



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:40 PM UTC

PDB ID : 9DL8 / pdb_00009dl8
Title : Structure of proline utilization A soaked with 4-methoxybenzyl alcohol
Authors : Tanner, J.J.; Meeks, K.R.
Deposited on : 2024-09-10
Resolution : 1.64 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

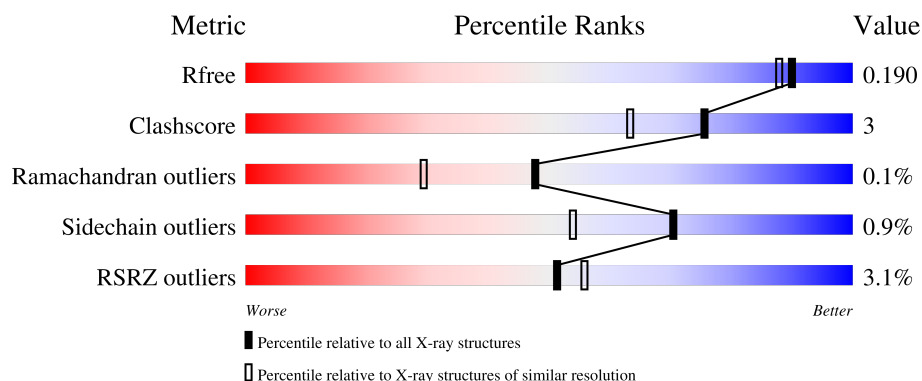
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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.



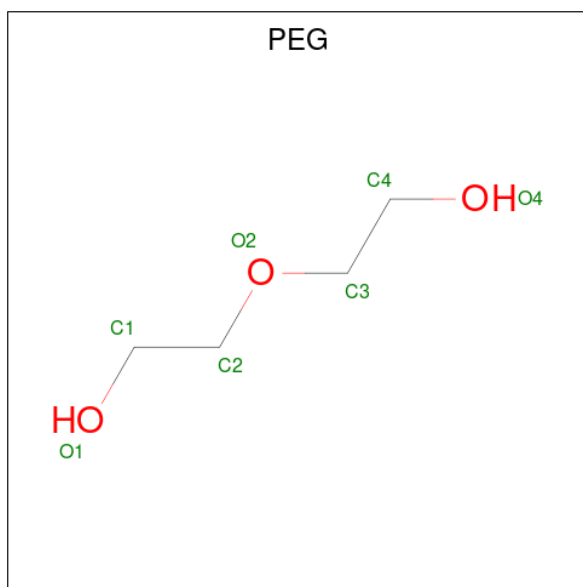
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	4% 92% 5%
1	B	1235	2% 89% 8%

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

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



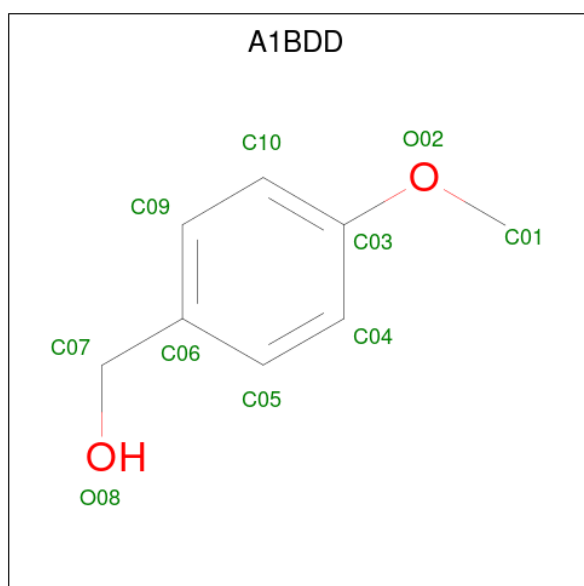
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

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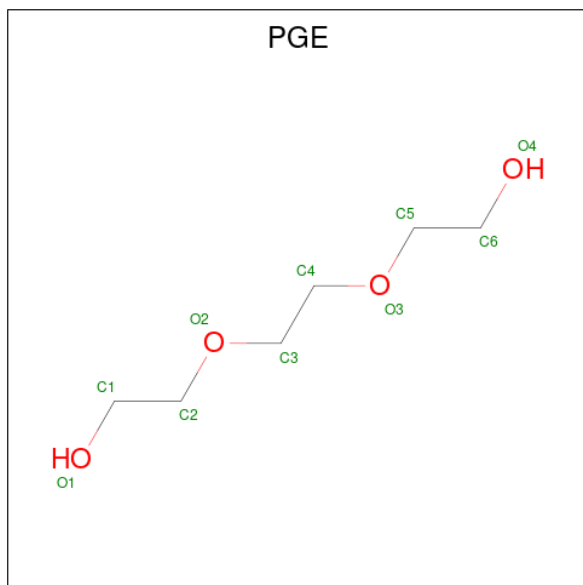
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total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

- Molecule 4 is (4-methoxyphenyl)methanol (CCD ID: A1BDD) (formula: C₈H₁₀O₂) (labeled as "Ligand of Interest" by depositor).



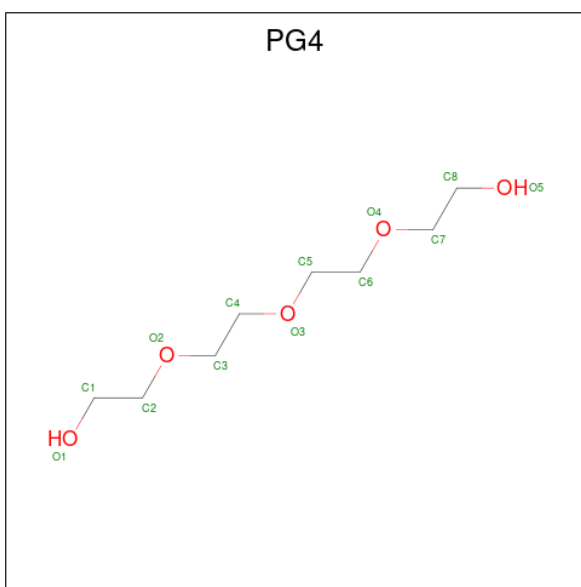
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	8	2		
4	B	1	Total	C	O	0	0
			10	8	2		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



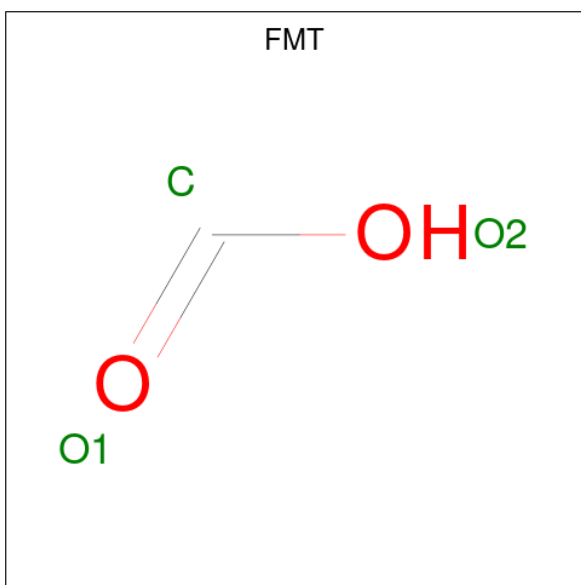
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



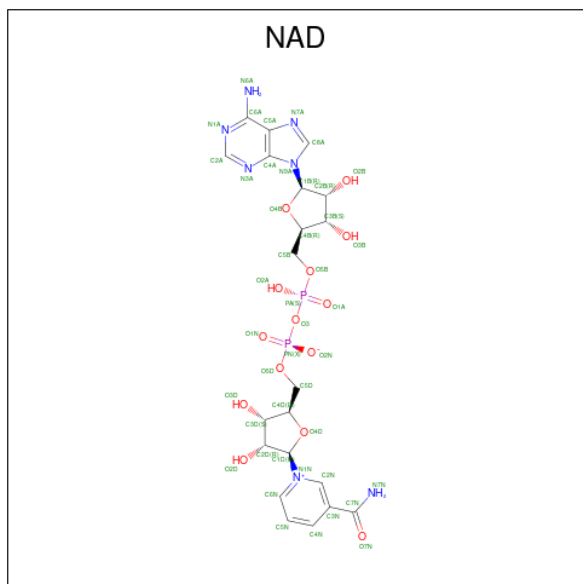
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



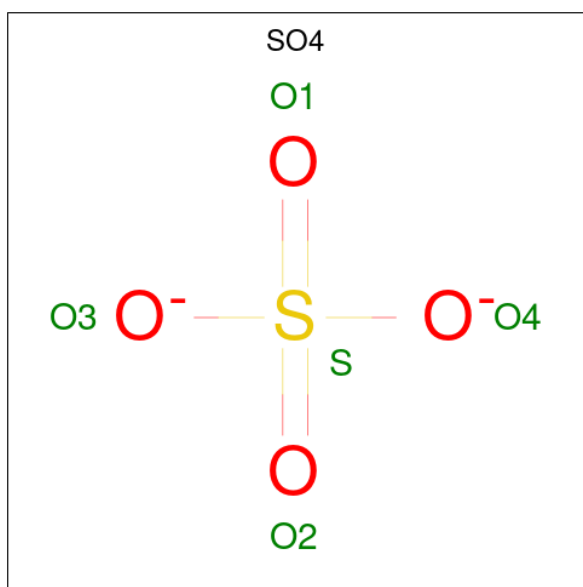
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 3 1 2	0	0
7	A	1	Total C O 3 1 2	0	0
7	A	1	Total C O 3 1 2	0	0
7	B	1	Total C O 3 1 2	0	0
7	B	1	Total C O 3 1 2	0	0
7	B	1	Total C O 3 1 2	0	0

- Molecule 8 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
8	A	1	Total C N O P 71 31 12 24 4	0	1
8	B	1	Total C N O P 44 21 7 14 2	0	0

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

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

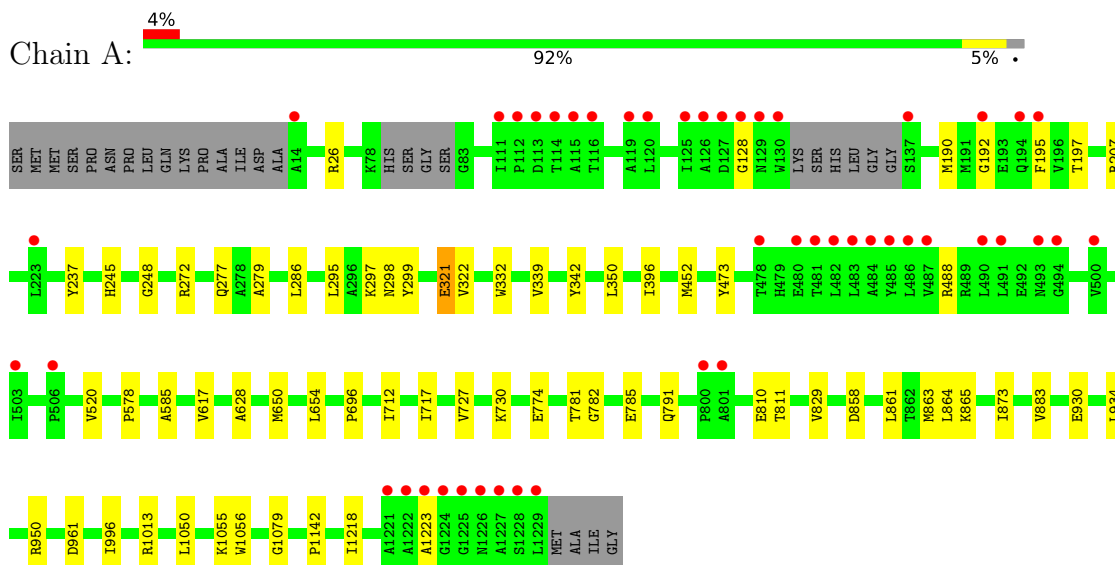
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	912	Total	O	0	0
			912	912		
11	B	892	Total	O	0	0
			892	892		

