



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:06 AM UTC

PDB ID : 3RJ9 / pdb_00003rj9
Title : Structure of alcohol dehydrogenase from *Drosophila lebanonesis* T114V mutant complexed with NAD⁺
Authors : Morgunova, E.; Wuxiuer, Y.; Cols, N.; Popov, A.; Sylte, I.; Karshikoff, A.; Gonzales-Duarte, R.; Ladenstein, R.; Winberg, J.O.
Deposited on : 2011-04-15
Resolution : 1.98 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:

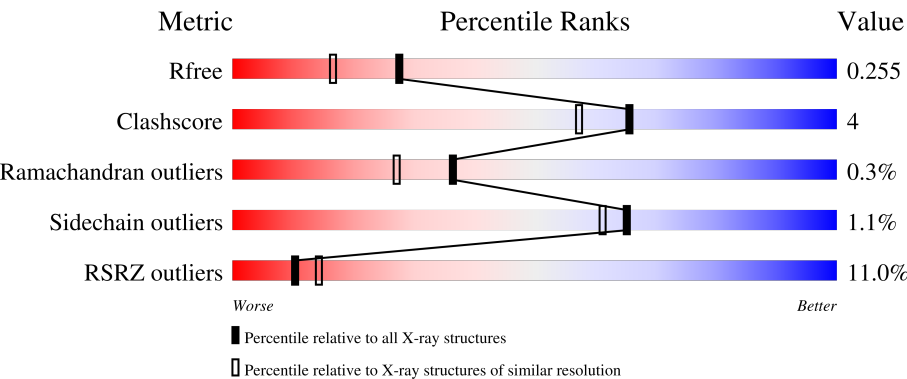
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	254	5% 91%9%
1	B	254	5% 85%14%
1	C	254	6% 91%9%
1	D	254	5% 90%9%

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Mol	Chain	Length	Quality of chain
1	E	254	23% 91% 8%
1	F	254	22% 91% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13060 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.

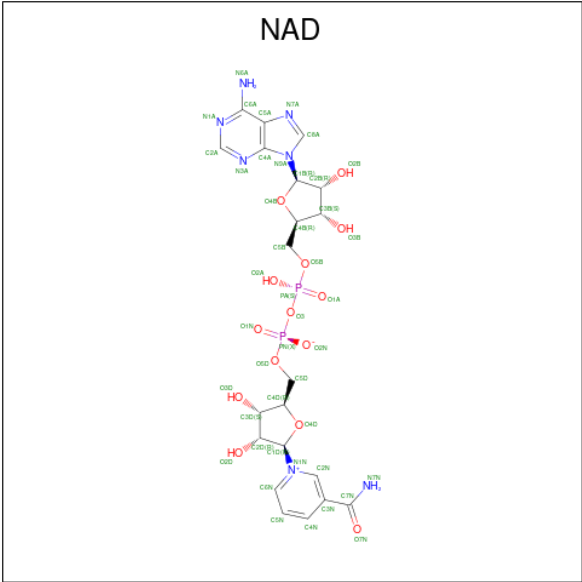
- Molecule 1 is a protein called Alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total 1963	C 1260	N 336	O 364	S 3	0	0	0
1	B	254	Total 1963	C 1260	N 336	O 364	S 3	0	0	0
1	C	254	Total 1963	C 1260	N 336	O 364	S 3	0	0	0
1	D	254	Total 1963	C 1260	N 336	O 364	S 3	5	0	0
1	E	254	Total 1963	C 1260	N 336	O 364	S 3	0	0	0
1	F	254	Total 1963	C 1260	N 336	O 364	S 3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	VAL	THR	engineered mutation	UNP P10807
B	114	VAL	THR	engineered mutation	UNP P10807
C	114	VAL	THR	engineered mutation	UNP P10807
D	114	VAL	THR	engineered mutation	UNP P10807
E	114	VAL	THR	engineered mutation	UNP P10807
F	114	VAL	THR	engineered mutation	UNP P10807

- 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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		
3	B	187	Total	O	0	0
			187	187		
3	C	220	Total	O	0	0
			220	220		
3	D	200	Total	O	0	0
			200	200		
3	E	120	Total	O	0	0
			120	120		
3	F	109	Total	O	0	0
			109	109		

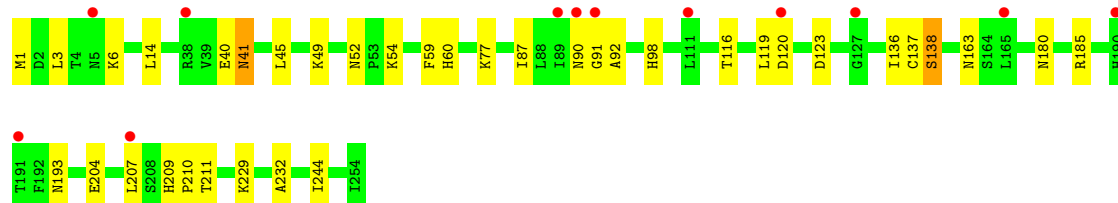
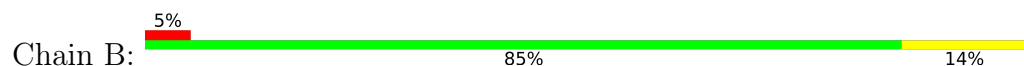
3 Residue-property plots [i](#)

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.

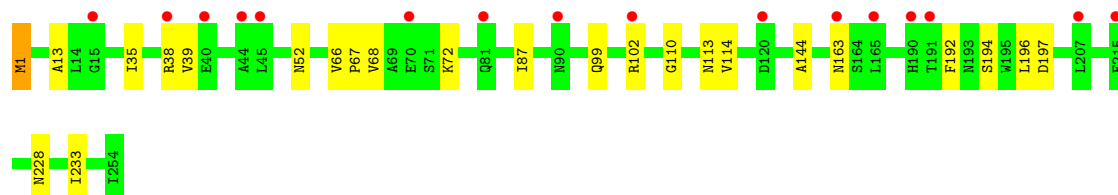
- Molecule 1: Alcohol dehydrogenase



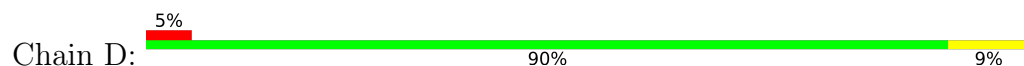
- Molecule 1: Alcohol dehydrogenase

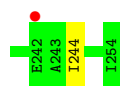


- Molecule 1: Alcohol dehydrogenase

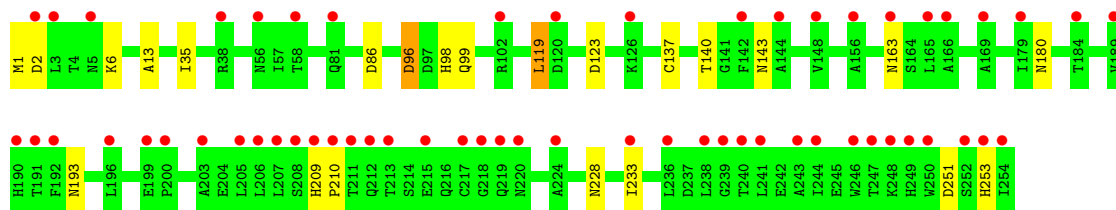
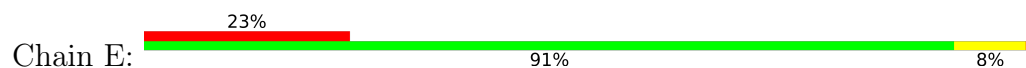


- Molecule 1: Alcohol dehydrogenase

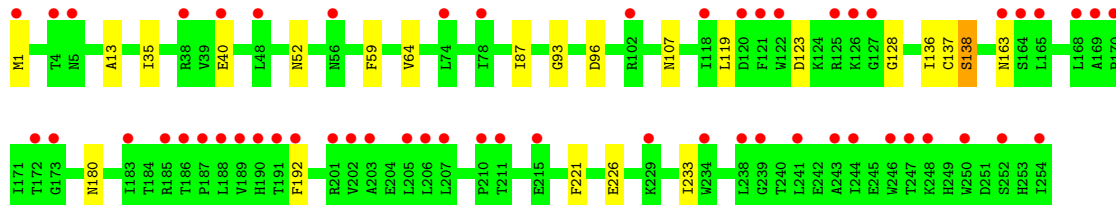
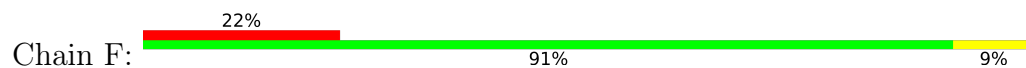




