



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 01:49 AM EDT

PDB ID : 2GVG
Title : Crystal Structure of human NMPRTase and its complex with NMN
Authors : Khan, J.A.; Tao, X.; Tong, L.
Deposited on : 2006-05-02
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

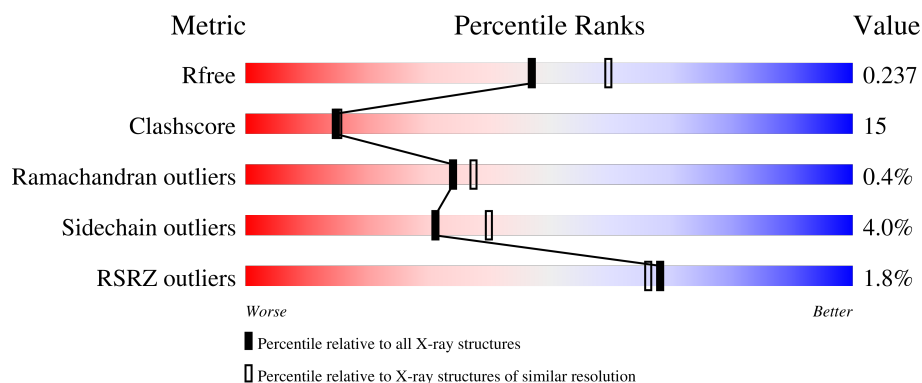
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	491	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>31%</div> <div>• 6%</div> </div> </div>
1	B	491	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• 5%</div> </div> </div>
1	C	491	<div> <div>4%</div> <div> <div></div> <div>59%</div> <div>33%</div> <div>• 6%</div> </div> </div>
1	D	491	<div> <div>0%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• 5%</div> </div> </div>
1	E	491	<div> <div></div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	491	 <p>% 71% 22% • 6%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	E	608	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23801 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 Nicotinamide phosphoribosyltransferase.

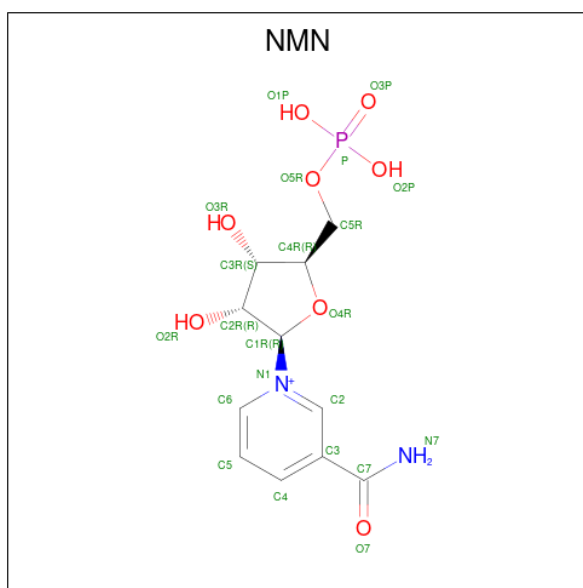
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3688	2376	609	696	7			
1	B	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	C	461	Total	C	N	O	S	0	0	0
			3688	2376	609	696	7			
1	D	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	E	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	F	463	Total	C	N	O	S	0	0	0
			3705	2385	612	701	7			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is BETA-NICOTINAMIDE RIBOSE MONOPHOSPHATE (three-letter code: NMN) (formula: $C_{11}H_{16}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	E	1	Total	C	N	O	P	0	0
			22	11	2	8	1		
3	F	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

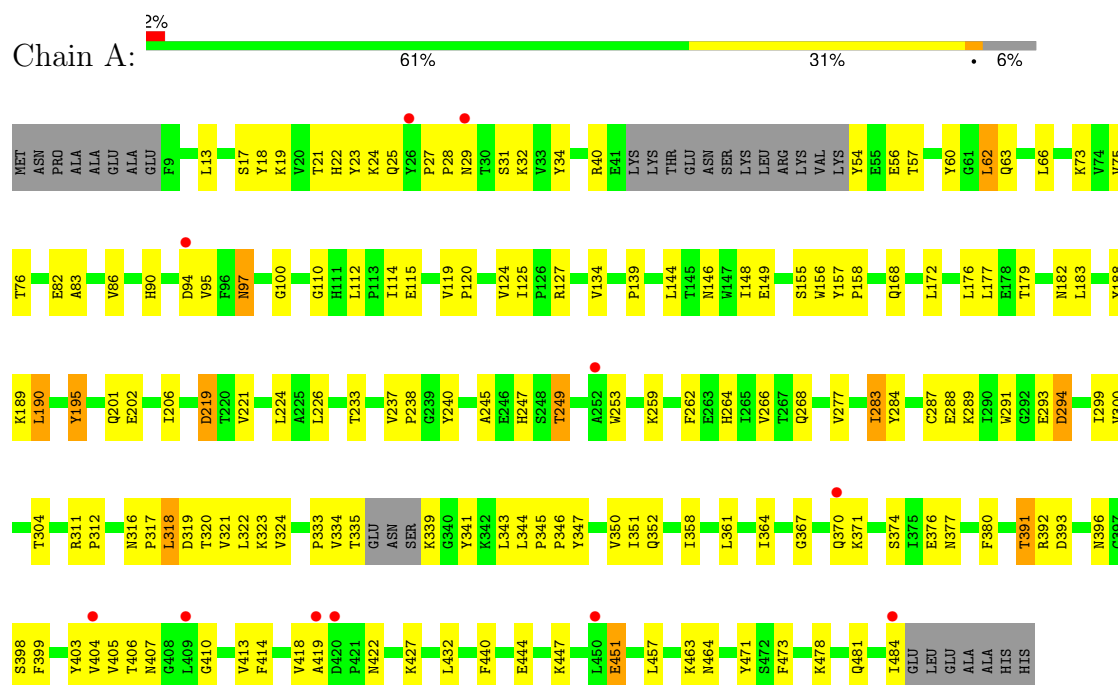
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	165	Total	O	0	0
			165	165		
4	C	125	Total	O	0	0
			125	125		
4	D	306	Total	O	0	0
			306	306		
4	E	280	Total	O	0	0
			280	280		
4	F	380	Total	O	0	0
			380	380		

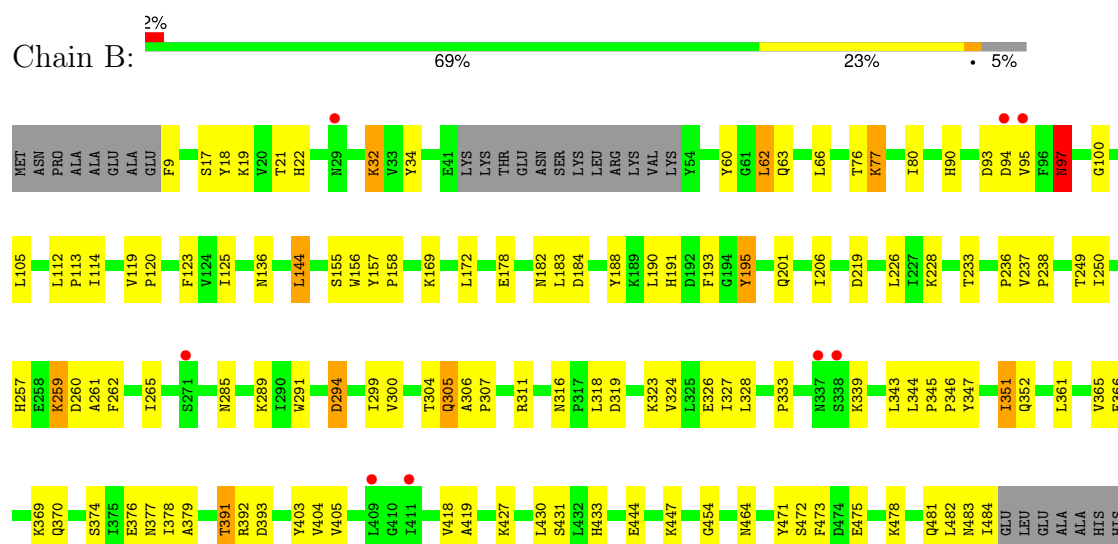
3 Residue-property plots

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.

