



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 AM UTC

PDB ID : 4BUR / pdb_00004bur
Title : Crystal structure of the reduced human Apoptosis inducing factor complexed with NAD
Authors : Martinez-Julvez, M.; Herguedas, B.; Hermoso, J.A.; Ferreira, P.; Villanueva, R.; Medina, M.
Deposited on : 2013-06-23
Resolution : 2.88 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

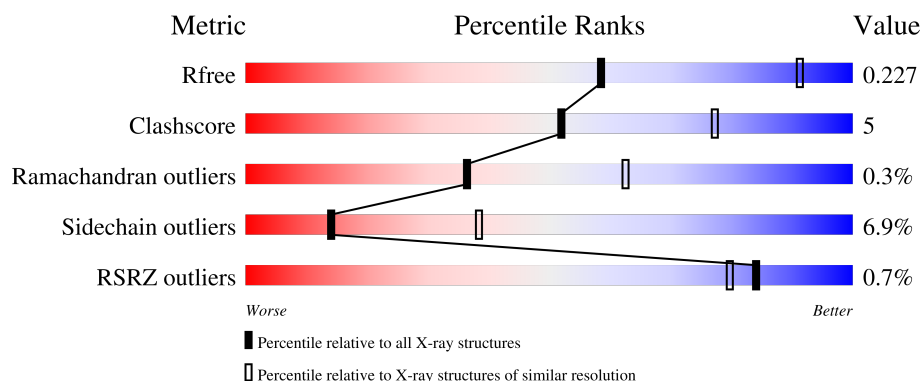
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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.

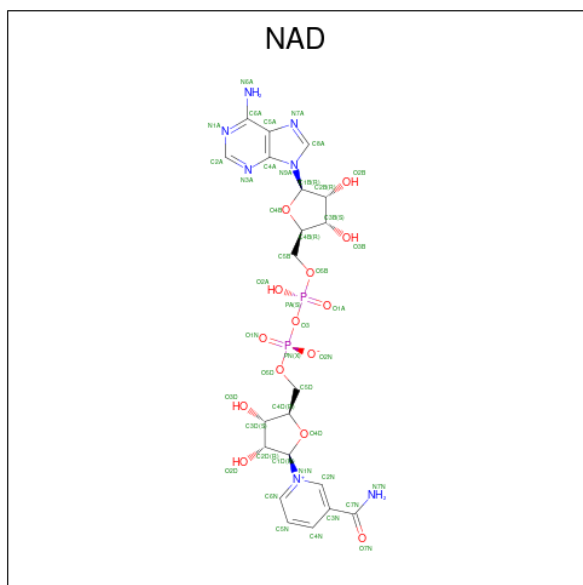
Mol	Chain	Length	Quality of chain
1	A	511	% 74% 13% • 12%
1	B	511	73% 14% • 12%
1	C	511	73% 13% • 13%
1	D	511	% 70% 14% • 15%

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 APOPTOSIS INDUCING FACTOR 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total 3475	C 2208	N 618	O 638	S 11	0	0	0
1	B	450	Total 3471	C 2205	N 616	O 639	S 11	0	0	0
1	C	446	Total 3452	C 2194	N 613	O 634	S 11	0	0	0
1	D	435	Total 3371	C 2147	N 599	O 614	S 11	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



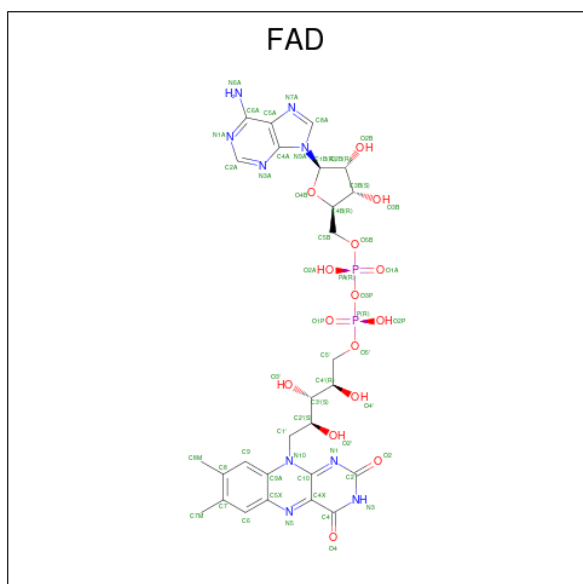
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

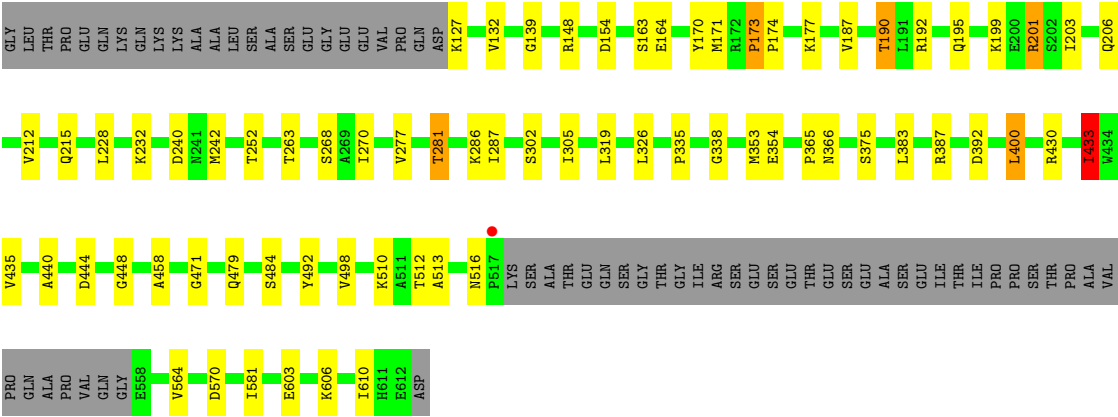
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



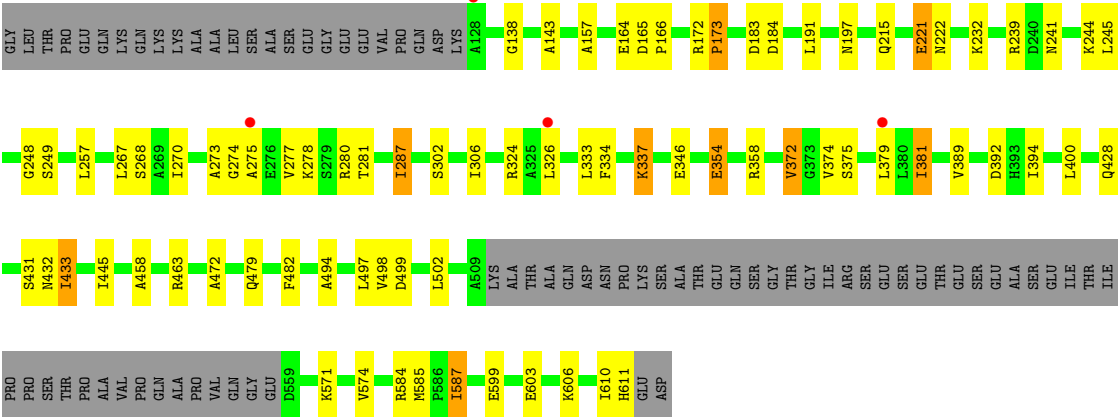
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	8	Total	O	0	0
			8	8		
5	C	7	Total	O	0	0
			7	7		



● Molecule 1: APOPTOSIS INDUCING FACTOR 1, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.77Å 120.77Å 343.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.88 40.00 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.88) 99.6 (40.00-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.230 0.176 , 0.227	Depositor DCC
R_{free} test set	4786 reflections (7.21%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14362	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: NAD, FAD, SO4

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	0.77	0/3546	0.98	8/4794 (0.2%)
1	B	0.72	0/3540	0.95	5/4785 (0.1%)
1	C	0.72	0/3522	0.96	6/4760 (0.1%)
1	D	0.71	0/3440	0.94	9/4648 (0.2%)
All	All	0.73	0/14048	0.96	28/18987 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	LEU	CA-C-N	-8.14	111.25	120.04
1	B	217	LEU	C-N-CA	-8.14	111.25	120.04
1	C	570	ASP	CB-CA-C	-6.89	108.63	116.63
1	A	178	GLU	N-CA-C	6.63	119.36	111.33
1	C	400	LEU	N-CA-C	6.43	119.67	109.50
1	A	552	GLN	N-CA-C	6.41	118.69	109.14
1	B	173	PRO	N-CA-C	6.38	118.48	110.70
1	C	433	ILE	N-CA-C	6.29	117.83	108.46
1	C	173	PRO	N-CA-C	6.15	118.20	110.70
1	A	334	PHE	CA-C-N	6.01	125.72	119.05
1	A	334	PHE	C-N-CA	6.01	125.72	119.05
1	C	206	GLN	N-CA-C	-6.00	101.81	110.40
1	D	585	MET	CA-C-N	-5.99	112.69	119.28
1	D	585	MET	C-N-CA	-5.99	112.69	119.28
1	A	513	ALA	N-CA-C	5.95	118.94	109.24
1	B	513	ALA	N-CA-C	5.93	118.31	109.59
1	D	334	PHE	CA-C-N	5.76	125.45	119.05
1	D	334	PHE	C-N-CA	5.76	125.45	119.05
1	B	471	GLY	N-CA-C	5.66	122.88	115.36
1	A	400	LEU	N-CA-C	5.47	118.48	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	PRO	N-CA-C	5.34	117.22	110.70
1	D	433	ILE	N-CA-C	5.34	116.41	108.46
1	C	471	GLY	N-CA-C	5.15	122.45	115.30
1	D	346	GLU	N-CA-C	5.14	116.57	111.07
1	D	472	ALA	N-CA-C	5.14	117.28	111.11
1	D	157	ALA	N-CA-C	5.12	117.73	110.10
1	A	173	PRO	CA-C-N	-5.04	114.42	119.56
1	A	173	PRO	C-N-CA	-5.04	114.42	119.56

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	3475	0	3509	34	0
1	B	3471	0	3505	45	0
1	C	3452	0	3487	29	0
1	D	3371	0	3418	35	0
2	A	88	0	52	0	0
2	B	88	0	52	2	0
2	C	88	0	52	0	0
2	D	88	0	52	1	0
3	A	53	0	31	4	0
3	B	53	0	31	5	0
3	C	53	0	31	1	0
3	D	53	0	31	4	0
4	D	5	0	0	0	0
5	A	9	0	0	1	0
5	B	8	0	0	0	0
5	C	7	0	0	1	0
All	All	14362	0	14251	145	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 5.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ILE:HA	1:A:611:HIS:C	2.04	0.81
1:B:589:ARG:HH11	1:B:589:ARG:HG3	1.48	0.78
1:D:584:ARG:HB3	1:D:587:ILE:HD12	1.63	0.78
1:A:445:ILE:HG12	5:A:2008:HOH:O	1.84	0.77
1:C:564:VAL:HG12	1:C:610:ILE:HD11	1.68	0.75
1:D:274:GLY:HA2	1:D:275:ALA:HB3	1.69	0.75
1:C:338:GLY:HA2	1:C:353:MET:HE3	1.70	0.73
1:B:221:GLU:O	1:B:222:ASN:HB2	1.89	0.72
1:C:201:ARG:HB2	1:C:201:ARG:HH11	1.56	0.70
1:B:450:ARG:HH12	1:B:479:GLN:NE2	1.91	0.69
1:B:484:SER:HB3	1:B:492:TYR:CE1	2.27	0.69
1:B:581:ILE:HD11	1:B:610:ILE:HD11	1.76	0.68
1:D:337:LYS:HE2	1:D:337:LYS:H	1.58	0.67
1:B:415:ASP:OD2	1:B:422:ARG:NH1	2.29	0.66
1:C:190:THR:HG22	1:C:192:ARG:H	1.59	0.66
1:B:282:THR:HG22	1:B:283:LEU:O	1.96	0.65
1:D:281:THR:HG22	1:D:394:ILE:HB	1.79	0.65
1:D:172:ARG:HH21	3:D:1612:FAD:PA	2.21	0.63
1:B:589:ARG:HH11	1:B:589:ARG:CG	2.12	0.62
1:B:609:ASN:O	1:B:610:ILE:HG13	2.00	0.61
1:C:195:GLN:HG2	1:C:199:LYS:O	2.01	0.61
1:B:430:ARG:H	1:B:433:ILE:HG22	1.65	0.60
1:A:450:ARG:HH12	1:A:479:GLN:HE21	1.48	0.60
1:B:571:LYS:HB3	1:B:597:GLN:HB3	1.82	0.60
1:C:484:SER:HB3	1:C:492:TYR:CE1	2.37	0.60
1:B:267:LEU:HD11	1:B:306:ILE:HG21	1.84	0.59
1:D:458:ALA:HB2	3:D:1612:FAD:H5'2	1.84	0.59
1:D:354:GLU:HG3	1:D:358:ARG:HH22	1.69	0.57
1:D:191:LEU:HD13	1:D:287:ILE:HD11	1.86	0.57
1:D:431:SER:O	1:D:432:ASN:HB2	2.06	0.56
1:A:450:ARG:HH12	1:A:479:GLN:NE2	2.03	0.56
1:B:428:GLN:HG3	1:B:434:TRP:CE2	2.39	0.56
1:A:276:GLU:HB3	1:A:374:VAL:HG21	1.87	0.55
1:A:282:THR:HG22	1:A:283:LEU:O	2.06	0.55
1:A:172:ARG:HH21	3:A:1612:FAD:PA	2.30	0.55
1:D:274:GLY:HA3	1:D:277:VAL:H	1.72	0.55
1:B:172:ARG:HH21	3:B:1612:FAD:PA	2.30	0.55
1:D:138:GLY:O	1:D:143:ALA:HB2	2.08	0.54
1:B:454:HIS:HD2	2:B:700:NAD:O7N	1.90	0.54
1:B:244:LYS:HG3	1:B:250:GLN:HE21	1.74	0.53
1:A:450:ARG:NH1	1:A:479:GLN:NE2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:SER:O	1:D:392:ASP:HB2	2.09	0.52
1:C:479:GLN:HG3	5:C:2006:HOH:O	2.10	0.51
1:B:261:GLY:HA2	1:B:438:ASP:HB2	1.91	0.51
1:B:571:LYS:CB	1:B:597:GLN:HB3	2.41	0.51
1:B:589:ARG:CG	1:B:589:ARG:NH1	2.72	0.51
1:B:164:GLU:HB2	3:B:1612:FAD:N3A	2.26	0.51
1:B:450:ARG:NH1	1:B:479:GLN:NE2	2.59	0.51
1:A:609:ASN:C	1:A:610:ILE:HG13	2.36	0.50
1:B:196:TRP:CH2	2:B:701:NAD:O2A	2.64	0.50
1:C:171:MET:HE3	1:C:201:ARG:HH21	1.74	0.50
1:A:183:ASP:OD1	1:A:183:ASP:N	2.39	0.50
1:A:264:PRO:HB2	1:A:283:LEU:HD13	1.92	0.50
1:C:139:GLY:HA3	1:C:163:SER:HB2	1.92	0.50
1:A:370:GLN:HB3	1:A:382:LYS:O	2.12	0.49
1:C:305:ILE:HD11	1:C:319:LEU:HD12	1.93	0.49
1:B:428:GLN:HG3	1:B:434:TRP:NE1	2.27	0.49
1:D:274:GLY:CA	1:D:275:ALA:HB3	2.40	0.49
1:C:173:PRO:HB2	1:C:174:PRO:HD3	1.95	0.49
1:D:165:ASP:HB2	1:D:166:PRO:HD2	1.95	0.49
1:A:258:ILE:HG23	1:A:260:THR:HG23	1.95	0.49
1:A:192:ARG:NH1	1:A:200:GLU:HG2	2.28	0.49
1:B:569:ARG:O	1:B:570:ASP:HB2	2.12	0.49
1:B:171:MET:O	1:B:203:ILE:HD11	2.12	0.48
1:D:499:ASP:HB3	1:D:502:LEU:HD12	1.94	0.48
1:A:484:SER:HB3	1:A:492:TYR:CE1	2.49	0.48
1:D:245:LEU:HD12	1:D:249:SER:HB2	1.94	0.48
1:A:584:ARG:HB3	1:A:587:ILE:HD12	1.95	0.48
1:B:172:ARG:N	1:B:173:PRO:CD	2.77	0.48
1:D:372:VAL:HG13	1:D:381:ILE:HG23	1.96	0.48
3:A:1612:FAD:C9	3:A:1612:FAD:O2'	2.62	0.47
1:D:482:PHE:CE1	1:D:494:ALA:HB3	2.49	0.47
1:D:606:LYS:HG2	1:D:611:HIS:CE1	2.48	0.47
1:A:244:LYS:HD3	1:A:250:GLN:HE21	1.80	0.47
1:C:335:PRO:O	1:C:366:ASN:HA	2.15	0.47
1:B:484:SER:HB3	1:B:492:TYR:CZ	2.50	0.47
1:C:242:MET:HG3	1:C:252:THR:HG22	1.97	0.47
1:B:512:THR:HG22	1:B:512:THR:O	2.15	0.46
1:B:575:GLY:O	1:B:576:ILE:HG13	2.16	0.46
1:B:496:GLY:HA3	1:B:575:GLY:HA2	1.98	0.46
1:C:458:ALA:HB2	3:C:1612:FAD:H5'2	1.98	0.46
1:D:267:LEU:HD11	1:D:306:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ALA:HB2	3:A:1612:FAD:H5'2	1.97	0.45
1:C:286:LYS:HB2	1:C:286:LYS:HE2	1.70	0.45
1:B:575:GLY:C	1:B:576:ILE:HG13	2.41	0.45
1:D:280:ARG:HB3	1:D:379:LEU:HD11	1.98	0.45
1:A:221:GLU:O	1:A:222:ASN:HB2	2.17	0.45
1:A:431:SER:O	1:A:432:ASN:HB2	2.17	0.44
1:D:458:ALA:CB	3:D:1612:FAD:H5'2	2.45	0.44
1:D:138:GLY:O	1:D:143:ALA:CB	2.66	0.44
1:A:296:ILE:HD13	1:A:393:HIS:CE1	2.52	0.44
1:B:241:ASN:HD21	1:B:432:ASN:HD22	1.65	0.44
1:D:281:THR:HA	1:D:394:ILE:O	2.18	0.44
1:A:268:SER:HA	1:A:271:ASP:HB2	1.99	0.44
1:B:426:GLU:O	1:B:427:LEU:HB2	2.18	0.44
1:B:430:ARG:N	1:B:433:ILE:HG22	2.30	0.44
1:C:430:ARG:HB2	1:C:433:ILE:HG23	1.99	0.44
1:A:450:ARG:NH1	1:A:479:GLN:HE21	2.13	0.44
1:A:455:HIS:HA	3:A:1612:FAD:H3'	2.00	0.43
1:B:172:ARG:HB2	3:B:1612:FAD:O2'	2.18	0.43
1:C:484:SER:HB3	1:C:492:TYR:CZ	2.53	0.43
1:A:484:SER:HB3	1:A:492:TYR:CZ	2.54	0.43
1:C:383:LEU:HD12	1:C:387:ARG:HB2	2.01	0.43
1:D:428:GLN:NE2	1:D:431:SER:HA	2.34	0.43
1:C:154:ASP:OD1	1:C:154:ASP:C	2.61	0.43
1:A:379:LEU:HD13	1:A:394:ILE:HG13	1.99	0.42
1:B:454:HIS:HB3	3:B:1612:FAD:O2	2.18	0.42
1:A:177:LYS:HB2	1:A:177:LYS:HZ3	1.84	0.42
1:A:276:GLU:O	1:A:280:ARG:NH1	2.52	0.42
1:C:270:ILE:HG21	1:C:281:THR:HG21	2.00	0.42
1:C:435:VAL:HG12	1:C:440:ALA:HB2	2.01	0.42
1:D:497:LEU:HD12	1:D:574:VAL:HB	2.02	0.42
1:D:164:GLU:OE2	1:D:232:LYS:HD2	2.20	0.42
1:B:401:GLU:OE2	1:B:402:PRO:HD2	2.19	0.42
1:D:274:GLY:HA2	1:D:275:ALA:CB	2.45	0.42
1:C:302:SER:O	1:C:392:ASP:HB2	2.18	0.42
1:B:379:LEU:HD13	1:B:394:ILE:HG13	2.02	0.42
1:C:164:GLU:HG3	1:C:232:LYS:HB2	2.02	0.42
1:B:173:PRO:HB2	1:B:174:PRO:HD3	2.02	0.42
1:B:458:ALA:HB2	3:B:1612:FAD:H5'2	2.02	0.42
1:C:338:GLY:HA2	1:C:353:MET:CE	2.47	0.42
1:D:244:LYS:HE2	1:D:248:GLY:HA2	2.00	0.42
1:A:610:ILE:CA	1:A:611:HIS:C	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:ASP:HB3	1:C:448:GLY:O	2.20	0.41
1:A:581:ILE:CD1	1:A:610:ILE:HD11	2.50	0.41
1:B:247:ASP:OD1	1:B:247:ASP:C	2.64	0.41
1:D:400:LEU:HD13	2:D:700:NAD:H4D	2.02	0.41
1:B:498:VAL:O	1:B:498:VAL:CG2	2.69	0.41
1:D:482:PHE:CZ	1:D:494:ALA:HB3	2.56	0.41
1:C:353:MET:HE1	1:C:365:PRO:HG3	2.02	0.41
1:C:603:GLU:O	1:C:606:LYS:HB2	2.20	0.41
1:D:172:ARG:N	1:D:173:PRO:CD	2.84	0.41
1:C:170:TYR:CZ	1:C:287:ILE:HG13	2.56	0.41
1:A:446:LYS:HE2	1:A:593:LYS:O	2.21	0.40
1:D:599:GLU:H	1:D:599:GLU:CD	2.30	0.40
1:A:401:GLU:OE1	1:A:401:GLU:HA	2.21	0.40
1:A:578:LEU:HD21	1:A:608:PHE:CE1	2.56	0.40
1:A:408:LYS:HE2	1:A:408:LYS:HB3	1.86	0.40
1:B:132:VAL:O	1:B:253:TYR:HA	2.22	0.40
1:B:570:ASP:HB3	1:B:571:LYS:H	1.68	0.40
1:C:240:ASP:HB3	1:C:242:MET:HE3	2.04	0.40
1:D:221:GLU:O	1:D:222:ASN:HB2	2.21	0.40
1:D:324:ARG:HH11	1:D:324:ARG:HB2	1.86	0.40
1:B:448:GLY:O	1:B:450:ARG:HG3	2.21	0.40
3:D:1612:FAD:H9	3:D:1612:FAD:H1'1	1.83	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	446/511 (87%)	417 (94%)	29 (6%)	0	100	100
1	B	446/511 (87%)	421 (94%)	22 (5%)	3 (1%)	18	44
1	C	442/511 (86%)	416 (94%)	25 (6%)	1 (0%)	43	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	431/511 (84%)	396 (92%)	34 (8%)	1 (0%)	43	70
All	All	1765/2044 (86%)	1650 (94%)	110 (6%)	5 (0%)	36	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	ASN
1	B	275	ALA
1	C	513	ALA
1	D	273	ALA
1	B	285	ARG

