Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2024 – 04:16 PM EST

PDB ID	:	9DL2
Title	:	Structure of proline utilization A complexed with 2,3-dihydro-1,4-benzodioxine-5-carboxylic acid
Authors	:	Tanner, J.J.; Meeks, K.R.
Deposited on	:	2024-09-10
Resolution	:	1.55 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:

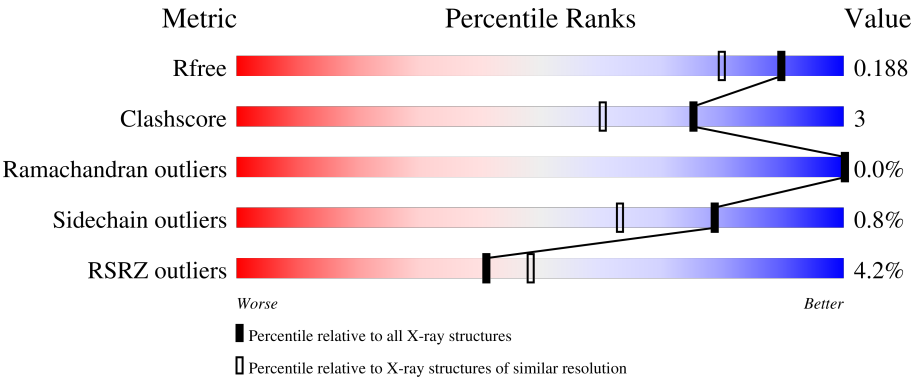
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (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 1.55 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	1935 (1.56-1.56)
Clashscore	180529	2073 (1.56-1.56)
Ramachandran outliers	177936	2037 (1.56-1.56)
Sidechain outliers	177891	2034 (1.56-1.56)
RSRZ outliers	164620	1935 (1.56-1.56)

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	3% 93% 5% ·
1	B	1235	6% 90% 8% ·

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20771 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.

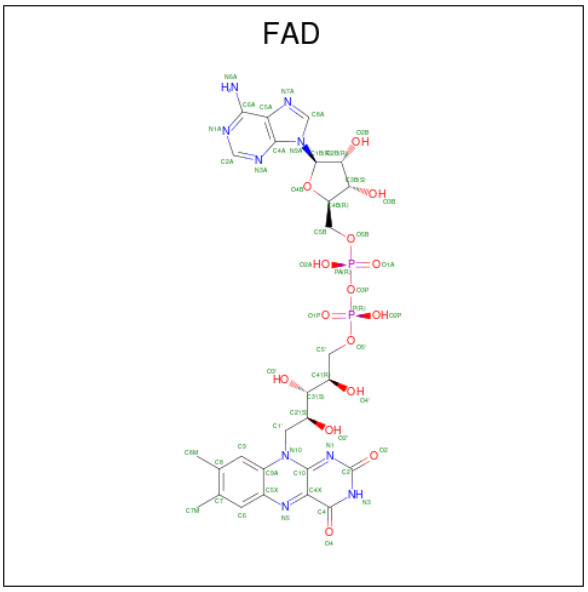
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1216	Total	C	N	O	S	0	25	0
			9102	5750	1615	1701	36			
1	B	1208	Total	C	N	O	S	0	16	0
			8918	5630	1595	1659	34			

There are 4 discrepancies between the modelled and reference sequences:

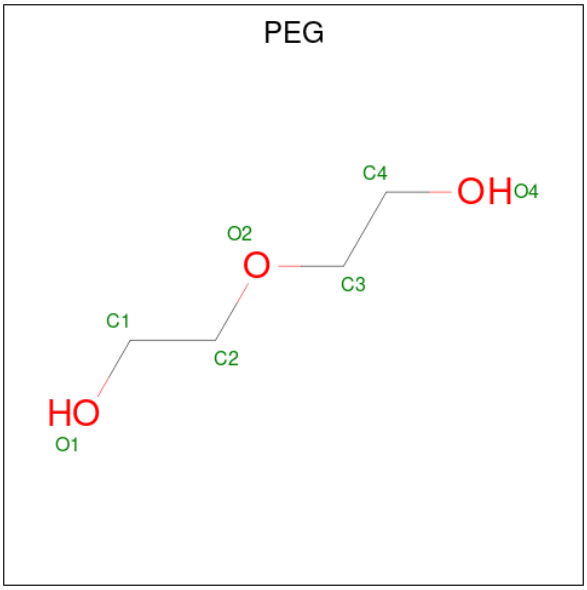
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- 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).



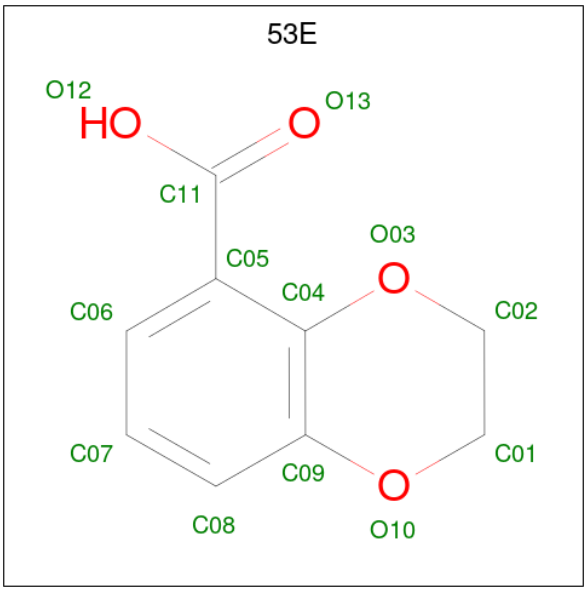
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			106	54	18	30	4		
2	B	1	Total	C	N	O	P	0	1
			106	54	18	30	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



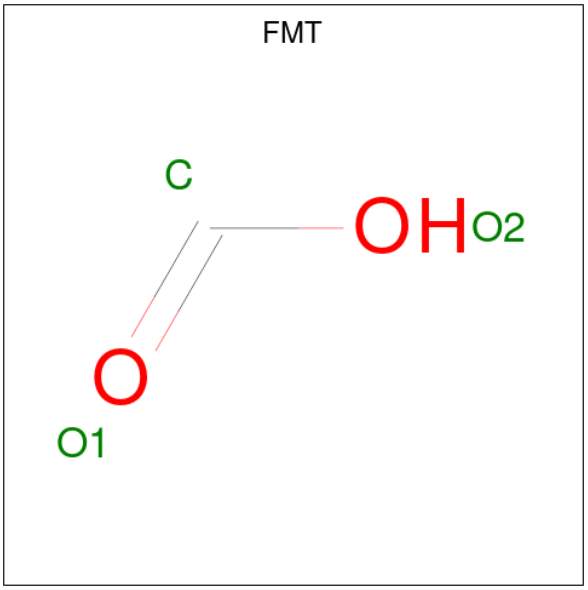
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			7	4	3			
3	A	1	Total	C	O		0	0
			7	4	3			
3	A	1	Total	C	O		0	0
			7	4	3			
3	B	1	Total	C	O		0	0
			7	4	3			
3	B	1	Total	C	O		0	0
			7	4	3			
3	B	1	Total	C	O		0	0
			7	4	3			

- Molecule 4 is 2,3-dihydro-1,4-benzodioxine-5-carboxylic acid (three-letter code: 53E) (formula: $C_9H_8O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 9 4	0	0
4	B	1	Total C O 13 9 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
5	A	1	Total C O 3 1 2	0	0

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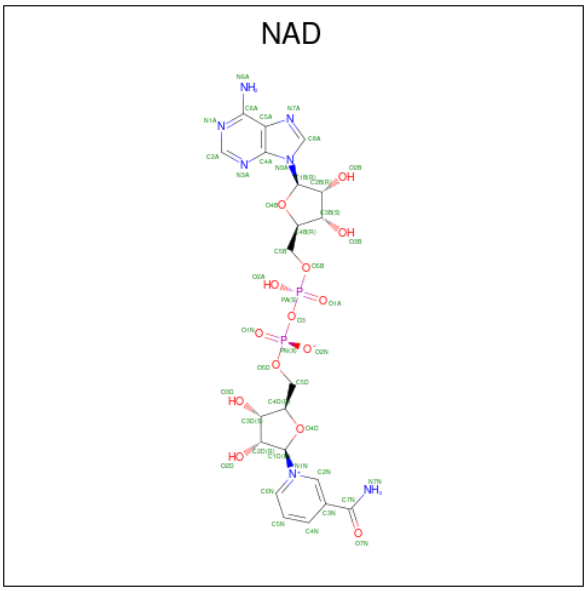
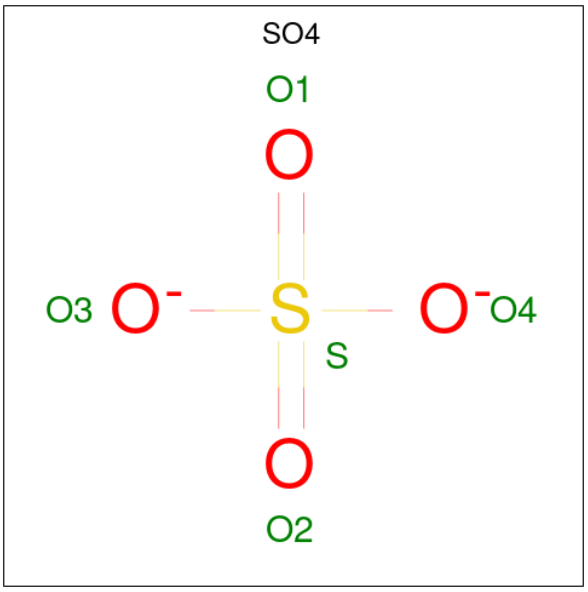
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0

- Molecule 6 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

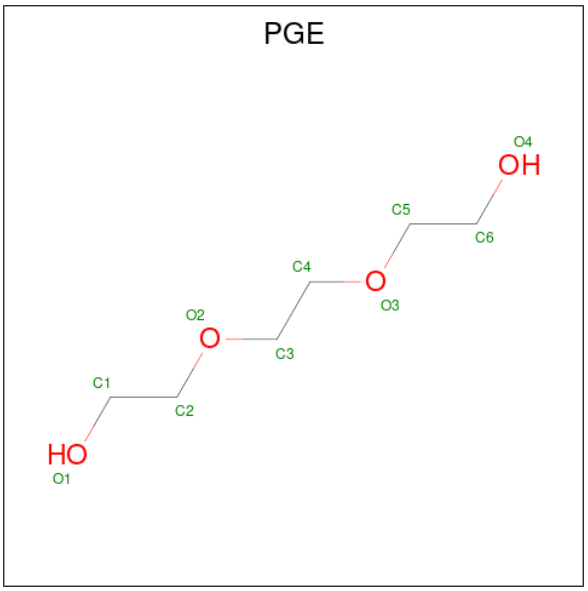


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0

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

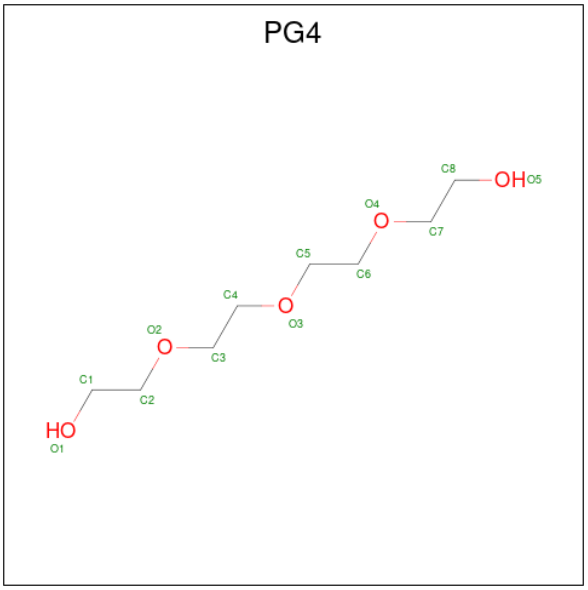
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mg 1 1	0	0
8	B	1	Total Mg 1 1	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 11 is water.

