



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:20 PM UTC

PDB ID : 5MIV / pdb_00005miv
Title : G307E variant of murine Apoptosis Inducing Factor in complex with NAD⁺
Authors : Sorrentino, L.; Cossu, F.; Aliverti, A.; Milani, M.; Mastrangelo, E.
Deposited on : 2016-11-29
Resolution : 3.10 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

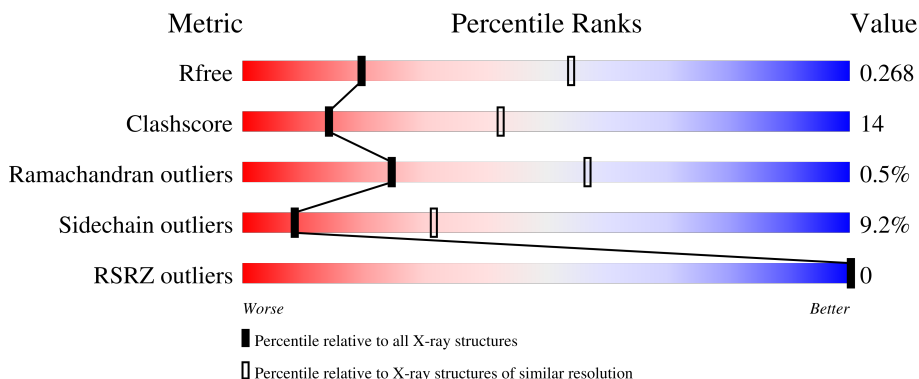
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	535	 61% 18% • 17%
1	C	535	 61% 18% •• 17%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7152 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.

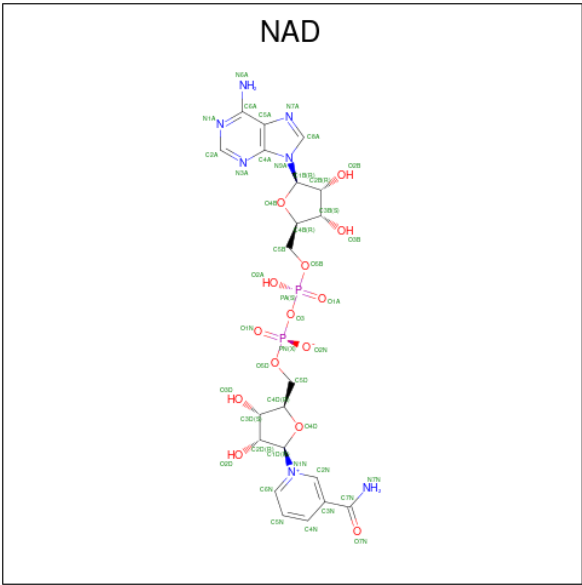
- Molecule 1 is a protein called Apoptosis-inducing factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3424	2179	606	628	11	0	0	0
1	C	442	3409	2170	602	626	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	GLU	GLY	engineered mutation	UNP Q9Z0X1
C	307	GLU	GLY	engineered mutation	UNP Q9Z0X1

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



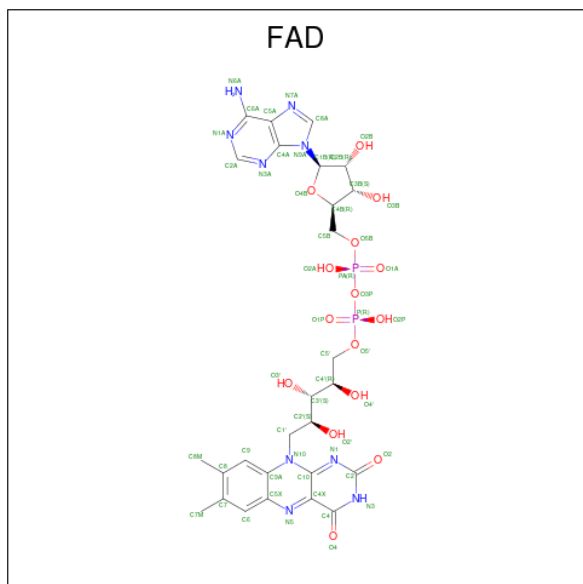
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	44	21	7	14	2	0	0

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

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



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

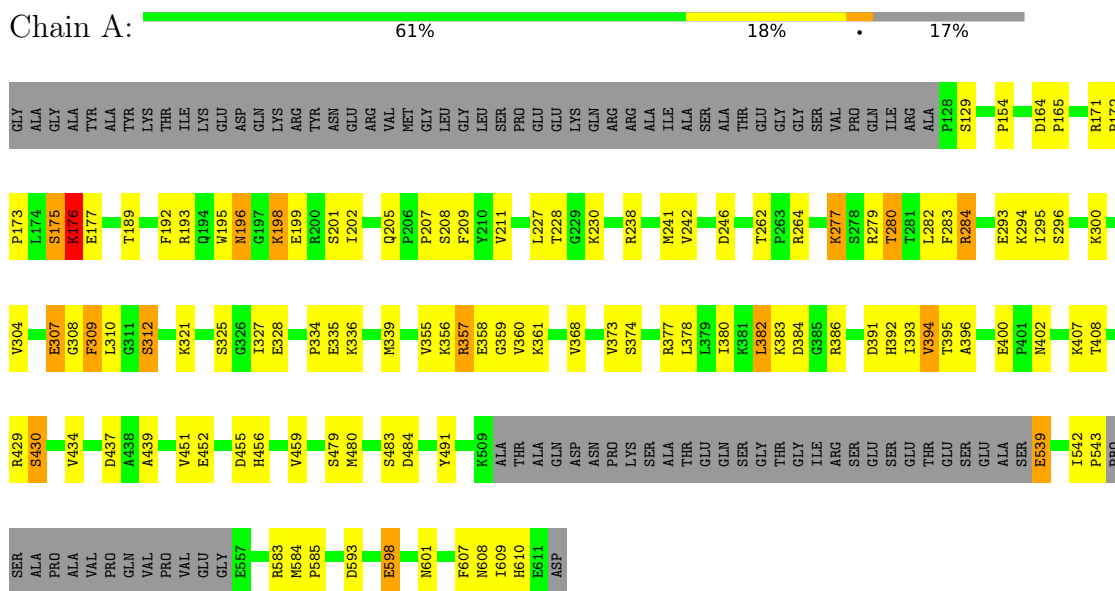
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 62 62	0	0
4	C	63	Total O 63 63	0	0