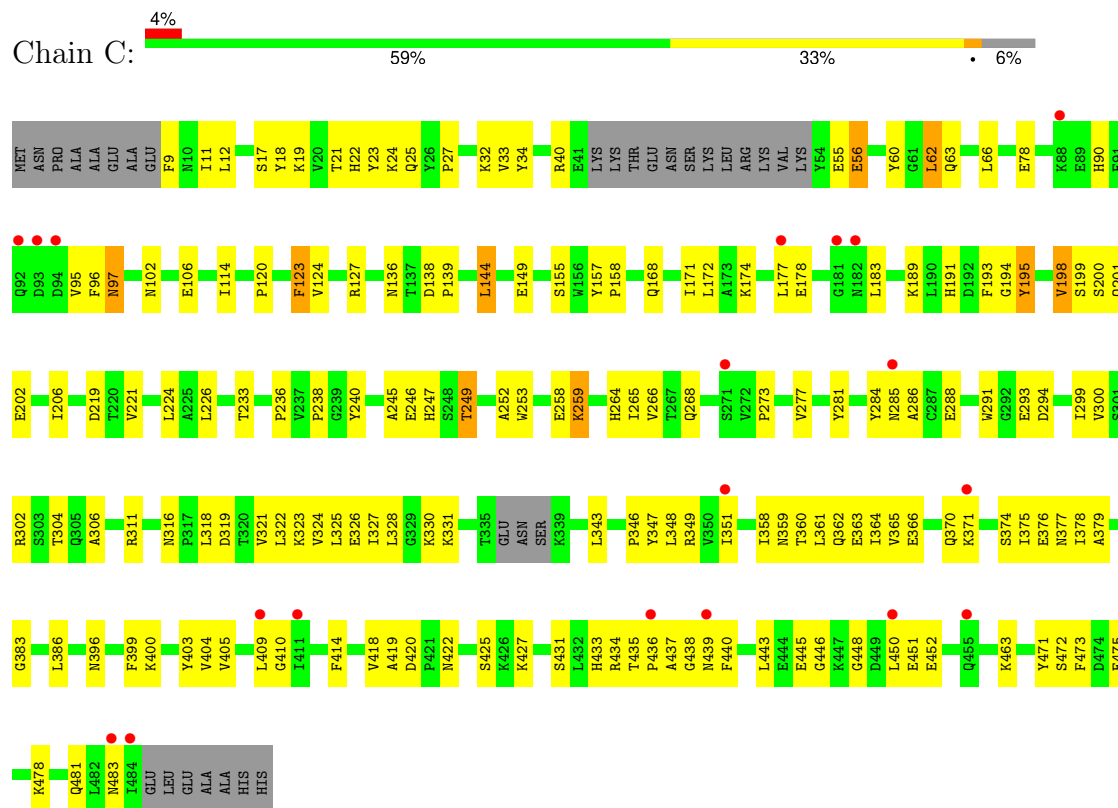
• Molecule 1: Nicotinamide phosphoribosyltransferase



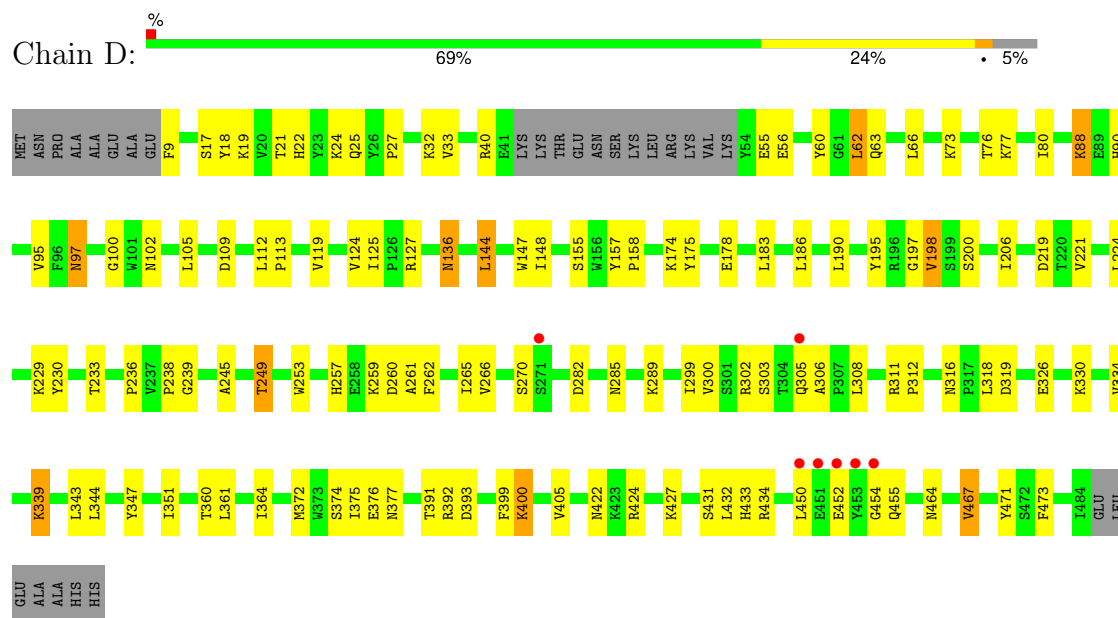
• Molecule 1: Nicotinamide phosphoribosyltransferase