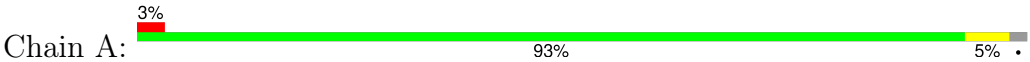
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1191	Total O 1191 1191	0	3
11	B	1120	Total O 1120 1120	0	3

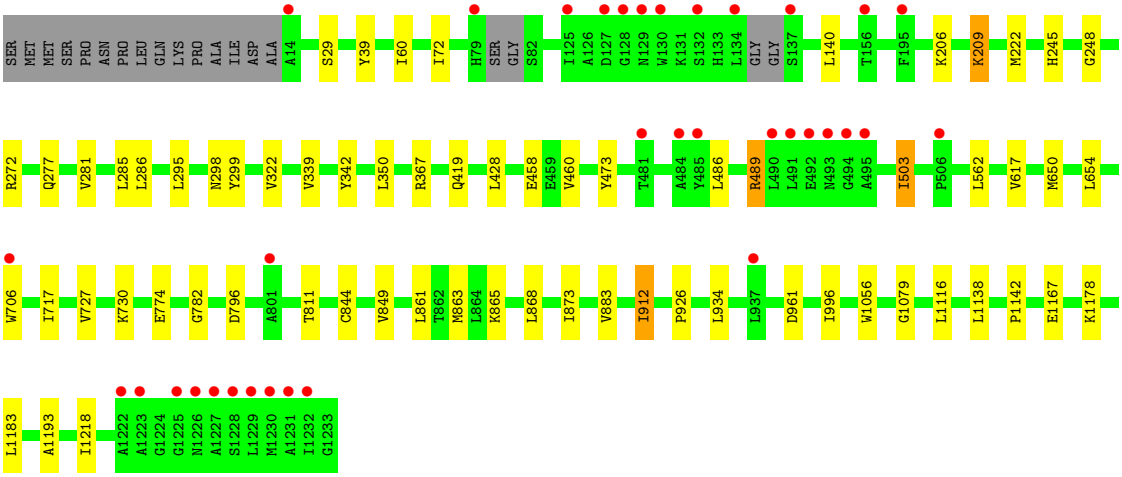
3 Residue-property plots (i)

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

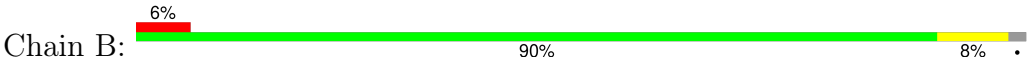
Chain A:

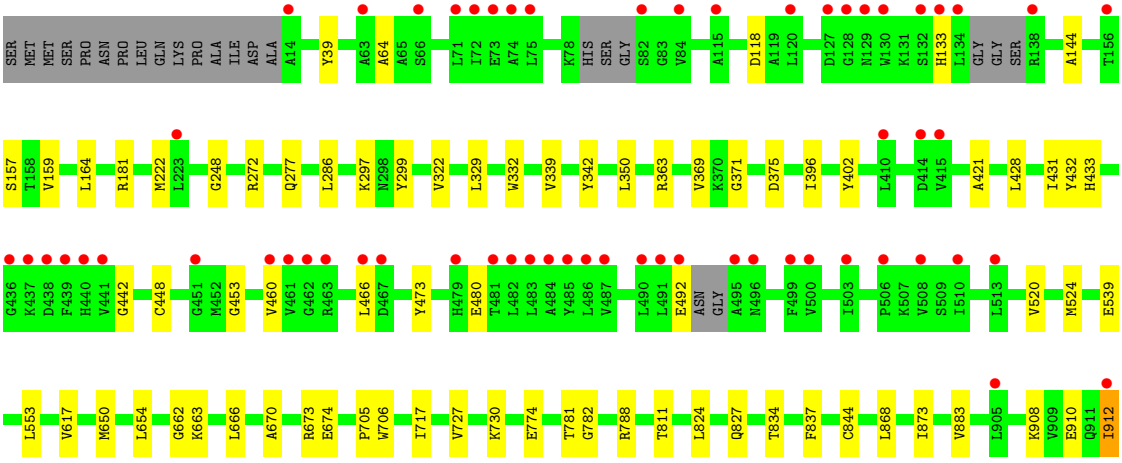


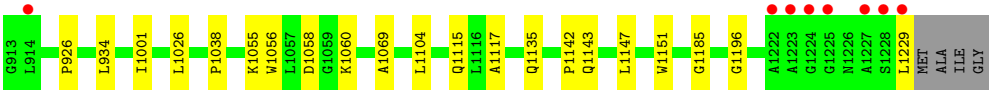


• Molecule 1: Bifunctional protein PutA

Chain B:






G913
L914
P926
L934
I1001
L1026
P1038
K1055
W1056
L1057
D1058
G1059
K1060
A1069
L1104
Q1115
L1116
A1117
Q1135
P1142
Q1143
L1147
W1151
G1185
G1196
A1222
A1223
G1224
G1225
N1226
A1227
S1228
L1229
MET
ALA
ILE
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.40Å 101.72Å 126.29Å 90.00° 106.23° 90.00°	Depositor
Resolution (Å)	46.90 – 1.55 46.90 – 1.55	Depositor EDS
% Data completeness (in resolution range)	94.5 (46.90-1.55) 98.2 (46.90-1.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.167 , 0.190 0.166 , 0.188	Depositor DCC
R_{free} test set	17581 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.8	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	20771	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 53E, FAD, PG4, SO4, PGE, PEG, 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	0.33	0/9336	0.60	0/12708
1	B	0.33	0/9122	0.61	0/12427
All	All	0.33	0/18458	0.60	0/25135

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

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	9102	0	9173	42	0
1	B	8918	0	8901	61	0
2	A	106	0	62	3	0
2	B	106	0	62	6	0
3	A	21	0	30	1	0
3	B	21	0	30	4	0
4	A	13	0	7	1	0
4	B	13	0	7	1	0
5	A	6	0	2	1	0
5	B	6	0	2	0	0
6	A	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	44	0	26	2	0
7	A	25	0	0	1	0
7	B	10	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	B	10	0	14	0	0
10	B	13	0	18	0	0
11	A	1191	0	0	7	0
11	B	1120	0	0	12	0
All	All	20771	0	18360	108	0

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

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:GLY:HA2	3:A:2002:PEG:H22	1.51	0.91
1:B:674:GLU:OE1	11:B:2101:HOH:O	1.98	0.81
1:B:673:ARG:HH11	3:B:2005:PEG:H41	1.46	0.78
1:A:473:TYR:HB2	2:A:2001[A]:FAD:HM72	1.69	0.73
1:B:873:ILE:HG13	1:B:883:VAL:HB	1.71	0.72
1:B:539:GLU:OE1	11:B:2102:HOH:O	2.10	0.70
1:A:339[B]:VAL:HG21	1:A:350:LEU:HD21	1.74	0.69
1:B:473:TYR:HB2	2:B:2001[B]:FAD:HM72	1.75	0.68
1:A:706:TRP:NE1	6:A:2008:NAD:O1N	2.27	0.68
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.76	0.68
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.27	0.67
1:B:339:VAL:HG21	1:B:350:LEU:HD21	1.76	0.67
1:A:281:VAL:HG13	1:A:285[B]:LEU:HD23	1.77	0.67
1:A:473:TYR:HB2	2:A:2001[B]:FAD:HM72	1.79	0.65
1:B:1196:GLY:HA3	3:B:2007:PEG:H22	1.78	0.65
1:B:473:TYR:HB2	2:B:2001[A]:FAD:HM72	1.80	0.63
1:A:796:ASP:HA	1:A:1178:LYS:NZ	2.16	0.61
7:A:2012:SO4:O4	11:A:2101:HOH:O	2.15	0.60
1:B:650:MET:O	1:B:654:LEU:HG	2.00	0.60
1:B:375[B]:ASP:OD1	11:B:2103:HOH:O	2.16	0.60
1:B:524[B]:MET:SD	11:B:2662:HOH:O	2.56	0.60
1:A:458:GLU:OE1	11:A:2102:HOH:O	2.16	0.59
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.84	0.59
1:B:663[B]:LYS:NZ	11:B:2105:HOH:O	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.86	0.58
1:A:1183:LEU:O	11:A:2103:HOH:O	2.16	0.58
1:A:222:MET:HG2	11:A:2115:HOH:O	2.03	0.57
1:B:844:CYS:SG	6:B:2010:NAD:C4N	2.92	0.56
1:B:480:GLU:O	11:B:2104:HOH:O	2.18	0.56
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.88	0.55
1:B:706:TRP:NE1	6:B:2010:NAD:O1N	2.38	0.55
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.89	0.55
1:A:650:MET:O	1:A:654:LEU:HG	2.07	0.55
1:A:473:TYR:CB	2:A:2001[B]:FAD:HM72	2.37	0.55
1:A:849:VAL:HG11	1:A:934:LEU:HD13	1.90	0.53
1:A:861[A]:LEU:HG	1:A:865:LYS:HE3	1.90	0.53
1:A:29:SER:HB2	5:A:2006:FMT:H	1.91	0.53
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.44	0.53
1:B:428:LEU:HD11	1:B:460:VAL:HG21	1.91	0.52
1:B:118:ASP:OD1	1:B:181:ARG:NH2	2.42	0.52
1:B:834[A]:THR:HG22	1:B:1001:ILE:HD11	1.92	0.51
1:B:473:TYR:CB	2:B:2001[A]:FAD:HM72	2.40	0.50
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	1.94	0.50
1:B:448:CYS:HB2	1:B:453:GLY:HA3	1.93	0.50
1:A:796:ASP:HA	1:A:1178:LYS:HZ1	1.76	0.50
1:A:298:ASN:ND2	11:A:2109:HOH:O	2.29	0.49
1:B:371:GLY:N	2:B:2001[B]:FAD:O2'	2.45	0.49
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.48	0.49
1:B:222:MET:HG2	11:B:2175:HOH:O	2.12	0.49
1:B:375[A]:ASP:OD1	1:B:1229:LEU:HB3	2.13	0.49
4:B:2004:53E:H3	11:B:2911:HOH:O	2.12	0.48
1:B:662:GLY:HA2	11:B:2167:HOH:O	2.13	0.48
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.94	0.48
1:A:1116[B]:LEU:HD11	1:A:1138:LEU:HD11	1.95	0.47
1:B:1058:ASP:OD1	11:B:2108:HOH:O	2.20	0.47
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.95	0.47
1:A:617:VAL:HG12	1:A:774:GLU:HB2	1.96	0.47
1:B:363:ARG:NH1	1:B:442:GLY:O	2.45	0.47
1:A:844:CYS:SG	6:A:2008:NAD:C4N	3.02	0.47
1:B:375[B]:ASP:OD1	11:B:2107:HOH:O	2.19	0.47
1:B:432:TYR:CZ	1:B:466:LEU:HD22	2.50	0.47
1:B:553:LEU:HD12	1:B:666[B]:LEU:HD13	1.96	0.46
1:B:788:ARG:NH2	1:B:1185:GLY:O	2.46	0.46
4:A:2003:53E:H3	11:A:2909:HOH:O	2.16	0.46
1:B:1143:GLN:O	1:B:1147:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562[A]:LEU:HD11	1:A:654:LEU:HD12	1.99	0.45
1:B:782:GLY:O	1:B:811:THR:HA	2.16	0.45
1:B:159:VAL:HG13	1:B:164:LEU:HD12	1.97	0.45
1:B:837:PHE:CE2	1:B:868:LEU:HD21	2.52	0.44
1:A:72:ILE:HG23	1:A:503:ILE:HD12	1.99	0.44
2:B:2001[A]:FAD:H9	2:B:2001[A]:FAD:H1'1	1.77	0.44
1:A:245:HIS:CE1	1:A:295:LEU:HD11	2.52	0.44
1:B:670:ALA:HB2	3:B:2005:PEG:H32	1.99	0.44
1:A:782:GLY:O	1:A:811:THR:HA	2.17	0.44
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.52	0.44
1:A:861[B]:LEU:HD22	1:A:865:LYS:HE3	2.00	0.43
1:A:717:ILE:HG12	1:A:727:VAL:HG11	2.01	0.43
1:B:705:PRO:HD3	1:B:781:THR:HB	2.00	0.42
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.02	0.42
1:B:837:PHE:CD2	1:B:868:LEU:HD21	2.54	0.42
1:B:144:ALA:HB3	1:B:159:VAL:CG2	2.50	0.42
1:B:396:ILE:HD11	1:B:520:VAL:HB	2.01	0.42
1:B:908:LYS:HE2	1:B:910:GLU:OE2	2.20	0.42
1:B:248:GLY:HA3	1:B:299:TYR:CG	2.55	0.42
1:A:367:ARG:HA	1:A:419:GLN:HB2	2.02	0.41
3:B:2007:PEG:H11	3:B:2007:PEG:H31	1.67	0.41
1:A:486:LEU:HD12	1:A:489:ARG:HG2	2.02	0.41
1:A:428:LEU:HD11	1:A:460:VAL:HG21	2.02	0.41
1:B:1069:ALA:HA	1:B:1117:ALA:HB1	2.02	0.41
2:B:2001[A]:FAD:H1'1	2:B:2001[A]:FAD:H4'	1.82	0.41
1:A:206:LYS:O	1:A:209:LYS:HG3	2.20	0.41
1:B:1060:LYS:HB3	1:B:1060:LYS:HE3	1.82	0.41
1:B:144:ALA:HB3	1:B:159:VAL:HG21	2.02	0.41
1:B:617:VAL:HG12	1:B:774:GLU:HB2	2.03	0.41
1:B:1104:LEU:HG	1:B:1115:GLN:HB3	2.02	0.41
1:A:868:LEU:HG	1:A:912:ILE:CG2	2.51	0.41
1:A:1167:GLU:HA	1:A:1193:ALA:O	2.21	0.41
1:B:272:ARG:HB3	1:B:277:GLN:HG3	2.03	0.41
1:B:492:GLU:HA	11:B:2338:HOH:O	2.20	0.41
1:A:912:ILE:HG12	1:A:926:PRO:HD2	2.03	0.41
1:B:912:ILE:HG12	1:B:926:PRO:HD2	2.03	0.41
1:A:863:MET:HE2	1:A:863:MET:HB2	1.88	0.40
1:B:402:TYR:HE1	1:B:431:ILE:HD11	1.86	0.40
1:A:60:ILE:HD12	11:A:2955:HOH:O	2.21	0.40
1:B:1135:GLN:HA	1:B:1151:TRP:CZ2	2.56	0.40
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:VAL:HG12	1:B:421:ALA:HB3	2.02	0.40
1:B:824:LEU:HD23	1:B:827:GLN:HG3	2.02	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	1235/1235 (100%)	1216 (98%)	19 (2%)	0	100 100
1	B	1216/1235 (98%)	1191 (98%)	24 (2%)	1 (0%)	48 26
All	All	2451/2470 (99%)	2407 (98%)	43 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	HIS