- Molecule 1: Alcohol dehydrogenase



- Molecule 1: Alcohol dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.32Å 94.83Å 139.01Å 90.00° 98.33° 90.00°	Depositor
Resolution (Å)	49.62 – 1.98 49.62 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.0 (49.62-1.98) 93.2 (49.62-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.256 0.208 , 0.255	Depositor DCC
R_{free} test set	2076 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.931	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13060	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.66	0/2002	0.84	0/2727
1	B	0.61	0/2002	0.87	2/2727 (0.1%)
1	C	0.67	0/2002	0.88	4/2727 (0.1%)
1	D	0.68	1/2002 (0.0%)	0.90	4/2727 (0.1%)
1	E	0.55	0/2002	0.83	0/2727
1	F	0.57	0/2002	0.86	5/2727 (0.2%)
All	All	0.63	1/12012 (0.0%)	0.86	15/16362 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	163	ASN	N-CA	6.81	1.54	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	ASN	CA-C-N	6.28	125.97	119.56
1	C	52	ASN	C-N-CA	6.28	125.97	119.56
1	F	192	PHE	N-CA-C	5.94	118.32	108.99
1	D	163	ASN	N-CA-C	5.84	118.39	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ASN	N-CA-C	5.36	117.20	111.36
1	F	52	ASN	CA-C-N	5.31	126.48	119.84
1	F	52	ASN	C-N-CA	5.31	126.48	119.84
1	B	41	ASN	CA-C-N	5.30	124.75	119.24
1	B	41	ASN	C-N-CA	5.30	124.75	119.24
1	C	192	PHE	N-CA-C	5.25	116.82	108.79
1	F	128	GLY	CA-C-N	5.22	125.67	120.04
1	F	128	GLY	C-N-CA	5.22	125.67	120.04
1	D	114	VAL	CB-CA-C	-5.12	105.22	112.14
1	D	52	ASN	CA-C-N	5.10	125.13	119.32
1	D	52	ASN	C-N-CA	5.10	125.13	119.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ALA	Peptide
1	C	144	ALA	Peptide

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	1963	0	2015	10	0
1	B	1963	0	2015	25	0
1	C	1963	0	2015	13	0
1	D	1963	0	2015	19	0
1	E	1963	0	2015	16	0
1	F	1963	0	2015	10	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
3	A	182	0	0	0	0
3	B	187	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	220	0	0	0	0
3	D	200	0	0	4	0
3	E	120	0	0	3	0
3	F	109	0	0	0	0
All	All	13060	0	12246	91	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 4.

All (91) 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:E:96:ASP:O	3:E:976:HOH:O	1.63	1.15
1:D:1:MET:HE2	1:D:87:ILE:HD11	1.49	0.92
1:B:1:MET:HE2	1:B:87:ILE:HD11	1.52	0.92
1:D:1:MET:HE3	1:D:3:LEU:HD23	1.61	0.80
1:D:100:ILE:HD11	3:D:320:HOH:O	1.80	0.80
1:B:52:ASN:OD1	1:B:54:LYS:HE3	1.95	0.65
1:A:209:HIS:HB3	1:A:210:PRO:HD2	1.79	0.64
1:D:1:MET:HE2	1:D:87:ILE:CD1	2.25	0.63
1:F:1:MET:HE2	1:F:87:ILE:HD11	1.81	0.63
1:D:13:ALA:HB3	1:D:35:ILE:HG23	1.81	0.62
1:C:38:ARG:HH11	2:C:850:NAD:C8A	2.13	0.61
1:B:90:ASN:HB3	3:B:1015:HOH:O	2.01	0.60
1:E:1:MET:HB2	1:E:228:ASN:HB2	1.83	0.60
1:C:38:ARG:NH1	2:C:850:NAD:C8A	2.68	0.56
1:E:137:CYS:HB2	1:E:180:ASN:OD1	2.05	0.56
1:B:137:CYS:HB2	1:B:180:ASN:OD1	2.07	0.55
1:D:190:HIS:CE1	3:D:406:HOH:O	2.59	0.55
1:F:136:ILE:HD11	1:F:221:PHE:HE2	1.73	0.54
1:E:96:ASP:C	3:E:976:HOH:O	2.32	0.54
1:C:110:GLY:O	1:C:114:VAL:HG23	2.09	0.53
1:E:163:ASN:HD21	1:E:233:ILE:HD11	1.75	0.52
1:C:68:VAL:CG1	1:C:72:LYS:HE3	2.43	0.49
1:D:119:LEU:O	1:D:123:ASP:HB2	2.13	0.49
1:E:98:HIS:CD2	1:E:193:ASN:HB3	2.47	0.49
1:A:1:MET:HE2	1:A:87:ILE:HD11	1.96	0.48
1:B:91:GLY:HA2	1:B:136:ILE:HD12	1.96	0.48
1:B:91:GLY:O	1:B:92:ALA:C	2.56	0.48
1:D:110:GLY:O	1:D:114:VAL:HG23	2.14	0.48
1:F:119:LEU:O	1:F:123:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:VAL:HB	1:C:67:PRO:HD2	1.95	0.47
1:B:60:HIS:HE1	1:B:77:LYS:NZ	2.13	0.47
1:B:119:LEU:O	1:B:123:ASP:HB2	2.14	0.47
1:B:163:ASN:ND2	3:B:459:HOH:O	2.48	0.47
1:E:209:HIS:HB3	1:E:210:PRO:CD	2.44	0.46
1:D:136:ILE:HD11	1:D:221:PHE:HE2	1.79	0.46
1:E:13:ALA:HB3	1:E:35:ILE:HG23	1.97	0.46
1:A:98:HIS:CD2	1:A:193:ASN:HB3	2.50	0.46
1:D:137:CYS:HB2	1:D:180:ASN:OD1	2.15	0.46
1:D:190:HIS:HE1	3:D:406:HOH:O	1.98	0.46
1:F:13:ALA:HB3	1:F:35:ILE:HG23	1.97	0.46
1:F:40:GLU:HG3	1:F:59:PHE:CE1	2.50	0.46
1:B:1:MET:HE3	1:B:3:LEU:HD23	1.98	0.46
1:D:45:LEU:HG	1:D:49:LYS:HE3	1.98	0.46
1:A:137:CYS:HB2	1:A:180:ASN:OD1	2.15	0.46
1:F:137:CYS:HB2	1:F:180:ASN:OD1	2.16	0.45
1:B:1:MET:CE	1:B:6:LYS:HG3	2.46	0.45
1:B:90:ASN:O	1:B:136:ILE:HG13	2.17	0.45
1:E:99:GLN:N	3:E:976:HOH:O	2.21	0.44
1:B:40:GLU:HG2	1:B:59:PHE:CE1	2.53	0.44
1:C:99:GLN:NE2	1:C:102:ARG:HD3	2.33	0.44
1:C:13:ALA:HB3	1:C:35:ILE:HG23	1.99	0.44
1:B:229:LYS:HB2	1:B:232:ALA:HB2	1.99	0.44
1:B:185:ARG:NH1	3:B:655:HOH:O	2.44	0.44
1:F:1:MET:HB3	1:F:226:GLU:HA	1.99	0.44
1:B:1:MET:HE3	1:B:6:LYS:HG3	1.98	0.43
1:D:45:LEU:O	1:D:49:LYS:HG3	2.17	0.43
1:B:98:HIS:CD2	1:B:193:ASN:HB3	2.53	0.43
1:C:163:ASN:HD21	1:C:233:ILE:HG12	1.83	0.43
1:B:209:HIS:HB3	1:B:210:PRO:HD2	2.01	0.43
1:A:196:LEU:HD21	1:B:116:THR:HG23	2.01	0.43
1:A:72:LYS:HD2	1:A:121:PHE:CE1	2.53	0.43
1:E:209:HIS:HB3	1:E:210:PRO:HD2	2.01	0.43
1:D:98:HIS:CD2	1:D:193:ASN:HB3	2.54	0.42
1:A:179:ILE:HG13	1:A:221:PHE:CE1	2.55	0.42
1:F:93:GLY:HA2	1:F:107:ASN:OD1	2.20	0.42
1:B:209:HIS:HB3	1:B:210:PRO:CD	2.49	0.42
1:C:1:MET:HB3	1:C:228:ASN:HB2	2.02	0.42
1:D:235:LYS:NZ	3:D:324:HOH:O	2.51	0.42
1:C:196:LEU:HD21	1:D:116:THR:HG23	2.00	0.42
1:A:195:TRP:O	1:A:198:VAL:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE2	1:C:87:ILE:HD11	2.01	0.42
1:D:54:LYS:HE3	1:D:54:LYS:H	1.85	0.42
1:B:14:LEU:HD13	1:B:41:ASN:HB3	2.01	0.41
1:D:1:MET:CE	1:D:6:LYS:HG3	2.49	0.41
1:E:119:LEU:O	1:E:123:ASP:HB2	2.20	0.41
1:C:194:SER:OG	1:C:197:ASP:HA	2.21	0.41
1:E:251:ASP:HB3	1:E:253:HIS:CE1	2.55	0.41
1:A:185:ARG:NH1	1:A:211:THR:OG1	2.52	0.41
1:E:2:ASP:O	1:E:6:LYS:NZ	2.52	0.41
1:E:6:LYS:HD2	1:E:86:ASP:CG	2.45	0.41
1:F:137:CYS:O	1:F:138:SER:HB2	2.20	0.41
1:B:137:CYS:O	1:B:138:SER:HB2	2.20	0.41
1:B:45:LEU:HG	1:B:49:LYS:HE2	2.03	0.41
1:C:68:VAL:HG12	1:C:72:LYS:HE3	2.03	0.41
1:A:33:PHE:HB3	1:A:57:ILE:HG12	2.02	0.41
1:B:91:GLY:CA	1:B:136:ILE:HD12	2.51	0.41
1:E:96:ASP:OD1	1:E:193:ASN:HB2	2.21	0.41
1:E:140:THR:HA	1:E:143:ASN:O	2.21	0.41
1:D:1:MET:HE1	1:D:6:LYS:HG3	2.03	0.41
1:F:163:ASN:HD21	1:F:233:ILE:HD11	1.87	0.40
1:B:185:ARG:NE	1:B:211:THR:OG1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	252/254 (99%)	242 (96%)	10 (4%)	0	100	100
1	B	252/254 (99%)	242 (96%)	9 (4%)	1 (0%)	30	20
1	C	252/254 (99%)	243 (96%)	9 (4%)	0	100	100
1	D	252/254 (99%)	243 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	252/254 (99%)	242 (96%)	9 (4%)	1 (0%)	30	20
1	F	252/254 (99%)	240 (95%)	10 (4%)	2 (1%)	16	7
All	All	1512/1524 (99%)	1452 (96%)	56 (4%)	4 (0%)	36	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	96	ASP
1	B	138	SER
1	E	96	ASP
1	F	138	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	216/216 (100%)	212 (98%)	4 (2%)	50	44
1	B	216/216 (100%)	212 (98%)	4 (2%)	50	44
1	C	216/216 (100%)	214 (99%)	2 (1%)	70	67
1	D	216/216 (100%)	214 (99%)	2 (1%)	70	67
1	E	216/216 (100%)	215 (100%)	1 (0%)	81	79
1	F	216/216 (100%)	215 (100%)	1 (0%)	81	79
All	All	1296/1296 (100%)	1282 (99%)	14 (1%)	65	61

