



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:38 PM UTC

PDB ID : 9DL2 / pdb_00009dl2
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

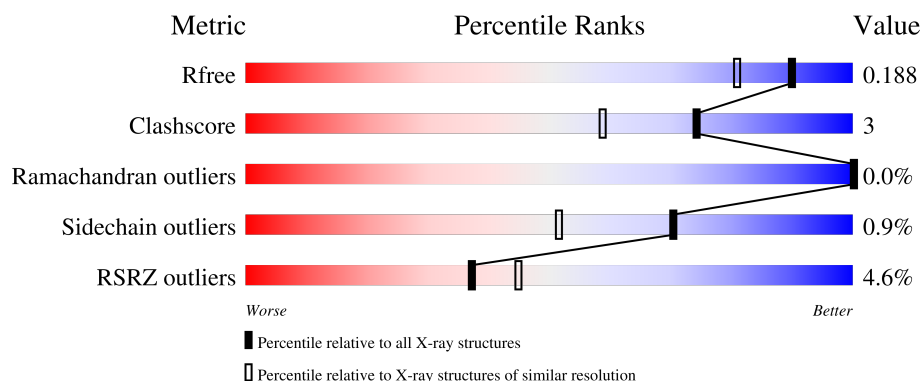
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1235	3% 93% 6%
1	B	1235	6% 89% 8%

2 Entry composition i

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.

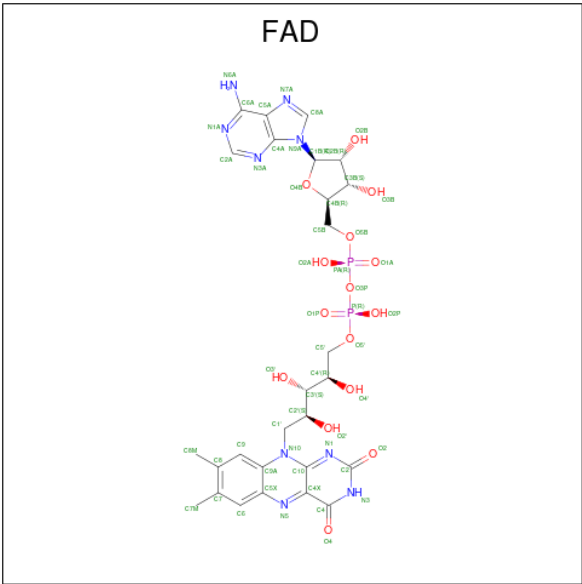
- Molecule 1 is a protein called Bifunctional protein PutA.

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:

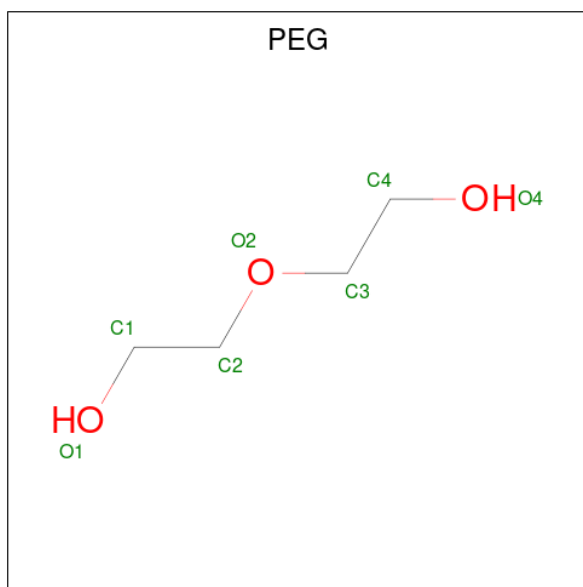
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP F7X6I3
A	0	MET	-	expression tag	UNP F7X6I3
B	-1	SER	-	expression tag	UNP F7X6I3
B	0	MET	-	expression tag	UNP F7X6I3

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



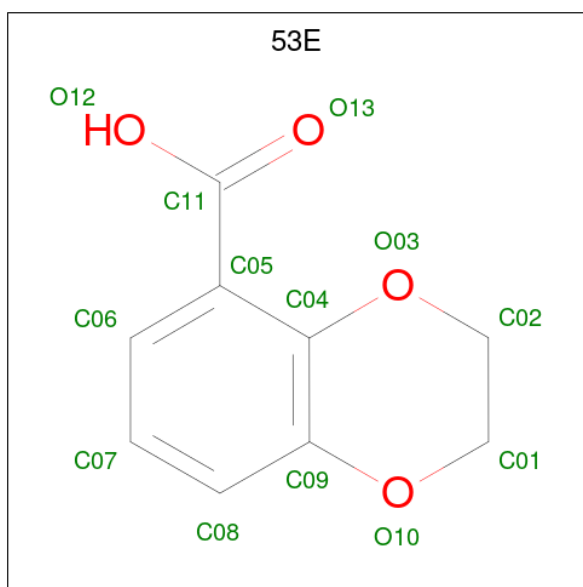
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			106	54	18	30	4	
2	B	1	Total	C	N	O	P	
			106	54	18	30	4	

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



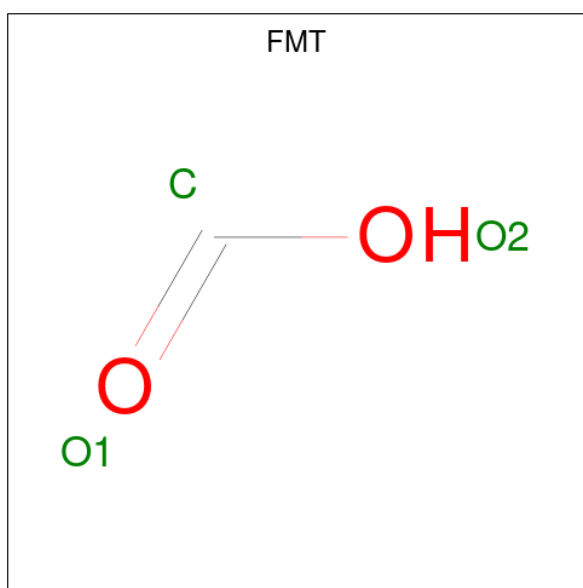
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			7	4	3	0	0
3	A	1	Total	C	O		
			7	4	3	0	0
3	A	1	Total	C	O		
			7	4	3	0	0
3	B	1	Total	C	O		
			7	4	3	0	0
3	B	1	Total	C	O		
			7	4	3	0	0
3	B	1	Total	C	O		
			7	4	3	0	0

- Molecule 4 is 2,3-dihydro-1,4-benzodioxine-5-carboxylic acid (CCD ID: 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	0	0
			13	9	4		
4	B	1	Total	C	O	0	0
			13	9	4		

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



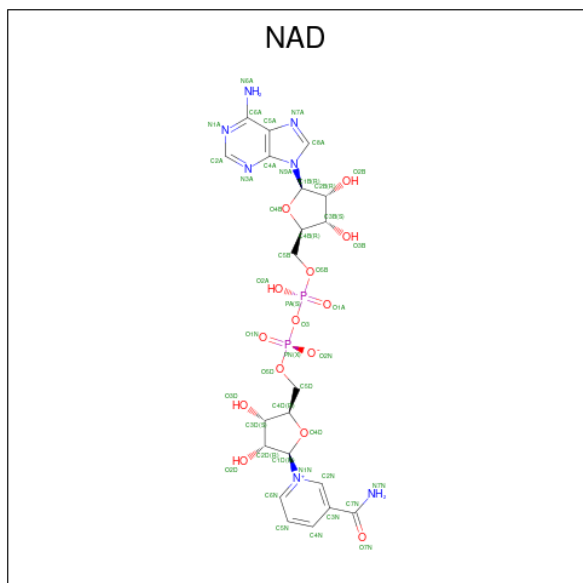
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		

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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 (CCD ID: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

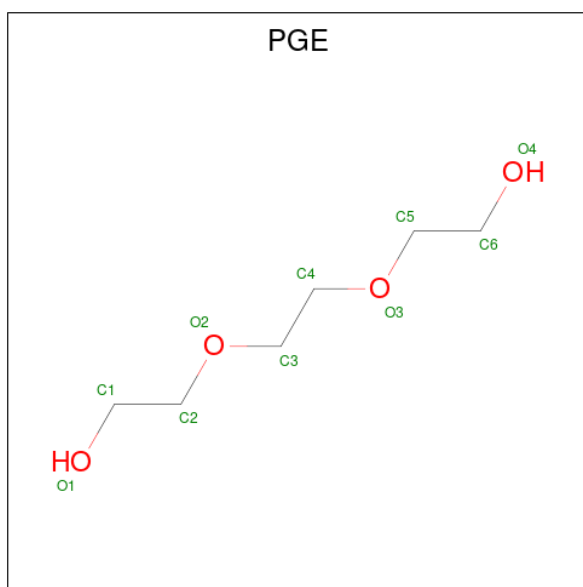


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

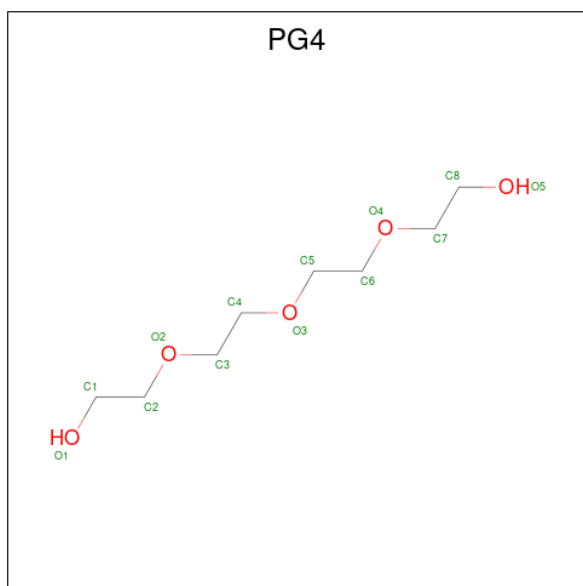
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