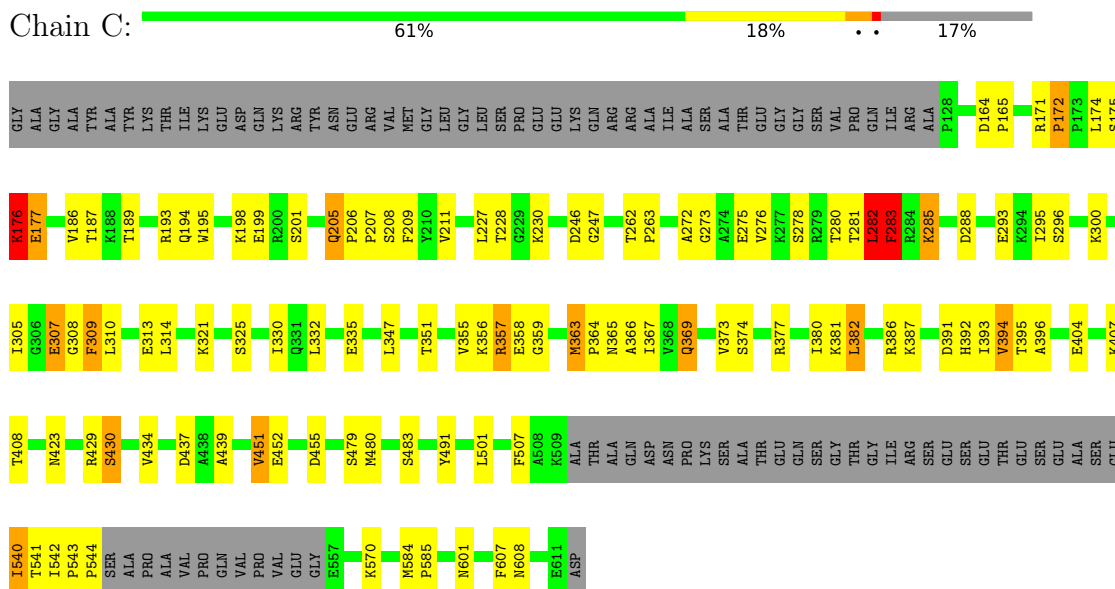
3 Residue-property plots

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



- Molecule 1: Apoptosis-inducing factor 1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.43Å 116.78Å 166.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.50 – 3.10 43.50 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.50-3.10) 99.5 (43.50-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.198 , 0.263 0.208 , 0.268	Depositor DCC
R_{free} test set	1322 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7152	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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	0.72	0/3492	0.98	6/4716 (0.1%)
1	C	0.72	1/3477 (0.0%)	1.00	12/4698 (0.3%)
All	All	0.72	1/6969 (0.0%)	0.99	18/9414 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	543	PRO	CA-C	5.45	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	LEU	N-CA-C	-9.05	93.67	109.06
1	C	543	PRO	N-CA-C	8.42	120.97	110.70
1	A	543	PRO	N-CA-CB	8.32	112.15	103.00
1	C	205	GLN	N-CA-C	8.17	115.34	108.07
1	C	607	PHE	N-CA-C	-7.89	95.87	108.73
1	C	172	PRO	N-CA-C	6.58	118.73	110.70
1	C	363	MET	CA-C-N	-6.15	114.43	120.52
1	C	363	MET	C-N-CA	-6.15	114.43	120.52
1	C	176	LYS	N-CA-C	6.11	123.81	110.80
1	C	283	PHE	N-CA-C	6.08	119.46	108.69
1	C	507	PHE	N-CA-C	5.68	117.88	109.69
1	A	283	PHE	N-CA-C	5.58	117.95	108.02
1	A	368	VAL	CB-CA-C	-5.37	102.49	111.29
1	A	309	PHE	CB-CA-C	-5.29	102.01	110.79
1	A	176	LYS	N-CA-C	5.26	122.01	110.80
1	A	610	HIS	N-CA-C	-5.23	104.79	110.91
1	C	177	GLU	N-CA-C	5.16	116.90	111.28
1	C	451	VAL	N-CA-C	5.09	115.36	107.78

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	3424	0	3457	89	1
1	C	3409	0	3448	99	1
2	A	44	0	26	10	0
2	C	44	0	26	9	0
3	A	53	0	31	12	0
3	C	53	0	31	10	0
4	A	62	0	0	18	0
4	C	63	0	0	11	0
All	All	7152	0	7019	200	1