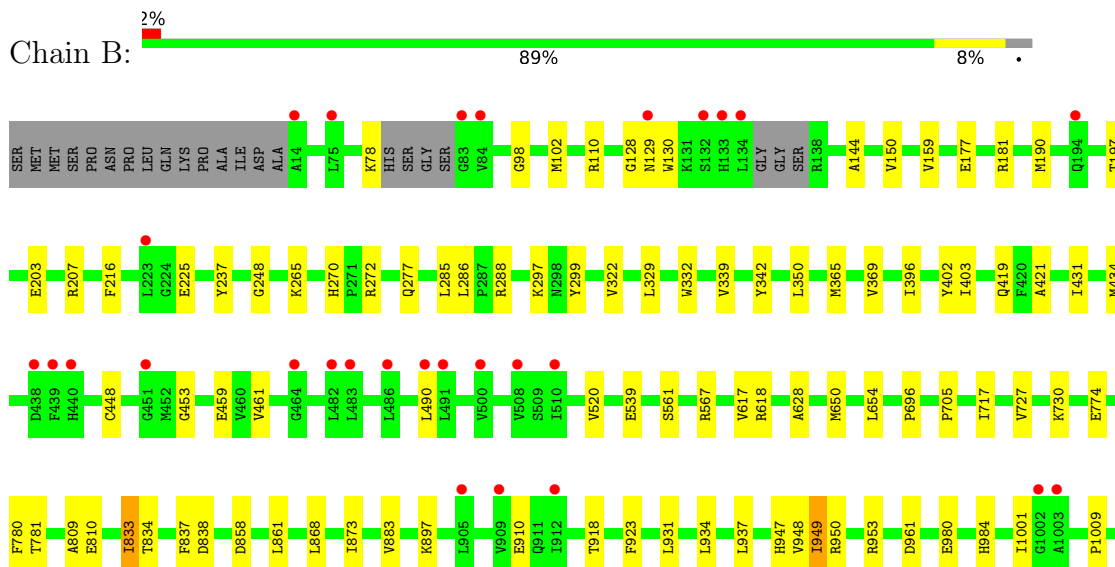
3 Residue-property plots [i](#)

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

• Molecule 1: Bifunctional protein PutA



• Molecule 1: Bifunctional protein PutA



K1021		L1050	K1055	D1058	R1070	G1079	L1104	H1114	K1178	G1196	L1207	A1221	ALA	ALA	GLY	GLY	ASN	ALA	SER	LEU	MET	ALA	ILE	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.75Å 101.30Å 125.20Å 90.00° 106.34° 90.00°	Depositor
Resolution (Å)	48.34 – 1.64 48.34 – 1.64	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.34-1.64) 98.8 (48.34-1.64)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.166 , 0.193 0.164 , 0.190	Depositor DCC
R_{free} test set	14566 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.8	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	20125	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 3.16% 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: PEG, NAD, A1BDD, SO4, FAD, PGE, FMT, MG, PG4

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	0/9127	0.45	0/12432
1	B	0.25	0/9068	0.46	0/12358
All	All	0.25	0/18195	0.45	0/24790

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8924	0	8907	39	0
1	B	8871	0	8853	64	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
3	A	91	0	130	5	0
3	B	63	0	90	7	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	10	0	14	0	0
5	B	20	0	28	1	0
6	A	26	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	26	0	36	2	0
7	A	9	0	3	0	0
7	B	9	0	3	0	0
8	A	71	0	38	0	0
8	B	44	0	26	1	0
9	A	20	0	0	2	0
9	B	10	0	0	0	0
10	B	1	0	0	0	0
11	A	912	0	0	8	0
11	B	892	0	0	9	0
All	All	20125	0	18226	110	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 (110) 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:1079:GLY:HA2	5:B:2003:PGE:H4	1.53	0.90
1:B:539:GLU:OE1	11:B:2101:HOH:O	1.98	0.80
1:A:1079:GLY:HA2	3:A:2003:PEG:H22	1.64	0.78
1:B:858:ASP:OD1	1:B:950:ARG:NH2	2.20	0.74
1:A:488:ARG:NE	1:A:1223:ALA:O	2.23	0.68
1:A:286:LEU:HD21	1:A:322:VAL:HG11	1.75	0.67
1:A:339:VAL:HG21	1:A:350:LEU:HD21	1.78	0.66
1:A:321[B]:GLU:OE1	11:A:2102:HOH:O	2.13	0.65
1:A:192:GLY:O	1:A:207:ARG:NH1	2.26	0.65
1:B:203:GLU:OE2	1:B:207:ARG:NH2	2.30	0.65
1:B:873:ILE:HG13	1:B:883:VAL:HB	1.78	0.64
1:B:339[A]:VAL:HG21	1:B:350:LEU:HD21	1.79	0.64
1:B:286:LEU:HD21	1:B:322:VAL:HG11	1.80	0.62
1:B:225:GLU:HB3	1:B:265:LYS:HD2	1.82	0.61
1:B:110:ARG:NH2	11:B:2104:HOH:O	2.27	0.61
1:B:297:LYS:HG3	1:B:332:TRP:HB2	1.83	0.60
9:A:2025:SO4:O1	11:A:2103:HOH:O	2.16	0.58
1:B:953:ARG:NH1	11:B:2111:HOH:O	2.37	0.58
1:A:996[B]:ILE:HD12	1:A:1218:ILE:HG12	1.86	0.57
1:A:829:VAL:HG21	1:A:863:MET:HE2	1.88	0.56
1:B:216:PHE:CE1	1:B:461[A]:VAL:HG21	2.41	0.56
1:B:78:LYS:NZ	1:B:459:GLU:OE2	2.37	0.55
1:B:197:THR:O	1:B:207:ARG:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:ASP:OD2	1:B:1055:LYS:NZ	2.39	0.54
1:A:298:ASN:ND2	11:A:2101:HOH:O	2.11	0.54
1:B:931:LEU:HB2	1:B:949:ILE:HG22	1.89	0.53
1:B:144:ALA:HB3	1:B:159:VAL:HG11	1.89	0.53
1:A:237:TYR:CZ	3:A:2002:PEG:H32	2.43	0.53
1:B:897:LYS:NZ	6:B:2012:PG4:H21	2.24	0.52
1:B:650:MET:O	1:B:654:LEU:HG	2.09	0.52
1:A:1055:LYS:NZ	1:B:961:ASP:OD2	2.36	0.52
1:B:567:ARG:NH2	11:B:2119:HOH:O	2.42	0.52
1:B:288:ARG:HD3	11:B:2425:HOH:O	2.11	0.50
1:B:237:TYR:CZ	3:B:2004:PEG:H22	2.47	0.49
1:B:834:THR:HG22	1:B:1001:ILE:HD11	1.93	0.49
1:B:403:ILE:HG23	1:B:434:MET:HE1	1.94	0.49
1:A:650:MET:O	1:A:654:LEU:HG	2.12	0.49
9:A:2024:SO4:O2	11:A:2104:HOH:O	2.20	0.49
1:B:297:LYS:HD2	1:B:329:LEU:HA	1.94	0.49
1:B:150:VAL:HG11	1:B:190:MET:HE1	1.95	0.48
1:B:617:VAL:HG12	1:B:774:GLU:HB2	1.96	0.48
1:B:837:PHE:CE2	1:B:868:LEU:HD21	2.48	0.48
1:B:618:ARG:NH2	11:B:2117:HOH:O	2.40	0.48
1:B:897:LYS:HZ2	6:B:2012:PG4:H21	1.77	0.48
1:B:1196:GLY:HA3	3:B:2006:PEG:H22	1.95	0.48
1:B:272:ARG:HB3	1:B:277:GLN:HG3	1.95	0.47
3:A:2002:PEG:H42	11:A:2140:HOH:O	2.15	0.47
1:B:833:ILE:HD13	1:B:868:LEU:HD23	1.97	0.47
1:A:473:TYR:HB2	2:A:2001:FAD:HM72	1.96	0.47
1:B:369:VAL:HG12	1:B:421:ALA:HB3	1.96	0.47
1:A:617:VAL:HG12	1:A:774:GLU:HB2	1.96	0.47
1:A:873:ILE:HG13	1:A:883:VAL:HB	1.97	0.47
2:B:2001:FAD:H9	2:B:2001:FAD:H1'1	1.75	0.47
1:A:1056:TRP:CD1	1:A:1142:PRO:HD3	2.50	0.46
1:A:578:PRO:HB2	1:A:585:ALA:HB3	1.96	0.46
1:A:26[A]:ARG:NH1	1:A:321[A]:GLU:HG2	2.31	0.46
1:A:717:ILE:HG12	1:A:727:VAL:HG11	1.98	0.46
1:A:1013:ARG:NH2	11:A:2142:HOH:O	2.49	0.46
1:A:861:LEU:HG	1:A:865:LYS:HE3	1.98	0.46
1:B:628:ALA:HB2	1:B:696:PRO:HG3	1.98	0.46
1:B:1207:LEU:HD21	3:B:2018:PEG:H31	1.98	0.46
1:A:245:HIS:CE1	1:A:295:LEU:HD11	2.51	0.45
3:A:2003:PEG:H21	3:A:2003:PEG:H42	1.73	0.45
1:A:628:ALA:HB2	1:A:696:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2018:PG4:H42	11:A:2256:HOH:O	2.15	0.45
3:B:2009:PEG:H12	11:B:2888:HOH:O	2.16	0.45
1:A:279:ALA:HA	3:A:2016:PEG:H31	1.97	0.45
1:B:128:GLY:O	1:B:130:TRP:N	2.50	0.45
1:B:402:TYR:HE1	1:B:431:ILE:HD11	1.82	0.45
1:A:858:ASP:CG	1:A:950:ARG:HH22	2.25	0.45
1:B:448:CYS:HB2	1:B:453:GLY:HA3	1.99	0.45
1:B:780:PHE:O	1:B:809:ALA:HA	2.16	0.45
1:A:297:LYS:HA	1:A:332:TRP:CD1	2.52	0.44
1:B:834:THR:O	1:B:838:ASP:HB3	2.18	0.44
3:B:2009:PEG:H11	3:B:2009:PEG:H31	1.68	0.44
1:B:365:MET:HE2	1:B:419:GLN:OE1	2.17	0.44
1:B:396:ILE:HD11	1:B:520:VAL:HB	2.00	0.44
1:B:717:ILE:HG12	1:B:727:VAL:HG11	2.00	0.44
1:B:810:GLU:OE1	11:B:2102:HOH:O	2.21	0.44
1:B:248:GLY:HA3	1:B:299:TYR:CG	2.53	0.43
1:A:452[A]:MET:HB2	1:A:452[A]:MET:HE3	1.81	0.43
1:B:1058:ASP:OD2	1:B:1070[B]:ARG:NH1	2.40	0.43
1:A:1050:LEU:C	1:A:1050:LEU:HD13	2.43	0.43
1:B:861:LEU:HD21	1:B:948:VAL:HG11	2.00	0.43
1:A:248:GLY:HA3	1:A:299:TYR:CG	2.53	0.43
1:A:782:GLY:O	1:A:811:THR:HA	2.18	0.43
1:A:712:ILE:HD13	1:A:781:THR:HG21	2.01	0.43
8:B:2019:NAD:H52A	11:B:2684:HOH:O	2.19	0.42
1:A:197:THR:O	1:A:207:ARG:HD2	2.20	0.42
1:B:1114:HIS:HD2	3:B:2018:PEG:O1	2.01	0.42
1:B:402:TYR:CE1	1:B:431:ILE:HD11	2.55	0.42
1:A:861:LEU:HD21	1:A:930:GLU:CD	2.45	0.41
1:B:270:HIS:HB2	1:B:285:LEU:HG	2.02	0.41
1:B:561[B]:SER:OG	3:B:2009:PEG:H31	2.20	0.41
1:A:396:ILE:HD11	1:A:520:VAL:HB	2.03	0.41
1:A:791:GLN:NE2	11:A:2113:HOH:O	2.33	0.41
1:B:1178:LYS:HB3	1:B:1178:LYS:HE3	1.88	0.41
1:A:272:ARG:HB3	1:A:277:GLN:HG3	2.02	0.41
1:B:628:ALA:CB	1:B:696:PRO:HG3	2.51	0.41
1:B:705:PRO:HD3	1:B:781:THR:HB	2.03	0.41
1:B:918:THR:HB	1:B:923:PHE:CD1	2.56	0.41
1:B:984:HIS:CD2	1:B:984:HIS:C	2.98	0.41
1:B:1009:PRO:HB2	1:B:1021:LYS:HD3	2.03	0.41
1:B:1050:LEU:C	1:B:1050:LEU:HD13	2.46	0.41
1:A:190:MET:HE2	1:A:195:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLY:O	1:B:102:MET:HG2	2.21	0.40
1:B:150:VAL:CG1	1:B:190:MET:HE1	2.50	0.40
1:B:937[B]:LEU:HD11	1:B:947:HIS:ND1	2.36	0.40
1:A:829:VAL:HG13	1:A:864[B]:LEU:HD23	2.02	0.40
1:B:177:GLU:OE2	1:B:181:ARG:NE	2.42	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	1217/1235 (98%)	1189 (98%)	27 (2%)	1 (0%)	48	29
1	B	1209/1235 (98%)	1183 (98%)	25 (2%)	1 (0%)	48	29
All	All	2426/2470 (98%)	2372 (98%)	52 (2%)	2 (0%)	48	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	GLY
1	B	129	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	889/951 (94%)	882 (99%)	7 (1%)	73	58
1	B	886/951 (93%)	877 (99%)	9 (1%)	68	49
All	All	1775/1902 (93%)	1759 (99%)	16 (1%)	70	54

