Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2024 – 04:21 PM EST

PDB ID	:	9DL9
Title	:	Structure of proline utilization A co-crystallized with 4-methoxybenzyl alcohol
Authors	:	Tanner, J.J.; Meeks, K.R.
Deposited on	:	2024-09-10
Resolution	:	1.32 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 (i) 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 (i)) were used in the production of this report:

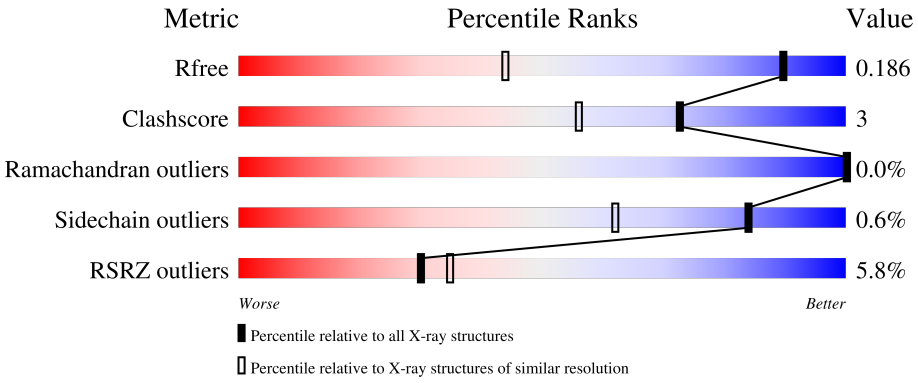
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.32 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}	164625	2202 (1.34-1.30)
Clashscore	180529	2378 (1.34-1.30)
Ramachandran outliers	177936	2325 (1.34-1.30)
Sidechain outliers	177891	2325 (1.34-1.30)
RSRZ outliers	164620	2199 (1.34-1.30)

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 <=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% 92% 6% ·
1	B	1235	6% 91% 7% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FMT	B	2007	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21273 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.

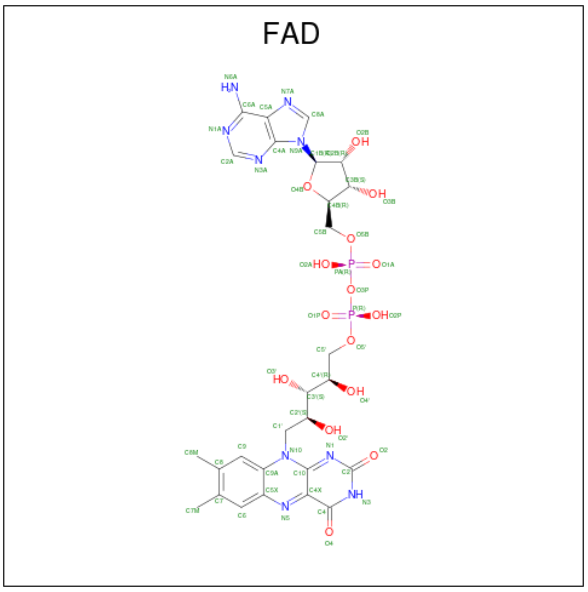
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1213	Total	C	N	O	S	0	27	0
			9097	5742	1625	1695	35			
1	B	1213	Total	C	N	O	S	0	25	0
			9080	5723	1630	1693	34			

There are 4 discrepancies between the modelled and reference sequences:

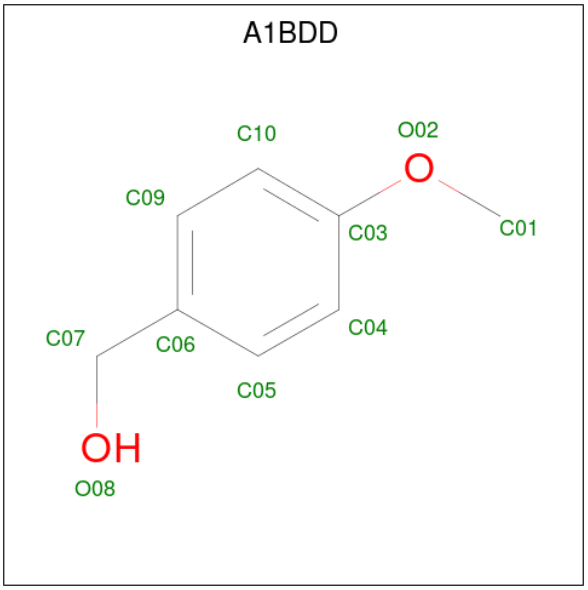
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



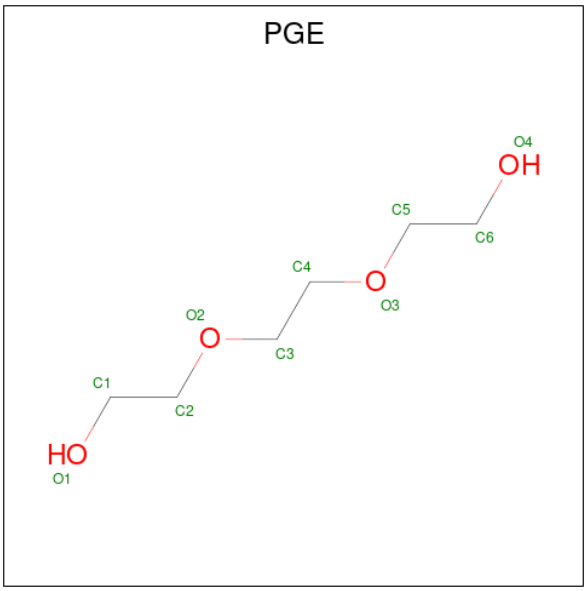
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			106	54	18	30	4		
2	B	1	Total	C	N	O	P	0	1
			106	54	18	30	4		

- Molecule 3 is (4-methoxyphenyl)methanol (three-letter code: A1BDD) (formula: $C_8H_{10}O_2$) (labeled as "Ligand of Interest" by depositor).



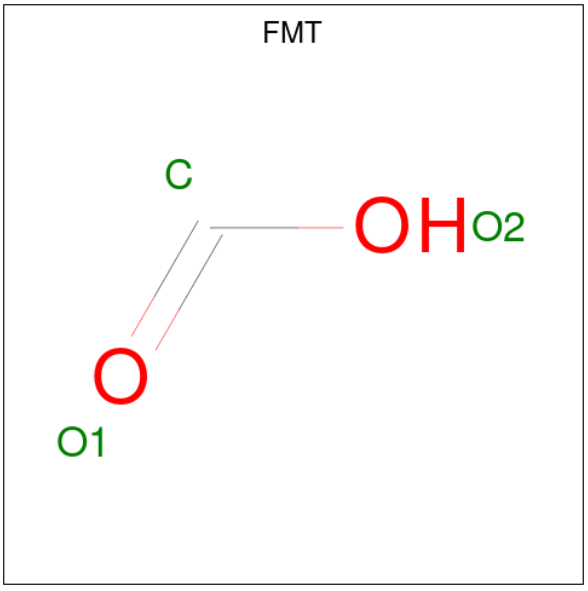
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	8	2		
3	B	1	Total	C	O	0	0
			10	8	2		
3	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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
4	B	1	Total C O 10 6 4	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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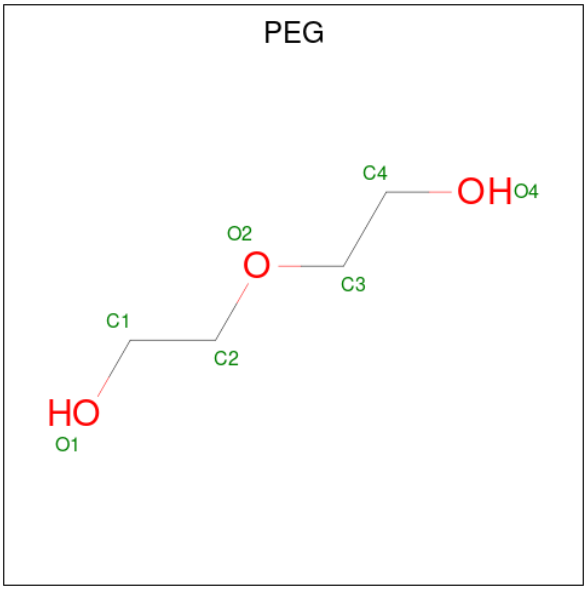
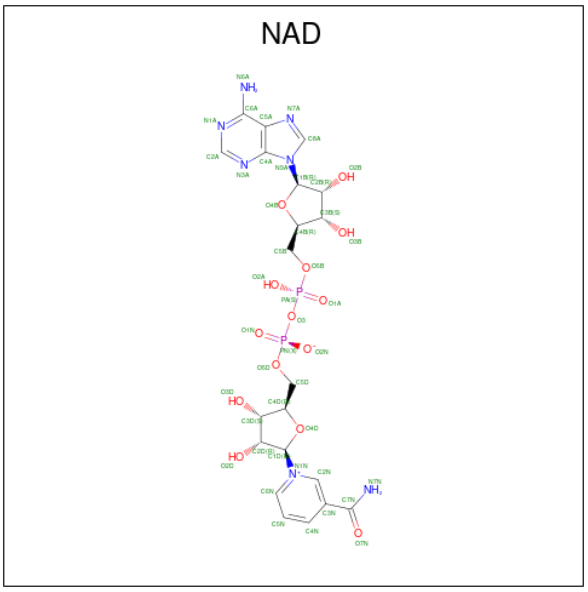
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



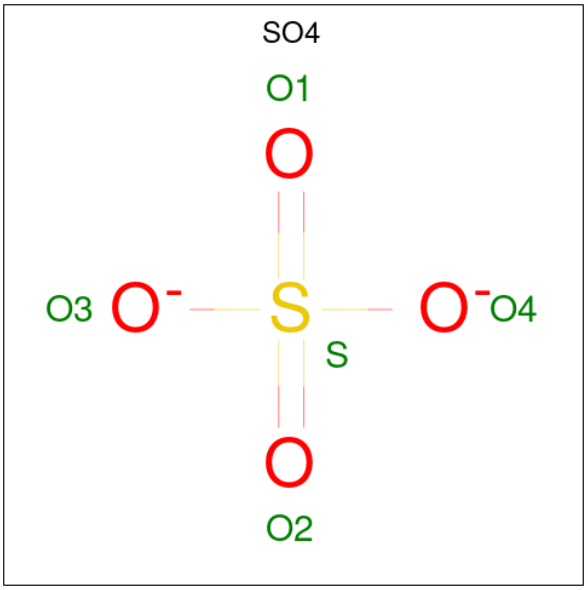
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- Molecule 7 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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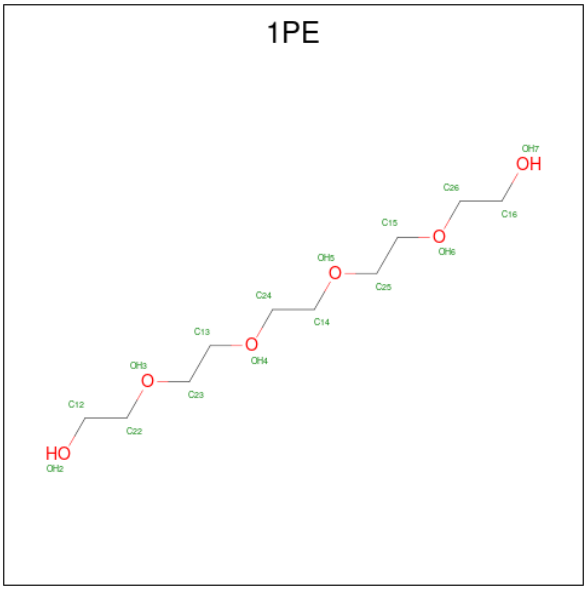
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 16 10 6	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1287	Total O 1287 1287	0	0

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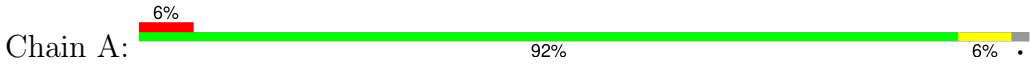
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1373	Total	O	0	4
			1373	1373		