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	367/419 (88%)	342 (93%)	25 (7%)	14	39
1	B	366/419 (87%)	346 (94%)	20 (6%)	19	48
1	C	365/419 (87%)	340 (93%)	25 (7%)	14	39
1	D	357/419 (85%)	327 (92%)	30 (8%)	10	29
All	All	1455/1676 (87%)	1355 (93%)	100 (7%)	14	38

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	SER
1	A	177	LYS
1	A	183	ASP
1	A	186	ASN
1	A	189	LYS
1	A	203	ILE
1	A	206	GLN
1	A	212	VAL
1	A	216	ASP

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Mol	Chain	Res	Type
1	A	228	LEU
1	A	263	THR
1	A	266	SER
1	A	268	SER
1	A	270	ILE
1	A	326	LEU
1	A	343	ILE
1	A	375	SER
1	A	405	GLU
1	A	408	LYS
1	A	433	ILE
1	A	446	LYS
1	A	571	LYS
1	A	591	ILE
1	A	602	ASN
1	A	610	ILE
1	B	127	LYS
1	B	177	LYS
1	B	209	SER
1	B	239	ARG
1	B	276	GLU
1	B	295	LYS
1	B	299	GLU
1	B	326	LEU
1	B	358	ARG
1	B	375	SER
1	B	408	LYS
1	B	433	ILE
1	B	446	LYS
1	B	498	VAL
1	B	510	LYS
1	B	564	VAL
1	B	568	LEU
1	B	571	LYS
1	B	587	ILE
1	B	589	ARG
1	C	127	LYS
1	C	132	VAL
1	C	148	ARG
1	C	177	LYS
1	C	187	VAL
1	C	190	THR

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Mol	Chain	Res	Type
1	C	201	ARG
1	C	203	ILE
1	C	212	VAL
1	C	215	GLN
1	C	228	LEU
1	C	263	THR
1	C	268	SER
1	C	277	VAL
1	C	281	THR
1	C	326	LEU
1	C	354	GLU
1	C	375	SER
1	C	400	LEU
1	C	433	ILE
1	C	498	VAL
1	C	510	LYS
1	C	512	THR
1	C	516	ASN
1	C	581	ILE
1	D	183	ASP
1	D	184	ASP
1	D	197	ASN
1	D	215	GLN
1	D	221	GLU
1	D	239	ARG
1	D	241	ASN
1	D	257	LEU
1	D	268	SER
1	D	270	ILE
1	D	278	LYS
1	D	287	ILE
1	D	326	LEU
1	D	333	LEU
1	D	337	LYS
1	D	354	GLU
1	D	372	VAL
1	D	374	VAL
1	D	375	SER
1	D	381	ILE
1	D	389	VAL
1	D	433	ILE
1	D	445	ILE

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Mol	Chain	Res	Type
1	D	463	ARG
1	D	479	GLN
1	D	498	VAL
1	D	571	LYS
1	D	587	ILE
1	D	603	GLU
1	D	610	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	197	ASN
1	A	250	GLN
1	A	366	ASN
1	A	428	GLN
1	A	478	HIS
1	A	479	GLN
1	A	556	GLN
1	B	219	HIS
1	B	250	GLN
1	B	432	ASN
1	B	454	HIS
1	B	457	HIS
1	B	478	HIS
1	B	479	GLN
1	B	516	ASN
1	C	215	GLN
1	C	241	ASN
1	C	332	GLN
1	C	339	ASN
1	C	403	ASN
1	C	432	ASN
1	C	478	HIS
1	C	583	ASN
1	C	597	GLN
1	C	609	ASN
1	D	222	ASN
1	D	428	GLN
1	D	478	HIS
1	D	580	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 ⓘ

13 ligands are modelled in this entry.

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	$\# Z > 2$
2	NAD	A	700	-	46,48,48	2.23	13 (28%)	64,73,73	1.92	14 (21%)
3	FAD	C	1612	-	58,58,58	1.95	16 (27%)	85,89,89	2.03	27 (31%)
2	NAD	B	701	-	46,48,48	2.42	13 (28%)	64,73,73	1.74	12 (18%)
2	NAD	B	700	-	46,48,48	1.97	11 (23%)	64,73,73	1.96	14 (21%)
3	FAD	A	1612	-	58,58,58	2.10	18 (31%)	85,89,89	2.23	28 (32%)
2	NAD	C	700	-	46,48,48	1.91	9 (19%)	64,73,73	1.98	16 (25%)
2	NAD	C	701	-	46,48,48	2.24	13 (28%)	64,73,73	1.73	12 (18%)
2	NAD	D	701	-	46,48,48	2.17	12 (26%)	64,73,73	2.09	15 (23%)
3	FAD	D	1612	-	58,58,58	2.03	17 (29%)	85,89,89	1.92	26 (30%)
2	NAD	A	701	-	46,48,48	2.38	11 (23%)	64,73,73	1.93	17 (26%)
3	FAD	B	1612	-	58,58,58	2.01	19 (32%)	85,89,89	1.99	28 (32%)
2	NAD	D	700	-	46,48,48	2.09	12 (26%)	64,73,73	1.80	13 (20%)
4	SO4	D	1613	-	4,4,4	0.57	0	6,6,6	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	700	-	-	8/30/62/62	0/5/5/5
3	FAD	C	1612	-	-	15/34/50/50	0/6/6/6
2	NAD	B	701	-	-	9/30/62/62	0/5/5/5
2	NAD	B	700	-	-	4/30/62/62	0/5/5/5
3	FAD	A	1612	-	-	10/34/50/50	0/6/6/6
2	NAD	C	700	-	-	4/30/62/62	0/5/5/5
2	NAD	C	701	-	-	10/30/62/62	0/5/5/5
2	NAD	D	701	-	-	8/30/62/62	0/5/5/5
3	FAD	D	1612	-	-	14/34/50/50	0/6/6/6
2	NAD	A	701	-	-	9/30/62/62	0/5/5/5
3	FAD	B	1612	-	-	14/34/50/50	0/6/6/6
2	NAD	D	700	-	-	2/30/62/62	0/5/5/5

