



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 06:55 PM UTC

PDB ID : 8H2A / pdb_00008h2a
Title : Crystal structure of alcohol dehydrogenase from Formosa agariphila
Authors : Brott, S.; Bornscheuer, U.T.; Nam, K.H.
Deposited on : 2022-10-05
Resolution : 2.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

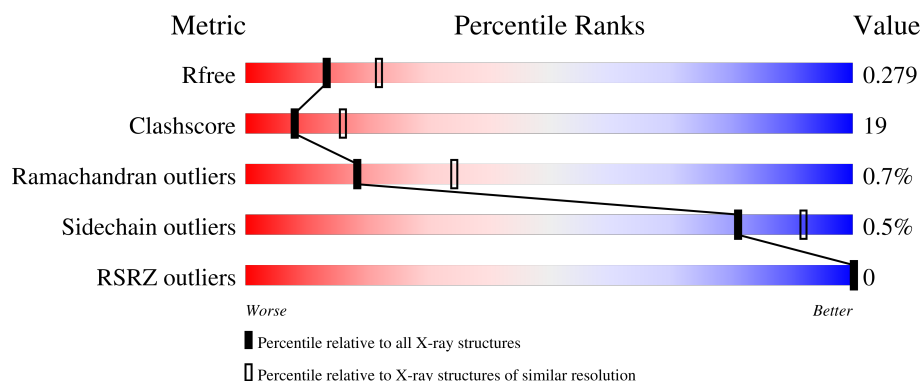
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	370	65% 32% ..
1	B	370	65% 33% ..
1	C	370	68% 28% ...
1	D	370	66% 31% ...
1	E	370	63% 34% ...

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Mol	Chain	Length	Quality of chain
1	F	370	 59% 36% ...
1	G	370	 64% 33% ...
1	H	370	 61% 34% . .

2 Entry composition

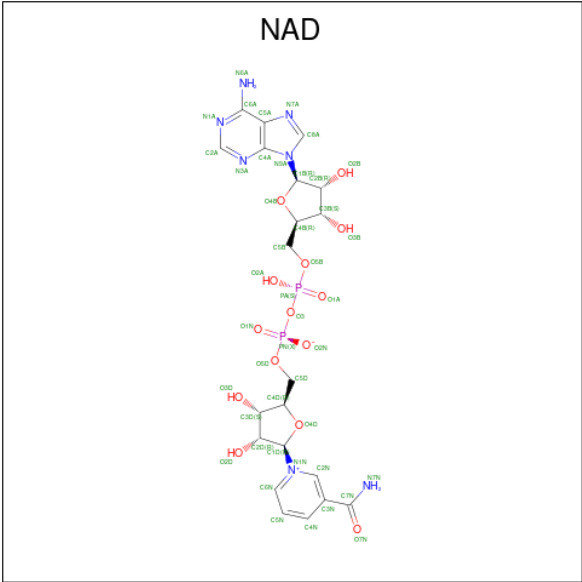
There are 4 unique types of molecules in this entry. The entry contains 22361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	366	Total	C	N	O	S	0	0	0
			2731	1718	459	532	22			
1	B	366	Total	C	N	O	S	0	0	0
			2739	1725	459	533	22			
1	C	363	Total	C	N	O	S	0	0	0
			2709	1704	456	528	21			
1	D	364	Total	C	N	O	S	0	0	0
			2717	1710	457	529	21			
1	E	364	Total	C	N	O	S	0	0	0
			2717	1710	457	529	21			
1	F	362	Total	C	N	O	S	0	0	0
			2705	1702	455	527	21			
1	G	365	Total	C	N	O	S	0	0	0
			2723	1713	458	531	21			
1	H	356	Total	C	N	O	S	0	0	0
			2664	1678	447	519	20			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: 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	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	Zn 2	0	0
3	E	2	Total 2	Zn 2	0	0
3	F	2	Total 2	Zn 2	0	0
3	G	2	Total 2	Zn 2	0	0
3	H	2	Total 2	Zn 2	0	0

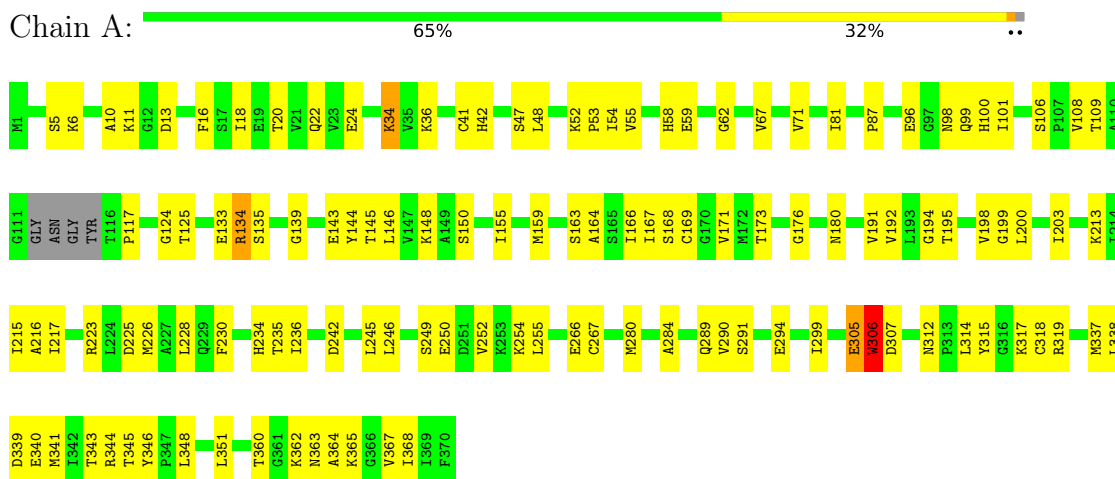
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total 37	O 37	0	0
4	B	41	Total 41	O 41	0	0
4	C	37	Total 37	O 37	0	0
4	D	36	Total 36	O 36	0	0
4	E	39	Total 39	O 39	0	0
4	F	34	Total 34	O 34	0	0
4	G	28	Total 28	O 28	0	0
4	H	36	Total 36	O 36	0	0

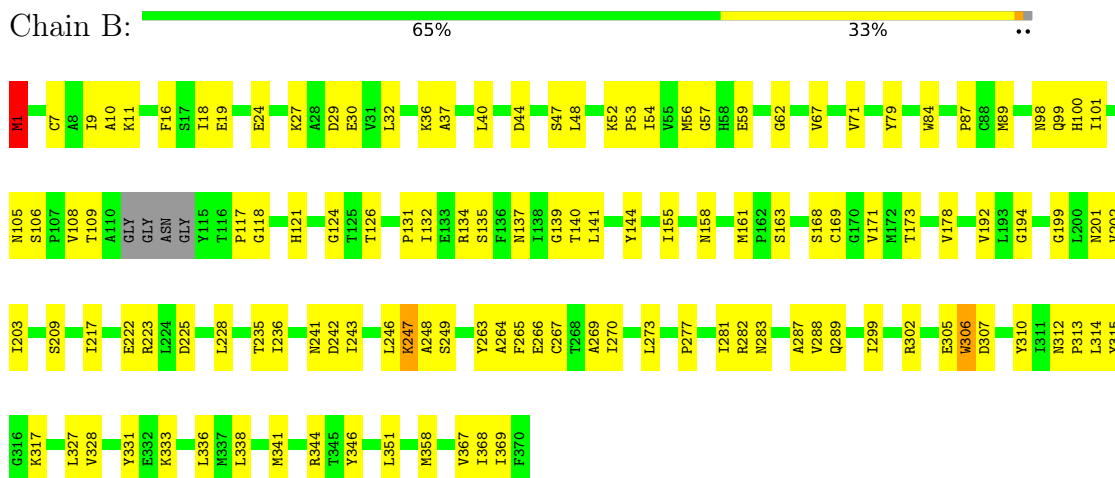
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Alcohol dehydrogenase



- Molecule 1: Alcohol dehydrogenase



- Molecule 1: Alcohol dehydrogenase





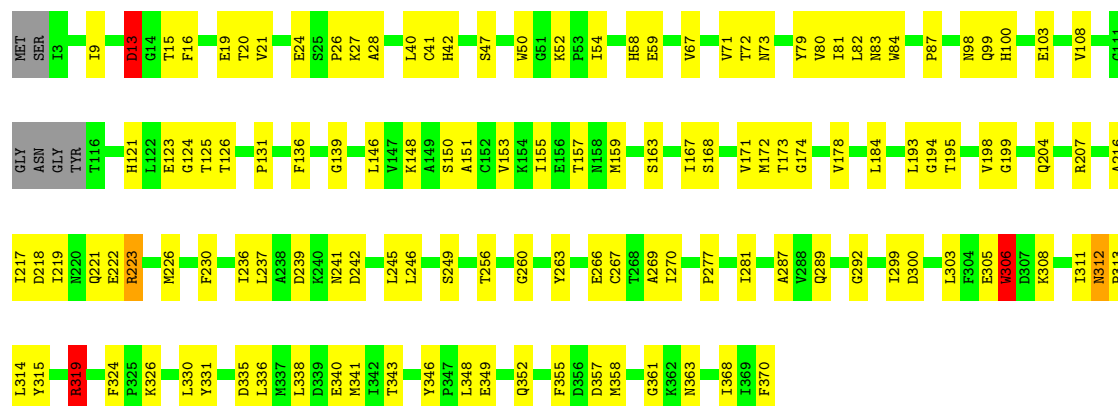
• Molecule 1: Alcohol dehydrogenase

Chain D: 66% 31% ...



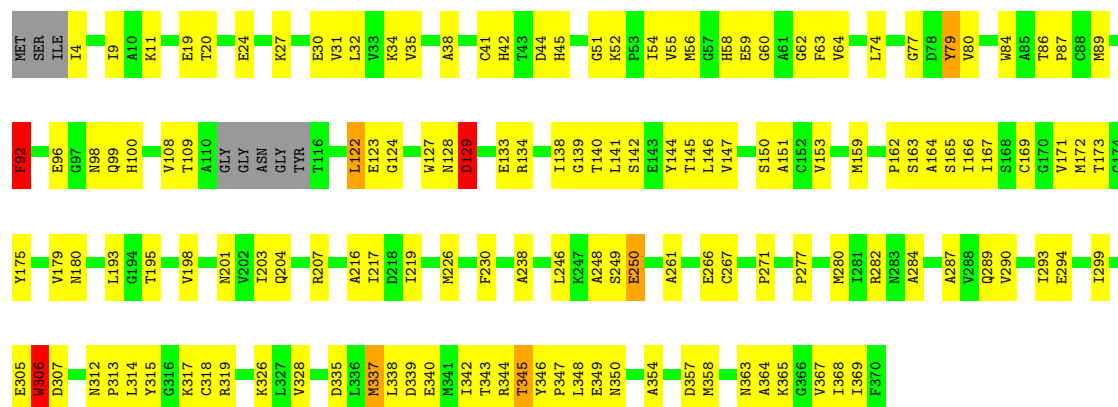
• Molecule 1: Alcohol dehydrogenase

Chain E: 63% 34% ...



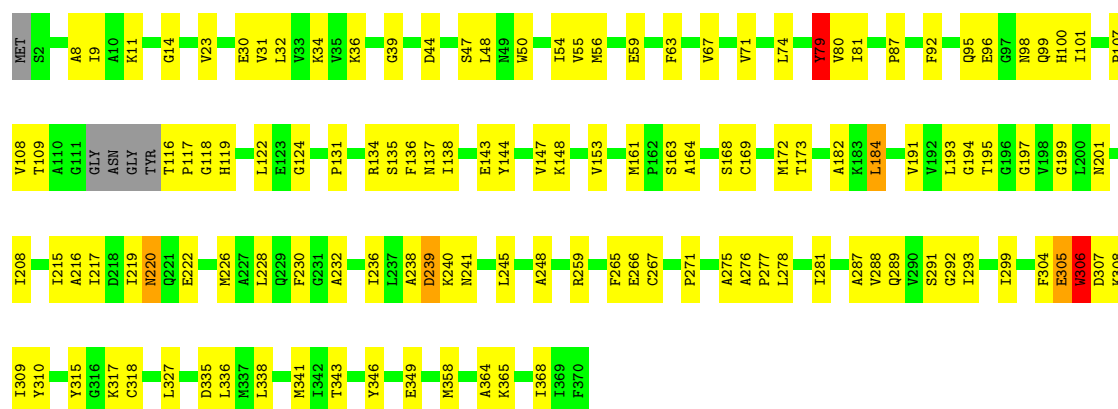
• Molecule 1: Alcohol dehydrogenase

Chain F: 59% 36% ...



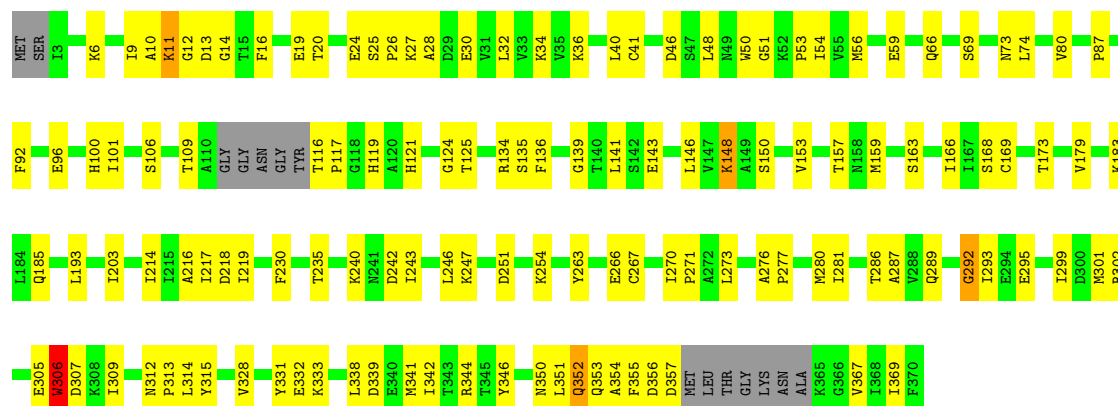
• Molecule 1: Alcohol dehydrogenase

Chain G: 64% 33% ...



