



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:19 AM UTC

PDB ID : 4E5N / pdb_00004e5n
Title : Thermostable phosphite dehydrogenase in complex with NAD
Authors : Zou, Y.; Zhang, H.; Nair, S.K.
Deposited on : 2012-03-14
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

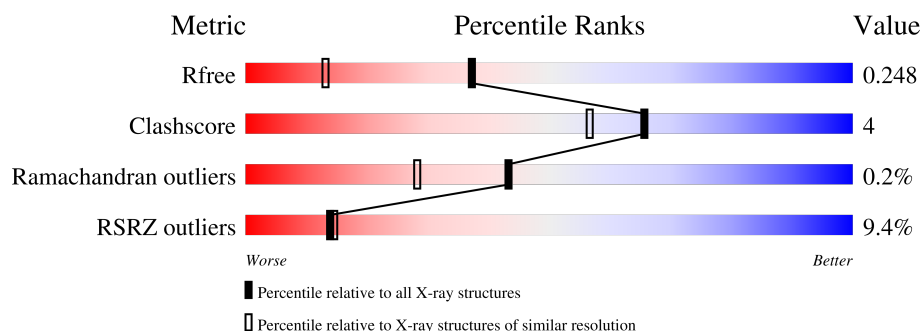
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	330	4% 91% 9%
1	B	330	6% 92% 8%
1	C	330	12% 91% 9%
1	D	330	4% 95% 5%
1	E	330	12% 90% 9%
1	F	330	2% 91% 8%

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Mol	Chain	Length	Quality of chain
1	G	330	4% 90% 9%
1	H	330	30% 91% 9%

2 Entry composition

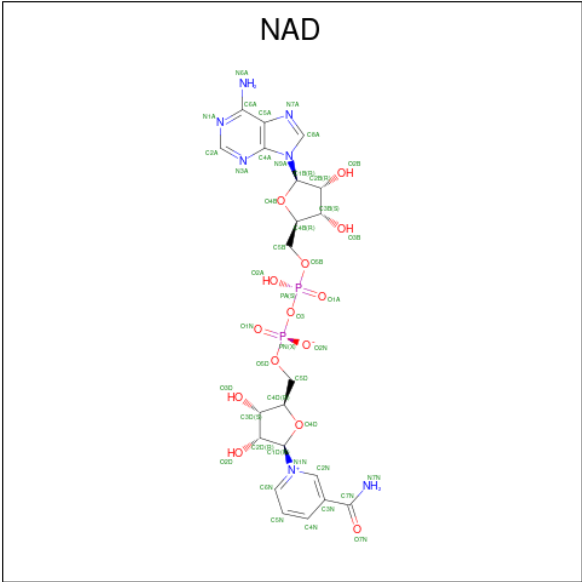
There are 3 unique types of molecules in this entry. The entry contains 22943 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thermostable phosphite dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2519	1591	456	457	15			
1	B	329	Total	C	N	O	S	0	0	0
			2519	1591	456	457	15			
1	C	330	Total	C	N	O	S	0	0	0
			2528	1597	458	458	15			
1	D	330	Total	C	N	O	S	0	0	0
			2524	1595	457	457	15			
1	E	328	Total	C	N	O	S	0	0	0
			2511	1586	455	456	14			
1	F	327	Total	C	N	O	S	0	0	0
			2504	1581	454	455	14			
1	G	328	Total	C	N	O	S	0	0	0
			2509	1584	455	456	14			
1	H	329	Total	C	N	O	S	0	0	0
			2519	1591	456	457	15			

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	347	Total	O	0	0
			347	347		
3	B	368	Total	O	0	0
			368	368		
3	C	210	Total	O	0	0
			210	210		
3	D	390	Total	O	0	0
			390	390		

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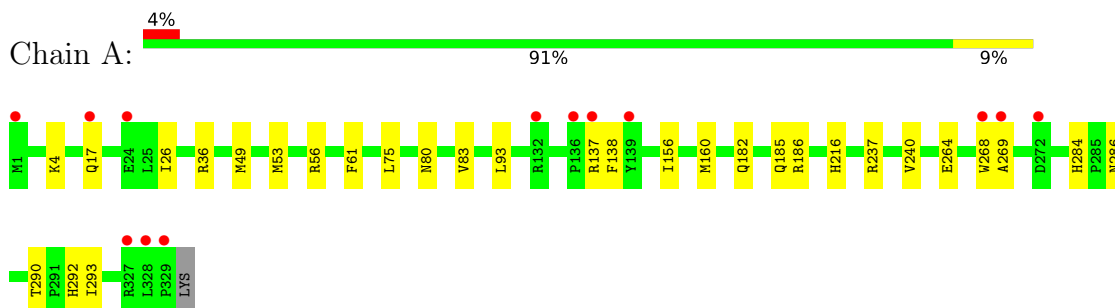
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	235	Total 235	O 235	0	0
3	F	370	Total 370	O 370	0	0
3	G	371	Total 371	O 371	0	0
3	H	167	Total 167	O 167	0	0

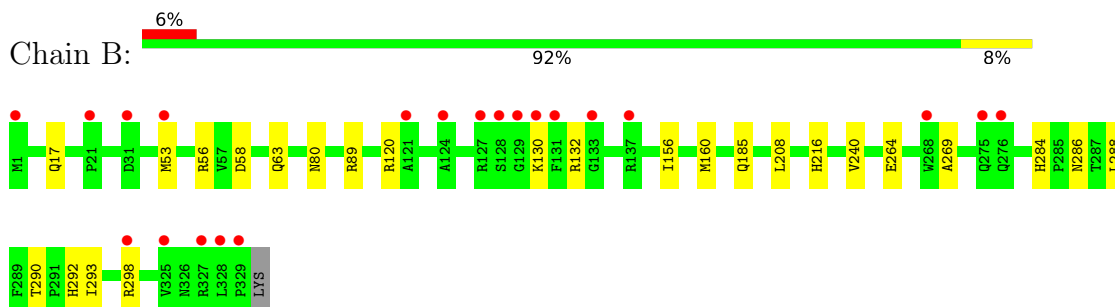
3 Residue-property plots [i](#)

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.

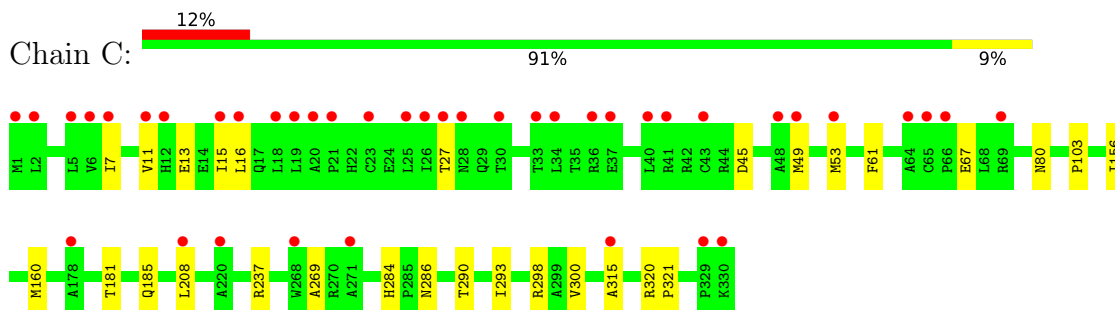
- Molecule 1: Thermostable phosphite dehydrogenase



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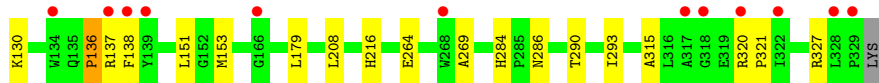
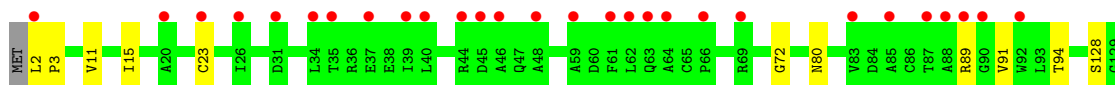
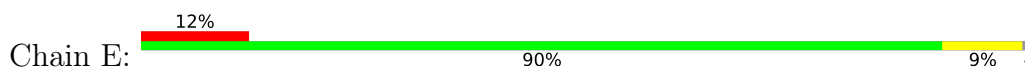


- Molecule 1: Thermostable phosphite dehydrogenase

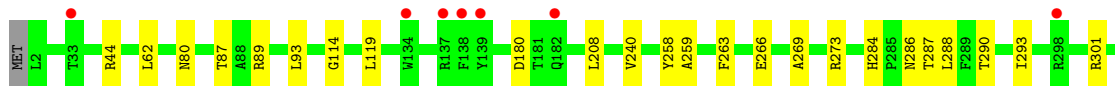
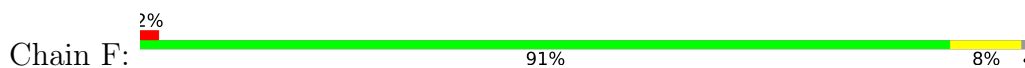




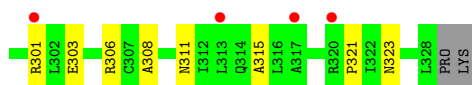
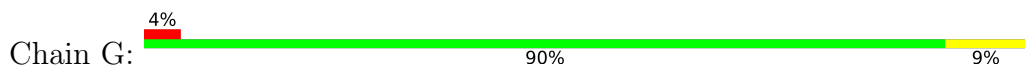
- Molecule 1: Thermostable phosphite dehydrogenase



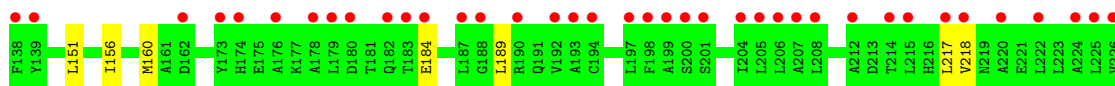
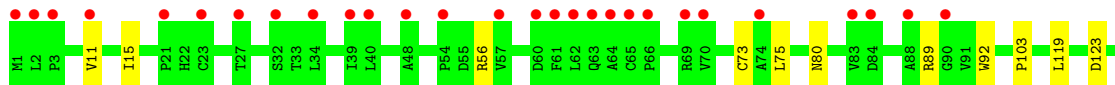
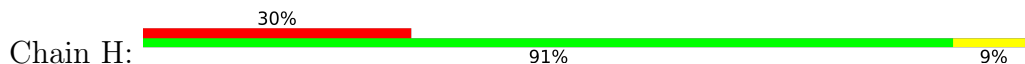
- Molecule 1: Thermostable phosphite dehydrogenase



- Molecule 1: Thermostable phosphite dehydrogenase



- Molecule 1: Thermostable phosphite dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.71Å 113.54Å 130.19Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70 25.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-1.70) 95.0 (25.00-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.247 (Not available) , 0.248	Depositor DCC
R_{free} test set	13626 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22943	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.3755e-04.*

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: 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	0.48	0/2566	0.76	0/3490
1	B	0.50	0/2566	0.76	0/3490
1	C	0.46	0/2575	0.76	0/3501
1	D	0.51	0/2571	0.77	0/3496
1	E	0.48	0/2558	0.79	0/3480
1	F	0.50	0/2550	0.77	0/3468
1	G	0.50	0/2555	0.77	0/3475
1	H	0.46	0/2566	0.77	0/3490
All	All	0.49	0/20507	0.77	0/27890

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2519	0	2540	22	0
1	B	2519	0	2540	22	0
1	C	2528	0	2553	18	0
1	D	2524	0	2547	15	0
1	E	2511	0	2528	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2504	0	2521	24	0
1	G	2509	0	2526	29	0
1	H	2519	0	2540	18	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	1	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	1	0
2	H	44	0	26	0	0
3	A	347	0	0	1	0
3	B	368	0	0	2	0
3	C	210	0	0	1	0
3	D	390	0	0	5	1
3	E	235	0	0	0	1
3	F	370	0	0	1	1
3	G	371	0	0	4	0
3	H	167	0	0	2	0
All	All	22943	0	20503	155	2

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 4.

