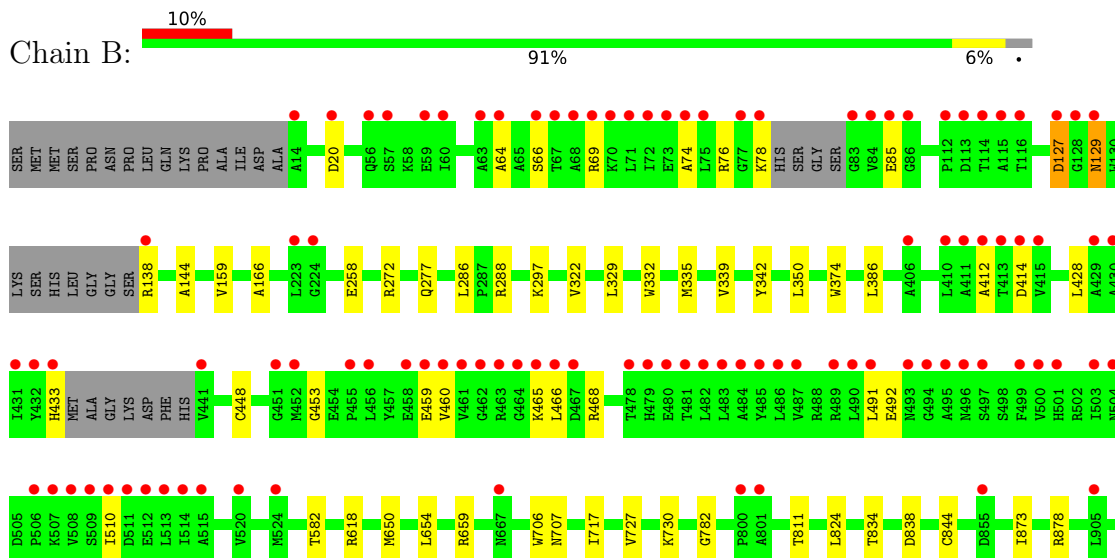
3 Residue-property plots [i](#)

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, α , β , γ	101.40Å 102.33Å 125.91Å 90.00° 106.53° 90.00°	Depositor
Resolution (Å)	51.38 – 1.70 51.38 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.8 (51.38-1.70) 97.8 (51.38-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.190 , 0.222 0.191 , 0.222	Depositor DCC
R_{free} test set	13392 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19406	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, TFB, PG4, PGE, NAD, MG

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	0.30	0/9113	0.49	0/12399
1	B	0.29	0/9061	0.50	0/12337
All	All	0.29	0/18174	0.50	0/24736