• Molecule 1: Nicotinamide phosphoribosyltransferase

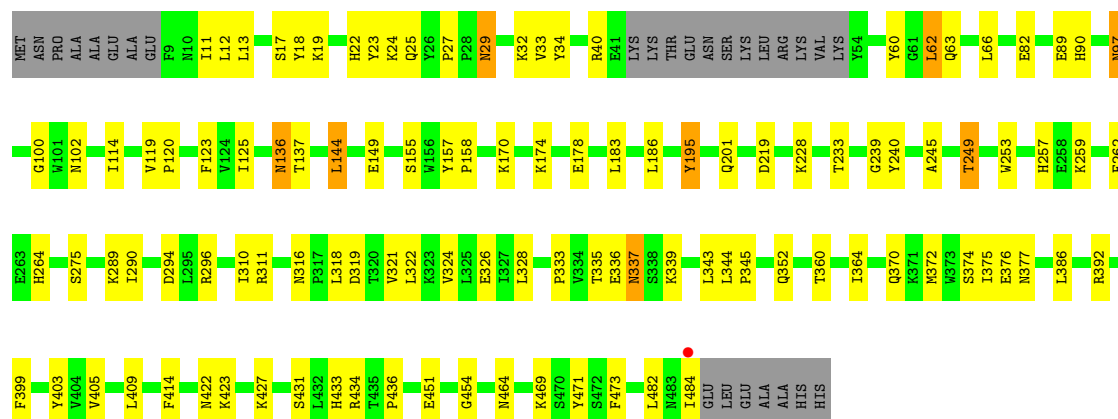


• Molecule 1: Nicotinamide phosphoribosyltransferase

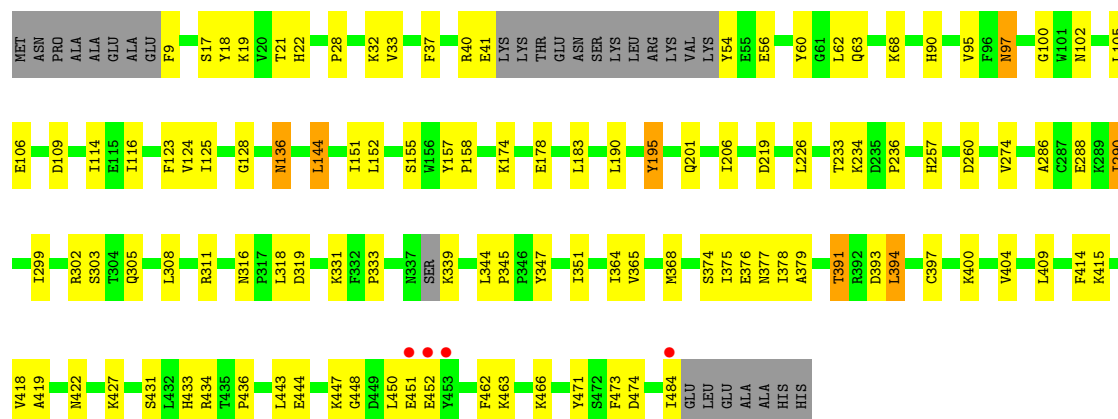


• Molecule 1: Nicotinamide phosphoribosyltransferase





● Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	253.07Å 101.37Å 148.20Å 90.00° 125.48° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 28.91 – 2.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.20) 92.3 (28.91-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.246 0.192 , 0.237	Depositor DCC
R_{free} test set	11237 reflections (7.47%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23801	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 39.91 % 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 2.9568e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NMN, PO4

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	0.32	0/3775	0.57	0/5115
1	B	0.32	0/3799	0.59	0/5149
1	C	0.31	0/3775	0.56	0/5115
1	D	0.37	0/3799	0.63	1/5149 (0.0%)
1	E	0.37	0/3799	0.64	0/5149
1	F	0.39	0/3792	0.64	0/5138
All	All	0.35	0/22739	0.61	1/30815 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	ARG	NE-CZ-NH1	-5.51	117.55	120.30

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	3688	0	3668	149	0
1	B	3711	0	3686	111	0
1	C	3688	0	3668	159	0
1	D	3711	0	3686	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3711	0	3686	98	0
1	F	3705	0	3680	93	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	22	0	12	0	0
3	B	22	0	12	0	0
3	C	22	0	12	1	0
3	D	22	0	12	1	0
3	E	22	0	12	1	0
3	F	22	0	12	1	0
4	A	139	0	0	9	0
4	B	165	0	0	8	0
4	C	125	0	0	10	0
4	D	306	0	0	14	0
4	E	280	0	0	9	0
4	F	380	0	0	14	0
All	All	23801	0	22146	678	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 15.

The worst 5 of 678 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:D:391:THR:HG22	1:D:393:ASP:H	1.19	1.08
1:A:63:GLN:HE22	1:A:471:TYR:H	1.03	0.99
1:D:25:GLN:HE21	1:E:249:THR:HG21	1.31	0.95
1:E:344:LEU:H	1:E:377:ASN:HD21	1.08	0.95
1:B:391:THR:HG23	1:B:393:ASP:H	1.31	0.93

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	455/491 (93%)	424 (93%)	30 (7%)	1 (0%)	47	55
1	B	460/491 (94%)	430 (94%)	29 (6%)	1 (0%)	47	55
1	C	455/491 (93%)	425 (93%)	26 (6%)	4 (1%)	17	16
1	D	460/491 (94%)	444 (96%)	15 (3%)	1 (0%)	47	55
1	E	460/491 (94%)	442 (96%)	16 (4%)	2 (0%)	34	37
1	F	457/491 (93%)	438 (96%)	18 (4%)	1 (0%)	47	55
All	All	2747/2946 (93%)	2603 (95%)	134 (5%)	10 (0%)	34	37

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	483	ASN
1	D	454	GLY
1	F	451	GLU
1	C	56	GLU
1	E	451	GLU

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	405/430 (94%)	389 (96%)	16 (4%)	31	40
1	B	408/430 (95%)	391 (96%)	17 (4%)	30	38
1	C	405/430 (94%)	393 (97%)	12 (3%)	41	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	408/430 (95%)	388 (95%)	20 (5%)	25	31
1	E	408/430 (95%)	390 (96%)	18 (4%)	28	35
1	F	407/430 (95%)	393 (97%)	14 (3%)	37	47
All	All	2441/2580 (95%)	2344 (96%)	97 (4%)	31	40

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	249	THR
1	E	144	LEU
1	D	339	LYS
1	E	18	TYR
1	E	249	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	407	ASN
1	F	257	HIS
1	D	201	GLN
1	F	201	GLN
1	F	464	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 monosaccharides in this entry.

5.6 Ligand geometry

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NMN	A	501	-	21,23,23	4.04	11 (52%)	27,34,34	3.45	12 (44%)
3	NMN	D	504	-	21,23,23	3.95	11 (52%)	27,34,34	3.37	10 (37%)
2	PO4	C	605	-	4,4,4	1.83	2 (50%)	6,6,6	0.45	0
2	PO4	D	607	-	4,4,4	1.84	2 (50%)	6,6,6	0.43	0
2	PO4	D	610	-	4,4,4	1.84	3 (75%)	6,6,6	0.46	0
2	PO4	F	611	-	4,4,4	1.58	0	6,6,6	0.48	0
3	NMN	B	502	-	21,23,23	4.02	11 (52%)	27,34,34	3.37	12 (44%)
2	PO4	B	604	-	4,4,4	1.72	0	6,6,6	0.46	0
2	PO4	F	612	-	4,4,4	1.80	2 (50%)	6,6,6	0.47	0
3	NMN	C	503	-	21,23,23	4.06	11 (52%)	27,34,34	3.32	11 (40%)
3	NMN	F	506	-	21,23,23	3.99	11 (52%)	27,34,34	3.49	12 (44%)
2	PO4	B	603	-	4,4,4	1.73	1 (25%)	6,6,6	0.46	0
2	PO4	E	609	-	4,4,4	1.73	2 (50%)	6,6,6	0.43	0
2	PO4	E	608	-	4,4,4	1.60	0	6,6,6	0.46	0
3	NMN	E	505	-	21,23,23	3.97	11 (52%)	27,34,34	3.40	12 (44%)
2	PO4	A	606	-	4,4,4	1.70	0	6,6,6	0.44	0
2	PO4	C	602	-	4,4,4	1.81	2 (50%)	6,6,6	0.45	0
2	PO4	A	601	-	4,4,4	1.57	0	6,6,6	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NMN	A	501	-	-	7/14/30/30	0/2/2/2
3	NMN	D	504	-	-	6/14/30/30	0/2/2/2
3	NMN	F	506	-	-	3/14/30/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NMN	C	503	-	-	7/14/30/30	0/2/2/2
3	NMN	E	505	-	-	3/14/30/30	0/2/2/2
3	NMN	B	502	-	-	5/14/30/30	0/2/2/2