All (155) 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:G:56:ARG:NH1	3:G:1263:HOH:O	2.05	0.82
1:G:311:ASN:HD21	1:G:323:ASN:H	1.30	0.79
1:B:298:ARG:O	3:B:1264:HOH:O	2.10	0.70
1:A:290:THR:HB	1:A:293:ILE:HG12	1.77	0.66
1:F:284:HIS:HD2	1:F:286:ASN:H	1.42	0.66
1:D:196:GLU:HG3	3:D:1050:HOH:O	1.96	0.66
1:A:284:HIS:HD2	1:A:286:ASN:H	1.42	0.65
1:F:326:ASN:HD22	1:F:326:ASN:H	1.44	0.65
1:G:50:MET:HE3	1:G:308:ALA:HB3	1.79	0.64
1:A:53:MET:HG2	1:A:292:HIS:CE1	2.32	0.64
1:G:185:GLN:NE2	3:G:997:HOH:O	2.24	0.64
1:A:53:MET:HE2	1:A:75:LEU:HD22	1.79	0.63
1:E:151:LEU:HG	1:E:208:LEU:HD21	1.80	0.63
1:G:295:SER:OG	1:G:301:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:HIS:HD2	1:D:286:ASN:H	1.47	0.62
1:D:139:TYR:CE1	1:G:301:ARG:HG3	2.36	0.61
1:B:298:ARG:C	1:B:298:ARG:HD3	2.26	0.60
1:A:49:MET:HE1	1:A:61:PHE:CE2	2.36	0.60
1:F:44:ARG:HD3	3:F:1005:HOH:O	2.01	0.60
1:F:80:ASN:ND2	1:F:269:ALA:H	2.00	0.59
1:G:284:HIS:HD2	1:G:286:ASN:H	1.49	0.59
1:D:303:GLU:OE2	1:D:306:ARG:NH1	2.36	0.59
1:A:284:HIS:CD2	1:A:286:ASN:H	2.19	0.59
1:E:11:VAL:CG1	1:E:15:ILE:HB	2.33	0.59
1:A:49:MET:HE1	1:A:61:PHE:HE2	1.67	0.59
1:A:36:ARG:NH2	1:A:56:ARG:HH21	2.00	0.58
1:E:216:HIS:HE1	1:E:264:GLU:OE1	1.86	0.58
1:A:4:LYS:HE2	1:A:26:ILE:HG13	1.86	0.58
1:F:208:LEU:HD21	1:F:240:VAL:HG11	1.85	0.57
1:C:49:MET:HE1	1:C:61:PHE:HE2	1.70	0.57
1:E:315:ALA:HB2	1:E:321:PRO:HG3	1.87	0.57
1:C:53:MET:HE1	1:C:237:ARG:NH2	2.20	0.57
1:D:196:GLU:OE1	3:D:1275:HOH:O	2.17	0.56
1:C:49:MET:HE1	1:C:61:PHE:CE2	2.40	0.56
1:G:303:GLU:OE1	1:G:306:ARG:NH1	2.39	0.55
1:D:119:LEU:HD21	1:G:288:LEU:HD21	1.88	0.55
1:F:114:GLY:HA2	1:F:119:LEU:HD12	1.88	0.55
1:F:314:GLN:HE22	1:F:322:ILE:H	1.52	0.55
1:F:314:GLN:HE22	1:F:322:ILE:HG12	1.70	0.55
1:C:181:THR:HG22	1:C:185:GLN:HE21	1.71	0.55
1:D:284:HIS:CD2	1:D:286:ASN:H	2.24	0.55
1:B:284:HIS:HD2	1:B:286:ASN:H	1.54	0.55
1:F:93:LEU:H	1:F:326:ASN:HD21	1.54	0.55
3:D:980:HOH:O	1:G:298:ARG:HA	2.08	0.54
1:D:139:TYR:HE1	1:G:301:ARG:HG3	1.72	0.54
1:C:298:ARG:HB2	3:C:979:HOH:O	2.07	0.53
1:G:311:ASN:ND2	1:G:323:ASN:H	2.02	0.53
1:C:156:ILE:HG22	1:C:160:MET:HE2	1.89	0.53
1:D:53:MET:HE3	3:D:1274:HOH:O	2.07	0.53
1:B:290:THR:HB	1:B:293:ILE:HG12	1.89	0.53
1:G:80:ASN:ND2	1:G:269:ALA:H	2.07	0.53
1:A:137:ARG:HG2	1:A:138:PHE:H	1.72	0.53
1:F:284:HIS:CD2	1:F:286:ASN:H	2.25	0.52
1:H:290:THR:HB	1:H:293:ILE:HG12	1.91	0.52
1:C:290:THR:HB	1:C:293:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:THR:HB	1:D:293:ILE:HG12	1.90	0.52
1:B:208:LEU:HD11	1:B:240:VAL:HG11	1.91	0.52
1:G:208:LEU:HD21	1:G:240:VAL:HG11	1.91	0.52
1:H:320:ARG:HH21	1:H:327:ARG:HG2	1.73	0.52
1:A:53:MET:HE2	1:A:53:MET:HA	1.92	0.51
1:C:284:HIS:HD2	1:C:286:ASN:H	1.57	0.51
1:G:69:ARG:HD2	3:G:1070:HOH:O	2.10	0.51
1:B:63:GLN:HE21	1:B:89:ARG:HH12	1.58	0.51
1:D:208:LEU:HD21	1:D:240:VAL:HG11	1.91	0.50
1:F:87:THR:HG22	1:F:326:ASN:HB2	1.93	0.50
1:A:156:ILE:HG22	1:A:160:MET:HE2	1.94	0.50
1:B:53:MET:HG2	1:B:292:HIS:CE1	2.47	0.50
1:G:303:GLU:OE2	1:G:306:ARG:NH1	2.45	0.49
1:C:53:MET:HE1	1:C:237:ARG:HH22	1.77	0.49
1:F:62:LEU:HB3	1:F:89:ARG:HD3	1.93	0.49
1:A:36:ARG:HH21	1:A:56:ARG:HH21	1.61	0.48
1:A:80:ASN:ND2	1:A:269:ALA:H	2.11	0.48
1:H:103:PRO:HG3	1:H:300:VAL:HG11	1.94	0.48
1:H:184:GLU:O	1:H:189:LEU:N	2.46	0.48
1:G:216:HIS:HE1	1:G:264:GLU:OE1	1.97	0.48
1:C:11:VAL:HG13	1:C:15:ILE:HB	1.95	0.48
1:G:284:HIS:CD2	1:G:286:ASN:H	2.29	0.48
1:E:89:ARG:HG3	1:E:91:VAL:HG23	1.96	0.48
1:A:216:HIS:HE1	1:A:264:GLU:OE1	1.95	0.48
1:B:216:HIS:HE1	1:B:264:GLU:OE1	1.96	0.48
1:E:284:HIS:CD2	1:E:286:ASN:H	2.32	0.48
1:H:11:VAL:CG1	1:H:15:ILE:HB	2.44	0.47
1:F:314:GLN:NE2	1:F:322:ILE:HG12	2.30	0.47
1:H:156:ILE:HG22	1:H:160:MET:HE2	1.96	0.47
1:D:80:ASN:ND2	1:D:269:ALA:H	2.13	0.47
1:E:290:THR:HB	1:E:293:ILE:HG12	1.97	0.46
1:C:208:LEU:HD22	2:C:800:NAD:C4A	2.45	0.46
1:A:83:VAL:HG22	1:A:93:LEU:CD2	2.46	0.46
1:G:315:ALA:HB2	1:G:321:PRO:HG3	1.97	0.46
1:E:284:HIS:HD2	1:E:286:ASN:H	1.62	0.46
1:G:303:GLU:CD	1:G:306:ARG:NH1	2.74	0.46
1:B:120:ARG:HD2	1:H:123:ASP:OD2	2.15	0.46
1:A:182:GLN:O	1:A:186:ARG:HG2	2.16	0.46
1:B:185:GLN:NE2	1:G:273:ARG:HH21	2.15	0.45
1:C:80:ASN:ND2	1:C:269:ALA:H	2.15	0.45
1:G:311:ASN:HD21	1:G:323:ASN:N	2.08	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:VAL:HB	1:H:241:VAL:HG12	1.99	0.45
1:B:63:GLN:NE2	1:B:89:ARG:HH12	2.14	0.45
1:H:56:ARG:HG3	1:H:268:TRP:HB2	1.99	0.45
1:A:17:GLN:CD	3:A:1236:HOH:O	2.59	0.45
1:E:80:ASN:ND2	1:E:269:ALA:H	2.14	0.45
1:E:136:PRO:O	1:E:138:PHE:N	2.44	0.45
1:B:284:HIS:CD2	1:B:286:ASN:H	2.33	0.44
1:F:263:PHE:O	1:F:266:GLU:HG2	2.17	0.44
2:G:800:NAD:H8A	3:G:1248:HOH:O	2.17	0.44
1:F:93:LEU:H	1:F:326:ASN:ND2	2.15	0.44
1:B:130:LYS:HE2	1:B:132:ARG:HH12	1.82	0.44
1:H:80:ASN:HD22	1:H:269:ALA:HB2	1.82	0.44
1:C:45:ASP:HA	1:C:67:GLU:HG3	2.00	0.44
1:H:151:LEU:HD21	1:H:217:LEU:HD22	2.00	0.44
1:B:208:LEU:CD1	1:B:240:VAL:HG11	2.48	0.43
1:B:288:LEU:HD21	1:H:119:LEU:HD21	2.00	0.43
1:B:156:ILE:HG22	1:B:160:MET:HE2	2.00	0.43
1:B:80:ASN:ND2	1:B:269:ALA:H	2.16	0.43
1:D:89:ARG:HD2	3:D:1007:HOH:O	2.18	0.43
1:E:128:SER:OG	1:E:130:LYS:HE2	2.18	0.43
1:E:3:PRO:O	1:E:23:CYS:HB2	2.18	0.43
1:E:72:GLY:HA2	1:E:94:THR:OG1	2.19	0.43
1:F:301:ARG:HD2	1:F:304:ILE:HD12	2.01	0.43
1:G:290:THR:HB	1:G:293:ILE:HG12	2.00	0.43
1:B:63:GLN:HE21	1:B:89:ARG:NH1	2.15	0.43
1:E:153:MET:HG2	1:E:179:LEU:HD11	2.02	0.42
1:G:150:PHE:CE1	1:G:205:LEU:HD12	2.55	0.42
1:B:17:GLN:HG2	3:B:1212:HOH:O	2.19	0.42
1:H:284:HIS:HA	1:H:285:PRO:HD3	1.85	0.42
1:A:237:ARG:O	1:A:240:VAL:HG22	2.20	0.42
1:F:314:GLN:NE2	1:F:322:ILE:H	2.17	0.42
1:E:320:ARG:HH21	1:E:327:ARG:NH1	2.17	0.42
1:F:87:THR:CG2	1:F:326:ASN:HB2	2.49	0.42
1:C:13:GLU:HA	1:C:16:LEU:HD12	2.01	0.42
1:H:89:ARG:NH2	3:H:1031:HOH:O	2.52	0.42
1:C:315:ALA:HB2	1:C:321:PRO:HG3	2.02	0.41
1:B:185:GLN:HE22	1:G:273:ARG:HE	1.67	0.41
1:C:320:ARG:HA	1:C:321:PRO:HD3	1.91	0.41
1:A:36:ARG:NH2	1:A:56:ARG:NH2	2.67	0.41
1:B:208:LEU:H	1:B:208:LEU:HD12	1.85	0.41
1:A:185:GLN:NE2	1:F:273:ARG:NH1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:CYS:HB3	1:H:75:LEU:HG	2.03	0.41
1:F:80:ASN:HD22	1:F:269:ALA:H	1.68	0.41
1:C:103:PRO:HG3	1:C:300:VAL:HG11	2.03	0.41
1:D:288:LEU:HD21	1:G:119:LEU:HD21	2.03	0.41
1:B:56:ARG:CZ	1:B:58:ASP:HB3	2.51	0.41
1:H:92:TRP:CH2	1:H:320:ARG:HG3	2.56	0.41
1:A:36:ARG:HH22	1:A:268:TRP:HB3	1.86	0.41
1:E:2:LEU:HB3	1:E:23:CYS:HA	2.02	0.41
1:D:123:ASP:OD1	1:G:120:ARG:CD	2.69	0.40
1:E:327:ARG:HD2	1:G:306:ARG:HD3	2.02	0.40
1:F:180:ASP:OD2	1:F:180:ASP:N	2.54	0.40
1:F:258:TYR:O	1:F:287:THR:HA	2.21	0.40
1:F:259:ALA:HA	1:F:288:LEU:O	2.22	0.40
1:F:290:THR:HB	1:F:293:ILE:HG12	2.03	0.40
1:C:7:ILE:HD12	1:C:27:THR:HG22	2.02	0.40
1:G:297:VAL:CG1	1:G:298:ARG:N	2.84	0.40
1:H:320:ARG:NH2	1:H:327:ARG:HG2	2.36	0.40
1:H:320:ARG:NH1	3:H:1043:HOH:O	2.55	0.40

