



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 08:42 pm GMT

PDB ID : 4BUR
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

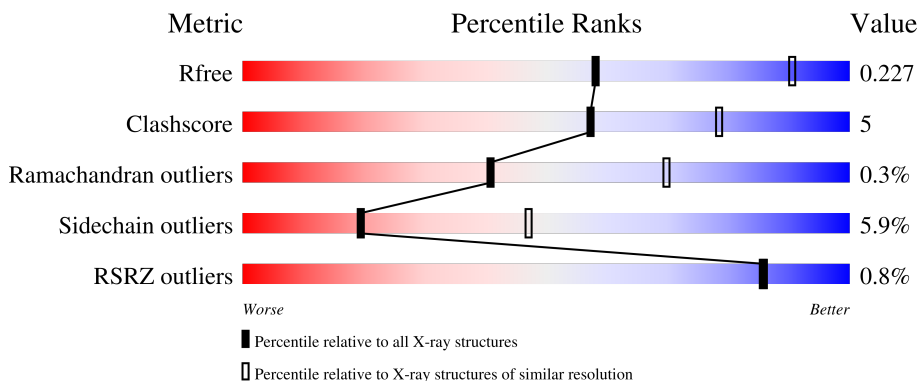
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (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	 75% 12% • 12%
1	B	511	 74% 13% • 12%
1	C	511	 74% 13% • 13%
1	D	511	 2% 71% 13% • 15%

2 Entry composition [i](#)

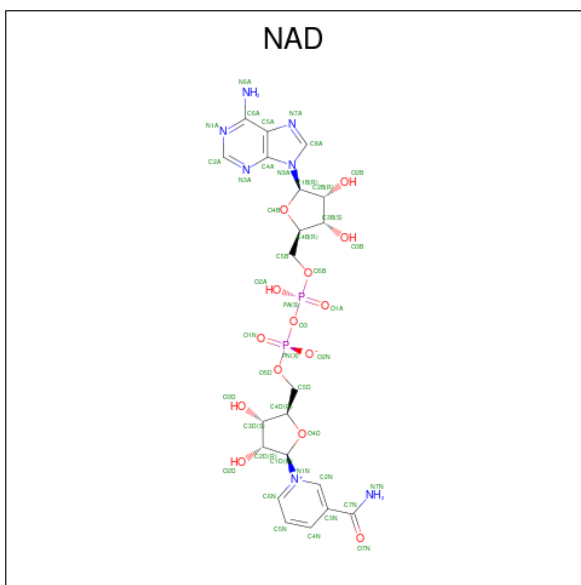
There are 5 unique types of molecules in this entry. The entry contains 14362 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called APOPTOSIS INDUCING FACTOR 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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 (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



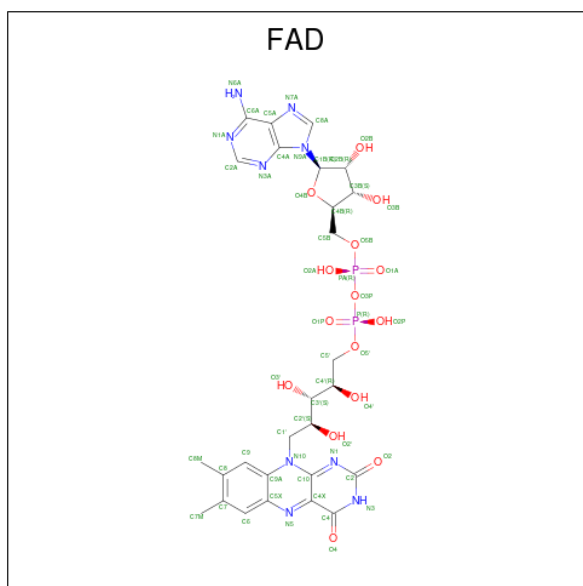
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0

Continued on next page...

Continued from previous page...

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 (three-letter code: 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 (three-letter code: 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.

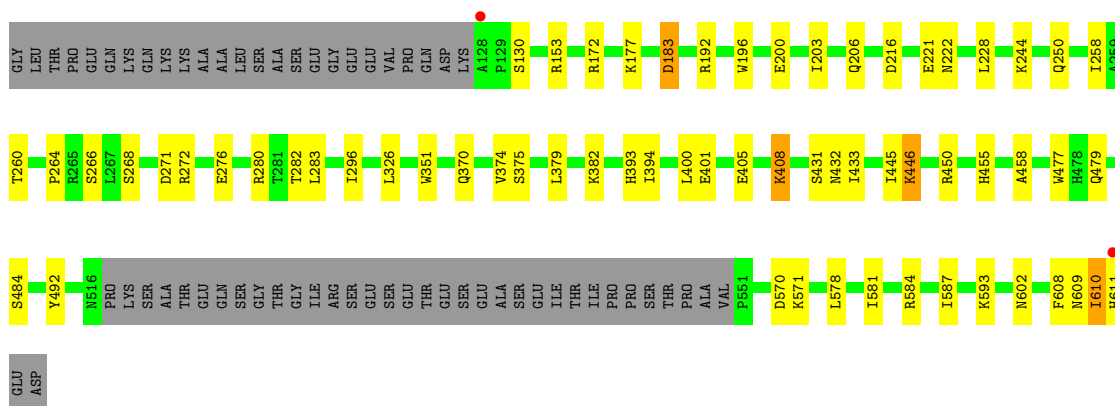
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	8	Total	O	0	0
			8	8		
5	C	7	Total	O	0	0
			7	7		

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.

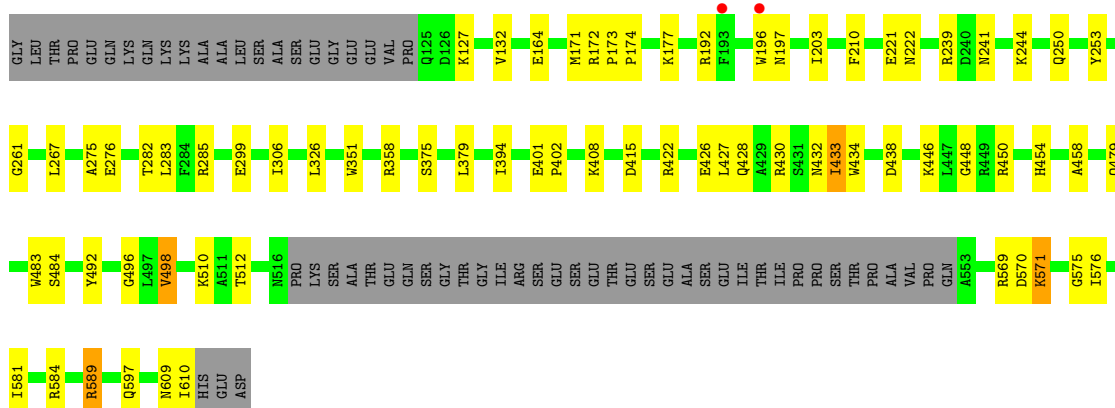
• Molecule 1: APOPTOSIS INDUCING FACTOR 1, MITOCHONDRIAL

Chain A: 



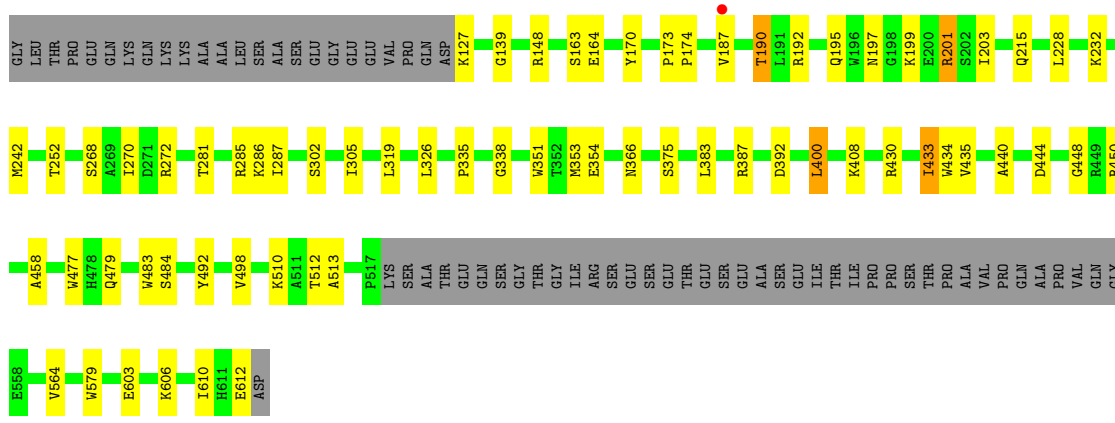
• Molecule 1: APOPTOSIS INDUCING FACTOR 1, MITOCHONDRIAL

Chain B: 

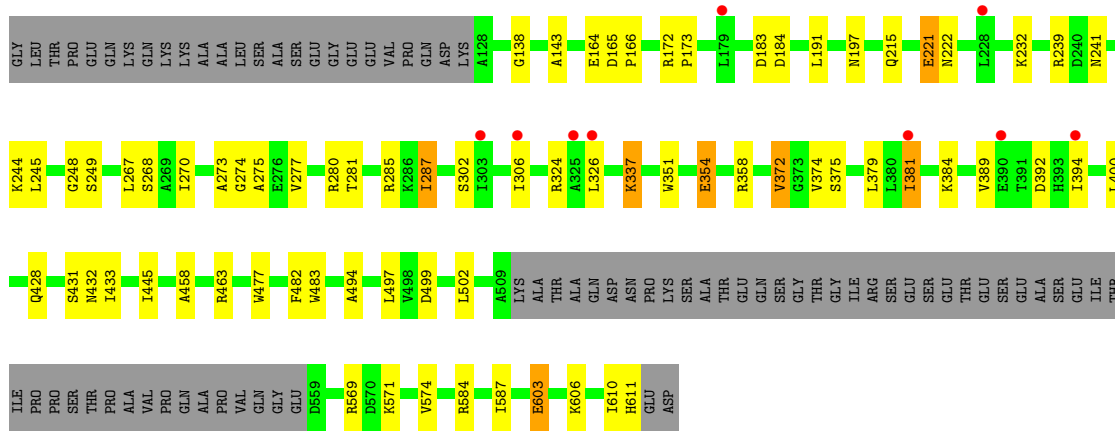


• Molecule 1: APOPTOSIS INDUCING FACTOR 1, MITOCHONDRIAL

Chain C: 



● 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 77.21 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.88) 99.7 (77.21-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.86Å)	Xtrriage
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	Xtrriage
Anisotropy	0.530	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SO4, NAD

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	0.58	3/3546 (0.1%)	0.71	2/4794 (0.0%)
1	B	0.55	2/3540 (0.1%)	0.67	0/4785
1	C	0.55	5/3522 (0.1%)	0.68	2/4760 (0.0%)
1	D	0.54	3/3440 (0.1%)	0.64	0/4648
All	All	0.56	13/14048 (0.1%)	0.67	4/18987 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	477	TRP	CD2-CE2	5.73	1.48	1.41
1	B	483	TRP	CD2-CE2	5.60	1.48	1.41
1	D	351	TRP	CD2-CE2	5.49	1.48	1.41
1	C	351	TRP	CD2-CE2	5.30	1.47	1.41
1	D	483	TRP	CD2-CE2	5.28	1.47	1.41
1	C	579	TRP	CD2-CE2	5.17	1.47	1.41
1	B	351	TRP	CD2-CE2	5.15	1.47	1.41
1	A	477	TRP	CD2-CE2	5.11	1.47	1.41
1	A	351	TRP	CD2-CE2	5.07	1.47	1.41
1	A	196	TRP	CD2-CE2	5.06	1.47	1.41
1	C	434	TRP	CD2-CE2	5.04	1.47	1.41
1	D	477	TRP	CD2-CE2	5.03	1.47	1.41
1	C	483	TRP	CD2-CE2	5.02	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	400	LEU	CA-CB-CG	6.94	131.27	115.30
1	A	400	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	400	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	400	LEU	CB-CG-CD2	-5.08	102.36	111.00

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	3475	0	3509	33	0
1	B	3471	0	3505	44	0
1	C	3452	0	3487	25	0
1	D	3371	0	3418	36	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	2	0
3	D	53	0	31	5	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	140	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 (140) 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: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:A:610:ILE:HA	1:A:611:HIS:C	2.04	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:B:221:GLU:O	1:B:222:ASN:HB2	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:285:ARG:NH1	3:D:1612:FAD:HM81	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:TRP:CH2	2:B:701:NAD:O2A	2.64	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:A:609:ASN:C	1:A:610:ILE:HG13	2.36	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:GLY:HA2	1:C:353:MET:CE	2.47	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: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: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:285:ARG:NH1	3:C:1612:FAD:HM81	2.34	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:D:244:LYS:HE2	1:D:248:GLY:HA2	2.00	0.42
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: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:A:610:ILE:CA	1:A:611:HIS:C	2.83	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:A:401:GLU:HA	1:A:401:GLU:OE1	2.21	0.41
1:C:170:TYR:CZ	1:C:287:ILE:HG13	2.56	0.41
1:B:575:GLY:C	1:B:576:ILE:HG13	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LYS:HE2	1:A:593:LYS:O	2.21	0.40
1:D:603:GLU:OE1	1:D:603: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: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%)	22	52
1	C	442/511 (86%)	416 (94%)	25 (6%)	1 (0%)	47	76
1	D	431/511 (84%)	396 (92%)	34 (8%)	1 (0%)	47	76
All	All	1765/2044 (86%)	1650 (94%)	110 (6%)	5 (0%)	41	70

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 [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	367/419 (88%)	347 (95%)	20 (5%)	22	51
1	B	366/419 (87%)	348 (95%)	18 (5%)	25	55
1	C	365/419 (87%)	343 (94%)	22 (6%)	19	46
1	D	357/419 (85%)	331 (93%)	26 (7%)	14	36
All	All	1455/1676 (87%)	1369 (94%)	86 (6%)	19	47

