



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:17 PM UTC

PDB ID : 9DL6 / pdb_00009dl6
Title : Structure of proline utilization A complexed with piperidine-3-carboxylic acid
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2024-09-10
Resolution : 1.42 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

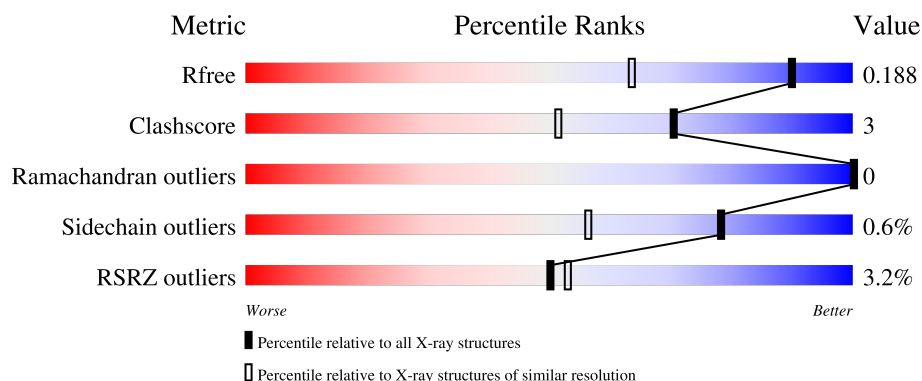
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

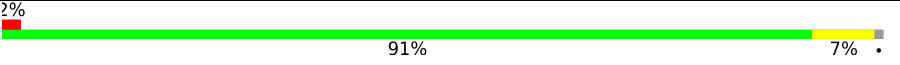
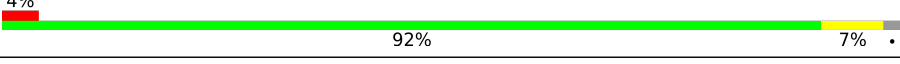
The reported resolution of this entry is 1.42 Å.

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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	 2% 91% 7% .
1	B	1235	 4% 92% 7% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FMT	A	2006	-	-	X	-
5	FMT	B	2006	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 21184 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.

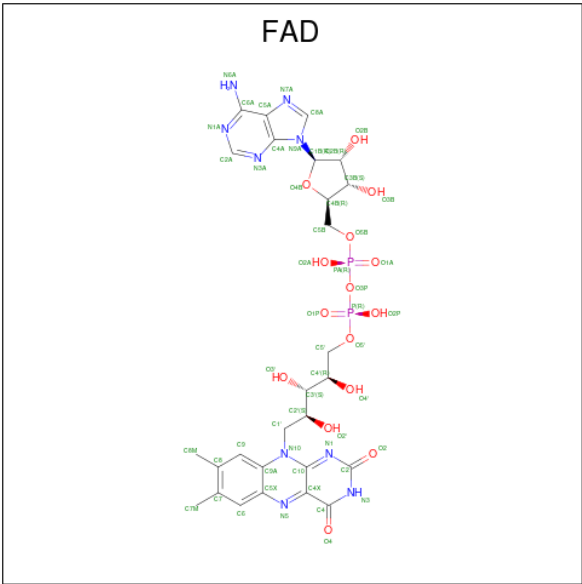
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1218	Total	C	N	O	S	0	26	0
			9174	5793	1641	1705	35			
1	B	1216	Total	C	N	O	S	0	24	0
			9095	5741	1634	1684	36			

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: $C_4H_{10}O_3$).



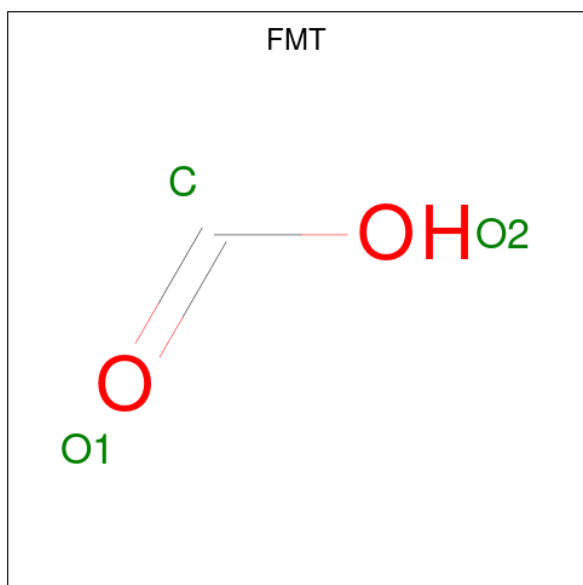
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			7	4	3	0	0
3	A	1	Total	C	O		
			7	4	3	0	0
3	A	1	Total	C	O		
			7	4	3	0	0
3	A	1	Total	C	O		
			7	4	3	0	0
3	B	1	Total	C	O		
			7	4	3	0	0
3	B	1	Total	C	O		
			7	4	3	0	0
3	B	1	Total	C	O		
			7	4	3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



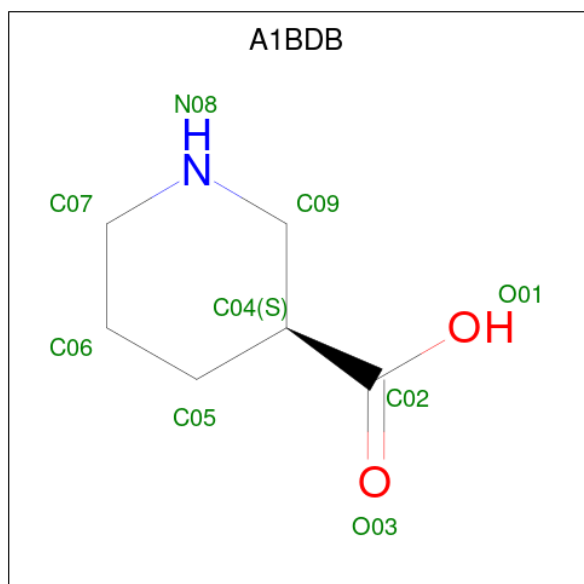
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		

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



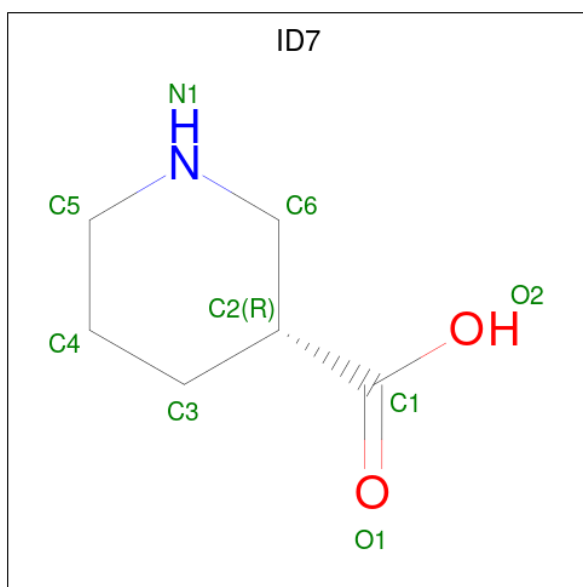
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is (3S)-piperidine-3-carboxylic acid (CCD ID: A1BDB) (formula: $C_6H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



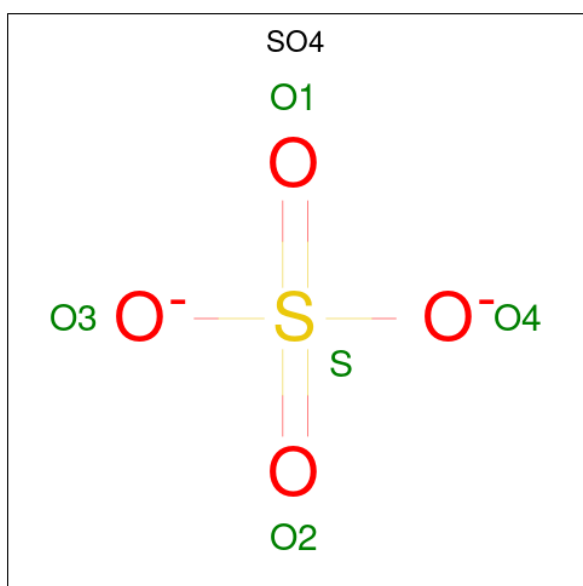
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	1
			9	6	1	2		
6	B	1	Total	C	N	O	0	1
			9	6	1	2		

- Molecule 7 is (3R)-piperidine-3-carboxylic acid (CCD ID: ID7) (formula: $C_6H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	1
			9	6	1	2		
7	B	1	Total	C	N	O	0	1
			9	6	1	2		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



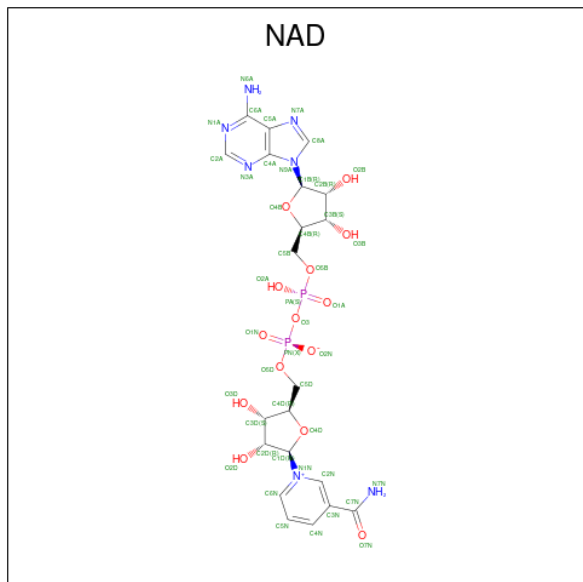
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 9 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

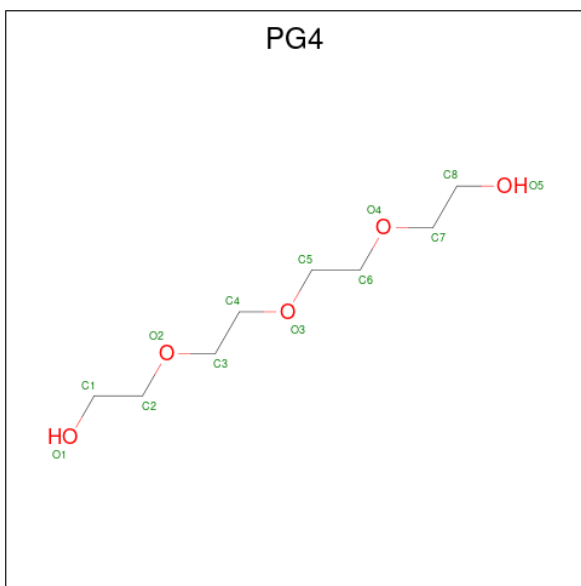


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
9	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 11 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

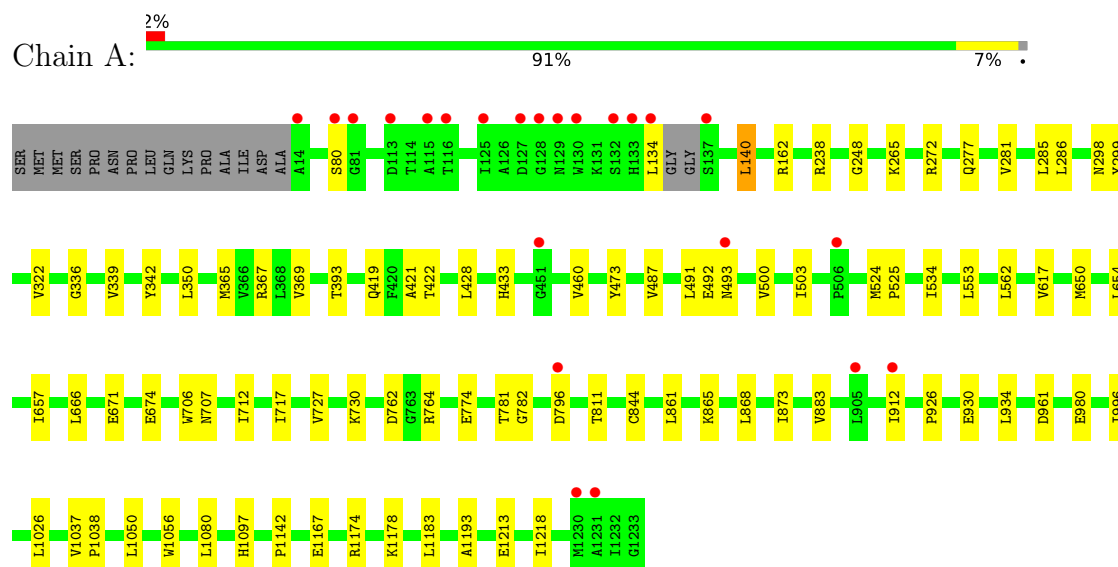
- Molecule 12 is water.