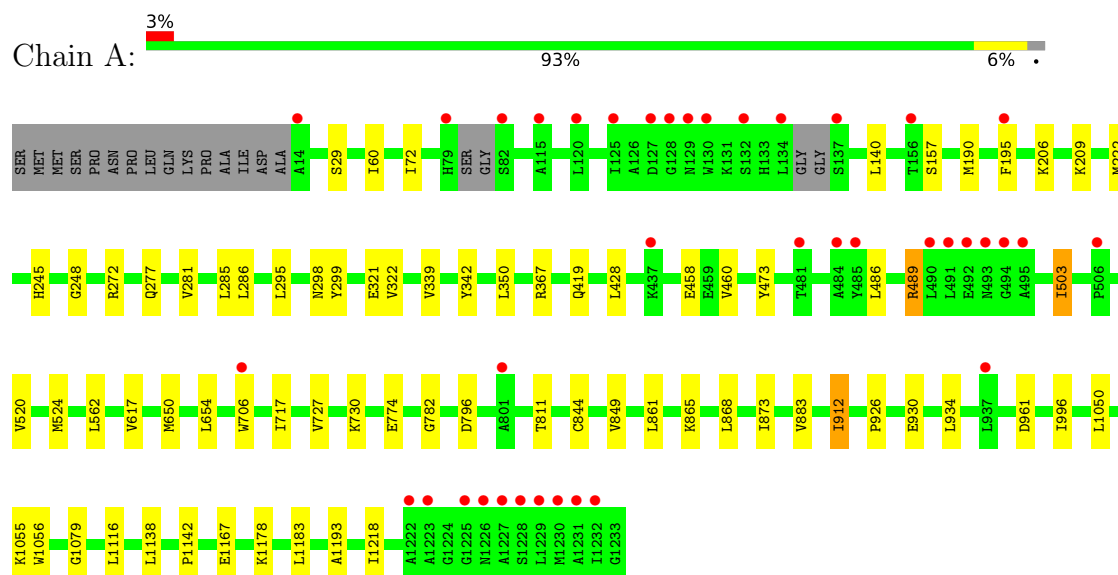
- Molecule 11 is water.

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

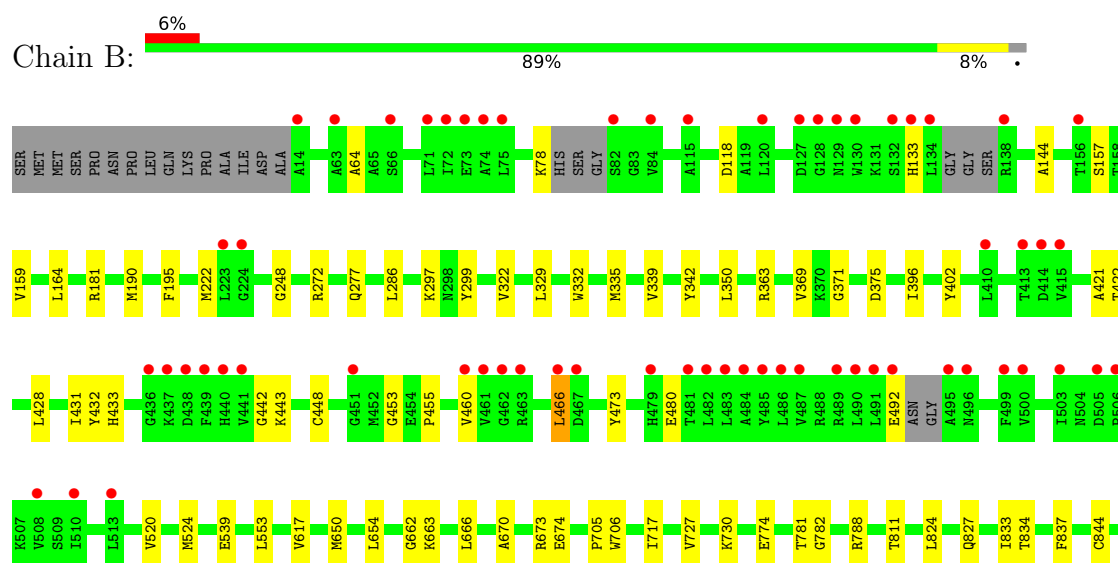
3 Residue-property plots

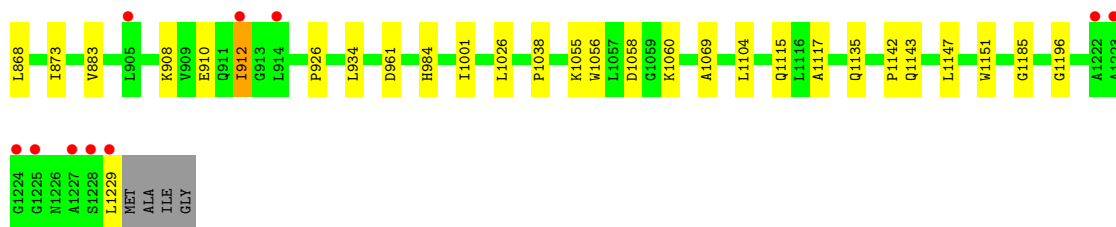
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Bifunctional protein PutA



• Molecule 1: Bifunctional protein PutA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ 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	17268 reflections (4.90%)	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	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FAD, PGE, 53E, FMT, MG, PG4, NAD, PEG

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	0.25	0/9336	0.45	0/12708
1	B	0.26	0/9122	0.48	2/12427 (0.0%)
All	All	0.25	0/18458	0.47	2/25135 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	LEU	CA-C-N	-6.93	113.51	122.79
1	B	466	LEU	C-N-CA	-6.93	113.51	122.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9102	0	9173	44	0
1	B	8918	0	8901	66	0
2	A	106	0	62	1	0
2	B	106	0	62	5	0
3	A	21	0	30	1	0
3	B	21	0	30	4	0
4	A	13	0	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	114	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 (114) 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: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: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:B:1196:GLY:HA3	3:B:2007:PEG:H22	1.78	0.65
1:B:663[B]:LYS:NZ	11:B:2105:HOH:O	2.19	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

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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:796:ASP:HA	1:A:1178:LYS:HZ1	1.72	0.54
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:B:473:TYR:HB2	2:B:2001[B]:FAD:HM72	1.91	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:A:473:TYR:HB2	2:A:2001[A]:FAD:HM71	1.91	0.51
1:B:834[A]:THR:HG22	1:B:1001:ILE:HD11	1.92	0.51
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: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:332:TRP:HZ3	1:B:335[B]:MET:HE2	1.80	0.47
1:B:422:THR:OG1	2:B:2001[A]:FAD:O1P	2.32	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:A:1055:LYS:NZ	1:B:961:ASP:OD2	2.41	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:332:TRP:CZ3	1:B:335[B]:MET:HE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:190:MET:HE2	1:A:195:PHE:CZ	2.51	0.45
1:B:159:VAL:HG13	1:B:164:LEU:HD12	1.97	0.45
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.42	0.44
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:A:861[A]:LEU:HD21	1:A:930:GLU:CD	2.44	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:78:LYS:NZ	1:B:455:PRO:O	2.53	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:984:HIS:C	1:B:984:HIS:CD2	2.97	0.42
1:A:520:VAL:HG12	1:A:524:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:190:MET:HE2	1:B:195:PHE:CZ	2.56	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
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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	70	51
1	B	882/951 (93%)	875 (99%)	7 (1%)	73	56
All	All	1803/1902 (95%)	1788 (99%)	15 (1%)	70	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LEU
1	A	157	SER
1	A	321	GLU
1	A	342	TYR
1	A	489	ARG
1	A	503	ILE
1	A	730	LYS
1	A	912	ILE
1	B	157	SER
1	B	342	TYR
1	B	443	LYS
1	B	730	LYS
1	B	833	ILE
1	B	912	ILE
1	B	934	LEU

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

Mol	Chain	Res	Type
1	A	143	ASN
1	A	419	GLN
1	A	440	HIS
1	A	1040	GLN
1	A	1114	HIS
1	B	419	GLN
1	B	479	HIS

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Mol	Chain	Res	Type
1	B	1114	HIS

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 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	$\# Z > 2$
3	PEG	B	2007	-	6,6,6	0.24	0	5,5,5	0.22	0
7	SO4	B	2012	-	4,4,4	0.69	0	6,6,6	0.14	0
5	FMT	B	2008	-	2,2,2	0.65	0	1,1,1	0.17	0
2	FAD	A	2001[B]	-	58,58,58	2.25	16 (27%)	85,89,89	1.78	18 (21%)
3	PEG	A	2007	-	6,6,6	0.25	0	5,5,5	0.22	0
7	SO4	B	2011	-	4,4,4	0.56	0	6,6,6	0.24	0
3	PEG	B	2005	-	6,6,6	0.35	0	5,5,5	0.45	0
3	PEG	B	2003	-	6,6,6	0.24	0	5,5,5	0.28	0
4	53E	A	2003	-	14,14,14	2.00	2 (14%)	18,19,19	1.00	1 (5%)
2	FAD	B	2001[B]	-	58,58,58	2.40	14 (24%)	85,89,89	1.77	20 (23%)
2	FAD	A	2001[A]	-	58,58,58	2.22	14 (24%)	85,89,89	1.75	19 (22%)
7	SO4	A	2012	-	4,4,4	0.64	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	A	2002	-	6,6,6	0.23	0	5,5,5	0.32	0
9	PGE	B	2002	-	9,9,9	0.33	0	8,8,8	0.40	0
5	FMT	B	2006	-	2,2,2	0.85	0	1,1,1	0.13	0
6	NAD	B	2010	8	46,48,48	2.37	10 (21%)	64,73,73	1.78	12 (18%)
2	FAD	B	2001[A]	-	58,58,58	2.22	14 (24%)	85,89,89	1.70	20 (23%)
6	NAD	A	2008	8	46,48,48	2.36	11 (23%)	64,73,73	1.86	14 (21%)
7	SO4	A	2010	-	4,4,4	0.66	0	6,6,6	0.29	0
10	PG4	B	2009	-	12,12,12	0.28	0	11,11,11	0.22	0
4	53E	B	2004	-	14,14,14	2.02	2 (14%)	18,19,19	0.59	0
5	FMT	A	2006	-	2,2,2	0.58	0	1,1,1	0.20	0
3	PEG	A	2005	-	6,6,6	0.26	0	5,5,5	0.17	0
5	FMT	A	2004	-	2,2,2	0.53	0	1,1,1	0.27	0
7	SO4	A	2009	-	4,4,4	0.55	0	6,6,6	0.23	0
7	SO4	A	2011	-	4,4,4	0.66	0	6,6,6	0.09	0
7	SO4	A	2013	-	4,4,4	0.67	0	6,6,6	0.18	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	PEG	B	2007	-	-	2/4/4/4	-
6	NAD	B	2010	8	-	4/30/62/62	0/5/5/5
2	FAD	B	2001[A]	-	-	5/34/50/50	0/6/6/6
6	NAD	A	2008	8	-	2/30/62/62	0/5/5/5
3	PEG	B	2005	-	-	3/4/4/4	-
3	PEG	B	2003	-	-	3/4/4/4	-
4	53E	B	2004	-	-	2/4/11/11	0/2/2/2
10	PG4	B	2009	-	-	3/10/10/10	-
4	53E	A	2003	-	-	4/4/11/11	0/2/2/2
2	FAD	B	2001[B]	-	-	9/34/50/50	0/6/6/6
2	FAD	A	2001[A]	-	-	7/34/50/50	0/6/6/6
3	PEG	A	2002	-	-	2/4/4/4	-
9	PGE	B	2002	-	-	1/7/7/7	-
3	PEG	A	2005	-	-	0/4/4/4	-
2	FAD	A	2001[B]	-	-	6/34/50/50	0/6/6/6
3	PEG	A	2007	-	-	3/4/4/4	-