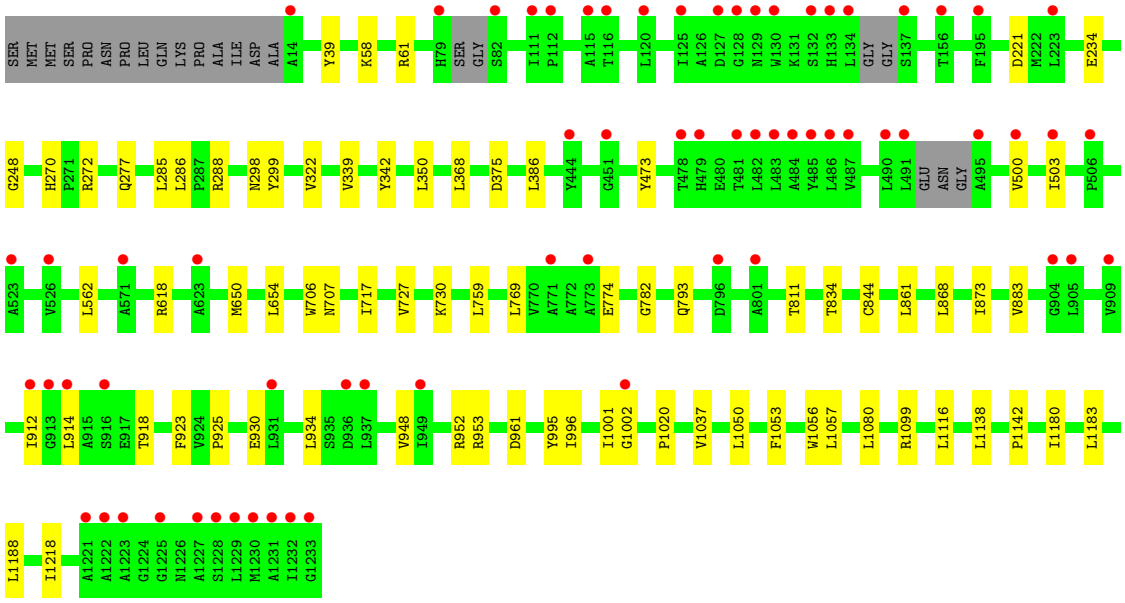
3 Residue-property plots (i)

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

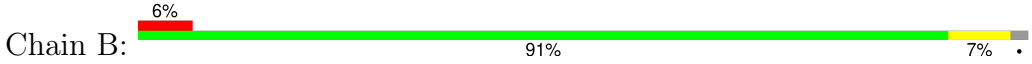
Chain A:

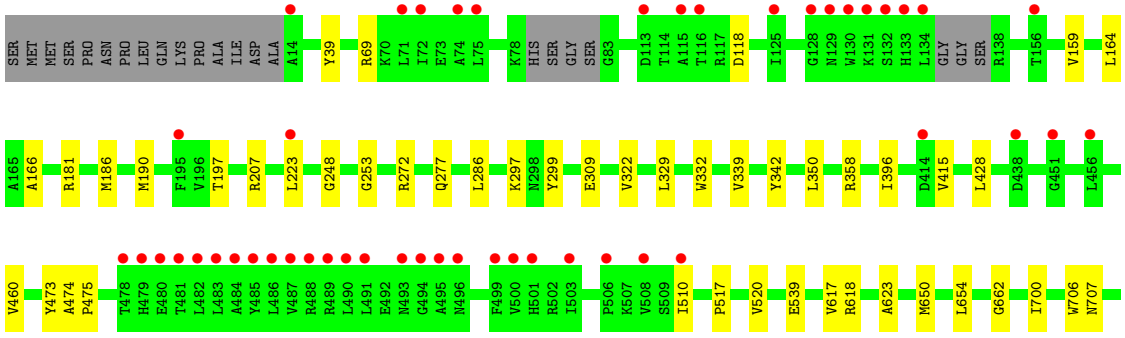


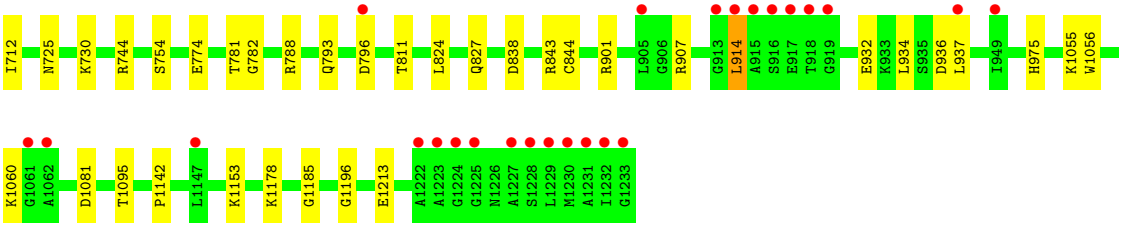


• Molecule 1: Bifunctional protein PutA

Chain B:






I712
N725
K730
R744
S754
E774
T781
G782
R788
Q793
D796
T811
L824
Q827
D838
R843
C844
R901
L905
G906
R907
G913
L914
A915
S916
E917
T918
G919
E932
K933
L934
S935
D936
L937
I949
H975
K1055
W1056
K1060
G1061
A1062
D1081
T1095
P1142
L1147
K1153
K1178
G1185
G1196
E1213
A1222
A1223
G1224
G1225
N1226
A1227
S1228
L1229
M1230
A1231
I1232
G1233

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.75Å 101.96Å 126.17Å 90.00° 106.32° 90.00°	Depositor
Resolution (Å)	46.99 – 1.32 46.99 – 1.32	Depositor EDS
% Data completeness (in resolution range)	93.3 (46.99-1.32) 94.2 (46.99-1.32)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.32Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.168 , 0.188 0.167 , 0.186	Depositor DCC
R_{free} test set	28852 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21273	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, A1BDD, 1PE, SO4, MG, PGE, FAD, PEG, NAD

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	0.34	0/9320	0.63	0/12686
1	B	0.36	0/9318	0.65	0/12681
All	All	0.35	0/18638	0.64	0/25367

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	744	ARG	Sidechain

5.2 Too-close contacts

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	9097	0	9168	52	0
1	B	9080	0	9135	60	0
2	A	106	0	62	4	0
2	B	106	0	62	4	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
4	A	10	0	14	0	0
4	B	20	0	28	0	0
5	A	3	0	1	1	0
5	B	9	0	3	4	0
6	A	14	0	20	0	0
6	B	7	0	10	2	0
7	A	44	0	26	2	0
7	B	44	0	26	2	0
8	A	20	0	0	1	0
8	B	5	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	B	16	0	22	0	0
11	A	1287	0	0	13	2
11	B	1373	0	0	16	2
All	All	21273	0	18577	115	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (115) 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:844:CYS:SG	7:B:2011:NAD:C4N	2.71	0.78
1:A:473:TYR:HB2	2:A:2001[B]:FAD:HM72	1.71	0.72
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.74	0.70
1:B:793:GLN:OE1	11:B:2101:HOH:O	2.12	0.68
1:A:339[A]:VAL:HG21	1:A:350:LEU:HD21	1.75	0.68
1:B:1213:GLU:HG3	5:B:2007:FMT:H	1.76	0.68
1:B:339[A]:VAL:HG21	1:B:350:LEU:HD21	1.75	0.68
1:B:473:TYR:HB2	2:B:2001[B]:FAD:HM72	1.76	0.67
1:A:793:GLN:OE1	11:A:2101:HOH:O	2.12	0.67
1:A:861[A]:LEU:HD21	1:A:948:VAL:HG11	1.76	0.67
1:B:297[B]:LYS:HD2	1:B:329:LEU:HA	1.76	0.67
1:A:473:TYR:HB2	2:A:2001[A]:FAD:HM72	1.78	0.66
1:A:234:GLU:OE2	11:A:2104:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:TYR:HB2	2:B:2001[A]:FAD:HM72	1.78	0.65
1:B:1213:GLU:H	5:B:2007:FMT:H	1.61	0.64
1:A:844:CYS:SG	7:A:2007:NAD:C4N	2.85	0.64
1:B:539:GLU:OE1	11:B:2103:HOH:O	2.15	0.63
8:A:2011:SO4:O4	11:A:2103:HOH:O	2.13	0.63
1:A:995:TYR:OH	11:A:2102:HOH:O	2.12	0.62
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.83	0.59
1:B:650:MET:O	1:B:654:LEU:HG	2.01	0.59
1:B:824:LEU:HD23	1:B:827[A]:GLN:HG3	1.85	0.59
1:B:907:ARG:NH1	1:B:936:ASP:OD2	2.37	0.57
1:B:1095[B]:THR:HG22	11:B:2884:HOH:O	2.06	0.56
1:B:1196:GLY:HA3	6:B:2003:PEG:H22	1.87	0.56
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.88	0.56
1:B:1213:GLU:CG	5:B:2007:FMT:H	2.36	0.56
1:B:1213:GLU:H	5:B:2007:FMT:C	2.18	0.55
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.89	0.55
1:B:197[B]:THR:HG21	1:B:474:ALA:HB1	1.88	0.55
1:A:618:ARG:NH2	11:A:2132:HOH:O	2.41	0.54
1:B:838:ASP:HB3	1:B:843:ARG:HH12	1.73	0.54
1:B:69[A]:ARG:HD3	1:B:510:ILE:HG21	1.90	0.53
1:B:844:CYS:SG	7:B:2011:NAD:C3N	2.96	0.53
1:A:1183:LEU:O	11:A:2105:HOH:O	2.18	0.53
1:A:873:ILE:HD13	1:A:912:ILE:HG21	1.89	0.53
1:B:662:GLY:HA2	11:B:2195:HOH:O	2.09	0.53
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.43	0.53
1:B:782:GLY:O	1:B:811:THR:HA	2.10	0.52
1:B:1060:LYS:NZ	11:B:2126:HOH:O	2.43	0.51
1:B:1081:ASP:OD1	11:B:2105:HOH:O	2.20	0.50
1:B:309:GLU:OE2	11:B:2104:HOH:O	2.19	0.50
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.40	0.50
1:A:782:GLY:O	1:A:811:THR:HA	2.13	0.49
1:B:223:LEU:HD21	1:B:475:PRO:HB3	1.93	0.49
1:A:562:LEU:HD11	1:A:654:LEU:HD12	1.94	0.48
1:B:618:ARG:NH2	11:B:2131:HOH:O	2.47	0.48
1:A:473:TYR:CB	2:A:2001[A]:FAD:HM72	2.43	0.48
1:A:375[B]:ASP:OD1	11:A:2106:HOH:O	2.20	0.48
1:A:844:CYS:SG	7:A:2007:NAD:C3N	3.02	0.48
1:B:197[B]:THR:HG22	1:B:475:PRO:O	2.13	0.48
1:B:706:TRP:CE3	1:B:707:ASN:HA	2.49	0.47
1:A:1116[B]:LEU:HD11	1:A:1138:LEU:HD11	1.96	0.47
1:B:623:ALA:HB2	1:B:754:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:ARG:NH1	11:B:2110:HOH:O	2.29	0.47
1:A:868:LEU:O	1:A:912:ILE:HD11	2.15	0.47
1:B:396:ILE:HD11	1:B:520:VAL:HB	1.97	0.47
1:A:759[A]:LEU:HD13	1:A:769:LEU:HD21	1.97	0.46
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.50	0.46
1:B:118:ASP:OD1	1:B:181:ARG:NH2	2.49	0.46
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.97	0.46
1:B:159:VAL:HG13	1:B:164:LEU:HD12	1.98	0.46
1:B:937:LEU:HD12	11:B:2969:HOH:O	2.14	0.46
1:A:995:TYR:OH	1:A:1002[A]:GLY:O	2.32	0.45
1:B:186:MET:O	1:B:190:MET:HG3	2.17	0.45
1:B:907:ARG:NH1	1:B:932:GLU:H	2.15	0.45
1:B:253:GLY:HA2	11:B:3076:HOH:O	2.17	0.45
1:B:788:ARG:NH2	1:B:1185:GLY:O	2.47	0.45
1:B:700[B]:ILE:HG12	1:B:725:ASN:HB3	1.99	0.44
1:B:796:ASP:OD1	1:B:1178:LYS:NZ	2.46	0.44
2:B:2001[A]:FAD:H9	2:B:2001[A]:FAD:H1'1	1.77	0.44
1:A:58:LYS:HD3	1:A:61:ARG:NH2	2.32	0.44
1:A:914:LEU:HD11	1:A:925:PRO:HD3	1.99	0.44
1:B:473:TYR:CB	2:B:2001[A]:FAD:HM72	2.47	0.44
1:A:650:MET:O	1:A:654:LEU:HG	2.18	0.44
1:A:953:ARG:HD3	11:A:2253:HOH:O	2.18	0.44
1:B:1153:LYS:O	11:B:2107:HOH:O	2.21	0.43
1:A:1037:VAL:HG11	1:B:166:ALA:HB1	2.00	0.43
1:A:500:VAL:O	1:A:503:ILE:HG22	2.18	0.43
1:B:712:ILE:HD13	1:B:781:THR:HG21	1.99	0.43
1:A:834:THR:HG22	1:A:1001[B]:ILE:HD11	2.00	0.43
6:B:2003:PEG:H11	6:B:2003:PEG:H31	1.55	0.43
1:B:1095[B]:THR:HG21	11:B:3019:HOH:O	2.17	0.43
1:A:58:LYS:HD3	1:A:61:ARG:HH22	1.83	0.43
1:A:618:ARG:HG2	1:A:774:GLU:OE2	2.19	0.43
1:A:1020:PRO:HA	11:A:2907:HOH:O	2.19	0.43
1:B:617:VAL:HG12	1:B:774:GLU:HB2	2.01	0.43
1:B:428:LEU:HD11	1:B:460:VAL:HG21	2.01	0.42
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.54	0.42
1:A:1180:ILE:HG23	1:A:1188:LEU:HD12	2.02	0.42
1:A:288:ARG:HD3	11:A:2514:HOH:O	2.19	0.42
1:A:918:THR:HB	1:A:923:PHE:CD1	2.54	0.42
2:A:2001[A]:FAD:H9	2:A:2001[A]:FAD:H1'1	1.70	0.42
1:A:298:ASN:ND2	11:A:2136:HOH:O	2.42	0.42
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.40	0.41
1:A:1080[A]:LEU:HD12	11:A:2852:HOH:O	2.20	0.41
1:A:221:ASP:HB2	1:A:473:TYR:CZ	2.54	0.41
1:A:270:HIS:HB2	1:A:285:LEU:HG	2.02	0.41
1:A:1099[B]:ARG:HD3	11:A:2894:HOH:O	2.20	0.41
1:B:358[A]:ARG:HG3	1:B:415:VAL:HG11	2.03	0.41
1:A:339[A]:VAL:HG23	1:A:368:LEU:HD12	2.03	0.41
1:A:386:LEU:HD22	5:A:2004:FMT:H	2.02	0.41
1:A:717:ILE:HG12	1:A:727:VAL:HG11	2.03	0.41
1:B:272:ARG:HB3	1:B:277:GLN:HG3	2.03	0.41
1:B:297[B]:LYS:HG3	1:B:332:TRP:HB2	2.02	0.41
1:B:396:ILE:HG13	1:B:517:PRO:HB3	2.03	0.41
1:A:861[B]:LEU:HD21	1:A:930:GLU:CD	2.42	0.40
1:B:248:GLY:HA3	1:B:299:TYR:CG	2.57	0.40
1:B:623:ALA:HB1	11:B:2481:HOH:O	2.21	0.40
1:B:827[B]:GLN:HG2	1:B:975:HIS:HE1	1.86	0.40
1:A:1053:PHE:CE2	1:A:1057:LEU:HD11	2.57	0.40
1:B:901:ARG:NH2	11:B:2153:HOH:O	2.52	0.40