All (2) 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)
3:F:997:HOH:O	3:F:1270:HOH:O[2_645]	2.13	0.07
3:D:1230:HOH:O	3:E:987:HOH:O[1_545]	2.15	0.05

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	327/330 (99%)	319 (98%)	8 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	327/330 (99%)	318 (97%)	9 (3%)	0	100	100
1	C	225/330 (68%)	216 (96%)	9 (4%)	0	100	100
1	D	328/330 (99%)	321 (98%)	7 (2%)	0	100	100
1	E	326/330 (99%)	313 (96%)	11 (3%)	2 (1%)	21	9
1	F	325/330 (98%)	318 (98%)	7 (2%)	0	100	100
1	G	326/330 (99%)	315 (97%)	9 (3%)	2 (1%)	21	9
1	H	327/330 (99%)	315 (96%)	11 (3%)	1 (0%)	36	22
All	All	2511/2640 (95%)	2435 (97%)	71 (3%)	5 (0%)	43	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	298	ARG
1	E	137	ARG
1	G	33	THR
1	E	136	PRO
1	H	228	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry

8 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	C	800	-	46,48,48	0.87	3 (6%)	64,73,73	1.57	10 (15%)
2	NAD	D	800	-	46,48,48	0.85	1 (2%)	64,73,73	1.59	8 (12%)
2	NAD	H	800	-	46,48,48	0.93	4 (8%)	64,73,73	1.50	9 (14%)
2	NAD	F	800	-	46,48,48	0.92	4 (8%)	64,73,73	1.56	9 (14%)
2	NAD	B	800	-	46,48,48	0.95	5 (10%)	64,73,73	1.66	9 (14%)
2	NAD	G	800	-	46,48,48	1.00	2 (4%)	64,73,73	1.61	11 (17%)
2	NAD	A	800	-	46,48,48	0.98	3 (6%)	64,73,73	1.55	9 (14%)
2	NAD	E	800	-	46,48,48	0.98	3 (6%)	64,73,73	1.56	9 (14%)

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	C	800	-	-	3/30/62/62	0/5/5/5
2	NAD	D	800	-	-	3/30/62/62	0/5/5/5
2	NAD	H	800	-	-	5/30/62/62	0/5/5/5
2	NAD	F	800	-	-	4/30/62/62	0/5/5/5
2	NAD	B	800	-	-	2/30/62/62	0/5/5/5
2	NAD	G	800	-	-	4/30/62/62	0/5/5/5
2	NAD	A	800	-	-	4/30/62/62	0/5/5/5
2	NAD	E	800	-	-	3/30/62/62	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	800	NAD	PA-O3	3.30	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	NAD	PN-O3	2.76	1.62	1.59
2	B	800	NAD	O4D-C1D	2.72	1.44	1.40
2	A	800	NAD	O4D-C1D	2.71	1.44	1.40
2	E	800	NAD	PA-O3	2.68	1.62	1.59
2	A	800	NAD	PN-O3	2.67	1.62	1.59
2	H	800	NAD	PN-O3	2.60	1.62	1.59
2	B	800	NAD	C8A-N7A	2.45	1.36	1.31
2	G	800	NAD	PN-O3	2.33	1.62	1.59
2	A	800	NAD	C8A-N7A	2.26	1.36	1.31
2	C	800	NAD	O4D-C1D	2.26	1.43	1.40
2	F	800	NAD	C8A-N7A	2.25	1.36	1.31
2	H	800	NAD	C8A-N7A	2.21	1.35	1.31
2	C	800	NAD	C5A-N7A	-2.17	1.35	1.39
2	F	800	NAD	O4D-C1D	2.12	1.43	1.40
2	H	800	NAD	PA-O3	2.12	1.61	1.59
2	F	800	NAD	PN-O3	2.12	1.61	1.59
2	D	800	NAD	C8A-N7A	2.10	1.35	1.31
2	F	800	NAD	C5A-N7A	-2.09	1.35	1.39
2	E	800	NAD	C8A-N7A	2.08	1.35	1.31
2	B	800	NAD	PA-O3	2.07	1.61	1.59
2	H	800	NAD	O4D-C1D	2.07	1.43	1.40
2	C	800	NAD	C8A-N7A	2.02	1.35	1.31
2	B	800	NAD	C4A-N9A	-2.01	1.33	1.37
2	B	800	NAD	C5A-N7A	-2.01	1.35	1.39

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	NAD	N3A-C2A-N1A	-5.32	120.52	128.58
2	B	800	NAD	N3A-C2A-N1A	-5.27	120.60	128.58
2	G	800	NAD	N3A-C2A-N1A	-5.25	120.63	128.58
2	D	800	NAD	N3A-C2A-N1A	-5.24	120.66	128.58
2	C	800	NAD	C5A-C4A-N3A	-5.17	119.59	126.72
2	E	800	NAD	N3A-C2A-N1A	-5.14	120.80	128.58
2	H	800	NAD	C5A-C4A-N3A	-5.12	119.67	126.72
2	F	800	NAD	N3A-C2A-N1A	-5.09	120.88	128.58
2	D	800	NAD	C5A-C4A-N3A	-5.04	119.78	126.72
2	C	800	NAD	N3A-C2A-N1A	-5.03	120.97	128.58
2	E	800	NAD	C5A-C4A-N3A	-4.98	119.85	126.72
2	F	800	NAD	C5A-C4A-N3A	-4.96	119.89	126.72
2	H	800	NAD	N3A-C2A-N1A	-4.96	121.07	128.58
2	G	800	NAD	C5A-C4A-N3A	-4.91	119.96	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	NAD	C5A-C4A-N3A	-4.79	120.12	126.72
2	B	800	NAD	C5A-C4A-N3A	-4.69	120.25	126.72
2	B	800	NAD	N9A-C8A-N7A	-4.15	108.05	113.94
2	D	800	NAD	N9A-C8A-N7A	-3.99	108.28	113.94
2	D	800	NAD	C2A-N3A-C4A	3.78	121.06	111.83
2	F	800	NAD	N9A-C8A-N7A	-3.75	108.61	113.94
2	E	800	NAD	N9A-C8A-N7A	-3.75	108.62	113.94
2	A	800	NAD	N9A-C8A-N7A	-3.74	108.62	113.94
2	H	800	NAD	N9A-C8A-N7A	-3.54	108.91	113.94
2	B	800	NAD	C2A-N3A-C4A	3.54	120.48	111.83
2	G	800	NAD	C2A-N3A-C4A	3.54	120.47	111.83
2	F	800	NAD	C2A-N3A-C4A	3.51	120.41	111.83
2	E	800	NAD	C2A-N3A-C4A	3.50	120.39	111.83
2	H	800	NAD	C2A-N3A-C4A	3.50	120.37	111.83
2	A	800	NAD	C2A-N3A-C4A	3.49	120.36	111.83
2	G	800	NAD	N9A-C8A-N7A	-3.48	108.99	113.94
2	C	800	NAD	C2A-N3A-C4A	3.46	120.27	111.83
2	B	800	NAD	C4A-N9A-C8A	3.39	109.30	105.74
2	C	800	NAD	N9A-C8A-N7A	-3.33	109.21	113.94
2	C	800	NAD	N3A-C4A-N9A	3.32	132.81	127.17
2	H	800	NAD	N3A-C4A-N9A	3.31	132.80	127.17
2	C	800	NAD	O4B-C1B-N9A	3.29	114.40	108.09
2	D	800	NAD	C4A-C5A-N7A	-3.27	106.85	110.58
2	E	800	NAD	N3A-C4A-N9A	3.24	132.68	127.17
2	F	800	NAD	N3A-C4A-N9A	3.11	132.46	127.17
2	D	800	NAD	C5A-N7A-C8A	3.06	108.25	103.45
2	G	800	NAD	N3A-C4A-N9A	3.06	132.37	127.17
2	B	800	NAD	N3A-C4A-N9A	3.02	132.31	127.17
2	D	800	NAD	N3A-C4A-N9A	2.98	132.24	127.17
2	A	800	NAD	N3A-C4A-N9A	2.98	132.23	127.17
2	B	800	NAD	O4B-C1B-N9A	2.94	113.75	108.09
2	B	800	NAD	C4A-C5A-N7A	-2.82	107.36	110.58
2	B	800	NAD	C5A-N7A-C8A	2.80	107.85	103.45
2	E	800	NAD	C4A-N9A-C8A	2.79	108.67	105.74
2	G	800	NAD	O4B-C1B-N9A	2.78	113.43	108.09
2	A	800	NAD	O4B-C1B-N9A	2.77	113.41	108.09
2	E	800	NAD	C5A-N7A-C8A	2.77	107.80	103.45
2	A	800	NAD	C4A-N9A-C8A	2.76	108.63	105.74
2	D	800	NAD	C4A-N9A-C8A	2.76	108.63	105.74
2	C	800	NAD	C4A-C5A-N7A	-2.74	107.44	110.58
2	E	800	NAD	C4A-C5A-N7A	-2.74	107.44	110.58
2	G	800	NAD	C4A-C5A-N7A	-2.74	107.45	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	800	NAD	C4A-N9A-C8A	2.74	108.61	105.74
2	F	800	NAD	C4A-C5A-N7A	-2.72	107.47	110.58
2	H	800	NAD	O4B-C1B-N9A	2.72	113.31	108.09
2	H	800	NAD	C4A-C5A-N7A	-2.69	107.50	110.58
2	F	800	NAD	C5A-N7A-C8A	2.67	107.65	103.45
2	H	800	NAD	C4A-N9A-C8A	2.64	108.50	105.74
2	H	800	NAD	C5A-N7A-C8A	2.61	107.56	103.45
2	G	800	NAD	C4A-N9A-C8A	2.57	108.44	105.74
2	C	800	NAD	C5A-N7A-C8A	2.57	107.49	103.45
2	A	800	NAD	C4A-C5A-N7A	-2.55	107.67	110.58
2	G	800	NAD	C5A-N7A-C8A	2.54	107.44	103.45
2	A	800	NAD	C5A-N7A-C8A	2.52	107.42	103.45
2	E	800	NAD	C3N-C7N-N7N	2.45	120.76	117.74
2	G	800	NAD	C6N-N1N-C2N	-2.44	119.81	121.88
2	G	800	NAD	C5N-C4N-C3N	-2.43	117.97	120.36
2	C	800	NAD	C4A-N9A-C8A	2.40	108.26	105.74
2	F	800	NAD	O4B-C1B-N9A	2.22	112.35	108.09
2	C	800	NAD	C6N-N1N-C2N	-2.00	120.17	121.88