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8948	0	8978	33	0
1	B	8879	0	8907	46	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	44	0	26	1	0
3	B	44	0	26	2	0
4	A	8	0	7	0	0
4	B	8	0	7	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	24	0	32	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	44	0	60	2	0
7	B	13	0	18	0	0
8	A	626	0	0	3	0
8	B	660	0	0	5	0
All	All	19406	0	18123	78	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 (78) 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:582:THR:HA	6:B:2005:PGE:H5	1.76	0.67
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.76	0.67
1:A:138:ARG:HE	1:A:142:VAL:HG21	1.61	0.66
1:B:844:CYS:SG	3:B:2002:NAD:C4N	2.83	0.66
1:B:20:ASP:OD2	1:B:878:ARG:NH1	2.29	0.65
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.30	0.62
1:A:861:LEU:HD22	1:A:865:LYS:HE3	1.81	0.62
1:B:332:TRP:HZ3	1:B:335:MET:HE2	1.64	0.62
1:A:844:CYS:SG	3:A:2002:NAD:C4N	2.87	0.62
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.82	0.61
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.81	0.60
1:B:288[B]:ARG:NE	8:B:2104:HOH:O	2.35	0.59
1:B:339:VAL:HG21	1:B:350:LEU:HD21	1.85	0.59
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.85	0.58
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.85	0.57
1:B:332:TRP:CZ3	1:B:335:MET:HE2	2.39	0.57
1:B:650:MET:O	1:B:654:LEU:HG	2.04	0.57
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.86	0.56
1:A:298:ASN:ND2	8:A:2104:HOH:O	2.35	0.55
1:A:69:ARG:NH2	1:A:511:ASP:OD1	2.40	0.54
1:A:449:LEU:HD23	1:A:473:TYR:HB3	1.90	0.53
1:B:459:GLU:OE1	1:B:465:LYS:NZ	2.42	0.53
1:A:785:GLU:CD	1:A:785:GLU:H	2.17	0.52
1:B:1143:GLN:O	1:B:1147:LEU:HG	2.11	0.51
1:A:281:VAL:HG13	1:A:285:LEU:HD23	1.93	0.51
1:B:69:ARG:HG3	1:B:510:ILE:HG21	1.92	0.50
1:B:127:ASP:N	1:B:127:ASP:OD1	2.45	0.49
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	1.94	0.49
1:B:448:CYS:HB2	1:B:453:GLY:HA3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:MET:O	1:A:654:LEU:HG	2.14	0.48
1:A:952:ARG:NH2	1:A:955:ASP:OD2	2.47	0.48
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.49	0.48
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.49	0.47
1:B:144:ALA:HB3	1:B:159:VAL:HG11	1.97	0.47
1:B:374:TRP:HZ3	1:B:1229:LEU:HB3	1.80	0.47
1:A:843:ARG:HH12	6:A:2006:PGE:H12	1.80	0.46
1:A:202:ARG:NH2	8:A:2113:HOH:O	2.47	0.46
1:A:782:GLY:O	1:A:811:THR:HA	2.16	0.46
1:B:466:LEU:O	1:B:468:ARG:NH1	2.49	0.46
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.51	0.46
1:B:844:CYS:SG	3:B:2002:NAD:C3N	3.04	0.46
1:A:1183:LEU:O	8:A:2101:HOH:O	2.20	0.45
1:B:918:THR:HB	1:B:923:PHE:CD1	2.52	0.44
1:A:1147:LEU:HD22	1:B:1147:LEU:HD22	2.00	0.44
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.99	0.44
1:A:120:LEU:O	1:A:125:ILE:HG12	2.17	0.44
1:B:428:LEU:HD11	1:B:460:VAL:HG21	2.00	0.43
1:A:918:THR:HB	1:A:923:PHE:CD1	2.54	0.43
1:B:824:LEU:HB2	1:B:977:ARG:HH21	1.83	0.43
1:A:396:ILE:HD11	1:A:520:VAL:HB	2.01	0.43
6:B:2008:PGE:H52	6:B:2008:PGE:H32	1.60	0.42
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	2.00	0.42
1:A:717:ILE:HG12	1:A:727:VAL:HG11	2.02	0.42
1:A:1037:VAL:HG11	1:B:166:ALA:HB1	2.01	0.42
1:B:74:ALA:O	1:B:78:LYS:HE3	2.19	0.42
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.55	0.42
1:B:873:ILE:HD11	1:B:912:ILE:HD11	2.01	0.42
1:B:127:ASP:C	1:B:129:ASN:H	2.27	0.42
1:B:491:LEU:HD12	1:B:1230:MET:SD	2.60	0.41
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.03	0.41
1:B:834:THR:O	1:B:838:ASP:HB3	2.20	0.41
2:B:2001:FAD:H1'1	2:B:2001:FAD:H9	1.82	0.41
1:B:659:ARG:HD3	8:B:2387:HOH:O	2.19	0.41
1:A:898:HIS:CE1	1:A:902:MET:HE3	2.55	0.41
1:B:272:ARG:HB3	1:B:277:GLN:HG3	2.02	0.41
1:B:460:VAL:HG22	1:B:466:LEU:HD12	2.02	0.41
1:B:618:ARG:NH1	8:B:2106:HOH:O	2.40	0.41
1:B:782:GLY:O	1:B:811:THR:HA	2.21	0.41
1:B:1070:ARG:HD3	8:B:2384:HOH:O	2.20	0.41
1:B:1050:LEU:C	1:B:1050:LEU:HD13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LEU:O	1:A:566:LEU:HG	2.21	0.41
1:A:1143:GLN:O	1:A:1147:LEU:HG	2.21	0.41
1:B:912:ILE:HD11	1:B:926:PRO:HD2	2.03	0.41
1:B:386:LEU:HD23	1:B:386:LEU:HA	1.92	0.40
1:A:695:GLY:HA2	1:A:696:PRO:HD3	1.95	0.40
1:B:412:ALA:C	1:B:414:ASP:H	2.29	0.40
1:A:297:LYS:HA	1:A:332:TRP:CD1	2.56	0.40
1:B:1020:PRO:HA	8:B:2164:HOH:O	2.21	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	1204/1235 (98%)	1178 (98%)	25 (2%)	1 (0%)	48	31
1	B	1202/1235 (97%)	1172 (98%)	29 (2%)	1 (0%)	48	31
All	All	2406/2470 (97%)	2350 (98%)	54 (2%)	2 (0%)	48	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	B	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	897/951 (94%)	891 (99%)	6 (1%)	76	69
1	B	892/951 (94%)	882 (99%)	10 (1%)	65	54
All	All	1789/1902 (94%)	1773 (99%)	16 (1%)	70	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	TYR
1	A	493	ASN
1	A	730	LYS
1	A	934	LEU
1	A	1197	GLU
1	A	1228	SER
1	B	66	SER
1	B	76	ARG
1	B	85	GLU
1	B	127	ASP
1	B	138	ARG
1	B	258	GLU
1	B	342	TYR
1	B	492	GLU
1	B	730	LYS
1	B	934	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	340	GLN
1	A	496	ASN
1	A	685	GLN
1	B	304	ASN
1	B	419	GLN
1	B	685	GLN
1	B	911	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
6	PGE	A	2005	-	9,9,9	0.62	0	8,8,8	0.76	0
6	PGE	A	2006	-	6,6,9	0.59	0	5,5,8	0.87	0
6	PGE	B	2008	-	9,9,9	0.69	0	8,8,8	0.84	0
2	FAD	B	2001	-	58,58,58	2.10	13 (22%)	85,89,89	1.78	21 (24%)
6	PGE	B	2006	-	6,6,9	0.55	0	5,5,8	0.69	0
6	PGE	B	2005	-	9,9,9	0.70	0	8,8,8	0.75	0
6	PGE	B	2009	-	6,6,9	0.52	0	5,5,8	0.63	0
7	PG4	B	2010	-	12,12,12	0.56	0	11,11,11	0.87	0
3	NAD	A	2002	5	46,48,48	2.07	9 (19%)	64,73,73	1.80	12 (18%)
3	NAD	B	2002	5	46,48,48	2.17	9 (19%)	64,73,73	1.87	9 (14%)
4	TFB	B	2003	-	8,8,8	1.62	2 (25%)	7,10,10	1.53	2 (28%)
2	FAD	A	2001	-	58,58,58	2.01	11 (18%)	85,89,89	1.66	16 (18%)
4	TFB	A	2003	-	8,8,8	1.56	2 (25%)	7,10,10	1.52	1 (14%)
6	PGE	B	2007	-	9,9,9	0.68	0	8,8,8	0.69	0
6	PGE	A	2007	-	6,6,9	0.55	0	5,5,8	0.92	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
6	PGE	A	2005	-	-	0/7/7/7	-
6	PGE	A	2006	-	-	1/4/4/7	-
6	PGE	B	2008	-	-	4/7/7/7	-
2	FAD	B	2001	-	-	4/34/50/50	0/6/6/6
6	PGE	B	2006	-	-	0/4/4/7	-
6	PGE	B	2005	-	-	4/7/7/7	-
6	PGE	B	2009	-	-	1/4/4/7	-
7	PG4	B	2010	-	-	2/10/10/10	-
3	NAD	A	2002	5	-	3/30/62/62	0/5/5/5
3	NAD	B	2002	5	-	3/30/62/62	0/5/5/5
4	TFB	B	2003	-	-	3/4/11/11	0/1/1/1
2	FAD	A	2001	-	-	3/34/50/50	0/6/6/6
4	TFB	A	2003	-	-	0/4/11/11	0/1/1/1
6	PGE	B	2007	-	-	1/7/7/7	-
6	PGE	A	2007	-	-	1/4/4/7	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	FAD	PA-O3P	-7.71	1.51	1.59
2	A	2001	FAD	PA-O3P	-7.33	1.51	1.59
3	B	2002	NAD	C2N-N1N	7.02	1.42	1.35
3	B	2002	NAD	PA-O3	-6.92	1.52	1.59
3	A	2002	NAD	PA-O3	-6.67	1.52	1.59
3	A	2002	NAD	C2N-N1N	6.49	1.42	1.35
2	A	2001	FAD	O4-C4	6.32	1.35	1.23
2	B	2001	FAD	O4-C4	6.29	1.35	1.23
2	B	2001	FAD	O2-C2	5.79	1.35	1.24
3	B	2002	NAD	C7N-N7N	5.66	1.43	1.33
3	A	2002	NAD	C7N-N7N	5.15	1.42	1.33
2	A	2001	FAD	O2-C2	4.72	1.33	1.24
3	B	2002	NAD	C6A-N6A	3.99	1.44	1.34
2	A	2001	FAD	C4X-N5	3.98	1.39	1.30
2	A	2001	FAD	C6A-N6A	3.87	1.44	1.34
2	B	2001	FAD	C4X-N5	3.84	1.39	1.30
2	B	2001	FAD	C6A-N6A	3.79	1.43	1.34
3	A	2002	NAD	C6A-N6A	3.73	1.43	1.34
2	A	2001	FAD	P-O3P	3.25	1.63	1.59
2	B	2001	FAD	P-O3P	3.16	1.62	1.59
4	A	2003	TFB	CB-CA	-3.16	1.45	1.52
4	B	2003	TFB	CB-CA	-2.98	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FAD	C2-N1	2.75	1.42	1.36
3	A	2002	NAD	C6N-N1N	2.58	1.41	1.35
2	A	2001	FAD	O2'-C2'	-2.58	1.37	1.43
2	A	2001	FAD	PA-O5B	-2.57	1.49	1.59
2	B	2001	FAD	C2-N1	2.52	1.42	1.36
3	A	2002	NAD	PA-O5B	-2.52	1.49	1.59
3	B	2002	NAD	C6N-N1N	2.50	1.41	1.35
2	B	2001	FAD	PA-O2A	-2.44	1.44	1.55
2	B	2001	FAD	O2'-C2'	-2.42	1.38	1.43
3	B	2002	NAD	O3D-C3D	-2.31	1.37	1.43
3	B	2002	NAD	PA-O5B	-2.30	1.50	1.59
3	A	2002	NAD	PA-O2A	-2.29	1.44	1.55
2	B	2001	FAD	C4A-N9A	2.28	1.42	1.37
2	A	2001	FAD	PA-O2A	-2.27	1.44	1.55
4	B	2003	TFB	OXT-C	2.26	1.28	1.22
2	B	2001	FAD	C10-N1	2.20	1.37	1.33
4	A	2003	TFB	OXT-C	2.15	1.28	1.22
3	A	2002	NAD	O4D-C4D	-2.12	1.40	1.45
2	A	2001	FAD	O4B-C4B	-2.06	1.40	1.45
3	B	2002	NAD	PA-O2A	-2.05	1.45	1.55
3	A	2002	NAD	PN-O3	2.05	1.61	1.59
2	B	2001	FAD	O2B-C2B	-2.04	1.37	1.43
2	B	2001	FAD	O4B-C4B	-2.03	1.40	1.45
3	B	2002	NAD	C4A-N9A	2.02	1.41	1.37