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NMN	C4-C3	8.63	1.52	1.39
3	B	502	NMN	C4-C3	8.62	1.52	1.39
3	C	503	NMN	C4-C3	8.23	1.51	1.39
3	E	505	NMN	C4-C3	8.23	1.51	1.39
3	C	503	NMN	C2-N1	8.16	1.43	1.35

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	506	NMN	C3-C7-N7	9.10	128.95	117.74
3	F	506	NMN	O7-C7-C3	-8.99	108.61	119.60
3	A	501	NMN	O7-C7-C3	-8.87	108.75	119.60
3	A	501	NMN	C3-C7-N7	8.77	128.54	117.74
3	E	505	NMN	C3-C7-N7	8.76	128.53	117.74

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NMN	C5R-O5R-P-O1P
3	A	501	NMN	C5R-O5R-P-O2P
3	B	502	NMN	C5R-O5R-P-O2P
3	C	503	NMN	C5R-O5R-P-O2P
3	C	503	NMN	C2R-C1R-N1-C2

There are no ring outliers.

7 monomers are involved in 7 short contacts:

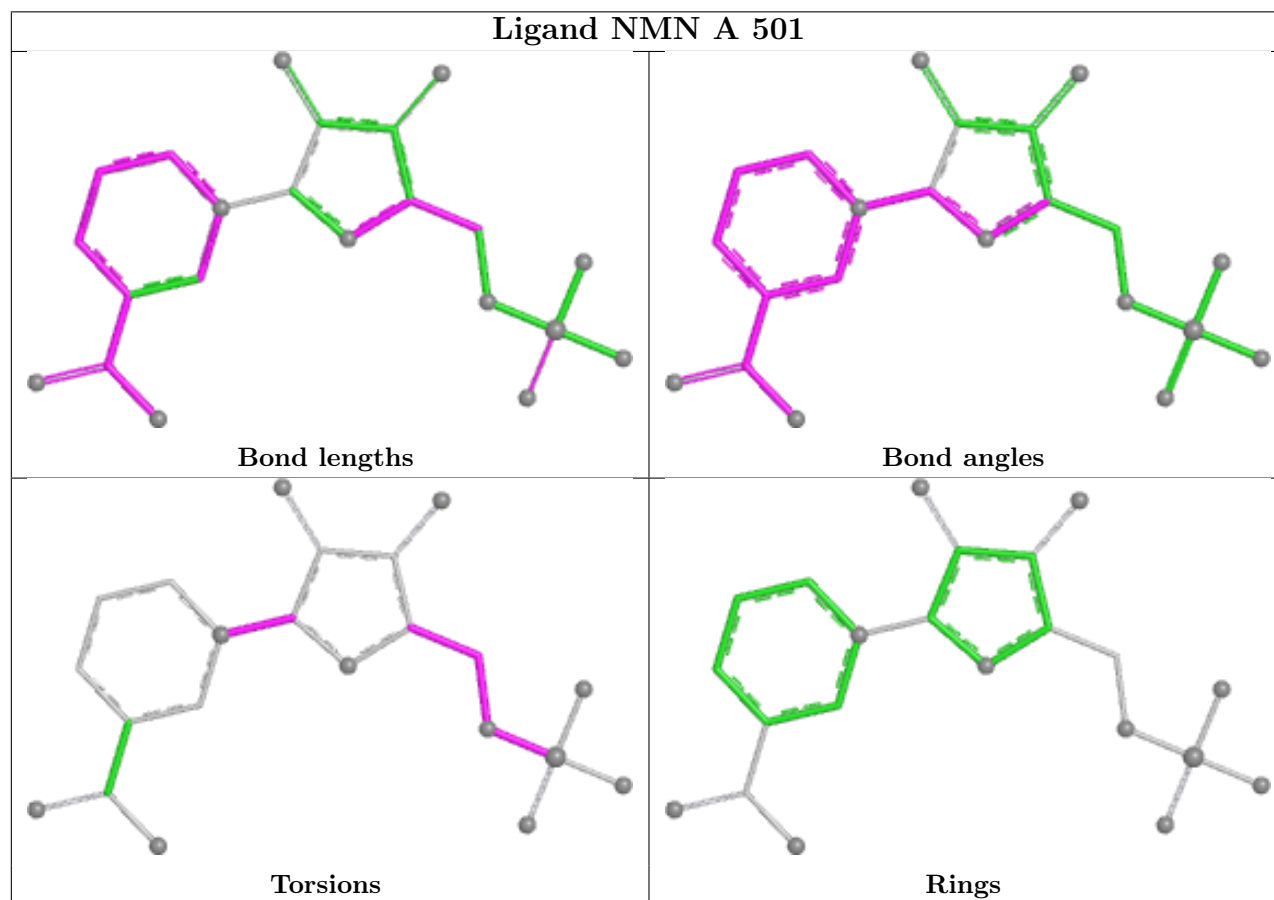
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	504	NMN	1	0
2	C	605	PO4	1	0
2	D	607	PO4	1	0
3	C	503	NMN	1	0

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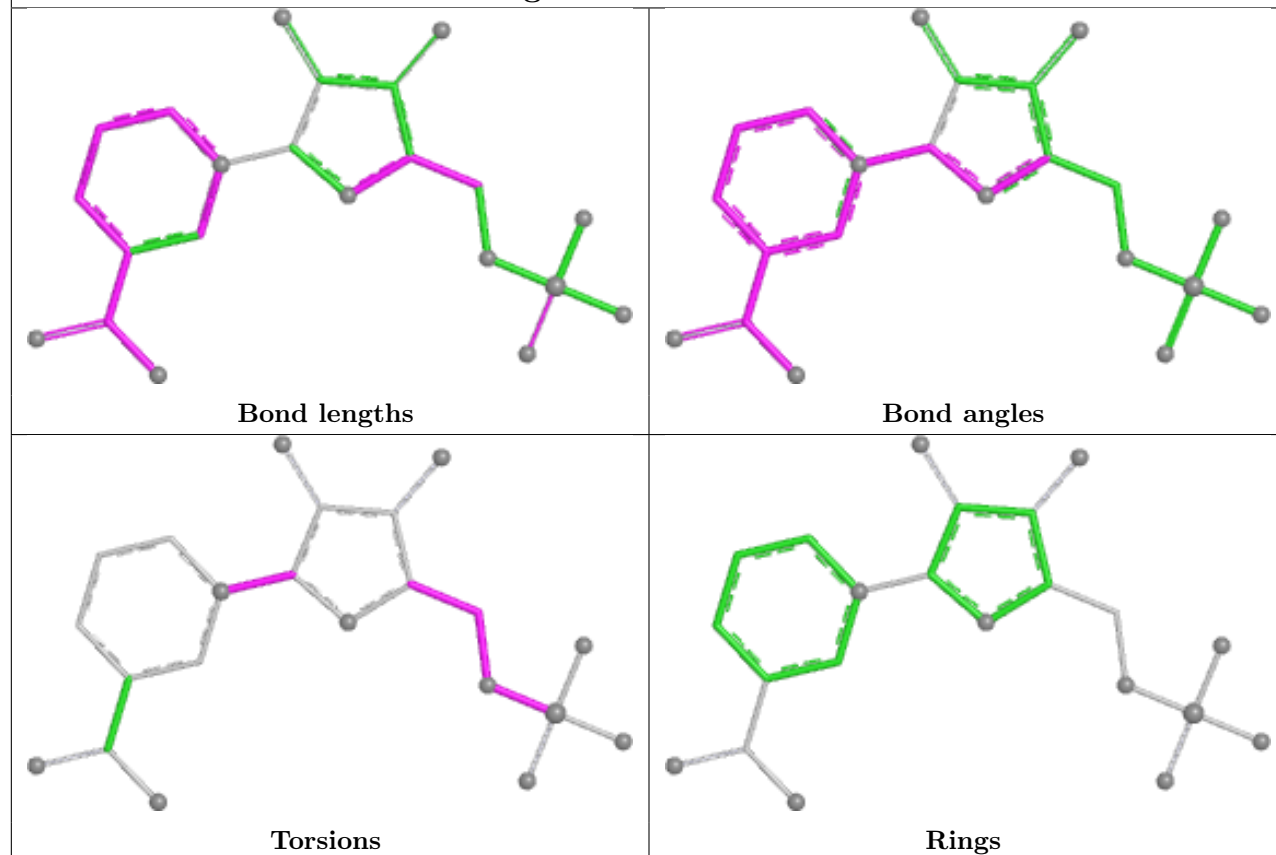
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	506	NMN	1	0
3	E	505	NMN	1	0
2	A	601	PO4	1	0