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 14.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLY:HA3	4:A:801:HOH:O	1.21	1.33
1:C:363:MET:CE	1:C:386:ARG:HH11	1.49	1.25
1:A:308:GLY:CA	4:A:801:HOH:O	1.77	1.22
1:C:283:PHE:HB2	1:C:288:ASP:CB	1.77	1.13
1:C:363:MET:HE3	1:C:386:ARG:HH11	0.99	1.13
1:A:175:SER:OG	3:A:702:FAD:HM71	1.50	1.11
1:C:283:PHE:HB2	1:C:288:ASP:HB3	1.24	1.10
1:C:283:PHE:CE1	1:C:314:LEU:HD11	1.87	1.09
1:C:363:MET:CE	1:C:386:ARG:NH1	2.15	1.07
1:C:307:GLU:HG3	1:C:335:GLU:OE1	1.52	1.06
1:C:363:MET:HE3	1:C:386:ARG:NH1	1.68	1.06
1:C:357:ARG:HB2	1:C:357:ARG:HH11	1.18	1.04
1:C:176:LYS:NZ	1:C:177:GLU:OE1	1.91	1.01
1:A:175:SER:OG	3:A:702:FAD:C7M	2.09	0.99
1:C:332:LEU:HD13	1:C:366:ALA:CB	1.95	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HH11	1:A:357:ARG:HB2	1.29	0.95
1:A:175:SER:HG	3:A:702:FAD:H6	1.31	0.94
1:C:332:LEU:HD13	1:C:366:ALA:HB1	1.50	0.93
1:C:283:PHE:HE1	1:C:314:LEU:HD11	1.26	0.91
1:A:175:SER:OG	3:A:702:FAD:H6	1.74	0.87
1:C:357:ARG:HH11	1:C:357:ARG:CB	1.88	0.85
1:A:328:GLU:HG3	1:A:361:LYS:CE	2.08	0.83
1:C:309:PHE:HB3	4:C:821:HOH:O	1.79	0.81
1:C:175:SER:OG	1:C:313:GLU:OE2	1.99	0.80
1:C:283:PHE:HB2	1:C:288:ASP:HB2	1.61	0.80
1:A:177:GLU:OE1	1:A:177:GLU:N	2.15	0.79
1:C:369:GLN:NE2	1:C:369:GLN:HA	1.97	0.79
1:A:357:ARG:HB2	1:A:357:ARG:NH1	1.98	0.78
1:C:282:LEU:HD12	1:C:282:LEU:O	1.84	0.77
1:A:356:LYS:O	1:A:359:GLY:N	2.18	0.76
1:C:283:PHE:CB	1:C:288:ASP:HB3	2.10	0.75
1:C:364:PRO:HG2	1:C:365:ASN:HD22	1.53	0.73
1:A:175:SER:HG	3:A:702:FAD:C6	2.00	0.72
1:A:176:LYS:HB3	1:A:177:GLU:OE1	1.89	0.72
1:A:175:SER:OG	3:A:702:FAD:C6	2.38	0.71
1:A:295:ILE:HG13	4:A:813:HOH:O	1.89	0.71
1:C:176:LYS:HG2	1:C:177:GLU:OE1	1.91	0.71
1:A:607:PHE:O	1:A:609:ILE:N	2.25	0.70
1:C:205:GLN:HB2	1:C:206:PRO:HD2	1.74	0.70
1:C:332:LEU:HB2	1:C:366:ALA:HB2	1.73	0.69
2:C:701:NAD:C5N	3:C:702:FAD:C5X	2.70	0.68
1:C:307:GLU:CG	1:C:335:GLU:OE1	2.38	0.68
1:A:175:SER:HG	3:A:702:FAD:HM71	1.58	0.68
1:A:294:LYS:HD3	4:A:813:HOH:O	1.95	0.67
1:A:154:PRO:HD2	4:A:827:HOH:O	1.94	0.67
1:A:328:GLU:HG3	1:A:361:LYS:HE3	1.78	0.66
1:C:355:VAL:O	1:C:358:GLU:HB2	1.96	0.66
1:C:357:ARG:HB2	1:C:357:ARG:NH1	2.02	0.66
1:A:358:GLU:HA	1:A:358:GLU:OE1	1.97	0.64
1:C:171:ARG:HD3	3:C:702:FAD:HM82	1.81	0.62
1:C:364:PRO:HG2	1:C:365:ASN:ND2	2.13	0.62
1:C:363:MET:HE2	1:C:386:ARG:NH1	2.13	0.62
1:C:381:LYS:C	1:C:382:LEU:HD23	2.24	0.62
1:C:357:ARG:HH11	1:C:357:ARG:CG	2.13	0.61
1:C:307:GLU:OE1	1:C:308:GLY:N	2.33	0.61
1:C:364:PRO:C	1:C:365:ASN:HD22	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ARG:NH2	3:A:702:FAD:O1A	2.34	0.61
1:A:357:ARG:HH11	1:A:357:ARG:CB	2.11	0.60
1:A:451:VAL:HB	1:A:456:HIS:CD2	2.37	0.60
1:A:328:GLU:CG	1:A:361:LYS:CE	2.74	0.60
1:A:238:ARG:NH1	4:A:802:HOH:O	2.35	0.60
1:C:367:ILE:HG23	1:C:367:ILE:O	2.01	0.59
1:C:483:SER:HB3	1:C:491:TYR:CE1	2.38	0.59
1:A:308:GLY:C	4:A:801:HOH:O	2.26	0.58
1:C:247:GLY:HA2	4:C:854:HOH:O	2.02	0.58
2:C:701:NAD:N7N	3:C:702:FAD:C2	2.68	0.57
1:C:608:ASN:ND2	4:C:804:HOH:O	2.38	0.56
1:A:584:MET:N	1:A:585:PRO:HD2	2.21	0.56
1:C:171:ARG:O	1:C:174:LEU:HG	2.05	0.56
1:C:309:PHE:C	4:C:821:HOH:O	2.49	0.56
1:C:501:LEU:CB	4:C:813:HOH:O	2.53	0.56
1:A:308:GLY:O	1:A:312:SER:OG	2.22	0.55
1:A:598:GLU:H	1:A:598:GLU:CD	2.15	0.55
1:C:295:ILE:HD13	1:C:392:HIS:CE1	2.43	0.54
1:C:584:MET:N	1:C:585:PRO:HD2	2.22	0.54
1:C:404:GLU:HG3	4:C:808:HOH:O	2.06	0.54
1:C:369:GLN:HA	1:C:369:GLN:HE21	1.70	0.54
1:C:272:ALA:HB3	1:C:276:VAL:HG21	1.89	0.54
1:C:483:SER:HB3	1:C:491:TYR:CZ	2.43	0.54
1:C:540:ILE:N	1:C:540:ILE:HD13	2.24	0.53
1:A:164:ASP:OD1	1:A:165:PRO:HD2	2.09	0.53
1:A:307:GLU:OE2	2:A:701:NAD:C4B	2.56	0.53
1:C:293:GLU:O	1:C:296:SER:OG	2.23	0.53
1:A:175:SER:OG	3:A:702:FAD:C7	2.57	0.53
2:C:701:NAD:C4N	3:C:702:FAD:N5	2.71	0.53
1:A:455:ASP:HB3	1:A:480:MET:O	2.09	0.53
1:C:483:SER:HA	4:C:801:HOH:O	2.09	0.53
1:C:227:LEU:HD21	1:C:230:LYS:HG3	1.90	0.52
2:A:701:NAD:N7N	3:A:702:FAD:C2	2.72	0.52
1:C:455:ASP:HB3	1:C:480:MET:O	2.09	0.52
1:A:264:ARG:NH2	4:A:805:HOH:O	2.43	0.52
1:A:483:SER:HB3	1:A:491:TYR:CE1	2.44	0.52
1:A:205:GLN:HG3	1:A:209:PHE:CD2	2.45	0.52
2:A:701:NAD:C7N	3:A:702:FAD:C4	2.88	0.52
1:A:434:VAL:HG12	1:A:439:ALA:HB2	1.91	0.52
1:C:357:ARG:NH1	1:C:357:ARG:CG	2.73	0.51
1:C:501:LEU:HB3	4:C:813:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:LYS:O	1:C:359:GLY:N	2.33	0.51
1:A:293:GLU:O	1:A:296:SER:OG	2.21	0.51
1:C:205:GLN:NE2	1:C:209:PHE:CD1	2.79	0.50
1:A:483:SER:HB3	1:A:491:TYR:CZ	2.46	0.50
1:A:539:GLU:HA	4:A:818:HOH:O	2.11	0.50
1:A:307:GLU:OE2	2:A:701:NAD:O4B	2.29	0.50
1:C:434:VAL:HG12	1:C:439:ALA:HB2	1.93	0.50
1:A:227:LEU:HD21	1:A:230:LYS:HG3	1.91	0.50
1:C:501:LEU:HB2	4:C:813:HOH:O	2.10	0.50
1:C:164:ASP:OD1	1:C:165:PRO:HD2	2.11	0.49
1:C:369:GLN:NE2	1:C:369:GLN:CA	2.73	0.49
1:C:542:ILE:HG22	1:C:544:PRO:HD2	1.93	0.49
1:C:366:ALA:O	1:C:367:ILE:HG22	2.12	0.49
1:A:355:VAL:O	1:A:358:GLU:CB	2.60	0.48
1:A:382:LEU:HG	1:A:384:ASP:HB3	1.95	0.48
1:A:309:PHE:H	1:A:309:PHE:HD1	1.61	0.48
1:A:339:MET:HE2	4:A:808:HOH:O	2.12	0.48
1:C:275:GLU:O	1:C:278:SER:OG	2.31	0.48
1:C:364:PRO:CG	1:C:365:ASN:HD22	2.26	0.48
1:A:328:GLU:CG	1:A:361:LYS:HE3	2.41	0.48
1:C:193:ARG:O	1:C:194:GLN:HG2	2.14	0.47
1:A:308:GLY:N	4:A:801:HOH:O	2.25	0.47
1:C:262:THR:HG23	1:C:263:PRO:HD2	1.97	0.47
1:C:209:PHE:CD1	1:C:209:PHE:C	2.93	0.47
1:C:364:PRO:C	1:C:365:ASN:ND2	2.72	0.47
1:A:295:ILE:HD13	1:A:392:HIS:CE1	2.50	0.47
1:A:177:GLU:HG2	1:A:192:PHE:CD2	2.49	0.47
1:A:355:VAL:O	1:A:358:GLU:N	2.47	0.46
1:C:364:PRO:CG	1:C:365:ASN:ND2	2.78	0.46
1:A:309:PHE:CD2	1:A:339:MET:HE1	2.50	0.46
1:C:363:MET:HE1	1:C:386:ARG:HH11	1.64	0.46
1:C:175:SER:OG	1:C:313:GLU:HB3	2.16	0.46
2:C:701:NAD:C6N	3:C:702:FAD:C9A	2.93	0.46
1:A:262:THR:HG22	1:A:402:ASN:OD1	2.16	0.46
1:A:437:ASP:HB3	1:A:452:GLU:HG2	1.98	0.46
1:A:173:PRO:HG2	1:A:202:ILE:HG22	1.98	0.46
1:A:246:ASP:OD1	1:A:246:ASP:C	2.59	0.46
1:A:307:GLU:H	1:A:307:GLU:HG3	1.56	0.46
1:A:377:ARG:NH2	1:A:391:ASP:OD1	2.49	0.46
1:C:273:GLY:O	1:C:276:VAL:HG22	2.16	0.46
1:A:452:GLU:HB3	2:A:701:NAD:O3D	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:ASP:HB3	1:C:452:GLU:HG2	1.97	0.45
1:A:327:ILE:HG21	4:A:807:HOH:O	2.15	0.45
1:C:364:PRO:HB2	1:C:365:ASN:ND2	2.30	0.45
1:A:400:GLU:HG3	4:A:826:HOH:O	2.16	0.45
1:C:246:ASP:OD1	1:C:246:ASP:C	2.60	0.45
1:C:363:MET:HE2	1:C:363:MET:HB3	1.65	0.45
1:C:176:LYS:NZ	1:C:177:GLU:CD	2.73	0.45
1:C:176:LYS:HG2	1:C:176:LYS:HZ3	1.65	0.45
1:C:285:LYS:HE3	4:C:825:HOH:O	2.17	0.45
1:C:307:GLU:CD	1:C:307:GLU:C	2.85	0.45
2:C:701:NAD:C4N	3:C:702:FAD:C5X	2.95	0.45
1:C:194:GLN:HB3	1:C:195:TRP:HA	1.98	0.44
1:A:380:ILE:HD11	1:A:393:ILE:HD11	1.99	0.44
1:A:294:LYS:HB3	4:A:813:HOH:O	2.17	0.44
1:C:172:PRO:HA	3:C:702:FAD:C6	2.47	0.44
1:C:355:VAL:O	1:C:358:GLU:N	2.48	0.44
1:A:198:LYS:HA	1:A:198:LYS:HD2	1.64	0.44
1:C:281:THR:O	1:C:394:VAL:HA	2.17	0.44
1:A:310:LEU:HB3	1:A:396:ALA:HB1	2.00	0.44
1:A:583:ARG:N	4:A:803:HOH:O	2.42	0.44
1:A:308:GLY:CA	2:A:701:NAD:H52A	2.48	0.44
1:A:607:PHE:O	1:A:609:ILE:HG13	2.18	0.44
1:A:277:LYS:HE3	1:A:280:THR:O	2.17	0.43
1:A:429:ARG:O	1:A:430:SER:C	2.61	0.43
1:C:283:PHE:CZ	1:C:314:LEU:HD21	2.54	0.43
1:A:593:ASP:HB2	4:A:828:HOH:O	2.17	0.43
1:C:355:VAL:O	1:C:356:LYS:C	2.61	0.43
1:A:308:GLY:HA3	2:A:701:NAD:H52A	1.99	0.43
1:C:377:ARG:NH1	1:C:391:ASP:OD1	2.51	0.43
1:A:171:ARG:N	1:A:172:PRO:CD	2.82	0.43
1:C:380:ILE:HD11	1:C:393:ILE:HD11	1.99	0.43
1:C:282:LEU:HD12	1:C:282:LEU:C	2.44	0.42
1:C:542:ILE:CD1	1:C:601:ASN:HD21	2.32	0.42
1:A:542:ILE:CD1	1:A:601:ASN:HD21	2.33	0.42
1:C:347:LEU:O	1:C:351:THR:OG1	2.30	0.42
1:A:294:LYS:CD	4:A:813:HOH:O	2.62	0.42
1:A:378:LEU:HD12	1:A:391:ASP:O	2.20	0.42
1:A:176:LYS:HD3	1:A:484:ASP:HB2	2.02	0.41
1:A:304:VAL:HG22	1:A:394:VAL:HG23	2.02	0.41
1:C:429:ARG:O	1:C:430:SER:C	2.62	0.41
2:C:701:NAD:C4N	3:C:702:FAD:C4X	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:701:NAD:O3	2:C:701:NAD:H3D	2.19	0.41
1:A:355:VAL:O	1:A:358:GLU:HB3	2.20	0.41
2:C:701:NAD:C3N	3:C:702:FAD:C4X	2.98	0.41
1:A:241:MET:HG2	1:A:242:VAL:N	2.35	0.41
1:A:334:PRO:HD2	2:A:701:NAD:H2A	2.02	0.41
1:A:335:GLU:HB3	4:A:836:HOH:O	2.20	0.41
1:C:310:LEU:HB3	1:C:396:ALA:HB1	2.02	0.41
2:C:701:NAD:C5N	3:C:702:FAD:C6	2.98	0.41
1:A:307:GLU:OE2	2:A:701:NAD:H4B	2.20	0.41
2:A:701:NAD:N7N	3:A:702:FAD:N3	2.68	0.41
1:A:382:LEU:HD21	1:A:386:ARG:HB2	2.02	0.41
1:A:455:ASP:O	1:A:459:VAL:HG23	2.20	0.41
1:A:196:ASN:OD1	1:A:196:ASN:C	2.65	0.40
1:C:364:PRO:CB	1:C:365:ASN:ND2	2.85	0.40
1:C:542:ILE:HD12	1:C:601:ASN:HD21	1.85	0.40
1:A:360:VAL:HG12	1:A:361:LYS:N	2.35	0.40
1:C:313:GLU:OE1	4:C:801:HOH:O	2.22	0.40
1:C:423:ASN:OD1	1:C:423:ASN:C	2.64	0.40
1:A:321:LYS:O	1:A:325:SER:N	2.55	0.40
1:C:186:VAL:HG13	1:C:187:THR:HG23	2.04	0.40
1:C:321:LYS:O	1:C:325:SER:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ARG:NH1	1:C:608:ASN:ND2[3_555]	1.95	0.25