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	SER
1	A	153	ARG
1	A	177	LYS
1	A	183	ASP
1	A	203	ILE
1	A	206	GLN
1	A	216	ASP
1	A	228	LEU
1	A	266	SER
1	A	272	ARG
1	A	326	LEU
1	A	375	SER
1	A	405	GLU
1	A	408	LYS
1	A	433	ILE
1	A	446	LYS
1	A	570	ASP
1	A	571	LYS
1	A	602	ASN
1	A	610	ILE
1	B	127	LYS
1	B	177	LYS
1	B	192	ARG
1	B	210	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	239	ARG
1	B	276	GLU
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	571	LYS
1	B	584	ARG
1	B	589	ARG
1	C	127	LYS
1	C	148	ARG
1	C	187	VAL
1	C	190	THR
1	C	197	ASN
1	C	201	ARG
1	C	203	ILE
1	C	215	GLN
1	C	228	LEU
1	C	268	SER
1	C	272	ARG
1	C	326	LEU
1	C	354	GLU
1	C	375	SER
1	C	400	LEU
1	C	408	LYS
1	C	433	ILE
1	C	450	ARG
1	C	498	VAL
1	C	510	LYS
1	C	512	THR
1	C	612	GLU
1	D	183	ASP
1	D	184	ASP
1	D	197	ASN
1	D	215	GLN
1	D	221	GLU
1	D	239	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	241	ASN
1	D	268	SER
1	D	270	ILE
1	D	287	ILE
1	D	326	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	384	LYS
1	D	389	VAL
1	D	433	ILE
1	D	445	ILE
1	D	463	ARG
1	D	569	ARG
1	D	571	LYS
1	D	603	GLU
1	D	610	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	197	ASN
1	A	250	GLN
1	A	403	ASN
1	A	428	GLN
1	A	479	GLN
1	B	250	GLN
1	B	403	ASN
1	B	432	ASN
1	B	454	HIS
1	B	457	HIS
1	B	479	GLN
1	C	215	GLN
1	C	609	ASN
1	D	222	ASN
1	D	403	ASN
1	D	428	GLN
1	D	602	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
3	FAD	D	1612	-	53,58,58	2.07	15 (28%)	68,89,89	1.84	17 (25%)
2	NAD	C	701	-	42,48,48	2.21	11 (26%)	50,73,73	1.51	6 (12%)
2	NAD	C	700	-	42,48,48	1.98	9 (21%)	50,73,73	1.65	7 (14%)
2	NAD	A	700	-	42,48,48	2.29	12 (28%)	50,73,73	1.64	7 (14%)
4	SO4	D	1613	-	4,4,4	0.49	0	6,6,6	0.26	0
2	NAD	A	701	-	42,48,48	2.08	8 (19%)	50,73,73	1.80	9 (18%)
3	FAD	B	1612	-	53,58,58	1.98	16 (30%)	68,89,89	1.85	20 (29%)
2	NAD	B	700	-	42,48,48	1.87	9 (21%)	50,73,73	1.70	5 (10%)
3	FAD	C	1612	-	53,58,58	1.96	14 (26%)	68,89,89	1.99	17 (25%)
3	FAD	A	1612	-	53,58,58	2.11	16 (30%)	68,89,89	2.04	20 (29%)
2	NAD	D	700	-	42,48,48	2.05	9 (21%)	50,73,73	1.54	6 (12%)
2	NAD	B	701	-	42,48,48	2.09	9 (21%)	50,73,73	1.45	5 (10%)
2	NAD	D	701	-	42,48,48	2.06	9 (21%)	50,73,73	1.85	8 (16%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	D	1612	-	-	12/30/50/50	0/6/6/6
2	NAD	C	701	-	-	8/26/62/62	0/5/5/5
2	NAD	C	700	-	-	4/26/62/62	0/5/5/5
2	NAD	A	700	-	-	8/26/62/62	0/5/5/5
2	NAD	A	701	-	-	6/26/62/62	0/5/5/5
3	FAD	B	1612	-	-	13/30/50/50	0/6/6/6
2	NAD	B	700	-	-	4/26/62/62	0/5/5/5
3	FAD	C	1612	-	-	12/30/50/50	0/6/6/6
3	FAD	A	1612	-	-	9/30/50/50	0/6/6/6
2	NAD	D	700	-	-	2/26/62/62	0/5/5/5
2	NAD	B	701	-	-	8/26/62/62	0/5/5/5
2	NAD	D	701	-	-	6/26/62/62	0/5/5/5

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	NAD	C3N-C7N	-7.58	1.39	1.50
2	C	701	NAD	C3N-C7N	-7.57	1.39	1.50
2	D	700	NAD	C3N-C7N	-6.53	1.40	1.50
2	C	700	NAD	C3N-C7N	-6.50	1.40	1.50
2	B	701	NAD	C3N-C7N	-6.43	1.40	1.50
2	B	700	NAD	C3N-C7N	-6.35	1.41	1.50
2	A	701	NAD	C2N-N1N	6.26	1.42	1.35
2	A	701	NAD	C3N-C7N	-6.22	1.41	1.50
2	D	701	NAD	C3N-C7N	-6.00	1.41	1.50
3	A	1612	FAD	C7M-C7	-5.89	1.39	1.51
2	D	701	NAD	C2N-N1N	5.78	1.42	1.35
2	B	701	NAD	C2A-N3A	5.74	1.41	1.32
2	C	701	NAD	C2A-N3A	5.72	1.41	1.32
2	D	700	NAD	C2A-N3A	5.69	1.41	1.32
2	B	701	NAD	C2N-N1N	5.67	1.41	1.35
3	D	1612	FAD	C8M-C8	-5.56	1.39	1.51
2	A	701	NAD	C2A-N3A	5.49	1.40	1.32
3	C	1612	FAD	C8M-C8	-5.48	1.40	1.51
3	C	1612	FAD	C7M-C7	-5.42	1.40	1.51
2	A	700	NAD	C2N-N1N	5.40	1.41	1.35
2	A	700	NAD	C2A-N3A	5.36	1.40	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	NAD	C2A-N3A	5.31	1.40	1.32
3	D	1612	FAD	C2A-N3A	5.22	1.40	1.32
2	C	701	NAD	C2N-N1N	5.22	1.41	1.35
2	C	700	NAD	C2A-N3A	5.20	1.40	1.32
2	D	700	NAD	C2N-N1N	5.16	1.41	1.35
3	D	1612	FAD	C7M-C7	-5.09	1.40	1.51
2	B	700	NAD	C2N-N1N	5.05	1.41	1.35
3	C	1612	FAD	C2A-N3A	5.01	1.40	1.32
3	B	1612	FAD	C7M-C7	-4.99	1.41	1.51
3	B	1612	FAD	C2A-N3A	4.95	1.40	1.32
3	A	1612	FAD	C2A-N3A	4.85	1.39	1.32
3	B	1612	FAD	C8M-C8	-4.85	1.41	1.51
3	A	1612	FAD	C8M-C8	-4.75	1.41	1.51
3	D	1612	FAD	C10-N1	4.67	1.42	1.33
2	B	700	NAD	C2A-N3A	4.43	1.39	1.32
3	A	1612	FAD	C5'-C4'	4.38	1.58	1.51
2	C	700	NAD	C2N-N1N	4.27	1.40	1.35
2	C	701	NAD	O4D-C1D	4.15	1.46	1.41
2	A	700	NAD	O4B-C1B	4.08	1.46	1.41
2	D	701	NAD	O4D-C1D	4.05	1.46	1.41
2	C	701	NAD	C2A-N1A	3.98	1.41	1.33
2	D	700	NAD	C2A-N1A	3.93	1.41	1.33
2	B	700	NAD	C2A-N1A	3.88	1.41	1.33
2	D	701	NAD	C2A-N1A	3.86	1.41	1.33
2	B	701	NAD	O4D-C1D	3.82	1.46	1.41
2	A	700	NAD	C2A-N1A	3.81	1.41	1.33
2	B	701	NAD	C2A-N1A	3.80	1.41	1.33
2	A	701	NAD	C2A-N1A	3.74	1.40	1.33
2	A	700	NAD	O4D-C1D	3.74	1.46	1.41
3	C	1612	FAD	C10-N1	3.71	1.40	1.33
3	A	1612	FAD	C10-N1	3.62	1.40	1.33
2	A	701	NAD	O4D-C1D	3.59	1.46	1.41
2	C	700	NAD	C2A-N1A	3.57	1.40	1.33
2	B	701	NAD	O4B-C1B	3.54	1.46	1.41
2	C	700	NAD	O4B-C1B	3.51	1.46	1.41
3	A	1612	FAD	O4B-C1B	3.42	1.45	1.41
3	C	1612	FAD	C2A-N1A	3.36	1.40	1.33
3	B	1612	FAD	C2A-N1A	3.33	1.40	1.33
3	B	1612	FAD	C10-N1	3.33	1.40	1.33
3	B	1612	FAD	C1'-N10	3.33	1.56	1.48
3	D	1612	FAD	C2-N1	3.32	1.44	1.36
3	D	1612	FAD	C2A-N1A	3.30	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1612	FAD	C5X-N5	-3.28	1.33	1.39
3	A	1612	FAD	P-O5'	3.27	1.72	1.59
2	C	700	NAD	C6N-N1N	3.24	1.43	1.35
3	A	1612	FAD	C4'-C3'	-3.22	1.47	1.53
3	C	1612	FAD	P-O5'	3.19	1.72	1.59
3	D	1612	FAD	C5'-C4'	3.16	1.56	1.51
3	B	1612	FAD	C5X-N5	-3.15	1.33	1.39
3	B	1612	FAD	C1'-C2'	3.14	1.57	1.52
2	D	701	NAD	C6N-N1N	3.11	1.43	1.35
3	B	1612	FAD	C2B-C1B	-3.08	1.49	1.53
2	D	700	NAD	O4D-C1D	3.07	1.45	1.41
3	D	1612	FAD	C2B-C1B	-3.01	1.49	1.53
2	C	700	NAD	C5A-C4A	-2.96	1.33	1.40
3	A	1612	FAD	C5A-C4A	-2.95	1.33	1.40
3	A	1612	FAD	C9A-N10	-2.92	1.36	1.41
2	A	700	NAD	C6N-N1N	2.91	1.42	1.35
2	A	701	NAD	C6N-N1N	2.91	1.42	1.35
2	D	700	NAD	C6N-N1N	2.89	1.42	1.35
3	C	1612	FAD	C9A-N10	-2.86	1.36	1.41
3	A	1612	FAD	C2B-C1B	-2.83	1.49	1.53
3	B	1612	FAD	C2'-C3'	2.82	1.58	1.53
3	C	1612	FAD	O4B-C1B	2.79	1.45	1.41
3	A	1612	FAD	C6A-C5A	-2.78	1.33	1.43
2	C	701	NAD	C6N-N1N	2.78	1.42	1.35
2	C	701	NAD	O4B-C1B	2.75	1.44	1.41
3	C	1612	FAD	C5'-C4'	2.70	1.55	1.51
2	B	700	NAD	C6N-N1N	2.68	1.41	1.35
3	A	1612	FAD	C2A-N1A	2.67	1.38	1.33
2	A	700	NAD	C5A-C4A	-2.67	1.33	1.40
3	A	1612	FAD	C5X-N5	-2.66	1.34	1.39
2	D	701	NAD	C6A-C5A	-2.65	1.33	1.43
2	D	700	NAD	C2D-C1D	-2.64	1.49	1.53
2	A	700	NAD	C2D-C1D	-2.63	1.49	1.53
2	A	701	NAD	C6A-C5A	-2.57	1.33	1.43
3	D	1612	FAD	C5A-C4A	-2.56	1.34	1.40
3	B	1612	FAD	C5'-C4'	2.53	1.55	1.51
2	B	700	NAD	O4B-C1B	2.53	1.44	1.41
3	B	1612	FAD	C5A-C4A	-2.51	1.34	1.40
3	C	1612	FAD	C4'-C3'	-2.51	1.48	1.53
2	A	700	NAD	C2B-C1B	-2.51	1.50	1.53
3	D	1612	FAD	C1'-C2'	2.45	1.56	1.52
3	D	1612	FAD	C6A-C5A	-2.45	1.34	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1612	FAD	C1'-N10	2.43	1.54	1.48
2	D	701	NAD	O4B-C1B	2.40	1.44	1.41
2	B	700	NAD	C5A-C4A	-2.40	1.34	1.40
2	C	701	NAD	C6A-C5A	-2.40	1.34	1.43
3	A	1612	FAD	C2-N1	2.37	1.42	1.36
3	B	1612	FAD	C6A-C5A	-2.37	1.34	1.43
3	C	1612	FAD	C4X-N5	2.37	1.35	1.30
2	C	700	NAD	C6A-C5A	-2.36	1.34	1.43
3	C	1612	FAD	C1'-N10	2.36	1.54	1.48
2	B	701	NAD	C6N-N1N	2.35	1.41	1.35
3	C	1612	FAD	C6A-C5A	-2.33	1.34	1.43
3	B	1612	FAD	P-O5'	2.31	1.68	1.59
2	A	701	NAD	C5A-C4A	-2.26	1.34	1.40
2	B	701	NAD	C5A-C4A	-2.26	1.34	1.40
2	D	701	NAD	C5A-C4A	-2.24	1.35	1.40
2	A	700	NAD	C6A-C5A	-2.19	1.35	1.43
2	B	701	NAD	C6A-C5A	-2.19	1.35	1.43
3	C	1612	FAD	C5A-C4A	-2.18	1.35	1.40
2	C	701	NAD	PA-O5B	2.18	1.68	1.59
2	B	700	NAD	O2B-C2B	2.16	1.48	1.43
3	D	1612	FAD	C4-N3	2.16	1.42	1.38
3	B	1612	FAD	C9A-N10	-2.15	1.37	1.41
3	B	1612	FAD	C4X-N5	2.15	1.34	1.30
2	A	700	NAD	O4B-C4B	-2.14	1.40	1.45
2	D	700	NAD	C6A-C5A	-2.12	1.35	1.43
2	D	700	NAD	C5A-C4A	-2.12	1.35	1.40
2	B	700	NAD	C6A-C5A	-2.12	1.35	1.43
2	C	701	NAD	C5A-C4A	-2.11	1.35	1.40
3	A	1612	FAD	C1'-N10	2.11	1.53	1.48
2	C	701	NAD	C2D-C1D	-2.10	1.50	1.53
3	D	1612	FAD	C4X-N5	2.08	1.34	1.30
2	C	700	NAD	C2D-C1D	-2.03	1.50	1.53