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

Mol	Chain	Res	Type
1	A	321[A]	GLU
1	A	321[B]	GLU
1	A	342	TYR
1	A	730	LYS
1	A	785	GLU
1	A	810[B]	GLU
1	A	934	LEU
1	B	342	TYR
1	B	490	LEU
1	B	730	LYS
1	B	833	ILE
1	B	910	GLU
1	B	934	LEU
1	B	949	ILE
1	B	980	GLU
1	B	1104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	827	GLN
1	B	340	GLN
1	B	667	ASN
1	B	872	HIS
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 49 ligands modelled in this entry, 1 is monoatomic - leaving 48 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PG4	B	2010	-	12,12,12	0.27	0	11,11,11	0.26	0
3	PEG	A	2015	-	6,6,6	0.23	0	5,5,5	0.27	0
8	NAD	B	2019	10	46,48,48	2.43	9 (19%)	64,73,73	1.79	13 (20%)
3	PEG	B	2011	-	6,6,6	0.23	0	5,5,5	0.24	0
3	PEG	B	2018	-	6,6,6	0.28	0	5,5,5	0.39	0
4	A1BDD	A	2009	-	10,10,10	0.62	0	12,12,12	0.69	0
7	FMT	B	2015	-	2,2,2	0.87	0	1,1,1	0.22	0
3	PEG	B	2005	-	6,6,6	0.27	0	5,5,5	0.34	0
3	PEG	B	2002	-	6,6,6	0.25	0	5,5,5	0.32	0
7	FMT	B	2017	-	2,2,2	0.62	0	1,1,1	0.22	0
2	FAD	B	2001	-	58,58,58	1.91	11 (18%)	85,89,89	1.82	19 (22%)
7	FMT	A	2019	-	2,2,2	0.63	0	1,1,1	0.22	0
7	FMT	A	2021	-	2,2,2	0.62	0	1,1,1	0.16	0
6	PG4	A	2018	-	12,12,12	0.31	0	11,11,11	0.44	0
3	PEG	A	2005	-	6,6,6	0.23	0	5,5,5	0.26	0
8	NAD	A	2022[B]	-	28,29,48	2.55	7 (25%)	43,45,73	2.04	11 (25%)
3	PEG	B	2007	-	6,6,6	0.26	0	5,5,5	0.34	0
5	PGE	B	2014	-	9,9,9	0.35	0	8,8,8	0.80	0
3	PEG	A	2003	-	6,6,6	0.22	0	5,5,5	0.51	0
5	PGE	A	2011	-	9,9,9	0.32	0	8,8,8	0.60	0
8	NAD	A	2022[A]	-	46,48,48	2.47	11 (23%)	64,73,73	1.91	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	A	2007	-	6,6,6	0.26	0	5,5,5	0.20	0
9	SO4	A	2025	-	4,4,4	0.63	0	6,6,6	0.19	0
3	PEG	B	2006	-	6,6,6	0.25	0	5,5,5	0.17	0
3	PEG	B	2009	-	6,6,6	0.23	0	5,5,5	0.29	0
5	PGE	B	2003	-	9,9,9	0.30	0	8,8,8	0.63	0
3	PEG	B	2004	-	6,6,6	0.24	0	5,5,5	0.34	0
9	SO4	B	2020	-	4,4,4	0.67	0	6,6,6	0.24	0
7	FMT	B	2013	-	2,2,2	0.64	0	1,1,1	0.33	0
9	SO4	B	2021	-	4,4,4	0.70	0	6,6,6	0.10	0
3	PEG	A	2017	-	6,6,6	0.27	0	5,5,5	0.38	0
4	A1BDD	B	2008	-	10,10,10	0.63	0	12,12,12	0.76	0
6	PG4	B	2012	-	12,12,12	0.28	0	11,11,11	0.28	0
3	PEG	A	2020	-	6,6,6	0.25	0	5,5,5	0.31	0
7	FMT	A	2014	-	2,2,2	0.51	0	1,1,1	0.24	0
3	PEG	A	2002	-	6,6,6	0.28	0	5,5,5	0.26	0
9	SO4	A	2026	-	4,4,4	0.64	0	6,6,6	0.07	0
9	SO4	A	2024	-	4,4,4	0.64	0	6,6,6	0.14	0
3	PEG	B	2016	-	6,6,6	0.24	0	5,5,5	0.37	0
3	PEG	A	2012	-	6,6,6	0.24	0	5,5,5	0.20	0
3	PEG	A	2008	-	6,6,6	0.23	0	5,5,5	0.21	0
6	PG4	A	2013	-	12,12,12	0.29	0	11,11,11	0.23	0
2	FAD	A	2001	-	58,58,58	2.08	12 (20%)	85,89,89	1.72	16 (18%)
9	SO4	A	2023	-	4,4,4	0.57	0	6,6,6	0.15	0
3	PEG	A	2016	-	6,6,6	0.27	0	5,5,5	0.32	0
3	PEG	A	2006	-	6,6,6	0.26	0	5,5,5	0.26	0
3	PEG	A	2010	-	6,6,6	0.26	0	5,5,5	0.22	0
3	PEG	A	2004	-	6,6,6	0.27	0	5,5,5	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
6	PG4	B	2010	-	-	1/10/10/10	-
3	PEG	A	2015	-	-	2/4/4/4	-
8	NAD	B	2019	10	-	2/30/62/62	0/5/5/5
3	PEG	B	2011	-	-	0/4/4/4	-
3	PEG	B	2018	-	-	0/4/4/4	-
4	A1BDD	A	2009	-	-	2/4/4/4	0/1/1/1
3	PEG	B	2005	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	2002	-	-	1/4/4/4	-
2	FAD	B	2001	-	-	3/34/50/50	0/6/6/6
6	PG4	A	2018	-	-	5/10/10/10	-
3	PEG	A	2005	-	-	3/4/4/4	-
8	NAD	A	2022[B]	-	-	1/16/32/62	0/3/3/5
3	PEG	B	2007	-	-	0/4/4/4	-
5	PGE	B	2014	-	-	2/7/7/7	-
3	PEG	A	2003	-	-	2/4/4/4	-
5	PGE	A	2011	-	-	7/7/7/7	-
8	NAD	A	2022[A]	-	-	4/30/62/62	0/5/5/5
3	PEG	A	2007	-	-	1/4/4/4	-
3	PEG	B	2006	-	-	2/4/4/4	-
3	PEG	B	2009	-	-	4/4/4/4	-
5	PGE	B	2003	-	-	5/7/7/7	-
3	PEG	B	2004	-	-	1/4/4/4	-
3	PEG	A	2017	-	-	0/4/4/4	-
4	A1BDD	B	2008	-	-	2/4/4/4	0/1/1/1
6	PG4	B	2012	-	-	7/10/10/10	-
3	PEG	A	2020	-	-	4/4/4/4	-
3	PEG	A	2002	-	-	1/4/4/4	-
3	PEG	B	2016	-	-	3/4/4/4	-
3	PEG	A	2012	-	-	1/4/4/4	-
3	PEG	A	2008	-	-	1/4/4/4	-
6	PG4	A	2013	-	-	8/10/10/10	-
2	FAD	A	2001	-	-	4/34/50/50	0/6/6/6
3	PEG	A	2016	-	-	3/4/4/4	-
3	PEG	A	2006	-	-	2/4/4/4	-
3	PEG	A	2010	-	-	0/4/4/4	-
3	PEG	A	2004	-	-	0/4/4/4	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2022[B]	NAD	PA-O3	-10.79	1.47	1.59
8	A	2022[A]	NAD	PA-O3	-10.61	1.48	1.59
8	B	2019	NAD	PA-O3	-10.06	1.48	1.59
2	A	2001	FAD	PA-O3P	-7.43	1.51	1.59
8	B	2019	NAD	C2N-N1N	7.07	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FAD	O4-C4	7.01	1.36	1.23
2	B	2001	FAD	O4-C4	6.24	1.35	1.23
8	A	2022[A]	NAD	C2N-N1N	6.17	1.41	1.35
8	A	2022[A]	NAD	C7N-N7N	5.80	1.43	1.33
2	B	2001	FAD	PA-O3P	-5.62	1.53	1.59
8	B	2019	NAD	C7N-N7N	5.40	1.42	1.33
2	B	2001	FAD	O2-C2	4.93	1.34	1.24
2	A	2001	FAD	O2-C2	4.60	1.33	1.24
2	B	2001	FAD	C4X-N5	4.11	1.39	1.30
2	A	2001	FAD	C6A-N6A	4.07	1.44	1.34
2	A	2001	FAD	C4X-N5	4.04	1.39	1.30
2	B	2001	FAD	C6A-N6A	3.98	1.44	1.34
8	A	2022[B]	NAD	C6A-N6A	3.89	1.44	1.34
8	A	2022[A]	NAD	C6A-N6A	3.87	1.44	1.34
8	B	2019	NAD	C6A-N6A	3.84	1.44	1.34
2	A	2001	FAD	P-O3P	3.35	1.63	1.59
2	B	2001	FAD	P-O3P	3.21	1.63	1.59
2	A	2001	FAD	O2'-C2'	-2.94	1.37	1.43
8	B	2019	NAD	C6N-N1N	2.92	1.42	1.35
8	A	2022[B]	NAD	PA-O5B	-2.86	1.48	1.59
8	A	2022[A]	NAD	C6N-N1N	2.71	1.41	1.35
8	A	2022[A]	NAD	PA-O5B	-2.69	1.48	1.59
2	A	2001	FAD	C2-N1	2.63	1.42	1.36
8	B	2019	NAD	PA-O5B	-2.54	1.49	1.59
2	B	2001	FAD	PA-O2A	-2.47	1.43	1.55
2	B	2001	FAD	O2'-C2'	-2.46	1.38	1.43
2	A	2001	FAD	PA-O5B	-2.34	1.50	1.59
2	B	2001	FAD	PA-O5B	-2.34	1.50	1.59
2	A	2001	FAD	O4B-C4B	-2.30	1.39	1.45
8	A	2022[A]	NAD	C4A-N9A	2.26	1.42	1.37
2	A	2001	FAD	PA-O2A	-2.25	1.44	1.55
8	B	2019	NAD	O3D-C3D	-2.24	1.37	1.43
2	B	2001	FAD	C2-N1	2.17	1.41	1.36
8	A	2022[B]	NAD	PA-O2A	-2.15	1.45	1.55
8	A	2022[A]	NAD	C2D-C3D	-2.14	1.47	1.53
2	A	2001	FAD	O4'-C4'	-2.12	1.38	1.43
8	A	2022[A]	NAD	PA-O2A	-2.10	1.45	1.55
8	A	2022[B]	NAD	C4A-N9A	2.09	1.42	1.37
2	B	2001	FAD	C10-N1	2.06	1.37	1.33
8	B	2019	NAD	C5A-C4A	2.06	1.42	1.39
8	A	2022[A]	NAD	C5A-C4A	2.05	1.42	1.39
8	B	2019	NAD	PA-O2A	-2.04	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2022[B]	NAD	C2B-C3B	-2.02	1.47	1.53
8	A	2022[B]	NAD	C5A-C4A	2.02	1.42	1.39
8	A	2022[A]	NAD	O3D-C3D	-2.02	1.38	1.43

