



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 5KMR / pdb_00005kmr
Title : The structure of type II NADH dehydrogenase from *Caldalkalibacillus thermarum* complexed with NAD⁺ at 3.0 angstrom resolution.
Authors : Cook, G.M.; Aragao, D.; Nakatani, Y.
Deposited on : 2016-06-27
Resolution : 3.00 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

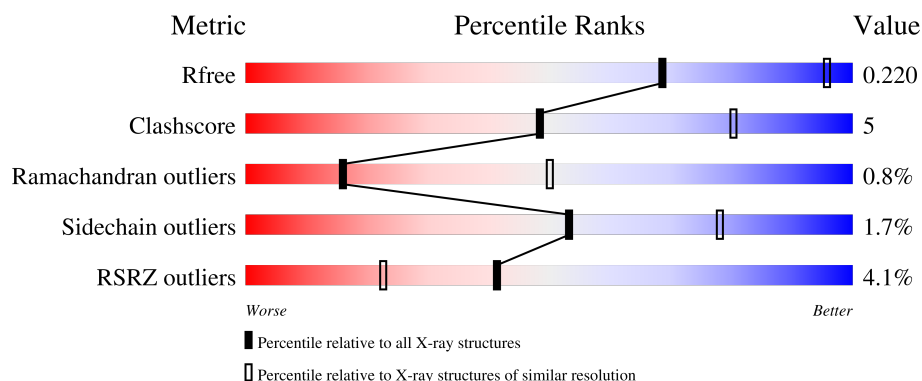
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	405	5% 79% 17% ..
1	B	405	3% 84% 12% .
1	C	405	7% 84% 13% .
1	D	405	% 85% 12% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11468 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 FAD-dependent pyridine nucleotide-disulfide oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	394	Total	C	N	O	S	0	0	0
			2845	1823	489	525	8			
1	A	393	Total	C	N	O	S	0	0	0
			2815	1809	485	513	8			
1	C	391	Total	C	N	O	S	0	0	0
			2640	1684	458	491	7			
1	D	394	Total	C	N	O	S	0	0	0
			2807	1798	483	518	8			

There are 24 discrepancies between the modelled and reference sequences:

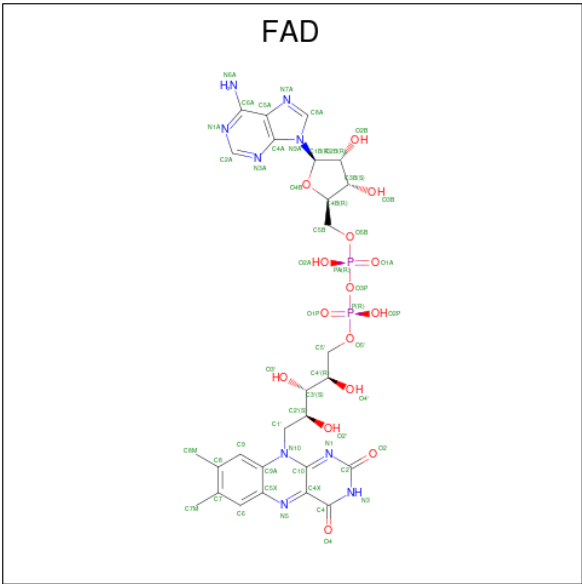
Chain	Residue	Modelled	Actual	Comment	Reference
B	400	HIS	-	expression tag	UNP F5L3B8
B	401	HIS	-	expression tag	UNP F5L3B8
B	402	HIS	-	expression tag	UNP F5L3B8
B	403	HIS	-	expression tag	UNP F5L3B8
B	404	HIS	-	expression tag	UNP F5L3B8
B	405	HIS	-	expression tag	UNP F5L3B8
A	400	HIS	-	expression tag	UNP F5L3B8
A	401	HIS	-	expression tag	UNP F5L3B8
A	402	HIS	-	expression tag	UNP F5L3B8
A	403	HIS	-	expression tag	UNP F5L3B8
A	404	HIS	-	expression tag	UNP F5L3B8
A	405	HIS	-	expression tag	UNP F5L3B8
C	400	HIS	-	expression tag	UNP F5L3B8
C	401	HIS	-	expression tag	UNP F5L3B8
C	402	HIS	-	expression tag	UNP F5L3B8
C	403	HIS	-	expression tag	UNP F5L3B8
C	404	HIS	-	expression tag	UNP F5L3B8
C	405	HIS	-	expression tag	UNP F5L3B8
D	400	HIS	-	expression tag	UNP F5L3B8
D	401	HIS	-	expression tag	UNP F5L3B8
D	402	HIS	-	expression tag	UNP F5L3B8

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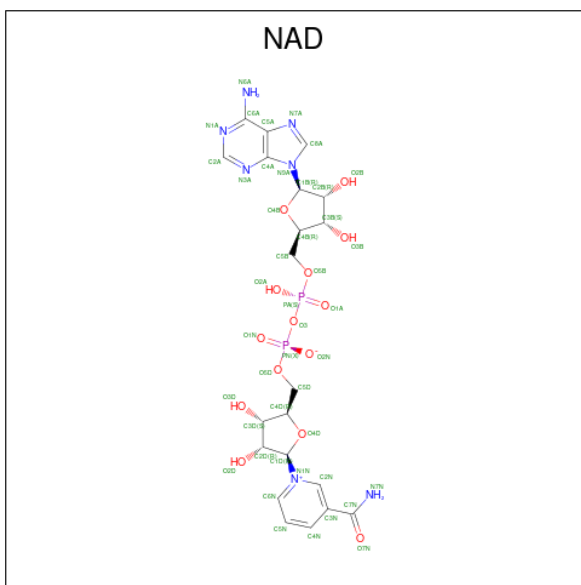
Chain	Residue	Modelled	Actual	Comment	Reference
D	403	HIS	-	expression tag	UNP F5L3B8
D	404	HIS	-	expression tag	UNP F5L3B8
D	405	HIS	-	expression tag	UNP F5L3B8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

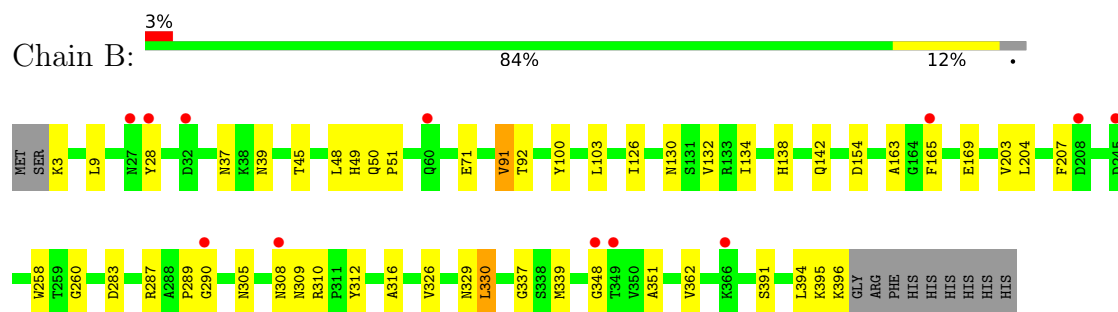
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total O 3 3	0	0
4	A	8	Total O 8 8	0	0
4	C	3	Total O 3 3	0	0
4	D	3	Total O 3 3	0	0

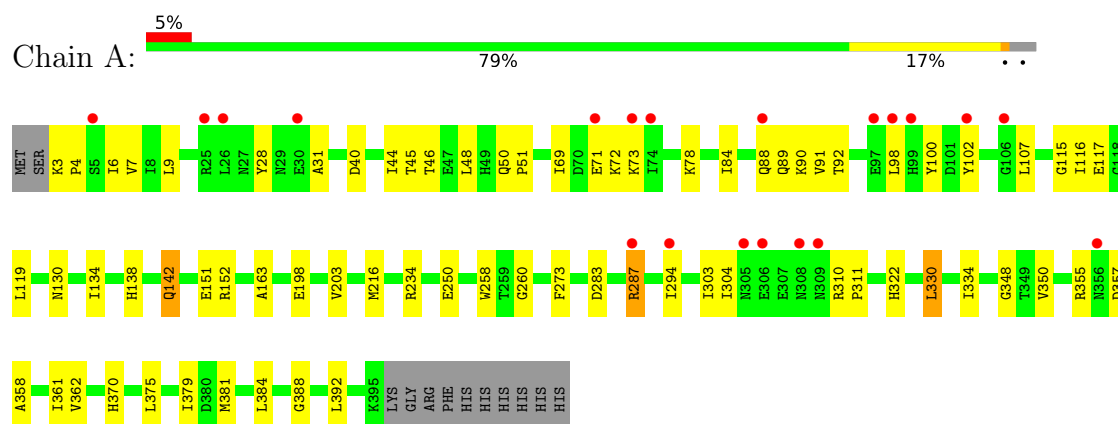
3 Residue-property plots [i](#)

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.

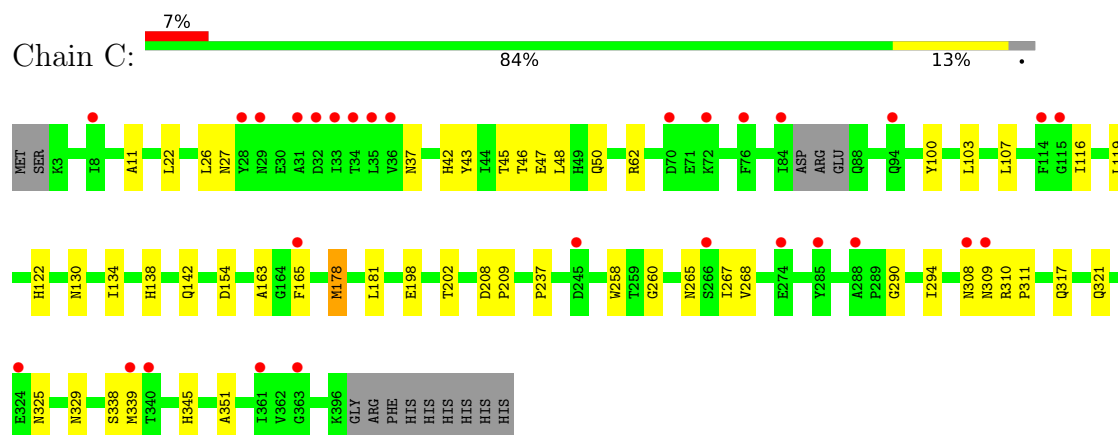
- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



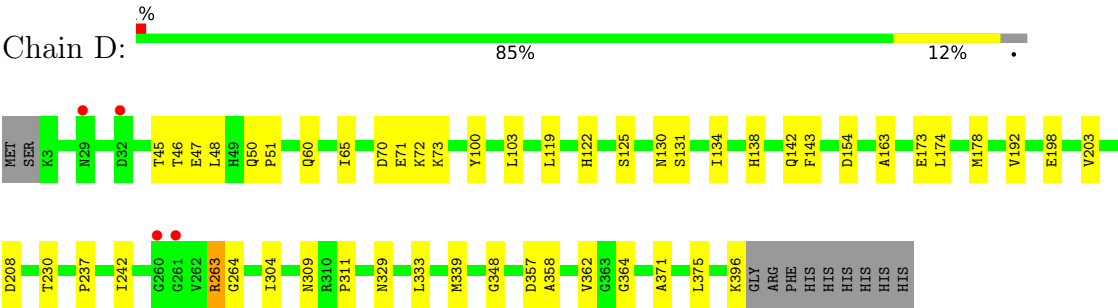
- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



- Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



● Molecule 1: FAD-dependent pyridine nucleotide-disulfide oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.06Å 114.21Å 130.96Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	43.64 – 3.00 43.64 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (43.64-3.00) 99.0 (43.64-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.237 , 0.254 (Not available) , 0.220	Depositor DCC
R_{free} test set	2134 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11468	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: FAD, 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	0.30	0/2873	0.79	4/3930 (0.1%)
1	B	0.30	0/2902	0.77	2/3967 (0.1%)
1	C	0.31	0/2688	0.80	1/3689 (0.0%)
1	D	0.30	0/2861	0.76	2/3910 (0.1%)
All	All	0.30	0/11324	0.78	9/15496 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	LYS	CA-C-N	-7.10	112.61	120.14
1	A	3	LYS	C-N-CA	-7.10	112.61	120.14
1	C	290	GLY	N-CA-C	-6.90	105.06	115.00
1	B	3	LYS	CA-C-N	-5.41	114.41	120.14
1	B	3	LYS	C-N-CA	-5.41	114.41	120.14
1	A	310	ARG	CA-C-N	5.38	125.58	120.31
1	A	310	ARG	C-N-CA	5.38	125.58	120.31
1	D	208	ASP	CA-C-N	5.20	125.00	119.28
1	D	208	ASP	C-N-CA	5.20	125.00	119.28

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	2815	0	2681	36	0
1	B	2845	0	2720	25	0
1	C	2640	0	2385	29	0
1	D	2807	0	2678	31	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
3	A	44	0	25	2	0
3	C	44	0	24	0	0
3	D	44	0	25	1	0
4	A	8	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
All	All	11468	0	10662	121	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 (121) 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:C:11:ALA:H	1:C:37:ASN:HD22	1.32	0.76
1:D:125:SER:O	1:D:131:SER:OG	2.07	0.70
1:C:325:ASN:ND2	1:C:329:ASN:OD1	2.24	0.70
1:C:103:LEU:HB3	1:C:294:ILE:HG13	1.74	0.69
1:A:348:GLY:HA3	1:A:362:VAL:HA	1.76	0.68
1:A:69:ILE:HG22	1:A:71:GLU:H	1.60	0.66
1:A:283:ASP:OD2	1:A:287:ARG:NE	2.25	0.65
1:D:198:GLU:OE2	3:D:602:NAD:O2B	2.16	0.63
1:A:71:GLU:O	1:A:73:LYS:N	2.28	0.62
1:D:333:LEU:HD13	1:D:339:MET:HE3	1.82	0.62
1:D:50:GLN:HA	1:D:173:GLU:HG2	1.83	0.61
1:D:178:MET:HE2	1:D:192:VAL:HG11	1.83	0.61
1:A:138:HIS:O	1:A:142:GLN:NE2	2.35	0.60
1:C:47:GLU:OE2	1:C:50:GLN:NE2	2.38	0.56
1:D:263:ARG:HD3	1:D:264:GLY:O	2.06	0.55
1:D:60:GLN:OE1	1:D:396:LYS:NZ	2.40	0.55
1:D:163:ALA:HB1	1:D:203:VAL:HG13	1.88	0.54
1:B:283:ASP:OD1	1:B:287:ARG:HG2	2.07	0.54
1:C:163:ALA:HB3	1:C:198:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASN:O	1:B:310:ARG:N	2.41	0.54
1:C:22:LEU:O	1:C:26:LEU:HG	2.08	0.53
1:B:45:THR:HA	1:B:48:LEU:HG	1.90	0.53
1:B:329:ASN:HB3	1:B:339:MET:HE2	1.91	0.52
1:B:316:ALA:HB2	2:B:601:FAD:H2'	1.92	0.51
1:D:45:THR:HA	1:D:48:LEU:HG	1.93	0.51
1:B:9:LEU:HD11	1:B:91:VAL:HG11	1.92	0.51
1:A:350:VAL:O	3:A:602:NAD:N7N	2.44	0.51
1:C:258:TRP:CZ2	1:C:260:GLY:HA3	2.47	0.50
1:B:348:GLY:HA3	1:B:362:VAL:HA	1.93	0.50
1:A:4:PRO:HD2	1:A:31:ALA:HA	1.94	0.50
1:C:265:ASN:O	1:C:268:VAL:HG12	2.12	0.50
1:C:165:PHE:CZ	1:C:351:ALA:HB2	2.47	0.49
1:C:46:THR:HA	2:C:601:FAD:C5X	2.43	0.49
1:C:138:HIS:O	1:C:142:GLN:HG2	2.13	0.49
1:D:348:GLY:HA3	1:D:362:VAL:HA	1.94	0.49
1:A:50:GLN:HB2	1:A:51:PRO:HD3	1.93	0.48
1:B:308:ASN:C	1:B:310:ARG:H	2.22	0.48
1:B:138:HIS:O	1:B:142:GLN:HG2	2.13	0.48
1:A:163:ALA:HB1	1:A:203:VAL:HG13	1.95	0.48
1:C:321:GLN:NE2	1:C:345:HIS:O	2.42	0.48
1:D:70:ASP:O	1:D:72:LYS:N	2.47	0.48
1:A:304:ILE:HA	1:A:311:PRO:HA	1.95	0.48
1:D:50:GLN:HB2	1:D:51:PRO:HD3	1.96	0.48
1:B:50:GLN:HB2	1:B:51:PRO:HD3	1.96	0.47
1:A:46:THR:HA	2:A:601:FAD:C5X	2.44	0.47
1:D:47:GLU:OE2	1:D:50:GLN:NE2	2.48	0.47
1:D:143:PHE:CE2	1:D:178:MET:HE1	2.50	0.47
1:C:45:THR:HA	1:C:48:LEU:HG	1.97	0.46
1:B:130:ASN:O	1:B:134:ILE:HG13	2.15	0.46
1:D:138:HIS:O	1:D:142:GLN:HG2	2.15	0.46
1:D:230:THR:HG21	1:D:242:ILE:HD12	1.97	0.46
1:B:305:ASN:ND2	1:B:312:TYR:OH	2.49	0.46
1:A:7:VAL:HG12	1:A:100:TYR:HB3	1.98	0.46
1:D:70:ASP:O	1:D:73:LYS:N	2.45	0.46
1:A:130:ASN:O	1:A:134:ILE:HG13	2.16	0.45
1:D:100:TYR:CD1	1:D:103:LEU:HB2	2.51	0.45
1:B:126:ILE:HG23	1:B:132:VAL:HG12	1.98	0.45
1:B:258:TRP:CZ2	1:B:260:GLY:HA3	2.52	0.45
1:C:11:ALA:O	1:C:42:HIS:ND1	2.50	0.45
1:C:154:ASP:OD1	1:C:154:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ASN:O	1:C:310:ARG:N	2.49	0.45
1:C:107:LEU:HD13	1:C:267:ILE:HD12	1.99	0.44
1:A:151:GLU:HG2	1:A:152:ARG:HG2	1.98	0.44
1:C:100:TYR:CD1	1:C:103:LEU:HB2	2.51	0.44
1:C:178:MET:HE3	1:C:178:MET:HA	1.99	0.44
1:A:45:THR:HA	1:A:48:LEU:HG	1.99	0.44
1:B:165:PHE:CE2	1:B:351:ALA:HB2	2.53	0.44
1:A:370:HIS:CD2	1:A:370:HIS:H	2.35	0.44
1:D:130:ASN:O	1:D:134:ILE:HG13	2.17	0.44
1:D:154:ASP:OD1	1:D:154:ASP:N	2.51	0.44
1:B:154:ASP:OD1	1:B:154:ASP:N	2.51	0.43
1:A:6:ILE:HG12	1:A:102:TYR:HB2	2.00	0.43
1:C:43:TYR:HA	1:C:62:ARG:HA	2.00	0.43
1:D:174:LEU:O	1:D:178:MET:HG2	2.18	0.43
1:D:357:ASP:OD1	1:D:358:ALA:N	2.51	0.43
1:A:40:ASP:HB3	1:A:78:LYS:HD2	1.99	0.43
1:B:100:TYR:CD1	1:B:103:LEU:HB2	2.54	0.43
1:C:116:ILE:HB	1:C:119:LEU:HD22	2.00	0.43
1:B:289:PRO:HA	1:B:290:GLY:HA2	1.61	0.43
1:A:116:ILE:HB	1:A:119:LEU:HD22	2.01	0.43
1:C:181:LEU:HD12	1:C:181:LEU:HA	1.90	0.43
1:D:46:THR:HA	2:D:601:FAD:C5X	2.49	0.43
1:A:44:ILE:HD11	1:A:384:LEU:HD21	2.01	0.43
1:C:122:HIS:CE1	1:C:237:PRO:HG3	2.54	0.43
1:B:394:LEU:O	1:B:396:LYS:N	2.44	0.42
1:C:310:ARG:HA	1:C:311:PRO:HD3	1.79	0.42
2:C:601:FAD:H8A	2:C:601:FAD:H2B	1.93	0.42
1:B:163:ALA:HB1	1:B:203:VAL:HG13	2.01	0.42
1:B:326:VAL:O	1:B:330:LEU:HB2	2.19	0.42
1:B:49:HIS:CD2	1:B:169:GLU:HB3	2.54	0.42
1:A:258:TRP:CZ2	1:A:260:GLY:HA3	2.54	0.42
1:A:9:LEU:HB3	1:A:107:LEU:HD21	2.01	0.42
1:A:198:GLU:OE2	3:A:602:NAD:O2B	2.38	0.42
1:A:273:PHE:HZ	1:A:294:ILE:HD13	1.84	0.42
1:C:130:ASN:O	1:C:134:ILE:HG13	2.19	0.42
1:D:304:ILE:HD13	1:D:311:PRO:HB3	2.02	0.42
1:D:119:LEU:HD12	1:D:119:LEU:HA	1.89	0.42
1:A:330:LEU:O	1:A:334:ILE:HG12	2.19	0.42
1:C:329:ASN:HB3	1:C:339:MET:HE2	2.01	0.42
1:A:388:GLY:HA3	1:A:392:LEU:HB2	2.01	0.42
1:A:375:LEU:O	1:A:379:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:ASN:HB3	1:D:339:MET:HE2	2.00	0.41
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.78	0.41
1:D:371:ALA:O	1:D:375:LEU:HD13	2.20	0.41
1:B:37:ASN:ND2	1:B:39:ASN:O	2.51	0.41
1:D:362:VAL:C	1:D:364:GLY:H	2.29	0.41
1:A:84:ILE:HD13	1:A:91:VAL:HG13	2.03	0.41
1:C:208:ASP:HA	1:C:209:PRO:HD3	1.96	0.41
1:A:117:GLU:HB3	1:A:234:ARG:HG3	2.01	0.41
1:A:357:ASP:OD1	1:A:358:ALA:N	2.54	0.41
1:C:11:ALA:H	1:C:37:ASN:ND2	2.08	0.41
1:D:143:PHE:CZ	1:D:178:MET:HE1	2.56	0.41
1:D:230:THR:HG22	1:D:242:ILE:HB	2.03	0.41
1:A:88:GLN:O	1:A:90:LYS:N	2.54	0.41
1:A:115:GLY:C	1:C:345:HIS:HE2	2.28	0.41
1:B:283:ASP:CG	1:B:287:ARG:HG2	2.46	0.40
1:A:355:ARG:HA	1:A:355:ARG:NE	2.36	0.40
1:B:204:LEU:O	1:B:207:PHE:HB2	2.21	0.40
1:D:122:HIS:CE1	1:D:237:PRO:HG3	2.56	0.40
1:A:303:ILE:HD12	1:A:322:HIS:HE2	1.87	0.40
1:A:216:MET:HE2	1:A:216:MET:HB3	1.86	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	391/405 (96%)	379 (97%)	9 (2%)	3 (1%)	16	50
1	B	392/405 (97%)	380 (97%)	7 (2%)	5 (1%)	9	38
1	C	387/405 (96%)	378 (98%)	7 (2%)	2 (0%)	24	60
1	D	392/405 (97%)	384 (98%)	6 (2%)	2 (0%)	24	60
All	All	1562/1620 (96%)	1521 (97%)	29 (2%)	12 (1%)	16	50