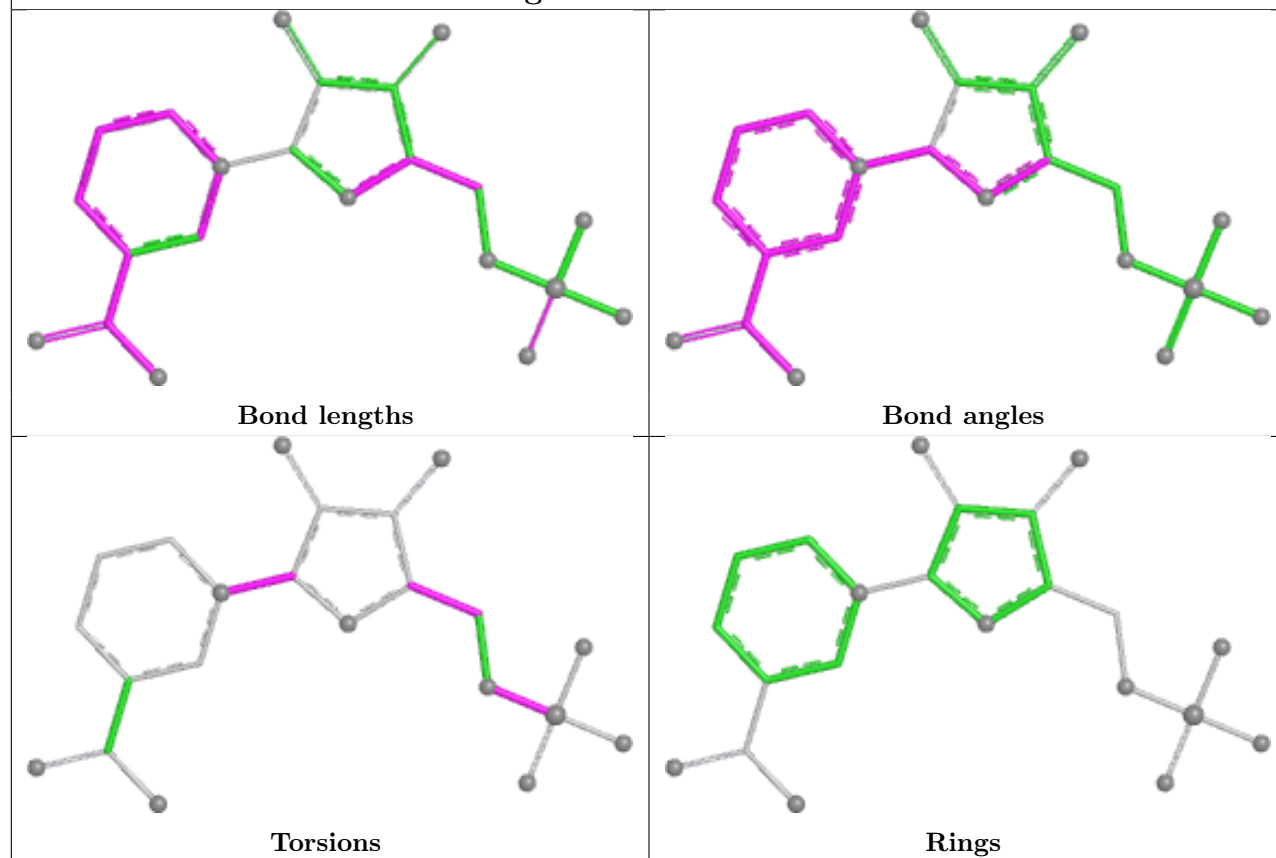
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