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	NAD	C3N-C7N	-7.66	1.39	1.50
2	C	701	NAD	C3N-C7N	-7.65	1.39	1.50
2	A	701	NAD	C2N-N1N	6.93	1.42	1.35
2	B	701	NAD	PN-O3	6.66	1.66	1.59
2	D	700	NAD	C3N-C7N	-6.60	1.40	1.50
2	C	700	NAD	C3N-C7N	-6.57	1.40	1.50
2	B	701	NAD	C3N-C7N	-6.50	1.40	1.50
2	B	700	NAD	C3N-C7N	-6.42	1.41	1.50
2	D	701	NAD	C2N-N1N	6.39	1.42	1.35
2	A	701	NAD	C3N-C7N	-6.29	1.41	1.50
3	A	1612	FAD	C7M-C7	-6.29	1.39	1.51
2	B	701	NAD	C2N-N1N	6.27	1.41	1.35
2	D	701	NAD	C3N-C7N	-6.07	1.41	1.50
2	A	700	NAD	C2N-N1N	5.96	1.41	1.35
3	D	1612	FAD	C8M-C8	-5.94	1.39	1.51
3	C	1612	FAD	C8M-C8	-5.85	1.40	1.51
3	C	1612	FAD	C7M-C7	-5.78	1.40	1.51
2	C	701	NAD	C2N-N1N	5.76	1.41	1.35
2	A	701	NAD	PN-O3	5.76	1.65	1.59
2	D	700	NAD	C2N-N1N	5.70	1.41	1.35
2	A	701	NAD	PA-O3	5.68	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	NAD	PA-O3	5.61	1.65	1.59
2	B	700	NAD	C2N-N1N	5.58	1.41	1.35
3	D	1612	FAD	C7M-C7	-5.43	1.40	1.51
3	B	1612	FAD	C7M-C7	-5.33	1.41	1.51
3	B	1612	FAD	C8M-C8	-5.18	1.41	1.51
3	A	1612	FAD	C8M-C8	-5.08	1.41	1.51
3	D	1612	FAD	C10-N1	4.73	1.42	1.33
2	C	700	NAD	C2N-N1N	4.72	1.40	1.35
2	C	701	NAD	O4D-C1D	4.55	1.46	1.40
3	A	1612	FAD	C5'-C4'	4.55	1.58	1.51
2	B	700	NAD	PN-O3	4.51	1.64	1.59
2	D	701	NAD	O4D-C1D	4.45	1.46	1.40
2	D	701	NAD	PA-O3	4.33	1.64	1.59
2	A	700	NAD	PN-O3	4.27	1.64	1.59
2	B	701	NAD	O4D-C1D	4.20	1.46	1.40
2	B	701	NAD	C2A-N3A	4.18	1.41	1.33
2	C	701	NAD	C2A-N3A	4.16	1.41	1.33
2	C	701	NAD	C2A-N1A	4.15	1.41	1.33
2	D	700	NAD	C2A-N3A	4.13	1.41	1.33
2	A	700	NAD	O4D-C1D	4.12	1.46	1.40
2	D	700	NAD	C2A-N1A	4.10	1.41	1.33
3	B	1612	FAD	P-O3P	4.06	1.63	1.59
2	B	700	NAD	C2A-N1A	4.05	1.41	1.33
2	D	701	NAD	C2A-N1A	4.03	1.41	1.33
2	A	700	NAD	C2A-N1A	3.98	1.41	1.33
2	A	701	NAD	O4D-C1D	3.97	1.46	1.40
2	B	701	NAD	C2A-N1A	3.96	1.41	1.33
2	A	701	NAD	C2A-N3A	3.95	1.40	1.33
2	A	701	NAD	C2A-N1A	3.91	1.40	1.33
2	A	700	NAD	C2A-N3A	3.83	1.40	1.33
2	D	701	NAD	C2A-N3A	3.78	1.40	1.33
3	C	1612	FAD	C10-N1	3.76	1.40	1.33
2	C	700	NAD	C2A-N1A	3.73	1.40	1.33
3	D	1612	FAD	C2A-N3A	3.71	1.40	1.33
2	C	700	NAD	C2A-N3A	3.68	1.40	1.33
3	A	1612	FAD	C10-N1	3.66	1.40	1.33
3	B	1612	FAD	C1'-N10	3.61	1.56	1.47
2	D	700	NAD	PN-O3	3.59	1.63	1.59
3	D	1612	FAD	C2-N1	3.53	1.44	1.36
3	C	1612	FAD	C2A-N3A	3.51	1.40	1.33
3	C	1612	FAD	C2A-N1A	3.50	1.40	1.33
2	C	700	NAD	C6N-N1N	3.50	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1612	FAD	C2A-N1A	3.47	1.40	1.33
3	B	1612	FAD	C2A-N3A	3.46	1.40	1.33
3	A	1612	FAD	C4'-C3'	-3.44	1.47	1.53
3	D	1612	FAD	C2A-N1A	3.44	1.40	1.33
3	D	1612	FAD	C5X-N5	-3.43	1.33	1.39
2	D	700	NAD	O4D-C1D	3.40	1.45	1.40
3	A	1612	FAD	C2A-N3A	3.37	1.39	1.33
3	B	1612	FAD	C10-N1	3.36	1.40	1.33
2	D	701	NAD	C6N-N1N	3.36	1.43	1.35
3	A	1612	FAD	P-O5'	3.36	1.72	1.59
2	C	700	NAD	C5A-C4A	-3.35	1.33	1.39
3	A	1612	FAD	C5A-C4A	-3.34	1.33	1.39
3	B	1612	FAD	C5X-N5	-3.30	1.33	1.39
2	C	701	NAD	PA-O3	3.29	1.63	1.59
3	D	1612	FAD	C5'-C4'	3.27	1.56	1.51
3	C	1612	FAD	P-O5'	3.27	1.72	1.59
2	C	701	NAD	PN-O3	3.26	1.63	1.59
2	D	700	NAD	PA-O3	3.22	1.63	1.59
3	B	1612	FAD	C1'-C2'	3.19	1.57	1.52
2	A	700	NAD	C6N-N1N	3.15	1.42	1.35
2	A	701	NAD	C6N-N1N	3.15	1.42	1.35
2	D	701	NAD	C5A-N7A	-3.15	1.33	1.39
2	D	700	NAD	C6N-N1N	3.13	1.42	1.35
2	C	701	NAD	C5A-N7A	-3.12	1.33	1.39
3	A	1612	FAD	C5A-N7A	-3.10	1.33	1.39
3	B	1612	FAD	C2'-C3'	3.06	1.58	1.53
3	A	1612	FAD	C8A-N9A	-3.04	1.32	1.37
2	C	701	NAD	C6N-N1N	3.01	1.42	1.35
2	B	700	NAD	C2A-N3A	2.99	1.39	1.33
3	A	1612	FAD	C9A-N10	-2.98	1.36	1.41
2	A	701	NAD	C5A-N7A	-2.97	1.33	1.39
3	C	1612	FAD	C5A-N7A	-2.97	1.33	1.39
2	A	700	NAD	C5A-C4A	-2.92	1.33	1.39
3	C	1612	FAD	C9A-N10	-2.92	1.36	1.41
2	B	700	NAD	C6N-N1N	2.90	1.41	1.35
2	C	700	NAD	C5A-N7A	-2.90	1.33	1.39
3	A	1612	FAD	C5A-C6A	-2.88	1.33	1.41
2	B	701	NAD	C5A-N7A	-2.87	1.33	1.39
2	B	701	NAD	C1B-N9A	2.86	1.54	1.46
3	D	1612	FAD	C5A-N7A	-2.85	1.33	1.39
3	C	1612	FAD	C5'-C4'	2.80	1.55	1.51
3	B	1612	FAD	C5A-N7A	-2.80	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1612	FAD	C2A-N1A	2.78	1.38	1.33
3	A	1612	FAD	C5X-N5	-2.78	1.34	1.39
3	D	1612	FAD	C5A-C4A	-2.76	1.34	1.39
2	D	701	NAD	C5A-C6A	-2.71	1.33	1.41
3	B	1612	FAD	C5A-C4A	-2.69	1.34	1.39
3	C	1612	FAD	C4'-C3'	-2.68	1.48	1.53
3	D	1612	FAD	C1'-N10	2.67	1.54	1.47
2	B	700	NAD	PA-O3	2.63	1.62	1.59
3	B	1612	FAD	C5'-C4'	2.62	1.55	1.51
2	A	701	NAD	C5A-C6A	-2.60	1.33	1.41
3	C	1612	FAD	C1'-N10	2.59	1.54	1.47
2	D	700	NAD	C5A-N7A	-2.59	1.34	1.39
2	B	701	NAD	C6N-N1N	2.56	1.41	1.35
3	A	1612	FAD	C2-N1	2.54	1.42	1.36
2	B	700	NAD	C5A-C4A	-2.53	1.34	1.39
2	C	700	NAD	C8A-N9A	-2.51	1.33	1.37
3	C	1612	FAD	C8A-N9A	-2.50	1.33	1.37
3	D	1612	FAD	C1'-C2'	2.49	1.56	1.52
3	D	1612	FAD	C5A-C6A	-2.44	1.34	1.41
3	B	1612	FAD	C8A-N9A	-2.38	1.33	1.37
2	C	701	NAD	C5A-C6A	-2.37	1.34	1.41
3	B	1612	FAD	P-O5'	2.36	1.68	1.59
3	A	1612	FAD	C1'-N10	2.33	1.53	1.47
3	B	1612	FAD	C5A-C6A	-2.33	1.34	1.41
2	D	701	NAD	PN-O3	2.33	1.62	1.59
2	A	701	NAD	C5A-C4A	-2.32	1.34	1.39
2	B	701	NAD	C5A-C4A	-2.32	1.34	1.39
2	C	700	NAD	C5A-C6A	-2.32	1.34	1.41
3	D	1612	FAD	PA-O3P	2.32	1.62	1.59
2	B	700	NAD	C8A-N9A	-2.31	1.33	1.37
3	A	1612	FAD	P-O3P	2.31	1.62	1.59
2	D	701	NAD	C5A-C4A	-2.29	1.35	1.39
2	A	700	NAD	C5A-N7A	-2.29	1.34	1.39
3	C	1612	FAD	C5A-C6A	-2.28	1.34	1.41
3	D	1612	FAD	C8A-N9A	-2.26	1.33	1.37
2	A	700	NAD	C4A-N9A	-2.25	1.33	1.37
2	C	701	NAD	PA-O5B	2.23	1.68	1.59
3	C	1612	FAD	C5A-C4A	-2.20	1.35	1.39
3	B	1612	FAD	C9A-N10	-2.20	1.37	1.41
2	D	700	NAD	C8A-N9A	-2.18	1.33	1.37
2	B	700	NAD	C5A-N7A	-2.17	1.35	1.39
3	A	1612	FAD	PA-O3P	2.17	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	NAD	O4B-C4B	-2.15	1.40	1.45
3	D	1612	FAD	C4-N3	2.13	1.42	1.38
3	B	1612	FAD	PA-O3P	2.13	1.61	1.59
3	C	1612	FAD	C4X-N5	2.12	1.35	1.30
2	D	700	NAD	C5A-C4A	-2.11	1.35	1.39
2	A	700	NAD	C5A-C6A	-2.09	1.35	1.41
2	C	701	NAD	C1B-N9A	2.09	1.52	1.46
2	C	701	NAD	C5A-C4A	-2.09	1.35	1.39
2	B	701	NAD	C5A-C6A	-2.09	1.35	1.41
2	B	700	NAD	O2B-C2B	2.07	1.48	1.43
3	B	1612	FAD	C2-N1	2.06	1.41	1.36
2	A	700	NAD	O4B-C1B	2.06	1.46	1.42
2	B	701	NAD	C8A-N9A	-2.04	1.34	1.37
3	D	1612	FAD	C4A-N9A	-2.03	1.33	1.37
3	C	1612	FAD	PA-O3P	2.02	1.61	1.59
2	D	701	NAD	C8A-N9A	-2.00	1.34	1.37
2	D	700	NAD	C5A-C6A	-2.00	1.35	1.41