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	700	NAD	N3A-C2A-N1A	-7.27	117.31	128.68
2	A	701	NAD	N3A-C2A-N1A	-7.23	117.38	128.68
2	D	700	NAD	N3A-C2A-N1A	-7.06	117.64	128.68
2	B	700	NAD	N3A-C2A-N1A	-7.01	117.72	128.68
2	D	701	NAD	N3A-C2A-N1A	-6.97	117.78	128.68
2	B	701	NAD	N3A-C2A-N1A	-6.94	117.84	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	NAD	N3A-C2A-N1A	-6.82	118.02	128.68
2	A	700	NAD	N3A-C2A-N1A	-6.76	118.12	128.68
3	A	1612	FAD	N3A-C2A-N1A	-6.60	118.36	128.68
3	C	1612	FAD	N3A-C2A-N1A	-6.47	118.56	128.68
3	B	1612	FAD	N3A-C2A-N1A	-6.44	118.62	128.68
3	D	1612	FAD	N3A-C2A-N1A	-6.32	118.80	128.68
2	B	700	NAD	C1B-N9A-C4A	-5.41	117.13	126.64
3	C	1612	FAD	O4B-C1B-C2B	-5.33	99.13	106.93
3	C	1612	FAD	C5'-C4'-C3'	-5.09	102.38	112.20
2	D	701	NAD	O5B-PA-O1A	-4.83	90.20	109.07
3	A	1612	FAD	C1'-C2'-C3'	4.80	123.20	109.79
3	A	1612	FAD	O3'-C3'-C4'	-4.59	97.73	108.81
2	D	701	NAD	O2A-PA-O5B	-4.54	86.64	107.75
3	B	1612	FAD	O4B-C1B-C2B	-4.44	100.44	106.93
3	B	1612	FAD	C1'-C2'-C3'	4.40	122.07	109.79
2	A	701	NAD	O4B-C1B-C2B	-4.24	100.74	106.93
3	B	1612	FAD	P-O3P-PA	-4.16	118.54	132.83
3	D	1612	FAD	O4B-C1B-C2B	-4.13	100.90	106.93
3	A	1612	FAD	C5'-C4'-C3'	-4.06	104.36	112.20
3	D	1612	FAD	C4-N3-C2	-4.02	118.22	125.64
2	A	700	NAD	C1B-N9A-C4A	-4.00	119.61	126.64
3	C	1612	FAD	C1'-C2'-C3'	3.94	120.81	109.79
2	A	701	NAD	C6N-N1N-C2N	-3.91	118.41	121.97
3	C	1612	FAD	C4-N3-C2	-3.89	118.45	125.64
3	A	1612	FAD	C4-N3-C2	-3.74	118.72	125.64
2	D	701	NAD	C1B-N9A-C4A	3.69	133.12	126.64
2	C	701	NAD	C6N-N1N-C2N	-3.66	118.64	121.97
3	A	1612	FAD	O5'-C5'-C4'	3.65	119.11	109.36
3	A	1612	FAD	C4-C4X-C10	3.64	122.91	116.79
3	D	1612	FAD	C1'-C2'-C3'	3.63	119.93	109.79
2	A	701	NAD	C1B-N9A-C4A	3.52	132.83	126.64
2	C	700	NAD	C1B-N9A-C4A	-3.50	120.50	126.64
3	D	1612	FAD	C4-C4X-C10	3.40	122.50	116.79
2	A	700	NAD	PN-O3-PA	-3.37	121.26	132.83
3	C	1612	FAD	C4X-C10-N1	-3.34	116.99	124.73
2	D	701	NAD	C6N-N1N-C2N	-3.32	118.95	121.97
3	C	1612	FAD	P-O3P-PA	-3.27	121.62	132.83
3	D	1612	FAD	C4X-C10-N1	-3.26	117.16	124.73
3	A	1612	FAD	C4X-C10-N1	-3.25	117.20	124.73
3	C	1612	FAD	C10-C4X-N5	-3.16	118.16	124.86
3	A	1612	FAD	P-O3P-PA	-3.12	122.14	132.83
3	C	1612	FAD	C4X-C10-N10	3.11	121.02	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1612	FAD	C4X-C4-N3	3.09	121.05	113.19
3	D	1612	FAD	C4X-C4-N3	3.00	120.80	113.19
2	A	701	NAD	C5A-C6A-N6A	-3.00	115.80	120.35
3	A	1612	FAD	C4X-C10-N10	2.98	120.84	116.48
3	D	1612	FAD	P-O3P-PA	-2.97	122.63	132.83
2	C	701	NAD	C5A-C6A-N6A	-2.96	115.85	120.35
2	D	701	NAD	C5A-C6A-N6A	-2.93	115.90	120.35
3	B	1612	FAD	C5'-C4'-C3'	-2.92	106.57	112.20
2	B	701	NAD	C6N-N1N-C2N	-2.89	119.34	121.97
3	D	1612	FAD	O2'-C2'-C3'	-2.88	102.10	109.10
2	C	700	NAD	O4D-C1D-C2D	-2.86	102.74	106.93
2	D	700	NAD	C6N-N1N-C2N	-2.83	119.39	121.97
3	D	1612	FAD	C9A-C5X-N5	-2.82	119.37	122.43
3	A	1612	FAD	C5A-C6A-N6A	-2.79	116.11	120.35
2	A	701	NAD	PN-O3-PA	-2.79	123.26	132.83
3	A	1612	FAD	C4'-C3'-C2'	2.77	119.13	113.36
3	A	1612	FAD	C10-C4X-N5	-2.75	119.01	124.86
2	A	700	NAD	O4D-C1D-C2D	-2.74	102.92	106.93
3	A	1612	FAD	O4B-C1B-C2B	-2.73	102.93	106.93
2	B	700	NAD	PN-O3-PA	-2.70	123.56	132.83
3	B	1612	FAD	C5A-C6A-N6A	-2.65	116.33	120.35
3	B	1612	FAD	C5X-C9A-N10	2.65	120.69	117.95
3	A	1612	FAD	C4X-C4-N3	2.61	119.83	113.19
2	D	701	NAD	PN-O3-PA	-2.60	123.91	132.83
3	B	1612	FAD	C4-N3-C2	-2.56	120.91	125.64
3	B	1612	FAD	C10-N1-C2	2.56	122.02	116.90
3	B	1612	FAD	C4X-C10-N10	2.54	120.19	116.48
3	D	1612	FAD	O4-C4-C4X	-2.54	119.87	126.60
3	B	1612	FAD	C4X-C10-N1	-2.51	118.89	124.73
2	A	700	NAD	C5A-C6A-N6A	-2.51	116.54	120.35
3	C	1612	FAD	O3'-C3'-C2'	2.50	114.85	108.81
3	D	1612	FAD	C6-C5X-C9A	2.49	122.47	118.94
2	B	700	NAD	C6N-N1N-C2N	-2.49	119.71	121.97
2	A	701	NAD	C3N-C7N-N7N	-2.47	114.79	117.75
3	C	1612	FAD	C4-C4X-C10	2.46	120.92	116.79
2	A	701	NAD	O7N-C7N-C3N	2.45	122.56	119.63
3	D	1612	FAD	C10-C4X-N5	-2.42	119.71	124.86
2	C	701	NAD	C2N-C3N-C4N	2.41	120.99	118.26
2	C	700	NAD	C5A-C6A-N6A	-2.40	116.70	120.35
3	B	1612	FAD	C9A-C5X-N5	-2.39	119.83	122.43
2	C	700	NAD	C3N-C7N-N7N	-2.39	114.89	117.75
3	B	1612	FAD	C4-C4X-C10	2.38	120.78	116.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1612	FAD	C4X-C4-N3	2.37	119.22	113.19
3	C	1612	FAD	O4-C4-N3	-2.37	115.58	120.12
2	D	700	NAD	C5A-C6A-N6A	-2.34	116.79	120.35
2	D	700	NAD	O4D-C1D-C2D	-2.33	103.53	106.93
2	C	701	NAD	C3B-C2B-C1B	2.32	104.47	100.98
2	B	700	NAD	C5A-C6A-N6A	-2.32	116.82	120.35
2	D	700	NAD	C3B-C2B-C1B	2.30	104.44	100.98
3	D	1612	FAD	C10-N1-C2	2.29	121.49	116.90
3	A	1612	FAD	C6-C5X-C9A	2.29	122.18	118.94
3	D	1612	FAD	C5X-N5-C4X	2.29	121.88	118.07
2	C	700	NAD	PN-O3-PA	-2.28	124.99	132.83
3	B	1612	FAD	C10-C4X-N5	-2.28	120.02	124.86
3	C	1612	FAD	C4A-C5A-N7A	-2.28	107.02	109.40
3	A	1612	FAD	C9A-C5X-N5	-2.27	119.97	122.43
3	B	1612	FAD	O4-C4-C4X	-2.24	120.65	126.60
3	C	1612	FAD	C10-N1-C2	2.24	121.39	116.90
3	B	1612	FAD	O3'-C3'-C2'	2.23	114.20	108.81
2	C	701	NAD	C3N-C7N-N7N	-2.23	115.08	117.75
3	A	1612	FAD	C4A-C5A-N7A	-2.20	107.11	109.40
3	C	1612	FAD	O5'-C5'-C4'	2.19	115.22	109.36
2	C	700	NAD	C6N-N1N-C2N	-2.19	119.98	121.97
3	D	1612	FAD	C5A-C6A-N6A	-2.17	117.05	120.35
2	D	701	NAD	O2A-PA-O1A	2.17	122.95	112.24
2	D	700	NAD	PN-O3-PA	-2.16	125.42	132.83
3	B	1612	FAD	C9A-N10-C10	-2.13	117.45	120.77
2	A	700	NAD	O2N-PN-O1N	2.13	122.75	112.24
3	D	1612	FAD	C5X-C9A-N10	2.12	120.14	117.95
3	B	1612	FAD	O3B-C3B-C4B	-2.11	104.95	111.05
2	A	700	NAD	C3N-C2N-N1N	-2.07	118.40	120.43
3	A	1612	FAD	O4-C4-C4X	-2.07	121.12	126.60
3	A	1612	FAD	C10-N1-C2	2.06	121.03	116.90
3	B	1612	FAD	C4'-C3'-C2'	2.06	117.65	113.36
3	C	1612	FAD	C9A-C5X-N5	-2.05	120.20	122.43
2	B	701	NAD	C5A-C6A-N6A	-2.03	117.26	120.35
2	A	701	NAD	C5D-C4D-C3D	-2.02	107.59	115.18
2	B	701	NAD	C3B-C2B-C1B	2.02	104.02	100.98
2	B	701	NAD	C4A-C5A-N7A	-2.01	107.30	109.40

There are no chirality outliers.

All (92) 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	C3B-C4B-C5B-O5B
2	A	701	NAD	O4D-C4D-C5D-O5D
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-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	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	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	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	O4B-C4B-C5B-O5B
2	A	701	NAD	C3B-C4B-C5B-O5B
2	C	701	NAD	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

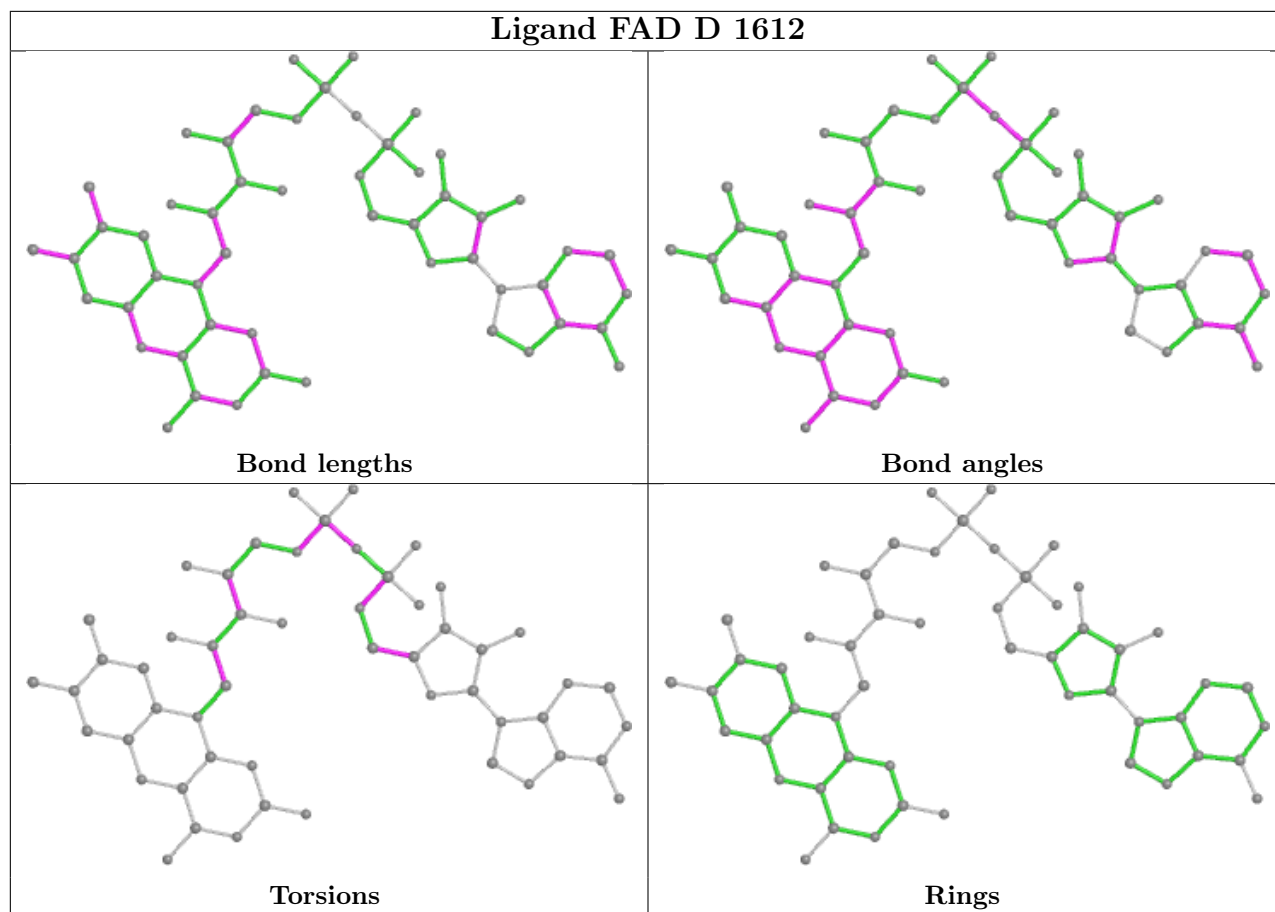
Mol	Chain	Res	Type	Atoms
2	D	700	NAD	PA-O3-PN-O2N
2	A	701	NAD	C5B-O5B-PA-O1A
2	D	700	NAD	C5B-O5B-PA-O1A
2	D	701	NAD	C5D-O5D-PN-O1N
2	C	701	NAD	C3D-C4D-C5D-O5D
2	D	701	NAD	C3D-C4D-C5D-O5D
3	D	1612	FAD	O4B-C4B-C5B-O5B