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	71	GLU
1	A	89	GLN
1	D	71	GLU
1	B	309	ASN
1	B	337	GLY
1	B	395	LYS
1	A	28	TYR
1	A	72	LYS
1	C	309	ASN
1	D	309	ASN
1	B	28	TYR
1	C	338	SER

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	262/329 (80%)	255 (97%)	7 (3%)	39	71
1	B	263/329 (80%)	259 (98%)	4 (2%)	57	80
1	C	222/329 (68%)	218 (98%)	4 (2%)	51	77
1	D	263/329 (80%)	261 (99%)	2 (1%)	73	86
All	All	1010/1316 (77%)	993 (98%)	17 (2%)	53	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	91	VAL
1	B	92	THR
1	B	330	LEU
1	B	391	SER
1	A	92	THR
1	A	142	GLN
1	A	250	GLU
1	A	287	ARG

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Mol	Chain	Res	Type
1	A	330	LEU
1	A	361	ILE
1	A	381	MET
1	C	27	ASN
1	C	178	MET
1	C	202	THR
1	C	317	GLN
1	D	65	ILE
1	D	263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	89	GLN
1	B	309	ASN
1	A	137	GLN
1	A	196	ASN
1	A	291	HIS
1	A	370	HIS
1	C	50	GLN
1	C	122	HIS
1	C	325	ASN
1	C	329	ASN
1	D	39	ASN
1	D	50	GLN
1	D	88	GLN
1	D	89	GLN
1	D	122	HIS
1	D	142	GLN
1	D	196	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	FAD	A	601	-	58,58,58	2.68	19 (32%)	85,89,89	2.22	23 (27%)
2	FAD	D	601	-	58,58,58	2.68	19 (32%)	85,89,89	2.23	23 (27%)
3	NAD	D	602	-	46,48,48	3.25	12 (26%)	64,73,73	1.68	12 (18%)
3	NAD	A	602	-	46,48,48	3.24	12 (26%)	64,73,73	1.70	11 (17%)
2	FAD	C	601	-	58,58,58	2.68	19 (32%)	85,89,89	2.24	25 (29%)
3	NAD	C	602	-	46,48,48	3.24	12 (26%)	64,73,73	1.65	12 (18%)
2	FAD	B	601	-	58,58,58	2.68	18 (31%)	85,89,89	2.23	23 (27%)

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	FAD	A	601	-	-	11/34/50/50	0/6/6/6
2	FAD	D	601	-	-	13/34/50/50	0/6/6/6
3	NAD	D	602	-	-	4/30/62/62	0/5/5/5
3	NAD	A	602	-	-	10/30/62/62	0/5/5/5
2	FAD	C	601	-	-	13/34/50/50	0/6/6/6
3	NAD	C	602	-	-	6/30/62/62	0/5/5/5
2	FAD	B	601	-	-	15/34/50/50	0/6/6/6

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAD	O4D-C1D	-10.92	1.26	1.40
3	C	602	NAD	O4D-C1D	-10.91	1.26	1.40
3	D	602	NAD	C2D-C3D	-10.86	1.23	1.53
3	D	602	NAD	O4D-C1D	-10.86	1.26	1.40
3	A	602	NAD	C2D-C3D	-10.83	1.24	1.53
3	C	602	NAD	C2D-C3D	-10.82	1.24	1.53
2	C	601	FAD	O4B-C1B	8.31	1.61	1.42
2	B	601	FAD	O4B-C1B	8.26	1.61	1.42
2	D	601	FAD	O4B-C1B	8.26	1.61	1.42
2	A	601	FAD	O4B-C1B	8.22	1.61	1.42
2	A	601	FAD	C2B-C1B	-7.70	1.29	1.53
2	D	601	FAD	C2B-C1B	-7.68	1.29	1.53
2	B	601	FAD	C2B-C1B	-7.65	1.29	1.53
3	C	602	NAD	C3B-C4B	-7.65	1.33	1.53
3	A	602	NAD	C3B-C4B	-7.64	1.33	1.53
3	D	602	NAD	C3B-C4B	-7.63	1.33	1.53
2	C	601	FAD	C2B-C1B	-7.62	1.29	1.53
3	A	602	NAD	C7N-N7N	7.42	1.46	1.33
3	D	602	NAD	C7N-N7N	7.36	1.46	1.33
3	C	602	NAD	C7N-N7N	7.35	1.46	1.33
2	D	601	FAD	C4X-N5	5.71	1.43	1.30
2	C	601	FAD	C4X-N5	5.71	1.43	1.30
2	A	601	FAD	C4X-N5	5.71	1.43	1.30
2	B	601	FAD	C4X-N5	5.70	1.43	1.30
2	C	601	FAD	C5X-N5	5.31	1.49	1.39
2	B	601	FAD	C5X-N5	5.27	1.49	1.39
2	D	601	FAD	C5X-N5	5.27	1.49	1.39
2	A	601	FAD	C5X-N5	5.26	1.49	1.39
3	D	602	NAD	O4B-C1B	-5.06	1.30	1.42
2	A	601	FAD	C10-N1	5.06	1.43	1.33
3	C	602	NAD	O4B-C1B	-5.05	1.30	1.42
2	B	601	FAD	C10-N1	5.03	1.43	1.33
2	D	601	FAD	C10-N1	5.02	1.43	1.33
2	C	601	FAD	C10-N1	4.98	1.43	1.33
3	A	602	NAD	O4B-C1B	-4.93	1.30	1.42
2	A	601	FAD	C6A-N6A	4.64	1.46	1.34
2	C	601	FAD	C6A-N6A	4.62	1.46	1.34
2	A	601	FAD	C2-N1	4.62	1.47	1.36
3	A	602	NAD	O3D-C3D	4.58	1.54	1.43
3	C	602	NAD	O3D-C3D	4.58	1.54	1.43
3	D	602	NAD	O3D-C3D	4.57	1.54	1.43
2	D	601	FAD	C2-N1	4.56	1.47	1.36
2	D	601	FAD	C6A-N6A	4.56	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C2-N1	4.56	1.47	1.36
2	B	601	FAD	C6A-N6A	4.55	1.45	1.34
2	C	601	FAD	C2-N1	4.51	1.46	1.36
3	D	602	NAD	O2B-C2B	-4.47	1.31	1.43
3	C	602	NAD	O2B-C2B	-4.39	1.32	1.43
3	A	602	NAD	O2B-C2B	-4.37	1.32	1.43
2	C	601	FAD	O4-C4	-4.36	1.15	1.23
2	B	601	FAD	O4-C4	-4.35	1.15	1.23
2	D	601	FAD	O4-C4	-4.32	1.15	1.23
2	A	601	FAD	O4-C4	-4.31	1.15	1.23
2	D	601	FAD	O2B-C2B	4.23	1.53	1.43
2	C	601	FAD	O2B-C2B	4.22	1.53	1.43
3	C	602	NAD	C6A-N6A	4.20	1.44	1.34
3	A	602	NAD	C6A-N6A	4.19	1.44	1.34
2	B	601	FAD	O2B-C2B	4.19	1.53	1.43
3	D	602	NAD	C6A-N6A	4.19	1.44	1.34
2	A	601	FAD	O2B-C2B	4.17	1.53	1.43
2	C	601	FAD	C10-N10	3.94	1.45	1.37
2	A	601	FAD	C10-N10	3.93	1.45	1.37
2	D	601	FAD	C10-N10	3.92	1.45	1.37
2	B	601	FAD	C10-N10	3.89	1.45	1.37
2	B	601	FAD	C2-N3	3.44	1.46	1.39
2	D	601	FAD	C2-N3	3.43	1.46	1.39
2	A	601	FAD	C2-N3	3.43	1.46	1.39
2	C	601	FAD	C2-N3	3.42	1.46	1.39
2	A	601	FAD	C8M-C8	3.34	1.57	1.51
2	C	601	FAD	C8M-C8	3.34	1.57	1.51
2	B	601	FAD	C8M-C8	3.33	1.57	1.51
2	D	601	FAD	C8M-C8	3.26	1.57	1.51
2	D	601	FAD	C7M-C7	2.89	1.56	1.51
2	C	601	FAD	C7M-C7	2.88	1.56	1.51
2	B	601	FAD	C7M-C7	2.87	1.56	1.51
2	A	601	FAD	C7M-C7	2.86	1.56	1.51
2	A	601	FAD	C9A-N10	2.85	1.46	1.41
2	B	601	FAD	C9A-N10	2.84	1.46	1.41
3	A	602	NAD	O4D-C4D	2.81	1.51	1.45
2	D	601	FAD	O4'-C4'	-2.79	1.37	1.43
2	C	601	FAD	C9A-N10	2.78	1.46	1.41
2	D	601	FAD	C9A-N10	2.77	1.45	1.41
3	D	602	NAD	O4D-C4D	2.74	1.51	1.45
2	C	601	FAD	O4'-C4'	-2.73	1.37	1.43
3	D	602	NAD	C5D-C4D	-2.73	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	O4'-C4'	-2.73	1.37	1.43
3	C	602	NAD	O4D-C4D	2.72	1.51	1.45
3	A	602	NAD	C5D-C4D	-2.71	1.43	1.51
3	C	602	NAD	C5D-C4D	-2.71	1.43	1.51
2	B	601	FAD	O4'-C4'	-2.69	1.37	1.43
3	D	602	NAD	O2D-C2D	2.67	1.49	1.43
3	A	602	NAD	O2D-C2D	2.62	1.49	1.43
3	C	602	NAD	O2D-C2D	2.62	1.49	1.43
2	B	601	FAD	C8A-N7A	2.43	1.36	1.31
2	D	601	FAD	C8A-N7A	2.41	1.36	1.31
2	A	601	FAD	C8A-N7A	2.40	1.36	1.31
2	C	601	FAD	C5'-C4'	2.36	1.55	1.51
2	B	601	FAD	C5'-C4'	2.36	1.55	1.51
2	C	601	FAD	C4-N3	2.35	1.43	1.38
2	C	601	FAD	C8A-N7A	2.34	1.36	1.31
2	B	601	FAD	C4-N3	2.32	1.43	1.38
3	C	602	NAD	O3B-C3B	2.30	1.48	1.43
3	A	602	NAD	O3B-C3B	2.30	1.48	1.43
2	D	601	FAD	C5'-C4'	2.29	1.54	1.51
2	A	601	FAD	C4-N3	2.29	1.43	1.38
3	D	602	NAD	O3B-C3B	2.26	1.48	1.43
2	A	601	FAD	C5'-C4'	2.25	1.54	1.51
2	D	601	FAD	C4-N3	2.23	1.43	1.38
2	D	601	FAD	C2A-N1A	2.04	1.37	1.33
2	C	601	FAD	C2A-N1A	2.04	1.37	1.33
2	A	601	FAD	C2A-N1A	2.01	1.37	1.33