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	436/535 (82%)	404 (93%)	30 (7%)	2 (0%)	24	57
1	C	436/535 (82%)	398 (91%)	36 (8%)	2 (0%)	24	57
All	All	872/1070 (82%)	802 (92%)	66 (8%)	4 (0%)	24	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	608	ASN
1	A	207	PRO
1	C	207	PRO
1	C	309	PHE

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	364/436 (84%)	329 (90%)	35 (10%)	8	30
1	C	363/436 (83%)	331 (91%)	32 (9%)	9	33
All	All	727/872 (83%)	660 (91%)	67 (9%)	8	31

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	SER
1	A	175	SER
1	A	176	LYS
1	A	189	THR
1	A	193	ARG
1	A	195	TRP
1	A	196	ASN
1	A	198	LYS
1	A	199	GLU
1	A	201	SER
1	A	208	SER
1	A	211	VAL

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Mol	Chain	Res	Type
1	A	228	THR
1	A	277	LYS
1	A	279	ARG
1	A	280	THR
1	A	282	LEU
1	A	284	ARG
1	A	300	LYS
1	A	307	GLU
1	A	312	SER
1	A	336	LYS
1	A	357	ARG
1	A	373	VAL
1	A	374	SER
1	A	382	LEU
1	A	383	LYS
1	A	394	VAL
1	A	395	THR
1	A	407	LYS
1	A	408	THR
1	A	430	SER
1	A	479	SER
1	A	539	GLU
1	A	598	GLU
1	C	176	LYS
1	C	189	THR
1	C	198	LYS
1	C	199	GLU
1	C	201	SER
1	C	208	SER
1	C	211	VAL
1	C	228	THR
1	C	280	THR
1	C	282	LEU
1	C	283	PHE
1	C	285	LYS
1	C	300	LYS
1	C	305	ILE
1	C	307	GLU
1	C	330	ILE
1	C	357	ARG
1	C	369	GLN
1	C	373	VAL

