wwPDB X-ray Structure Validation Summary Report (i)

Oct 28, 2024 – 12:31 pm GMT

PDB ID	:	6ZTH
Title	:	Phospholipase PlaB from Legionella pneumophila
Authors	:	Diwo, M.G.; Flieger, A.; Blankenfeldt, W.
Deposited on	:	2020-07-20
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

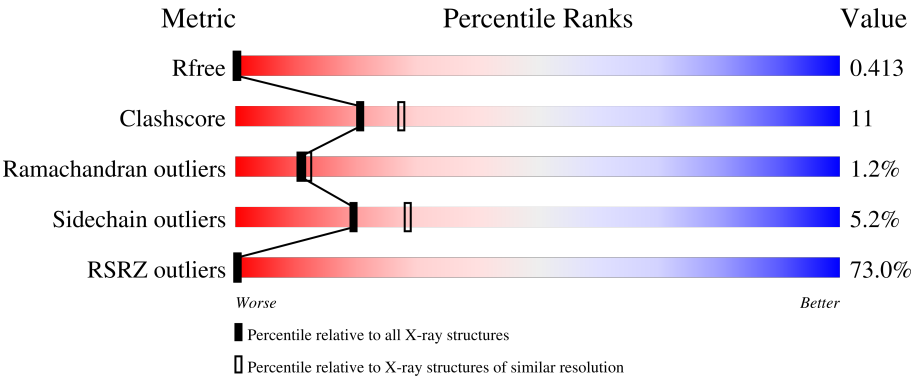
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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 <=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	489	66% 72% 23%
1	B	489	67% 72% 22%
1	C	489	69% 73% 20%
1	D	489	72% 71% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 30812 atoms, of which 14970 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 PlaB phospholipase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	470	Total	C	H	N	O	S	Se	0	7	0
			7444	2372	3694	661	699	5	13			
1	B	470	Total	C	H	N	O	S	Se	0	1	0
			7417	2360	3683	661	695	5	13			
1	C	467	Total	C	H	N	O	S	Se	0	2	0
			7417	2358	3697	657	687	5	13			
1	D	474	Total	C	H	N	O	S	Se	1	0	0
			7431	2369	3688	658	698	5	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MSE	-	initiating methionine	UNP A0A378K488
A	-13	ALA	-	expression tag	UNP A0A378K488
A	-12	SER	-	expression tag	UNP A0A378K488
A	-11	TRP	-	expression tag	UNP A0A378K488
A	-10	SER	-	expression tag	UNP A0A378K488
A	-9	HIS	-	expression tag	UNP A0A378K488
A	-8	PRO	-	expression tag	UNP A0A378K488
A	-7	GLN	-	expression tag	UNP A0A378K488
A	-6	PHE	-	expression tag	UNP A0A378K488
A	-5	GLU	-	expression tag	UNP A0A378K488
A	-4	LYS	-	expression tag	UNP A0A378K488
A	-3	GLY	-	expression tag	UNP A0A378K488
A	-2	ALA	-	expression tag	UNP A0A378K488
A	-1	GLY	-	expression tag	UNP A0A378K488
A	0	THR	-	expression tag	UNP A0A378K488
A	203	ASN	ASP	conflict	UNP A0A378K488
B	-14	MSE	-	initiating methionine	UNP A0A378K488
B	-13	ALA	-	expression tag	UNP A0A378K488
B	-12	SER	-	expression tag	UNP A0A378K488
B	-11	TRP	-	expression tag	UNP A0A378K488
B	-10	SER	-	expression tag	UNP A0A378K488

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP A0A378K488
B	-8	PRO	-	expression tag	UNP A0A378K488
B	-7	GLN	-	expression tag	UNP A0A378K488
B	-6	PHE	-	expression tag	UNP A0A378K488
B	-5	GLU	-	expression tag	UNP A0A378K488
B	-4	LYS	-	expression tag	UNP A0A378K488
B	-3	GLY	-	expression tag	UNP A0A378K488
B	-2	ALA	-	expression tag	UNP A0A378K488
B	-1	GLY	-	expression tag	UNP A0A378K488
B	0	THR	-	expression tag	UNP A0A378K488
B	203	ASN	ASP	conflict	UNP A0A378K488
C	-14	MSE	-	initiating methionine	UNP A0A378K488
C	-13	ALA	-	expression tag	UNP A0A378K488
C	-12	SER	-	expression tag	UNP A0A378K488
C	-11	TRP	-	expression tag	UNP A0A378K488
C	-10	SER	-	expression tag	UNP A0A378K488
C	-9	HIS	-	expression tag	UNP A0A378K488
C	-8	PRO	-	expression tag	UNP A0A378K488
C	-7	GLN	-	expression tag	UNP A0A378K488
C	-6	PHE	-	expression tag	UNP A0A378K488
C	-5	GLU	-	expression tag	UNP A0A378K488
C	-4	LYS	-	expression tag	UNP A0A378K488
C	-3	GLY	-	expression tag	UNP A0A378K488
C	-2	ALA	-	expression tag	UNP A0A378K488
C	-1	GLY	-	expression tag	UNP A0A378K488
C	0	THR	-	expression tag	UNP A0A378K488
C	203	ASN	ASP	conflict	UNP A0A378K488
D	-14	MSE	-	initiating methionine	UNP A0A378K488
D	-13	ALA	-	expression tag	UNP A0A378K488
D	-12	SER	-	expression tag	UNP A0A378K488
D	-11	TRP	-	expression tag	UNP A0A378K488
D	-10	SER	-	expression tag	UNP A0A378K488
D	-9	HIS	-	expression tag	UNP A0A378K488
D	-8	PRO	-	expression tag	UNP A0A378K488
D	-7	GLN	-	expression tag	UNP A0A378K488
D	-6	PHE	-	expression tag	UNP A0A378K488
D	-5	GLU	-	expression tag	UNP A0A378K488
D	-4	LYS	-	expression tag	UNP A0A378K488
D	-3	GLY	-	expression tag	UNP A0A378K488
D	-2	ALA	-	expression tag	UNP A0A378K488
D	-1	GLY	-	expression tag	UNP A0A378K488
D	0	THR	-	expression tag	UNP A0A378K488

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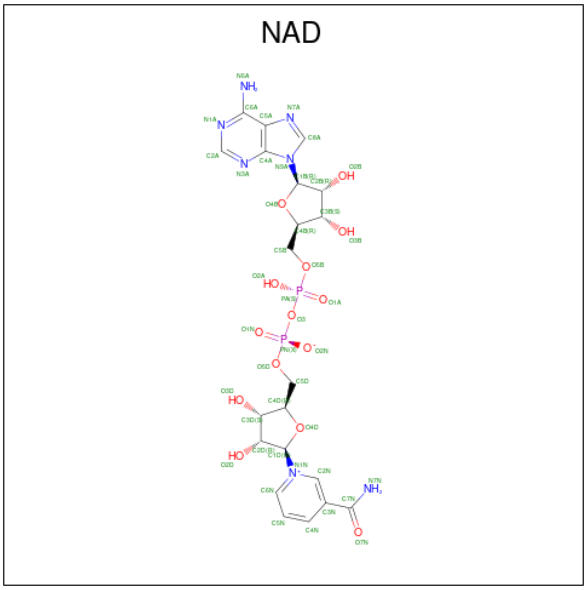
Chain	Residue	Modelled	Actual	Comment	Reference
D	203	ASN	ASP	conflict	UNP A0A378K488

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
2	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is water.

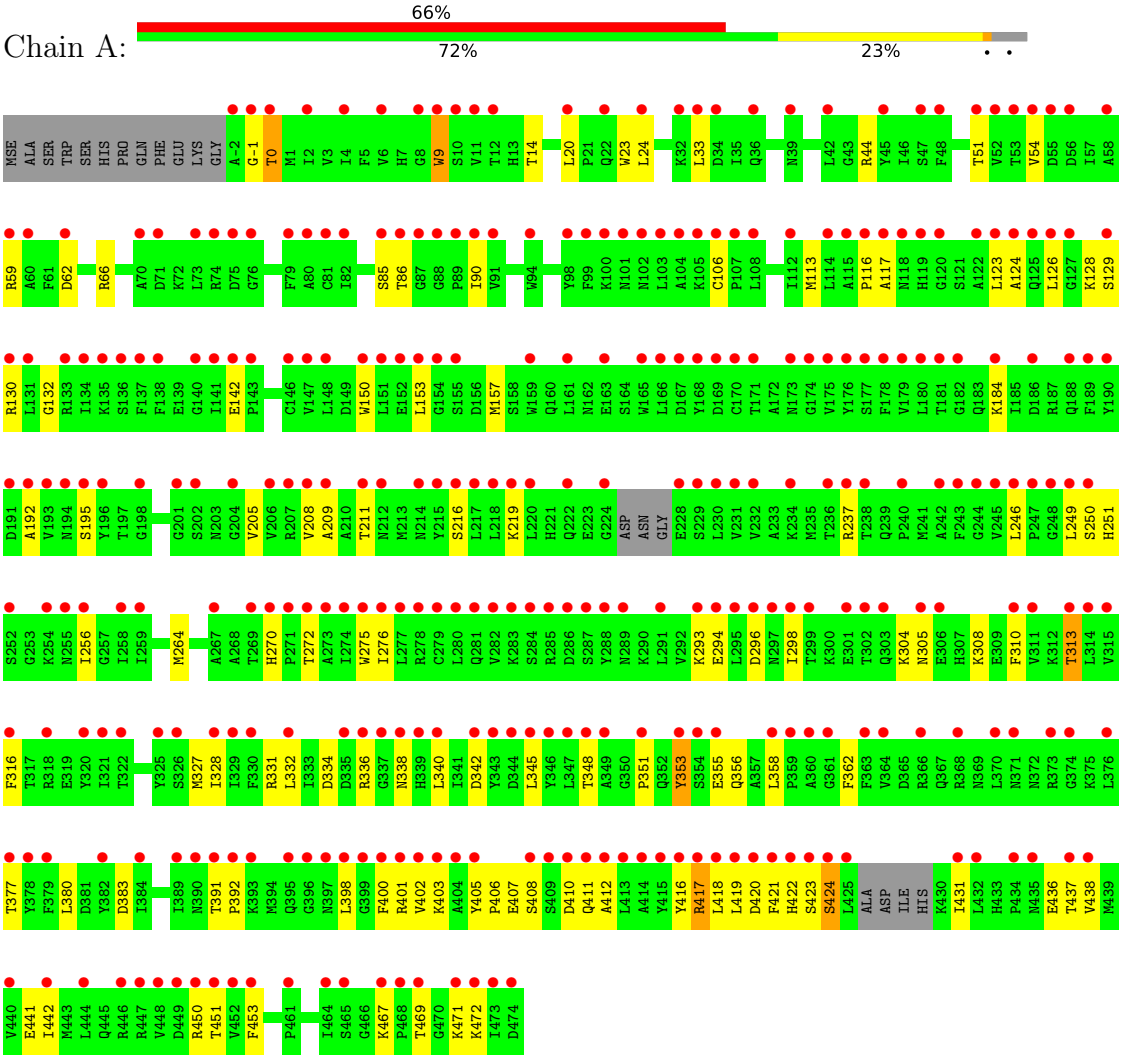
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	131	Total O 131 131	0	0
3	B	125	Total O 125 125	0	0
3	C	148	Total O 148 148	0	0
3	D	139	Total O 139 139	0	0

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.