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	NAD	N3A-C2A-N1A	-7.45	117.31	128.58
2	A	701	NAD	N3A-C2A-N1A	-7.40	117.38	128.58
2	D	700	NAD	N3A-C2A-N1A	-7.23	117.64	128.58
2	B	700	NAD	N3A-C2A-N1A	-7.18	117.72	128.58
2	D	701	NAD	N3A-C2A-N1A	-7.13	117.78	128.58
2	B	701	NAD	N3A-C2A-N1A	-7.10	117.84	128.58
2	C	701	NAD	N3A-C2A-N1A	-6.98	118.02	128.58
2	A	700	NAD	N3A-C2A-N1A	-6.91	118.12	128.58
3	A	1612	FAD	N3A-C2A-N1A	-6.75	118.36	128.58
3	C	1612	FAD	N3A-C2A-N1A	-6.62	118.56	128.58
3	B	1612	FAD	N3A-C2A-N1A	-6.58	118.62	128.58
3	D	1612	FAD	N3A-C2A-N1A	-6.46	118.80	128.58
3	B	1612	FAD	O4B-C1B-N9A	-5.67	97.20	108.09
2	A	700	NAD	N9A-C8A-N7A	-5.46	106.19	113.94
2	C	700	NAD	N9A-C8A-N7A	-5.45	106.20	113.94
2	B	700	NAD	N9A-C8A-N7A	-5.34	106.36	113.94
3	A	1612	FAD	C5A-C4A-N3A	-5.31	119.41	126.72
3	C	1612	FAD	C5'-C4'-C3'	-5.22	102.38	112.22
3	A	1612	FAD	C1'-C2'-C3'	4.99	123.20	109.66
2	D	701	NAD	O2A-PA-O3	4.96	120.69	107.27
3	A	1612	FAD	O3'-C3'-C4'	-4.93	97.73	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1612	FAD	N9A-C8A-N7A	-4.89	107.00	113.94
3	C	1612	FAD	C5A-C4A-N3A	-4.82	120.07	126.72
3	D	1612	FAD	C5A-C4A-N3A	-4.81	120.09	126.72
2	C	701	NAD	C5A-C4A-N3A	-4.80	120.11	126.72
2	B	701	NAD	C5A-C4A-N3A	-4.76	120.16	126.72
2	D	701	NAD	O5B-PA-O1A	-4.73	90.20	108.94
3	B	1612	FAD	C5A-C4A-N3A	-4.64	120.33	126.72
2	D	701	NAD	O2A-PA-O5B	-4.62	86.64	107.57
3	B	1612	FAD	C1'-C2'-C3'	4.58	122.07	109.66
3	A	1612	FAD	O4B-C1B-N9A	-4.49	99.47	108.09
2	A	700	NAD	C4D-O4D-C1D	-4.38	105.92	109.92
2	D	701	NAD	C5A-C4A-N3A	-4.31	120.79	126.72
2	B	700	NAD	C4A-N9A-C8A	4.28	110.23	105.74
2	D	700	NAD	N9A-C8A-N7A	-4.25	107.91	113.94
3	D	1612	FAD	C4-N3-C2	-4.18	118.22	125.64
3	A	1612	FAD	C5'-C4'-C3'	-4.17	104.36	112.22
2	A	701	NAD	C5A-C4A-N3A	-4.16	120.99	126.72
2	D	700	NAD	C5A-C4A-N3A	-4.15	121.00	126.72
3	C	1612	FAD	C1'-C2'-C3'	4.11	120.81	109.66
2	A	701	NAD	C6N-N1N-C2N	-4.08	118.41	121.88
2	B	700	NAD	C4A-N9A-C1B	-4.06	117.13	126.63
3	C	1612	FAD	C4-N3-C2	-4.05	118.45	125.64
2	A	700	NAD	C4A-N9A-C8A	4.03	109.97	105.74
2	C	700	NAD	C5A-C4A-N3A	-3.99	121.22	126.72
3	B	1612	FAD	N9A-C8A-N7A	-3.96	108.31	113.94
3	D	1612	FAD	N9A-C8A-N7A	-3.91	108.39	113.94
3	A	1612	FAD	C4-N3-C2	-3.90	118.72	125.64
2	C	700	NAD	C5A-N7A-C8A	3.87	109.53	103.45
2	C	701	NAD	C6N-N1N-C2N	-3.80	118.64	121.88
2	B	701	NAD	N9A-C8A-N7A	-3.79	108.56	113.94
3	D	1612	FAD	C1'-C2'-C3'	3.79	119.93	109.66
2	D	701	NAD	N9A-C8A-N7A	-3.71	108.67	113.94
3	A	1612	FAD	C5A-N7A-C8A	3.68	109.23	103.45
3	A	1612	FAD	O5'-C5'-C4'	3.65	119.11	109.36
3	C	1612	FAD	N9A-C8A-N7A	-3.61	108.82	113.94
2	D	701	NAD	C1B-N9A-C8A	-3.59	119.12	127.09
2	A	701	NAD	N9A-C8A-N7A	-3.59	108.84	113.94
2	C	700	NAD	C4A-N9A-C8A	3.56	109.47	105.74
2	B	700	NAD	C5A-N7A-C8A	3.55	109.04	103.45
3	C	1612	FAD	O4B-C1B-C2B	-3.50	99.13	106.62
2	A	701	NAD	C1B-N9A-C8A	-3.49	119.35	127.09
3	A	1612	FAD	C4-C4X-C10	3.49	122.91	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1612	FAD	C2A-N3A-C4A	3.48	120.34	111.83
2	C	700	NAD	C2A-N3A-C4A	3.46	120.28	111.83
2	B	701	NAD	C2A-N3A-C4A	3.45	120.26	111.83
2	A	700	NAD	C5A-N7A-C8A	3.45	108.87	103.45
2	D	701	NAD	C6N-N1N-C2N	-3.44	118.95	121.88
2	B	700	NAD	C5A-C4A-N3A	-3.42	122.01	126.72
2	C	701	NAD	C2A-N3A-C4A	3.40	120.13	111.83
2	A	700	NAD	C5A-C4A-N3A	-3.39	122.04	126.72
2	D	700	NAD	C2A-N3A-C4A	3.37	120.07	111.83
3	A	1612	FAD	C4'-C3'-C2'	3.34	119.13	113.57
2	A	701	NAD	C2A-N3A-C4A	3.32	119.95	111.83
3	D	1612	FAD	C2A-N3A-C4A	3.30	119.88	111.83
3	B	1612	FAD	C2A-N3A-C4A	3.29	119.86	111.83
3	C	1612	FAD	C10-C4X-N5	-3.26	118.16	124.81
3	C	1612	FAD	C2A-N3A-C4A	3.25	119.76	111.83
3	D	1612	FAD	C4-C4X-C10	3.25	122.50	116.93
2	C	701	NAD	N9A-C8A-N7A	-3.24	109.33	113.94
2	B	700	NAD	C2A-N3A-C4A	3.24	119.75	111.83
2	B	701	NAD	C5A-N7A-C8A	3.22	108.51	103.45
3	C	1612	FAD	C4X-C10-N10	3.17	121.02	116.48
2	D	701	NAD	C2A-N3A-C4A	3.16	119.56	111.83
2	D	700	NAD	C5A-N7A-C8A	3.14	108.38	103.45
2	A	700	NAD	C2A-N3A-C4A	3.14	119.50	111.83
3	C	1612	FAD	C4A-C5A-N7A	-3.11	107.02	110.58
3	C	1612	FAD	C4X-C10-N1	-3.10	116.99	124.59
3	A	1612	FAD	N3A-C4A-N9A	3.10	132.44	127.17
3	C	1612	FAD	C4X-C4-N3	3.06	121.05	113.25
3	D	1612	FAD	O2'-C2'-C3'	-3.06	102.10	109.25
3	A	1612	FAD	C4X-C10-N10	3.05	120.84	116.48
3	A	1612	FAD	C4A-C5A-N7A	-3.04	107.11	110.58
3	D	1612	FAD	C4X-C10-N1	-3.03	117.16	124.59
2	A	701	NAD	C5A-C6A-N6A	-3.02	115.80	123.29
3	A	1612	FAD	C4X-C10-N1	-3.02	117.20	124.59
3	B	1612	FAD	C5X-C9A-N10	3.01	120.69	117.97
2	A	700	NAD	C4A-N9A-C1B	-3.00	119.61	126.63
2	C	701	NAD	C5A-C6A-N6A	-3.00	115.85	123.29
3	C	1612	FAD	C5A-N7A-C8A	3.00	108.16	103.45
3	B	1612	FAD	C5'-C4'-C3'	-2.99	106.57	112.22
2	B	701	NAD	C6N-N1N-C2N	-2.98	119.34	121.88
2	D	701	NAD	C5A-C6A-N6A	-2.98	115.90	123.29
3	D	1612	FAD	C4X-C4-N3	2.97	120.80	113.25
3	B	1612	FAD	C5A-N7A-C8A	2.96	108.10	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAD	C4B-O4B-C1B	-2.96	102.94	109.47
3	D	1612	FAD	C5A-N7A-C8A	2.92	108.04	103.45
2	D	700	NAD	C6N-N1N-C2N	-2.92	119.39	121.88
3	D	1612	FAD	C9A-C5X-N5	-2.91	119.37	122.45
3	A	1612	FAD	C5A-C6A-N6A	-2.90	116.11	123.29
3	B	1612	FAD	O4B-C1B-C2B	-2.88	100.44	106.62
3	A	1612	FAD	C6A-C5A-C4A	2.87	121.10	117.18
2	B	701	NAD	C4A-C5A-N7A	-2.87	107.30	110.58
3	A	1612	FAD	C10-C4X-N5	-2.84	119.01	124.81
2	C	701	NAD	N3A-C4A-N9A	2.83	131.98	127.17
2	D	701	NAD	C6A-C5A-C4A	2.82	121.03	117.18
2	C	700	NAD	C4A-C5A-N7A	-2.81	107.36	110.58
3	B	1612	FAD	C5A-C6A-N6A	-2.81	116.33	123.29
3	C	1612	FAD	C6A-C5A-C4A	2.78	120.97	117.18
2	D	701	NAD	N3A-C4A-N9A	2.77	131.88	127.17
2	D	701	NAD	C4A-N9A-C1B	2.77	133.12	126.63
3	C	1612	FAD	C5A-C4A-N9A	2.76	108.82	105.81
2	A	701	NAD	O4B-C1B-C2B	-2.75	100.74	106.62
3	D	1612	FAD	C4A-C5A-N7A	-2.73	107.46	110.58
2	A	700	NAD	C5A-C6A-N6A	-2.73	116.54	123.29
2	D	701	NAD	C5A-N7A-C8A	2.72	107.73	103.45
2	A	701	NAD	N3A-C4A-N9A	2.71	131.78	127.17
3	B	1612	FAD	N3A-C4A-N9A	2.71	131.77	127.17
2	C	701	NAD	C6A-C5A-C4A	2.69	120.84	117.18
2	B	701	NAD	C6A-C5A-C4A	2.68	120.84	117.18
2	D	700	NAD	C4A-N9A-C8A	2.68	108.55	105.74
3	D	1612	FAD	O4B-C1B-C2B	-2.67	100.90	106.62
2	C	701	NAD	C5A-N7A-C8A	2.67	107.64	103.45
3	B	1612	FAD	C4-N3-C2	-2.66	120.91	125.64
2	C	700	NAD	C5A-C6A-N6A	-2.66	116.70	123.29
2	B	700	NAD	C4D-O4D-C1D	-2.65	107.50	109.92
2	A	701	NAD	C4A-N9A-C1B	2.65	132.83	126.63
3	A	1612	FAD	C4A-N9A-C8A	2.64	108.51	105.74
2	D	700	NAD	C5A-C6A-N6A	-2.62	116.79	123.29
2	C	700	NAD	C4A-N9A-C1B	-2.62	120.50	126.63
2	C	700	NAD	C4D-O4D-C1D	-2.62	107.53	109.92
2	B	700	NAD	C5A-C6A-N6A	-2.61	116.82	123.29
3	D	1612	FAD	C6A-C5A-C4A	2.61	120.74	117.18
3	C	1612	FAD	O3'-C3'-C2'	2.61	114.85	108.93
2	B	700	NAD	C4A-C5A-N7A	-2.60	107.61	110.58
2	D	700	NAD	C4A-C5A-N7A	-2.60	107.61	110.58
3	B	1612	FAD	C4X-C10-N10	2.59	120.19	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1612	FAD	C4X-C4-N3	2.58	119.83	113.25
2	B	700	NAD	C6N-N1N-C2N	-2.55	119.71	121.88
3	D	1612	FAD	C5A-C4A-N9A	2.53	108.57	105.81
3	B	1612	FAD	C6A-C5A-C4A	2.53	120.63	117.18
3	D	1612	FAD	O4-C4-C4X	-2.52	119.87	126.53
2	D	700	NAD	N3A-C4A-N9A	2.52	131.45	127.17
3	D	1612	FAD	C5A-C6A-N6A	-2.52	117.05	123.29
2	B	700	NAD	C1B-N9A-C8A	2.50	132.63	127.09
3	D	1612	FAD	C10-C4X-N5	-2.50	119.71	124.81
2	B	701	NAD	N3A-C4A-N9A	2.49	131.41	127.17
3	D	1612	FAD	C6-C5X-C9A	2.49	122.47	119.05
2	A	701	NAD	C5A-N7A-C8A	2.48	107.35	103.45
3	B	1612	FAD	C9A-C5X-N5	-2.47	119.83	122.45
2	C	700	NAD	N3A-C4A-N9A	2.46	131.36	127.17
3	B	1612	FAD	C4A-C5A-N7A	-2.46	107.78	110.58
3	D	1612	FAD	N3A-C4A-N9A	2.45	131.33	127.17
3	B	1612	FAD	C4'-C3'-C2'	2.45	117.65	113.57
2	A	700	NAD	C4A-C5A-N7A	-2.45	107.78	110.58
2	D	700	NAD	C4B-O4B-C1B	-2.44	104.08	109.47
2	B	701	NAD	C5A-C6A-N6A	-2.43	117.26	123.29
2	A	701	NAD	O7N-C7N-C3N	2.43	122.56	119.60
3	C	1612	FAD	O4-C4-N3	-2.41	115.58	120.11
3	D	1612	FAD	C5X-C9A-N10	2.40	120.14	117.97
2	B	701	NAD	C5A-C4A-N9A	2.40	108.43	105.81
2	A	701	NAD	C3N-C7N-N7N	-2.40	114.79	117.74
2	A	701	NAD	C6A-C5A-C4A	2.39	120.44	117.18
3	B	1612	FAD	C10-N1-C2	2.39	122.02	116.85
2	B	700	NAD	N3A-C4A-N9A	2.39	131.22	127.17
3	D	1612	FAD	O4B-C1B-N9A	-2.37	103.54	108.09
2	C	701	NAD	C2N-C3N-C4N	2.35	120.99	118.26
3	B	1612	FAD	C10-C4X-N5	-2.35	120.02	124.81
3	B	1612	FAD	C4X-C4-N3	2.34	119.22	113.25
3	D	1612	FAD	C5X-N5-C4X	2.34	121.88	118.09
3	A	1612	FAD	C9A-C5X-N5	-2.34	119.97	122.45
3	C	1612	FAD	C4-C4X-C10	2.33	120.92	116.93
3	B	1612	FAD	C4X-C10-N1	-2.32	118.89	124.59
3	B	1612	FAD	O3'-C3'-C2'	2.32	114.20	108.93
3	C	1612	FAD	N3A-C4A-N9A	2.32	131.10	127.17
2	C	700	NAD	C3N-C7N-N7N	-2.31	114.89	117.74
3	A	1612	FAD	C6-C5X-C9A	2.28	122.18	119.05
2	D	701	NAD	O2A-PA-O1A	2.26	122.95	112.44
2	A	700	NAD	C4B-O4B-C1B	-2.25	104.50	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	NAD	O2N-PN-O3	2.25	113.35	107.27
3	B	1612	FAD	C4-C4X-C10	2.25	120.78	116.93
2	C	700	NAD	C6N-N1N-C2N	-2.23	119.98	121.88
3	B	1612	FAD	O4-C4-C4X	-2.23	120.65	126.53
2	A	700	NAD	O2A-PA-O3	2.23	113.30	107.27
2	A	700	NAD	O2N-PN-O1N	2.22	122.75	112.44
3	C	1612	FAD	O5'-C5'-C4'	2.19	115.22	109.36
3	B	1612	FAD	C9A-N10-C10	-2.16	117.45	120.75
2	C	701	NAD	C3N-C7N-N7N	-2.16	115.08	117.74
3	D	1612	FAD	C10-N1-C2	2.14	121.49	116.85
3	C	1612	FAD	C5A-C6A-N6A	-2.14	118.00	123.29
3	B	1612	FAD	O3B-C3B-C4B	-2.14	104.95	111.08
3	A	1612	FAD	C5A-C4A-N9A	2.14	108.14	105.81
2	A	700	NAD	N3A-C4A-N9A	2.13	130.78	127.17
3	C	1612	FAD	C9A-C5X-N5	-2.12	120.20	122.45
2	A	701	NAD	C5D-C4D-C3D	-2.12	107.59	115.21
2	A	701	NAD	C2B-C1B-N9A	2.10	118.52	113.30
3	C	1612	FAD	C10-N1-C2	2.10	121.39	116.85
3	C	1612	FAD	O2P-P-O3P	-2.09	101.62	107.27
3	A	1612	FAD	C5A-C6A-N1A	2.09	122.82	117.51
2	C	700	NAD	O2A-PA-O3	2.08	112.88	107.27
2	C	700	NAD	C5A-C6A-N1A	2.07	122.77	117.51
3	A	1612	FAD	C5X-C9A-N10	2.07	119.84	117.97
2	C	701	NAD	C4A-C5A-N7A	-2.07	108.22	110.58
2	B	701	NAD	O4B-C1B-N9A	2.06	112.04	108.09
3	A	1612	FAD	O4-C4-C4X	-2.05	121.12	126.53
2	D	700	NAD	C6A-C5A-C4A	2.05	119.98	117.18
3	D	1612	FAD	C5A-C6A-N1A	2.05	122.72	117.51
3	B	1612	FAD	C4A-N9A-C8A	2.04	107.88	105.74
3	C	1612	FAD	O3'-C3'-C4'	-2.03	104.32	108.93
2	C	700	NAD	O2N-PN-O1N	2.03	121.87	112.44
3	C	1612	FAD	C5X-C9A-N10	2.01	119.78	117.97
2	D	700	NAD	C5B-C4B-C3B	-2.01	107.99	115.21

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	NAD	C5B-O5B-PA-O1A
2	A	700	NAD	C5B-O5B-PA-O2A
2	A	700	NAD	C5B-O5B-PA-O3
2	A	701	NAD	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	A	701	NAD	C3D-C4D-C5D-O5D
2	B	700	NAD	C5B-O5B-PA-O2A
2	B	700	NAD	C5B-O5B-PA-O3
2	B	701	NAD	C5B-O5B-PA-O1A
2	B	701	NAD	C5B-O5B-PA-O3
2	B	701	NAD	C5D-O5D-PN-O1N
2	C	700	NAD	C5B-O5B-PA-O2A
2	C	700	NAD	C5B-O5B-PA-O3
2	C	701	NAD	C5D-O5D-PN-O3
2	C	701	NAD	C5D-O5D-PN-O1N
2	C	701	NAD	C5D-O5D-PN-O2N
2	D	701	NAD	PA-O3-PN-O5D
3	A	1612	FAD	C1'-C2'-C3'-O3'
3	A	1612	FAD	C1'-C2'-C3'-C4'
3	A	1612	FAD	O2'-C2'-C3'-O3'
3	A	1612	FAD	O2'-C2'-C3'-C4'
3	A	1612	FAD	C5'-O5'-P-O1P
3	A	1612	FAD	C5'-O5'-P-O3P
3	B	1612	FAD	C1'-C2'-C3'-O3'
3	B	1612	FAD	C1'-C2'-C3'-C4'
3	B	1612	FAD	C5'-O5'-P-O1P
3	B	1612	FAD	C5'-O5'-P-O2P
3	B	1612	FAD	C5'-O5'-P-O3P
3	B	1612	FAD	PA-O3P-P-O5'
3	C	1612	FAD	C1'-C2'-C3'-O3'
3	C	1612	FAD	C1'-C2'-C3'-C4'
3	C	1612	FAD	C5'-O5'-P-O1P
3	C	1612	FAD	C5'-O5'-P-O2P
3	C	1612	FAD	C5'-O5'-P-O3P
3	D	1612	FAD	C5B-O5B-PA-O3P
3	D	1612	FAD	N10-C1'-C2'-O2'
3	D	1612	FAD	N10-C1'-C2'-C3'
3	D	1612	FAD	C2'-C3'-C4'-O4'
3	D	1612	FAD	C2'-C3'-C4'-C5'
3	D	1612	FAD	O3'-C3'-C4'-O4'
3	D	1612	FAD	O3'-C3'-C4'-C5'
3	D	1612	FAD	C5'-O5'-P-O1P
3	D	1612	FAD	C5'-O5'-P-O2P
3	D	1612	FAD	C5'-O5'-P-O3P
3	B	1612	FAD	C2'-C3'-C4'-O4'
2	A	700	NAD	C3B-C4B-C5B-O5B
2	A	700	NAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	A	701	NAD	C3B-C4B-C5B-O5B
2	C	701	NAD	O4B-C4B-C5B-O5B
3	B	1612	FAD	C2'-C3'-C4'-C5'
3	C	1612	FAD	C2'-C3'-C4'-O4'
2	A	701	NAD	O4B-C4B-C5B-O5B
3	C	1612	FAD	C2'-C3'-C4'-C5'
2	B	701	NAD	O4D-C4D-C5D-O5D
3	C	1612	FAD	O2'-C2'-C3'-O3'
2	B	701	NAD	C3D-C4D-C5D-O5D
2	B	701	NAD	PA-O3-PN-O1N
2	D	701	NAD	PN-O3-PA-O1A
2	A	700	NAD	PN-O3-PA-O5B
3	A	1612	FAD	PA-O3P-P-O5'
3	C	1612	FAD	PA-O3P-P-O5'
3	D	1612	FAD	PA-O3P-P-O5'
3	C	1612	FAD	O2'-C2'-C3'-C4'
3	C	1612	FAD	C2B-C1B-N9A-C8A
2	C	700	NAD	PA-O3-PN-O2N
2	C	701	NAD	PA-O3-PN-O1N
3	C	1612	FAD	P-O3P-PA-O1A
3	B	1612	FAD	N10-C1'-C2'-O2'
2	B	700	NAD	C3B-C4B-C5B-O5B
2	C	701	NAD	C2B-C1B-N9A-C8A
2	D	701	NAD	O4B-C4B-C5B-O5B
2	A	701	NAD	C5B-O5B-PA-O1A
2	D	700	NAD	C5B-O5B-PA-O1A
2	D	701	NAD	C5D-O5D-PN-O1N
3	A	1612	FAD	C5'-O5'-P-O2P
3	B	1612	FAD	O3'-C3'-C4'-C5'
2	B	701	NAD	PA-O3-PN-O2N
3	B	1612	FAD	O3'-C3'-C4'-O4'
2	D	701	NAD	C2B-C1B-N9A-C8A
2	C	701	NAD	O4D-C4D-C5D-O5D
2	D	701	NAD	O4D-C4D-C5D-O5D
2	D	701	NAD	C2B-C1B-N9A-C4A
2	D	701	NAD	O4B-C1B-N9A-C8A
2	C	701	NAD	C3B-C4B-C5B-O5B
2	A	700	NAD	PA-O3-PN-O2N
2	C	700	NAD	PA-O3-PN-O1N
2	A	701	NAD	PN-O3-PA-O5B
2	A	700	NAD	O4D-C4D-C5D-O5D
2	A	701	NAD	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
3	B	1612	FAD	O2'-C2'-C3'-O3'
2	C	701	NAD	C3D-C4D-C5D-O5D
2	B	701	NAD	C2B-C1B-N9A-C8A
2	B	700	NAD	PA-O3-PN-O1N
2	D	700	NAD	PA-O3-PN-O2N
2	A	701	NAD	O4B-C1B-N9A-C8A
3	C	1612	FAD	O4B-C4B-C5B-O5B
3	C	1612	FAD	O3'-C3'-C4'-C5'
3	A	1612	FAD	C2B-C1B-N9A-C8A
3	D	1612	FAD	C2B-C1B-N9A-C8A
2	A	701	NAD	PN-O3-PA-O2A
2	C	701	NAD	PA-O3-PN-O2N
3	A	1612	FAD	P-O3P-PA-O2A
3	B	1612	FAD	P-O3P-PA-O1A
3	B	1612	FAD	P-O3P-PA-O2A
3	C	1612	FAD	P-O3P-PA-O2A
3	D	1612	FAD	P-O3P-PA-O1A
3	D	1612	FAD	P-O3P-PA-O2A
2	B	701	NAD	O4B-C4B-C5B-O5B