All (83) 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
2	A	2001[A]	FAD	C6A-N6A	4.10	1.44	1.34
2	B	2001[B]	FAD	C4X-N5	4.07	1.39	1.30
2	A	2001[B]	FAD	C6A-N6A	4.06	1.44	1.34
2	B	2001[B]	FAD	C6A-N6A	4.03	1.44	1.34
2	B	2001[A]	FAD	C6A-N6A	3.95	1.44	1.34
6	B	2010	NAD	C6A-N6A	3.92	1.44	1.34
6	A	2008	NAD	C6A-N6A	3.75	1.43	1.34
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	A	2001[B]	FAD	P-O3P	2.95	1.62	1.59
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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	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	B	2001[A]	FAD	C10-N1	2.44	1.38	1.33
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
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
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
6	B	2010	NAD	C4A-N9A	2.15	1.42	1.37
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	C4A-N9A	2.11	1.42	1.37
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
2	A	2001[B]	FAD	C5A-C4A	2.02	1.42	1.39
6	A	2008	NAD	PA-O2A	-2.02	1.46	1.55
6	B	2010	NAD	O3D-C3D	-2.02	1.38	1.43
2	A	2001[A]	FAD	C5A-C4A	2.02	1.42	1.39
6	B	2010	NAD	C5A-C4A	2.01	1.42	1.39

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2008	NAD	N3A-C2A-N1A	-6.05	119.43	128.58
6	B	2010	NAD	N3A-C2A-N1A	-5.99	119.52	128.58
2	B	2001[A]	FAD	N3A-C2A-N1A	-5.78	119.83	128.58
2	B	2001[B]	FAD	N3A-C2A-N1A	-5.66	120.01	128.58
2	A	2001[A]	FAD	N3A-C2A-N1A	-5.57	120.15	128.58
2	A	2001[B]	FAD	N3A-C2A-N1A	-5.55	120.17	128.58
2	B	2001[B]	FAD	O2P-P-O3P	-5.25	93.09	107.27
6	B	2010	NAD	C5A-C4A-N3A	-5.08	119.72	126.72
6	A	2008	NAD	C5A-C4A-N3A	-4.96	119.89	126.72
2	B	2001[B]	FAD	C5A-C4A-N3A	-4.70	120.24	126.72
2	A	2001[A]	FAD	C5A-C4A-N3A	-4.66	120.30	126.72
2	A	2001[B]	FAD	C5A-C4A-N3A	-4.60	120.39	126.72
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	B	2001[A]	FAD	C5A-C4A-N3A	-4.32	120.77	126.72
6	A	2008	NAD	N3A-C4A-N9A	4.31	134.50	127.17
6	B	2010	NAD	N3A-C4A-N9A	4.18	134.27	127.17
2	A	2001[B]	FAD	O2P-P-O3P	-3.98	96.51	107.27
2	A	2001[A]	FAD	N3A-C4A-N9A	3.98	133.93	127.17
2	A	2001[B]	FAD	N3A-C4A-N9A	3.94	133.86	127.17
2	B	2001[B]	FAD	N3A-C4A-N9A	3.91	133.82	127.17
2	A	2001[A]	FAD	O2P-P-O3P	-3.90	96.72	107.27
2	A	2001[B]	FAD	C5A-N7A-C8A	3.90	109.59	103.45
2	A	2001[A]	FAD	C5A-N7A-C8A	3.90	109.58	103.45
6	A	2008	NAD	C5A-N7A-C8A	3.82	109.46	103.45
2	A	2001[A]	FAD	C4-C4X-N5	3.82	123.48	118.21
6	B	2010	NAD	C2A-N3A-C4A	3.78	121.07	111.83
6	B	2010	NAD	C5A-N7A-C8A	3.72	109.30	103.45
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
2	A	2001[B]	FAD	C4-C4X-N5	3.63	123.22	118.21
2	B	2001[B]	FAD	C5A-N7A-C8A	3.61	109.12	103.45
2	B	2001[A]	FAD	N3A-C4A-N9A	3.60	133.28	127.17
6	A	2008	NAD	C2A-N3A-C4A	3.59	120.61	111.83
2	B	2001[B]	FAD	O2A-PA-O3P	-3.57	97.62	107.27
2	B	2001[B]	FAD	C2A-N3A-C4A	3.49	120.35	111.83
2	A	2001[A]	FAD	C2A-N3A-C4A	3.40	120.14	111.83
2	B	2001[A]	FAD	C5A-N7A-C8A	3.39	108.77	103.45
2	B	2001[B]	FAD	O3P-P-O1P	3.39	120.89	110.70
2	A	2001[B]	FAD	C2A-N3A-C4A	3.38	120.07	111.83
2	A	2001[A]	FAD	C4-N3-C2	-3.36	119.67	125.64
2	A	2001[B]	FAD	N9A-C8A-N7A	-3.35	109.18	113.94
2	B	2001[A]	FAD	C2A-N3A-C4A	3.35	120.00	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001[A]	FAD	N9A-C8A-N7A	-3.33	109.20	113.94
6	A	2008	NAD	N9A-C8A-N7A	-3.23	109.35	113.94
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
6	B	2010	NAD	N9A-C8A-N7A	-3.06	109.60	113.94
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
6	B	2010	NAD	C4A-C5A-N7A	-2.92	107.25	110.58
2	A	2001[B]	FAD	C4A-C5A-N7A	-2.90	107.26	110.58
2	B	2001[B]	FAD	N9A-C8A-N7A	-2.89	109.84	113.94
2	A	2001[A]	FAD	C4X-C4-N3	2.88	120.60	113.25
2	A	2001[A]	FAD	C4A-C5A-N7A	-2.88	107.29	110.58
2	B	2001[A]	FAD	N9A-C8A-N7A	-2.79	109.97	113.94
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	C4A-C5A-N7A	-2.73	107.46	110.58
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	C4A-C5A-N7A	-2.62	107.58	110.58
6	A	2008	NAD	C4A-C5A-N7A	-2.61	107.60	110.58
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	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
2	A	2001[B]	FAD	C4A-N9A-C8A	2.37	108.22	105.74
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	A	2001[A]	FAD	C4A-N9A-C8A	2.30	108.16	105.74
2	B	2001[B]	FAD	C10-C4X-N5	-2.30	120.11	124.81
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
6	A	2008	NAD	C4A-N9A-C8A	2.14	107.98	105.74
2	A	2001[A]	FAD	C4X-C10-N1	-2.12	119.40	124.59
2	B	2001[A]	FAD	C2A-N1A-C6A	2.10	122.18	118.73
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
6	A	2008	NAD	C2A-N1A-C6A	2.01	122.04	118.73
2	A	2001[A]	FAD	C9-C9A-N10	-2.01	119.15	121.85
6	B	2010	NAD	C4A-N9A-C8A	2.01	107.85	105.74
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 (56) 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'

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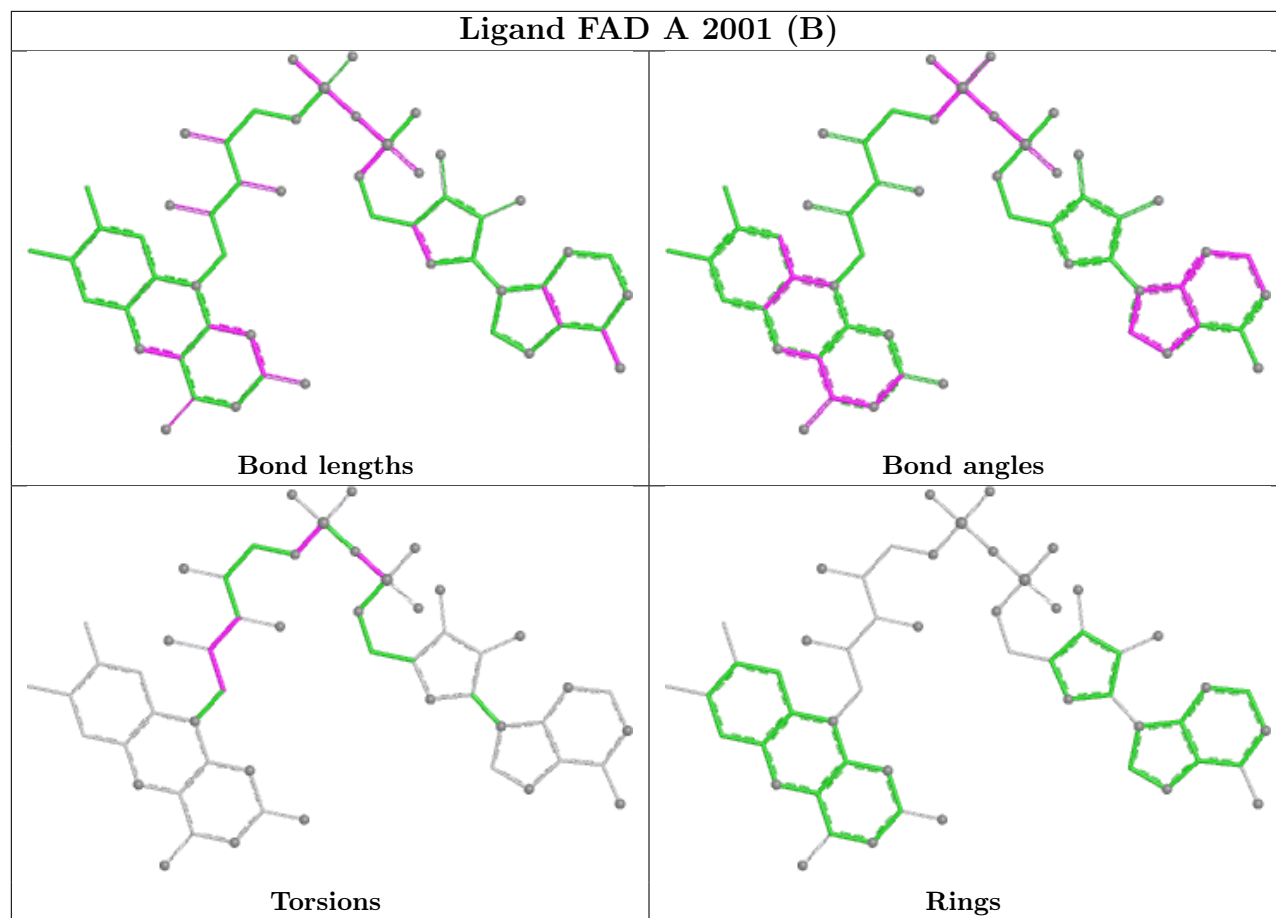
Mol	Chain	Res	Type	Atoms
3	A	2007	PEG	O1-C1-C2-O2
2	A	2001[A]	FAD	O3'-C3'-C4'-C5'
3	A	2002	PEG	O2-C3-C4-O4
4	B	2004	53E	C04-C05-C11-O13
2	B	2001[B]	FAD	C3B-C4B-C5B-O5B
3	A	2002	PEG	C4-C3-O2-C2
3	B	2005	PEG	O2-C3-C4-O4
3	B	2007	PEG	C1-C2-O2-C3
10	B	2009	PG4	O1-C1-C2-O2
3	B	2007	PEG	O1-C1-C2-O2
2	A	2001[A]	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'
6	B	2010	NAD	C2B-C1B-N9A-C8A
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
6	B	2010	NAD	O4B-C1B-N9A-C8A