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	NAD	O4D-C1D-N1N-C2N
2	A	800	NAD	O4D-C1D-N1N-C6N
2	B	800	NAD	O4D-C1D-N1N-C2N
2	B	800	NAD	O4D-C1D-N1N-C6N
2	C	800	NAD	O4D-C1D-N1N-C2N
2	C	800	NAD	O4D-C1D-N1N-C6N
2	D	800	NAD	O4D-C1D-N1N-C2N
2	D	800	NAD	O4D-C1D-N1N-C6N
2	E	800	NAD	O4D-C1D-N1N-C6N
2	F	800	NAD	O4D-C1D-N1N-C2N
2	F	800	NAD	O4D-C1D-N1N-C6N
2	G	800	NAD	O4D-C1D-N1N-C2N
2	G	800	NAD	O4D-C1D-N1N-C6N
2	H	800	NAD	O4D-C1D-N1N-C2N
2	H	800	NAD	O4D-C1D-N1N-C6N
2	D	800	NAD	C2D-C1D-N1N-C2N
2	G	800	NAD	C2D-C1D-N1N-C2N
2	H	800	NAD	C2D-C1D-N1N-C2N
2	H	800	NAD	C2D-C1D-N1N-C6N

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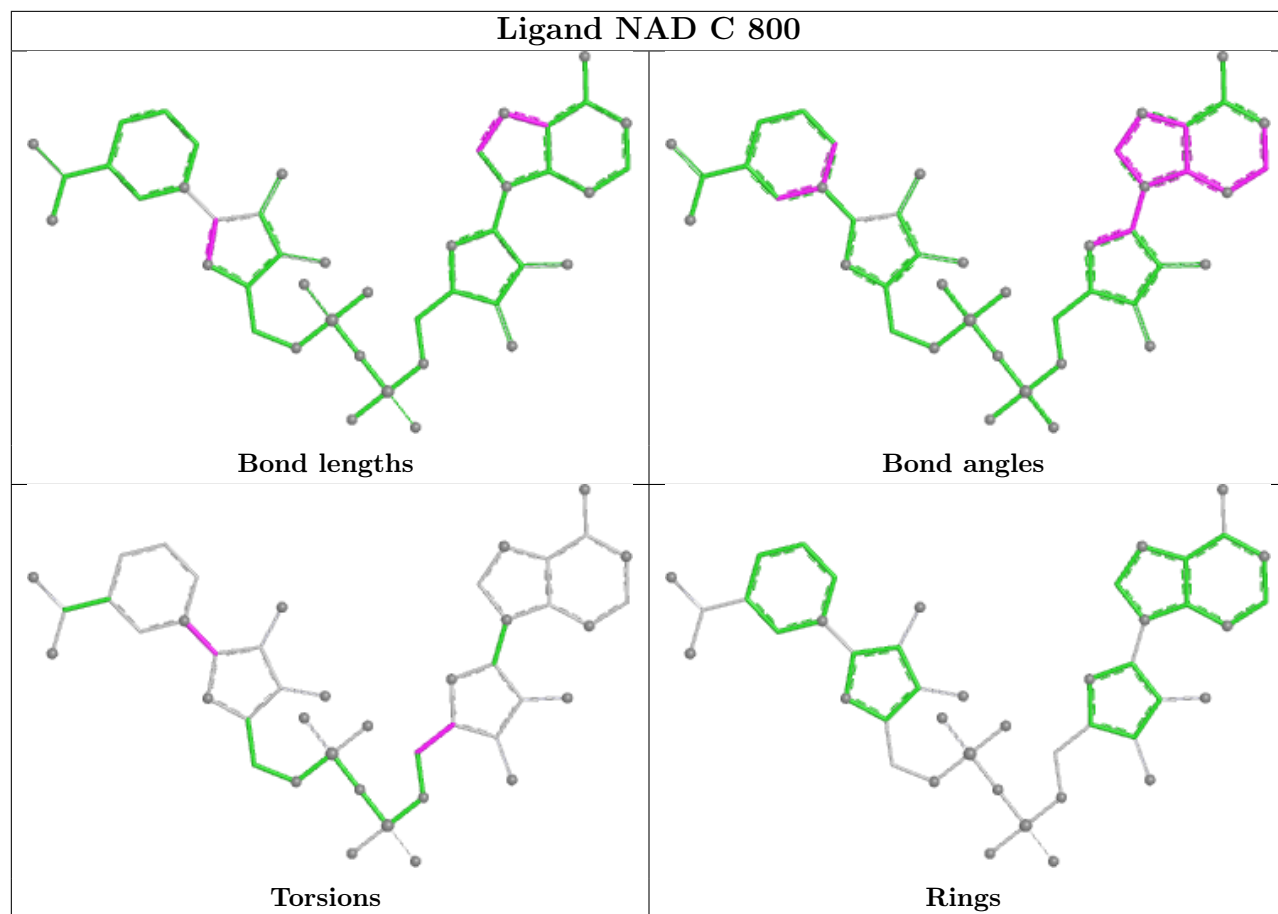
Mol	Chain	Res	Type	Atoms
2	C	800	NAD	O4B-C4B-C5B-O5B
2	E	800	NAD	O4D-C1D-N1N-C2N
2	G	800	NAD	O4B-C4B-C5B-O5B
2	E	800	NAD	O4B-C4B-C5B-O5B
2	H	800	NAD	O4B-C4B-C5B-O5B
2	A	800	NAD	O4B-C4B-C5B-O5B
2	A	800	NAD	C2B-C1B-N9A-C8A
2	F	800	NAD	C2B-C1B-N9A-C8A
2	F	800	NAD	O4B-C4B-C5B-O5B

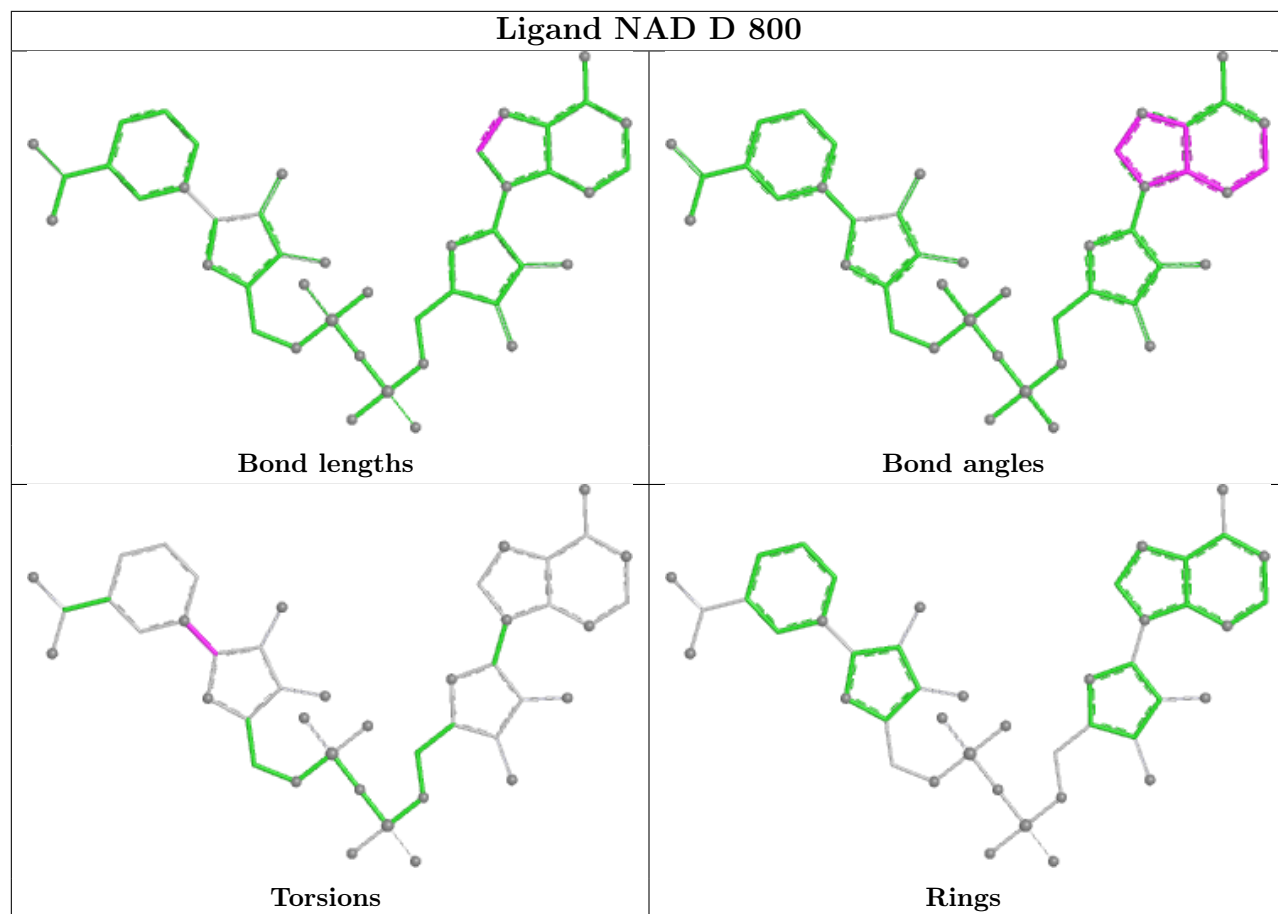
There are no ring outliers.