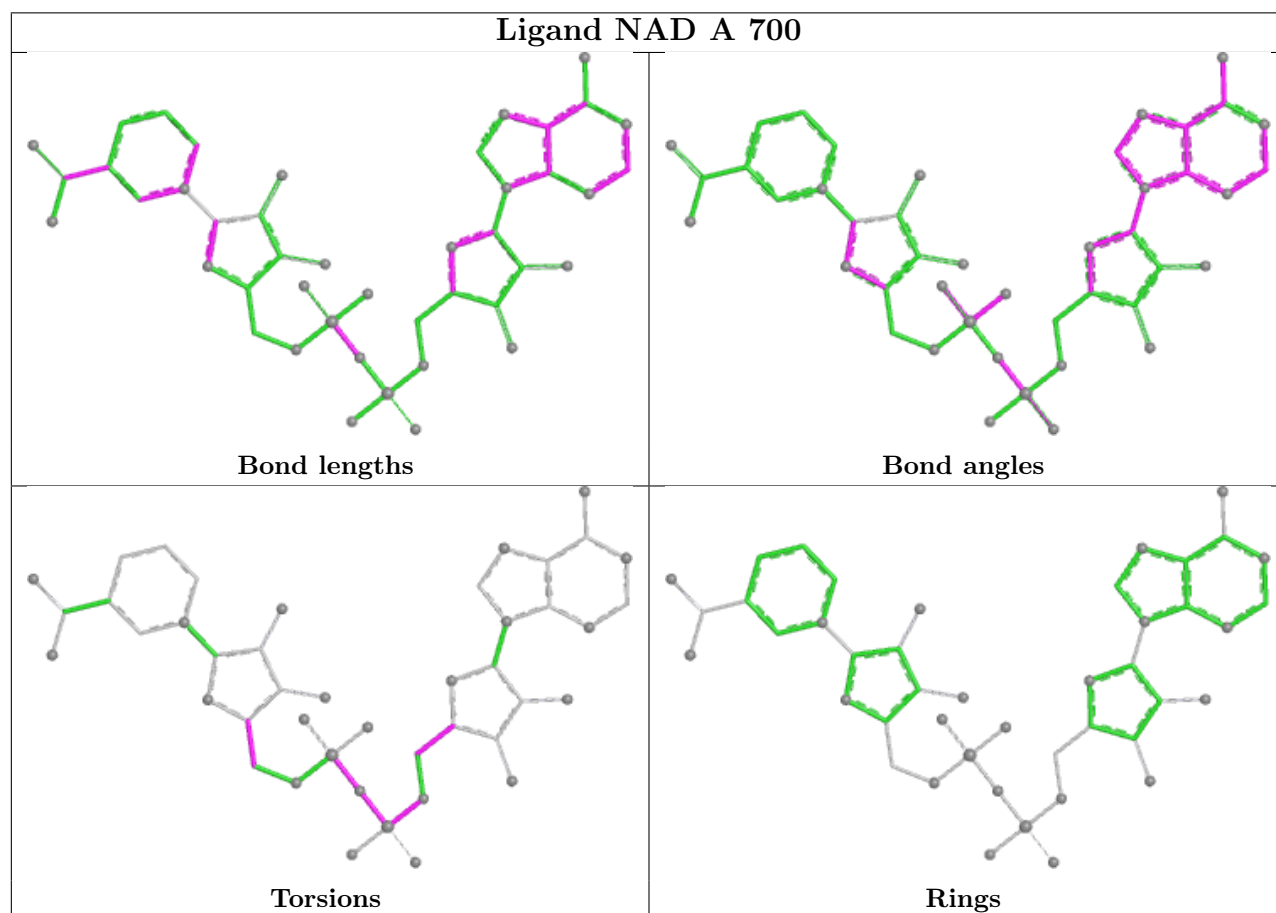
There are no ring outliers.

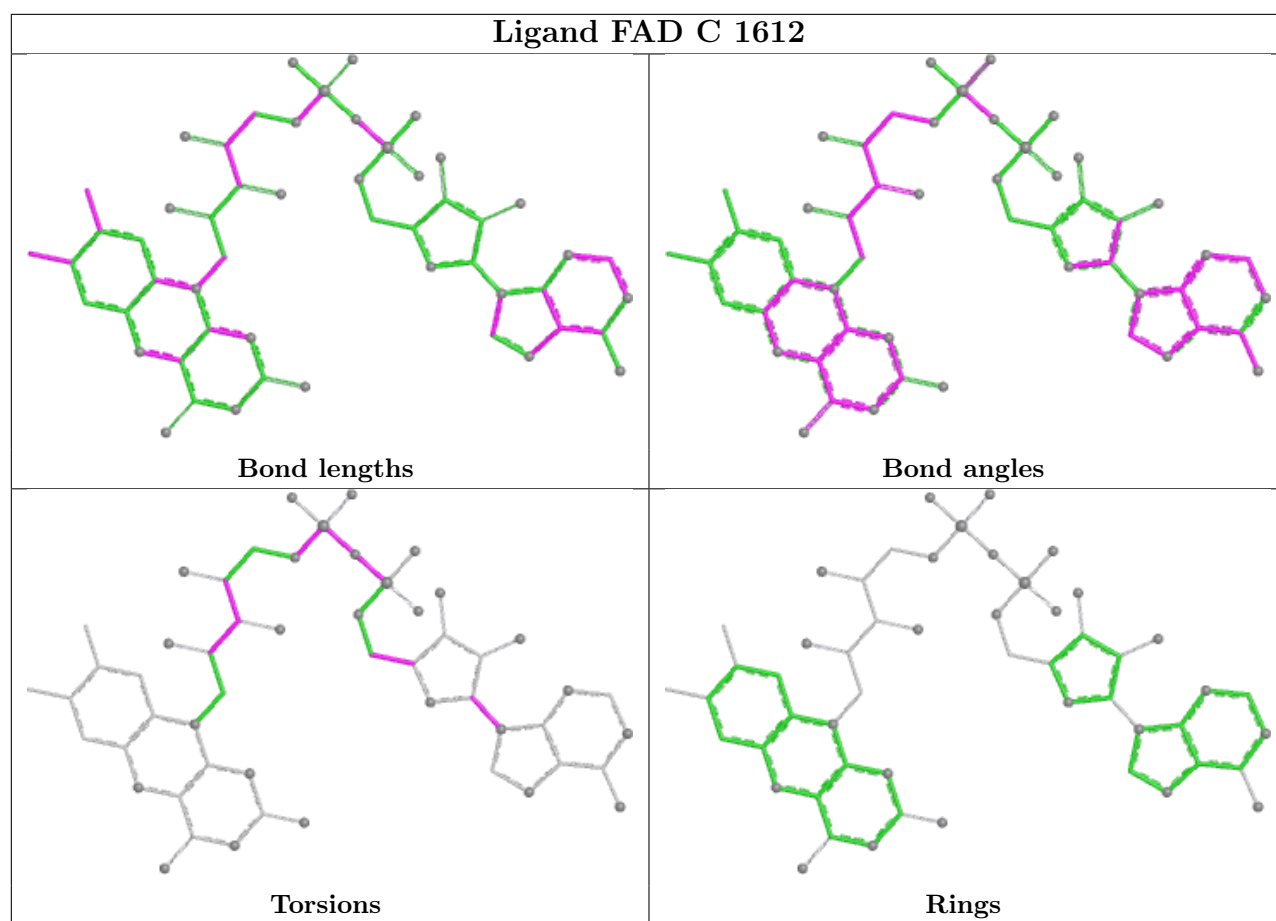
7 monomers are involved in 17 short contacts:

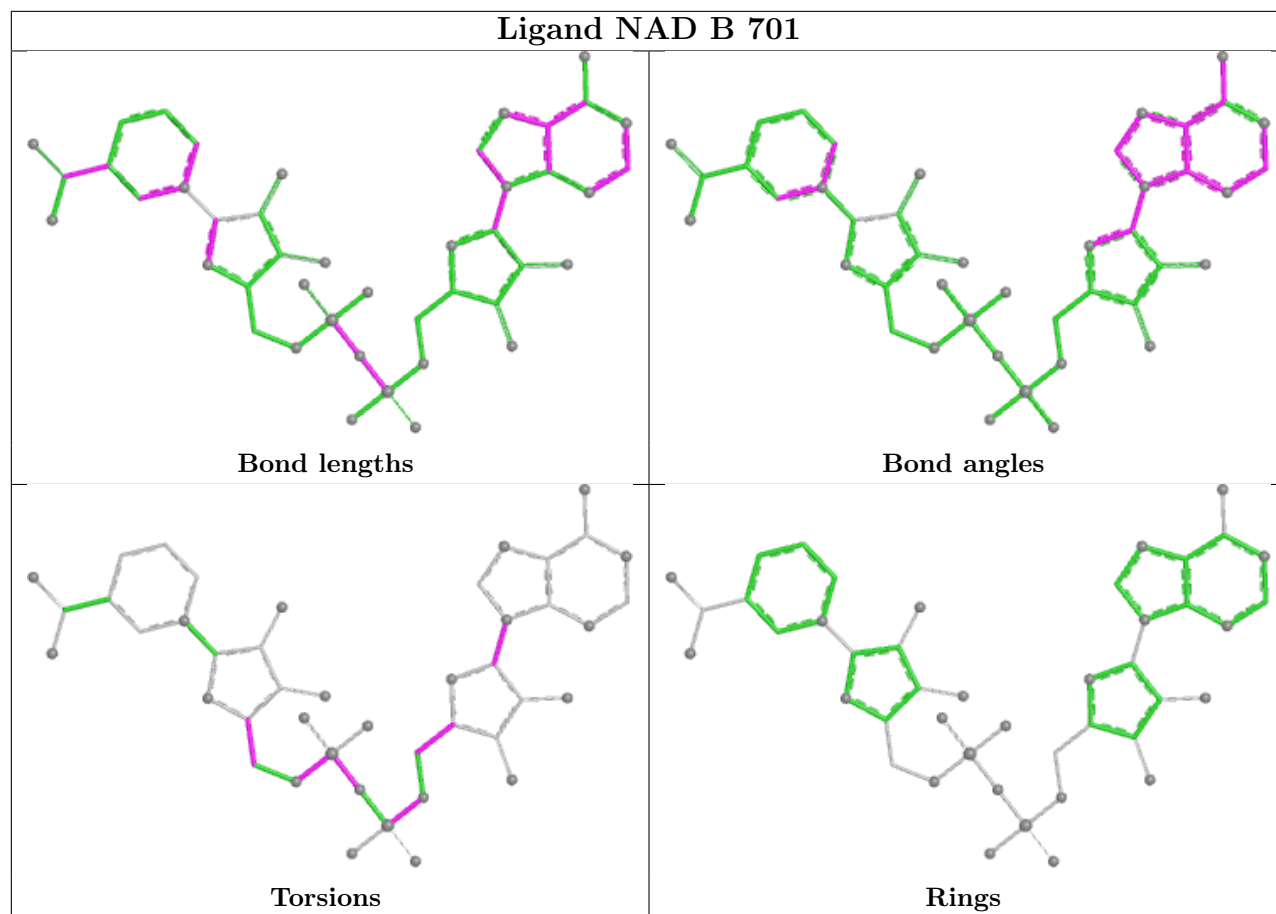
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1612	FAD	1	0
2	B	701	NAD	1	0
2	B	700	NAD	1	0
3	A	1612	FAD	4	0
3	D	1612	FAD	4	0
3	B	1612	FAD	5	0
2	D	700	NAD	1	0

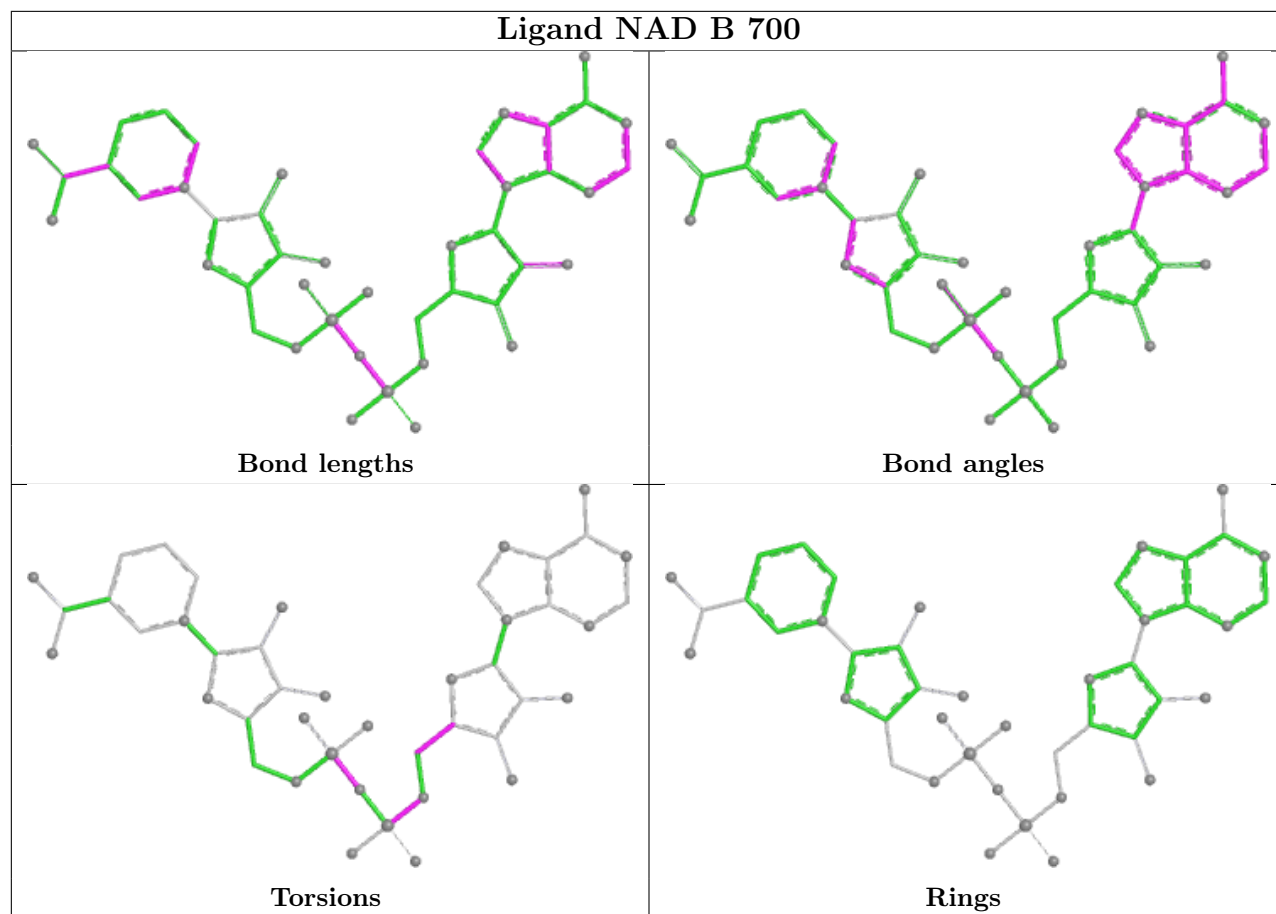
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

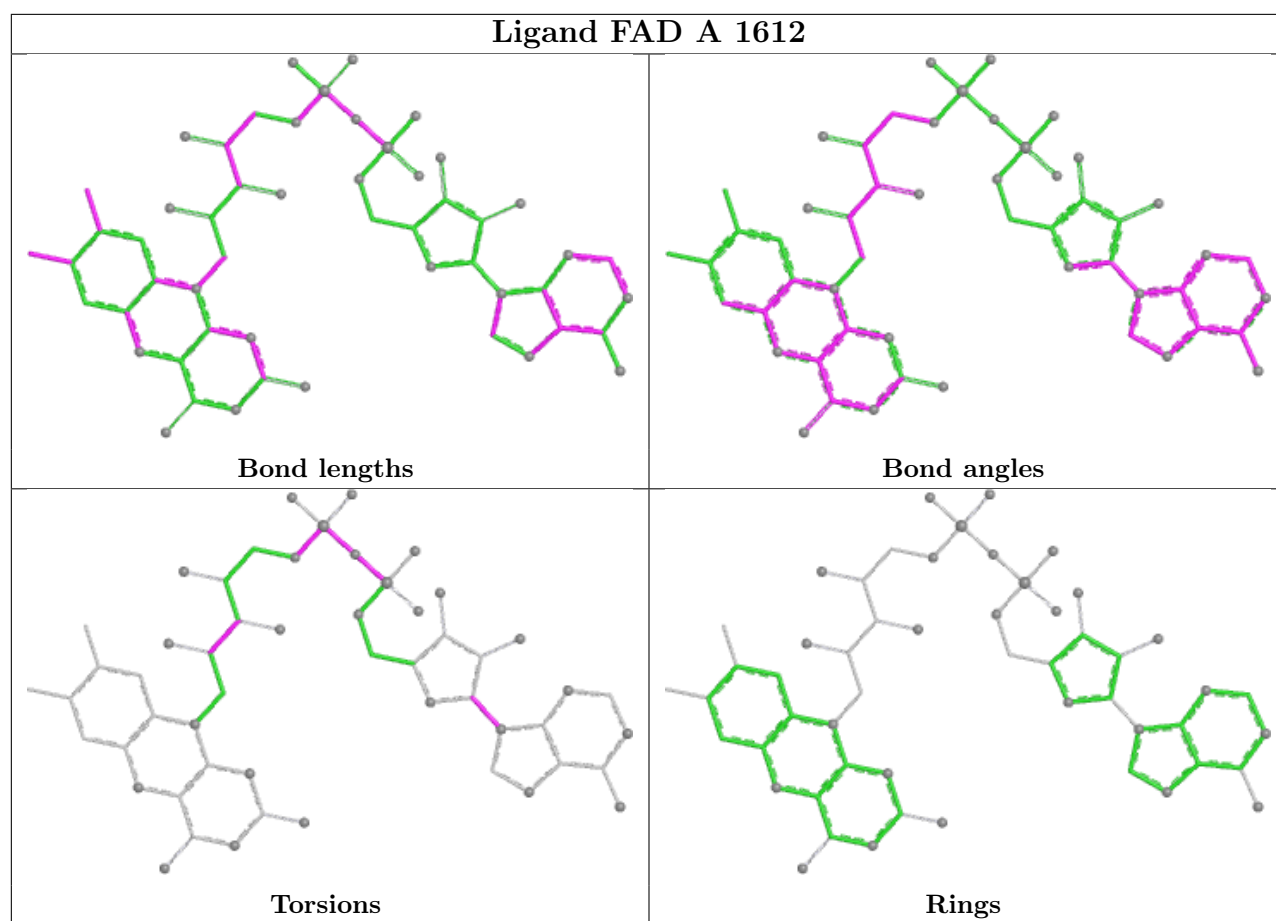
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