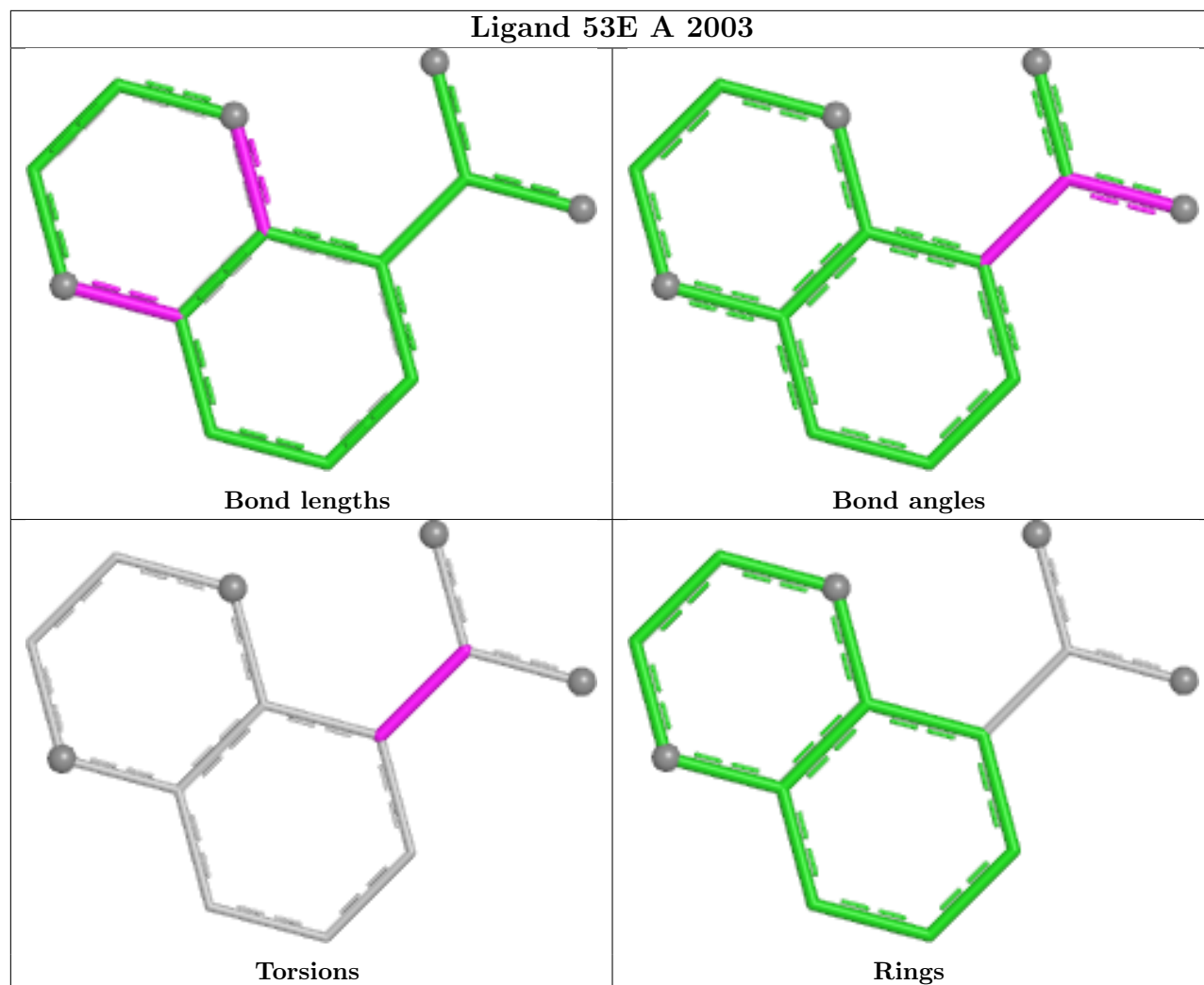
There are no ring outliers.

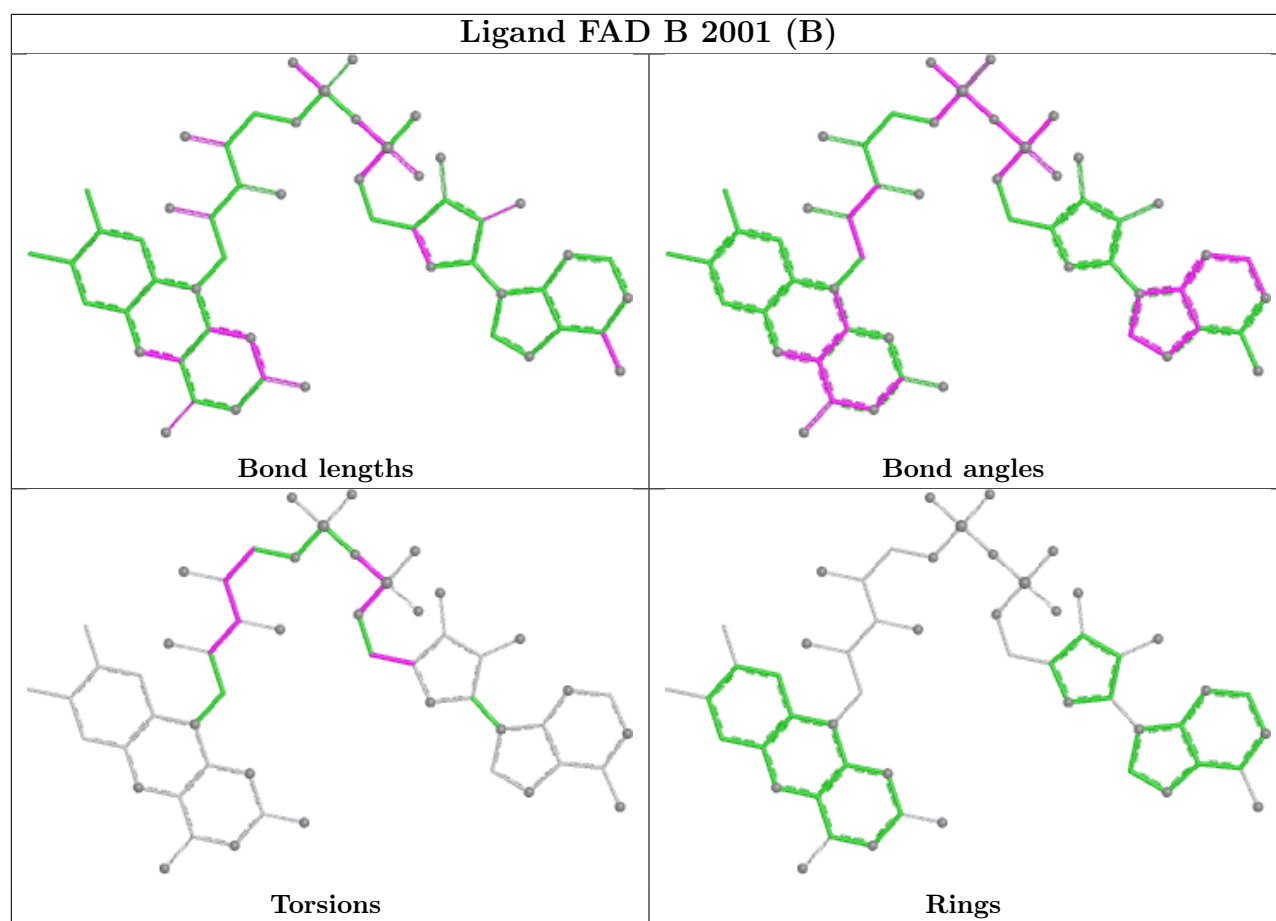
12 monomers are involved in 19 short contacts:

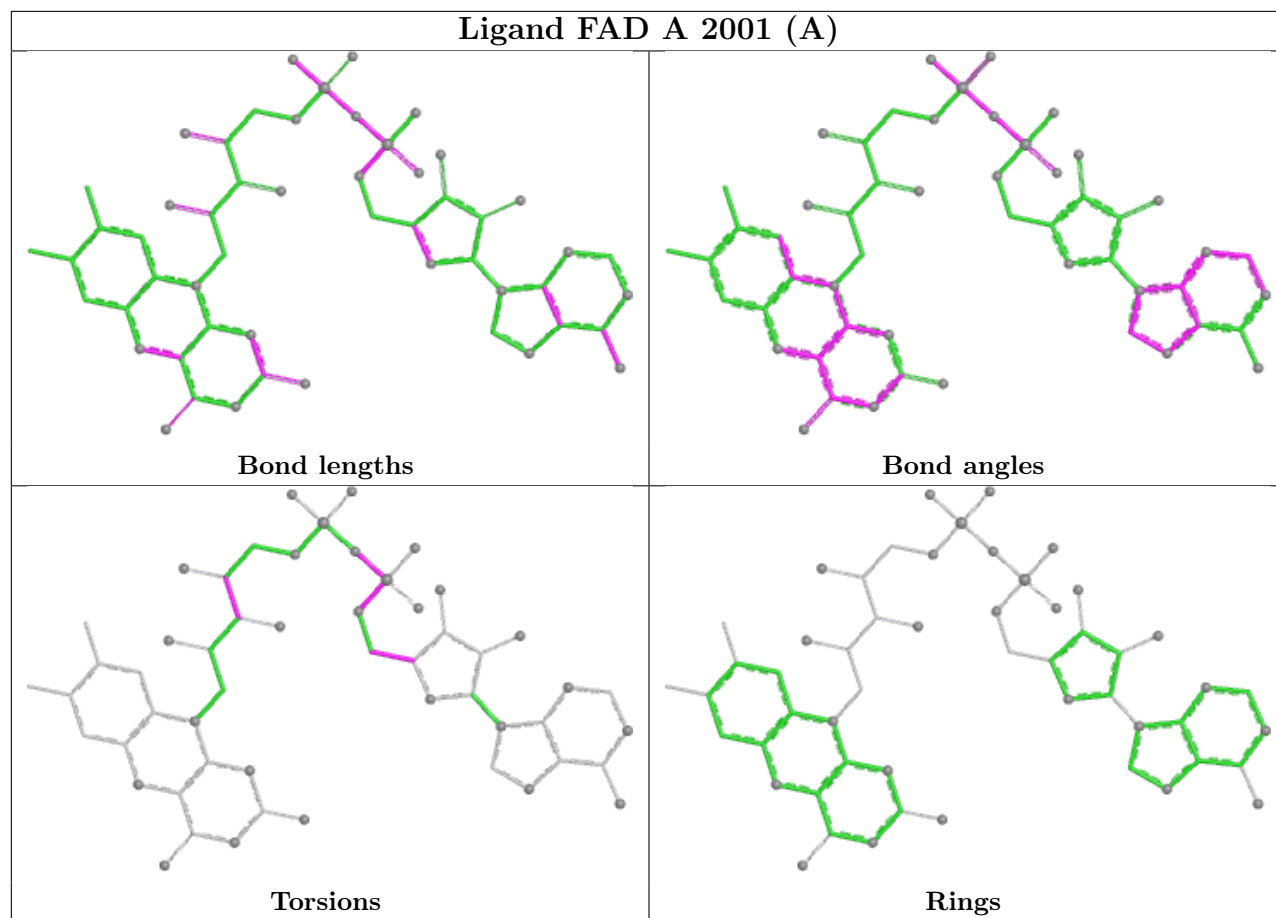
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2007	PEG	2	0
3	B	2005	PEG	2	0
4	A	2003	53E	1	0
2	B	2001[B]	FAD	2	0
2	A	2001[A]	FAD	1	0
7	A	2012	SO4	1	0
3	A	2002	PEG	1	0
6	B	2010	NAD	2	0
2	B	2001[A]	FAD	3	0
6	A	2008	NAD	2	0
4	B	2004	53E	1	0
5	A	2006	FMT	1	0

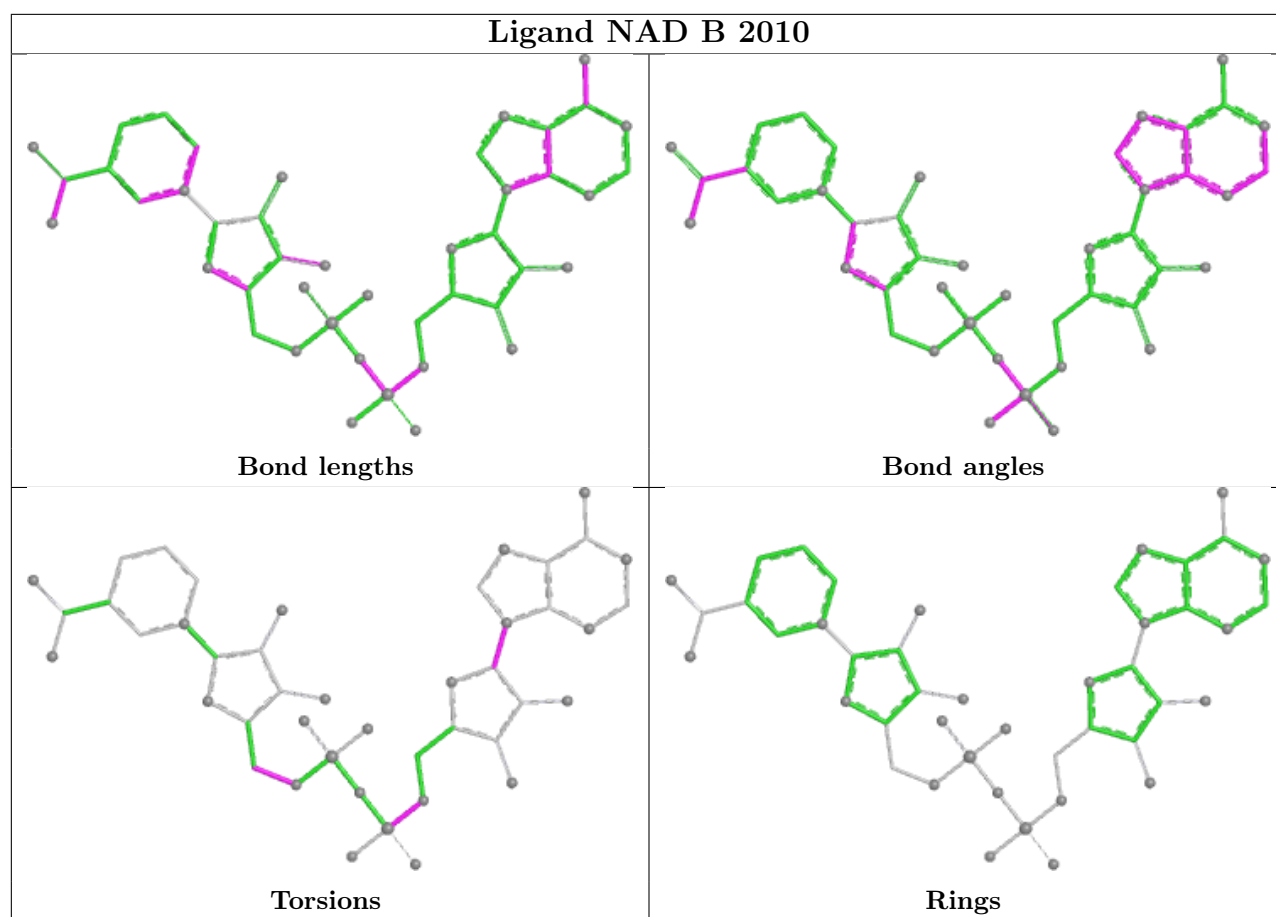
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