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	NAD	N3A-C2A-N1A	-6.15	119.28	128.58
3	B	2002	NAD	N3A-C2A-N1A	-6.04	119.43	128.58
3	B	2002	NAD	C5A-C4A-N3A	-5.64	118.95	126.72
2	B	2001	FAD	N3A-C2A-N1A	-5.56	120.16	128.58
2	A	2001	FAD	N3A-C2A-N1A	-5.22	120.68	128.58
2	B	2001	FAD	O2P-P-O3P	-4.95	93.89	107.27
3	B	2002	NAD	N3A-C4A-N9A	4.74	135.24	127.17
3	A	2002	NAD	C5A-C4A-N3A	-4.57	120.42	126.72
3	B	2002	NAD	C5A-N7A-C8A	4.48	110.50	103.45
2	B	2001	FAD	C5A-C4A-N3A	-4.26	120.85	126.72
2	A	2001	FAD	C5A-C4A-N3A	-4.15	121.00	126.72
3	B	2002	NAD	N9A-C8A-N7A	-4.13	108.07	113.94
2	B	2001	FAD	O3P-P-O1P	4.13	123.12	110.70
3	A	2002	NAD	C5A-N7A-C8A	4.11	109.91	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	NAD	C2A-N3A-C4A	3.91	121.37	111.83
3	A	2002	NAD	N3A-C4A-N9A	3.83	133.68	127.17
2	A	2001	FAD	C5A-N7A-C8A	3.74	109.32	103.45
2	B	2001	FAD	O2-C2-N1	-3.72	115.62	121.80
3	A	2002	NAD	N9A-C8A-N7A	-3.69	108.70	113.94
2	B	2001	FAD	C5A-N7A-C8A	3.65	109.19	103.45
2	A	2001	FAD	C4-C4X-N5	3.61	123.19	118.21
2	A	2001	FAD	N9A-C8A-N7A	-3.61	108.82	113.94
3	A	2002	NAD	C2A-N3A-C4A	3.54	120.47	111.83
3	A	2002	NAD	C4D-O4D-C1D	-3.53	106.69	109.92
2	B	2001	FAD	N3A-C4A-N9A	3.46	133.04	127.17
2	A	2001	FAD	C4-N3-C2	-3.36	119.67	125.64
2	A	2001	FAD	C4X-C4-N3	3.34	121.74	113.25
2	A	2001	FAD	N3A-C4A-N9A	3.22	132.64	127.17
3	B	2002	NAD	C4A-C5A-N7A	-3.20	106.92	110.58
2	A	2001	FAD	C2A-N3A-C4A	3.10	119.40	111.83
2	B	2001	FAD	O2A-PA-O3P	-3.08	98.93	107.27
2	B	2001	FAD	C2A-N3A-C4A	3.08	119.35	111.83
2	A	2001	FAD	O2P-P-O3P	-3.03	99.09	107.27
3	A	2002	NAD	C4A-C5A-N7A	-2.96	107.20	110.58
2	B	2001	FAD	C4A-C5A-N7A	-2.95	107.21	110.58
3	B	2002	NAD	C4D-O4D-C1D	-2.95	107.23	109.92
2	A	2001	FAD	C4A-C5A-N7A	-2.92	107.24	110.58
3	B	2002	NAD	C4A-N9A-C8A	2.84	108.72	105.74
2	B	2001	FAD	C2A-N1A-C6A	2.66	123.10	118.73
4	A	2003	TFB	OB-C-CA	2.64	119.56	112.71
4	B	2003	TFB	CB-CA-C	-2.58	108.85	113.00
2	A	2001	FAD	O4-C4-C4X	-2.52	119.89	126.53
3	A	2002	NAD	C4A-N9A-C8A	2.44	108.30	105.74
2	B	2001	FAD	C4-C4X-N5	2.42	121.55	118.21
2	A	2001	FAD	C4A-N9A-C8A	2.38	108.23	105.74
3	A	2002	NAD	C3N-C7N-N7N	2.37	120.66	117.74
2	B	2001	FAD	C5X-C9A-N10	2.34	120.09	117.97
2	B	2001	FAD	C4-N3-C2	-2.32	121.53	125.64
2	B	2001	FAD	N9A-C8A-N7A	-2.31	110.65	113.94
2	B	2001	FAD	O4-C4-C4X	-2.31	120.43	126.53
2	B	2001	FAD	O2P-P-O5'	-2.31	97.09	107.57
2	B	2001	FAD	C4X-C10-N10	2.31	119.79	116.48
2	A	2001	FAD	C4X-C10-N10	2.28	119.75	116.48
2	B	2001	FAD	O2A-PA-O5B	-2.25	97.39	107.57
4	B	2003	TFB	OB-C-CA	2.18	118.39	112.71
2	B	2001	FAD	O2A-PA-O1A	2.15	122.45	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	NAD	O5B-PA-O1A	2.14	117.43	108.94
2	A	2001	FAD	O3P-P-O1P	2.12	117.08	110.70
2	B	2001	FAD	C4X-C4-N3	2.10	118.59	113.25
2	A	2001	FAD	O5B-PA-O1A	2.06	117.12	108.94
3	A	2002	NAD	C2A-N1A-C6A	2.03	122.07	118.73