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	FAD	N3A-C2A-N1A	-6.39	118.91	128.58
8	A	2022[B]	NAD	N3A-C2A-N1A	-5.72	119.92	128.58
8	B	2019	NAD	N3A-C2A-N1A	-5.70	119.95	128.58
8	A	2022[A]	NAD	N3A-C2A-N1A	-5.64	120.04	128.58
2	A	2001	FAD	N3A-C2A-N1A	-5.37	120.46	128.58
8	A	2022[A]	NAD	C5A-C4A-N3A	-5.20	119.56	126.72
8	B	2019	NAD	C5A-C4A-N3A	-5.15	119.62	126.72
8	A	2022[B]	NAD	C5A-C4A-N3A	-5.07	119.73	126.72
2	B	2001	FAD	C5A-C4A-N3A	-4.75	120.18	126.72
2	A	2001	FAD	C5A-C4A-N3A	-4.50	120.52	126.72
8	A	2022[A]	NAD	C4D-O4D-C1D	-4.43	105.87	109.92
8	B	2019	NAD	N3A-C4A-N9A	4.34	134.54	127.17
8	A	2022[A]	NAD	N3A-C4A-N9A	4.24	134.37	127.17
8	A	2022[A]	NAD	O2A-PA-O3	-4.18	95.96	107.27
8	A	2022[B]	NAD	N3A-C4A-N9A	4.17	134.26	127.17
8	B	2019	NAD	C5A-N7A-C8A	3.97	109.69	103.45
8	A	2022[A]	NAD	C5A-N7A-C8A	3.90	109.58	103.45
8	A	2022[B]	NAD	C5A-N7A-C8A	3.88	109.56	103.45
2	A	2001	FAD	C5A-N7A-C8A	3.82	109.46	103.45
2	B	2001	FAD	C2A-N3A-C4A	3.81	121.13	111.83
2	A	2001	FAD	O2P-P-O3P	-3.80	97.01	107.27
2	B	2001	FAD	O2P-P-O3P	-3.78	97.04	107.27
2	B	2001	FAD	N3A-C4A-N9A	3.77	133.58	127.17
2	A	2001	FAD	N3A-C4A-N9A	3.76	133.56	127.17
8	A	2022[B]	NAD	O2A-PA-O3	-3.75	97.14	107.27
8	B	2019	NAD	C2A-N3A-C4A	3.70	120.87	111.83
2	A	2001	FAD	C4-C4X-N5	3.64	123.24	118.21
8	A	2022[A]	NAD	C2A-N3A-C4A	3.59	120.59	111.83
8	A	2022[B]	NAD	C2A-N3A-C4A	3.58	120.58	111.83
2	B	2001	FAD	C5A-N7A-C8A	3.57	109.06	103.45
2	A	2001	FAD	C4-N3-C2	-3.48	119.45	125.64
8	B	2019	NAD	N9A-C8A-N7A	-3.41	109.10	113.94
2	A	2001	FAD	N9A-C8A-N7A	-3.35	109.19	113.94
2	A	2001	FAD	C2A-N3A-C4A	3.34	119.99	111.83
8	B	2019	NAD	C6N-N1N-C2N	-3.27	119.10	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2022[B]	NAD	N9A-C8A-N7A	-3.18	109.43	113.94
2	B	2001	FAD	N9A-C8A-N7A	-3.15	109.47	113.94
2	B	2001	FAD	C4-N3-C2	-3.13	120.09	125.64
8	A	2022[A]	NAD	N9A-C8A-N7A	-3.10	109.54	113.94
8	B	2019	NAD	C4A-C5A-N7A	-2.99	107.17	110.58
2	B	2001	FAD	O2-C2-N1	-2.98	116.85	121.80
2	B	2001	FAD	C9-C9A-N10	-2.95	117.88	121.85
2	A	2001	FAD	C4A-C5A-N7A	-2.94	107.22	110.58
8	A	2022[A]	NAD	C4A-C5A-N7A	-2.94	107.22	110.58
8	A	2022[B]	NAD	C4A-C5A-N7A	-2.92	107.25	110.58
2	A	2001	FAD	C4X-C4-N3	2.85	120.50	113.25
2	B	2001	FAD	C4-C4X-N5	2.81	122.09	118.21
2	B	2001	FAD	O3P-P-O1P	2.80	119.12	110.70
8	A	2022[A]	NAD	C3N-C7N-N7N	2.79	121.18	117.74
2	B	2001	FAD	C4X-C4-N3	2.73	120.19	113.25
2	B	2001	FAD	O4-C4-C4X	-2.66	119.52	126.53
2	B	2001	FAD	C4A-C5A-N7A	-2.61	107.59	110.58
2	A	2001	FAD	C4X-C10-N10	2.58	120.18	116.48
8	A	2022[A]	NAD	O3-PA-O1A	2.58	118.48	110.70
8	B	2019	NAD	O2A-PA-O5B	-2.57	95.90	107.57
2	A	2001	FAD	C10-C4X-N5	-2.54	119.63	124.81
2	B	2001	FAD	C4X-C10-N10	2.41	119.94	116.48
8	A	2022[A]	NAD	O5B-PA-O1A	2.40	118.44	108.94
2	B	2001	FAD	C5X-C9A-N10	2.39	120.13	117.97
2	A	2001	FAD	O3P-P-O1P	2.37	117.84	110.70
2	A	2001	FAD	C4A-N9A-C8A	2.36	108.22	105.74
8	A	2022[B]	NAD	O2A-PA-O5B	-2.35	96.90	107.57
8	B	2019	NAD	C4A-N9A-C8A	2.35	108.21	105.74
2	A	2001	FAD	C2'-C1'-N10	2.35	121.30	110.20
2	B	2001	FAD	C2A-N1A-C6A	2.35	122.58	118.73
2	B	2001	FAD	C2'-C1'-N10	2.29	121.04	110.20
8	A	2022[B]	NAD	O5B-PA-O1A	2.24	117.81	108.94
8	A	2022[B]	NAD	O3-PA-O1A	2.09	117.00	110.70
8	B	2019	NAD	O5B-PA-O1A	2.07	117.16	108.94
8	B	2019	NAD	O2A-PA-O3	-2.07	101.67	107.27
8	A	2022[A]	NAD	O2A-PA-O5B	-2.07	98.18	107.57
8	B	2019	NAD	C2N-C3N-C4N	2.03	120.62	118.26

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	FAD	P-O3P-PA-O5B
2	A	2001	FAD	N10-C1'-C2'-O2'
2	A	2001	FAD	N10-C1'-C2'-C3'
2	B	2001	FAD	P-O3P-PA-O5B
2	B	2001	FAD	N10-C1'-C2'-O2'
2	B	2001	FAD	N10-C1'-C2'-C3'
8	A	2022[A]	NAD	PN-O3-PA-O5B
8	A	2022[B]	NAD	C5B-O5B-PA-O3
4	B	2008	A1BDD	C10-C03-O02-C01
4	B	2008	A1BDD	C04-C03-O02-C01
5	B	2003	PGE	C4-C3-O2-C2
6	A	2013	PG4	C6-C5-O3-C4
5	A	2011	PGE	C4-C3-O2-C2
3	B	2005	PEG	O2-C3-C4-O4
6	A	2013	PG4	O2-C3-C4-O3
6	B	2012	PG4	O2-C3-C4-O3
3	A	2007	PEG	O1-C1-C2-O2
3	B	2006	PEG	O1-C1-C2-O2
5	A	2011	PGE	O2-C3-C4-O3
6	B	2012	PG4	O3-C5-C6-O4
3	A	2003	PEG	O2-C3-C4-O4
3	A	2015	PEG	O1-C1-C2-O2
3	A	2020	PEG	O1-C1-C2-O2
3	A	2020	PEG	O2-C3-C4-O4
3	B	2004	PEG	O1-C1-C2-O2
5	A	2011	PGE	O1-C1-C2-O2
3	A	2015	PEG	O2-C3-C4-O4
3	A	2016	PEG	O2-C3-C4-O4
5	B	2003	PGE	O3-C5-C6-O4
6	A	2013	PG4	O4-C7-C8-O5
6	B	2012	PG4	O1-C1-C2-O2
6	A	2013	PG4	O3-C5-C6-O4
6	A	2013	PG4	O1-C1-C2-O2
3	A	2005	PEG	O1-C1-C2-O2
6	B	2012	PG4	O4-C7-C8-O5
3	B	2016	PEG	C4-C3-O2-C2
3	B	2009	PEG	C1-C2-O2-C3
5	A	2011	PGE	O3-C5-C6-O4
6	A	2013	PG4	C4-C3-O2-C2
3	B	2005	PEG	O1-C1-C2-O2
3	A	2005	PEG	C4-C3-O2-C2
6	A	2018	PG4	C4-C3-O2-C2
3	B	2006	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	A	2011	PGE	C1-C2-O2-C3
6	B	2012	PG4	C1-C2-O2-C3
5	B	2014	PGE	O3-C5-C6-O4
3	A	2003	PEG	C4-C3-O2-C2
3	A	2016	PEG	C4-C3-O2-C2
5	B	2003	PGE	C1-C2-O2-C3
3	A	2012	PEG	C4-C3-O2-C2
8	B	2019	NAD	C2B-C1B-N9A-C8A
3	A	2006	PEG	C4-C3-O2-C2
6	A	2018	PG4	C5-C6-O4-C7
3	B	2009	PEG	O1-C1-C2-O2
3	B	2016	PEG	O2-C3-C4-O4
5	B	2003	PGE	O1-C1-C2-O2
3	A	2005	PEG	O2-C3-C4-O4
6	A	2018	PG4	C8-C7-O4-C6
6	A	2018	PG4	O1-C1-C2-O2
3	A	2016	PEG	C1-C2-O2-C3
5	B	2014	PGE	O2-C3-C4-O3
2	A	2001	FAD	C3B-C4B-C5B-O5B
3	B	2009	PEG	O2-C3-C4-O4
3	B	2016	PEG	C1-C2-O2-C3
3	B	2002	PEG	C4-C3-O2-C2
3	A	2020	PEG	C1-C2-O2-C3
3	A	2008	PEG	O2-C3-C4-O4
6	A	2018	PG4	C6-C5-O3-C4
8	A	2022[A]	NAD	C4D-C5D-O5D-PN
6	B	2012	PG4	C4-C3-O2-C2
3	A	2006	PEG	C1-C2-O2-C3
3	B	2009	PEG	C4-C3-O2-C2
5	B	2003	PGE	O2-C3-C4-O3
6	A	2013	PG4	C8-C7-O4-C6
6	B	2010	PG4	C8-C7-O4-C6
3	A	2020	PEG	C4-C3-O2-C2
4	A	2009	A1BDD	C10-C03-O02-C01
6	A	2013	PG4	C5-C6-O4-C7
4	A	2009	A1BDD	C04-C03-O02-C01
3	A	2002	PEG	C4-C3-O2-C2
5	A	2011	PGE	C3-C4-O3-C5
5	A	2011	PGE	C6-C5-O3-C4
8	B	2019	NAD	O4B-C1B-N9A-C8A
8	A	2022[A]	NAD	C2B-C1B-N9A-C8A
6	B	2012	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
8	A	2022[A]	NAD	O4B-C1B-N9A-C8A