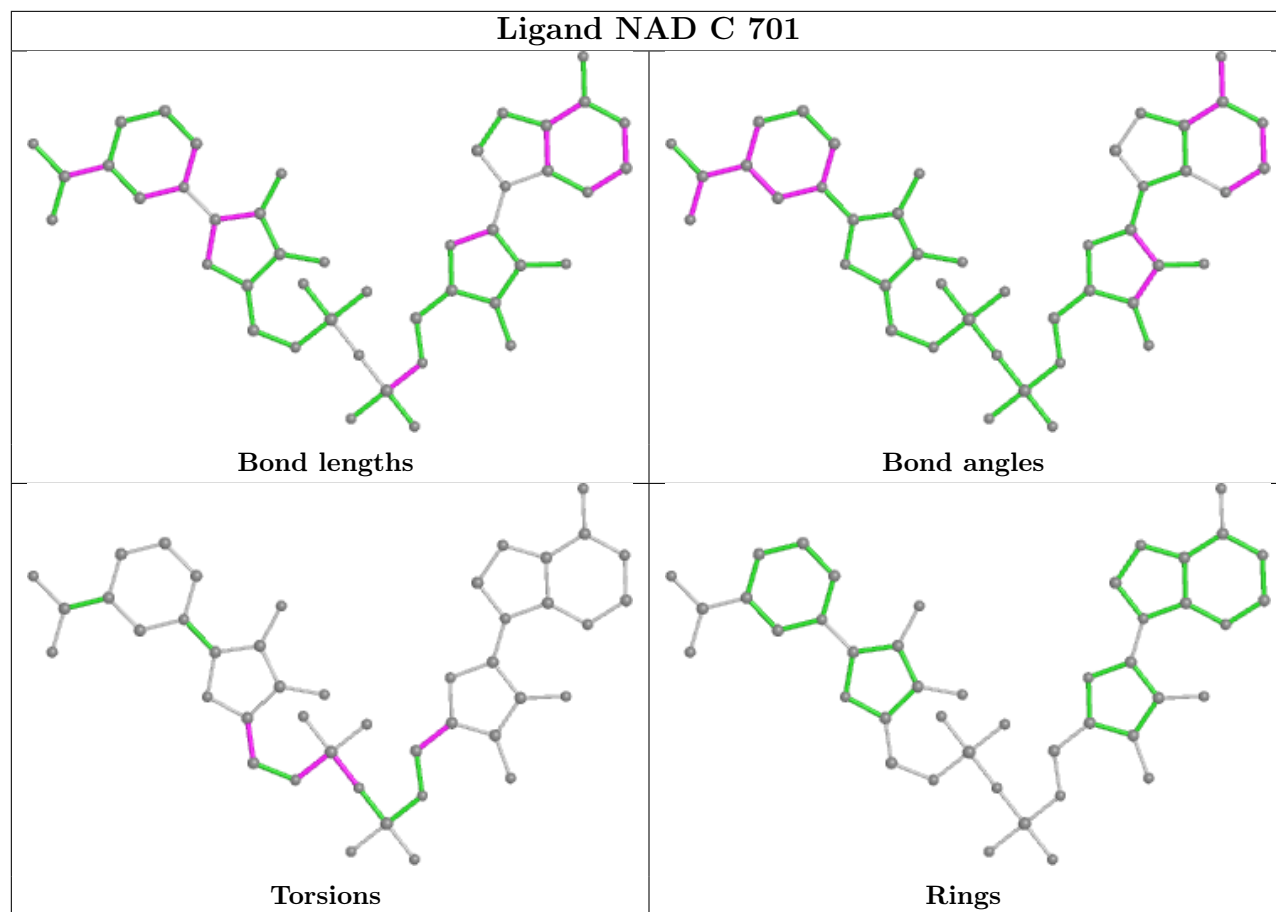
There are no ring outliers.

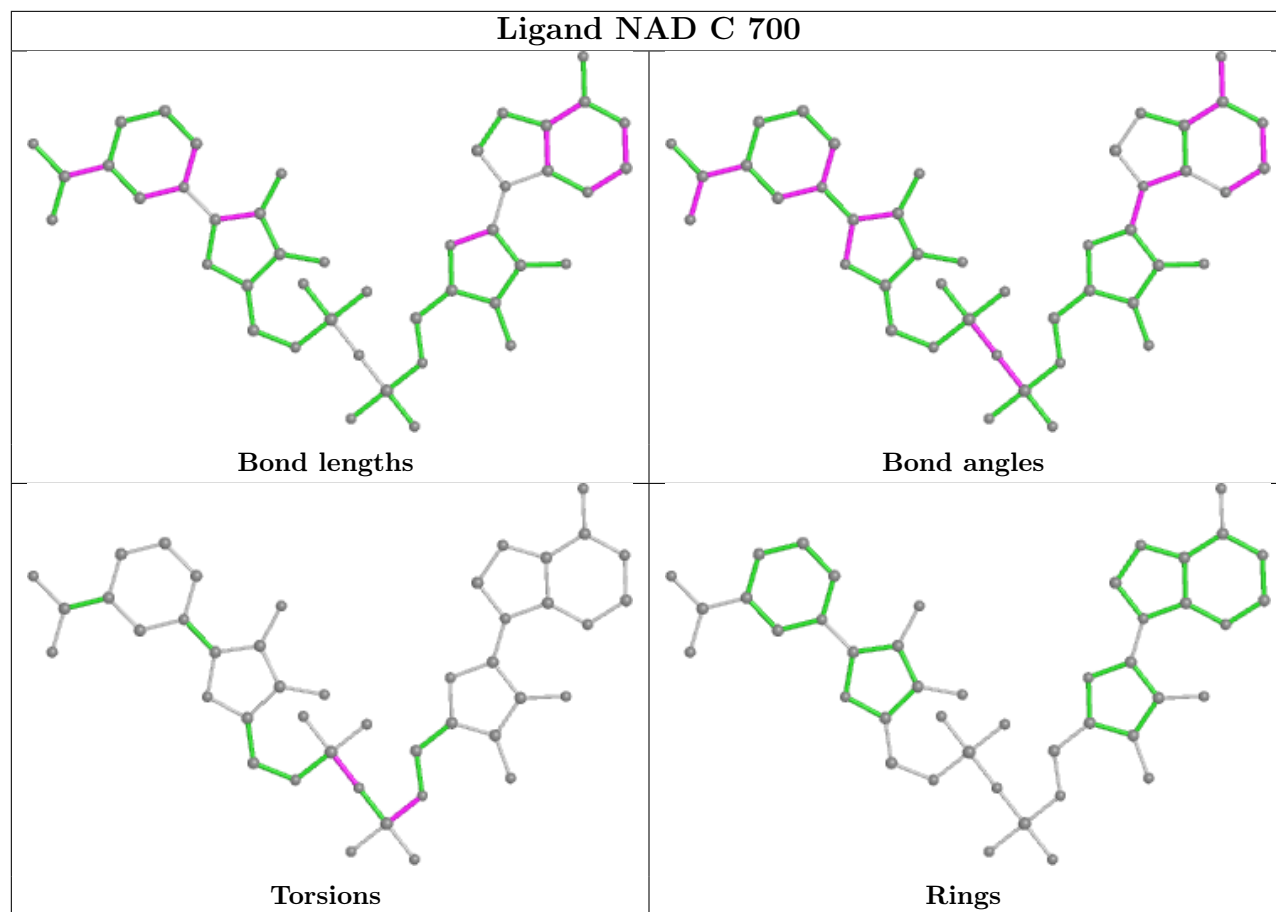
7 monomers are involved in 19 short contacts:

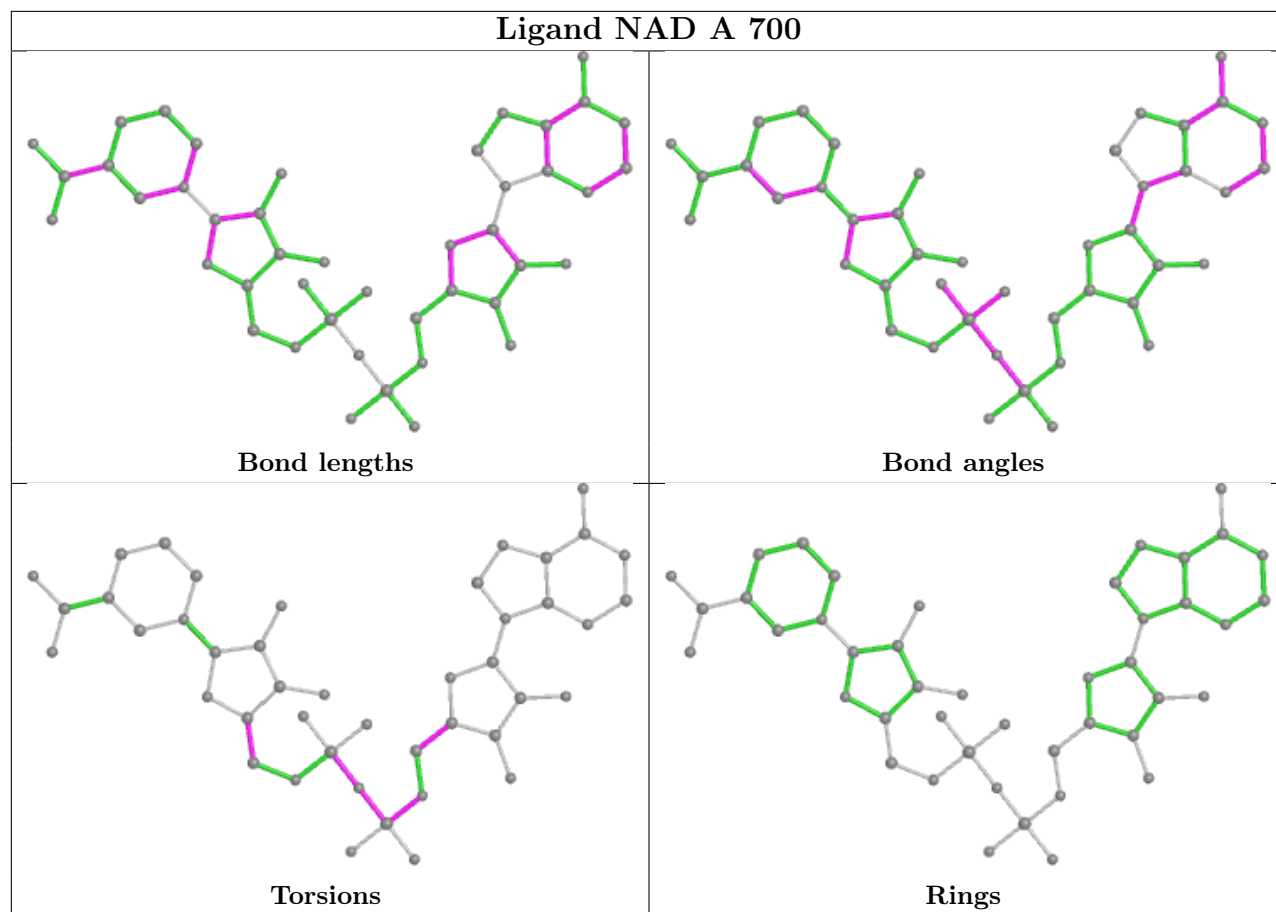
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1612	FAD	5	0
3	B	1612	FAD	5	0
2	B	700	NAD	1	0
3	C	1612	FAD	2	0
3	A	1612	FAD	4	0
2	D	700	NAD	1	0
2	B	701	NAD	1	0