There are no chirality outliers.

All (30) torsion outliers are listed below:

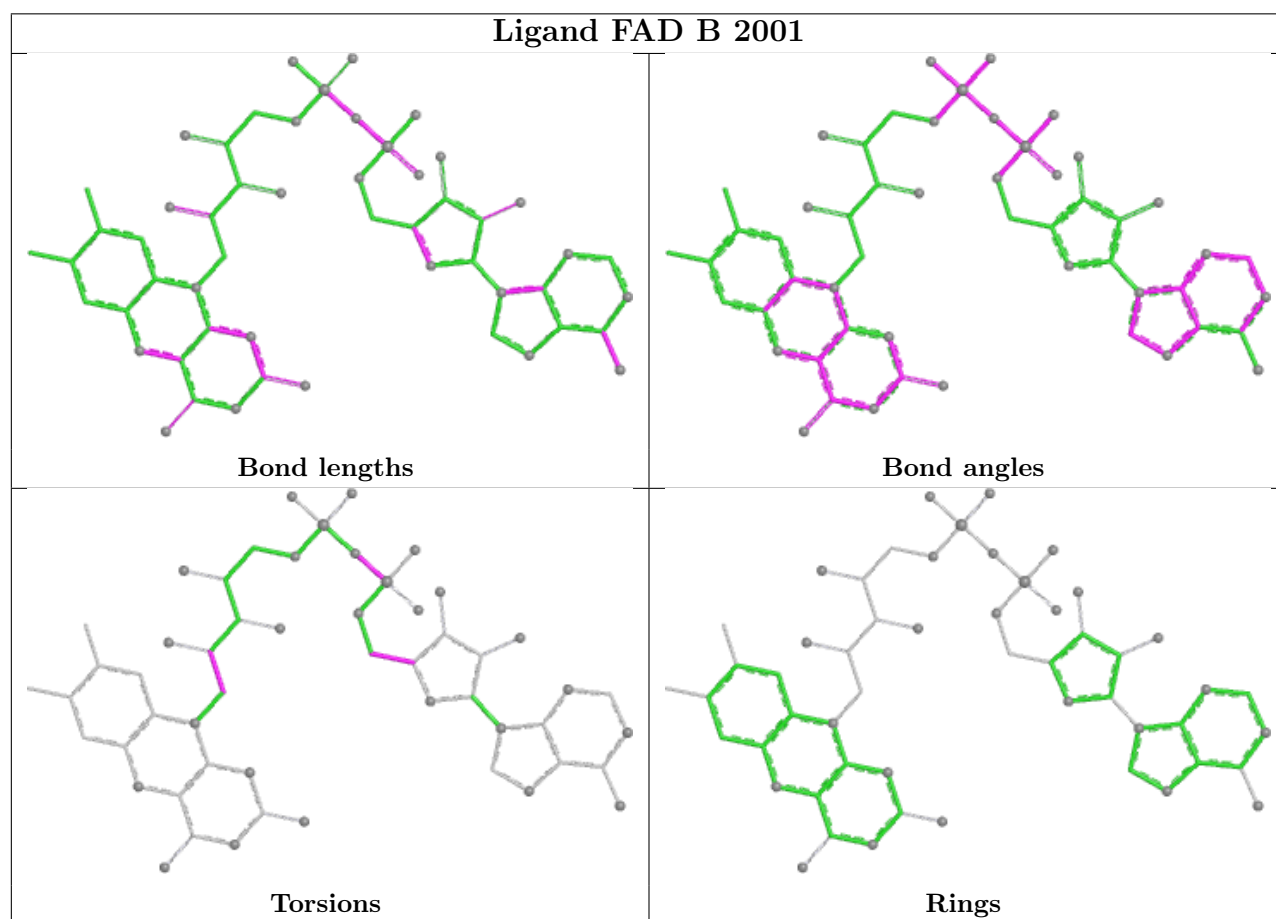
Mol	Chain	Res	Type	Atoms
2	A	2001	FAD	P-O3P-PA-O5B
2	A	2001	FAD	N10-C1'-C2'-O2'
2	A	2001	FAD	N10-C1'-C2'-C3'
2	B	2001	FAD	N10-C1'-C2'-O2'
2	B	2001	FAD	N10-C1'-C2'-C3'
6	B	2008	PGE	C3-C4-O3-C5
6	B	2005	PGE	O2-C3-C4-O3
4	B	2003	TFB	OXT-C-CA-CB
6	A	2007	PGE	C1-C2-O2-C3
7	B	2010	PG4	O4-C7-C8-O5
2	B	2001	FAD	P-O3P-PA-O5B
6	B	2005	PGE	C1-C2-O2-C3
3	A	2002	NAD	C2B-C1B-N9A-C8A
3	B	2002	NAD	C2B-C1B-N9A-C8A
4	B	2003	TFB	OB-C-CA-CB
3	A	2002	NAD	C4D-C5D-O5D-PN
3	B	2002	NAD	C4D-C5D-O5D-PN
6	B	2008	PGE	O2-C3-C4-O3
6	B	2008	PGE	C1-C2-O2-C3
6	B	2005	PGE	O3-C5-C6-O4
6	B	2007	PGE	O1-C1-C2-O2
2	B	2001	FAD	C3B-C4B-C5B-O5B
6	A	2006	PGE	C1-C2-O2-C3
7	B	2010	PG4	O3-C5-C6-O4
6	B	2009	PGE	C3-C4-O3-C5
3	A	2002	NAD	O4B-C1B-N9A-C8A
6	B	2005	PGE	C6-C5-O3-C4
3	B	2002	NAD	O4B-C1B-N9A-C8A
6	B	2008	PGE	C6-C5-O3-C4
4	B	2003	TFB	OXT-C-CA-OA