• Molecule 1: Alcohol dehydrogenase

Chain H: 61% 34% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.49Å 157.20Å 98.57Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	48.19 – 2.50 48.19 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.19-2.50) 97.3 (48.19-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.225 , 0.278 0.227 , 0.279	Depositor DCC
R_{free} test set	1981 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.398 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22361	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.90% 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: ZN, 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	0.47	1/2776 (0.0%)	0.76	3/3764 (0.1%)
1	B	0.52	1/2785 (0.0%)	0.79	4/3777 (0.1%)
1	C	0.44	0/2754	0.82	7/3735 (0.2%)
1	D	0.47	0/2762	0.81	11/3746 (0.3%)
1	E	0.45	0/2762	0.77	3/3746 (0.1%)
1	F	0.50	1/2750 (0.0%)	0.90	14/3730 (0.4%)
1	G	0.45	0/2768	0.74	3/3754 (0.1%)
1	H	0.49	1/2708 (0.0%)	0.81	3/3673 (0.1%)
All	All	0.47	4/22065 (0.0%)	0.80	48/29925 (0.2%)

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	B	0	2
1	C	0	2
1	D	0	3
1	E	0	3
1	F	0	4
1	G	0	3
All	All	0	18

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MET	CA-C	6.55	1.66	1.52
1	F	337	MET	SD-CE	-5.77	1.65	1.79
1	A	34	LYS	CE-NZ	5.41	1.65	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	11	LYS	CA-CB	5.30	1.60	1.53

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	289	GLN	N-CA-C	-11.29	90.33	108.73
1	C	358	MET	CB-CG-SD	-8.53	87.11	112.70
1	C	289	GLN	CB-CA-C	-8.22	96.87	110.19
1	F	129	ASP	CB-CG-OD2	-8.18	99.58	118.40
1	D	207	ARG	NE-CZ-NH2	8.14	126.52	119.20

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	GLU	Peptide
1	B	1	MET	Mainchain
1	B	79	TYR	Sidechain
1	C	289	GLN	Sidechain
1	C	79	TYR	Sidechain

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	2731	0	2726	110	2
1	B	2739	0	2732	109	1
1	C	2709	0	2698	98	1
1	D	2717	0	2709	93	1
1	E	2717	0	2709	115	1
1	F	2705	0	2695	151	1
1	G	2723	0	2714	108	0
1	H	2664	0	2651	123	0
2	A	44	0	26	5	0
2	B	44	0	26	2	0
2	C	44	0	26	3	0
2	D	44	0	26	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	44	0	26	6	0
2	F	44	0	26	2	0
2	G	44	0	26	4	0
2	H	44	0	26	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	37	0	0	10	0
4	B	41	0	0	14	0
4	C	37	0	0	11	0
4	D	36	0	0	9	0
4	E	39	0	0	10	1
4	F	34	0	0	13	0
4	G	28	0	0	6	0
4	H	36	0	0	11	0
All	All	22361	0	21842	854	4

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 19.

The worst 5 of 854 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:27:LYS:HG3	1:E:28:ALA:H	1.16	1.08
1:C:289:GLN:OE1	1:C:312:ASN:ND2	1.85	1.07
1:F:312:ASN:ND2	4:F:501:HOH:O	1.94	1.00
1:E:40:LEU:HB3	1:E:358:MET:HE1	1.52	0.92
1:E:173:THR:HG22	1:E:315:TYR:HA	1.53	0.91

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ARG:NH2	1:E:357:ASP:OD2[1_554]	1.97	0.23
1:C:349:GLU:OE2	1:D:344:ARG:NH2[2_546]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASN:ND2	1:F:129:ASP:O[1_455]	2.08	0.12
1:A:339:ASP:O	4:E:503:HOH:O[1_554]	2.11	0.09

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	362/370 (98%)	345 (95%)	15 (4%)	2 (1%)	21	38
1	B	362/370 (98%)	335 (92%)	26 (7%)	1 (0%)	36	55
1	C	359/370 (97%)	341 (95%)	16 (4%)	2 (1%)	21	38
1	D	360/370 (97%)	336 (93%)	20 (6%)	4 (1%)	11	22
1	E	360/370 (97%)	341 (95%)	16 (4%)	3 (1%)	16	31
1	F	358/370 (97%)	338 (94%)	17 (5%)	3 (1%)	16	31
1	G	361/370 (98%)	344 (95%)	15 (4%)	2 (1%)	21	38
1	H	350/370 (95%)	335 (96%)	12 (3%)	3 (1%)	14	27
All	All	2872/2960 (97%)	2715 (94%)	137 (5%)	20 (1%)	18	34

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	TRP
1	B	306	TRP
1	C	306	TRP
1	D	306	TRP
1	D	356	ASP

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	296/298 (99%)	296 (100%)	0	100	100
1	B	297/298 (100%)	297 (100%)	0	100	100
1	C	293/298 (98%)	291 (99%)	2 (1%)	76	89
1	D	294/298 (99%)	292 (99%)	2 (1%)	76	89
1	E	294/298 (99%)	292 (99%)	2 (1%)	76	89
1	F	293/298 (98%)	291 (99%)	2 (1%)	76	89
1	G	295/298 (99%)	293 (99%)	2 (1%)	76	89
1	H	289/298 (97%)	288 (100%)	1 (0%)	86	94
All	All	2351/2384 (99%)	2340 (100%)	11 (0%)	81	92

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	92	PHE
1	G	220	ASN
1	H	306	TRP
1	G	306	TRP
1	E	306	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	234	HIS
1	H	312	ASN
1	F	221	GLN
1	H	98	ASN
1	F	95	GLN

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 ⓘ

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 for Mogul analysis.

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	E	401	-	46,48,48	4.18	17 (36%)	64,73,73	1.91	16 (25%)
2	NAD	A	401	-	46,48,48	4.18	19 (41%)	64,73,73	1.74	14 (21%)
2	NAD	D	401	-	46,48,48	3.95	15 (32%)	64,73,73	1.87	13 (20%)
2	NAD	B	401	-	46,48,48	4.04	15 (32%)	64,73,73	1.87	16 (25%)
2	NAD	C	401	-	46,48,48	4.13	17 (36%)	64,73,73	1.70	15 (23%)
2	NAD	F	401	-	46,48,48	3.99	17 (36%)	64,73,73	1.86	13 (20%)
2	NAD	G	401	-	46,48,48	3.91	16 (34%)	64,73,73	1.96	18 (28%)
2	NAD	H	401	-	46,48,48	4.04	16 (34%)	64,73,73	2.10	18 (28%)

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	E	401	-	-	7/30/62/62	0/5/5/5
2	NAD	A	401	-	-	4/30/62/62	0/5/5/5
2	NAD	D	401	-	-	18/30/62/62	0/5/5/5
2	NAD	B	401	-	-	6/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	C	401	-	-	10/30/62/62	0/5/5/5
2	NAD	F	401	-	-	7/30/62/62	0/5/5/5
2	NAD	G	401	-	-	8/30/62/62	0/5/5/5
2	NAD	H	401	-	-	11/30/62/62	0/5/5/5

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	NAD	O4D-C1D	16.42	1.62	1.40
2	E	401	NAD	O4D-C1D	16.37	1.62	1.40
2	D	401	NAD	O4D-C1D	16.05	1.62	1.40
2	A	401	NAD	O4D-C1D	15.82	1.61	1.40
2	F	401	NAD	O4D-C1D	15.81	1.61	1.40

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	NAD	C5A-C4A-N3A	-6.11	118.30	126.72
2	B	401	NAD	N3A-C2A-N1A	-6.02	119.46	128.58
2	E	401	NAD	N3A-C2A-N1A	-6.01	119.49	128.58
2	G	401	NAD	C5A-C4A-N3A	-5.64	118.94	126.72
2	A	401	NAD	N3A-C2A-N1A	-5.58	120.14	128.58

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C2N

There are no ring outliers.

8 monomers are involved in 30 short contacts:

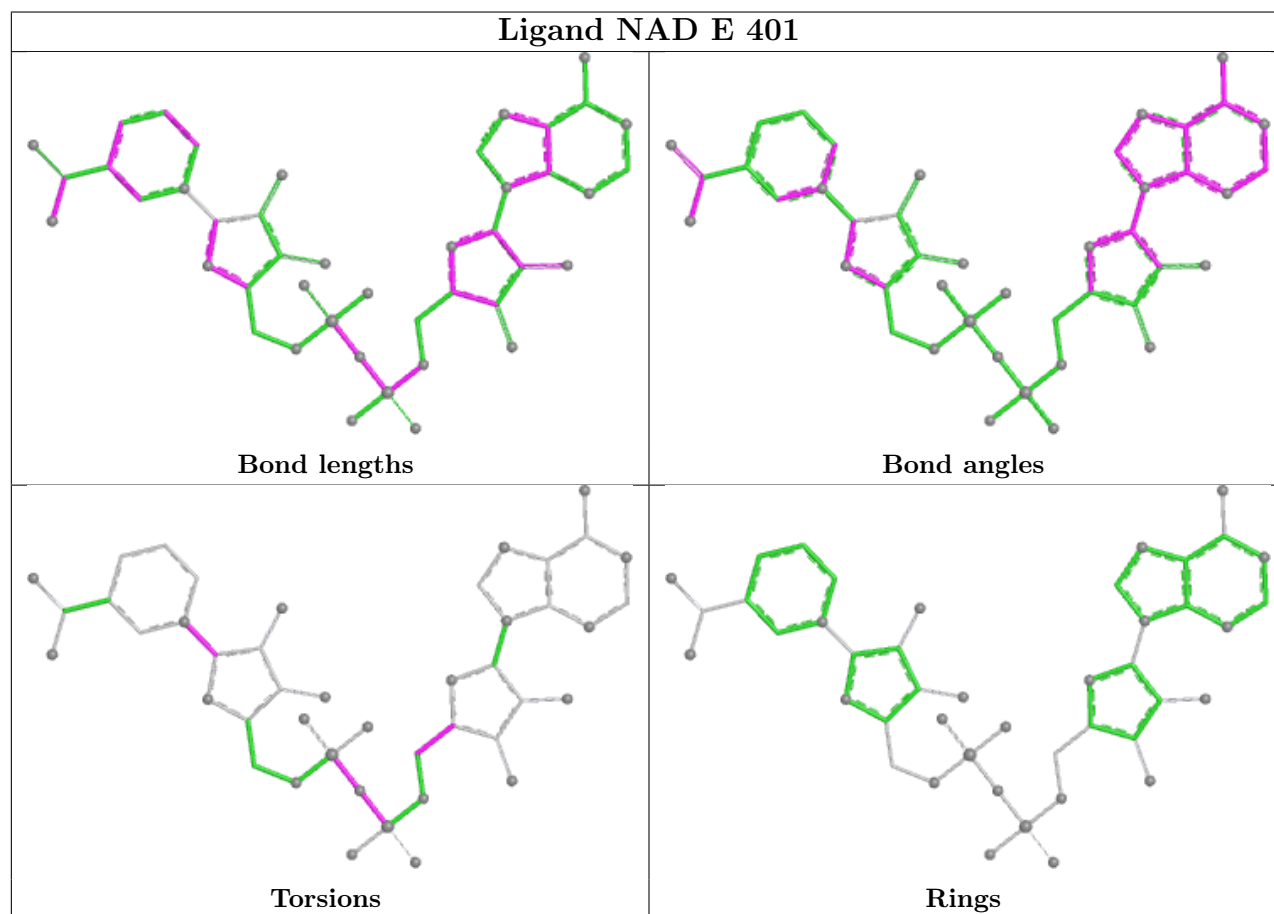
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	NAD	6	0
2	A	401	NAD	5	0
2	D	401	NAD	4	0

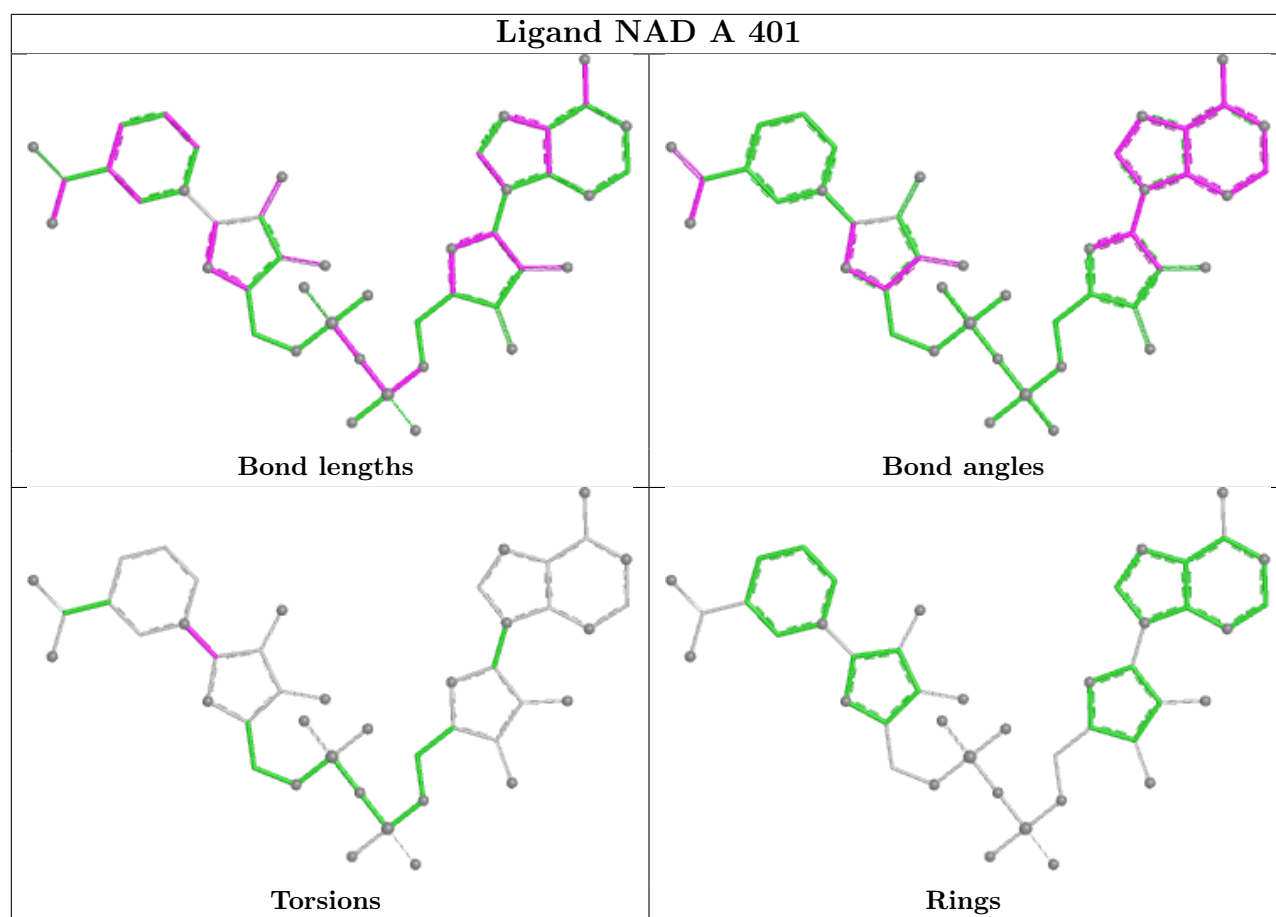
Continued on next page...