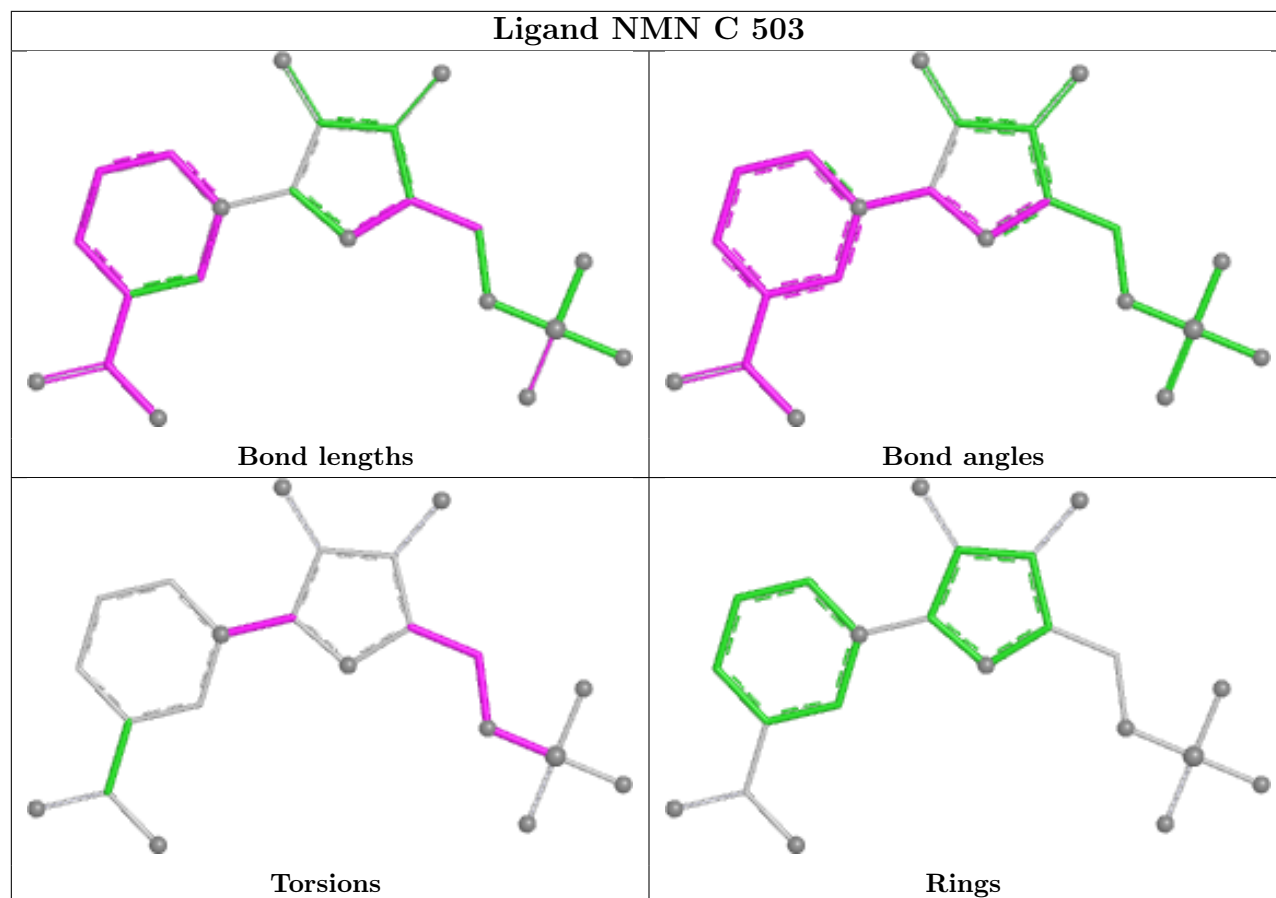
Ligand NMN D 504



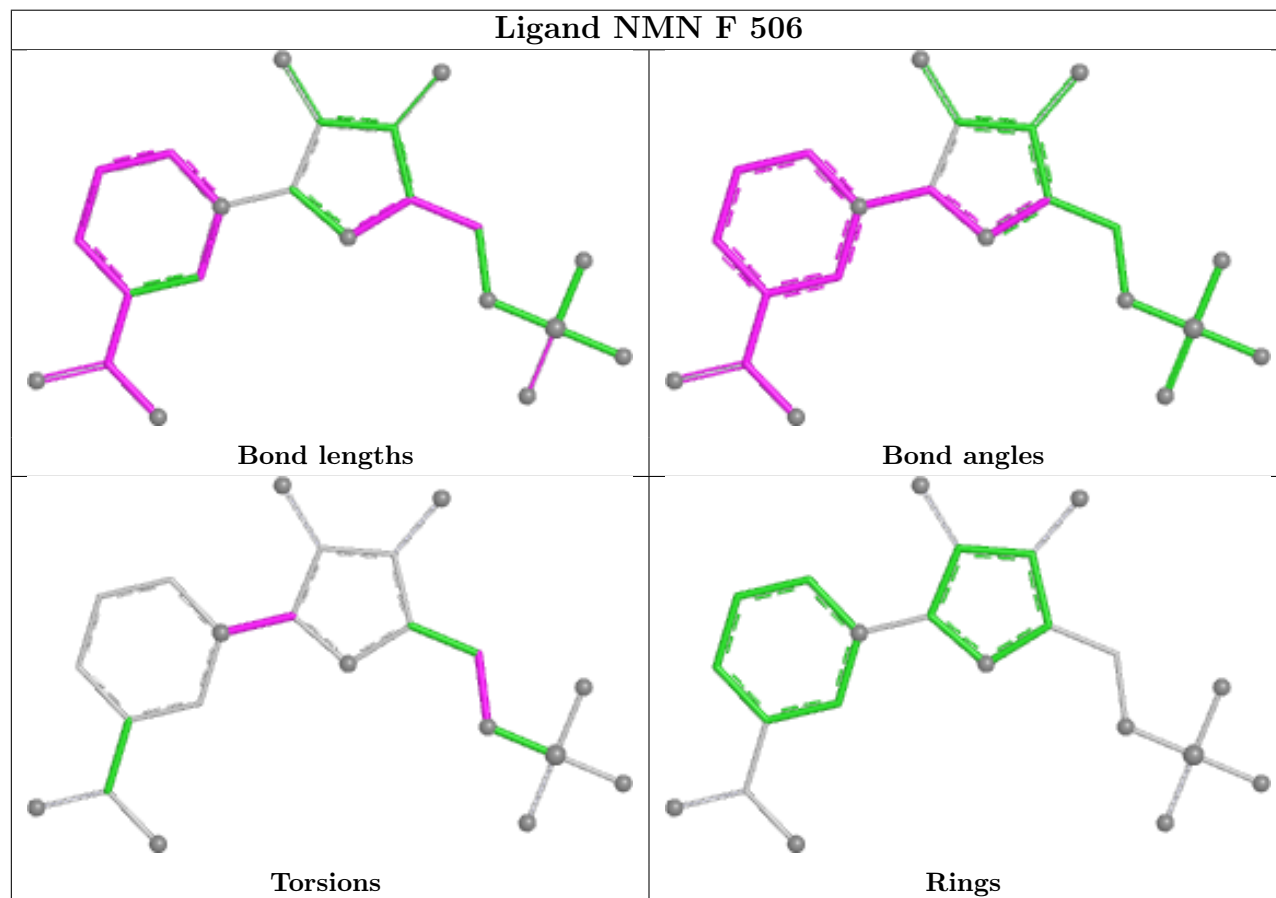
Ligand NMN B 502

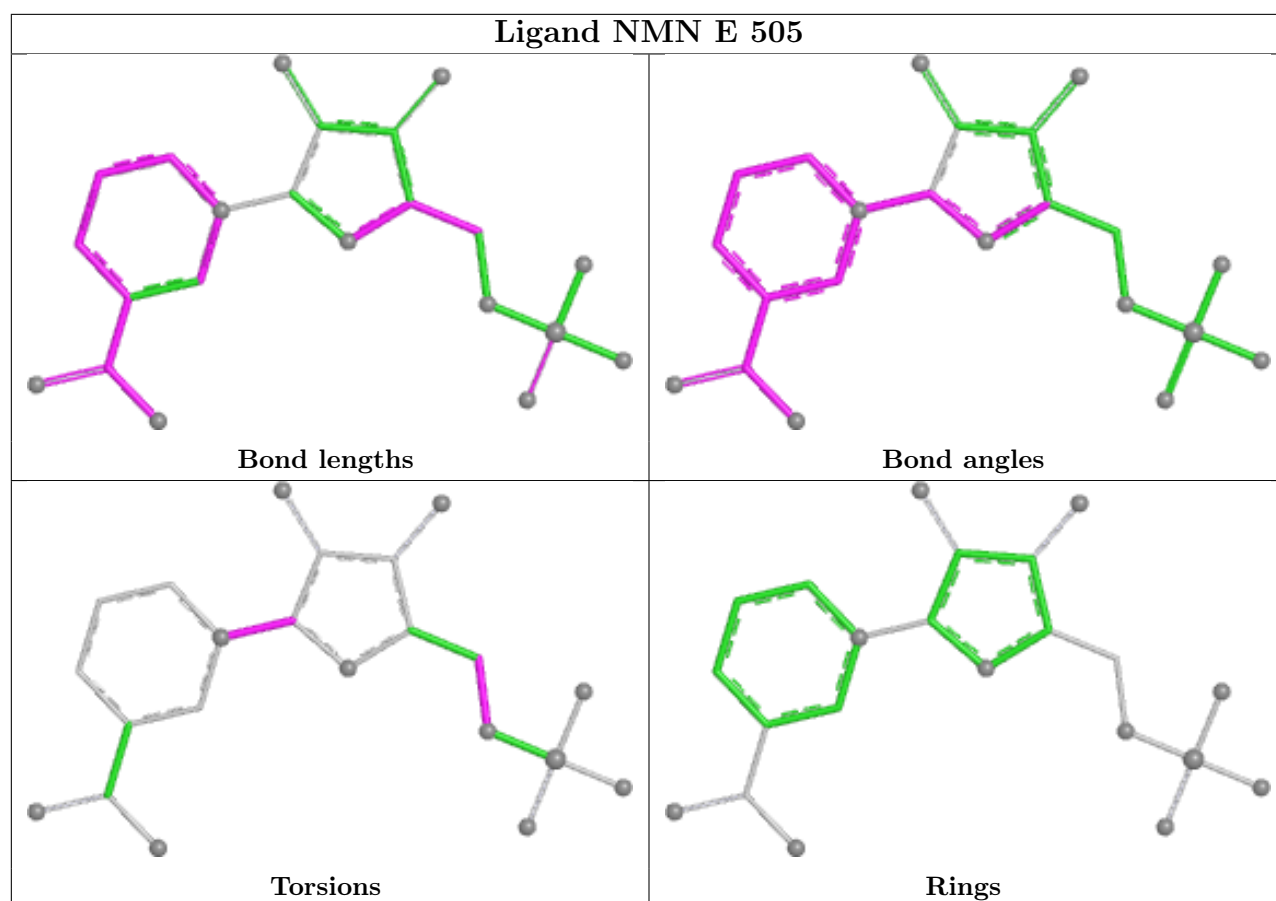


Ligand NMN C 503



Ligand NMN F 506





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	461/491 (93%)	0.13	11 (2%) 59 56	22, 39, 53, 67	0
1	B	464/491 (94%)	-0.04	8 (1%) 70 68	19, 36, 53, 66	0
1	C	461/491 (93%)	0.34	19 (4%) 37 35	21, 42, 67, 81	0
1	D	464/491 (94%)	-0.38	7 (1%) 73 72	14, 23, 38, 69	0
1	E	464/491 (94%)	-0.37	1 (0%) 95 94	14, 24, 38, 57	0
1	F	463/491 (94%)	-0.46	4 (0%) 84 83	11, 20, 36, 64	0
All	All	2777/2946 (94%)	-0.13	50 (1%) 68 66	11, 30, 55, 81	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	484	ILE	7.4
1	A	484	ILE	4.6
1	B	338	SER	4.5
1	A	29	ASN	4.4
1	A	409	LEU	4.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

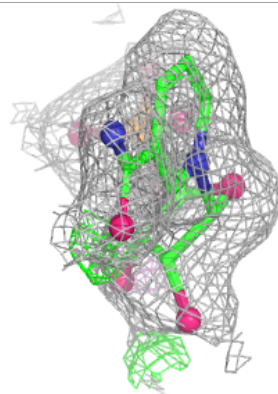
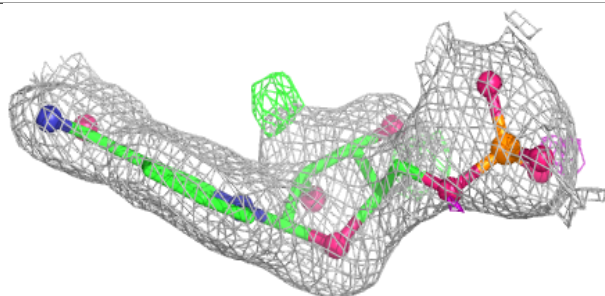
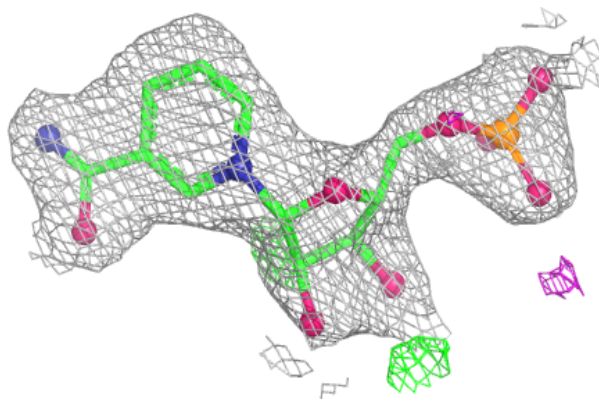