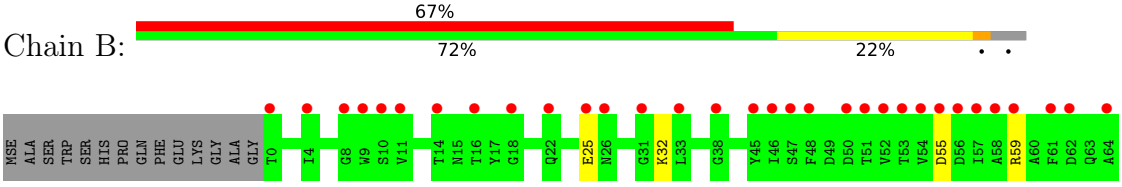
• Molecule 1: PlaB phospholipase

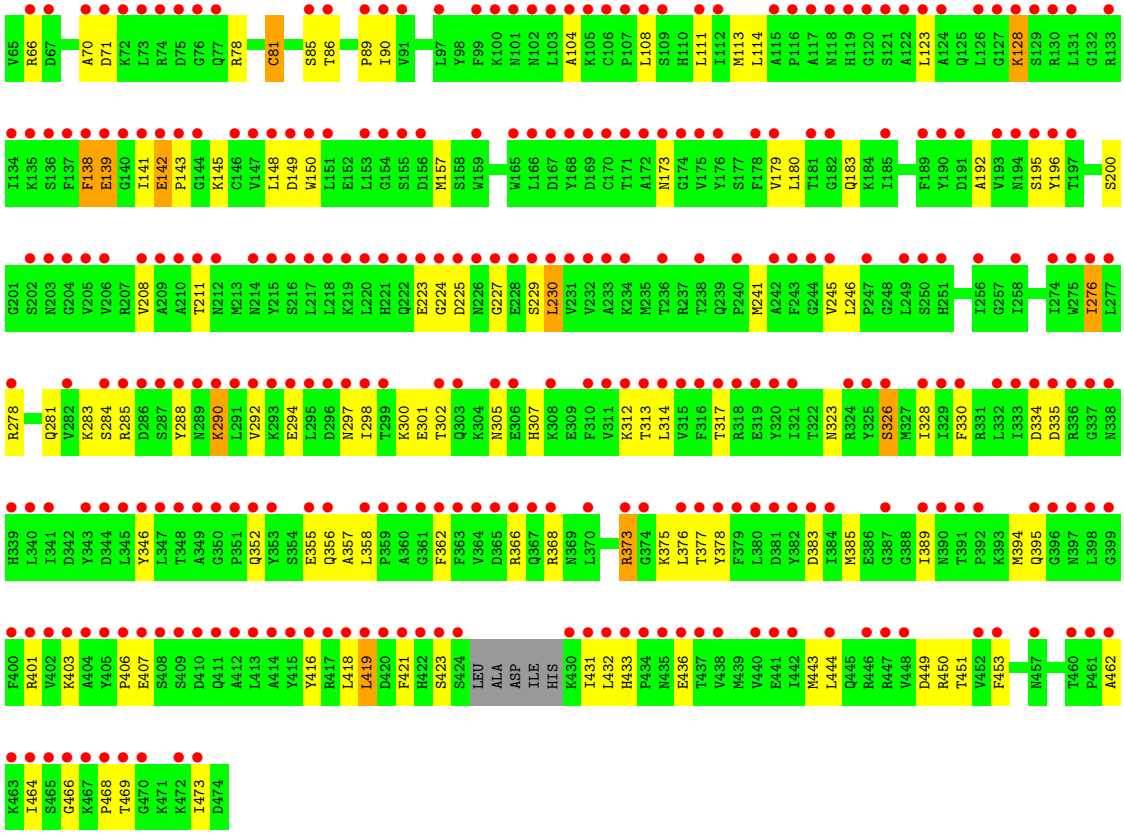
Chain A:



• Molecule 1: PlaB phospholipase

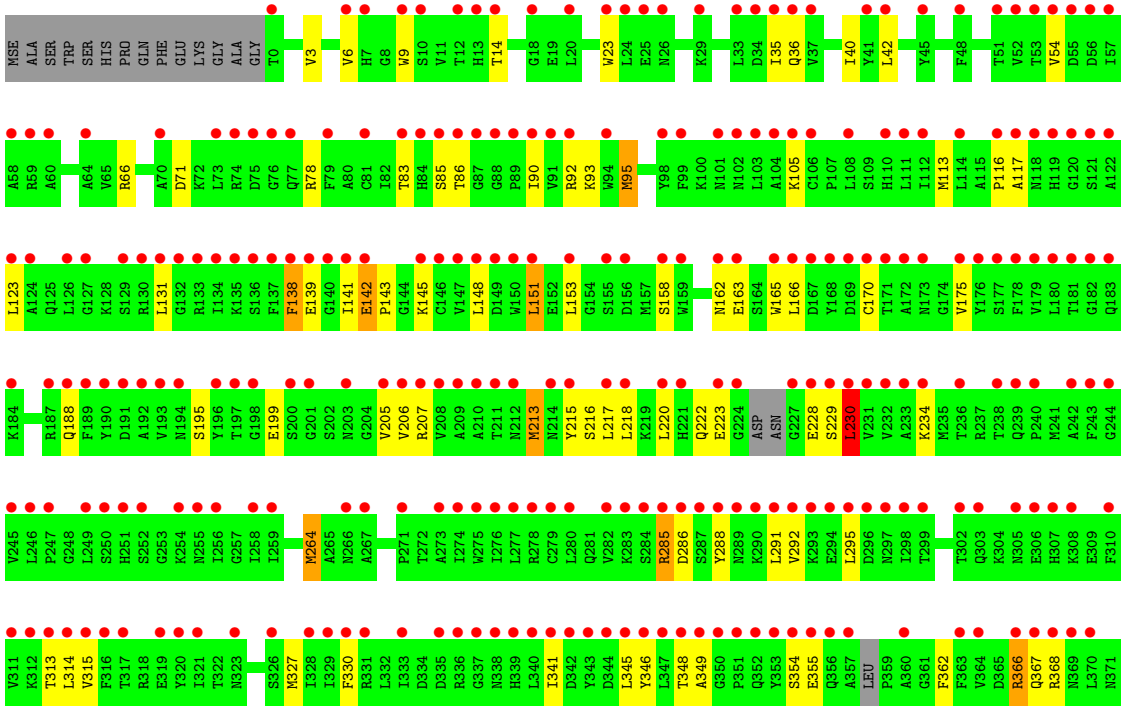
Chain B:

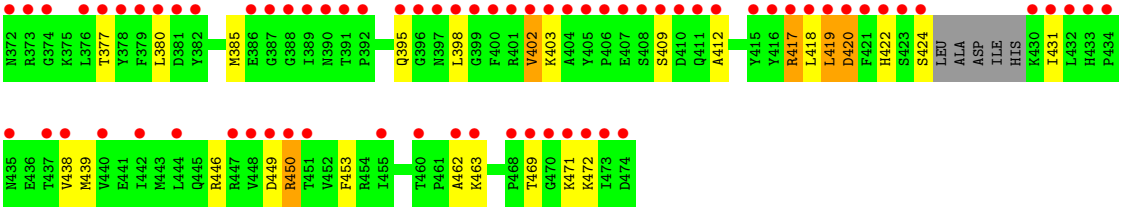




• Molecule 1: PlaB phospholipase

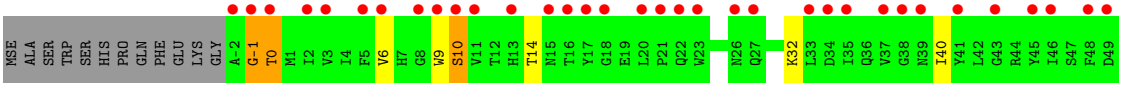
Chain C:

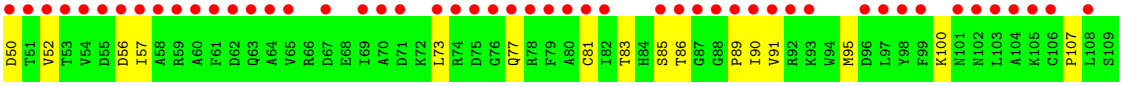


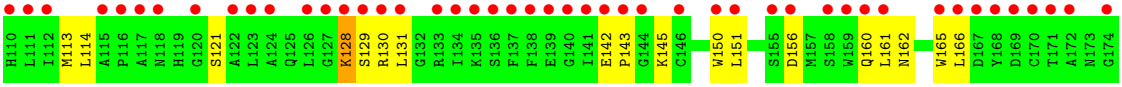


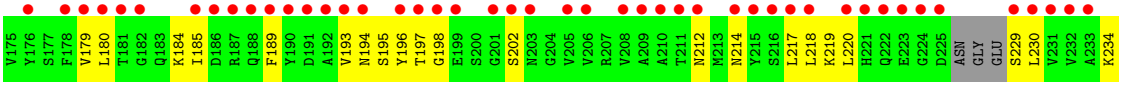
• Molecule 1: PlaB phospholipase

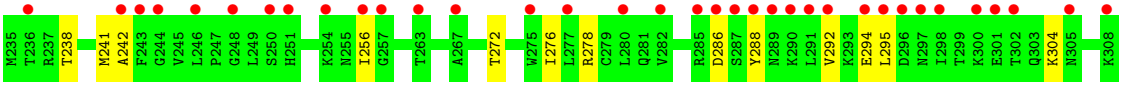
Chain D:

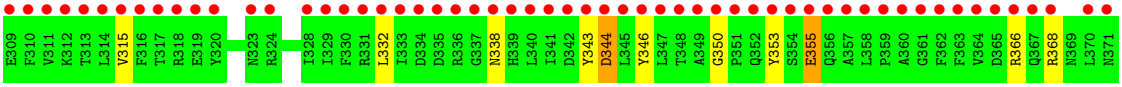


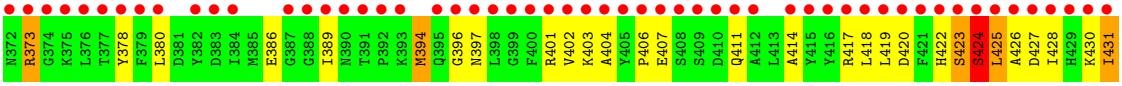


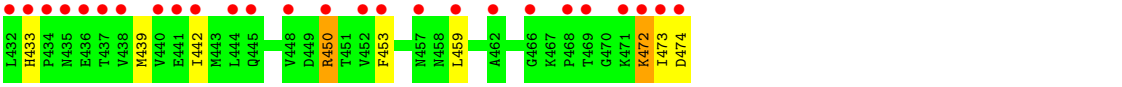












4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.81Å 170.58Å 93.48Å 90.00° 92.86° 90.00°	Depositor
Resolution (Å)	49.24 – 2.30 49.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.24-2.30) 99.7 (49.24-2.30)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.29Å)	Xtriage
Refinement program	PHENIX dev_3922	Depositor
R, R_{free}	0.364 , 0.413 0.363 , 0.413	Depositor DCC
R_{free} test set	5259 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	30812	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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 40.38 % 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 2.7605e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.27	0/3858	0.47	0/5192
1	B	0.25	0/3800	0.47	0/5115
1	C	0.26	0/3788	0.45	0/5094
1	D	0.49	2/3807 (0.1%)	0.47	1/5130 (0.0%)
All	All	0.33	2/15253 (0.0%)	0.47	1/20531 (0.0%)

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
1	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	424	SER	CB-OG	-23.99	1.11	1.42
1	D	431	ILE	CG1-CD1	-8.62	0.91	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	431	ILE	CB-CG1-CD1	6.52	132.16	113.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	423	SER	Peptide
1	C	230	LEU	Peptide
1	D	424	SER	Peptide

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	3750	3694	3662	79	0
1	B	3734	3683	3700	77	0
1	C	3720	3697	3701	75	0
1	D	3743	3688	3689	106	0
2	A	88	52	51	6	0
2	B	88	52	49	1	0
2	C	88	52	50	4	0
2	D	88	52	52	12	0
3	A	131	0	0	15	0
3	B	125	0	0	11	1
3	C	148	0	0	7	0
3	D	139	0	0	11	1
All	All	15842	14970	14954	333	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 333 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:431:ILE:CD1	1:D:431:ILE:CB	2.24	1.14
1:D:431:ILE:CG1	1:D:431:ILE:HD11	1.53	1.05
1:D:431:ILE:CG1	1:D:431:ILE:HD12	1.53	1.02
1:D:431:ILE:CG1	1:D:431:ILE:HD13	1.53	1.02
1:D:431:ILE:CD1	1:D:431:ILE:HG13	1.48	0.99

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:790:HOH:O	3:D:652:HOH:O[1_655]	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	471/489 (96%)	445 (94%)	22 (5%)	4 (1%)	16	20
1	B	467/489 (96%)	434 (93%)	27 (6%)	6 (1%)	10	11
1	C	461/489 (94%)	437 (95%)	18 (4%)	6 (1%)	10	11
1	D	470/489 (96%)	439 (93%)	25 (5%)	6 (1%)	10	11
All	All	1869/1956 (96%)	1755 (94%)	92 (5%)	22 (1%)	11	12

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	THR
1	A	412	ALA
1	B	139	GLU
1	B	229	SER
1	C	138	PHE

5.3.2 Protein sidechains (i)

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	407/408 (100%)	385 (95%)	22 (5%)	18	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	403/408 (99%)	385 (96%)	18 (4%)	23 34
1	C	402/408 (98%)	374 (93%)	28 (7%)	12 17
1	D	401/408 (98%)	382 (95%)	19 (5%)	22 32
All	All	1613/1632 (99%)	1526 (95%)	87 (5%)	19 27

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	367	GLN
1	D	81	CYS
1	C	417	ARG
1	C	463[A]	LYS
1	D	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	270	HIS
1	A	356	GLN
1	B	281	GLN
1	C	305	ASN

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 (i)

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	501	-	42,48,48	4.73	19 (45%)	50,73,73	1.77	6 (12%)
2	NAD	A	501	-	42,48,48	4.72	19 (45%)	50,73,73	1.81	10 (20%)
2	NAD	D	501	-	42,48,48	4.70	19 (45%)	50,73,73	1.76	7 (14%)
2	NAD	B	601	-	42,48,48	4.85	19 (45%)	50,73,73	1.76	10 (20%)
2	NAD	C	502	-	42,48,48	5.04	19 (45%)	50,73,73	1.82	9 (18%)
2	NAD	D	502	-	42,48,48	4.71	19 (45%)	50,73,73	1.82	11 (22%)
2	NAD	A	502	-	42,48,48	5.05	19 (45%)	50,73,73	1.80	10 (20%)
2	NAD	B	602	-	42,48,48	4.83	19 (45%)	50,73,73	1.75	9 (18%)

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	501	-	-	3/26/62/62	0/5/5/5
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
2	NAD	D	501	-	-	2/26/62/62	0/5/5/5
2	NAD	B	601	-	-	4/26/62/62	0/5/5/5
2	NAD	C	502	-	-	6/26/62/62	0/5/5/5
2	NAD	D	502	-	-	3/26/62/62	0/5/5/5
2	NAD	A	502	-	-	4/26/62/62	0/5/5/5
2	NAD	B	602	-	-	2/26/62/62	0/5/5/5

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAD	C2B-C1B	-18.51	1.25	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	NAD	C2B-C1B	-18.32	1.26	1.53
2	B	601	NAD	C2B-C1B	-17.30	1.27	1.53
2	B	602	NAD	C2B-C1B	-17.15	1.27	1.53
2	C	501	NAD	C2B-C1B	-16.37	1.28	1.53

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	502	NAD	C5A-C6A-N6A	7.17	131.25	120.35
2	C	502	NAD	C5A-C6A-N6A	7.16	131.23	120.35
2	D	501	NAD	C5A-C6A-N6A	7.13	131.19	120.35
2	C	501	NAD	C5A-C6A-N6A	7.05	131.07	120.35
2	A	501	NAD	C5A-C6A-N6A	6.78	130.66	120.35

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	PN-O3-PA-O5B
2	A	502	NAD	C5D-O5D-PN-O1N
2	A	502	NAD	O4D-C1D-N1N-C6N
2	B	601	NAD	C5D-O5D-PN-O3
2	B	601	NAD	C5D-O5D-PN-O1N

There are no ring outliers.

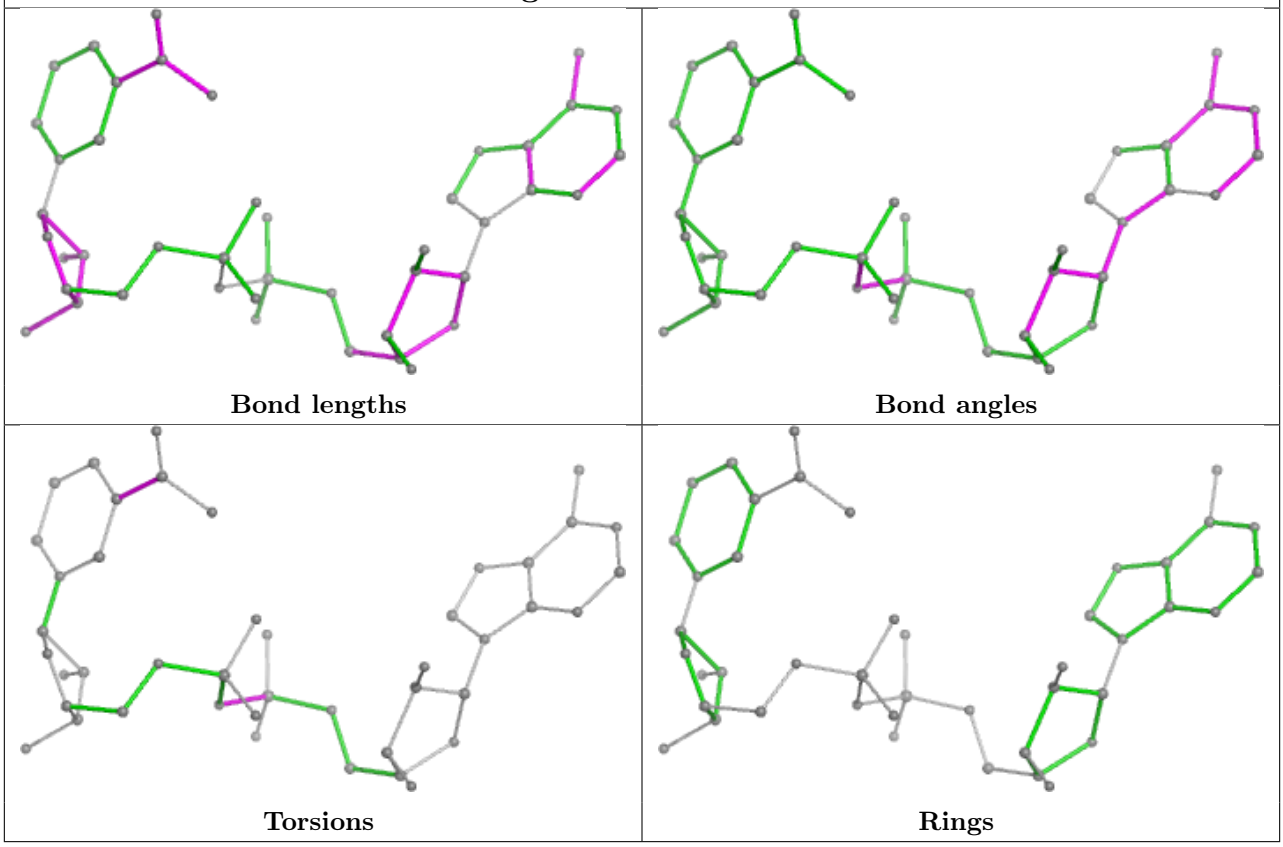
7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAD	3	0
2	A	501	NAD	3	0
2	D	501	NAD	6	0
2	C	502	NAD	1	0
2	D	502	NAD	7	0
2	A	502	NAD	3	0
2	B	602	NAD	1	0