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	921/951 (97%)	913 (99%)	8 (1%)	75 58
1	B	882/951 (93%)	876 (99%)	6 (1%)	81 67
All	All	1803/1902 (95%)	1789 (99%)	14 (1%)	79 63

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

Mol	Chain	Res	Type
1	A	39	TYR
1	A	140	LEU
1	A	209	LYS
1	A	342	TYR
1	A	489	ARG
1	A	503	ILE
1	A	730	LYS
1	A	912	ILE
1	B	39	TYR
1	B	157	SER
1	B	342	TYR
1	B	730	LYS
1	B	912	ILE
1	B	934	LEU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	SO4	A	2012	-	4,4,4	0.64	0	6,6,6	0.12	0
7	SO4	A	2010	-	4,4,4	0.66	0	6,6,6	0.29	0
3	PEG	B	2005	-	6,6,6	0.35	0	5,5,5	0.45	0
5	FMT	A	2004	-	2,2,2	0.53	0	1,1,1	0.27	0
3	PEG	B	2007	-	6,6,6	0.24	0	5,5,5	0.22	0
6	NAD	A	2008	8	42,48,48	2.43	11 (26%)	50,73,73	1.72	7 (14%)
3	PEG	B	2003	-	6,6,6	0.24	0	5,5,5	0.28	0
5	FMT	B	2006	-	2,2,2	0.85	0	1,1,1	0.13	0
7	SO4	A	2013	-	4,4,4	0.67	0	6,6,6	0.18	0
7	SO4	B	2012	-	4,4,4	0.69	0	6,6,6	0.14	0
3	PEG	A	2002	-	6,6,6	0.23	0	5,5,5	0.32	0
6	NAD	B	2010	8	42,48,48	2.42	9 (21%)	50,73,73	1.57	6 (12%)
4	53E	B	2004	-	14,14,14	2.02	2 (14%)	18,19,19	0.59	0
2	FAD	A	2001[B]	-	54,58,58	2.30	17 (31%)	71,89,89	1.63	12 (16%)
2	FAD	B	2001[B]	-	54,58,58	2.46	16 (29%)	71,89,89	1.65	15 (21%)
3	PEG	A	2007	-	6,6,6	0.25	0	5,5,5	0.22	0
7	SO4	A	2011	-	4,4,4	0.66	0	6,6,6	0.09	0
5	FMT	B	2008	-	2,2,2	0.65	0	1,1,1	0.17	0
7	SO4	A	2009	-	4,4,4	0.55	0	6,6,6	0.23	0
5	FMT	A	2006	-	2,2,2	0.58	0	1,1,1	0.20	0
2	FAD	A	2001[A]	-	54,58,58	2.27	15 (27%)	71,89,89	1.60	13 (18%)
2	FAD	B	2001[A]	-	54,58,58	2.28	16 (29%)	71,89,89	1.61	14 (19%)
10	PG4	B	2009	-	12,12,12	0.28	0	11,11,11	0.22	0
4	53E	A	2003	-	14,14,14	2.00	2 (14%)	18,19,19	1.00	1 (5%)
9	PGE	B	2002	-	9,9,9	0.33	0	8,8,8	0.40	0
7	SO4	B	2011	-	4,4,4	0.56	0	6,6,6	0.24	0
3	PEG	A	2005	-	6,6,6	0.26	0	5,5,5	0.17	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
2	FAD	B	2001[A]	-	-	5/30/50/50	0/6/6/6
3	PEG	B	2003	-	-	3/4/4/4	-
2	FAD	B	2001[B]	-	-	9/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	2007	-	-	2/4/4/4	-
10	PG4	B	2009	-	-	3/10/10/10	-
3	PEG	B	2005	-	-	3/4/4/4	-
4	53E	A	2003	-	-	4/4/11/11	0/2/2/2
3	PEG	A	2002	-	-	2/4/4/4	-
3	PEG	A	2007	-	-	3/4/4/4	-
6	NAD	B	2010	8	-	2/26/62/62	0/5/5/5
9	PGE	B	2002	-	-	1/7/7/7	-
6	NAD	A	2008	8	-	2/26/62/62	0/5/5/5
4	53E	B	2004	-	-	2/4/11/11	0/2/2/2
2	FAD	A	2001[A]	-	-	7/30/50/50	0/6/6/6
3	PEG	A	2005	-	-	0/4/4/4	-
2	FAD	A	2001[B]	-	-	6/30/50/50	0/6/6/6

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001[B]	FAD	PA-O3P	-10.30	1.48	1.59
6	A	2008	NAD	PA-O3	-9.83	1.48	1.59
6	B	2010	NAD	PA-O3	-9.58	1.49	1.59
2	A	2001[B]	FAD	PA-O3P	-9.20	1.49	1.59
2	B	2001[A]	FAD	PA-O3P	-9.05	1.49	1.59
2	A	2001[A]	FAD	PA-O3P	-8.65	1.50	1.59
2	B	2001[B]	FAD	O4-C4	7.40	1.37	1.23
2	A	2001[B]	FAD	O4-C4	6.92	1.36	1.23
2	A	2001[A]	FAD	O4-C4	6.87	1.36	1.23
2	B	2001[A]	FAD	O4-C4	6.81	1.36	1.23
6	B	2010	NAD	C2N-N1N	6.48	1.42	1.35
2	B	2001[B]	FAD	O2-C2	6.06	1.36	1.24
6	A	2008	NAD	C2N-N1N	5.78	1.41	1.35
2	B	2001[A]	FAD	O2-C2	5.78	1.35	1.24
6	A	2008	NAD	C7N-N7N	5.77	1.43	1.33
6	B	2010	NAD	C7N-N7N	5.74	1.43	1.33
4	B	2004	53E	O10-C09	5.72	1.44	1.37
4	A	2003	53E	O10-C09	5.53	1.43	1.37
2	A	2001[B]	FAD	O2-C2	4.98	1.34	1.24
2	A	2001[A]	FAD	O2-C2	4.81	1.33	1.24
2	A	2001[B]	FAD	C4X-N5	4.44	1.40	1.30
2	B	2001[A]	FAD	C4X-N5	4.26	1.40	1.30
2	A	2001[A]	FAD	C4X-N5	4.16	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001[B]	FAD	C4X-N5	4.07	1.39	1.30
2	A	2001[A]	FAD	P-O3P	3.65	1.63	1.59
4	A	2003	53E	O03-C04	3.52	1.43	1.37
4	B	2004	53E	O03-C04	3.31	1.42	1.37
2	B	2001[B]	FAD	C2-N1	3.31	1.44	1.36
2	A	2001[A]	FAD	C2-N1	3.05	1.43	1.36
2	B	2001[A]	FAD	C2A-N3A	2.99	1.36	1.32
2	A	2001[A]	FAD	C6A-N6A	2.96	1.44	1.34
2	A	2001[B]	FAD	P-O3P	2.95	1.62	1.59
2	A	2001[B]	FAD	C6A-N6A	2.93	1.44	1.34
2	B	2001[B]	FAD	C2A-N3A	2.92	1.36	1.32
2	B	2001[B]	FAD	C6A-N6A	2.91	1.44	1.34
2	B	2001[A]	FAD	C2-N1	2.90	1.43	1.36
2	A	2001[B]	FAD	PA-O5B	-2.89	1.48	1.59
2	A	2001[A]	FAD	PA-O5B	-2.88	1.48	1.59
2	A	2001[A]	FAD	O2'-C2'	-2.86	1.37	1.43
2	B	2001[A]	FAD	C6A-N6A	2.85	1.44	1.34
6	B	2010	NAD	C6A-N6A	2.83	1.44	1.34
2	A	2001[B]	FAD	C2-N1	2.82	1.43	1.36
2	B	2001[B]	FAD	PA-O5B	-2.76	1.48	1.59
6	A	2008	NAD	C2A-N3A	2.71	1.36	1.32
6	B	2010	NAD	C2A-N3A	2.71	1.36	1.32
6	A	2008	NAD	PA-O5B	-2.71	1.48	1.59
2	B	2001[B]	FAD	O2'-C2'	-2.71	1.37	1.43
6	A	2008	NAD	C6A-N6A	2.71	1.43	1.34
2	A	2001[A]	FAD	C2A-N3A	2.68	1.36	1.32
2	B	2001[B]	FAD	C10-N1	2.64	1.38	1.33
6	B	2010	NAD	C6N-N1N	2.62	1.41	1.35
2	A	2001[B]	FAD	C2A-N3A	2.60	1.36	1.32
2	B	2001[B]	FAD	O4'-C4'	-2.59	1.37	1.43
6	A	2008	NAD	C6N-N1N	2.59	1.41	1.35
2	B	2001[A]	FAD	PA-O5B	-2.57	1.49	1.59
2	A	2001[B]	FAD	O4'-C4'	-2.57	1.37	1.43
2	A	2001[A]	FAD	O4'-C4'	-2.55	1.38	1.43
2	A	2001[B]	FAD	O2'-C2'	-2.54	1.38	1.43
2	B	2001[A]	FAD	O2'-C2'	-2.49	1.38	1.43
6	B	2010	NAD	PA-O5B	-2.45	1.49	1.59
2	A	2001[B]	FAD	C1B-N9A	-2.44	1.43	1.49
2	B	2001[A]	FAD	C10-N1	2.44	1.38	1.33
2	A	2001[A]	FAD	C1B-N9A	-2.40	1.44	1.49
2	B	2001[A]	FAD	O4B-C4B	-2.40	1.39	1.45
2	A	2001[B]	FAD	O4B-C4B	-2.35	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001[A]	FAD	C1B-N9A	-2.35	1.44	1.49
2	B	2001[B]	FAD	O4B-C4B	-2.34	1.39	1.45
2	B	2001[A]	FAD	O4'-C4'	-2.33	1.38	1.43
2	A	2001[A]	FAD	O4B-C4B	-2.31	1.39	1.45
2	A	2001[B]	FAD	C10-N1	2.29	1.37	1.33
2	B	2001[B]	FAD	PA-O2A	-2.25	1.44	1.55
2	B	2001[B]	FAD	C1B-N9A	-2.23	1.44	1.49
6	A	2008	NAD	O3D-C3D	-2.21	1.37	1.43
2	A	2001[A]	FAD	PA-O2A	-2.21	1.45	1.55
2	A	2001[B]	FAD	PA-O2A	-2.19	1.45	1.55
2	B	2001[B]	FAD	O2B-C2B	-2.17	1.37	1.43
2	B	2001[A]	FAD	PA-O2A	-2.17	1.45	1.55
2	B	2001[A]	FAD	O2B-C2B	-2.14	1.37	1.43
2	B	2001[B]	FAD	P-O1P	2.11	1.58	1.50
6	B	2010	NAD	O4D-C4D	-2.11	1.40	1.45
6	A	2008	NAD	C2D-C3D	-2.10	1.47	1.53
6	A	2008	NAD	O4D-C4D	-2.10	1.40	1.45
2	A	2001[A]	FAD	P-O1P	2.09	1.58	1.50
2	A	2001[B]	FAD	P-O1P	2.06	1.57	1.50
2	B	2001[A]	FAD	P-O1P	2.04	1.57	1.50
2	A	2001[B]	FAD	O3'-C3'	-2.03	1.37	1.43
6	A	2008	NAD	PA-O2A	-2.02	1.46	1.55
6	B	2010	NAD	O3D-C3D	-2.02	1.38	1.43