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	PO4	E	608	5/5	0.60	0.53	87,88,89,90	0
3	NMN	A	501	22/22	0.93	0.19	27,37,40,42	0
3	NMN	B	502	22/22	0.93	0.20	26,38,41,47	0
3	NMN	C	503	22/22	0.94	0.18	36,39,41,43	0
3	NMN	D	504	22/22	0.94	0.19	16,26,31,33	0
3	NMN	E	505	22/22	0.94	0.19	17,31,42,46	0
3	NMN	F	506	22/22	0.95	0.17	9,28,34,37	0
2	PO4	A	606	5/5	0.96	0.14	49,51,52,52	0
2	PO4	A	601	5/5	0.96	0.10	31,34,34,35	0
2	PO4	C	602	5/5	0.98	0.17	47,48,49,50	0
2	PO4	D	610	5/5	0.98	0.12	33,34,36,37	0
2	PO4	B	604	5/5	0.98	0.10	36,36,37,37	0
2	PO4	B	603	5/5	0.99	0.15	27,28,30,30	0
2	PO4	C	605	5/5	0.99	0.13	35,36,38,40	0
2	PO4	E	609	5/5	0.99	0.10	22,22,23,24	0
2	PO4	F	612	5/5	0.99	0.08	27,27,29,30	0
2	PO4	D	607	5/5	0.99	0.11	15,15,17,19	0
2	PO4	F	611	5/5	1.00	0.08	16,17,19,20	0

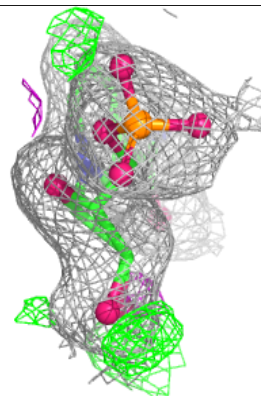
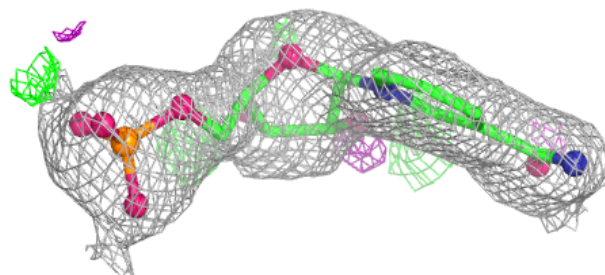
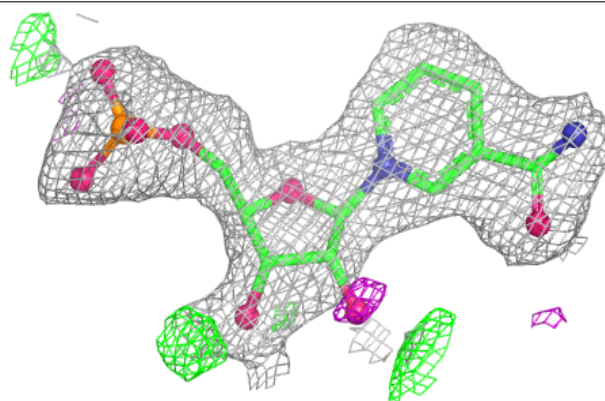
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NMN A 501:

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

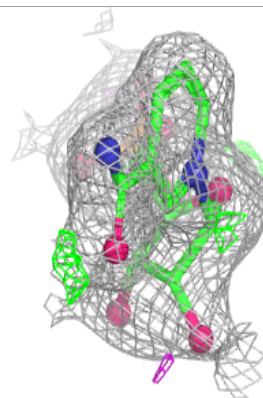
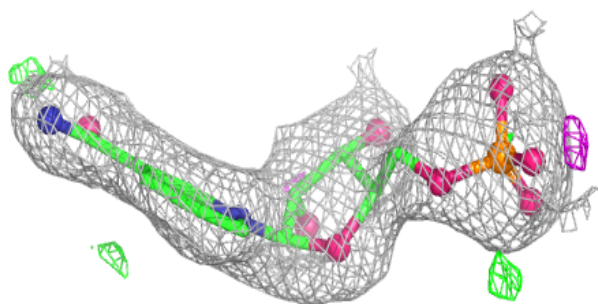
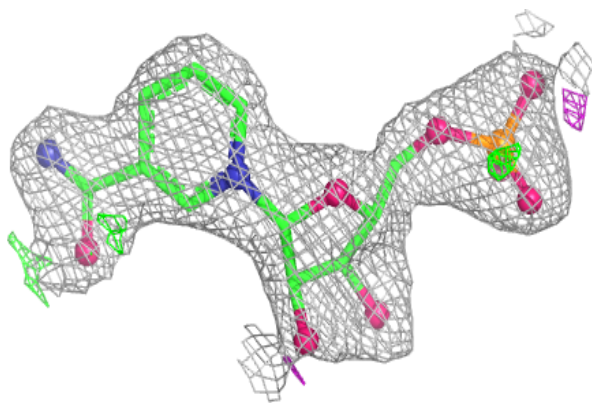
**Electron density around NMN B 502:**

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

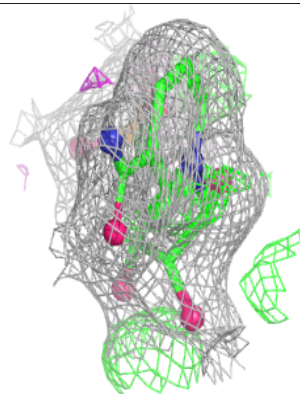
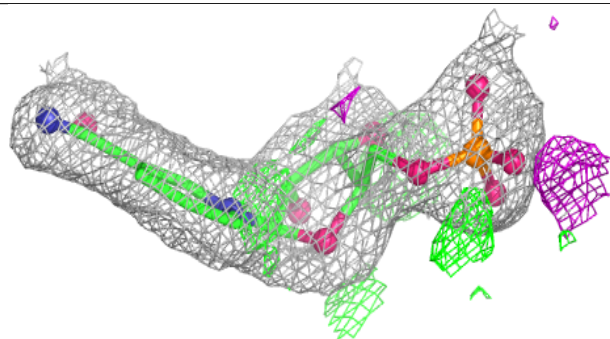
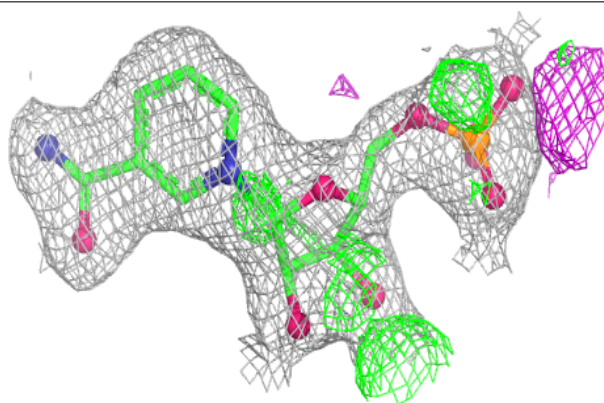


Electron density around NMN C 503:

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

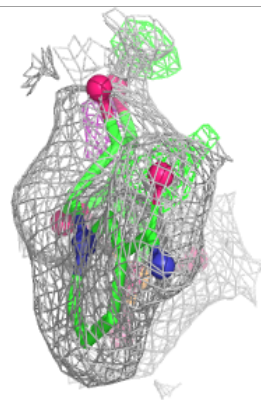
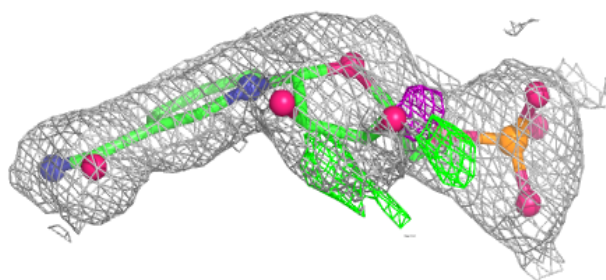
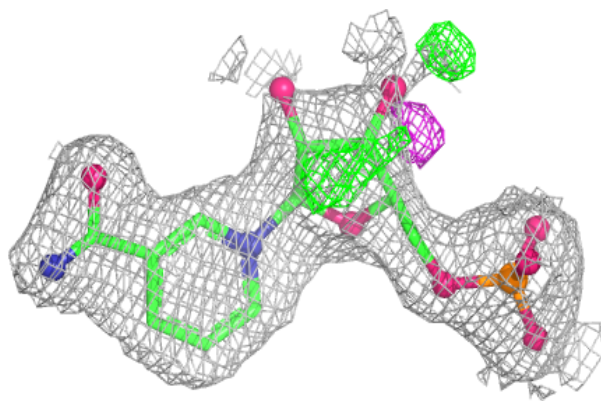
**Electron density around NMN D 504:**

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

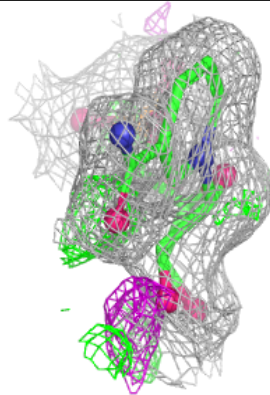
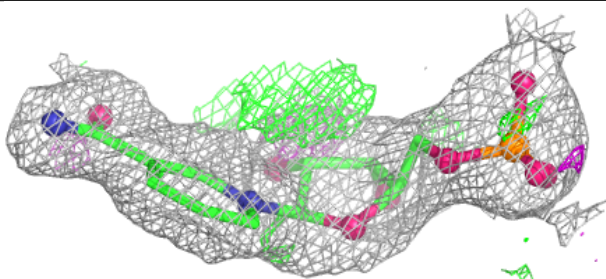
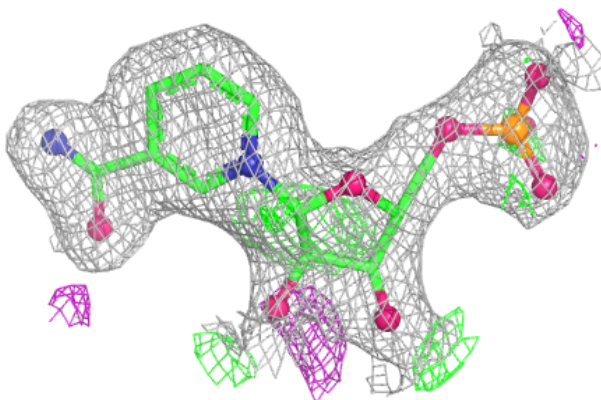


Electron density around NMN E 505:

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

**Electron density around NMN F 506:**

$2mF_o-DF_c$ (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.