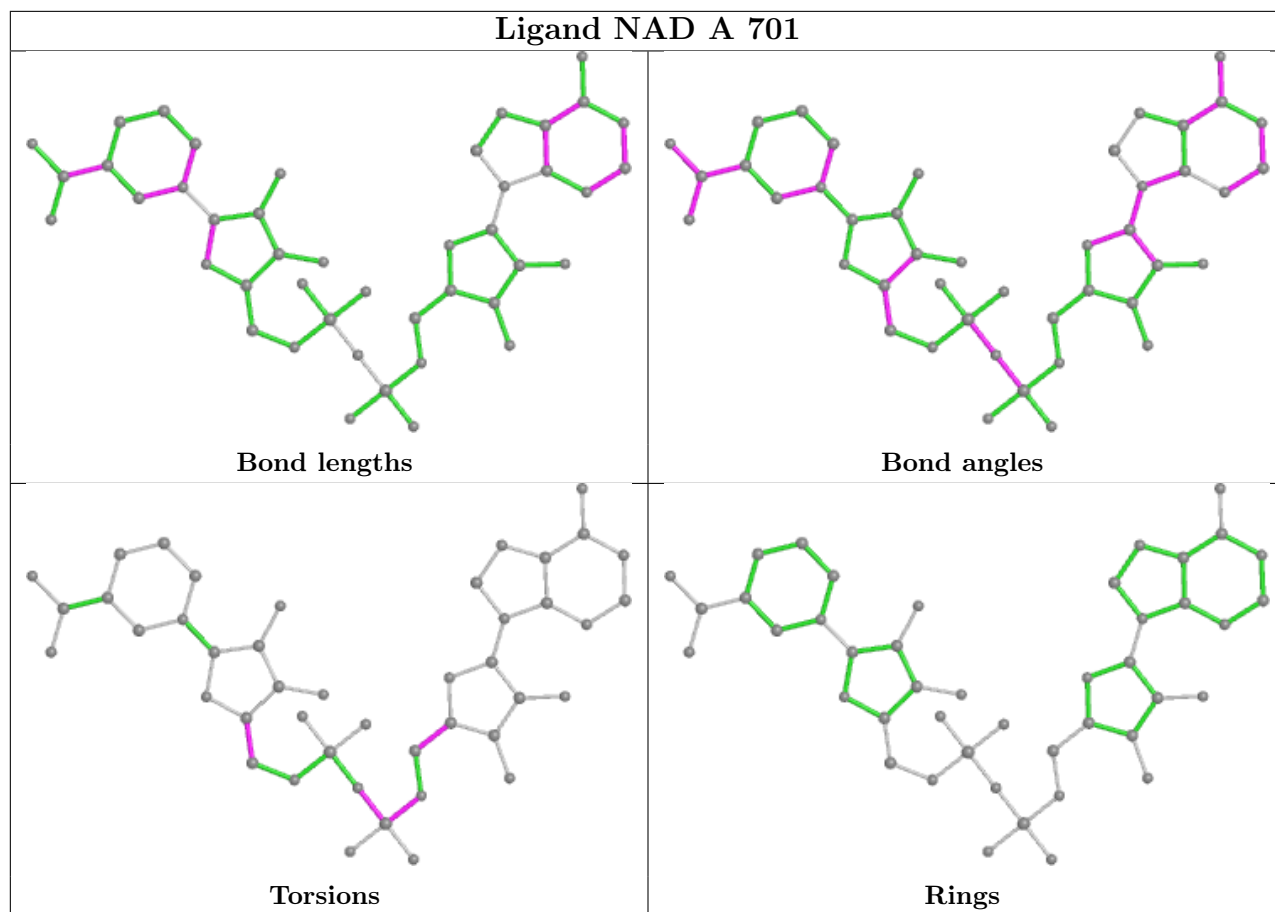
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