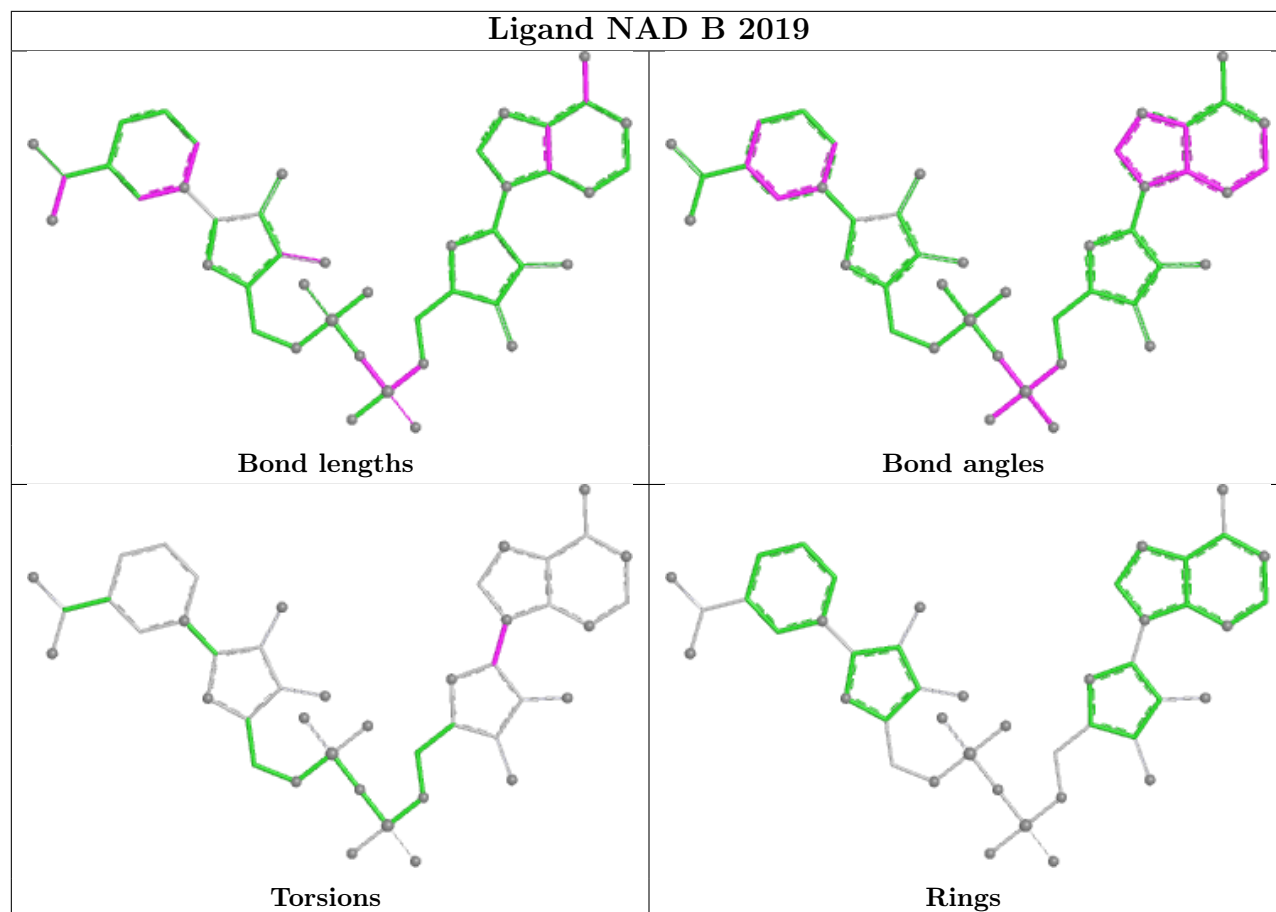
There are no ring outliers.

15 monomers are involved in 21 short contacts:

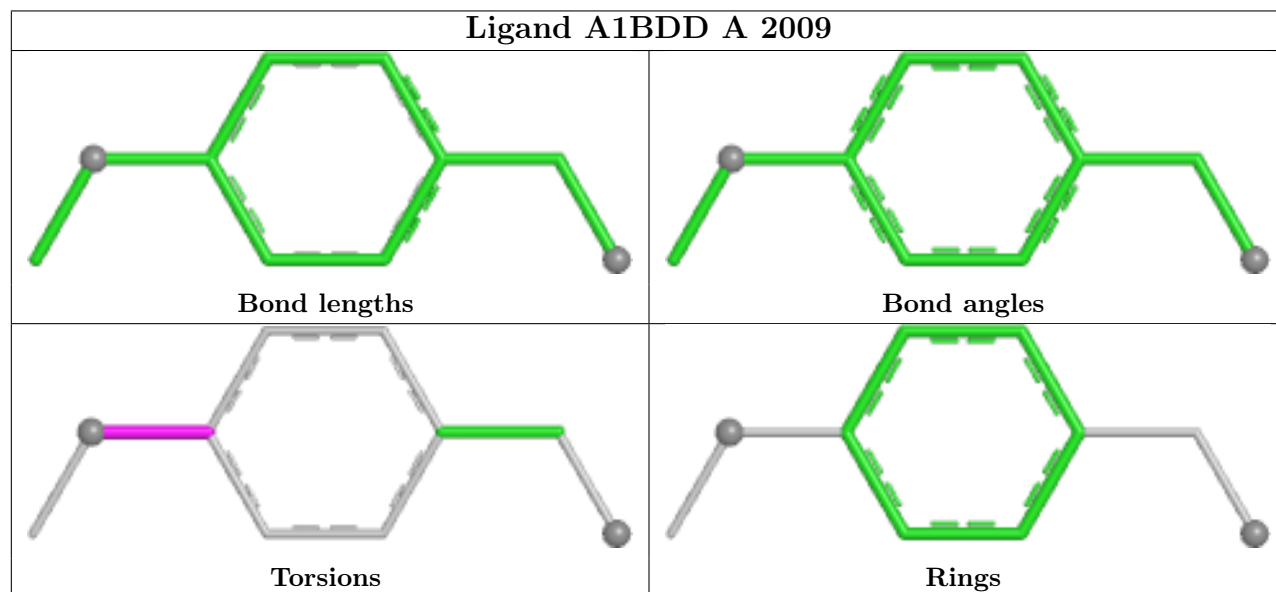
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	2019	NAD	1	0
3	B	2018	PEG	2	0
2	B	2001	FAD	1	0
6	A	2018	PG4	1	0
3	A	2003	PEG	2	0
9	A	2025	SO4	1	0
3	B	2006	PEG	1	0
3	B	2009	PEG	3	0
5	B	2003	PGE	1	0
3	B	2004	PEG	1	0
6	B	2012	PG4	2	0
3	A	2002	PEG	2	0
9	A	2024	SO4	1	0
2	A	2001	FAD	1	0
3	A	2016	PEG	1	0