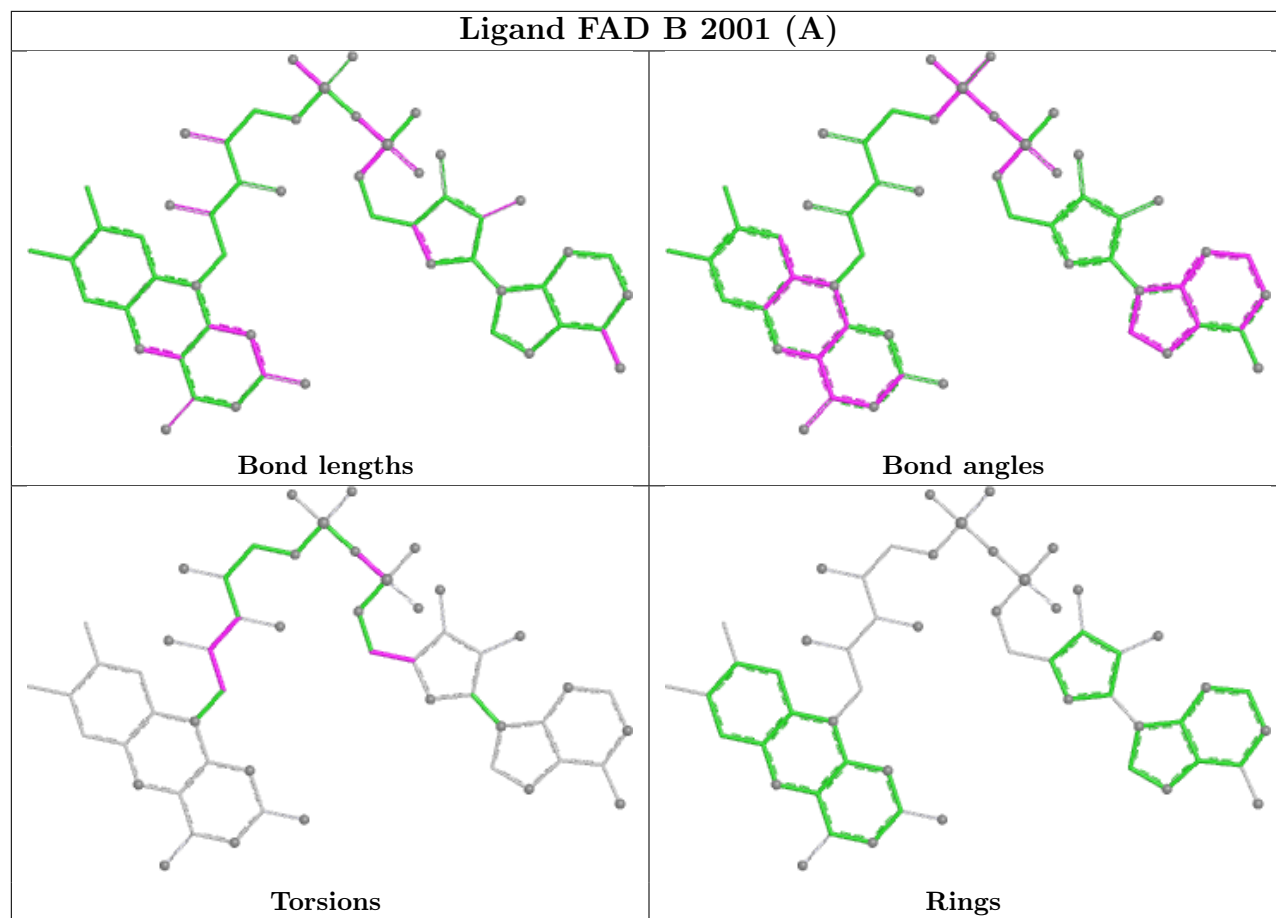


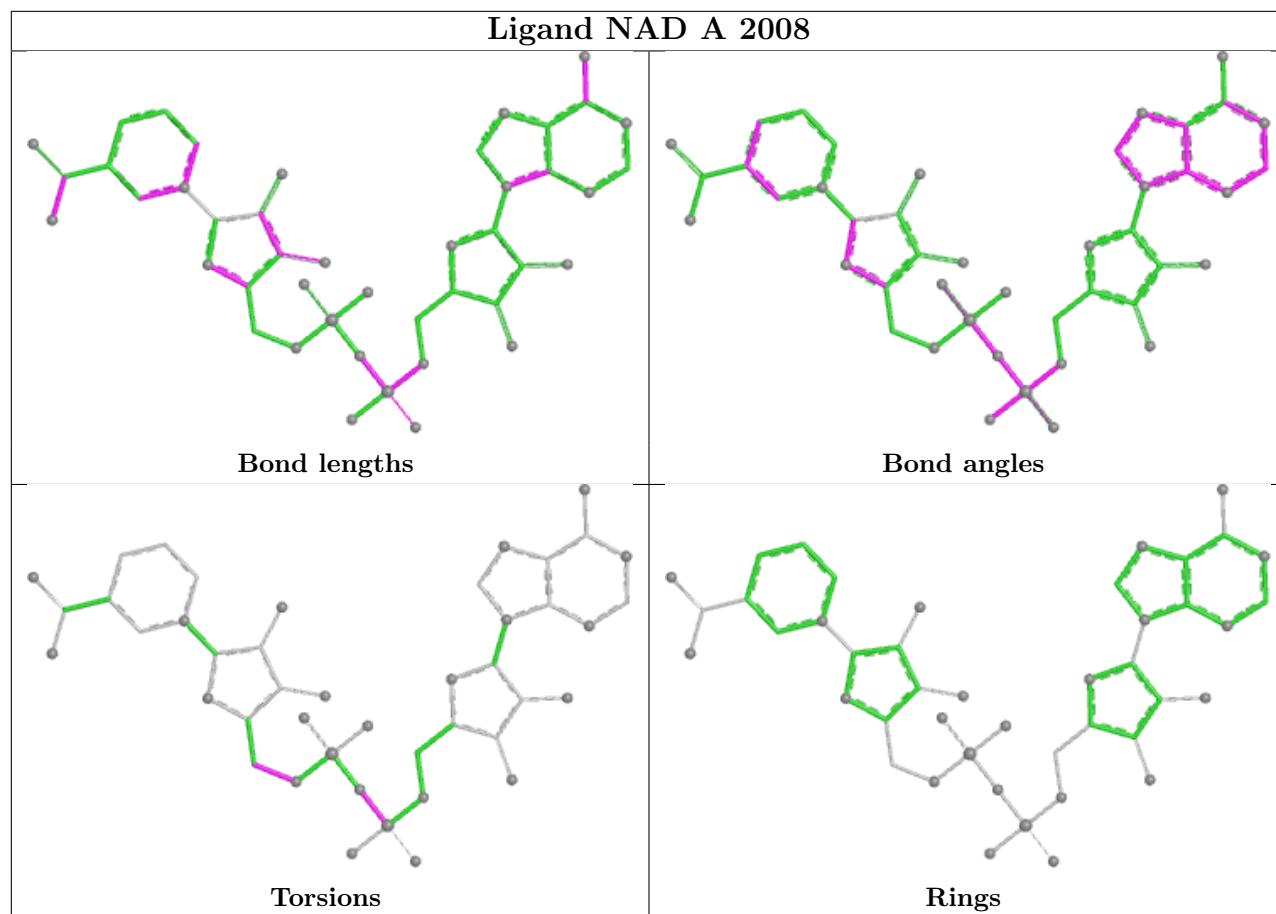


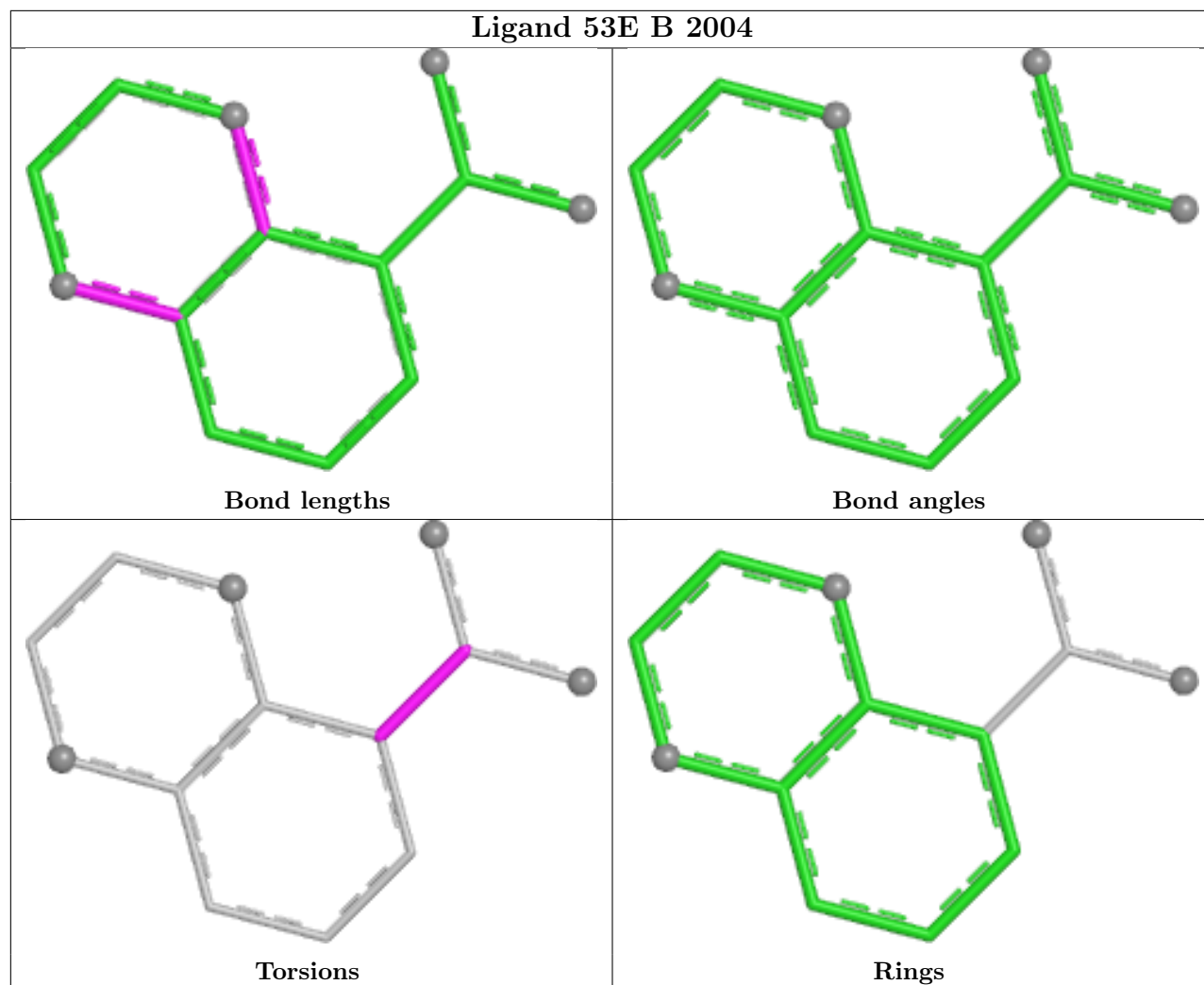












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1216/1235 (98%)	0.07	39 (3%)	50	59	10, 24, 41, 67	25 (2%)
1	B	1208/1235 (97%)	0.23	72 (5%)	27	33	11, 25, 48, 68	16 (1%)
All	All	2424/2470 (98%)	0.15	111 (4%)	37	45	10, 24, 45, 68	41 (1%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	VAL	6.0
1	B	500	VAL	5.6
1	B	491	LEU	5.4
1	B	912	ILE	5.1
1	B	1223	ALA	4.9
1	B	439	PHE	4.8
1	B	1222	ALA	4.8
1	B	495	ALA	4.4
1	B	490	LEU	4.4
1	B	487	VAL	4.4
1	A	493	ASN	4.3
1	A	1230	MET	4.1
1	B	223	LEU	4.0
1	B	486	LEU	4.0
1	B	1229	LEU	3.9
1	A	1222	ALA	3.8
1	A	134	LEU	3.7
1	B	466	LEU	3.7
1	B	482	LEU	3.5
1	A	490	LEU	3.4
1	A	132	SER	3.4
1	B	485	TYR	3.3
1	B	1227	ALA	3.3
1	A	127	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	66	SER	3.3
1	B	484	ALA	3.3
1	B	156	THR	3.2
1	B	128	GLY	3.2
1	B	481	THR	3.1
1	A	1225	GLY	3.1
1	B	479	HIS	3.1
1	B	510	ILE	3.1
1	A	1223	ALA	3.1
1	B	415	VAL	3.0
1	B	1224	GLY	3.0
1	B	492	GLU	3.0
1	A	129	ASN	3.0
1	B	438	ASP	3.0
1	A	1227	ALA	2.9
1	B	14	ALA	2.9
1	A	494	GLY	2.9
1	B	63	ALA	2.9
1	A	491	LEU	2.9
1	B	129	ASN	2.8
1	B	134	LEU	2.8
1	B	436	GLY	2.8
1	A	1229	LEU	2.8
1	B	914	LEU	2.8
1	A	137	SER	2.8
1	A	14	ALA	2.7
1	A	1232	ILE	2.7
1	B	1228	SER	2.7
1	B	462	GLY	2.6
1	B	1225	GLY	2.6
1	B	440	HIS	2.6
1	A	492	GLU	2.6
1	A	156	THR	2.6
1	B	132	SER	2.6
1	A	506	PRO	2.6
1	A	706	TRP	2.6
1	A	485	TYR	2.6
1	B	467	ASP	2.6
1	B	414	ASP	2.5
1	A	1228	SER	2.5
1	A	128	GLY	2.5
1	B	82	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	72	ILE	2.5
1	B	503	ILE	2.5
1	B	513	LEU	2.5
1	A	481	THR	2.5
1	B	441	VAL	2.5
1	A	495	ALA	2.4
1	B	74	ALA	2.4
1	B	410	LEU	2.4
1	A	130	TRP	2.4
1	A	79	HIS	2.4
1	B	499	PHE	2.4
1	A	1231	ALA	2.4
1	A	125	ILE	2.4
1	B	84	VAL	2.3
1	B	461	VAL	2.3
1	A	937	LEU	2.3
1	B	905	LEU	2.3
1	B	463	ARG	2.3
1	B	127	ASP	2.3
1	B	133	HIS	2.3
1	A	484	ALA	2.2
1	B	115	ALA	2.2
1	B	496	ASN	2.2
1	A	801	ALA	2.2
1	B	506	PRO	2.2
1	B	130	TRP	2.2
1	A	1226	ASN	2.2
1	A	195	PHE	2.2
1	B	73	GLU	2.2
1	B	75	LEU	2.1
1	B	120	LEU	2.1
1	B	483	LEU	2.1
1	B	451	GLY	2.1
1	B	138	ARG	2.1
1	B	224	GLY	2.1
1	B	71	LEU	2.1
1	B	460	VAL	2.1
1	B	413	THR	2.1
1	B	437	LYS	2.1
1	B	505	ASP	2.1
1	A	437	LYS	2.0
1	A	115	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	489	ARG	2.0
1	A	120	LEU	2.0
1	A	82	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