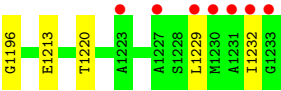
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1229	Total	O	0	4
			1229	1229		
12	B	1193	Total	O	0	4
			1193	1193		

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.51Å 101.83Å 126.55Å 90.00° 106.43° 90.00°	Depositor
Resolution (Å)	45.85 – 1.42 45.85 – 1.42	Depositor EDS
% Data completeness (in resolution range)	90.5 (45.85-1.42) 91.3 (45.85-1.42)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.42Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.167 , 0.189 0.167 , 0.188	Depositor DCC
R_{free} test set	20793 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.3	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	21184	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1BDB, SO4, PG4, ID7, PGE, FMT, NAD, FAD, MG, 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	0.26	0/9416	0.46	0/12808
1	B	0.26	0/9327	0.47	0/12692
All	All	0.26	0/18743	0.47	0/25500

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	9174	0	9293	60	0
1	B	9095	0	9169	62	0
2	A	106	0	62	4	0
2	B	106	0	62	7	0
3	A	28	0	40	1	0
3	B	21	0	30	2	0
4	A	20	0	28	1	0
4	B	20	0	28	1	0
5	A	12	0	4	6	0
5	B	6	0	2	5	0
6	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	9	0	0	1	0
7	A	9	0	0	1	0
7	B	9	0	0	1	0
8	A	25	0	0	0	0
8	B	10	0	0	0	0
9	A	44	0	26	2	0
9	B	44	0	26	2	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	B	13	0	18	3	0
12	A	1229	0	0	6	0
12	B	1193	0	0	10	0
All	All	21184	0	18788	128	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 (128) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:CYS:SG	9:B:2014:NAD:C4N	2.77	0.72
1:B:1213:GLU:HG3	5:B:2006:FMT:H	1.71	0.72
1:B:834[A]:THR:HG22	1:B:1001:ILE:HD11	1.72	0.70
1:A:674:GLU:OE2	7:A:2012[B]:ID7:N1	2.25	0.70
1:B:339[A]:VAL:HG21	1:B:350:LEU:HD21	1.75	0.69
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.75	0.69
1:B:539:GLU:OE1	12:B:2101:HOH:O	2.09	0.68
1:A:844:CYS:SG	9:A:2018:NAD:C4N	2.82	0.67
1:B:524[B]:MET:SD	12:B:2789:HOH:O	2.51	0.67
1:B:414:ASP:O	12:B:2102:HOH:O	2.12	0.67
1:A:339[A]:VAL:HG21	1:A:350:LEU:HD21	1.77	0.66
1:A:281:VAL:HG13	1:A:285[B]:LEU:HD23	1.78	0.66
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.78	0.66
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.29	0.65
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.78	0.65
1:A:796:ASP:OD1	1:A:1178:LYS:NZ	2.31	0.64
5:B:2009:FMT:O1	12:B:2103:HOH:O	2.15	0.64
1:B:332:TRP:HZ3	1:B:335[A]:MET:HE2	1.63	0.64
1:B:1196:GLY:HA3	3:B:2005:PEG:H22	1.81	0.62
1:B:618[A]:ARG:NH2	12:B:2112:HOH:O	2.33	0.61
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:GLU:OE2	6:B:2010[A]:A1BDB:N08	2.35	0.59
1:B:650:MET:O	1:B:654:LEU:HG	2.04	0.57
1:B:1213:GLU:H	5:B:2006:FMT:H	1.68	0.57
1:B:1229[A]:LEU:HD23	1:B:1232:ILE:HD12	1.84	0.57
1:A:473:TYR:HB2	2:A:2001[A]:FAD:HM71	1.85	0.57
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.87	0.57
1:B:674:GLU:OE2	7:B:2011[B]:ID7:N1	2.39	0.55
2:A:2001[A]:FAD:H8A	12:A:2770:HOH:O	2.07	0.55
1:B:1213:GLU:CG	5:B:2006:FMT:H	2.38	0.54
1:A:1183:LEU:O	12:A:2101:HOH:O	2.18	0.54
1:B:332:TRP:CZ3	1:B:335[A]:MET:HE2	2.42	0.54
1:B:473:TYR:HB2	2:B:2001[B]:FAD:HM71	1.90	0.54
1:A:134:LEU:HB3	1:A:140[B]:LEU:HD21	1.90	0.54
1:A:1213:GLU:H	5:A:2006:FMT:C	2.23	0.52
1:A:553:LEU:HD12	1:A:666:LEU:HD13	1.92	0.50
1:B:844:CYS:SG	9:B:2014:NAD:C3N	3.00	0.50
1:A:717:ILE:HG12	1:A:727:VAL:HG11	1.94	0.50
1:A:1174:ARG:HG2	1:A:1178:LYS:HE2	1.95	0.49
1:B:897:LYS:HZ1	11:B:2004:PG4:H42	1.77	0.49
1:A:650:MET:O	1:A:654:LEU:HG	2.13	0.49
1:A:868:LEU:O	1:A:912:ILE:HD11	2.14	0.48
1:A:1213:GLU:CG	5:A:2006:FMT:H	2.43	0.48
1:B:897:LYS:HZ3	11:B:2004:PG4:C7	2.27	0.48
1:A:844:CYS:SG	9:A:2018:NAD:C3N	3.02	0.48
1:B:1213:GLU:H	5:B:2006:FMT:C	2.26	0.48
1:B:617:VAL:HG12	1:B:774:GLU:HB2	1.96	0.48
1:A:782:GLY:O	1:A:811:THR:HA	2.14	0.48
1:A:796:ASP:HA	1:A:1178:LYS:NZ	2.29	0.48
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.96	0.48
1:B:853:GLN:OE1	12:B:2104:HOH:O	2.20	0.47
1:B:788:ARG:NH2	1:B:1185:GLY:O	2.45	0.47
1:B:782:GLY:O	1:B:811:THR:HA	2.14	0.47
1:A:428:LEU:HD11	1:A:460:VAL:HG21	1.96	0.47
1:B:19:ALA:O	1:B:567:ARG:NH2	2.43	0.47
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.50	0.47
1:B:69:ARG:NH2	1:B:511:ASP:OD1	2.47	0.47
1:A:562[A]:LEU:HD11	1:A:654:LEU:HD12	1.96	0.46
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.50	0.46
1:B:309:GLU:OE2	12:B:2105:HOH:O	2.21	0.46
1:A:1097:HIS:NE2	4:A:2003:PGE:H2	2.29	0.46
1:A:657:ILE:HD13	1:A:671[A]:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1056:TRP:CD1	1:B:1142:PRO:HD3	2.51	0.46
1:B:422:THR:OG1	2:B:2001[A]:FAD:O1P	2.33	0.46
1:A:422:THR:OG1	2:A:2001[B]:FAD:O1P	2.33	0.45
1:A:1080[A]:LEU:HD12	12:A:2879:HOH:O	2.15	0.45
1:B:374:TRP:HZ3	1:B:1229[A]:LEU:HB3	1.81	0.45
1:A:912:ILE:HD12	1:A:926:PRO:HB2	1.99	0.45
1:A:1213:GLU:HG3	5:A:2006:FMT:H	1.99	0.45
1:A:298:ASN:ND2	12:A:2110:HOH:O	2.34	0.45
1:B:363:ARG:NH1	1:B:442:GLY:O	2.44	0.45
1:B:448:CYS:HB2	1:B:453:GLY:HA3	1.98	0.45
1:B:1042:SER:O	1:B:1080[A]:LEU:HD13	2.17	0.45
1:B:524[A]:MET:HE3	1:B:525:PRO:HD2	1.99	0.44
1:B:118:ASP:OD1	1:B:181:ARG:NH2	2.49	0.44
1:A:433:HIS:HA	3:A:2005:PEG:H31	2.00	0.44
1:A:493:ASN:HB3	1:A:500:VAL:HB	2.00	0.44
1:A:657:ILE:HD13	1:A:671[B]:GLU:HG2	2.00	0.44
1:B:1026:LEU:HD23	1:B:1038:PRO:HG2	1.99	0.44
1:A:272:ARG:HB3	1:A:277:GLN:HG3	1.99	0.44
1:A:367:ARG:HA	1:A:419:GLN:HB2	2.00	0.44
1:B:248:GLY:HA3	1:B:299:TYR:CG	2.53	0.44
1:B:64:ALA:HA	1:B:433:HIS:CD2	2.52	0.43
1:B:272:ARG:HB3	1:B:277:GLN:HG3	2.00	0.43
2:B:2001[A]:FAD:H4'	2:B:2001[A]:FAD:H1'1	1.78	0.43
2:B:2001[B]:FAD:H8A	12:B:2759:HOH:O	2.17	0.43
1:A:487:VAL:O	1:A:491[B]:LEU:HG	2.18	0.43
1:B:1172:ARG:HH12	4:B:2007:PGE:H2	1.81	0.43
2:B:2001[A]:FAD:H8A	12:B:2759:HOH:O	2.17	0.43
3:B:2005:PEG:H11	3:B:2005:PEG:H31	1.55	0.43
1:A:238[B]:ARG:HH21	5:A:2007:FMT:H	1.83	0.43
1:B:1091[B]:ARG:HG3	1:B:1220:THR:HG21	2.00	0.43
1:A:1167:GLU:HA	1:A:1193:ALA:O	2.19	0.43
1:A:861[A]:LEU:HG	1:A:865:LYS:HE3	2.01	0.42
1:B:428:LEU:HD11	1:B:460:VAL:HG21	2.00	0.42
1:B:1069:ALA:HA	1:B:1117:ALA:HB1	2.01	0.42
1:A:617:VAL:HG12	1:A:774:GLU:HB2	2.01	0.42
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.44	0.42
1:A:712:ILE:HD13	1:A:781:THR:HG21	2.02	0.42
1:A:706:TRP:CE3	1:A:707:ASN:HA	2.54	0.42
1:A:873:ILE:HD13	1:A:912:ILE:HG21	2.02	0.42
1:A:1026:LEU:HD23	1:A:1038:PRO:HG2	2.01	0.42
1:A:265:LYS:HE3	12:A:2429:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:HB	1:A:534:ILE:HD12	2.02	0.41
1:A:369:VAL:HG12	1:A:421:ALA:HB3	2.02	0.41
1:B:824:LEU:HD23	1:B:827:GLN:HG3	2.02	0.41
1:A:492:GLU:HB3	2:A:2001[A]:FAD:H4'	2.02	0.41
5:A:2008:FMT:O1	12:A:2102:HOH:O	2.22	0.41
1:B:336:GLY:HA2	1:B:365:MET:O	2.20	0.41
1:B:1060:LYS:HE3	1:B:1060:LYS:HB2	1.80	0.41
1:A:861[A]:LEU:HD21	1:A:930:GLU:CD	2.46	0.41
1:A:861[B]:LEU:HD22	1:A:865:LYS:HE3	2.01	0.41
1:B:984:HIS:C	1:B:984:HIS:CD2	2.98	0.41
1:A:524:MET:HE3	1:A:525:PRO:HD2	2.02	0.41
1:A:1037:VAL:HG11	1:B:166:ALA:HB1	2.02	0.41
1:B:338:VAL:HG22	1:B:367:ARG:HB3	2.02	0.41
1:B:897:LYS:HZ1	11:B:2004:PG4:H22	1.86	0.41
1:A:762:ASP:OD1	1:A:764:ARG:HB2	2.20	0.41
1:A:1213:GLU:H	5:A:2006:FMT:H	1.85	0.41
1:B:1080[A]:LEU:HD12	12:B:2784:HOH:O	2.20	0.41
2:B:2001[B]:FAD:HM73	2:B:2001[B]:FAD:HM81	1.89	0.41
1:B:498:SER:HA	2:B:2001[B]:FAD:O1A	2.21	0.40
1:A:162[B]:ARG:HD2	1:A:980:GLU:OE2	2.21	0.40
1:A:336:GLY:HA2	1:A:365:MET:O	2.21	0.40
1:B:223:LEU:HB3	1:B:481:THR:HG22	2.02	0.40
1:B:225:GLU:HB3	1:B:265:LYS:HD2	2.04	0.40
1:B:531:HIS:CE1	1:B:1232:ILE:HG23	2.57	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	1241/1235 (100%)	1224 (99%)	17 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1237/1235 (100%)	1214 (98%)	23 (2%)	0	100	100
All	All	2478/2470 (100%)	2438 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	932/951 (98%)	925 (99%)	7 (1%)	73	47
1	B	913/951 (96%)	909 (100%)	4 (0%)	84	67
All	All	1845/1902 (97%)	1834 (99%)	11 (1%)	78	56

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	SER
1	A	140[A]	LEU
1	A	140[B]	LEU
1	A	342	TYR
1	A	503	ILE
1	A	730	LYS
1	A	934	LEU
1	B	342	TYR
1	B	730	LYS
1	B	833	ILE
1	B	934	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	872	HIS
1	A	1114	HIS

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Mol	Chain	Res	Type
1	B	667	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 2 are monoatomic - leaving 35 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$
5	FMT	A	2006	-	2,2,2	0.54	0	1,1,1	0.35	0
7	ID7	B	2011[B]	-	8,9,9	2.71	2 (25%)	9,11,11	1.23	0
5	FMT	B	2009	-	2,2,2	0.61	0	1,1,1	0.14	0
3	PEG	A	2002	-	6,6,6	0.26	0	5,5,5	0.14	0
6	A1BDB	B	2010[A]	-	8,9,9	1.41	1 (12%)	9,11,11	1.27	1 (11%)
5	FMT	A	2008	-	2,2,2	0.58	0	1,1,1	0.25	0
7	ID7	A	2012[B]	-	8,9,9	2.68	2 (25%)	9,11,11	1.43	1 (11%)
8	SO4	B	2013	-	4,4,4	0.68	0	6,6,6	0.11	0
2	FAD	B	2001[B]	-	58,58,58	2.33	15 (25%)	85,89,89	1.91	22 (25%)
2	FAD	B	2001[A]	-	58,58,58	2.25	14 (24%)	85,89,89	1.71	21 (24%)
5	FMT	B	2006	-	2,2,2	0.65	0	1,1,1	0.41	0
8	SO4	A	2014	-	4,4,4	0.62	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGE	B	2007	-	9,9,9	0.34	0	8,8,8	0.43	0
8	SO4	A	2017	-	4,4,4	0.67	0	6,6,6	0.10	0
4	PGE	A	2010	-	9,9,9	0.32	0	8,8,8	0.37	0
3	PEG	A	2005	-	6,6,6	0.24	0	5,5,5	0.21	0
8	SO4	A	2013	-	4,4,4	0.54	0	6,6,6	0.30	0
3	PEG	A	2004	-	6,6,6	0.23	0	5,5,5	0.30	0
5	FMT	A	2007	-	2,2,2	0.72	0	1,1,1	0.48	0
4	PGE	B	2002	-	9,9,9	0.34	0	8,8,8	0.49	0
4	PGE	A	2003	-	9,9,9	0.32	0	8,8,8	0.48	0
11	PG4	B	2004	-	12,12,12	0.31	0	11,11,11	0.33	0
3	PEG	B	2005	-	6,6,6	0.24	0	5,5,5	0.25	0
9	NAD	A	2018	10	46,48,48	3.64	20 (43%)	64,73,73	2.00	14 (21%)
8	SO4	A	2016	-	4,4,4	0.67	0	6,6,6	0.07	0
8	SO4	A	2015	-	4,4,4	0.68	0	6,6,6	0.24	0
5	FMT	A	2020	-	2,2,2	0.63	0	1,1,1	0.26	0
3	PEG	B	2008	-	6,6,6	0.23	0	5,5,5	0.27	0
2	FAD	A	2001[A]	-	58,58,58	2.22	13 (22%)	85,89,89	2.04	20 (23%)
2	FAD	A	2001[B]	-	58,58,58	2.24	14 (24%)	85,89,89	1.81	22 (25%)
3	PEG	A	2009	-	6,6,6	0.26	0	5,5,5	0.20	0
3	PEG	B	2003	-	6,6,6	0.25	0	5,5,5	0.26	0
9	NAD	B	2014	10	46,48,48	3.52	18 (39%)	64,73,73	2.05	11 (17%)
8	SO4	B	2012	-	4,4,4	0.59	0	6,6,6	0.29	0
6	A1BDB	A	2011[A]	-	8,9,9	1.45	1 (12%)	9,11,11	1.31	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ID7	B	2011[B]	-	-	0/4/12/12	0/1/1/1
3	PEG	A	2002	-	-	0/4/4/4	-
6	A1BDB	B	2010[A]	-	-	0/4/12/12	1/1/1/1
7	ID7	A	2012[B]	-	-	2/4/12/12	0/1/1/1
2	FAD	B	2001[B]	-	-	17/34/50/50	0/6/6/6
2	FAD	B	2001[A]	-	-	8/34/50/50	0/6/6/6
4	PGE	B	2007	-	-	3/7/7/7	-
4	PGE	A	2010	-	-	2/7/7/7	-
3	PEG	A	2005	-	-	2/4/4/4	-
3	PEG	A	2004	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	B	2002	-	-	1/7/7/7	-
4	PGE	A	2003	-	-	4/7/7/7	-
11	PG4	B	2004	-	-	4/10/10/10	-
3	PEG	B	2005	-	-	2/4/4/4	-
9	NAD	A	2018	10	-	6/30/62/62	0/5/5/5
3	PEG	B	2008	-	-	1/4/4/4	-
2	FAD	A	2001[A]	-	-	15/34/50/50	0/6/6/6
2	FAD	A	2001[B]	-	-	9/34/50/50	0/6/6/6
3	PEG	A	2009	-	-	1/4/4/4	-
3	PEG	B	2003	-	-	0/4/4/4	-
9	NAD	B	2014	10	-	5/30/62/62	0/5/5/5
6	A1BDB	A	2011[A]	-	-	0/4/12/12	1/1/1/1