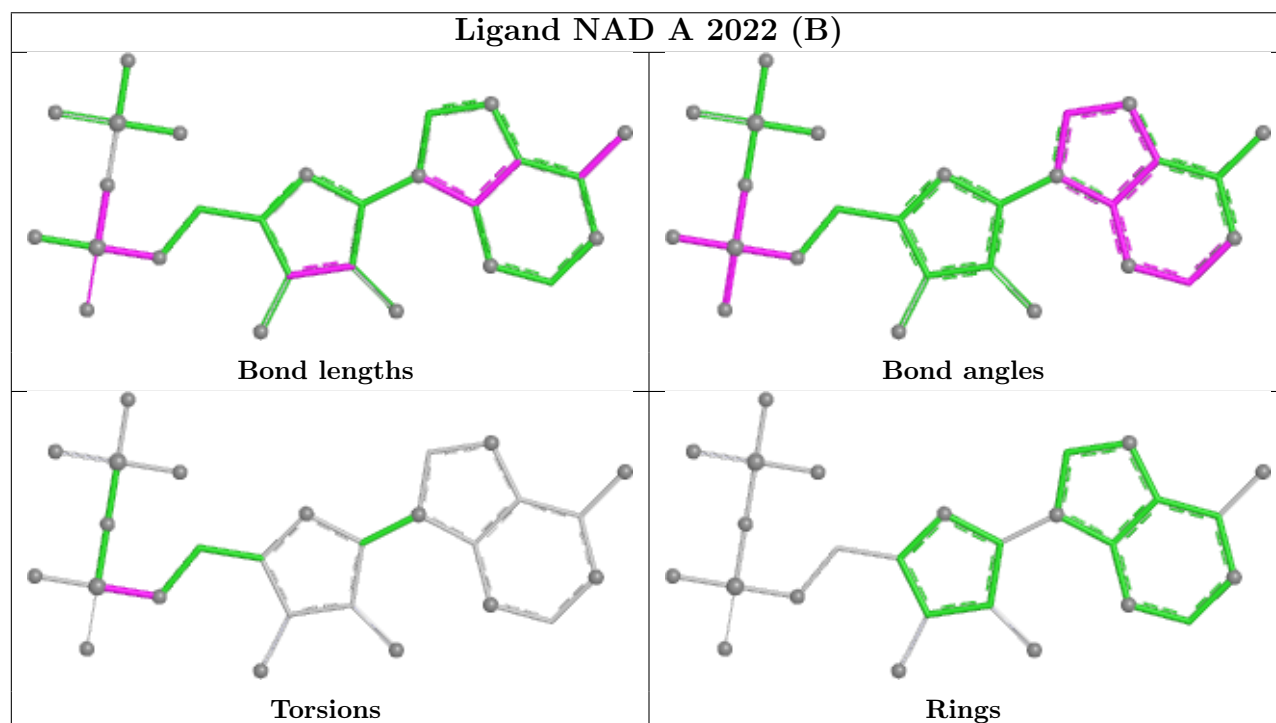
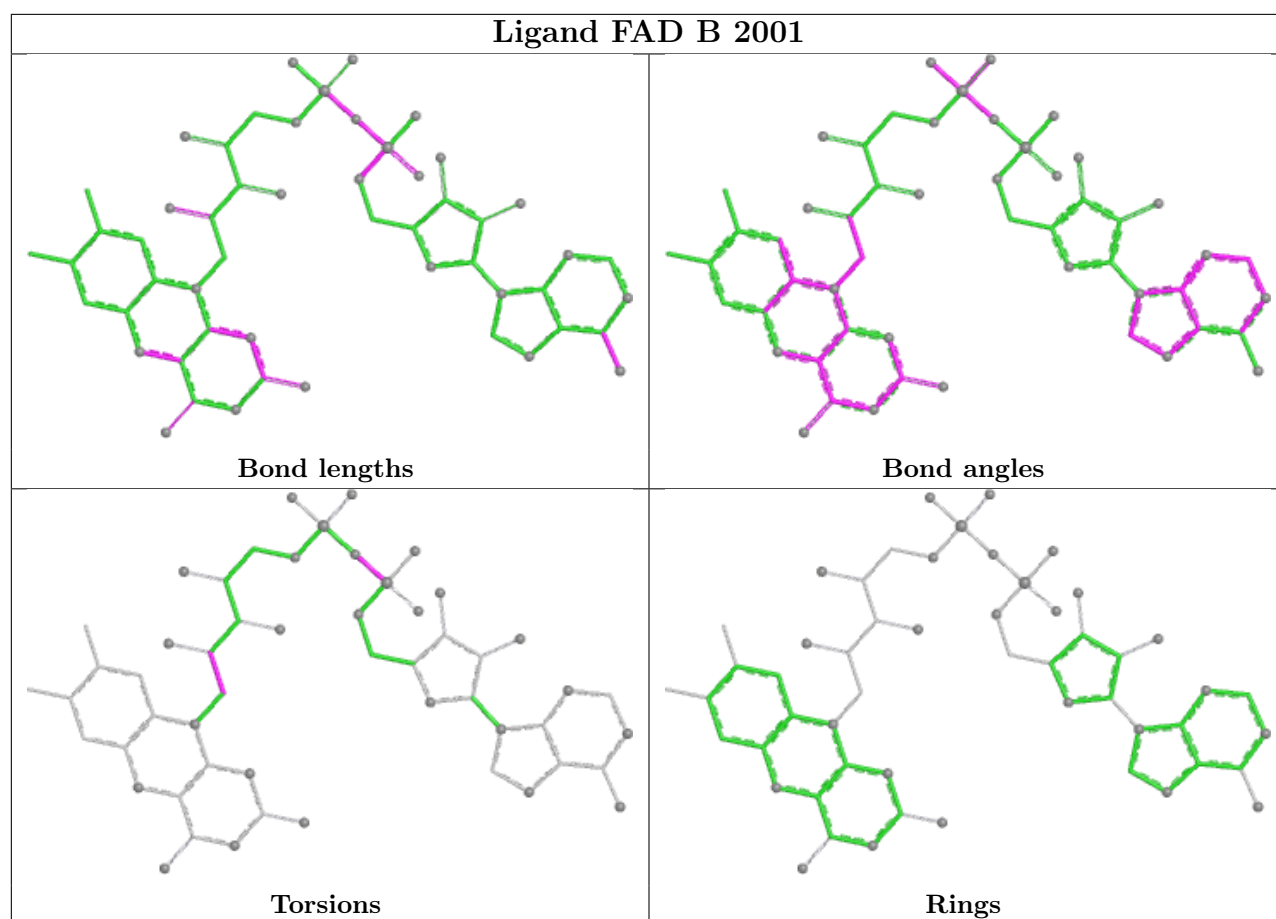
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand NAD B 2019