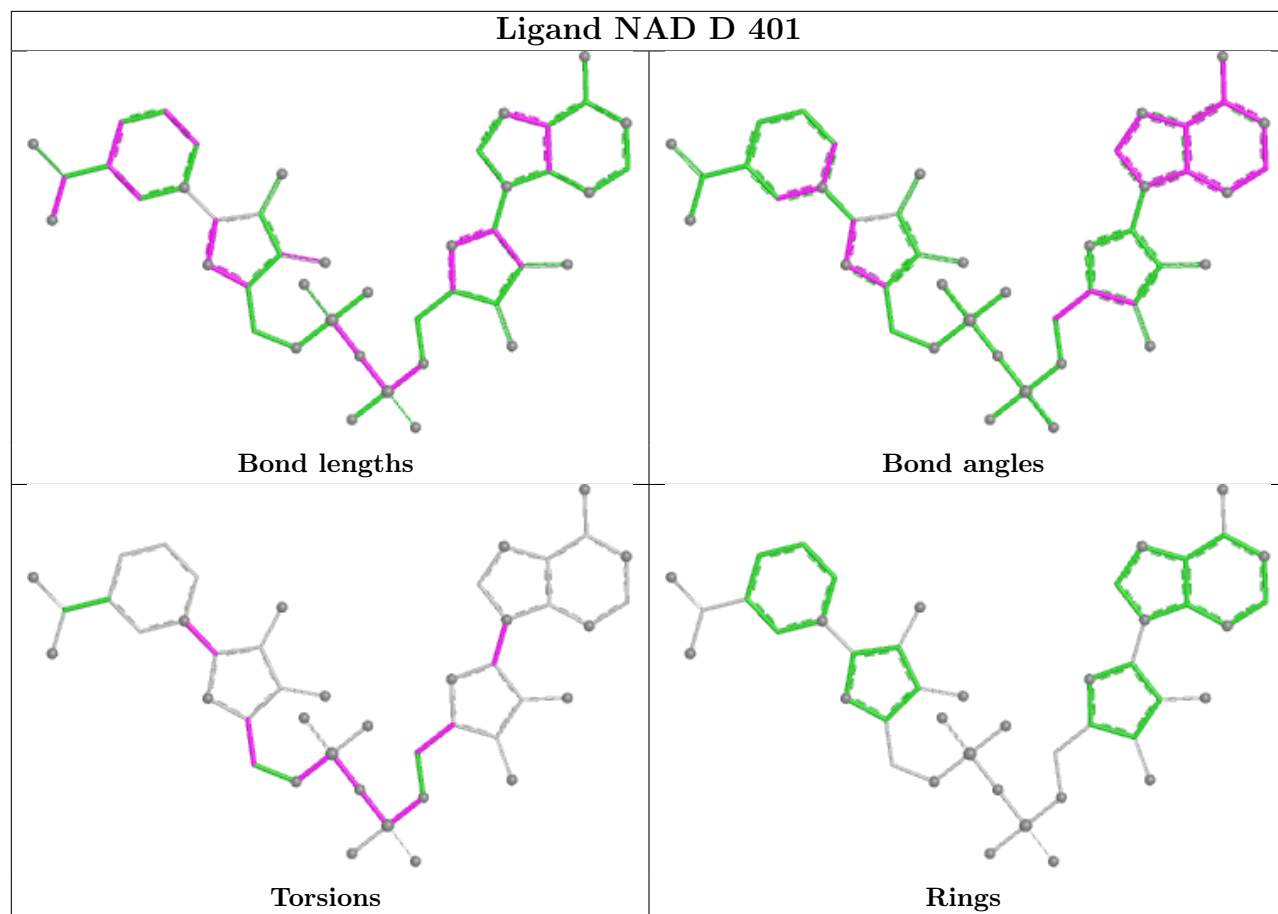
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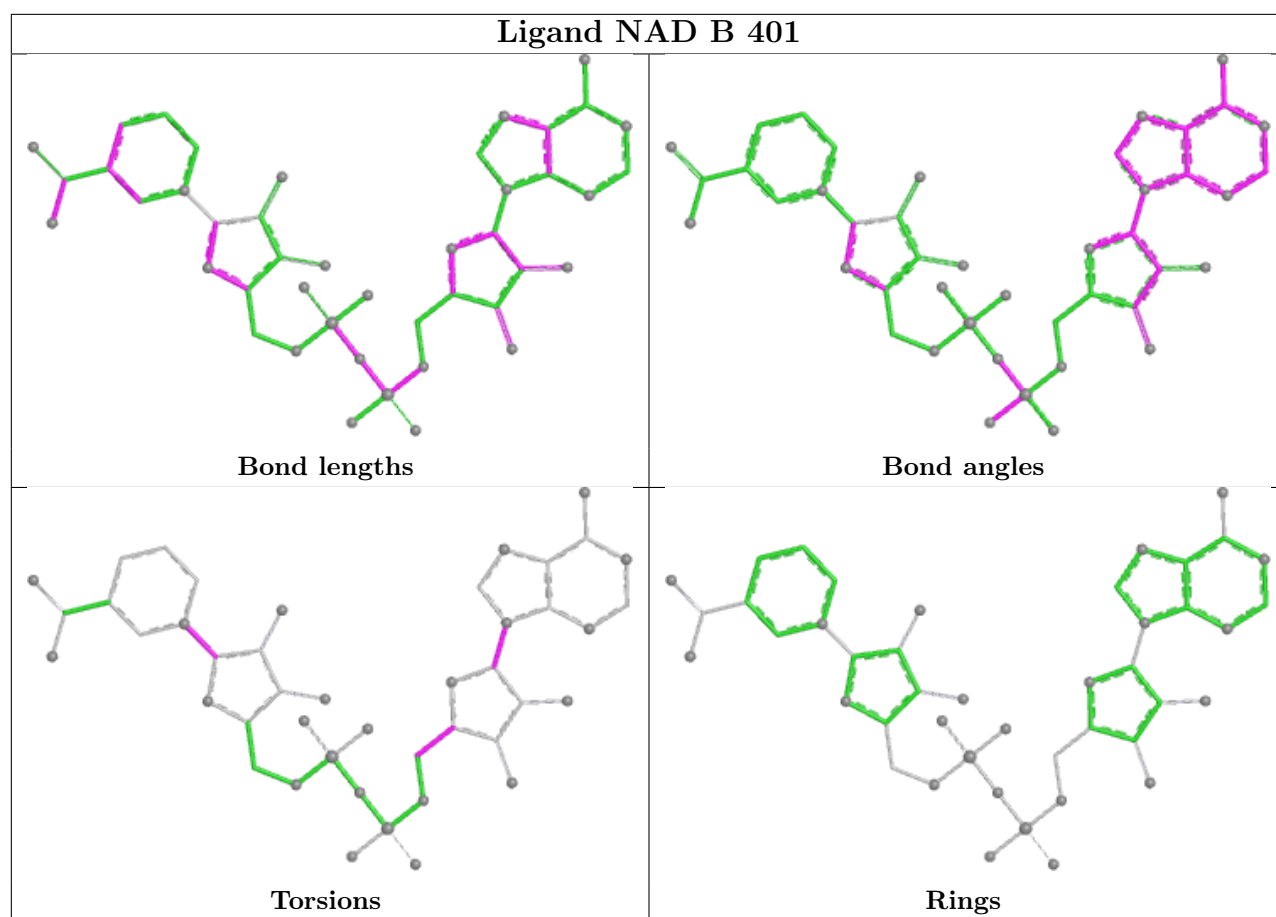
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAD	2	0
2	C	401	NAD	3	0
2	F	401	NAD	2	0
2	G	401	NAD	4	0
2	H	401	NAD	4	0

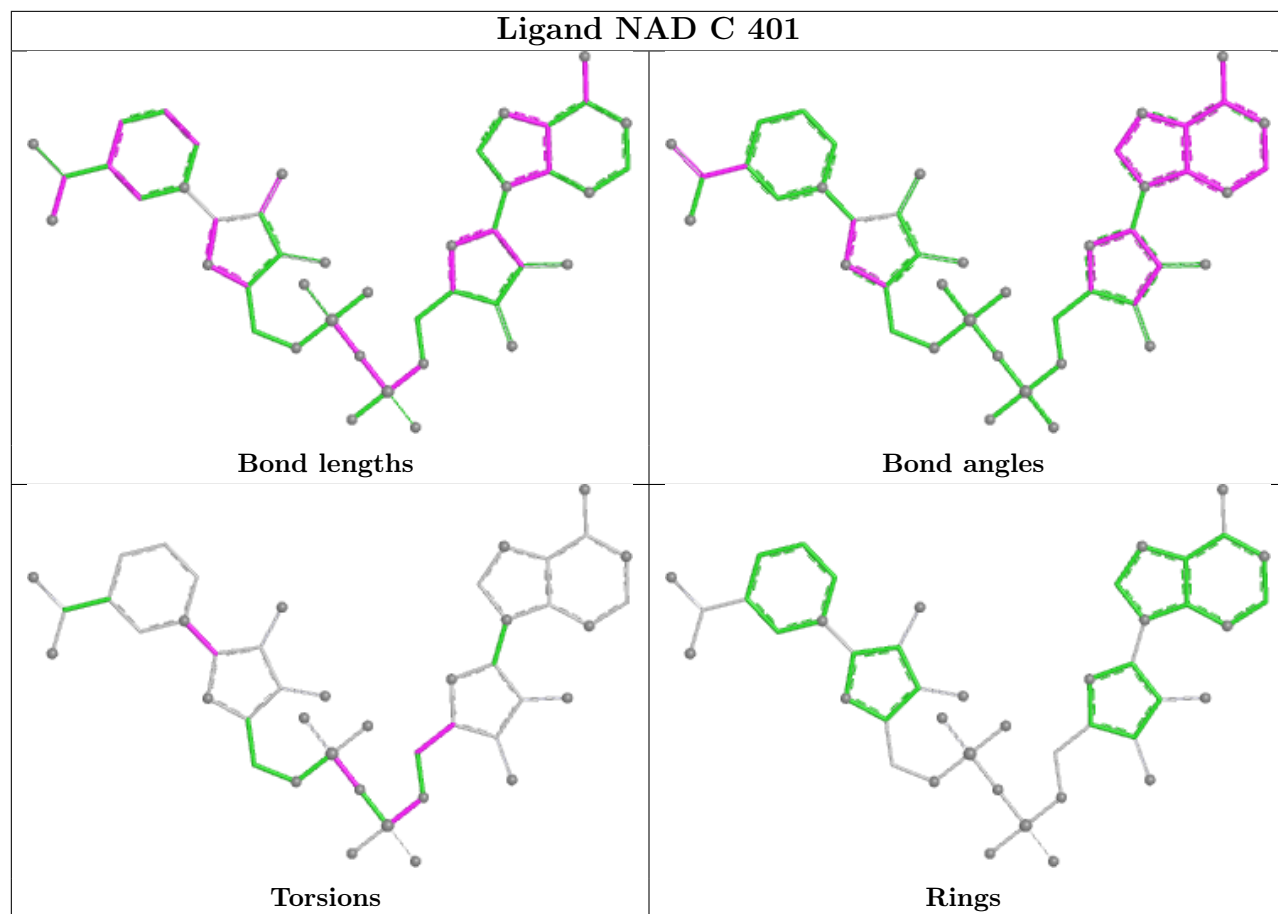
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