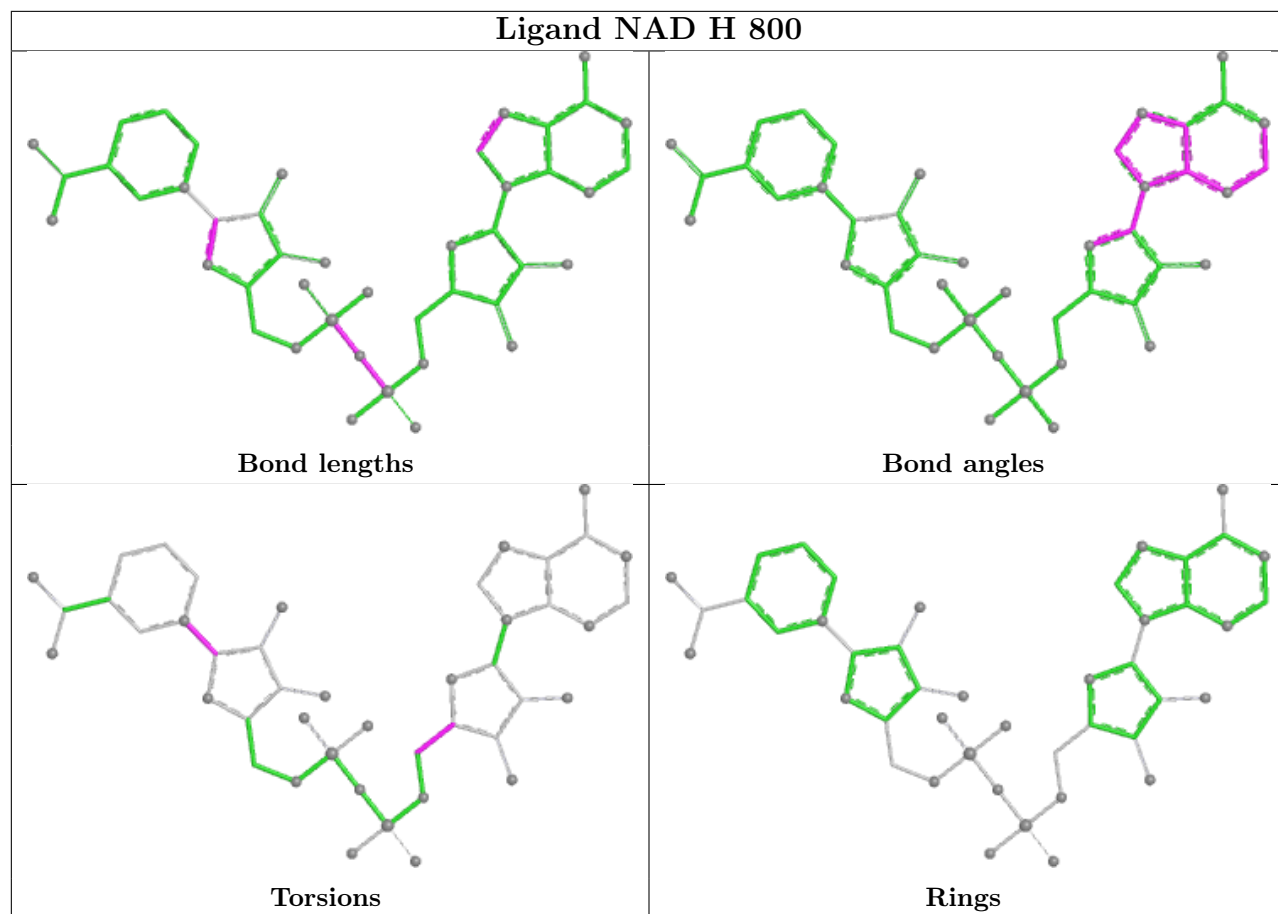
2 monomers are involved in 2 short contacts:

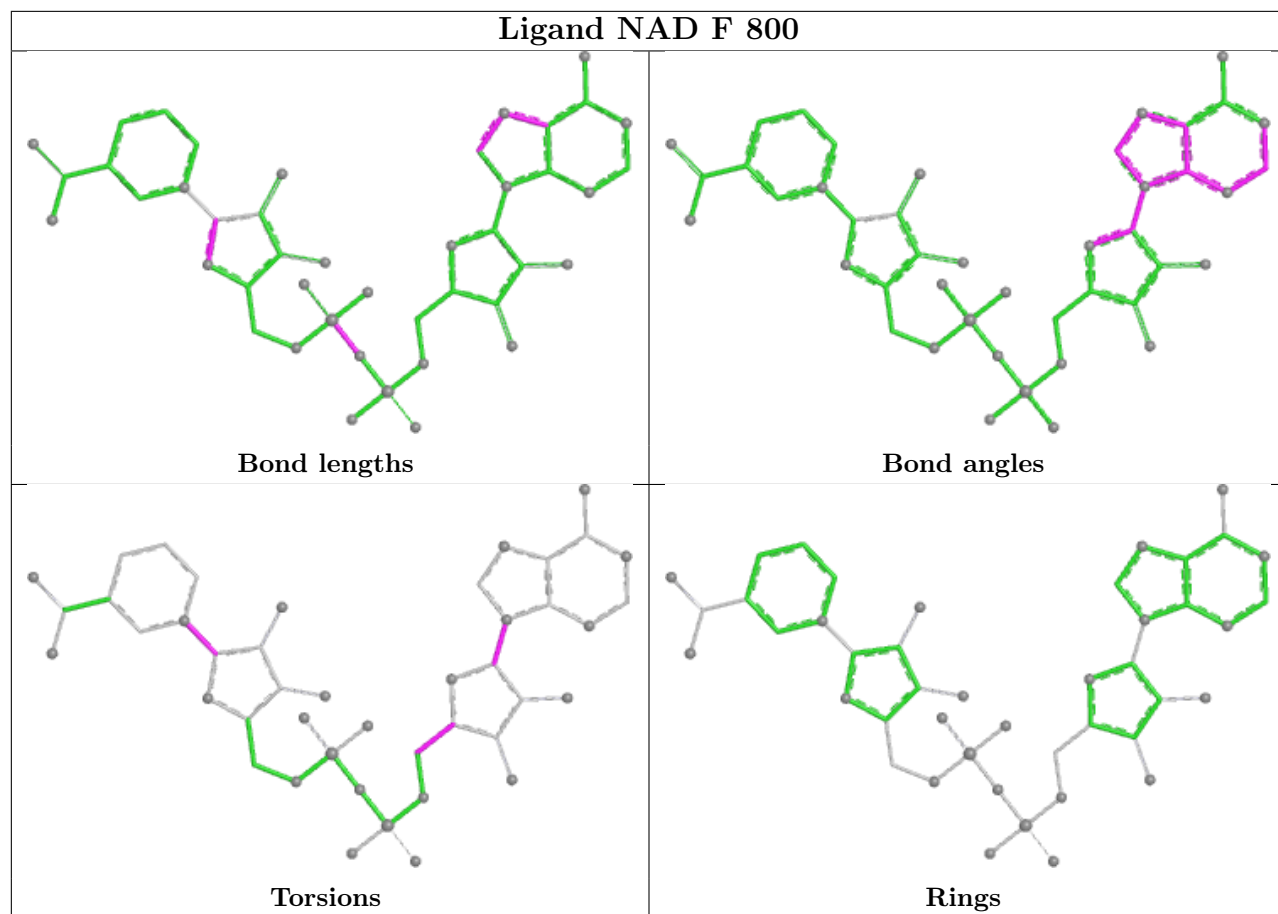
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	800	NAD	1	0
2	G	800	NAD	1	0

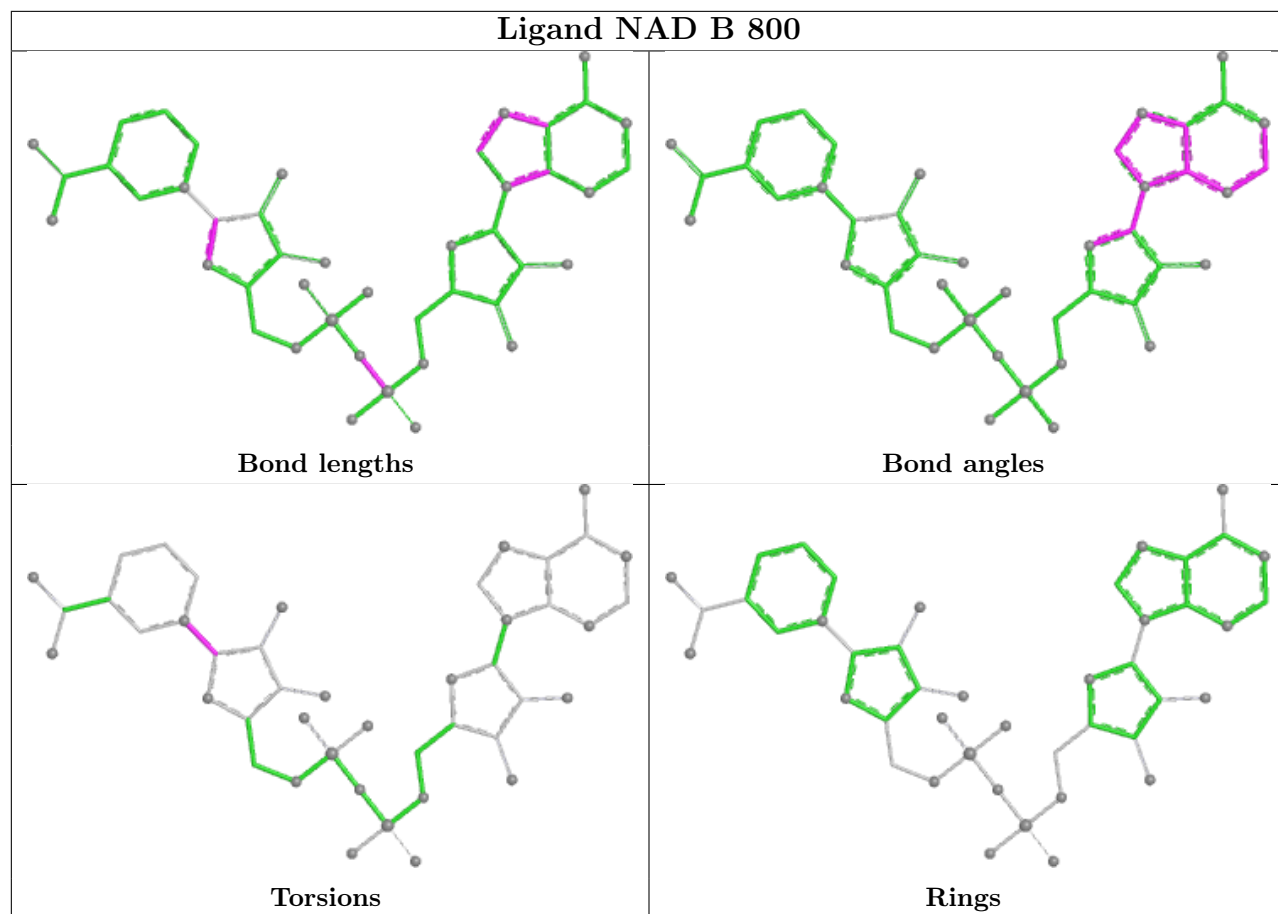
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