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C7M-C7-C6	-9.07	103.59	119.57
2	B	601	FAD	C7M-C7-C6	-9.00	103.72	119.57
2	A	601	FAD	C7M-C7-C6	-8.98	103.75	119.57
2	D	601	FAD	C7M-C7-C6	-8.96	103.79	119.57
2	D	601	FAD	C7M-C7-C8	7.62	136.33	120.76
2	B	601	FAD	C7M-C7-C8	7.62	136.33	120.76
2	C	601	FAD	C7M-C7-C8	7.62	136.32	120.76
2	A	601	FAD	C7M-C7-C8	7.59	136.26	120.76
2	B	601	FAD	N3A-C2A-N1A	-5.75	119.88	128.58
2	D	601	FAD	N3A-C2A-N1A	-5.70	119.95	128.58
2	A	601	FAD	N3A-C2A-N1A	-5.70	119.95	128.58
2	C	601	FAD	N3A-C2A-N1A	-5.63	120.07	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	N6A-C6A-N1A	-5.45	106.23	118.38
2	D	601	FAD	N6A-C6A-N1A	-5.39	106.38	118.38
2	A	601	FAD	N6A-C6A-N1A	-5.33	106.50	118.38
2	C	601	FAD	N6A-C6A-N1A	-5.30	106.58	118.38
3	A	602	NAD	C4D-O4D-C1D	-5.20	105.16	109.92
3	C	602	NAD	C5A-C4A-N3A	-5.19	119.57	126.72
3	D	602	NAD	C5A-C4A-N3A	-5.19	119.58	126.72
3	A	602	NAD	C5A-C4A-N3A	-5.18	119.58	126.72
2	C	601	FAD	C5A-C4A-N3A	-4.92	119.94	126.72
2	B	601	FAD	C5A-C4A-N3A	-4.84	120.05	126.72
2	D	601	FAD	C5A-C4A-N3A	-4.77	120.15	126.72
2	A	601	FAD	C5A-C4A-N3A	-4.77	120.15	126.72
3	D	602	NAD	N3A-C2A-N1A	-4.52	121.74	128.58
3	C	602	NAD	N3A-C2A-N1A	-4.45	121.84	128.58
3	A	602	NAD	N3A-C2A-N1A	-4.44	121.86	128.58
2	D	601	FAD	N9A-C8A-N7A	-4.27	107.88	113.94
2	B	601	FAD	N9A-C8A-N7A	-4.27	107.89	113.94
2	C	601	FAD	N9A-C8A-N7A	-4.21	107.96	113.94
2	B	601	FAD	C5A-C6A-N6A	4.19	133.66	123.29
2	A	601	FAD	N9A-C8A-N7A	-4.18	108.00	113.94
2	A	601	FAD	C5A-C6A-N6A	4.16	133.58	123.29
2	D	601	FAD	C5A-C6A-N6A	4.16	133.58	123.29
2	C	601	FAD	C5A-C6A-N6A	4.11	133.47	123.29
3	D	602	NAD	C4D-O4D-C1D	-4.08	106.19	109.92
3	D	602	NAD	N3A-C4A-N9A	4.03	134.03	127.17
3	C	602	NAD	N3A-C4A-N9A	4.02	134.00	127.17
3	A	602	NAD	N3A-C4A-N9A	3.96	133.90	127.17
3	C	602	NAD	C4D-O4D-C1D	-3.76	106.48	109.92
3	D	602	NAD	N9A-C8A-N7A	-3.67	108.73	113.94
3	C	602	NAD	N9A-C8A-N7A	-3.66	108.74	113.94
3	A	602	NAD	N9A-C8A-N7A	-3.64	108.78	113.94
3	D	602	NAD	C2A-N3A-C4A	3.49	120.36	111.83
3	A	602	NAD	C2A-N3A-C4A	3.45	120.25	111.83
3	C	602	NAD	C2A-N3A-C4A	3.43	120.20	111.83
2	B	601	FAD	C2A-N3A-C4A	3.40	120.14	111.83
2	C	601	FAD	C4-N3-C2	-3.38	119.64	125.64
2	C	601	FAD	C2A-N3A-C4A	3.36	120.04	111.83
2	A	601	FAD	C2A-N3A-C4A	3.35	120.01	111.83
2	D	601	FAD	C2A-N3A-C4A	3.35	120.01	111.83
2	A	601	FAD	C4-N3-C2	-3.34	119.72	125.64
2	D	601	FAD	C4-N3-C2	-3.33	119.73	125.64
2	B	601	FAD	C4-N3-C2	-3.31	119.76	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C8M-C8-C9	3.29	125.36	119.57
2	A	601	FAD	C8M-C8-C9	3.23	125.27	119.57
2	B	601	FAD	C8M-C8-C9	3.15	125.12	119.57
2	C	601	FAD	C4'-C3'-C2'	-3.11	108.40	113.57
2	A	601	FAD	C4'-C3'-C2'	-3.04	108.51	113.57
2	C	601	FAD	C8M-C8-C7	-3.00	114.63	120.76
2	A	601	FAD	C8M-C8-C7	-3.00	114.64	120.76
2	D	601	FAD	C8M-C8-C9	2.99	124.84	119.57
3	D	602	NAD	C4A-N9A-C8A	2.96	108.84	105.74
2	B	601	FAD	C8M-C8-C7	-2.95	114.73	120.76
3	C	602	NAD	C5A-N7A-C8A	2.94	108.07	103.45
3	A	602	NAD	C5A-N7A-C8A	2.94	108.06	103.45
3	C	602	NAD	C4A-N9A-C8A	2.93	108.81	105.74
2	C	601	FAD	N3A-C4A-N9A	2.90	132.11	127.17
3	D	602	NAD	C5A-N7A-C8A	2.89	108.00	103.45
2	D	601	FAD	C8M-C8-C7	-2.88	114.88	120.76
3	A	602	NAD	C4A-N9A-C8A	2.87	108.76	105.74
2	C	601	FAD	C5A-N7A-C8A	2.85	107.93	103.45
2	B	601	FAD	C5A-N7A-C8A	2.85	107.93	103.45
2	D	601	FAD	C5A-N7A-C8A	2.84	107.91	103.45
2	A	601	FAD	C5A-N7A-C8A	2.81	107.87	103.45
2	B	601	FAD	N3A-C4A-N9A	2.78	131.90	127.17
2	D	601	FAD	C5X-C9A-N10	2.76	120.46	117.97
2	D	601	FAD	N3A-C4A-N9A	2.75	131.84	127.17
2	A	601	FAD	N3A-C4A-N9A	2.73	131.81	127.17
2	D	601	FAD	C4'-C3'-C2'	-2.72	109.04	113.57
2	C	601	FAD	C4X-C4-N3	2.59	119.84	113.25
2	B	601	FAD	C5X-C9A-N10	2.57	120.29	117.97
2	D	601	FAD	C4X-C4-N3	2.57	119.80	113.25
2	C	601	FAD	C4X-C10-N10	2.57	120.16	116.48
2	A	601	FAD	C4X-C4-N3	2.55	119.75	113.25
2	B	601	FAD	C4X-C4-N3	2.54	119.71	113.25
2	A	601	FAD	C5X-C9A-N10	2.52	120.25	117.97
2	D	601	FAD	C9A-C5X-N5	-2.51	119.79	122.45
2	D	601	FAD	O4-C4-C4X	-2.49	119.96	126.53
2	B	601	FAD	C4X-C10-N10	2.49	120.04	116.48
2	C	601	FAD	C5X-C9A-N10	2.49	120.22	117.97
2	C	601	FAD	C10-C4X-N5	-2.49	119.73	124.81
2	B	601	FAD	O4-C4-C4X	-2.44	120.09	126.53
2	B	601	FAD	C10-C4X-N5	-2.43	119.84	124.81
2	A	601	FAD	C10-C4X-N5	-2.43	119.84	124.81
2	C	601	FAD	C3B-C2B-C1B	2.43	106.06	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	O4-C4-C4X	-2.42	120.14	126.53
2	A	601	FAD	O4-C4-C4X	-2.40	120.18	126.53
2	B	601	FAD	C4'-C3'-C2'	-2.38	109.60	113.57
2	A	601	FAD	C9A-C5X-N5	-2.37	119.94	122.45
2	A	601	FAD	C4X-C10-N10	2.37	119.88	116.48
3	A	602	NAD	C4A-C5A-N7A	-2.36	107.88	110.58
2	D	601	FAD	C10-C4X-N5	-2.36	120.00	124.81
3	A	602	NAD	O4B-C4B-C3B	2.34	109.80	105.15
2	D	601	FAD	C4X-C10-N10	2.34	119.83	116.48
2	B	601	FAD	C9A-C5X-N5	-2.33	119.98	122.45
2	D	601	FAD	C4A-N9A-C8A	2.32	108.17	105.74
3	C	602	NAD	C4A-C5A-N7A	-2.30	107.95	110.58
2	B	601	FAD	C4A-N9A-C8A	2.29	108.14	105.74
3	D	602	NAD	O4B-C1B-C2B	-2.28	101.75	106.62
2	C	601	FAD	C4A-N9A-C8A	2.28	108.13	105.74
2	B	601	FAD	C4A-C5A-N7A	-2.26	107.99	110.58
2	A	601	FAD	C4A-C5A-N7A	-2.25	108.01	110.58
2	C	601	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
2	C	601	FAD	C9A-C5X-N5	-2.23	120.08	122.45
2	D	601	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
2	A	601	FAD	C4A-N9A-C8A	2.23	108.08	105.74
3	D	602	NAD	C4A-C5A-N7A	-2.23	108.04	110.58
3	D	602	NAD	C5B-C4B-C3B	-2.23	107.20	115.21
3	D	602	NAD	O4B-C4B-C3B	2.22	109.56	105.15
3	C	602	NAD	C5B-C4B-C3B	-2.15	107.47	115.21
3	C	602	NAD	O4B-C4B-C3B	2.14	109.40	105.15
3	C	602	NAD	C2D-C3D-C4D	2.08	106.63	102.61
3	A	602	NAD	C5B-C4B-C3B	-2.07	107.77	115.21
2	B	601	FAD	C5A-C4A-N9A	2.06	108.06	105.81
2	A	601	FAD	C5A-C4A-N9A	2.04	108.03	105.81
2	C	601	FAD	C6A-C5A-C4A	2.02	119.94	117.18
2	D	601	FAD	C5A-C4A-N9A	2.02	108.01	105.81
2	C	601	FAD	C4X-C10-N1	-2.01	119.66	124.59