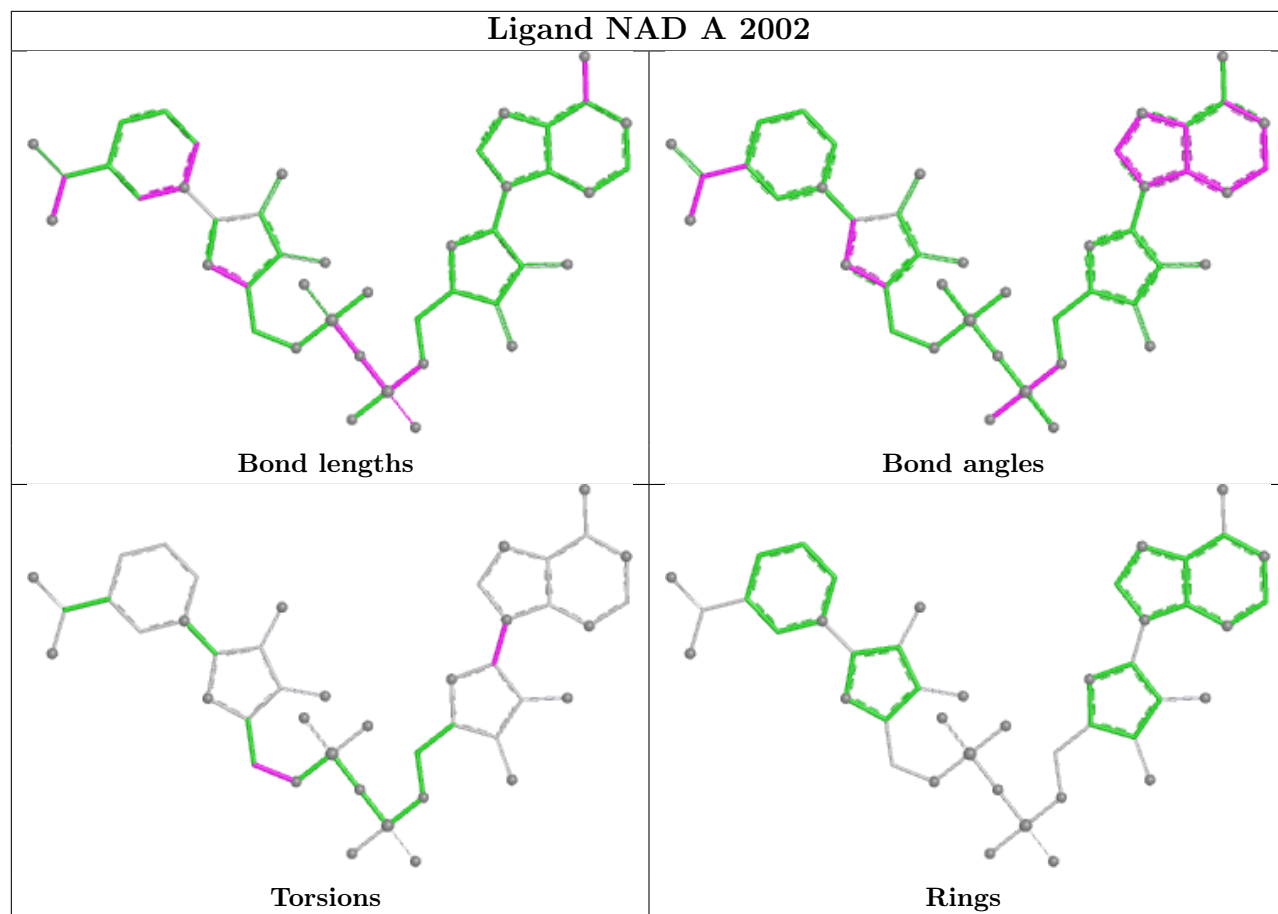
There are no ring outliers.

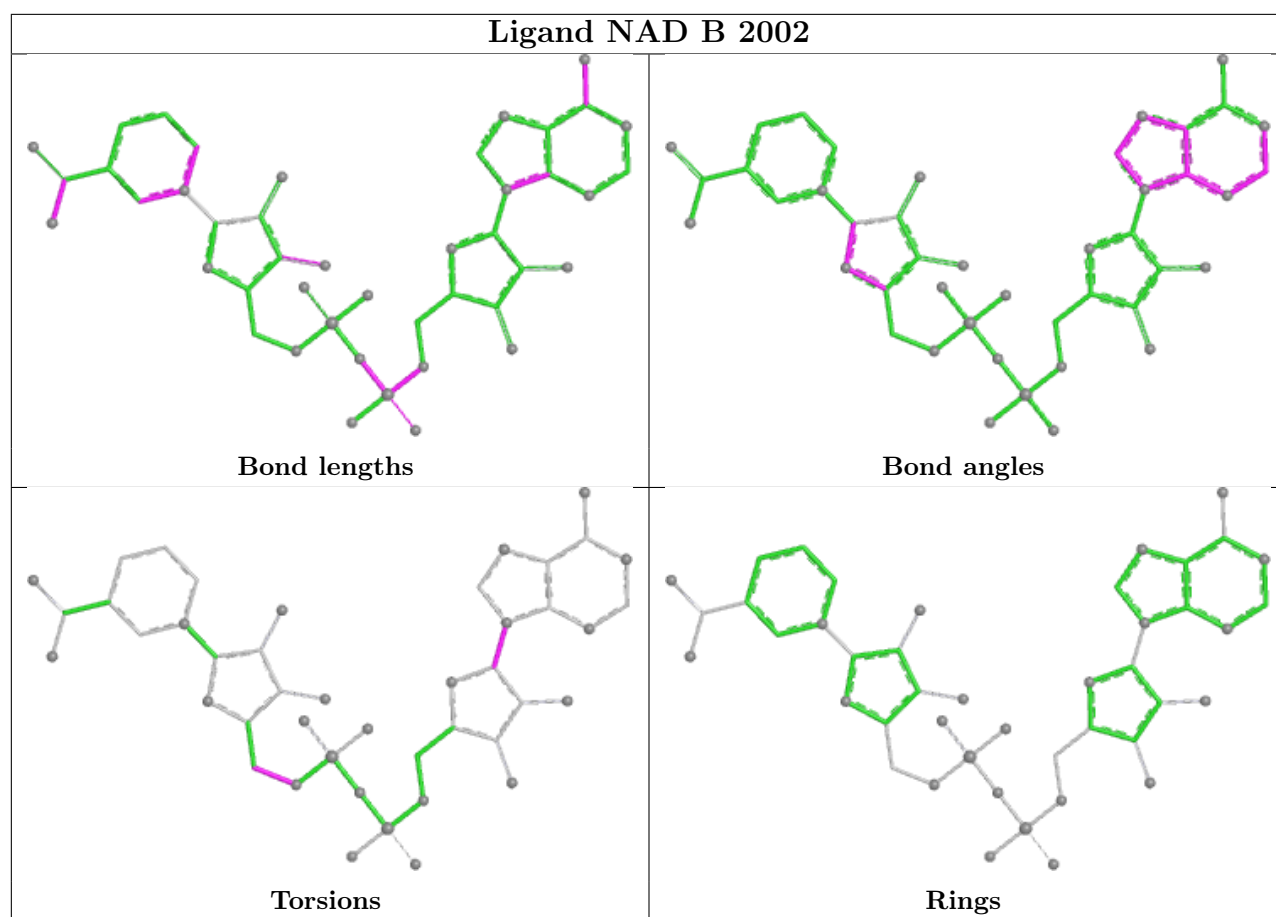
6 monomers are involved in 7 short contacts:

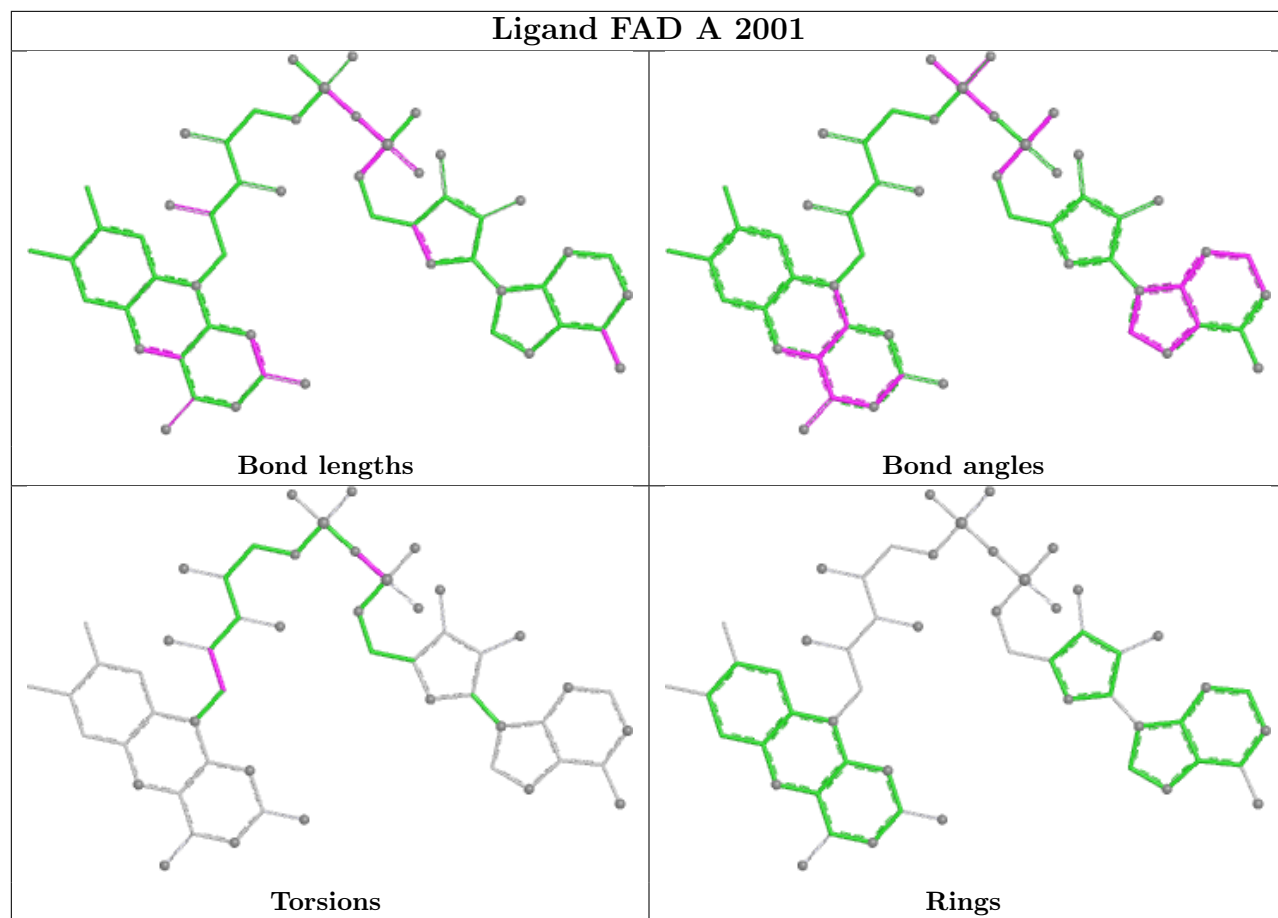
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2006	PGE	1	0
6	B	2008	PGE	1	0
2	B	2001	FAD	1	0
6	B	2005	PGE	1	0
3	A	2002	NAD	1	0
3	B	2002	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	1207/1235 (97%)	0.20	69 (5%)	29 32	8, 18, 39, 67	3 (0%)
1	B	1200/1235 (97%)	0.33	123 (10%)	12 12	6, 18, 43, 63	8 (0%)
All	All	2407/2470 (97%)	0.27	192 (7%)	18 19	6, 18, 41, 67	11 (0%)