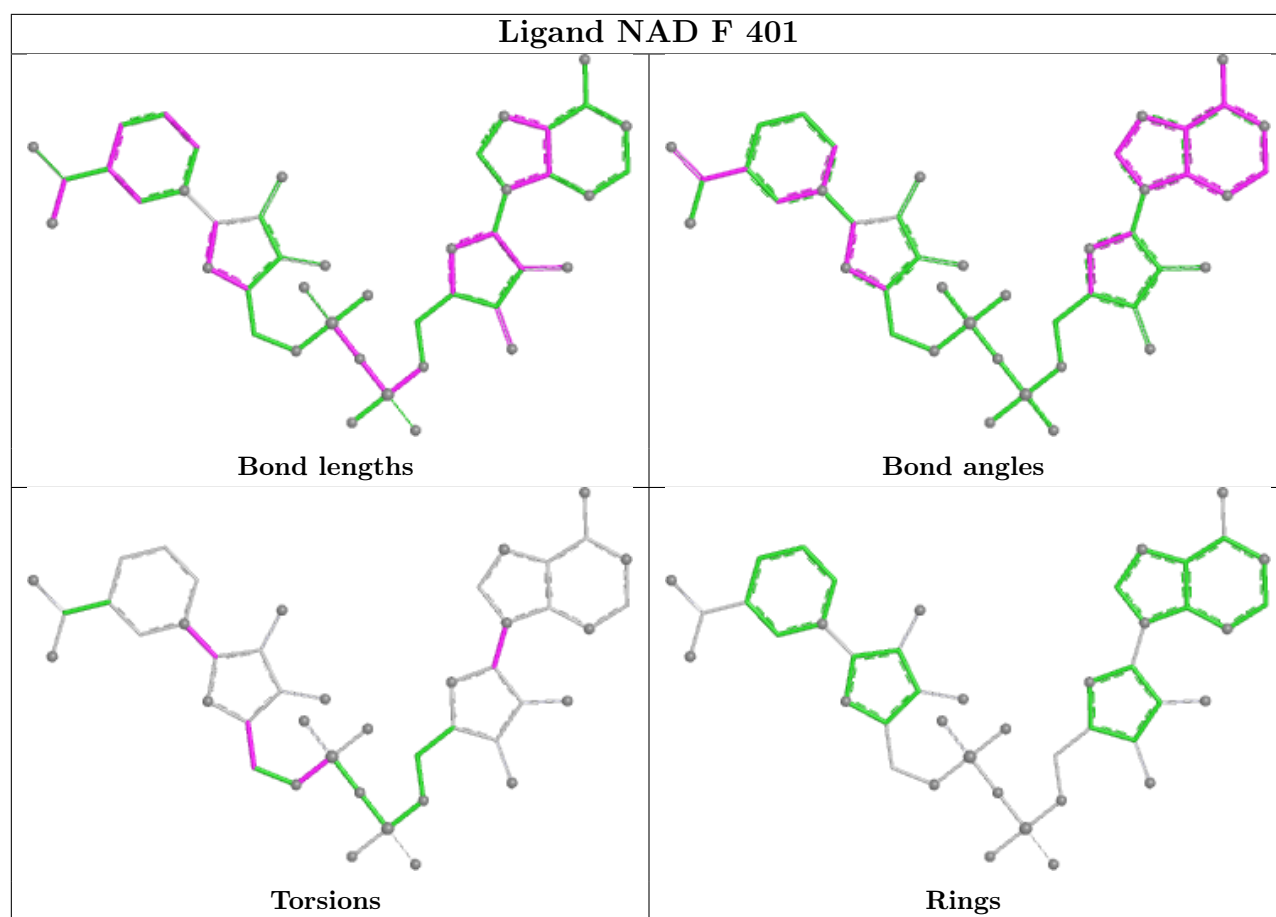


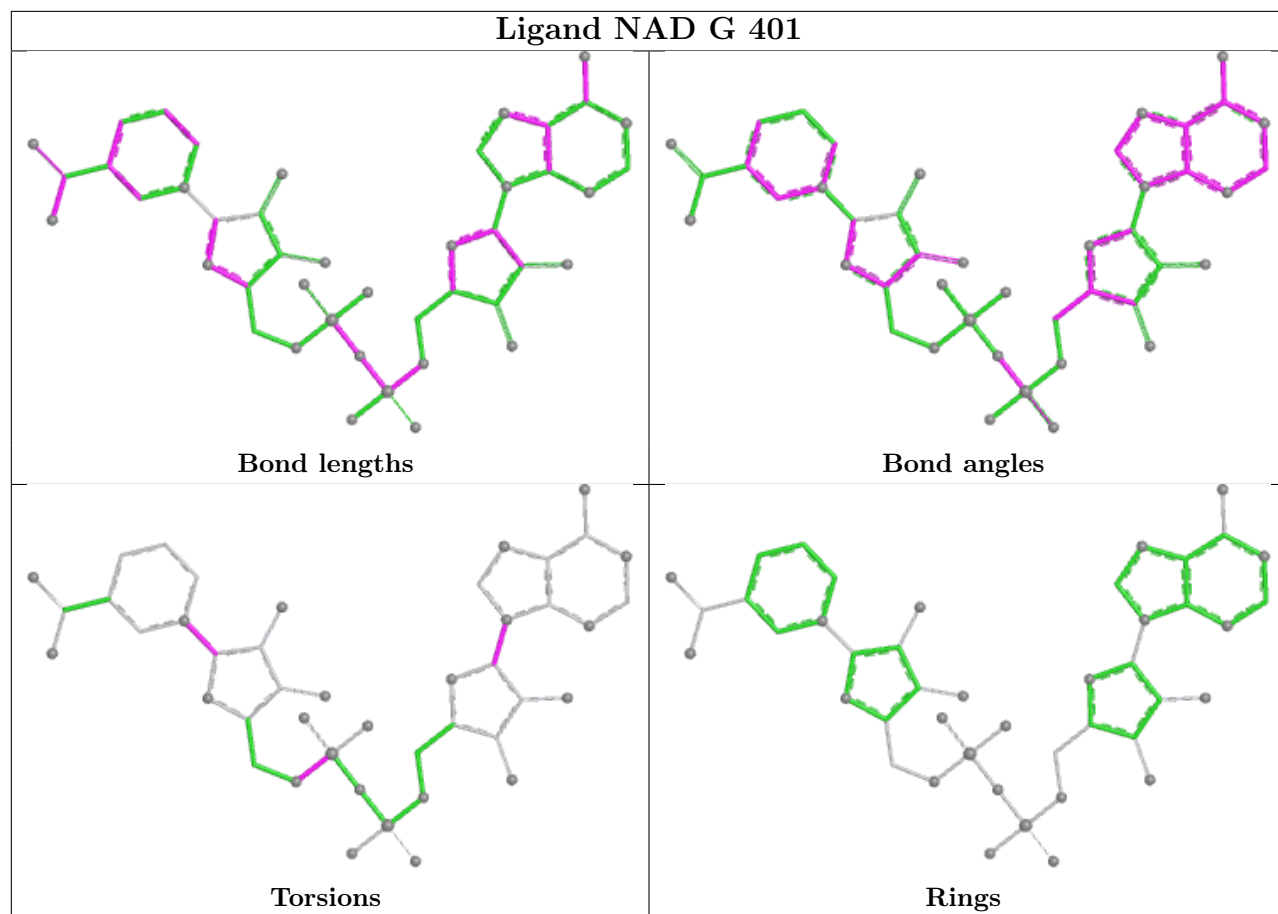


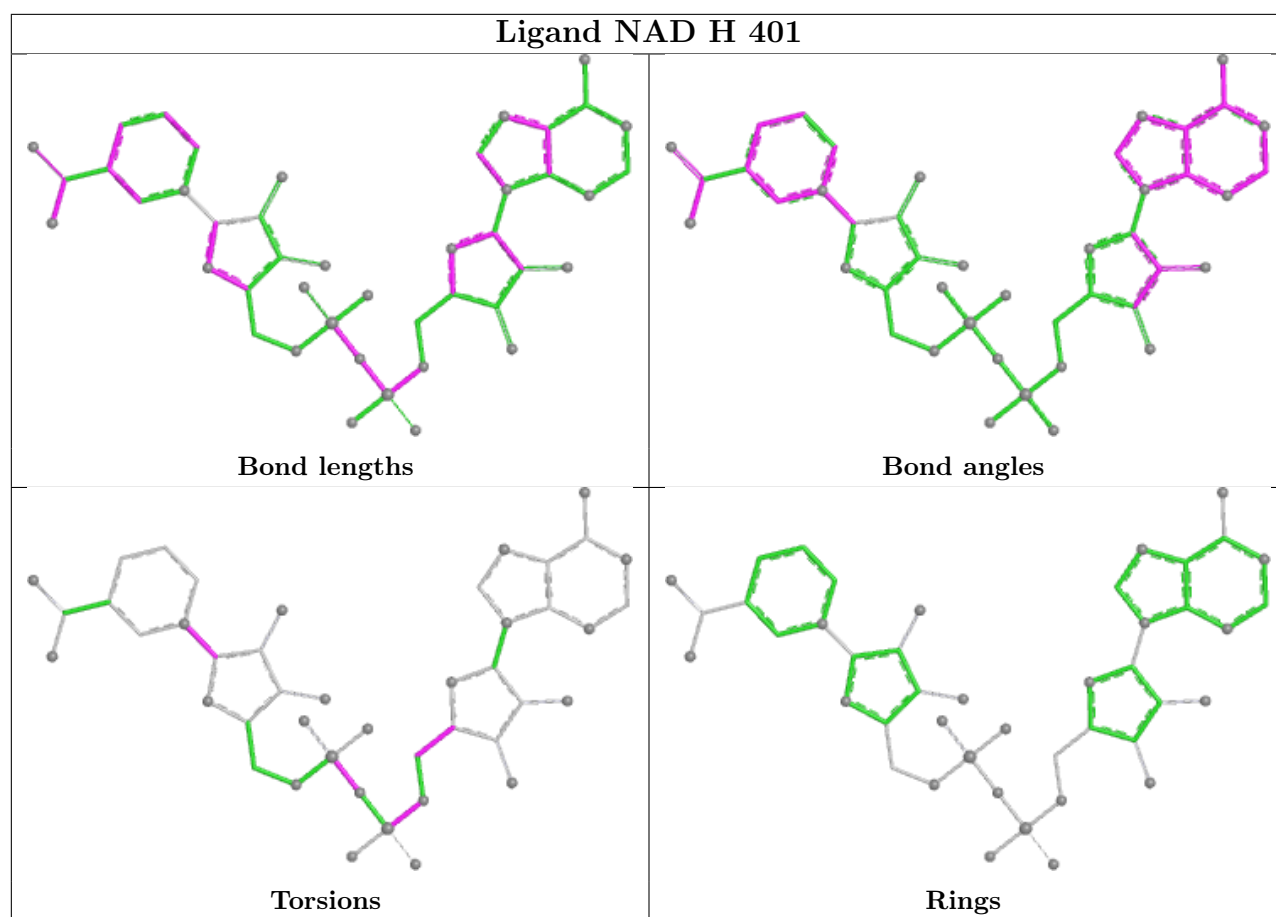












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	366/370 (98%)	-1.16	0 100 100	33, 46, 62, 76	0
1	B	366/370 (98%)	-1.16	0 100 100	31, 43, 58, 74	0
1	C	363/370 (98%)	-1.07	0 100 100	35, 53, 72, 83	0
1	D	364/370 (98%)	-1.08	0 100 100	36, 51, 75, 90	0
1	E	364/370 (98%)	-1.13	0 100 100	33, 46, 61, 73	0
1	F	362/370 (97%)	-1.01	0 100 100	35, 55, 84, 91	0
1	G	365/370 (98%)	-1.09	0 100 100	32, 46, 61, 75	0
1	H	356/370 (96%)	-1.07	0 100 100	35, 53, 79, 88	0
All	All	2906/2960 (98%)	-1.10	0 100 100	31, 48, 74, 91	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

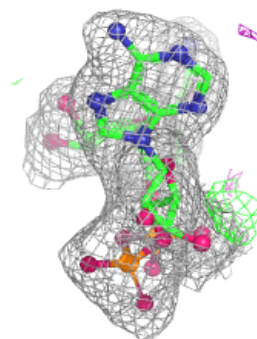
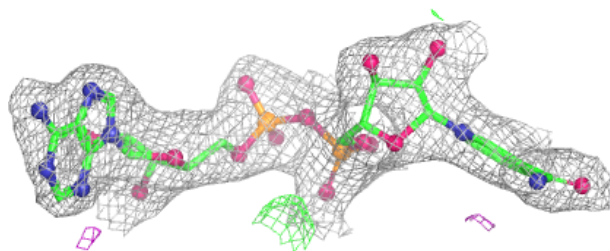
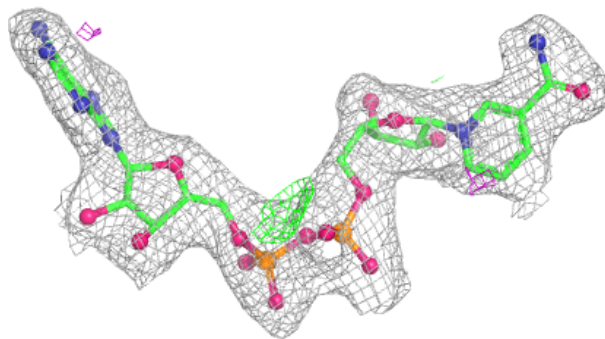
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	401	44/44	0.99	0.04	29,43,49,57	0
2	NAD	B	401	44/44	0.99	0.04	35,44,49,54	0
2	NAD	C	401	44/44	0.99	0.04	36,53,58,66	0
2	NAD	D	401	44/44	0.99	0.04	34,50,59,62	0
2	NAD	E	401	44/44	0.99	0.04	40,48,54,61	0
2	NAD	F	401	44/44	0.99	0.04	44,54,59,61	0
2	NAD	G	401	44/44	0.99	0.04	38,45,52,54	0
2	NAD	H	401	44/44	0.99	0.04	39,52,60,64	0
3	ZN	A	402	1/1	0.99	0.04	83,83,83,83	0
3	ZN	B	402	1/1	0.99	0.02	68,68,68,68	0
3	ZN	C	402	1/1	0.99	0.03	71,71,71,71	0
3	ZN	D	402	1/1	0.99	0.03	71,71,71,71	0
3	ZN	E	402	1/1	0.99	0.03	78,78,78,78	0
3	ZN	F	402	1/1	0.99	0.03	89,89,89,89	0
3	ZN	G	402	1/1	0.99	0.02	62,62,62,62	0
3	ZN	D	403	1/1	1.00	0.02	53,53,53,53	0
3	ZN	A	403	1/1	1.00	0.01	61,61,61,61	0
3	ZN	E	403	1/1	1.00	0.01	53,53,53,53	0
3	ZN	C	403	1/1	1.00	0.01	57,57,57,57	0
3	ZN	F	403	1/1	1.00	0.02	60,60,60,60	0
3	ZN	B	403	1/1	1.00	0.01	56,56,56,56	0
3	ZN	G	403	1/1	1.00	0.02	62,62,62,62	0
3	ZN	H	402	1/1	1.00	0.02	83,83,83,83	0
3	ZN	H	403	1/1	1.00	0.02	57,57,57,57	0

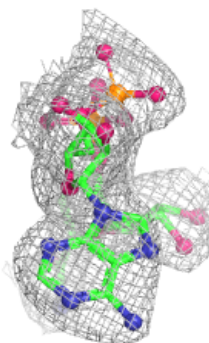
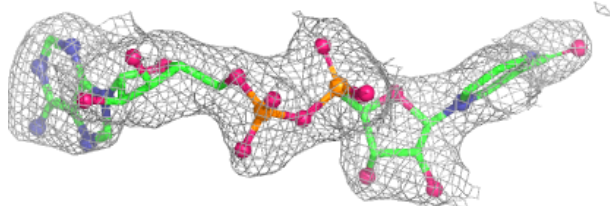
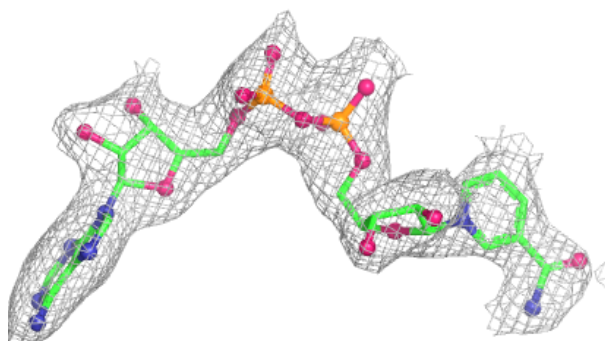
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 401:

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

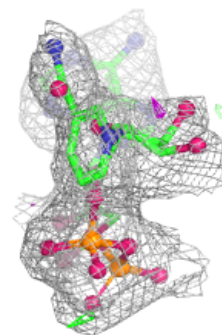
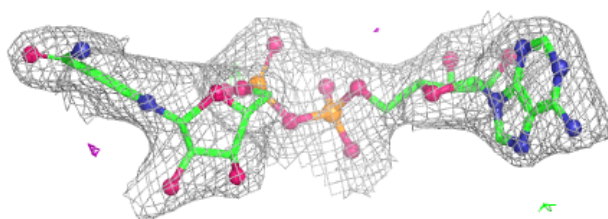
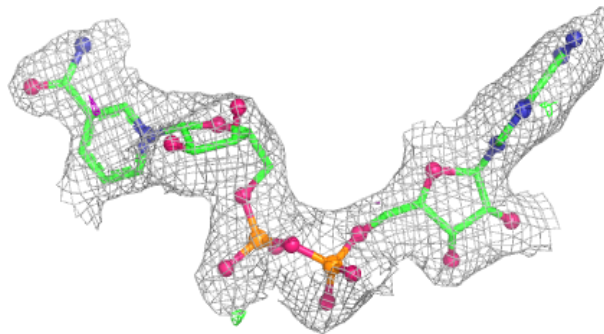
**Electron density around NAD B 401:**

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and green (positive)

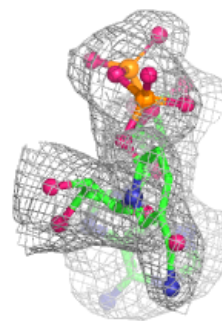
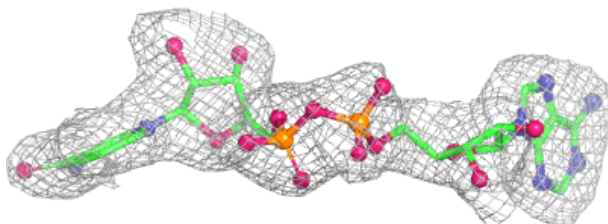
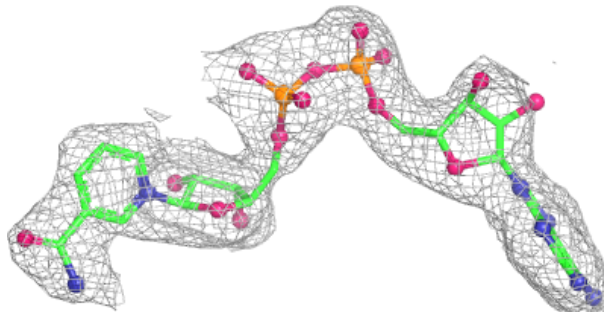


Electron density around NAD C 401:

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

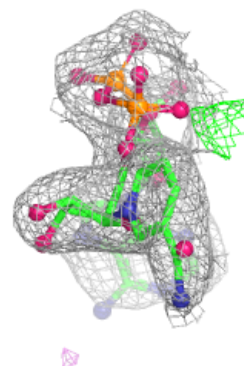
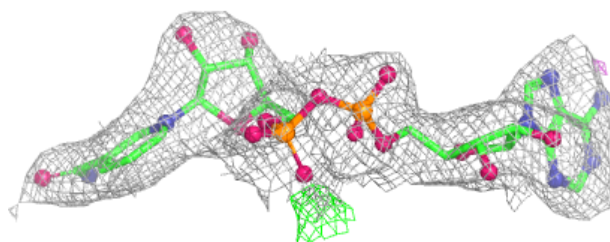
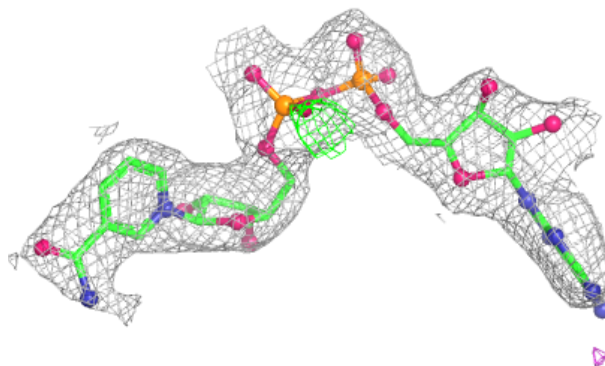
**Electron density around NAD D 401:**