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Mol	Chain	Res	Type
1	C	374	SER
1	C	382	LEU
1	C	387	LYS
1	C	394	VAL
1	C	395	THR
1	C	407	LYS
1	C	408	THR
1	C	430	SER
1	C	451	VAL
1	C	479	SER
1	C	540	ILE
1	C	541	THR
1	C	570	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	GLN
1	A	392	HIS
1	A	456	HIS
1	A	477	HIS
1	A	601	ASN
1	C	323	GLN
1	C	338	ASN
1	C	349	ASN
1	C	365	ASN
1	C	392	HIS
1	C	601	ASN
1	C	608	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	701	-	46,48,48	1.21	3 (6%)	64,73,73	1.77	15 (23%)
3	FAD	C	702	-	58,58,58	1.80	11 (18%)	85,89,89	1.71	18 (21%)
2	NAD	C	701	-	46,48,48	1.20	5 (10%)	64,73,73	1.61	11 (17%)
3	FAD	A	702	-	58,58,58	1.66	11 (18%)	85,89,89	1.66	17 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	701	-	-	13/30/62/62	0/5/5/5
3	FAD	C	702	-	-	7/34/50/50	0/6/6/6
2	NAD	C	701	-	-	15/30/62/62	0/5/5/5
3	FAD	A	702	-	-	6/34/50/50	0/6/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	FAD	P-O3P	6.14	1.66	1.59
3	A	702	FAD	P-O3P	5.18	1.65	1.59
3	C	702	FAD	C5A-C4A	5.06	1.48	1.39
3	C	702	FAD	C9A-C5X	5.04	1.49	1.41
3	A	702	FAD	C9A-C5X	5.04	1.49	1.41
2	A	701	NAD	C5A-C4A	5.00	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	FAD	PA-O3P	4.93	1.64	1.59
2	C	701	NAD	C5A-C4A	4.68	1.47	1.39
3	A	702	FAD	PA-O3P	4.43	1.64	1.59
3	A	702	FAD	C5A-C4A	4.08	1.46	1.39
3	C	702	FAD	C8-C7	3.07	1.48	1.40
3	A	702	FAD	C8-C7	3.06	1.48	1.40
3	A	702	FAD	C5X-N5	-3.03	1.33	1.39
2	A	701	NAD	C5A-C6A	2.81	1.48	1.41
2	C	701	NAD	C5A-C6A	2.69	1.48	1.41
3	C	702	FAD	C5A-N7A	-2.69	1.34	1.39
3	A	702	FAD	C5A-N7A	-2.67	1.34	1.39
2	C	701	NAD	C8A-N7A	2.59	1.36	1.31
2	A	701	NAD	C8A-N7A	2.53	1.36	1.31
3	A	702	FAD	C8A-N7A	2.49	1.36	1.31
3	C	702	FAD	C4A-N9A	-2.25	1.33	1.37
3	A	702	FAD	C5A-C6A	2.24	1.47	1.41
2	C	701	NAD	O4D-C1D	2.18	1.43	1.40
3	C	702	FAD	C10-N10	2.18	1.42	1.37
3	C	702	FAD	C5X-N5	-2.10	1.35	1.39
3	C	702	FAD	C8A-N7A	2.08	1.35	1.31
3	A	702	FAD	C4-N3	-2.06	1.35	1.38
3	C	702	FAD	C5A-C6A	2.05	1.46	1.41
3	A	702	FAD	C4A-N9A	-2.03	1.33	1.37
2	C	701	NAD	C5A-N7A	-2.01	1.35	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	C5A-C4A-N3A	-6.20	118.18	126.72
2	A	701	NAD	C5A-C4A-N3A	-5.35	119.36	126.72
2	C	701	NAD	C5A-C4A-N3A	-5.27	119.46	126.72
3	A	702	FAD	N3A-C4A-N9A	4.73	135.21	127.17
3	C	702	FAD	O4B-C1B-N9A	4.48	116.70	108.09
2	A	701	NAD	N3A-C4A-N9A	4.40	134.64	127.17
2	C	701	NAD	N3A-C4A-N9A	4.40	134.64	127.17
3	C	702	FAD	N3A-C2A-N1A	-4.22	122.19	128.58
3	C	702	FAD	N3A-C4A-N9A	4.05	134.05	127.17
2	A	701	NAD	N3A-C2A-N1A	-3.99	122.55	128.58
3	A	702	FAD	C2A-N3A-C4A	3.99	121.56	111.83
2	C	701	NAD	N3A-C2A-N1A	-3.93	122.63	128.58
3	C	702	FAD	O4-C4-C4X	-3.92	116.19	126.53
2	C	701	NAD	C2A-N3A-C4A	3.86	121.26	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAD	C2A-N3A-C4A	3.83	121.18	111.83
3	C	702	FAD	C5A-C4A-N3A	-3.69	121.64	126.72
3	A	702	FAD	O2-C2-N1	-3.64	115.75	121.80
2	A	701	NAD	O2N-PN-O3	3.52	116.79	107.27
3	A	702	FAD	N3A-C2A-N1A	-3.50	123.29	128.58
2	A	701	NAD	O4B-C1B-N9A	3.34	114.51	108.09
3	C	702	FAD	C2B-C1B-N9A	-3.16	105.45	113.30
2	C	701	NAD	C4A-N9A-C8A	3.15	109.05	105.74
3	A	702	FAD	C4A-C5A-N7A	-3.10	107.03	110.58
3	C	702	FAD	N6A-C6A-N1A	3.08	125.25	118.38
3	A	702	FAD	C9A-N10-C10	-3.07	116.08	120.75
2	A	701	NAD	O3-PA-O1A	-3.01	101.65	110.70
3	C	702	FAD	C2A-N3A-C4A	3.01	119.17	111.83
2	A	701	NAD	C4A-C5A-N7A	-3.00	107.15	110.58
3	C	702	FAD	C4A-N9A-C8A	3.00	108.89	105.74
3	C	702	FAD	O4-C4-N3	2.99	125.74	120.11
3	A	702	FAD	C4X-C10-N10	2.92	120.66	116.48
3	C	702	FAD	C10-N1-C2	2.89	123.11	116.85
3	C	702	FAD	C2A-N1A-C6A	2.88	123.47	118.73
2	C	701	NAD	C3N-C7N-N7N	2.87	121.28	117.74
3	A	702	FAD	O4-C4-C4X	-2.85	119.01	126.53
2	C	701	NAD	C4A-C5A-N7A	-2.85	107.33	110.58
2	A	701	NAD	C4A-N9A-C8A	2.78	108.66	105.74
3	C	702	FAD	C4X-C10-N1	-2.73	117.91	124.59
3	C	702	FAD	O2-C2-N1	-2.67	117.36	121.80
2	A	701	NAD	O2A-PA-O1A	2.57	124.40	112.44
2	A	701	NAD	C5A-N7A-C8A	2.50	107.38	103.45
2	C	701	NAD	C6A-C5A-N7A	2.42	136.75	132.09
3	C	702	FAD	C5A-C6A-N6A	-2.39	117.37	123.29
3	A	702	FAD	C5A-N7A-C8A	2.38	107.19	103.45
2	C	701	NAD	N9A-C8A-N7A	-2.35	110.61	113.94
3	A	702	FAD	C4A-N9A-C8A	2.34	108.19	105.74
2	C	701	NAD	C5A-N7A-C8A	2.34	107.12	103.45
2	A	701	NAD	C6A-C5A-N7A	2.32	136.57	132.09
3	A	702	FAD	O4'-C4'-C5'	-2.32	104.86	109.99
3	C	702	FAD	C4A-N9A-C1B	-2.29	121.27	126.63
2	A	701	NAD	C2A-N1A-C6A	2.25	122.42	118.73
3	C	702	FAD	O3B-C3B-C4B	2.24	117.52	111.08
2	C	701	NAD	O2N-PN-O1N	2.24	122.87	112.44
3	A	702	FAD	O3P-PA-O1A	-2.24	103.98	110.70
2	A	701	NAD	N9A-C8A-N7A	-2.20	110.81	113.94
3	A	702	FAD	C5X-C9A-N10	2.17	119.93	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	C4X-C10-N1	-2.16	119.29	124.59
3	A	702	FAD	N9A-C8A-N7A	-2.09	110.97	113.94
3	C	702	FAD	O2A-PA-O1A	2.08	122.11	112.44
3	A	702	FAD	O4-C4-N3	2.04	123.95	120.11
2	A	701	NAD	C3B-C2B-C1B	2.02	105.29	101.46