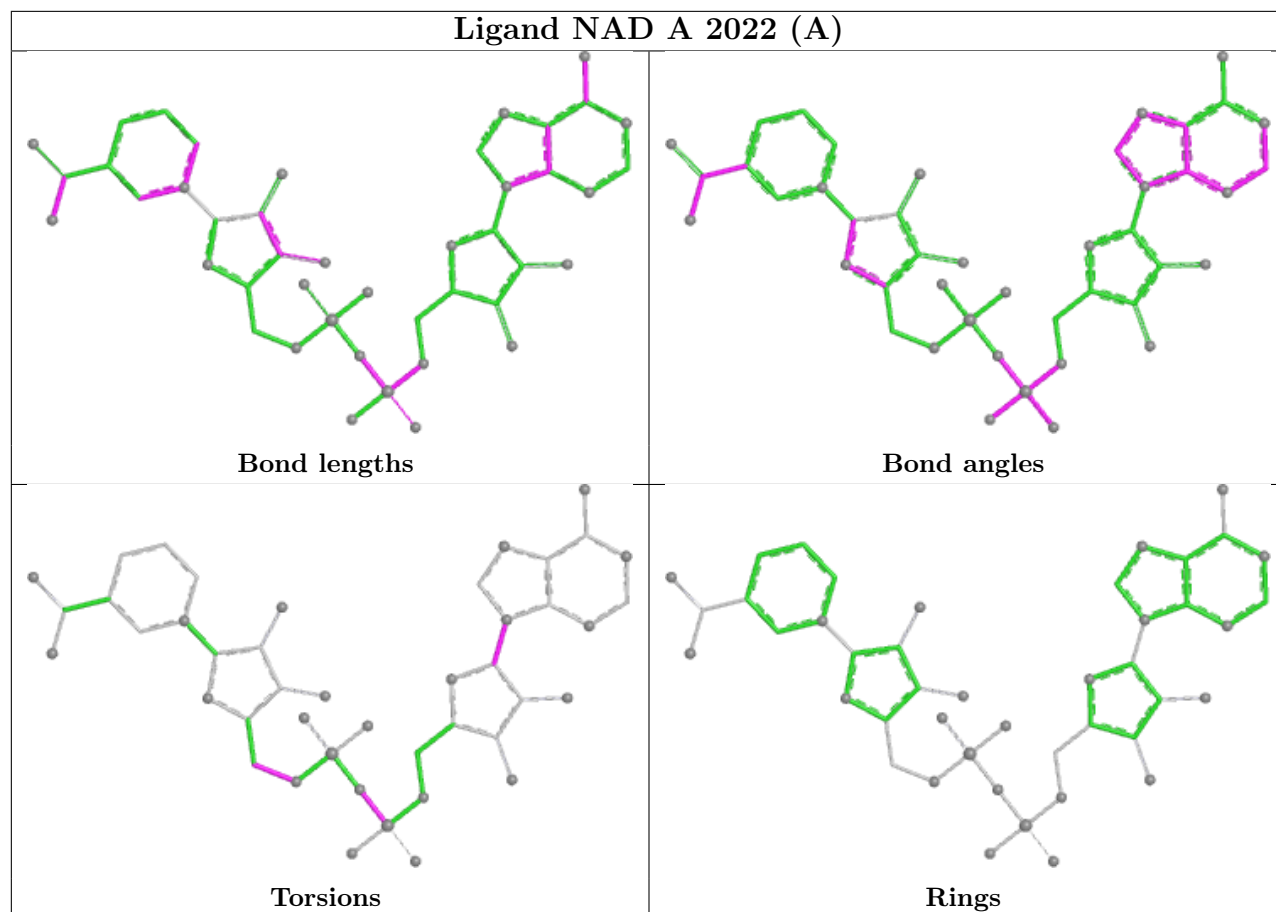


Ligand A1BDD A 2009

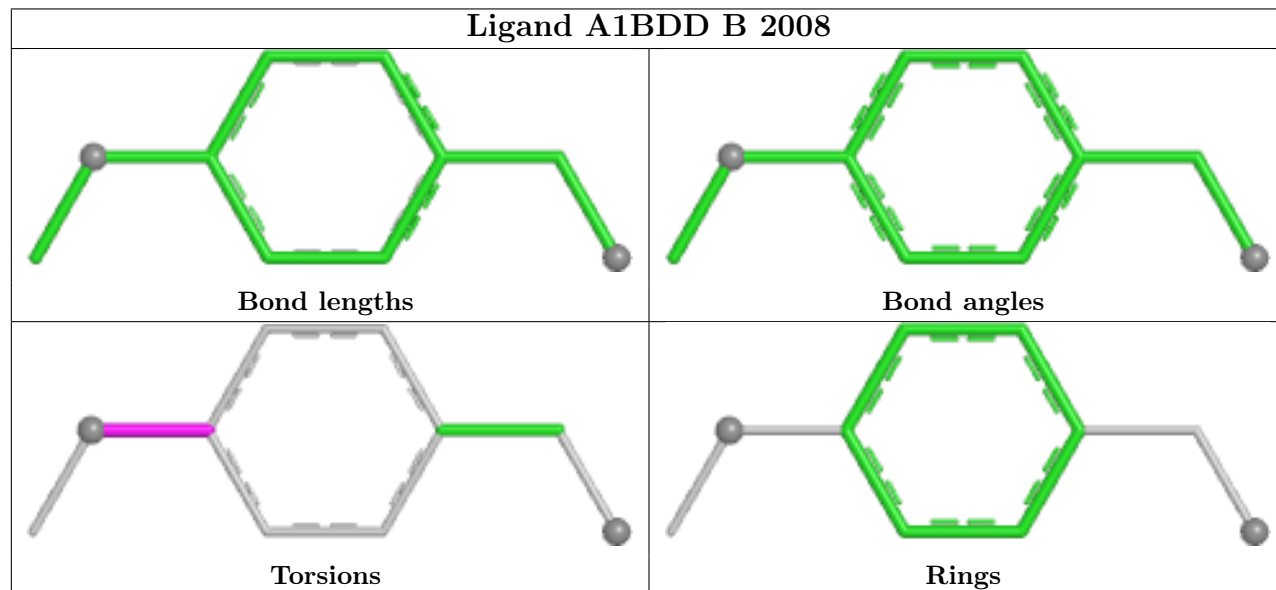


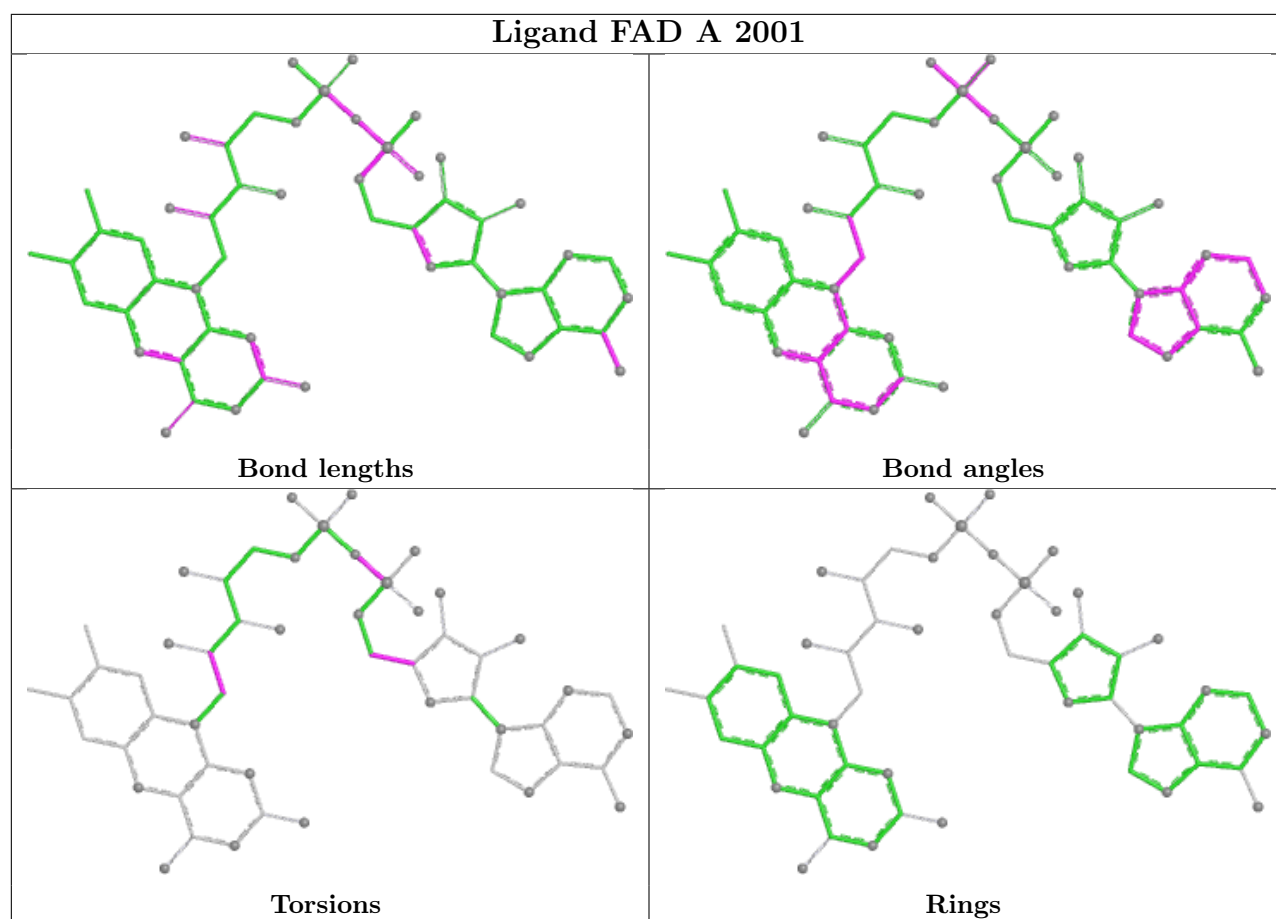


Ligand NAD A 2022 (A)



Ligand A1BDD B 2008





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	1206/1235 (97%)	-0.03	47 (3%)	43 48	10, 23, 45, 81	18 (1%)
1	B	1201/1235 (97%)	-0.02	28 (2%)	61 66	10, 24, 43, 81	13 (1%)
All	All	2407/2470 (97%)	-0.02	75 (3%)	51 56	10, 24, 44, 81	31 (1%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1223	ALA	5.2
1	A	1222	ALA	5.1
1	A	482	LEU	5.1
1	A	1224	GLY	4.6
1	B	129	ASN	4.2
1	A	111	ILE	3.9
1	A	114	THR	3.9
1	A	116	THR	3.6
1	A	484	ALA	3.6
1	A	130	TRP	3.5
1	A	1229	LEU	3.5
1	A	494	GLY	3.5
1	A	129	ASN	3.4
1	A	14	ALA	3.4
1	A	483	LEU	3.3
1	B	482	LEU	3.3
1	B	134	LEU	3.2
1	B	905	LEU	3.2
1	B	132	SER	3.2
1	B	14	ALA	3.1
1	A	500	VAL	3.1
1	A	801	ALA	3.1
1	A	1228	SER	3.1
1	A	493	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	912	ILE	3.0
1	A	487	VAL	3.0
1	A	491	LEU	3.0
1	A	1226	ASN	3.0
1	A	223	LEU	3.0
1	A	481	THR	2.9
1	A	115	ALA	2.9
1	B	464	GLY	2.9
1	A	112	PRO	2.9
1	A	125	ILE	2.9
1	B	500	VAL	2.8
1	A	1227	ALA	2.8
1	B	84	VAL	2.8
1	A	485	TYR	2.8
1	B	223	LEU	2.7
1	A	137	SER	2.7
1	A	490	LEU	2.7
1	A	192	GLY	2.7
1	A	480	GLU	2.6
1	A	127	ASP	2.5
1	B	486	LEU	2.5
1	B	510	ILE	2.5
1	A	1225	GLY	2.5
1	A	119	ALA	2.5
1	B	1003	ALA	2.5
1	A	120	LEU	2.4
1	A	486	LEU	2.4
1	A	506	PRO	2.4
1	B	483	LEU	2.4
1	B	490	LEU	2.4
1	A	126	ALA	2.4
1	A	503	ILE	2.4
1	B	440	HIS	2.4
1	B	451	GLY	2.4
1	B	194	GLN	2.4
1	B	439	PHE	2.4
1	B	438	ASP	2.3
1	B	491	LEU	2.3
1	A	194	GLN	2.3
1	B	133	HIS	2.3
1	B	508	VAL	2.3
1	B	909	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	83	GLY	2.3
1	A	113	ASP	2.2
1	A	1221	ALA	2.2
1	A	128	GLY	2.2
1	B	75	LEU	2.2
1	A	478	THR	2.2
1	B	1002	GLY	2.1
1	A	195	PHE	2.1
1	A	800	PRO	2.1

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
5	PGE	A	2011	10/10	0.73	0.18	41,45,49,49	0
7	FMT	A	2021	3/3	0.74	0.17	32,32,36,37	3
8	NAD	A	2022[A]	44/44	0.74	0.17	22,29,33,35	44
8	NAD	A	2022[B]	27/44	0.74	0.17	29,32,34,37	27
3	PEG	A	2010	7/7	0.79	0.16	41,44,49,49	0
3	PEG	B	2011	7/7	0.79	0.17	40,41,47,47	0
7	FMT	B	2017	3/3	0.80	0.13	46,46,47,52	0
6	PG4	B	2012	13/13	0.80	0.16	37,47,54,57	0
3	PEG	A	2005	7/7	0.80	0.15	43,44,49,53	0
3	PEG	A	2016	7/7	0.81	0.13	35,43,49,51	0
3	PEG	A	2008	7/7	0.81	0.14	30,37,46,46	0
3	PEG	B	2018	7/7	0.81	0.15	33,39,42,45	0
6	PG4	A	2013	13/13	0.82	0.14	34,43,48,49	0
3	PEG	B	2016	7/7	0.82	0.16	43,48,49,50	0

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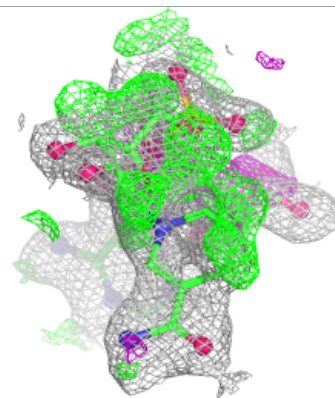
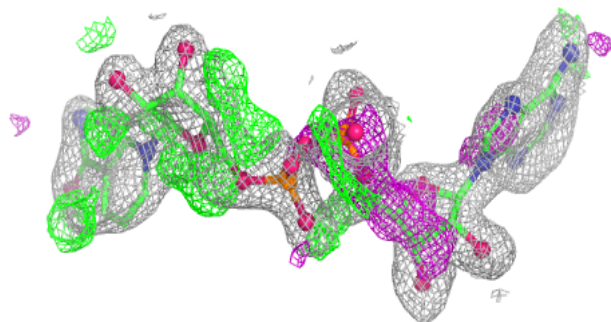
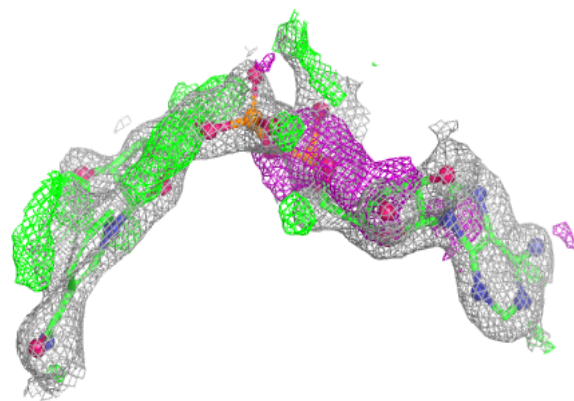
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	B	2004	7/7	0.83	0.16	35,41,49,49	0
3	PEG	A	2017	7/7	0.84	0.12	32,33,39,41	0
3	PEG	A	2015	7/7	0.84	0.14	39,42,45,54	0
3	PEG	A	2020	7/7	0.85	0.12	36,43,47,47	0
7	FMT	A	2019	3/3	0.85	0.14	34,34,40,42	3
3	PEG	A	2004	7/7	0.86	0.14	27,29,33,35	0
3	PEG	B	2006	7/7	0.87	0.12	38,43,50,51	0
5	PGE	B	2014	10/10	0.87	0.13	26,34,38,41	0
4	A1BDD	A	2009	10/10	0.87	0.15	25,29,35,36	10
3	PEG	A	2007	7/7	0.88	0.11	38,41,46,48	0
5	PGE	B	2003	10/10	0.88	0.12	24,37,45,48	0
3	PEG	B	2005	7/7	0.88	0.12	32,41,44,47	0
3	PEG	A	2012	7/7	0.88	0.11	39,45,51,54	0
3	PEG	B	2009	7/7	0.88	0.11	33,36,44,47	0
3	PEG	B	2007	7/7	0.89	0.11	34,39,49,49	0
3	PEG	A	2002	7/7	0.89	0.12	30,33,44,45	0
6	PG4	A	2018	13/13	0.89	0.12	22,28,38,40	0
3	PEG	B	2002	7/7	0.90	0.11	27,32,36,44	0
3	PEG	A	2006	7/7	0.91	0.10	37,38,44,50	0
8	NAD	B	2019	44/44	0.91	0.11	20,25,31,34	44
9	SO4	A	2024	5/5	0.91	0.11	41,41,48,49	5
9	SO4	A	2025	5/5	0.91	0.10	39,40,45,51	5
3	PEG	A	2003	7/7	0.92	0.10	22,30,37,44	0
4	A1BDD	B	2008	10/10	0.92	0.11	24,26,33,36	10
7	FMT	B	2015	3/3	0.92	0.12	19,19,25,35	3
9	SO4	A	2026	5/5	0.92	0.10	25,29,34,37	5
7	FMT	B	2013	3/3	0.94	0.14	40,40,40,41	0
6	PG4	B	2010	13/13	0.95	0.09	18,24,37,38	0
7	FMT	A	2014	3/3	0.96	0.09	21,21,31,32	0
9	SO4	B	2021	5/5	0.96	0.08	31,34,37,45	5
2	FAD	A	2001	53/53	0.97	0.06	16,22,25,26	0
2	FAD	B	2001	53/53	0.97	0.06	17,20,24,26	0
10	MG	B	2022	1/1	0.98	0.10	33,33,33,33	0
9	SO4	A	2023	5/5	0.99	0.05	20,21,23,24	0
9	SO4	B	2020	5/5	0.99	0.05	19,22,25,27	0