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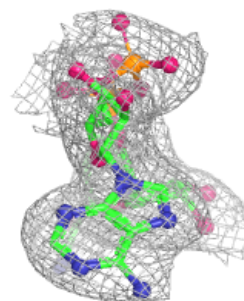
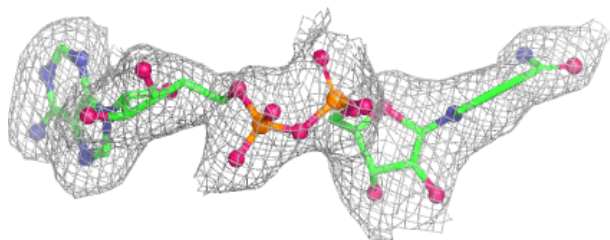
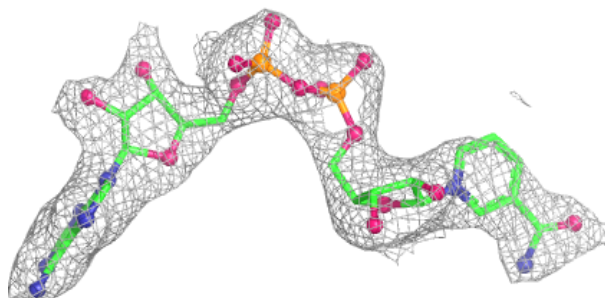


Electron density around NAD E 401:

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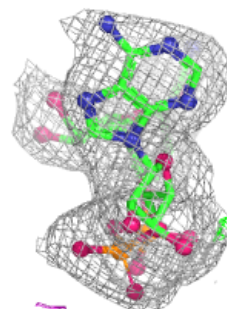
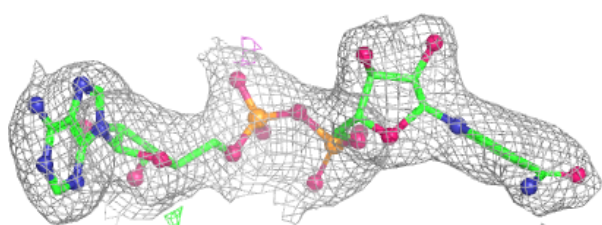
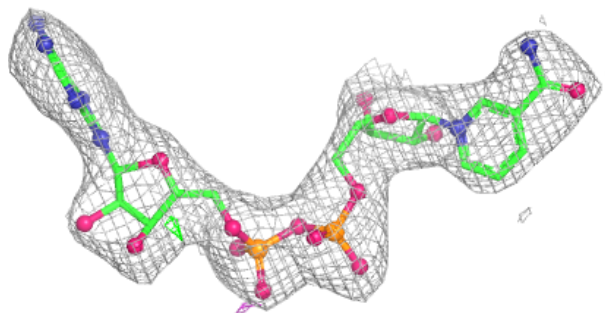
**Electron density around NAD F 401:**

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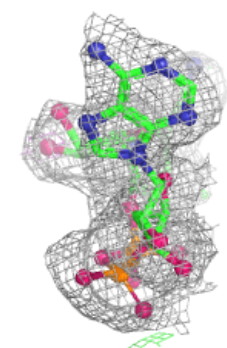
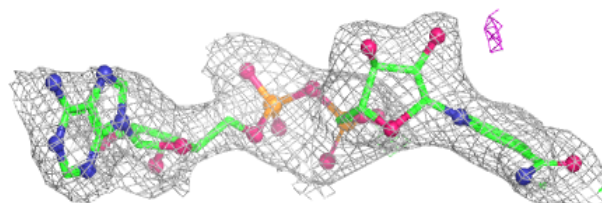
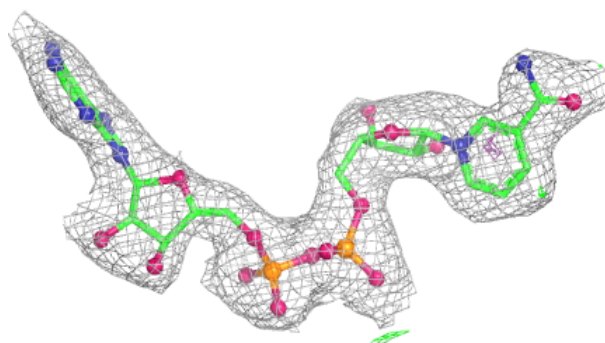


Electron density around NAD G 401:

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and green (positive)

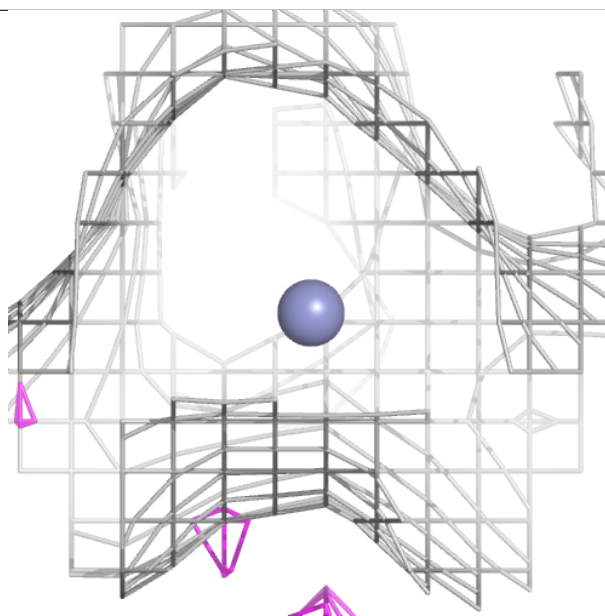
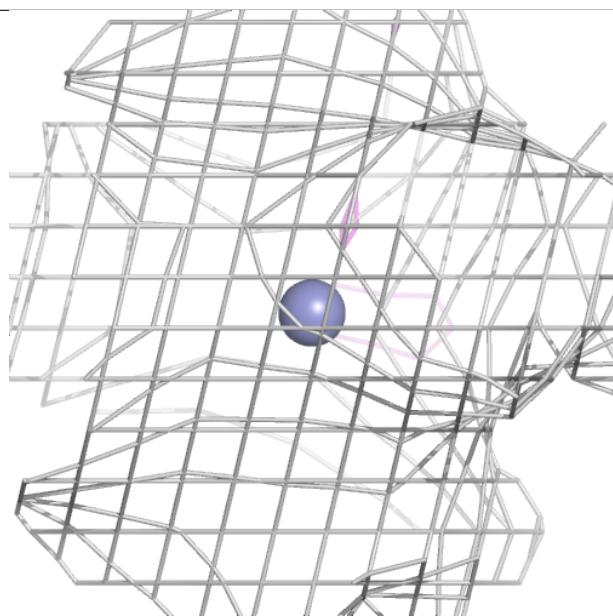
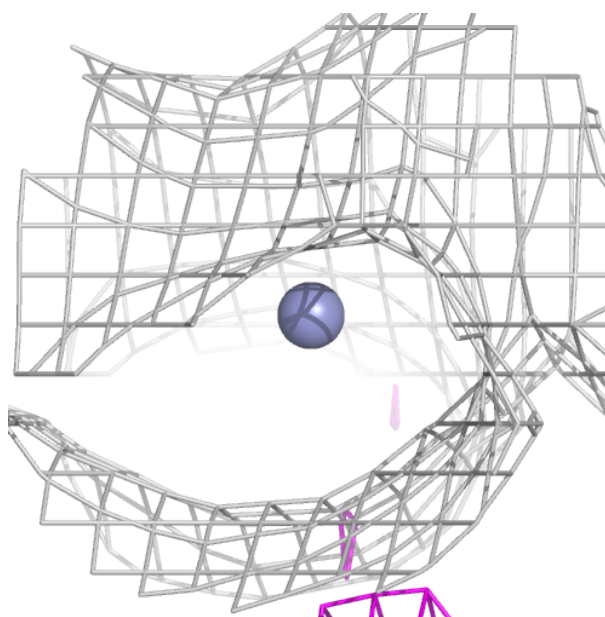
**Electron density around NAD H 401:**

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and green (positive)



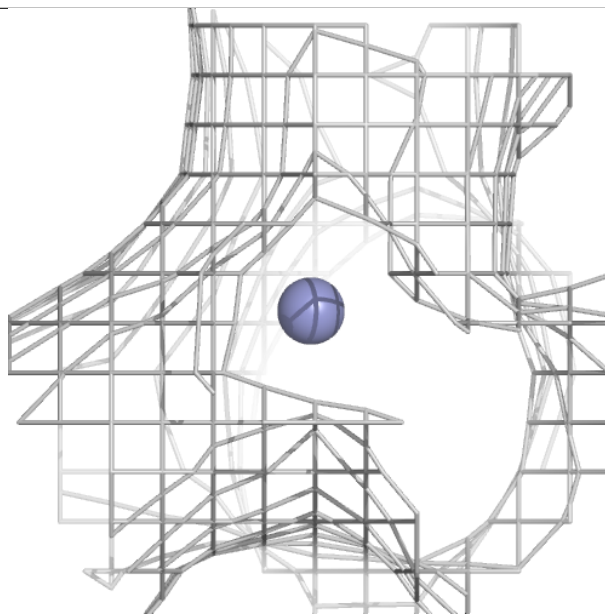
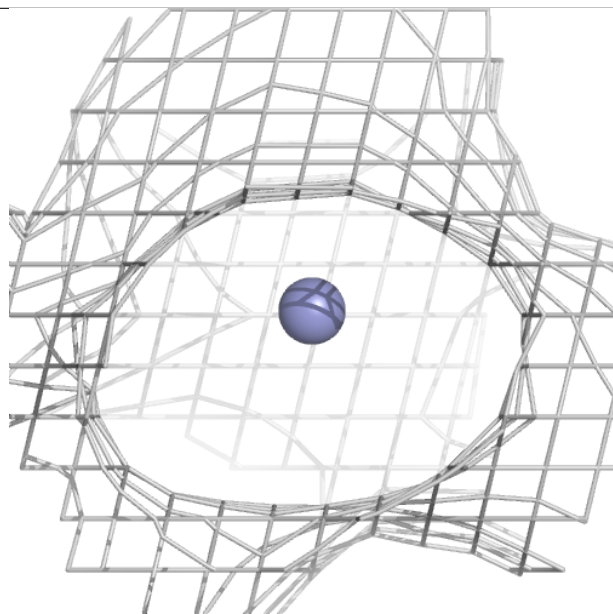
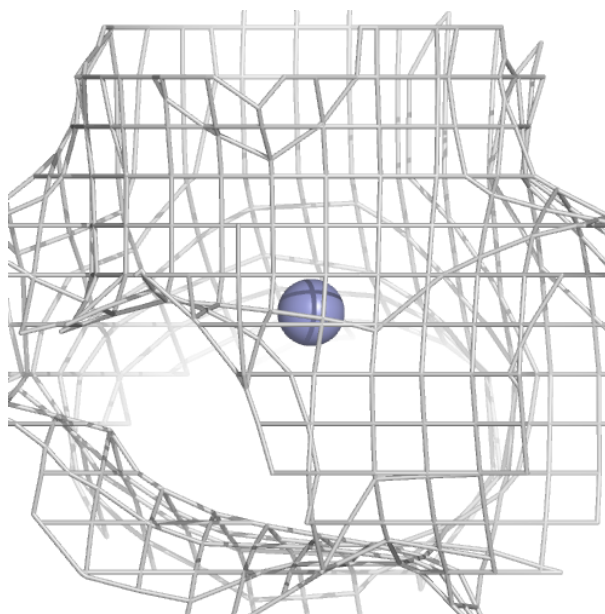
Electron density around ZN A 402:

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



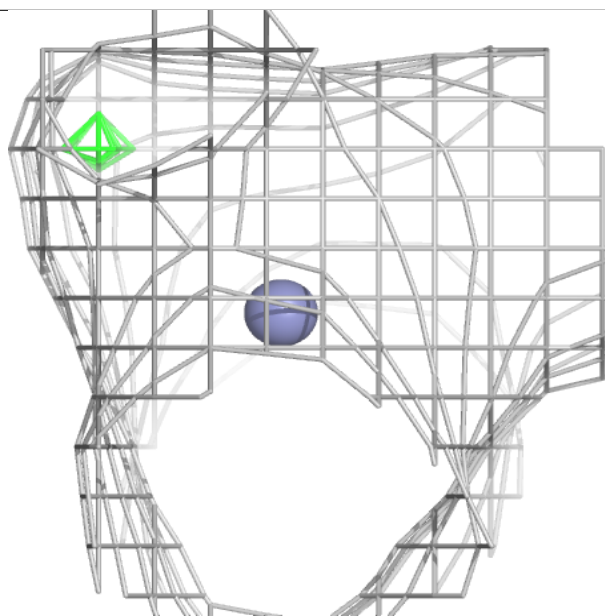
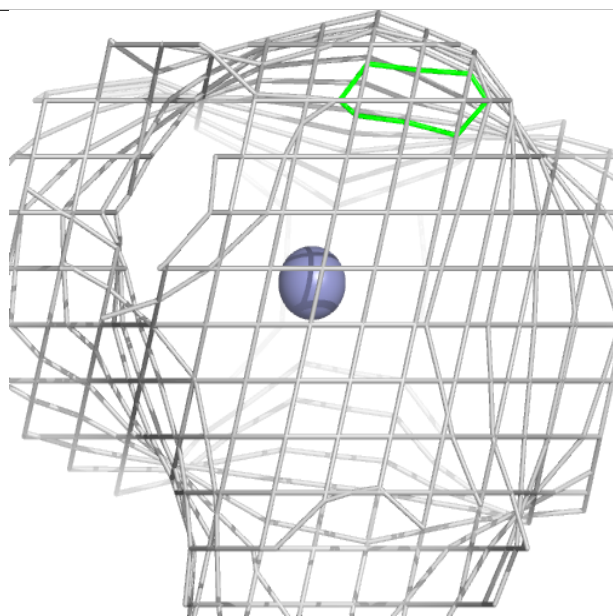
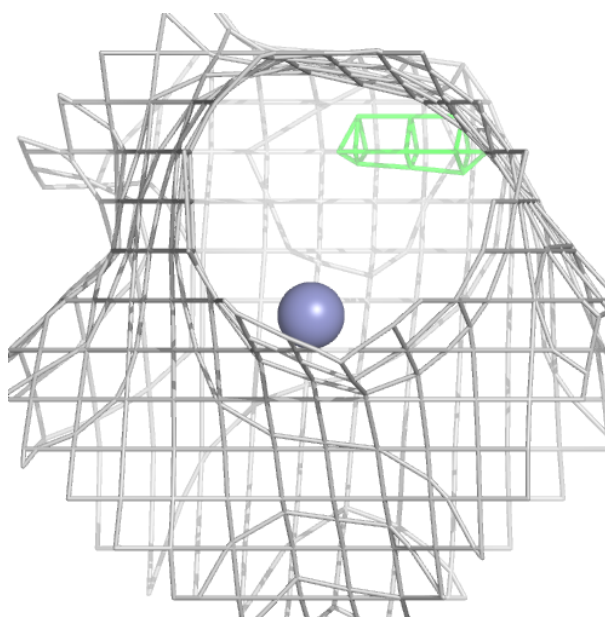
Electron density around ZN B 402:

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and green (positive)