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	P-O3P-PA-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O2A
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	C5B-O5B-PA-O3P
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C2'-C3'-C4'-O4'
2	C	601	FAD	C2'-C3'-C4'-C5'
2	C	601	FAD	O3'-C3'-C4'-C5'
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	P-O3P-PA-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
3	A	602	NAD	C5D-O5D-PN-O3
3	A	602	NAD	C5D-O5D-PN-O2N
2	C	601	FAD	O3'-C3'-C4'-O4'
2	C	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	C2'-C3'-C4'-O4'
3	C	602	NAD	O4B-C4B-C5B-O5B
3	D	602	NAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C2'-C3'-C4'-C5'
3	C	602	NAD	C3B-C4B-C5B-O5B
3	D	602	NAD	C3B-C4B-C5B-O5B
2	A	601	FAD	O3'-C3'-C4'-C5'
3	A	602	NAD	O4B-C4B-C5B-O5B
3	C	602	NAD	O4D-C4D-C5D-O5D
2	C	601	FAD	P-O3P-PA-O5B
3	A	602	NAD	PA-O3-PN-O5D
3	C	602	NAD	PA-O3-PN-O5D
3	D	602	NAD	PA-O3-PN-O5D
2	D	601	FAD	C2'-C3'-C4'-O4'
3	A	602	NAD	C3B-C4B-C5B-O5B
3	C	602	NAD	C3D-C4D-C5D-O5D
2	D	601	FAD	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
2	D	601	FAD	C2'-C3'-C4'-C5'
2	D	601	FAD	PA-O3P-P-O1P
2	B	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	C5'-O5'-P-O3P
3	A	602	NAD	C5D-O5D-PN-O1N
2	B	601	FAD	C4'-C5'-O5'-P
2	C	601	FAD	C4'-C5'-O5'-P
2	D	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	C4'-C5'-O5'-P
2	B	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	C	601	FAD	C4B-C5B-O5B-PA
2	B	601	FAD	PA-O3P-P-O1P
3	A	602	NAD	C3D-C4D-C5D-O5D
2	C	601	FAD	C2B-C1B-N9A-C8A
2	B	601	FAD	PA-O3P-P-O2P
3	A	602	NAD	PN-O3-PA-O1A
3	C	602	NAD	PN-O3-PA-O2A
2	A	601	FAD	PA-O3P-P-O2P
2	D	601	FAD	PA-O3P-P-O2P
3	A	602	NAD	PN-O3-PA-O2A
3	D	602	NAD	PN-O3-PA-O2A
3	A	602	NAD	O4D-C4D-C5D-O5D

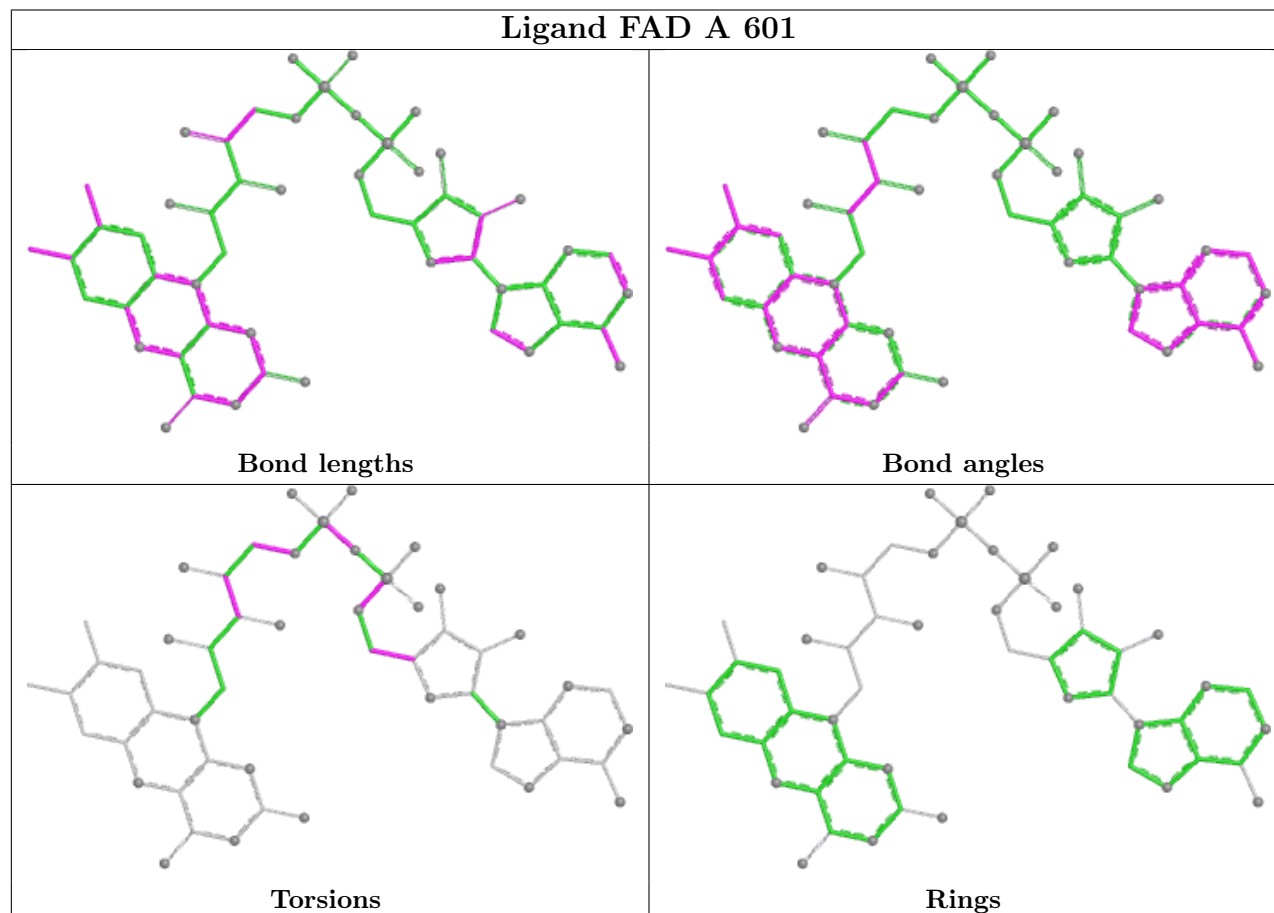
There are no ring outliers.

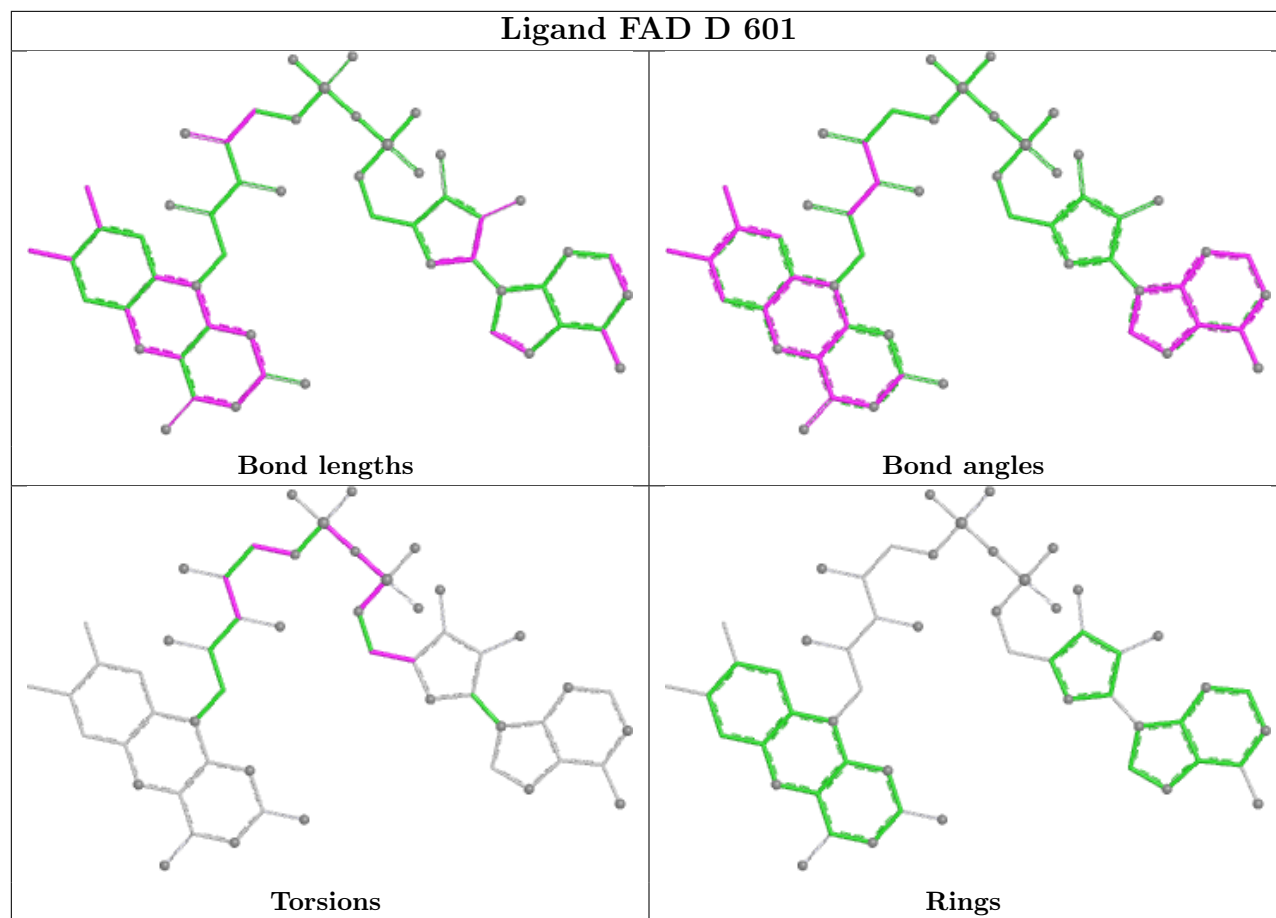
6 monomers are involved in 8 short contacts:

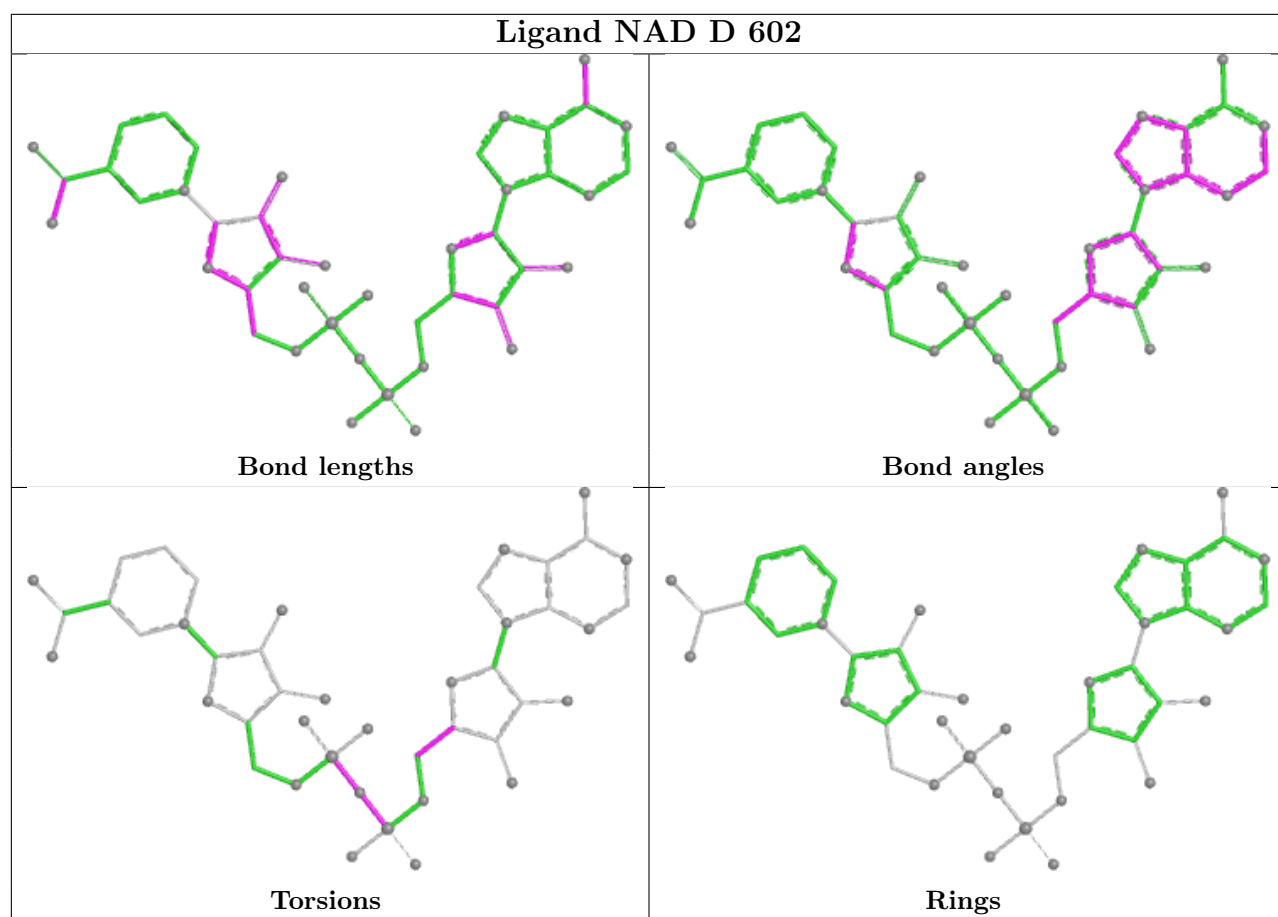
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	1	0
2	D	601	FAD	1	0
3	D	602	NAD	1	0
3	A	602	NAD	2	0
2	C	601	FAD	2	0
2	B	601	FAD	1	0

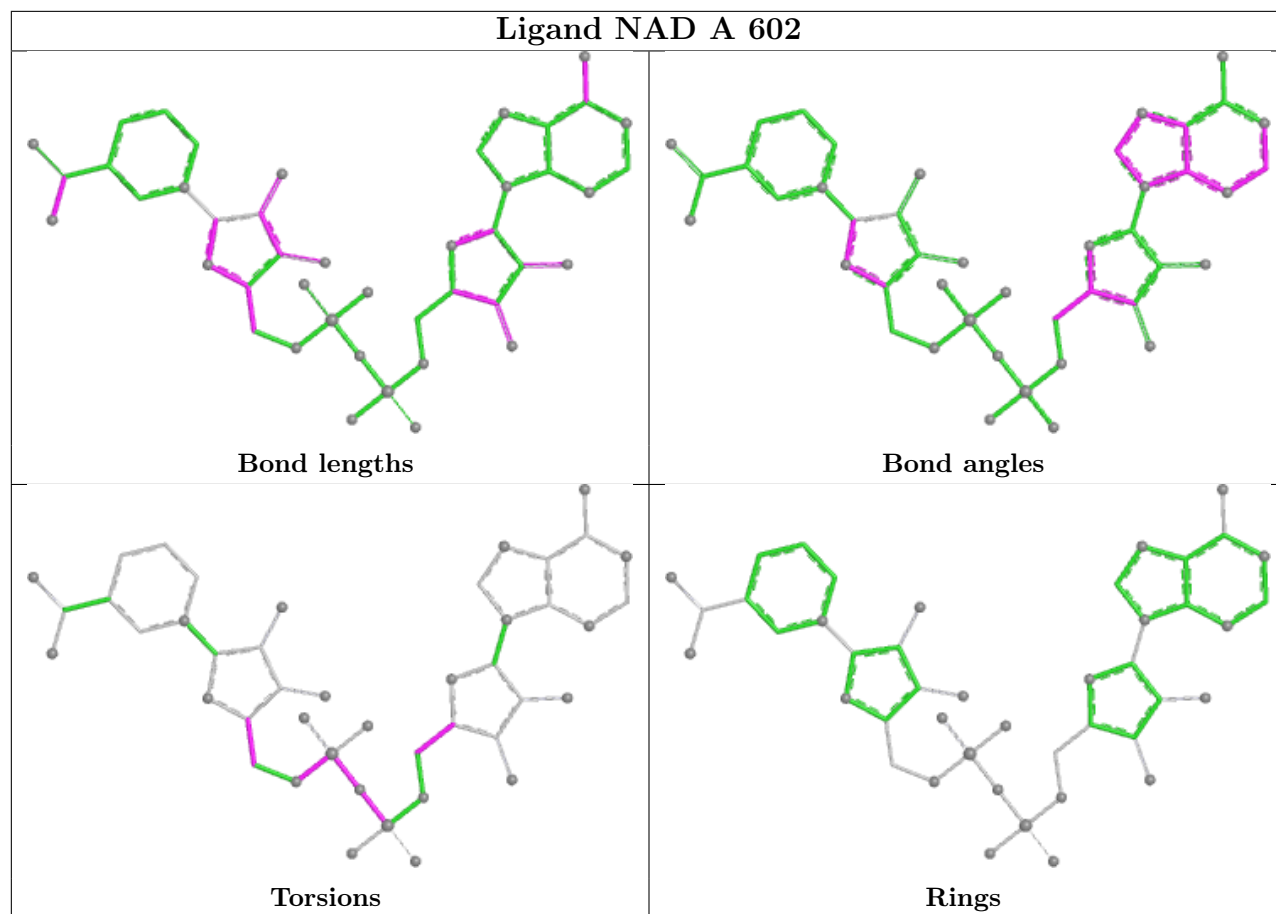
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

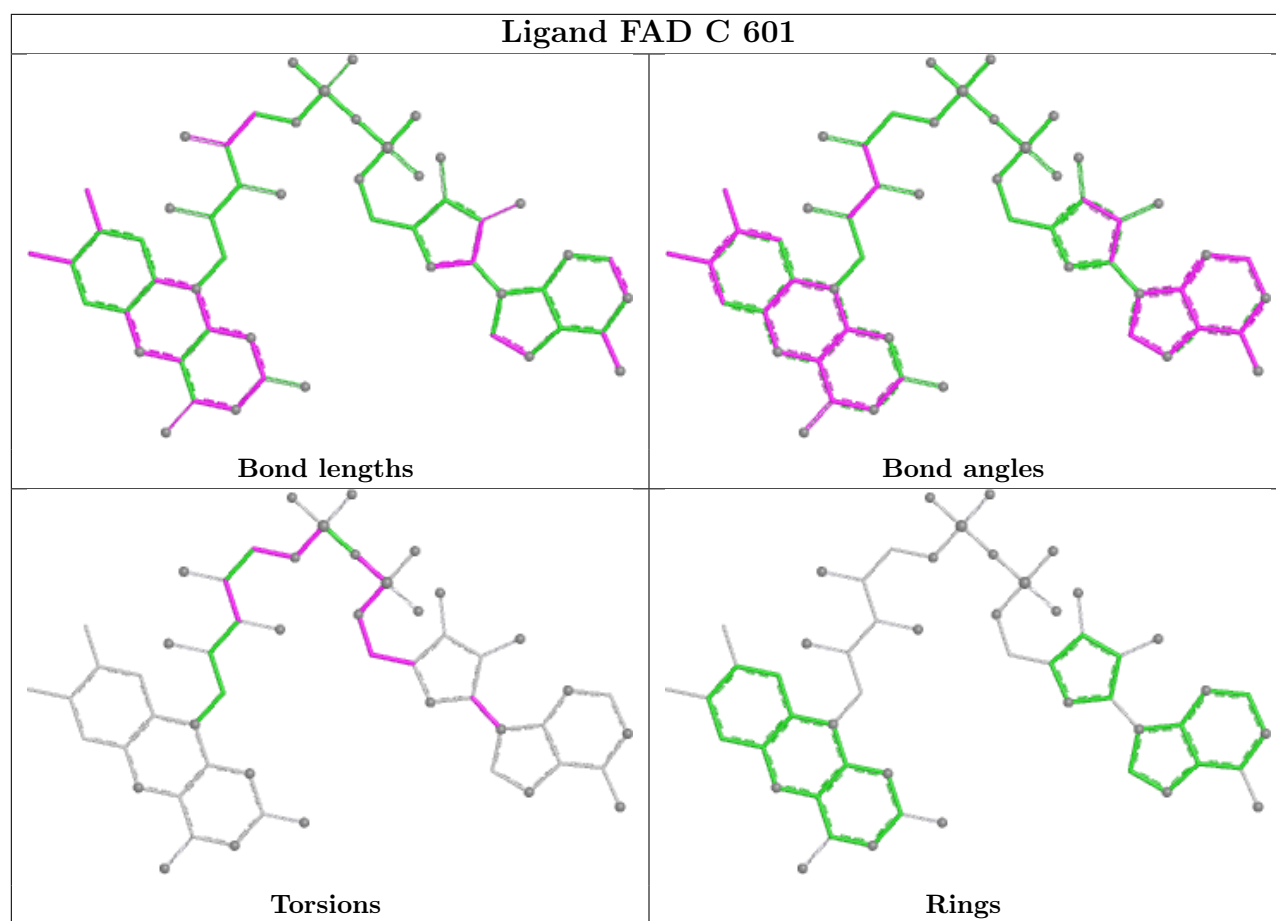
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