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	77	LYS
1	A	185	ARG
1	A	207	LEU
1	B	120	ASP
1	B	204	GLU

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Mol	Chain	Res	Type
1	B	207	LEU
1	B	244	ILE
1	C	1	MET
1	C	39	VAL
1	D	54	LYS
1	D	244	ILE
1	E	119	LEU
1	F	64	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	163	ASN
1	A	193	ASN
1	A	228	ASN
1	B	32	ASN
1	B	56	ASN
1	B	60	HIS
1	B	90	ASN
1	B	99	GLN
1	B	146	HIS
1	B	163	ASN
1	B	190	HIS
1	B	209	HIS
1	C	56	ASN
1	C	99	GLN
1	C	163	ASN
1	C	190	HIS
1	C	193	ASN
1	C	228	ASN
1	D	56	ASN
1	D	90	ASN
1	D	190	HIS
1	D	209	HIS
1	D	253	HIS
1	E	56	ASN
1	E	90	ASN
1	E	163	ASN
1	E	209	HIS
1	E	219	GLN
1	E	253	HIS

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Mol	Chain	Res	Type
1	F	90	ASN
1	F	163	ASN
1	F	190	HIS
1	F	193	ASN
1	F	209	HIS
1	F	228	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	850	-	46,48,48	0.94	3 (6%)	64,73,73	1.58	9 (14%)
2	NAD	F	850	-	46,48,48	0.99	4 (8%)	64,73,73	1.68	11 (17%)
2	NAD	D	850	-	46,48,48	0.96	4 (8%)	64,73,73	1.65	12 (18%)
2	NAD	B	850	-	46,48,48	0.95	3 (6%)	64,73,73	1.68	11 (17%)
2	NAD	A	850	-	46,48,48	0.89	1 (2%)	64,73,73	1.57	9 (14%)
2	NAD	E	850	-	46,48,48	0.82	2 (4%)	64,73,73	1.62	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	850	-	-	7/30/62/62	0/5/5/5
2	NAD	F	850	-	-	8/30/62/62	0/5/5/5
2	NAD	D	850	-	-	7/30/62/62	0/5/5/5
2	NAD	B	850	-	-	7/30/62/62	0/5/5/5
2	NAD	A	850	-	-	8/30/62/62	0/5/5/5
2	NAD	E	850	-	-	8/30/62/62	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	850	NAD	PA-O3	2.76	1.62	1.59
2	F	850	NAD	PN-O3	2.70	1.62	1.59
2	D	850	NAD	O4D-C1D	2.64	1.44	1.40
2	E	850	NAD	O4D-C1D	2.55	1.44	1.40
2	C	850	NAD	O4D-C1D	2.51	1.44	1.40
2	A	850	NAD	O4D-C1D	2.48	1.44	1.40
2	B	850	NAD	C8A-N7A	2.36	1.36	1.31
2	C	850	NAD	PN-O3	2.36	1.62	1.59
2	B	850	NAD	PA-O3	2.27	1.61	1.59
2	D	850	NAD	C8A-N7A	2.24	1.36	1.31
2	B	850	NAD	O4D-C1D	2.21	1.43	1.40
2	F	850	NAD	O4D-C1D	2.16	1.43	1.40
2	F	850	NAD	C8A-N7A	2.14	1.35	1.31
2	C	850	NAD	C8A-N7A	2.12	1.35	1.31
2	E	850	NAD	C8A-N7A	2.12	1.35	1.31
2	D	850	NAD	PA-O3	2.07	1.61	1.59
2	D	850	NAD	C4A-N3A	2.06	1.38	1.34

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	850	NAD	N3A-C2A-N1A	-5.41	120.39	128.58
2	F	850	NAD	N3A-C2A-N1A	-5.40	120.41	128.58
2	C	850	NAD	N3A-C2A-N1A	-5.39	120.42	128.58
2	E	850	NAD	N3A-C2A-N1A	-5.33	120.52	128.58
2	A	850	NAD	N3A-C2A-N1A	-5.07	120.91	128.58
2	E	850	NAD	C5A-C4A-N3A	-5.02	119.80	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	850	NAD	C5A-C4A-N3A	-5.01	119.82	126.72
2	B	850	NAD	O4B-C1B-N9A	4.96	117.61	108.09
2	F	850	NAD	C5A-C4A-N3A	-4.95	119.91	126.72
2	B	850	NAD	N3A-C2A-N1A	-4.91	121.16	128.58
2	D	850	NAD	C5A-C4A-N3A	-4.69	120.25	126.72
2	C	850	NAD	C5A-C4A-N3A	-4.30	120.79	126.72
2	A	850	NAD	C5A-C4A-N3A	-4.28	120.83	126.72
2	D	850	NAD	N9A-C8A-N7A	-3.92	108.38	113.94
2	C	850	NAD	O4B-C1B-N9A	3.89	115.56	108.09
2	F	850	NAD	N9A-C8A-N7A	-3.63	108.78	113.94
2	F	850	NAD	C2A-N3A-C4A	3.58	120.57	111.83
2	D	850	NAD	O4B-C1B-N9A	3.51	114.83	108.09
2	E	850	NAD	C2A-N3A-C4A	3.49	120.34	111.83
2	A	850	NAD	C4A-N9A-C8A	3.47	109.38	105.74
2	E	850	NAD	N9A-C8A-N7A	-3.47	109.02	113.94
2	B	850	NAD	N3A-C4A-N9A	3.45	133.03	127.17
2	F	850	NAD	O4B-C1B-N9A	3.45	114.71	108.09
2	E	850	NAD	O4B-C1B-N9A	3.44	114.70	108.09
2	B	850	NAD	N9A-C8A-N7A	-3.44	109.06	113.94
2	A	850	NAD	N3A-C4A-N9A	3.42	132.98	127.17
2	D	850	NAD	C2A-N3A-C4A	3.41	120.16	111.83
2	C	850	NAD	N9A-C8A-N7A	-3.40	109.11	113.94
2	E	850	NAD	N3A-C4A-N9A	3.39	132.94	127.17
2	A	850	NAD	N9A-C8A-N7A	-3.39	109.12	113.94
2	A	850	NAD	C3N-C7N-N7N	3.39	121.92	117.74
2	B	850	NAD	C2A-N3A-C4A	3.36	120.04	111.83
2	F	850	NAD	N3A-C4A-N9A	3.36	132.88	127.17
2	C	850	NAD	C2A-N3A-C4A	3.24	119.74	111.83
2	D	850	NAD	N3A-C4A-N9A	3.22	132.64	127.17
2	D	850	NAD	C4A-N9A-C8A	3.20	109.10	105.74
2	F	850	NAD	C4A-N9A-C8A	3.17	109.07	105.74
2	A	850	NAD	C2A-N3A-C4A	3.04	119.26	111.83
2	C	850	NAD	C4A-N9A-C8A	2.92	108.81	105.74
2	C	850	NAD	N3A-C4A-N9A	2.88	132.06	127.17
2	F	850	NAD	C4A-C5A-N7A	-2.74	107.45	110.58
2	B	850	NAD	C4A-N9A-C8A	2.72	108.59	105.74
2	D	850	NAD	C5A-N7A-C8A	2.68	107.66	103.45
2	E	850	NAD	C4A-N9A-C8A	2.63	108.50	105.74
2	B	850	NAD	C3N-C7N-N7N	2.59	120.93	117.74
2	F	850	NAD	C5A-N7A-C8A	2.57	107.48	103.45
2	E	850	NAD	C5A-N7A-C8A	2.53	107.43	103.45
2	F	850	NAD	C3N-C7N-N7N	2.52	120.84	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	850	NAD	O7N-C7N-N7N	-2.49	119.02	122.62
2	B	850	NAD	O2N-PN-O3	2.48	113.97	107.27
2	D	850	NAD	C4A-C5A-N7A	-2.46	107.77	110.58
2	E	850	NAD	C4A-C5A-N7A	-2.44	107.79	110.58
2	A	850	NAD	C5A-N7A-C8A	2.25	106.99	103.45
2	B	850	NAD	C5A-N7A-C8A	2.25	106.98	103.45
2	C	850	NAD	C4A-C5A-N7A	-2.23	108.03	110.58
2	C	850	NAD	C5A-N7A-C8A	2.19	106.89	103.45
2	D	850	NAD	C3N-C7N-N7N	2.15	120.39	117.74
2	D	850	NAD	O2A-PA-O1A	2.14	122.41	112.44
2	B	850	NAD	C4A-C5A-N7A	-2.08	108.21	110.58
2	F	850	NAD	C6N-N1N-C2N	-2.02	120.16	121.88
2	D	850	NAD	C2A-N1A-C6A	2.01	122.03	118.73