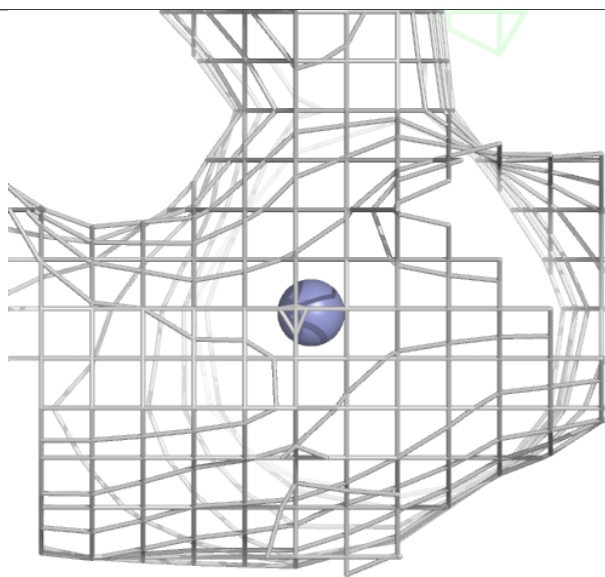
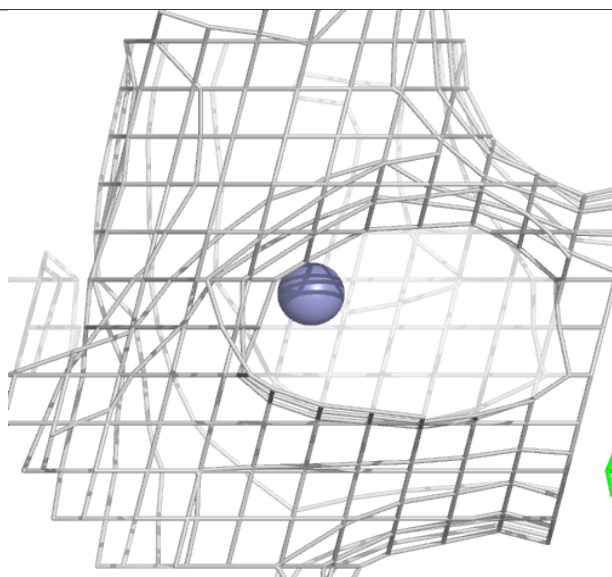
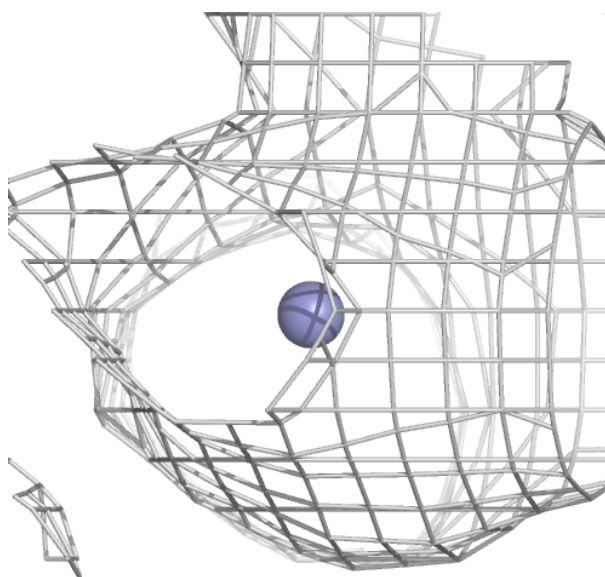
Electron density around ZN C 402:

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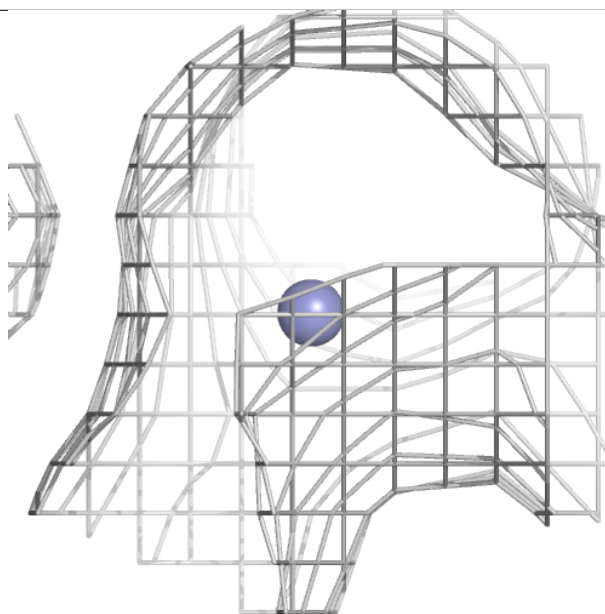
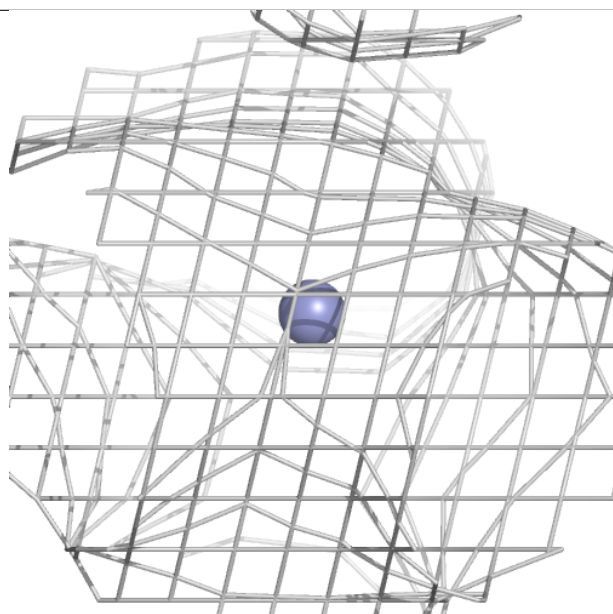
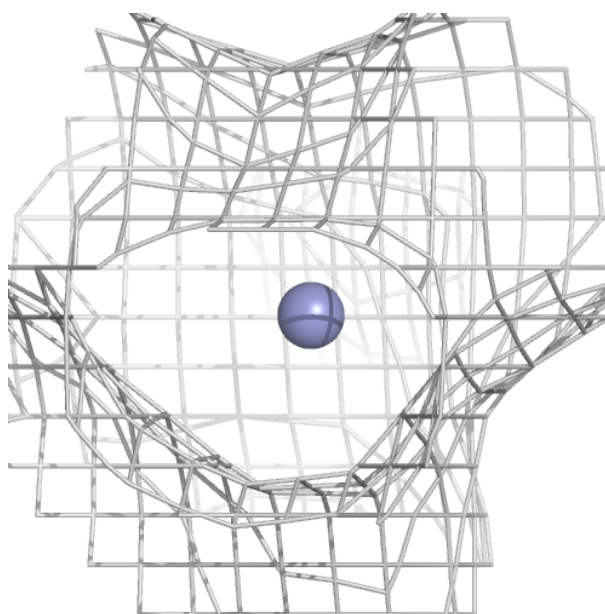
Electron density around ZN D 402:

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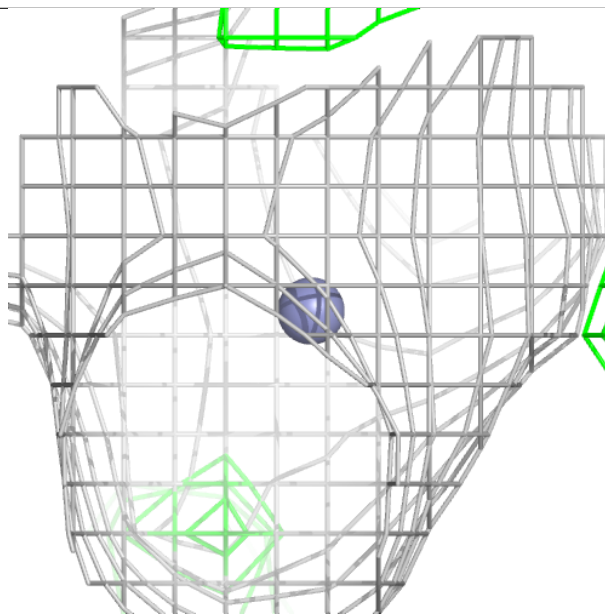
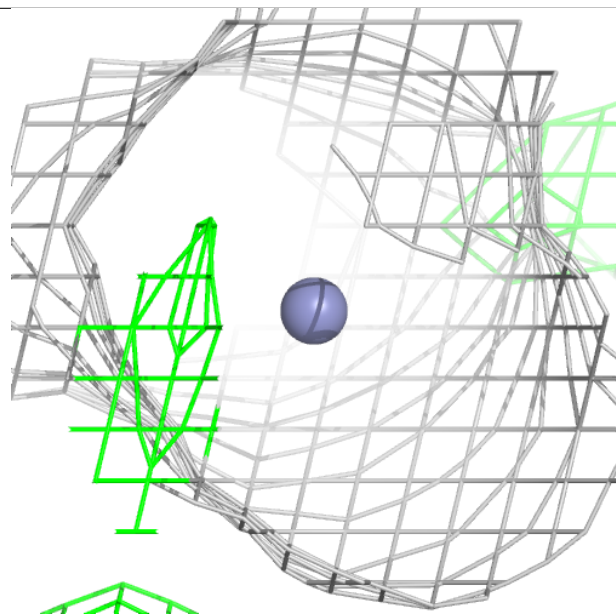
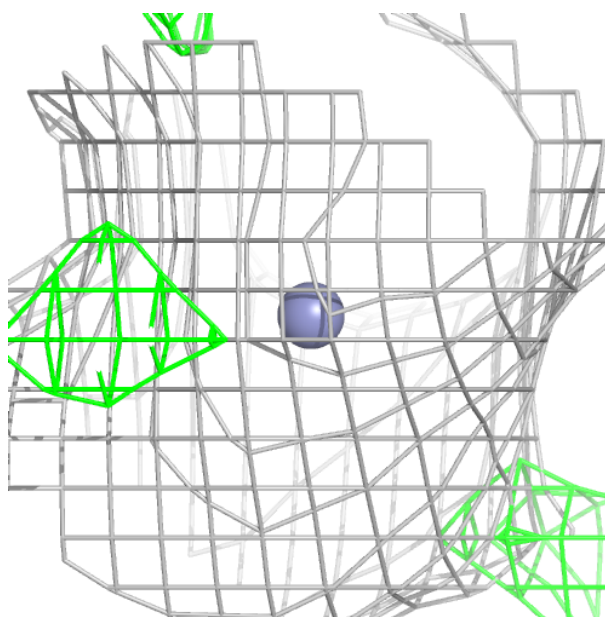
Electron density around ZN E 402:

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and green (positive)



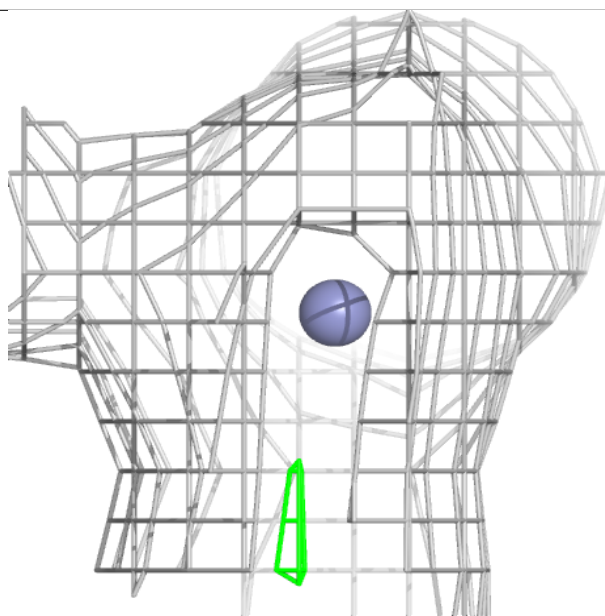
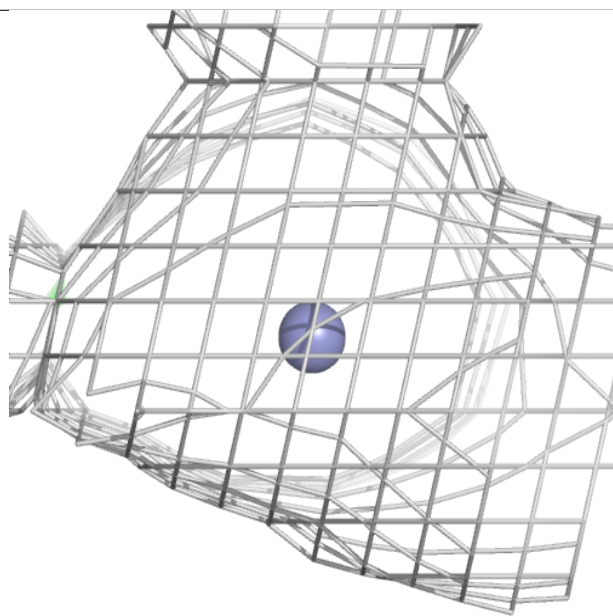
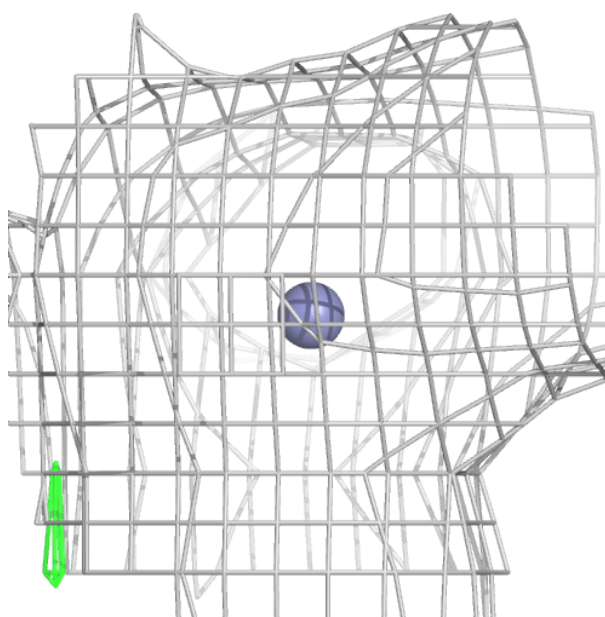
Electron density around ZN F 402:

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and green (positive)