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001[B]	FAD	PA-O3P	-10.39	1.48	1.59
2	B	2001[A]	FAD	PA-O3P	-9.62	1.49	1.59
9	B	2014	NAD	O4D-C1D	-9.36	1.28	1.40
2	A	2001[A]	FAD	PA-O3P	-9.13	1.49	1.59
9	A	2018	NAD	O4D-C1D	-9.10	1.28	1.40
9	B	2014	NAD	C3B-C4B	-8.51	1.31	1.53
9	A	2018	NAD	PN-O3	8.49	1.68	1.59
9	A	2018	NAD	C3B-C4B	-8.43	1.31	1.53
9	B	2014	NAD	C7N-N7N	8.27	1.48	1.33
9	A	2018	NAD	C7N-N7N	8.05	1.47	1.33
2	A	2001[B]	FAD	PA-O3P	-7.73	1.51	1.59
9	A	2018	NAD	C3D-C4D	-7.58	1.33	1.53
9	B	2014	NAD	C3D-C4D	-7.10	1.35	1.53
9	B	2014	NAD	PN-O3	7.09	1.67	1.59
9	A	2018	NAD	O4B-C4B	7.01	1.60	1.45
2	B	2001[B]	FAD	O4-C4	6.98	1.36	1.23
2	A	2001[B]	FAD	O4-C4	6.89	1.36	1.23
9	B	2014	NAD	O4D-C4D	6.85	1.60	1.45
9	A	2018	NAD	O4D-C4D	6.84	1.60	1.45
9	B	2014	NAD	O4B-C4B	6.77	1.60	1.45
2	B	2001[A]	FAD	O4-C4	6.76	1.36	1.23
7	B	2011[B]	ID7	C6-N1	6.43	1.63	1.47
7	A	2012[B]	ID7	C6-N1	6.39	1.62	1.47
2	A	2001[A]	FAD	O4-C4	6.31	1.35	1.23
9	A	2018	NAD	C6A-N6A	5.85	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001[B]	FAD	O2-C2	5.79	1.35	1.24
9	B	2014	NAD	C6A-N6A	5.77	1.48	1.34
2	B	2001[B]	FAD	O2-C2	5.33	1.34	1.24
2	B	2001[A]	FAD	O2-C2	5.12	1.34	1.24
2	A	2001[A]	FAD	O2-C2	5.03	1.34	1.24
2	A	2001[B]	FAD	C4X-N5	4.55	1.40	1.30
2	B	2001[A]	FAD	C4X-N5	4.22	1.39	1.30
9	B	2014	NAD	O3D-C3D	4.16	1.53	1.43
2	A	2001[A]	FAD	C6A-N6A	4.14	1.44	1.34
2	A	2001[B]	FAD	C6A-N6A	4.07	1.44	1.34
2	B	2001[B]	FAD	C6A-N6A	4.03	1.44	1.34
2	B	2001[B]	FAD	C4X-N5	4.01	1.39	1.30
2	B	2001[A]	FAD	C6A-N6A	4.00	1.44	1.34
9	A	2018	NAD	O3D-C3D	3.90	1.52	1.43
2	A	2001[A]	FAD	C4X-N5	3.86	1.39	1.30
9	B	2014	NAD	C3N-C7N	3.80	1.56	1.50
2	A	2001[A]	FAD	P-O3P	3.66	1.63	1.59
9	A	2018	NAD	C3N-C7N	3.62	1.56	1.50
2	A	2001[B]	FAD	P-O3P	3.47	1.63	1.59
9	A	2018	NAD	O4B-C1B	-3.39	1.34	1.42
9	A	2018	NAD	C2N-N1N	3.37	1.38	1.35
2	A	2001[B]	FAD	C2-N1	3.16	1.43	1.36
9	A	2018	NAD	PA-O3	3.15	1.62	1.59
9	B	2014	NAD	O4B-C1B	-3.15	1.34	1.42
9	B	2014	NAD	C2N-N1N	3.11	1.38	1.35
2	A	2001[B]	FAD	O2'-C2'	-3.09	1.36	1.43
2	A	2001[A]	FAD	O2'-C2'	-3.01	1.37	1.43
9	A	2018	NAD	O3B-C3B	2.91	1.50	1.43
2	B	2001[B]	FAD	C2-N1	2.90	1.43	1.36
2	A	2001[B]	FAD	PA-O5B	-2.84	1.48	1.59
9	B	2014	NAD	O3B-C3B	2.82	1.49	1.43
9	A	2018	NAD	O7N-C7N	-2.80	1.18	1.24
2	A	2001[A]	FAD	C2-N1	2.80	1.43	1.36
2	B	2001[A]	FAD	C2-N1	2.80	1.43	1.36
2	A	2001[A]	FAD	PA-O5B	-2.80	1.48	1.59
2	B	2001[B]	FAD	O2'-C2'	-2.78	1.37	1.43
9	A	2018	NAD	C5A-C4A	-2.76	1.34	1.39
2	B	2001[A]	FAD	O2'-C2'	-2.73	1.37	1.43
6	A	2011[A]	A1BDB	C04-C02	2.65	1.56	1.51
9	B	2014	NAD	C2A-N1A	2.63	1.38	1.33
6	B	2010[A]	A1BDB	C04-C02	2.61	1.56	1.51
2	A	2001[B]	FAD	C10-N1	2.60	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001[B]	FAD	O4'-C4'	-2.59	1.37	1.43
9	A	2018	NAD	C2A-N1A	2.57	1.38	1.33
7	B	2011[B]	ID7	C2-C1	2.54	1.56	1.51
2	B	2001[B]	FAD	P-O3P	2.49	1.62	1.59
2	B	2001[A]	FAD	O4'-C4'	-2.47	1.38	1.43
2	A	2001[B]	FAD	O4B-C4B	-2.43	1.39	1.45
2	B	2001[A]	FAD	O4B-C4B	-2.42	1.39	1.45
2	B	2001[B]	FAD	O4B-C4B	-2.41	1.39	1.45
9	B	2014	NAD	O7N-C7N	-2.38	1.19	1.24
2	B	2001[A]	FAD	PA-O5B	-2.37	1.50	1.59
2	B	2001[B]	FAD	PA-O5B	-2.36	1.50	1.59
7	A	2012[B]	ID7	C2-C1	2.35	1.55	1.51
2	B	2001[B]	FAD	P-O1P	2.35	1.58	1.50
2	A	2001[A]	FAD	O4B-C4B	-2.34	1.39	1.45
2	B	2001[A]	FAD	PA-O2A	-2.33	1.44	1.55
9	A	2018	NAD	C8A-N9A	-2.31	1.33	1.37
2	B	2001[A]	FAD	C10-N1	2.29	1.37	1.33
2	B	2001[A]	FAD	O2B-C2B	-2.27	1.37	1.43
2	B	2001[B]	FAD	O4'-C4'	-2.25	1.38	1.43
2	B	2001[B]	FAD	O2B-C2B	-2.25	1.37	1.43
9	B	2014	NAD	C5A-N7A	-2.25	1.35	1.39
2	B	2001[B]	FAD	PA-O2A	-2.25	1.44	1.55
2	A	2001[B]	FAD	PA-O2A	-2.23	1.45	1.55
2	B	2001[B]	FAD	C10-N1	2.18	1.37	1.33
2	A	2001[A]	FAD	PA-O2A	-2.17	1.45	1.55
2	B	2001[A]	FAD	O3'-C3'	-2.15	1.37	1.43
2	A	2001[A]	FAD	O4'-C4'	-2.14	1.38	1.43
2	A	2001[B]	FAD	O3'-C3'	-2.12	1.37	1.43
9	A	2018	NAD	C5A-N7A	-2.06	1.35	1.39
9	B	2014	NAD	C8A-N9A	-2.05	1.34	1.37
2	A	2001[A]	FAD	P-O1P	2.04	1.57	1.50
9	A	2018	NAD	O2B-C2B	-2.02	1.37	1.43
9	B	2014	NAD	C5A-C4A	-2.01	1.35	1.39

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001[A]	FAD	C5'-C4'-C3'	-8.00	97.13	112.22
9	B	2014	NAD	N3A-C2A-N1A	-6.08	119.38	128.58
2	A	2001[B]	FAD	N3A-C2A-N1A	-6.07	119.39	128.58
9	B	2014	NAD	C5A-C4A-N3A	-5.78	118.76	126.72
2	B	2001[B]	FAD	N3A-C2A-N1A	-5.61	120.10	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2018	NAD	C4A-N9A-C1B	-5.56	113.63	126.63
2	B	2001[A]	FAD	N3A-C2A-N1A	-5.54	120.20	128.58
2	A	2001[A]	FAD	N3A-C2A-N1A	-5.52	120.22	128.58
2	B	2001[B]	FAD	C5'-C4'-C3'	-5.36	102.11	112.22
9	A	2018	NAD	N3A-C2A-N1A	-5.35	120.48	128.58
2	A	2001[A]	FAD	C5A-C4A-N3A	-5.14	119.64	126.72
9	A	2018	NAD	N9A-C8A-N7A	-5.05	106.78	113.94
9	B	2014	NAD	N9A-C8A-N7A	-5.01	106.83	113.94
2	B	2001[B]	FAD	O2A-PA-O3P	-4.96	93.86	107.27
9	B	2014	NAD	C4A-N9A-C1B	-4.82	115.35	126.63
9	A	2018	NAD	C5A-C4A-N3A	-4.76	120.16	126.72
9	A	2018	NAD	C4D-O4D-C1D	-4.75	105.58	109.92
9	B	2014	NAD	N3A-C4A-N9A	4.56	134.93	127.17
2	B	2001[B]	FAD	C5A-C4A-N3A	-4.49	120.54	126.72
2	A	2001[B]	FAD	C5A-C4A-N3A	-4.41	120.65	126.72
2	B	2001[A]	FAD	C5A-C4A-N3A	-4.30	120.80	126.72
9	A	2018	NAD	C1B-N9A-C8A	4.27	136.56	127.09
2	B	2001[B]	FAD	O2P-P-O3P	-4.21	95.90	107.27
2	A	2001[A]	FAD	O5'-P-O1P	4.04	124.96	108.94
2	A	2001[A]	FAD	N3A-C4A-N9A	4.03	134.02	127.17
9	B	2014	NAD	C2A-N3A-C4A	4.02	121.65	111.83
2	A	2001[A]	FAD	O2P-P-O3P	-4.01	96.43	107.27
2	A	2001[B]	FAD	C4-C4X-N5	3.95	123.66	118.21
9	A	2018	NAD	C4A-N9A-C8A	3.84	109.77	105.74
9	B	2014	NAD	C4A-N9A-C8A	3.81	109.74	105.74
2	A	2001[A]	FAD	C5A-N7A-C8A	3.75	109.34	103.45
2	A	2001[B]	FAD	N3A-C4A-N9A	3.74	133.52	127.17
9	A	2018	NAD	N3A-C4A-N9A	3.72	133.50	127.17
2	A	2001[A]	FAD	C4-C4X-N5	3.68	123.29	118.21
2	A	2001[B]	FAD	C5A-N7A-C8A	3.63	109.15	103.45
2	B	2001[B]	FAD	N3A-C4A-N9A	3.59	133.28	127.17
2	A	2001[A]	FAD	C2A-N3A-C4A	3.58	120.58	111.83
2	A	2001[B]	FAD	C2A-N3A-C4A	3.54	120.47	111.83
9	B	2014	NAD	C1B-N9A-C8A	3.49	134.84	127.09
2	B	2001[A]	FAD	N3A-C4A-N9A	3.49	133.10	127.17
2	B	2001[B]	FAD	C5A-N7A-C8A	3.48	108.92	103.45
2	A	2001[A]	FAD	O2P-P-O5'	-3.46	91.88	107.57
2	B	2001[B]	FAD	C2A-N3A-C4A	3.39	120.12	111.83
2	B	2001[A]	FAD	C5A-N7A-C8A	3.38	108.76	103.45
9	B	2014	NAD	C5A-N7A-C8A	3.36	108.72	103.45
2	A	2001[B]	FAD	N9A-C8A-N7A	-3.31	109.25	113.94
2	A	2001[A]	FAD	O2A-PA-O3P	-3.30	98.36	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001[B]	FAD	C4X-C4-N3	3.30	121.64	113.25
2	B	2001[A]	FAD	C2A-N3A-C4A	3.28	119.84	111.83
2	B	2001[A]	FAD	O2P-P-O3P	-3.28	98.42	107.27
9	A	2018	NAD	C5A-N7A-C8A	3.27	108.59	103.45
9	B	2014	NAD	C4D-O4D-C1D	-3.23	106.96	109.92
2	A	2001[B]	FAD	C5X-C9A-N10	3.21	120.87	117.97
2	B	2001[B]	FAD	C4-C4X-N5	3.16	122.58	118.21
9	A	2018	NAD	C2A-N3A-C4A	3.07	119.32	111.83
2	A	2001[A]	FAD	C4-N3-C2	-3.04	120.24	125.64
2	A	2001[A]	FAD	N9A-C8A-N7A	-3.02	109.65	113.94
2	A	2001[A]	FAD	C4A-C5A-N7A	-3.00	107.15	110.58
2	B	2001[A]	FAD	C9-C9A-N10	-2.98	117.84	121.85
2	B	2001[B]	FAD	C4-N3-C2	-2.96	120.39	125.64
2	B	2001[A]	FAD	C4-C4X-N5	2.95	122.29	118.21
2	B	2001[A]	FAD	O5'-P-O1P	2.90	120.45	108.94
2	A	2001[B]	FAD	O5'-P-O1P	2.86	120.26	108.94
2	B	2001[B]	FAD	N9A-C8A-N7A	-2.83	109.92	113.94
2	B	2001[A]	FAD	N9A-C8A-N7A	-2.80	109.97	113.94
2	A	2001[B]	FAD	O2P-P-O3P	-2.79	99.73	107.27
2	B	2001[B]	FAD	O2-C2-N1	-2.77	117.20	121.80
2	A	2001[B]	FAD	C9-C9A-N10	-2.77	118.13	121.85
2	A	2001[B]	FAD	O2A-PA-O3P	-2.76	99.81	107.27
2	B	2001[B]	FAD	C4A-C5A-N7A	-2.75	107.44	110.58
2	B	2001[B]	FAD	O3P-P-O1P	2.75	118.97	110.70
2	B	2001[A]	FAD	C5X-C9A-N10	2.74	120.45	117.97
2	B	2001[A]	FAD	C4-N3-C2	-2.72	120.81	125.64
2	A	2001[A]	FAD	C4X-C4-N3	2.67	120.06	113.25
2	A	2001[B]	FAD	C4-N3-C2	-2.67	120.91	125.64
2	B	2001[A]	FAD	C4A-C5A-N7A	-2.66	107.53	110.58
2	A	2001[B]	FAD	C4A-C5A-N7A	-2.66	107.54	110.58
2	A	2001[A]	FAD	O3P-P-O1P	2.63	118.61	110.70
2	A	2001[B]	FAD	O4-C4-C4X	-2.62	119.62	126.53
2	B	2001[B]	FAD	O2P-P-O5'	-2.61	95.74	107.57
9	A	2018	NAD	C2N-C3N-C4N	2.60	121.28	118.26
2	B	2001[A]	FAD	C4X-C4-N3	2.55	119.75	113.25
2	B	2001[B]	FAD	C4X-C10-N10	2.50	120.06	116.48
2	A	2001[B]	FAD	O3P-P-O1P	2.48	118.15	110.70
9	A	2018	NAD	O2N-PN-O3	2.46	113.91	107.27
2	A	2001[A]	FAD	O4-C4-C4X	-2.45	120.06	126.53
6	B	2010[A]	A1BDB	O01-C02-C04	2.44	120.49	114.16
2	B	2001[B]	FAD	C10-C4X-N5	-2.38	119.95	124.81
2	A	2001[B]	FAD	C4A-N9A-C8A	2.37	108.23	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001[B]	FAD	O4-C4-C4X	-2.34	120.35	126.53
2	B	2001[A]	FAD	O2A-PA-O3P	-2.34	100.95	107.27
2	B	2001[B]	FAD	C4X-C4-N3	2.32	119.16	113.25
2	B	2001[A]	FAD	O4-C4-C4X	-2.32	120.41	126.53
2	A	2001[B]	FAD	O2P-P-O5'	-2.31	97.10	107.57
2	A	2001[B]	FAD	C9A-C5X-N5	-2.28	120.03	122.45
7	A	2012[B]	ID7	O2-C1-C2	2.27	120.06	114.16
9	A	2018	NAD	C6A-C5A-C4A	2.27	120.28	117.18
2	A	2001[A]	FAD	C4X-C10-N10	2.26	119.72	116.48
2	B	2001[A]	FAD	O2A-PA-O5B	-2.26	97.33	107.57
2	B	2001[B]	FAD	C9-C9A-N10	-2.25	118.82	121.85
2	A	2001[B]	FAD	C2A-N1A-C6A	2.24	122.41	118.73
2	A	2001[A]	FAD	C10-C4X-N5	-2.21	120.30	124.81
9	B	2014	NAD	C2B-C1B-N9A	-2.20	107.84	113.30
2	B	2001[B]	FAD	O3P-PA-O1A	2.14	117.13	110.70
2	B	2001[A]	FAD	O3P-P-O1P	2.13	117.12	110.70
2	B	2001[A]	FAD	O3P-PA-O1A	2.12	117.08	110.70
2	B	2001[B]	FAD	O5B-PA-O1A	2.08	117.16	108.94
2	A	2001[A]	FAD	C9-C9A-N10	-2.06	119.08	121.85
6	A	2011[A]	A1BDB	O01-C02-C04	2.05	119.48	114.16
2	A	2001[B]	FAD	C10-N1-C2	2.05	121.28	116.85
9	A	2018	NAD	O4B-C1B-C2B	-2.03	102.27	106.62
2	B	2001[A]	FAD	C4X-C10-N10	2.00	119.35	116.48
2	B	2001[A]	FAD	C2A-N1A-C6A	2.00	122.02	118.73