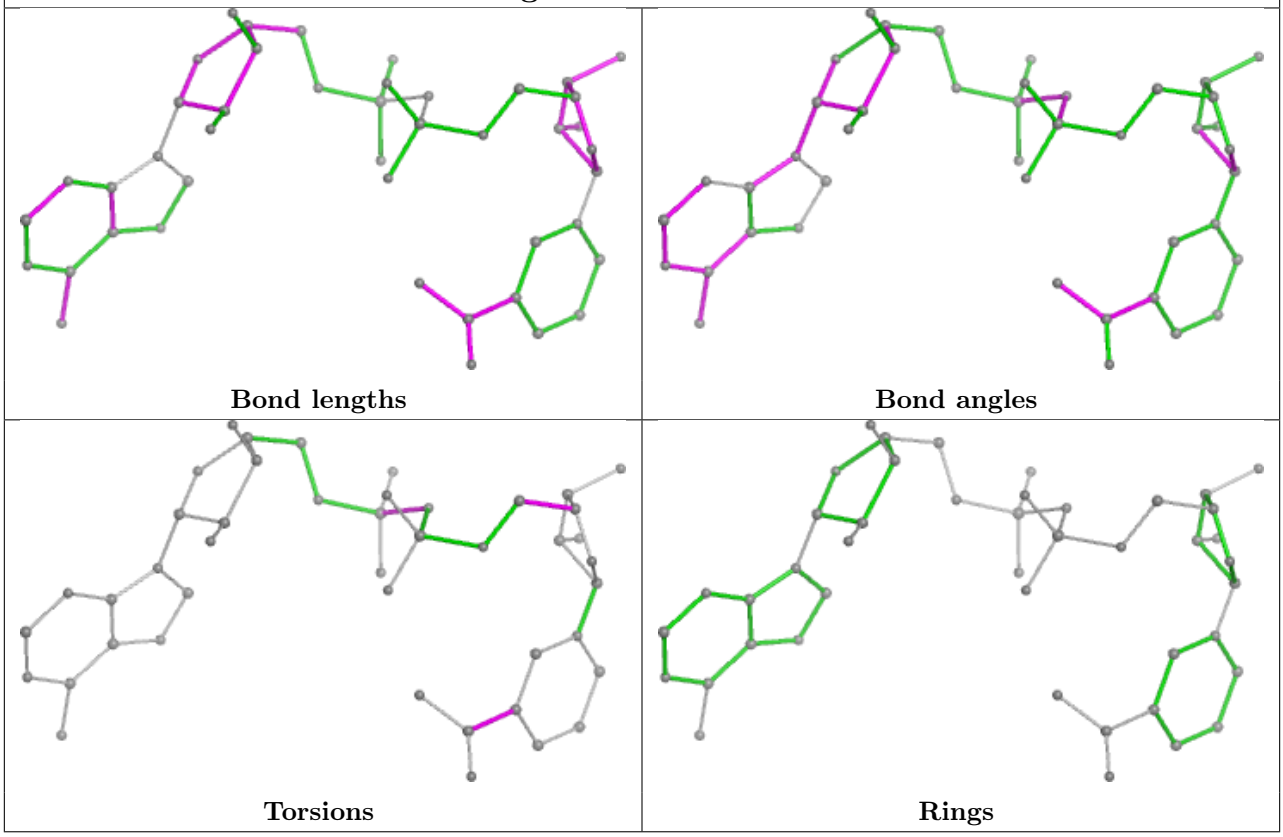
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