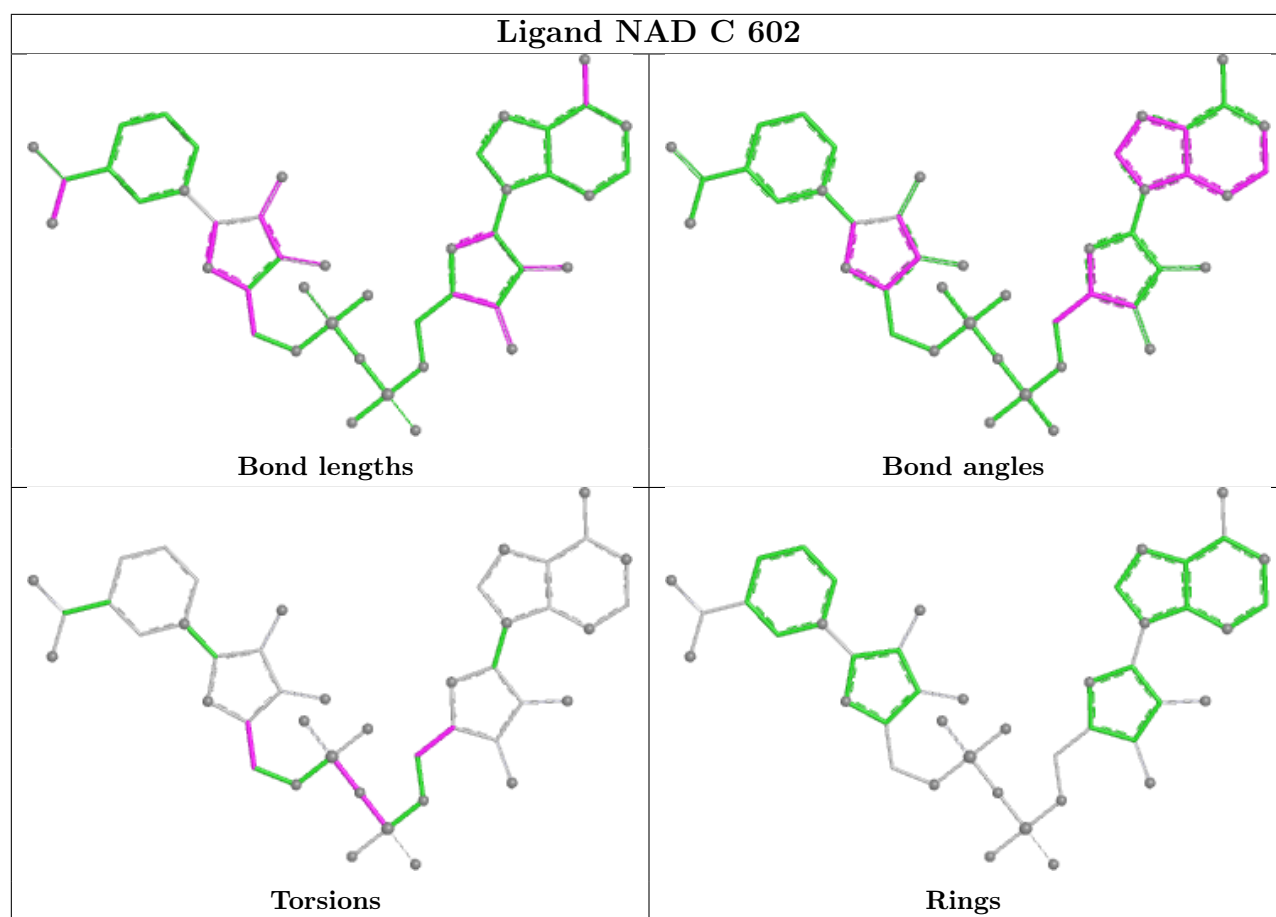


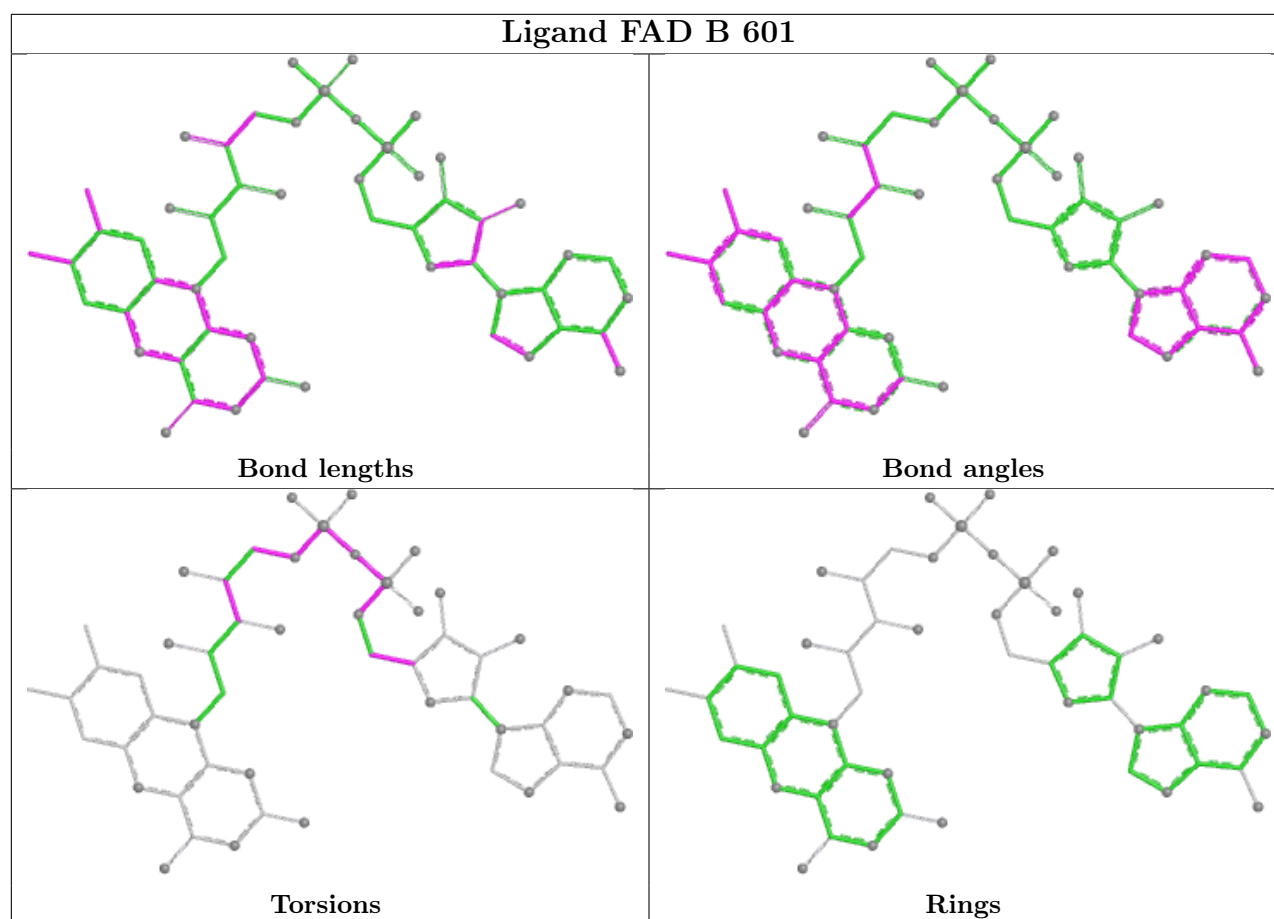












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/405 (97%)	0.51	20 (5%) 33 17	50, 73, 102, 117	0
1	B	394/405 (97%)	0.34	12 (3%) 52 30	52, 73, 97, 125	0
1	C	391/405 (96%)	0.69	29 (7%) 20 10	58, 84, 114, 127	0
1	D	394/405 (97%)	0.23	4 (1%) 79 59	57, 72, 93, 102	0
All	All	1572/1620 (97%)	0.44	65 (4%) 41 23	50, 75, 105, 127	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	GLY	4.3
1	C	165	PHE	3.9
1	A	102	TYR	3.6
1	C	35	LEU	3.3
1	C	70	ASP	3.2
1	C	33	ILE	3.2
1	A	25	ARG	3.1
1	C	94	GLN	3.1
1	A	99	HIS	3.0
1	C	76	PHE	2.9
1	A	74	ILE	2.9
1	A	287	ARG	2.9
1	C	32	ASP	2.8
1	A	71	GLU	2.8
1	B	28	TYR	2.8
1	C	34	THR	2.8
1	C	29	ASN	2.8
1	C	285	TYR	2.8
1	C	31	ALA	2.8
1	C	288	ALA	2.7
1	C	266	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	366	LYS	2.6
1	B	208	ASP	2.6
1	C	8	ILE	2.6
1	A	30	GLU	2.6
1	C	309	ASN	2.5
1	A	306	GLU	2.5
1	B	290	GLY	2.5
1	C	363	GLY	2.5
1	A	106	GLY	2.4
1	C	72	LYS	2.4
1	C	84	ILE	2.4
1	A	26	LEU	2.4
1	A	97	GLU	2.4
1	C	324	GLU	2.4
1	B	349	THR	2.3
1	D	261	GLY	2.3
1	B	165	PHE	2.3
1	A	356	ASN	2.3
1	B	348	GLY	2.3
1	A	309	ASN	2.2
1	A	308	ASN	2.2
1	C	245	ASP	2.2
1	B	27	ASN	2.2
1	B	308	ASN	2.2
1	D	260	GLY	2.2
1	A	98	LEU	2.1
1	A	305	ASN	2.1
1	C	28	TYR	2.1
1	C	114	PHE	2.1
1	C	308	ASN	2.1
1	B	60	GLN	2.1
1	A	88	GLN	2.1
1	D	29	ASN	2.1
1	B	245	ASP	2.1
1	C	339	MET	2.1
1	C	361	ILE	2.1
1	C	340	THR	2.1
1	C	274	GLU	2.1
1	C	36	VAL	2.0
1	A	5	SER	2.0
1	D	32	ASP	2.0
1	A	73	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	294	ILE	2.0
1	B	32	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

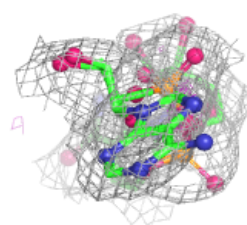
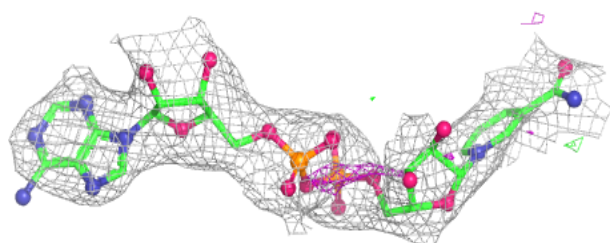
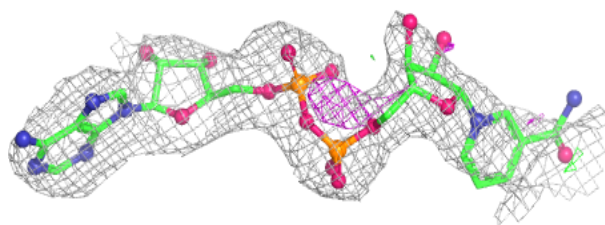
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	C	602	44/44	0.87	0.12	79,84,95,105	0
3	NAD	D	602	44/44	0.91	0.10	69,72,78,88	0
2	FAD	A	601	53/53	0.92	0.12	57,63,73,78	0
3	NAD	A	602	44/44	0.92	0.09	61,66,69,84	0
2	FAD	C	601	53/53	0.93	0.12	72,80,87,95	0
2	FAD	B	601	53/53	0.93	0.10	52,59,65,75	0
2	FAD	D	601	53/53	0.94	0.09	57,62,73,77	0