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001[A]	FAD	C5B-O5B-PA-O1A
2	A	2001[A]	FAD	C5B-O5B-PA-O3P
2	A	2001[A]	FAD	P-O3P-PA-O5B
2	A	2001[A]	FAD	C2'-C3'-C4'-O4'
2	A	2001[A]	FAD	C2'-C3'-C4'-C5'
2	A	2001[A]	FAD	O3'-C3'-C4'-C5'
2	A	2001[A]	FAD	C5'-O5'-P-O1P
2	A	2001[A]	FAD	C5'-O5'-P-O3P
2	A	2001[B]	FAD	P-O3P-PA-O5B
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

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Mol	Chain	Res	Type	Atoms
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-O1A
2	B	2001[B]	FAD	C5B-O5B-PA-O3P
2	B	2001[B]	FAD	C1'-C2'-C3'-C4'
2	B	2001[B]	FAD	C2'-C3'-C4'-O4'
2	B	2001[B]	FAD	O3'-C3'-C4'-O4'
2	B	2001[B]	FAD	C5'-O5'-P-O1P
2	B	2001[B]	FAD	C5'-O5'-P-O2P
2	B	2001[B]	FAD	C5'-O5'-P-O3P
7	A	2012[B]	ID7	O2-C1-C2-C6
9	A	2018	NAD	C5B-O5B-PA-O1A
2	B	2001[B]	FAD	O3'-C3'-C4'-C5'
2	B	2001[B]	FAD	C2'-C3'-C4'-C5'
11	B	2004	PG4	O3-C5-C6-O4
3	B	2005	PEG	C1-C2-O2-C3
2	A	2001[A]	FAD	O3'-C3'-C4'-O4'
4	B	2007	PGE	O2-C3-C4-O3
4	A	2003	PGE	O1-C1-C2-O2
4	B	2002	PGE	O1-C1-C2-O2
11	B	2004	PG4	O1-C1-C2-O2
3	A	2005	PEG	O2-C3-C4-O4
11	B	2004	PG4	O4-C7-C8-O5
3	B	2005	PEG	O1-C1-C2-O2
4	A	2010	PGE	O3-C5-C6-O4
2	A	2001[A]	FAD	C3B-C4B-C5B-O5B
2	A	2001[B]	FAD	O2'-C2'-C3'-O3'
3	B	2008	PEG	O1-C1-C2-O2
9	A	2018	NAD	C3D-C4D-C5D-O5D
2	A	2001[B]	FAD	O2'-C2'-C3'-C4'
2	B	2001[B]	FAD	O2'-C2'-C3'-C4'
4	B	2007	PGE	C3-C4-O3-C5
2	B	2001[A]	FAD	P-O3P-PA-O5B
2	B	2001[B]	FAD	PA-O3P-P-O5'
4	A	2003	PGE	C6-C5-O3-C4
11	B	2004	PG4	C6-C5-O3-C4
2	A	2001[B]	FAD	C1'-C2'-C3'-O3'
2	B	2001[A]	FAD	C1'-C2'-C3'-O3'
7	A	2012[B]	ID7	O1-C1-C2-C6
4	B	2007	PGE	C1-C2-O2-C3
9	A	2018	NAD	C4D-C5D-O5D-PN

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Mol	Chain	Res	Type	Atoms
9	A	2018	NAD	C2B-C1B-N9A-C8A
9	B	2014	NAD	C2B-C1B-N9A-C8A
4	A	2003	PGE	C1-C2-O2-C3
2	A	2001[A]	FAD	C5B-O5B-PA-O2A
2	A	2001[A]	FAD	C5'-O5'-P-O2P
2	A	2001[B]	FAD	C5'-O5'-P-O1P
2	B	2001[B]	FAD	C5B-O5B-PA-O2A
9	B	2014	NAD	C5B-O5B-PA-O1A
2	B	2001[A]	FAD	O2'-C2'-C3'-C4'
9	B	2014	NAD	C4D-C5D-O5D-PN
3	A	2004	PEG	C4-C3-O2-C2
2	A	2001[A]	FAD	O4B-C4B-C5B-O5B
2	B	2001[B]	FAD	C3B-C4B-C5B-O5B
3	A	2009	PEG	C1-C2-O2-C3
2	B	2001[A]	FAD	O2'-C2'-C3'-O3'
4	A	2010	PGE	C3-C4-O3-C5
9	A	2018	NAD	O4D-C4D-C5D-O5D
2	B	2001[B]	FAD	P-O3P-PA-O5B
3	A	2005	PEG	C1-C2-O2-C3
9	B	2014	NAD	C2B-C1B-N9A-C4A
2	A	2001[A]	FAD	P-O3P-PA-O1A
2	B	2001[B]	FAD	PA-O3P-P-O2P
2	B	2001[A]	FAD	C3B-C4B-C5B-O5B
9	A	2018	NAD	C2B-C1B-N9A-C4A
9	B	2014	NAD	C3D-C4D-C5D-O5D
2	A	2001[A]	FAD	C4'-C5'-O5'-P
4	A	2003	PGE	O2-C3-C4-O3
2	B	2001[B]	FAD	P-O3P-PA-O1A

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2011[A]	A1BDB	C04-C05-C06-C07-C09-N08
6	B	2010[A]	A1BDB	C04-C05-C06-C07-C09-N08

19 monomers are involved in 37 short contacts:

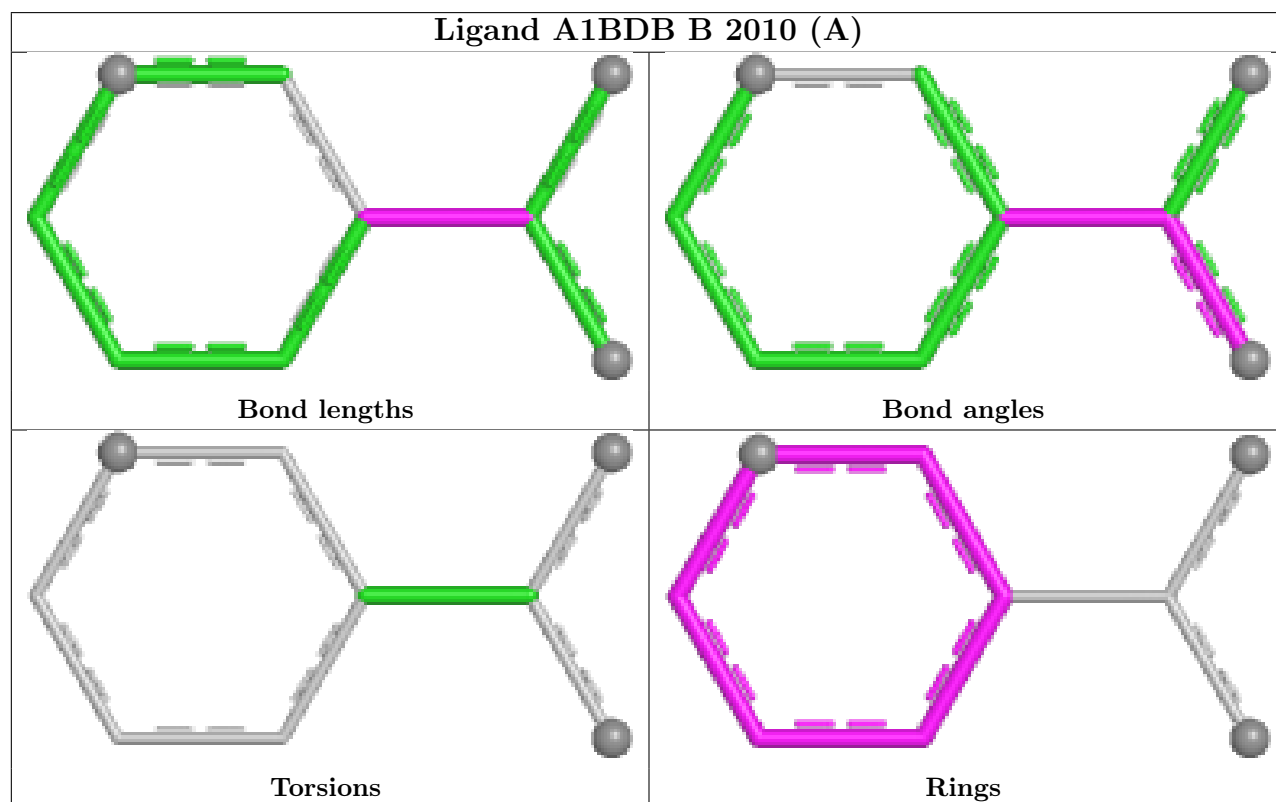
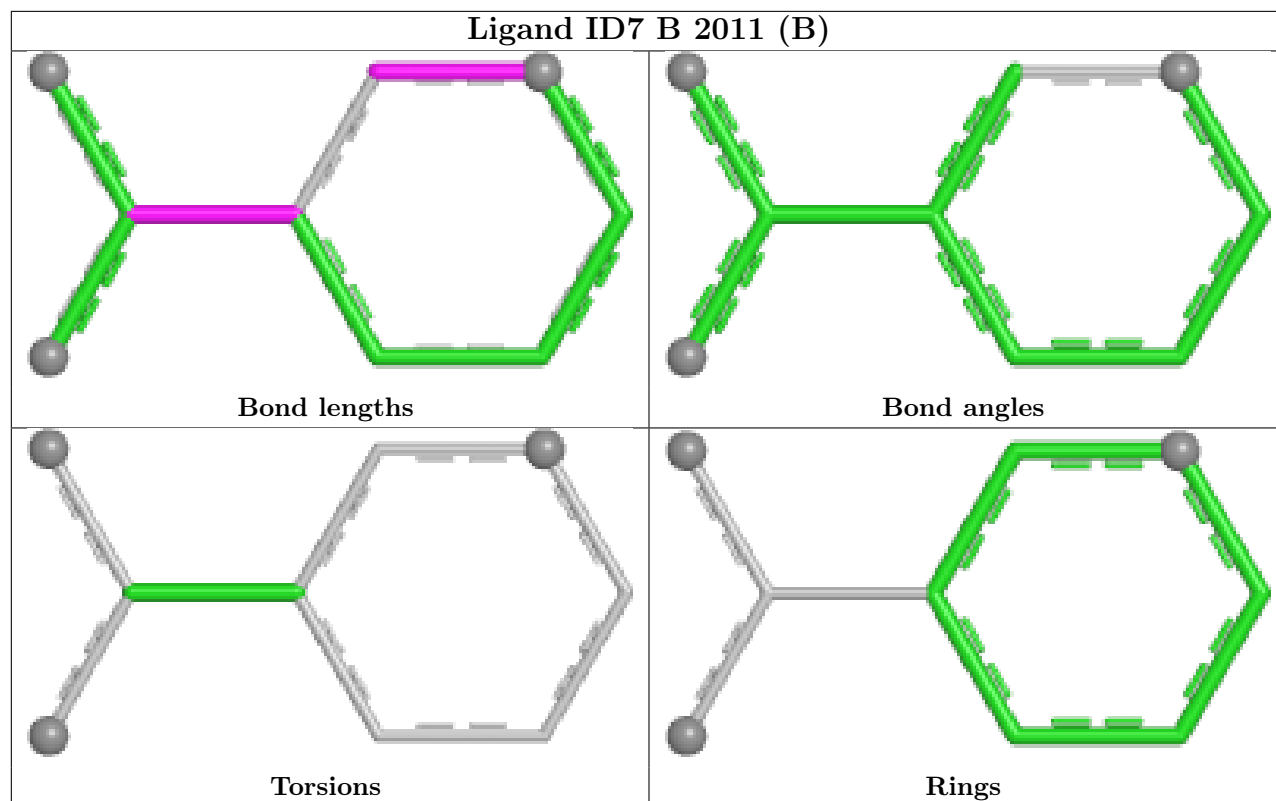
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2006	FMT	4	0
7	B	2011[B]	ID7	1	0
5	B	2009	FMT	1	0
6	B	2010[A]	A1BDB	1	0