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	2008	NAD	N3A-C2A-N1A	-6.81	119.43	128.67
6	B	2010	NAD	N3A-C2A-N1A	-6.74	119.52	128.67
2	B	2001[A]	FAD	N3A-C2A-N1A	-6.52	119.83	128.67
2	B	2001[B]	FAD	N3A-C2A-N1A	-6.38	120.01	128.67
2	A	2001[A]	FAD	N3A-C2A-N1A	-6.28	120.15	128.67
2	A	2001[B]	FAD	N3A-C2A-N1A	-6.26	120.17	128.67
2	B	2001[B]	FAD	O2P-P-O3P	-5.25	93.09	107.27
6	A	2008	NAD	C4B-O4B-C1B	-4.45	105.85	109.92
2	B	2001[A]	FAD	O2P-P-O3P	-4.39	95.40	107.27
6	A	2008	NAD	C4D-O4D-C1D	-4.37	105.92	109.92
2	A	2001[B]	FAD	O2P-P-O3P	-3.98	96.51	107.27
2	A	2001[A]	FAD	O2P-P-O3P	-3.90	96.72	107.27
2	A	2001[A]	FAD	C4-C4X-N5	3.82	123.48	118.21
6	A	2008	NAD	O2A-PA-O3	-3.72	97.21	107.27
6	B	2010	NAD	C4D-O4D-C1D	-3.68	106.55	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001[B]	FAD	C4-C4X-N5	3.63	123.22	118.21
2	B	2001[B]	FAD	O2A-PA-O3P	-3.57	97.62	107.27
2	B	2001[B]	FAD	O3P-P-O1P	3.39	120.89	110.70
2	A	2001[A]	FAD	C4-N3-C2	-3.36	119.67	125.64
6	B	2010	NAD	C4B-O4B-C1B	-3.29	106.91	109.92
2	B	2001[A]	FAD	O3P-P-O1P	3.17	120.23	110.70
2	A	2001[B]	FAD	C4X-C4-N3	3.11	121.16	113.25
2	B	2001[A]	FAD	C4-C4X-N5	2.98	122.33	118.21
2	A	2001[B]	FAD	C4-N3-C2	-2.95	120.40	125.64
2	A	2001[A]	FAD	C4X-C4-N3	2.88	120.60	113.25
2	A	2001[B]	FAD	C9-C9A-N10	-2.79	118.11	121.85
2	A	2001[A]	FAD	O2A-PA-O3P	-2.76	99.82	107.27
2	A	2001[B]	FAD	O2A-PA-O3P	-2.75	99.85	107.27
2	B	2001[B]	FAD	C4-C4X-N5	2.72	121.97	118.21
2	A	2001[B]	FAD	O4-C4-C4X	-2.71	119.37	126.53
2	A	2001[B]	FAD	C5X-C9A-N10	2.63	120.35	117.97
2	A	2001[A]	FAD	C4X-C10-N10	2.63	120.24	116.48
2	B	2001[A]	FAD	C4B-O4B-C1B	-2.62	107.52	109.92
2	A	2001[B]	FAD	O3P-P-O1P	2.59	118.49	110.70
2	B	2001[A]	FAD	C9-C9A-N10	-2.58	118.38	121.85
2	A	2001[A]	FAD	C10-C4X-N5	-2.58	119.55	124.81
2	B	2001[B]	FAD	C4-N3-C2	-2.57	121.07	125.64
6	A	2008	NAD	O5B-PA-O1A	2.50	118.83	108.94
2	A	2001[B]	FAD	C4B-O4B-C1B	-2.48	107.65	109.92
2	A	2001[A]	FAD	C4B-O4B-C1B	-2.48	107.66	109.92
2	B	2001[A]	FAD	C4X-C4-N3	2.48	119.56	113.25
2	B	2001[A]	FAD	O2A-PA-O3P	-2.46	100.64	107.27
2	A	2001[A]	FAD	O3P-P-O1P	2.41	117.97	110.70
2	A	2001[B]	FAD	O5'-P-O1P	2.38	118.35	108.94
2	B	2001[A]	FAD	C5X-C9A-N10	2.37	120.11	117.97
6	B	2010	NAD	C3N-C7N-N7N	2.34	120.62	117.74
2	B	2001[A]	FAD	C4-N3-C2	-2.32	121.52	125.64
2	B	2001[B]	FAD	C4X-C4-N3	2.32	119.15	113.25
2	B	2001[B]	FAD	C10-C4X-N5	-2.30	120.11	124.81
2	B	2001[B]	FAD	C4B-O4B-C1B	-2.28	107.84	109.92
2	B	2001[B]	FAD	O3P-PA-O1A	2.24	117.45	110.70
6	B	2010	NAD	O2A-PA-O3	-2.23	101.24	107.27
2	B	2001[B]	FAD	C1'-C2'-C3'	2.22	115.67	109.66
2	B	2001[B]	FAD	O5'-P-O1P	2.21	117.70	108.94
2	B	2001[A]	FAD	O4-C4-C4X	-2.21	120.70	126.53
2	B	2001[B]	FAD	C4X-C10-N10	2.19	119.62	116.48
2	B	2001[A]	FAD	C4X-C10-N10	2.19	119.62	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001[A]	FAD	O2A-PA-O5B	-2.19	97.66	107.57
2	B	2001[B]	FAD	O2A-PA-O5B	-2.16	97.76	107.57
4	A	2003	53E	O12-C11-C05	2.15	121.39	115.28
2	A	2001[A]	FAD	C4X-C10-N1	-2.12	119.40	124.59
2	B	2001[B]	FAD	O4-C4-C4X	-2.06	121.09	126.53
6	B	2010	NAD	O3-PA-O1A	2.05	116.86	110.70
2	B	2001[A]	FAD	O5'-P-O1P	2.02	116.94	108.94
6	A	2008	NAD	C2N-C3N-C4N	2.02	120.61	118.26
2	A	2001[A]	FAD	C9-C9A-N10	-2.01	119.15	121.85
6	A	2008	NAD	O2N-PN-O3	2.01	112.70	107.27
2	A	2001[A]	FAD	O4-C4-C4X	-2.00	121.25	126.53

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001[B]	FAD	N10-C1'-C2'-O2'
2	A	2001[B]	FAD	N10-C1'-C2'-C3'
2	A	2001[B]	FAD	C1'-C2'-C3'-C4'
2	A	2001[B]	FAD	C5'-O5'-P-O2P
2	B	2001[A]	FAD	P-O3P-PA-O5B
2	B	2001[A]	FAD	N10-C1'-C2'-O2'
2	B	2001[A]	FAD	N10-C1'-C2'-C3'
2	B	2001[A]	FAD	C1'-C2'-C3'-C4'
2	B	2001[B]	FAD	C5B-O5B-PA-O3P
2	B	2001[B]	FAD	C1'-C2'-C3'-C4'
6	A	2008	NAD	PN-O3-PA-O5B
2	A	2001[A]	FAD	C2'-C3'-C4'-O4'
4	A	2003	53E	C04-C05-C11-O12
2	A	2001[A]	FAD	C2'-C3'-C4'-C5'
4	A	2003	53E	C04-C05-C11-O13
3	B	2005	PEG	O1-C1-C2-O2
4	B	2004	53E	C04-C05-C11-O12
2	A	2001[A]	FAD	O3'-C3'-C4'-O4'
3	A	2007	PEG	O1-C1-C2-O2
2	A	2001[A]	FAD	O3'-C3'-C4'-C5'
3	A	2002	PEG	O2-C3-C4-O4
4	B	2004	53E	C04-C05-C11-O13
2	B	2001[B]	FAD	C3B-C4B-C5B-O5B
3	A	2002	PEG	C4-C3-O2-C2
3	B	2005	PEG	O2-C3-C4-O4
3	B	2007	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
10	B	2009	PG4	O1-C1-C2-O2
3	B	2007	PEG	O1-C1-C2-O2
2	A	2001[A]	FAD	P-O3P-PA-O5B
2	A	2001[B]	FAD	P-O3P-PA-O5B
2	B	2001[B]	FAD	P-O3P-PA-O5B
2	B	2001[B]	FAD	C1'-C2'-C3'-O3'
3	B	2003	PEG	O2-C3-C4-O4
2	B	2001[B]	FAD	C3'-C4'-C5'-O5'
3	B	2005	PEG	C1-C2-O2-C3
3	B	2003	PEG	C1-C2-O2-C3
10	B	2009	PG4	C1-C2-O2-C3
3	A	2007	PEG	C4-C3-O2-C2
2	A	2001[A]	FAD	C5B-O5B-PA-O3P
2	A	2001[B]	FAD	C5'-O5'-P-O1P
6	B	2010	NAD	C5B-O5B-PA-O1A
6	A	2008	NAD	C4D-C5D-O5D-PN
6	B	2010	NAD	C4D-C5D-O5D-PN
2	A	2001[A]	FAD	C3B-C4B-C5B-O5B
2	B	2001[B]	FAD	O4B-C4B-C5B-O5B
3	B	2003	PEG	C4-C3-O2-C2
3	A	2007	PEG	O2-C3-C4-O4
9	B	2002	PGE	O2-C3-C4-O3
2	B	2001[B]	FAD	C2'-C3'-C4'-O4'
2	B	2001[B]	FAD	O4'-C4'-C5'-O5'
4	A	2003	53E	C06-C05-C11-O12
10	B	2009	PG4	C4-C3-O2-C2
4	A	2003	53E	C06-C05-C11-O13
2	B	2001[A]	FAD	C3B-C4B-C5B-O5B

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2012	SO4	1	0
3	B	2005	PEG	2	0
3	B	2007	PEG	2	0
6	A	2008	NAD	2	0
3	A	2002	PEG	1	0
6	B	2010	NAD	2	0
4	B	2004	53E	1	0
2	A	2001[B]	FAD	2	0
2	B	2001[B]	FAD	2	0

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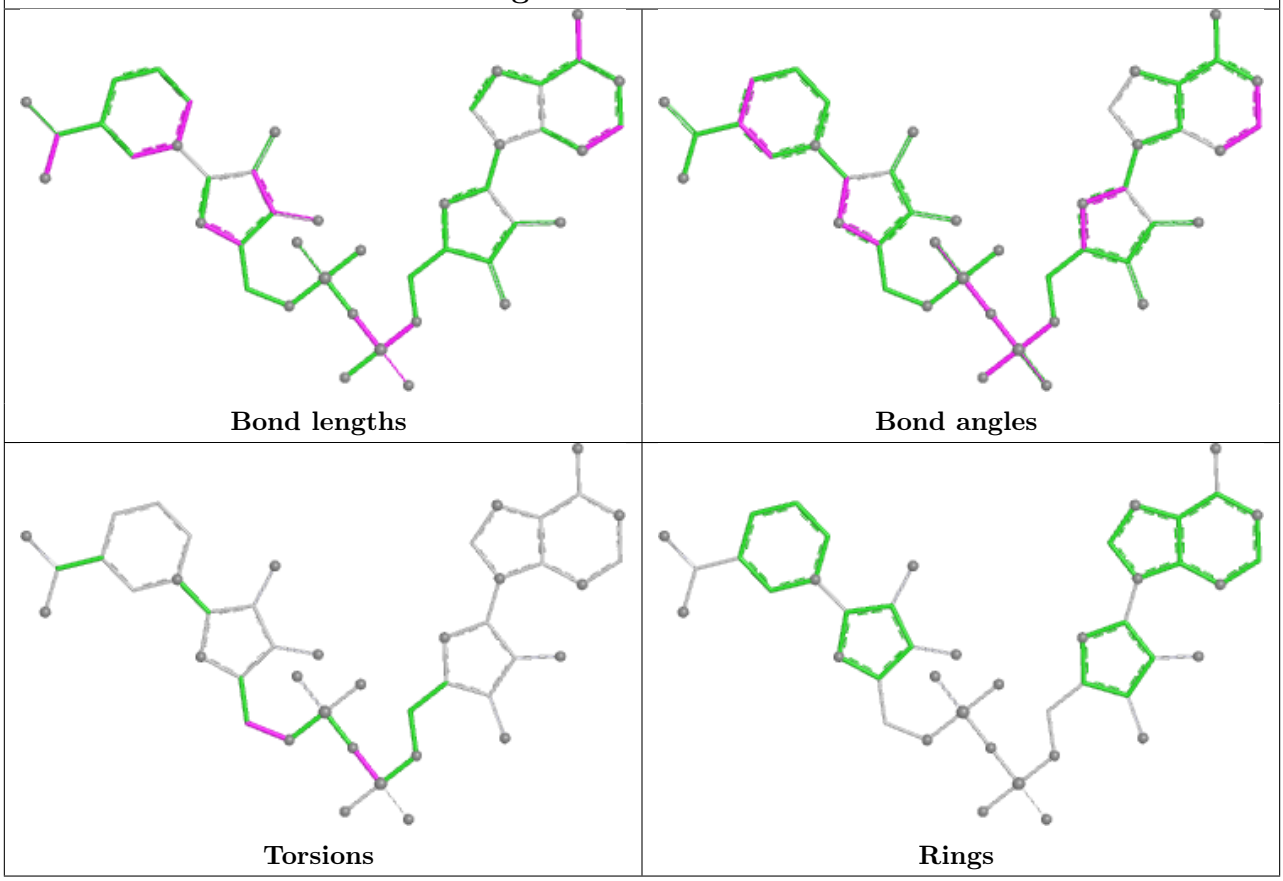
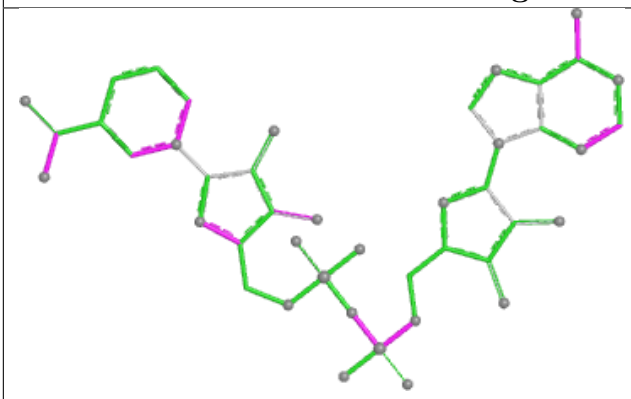
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2006	FMT	1	0
2	A	2001[A]	FAD	1	0
2	B	2001[A]	FAD	4	0
4	A	2003	53E	1	0

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.