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	850	NAD	PN-O3-PA-O5B
2	A	850	NAD	C5D-O5D-PN-O3
2	A	850	NAD	C5D-O5D-PN-O1N
2	A	850	NAD	C5D-O5D-PN-O2N
2	A	850	NAD	O4D-C1D-N1N-C2N
2	B	850	NAD	C5D-O5D-PN-O3
2	B	850	NAD	C5D-O5D-PN-O1N
2	B	850	NAD	C5D-O5D-PN-O2N
2	B	850	NAD	O4D-C1D-N1N-C2N
2	C	850	NAD	C5D-O5D-PN-O3
2	C	850	NAD	C5D-O5D-PN-O2N
2	C	850	NAD	O4D-C1D-N1N-C2N
2	D	850	NAD	C5D-O5D-PN-O3
2	D	850	NAD	C5D-O5D-PN-O2N
2	D	850	NAD	O4D-C1D-N1N-C2N
2	E	850	NAD	C5D-O5D-PN-O3
2	E	850	NAD	C5D-O5D-PN-O1N
2	E	850	NAD	C5D-O5D-PN-O2N
2	E	850	NAD	O4D-C1D-N1N-C2N
2	F	850	NAD	PN-O3-PA-O5B
2	F	850	NAD	C5D-O5D-PN-O3
2	F	850	NAD	C5D-O5D-PN-O1N
2	F	850	NAD	C5D-O5D-PN-O2N
2	F	850	NAD	O4D-C1D-N1N-C2N

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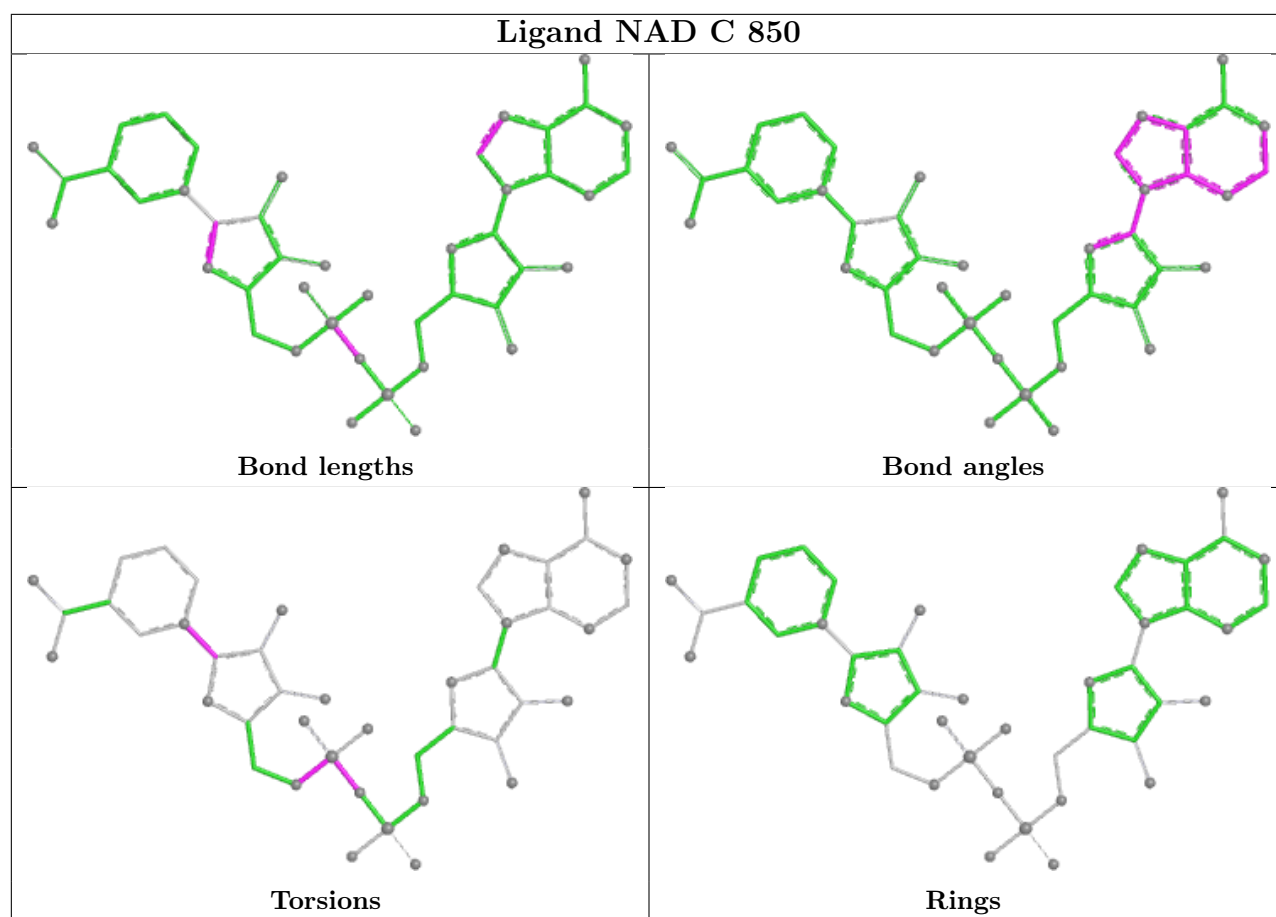
Mol	Chain	Res	Type	Atoms
2	A	850	NAD	PA-O3-PN-O1N
2	F	850	NAD	PA-O3-PN-O1N
2	E	850	NAD	PN-O3-PA-O5B
2	B	850	NAD	PA-O3-PN-O2N
2	D	850	NAD	PA-O3-PN-O2N
2	E	850	NAD	PA-O3-PN-O1N
2	C	850	NAD	C5D-O5D-PN-O1N
2	D	850	NAD	C5D-O5D-PN-O1N
2	A	850	NAD	PA-O3-PN-O2N
2	C	850	NAD	PA-O3-PN-O2N
2	E	850	NAD	PA-O3-PN-O2N
2	F	850	NAD	PA-O3-PN-O2N
2	A	850	NAD	O4D-C1D-N1N-C6N
2	B	850	NAD	O4D-C1D-N1N-C6N
2	C	850	NAD	O4D-C1D-N1N-C6N
2	D	850	NAD	O4D-C1D-N1N-C6N
2	E	850	NAD	O4D-C1D-N1N-C6N
2	F	850	NAD	O4D-C1D-N1N-C6N
2	B	850	NAD	PA-O3-PN-O1N
2	C	850	NAD	PA-O3-PN-O1N
2	D	850	NAD	PA-O3-PN-O1N

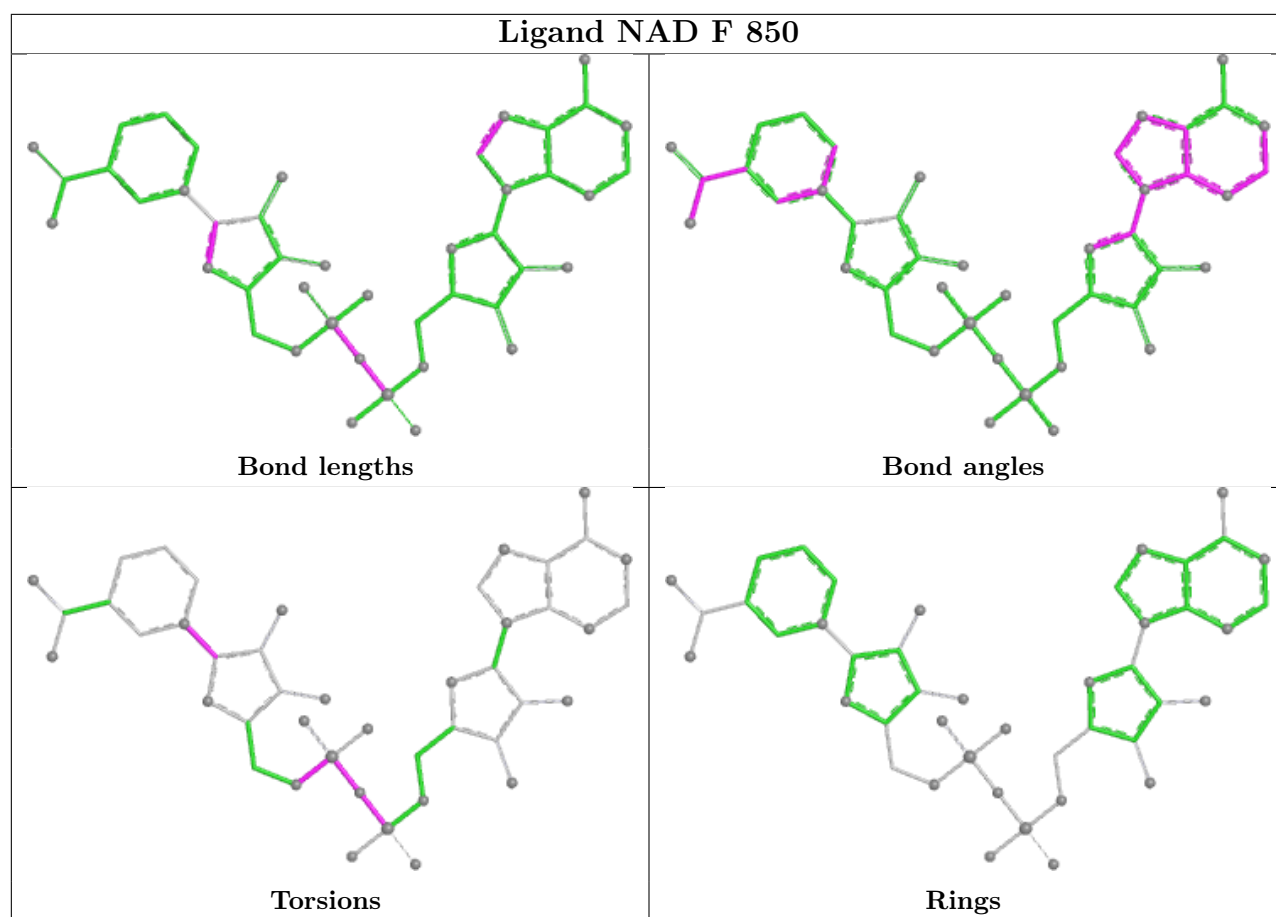
There are no ring outliers.