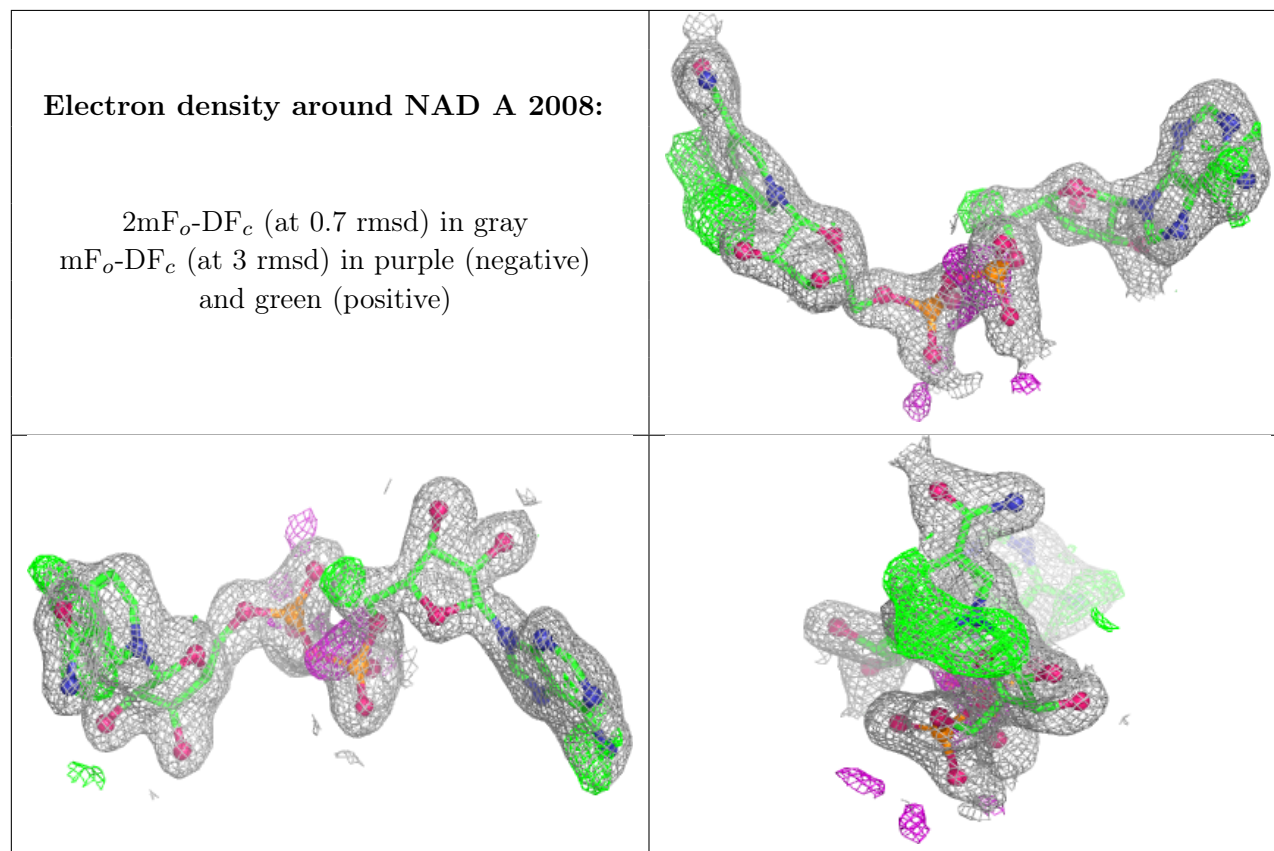
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	A	2007	7/7	0.79	0.15	44,48,55,60	0
3	PEG	A	2005	7/7	0.80	0.14	34,37,41,49	0
3	PEG	B	2007	7/7	0.83	0.15	37,46,52,54	0
7	SO4	A	2013	5/5	0.83	0.13	41,43,52,67	5
3	PEG	B	2003	7/7	0.85	0.12	33,39,46,50	0
7	SO4	B	2012	5/5	0.85	0.12	29,29,39,49	5
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	0.12	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
7	SO4	A	2012	5/5	0.92	0.11	36,39,49,52	5
8	MG	A	2014	1/1	0.93	0.17	45,45,45,45	0
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

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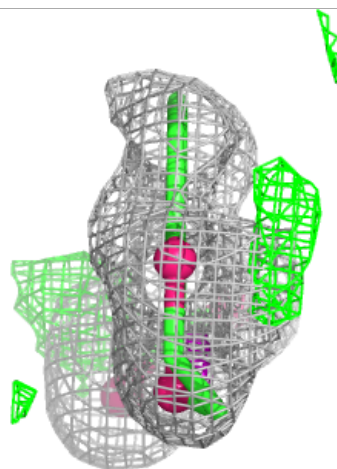
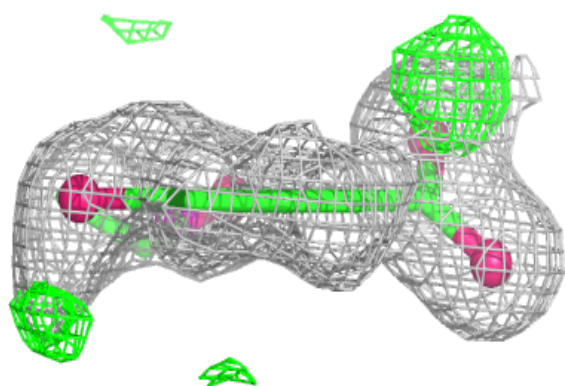
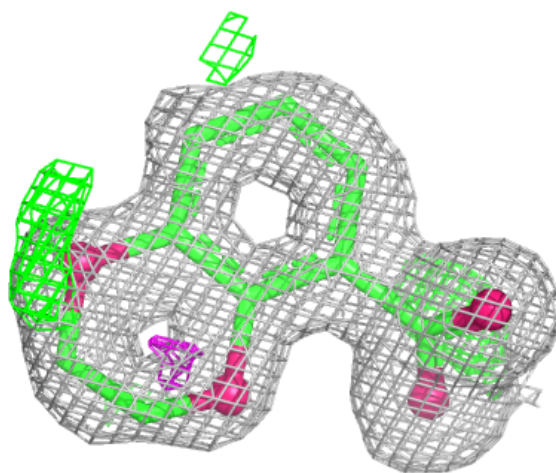
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	2001[B]	53/53	0.94	0.08	18,22,28,29	53
2	FAD	A	2001[A]	53/53	0.95	0.07	16,21,25,26	53
8	MG	B	2013	1/1	0.95	0.12	38,38,38,38	0
5	FMT	B	2006	3/3	0.95	0.14	15,15,34,38	0
2	FAD	A	2001[B]	53/53	0.95	0.07	16,21,25,27	53
5	FMT	A	2004	3/3	0.96	0.10	24,24,32,34	0
7	SO4	A	2010	5/5	0.96	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.