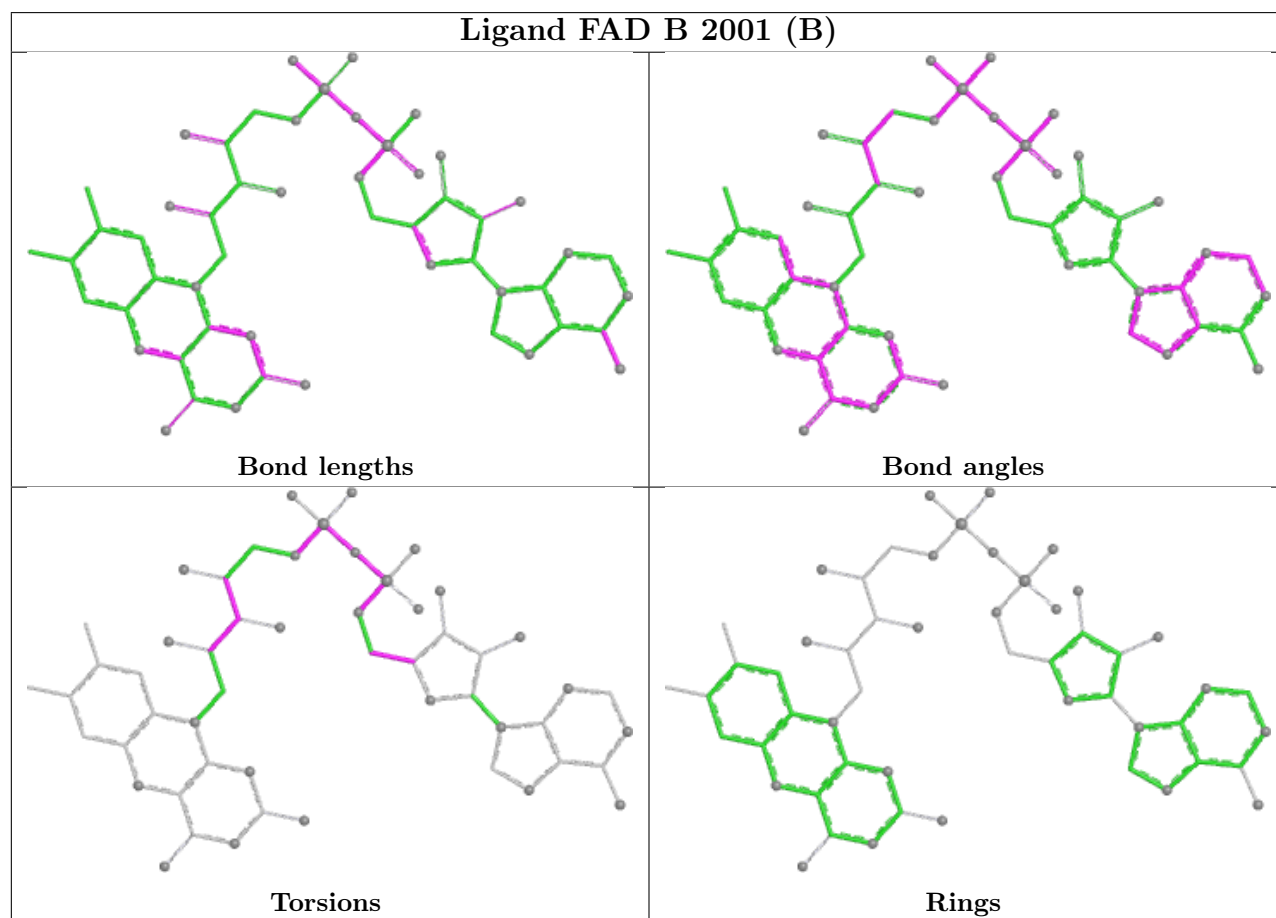
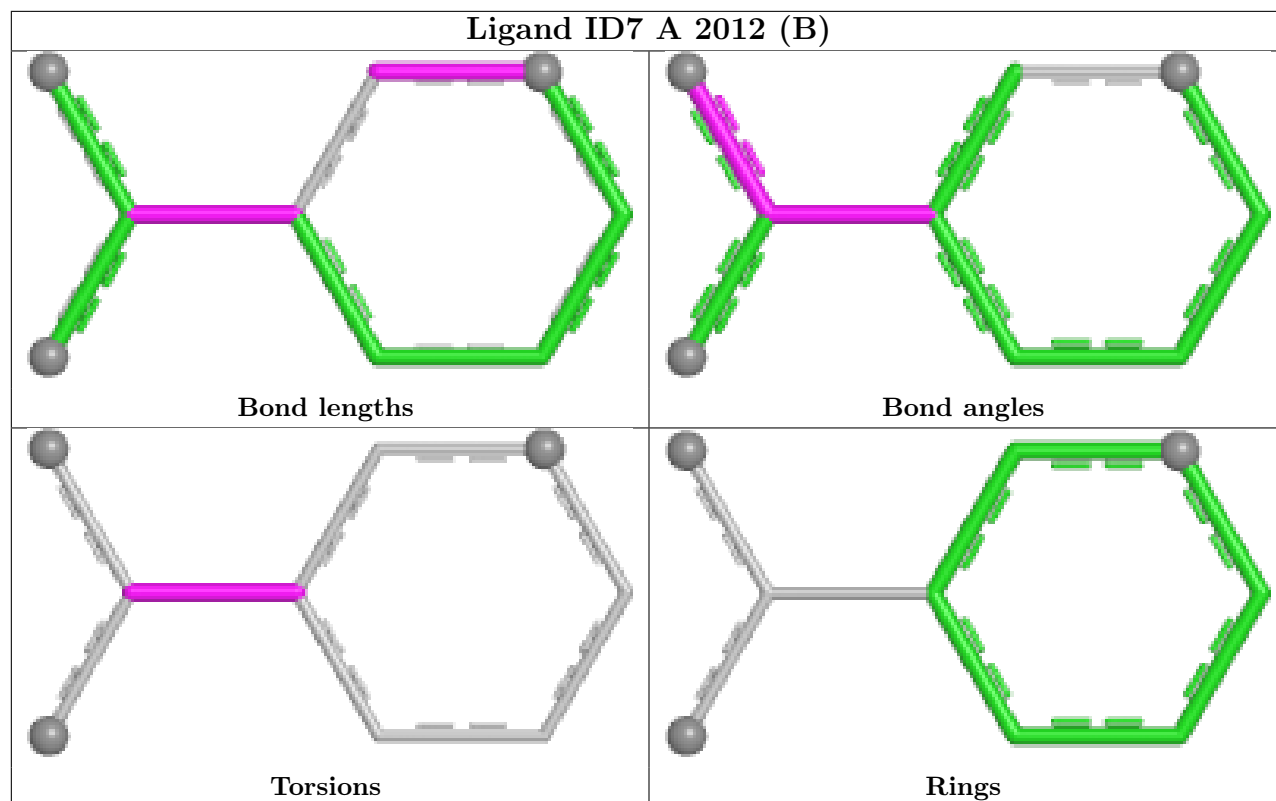
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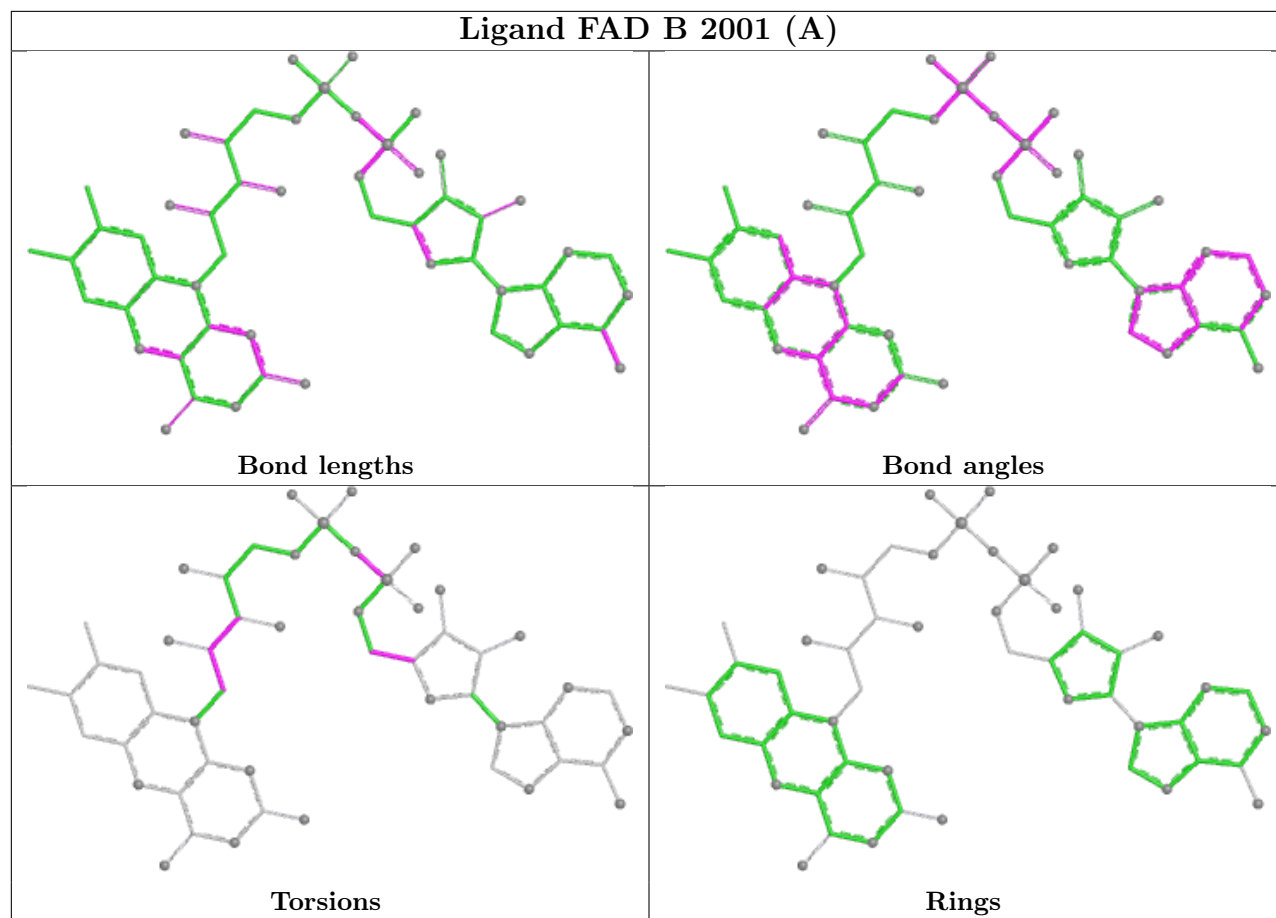
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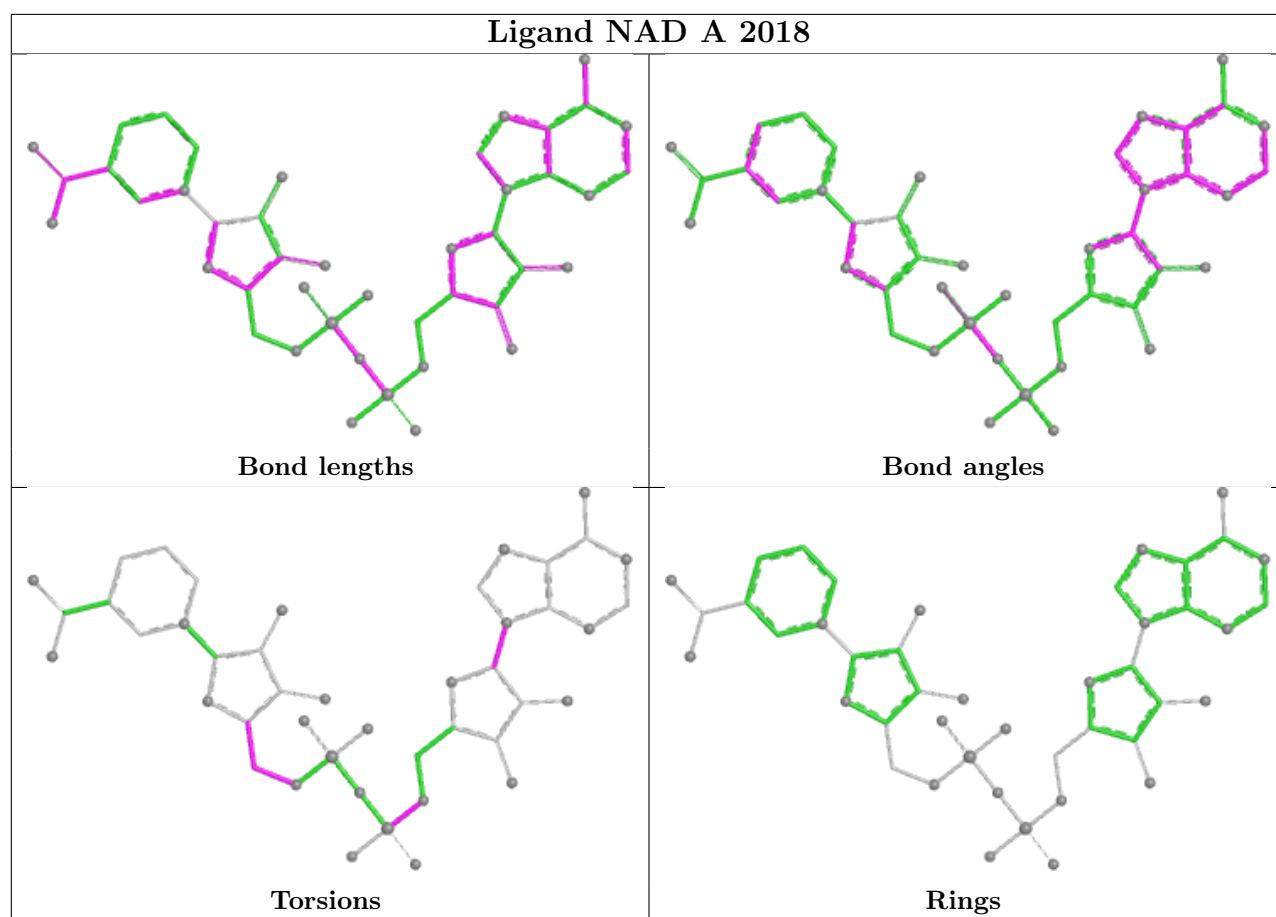
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2008	FMT	1	0
7	A	2012[B]	ID7	1	0
2	B	2001[B]	FAD	4	0
2	B	2001[A]	FAD	3	0
5	B	2006	FMT	4	0
4	B	2007	PGE	1	0
3	A	2005	PEG	1	0
5	A	2007	FMT	1	0
4	A	2003	PGE	1	0
11	B	2004	PG4	3	0
3	B	2005	PEG	2	0
9	A	2018	NAD	2	0
2	A	2001[A]	FAD	3	0
2	A	2001[B]	FAD	1	0
9	B	2014	NAD	2	0