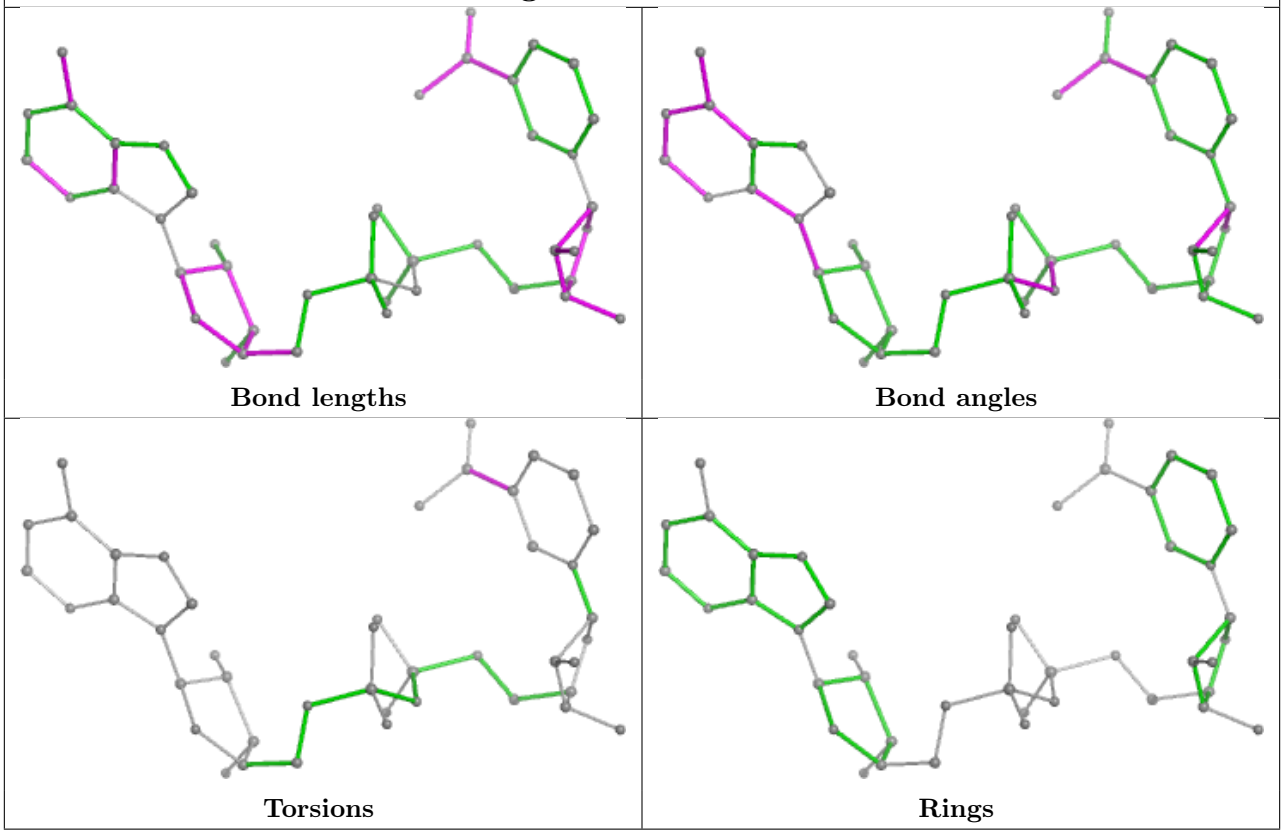
Ligand NAD C 501



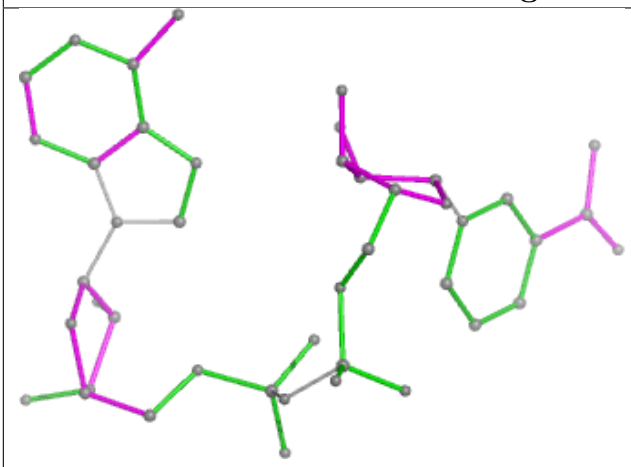
Ligand NAD A 501



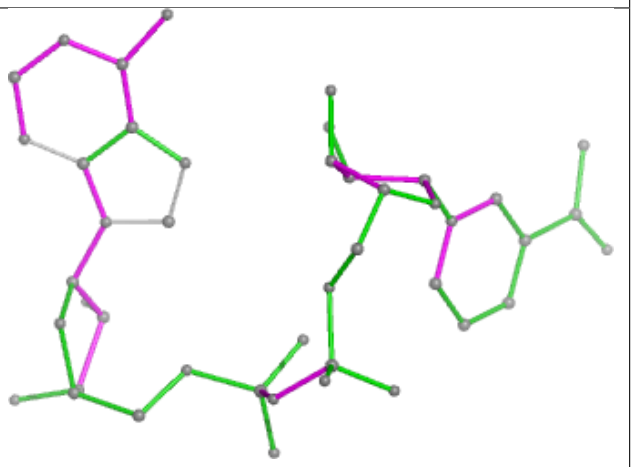
Ligand NAD D 501



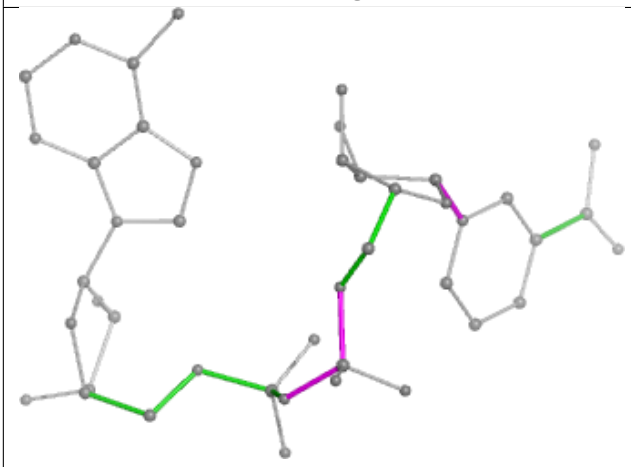
Ligand NAD B 601



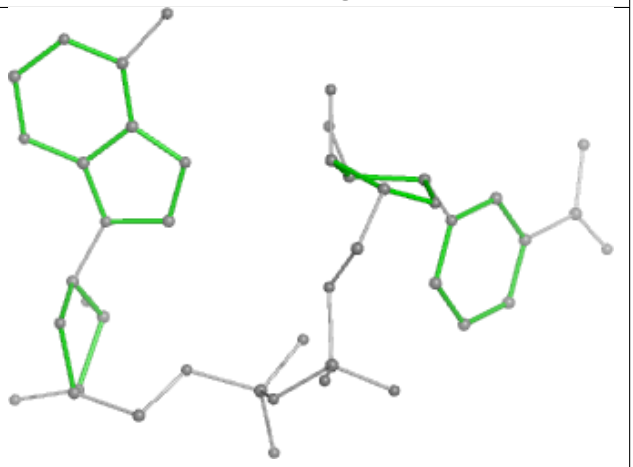
Bond lengths



Bond angles

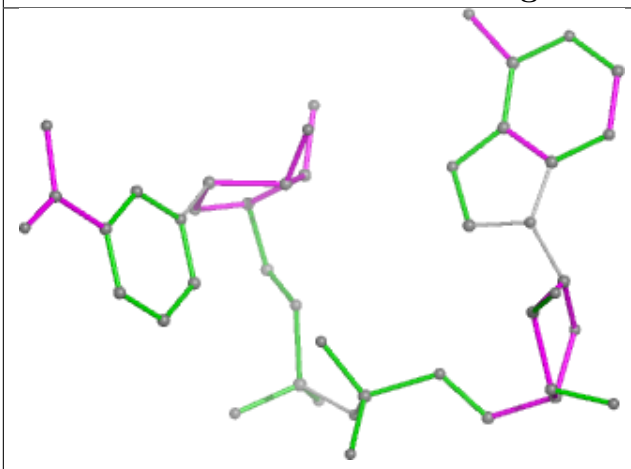


Torsions

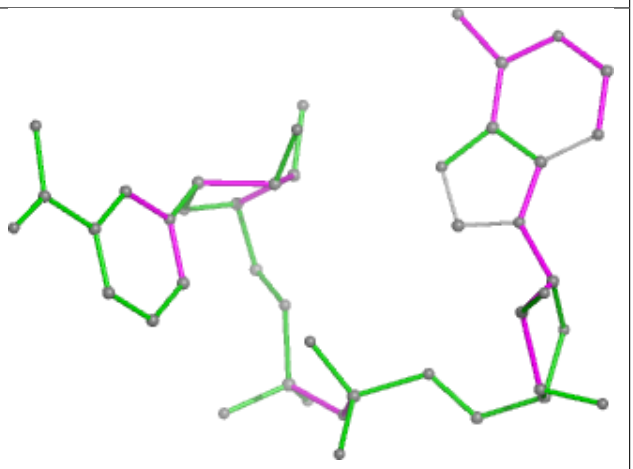


Rings

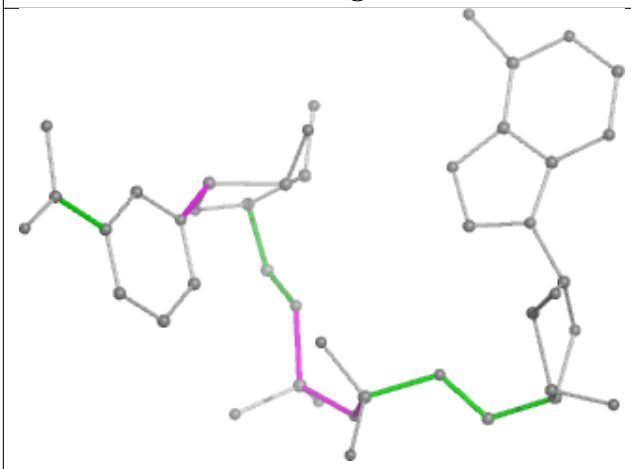
Ligand NAD C 502



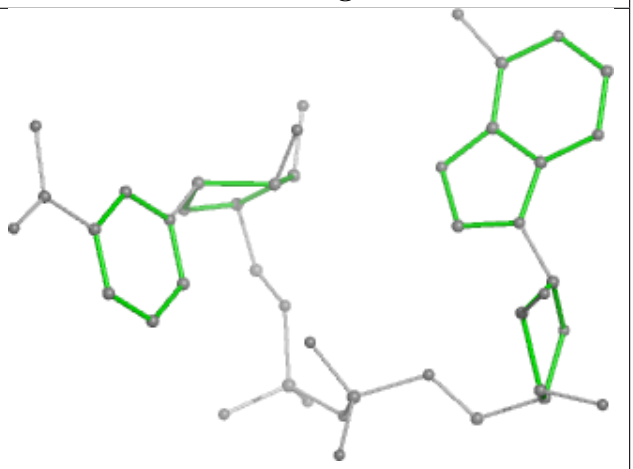
Bond lengths



Bond angles

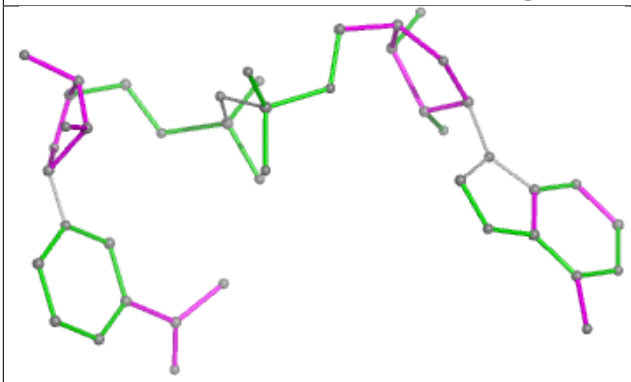


Torsions

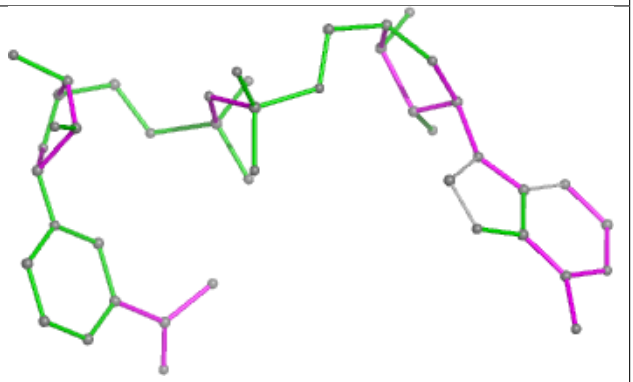


Rings

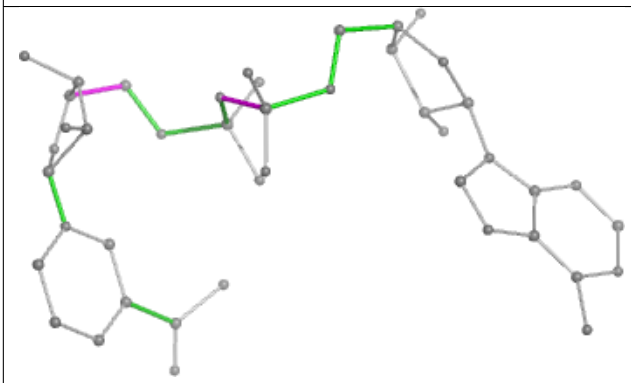
Ligand NAD D 502



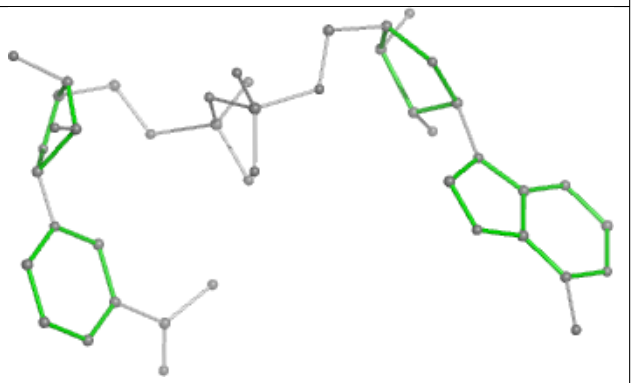
Bond lengths



Bond angles

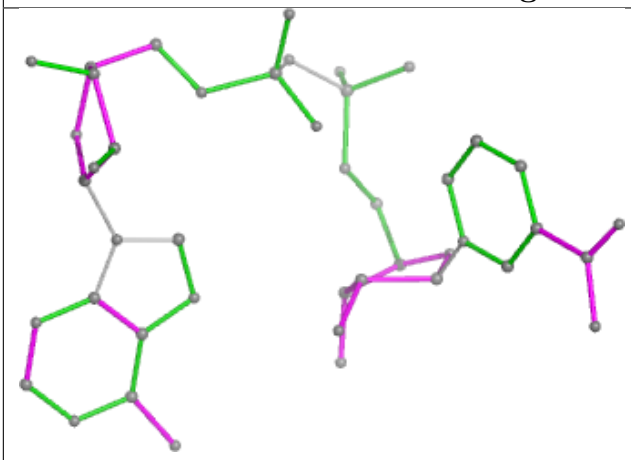


Torsions

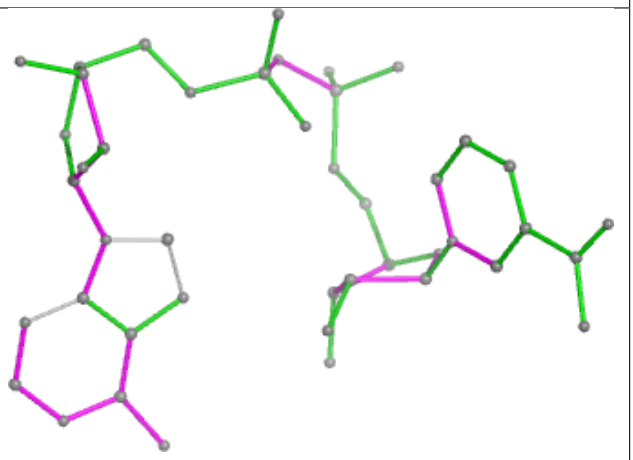


Rings

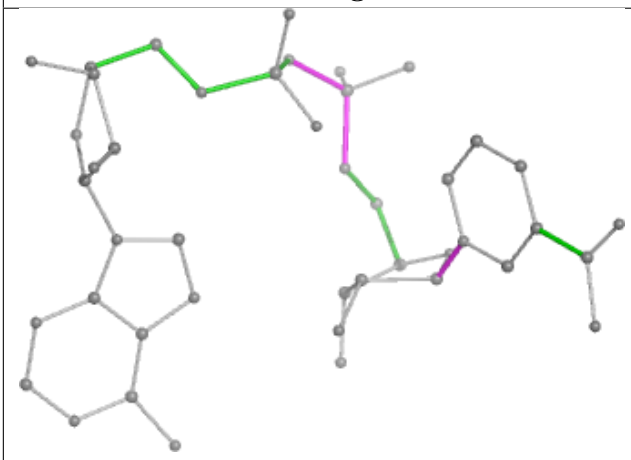
Ligand NAD A 502



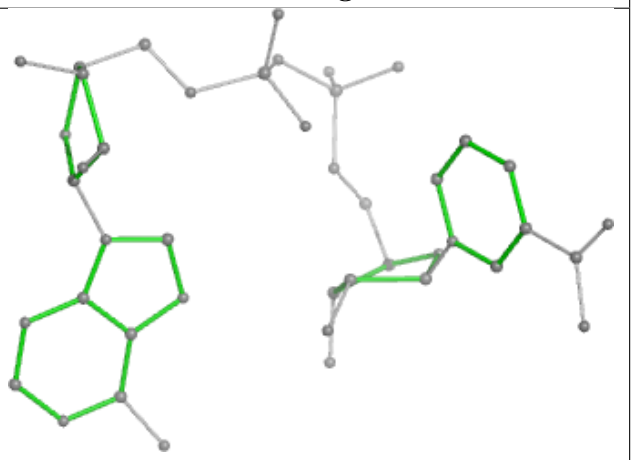
Bond lengths



Bond angles

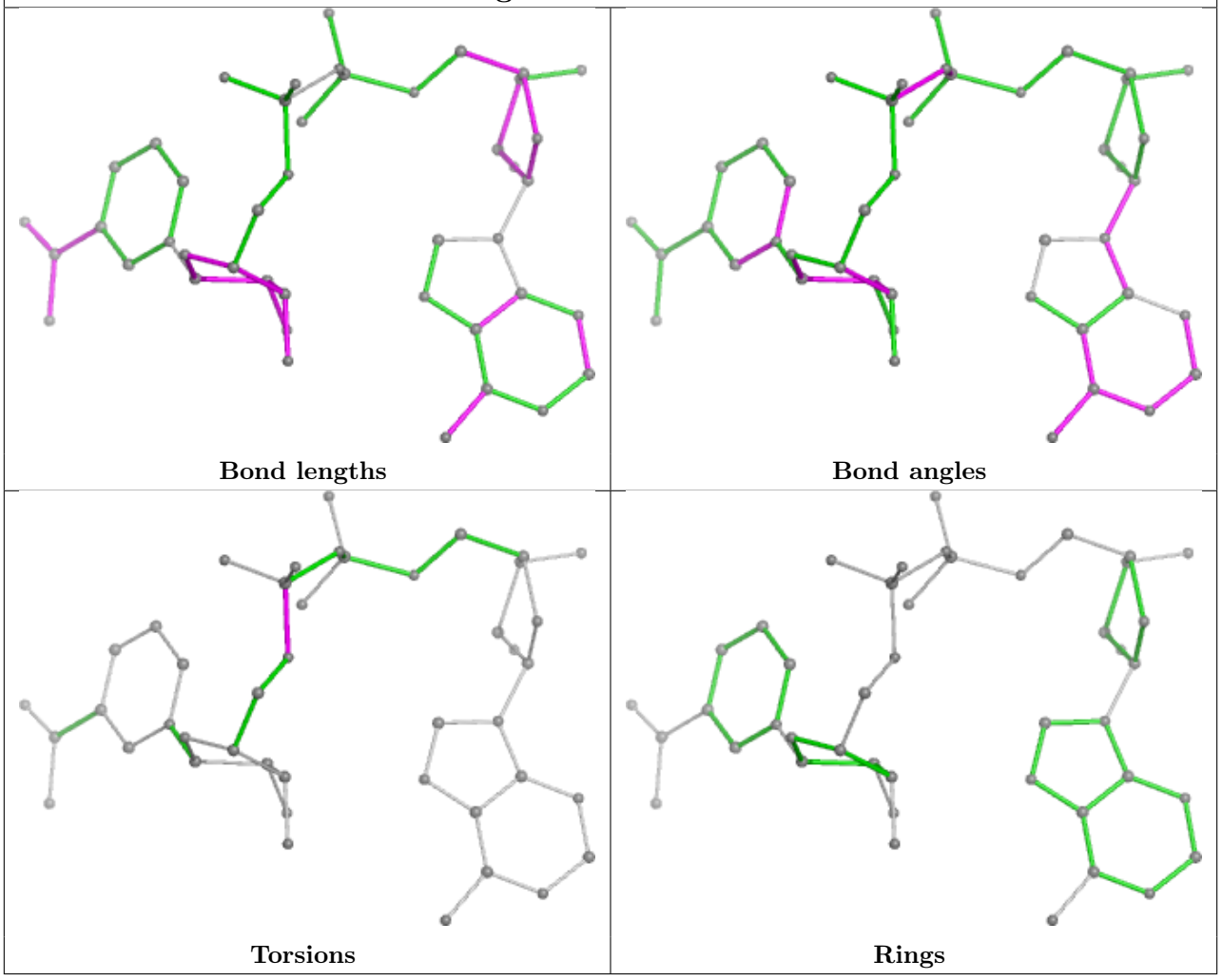


Torsions



Rings

Ligand NAD B 602