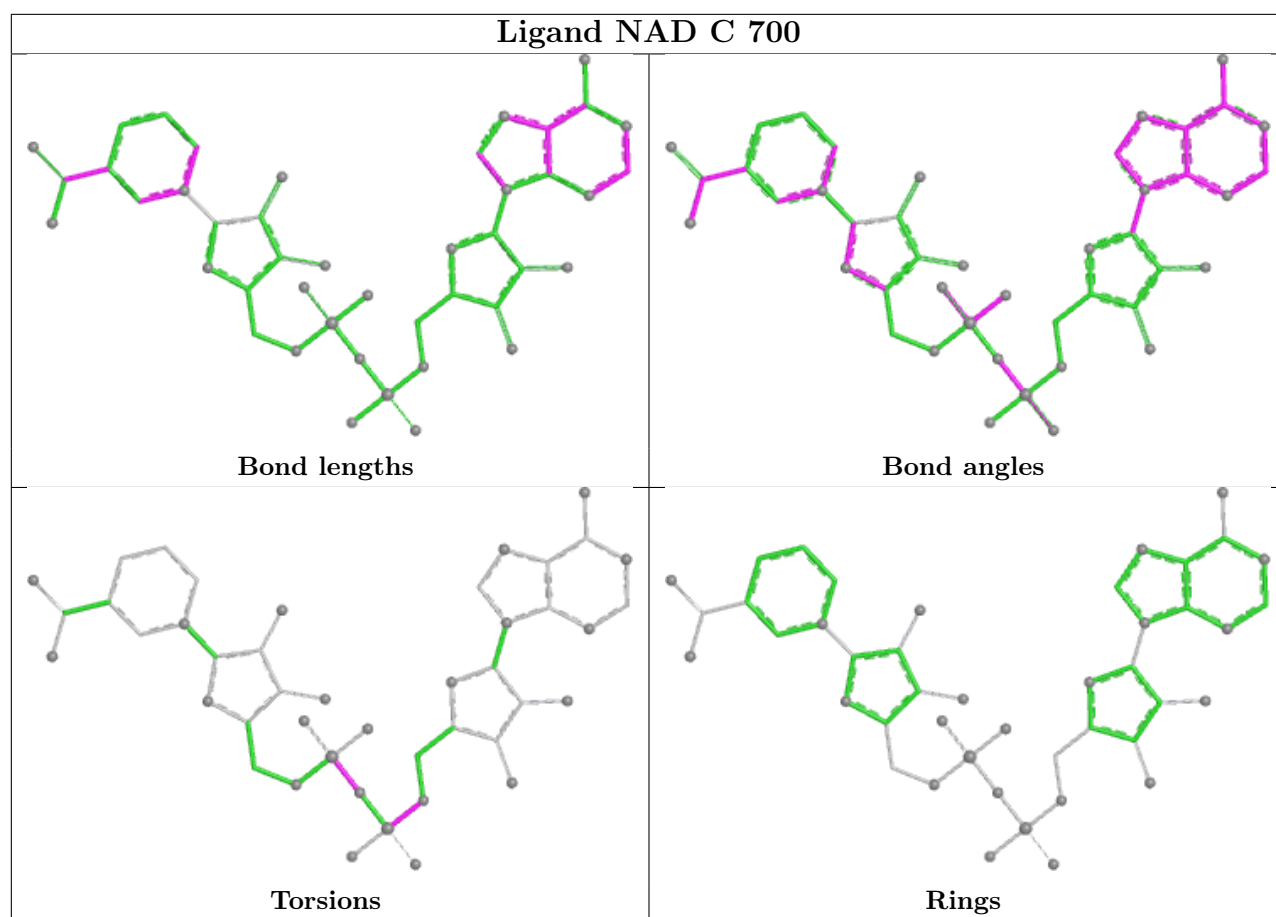


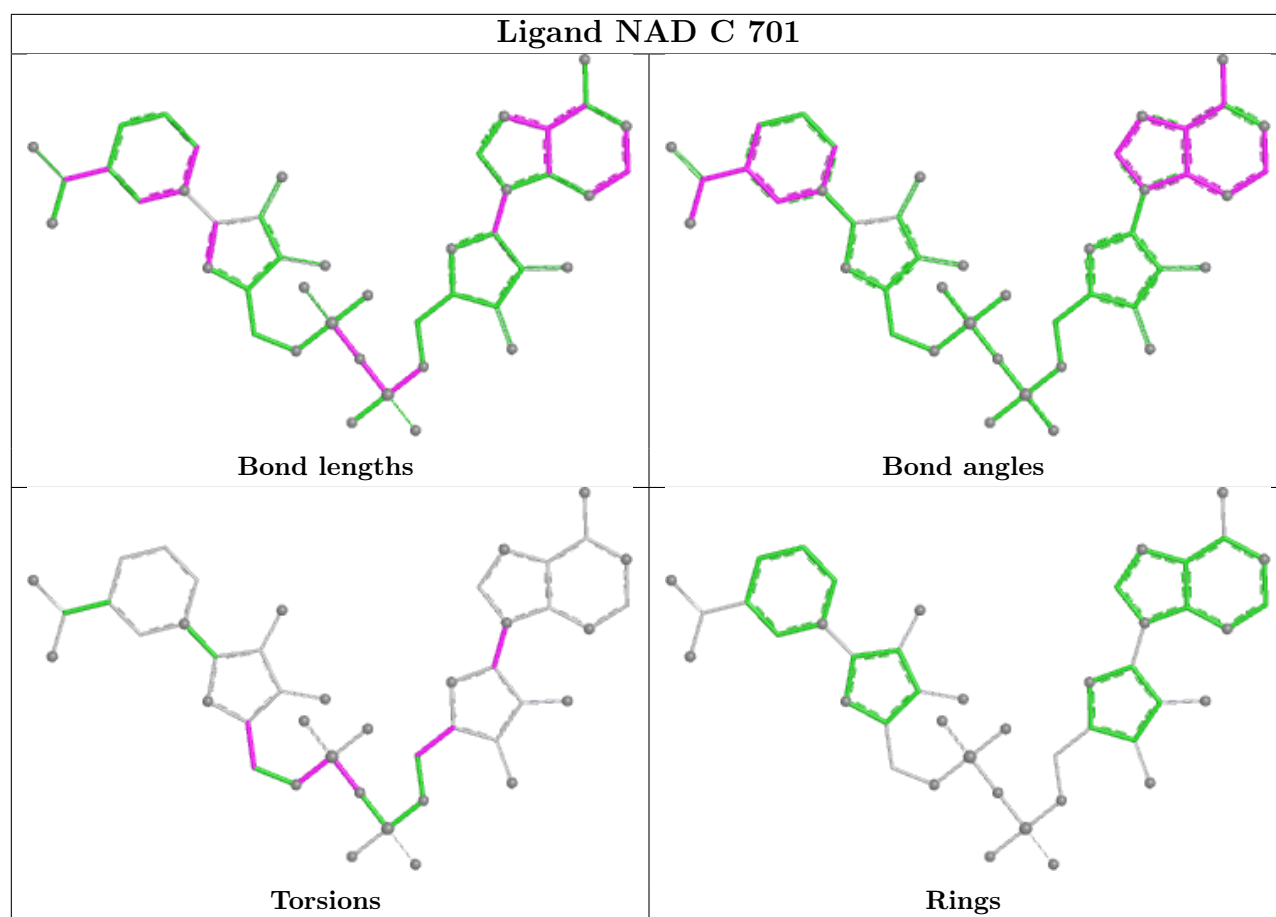


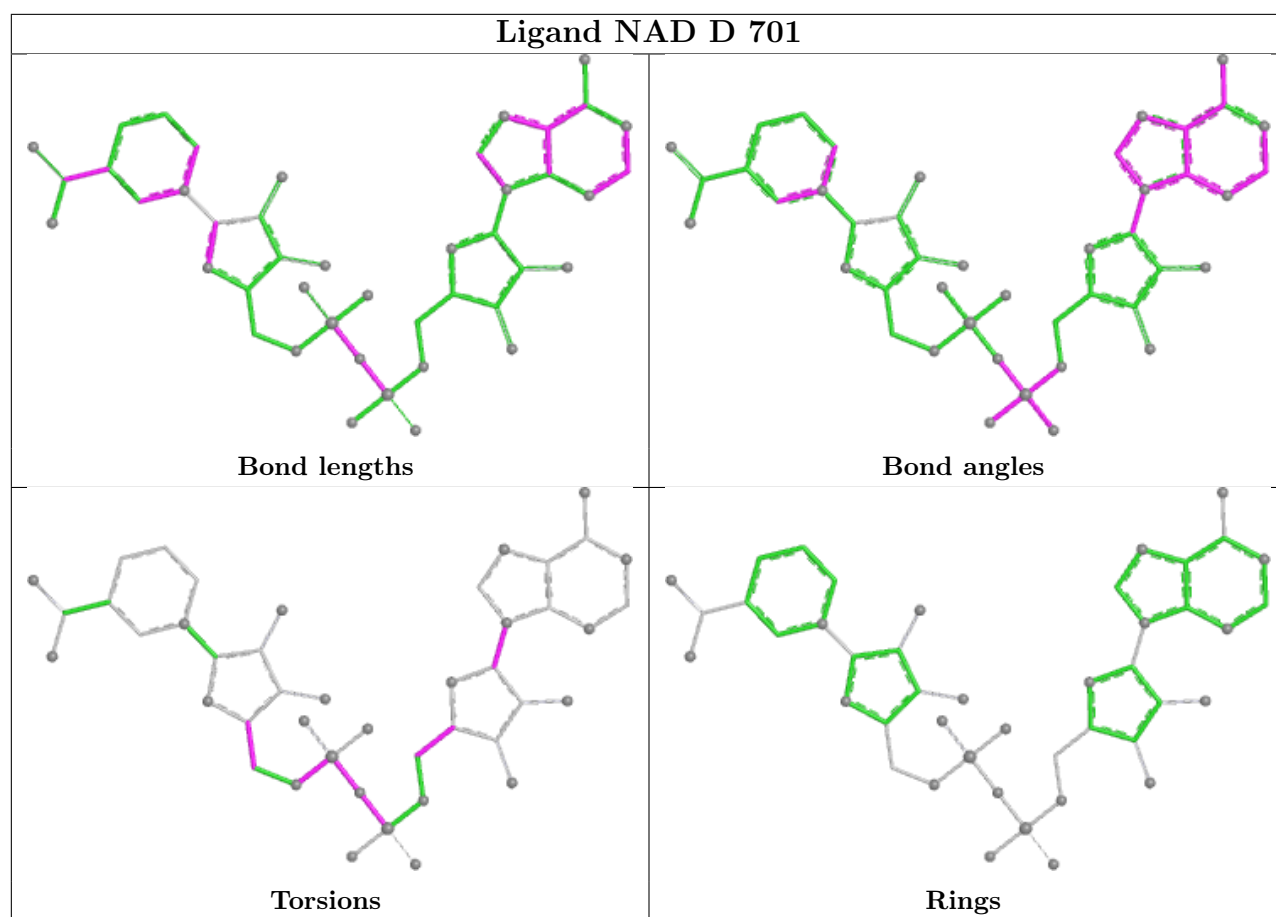


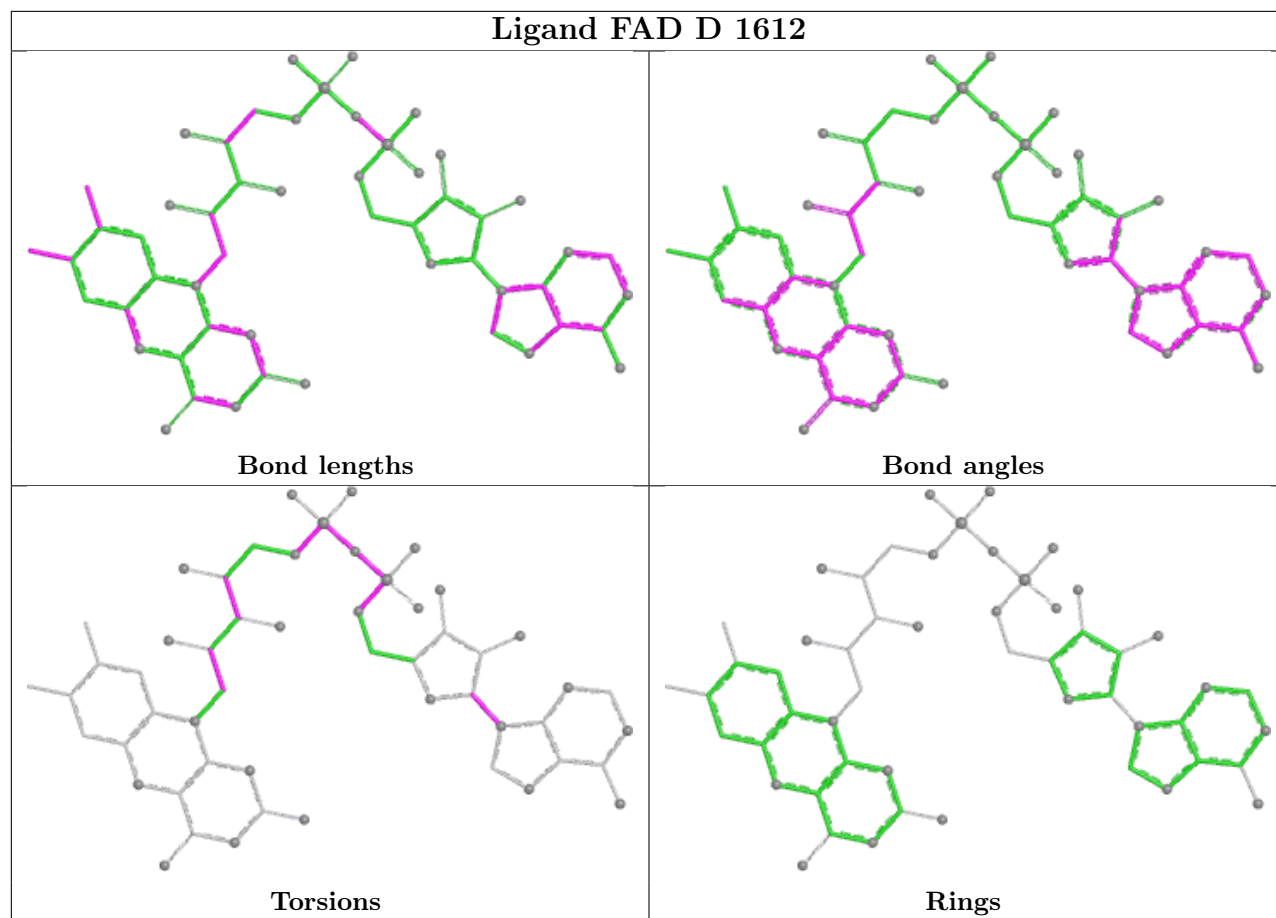


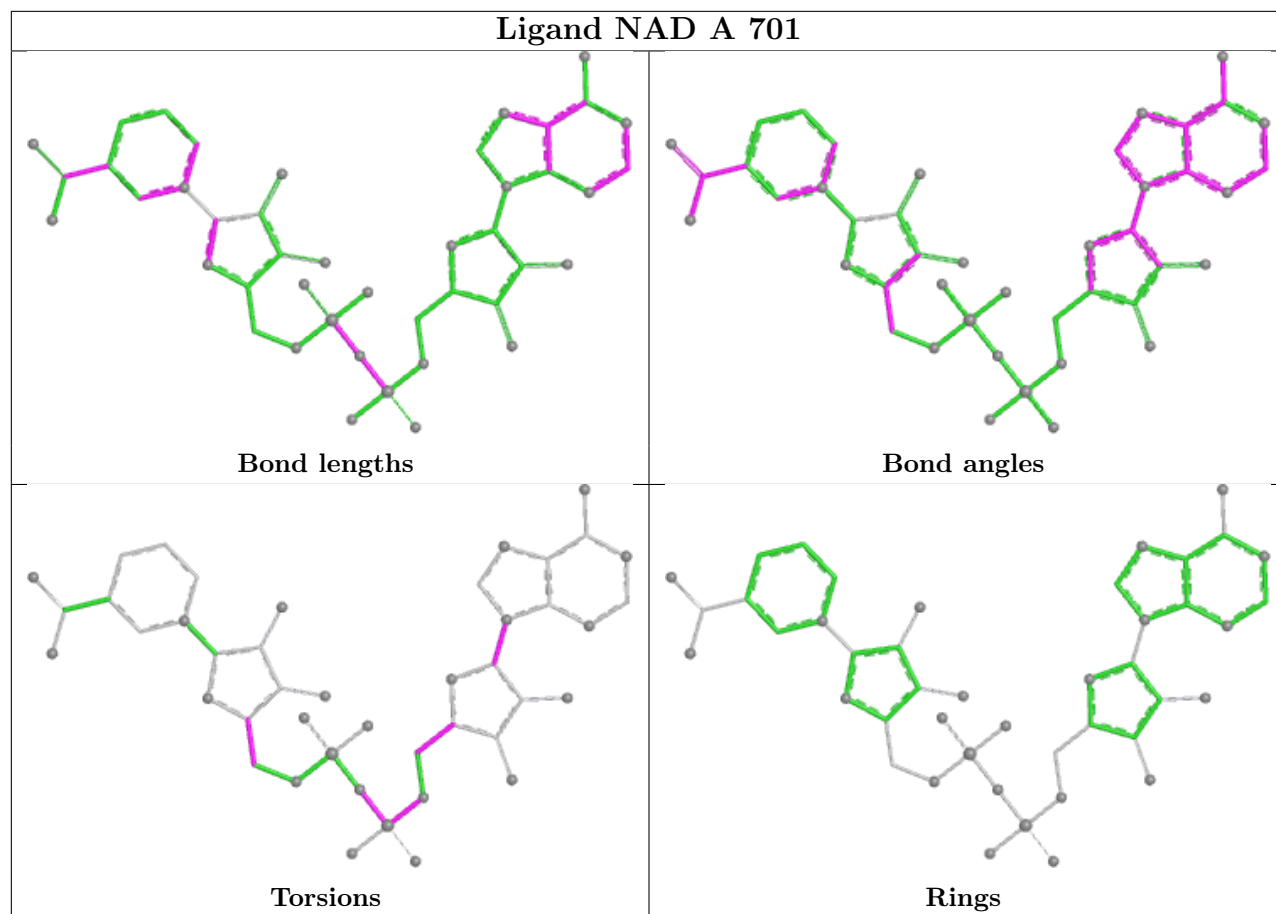


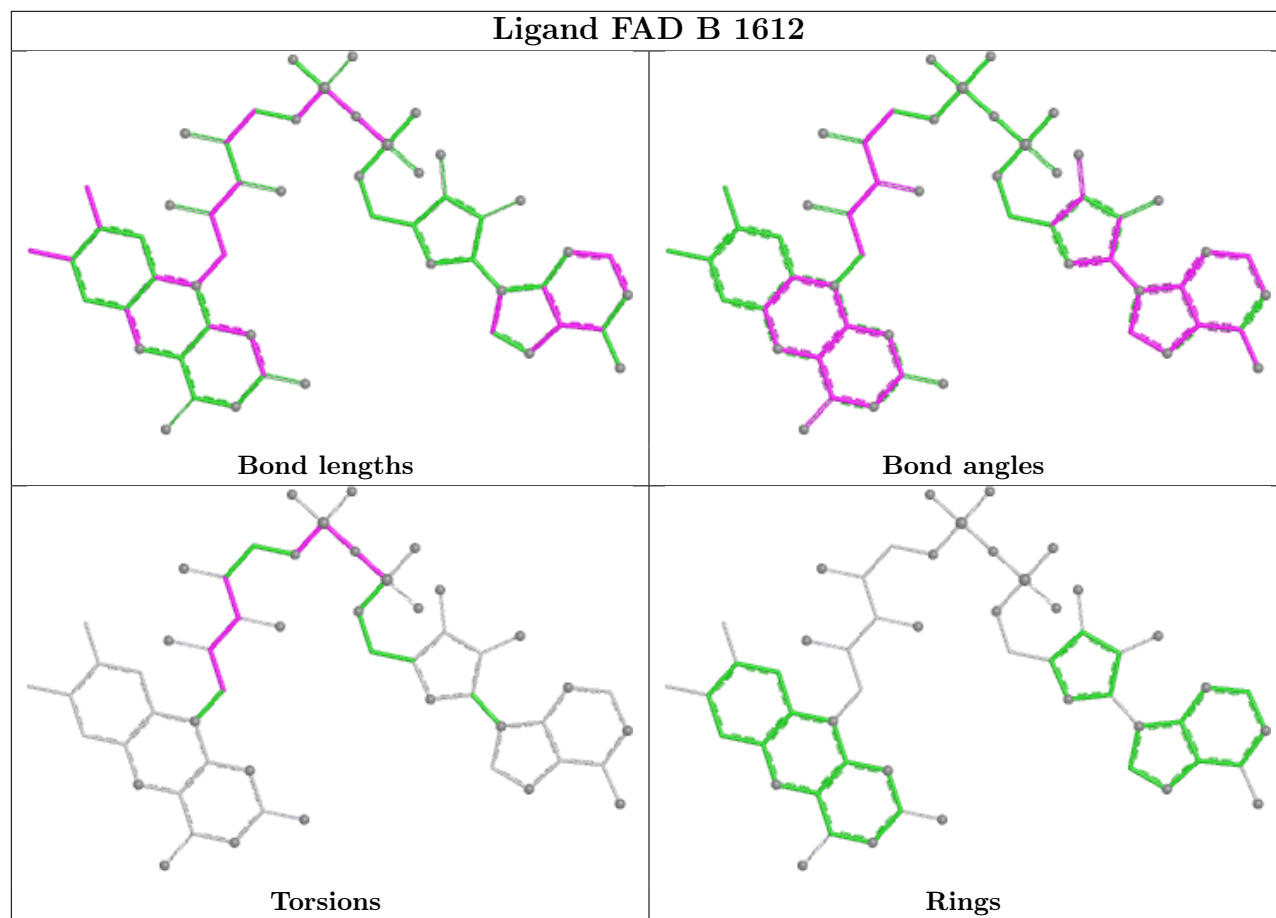


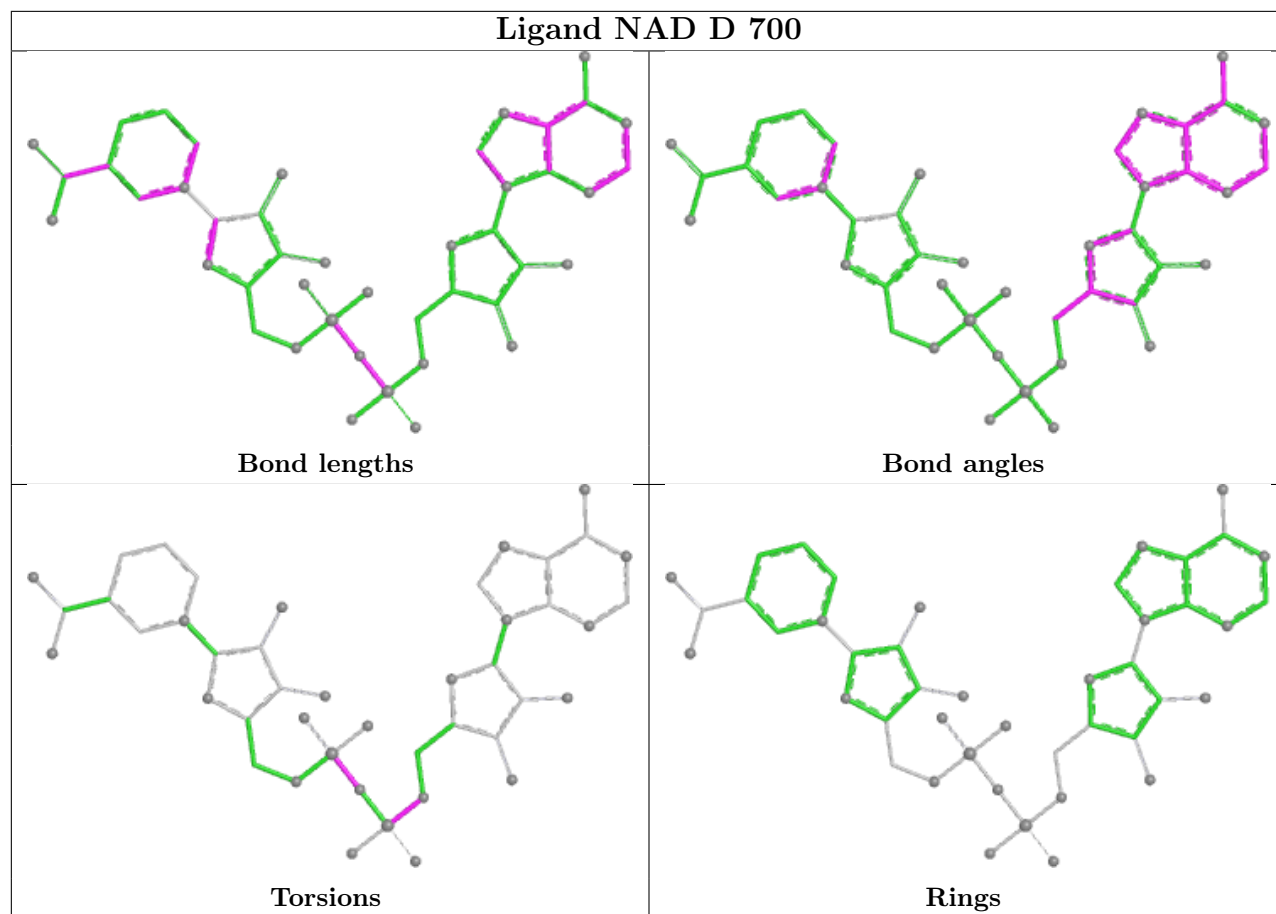












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	450/511 (88%)	-0.71	6 (1%) 75 68	27, 42, 74, 111	0
1	B	450/511 (88%)	-0.61	2 (0%) 88 86	30, 51, 81, 116	0
1	C	446/511 (87%)	-0.57	1 (0%) 91 89	30, 52, 84, 100	0
1	D	435/511 (85%)	-0.21	4 (0%) 81 75	39, 67, 104, 123	0
All	All	1781/2044 (87%)	-0.53	13 (0%) 84 80	27, 53, 91, 123	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	511	ALA	3.8
1	C	517	PRO	3.6
1	A	611	HIS	3.3
1	A	512	THR	3.3
1	A	128	ALA	3.1
1	D	128	ALA	2.9
1	D	326	LEU	2.8
1	B	125	GLN	2.7
1	A	553	ALA	2.6
1	B	553	ALA	2.3
1	D	275	ALA	2.3