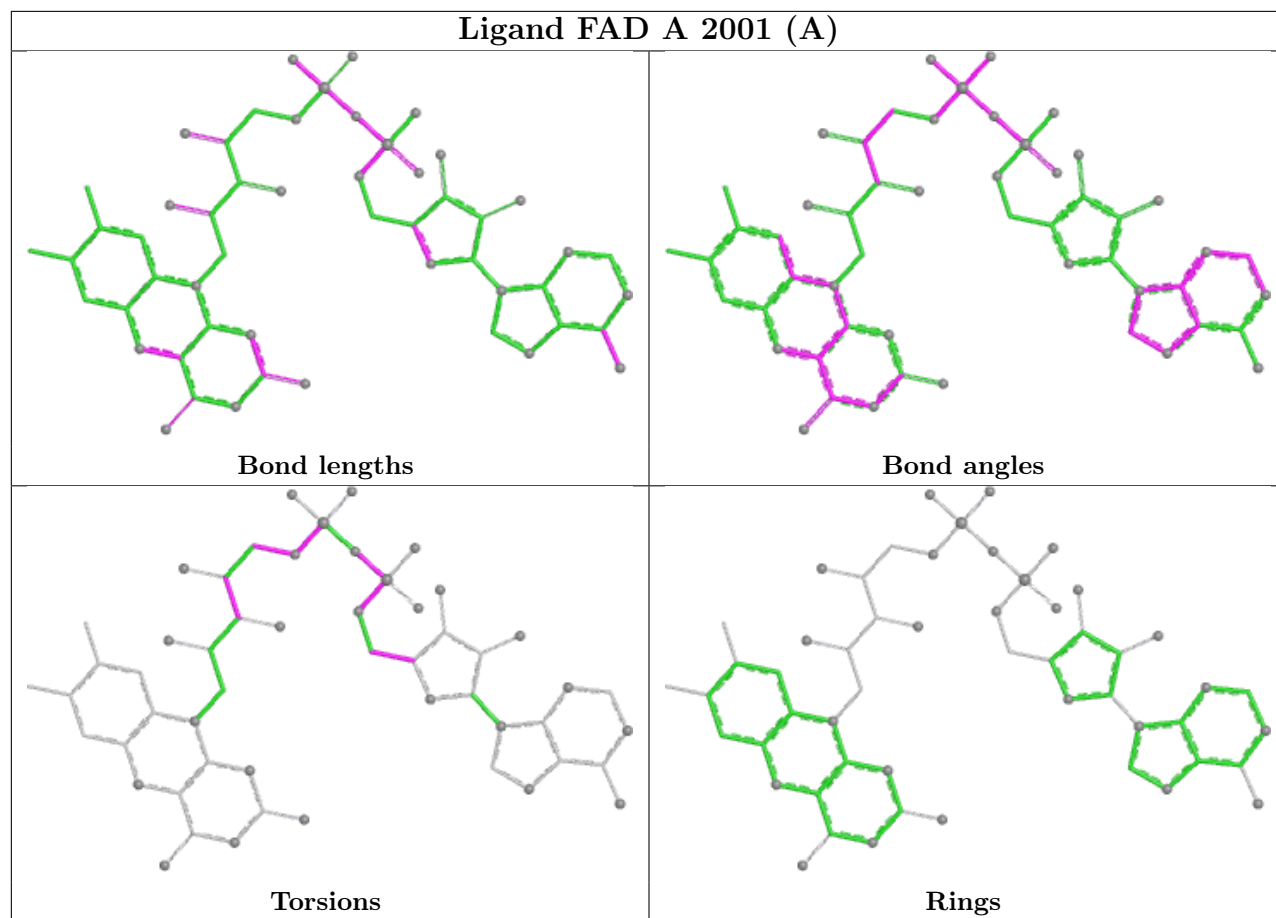
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