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, 95^{th} 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	457/489 (93%)	2.76	321 (70%)	0	0	19, 35, 56, 82	3 (0%)
1	B	457/489 (93%)	2.89	327 (71%)	0	0	17, 39, 65, 91	1 (0%)
1	C	454/489 (92%)	2.94	338 (74%)	0	0	22, 37, 61, 98	2 (0%)
1	D	461/489 (94%)	3.09	350 (75%)	0	0	25, 41, 65, 97	0
All	All	1829/1956 (93%)	2.92	1336 (73%)	0	0	17, 38, 62, 98	6 (0%)

The worst 5 of 1336 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	GLY	11.7
1	B	138	PHE	11.5
1	C	424	SER	11.1
1	D	427	ASP	10.8
1	D	399	GLY	9.5

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 monosaccharides in this entry.

6.4 Ligands

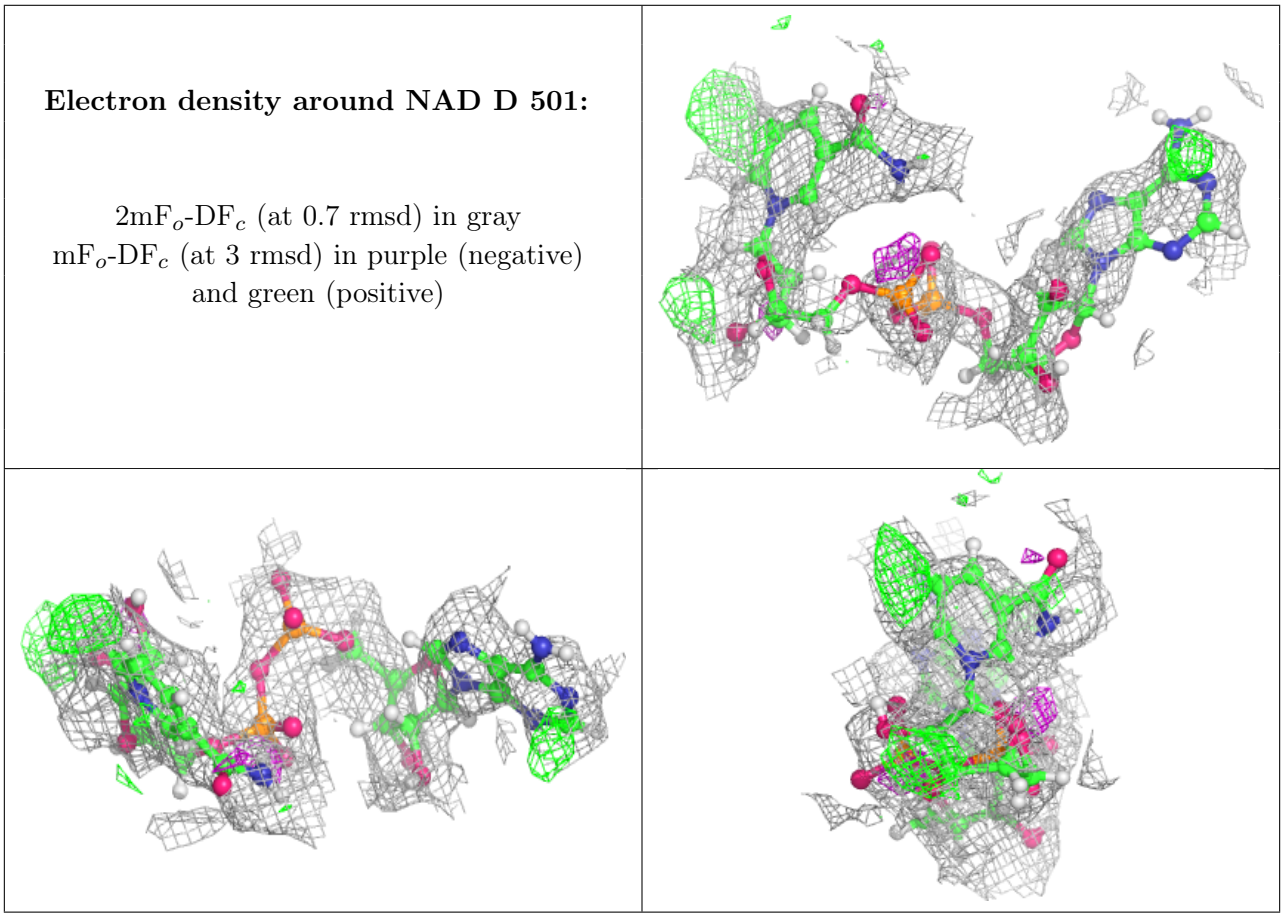
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	D	501	44/44	0.57	0.30	23,48,62,69	70
2	NAD	D	502	44/44	0.61	0.33	22,34,44,53	70
2	NAD	A	501	44/44	0.63	0.23	22,38,52,55	0
2	NAD	C	501	44/44	0.69	0.27	15,30,43,49	70
2	NAD	B	601	44/44	0.72	0.23	21,38,51,57	70
2	NAD	B	602	44/44	0.74	0.23	10,28,39,46	0
2	NAD	A	502	44/44	0.76	0.20	18,31,45,55	70
2	NAD	C	502	44/44	0.86	0.16	6,24,34,41	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.