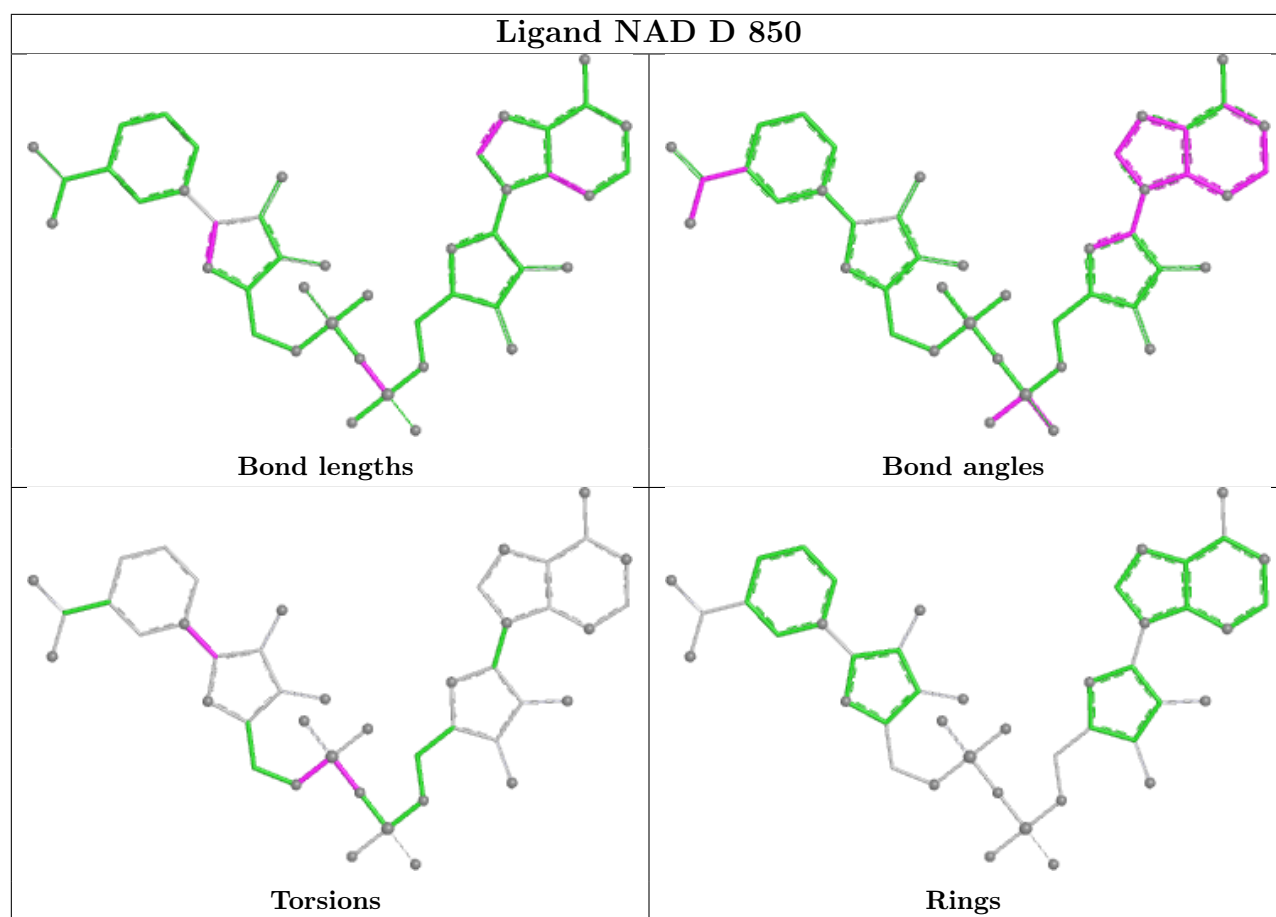
1 monomer is involved in 2 short contacts:

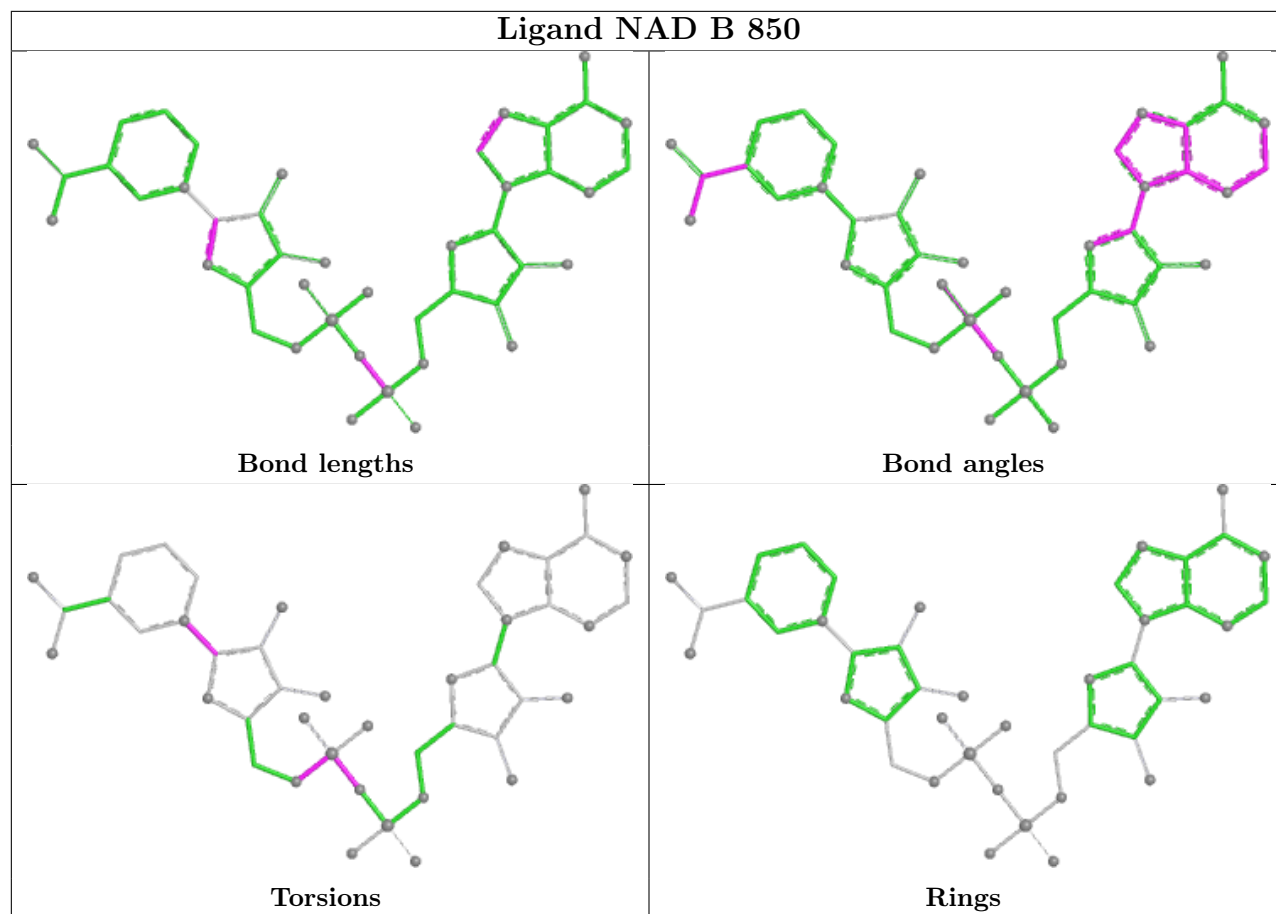
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	850	NAD	2	0