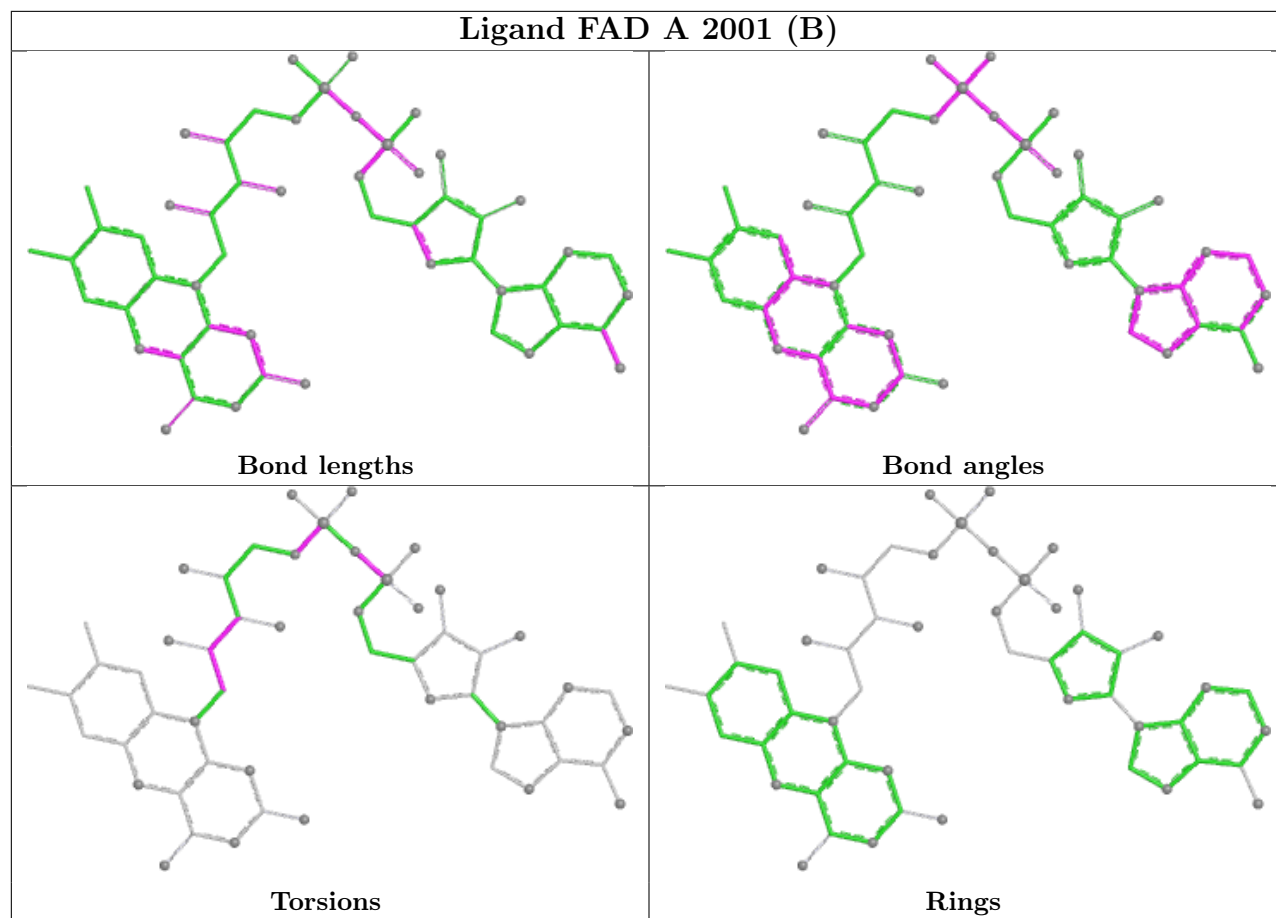




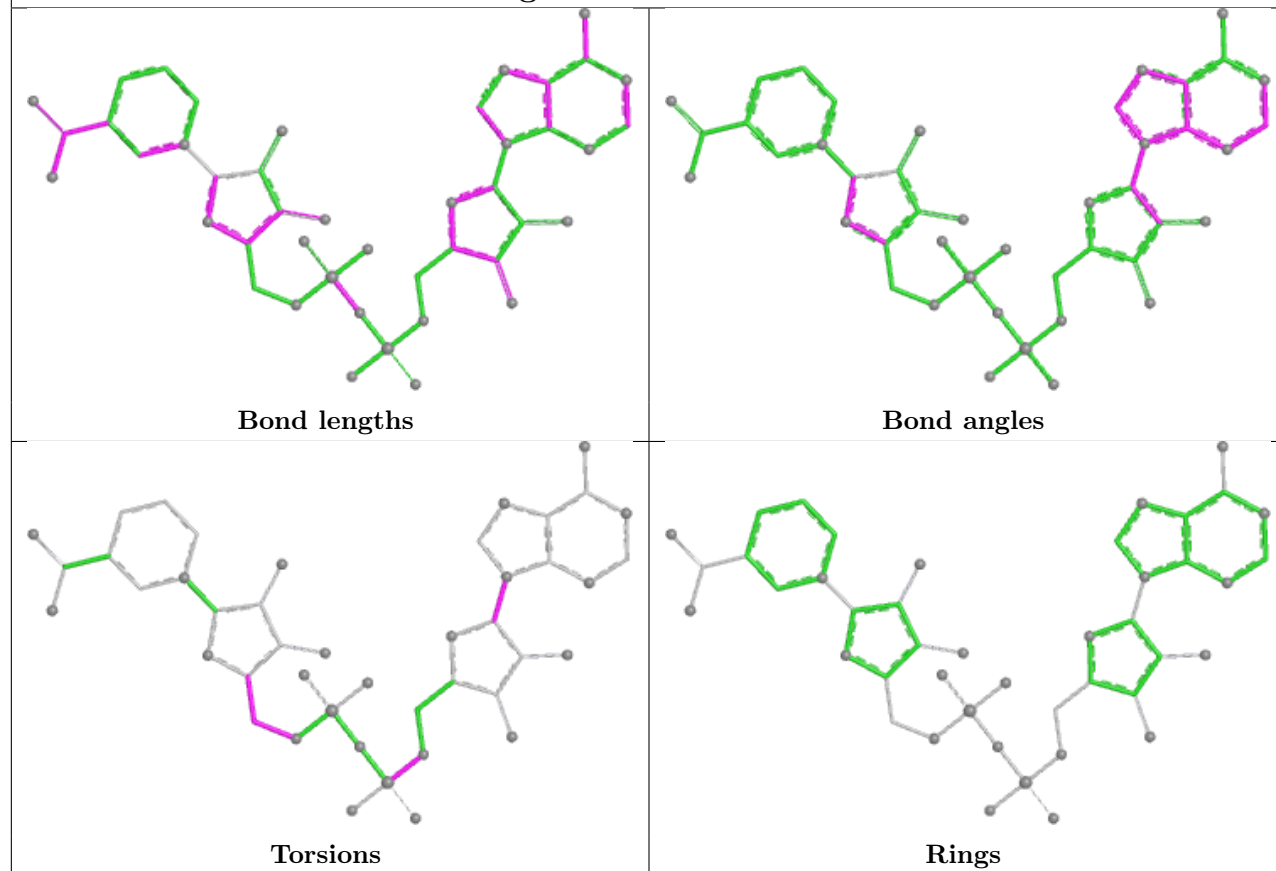




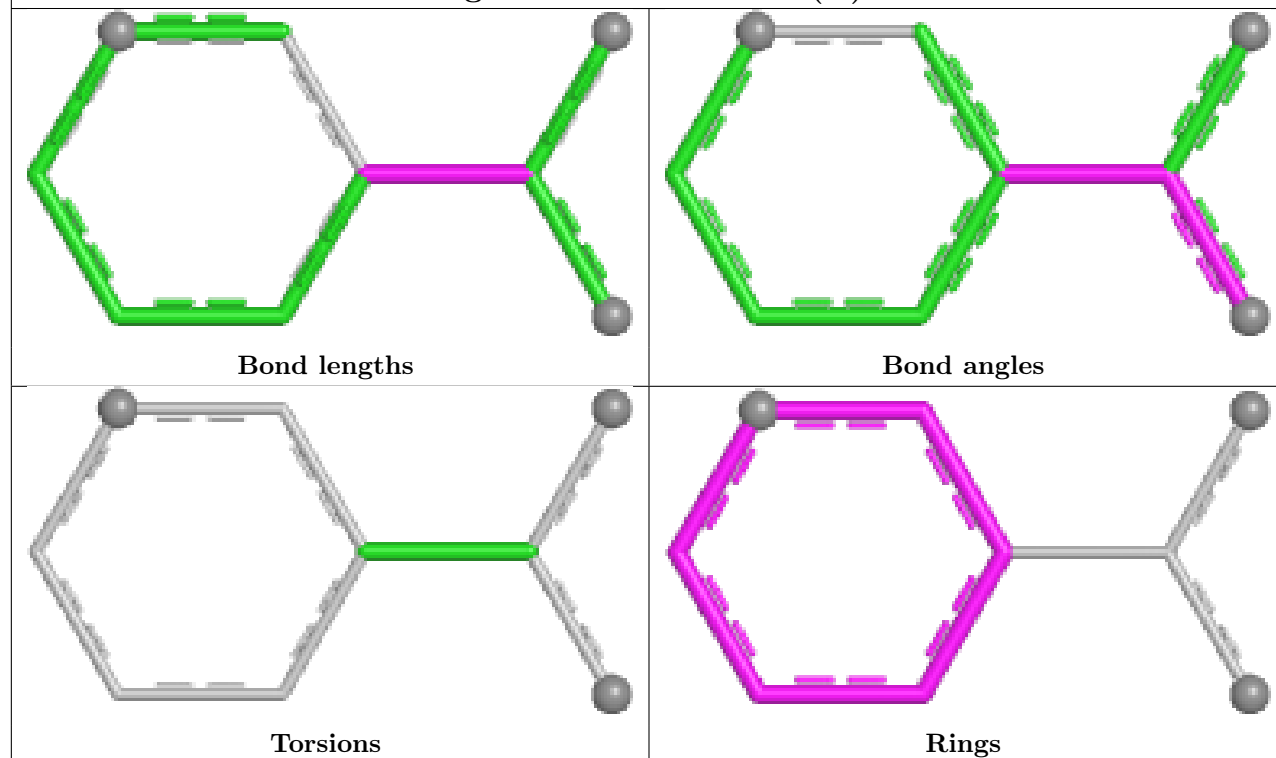




Ligand NAD B 2014



Ligand A1BDB A 2011 (A)



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, 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	1218/1235 (98%)	0.07	23 (1%) 66 70	10, 24, 40, 65	26 (2%)
1	B	1216/1235 (98%)	0.16	55 (4%) 38 40	10, 23, 43, 76	24 (1%)
All	All	2434/2470 (98%)	0.12	78 (3%) 50 53	10, 24, 42, 76	50 (2%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	912	ILE	5.2
1	B	491[A]	LEU	4.2
1	B	1230	MET	4.1
1	B	80	SER	4.1
1	B	129	ASN	3.9
1	B	914	LEU	3.9
1	A	14	ALA	3.8
1	B	494	GLY	3.8
1	B	1229[A]	LEU	3.6
1	B	915	ALA	3.6
1	A	81	GLY	3.6
1	B	79	HIS	3.6
1	A	912	ILE	3.5
1	B	438	ASP	3.4
1	A	129	ASN	3.3
1	B	1233	GLY	3.3
1	B	414	ASP	3.2
1	A	506	PRO	3.2
1	B	415	VAL	3.2
1	B	1232	ILE	3.2
1	B	1231	ALA	3.2
1	A	132	SER	3.1
1	B	128	GLY	3.1
1	A	127	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	913	GLY	3.0
1	B	156	THR	3.0
1	B	508	VAL	3.0
1	A	134	LEU	3.0
1	B	492	GLU	2.9
1	A	493	ASN	2.9
1	B	132	SER	2.9
1	B	493	ASN	2.9
1	B	439	PHE	2.8
1	B	77	GLY	2.8
1	B	134	LEU	2.8
1	B	504	ASN	2.8
1	A	128	GLY	2.7
1	B	223	LEU	2.6
1	B	74	ALA	2.6
1	B	495	ALA	2.6
1	B	131	LYS	2.5
1	A	115	ALA	2.5
1	B	75	LEU	2.5
1	B	485	TYR	2.5
1	B	503	ILE	2.5
1	A	451	GLY	2.5
1	B	500	VAL	2.4
1	B	916	SER	2.4
1	A	125	ILE	2.4
1	B	918	THR	2.4
1	B	138	ARG	2.3
1	B	412	ALA	2.3
1	B	1223	ALA	2.3
1	A	137	SER	2.3
1	A	796	ASP	2.3
1	A	80	SER	2.3
1	B	224	GLY	2.2
1	B	1140	ASN	2.2
1	B	1227	ALA	2.2
1	A	1230	MET	2.2
1	B	19	ALA	2.2
1	B	63	ALA	2.2
1	A	113	ASP	2.2
1	B	436	GLY	2.1
1	B	451	GLY	2.1
1	A	1231	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	64	ALA	2.1
1	A	130	TRP	2.1
1	B	66	SER	2.1
1	B	84	VAL	2.1
1	B	441	VAL	2.1
1	B	510	ILE	2.1
1	A	133	HIS	2.1
1	B	130	TRP	2.1
1	B	115	ALA	2.0
1	A	905	LEU	2.0
1	B	120	LEU	2.0
1	A	116	THR	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	B	2005	7/7	0.73	0.18	34,43,50,54	0
3	PEG	A	2005	7/7	0.76	0.17	39,42,47,56	0
3	PEG	A	2004	7/7	0.76	0.15	35,39,46,48	0
4	PGE	A	2003	10/10	0.78	0.19	35,38,43,45	10
8	SO4	B	2013	5/5	0.78	0.13	48,50,59,59	5
11	PG4	B	2004	13/13	0.79	0.18	29,36,45,50	13
4	PGE	B	2007	10/10	0.80	0.15	28,43,49,51	0
5	FMT	A	2006	3/3	0.84	0.15	16,16,23,25	3
3	PEG	A	2009	7/7	0.85	0.12	39,41,48,51	0
3	PEG	A	2002	7/7	0.86	0.12	28,35,38,44	0
5	FMT	A	2007	3/3	0.86	0.15	15,15,25,31	3

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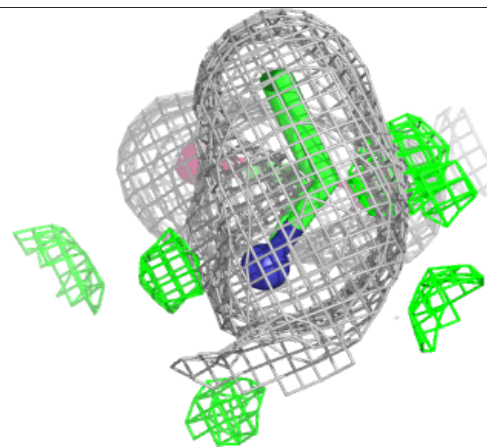
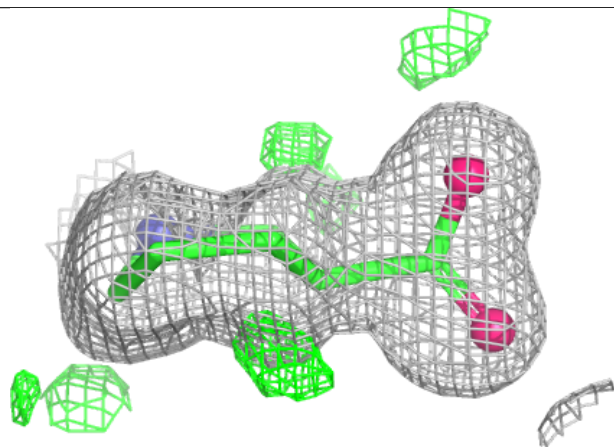
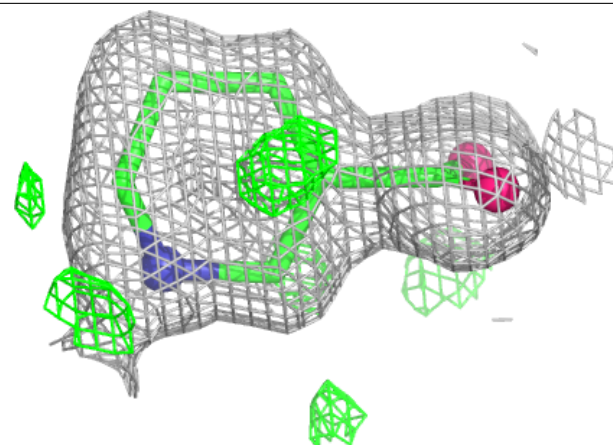
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	A1BDB	B	2010[A]	9/9	0.88	0.10	19,23,25,25	9
3	PEG	B	2003	7/7	0.88	0.11	34,39,43,46	0
5	FMT	B	2006	3/3	0.88	0.13	20,20,22,23	3
8	SO4	A	2016	5/5	0.89	0.09	52,52,55,56	5
6	A1BDB	A	2011[A]	9/9	0.89	0.11	21,24,28,30	9
3	PEG	B	2008	7/7	0.89	0.10	38,44,49,50	0
4	PGE	A	2010	10/10	0.90	0.11	28,36,40,43	0
8	SO4	A	2017	5/5	0.90	0.11	30,33,37,37	5
8	SO4	A	2015	5/5	0.91	0.11	32,35,39,49	5
4	PGE	B	2002	10/10	0.93	0.09	29,35,41,41	0
5	FMT	A	2008	3/3	0.93	0.10	15,15,34,36	3
5	FMT	B	2009	3/3	0.94	0.14	10,10,34,37	3
7	ID7	A	2012[B]	9/9	0.94	0.09	20,24,28,31	9
7	ID7	B	2011[B]	9/9	0.94	0.08	18,23,24,26	9
5	FMT	A	2020	3/3	0.94	0.08	37,37,40,40	0
2	FAD	B	2001[A]	53/53	0.95	0.07	15,20,24,25	53
9	NAD	A	2018	44/44	0.95	0.08	16,24,28,32	0
10	MG	A	2019	1/1	0.95	0.13	30,30,30,30	0
10	MG	B	2015	1/1	0.95	0.15	31,31,31,31	0
2	FAD	B	2001[B]	53/53	0.95	0.07	16,20,25,26	53
9	NAD	B	2014	44/44	0.96	0.07	15,18,22,29	0
8	SO4	A	2014	5/5	0.96	0.09	26,29,37,41	5
2	FAD	A	2001[B]	53/53	0.96	0.07	15,18,23,23	53
2	FAD	A	2001[A]	53/53	0.96	0.07	14,19,22,30	53
8	SO4	A	2013	5/5	0.99	0.05	20,20,23,24	0
8	SO4	B	2012	5/5	0.99	0.04	17,17,21,22	0

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

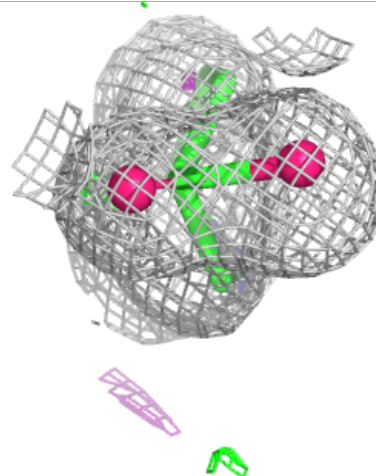
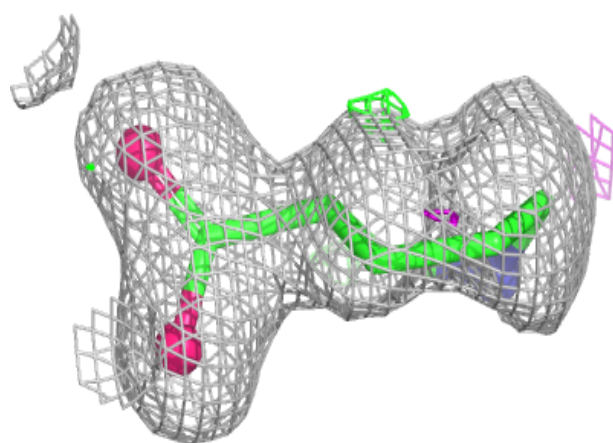
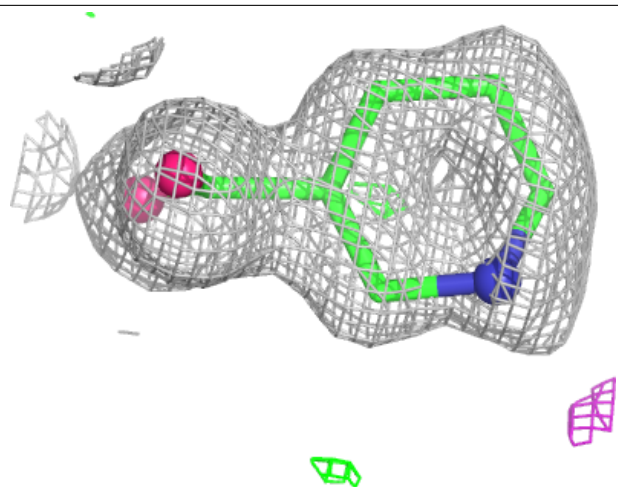
Electron density around A1BDB B 2010 (A):