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	485	TYR	9.7
1	B	462	GLY	6.5
1	B	1227	ALA	6.3
1	A	1230	MET	6.1
1	B	481	THR	6.1
1	B	484	ALA	6.1
1	A	1231	ALA	5.9
1	B	912	ILE	5.6
1	B	482	LEU	5.6
1	A	129	ASN	5.5
1	A	115	ALA	5.4
1	B	508	VAL	5.2
1	A	479	HIS	4.9
1	A	114	THR	4.8
1	B	500	VAL	4.8
1	A	480	GLU	4.6
1	B	483	LEU	4.6
1	A	112	PRO	4.6
1	A	130	TRP	4.5
1	B	1231	ALA	4.5
1	A	483	LEU	4.4
1	B	74	ALA	4.4
1	B	506	PRO	4.3
1	B	486	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	493	ASN	4.1
1	B	415	VAL	4.1
1	B	1230	MET	4.1
1	A	119	ALA	4.1
1	B	464	GLY	4.1
1	B	1229	LEU	4.1
1	B	67	THR	4.0
1	B	463	ARG	4.0
1	A	481	THR	4.0
1	B	66	SER	4.0
1	A	1224	GLY	4.0
1	A	14	ALA	3.9
1	B	491	LEU	3.8
1	B	414	ASP	3.8
1	A	156	THR	3.8
1	A	116	THR	3.8
1	B	429	ALA	3.7
1	A	111	ILE	3.7
1	A	491	LEU	3.7
1	B	507	LYS	3.7
1	B	510	ILE	3.7
1	A	1227	ALA	3.7
1	B	63	ALA	3.7
1	B	115	ALA	3.7
1	B	915	ALA	3.7
1	B	494	GLY	3.7
1	B	479	HIS	3.6
1	A	493	ASN	3.6
1	B	499	PHE	3.5
1	B	452	MET	3.5
1	A	192	GLY	3.5
1	B	430	ALA	3.4
1	B	72	ILE	3.4
1	B	1228	SER	3.4
1	A	506	PRO	3.4
1	B	129	ASN	3.3
1	A	127	ASP	3.3
1	A	125	ILE	3.3
1	B	71	LEU	3.3
1	A	128	GLY	3.2
1	B	14	ALA	3.2
1	B	68	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	935	SER	3.2
1	A	525	PRO	3.2
1	A	482	LEU	3.2
1	B	59	GLU	3.2
1	A	1223	ALA	3.2
1	B	1222	ALA	3.2
1	B	20	ASP	3.1
1	A	1229	LEU	3.1
1	B	75	LEU	3.1
1	B	509	SER	3.1
1	B	913	GLY	3.0
1	B	69	ARG	3.0
1	B	914	LEU	3.0
1	B	451	GLY	3.0
1	A	1226	ASN	3.0
1	B	77	GLY	3.0
1	B	1224	GLY	3.0
1	B	458	GLU	3.0
1	A	905	LEU	3.0
1	B	465	LYS	2.9
1	B	490	LEU	2.9
1	B	496	ASN	2.9
1	A	484	ALA	2.9
1	A	110	ARG	2.8
1	A	138	ARG	2.8
1	B	460	VAL	2.8
1	B	487	VAL	2.8
1	A	796	ASP	2.8
1	B	83	GLY	2.8
1	B	524	MET	2.8
1	B	128	GLY	2.8
1	B	84	VAL	2.8
1	B	441	VAL	2.8
1	B	60	ILE	2.8
1	B	113	ASP	2.8
1	B	455	PRO	2.8
1	B	461	VAL	2.8
1	B	478	THR	2.8
1	B	501	HIS	2.8
1	B	495	ALA	2.7
1	B	456	LEU	2.7
1	B	917	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	938	GLN	2.7
1	A	934	LEU	2.7
1	B	432	TYR	2.7
1	B	905	LEU	2.7
1	B	413	THR	2.7
1	A	801	ALA	2.7
1	B	800	PRO	2.7
1	B	73	GLU	2.7
1	A	84	VAL	2.7
1	B	223	LEU	2.7
1	B	467	ASP	2.7
1	B	412	ALA	2.6
1	A	490	LEU	2.6
1	B	138	ARG	2.6
1	A	109	LEU	2.6
1	B	466	LEU	2.6
1	B	1223	ALA	2.6
1	A	155	LEU	2.5
1	A	1228	SER	2.5
1	B	410	LEU	2.5
1	B	64	ALA	2.5
1	A	478	THR	2.5
1	B	1226	ASN	2.5
1	A	937	LEU	2.5
1	B	937	LEU	2.5
1	B	411	ALA	2.5
1	B	1225	GLY	2.5
1	B	56	GLN	2.5
1	B	503	ILE	2.5
1	A	118	ASP	2.4
1	A	1002	GLY	2.4
1	B	667	ASN	2.4
1	A	153	GLY	2.4
1	B	520	VAL	2.4
1	B	127	ASP	2.4
1	B	497	SER	2.4
1	B	513	LEU	2.4
1	A	85	GLU	2.4
1	B	512	GLU	2.4
1	B	489	ARG	2.4
1	B	85	GLU	2.3
1	B	511	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	855	ASP	2.3
1	B	1147	LEU	2.3
1	B	70	LYS	2.3
1	B	78	LYS	2.3
1	B	112	PRO	2.3
1	A	1003	ALA	2.3
1	B	57	SER	2.3
1	B	459	GLU	2.3
1	B	480	GLU	2.3
1	A	901	ARG	2.3
1	B	224	GLY	2.3
1	A	120	LEU	2.3
1	A	77	GLY	2.3
1	B	116	THR	2.2
1	B	515	ALA	2.2
1	A	189	ARG	2.2
1	A	486	LEU	2.2
1	A	123	ASP	2.2
1	B	919	GLY	2.2
1	A	508	VAL	2.2
1	B	1059	GLY	2.2
1	A	87	LEU	2.1
1	A	800	PRO	2.1
1	B	514	ILE	2.1
1	A	83	GLY	2.1
1	A	86	GLY	2.1
1	B	86	GLY	2.1
1	A	124	LYS	2.1
1	B	504	ASN	2.1
1	B	916	SER	2.1
1	B	431	ILE	2.1
1	A	494	GLY	2.1
1	A	904	GLY	2.1
1	B	801	ALA	2.1
1	A	894	ASN	2.1
1	B	114	THR	2.1
1	B	433	HIS	2.1
1	A	186	MET	2.0
1	A	113	ASP	2.0
1	B	1144	THR	2.0
1	B	406	ALA	2.0
1	A	66	SER	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](#)