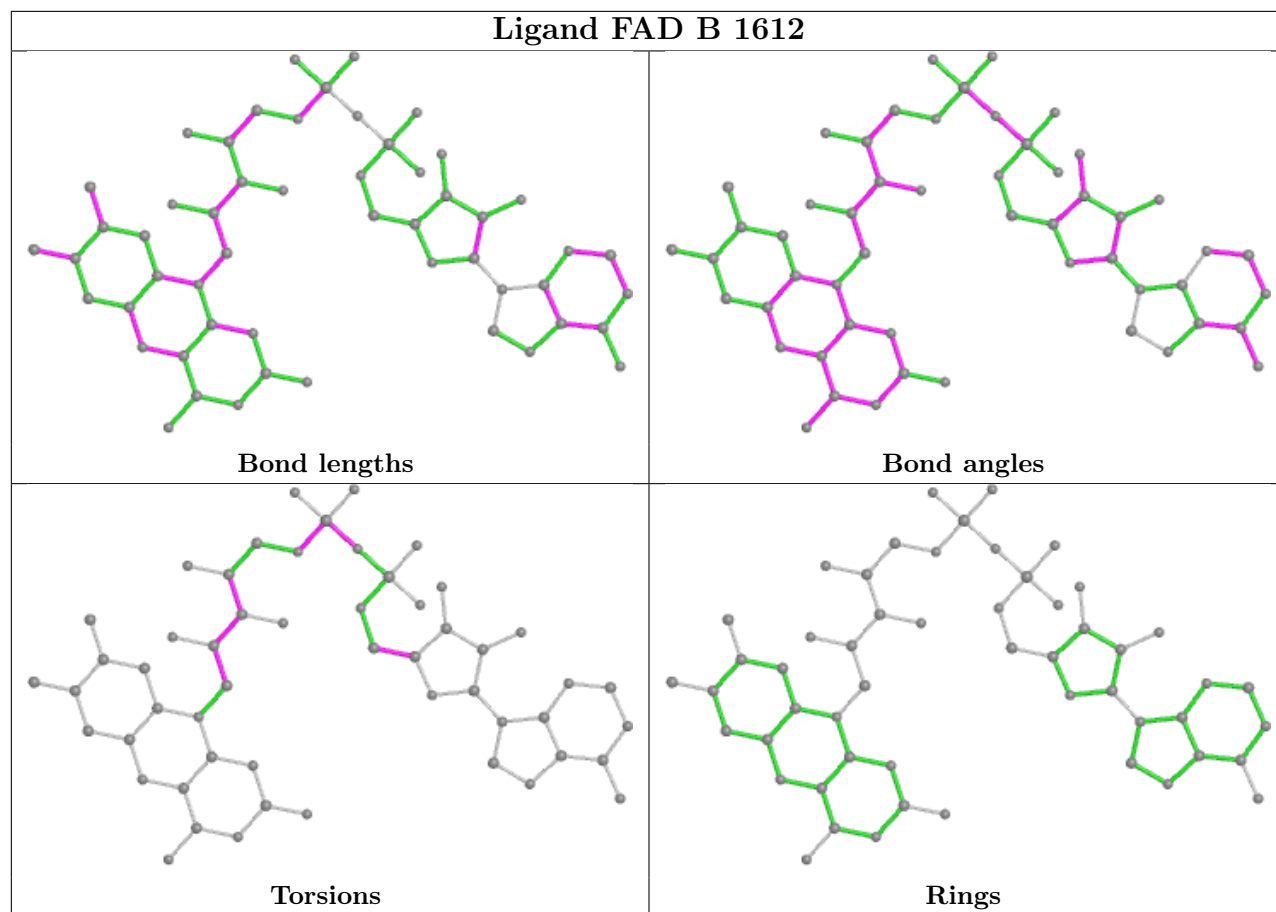


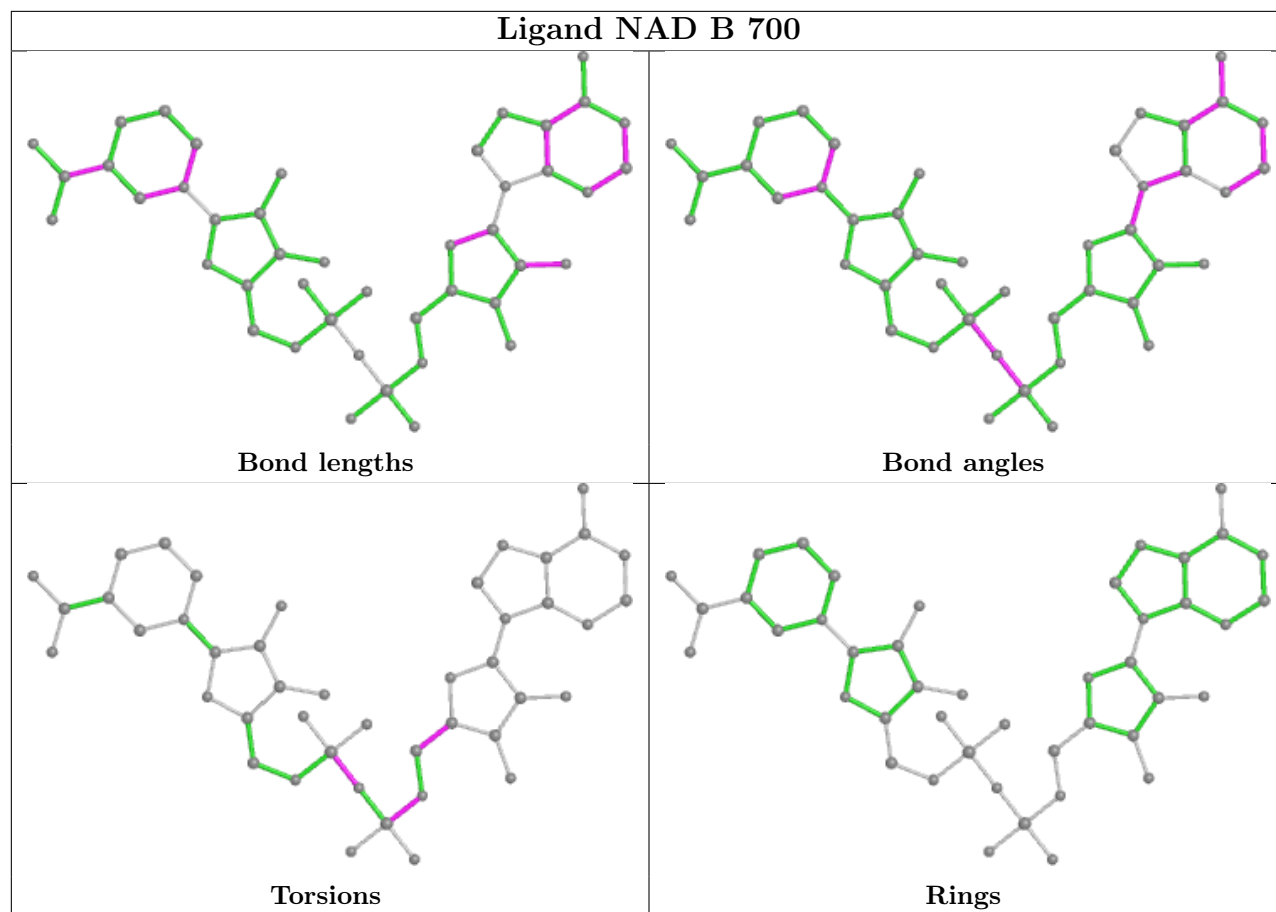


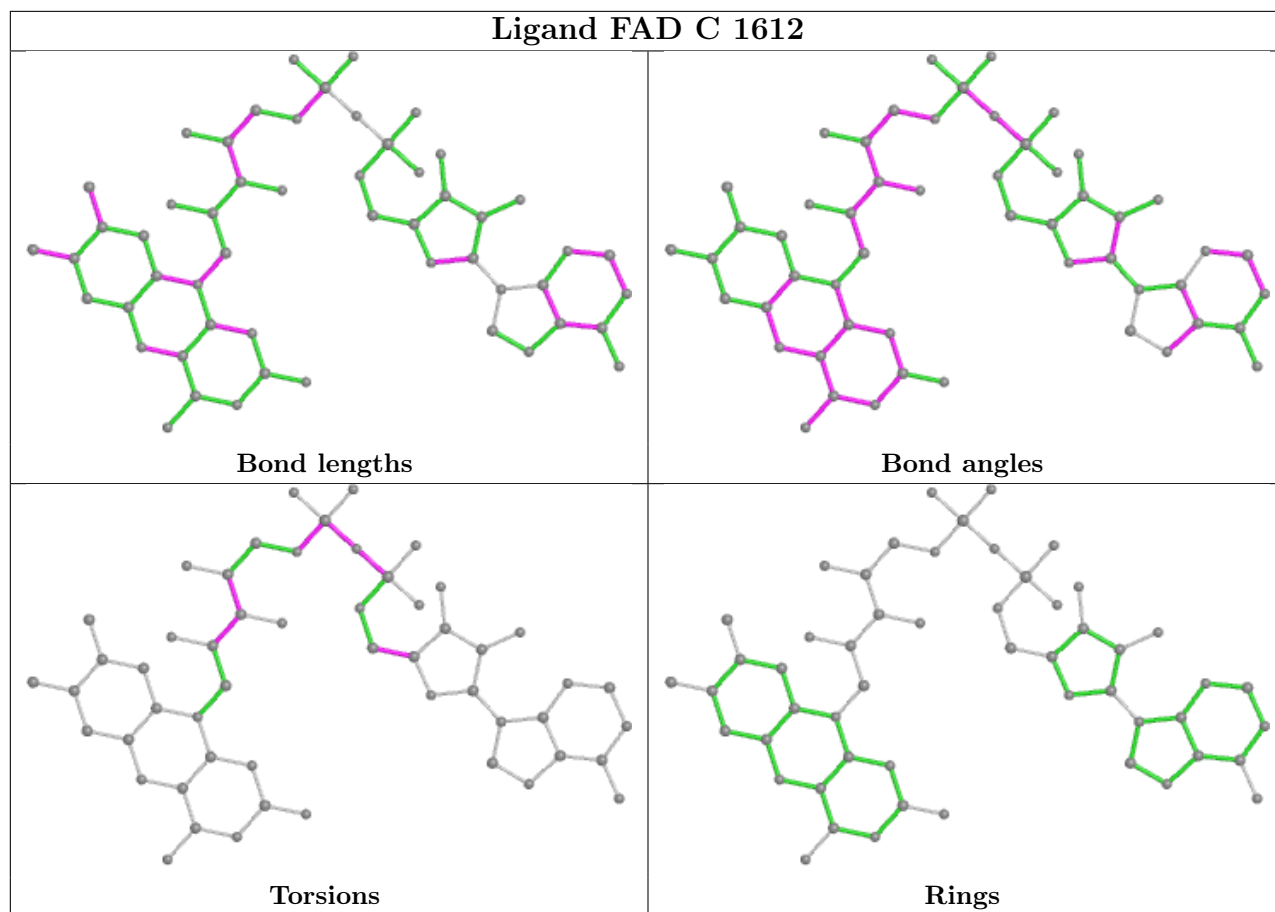


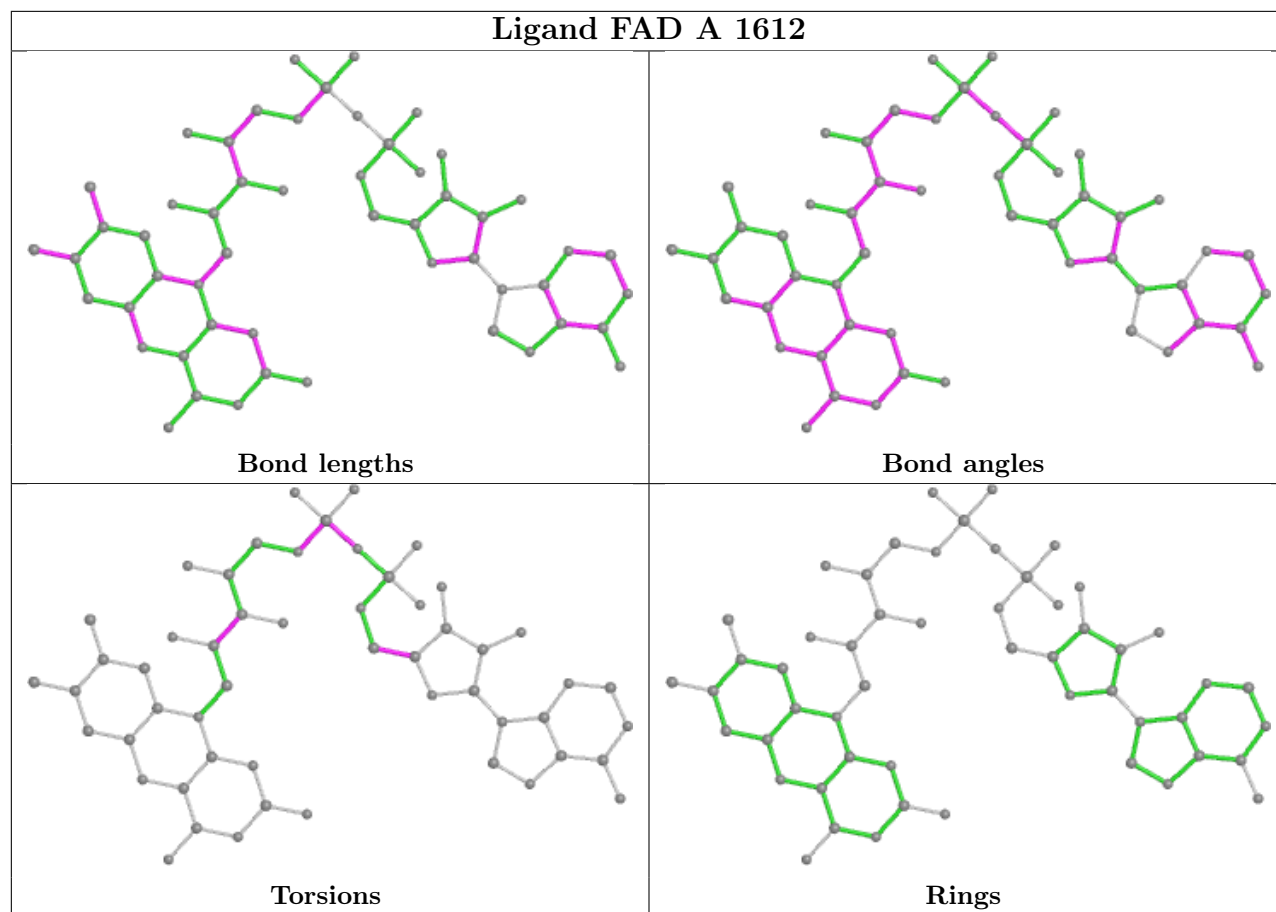


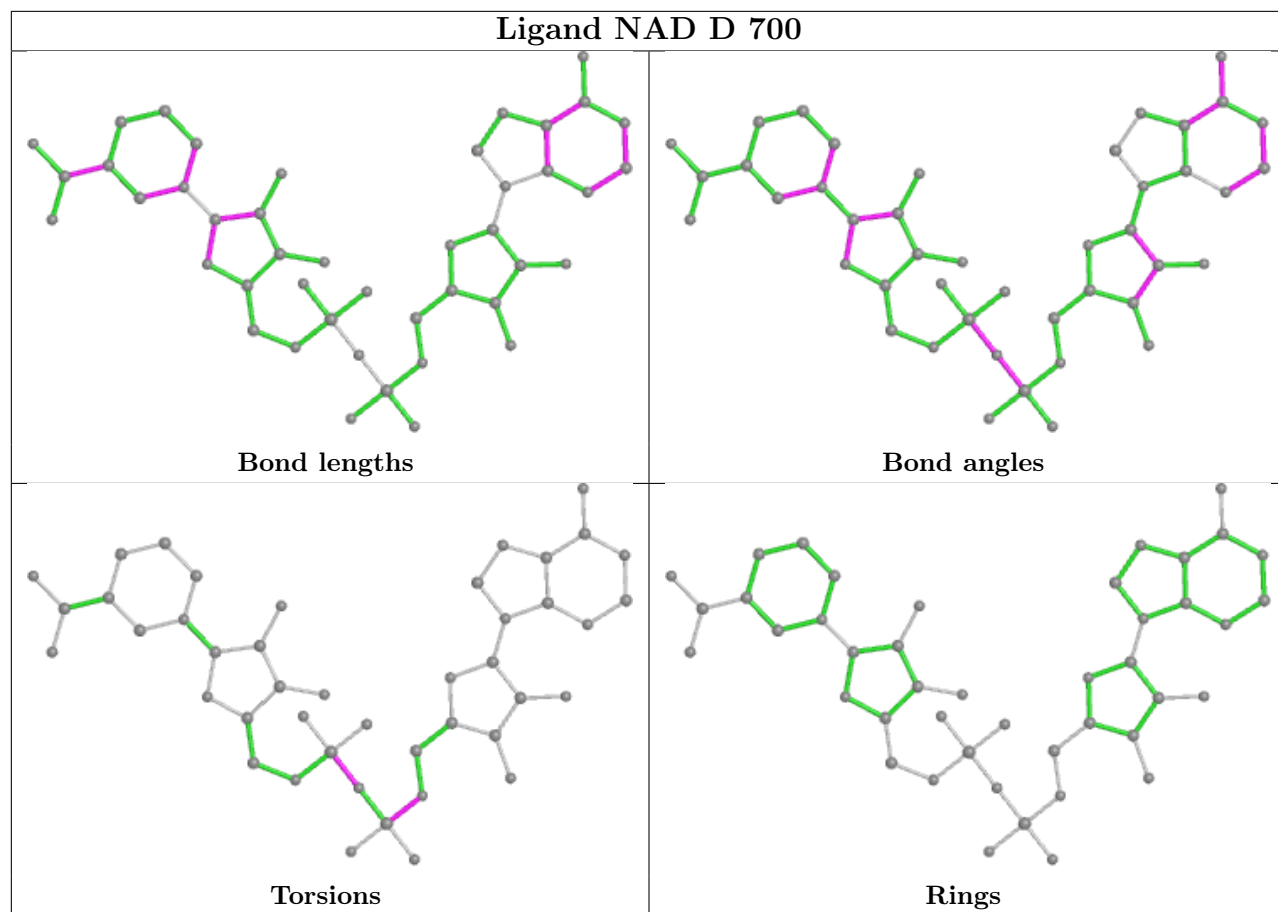


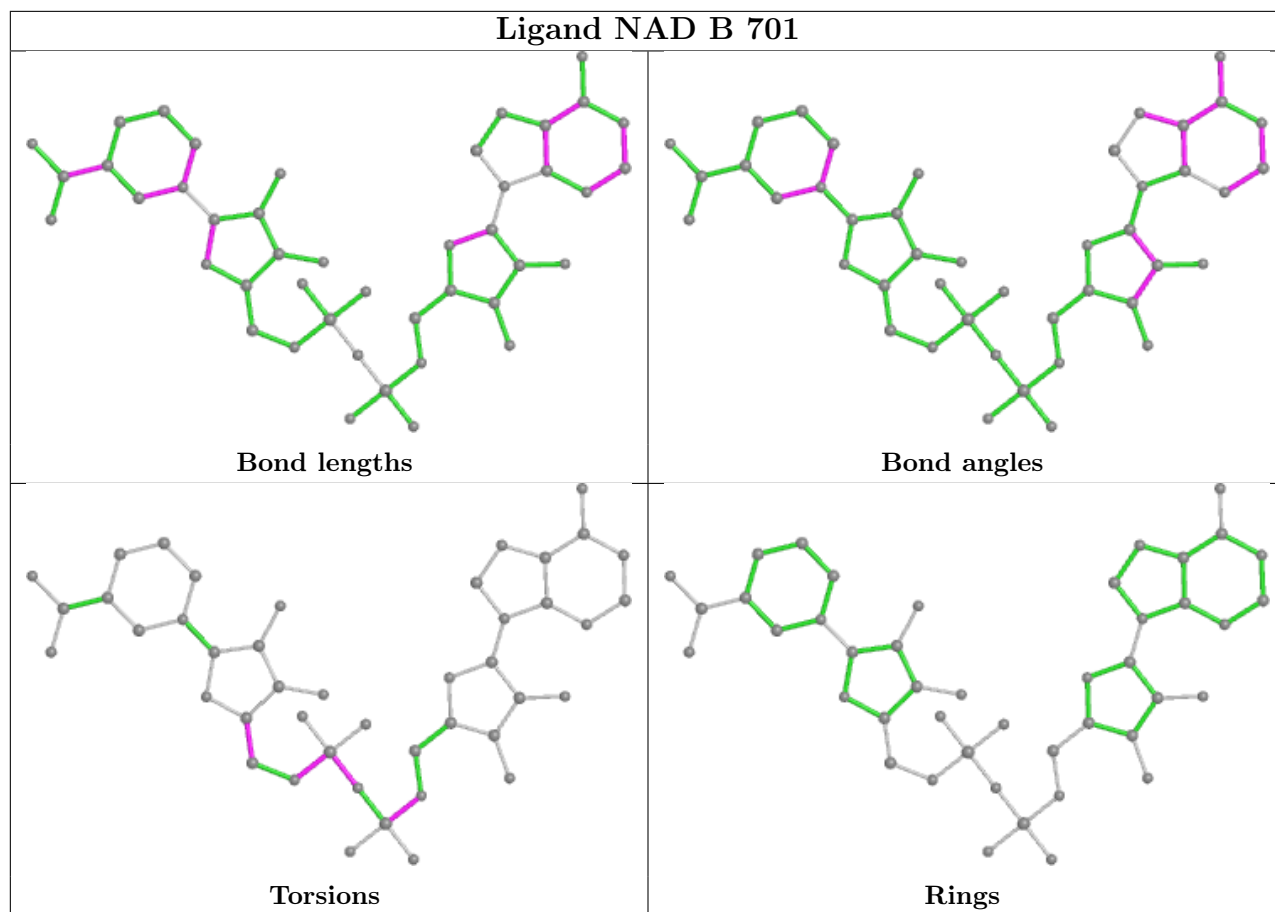


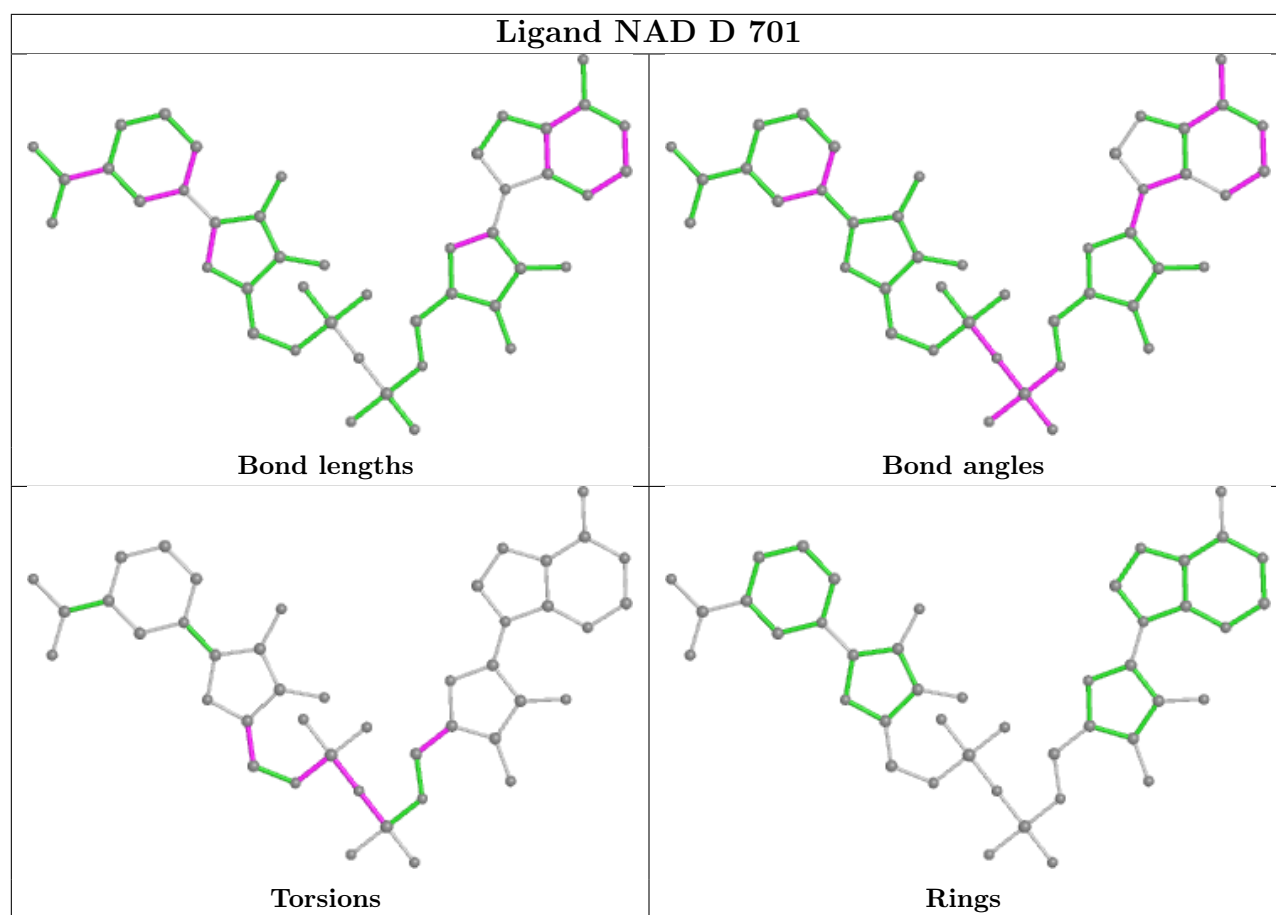












5.7 Other polymers [i](#)

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%)	0.11	2 (0%) 92 92	27, 42, 74, 111	0
1	B	450/511 (88%)	0.18	2 (0%) 92 92	30, 51, 81, 116	0
1	C	446/511 (87%)	0.16	1 (0%) 95 95	30, 52, 84, 100	0
1	D	435/511 (85%)	0.38	9 (2%) 63 62	39, 67, 104, 123	0
All	All	1781/2044 (87%)	0.21	14 (0%) 86 86	27, 53, 91, 123	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	LEU	2.6
1	A	128	ALA	2.6
1	D	325	ALA	2.5
1	A	611	HIS	2.4
1	D	326	LEU	2.4
1	B	193	PHE	2.3
1	D	390	GLU	2.3
1	D	303	ILE	2.2
1	B	196	TRP	2.2
1	D	394	ILE	2.1
1	D	228	LEU	2.1
1	C	187	VAL	2.1
1	D	306	ILE	2.0
1	D	381	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

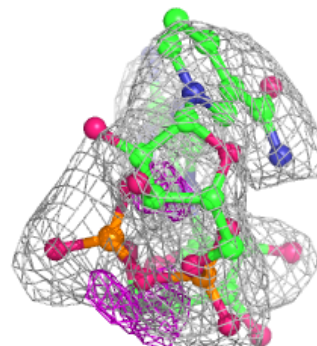
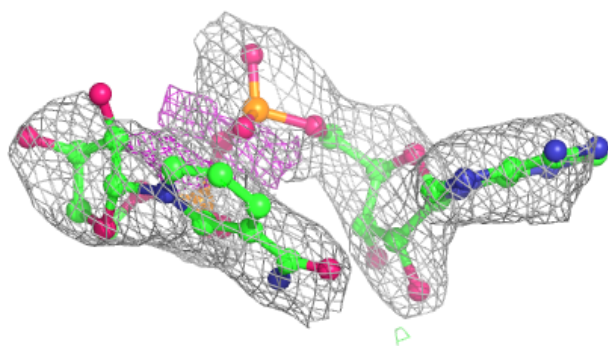
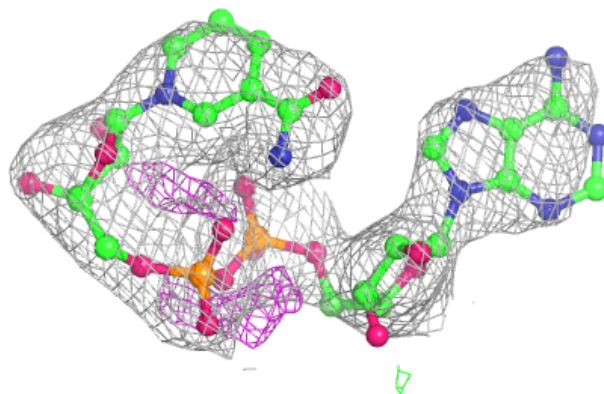
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	D	1613	5/5	0.90	0.17	72,74,86,89	0
2	NAD	B	701	44/44	0.92	0.28	74,102,110,116	0
2	NAD	A	701	44/44	0.93	0.25	71,87,104,112	0