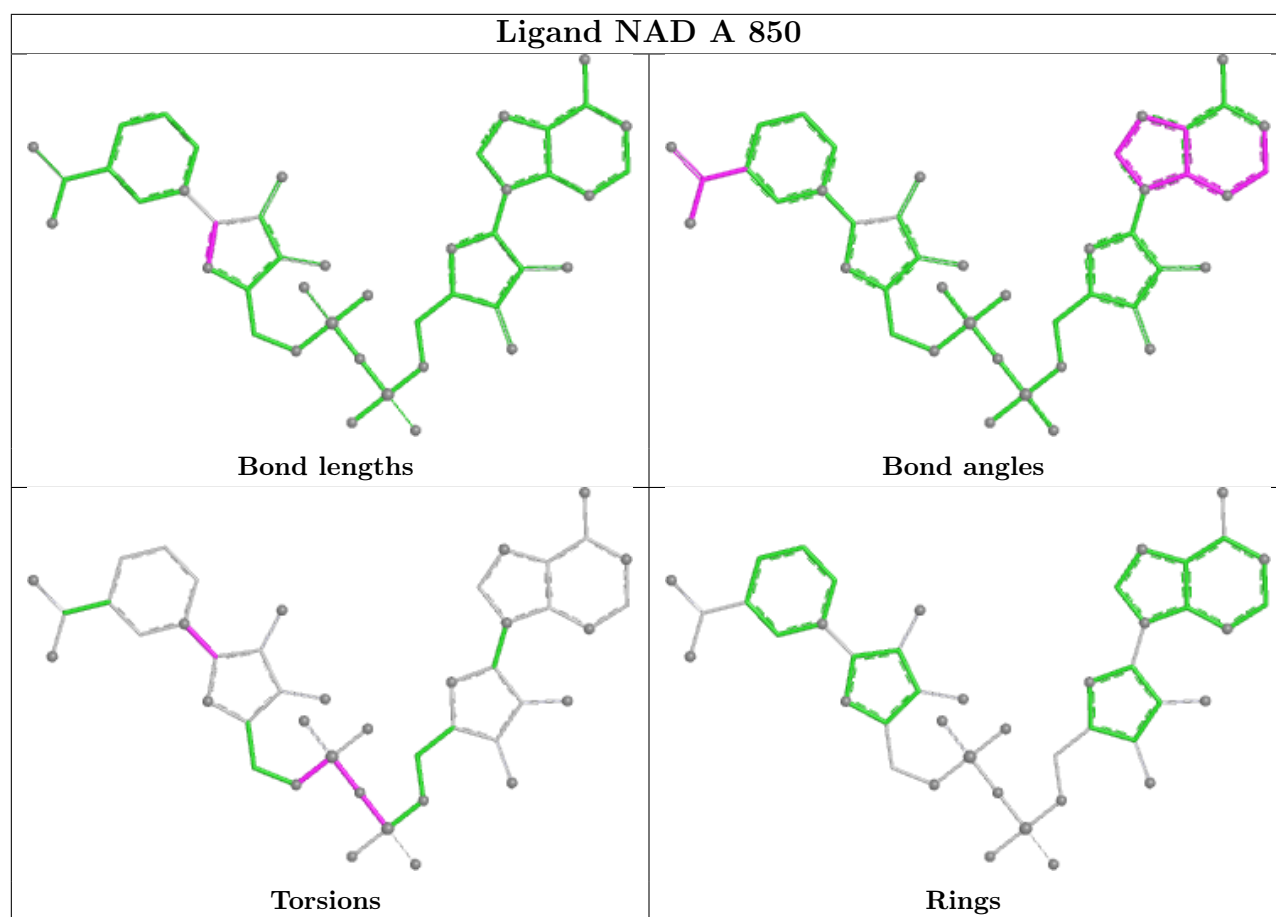
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