All (2) 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)
11:A:3060:HOH:O	11:B:2107:HOH:O[1_455]	2.09	0.11
11:A:2112:HOH:O	11:B:3106:HOH:O[2_556]	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	1232/1235 (100%)	1212 (98%)	20 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1233/1235 (100%)	1207 (98%)	25 (2%)	1 (0%)	48 19
All	All	2465/2470 (100%)	2419 (98%)	45 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	914	LEU

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	918/951 (96%)	913 (100%)	5 (0%)	86 67
1	B	916/951 (96%)	911 (100%)	5 (0%)	86 67
All	All	1834/1902 (96%)	1824 (100%)	10 (0%)	84 67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	TYR
1	A	342	TYR
1	A	730	LYS
1	A	934	LEU
1	A	952	ARG
1	B	39	TYR
1	B	342	TYR
1	B	730	LYS
1	B	914	LEU
1	B	934	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	A	298	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
3	A1BDD	A	2002	-	10,10,10	0.60	0	12,12,12	0.74	0
7	NAD	B	2011	9	42,48,48	2.03	7 (16%)	50,73,73	1.53	3 (6%)
5	FMT	B	2007	-	2,2,2	0.63	0	1,1,1	0.44	0
2	FAD	B	2001[A]	-	54,58,58	1.99	13 (24%)	71,89,89	1.48	12 (16%)
5	FMT	A	2004	-	2,2,2	0.52	0	1,1,1	0.26	0
2	FAD	B	2001[B]	-	54,58,58	2.41	16 (29%)	71,89,89	1.52	11 (15%)
5	FMT	B	2006	-	2,2,2	0.61	0	1,1,1	0.20	0
8	SO4	A	2011	-	4,4,4	0.67	0	6,6,6	0.09	0
5	FMT	B	2008	-	2,2,2	0.81	0	1,1,1	0.33	0
4	PGE	B	2009	-	9,9,9	0.32	0	8,8,8	0.54	0
3	A1BDD	B	2004	-	10,10,10	0.64	0	12,12,12	0.75	0
6	PEG	A	2005	-	6,6,6	0.24	0	5,5,5	0.19	0
8	SO4	A	2008	-	4,4,4	0.54	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	SO4	A	2009	-	4,4,4	0.64	0	6,6,6	0.23	0
4	PGE	B	2005	-	9,9,9	0.34	0	8,8,8	0.51	0
6	PEG	B	2003	-	6,6,6	0.24	0	5,5,5	0.33	0
8	SO4	A	2010	-	4,4,4	0.66	0	6,6,6	0.08	0
3	A1BDD	B	2002	-	10,10,10	0.64	0	12,12,12	0.58	0
7	NAD	A	2007	9	42,48,48	2.21	12 (28%)	50,73,73	1.58	5 (10%)
4	PGE	A	2003	-	9,9,9	0.32	0	8,8,8	0.44	0
6	PEG	A	2006	-	6,6,6	0.26	0	5,5,5	0.24	0
2	FAD	A	2001[A]	-	54,58,58	2.14	14 (25%)	71,89,89	1.57	12 (16%)
2	FAD	A	2001[B]	-	54,58,58	2.23	15 (27%)	71,89,89	1.45	10 (14%)
8	SO4	B	2012	-	4,4,4	0.58	0	6,6,6	0.40	0
10	1PE	B	2010	-	15,15,15	0.28	0	14,14,14	0.22	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
3	A1BDD	B	2002	-	-	0/4/4/4	0/1/1/1
7	NAD	A	2007	9	-	1/26/62/62	0/5/5/5
2	FAD	B	2001[A]	-	-	3/30/50/50	0/6/6/6
4	PGE	A	2003	-	-	4/7/7/7	-
4	PGE	B	2009	-	-	3/7/7/7	-
2	FAD	B	2001[B]	-	-	8/30/50/50	0/6/6/6
6	PEG	A	2006	-	-	2/4/4/4	-
3	A1BDD	B	2004	-	-	2/4/4/4	0/1/1/1
6	PEG	A	2005	-	-	1/4/4/4	-
2	FAD	A	2001[A]	-	-	2/30/50/50	0/6/6/6
2	FAD	A	2001[B]	-	-	12/30/50/50	0/6/6/6
4	PGE	B	2005	-	-	1/7/7/7	-
10	1PE	B	2010	-	-	4/13/13/13	-
6	PEG	B	2003	-	-	3/4/4/4	-
3	A1BDD	A	2002	-	-	2/4/4/4	0/1/1/1
7	NAD	B	2011	9	-	1/26/62/62	0/5/5/5

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001[B]	FAD	PA-O3P	-10.01	1.48	1.59
2	A	2001[B]	FAD	PA-O3P	-9.08	1.49	1.59
2	A	2001[A]	FAD	PA-O3P	-8.30	1.50	1.59
2	B	2001[A]	FAD	PA-O3P	-7.51	1.51	1.59
7	B	2011	NAD	PA-O3	-7.21	1.51	1.59
2	B	2001[B]	FAD	O4-C4	7.14	1.37	1.23
7	A	2007	NAD	PA-O3	-7.07	1.51	1.59
7	A	2007	NAD	C2N-N1N	6.88	1.42	1.35
2	A	2001[B]	FAD	O4-C4	6.57	1.36	1.23
2	A	2001[A]	FAD	O4-C4	6.52	1.35	1.23
2	B	2001[A]	FAD	O4-C4	6.03	1.35	1.23
2	B	2001[B]	FAD	O2-C2	5.77	1.35	1.24
7	B	2011	NAD	C2N-N1N	5.71	1.41	1.35
7	A	2007	NAD	C7N-N7N	4.89	1.42	1.33
2	A	2001[B]	FAD	O2-C2	4.76	1.33	1.24
7	B	2011	NAD	C7N-N7N	4.60	1.41	1.33
2	A	2001[A]	FAD	O2-C2	4.31	1.32	1.24
2	B	2001[A]	FAD	O2-C2	4.25	1.32	1.24
2	A	2001[A]	FAD	C4X-N5	4.05	1.39	1.30
2	B	2001[B]	FAD	C4X-N5	4.01	1.39	1.30
2	A	2001[B]	FAD	C4X-N5	3.73	1.38	1.30
2	B	2001[A]	FAD	C4X-N5	3.68	1.38	1.30
2	B	2001[B]	FAD	C2-N1	3.25	1.44	1.36
2	A	2001[A]	FAD	PA-O5B	-3.04	1.47	1.59
2	A	2001[B]	FAD	O2'-C2'	-2.97	1.37	1.43
2	B	2001[B]	FAD	C6A-N6A	2.96	1.44	1.34
2	A	2001[B]	FAD	C6A-N6A	2.91	1.44	1.34
2	A	2001[A]	FAD	C6A-N6A	2.89	1.44	1.34
2	A	2001[B]	FAD	C2-N1	2.88	1.43	1.36
2	A	2001[A]	FAD	P-O3P	2.88	1.62	1.59
2	A	2001[B]	FAD	P-O3P	2.88	1.62	1.59
7	B	2011	NAD	C6A-N6A	2.83	1.44	1.34
2	B	2001[A]	FAD	C6A-N6A	2.83	1.44	1.34
7	A	2007	NAD	C2A-N3A	2.78	1.36	1.32
2	B	2001[B]	FAD	O2'-C2'	-2.74	1.37	1.43
2	A	2001[A]	FAD	O2'-C2'	-2.73	1.37	1.43
7	A	2007	NAD	C6A-N6A	2.71	1.43	1.34
2	B	2001[B]	FAD	C2A-N3A	2.67	1.36	1.32
2	A	2001[B]	FAD	C2A-N3A	2.66	1.36	1.32
2	B	2001[B]	FAD	PA-O5B	-2.64	1.49	1.59
2	A	2001[B]	FAD	PA-O5B	-2.64	1.49	1.59
2	A	2001[A]	FAD	C2A-N3A	2.61	1.36	1.32
7	A	2007	NAD	C6N-N1N	2.60	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001[B]	FAD	O4'-C4'	-2.55	1.38	1.43
2	B	2001[A]	FAD	O2'-C2'	-2.53	1.38	1.43
2	B	2001[B]	FAD	O4'-C4'	-2.52	1.38	1.43
2	A	2001[A]	FAD	O4'-C4'	-2.50	1.38	1.43
2	B	2001[A]	FAD	C2A-N3A	2.49	1.35	1.32
2	B	2001[B]	FAD	C10-N1	2.48	1.38	1.33
2	B	2001[B]	FAD	C1B-N9A	-2.36	1.44	1.49
2	B	2001[A]	FAD	C1B-N9A	-2.33	1.44	1.49
2	B	2001[B]	FAD	O2B-C2B	-2.32	1.37	1.43
7	A	2007	NAD	PA-O5B	-2.32	1.50	1.59
2	B	2001[B]	FAD	O4B-C4B	-2.31	1.39	1.45
2	A	2001[A]	FAD	C2-N1	2.30	1.41	1.36
7	A	2007	NAD	C1B-N9A	-2.29	1.44	1.49
7	A	2007	NAD	O3D-C3D	-2.28	1.37	1.43
2	A	2001[A]	FAD	C1B-N9A	-2.25	1.44	1.49
2	B	2001[B]	FAD	PA-O2A	-2.25	1.44	1.55
2	A	2001[A]	FAD	O4B-C4B	-2.25	1.40	1.45
2	A	2001[B]	FAD	O4B-C4B	-2.25	1.40	1.45
2	B	2001[A]	FAD	O2B-C2B	-2.24	1.37	1.43
7	A	2007	NAD	C2D-C3D	-2.23	1.47	1.53
2	A	2001[B]	FAD	C1B-N9A	-2.22	1.44	1.49
7	B	2011	NAD	C2A-N3A	2.22	1.35	1.32
7	A	2007	NAD	C2B-C3B	-2.20	1.47	1.53
2	B	2001[A]	FAD	O4B-C4B	-2.17	1.40	1.45
2	B	2001[A]	FAD	P-O3P	2.17	1.61	1.59
2	A	2001[B]	FAD	PA-O2A	-2.12	1.45	1.55
7	A	2007	NAD	O4D-C4D	-2.12	1.40	1.45
2	A	2001[B]	FAD	C10-N1	2.11	1.37	1.33
7	B	2011	NAD	C6N-N1N	2.09	1.40	1.35
7	B	2011	NAD	C1B-N9A	-2.07	1.44	1.49
2	B	2001[A]	FAD	O3'-C3'	-2.05	1.37	1.43
2	A	2001[A]	FAD	O3'-C3'	-2.05	1.37	1.43
2	B	2001[B]	FAD	P-O1P	2.04	1.57	1.50
2	B	2001[A]	FAD	C2-N1	2.02	1.41	1.36