2	NAD	D	701	44/44	0.94	0.25	71,97,111,112	0
2	NAD	C	701	44/44	0.96	0.22	61,70,81,86	0
2	NAD	D	700	44/44	0.96	0.19	36,57,79,82	0
3	FAD	D	1612	53/53	0.97	0.21	38,53,63,67	0
2	NAD	C	700	44/44	0.98	0.20	30,41,56,60	0
3	FAD	A	1612	53/53	0.98	0.20	22,33,40,43	0
3	FAD	B	1612	53/53	0.98	0.21	29,43,50,52	0
3	FAD	C	1612	53/53	0.98	0.20	30,39,50,54	0
2	NAD	B	700	44/44	0.98	0.19	27,41,49,49	0
2	NAD	A	700	44/44	0.98	0.19	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.

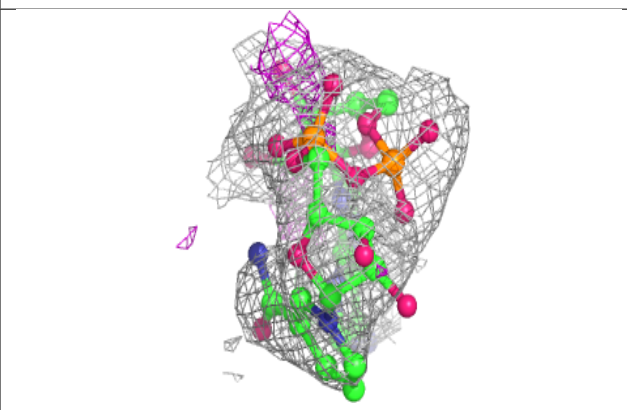
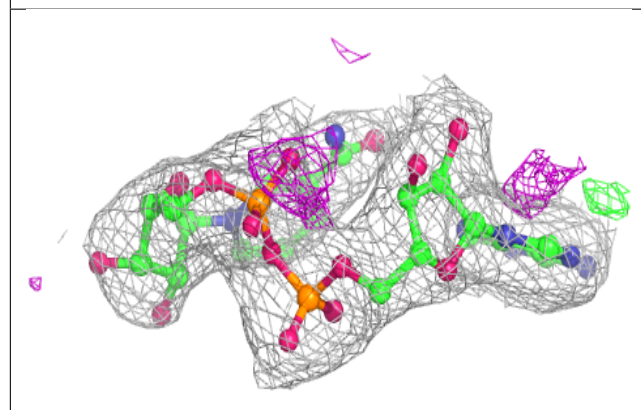
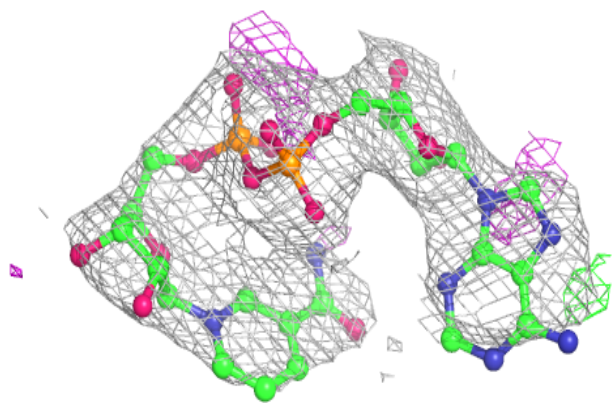
Electron density around NAD B 701:

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

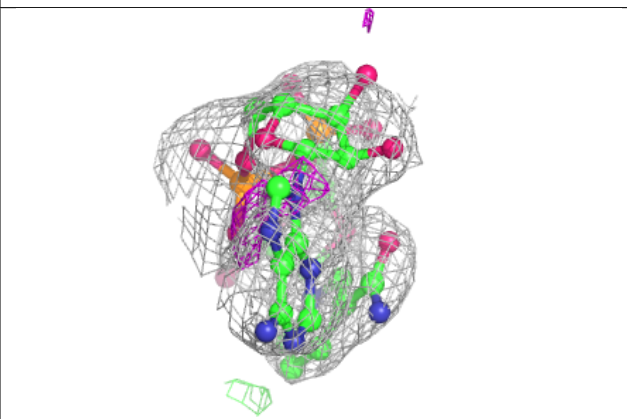
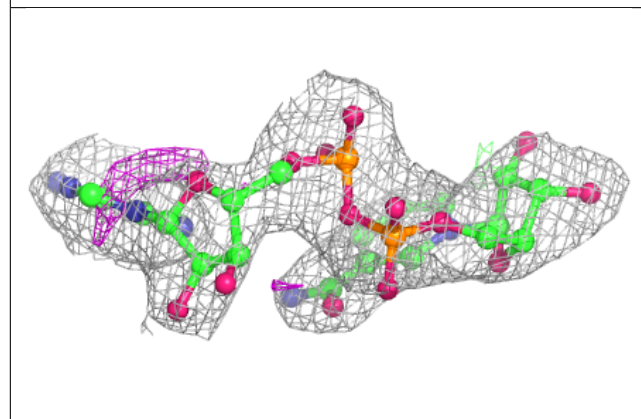
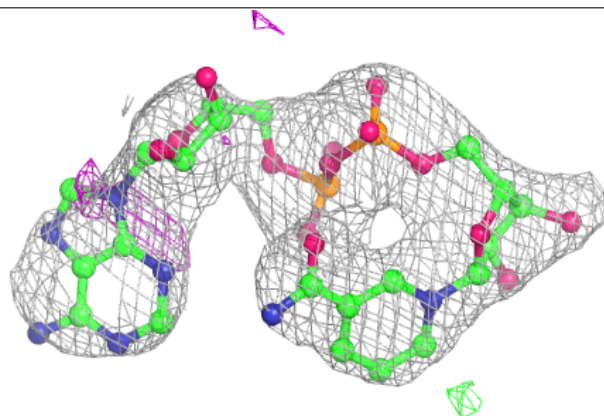


Electron density around NAD A 701:

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

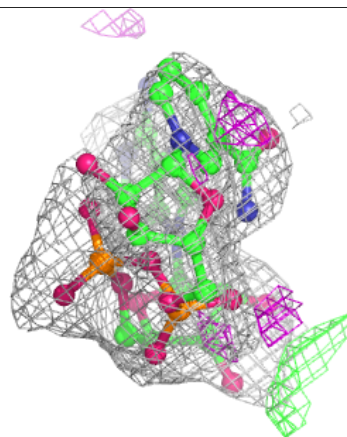
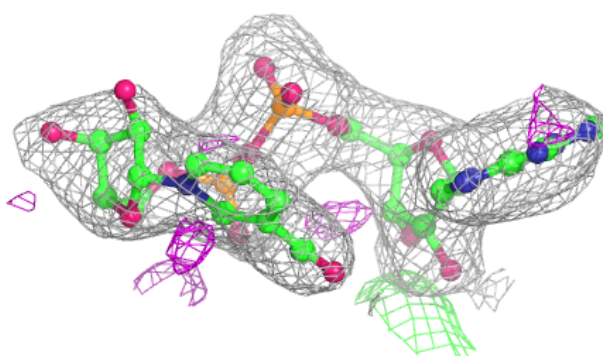
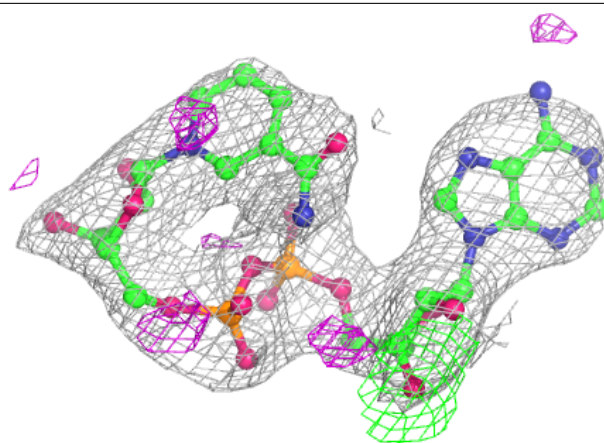
**Electron density around NAD D 701:**

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

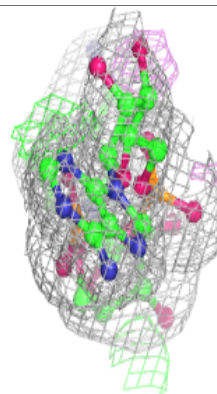
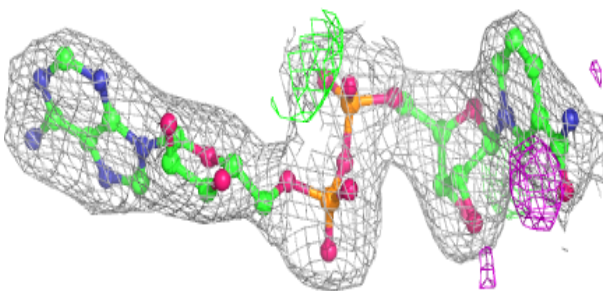
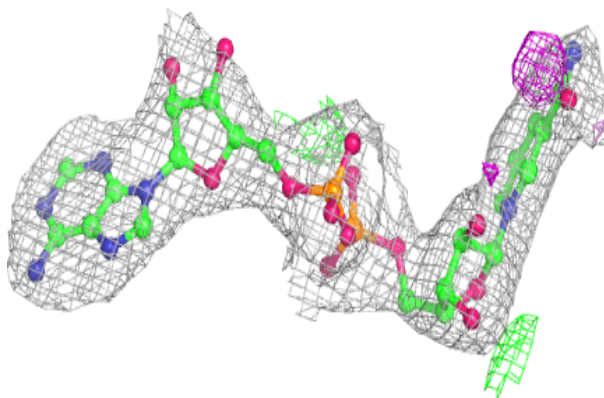