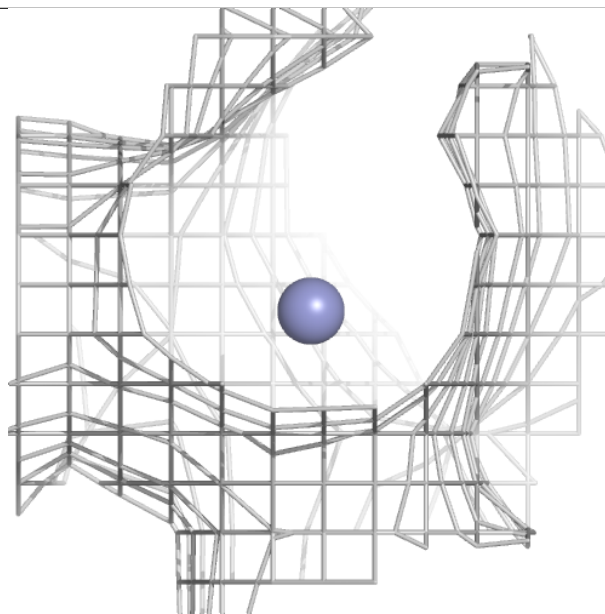
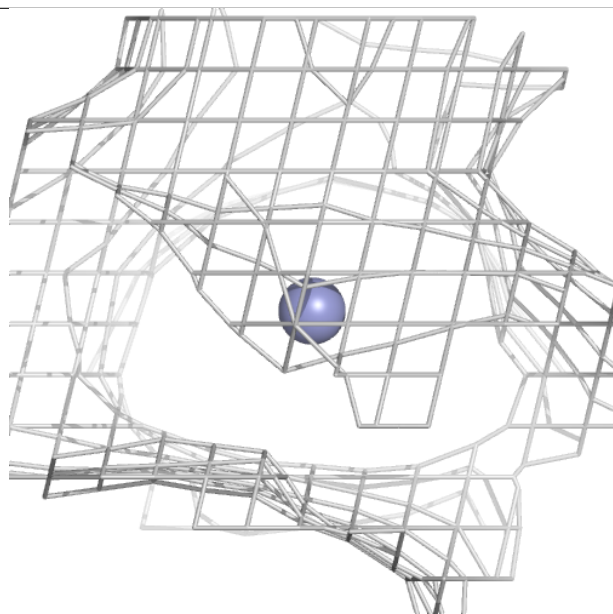
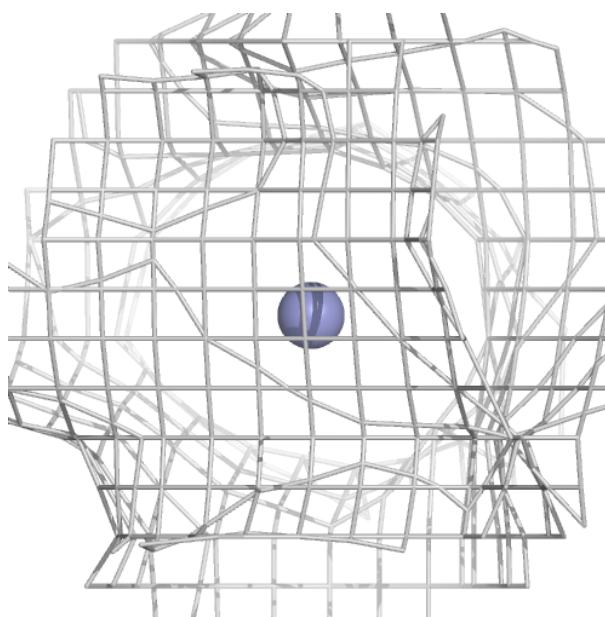
Electron density around ZN G 402:

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



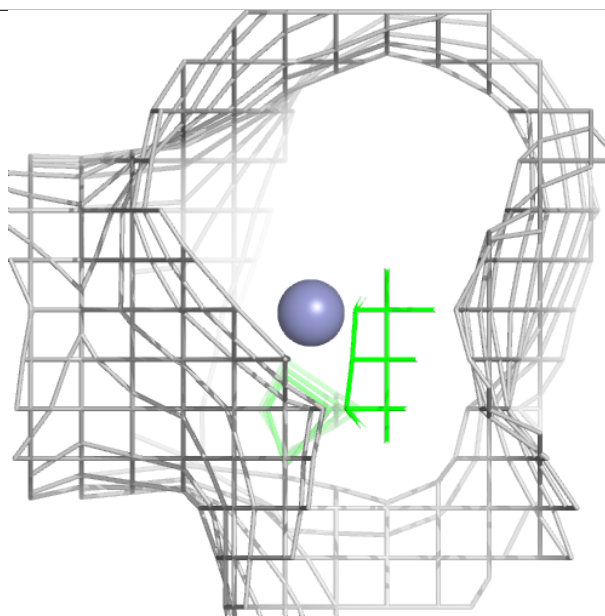
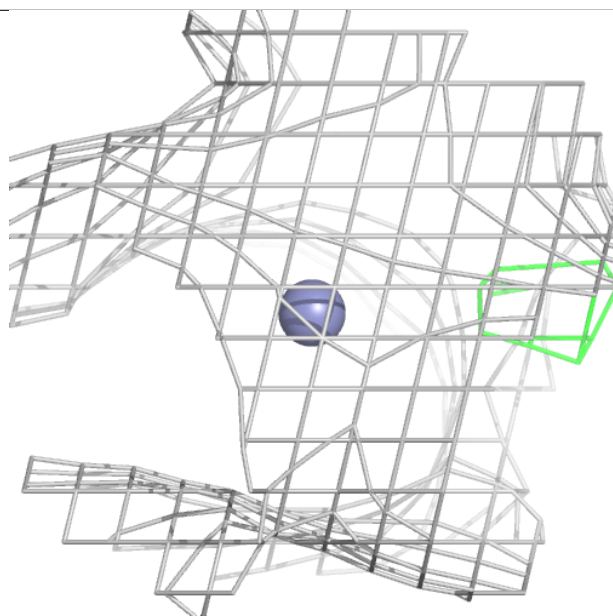
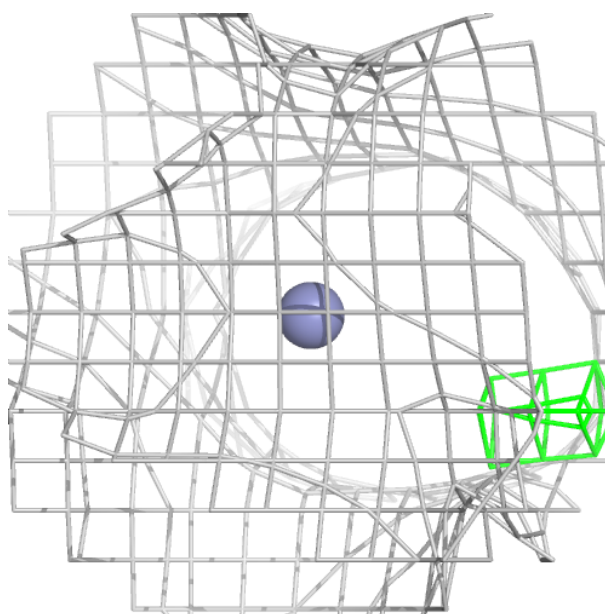
Electron density around ZN D 403:

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



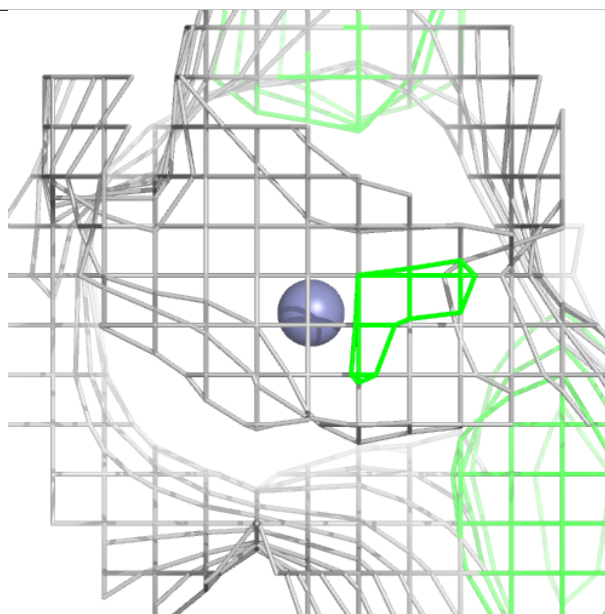
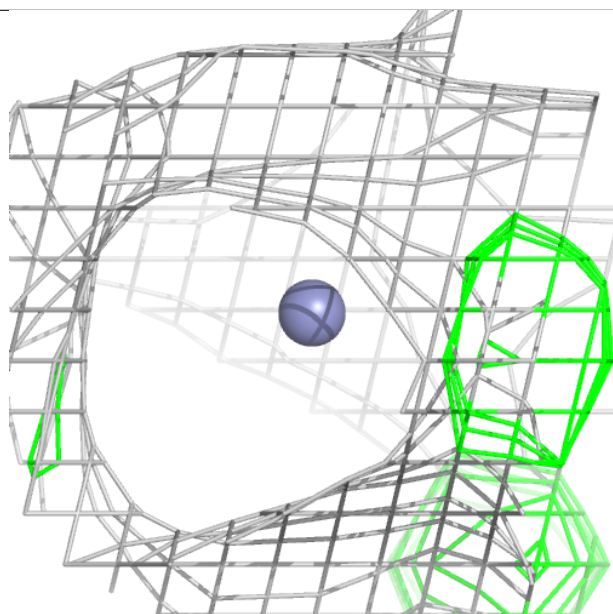
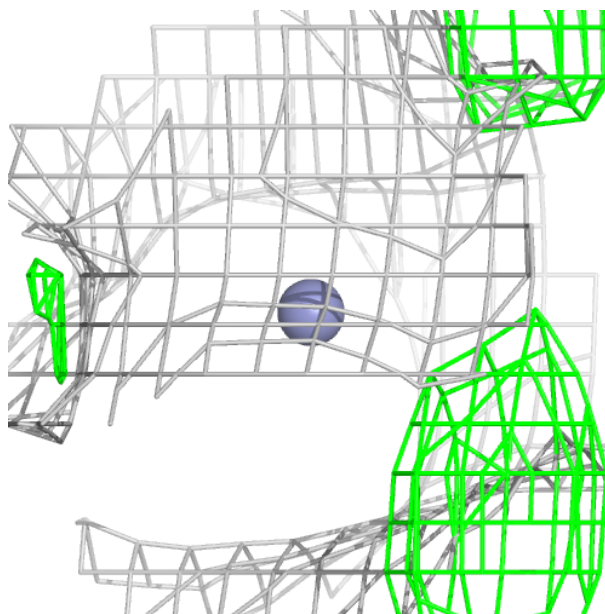
Electron density around ZN A 403:

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



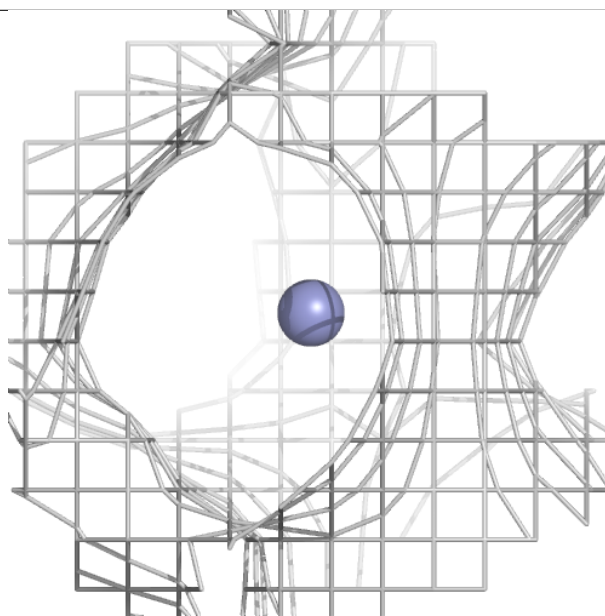
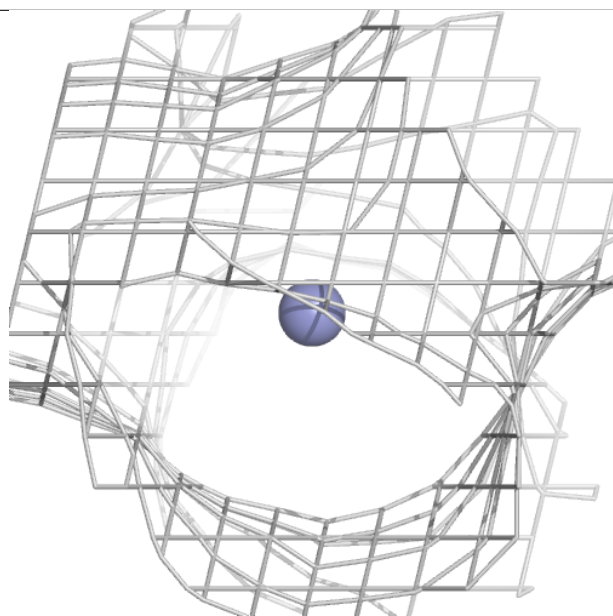
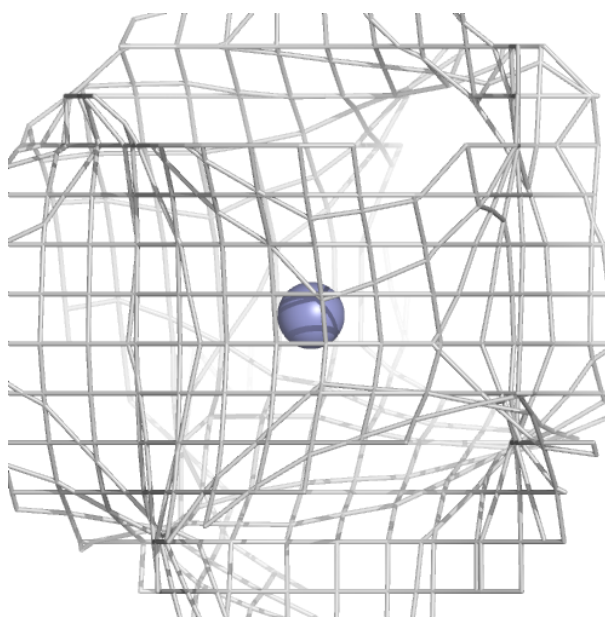
Electron density around ZN E 403:

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



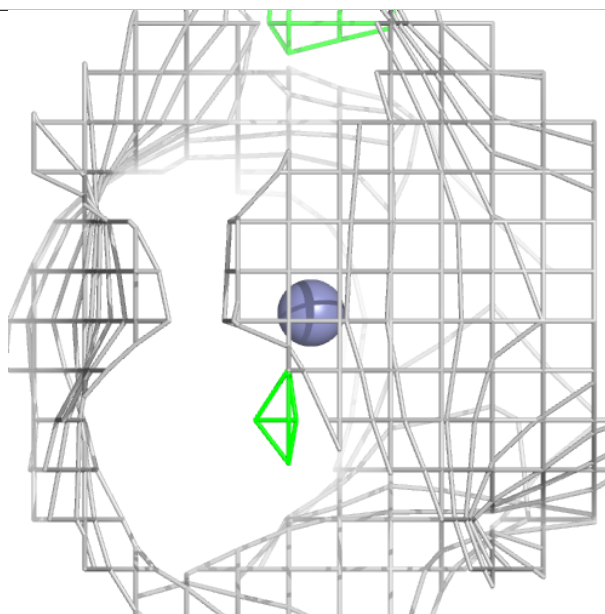
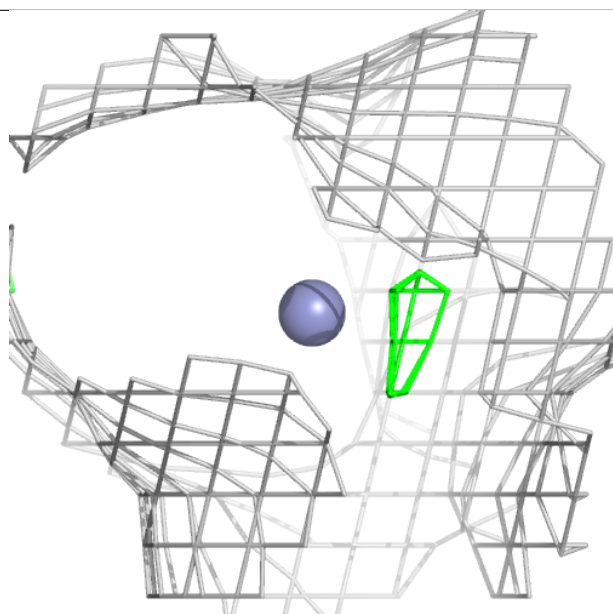
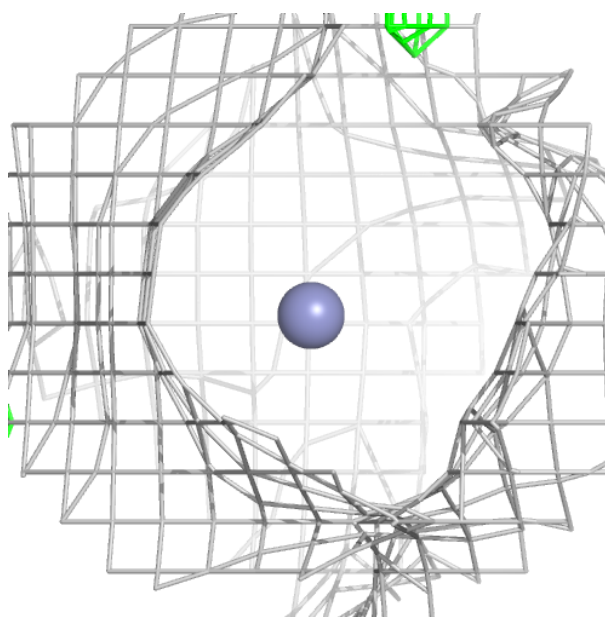
Electron density around ZN C 403:

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



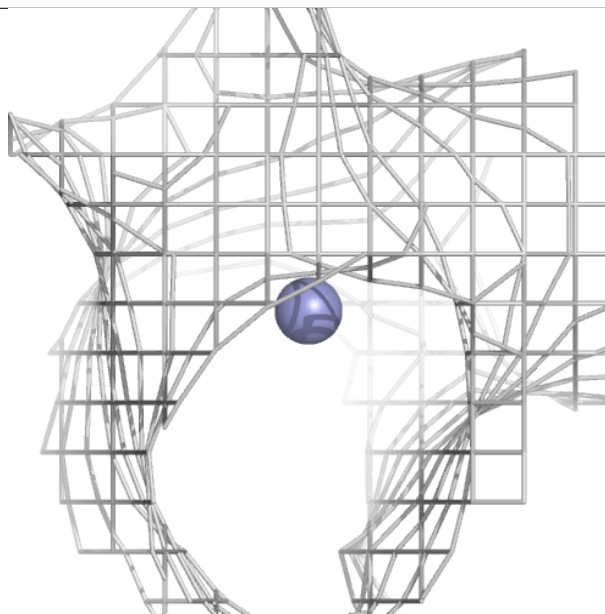
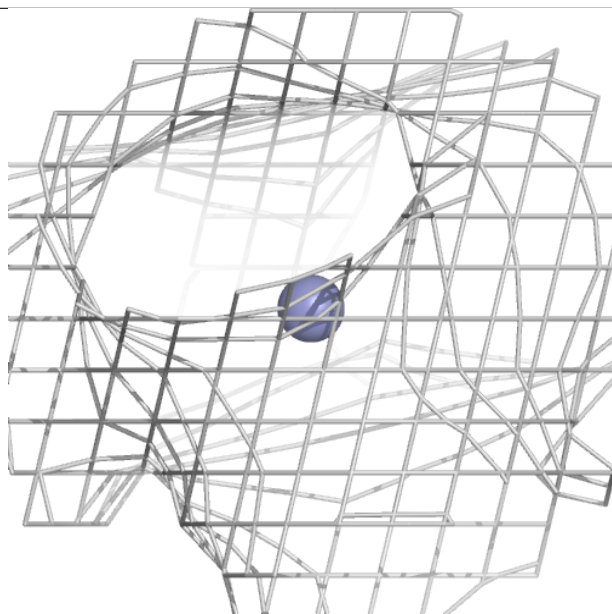
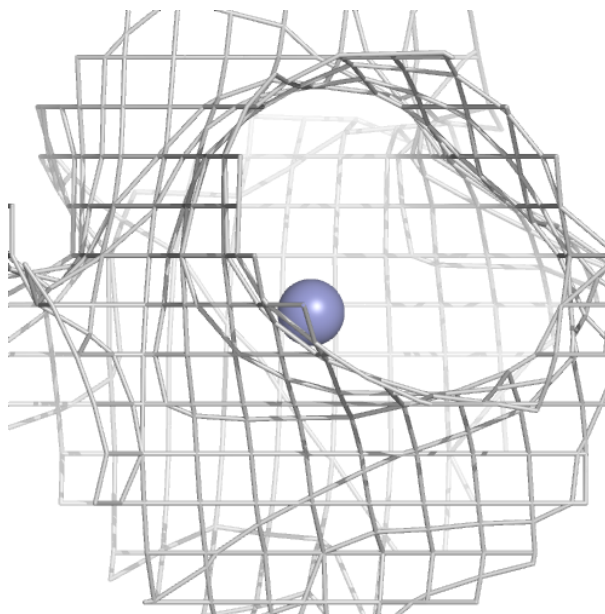
Electron density around ZN F 403:

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



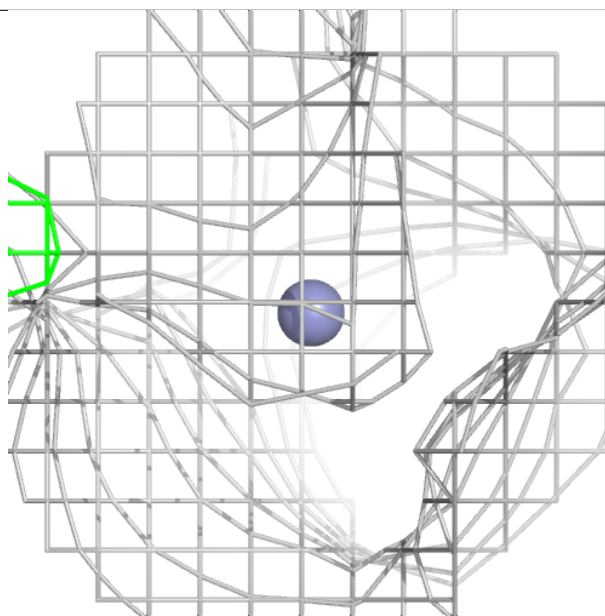
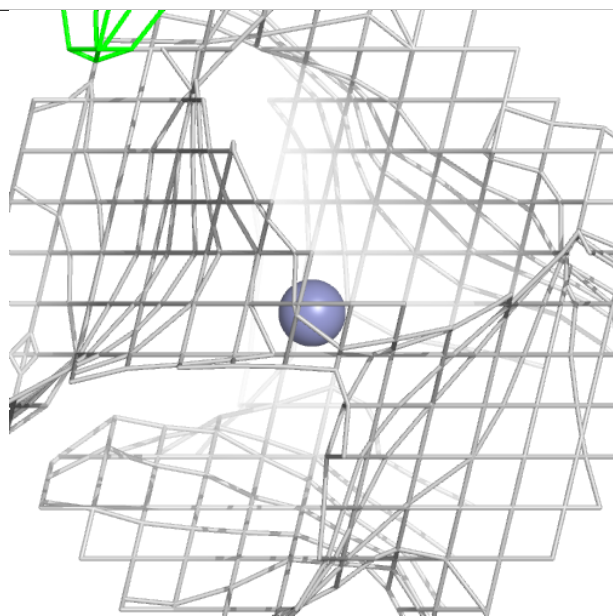
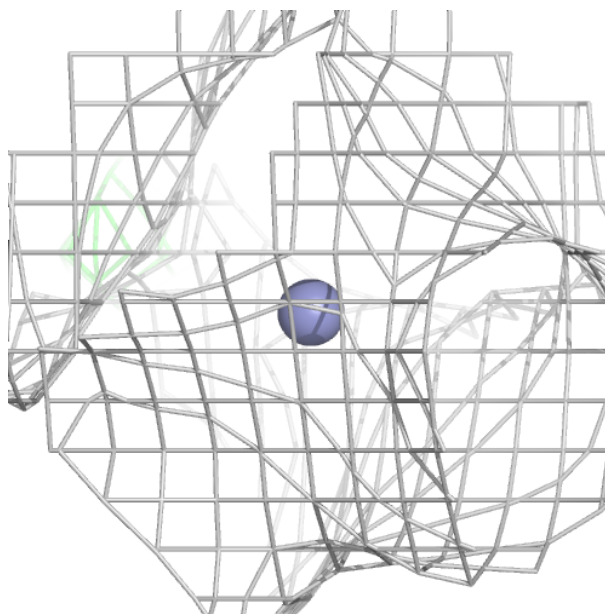
Electron density around ZN B 403:

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



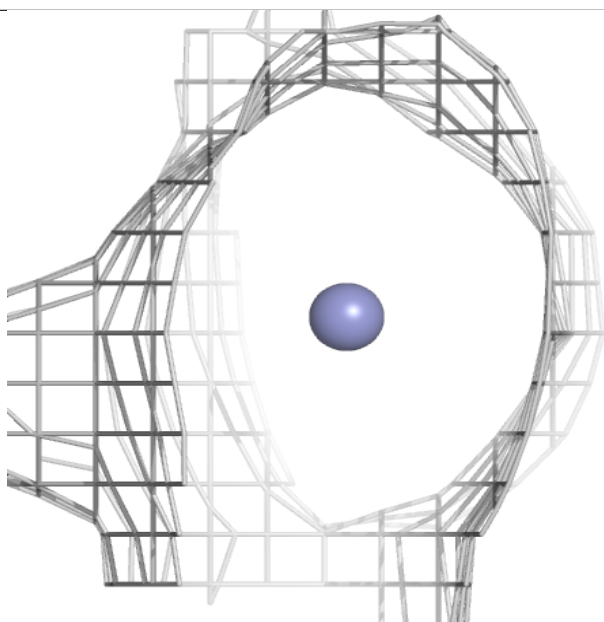
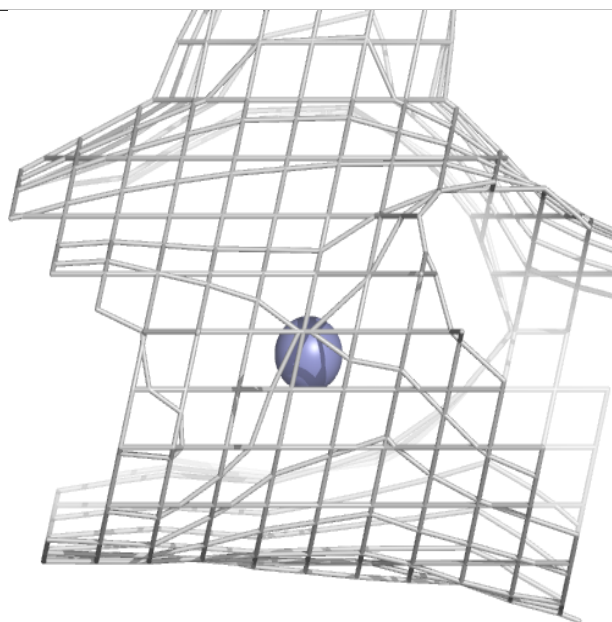
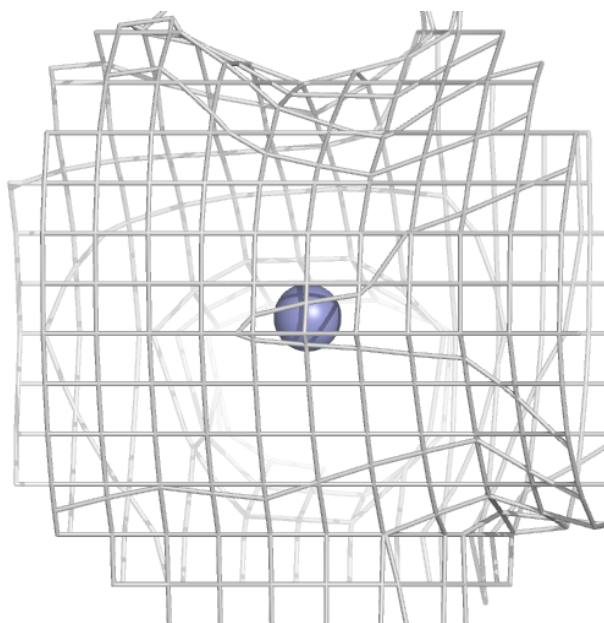
Electron density around ZN G 403:

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



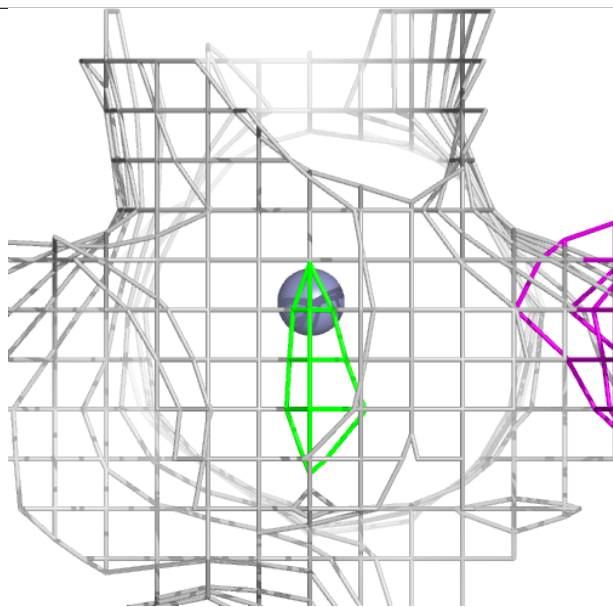
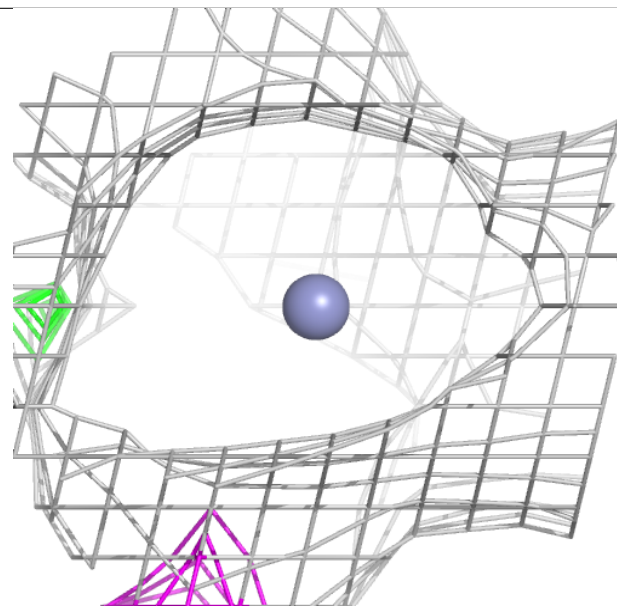
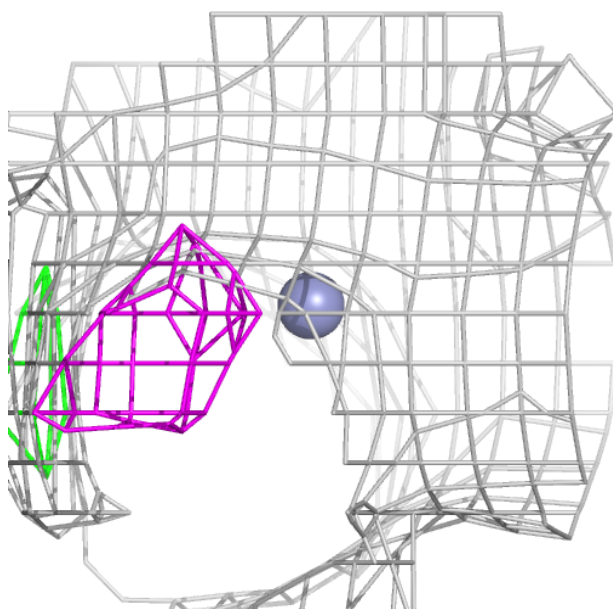
Electron density around ZN H 402:

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



Electron density around ZN H 403:

$2mF_o-DF_c$ (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.