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	2011	NAD	N3A-C2A-N1A	-7.47	118.53	128.67
7	A	2007	NAD	N3A-C2A-N1A	-6.65	119.64	128.67
2	A	2001[A]	FAD	N3A-C2A-N1A	-6.34	120.07	128.67
2	A	2001[B]	FAD	N3A-C2A-N1A	-6.28	120.15	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001[B]	FAD	N3A-C2A-N1A	-6.08	120.41	128.67
2	B	2001[A]	FAD	N3A-C2A-N1A	-5.83	120.76	128.67
7	A	2007	NAD	C4B-O4B-C1B	-5.14	105.22	109.92
2	B	2001[B]	FAD	O2P-P-O3P	-4.44	95.28	107.27
7	B	2011	NAD	C4B-O4B-C1B	-4.27	106.01	109.92
2	A	2001[A]	FAD	C4-C4X-N5	3.90	123.60	118.21
2	A	2001[B]	FAD	O2P-P-O3P	-3.48	97.86	107.27
2	B	2001[A]	FAD	C4X-C10-N10	3.19	121.05	116.48
2	B	2001[A]	FAD	O2-C2-N1	-3.12	116.61	121.80
2	A	2001[A]	FAD	C5X-C9A-N10	3.06	120.73	117.97
2	A	2001[B]	FAD	C4-N3-C2	-3.02	120.28	125.64
2	A	2001[A]	FAD	C4X-C4-N3	3.01	120.92	113.25
2	A	2001[A]	FAD	C9-C9A-N10	-2.90	117.95	121.85
2	B	2001[B]	FAD	C4-C4X-N5	2.85	122.15	118.21
2	B	2001[A]	FAD	C4-N3-C2	-2.80	120.66	125.64
2	A	2001[A]	FAD	O5'-P-O1P	2.80	120.04	108.94
2	B	2001[A]	FAD	C4-C4X-N5	2.78	122.05	118.21
2	A	2001[B]	FAD	C4-C4X-N5	2.77	122.03	118.21
2	B	2001[B]	FAD	O3P-P-O1P	2.73	118.93	110.70
2	A	2001[B]	FAD	C4X-C4-N3	2.73	120.20	113.25
2	A	2001[A]	FAD	C4-N3-C2	-2.68	120.89	125.64
2	B	2001[B]	FAD	C4-N3-C2	-2.62	120.99	125.64
2	B	2001[B]	FAD	O2A-PA-O3P	-2.60	100.24	107.27
2	B	2001[B]	FAD	C4X-C4-N3	2.52	119.68	113.25
7	A	2007	NAD	C4D-O4D-C1D	-2.47	107.66	109.92
2	A	2001[B]	FAD	O2A-PA-O3P	-2.44	100.67	107.27
2	A	2001[A]	FAD	O2P-P-O3P	-2.44	100.67	107.27
2	B	2001[A]	FAD	C2'-C1'-N10	2.41	121.61	110.20
2	A	2001[A]	FAD	C4A-C5A-N7A	-2.41	106.79	109.34
7	B	2011	NAD	C4A-C5A-N7A	-2.38	106.82	109.34
2	B	2001[B]	FAD	O4-C4-C4X	-2.38	120.24	126.53
2	A	2001[B]	FAD	C5X-C9A-N10	2.38	120.12	117.97
2	B	2001[A]	FAD	C9-C9A-N10	-2.36	118.68	121.85
7	A	2007	NAD	C1B-N9A-C4A	-2.34	122.53	126.64
2	A	2001[A]	FAD	C4B-O4B-C1B	-2.32	107.80	109.92
2	A	2001[B]	FAD	O4-C4-C4X	-2.27	120.55	126.53
2	A	2001[B]	FAD	C4A-C5A-N7A	-2.25	106.96	109.34
2	B	2001[B]	FAD	C10-C4X-N5	-2.22	120.28	124.81
2	B	2001[A]	FAD	C5X-C9A-N10	2.20	119.95	117.97
2	A	2001[A]	FAD	C2'-C1'-N10	2.19	120.57	110.20
2	B	2001[B]	FAD	O5'-P-O1P	2.19	117.62	108.94
2	A	2001[B]	FAD	C9-C9A-N10	-2.19	118.91	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001[A]	FAD	C4X-C4-N3	2.13	118.68	113.25
7	A	2007	NAD	O2N-PN-O3	2.12	113.02	107.27
2	B	2001[A]	FAD	C10-C4X-N5	-2.12	120.48	124.81
2	A	2001[A]	FAD	O4-C4-C4X	-2.08	121.05	126.53
2	B	2001[A]	FAD	O4-C4-C4X	-2.02	121.20	126.53
2	B	2001[A]	FAD	C5'-C4'-C3'	-2.01	108.42	112.22
2	B	2001[B]	FAD	C4B-O4B-C1B	-2.00	108.09	109.92

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001[A]	FAD	N10-C1'-C2'-O2'
2	A	2001[A]	FAD	N10-C1'-C2'-C3'
2	A	2001[B]	FAD	C5B-O5B-PA-O1A
2	A	2001[B]	FAD	C5B-O5B-PA-O3P
2	B	2001[A]	FAD	N10-C1'-C2'-O2'
2	B	2001[A]	FAD	N10-C1'-C2'-C3'
2	B	2001[B]	FAD	P-O3P-PA-O5B
3	A	2002	A1BDD	C04-C03-O02-C01
3	A	2002	A1BDD	C10-C03-O02-C01
3	B	2004	A1BDD	C04-C03-O02-C01
2	B	2001[B]	FAD	C3B-C4B-C5B-O5B
6	B	2003	PEG	C1-C2-O2-C3
3	B	2004	A1BDD	C10-C03-O02-C01
2	B	2001[B]	FAD	C2'-C3'-C4'-O4'
2	A	2001[B]	FAD	C3B-C4B-C5B-O5B
2	B	2001[B]	FAD	O3'-C3'-C4'-C5'
2	B	2001[B]	FAD	C2'-C3'-C4'-C5'
2	B	2001[B]	FAD	O3'-C3'-C4'-O4'
6	B	2003	PEG	O1-C1-C2-O2
2	A	2001[B]	FAD	C2'-C3'-C4'-O4'
6	B	2003	PEG	O2-C3-C4-O4
4	A	2003	PGE	O2-C3-C4-O3
10	B	2010	1PE	OH7-C16-C26-OH6
2	B	2001[B]	FAD	O4B-C4B-C5B-O5B
2	A	2001[B]	FAD	P-O3P-PA-O5B
2	B	2001[A]	FAD	P-O3P-PA-O5B
4	A	2003	PGE	O3-C5-C6-O4
2	A	2001[B]	FAD	O4B-C4B-C5B-O5B
6	A	2005	PEG	C1-C2-O2-C3
4	B	2009	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	2006	PEG	O1-C1-C2-O2
2	A	2001[B]	FAD	C2'-C3'-C4'-C5'
7	A	2007	NAD	C4D-C5D-O5D-PN
7	B	2011	NAD	C4D-C5D-O5D-PN
4	A	2003	PGE	C3-C4-O3-C5
2	A	2001[B]	FAD	C5B-O5B-PA-O2A
2	B	2001[B]	FAD	C5B-O5B-PA-O3P
4	B	2009	PGE	C4-C3-O2-C2
10	B	2010	1PE	C25-C15-OH6-C26
4	B	2005	PGE	O2-C3-C4-O3
2	A	2001[B]	FAD	O3'-C3'-C4'-O4'
2	A	2001[B]	FAD	O3'-C3'-C4'-C5'
2	A	2001[B]	FAD	P-O3P-PA-O1A
2	A	2001[B]	FAD	C4'-C5'-O5'-P
6	A	2006	PEG	C1-C2-O2-C3
4	A	2003	PGE	O1-C1-C2-O2
10	B	2010	1PE	C13-C23-OH3-C22
10	B	2010	1PE	C15-C25-OH5-C14
4	B	2009	PGE	C3-C4-O3-C5

There are no ring outliers.

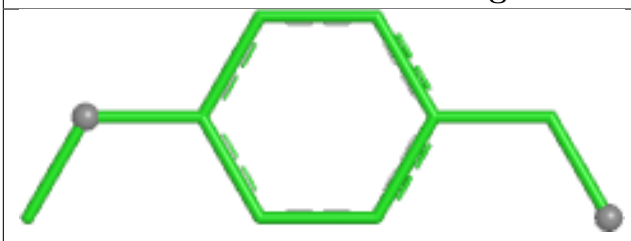
10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2011	NAD	2	0
5	B	2007	FMT	4	0
2	B	2001[A]	FAD	3	0
5	A	2004	FMT	1	0
2	B	2001[B]	FAD	1	0
8	A	2011	SO4	1	0
6	B	2003	PEG	2	0
7	A	2007	NAD	2	0
2	A	2001[A]	FAD	3	0
2	A	2001[B]	FAD	1	0

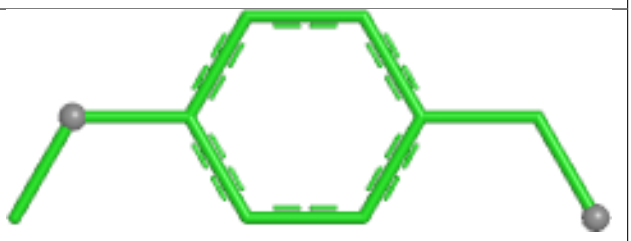
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