1	A	551	PRO	2.2
1	D	379	LEU	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](#)

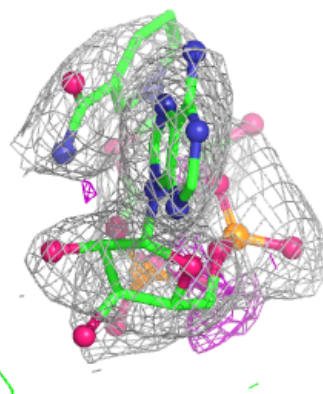
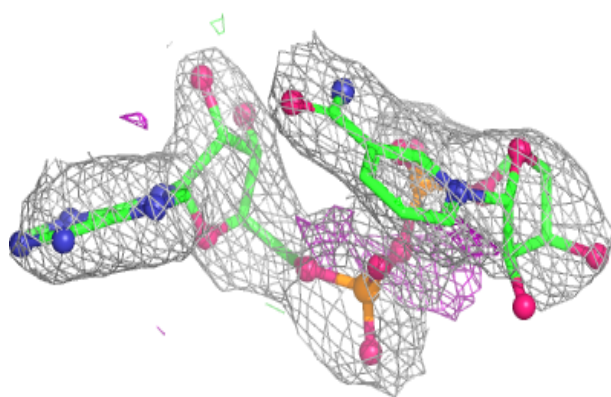
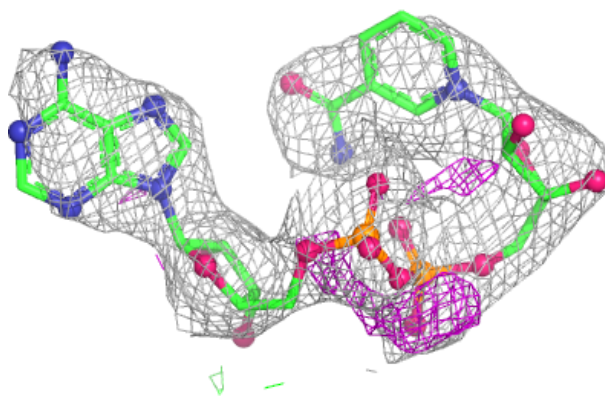
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	D	1613	5/5	0.86	0.10	72,74,86,89	0
2	NAD	B	701	44/44	0.89	0.10	74,102,110,116	0
2	NAD	D	701	44/44	0.91	0.10	71,97,111,112	0
2	NAD	A	701	44/44	0.91	0.10	71,87,104,112	0
2	NAD	C	701	44/44	0.94	0.08	61,70,81,86	0
3	FAD	D	1612	53/53	0.96	0.07	38,53,63,67	0
2	NAD	D	700	44/44	0.96	0.07	36,57,79,82	0
3	FAD	B	1612	53/53	0.97	0.06	29,43,50,52	0
2	NAD	C	700	44/44	0.98	0.06	30,41,56,60	0
3	FAD	C	1612	53/53	0.98	0.06	30,39,50,54	0
2	NAD	B	700	44/44	0.98	0.05	27,41,49,49	0
3	FAD	A	1612	53/53	0.98	0.05	22,33,40,43	0
2	NAD	A	700	44/44	0.99	0.05	23,33,47,47	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.