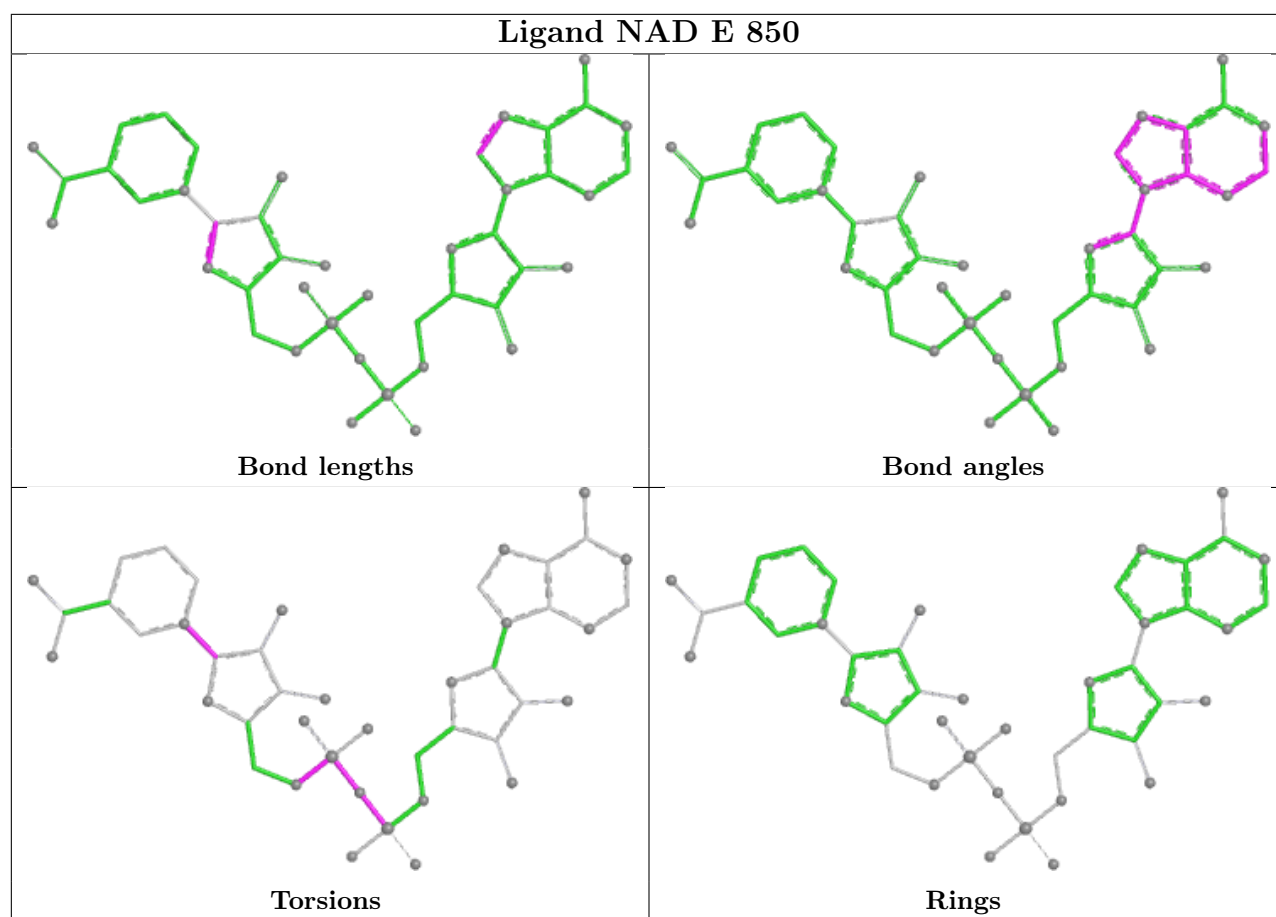












5.7 Other polymers [i](#)

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	254/254 (100%)	0.49	12 (4%)	36 46	12, 24, 38, 45	9 (3%)
1	B	254/254 (100%)	0.44	12 (4%)	36 46	12, 24, 36, 41	11 (4%)
1	C	254/254 (100%)	0.33	16 (6%)	26 34	10, 22, 34, 39	11 (4%)
1	D	254/254 (100%)	0.34	12 (4%)	36 46	2, 22, 34, 39	10 (3%)
1	E	254/254 (100%)	1.28	59 (23%)	2 2	8, 36, 51, 54	11 (4%)
1	F	254/254 (100%)	1.30	56 (22%)	2 2	12, 34, 50, 54	11 (4%)
All	All	1524/1524 (100%)	0.70	167 (10%)	10 14	2, 27, 44, 54	63 (4%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	38	ARG	8.2
1	E	38	ARG	8.0
1	B	38	ARG	6.7
1	E	199	GLU	6.7
1	D	38	ARG	6.3
1	C	38	ARG	6.1
1	F	207	LEU	6.1
1	E	207	LEU	5.9
1	F	191	THR	5.6
1	F	56	ASN	5.5
1	B	89	ILE	5.2
1	E	56	ASN	5.1
1	B	90	ASN	5.1
1	D	207	LEU	5.0
1	D	163	ASN	5.0
1	F	165	LEU	4.9
1	E	238	LEU	4.8
1	D	191	THR	4.7
1	F	188	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	189	VAL	4.5
1	E	165	LEU	4.3
1	F	206	LEU	4.3
1	E	241	LEU	4.2
1	D	5	ASN	4.0
1	B	207	LEU	4.0
1	F	205	LEU	4.0
1	A	191	THR	4.0
1	C	165	LEU	3.9
1	F	250	TRP	3.9
1	E	250	TRP	3.8
1	F	190	HIS	3.7
1	A	185	ARG	3.7
1	F	239	GLY	3.7
1	C	207	LEU	3.7
1	E	126	LYS	3.7
1	A	54	LYS	3.6
1	E	210	PRO	3.6
1	E	209	HIS	3.6
1	F	252	SER	3.6
1	F	192	PHE	3.6
1	A	207	LEU	3.6
1	E	190	HIS	3.5
1	F	1	MET	3.4
1	F	244	ILE	3.4
1	B	190	HIS	3.3
1	F	215	GLU	3.3
1	D	165	LEU	3.3
1	F	173	GLY	3.3
1	F	183	ILE	3.2
1	F	254	ILE	3.2
1	E	244	ILE	3.2
1	E	189	VAL	3.2
1	E	215	GLU	3.2
1	B	111	LEU	3.2
1	E	243	ALA	3.1
1	F	247	THR	3.1
1	F	246	TRP	3.1
1	A	5	ASN	3.1
1	E	217	CYS	3.1
1	A	165	LEU	3.1
1	F	163	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	254	ILE	3.0
1	B	165	LEU	3.0
1	E	81	GLN	3.0
1	E	248	LYS	3.0
1	F	202	VAL	3.0
1	E	192	PHE	3.0
1	F	243	ALA	3.0
1	E	252	SER	3.0
1	A	190	HIS	3.0
1	E	196	LEU	2.9
1	F	238	LEU	2.9
1	F	78	ILE	2.9
1	F	168	LEU	2.9
1	E	213	THR	2.9
1	F	121	PHE	2.9
1	C	163	ASN	2.8
1	E	224	ALA	2.8
1	F	120	ASP	2.8
1	F	201	ARG	2.8
1	F	169	ALA	2.8
1	E	191	THR	2.8
1	F	126	LYS	2.8
1	F	186	THR	2.8
1	C	190	HIS	2.7
1	D	126	LYS	2.7
1	D	190	HIS	2.7
1	E	239	GLY	2.7
1	E	206	LEU	2.7
1	E	219	GLN	2.7
1	E	169	ALA	2.7
1	E	203	ALA	2.7
1	B	120	ASP	2.7
1	B	191	THR	2.7
1	C	90	ASN	2.7
1	F	118	ILE	2.7
1	E	142	PHE	2.6
1	C	120	ASP	2.6
1	F	229	LYS	2.6
1	F	210	PRO	2.6
1	C	81	GLN	2.6
1	D	120	ASP	2.6
1	E	3	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	127	GLY	2.5
1	E	240	THR	2.5
1	C	45	LEU	2.5
1	C	70	GLU	2.5
1	C	215	GLU	2.5
1	F	48	LEU	2.5
1	F	5	ASN	2.5
1	F	164	SER	2.5
1	E	179	ILE	2.4
1	C	191	THR	2.4
1	E	156	ALA	2.4
1	E	253	HIS	2.4
1	A	56	ASN	2.4
1	F	241	LEU	2.4
1	E	2	ASP	2.4
1	E	211	THR	2.4
1	E	166	ALA	2.4
1	B	127	GLY	2.4
1	F	248	LYS	2.4
1	E	120	ASP	2.3
1	E	102	ARG	2.3
1	F	74	LEU	2.3
1	E	247	THR	2.3
1	B	5	ASN	2.3
1	E	200	PRO	2.3
1	E	218	GLY	2.3
1	E	208	SER	2.3
1	E	205	LEU	2.3
1	F	234	TRP	2.3
1	E	249	HIS	2.3
1	D	1	MET	2.3
1	C	44	ALA	2.3
1	E	246	TRP	2.2
1	B	91	GLY	2.2
1	F	170	PRO	2.2
1	F	187	PRO	2.2
1	A	55	VAL	2.2
1	E	163	ASN	2.2
1	A	1	MET	2.2
1	F	102	ARG	2.2
1	F	211	THR	2.2
1	E	220	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	203	ALA	2.2
1	C	102	ARG	2.2
1	F	40	GLU	2.1
1	E	233	ILE	2.1
1	F	125	ARG	2.1
1	C	40	GLU	2.1
1	E	5	ASN	2.1
1	E	144	ALA	2.1
1	E	184	THR	2.1
1	F	122	TRP	2.1
1	A	102	ARG	2.1
1	F	185	ARG	2.1
1	E	236	LEU	2.1
1	D	208	SER	2.0
1	F	172	THR	2.0
1	A	219	GLN	2.0
1	E	212	GLN	2.0
1	E	148	VAL	2.0
1	D	242	GLU	2.0
1	C	15	GLY	2.0
1	E	58	THR	2.0
1	F	4	THR	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.

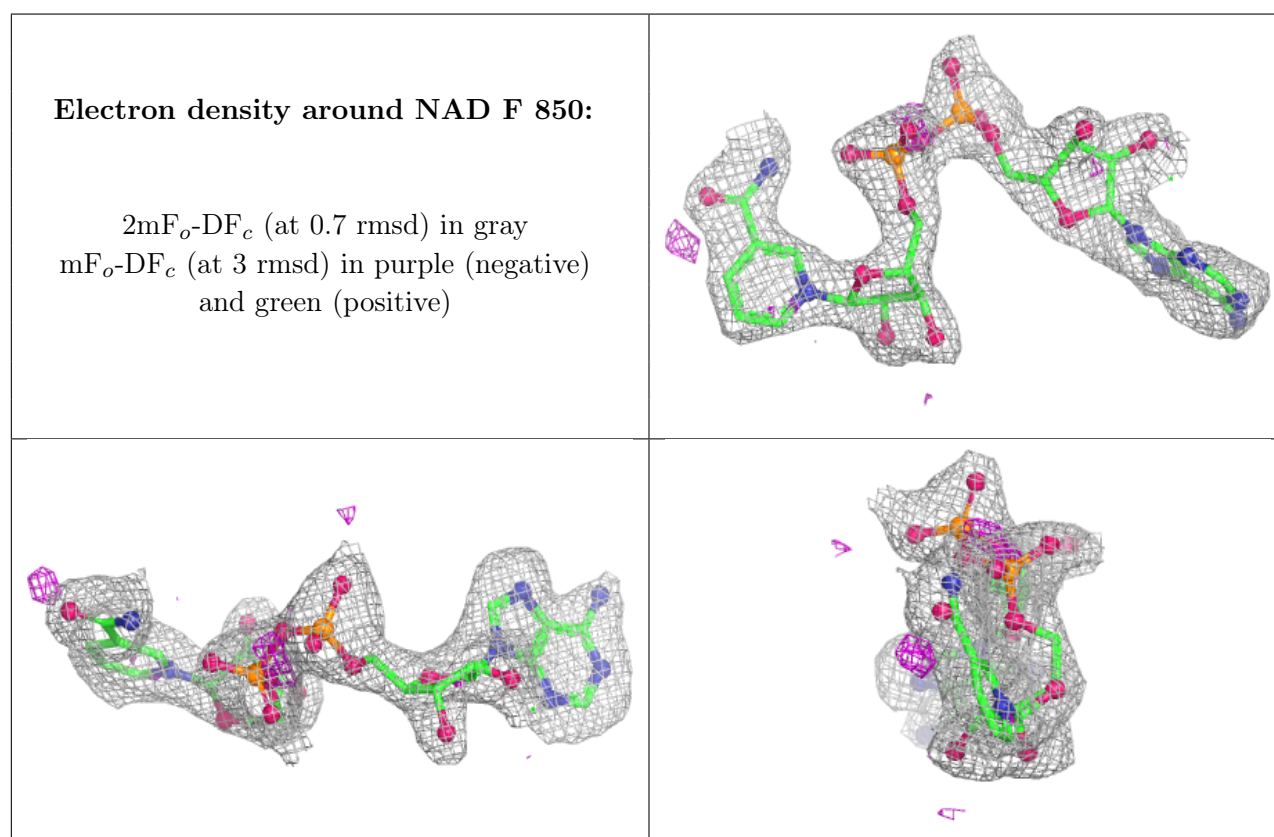
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAD	F	850	44/44	0.89	0.10	39,41,42,43	0

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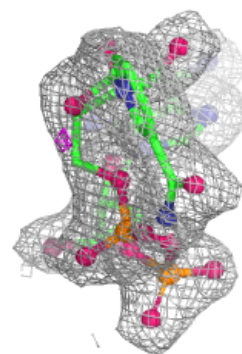
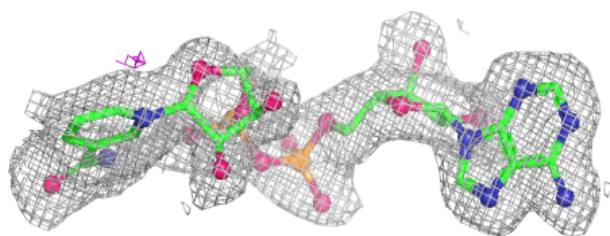
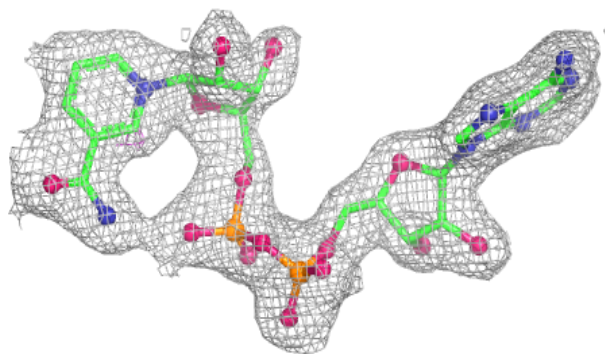
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	E	850	44/44	0.95	0.07	25,31,33,35	0
2	NAD	D	850	44/44	0.95	0.07	20,22,24,26	0
2	NAD	A	850	44/44	0.96	0.06	18,20,22,24	0
2	NAD	B	850	44/44	0.96	0.06	19,24,25,26	0
2	NAD	C	850	44/44	0.96	0.06	20,22,25,26	0

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.