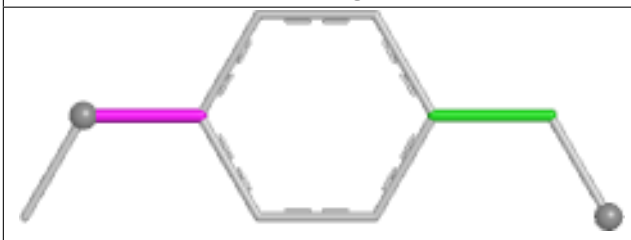
Ligand A1BDD A 2002



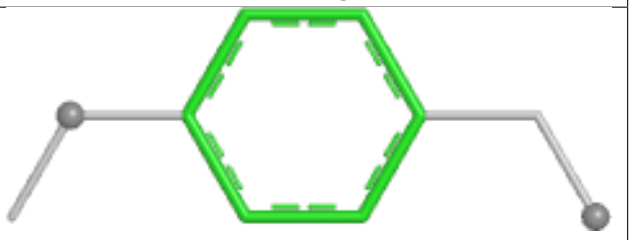
Bond lengths



Bond angles

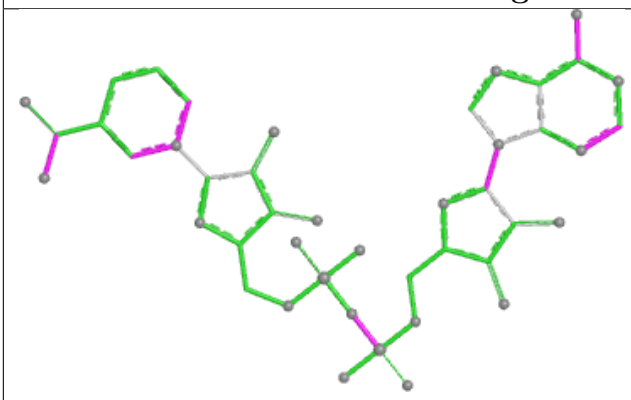


Torsions

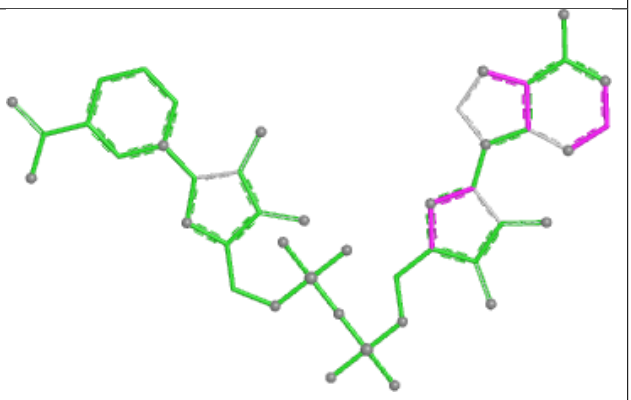


Rings

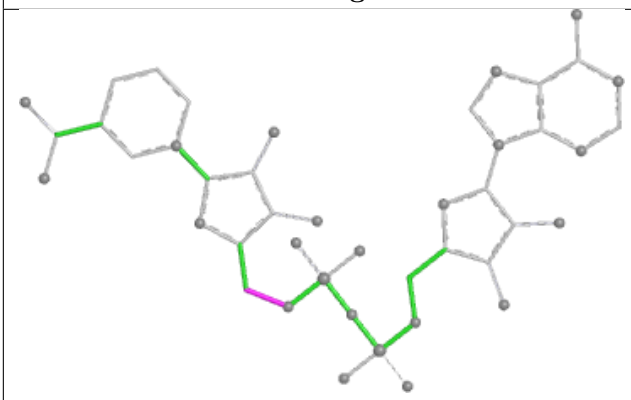
Ligand NAD B 2011



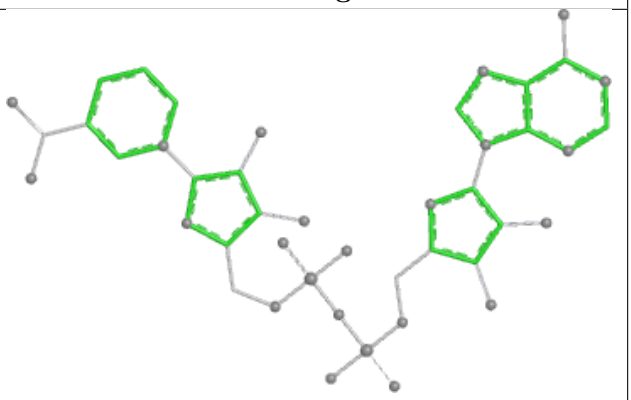
Bond lengths



Bond angles

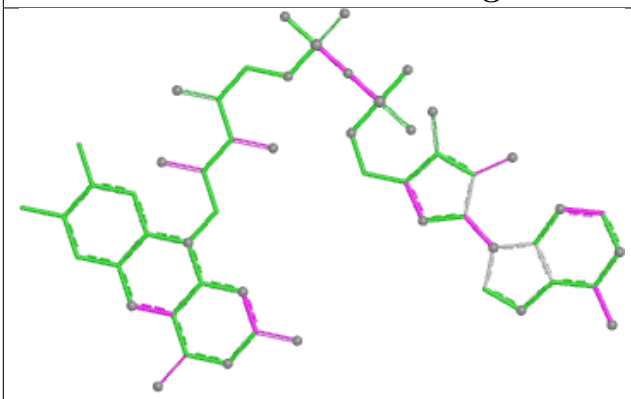


Torsions

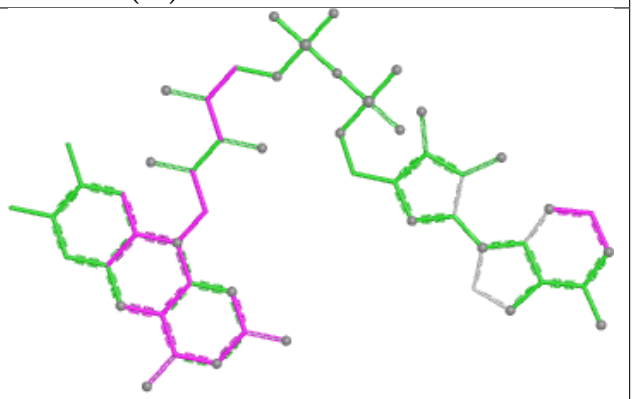


Rings

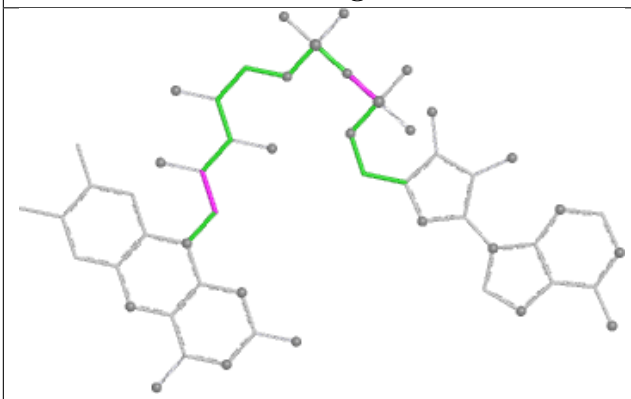
Ligand FAD B 2001 (A)



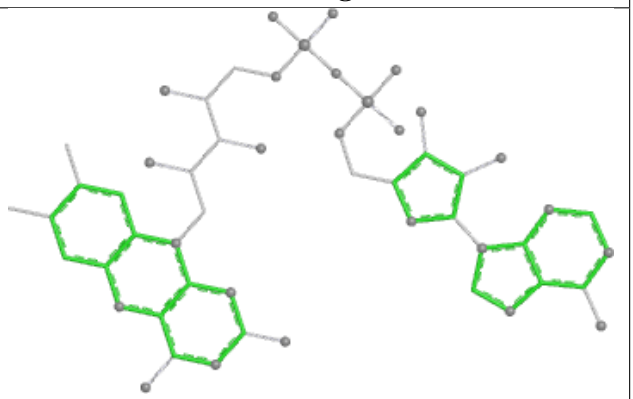
Bond lengths



Bond angles

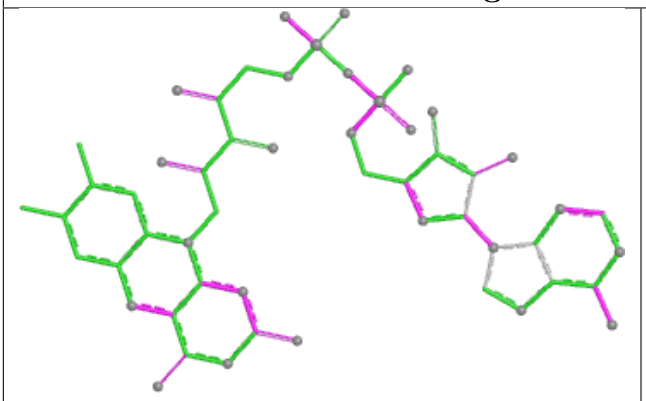


Torsions

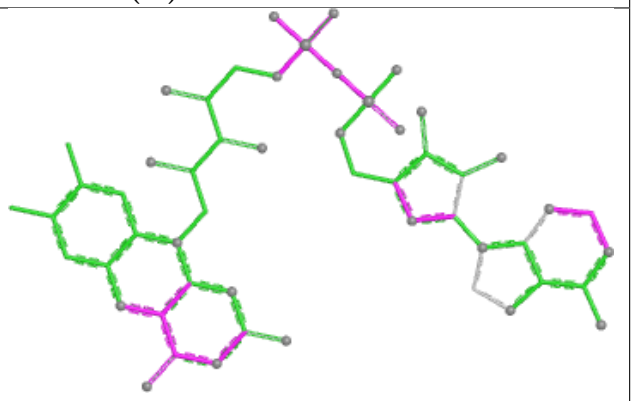


Rings

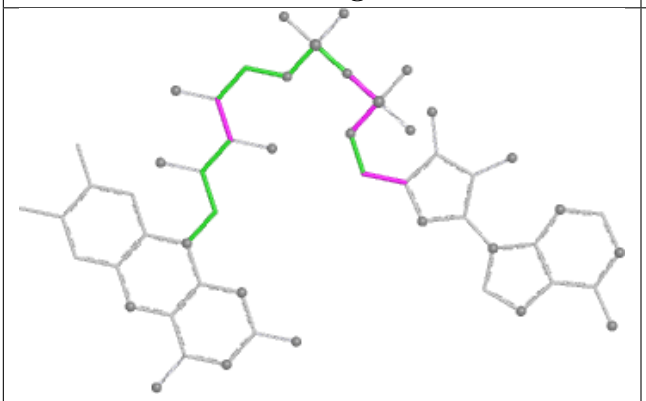
Ligand FAD B 2001 (B)