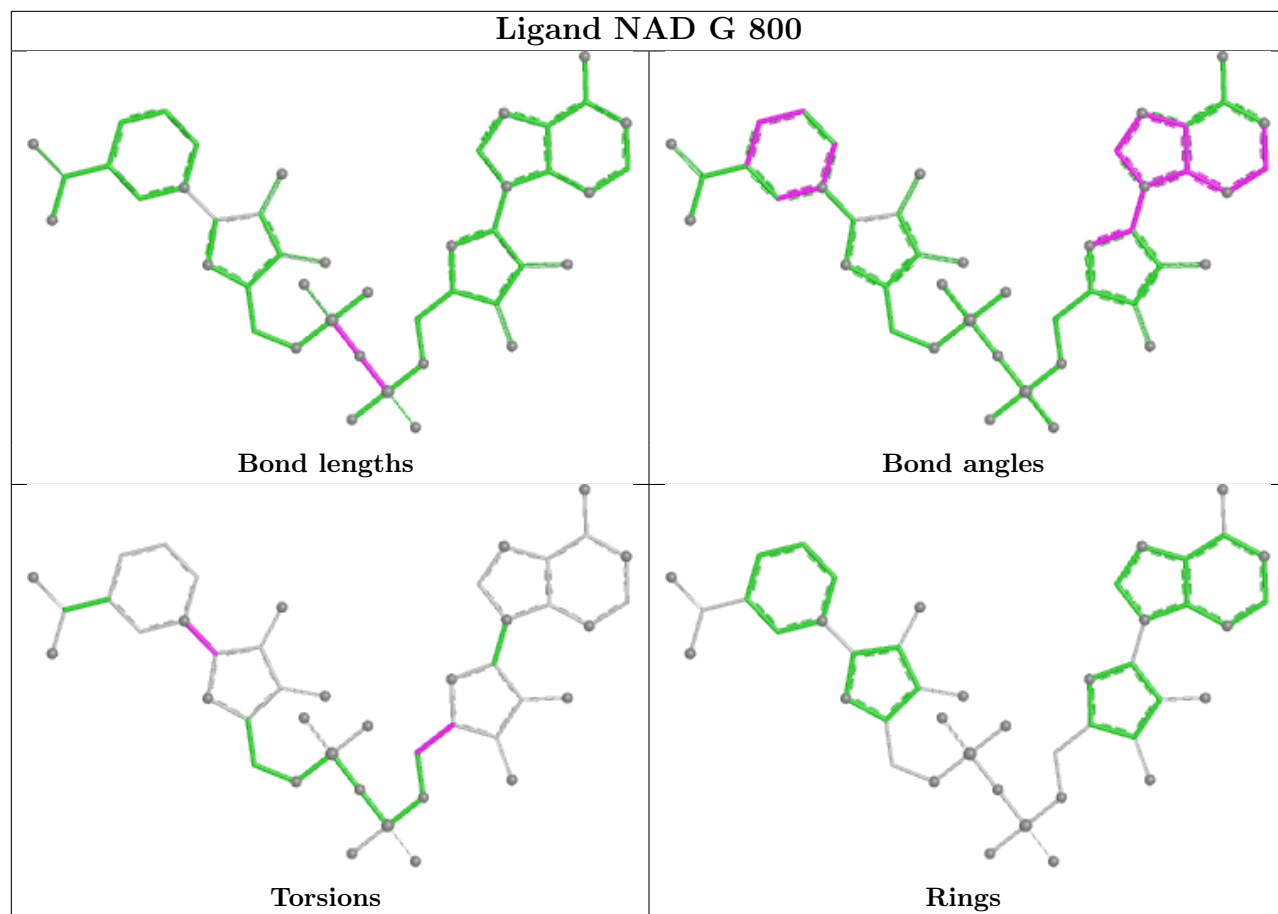


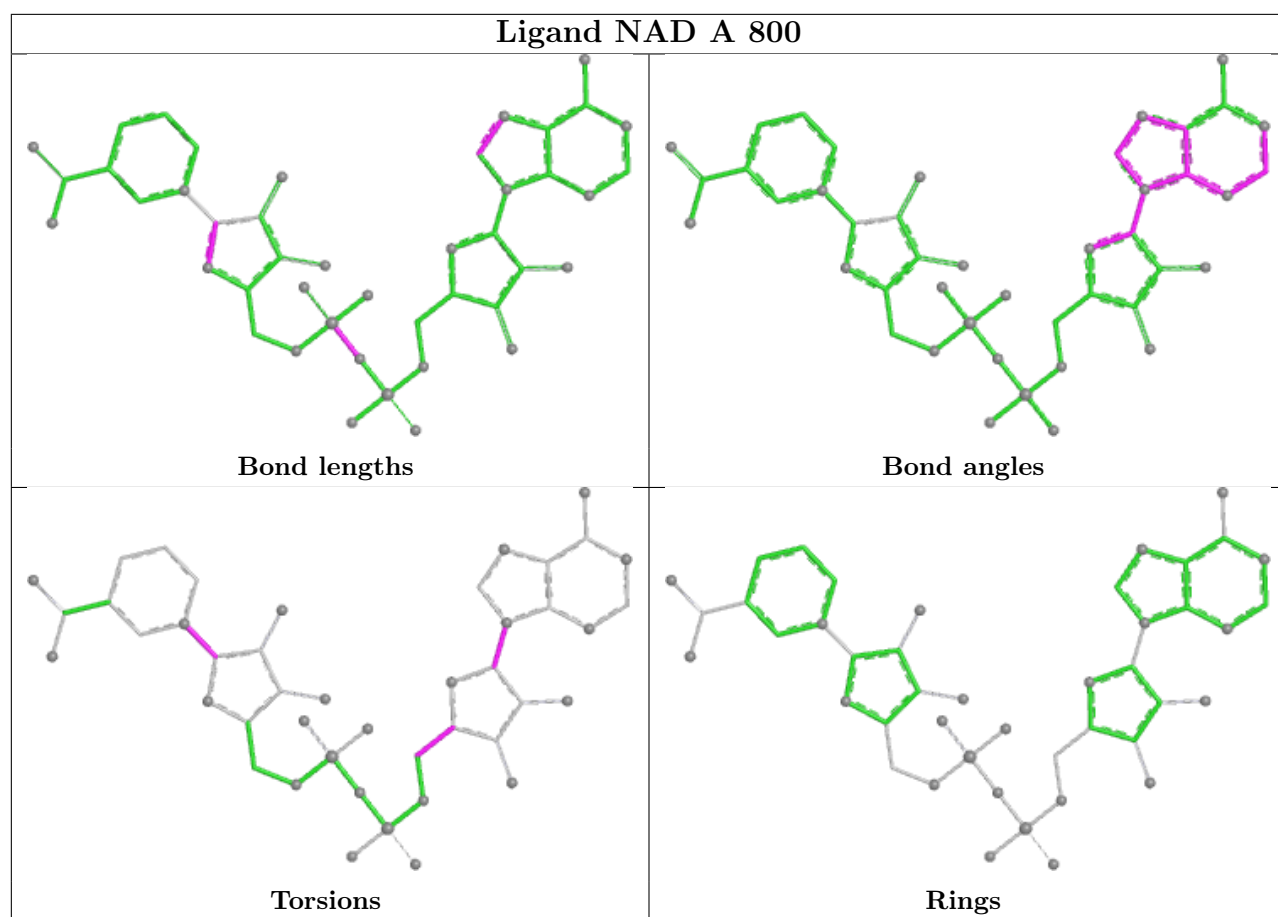


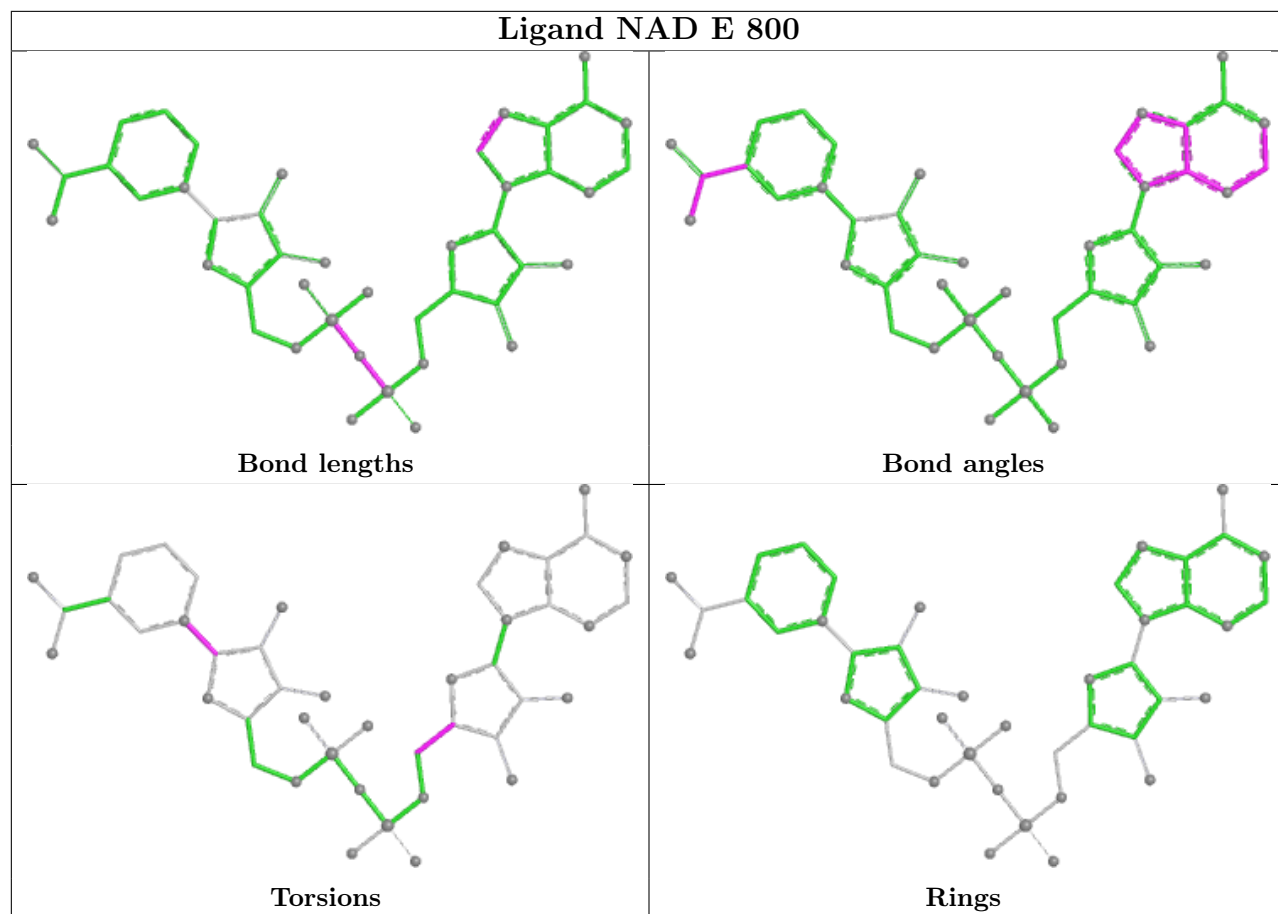












5.7 Other polymers [i](#)

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 ⓘ

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	329/330 (99%)	0.34	13 (3%) 42 46	17, 24, 37, 47	0
1	B	329/330 (99%)	0.32	21 (6%) 25 27	15, 23, 39, 52	0
1	C	330/330 (100%)	0.82	41 (12%) 8 8	19, 31, 55, 61	0
1	D	330/330 (100%)	0.13	13 (3%) 43 47	14, 21, 36, 45	0
1	E	328/330 (99%)	0.75	40 (12%) 8 8	17, 29, 53, 64	0
1	F	327/330 (99%)	0.20	7 (2%) 63 68	16, 24, 37, 46	0
1	G	328/330 (99%)	0.30	13 (3%) 42 46	14, 22, 38, 43	0
1	H	329/330 (99%)	1.63	99 (30%) 1 1	24, 40, 60, 65	0
All	All	2630/2640 (99%)	0.56	247 (9%) 14 14	14, 26, 50, 65	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	183	THR	5.0
1	C	15	ILE	5.0
1	H	268	TRP	5.0
1	C	26	ILE	4.8
1	H	192	VAL	4.8
1	B	328	LEU	4.7
1	C	1	MET	4.6
1	H	329	PRO	4.5
1	D	297	VAL	4.3
1	G	31	ASP	4.3
1	A	136	PRO	4.3
1	H	64	ALA	4.2
1	H	193	ALA	4.1
1	A	139	TYR	4.1
1	B	329	PRO	4.1
1	G	136	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	178	ALA	4.0
1	E	88	ALA	4.0
1	D	134	TRP	3.9
1	G	32	SER	3.8
1	E	40	LEU	3.8
1	C	21	PRO	3.8
1	B	298	ARG	3.8
1	F	182	GLN	3.8
1	C	2	LEU	3.7
1	E	137	ARG	3.7
1	H	1	MET	3.7
1	D	31	ASP	3.6
1	E	64	ALA	3.6
1	H	48	ALA	3.5
1	E	63	GLN	3.5
1	E	59	ALA	3.5
1	H	2	LEU	3.5
1	H	182	GLN	3.5
1	H	271	ALA	3.4
1	F	138	PHE	3.4
1	B	1	MET	3.4
1	C	16	LEU	3.4
1	C	40	LEU	3.4
1	C	268	TRP	3.4
1	H	139	TYR	3.3
1	E	34	LEU	3.3
1	C	6	VAL	3.3
1	H	328	LEU	3.3
1	H	180	ASP	3.3
1	C	65	CYS	3.3
1	E	37	GLU	3.2
1	H	83	VAL	3.2
1	E	139	TYR	3.2
1	H	222	LEU	3.2
1	C	329	PRO	3.1
1	D	32	SER	3.1
1	C	18	LEU	3.1
1	E	328	LEU	3.1
1	H	187	LEU	3.1
1	C	271	ALA	3.1
1	E	45	ASP	3.1
1	C	178	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	188	GLY	3.0
1	H	173	TYR	3.0
1	H	199	ALA	3.0
1	H	217	LEU	3.0
1	H	23	CYS	3.0
1	H	21	PRO	3.0
1	C	19	LEU	3.0
1	H	179	LEU	3.0
1	C	28	ASN	3.0
1	B	31	ASP	2.9
1	H	260	ALA	2.9
1	E	44	ARG	2.9
1	H	57	VAL	2.9
1	A	1	MET	2.9
1	G	320	ARG	2.8
1	H	220	ALA	2.8
1	H	34	LEU	2.8
1	E	26	ILE	2.8
1	E	322	ILE	2.8
1	D	178	ALA	2.8
1	H	39	ILE	2.8
1	H	174	HIS	2.8
1	E	39	ILE	2.8
1	H	176	ALA	2.7
1	H	280	ALA	2.7
1	B	127	ARG	2.7
1	B	327	ARG	2.7
1	C	66	PRO	2.7
1	H	226	VAL	2.7
1	C	36	ARG	2.7
1	F	137	ARG	2.7
1	H	61	PHE	2.7
1	C	208	LEU	2.7
1	H	247	LEU	2.7
1	H	318	GLY	2.7
1	H	267	ASP	2.7
1	A	269	ALA	2.7
1	H	207	ALA	2.7
1	E	329	PRO	2.6
1	G	138	PHE	2.6
1	C	25	LEU	2.6
1	A	268	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	134	TRP	2.6
1	E	31	ASP	2.6
1	H	84	ASP	2.6
1	C	220	ALA	2.6
1	G	317	ALA	2.6
1	E	90	GLY	2.6
1	H	198	PHE	2.6
1	C	23	CYS	2.6
1	D	179	LEU	2.6
1	D	298	ARG	2.6
1	E	317	ALA	2.6
1	G	20	ALA	2.6
1	H	66	PRO	2.6
1	C	30	THR	2.6
1	C	41	ARG	2.6
1	H	253	GLY	2.6
1	B	131	PHE	2.6
1	E	2	LEU	2.6
1	H	88	ALA	2.6