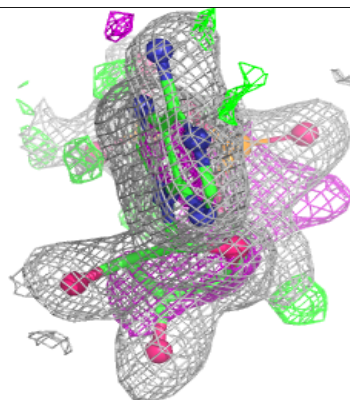
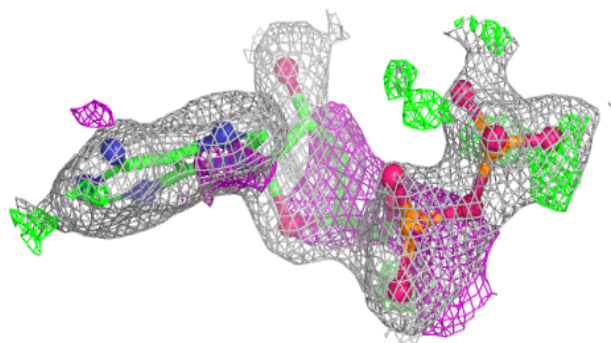
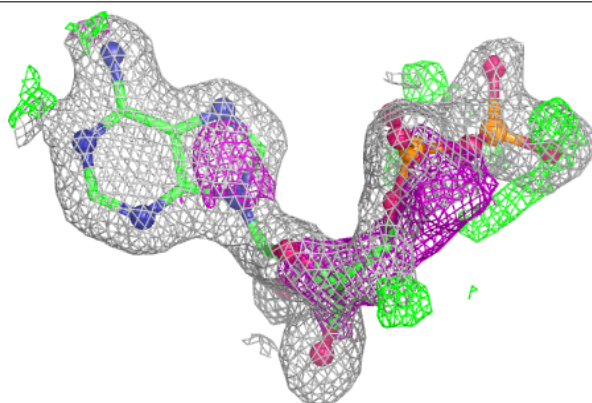
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 2022 (A):

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

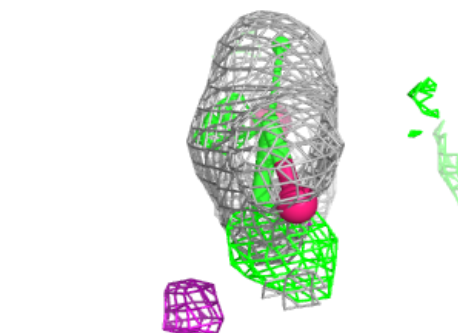
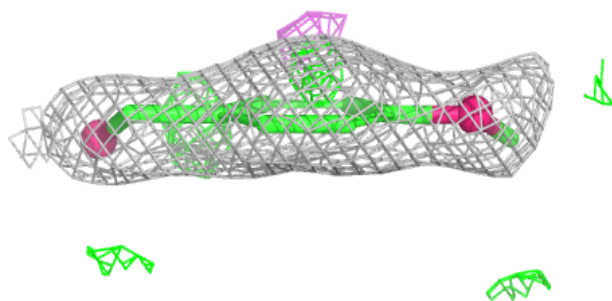
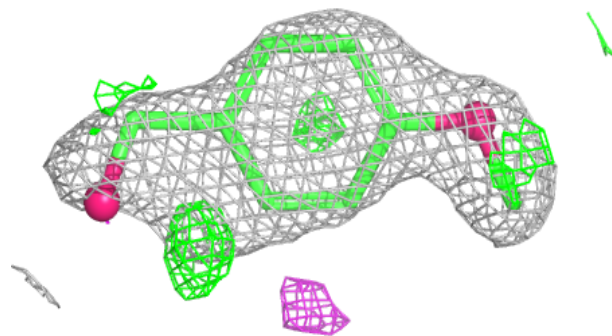
**Electron density around NAD A 2022 (B):**

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

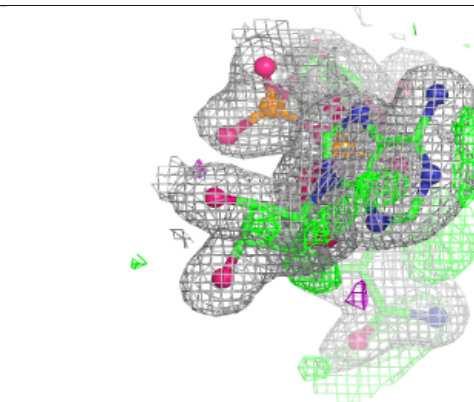
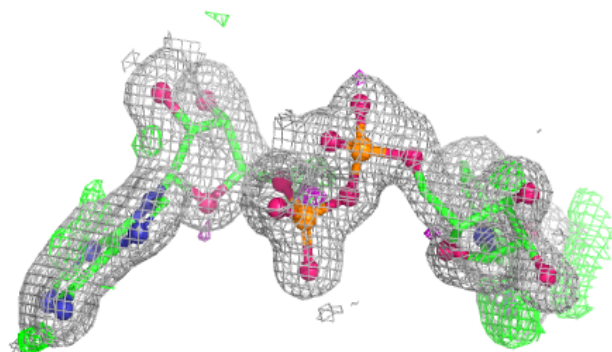
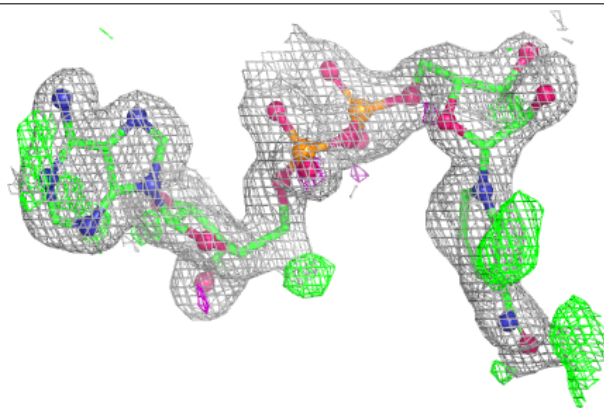


Electron density around A1BDD A 2009:

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

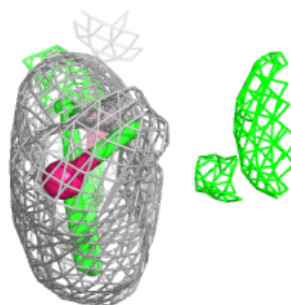
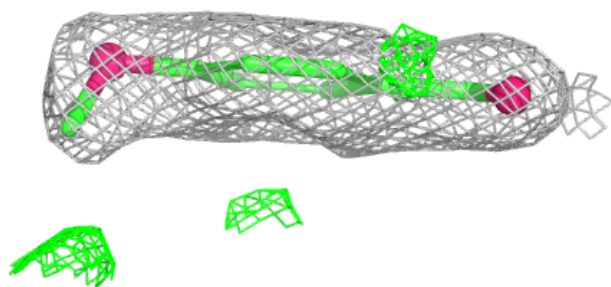
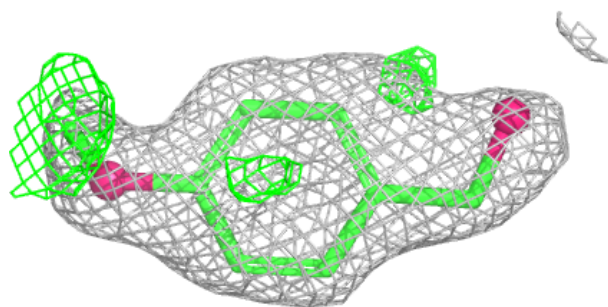
**Electron density around NAD B 2019:**

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

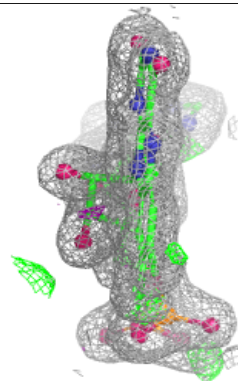
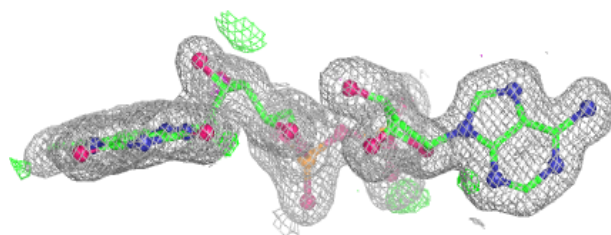
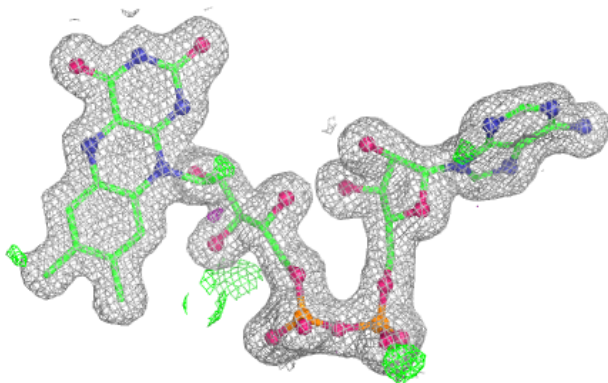


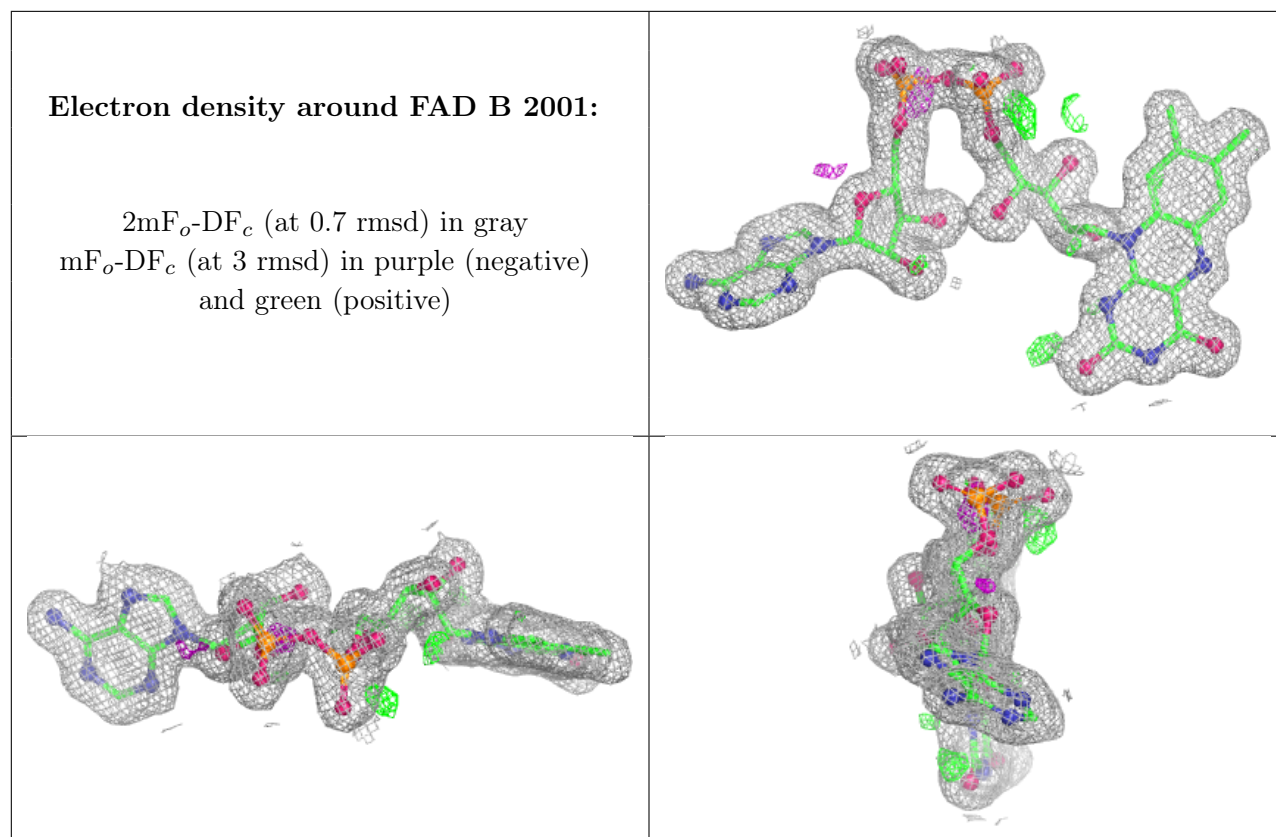
Electron density around A1BDD B 2008:

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

**Electron density around FAD A 2001:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.