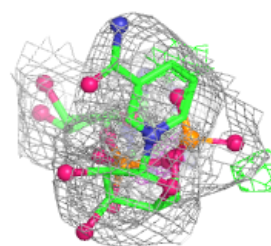
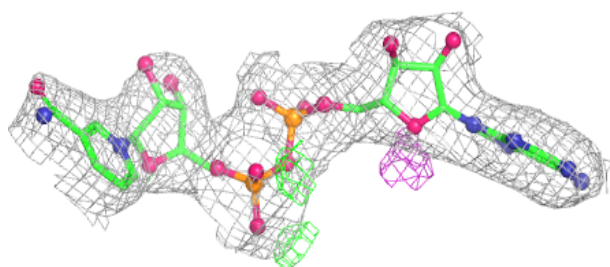
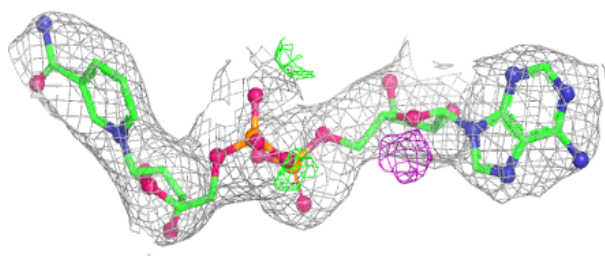
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 602:

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

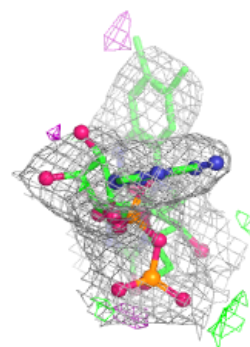
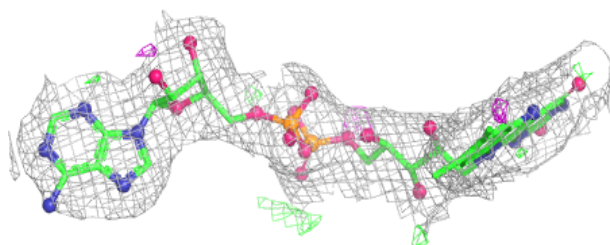
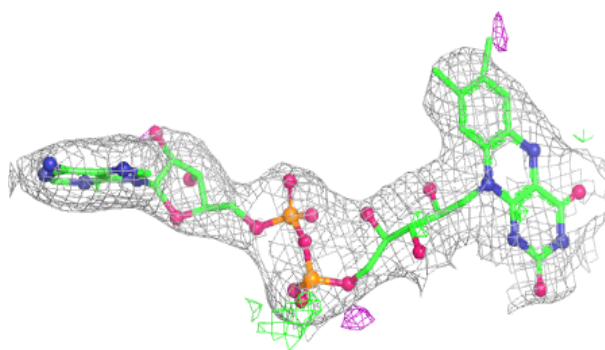
**Electron density around NAD D 602:**

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

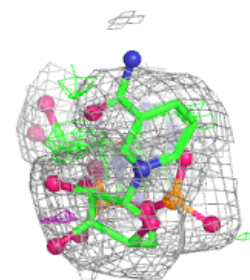
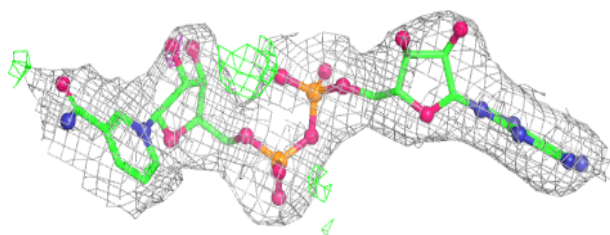
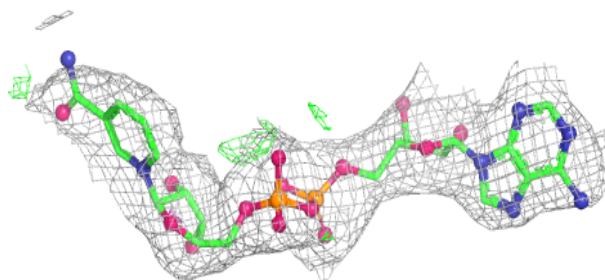


Electron density around FAD A 601:

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

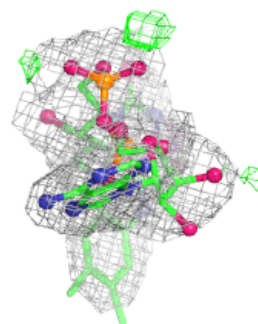
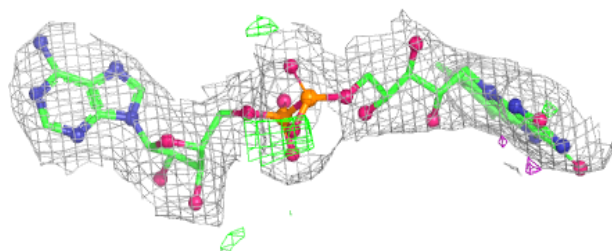
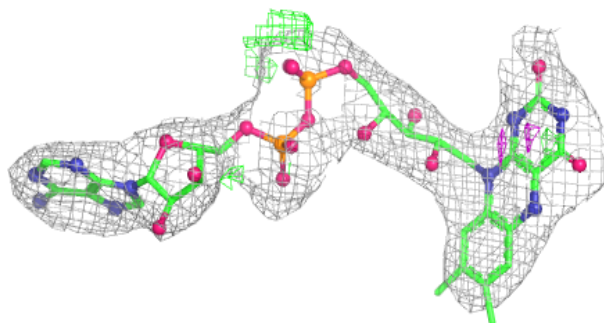
**Electron density around NAD A 602:**

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

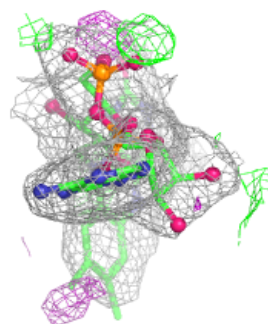
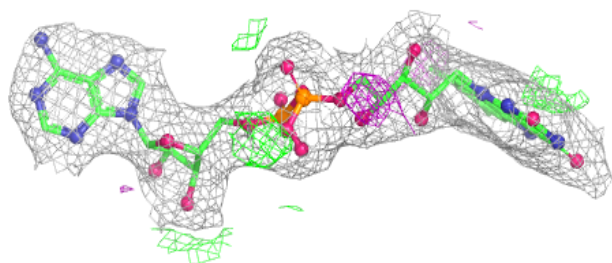
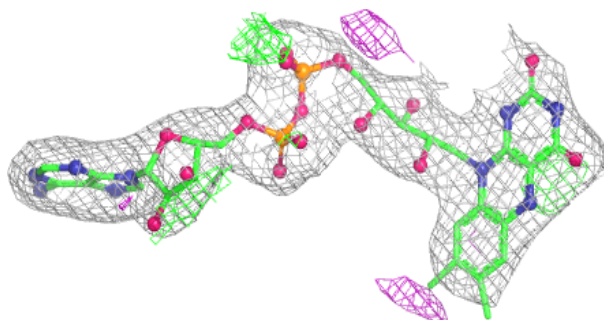


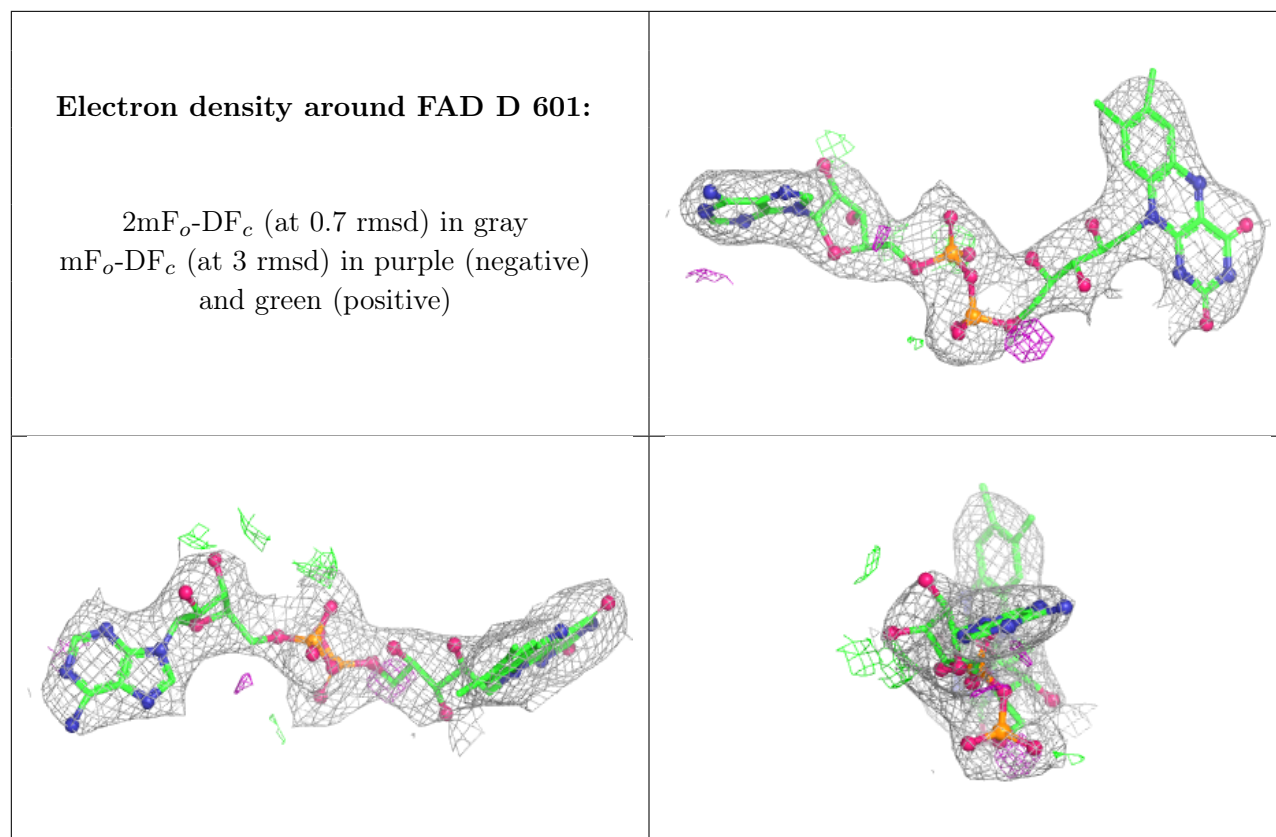
Electron density around FAD C 601:

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

**Electron density around FAD B 601:**

$2mF_o-DF_c$ (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.