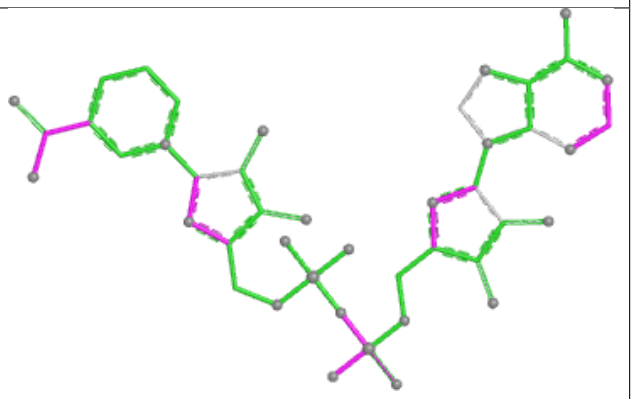
Ligand NAD A 2008



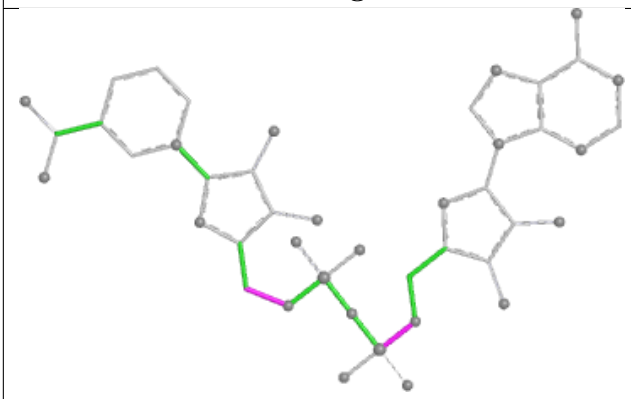
Ligand NAD B 2010



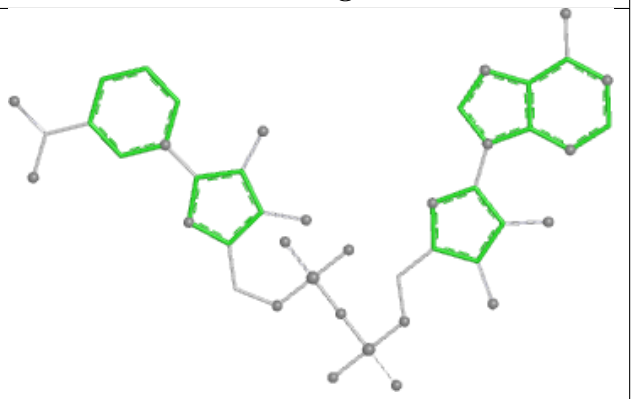
Bond lengths



Bond angles

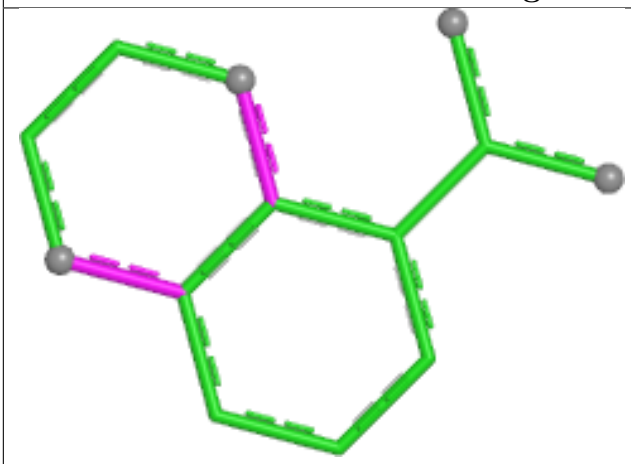


Torsions

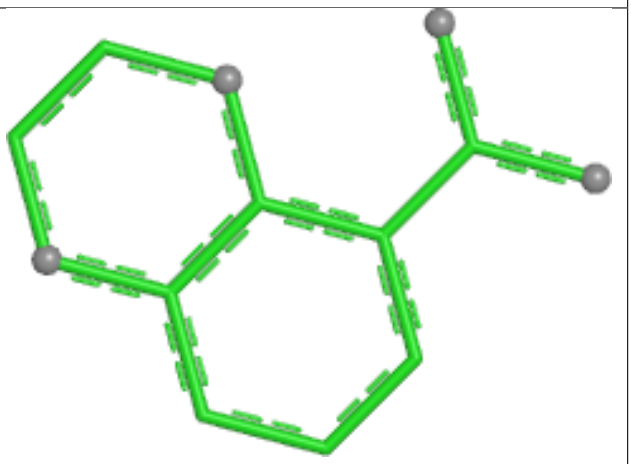


Rings

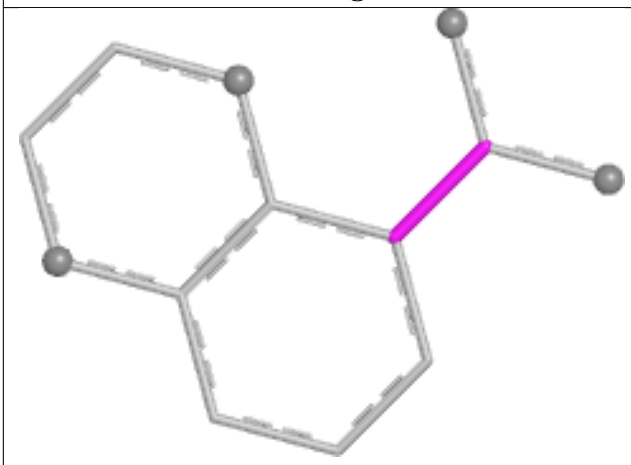
Ligand 53E B 2004



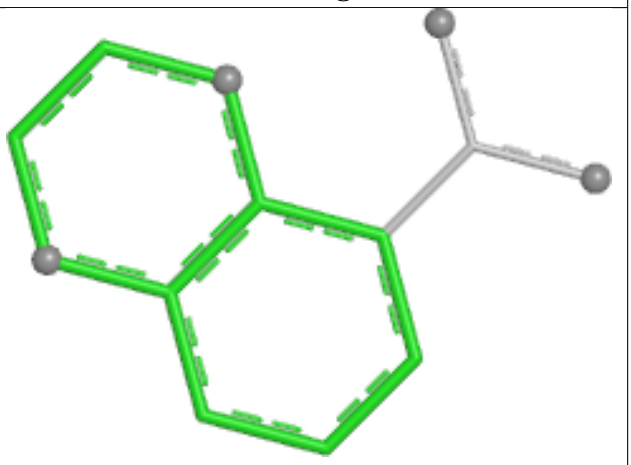
Bond lengths



Bond angles

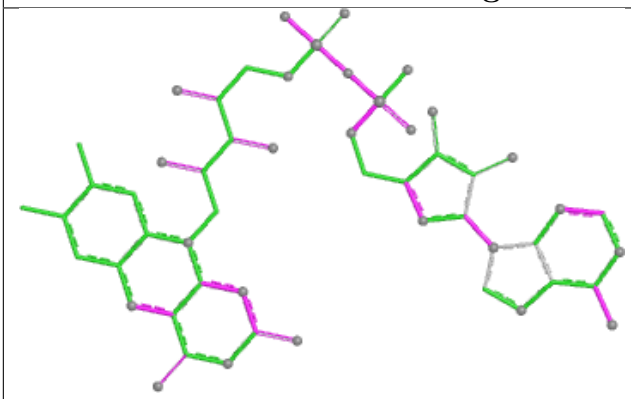


Torsions

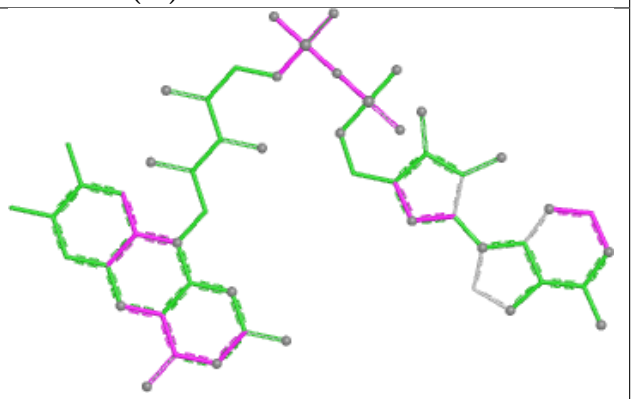


Rings

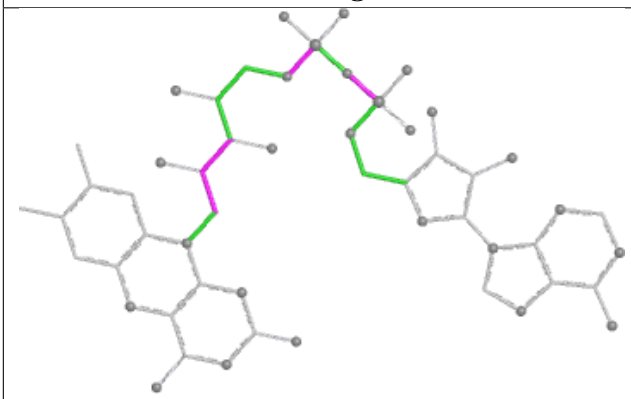
Ligand FAD A 2001 (B)



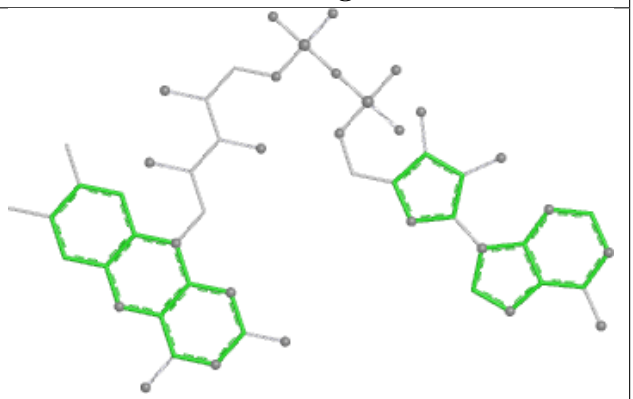
Bond lengths



Bond angles

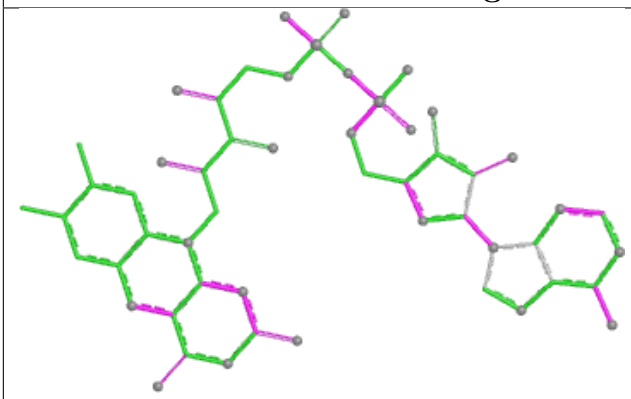


Torsions

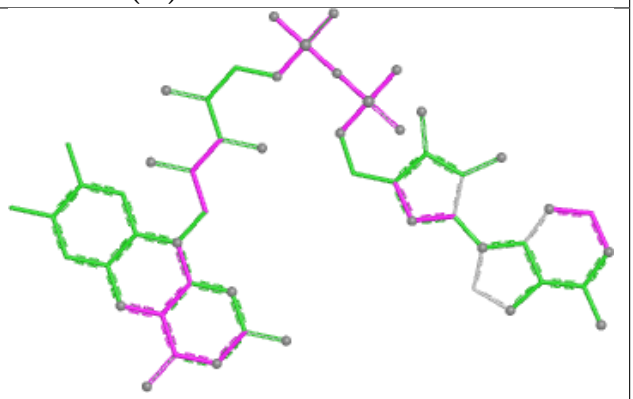


Rings

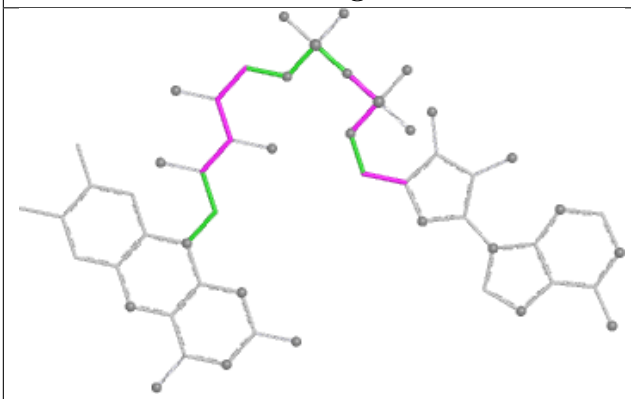
Ligand FAD B 2001 (B)