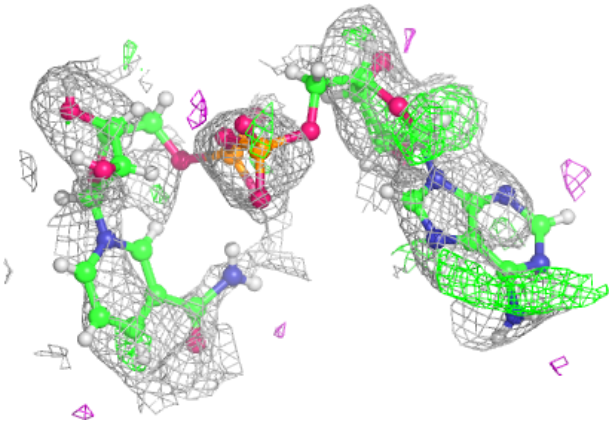
Electron density around NAD D 501:

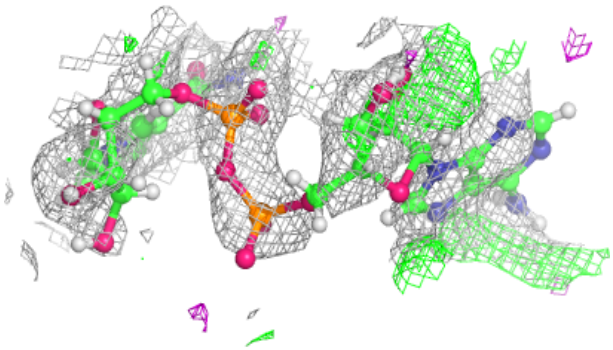
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

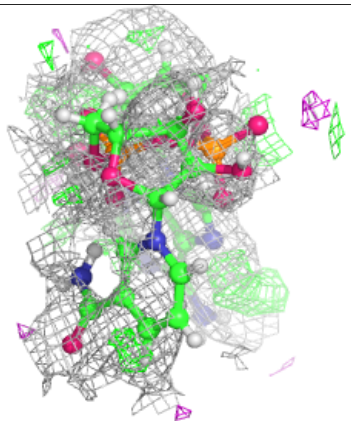


Electron density around NAD D 502:

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

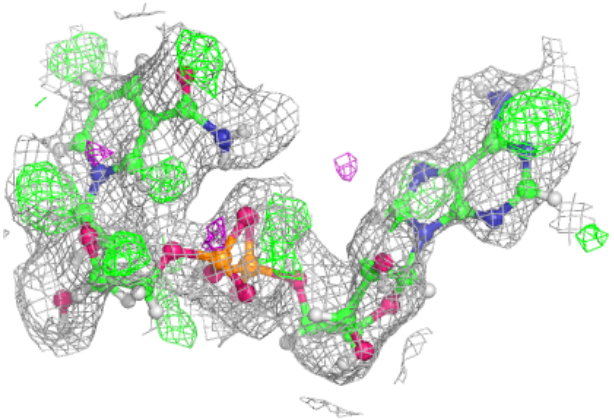


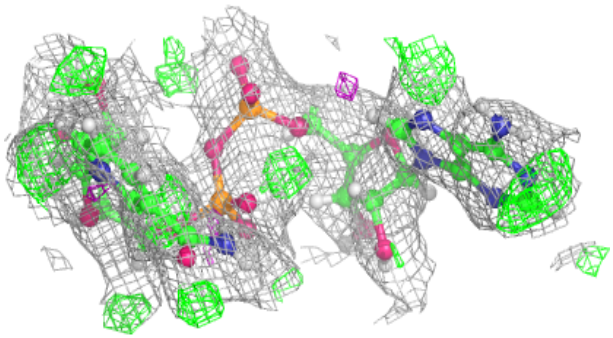


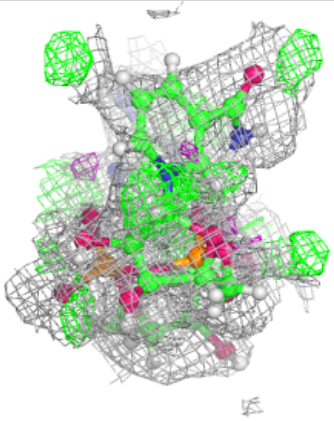


Electron density around NAD A 501:

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

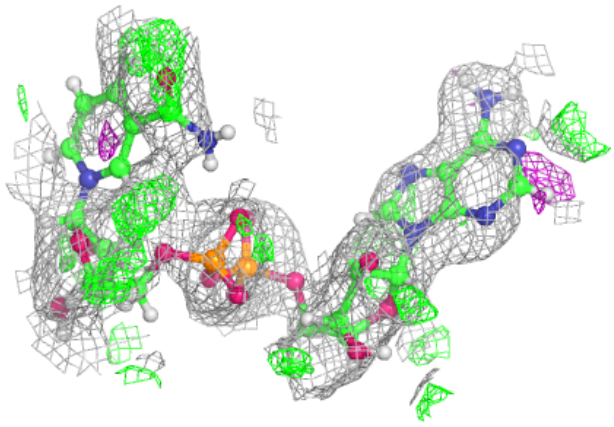


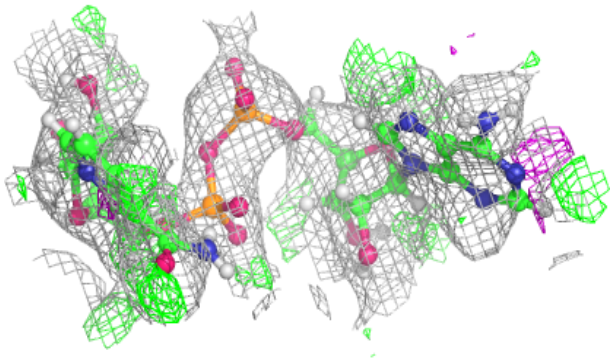


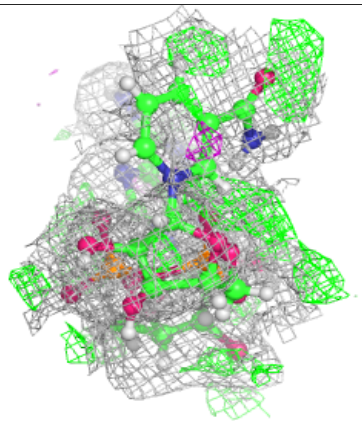


Electron density around NAD C 501:

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

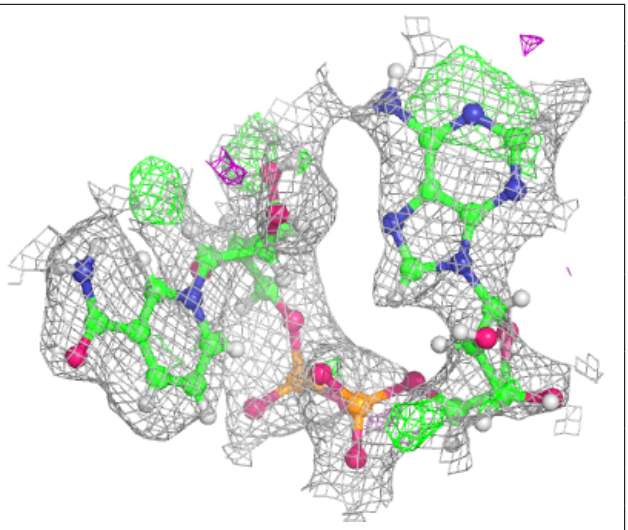


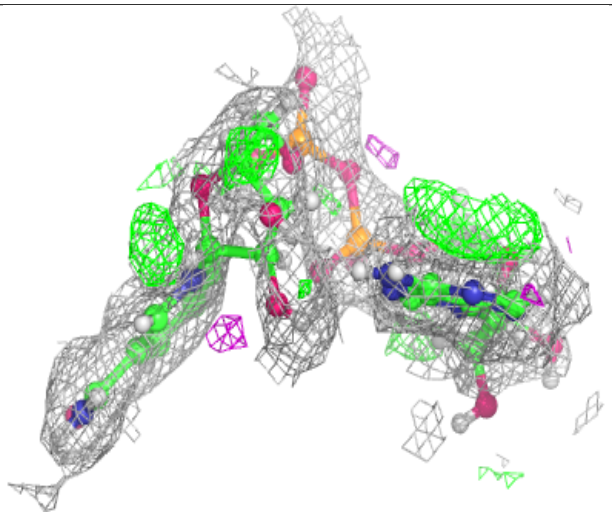


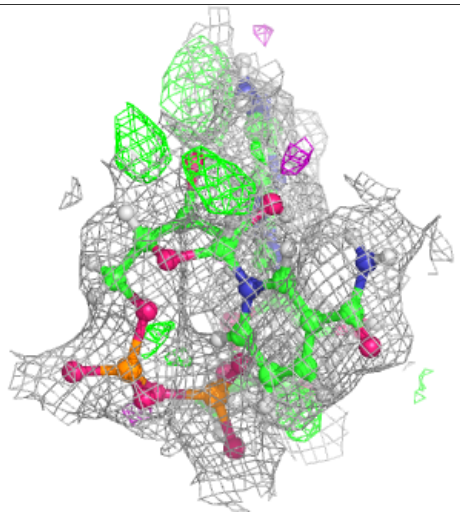


Electron density around NAD B 601:

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

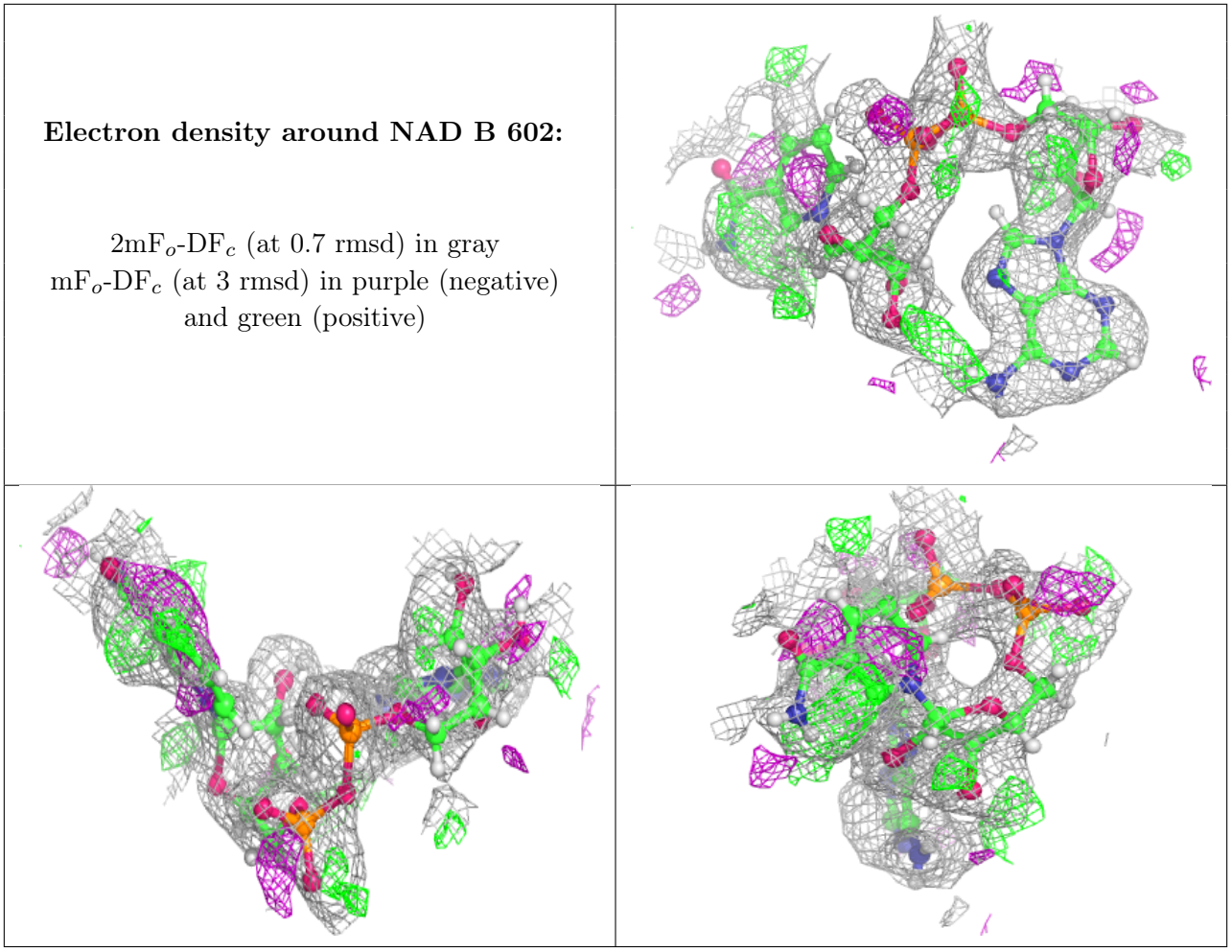






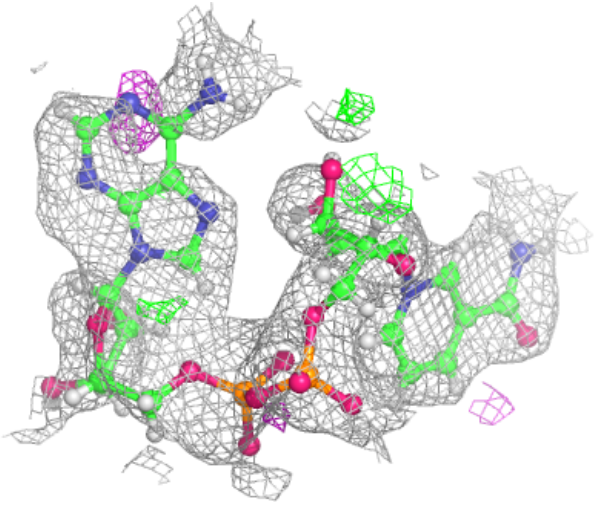
Electron density around NAD B 602:

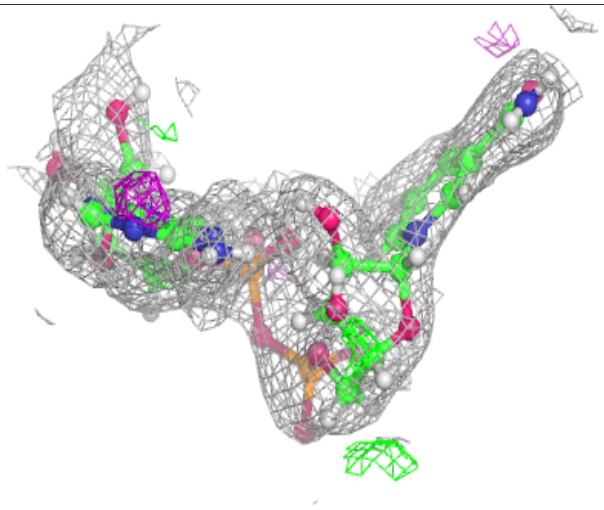
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

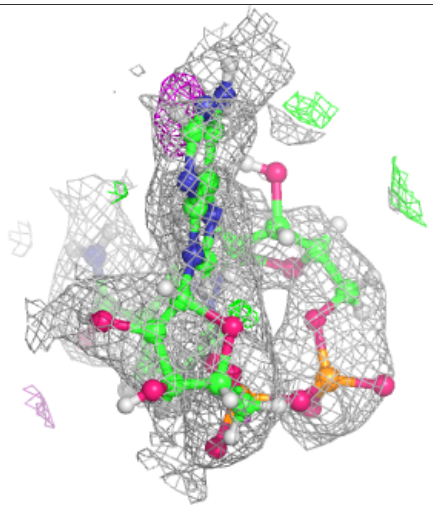


Electron density around NAD A 502:

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

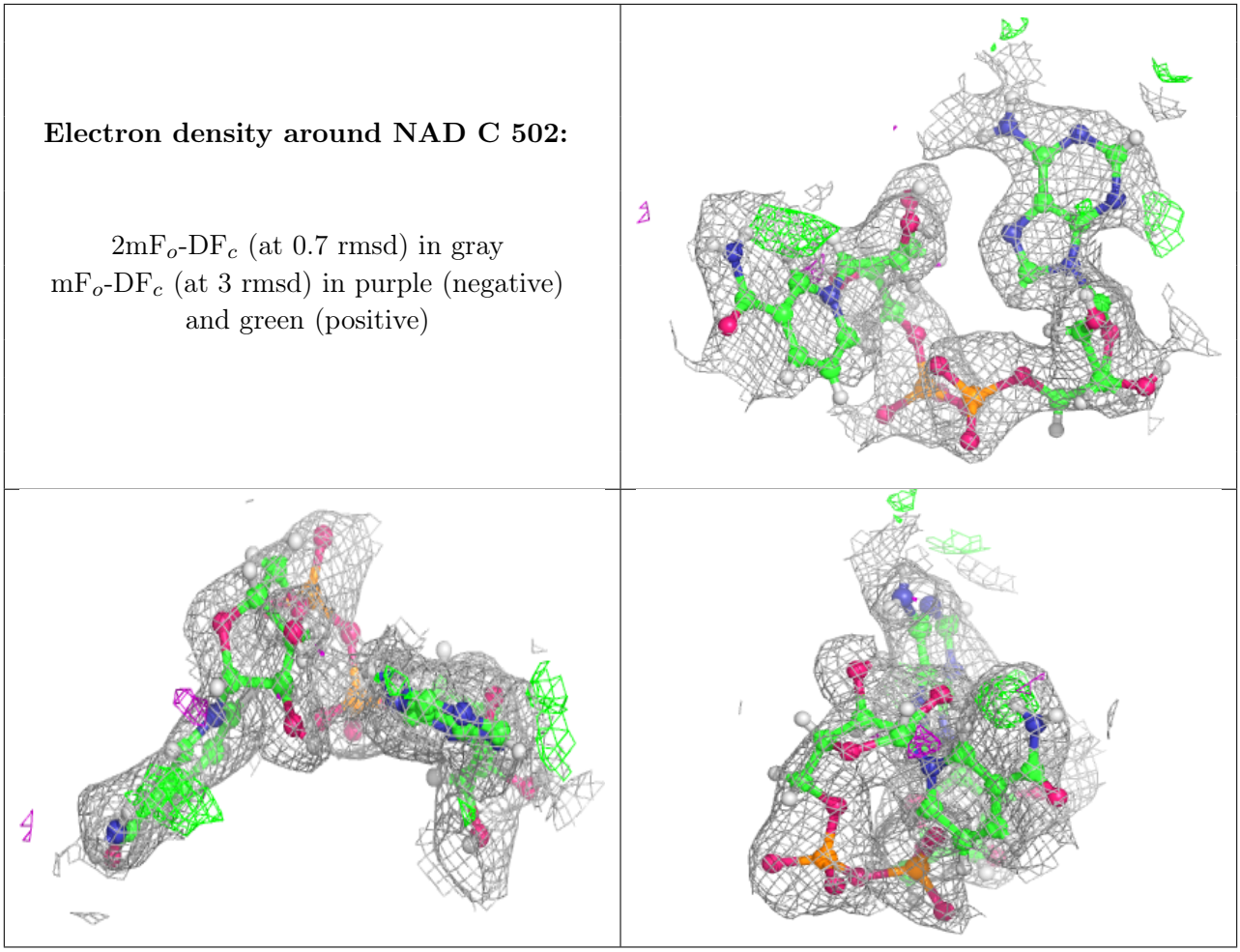






Electron density around NAD C 502:

$2mF_o$-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.