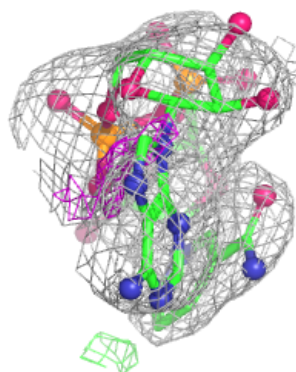
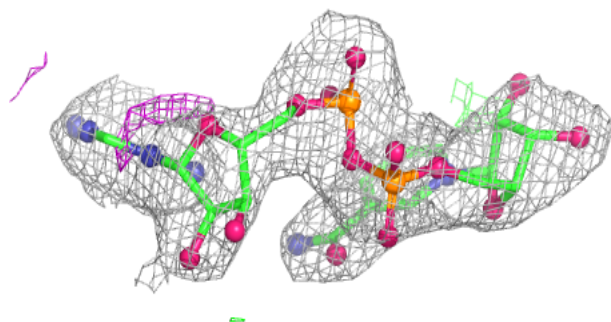
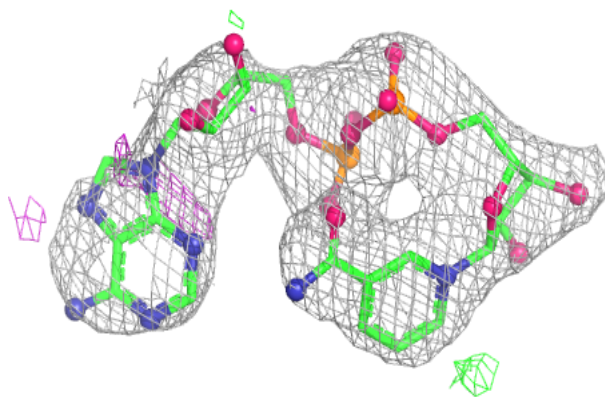
Electron density around NAD B 701:

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

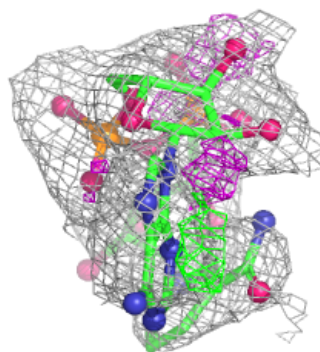
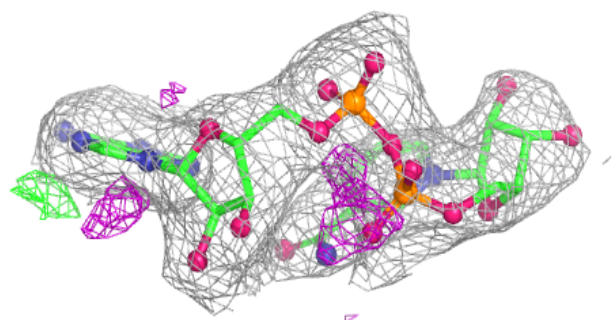
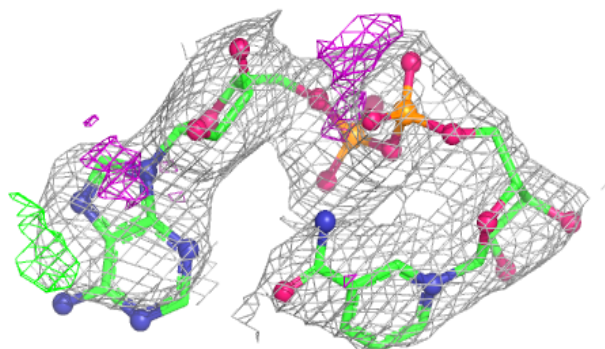


Electron density around NAD D 701:

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

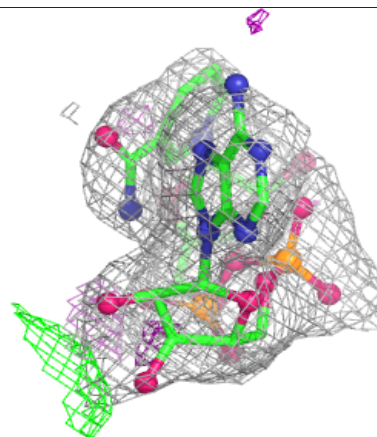
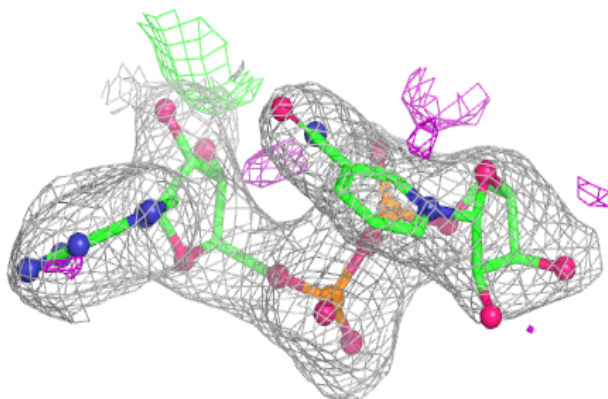
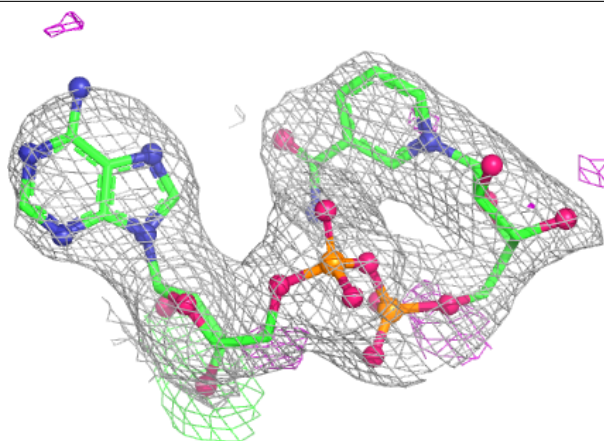
**Electron density around NAD A 701:**

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

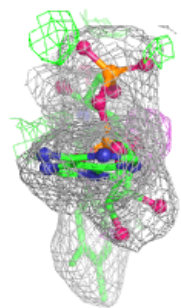
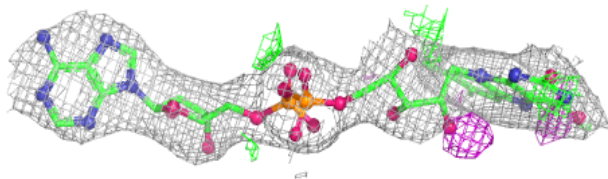
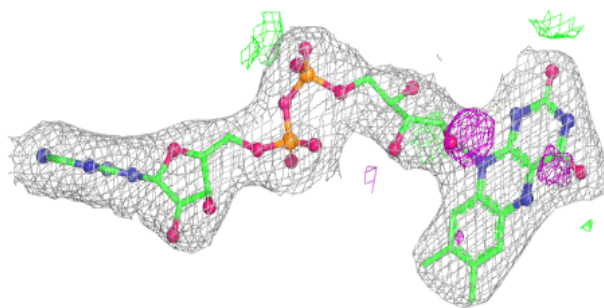


Electron density around NAD C 701:

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

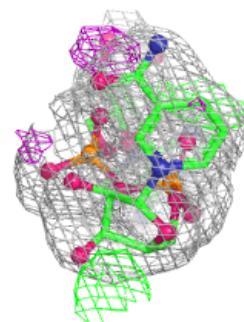
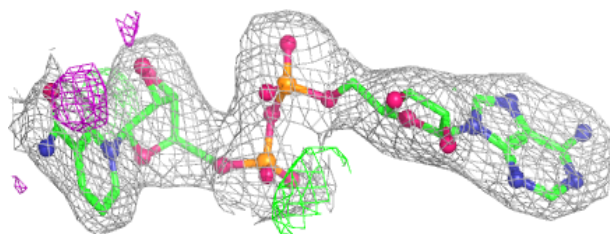
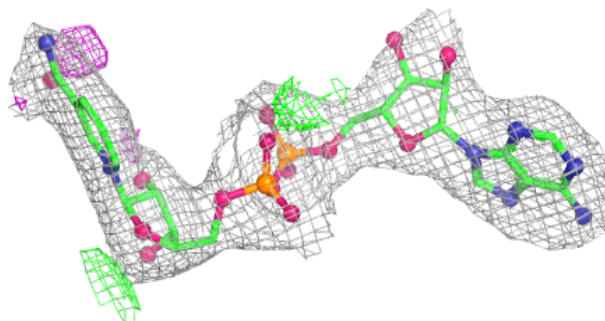
**Electron density around FAD D 1612:**

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

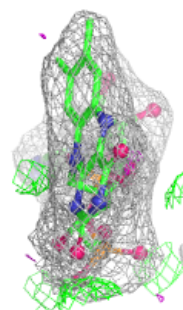
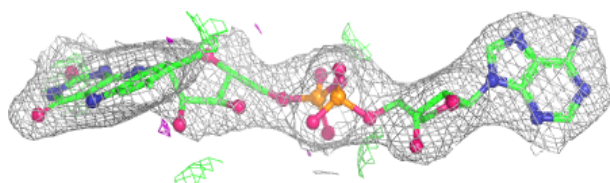
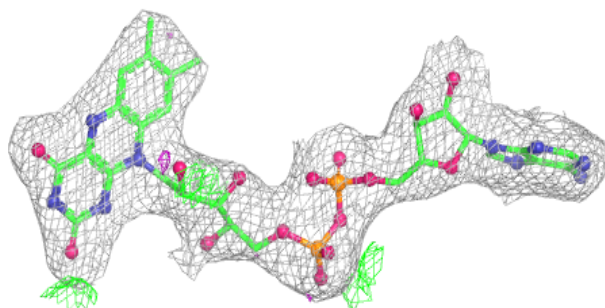


Electron density around NAD D 700:

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

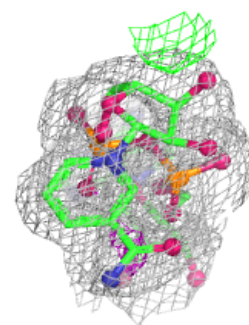
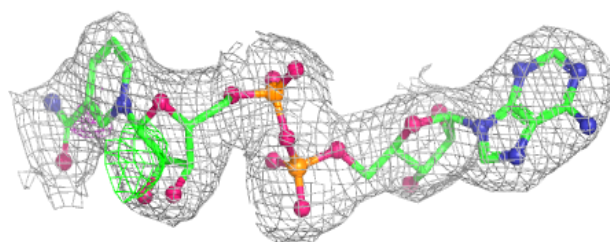
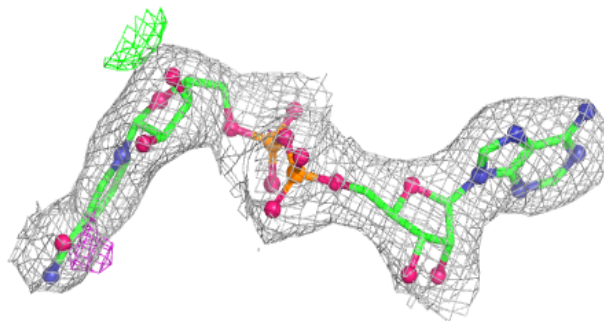
**Electron density around FAD B 1612:**

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

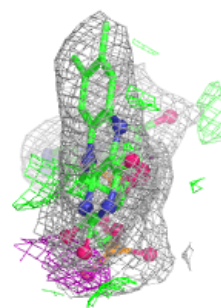
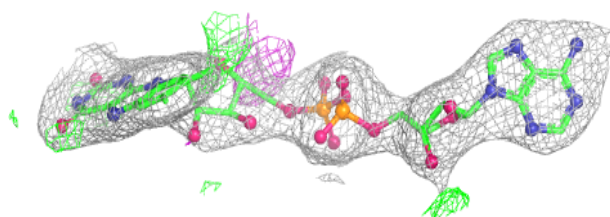
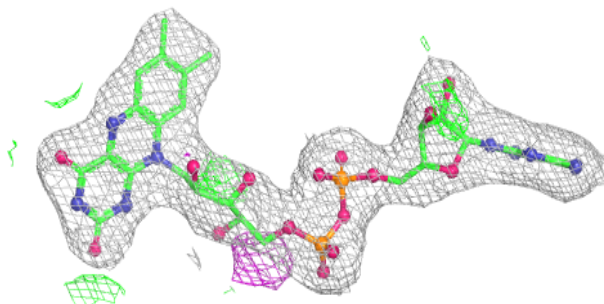


Electron density around NAD C 700:

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

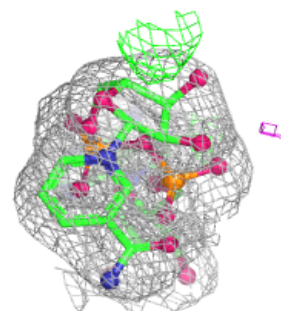
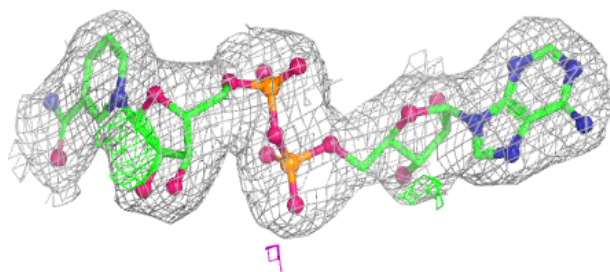
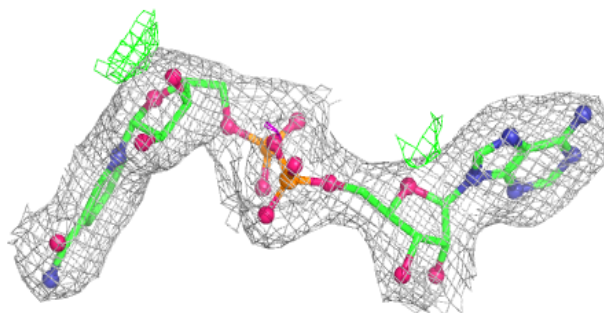
**Electron density around FAD C 1612:**

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

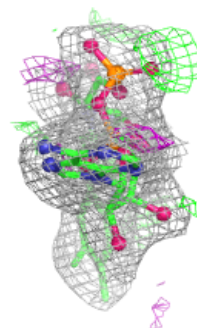
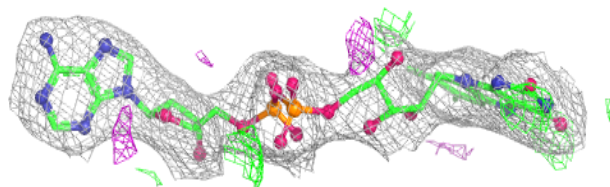
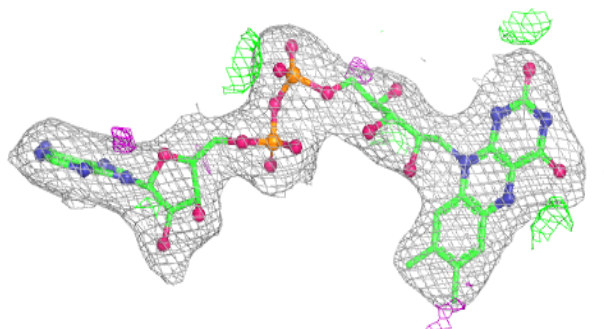


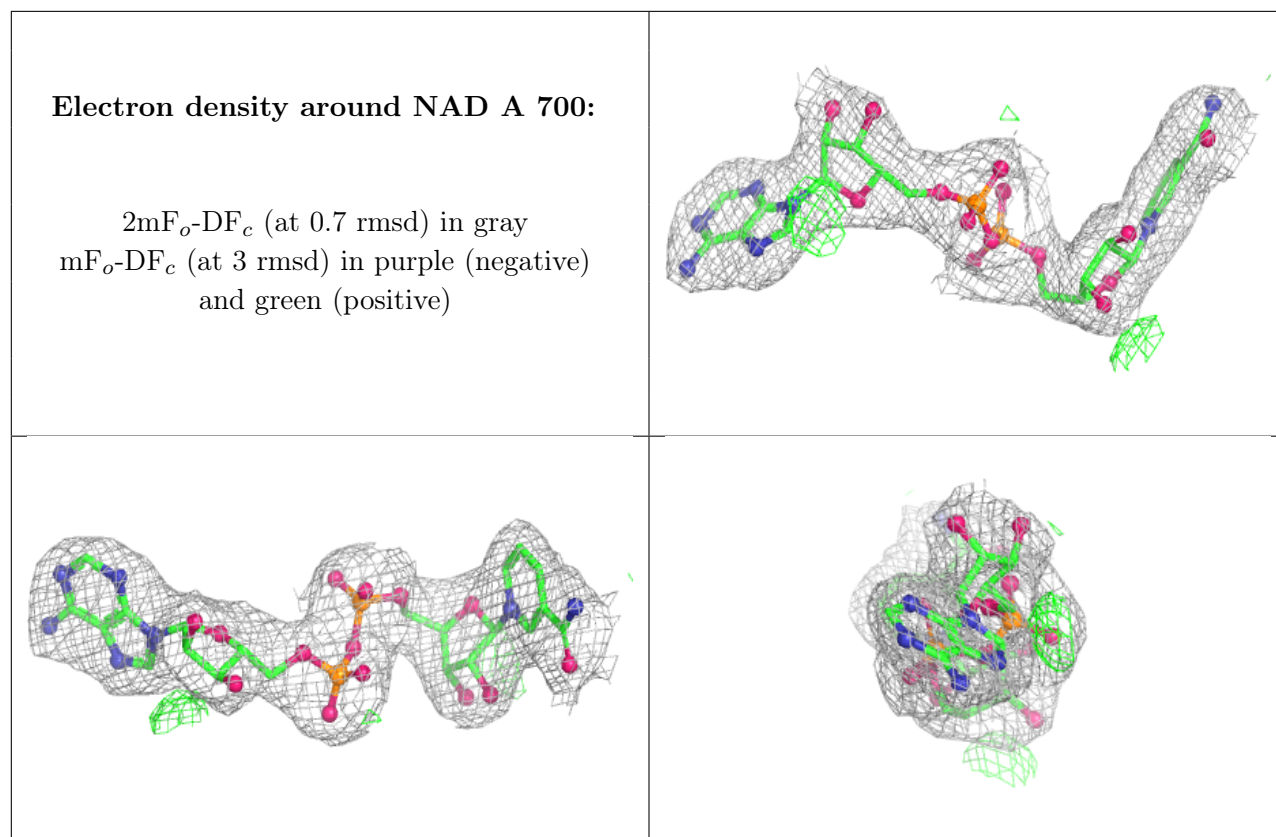
Electron density around NAD B 700:

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

**Electron density around FAD A 1612:**

$2mF_o-DF_c$ (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.