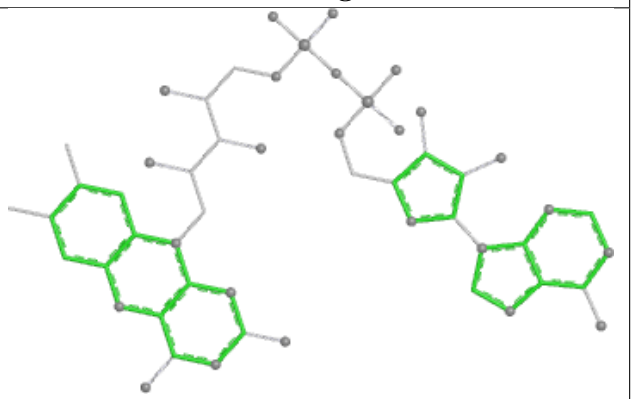
Bond lengths



Bond angles

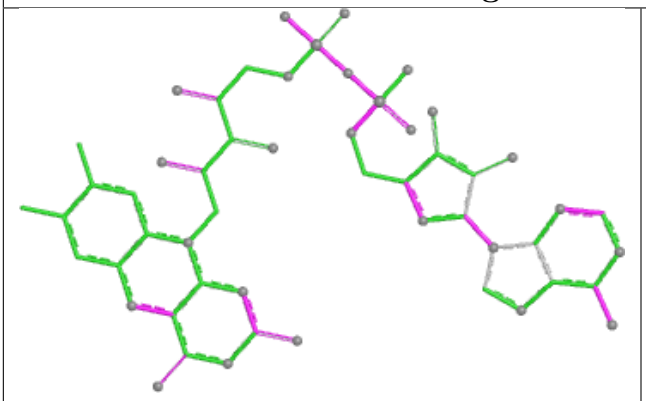


Torsions

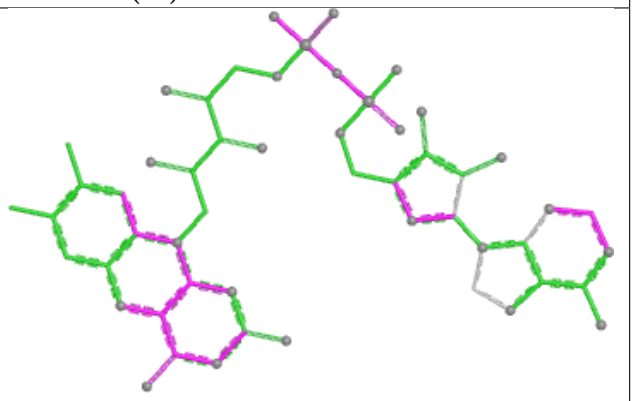


Rings

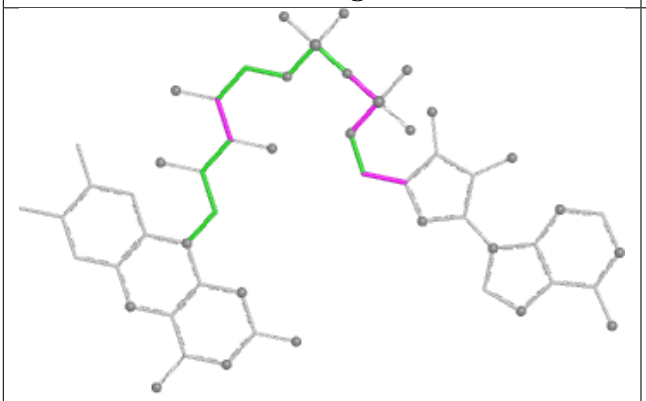
Ligand FAD A 2001 (A)



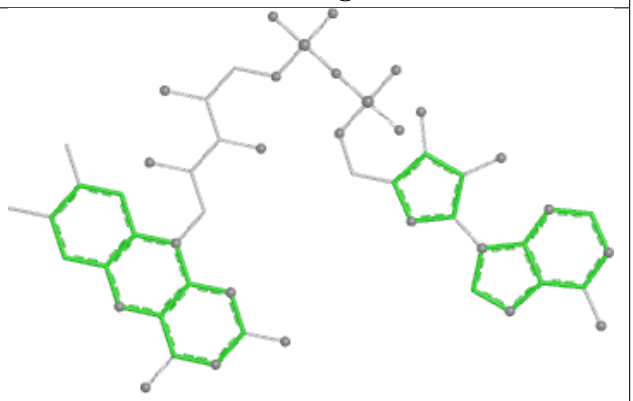
Bond lengths



Bond angles

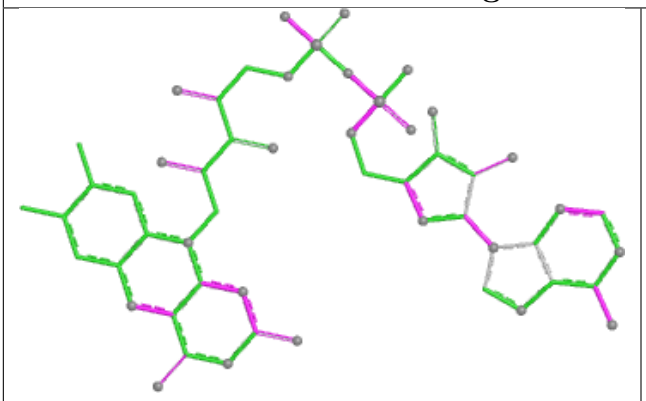


Torsions

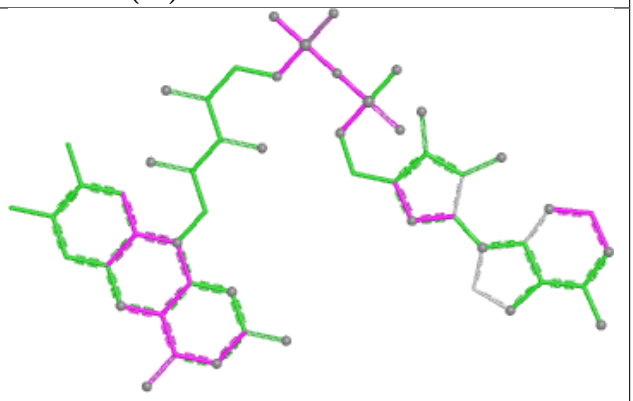


Rings

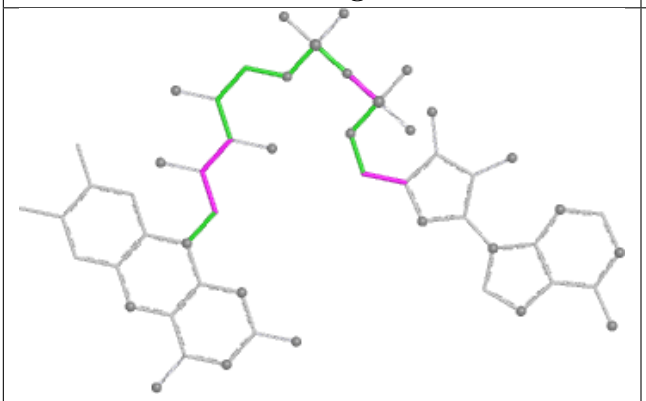
Ligand FAD B 2001 (A)



Bond lengths



Bond angles



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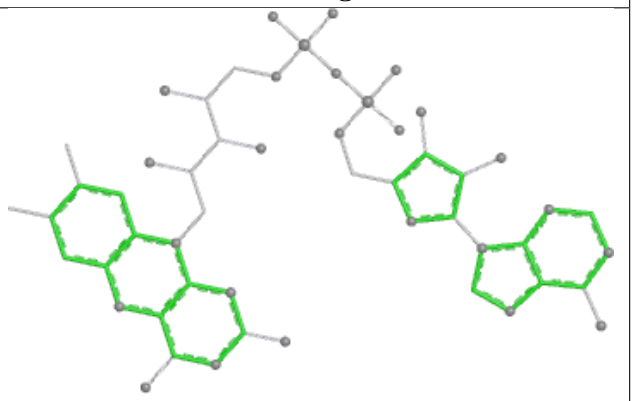
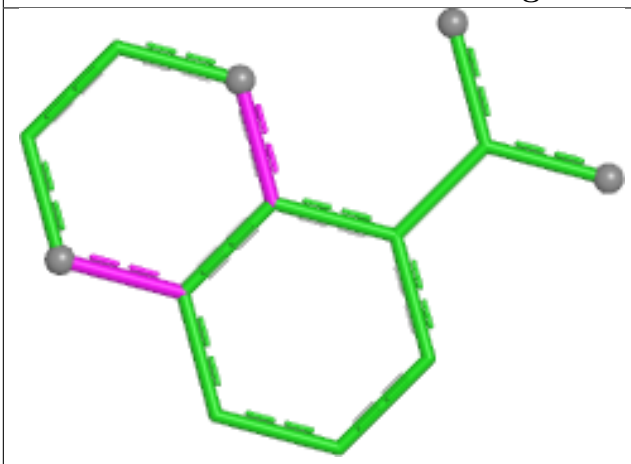
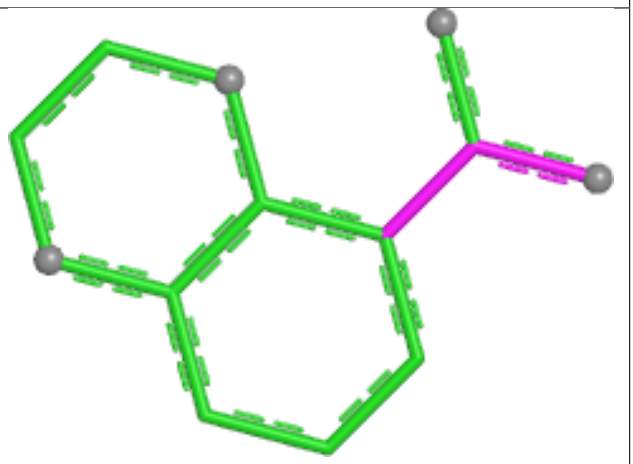