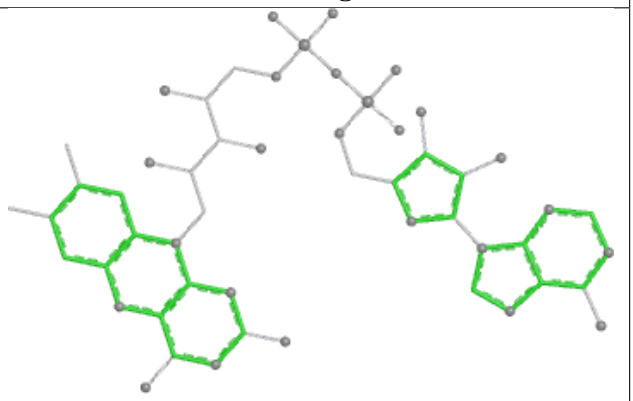
Bond lengths



Bond angles

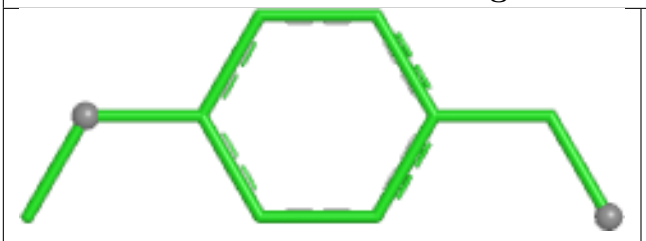


Torsions

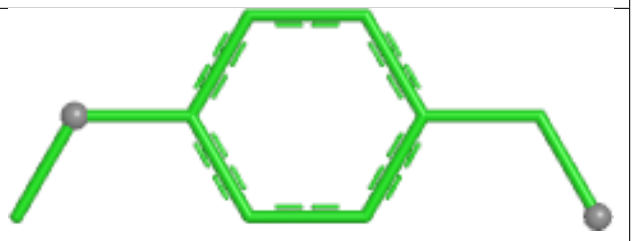


Rings

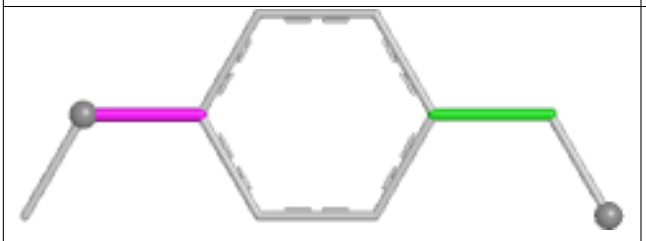
Ligand A1BDD B 2004



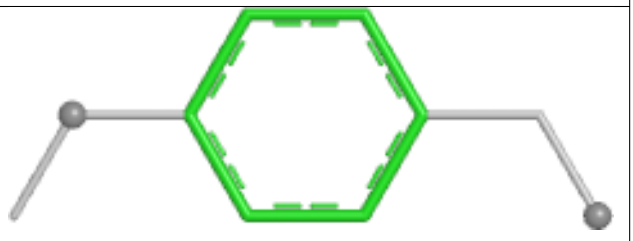
Bond lengths



Bond angles

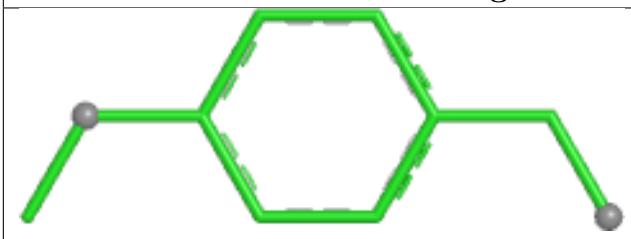


Torsions

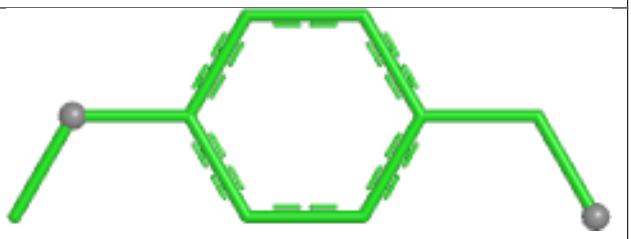


Rings

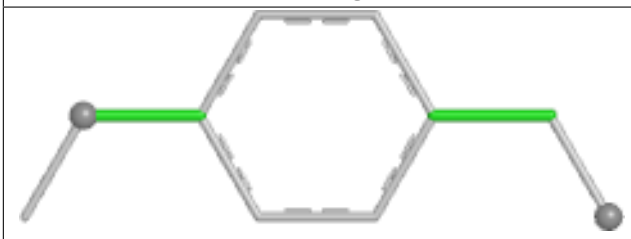
Ligand A1BDD B 2002



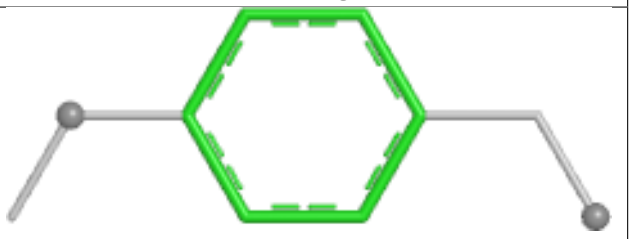
Bond lengths



Bond angles

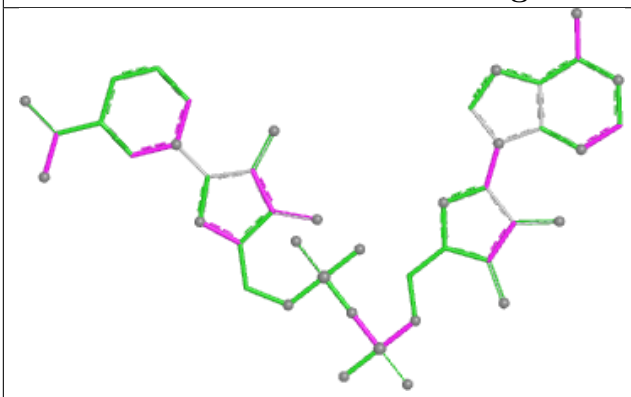


Torsions

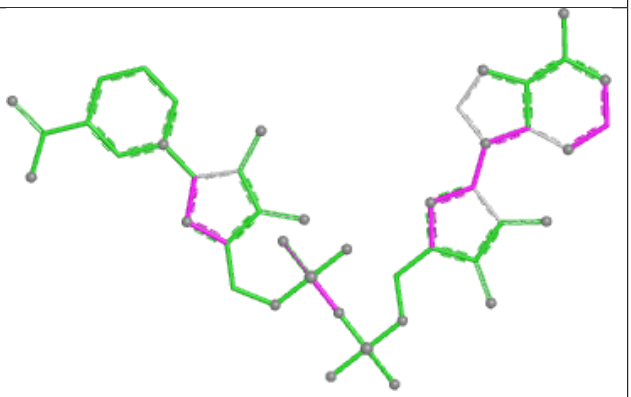


Rings

Ligand NAD A 2007



Bond lengths



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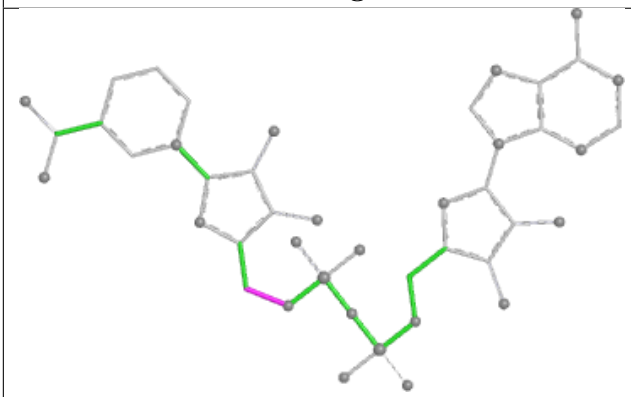

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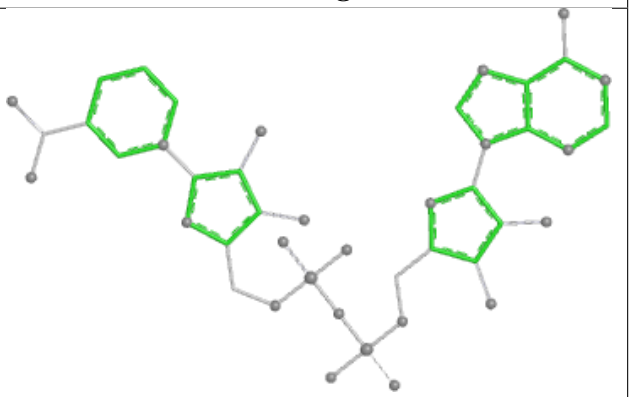
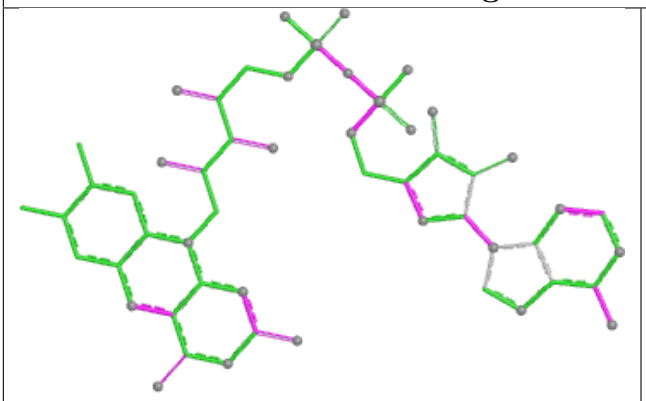
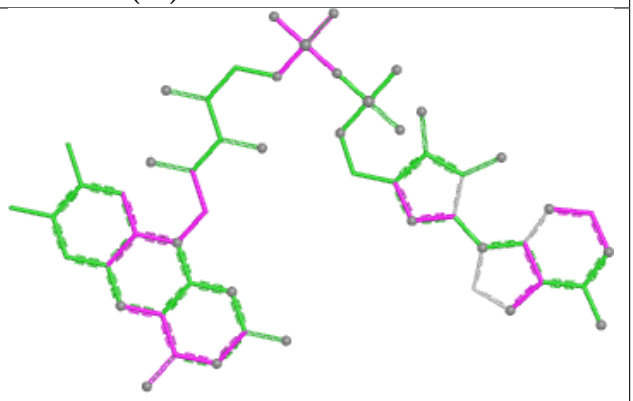


Rings

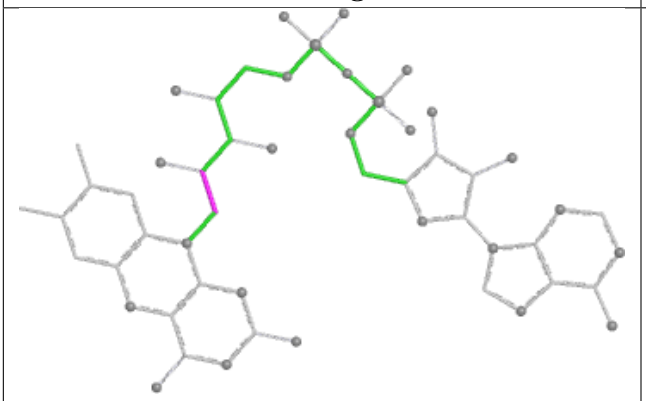
Ligand FAD A 2001 (A)