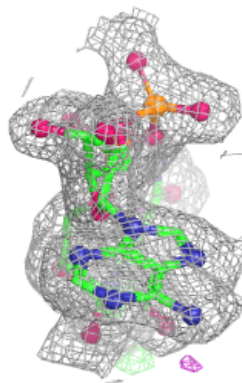
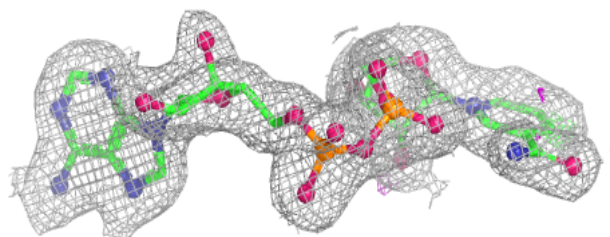
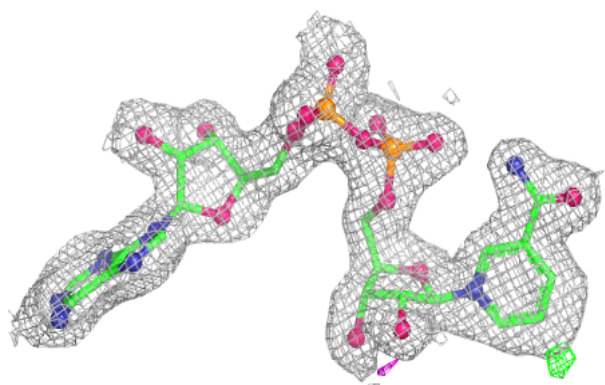


Electron density around NAD E 850:

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

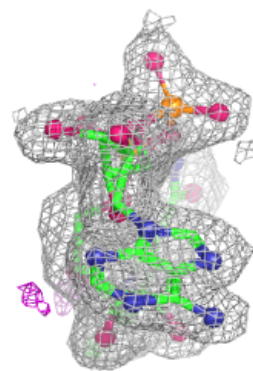
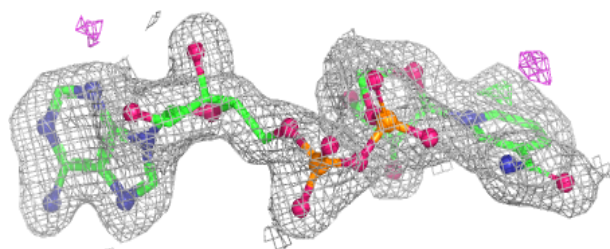
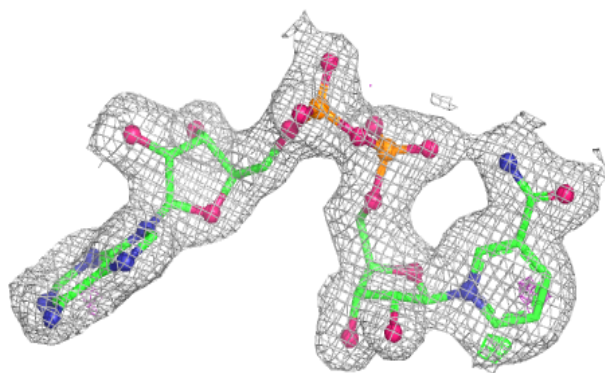
**Electron density around NAD D 850:**

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

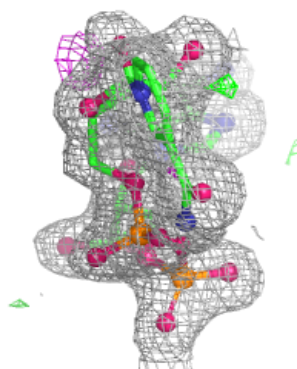
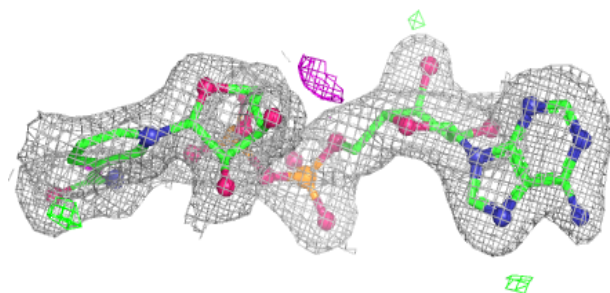
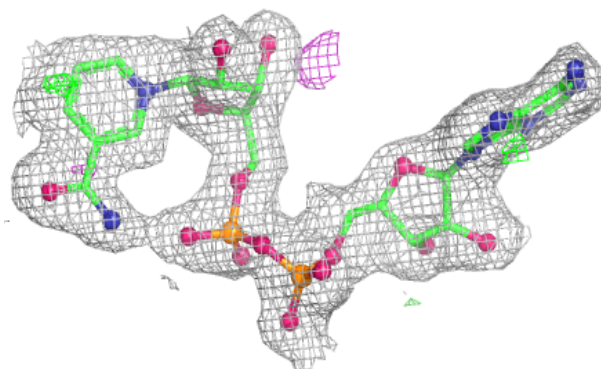


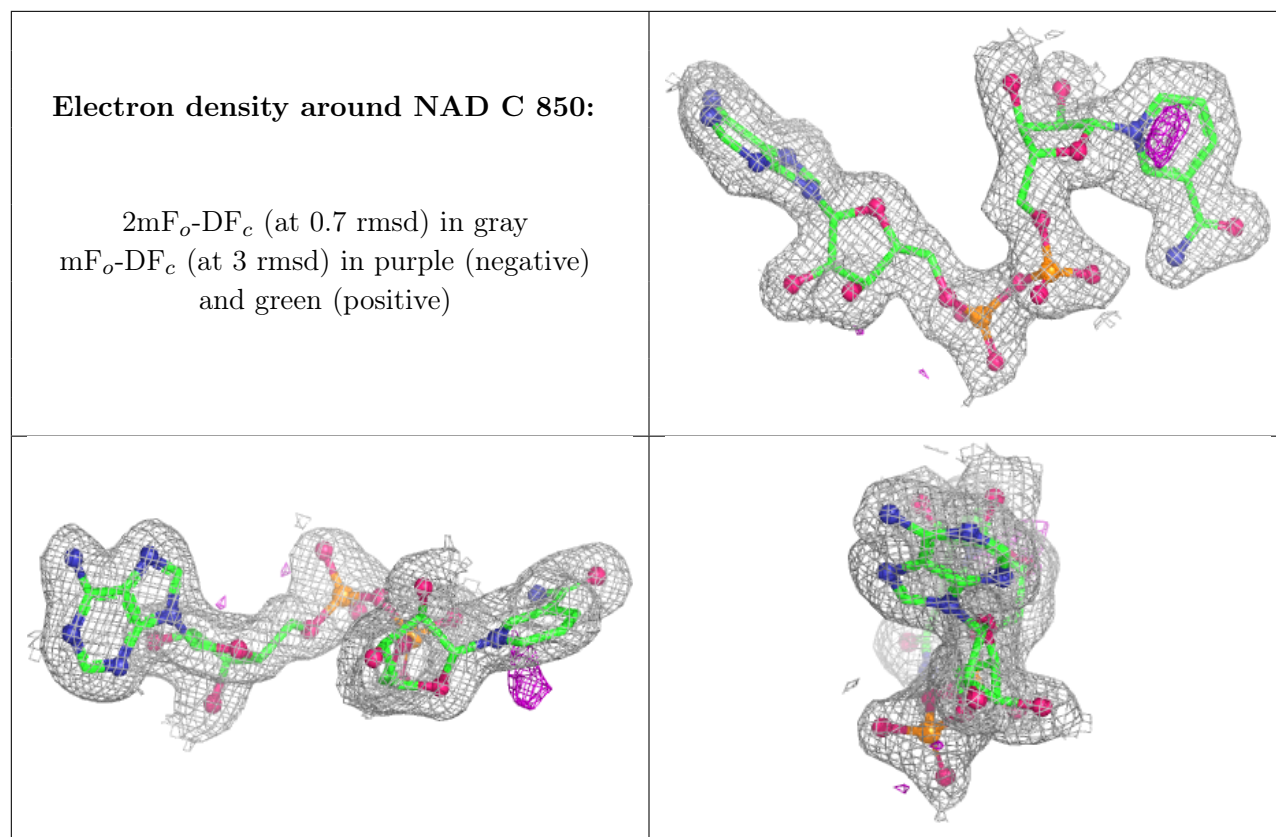
Electron density around NAD A 850:

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

**Electron density around NAD B 850:**

$2mF_o-DF_c$ (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.