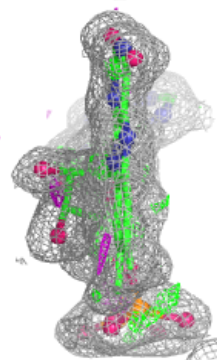
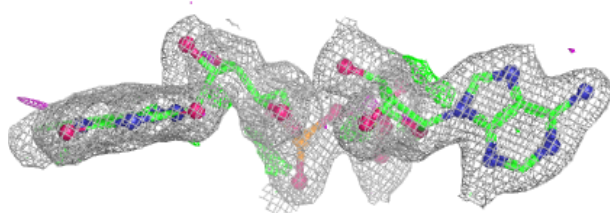
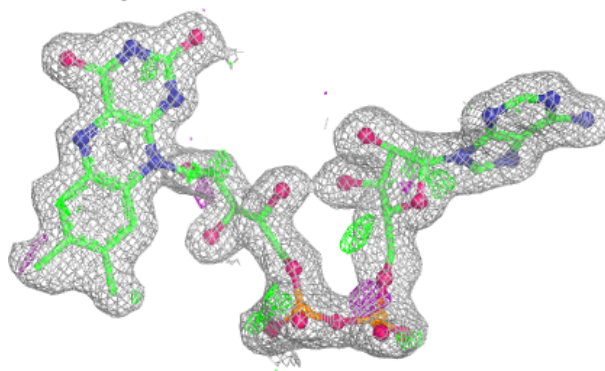
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	PG4	B	2010	13/13	0.80	0.21	33,42,52,54	0
6	PGE	B	2008	10/10	0.83	0.16	30,43,45,46	0
6	PGE	A	2006	7/10	0.84	0.15	31,44,46,49	0
6	PGE	A	2005	10/10	0.87	0.13	23,36,47,51	0
6	PGE	B	2006	7/10	0.88	0.12	23,34,41,45	0
4	TFB	B	2003	8/8	0.88	0.12	24,25,28,34	8
6	PGE	B	2005	10/10	0.88	0.13	31,41,45,50	0
6	PGE	A	2007	7/10	0.91	0.13	20,33,40,42	0
6	PGE	B	2007	10/10	0.91	0.12	24,34,41,43	0
6	PGE	B	2009	7/10	0.94	0.12	15,31,39,44	0
2	FAD	B	2001	53/53	0.94	0.09	12,19,23,25	0
3	NAD	A	2002	44/44	0.96	0.06	13,16,19,26	0
3	NAD	B	2002	44/44	0.96	0.06	9,13,17,30	0
4	TFB	A	2003	8/8	0.97	0.08	17,18,20,20	0
2	FAD	A	2001	53/53	0.97	0.06	9,13,17,19	0
5	MG	B	2004	1/1	0.97	0.07	23,23,23,23	0
5	MG	A	2004	1/1	0.98	0.07	23,23,23,23	0

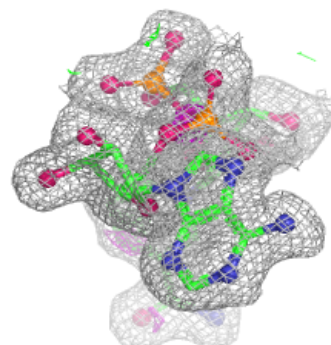
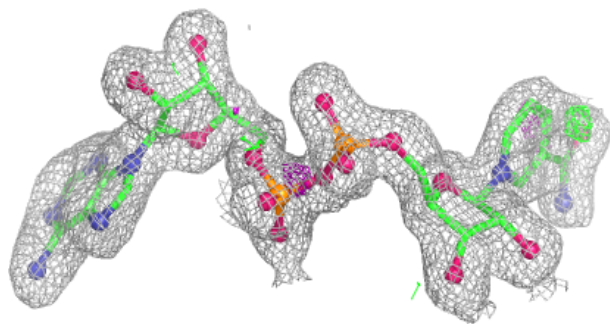
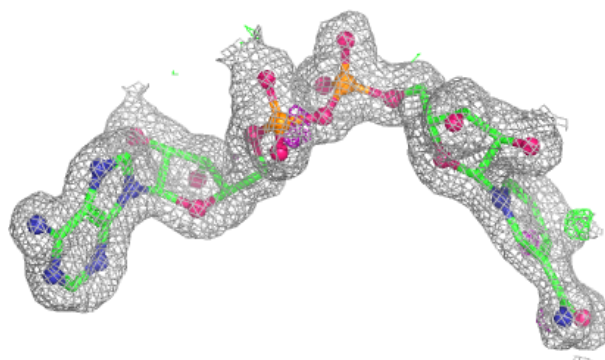
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 2001:

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

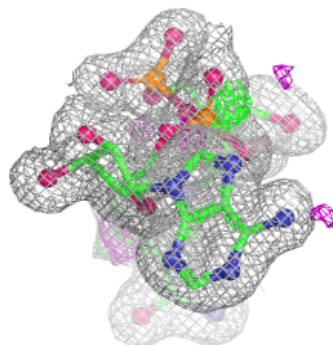
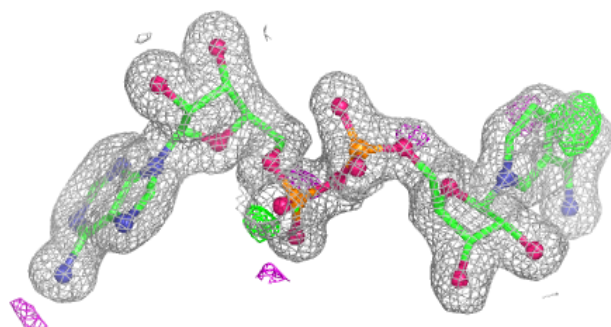
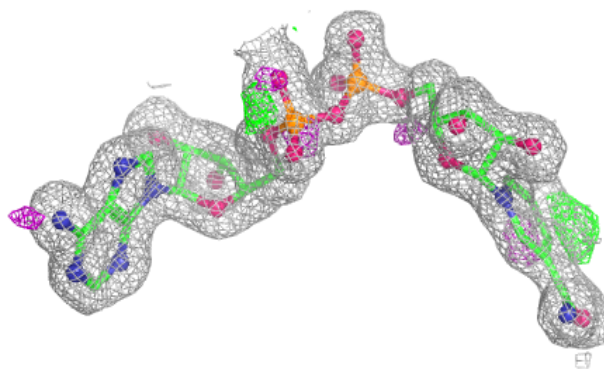
**Electron density around NAD A 2002:**

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

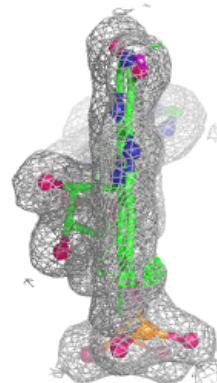
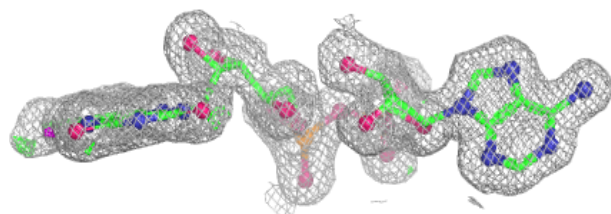
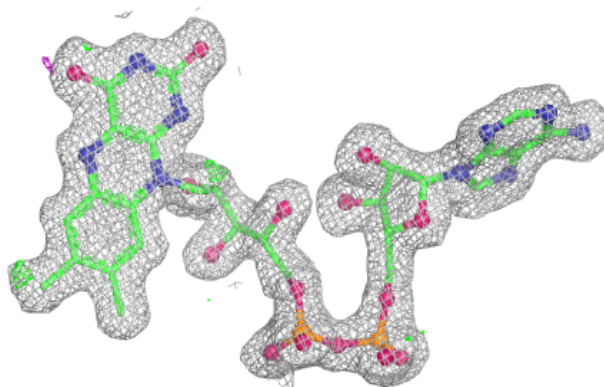


Electron density around NAD B 2002:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.