1	F	33	THR	2.5
1	H	200	SER	2.5
1	H	250	LEU	2.5
1	F	298	ARG	2.5
1	H	218	VAL	2.5
1	C	20	ALA	2.5
1	D	136	PRO	2.5
1	H	3	PRO	2.5
1	C	27	THR	2.5
1	E	92	TRP	2.5
1	H	201	SER	2.5
1	C	37	GLU	2.5
1	G	139	TYR	2.5
1	H	63	GLN	2.5
1	E	85	ALA	2.5
1	H	204	ILE	2.5
1	H	228	PRO	2.5
1	H	244	ALA	2.5
1	H	269	ALA	2.5
1	B	275	GLN	2.5
1	E	62	LEU	2.5
1	H	208	LEU	2.5
1	H	316	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	124	ALA	2.5
1	F	139	TYR	2.5
1	B	129	GLY	2.5
1	H	90	GLY	2.5
1	C	49	MET	2.5
1	D	196	GLU	2.5
1	H	327	ARG	2.5
1	C	330	LYS	2.4
1	H	40	LEU	2.4
1	H	184	GLU	2.4
1	D	1	MET	2.4
1	D	133	GLY	2.4
1	H	282	LEU	2.4
1	E	61	PHE	2.4
1	E	138	PHE	2.4
1	H	299	ALA	2.4
1	H	324	ALA	2.4
1	H	60	ASP	2.4
1	A	24	GLU	2.4
1	B	128	SER	2.4
1	E	66	PRO	2.4
1	H	54	PRO	2.4
1	H	205	LEU	2.4
1	H	206	LEU	2.4
1	H	249	ALA	2.4
1	H	138	PHE	2.4
1	D	180	ASP	2.4
1	A	327	ARG	2.4
1	G	298	ARG	2.4
1	H	190	ARG	2.4
1	B	133	GLY	2.3
1	E	166	GLY	2.3
1	C	34	LEU	2.3
1	E	20	ALA	2.3
1	H	197	LEU	2.3
1	E	134	TRP	2.3
1	B	276	GLN	2.3
1	H	212	ALA	2.3
1	H	224	ALA	2.3
1	C	11	VAL	2.3
1	H	27	THR	2.3
1	A	17	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	275	GLN	2.3
1	A	137	ARG	2.3
1	E	83	VAL	2.3
1	A	329	PRO	2.2
1	B	137	ARG	2.2
1	G	301	ARG	2.2
1	C	7	ILE	2.2
1	H	285	PRO	2.2
1	A	132	ARG	2.2
1	E	268	TRP	2.2
1	F	134	TRP	2.2
1	C	43	CYS	2.2
1	H	194	CYS	2.2
1	C	5	LEU	2.2
1	E	89	ARG	2.2
1	G	41	ARG	2.2
1	B	21	PRO	2.2
1	H	70	VAL	2.2
1	H	325	VAL	2.2
1	A	272	ASP	2.2
1	C	48	ALA	2.2
1	E	46	ALA	2.2
1	A	328	LEU	2.2
1	D	139	TYR	2.2
1	C	33	THR	2.2
1	H	257	GLY	2.1
1	C	53	MET	2.1
1	H	162	ASP	2.1
1	H	214	THR	2.1
1	H	263	PHE	2.1
1	H	272	ASP	2.1
1	H	69	ARG	2.1
1	H	252	ARG	2.1
1	C	315	ALA	2.1
1	H	65	CYS	2.1
1	H	215	LEU	2.1
1	E	69	ARG	2.1
1	E	87	THR	2.1
1	C	12	HIS	2.1
1	B	130	LYS	2.1
1	B	325	VAL	2.1
1	H	262	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	53	MET	2.1
1	E	23	CYS	2.1
1	H	251	GLU	2.1
1	E	35	THR	2.1
1	B	268	TRP	2.1
1	H	277	ILE	2.1
1	E	318	GLY	2.0
1	B	121	ALA	2.0
1	C	64	ALA	2.0
1	H	265	MET	2.0
1	E	320	ARG	2.0
1	H	11	VAL	2.0
1	H	278	ASP	2.0
1	C	69	ARG	2.0
1	G	313	LEU	2.0
1	H	62	LEU	2.0
1	H	225	LEU	2.0
1	E	48	ALA	2.0
1	H	74	ALA	2.0
1	H	245	ALA	2.0
1	H	32	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	NAD	H	800	44/44	0.88	0.12	35,38,47,47	0
2	NAD	E	800	44/44	0.96	0.06	21,24,27,29	0

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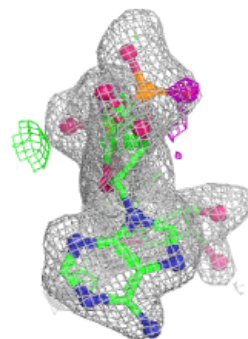
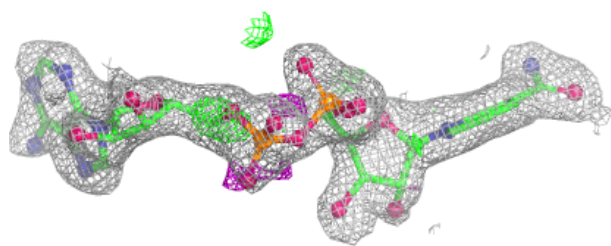
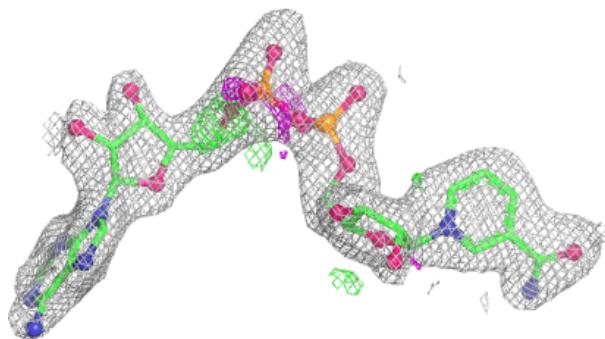
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	C	800	44/44	0.96	0.07	21,24,33,34	0
2	NAD	A	800	44/44	0.97	0.05	18,22,25,25	0
2	NAD	F	800	44/44	0.97	0.05	18,19,23,24	0
2	NAD	G	800	44/44	0.97	0.05	15,18,21,22	0
2	NAD	D	800	44/44	0.97	0.05	16,18,22,23	0
2	NAD	B	800	44/44	0.98	0.05	13,16,18,21	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.