Rings

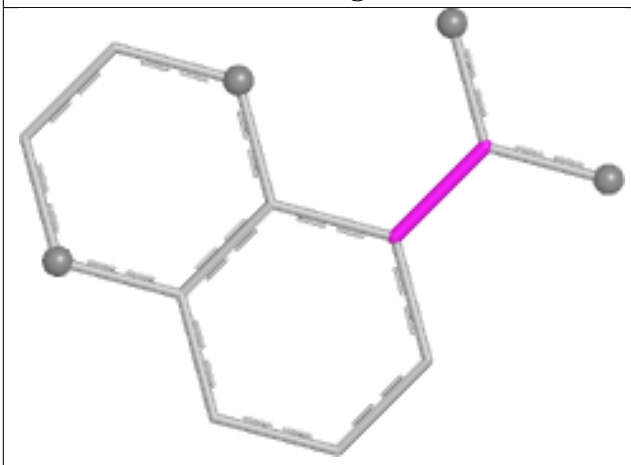
Ligand 53E A 2003



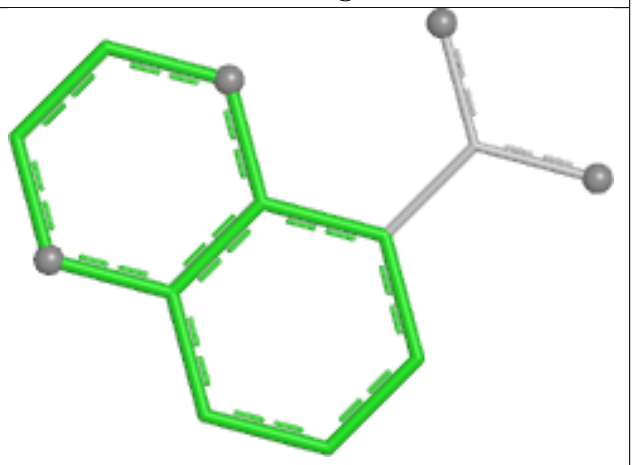
Bond lengths



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	1216/1235 (98%)	0.02	35 (2%) 54 61	10, 24, 41, 67	25 (2%)
1	B	1208/1235 (97%)	0.18	68 (5%) 31 37	11, 25, 48, 68	16 (1%)
All	All	2424/2470 (98%)	0.10	103 (4%) 41 48	10, 24, 45, 68	41 (1%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	VAL	5.8
1	B	500	VAL	5.4
1	B	491	LEU	5.3
1	B	912	ILE	4.9
1	B	439	PHE	4.7
1	B	1223	ALA	4.7
1	B	1222	ALA	4.6
1	B	487	VAL	4.2
1	B	490	LEU	4.2
1	B	495	ALA	4.2
1	A	493	ASN	4.2
1	A	1230	MET	4.1
1	B	486	LEU	3.9
1	B	223	LEU	3.8
1	B	1229	LEU	3.8
1	A	1222	ALA	3.7
1	A	134	LEU	3.6
1	B	466	LEU	3.5
1	A	490	LEU	3.3
1	B	482	LEU	3.3
1	A	132	SER	3.3
1	A	127	ASP	3.2
1	B	485	TYR	3.2
1	B	156	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	484	ALA	3.1
1	B	1227	ALA	3.1
1	B	66	SER	3.1
1	B	128	GLY	3.1
1	A	1225	GLY	3.0
1	B	481	THR	3.0
1	B	510	ILE	3.0
1	B	479	HIS	3.0
1	B	492	GLU	3.0
1	B	415	VAL	2.9
1	B	1224	GLY	2.9
1	A	1223	ALA	2.9
1	A	129	ASN	2.9
1	B	438	ASP	2.9
1	A	1227	ALA	2.9
1	B	14	ALA	2.8
1	B	63	ALA	2.8
1	A	491	LEU	2.8
1	A	494	GLY	2.7
1	B	129	ASN	2.7
1	B	134	LEU	2.7
1	B	436	GLY	2.7
1	A	1229	LEU	2.7
1	B	914	LEU	2.7
1	A	137	SER	2.7
1	A	14	ALA	2.7
1	A	1232	ILE	2.7
1	B	1228	SER	2.6
1	A	492	GLU	2.6
1	B	462	GLY	2.6
1	B	1225	GLY	2.6
1	B	440	HIS	2.6
1	A	156	THR	2.5
1	B	132	SER	2.5
1	B	467	ASP	2.5
1	A	706	TRP	2.5
1	A	506	PRO	2.5
1	B	414	ASP	2.5
1	A	485	TYR	2.4
1	A	1228	SER	2.4
1	B	72	ILE	2.4
1	B	513	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	82	SER	2.4
1	B	503	ILE	2.4
1	A	128	GLY	2.4
1	B	441	VAL	2.4
1	A	481	THR	2.4
1	B	410	LEU	2.3
1	A	130	TRP	2.3
1	B	74	ALA	2.3
1	B	499	PHE	2.3
1	A	79	HIS	2.3
1	A	495	ALA	2.3
1	B	84	VAL	2.3
1	B	461	VAL	2.3
1	A	125	ILE	2.3
1	B	463	ARG	2.2
1	A	1231	ALA	2.2
1	A	937	LEU	2.2
1	B	127	ASP	2.2
1	B	905	LEU	2.2
1	B	133	HIS	2.2
1	B	496	ASN	2.2
1	A	484	ALA	2.1
1	B	115	ALA	2.1
1	B	506	PRO	2.1
1	A	801	ALA	2.1
1	A	195	PHE	2.1
1	B	138	ARG	2.1
1	B	130	TRP	2.1
1	A	1226	ASN	2.1
1	B	73	GLU	2.1
1	B	71	LEU	2.1
1	B	75	LEU	2.1
1	B	120	LEU	2.1
1	B	451	GLY	2.1
1	B	483	LEU	2.0
1	B	437	LYS	2.0
1	B	460	VAL	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.

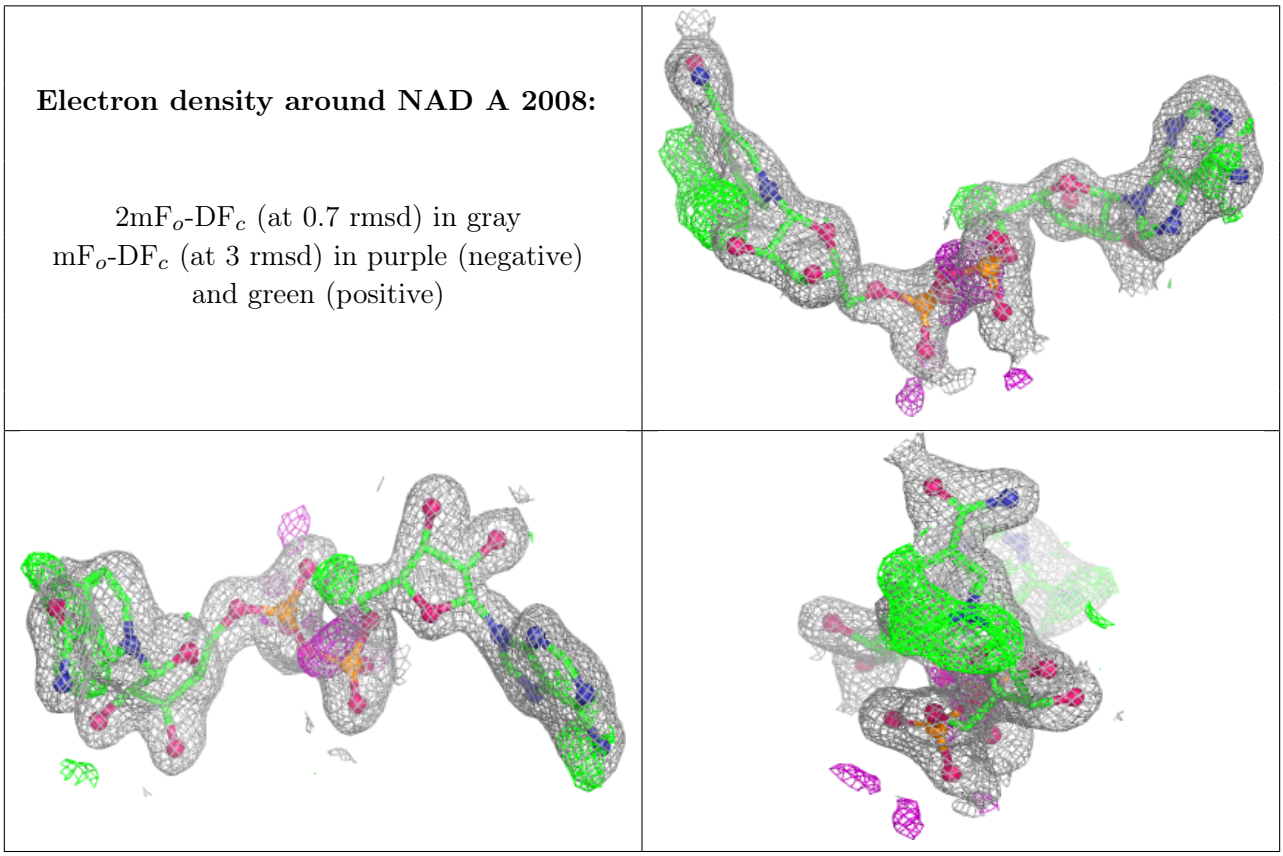
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	A	2007	7/7	0.78	0.15	44,48,55,60	0
3	PEG	A	2005	7/7	0.80	0.14	34,37,41,49	0
3	PEG	B	2007	7/7	0.83	0.15	37,46,52,54	0
7	SO4	A	2013	5/5	0.83	0.13	41,43,52,67	5
7	SO4	B	2012	5/5	0.85	0.12	29,29,39,49	5
3	PEG	B	2003	7/7	0.86	0.12	33,39,46,50	0
3	PEG	A	2002	7/7	0.87	0.12	26,34,43,45	0
6	NAD	A	2008	44/44	0.87	0.13	21,29,35,36	44
3	PEG	B	2005	7/7	0.88	0.12	28,35,41,45	0
7	SO4	A	2011	5/5	0.88	0.09	51,52,53,61	5
5	FMT	B	2008	3/3	0.89	0.11	32,32,33,36	0
4	53E	A	2003	13/13	0.90	0.12	21,29,37,38	13
10	PG4	B	2009	13/13	0.91	0.11	35,42,48,48	0
6	NAD	B	2010	44/44	0.92	0.10	19,22,25,34	44
5	FMT	A	2006	3/3	0.92	0.08	36,36,46,51	0
8	MG	A	2014	1/1	0.92	0.17	45,45,45,45	0
7	SO4	A	2012	5/5	0.92	0.11	36,39,49,52	5
2	FAD	B	2001[A]	53/53	0.94	0.08	18,22,27,30	53
4	53E	B	2004	13/13	0.94	0.09	20,24,28,34	13
9	PGE	B	2002	10/10	0.94	0.08	32,38,43,44	0
2	FAD	B	2001[B]	53/53	0.94	0.08	18,22,28,29	53
2	FAD	A	2001[A]	53/53	0.95	0.07	16,21,25,26	53
5	FMT	B	2006	3/3	0.95	0.14	15,15,34,38	0
8	MG	B	2013	1/1	0.95	0.12	38,38,38,38	0
2	FAD	A	2001[B]	53/53	0.95	0.07	16,21,25,27	53
5	FMT	A	2004	3/3	0.95	0.10	24,24,32,34	0
7	SO4	A	2010	5/5	0.97	0.08	25,30,37,40	5
7	SO4	B	2011	5/5	0.99	0.04	18,18,22,22	0
7	SO4	A	2009	5/5	0.99	0.04	20,20,23,25	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.

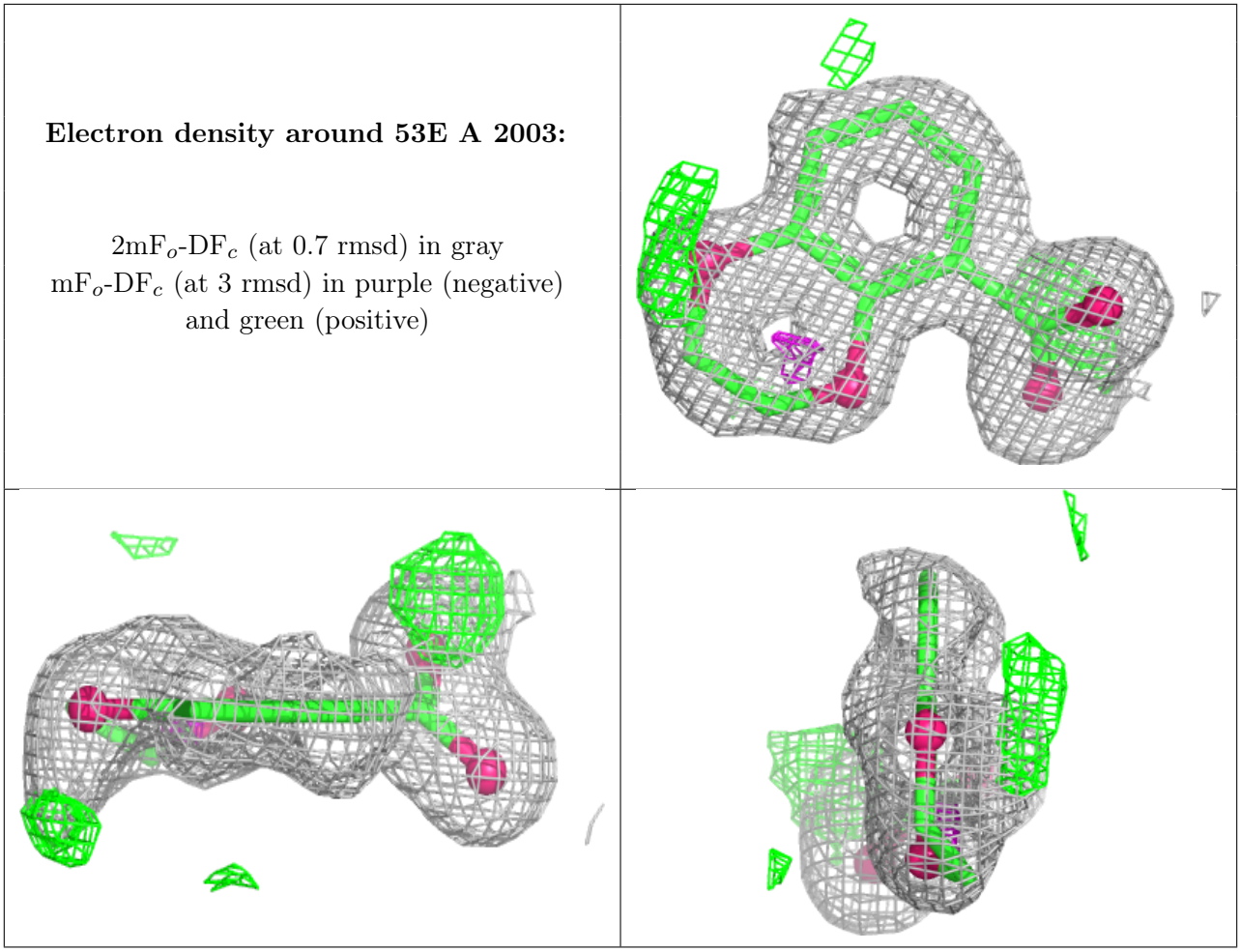
Electron density around NAD A 2008:

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



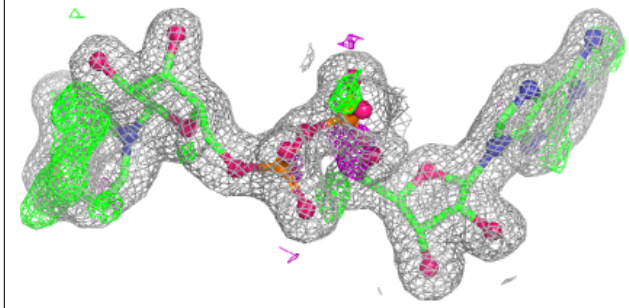
Electron density around 53E A 2003:

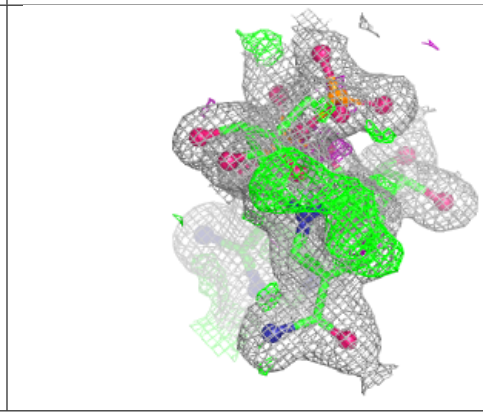
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

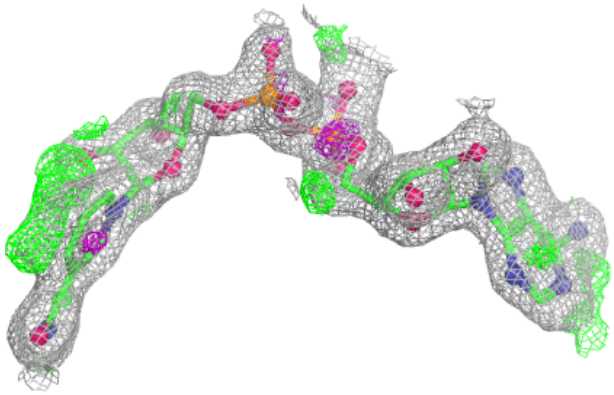


Electron density around NAD B 2010:

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

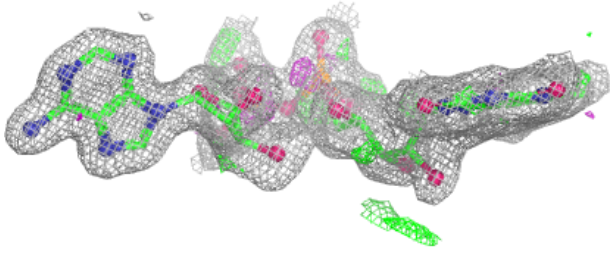


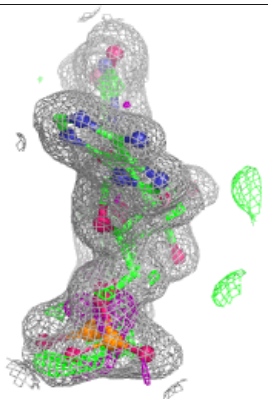


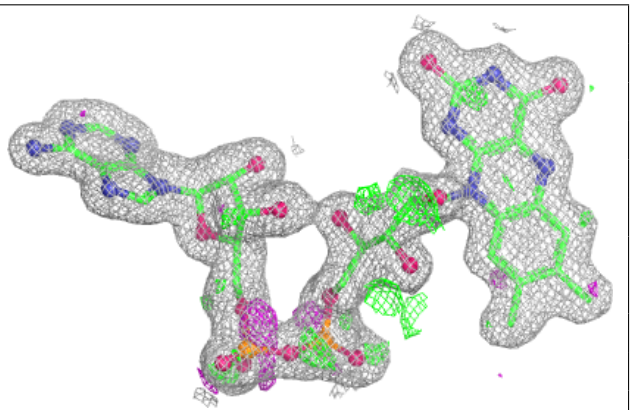


Electron density around FAD B 2001 (A):

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

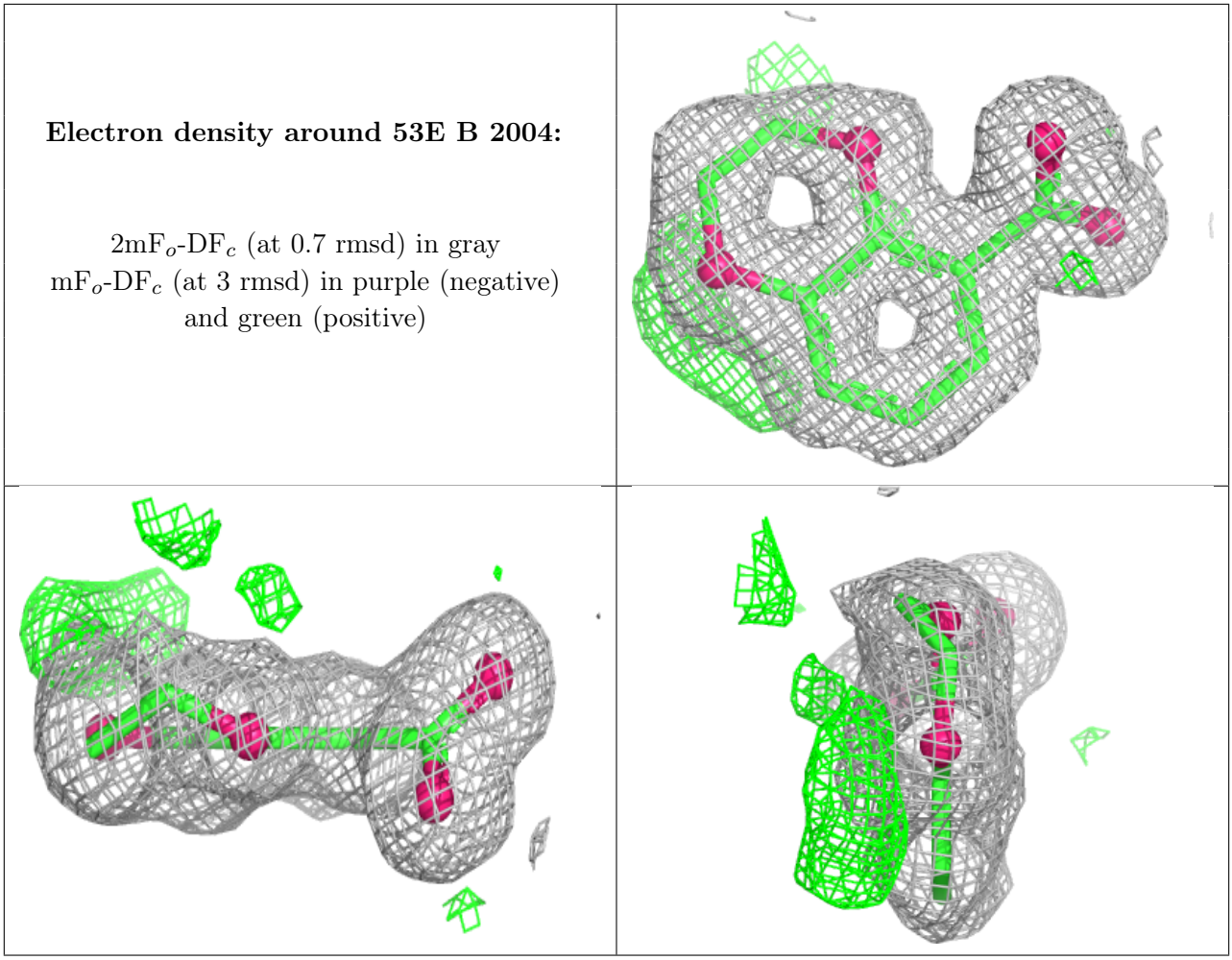






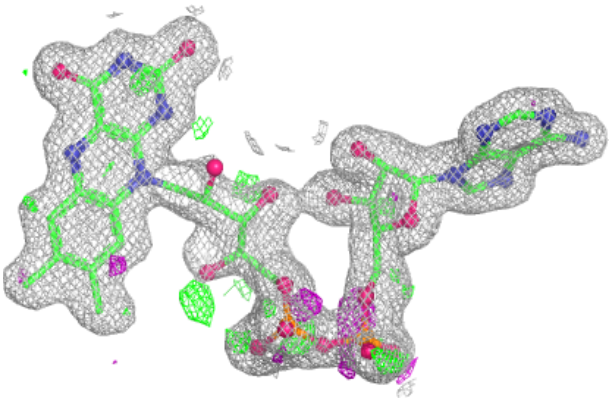
Electron density around 53E B 2004:

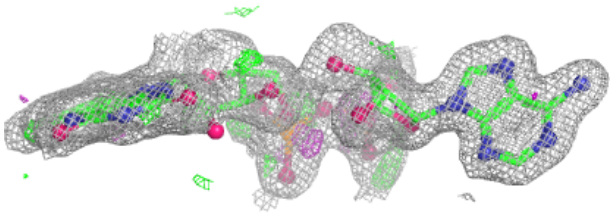
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

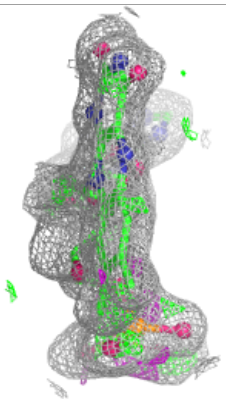


Electron density around FAD B 2001 (B):

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

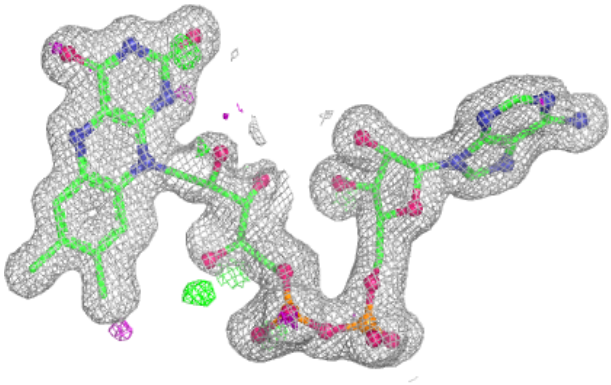


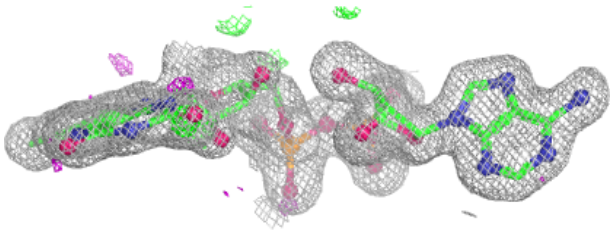


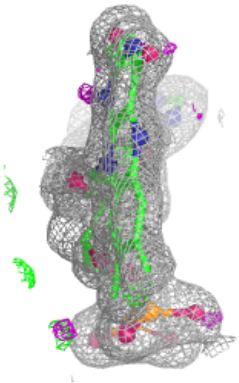


Electron density around FAD A 2001 (A):

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

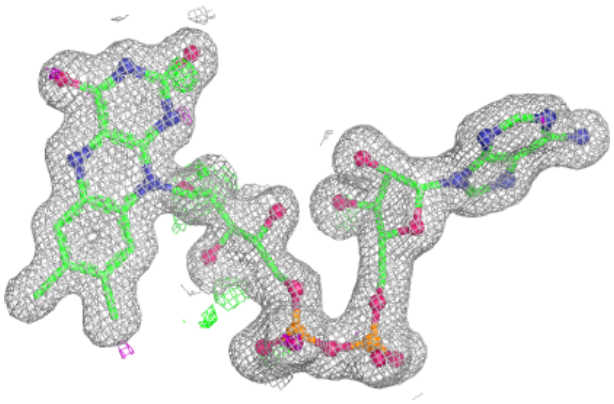


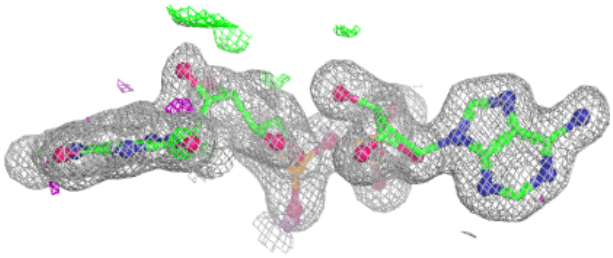


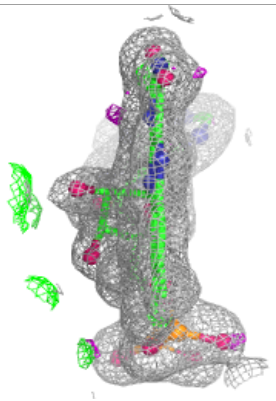


Electron density around FAD A 2001 (B):

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







6.5 Other polymers

There are no such residues in this entry.