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NAD	C5B-O5B-PA-O1A
2	A	701	NAD	C5B-O5B-PA-O3
2	A	701	NAD	PN-O3-PA-O5B
2	A	701	NAD	C5D-O5D-PN-O3
2	A	701	NAD	C5D-O5D-PN-O2N
2	C	701	NAD	C5B-O5B-PA-O1A
2	C	701	NAD	O4D-C1D-N1N-C2N
3	A	702	FAD	PA-O3P-P-O5'
3	C	702	FAD	PA-O3P-P-O5'
3	C	702	FAD	O4B-C4B-C5B-O5B
2	A	701	NAD	O4B-C4B-C5B-O5B
2	A	701	NAD	C3B-C4B-C5B-O5B
2	C	701	NAD	O4B-C4B-C5B-O5B
3	C	702	FAD	C3B-C4B-C5B-O5B
2	A	701	NAD	C4B-C5B-O5B-PA
2	C	701	NAD	C3B-C4B-C5B-O5B
2	C	701	NAD	O4D-C4D-C5D-O5D
2	C	701	NAD	C3D-C4D-C5D-O5D
2	C	701	NAD	C4B-C5B-O5B-PA
2	C	701	NAD	PN-O3-PA-O5B
2	C	701	NAD	C2B-C1B-N9A-C8A
2	A	701	NAD	O4B-C1B-N9A-C8A
3	A	702	FAD	O4B-C4B-C5B-O5B
2	A	701	NAD	C2B-C1B-N9A-C8A
3	A	702	FAD	C2B-C1B-N9A-C8A
3	C	702	FAD	N10-C1'-C2'-O2'
2	A	701	NAD	C5D-O5D-PN-O1N
2	C	701	NAD	C5B-O5B-PA-O2A
2	C	701	NAD	C5B-O5B-PA-O3
2	C	701	NAD	PN-O3-PA-O1A
3	C	702	FAD	P-O3P-PA-O2A
2	C	701	NAD	C2B-C1B-N9A-C4A

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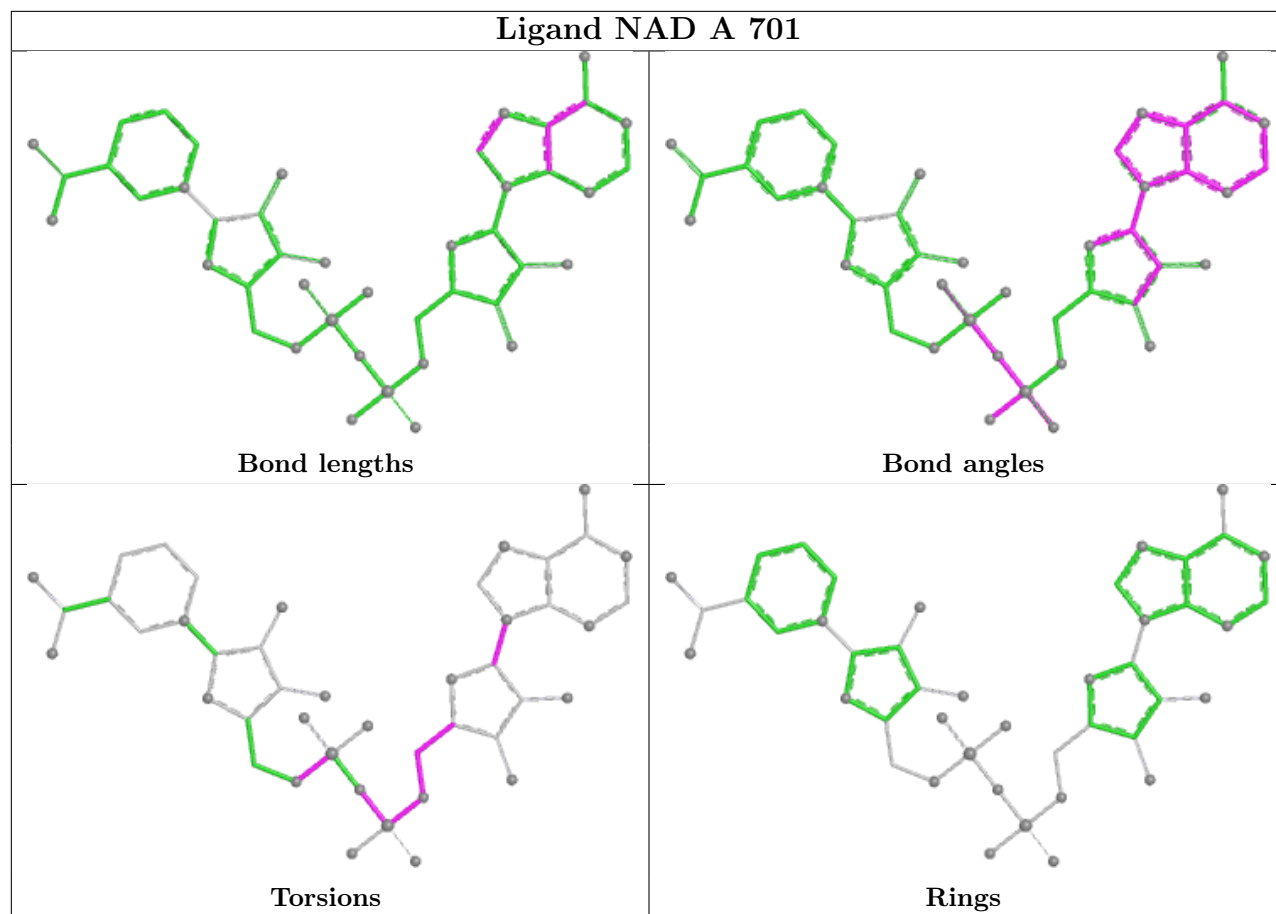
Mol	Chain	Res	Type	Atoms
3	A	702	FAD	C3B-C4B-C5B-O5B
2	A	701	NAD	O4B-C1B-N9A-C4A
2	C	701	NAD	C4D-C5D-O5D-PN
3	C	702	FAD	P-O3P-PA-O1A
3	A	702	FAD	O4B-C1B-N9A-C8A
2	C	701	NAD	O4B-C1B-N9A-C8A
2	A	701	NAD	C2B-C1B-N9A-C4A
3	A	702	FAD	C2B-C1B-N9A-C4A
3	C	702	FAD	C2B-C1B-N9A-C8A

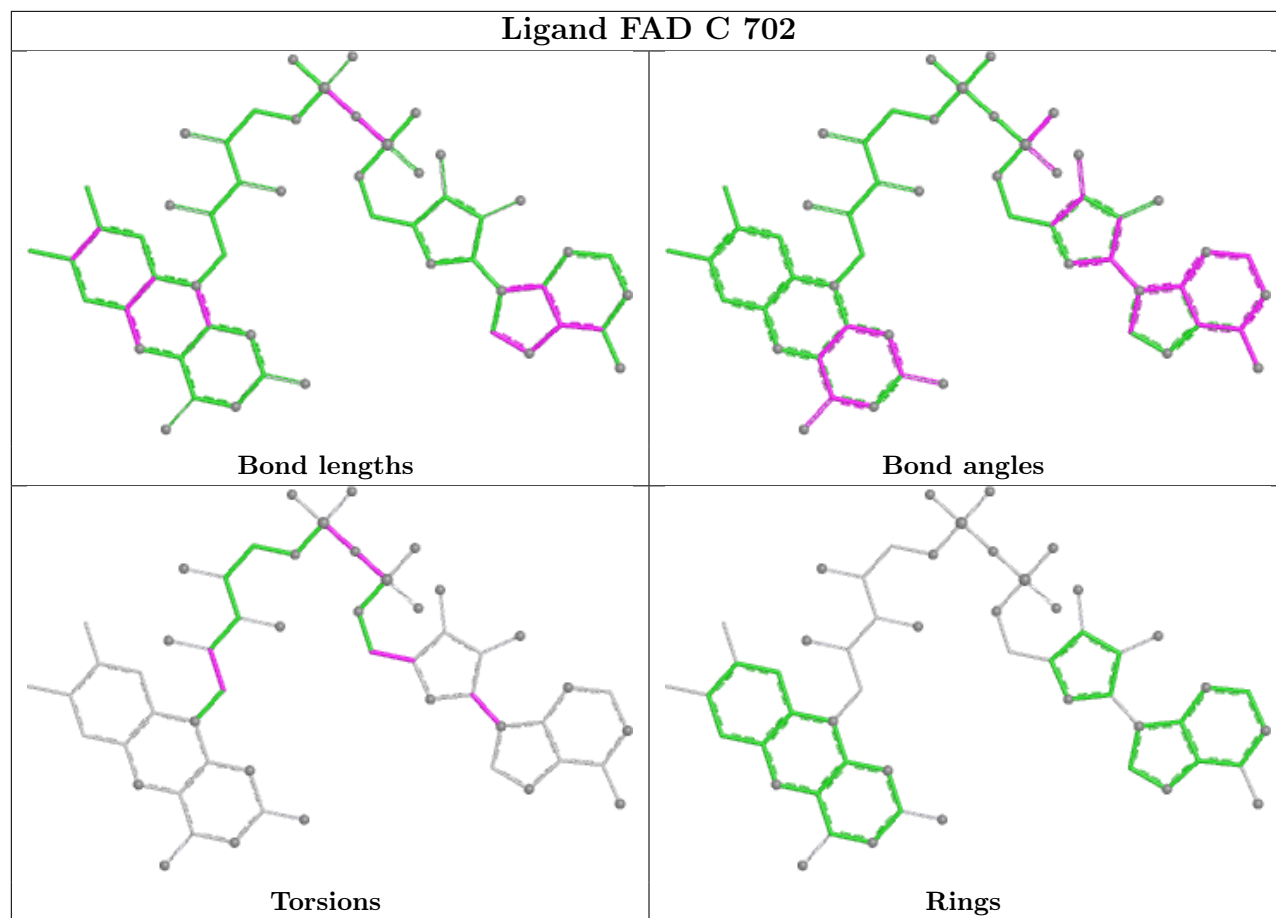
There are no ring outliers.