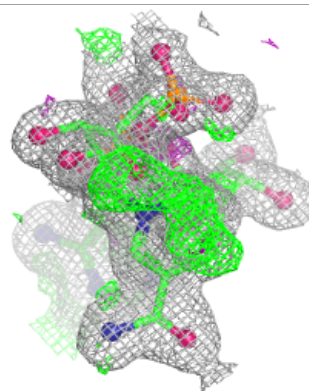
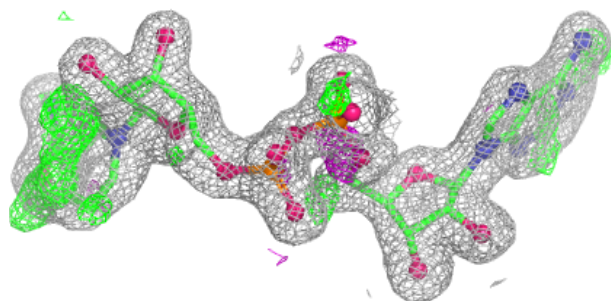
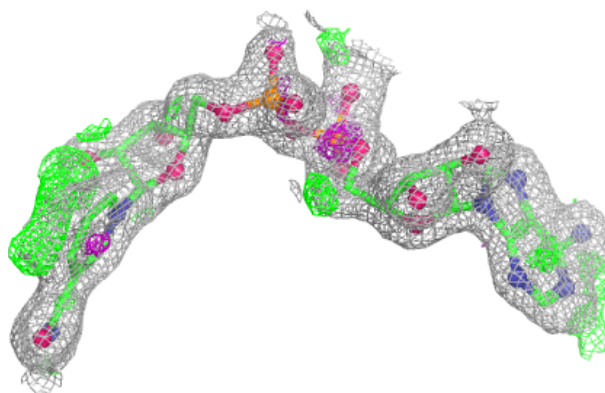
Electron density around 53E A 2003:

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

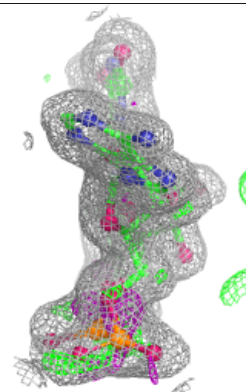
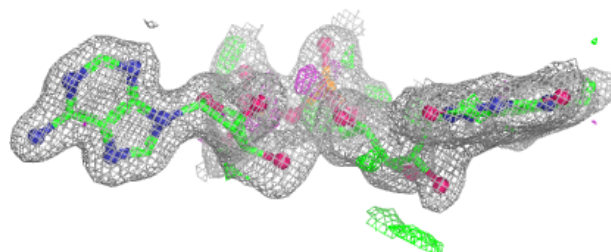
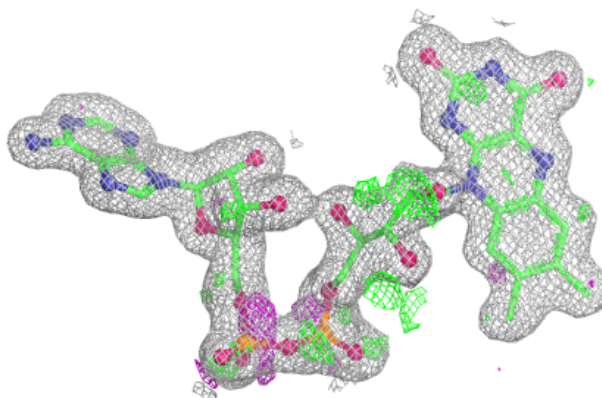


Electron density around NAD B 2010:

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

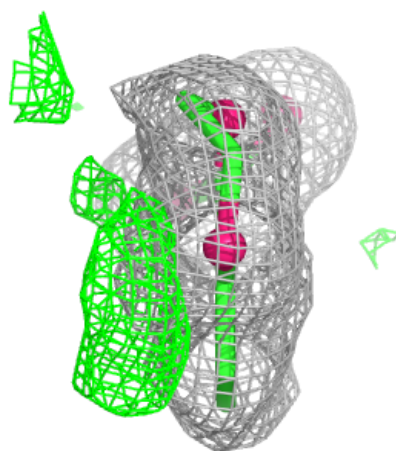
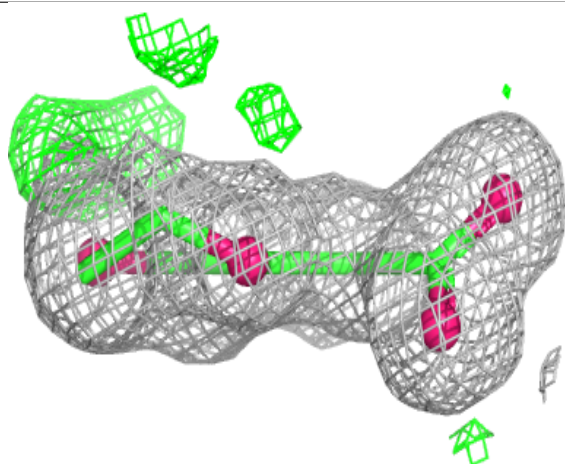
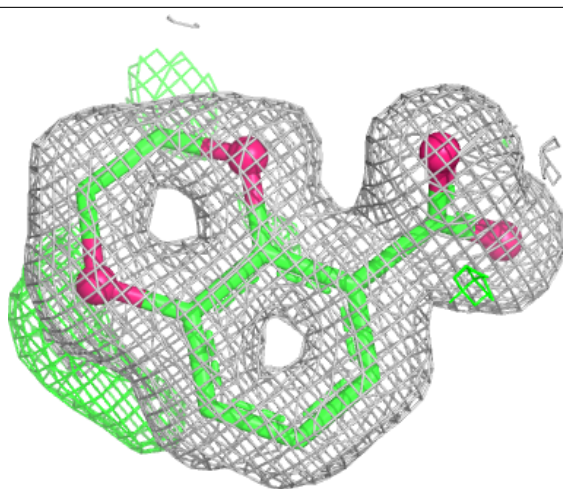
**Electron density around FAD B 2001 (A):**

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



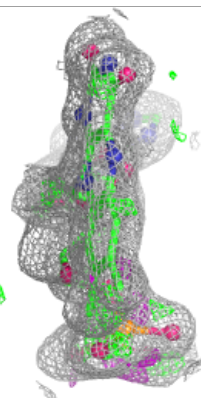
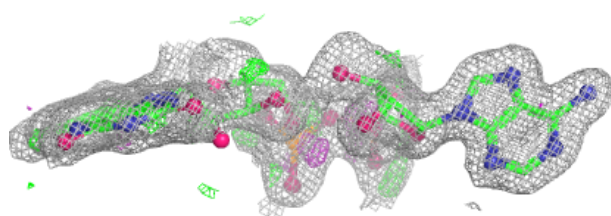
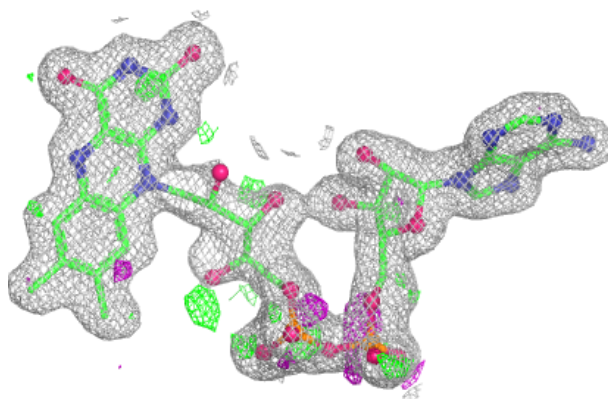
Electron density around 53E B 2004:

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

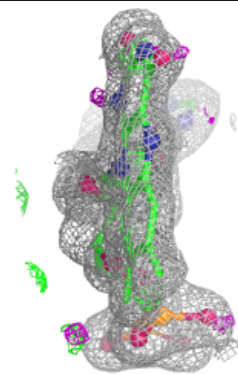
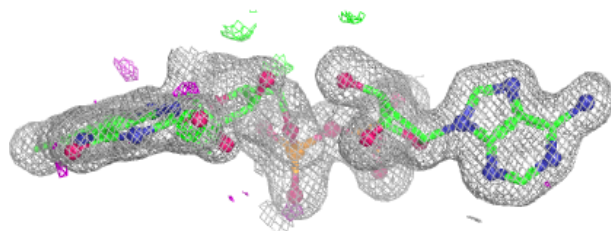
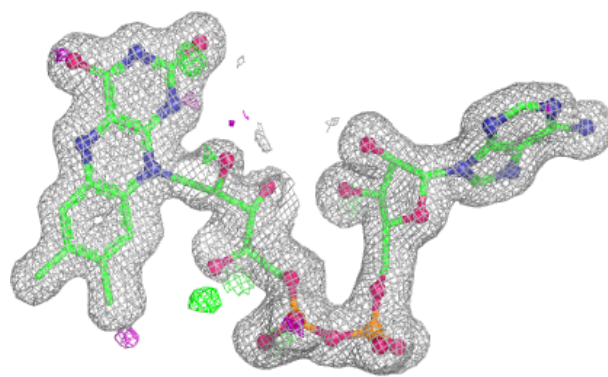


Electron density around FAD B 2001 (B):

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

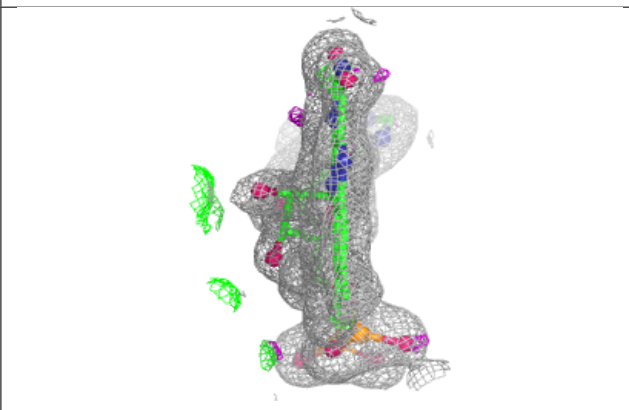
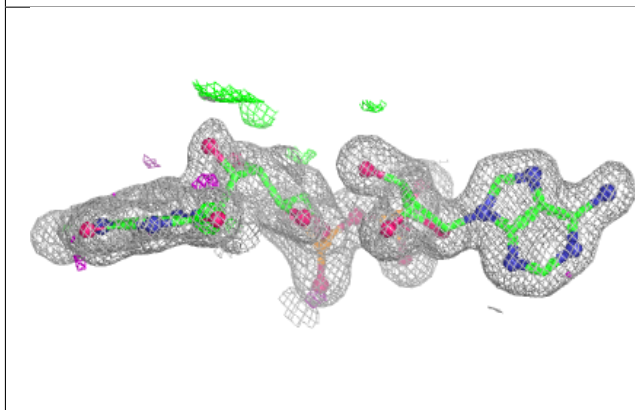
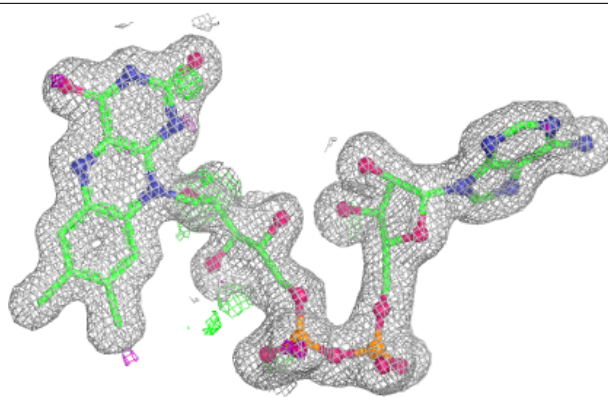
**Electron density around FAD A 2001 (A):**

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.