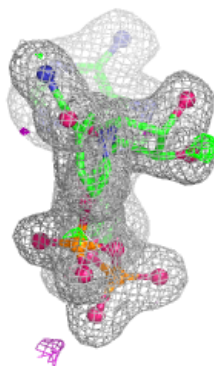
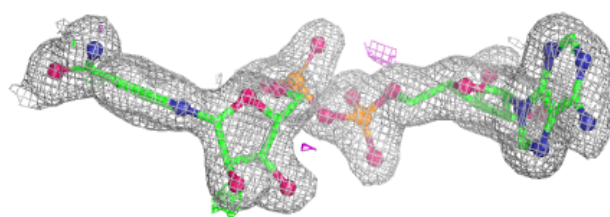
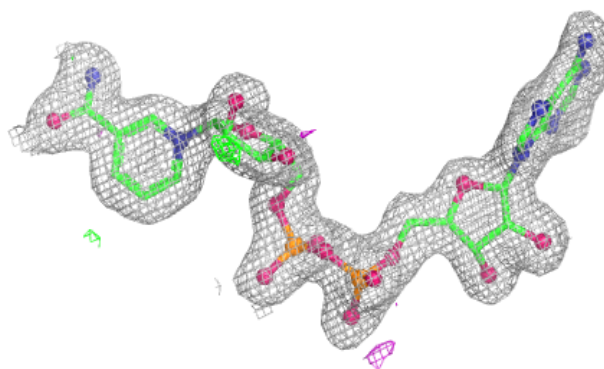
Electron density around NAD H 800:

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

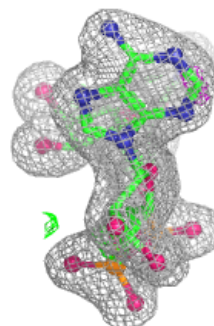
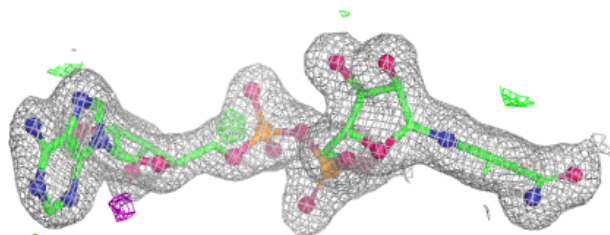
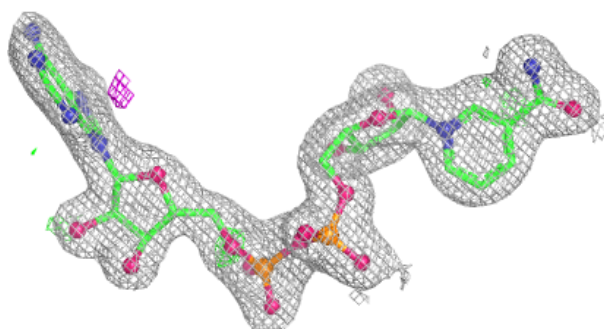


Electron density around NAD E 800:

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

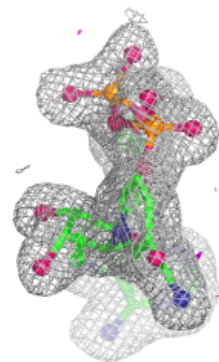
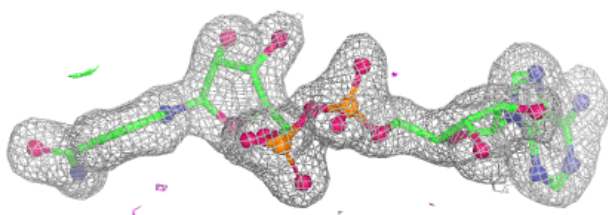
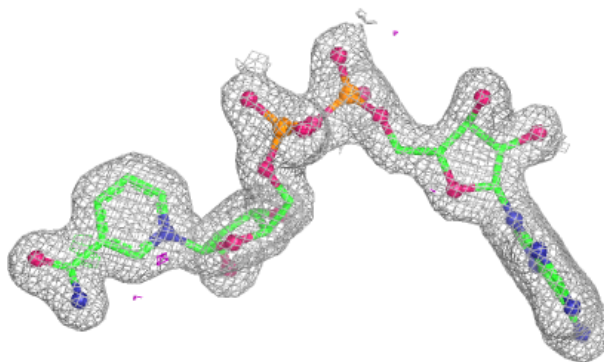
**Electron density around NAD C 800:**

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

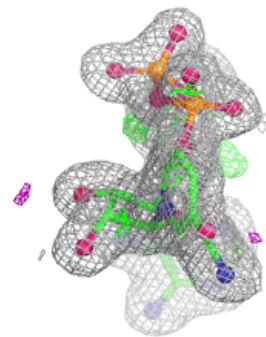
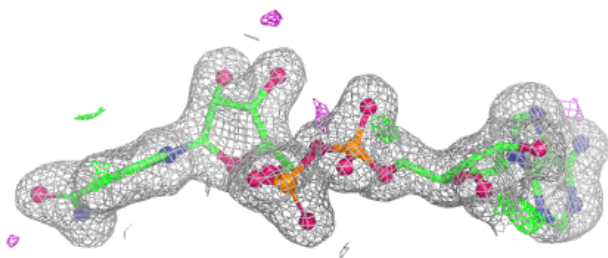
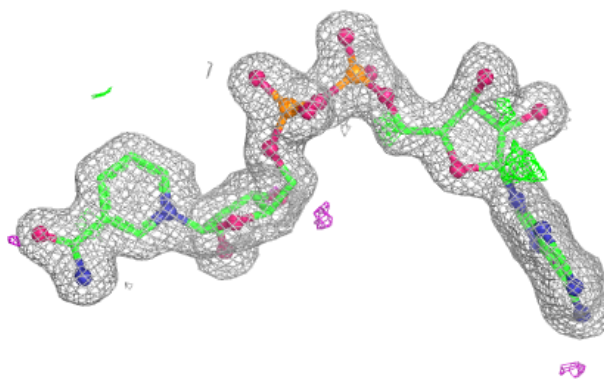


Electron density around NAD A 800:

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

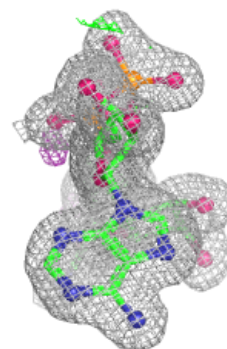
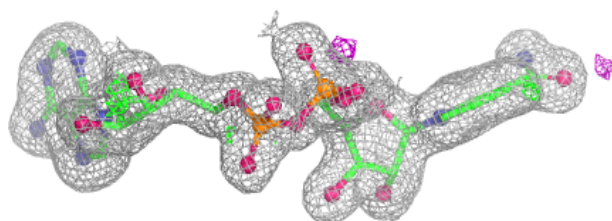
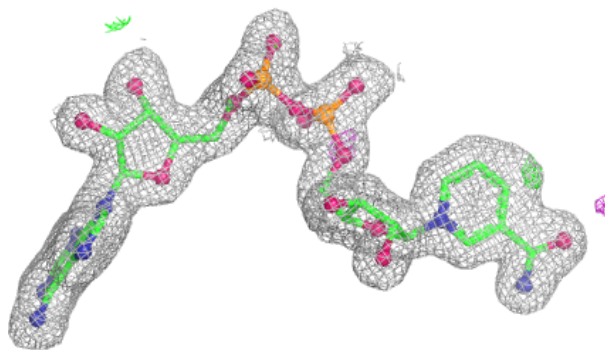
**Electron density around NAD F 800:**

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

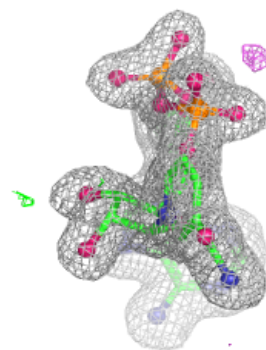
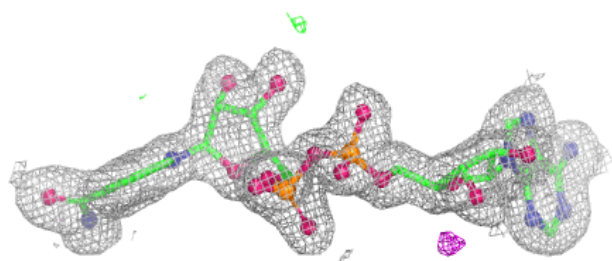
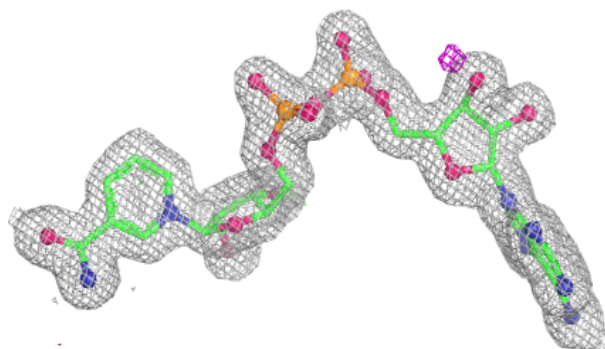


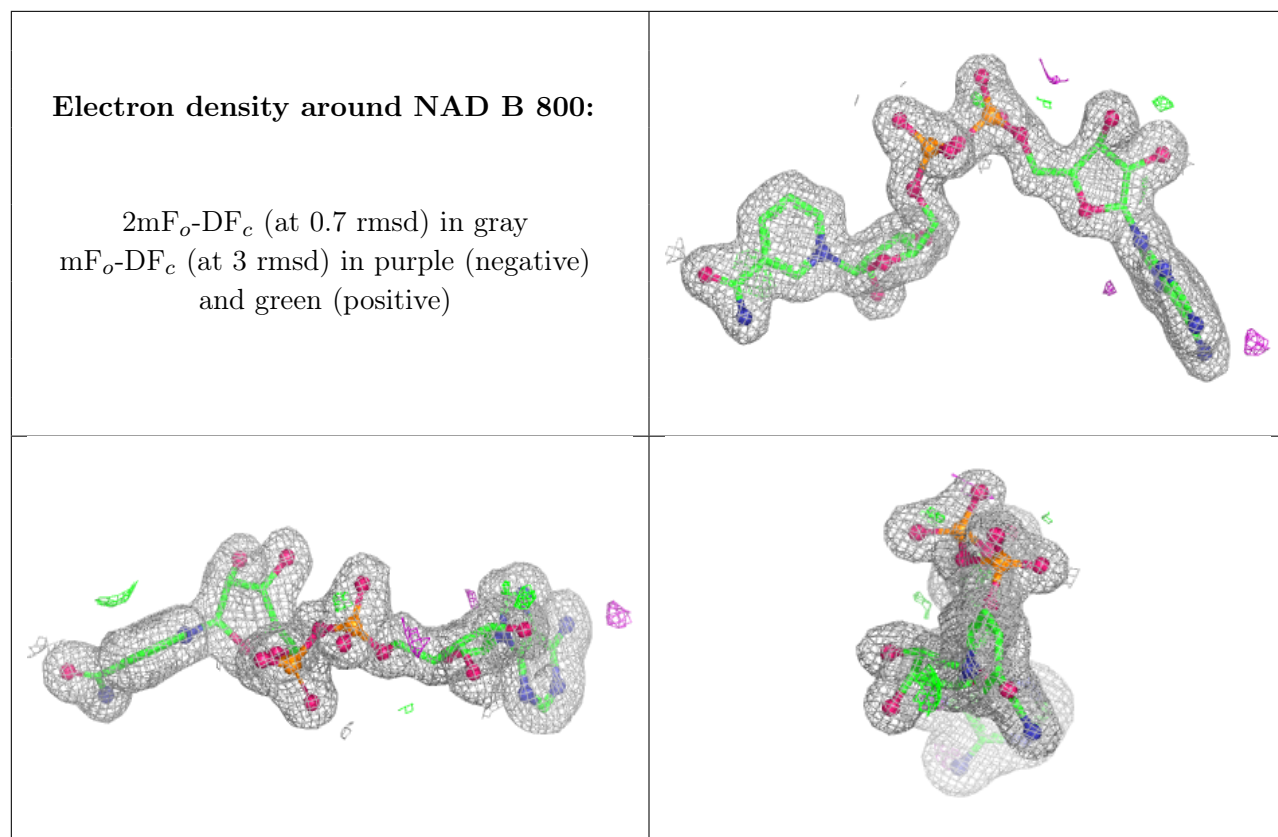
Electron density around NAD G 800:

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

**Electron density around NAD D 800:**

$2mF_o-DF_c$ (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.