Electron density around NAD C 701:

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

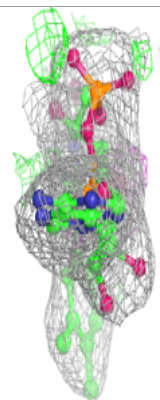
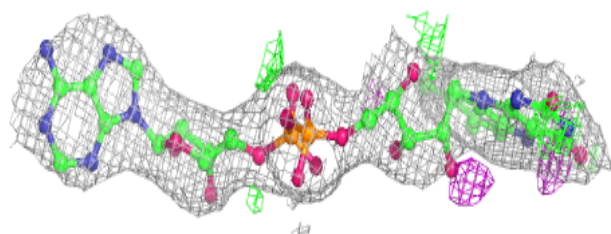
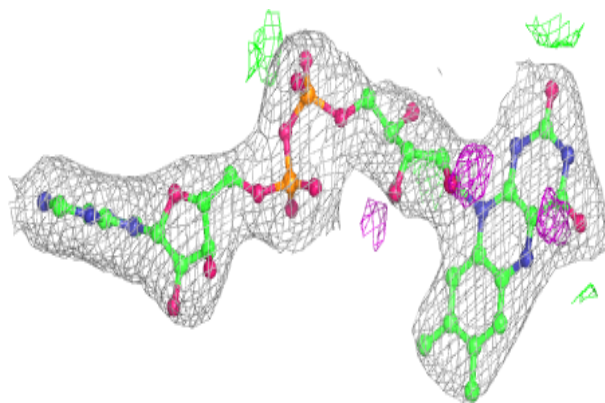
**Electron density around NAD D 700:**

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

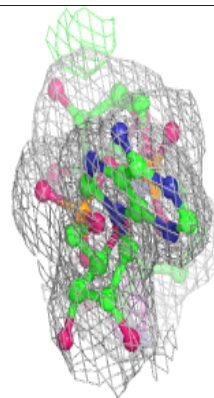
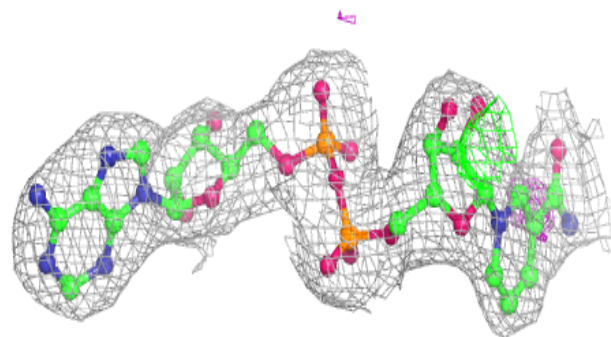
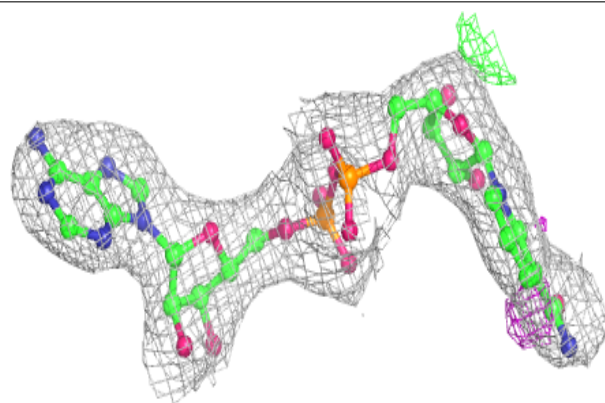


Electron density around FAD D 1612:

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

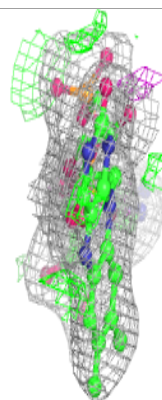
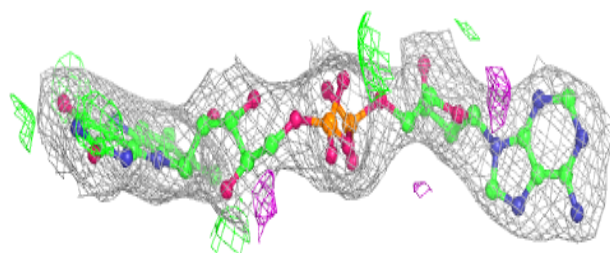
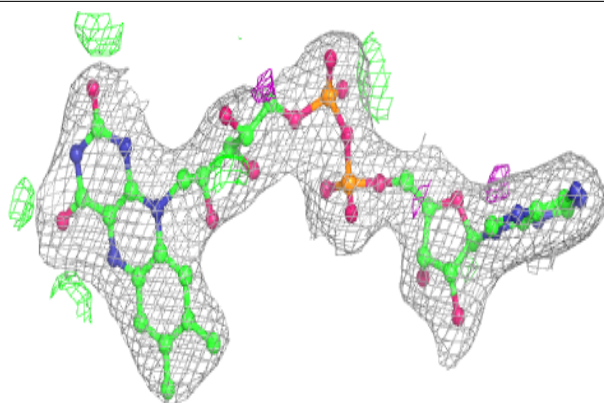
**Electron density around NAD C 700:**

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

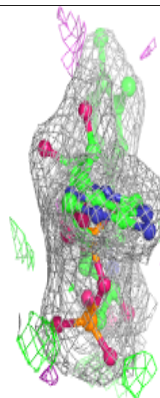
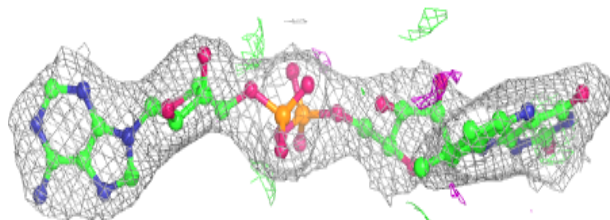
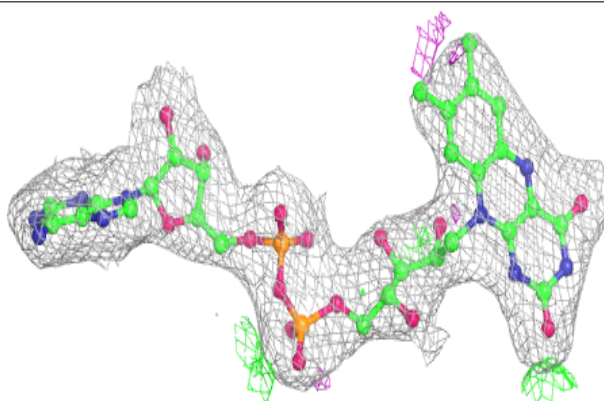


Electron density around FAD A 1612:

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

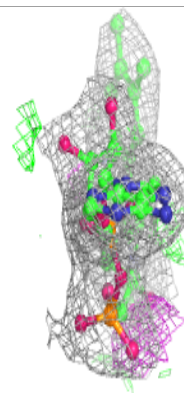
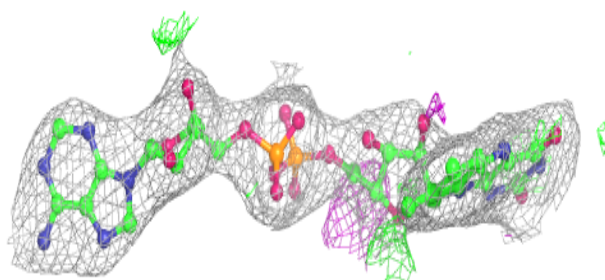
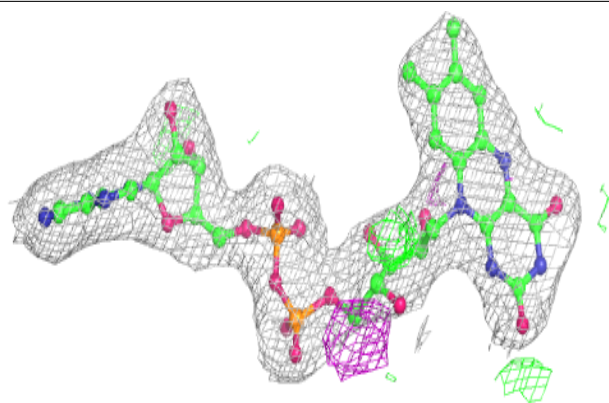
**Electron density around FAD B 1612:**

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

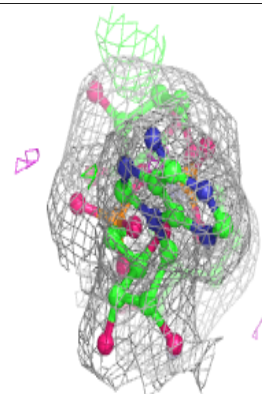
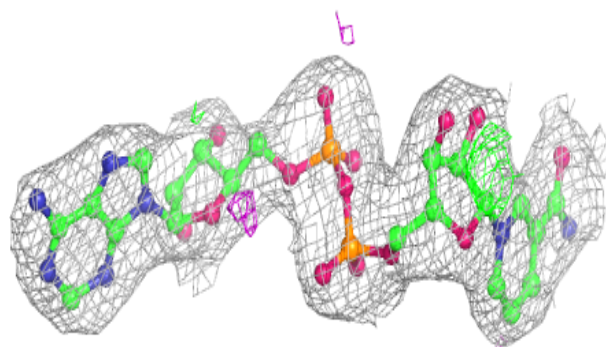
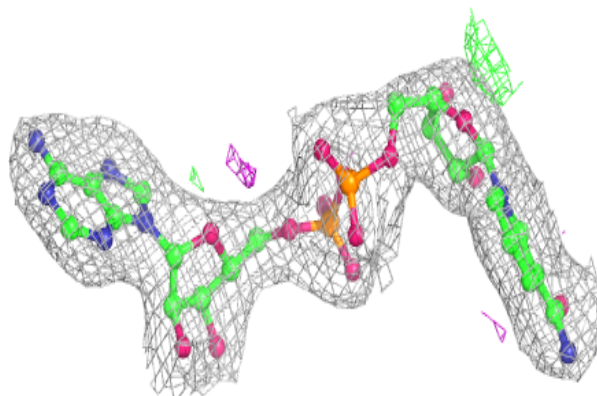


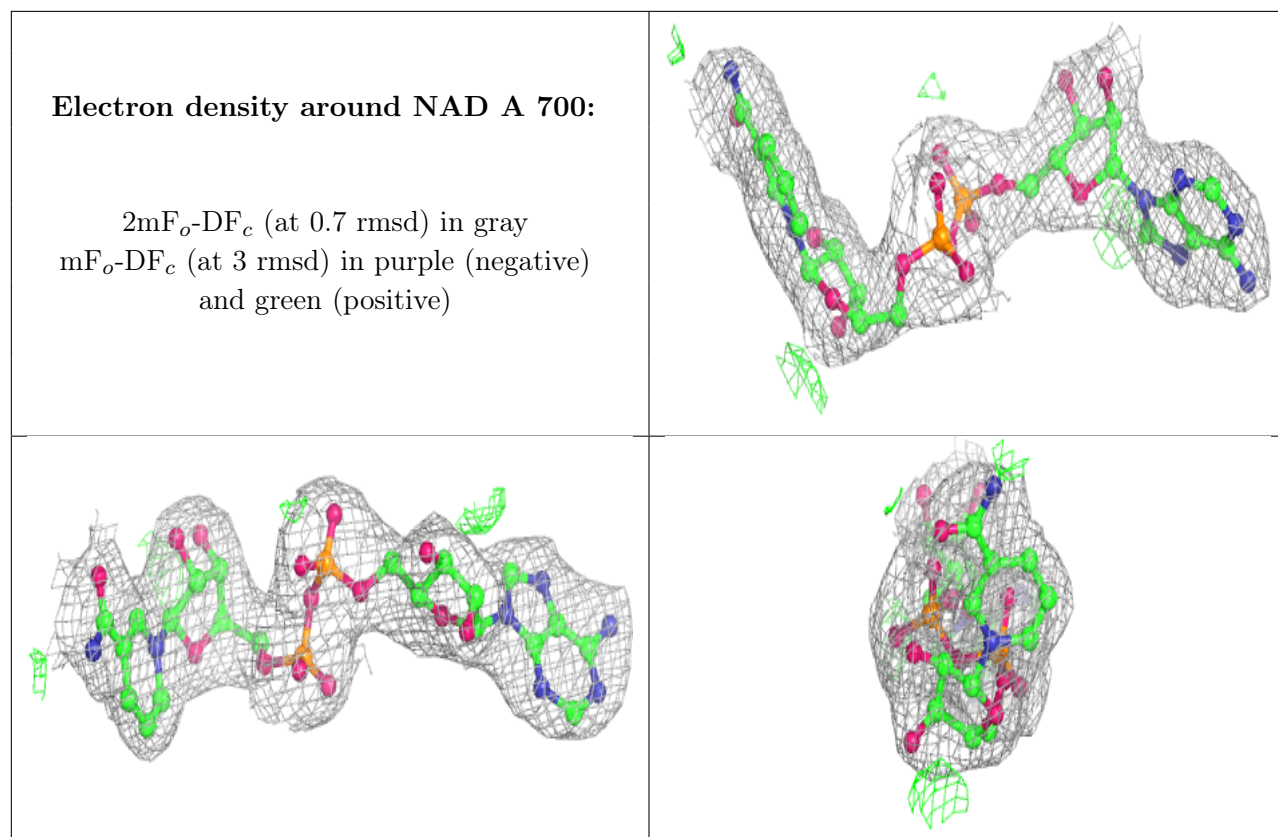
Electron density around FAD C 1612:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.