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



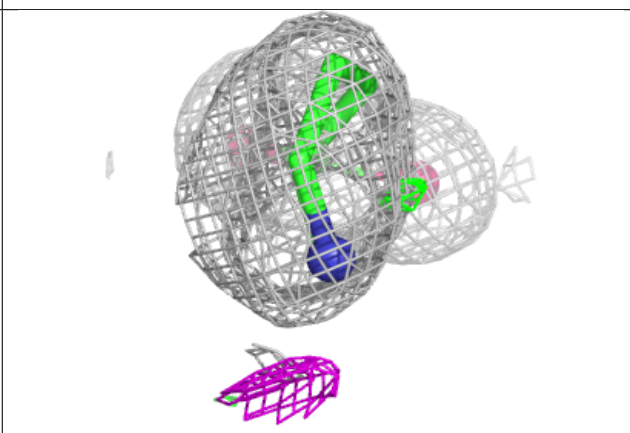
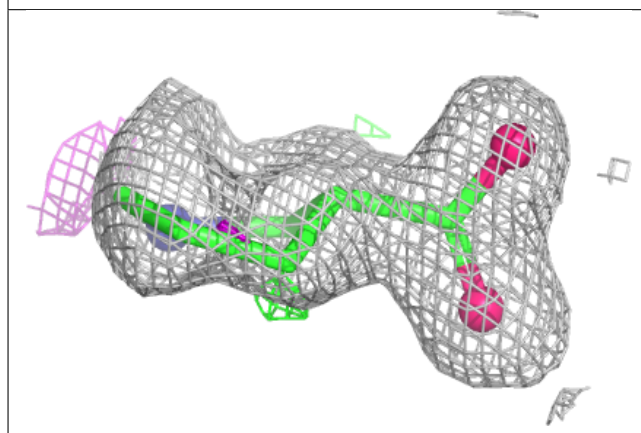
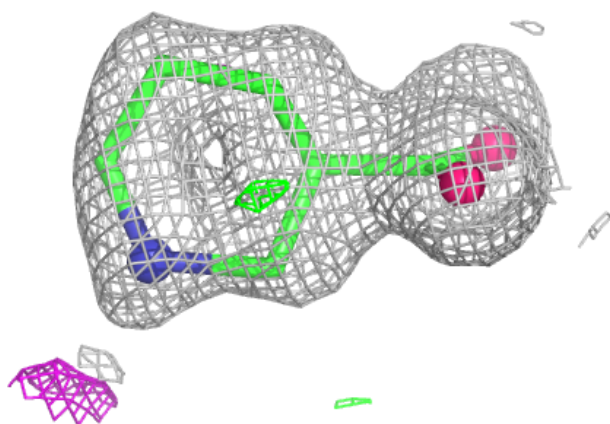
Electron density around A1BDB A 2011 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



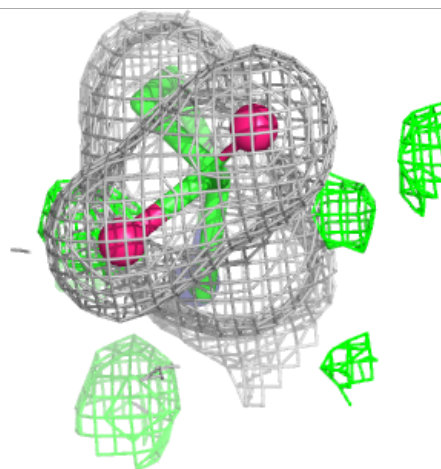
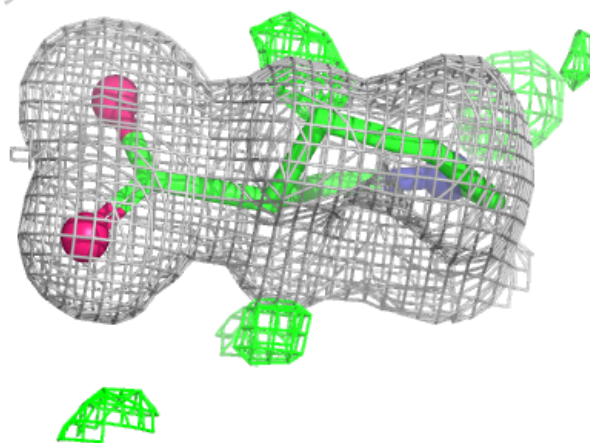
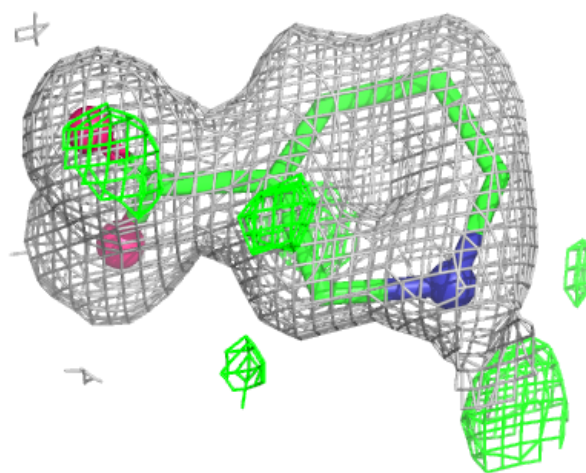
Electron density around ID7 A 2012 (B):

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



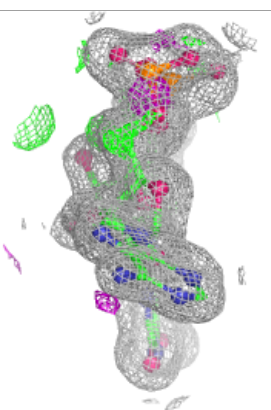
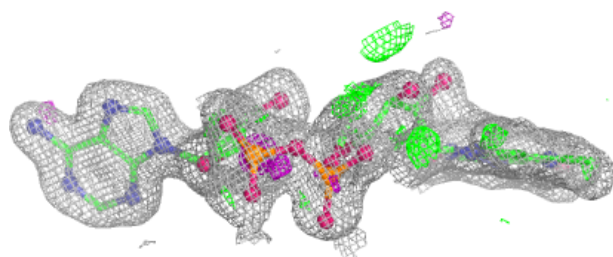
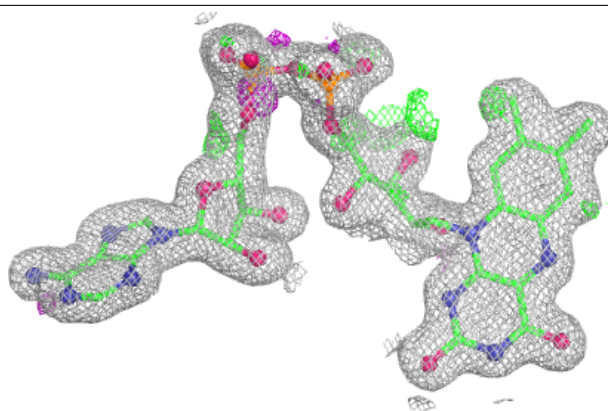
Electron density around ID7 B 2011 (B):

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

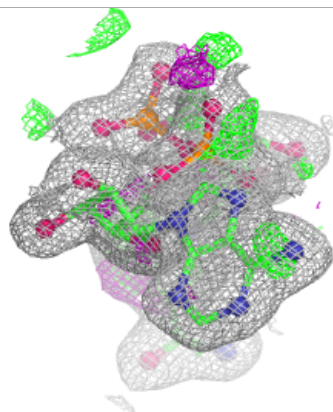
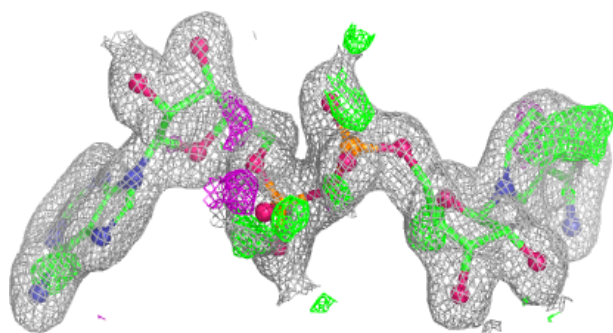
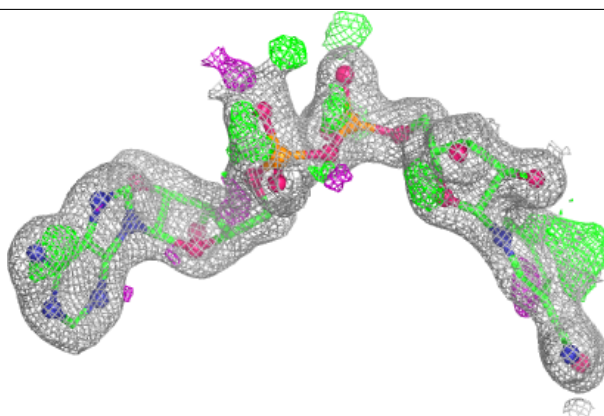


Electron density around FAD B 2001 (A):

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

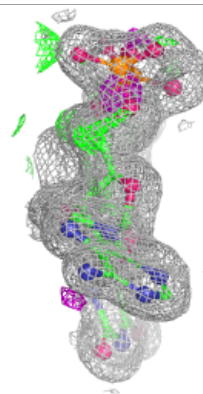
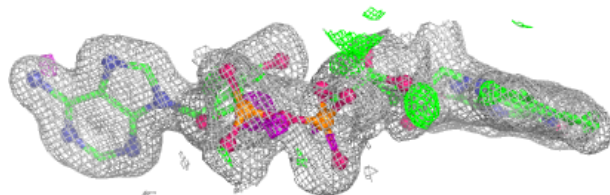
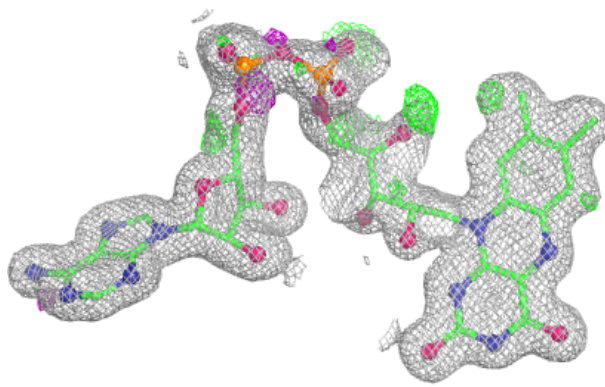
**Electron density around NAD A 2018:**

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and green (positive)

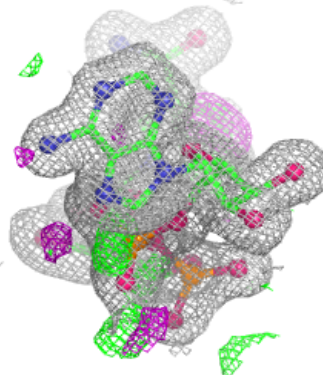
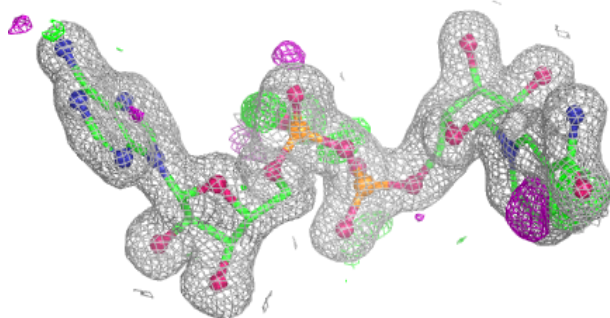
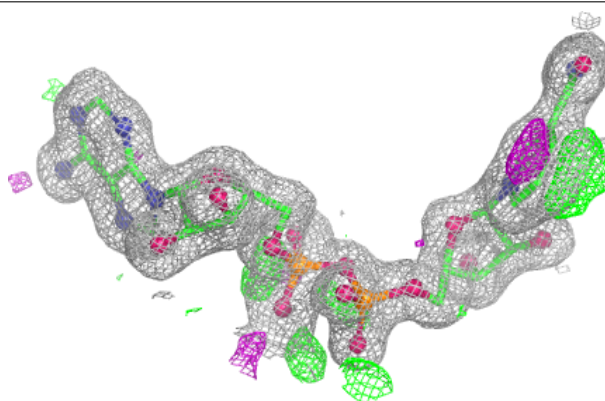


Electron density around FAD B 2001 (B):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

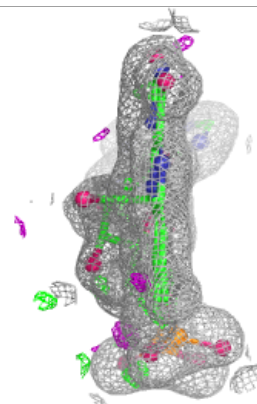
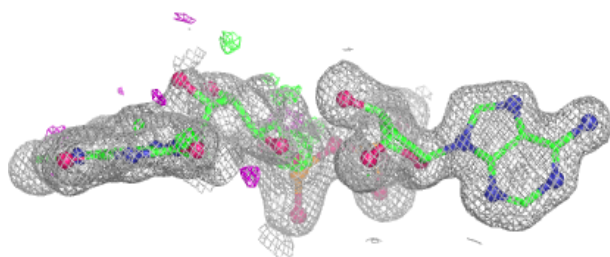
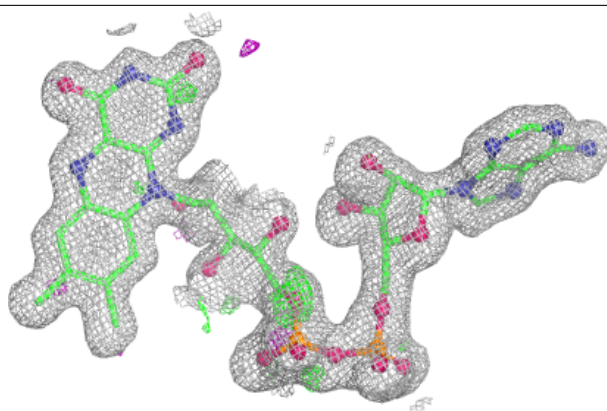
**Electron density around NAD B 1414:**

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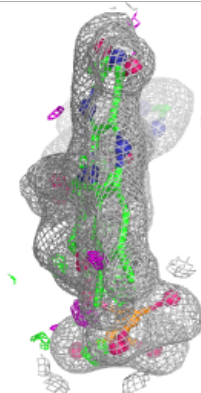
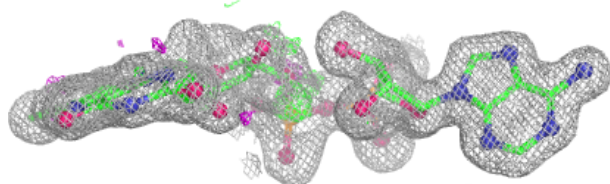
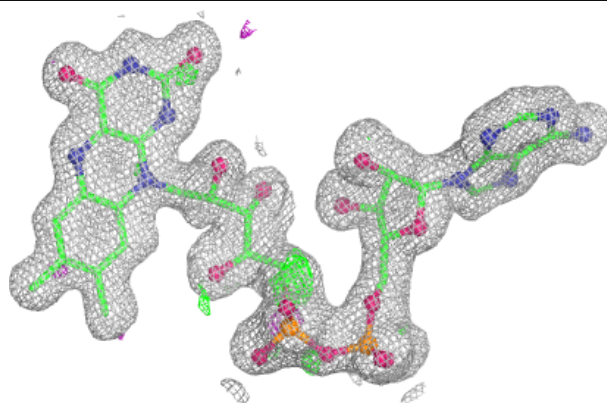


Electron density around FAD A 2001 (B):

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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)



6.5 Other polymers [i](#)

There are no such residues in this entry.