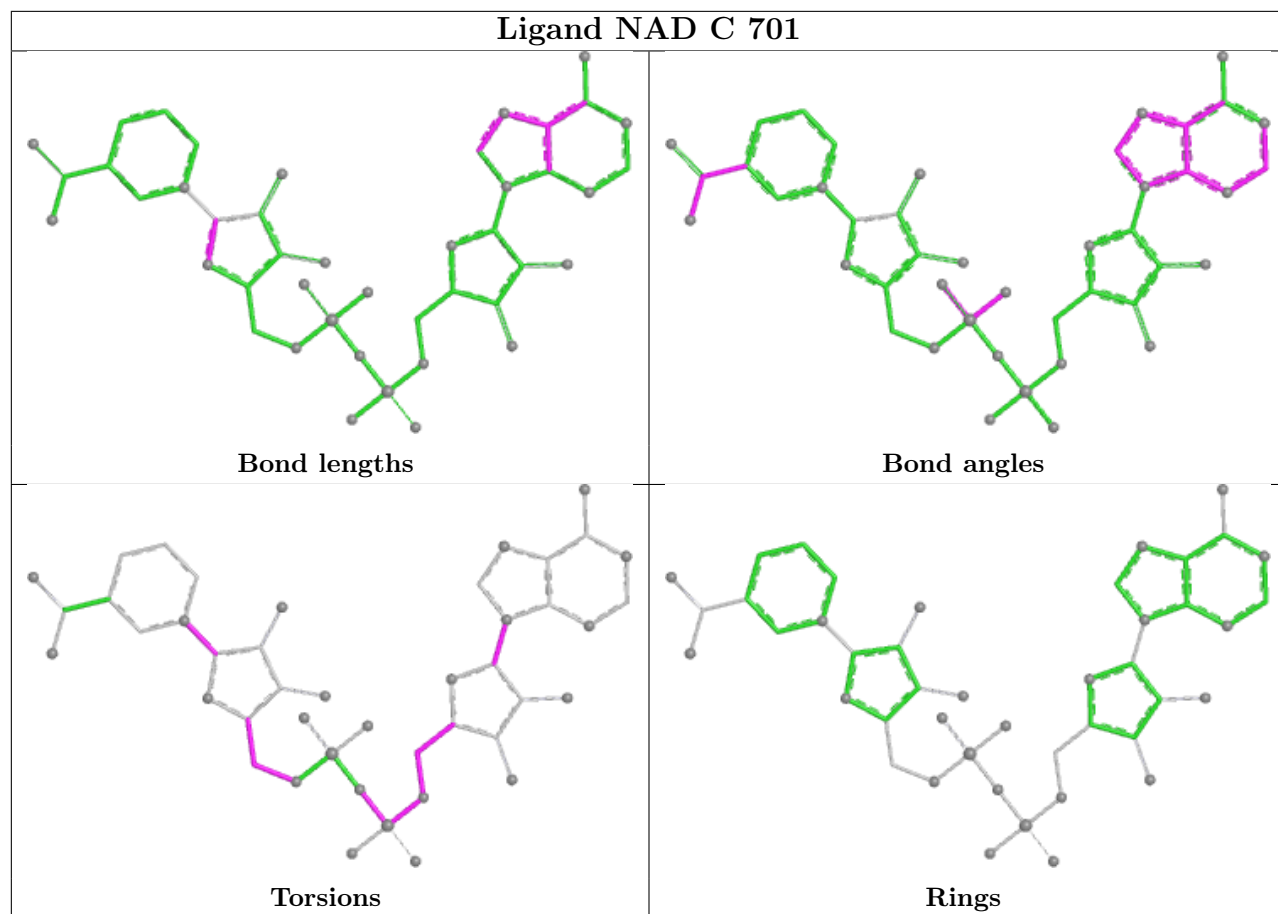
4 monomers are involved in 30 short contacts:

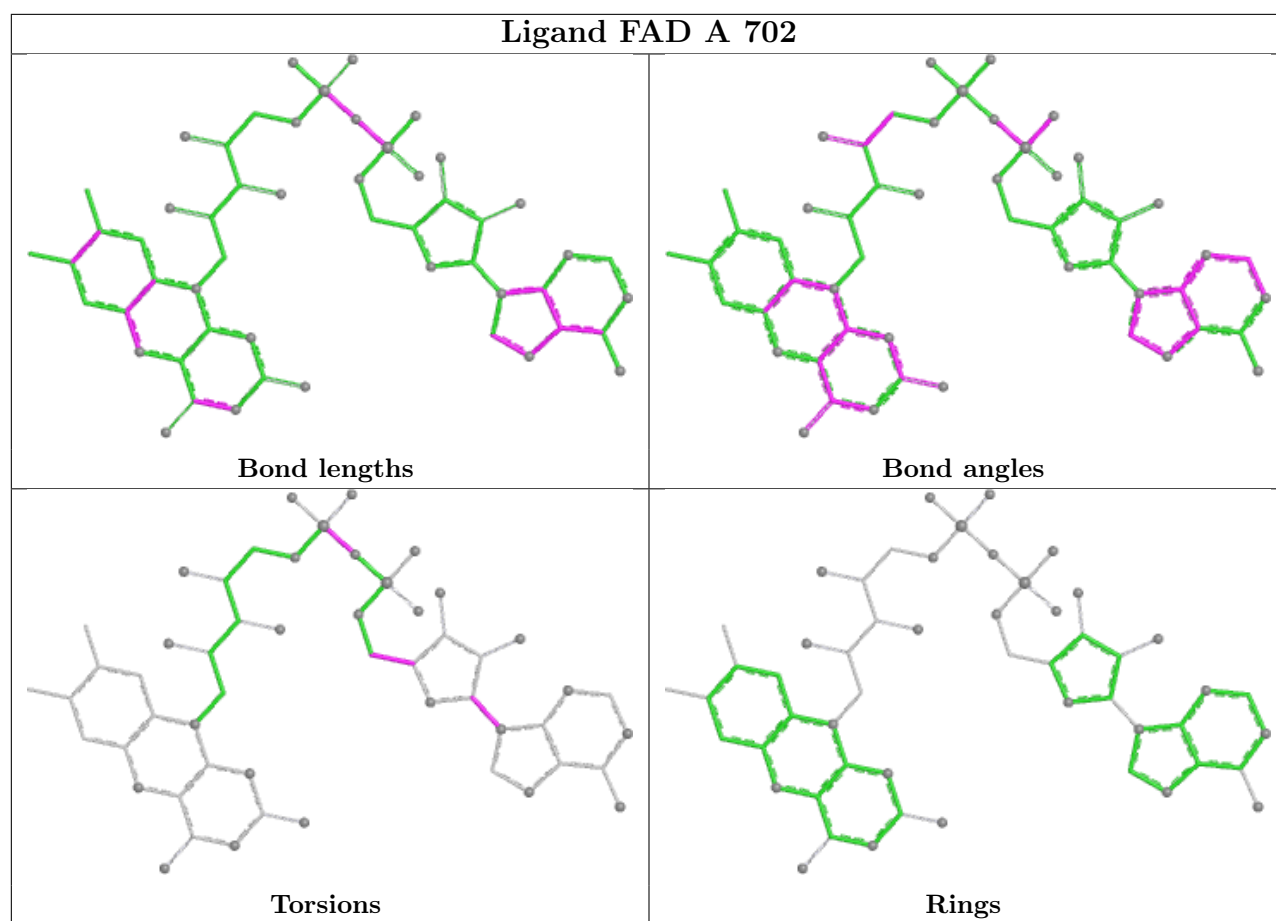
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	NAD	10	0
3	C	702	FAD	10	0
2	C	701	NAD	9	0
3	A	702	FAD	12	0