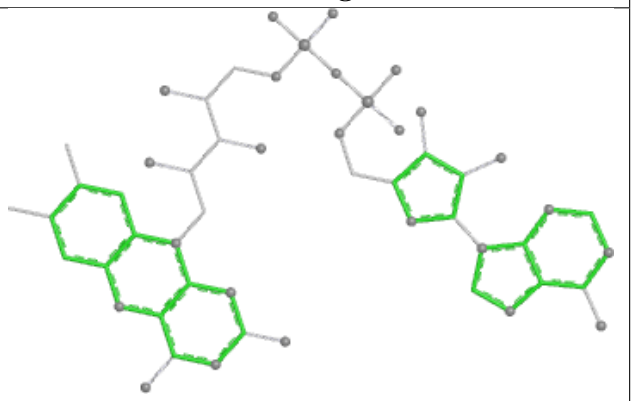
Bond lengths



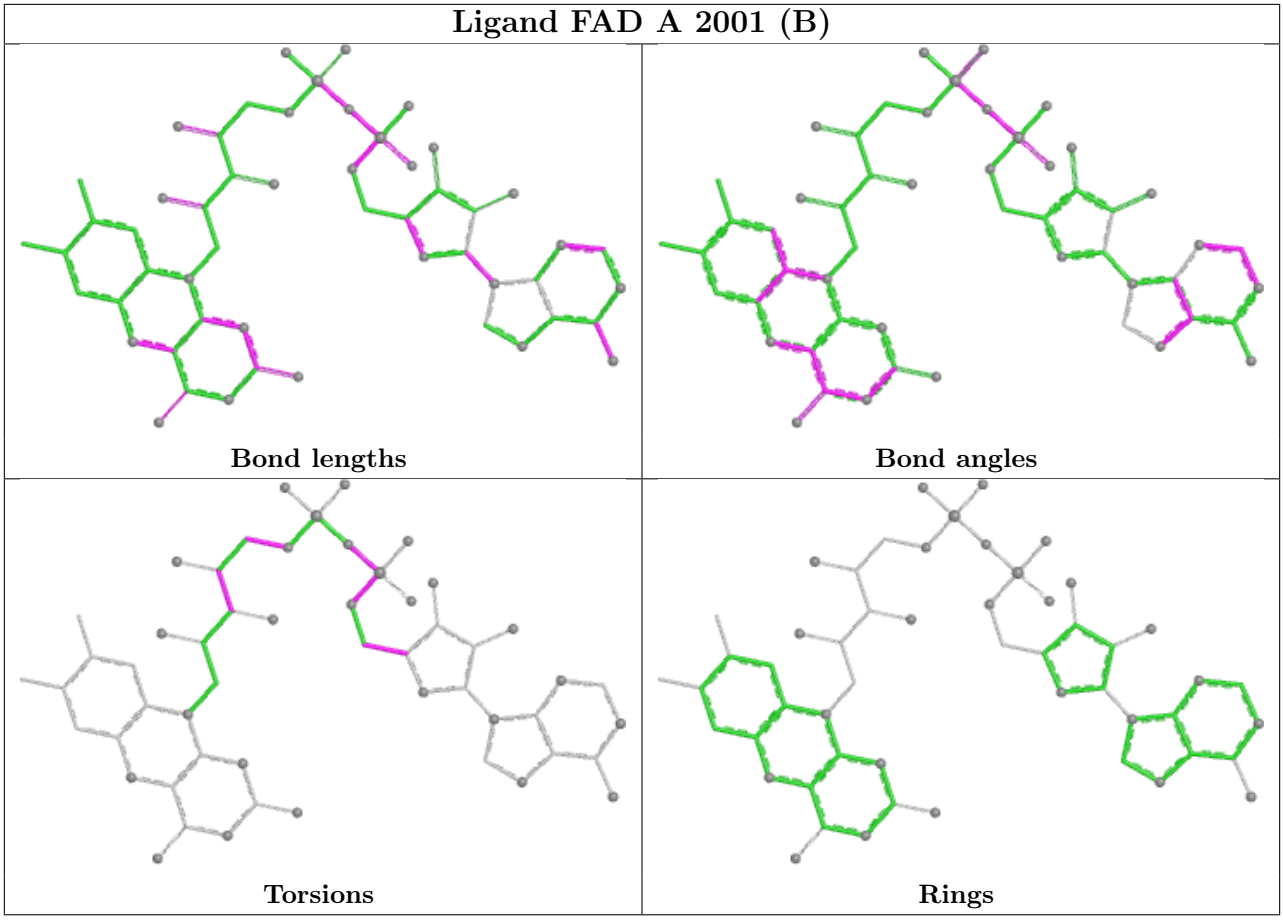
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	1213/1235 (98%)	0.42	68 (5%)	31	36	8, 22, 39, 59	39 (3%)
1	B	1213/1235 (98%)	0.33	73 (6%)	29	33	9, 20, 40, 67	37 (3%)
All	All	2426/2470 (98%)	0.38	141 (5%)	30	35	8, 21, 39, 67	76 (3%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	LEU	9.0
1	B	1229	LEU	6.5
1	B	914	LEU	6.4
1	B	1232	ILE	6.3
1	B	490	LEU	6.1
1	B	1231	ALA	5.9
1	B	915	ALA	5.8
1	B	487	VAL	5.3
1	A	156	THR	5.1
1	B	484	ALA	5.0
1	B	485	TYR	5.0
1	A	1232	ILE	4.8
1	B	918	THR	4.8
1	B	1222	ALA	4.8
1	B	913	GLY	4.7
1	A	490	LEU	4.7
1	A	491	LEU	4.7
1	B	481	THR	4.6
1	B	508	VAL	4.6
1	B	486	LEU	4.5
1	A	1229	LEU	4.5
1	A	82	SER	4.4
1	B	134	LEU	4.4
1	B	500	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	482	LEU	4.3
1	B	1233	GLY	4.2
1	A	134	LEU	4.2
1	B	1230	MET	4.1
1	B	494	GLY	4.0
1	B	488	ARG	4.0
1	A	485	TYR	4.0
1	B	128	GLY	3.8
1	A	484	ALA	3.8
1	A	905	LEU	3.8
1	B	479	HIS	3.8
1	B	1227	ALA	3.7
1	B	478	THR	3.7
1	B	1228	SER	3.7
1	A	137	SER	3.7
1	B	483	LEU	3.6
1	B	493	ASN	3.6
1	B	1223	ALA	3.6
1	A	125	ILE	3.5
1	B	223	LEU	3.5
1	A	500	VAL	3.5
1	A	14	ALA	3.4
1	B	129	ASN	3.4
1	B	132	SER	3.3
1	A	223	LEU	3.3
1	A	1233	GLY	3.3
1	B	133	HIS	3.3
1	A	1231	ALA	3.2
1	B	495	ALA	3.2
1	A	571	ALA	3.2
1	A	127	ASP	3.2
1	A	912	ILE	3.2
1	A	495	ALA	3.2
1	A	482	LEU	3.1
1	B	510	ILE	3.1
1	A	1221	ALA	3.1
1	B	14	ALA	3.1
1	A	133	HIS	3.0
1	B	917	GLU	3.0
1	A	481	THR	2.9
1	A	904	GLY	2.9
1	B	916	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	487	VAL	2.8
1	A	503	ILE	2.8
1	A	116	THR	2.8
1	B	115	ALA	2.8
1	A	1222	ALA	2.8
1	A	130	TRP	2.8
1	A	79	HIS	2.8
1	A	1227	ALA	2.8
1	B	414	ASP	2.7
1	A	115	ALA	2.7
1	B	125	ILE	2.7
1	A	506	PRO	2.7
1	A	111	ILE	2.7
1	A	937	LEU	2.7
1	A	195	PHE	2.6
1	B	796	ASP	2.6
1	A	1223	ALA	2.6
1	A	916	SER	2.6
1	A	913	GLY	2.5
1	B	489	ARG	2.5
1	A	483	LEU	2.5
1	A	478	THR	2.5
1	A	801	ALA	2.5
1	B	131	LYS	2.5
1	B	496	ASN	2.4
1	B	503	ILE	2.4
1	B	1147	LEU	2.4
1	B	116	THR	2.4
1	B	905	LEU	2.4
1	B	1224	GLY	2.4
1	A	112	PRO	2.4
1	B	506	PRO	2.4
1	A	451	GLY	2.4
1	B	156	THR	2.3
1	A	128	GLY	2.3
1	A	1225	GLY	2.3
1	B	1225	GLY	2.3
1	A	132	SER	2.3
1	B	480	GLU	2.3
1	B	195	PHE	2.3
1	A	949	ILE	2.3
1	B	499	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	501	HIS	2.2
1	B	72	ILE	2.2
1	B	949	ILE	2.2
1	B	130	TRP	2.2
1	A	523	ALA	2.2
1	A	909	VAL	2.2
1	A	486	LEU	2.2
1	A	771	ALA	2.2
1	A	526	VAL	2.2
1	A	1228	SER	2.2
1	A	120	LEU	2.2
1	A	129	ASN	2.2
1	A	914	LEU	2.2
1	A	931	LEU	2.2
1	B	75	LEU	2.2
1	B	456	LEU	2.1
1	B	451	GLY	2.1
1	A	623	ALA	2.1
1	A	773	ALA	2.1
1	B	1061	GLY	2.1
1	B	937	LEU	2.1
1	A	444	TYR	2.1
1	A	1230	MET	2.1
1	A	936	ASP	2.1
1	A	1002[A]	GLY	2.1
1	B	74	ALA	2.0
1	B	71	LEU	2.0
1	A	796	ASP	2.0
1	B	438	ASP	2.0
1	B	919	GLY	2.0
1	A	479	HIS	2.0
1	B	1062	ALA	2.0
1	B	113	ASP	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)

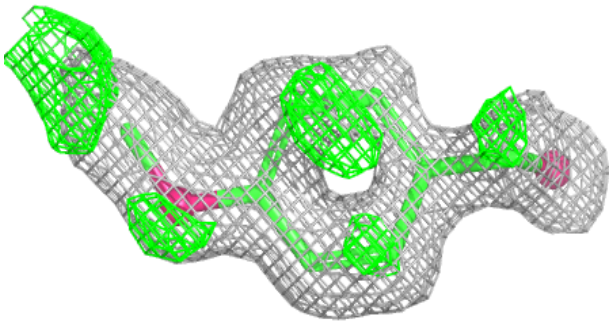
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

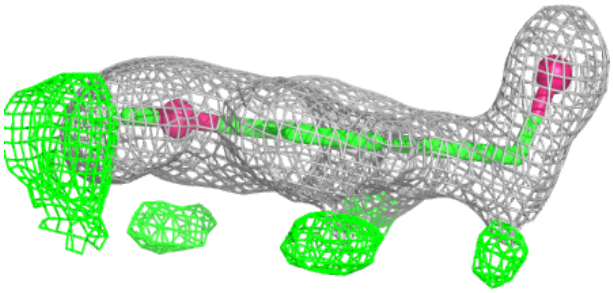
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGE	B	2009	10/10	0.74	0.15	34,43,47,50	0
6	PEG	A	2005	7/7	0.80	0.14	27,37,42,43	0
6	PEG	A	2006	7/7	0.80	0.13	41,43,46,54	0
6	PEG	B	2003	7/7	0.83	0.14	28,35,44,44	0
4	PGE	A	2003	10/10	0.84	0.13	30,41,43,49	0
4	PGE	B	2005	10/10	0.87	0.12	30,36,43,45	0
10	1PE	B	2010	16/16	0.87	0.13	28,38,47,48	0
3	A1BDD	B	2002	10/10	0.89	0.12	19,21,24,25	10
5	FMT	B	2006	3/3	0.90	0.12	20,20,21,28	3
5	FMT	A	2004	3/3	0.92	0.10	21,21,36,36	0
3	A1BDD	A	2002	10/10	0.92	0.12	17,21,27,30	10
5	FMT	B	2007	3/3	0.92	0.11	14,14,18,19	3
8	SO4	A	2010	5/5	0.92	0.10	38,42,45,47	5
8	SO4	A	2011	5/5	0.92	0.13	30,35,45,45	5
5	FMT	B	2008	3/3	0.92	0.10	14,14,32,35	0
3	A1BDD	B	2004	10/10	0.94	0.09	16,19,29,29	10
8	SO4	A	2009	5/5	0.96	0.08	22,28,35,38	5
2	FAD	A	2001[B]	53/53	0.96	0.07	15,19,21,23	53
2	FAD	A	2001[A]	53/53	0.96	0.07	14,18,22,24	53
7	NAD	A	2007	44/44	0.96	0.08	16,21,25,30	0
2	FAD	B	2001[A]	53/53	0.97	0.07	14,17,21,23	53
9	MG	B	2013	1/1	0.97	0.11	23,23,23,23	0
2	FAD	B	2001[B]	53/53	0.97	0.07	14,17,21,23	53
9	MG	A	2012	1/1	0.98	0.11	26,26,26,26	0
7	NAD	B	2011	44/44	0.98	0.06	13,15,18,29	0
8	SO4	B	2012	5/5	0.98	0.06	16,17,21,22	0
8	SO4	A	2008	5/5	0.99	0.05	18,18,22,22	0

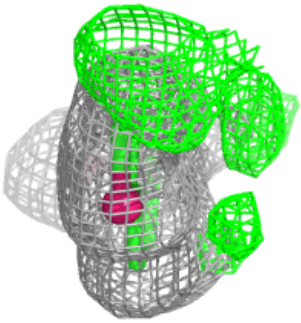
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BDD 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)

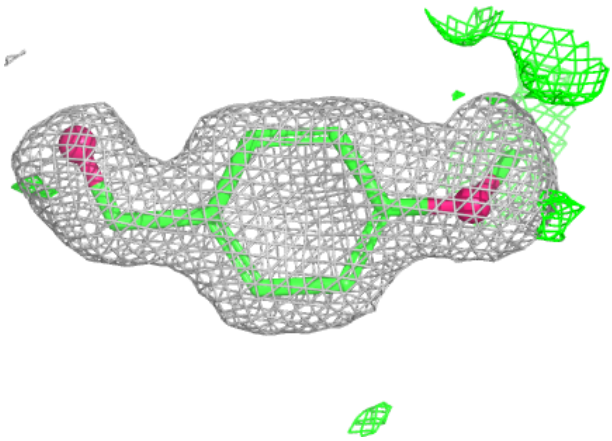


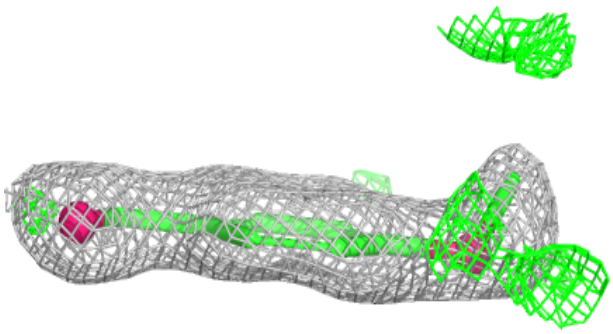


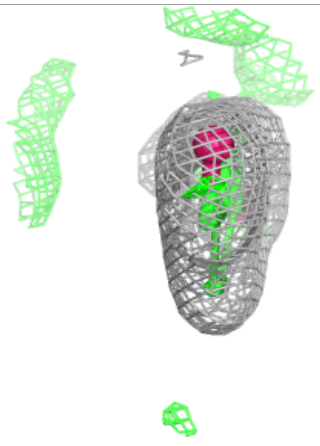


Electron density around A1BDD A 2002:

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

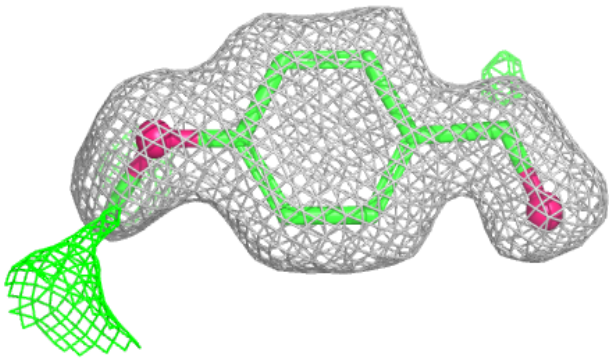


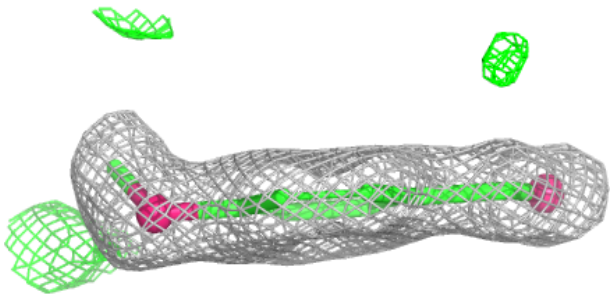


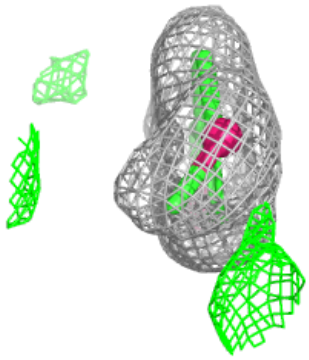


Electron density around A1BDD B 2004:

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

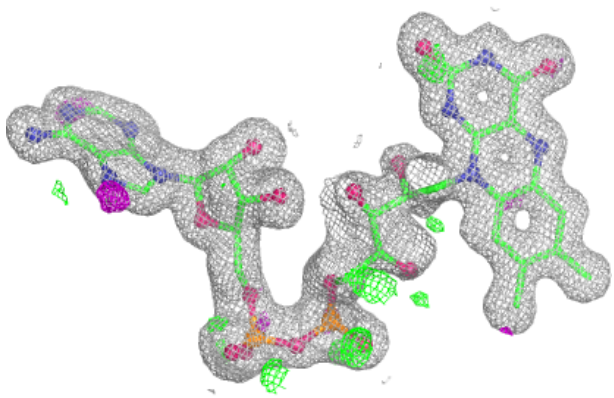


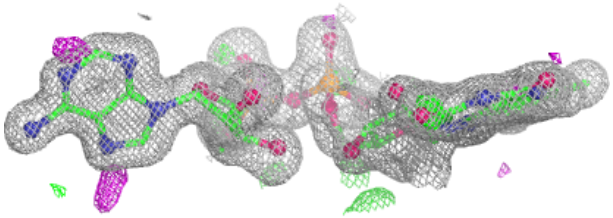


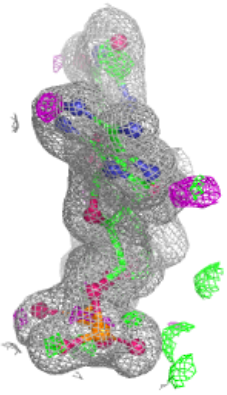


Electron density around FAD A 2001 (B):

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

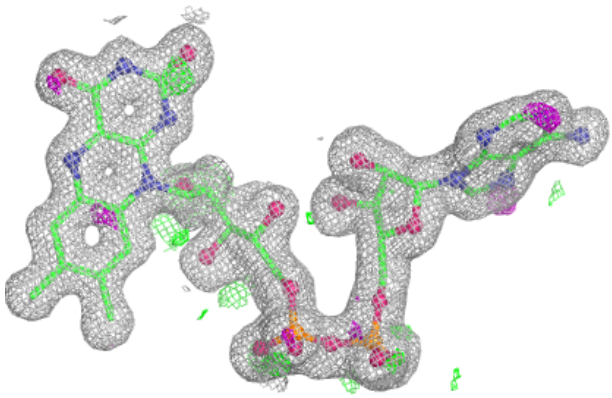


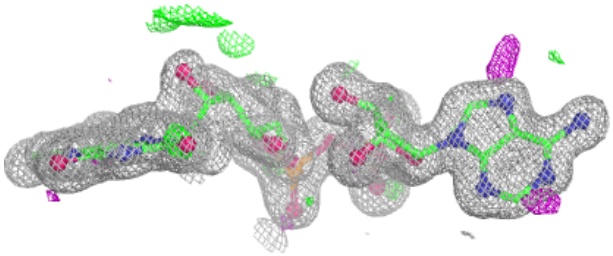


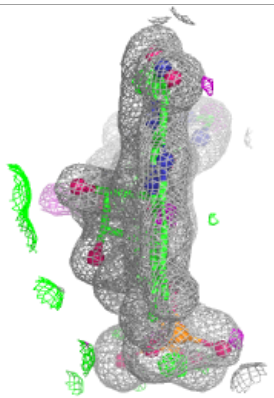


Electron density around FAD A 2001 (A):

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

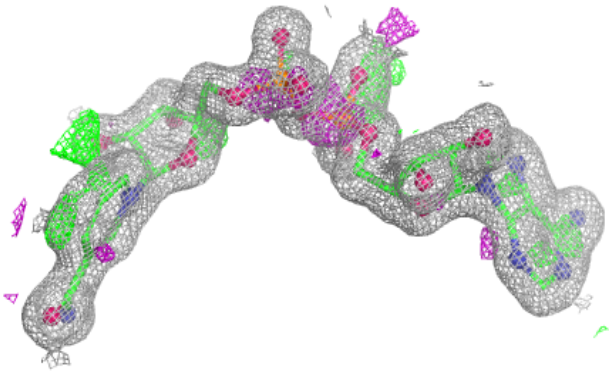


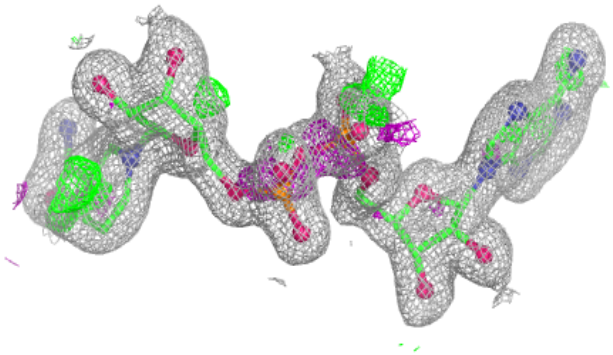


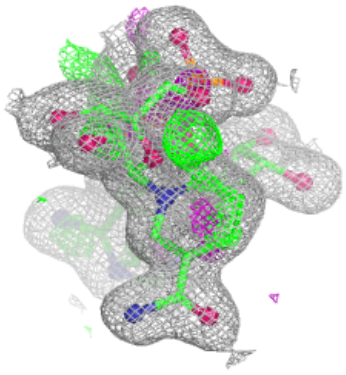


Electron density around NAD A 2007:

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

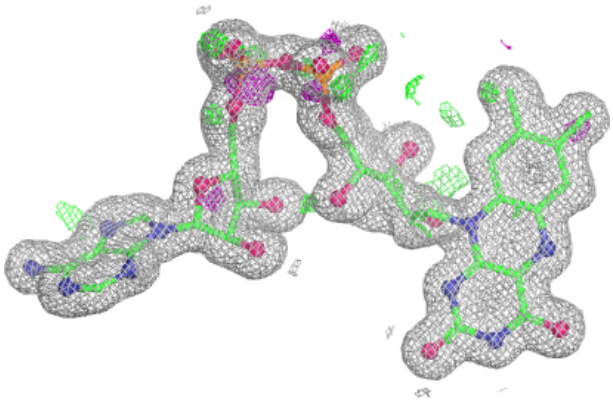


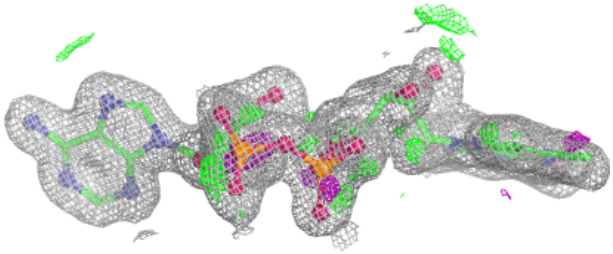


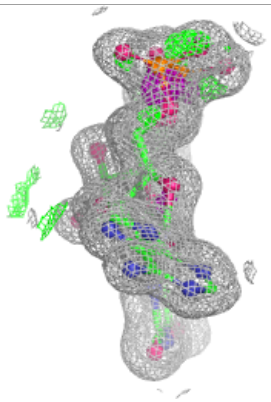


Electron density around FAD B 2001 (A):

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

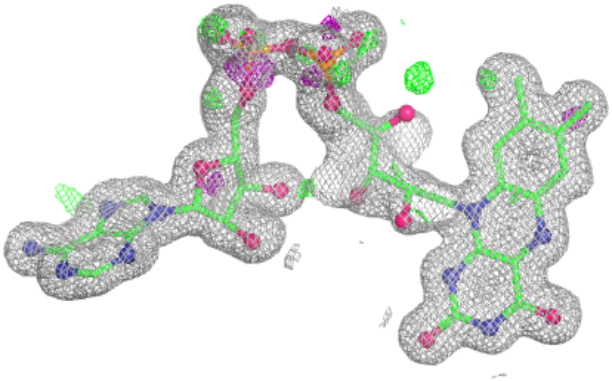


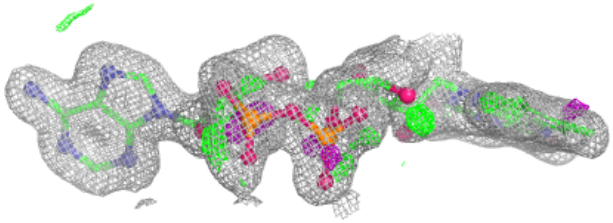


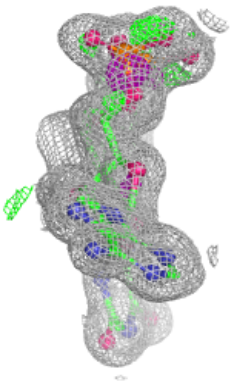


Electron density around FAD B 2001 (B):

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

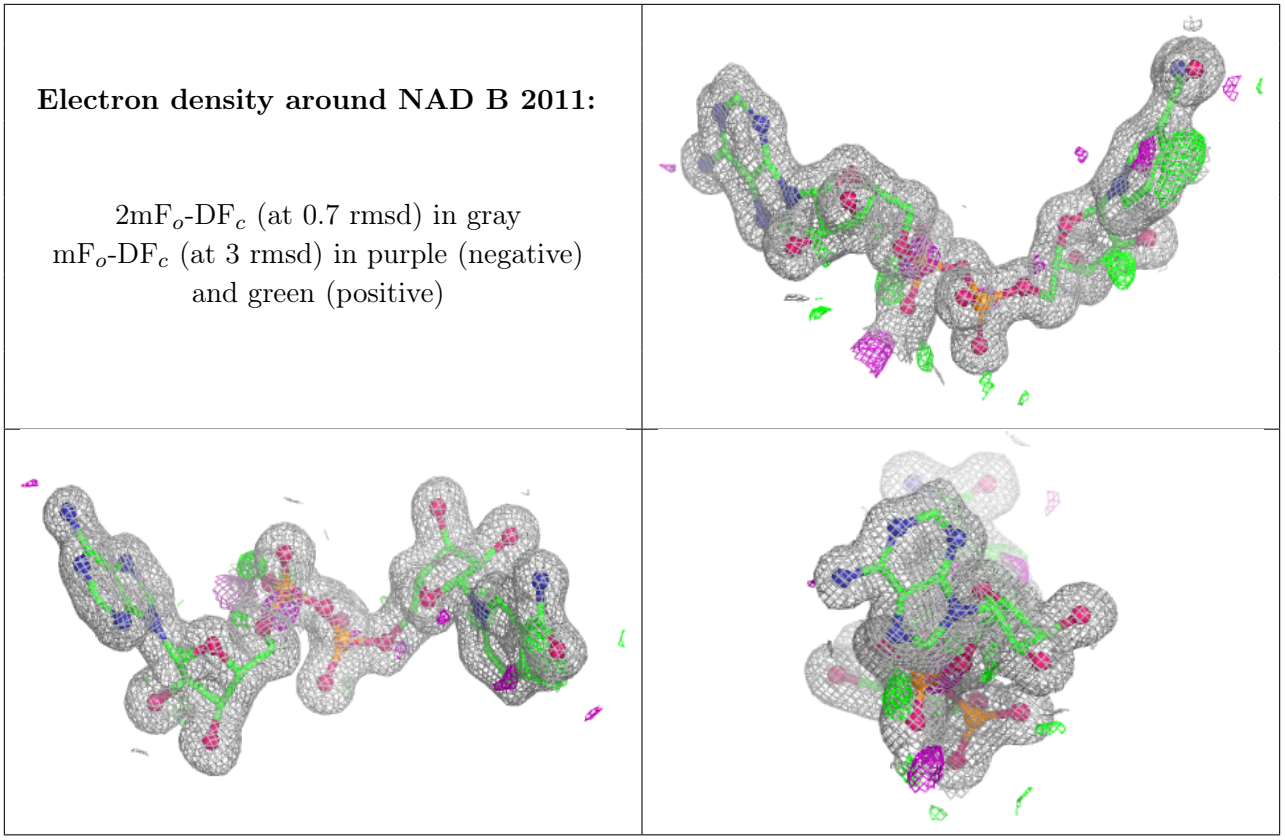






Electron density around NAD B 2011:

$2mF_o$-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.