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	442/535 (82%)	-0.56	0 100 100	51, 87, 134, 153	0
1	C	442/535 (82%)	-0.38	0 100 100	58, 98, 134, 170	0
All	All	884/1070 (82%)	-0.47	0 100 100	51, 94, 134, 170	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

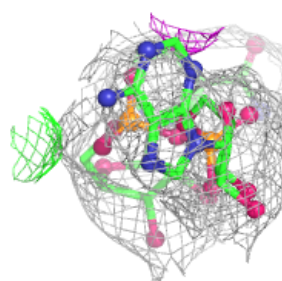
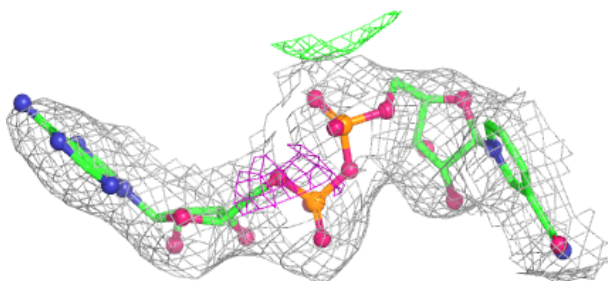
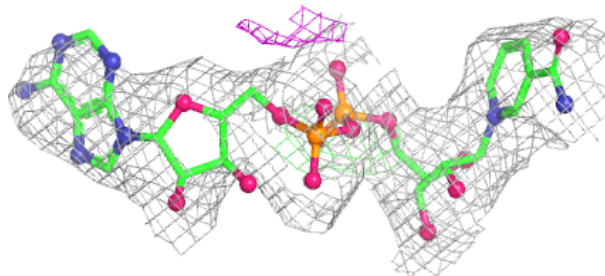
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	A	701	44/44	0.96	0.06	64,82,135,140	0
2	NAD	C	701	44/44	0.96	0.07	63,77,140,143	0
3	FAD	C	702	53/53	0.96	0.07	61,80,97,108	0
3	FAD	A	702	53/53	0.97	0.06	52,68,79,88	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

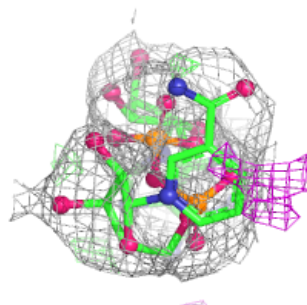
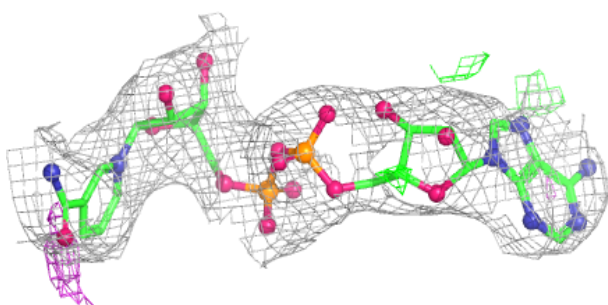
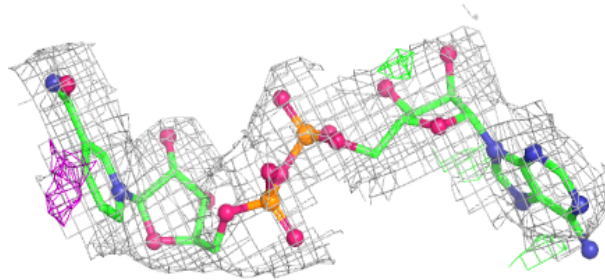
Electron density around NAD A 701:

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



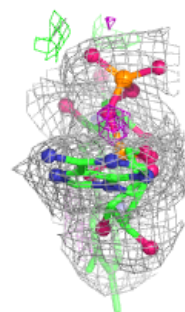
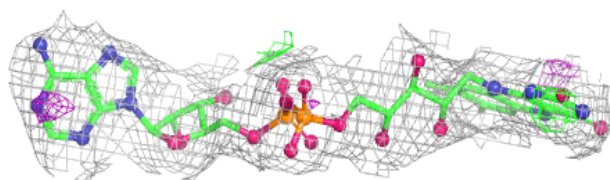
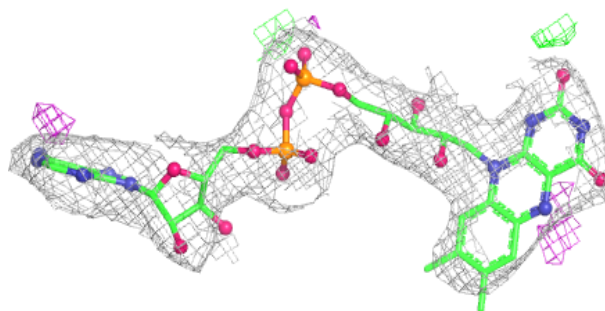
Electron density around NAD C 701:

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

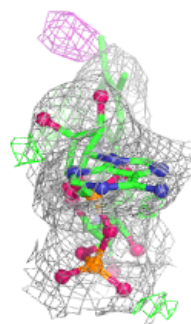
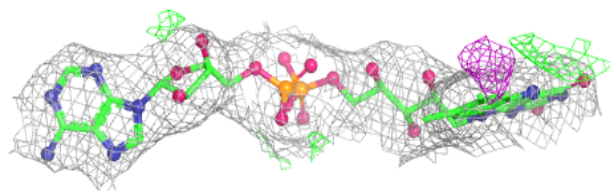
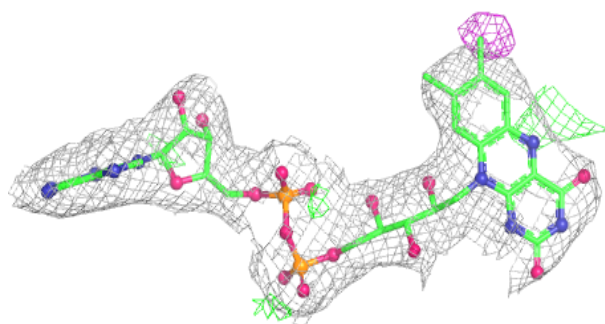


Electron density around FAD C 702:

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

**Electron density around FAD A 702:**

$2mF_o-DF_c$ (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.