



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 05:31 AM UTC

PDB ID : 8S3B / pdb_00008s3b
Title : Crystal structure of Medicago truncatula glutamate dehydrogenase 2 in complex with 3-(1H-Tetrazol-5-yl)benzoic acid and NAD
Authors : Grzechowiak, M.; Ruszkowski, M.
Deposited on : 2024-02-19
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 ⓘ 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

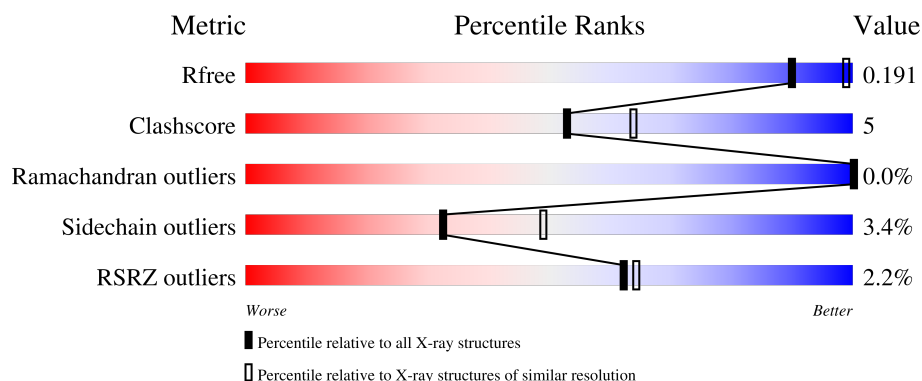
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



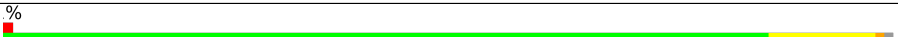
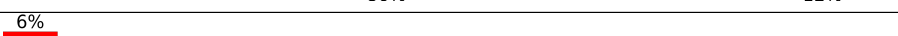
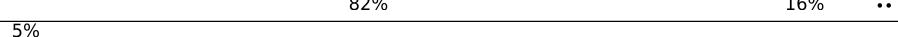
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 $\leq 5\%$. 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	414	 87% 11% ..
1	B	414	 86% 11% ..
1	C	414	 87% 11% ..
1	D	414	 85% 13% .
1	E	414	 87% 11% ..

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Mol	Chain	Length	Quality of chain	
1	F	414		86% 12% ..
1	G	414		83% 15% ..
1	H	414		87% 11% ..
1	I	414		86% 12% ..
1	J	414		82% 16% ..
1	K	414		82% 15% ..
1	L	414		84% 14% ..

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	A1H40	A	601	-	X	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 39595 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	1	0
			3135	1978	550	592	15			
1	B	410	Total	C	N	O	S	0	0	0
			3126	1973	548	590	15			
1	C	410	Total	C	N	O	S	0	0	0
			3126	1973	548	590	15			
1	D	412	Total	C	N	O	S	0	0	0
			3139	1981	550	592	16			
1	E	409	Total	C	N	O	S	0	0	0
			3118	1969	546	588	15			
1	F	410	Total	C	N	O	S	0	0	0
			3126	1973	548	590	15			
1	G	410	Total	C	N	O	S	0	1	0
			3135	1978	550	592	15			
1	H	410	Total	C	N	O	S	0	1	0
			3137	1979	552	591	15			
1	I	409	Total	C	N	O	S	0	0	0
			3118	1969	546	588	15			
1	J	409	Total	C	N	O	S	0	0	0
			3118	1969	546	588	15			
1	K	408	Total	C	N	O	S	0	0	0
			3113	1966	545	587	15			
1	L	409	Total	C	N	O	S	0	0	0
			3118	1969	546	588	15			

There are 36 discrepancies between the modelled and reference sequences:

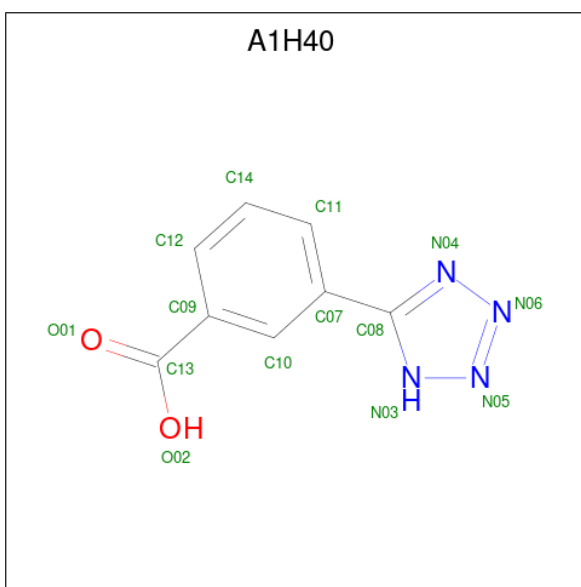
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP G7JYL4
A	-1	ASN	-	expression tag	UNP G7JYL4
A	0	ALA	-	expression tag	UNP G7JYL4
B	-2	SER	-	expression tag	UNP G7JYL4
B	-1	ASN	-	expression tag	UNP G7JYL4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP G7JYL4
C	-2	SER	-	expression tag	UNP G7JYL4
C	-1	ASN	-	expression tag	UNP G7JYL4
C	0	ALA	-	expression tag	UNP G7JYL4
D	-2	SER	-	expression tag	UNP G7JYL4
D	-1	ASN	-	expression tag	UNP G7JYL4
D	0	ALA	-	expression tag	UNP G7JYL4
E	-2	SER	-	expression tag	UNP G7JYL4
E	-1	ASN	-	expression tag	UNP G7JYL4
E	0	ALA	-	expression tag	UNP G7JYL4
F	-2	SER	-	expression tag	UNP G7JYL4
F	-1	ASN	-	expression tag	UNP G7JYL4
F	0	ALA	-	expression tag	UNP G7JYL4
G	-2	SER	-	expression tag	UNP G7JYL4
G	-1	ASN	-	expression tag	UNP G7JYL4
G	0	ALA	-	expression tag	UNP G7JYL4
H	-2	SER	-	expression tag	UNP G7JYL4
H	-1	ASN	-	expression tag	UNP G7JYL4
H	0	ALA	-	expression tag	UNP G7JYL4
I	-2	SER	-	expression tag	UNP G7JYL4
I	-1	ASN	-	expression tag	UNP G7JYL4
I	0	ALA	-	expression tag	UNP G7JYL4
J	-2	SER	-	expression tag	UNP G7JYL4
J	-1	ASN	-	expression tag	UNP G7JYL4
J	0	ALA	-	expression tag	UNP G7JYL4
K	-2	SER	-	expression tag	UNP G7JYL4
K	-1	ASN	-	expression tag	UNP G7JYL4
K	0	ALA	-	expression tag	UNP G7JYL4
L	-2	SER	-	expression tag	UNP G7JYL4
L	-1	ASN	-	expression tag	UNP G7JYL4
L	0	ALA	-	expression tag	UNP G7JYL4

- Molecule 2 is 3-(1 {H}-1,2,3,4-tetrazol-5-yl)benzoic acid (CCD ID: A1H40) (formula: C₈H₆N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	4	2		
2	B	1	Total	C	N	O	0	0
			14	8	4	2		
2	C	1	Total	C	N	O	0	0
			14	8	4	2		
2	D	1	Total	C	N	O	0	0
			14	8	4	2		
2	H	1	Total	C	N	O	0	0
			14	8	4	2		
2	K	1	Total	C	N	O	0	0
			14	8	4	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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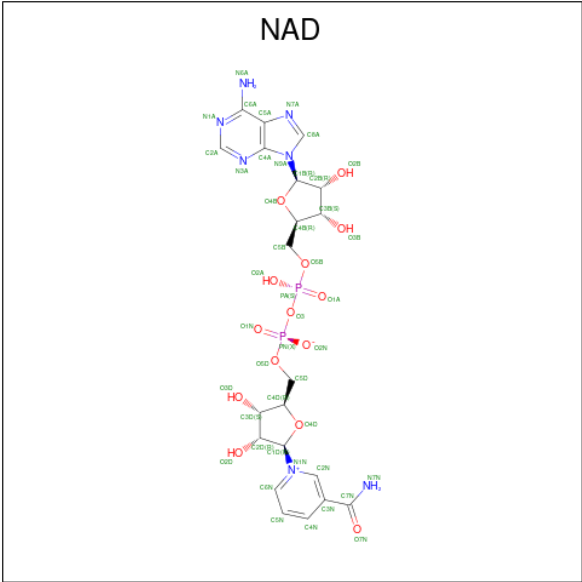
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	G	1	Total 4	C 2	O 2	0	0
3	H	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	I	1	Total 4	C 2	O 2	0	0
3	J	1	Total 4	C 2	O 2	0	0
3	K	1	Total 4	C 2	O 2	0	0
3	K	1	Total 4	C 2	O 2	0	0
3	K	1	Total 4	C 2	O 2	0	0
3	L	1	Total 4	C 2	O 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



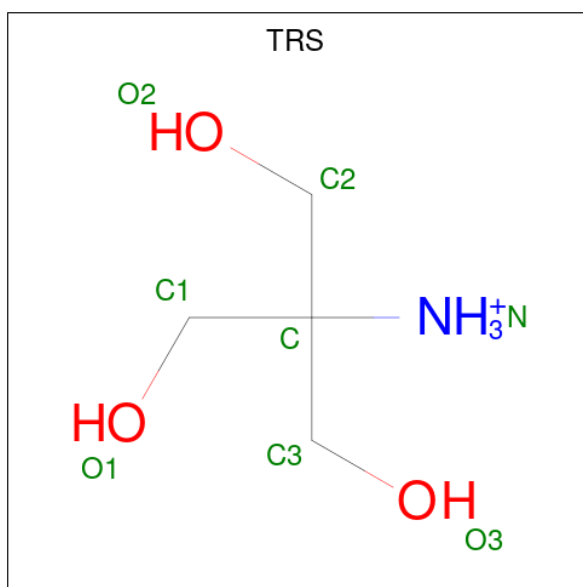
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	G	1	Total	C	O	0	0
			7	4	3		
4	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 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
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
5	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		
6	G	1	Total	C	N	O	0	0
			8	4	1	3		
6	H	1	Total	C	N	O	0	0
			8	4	1	3		
6	I	1	Total	C	N	O	0	0
			8	4	1	3		
6	K	1	Total	C	N	O	0	0
			8	4	1	3		
6	L	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

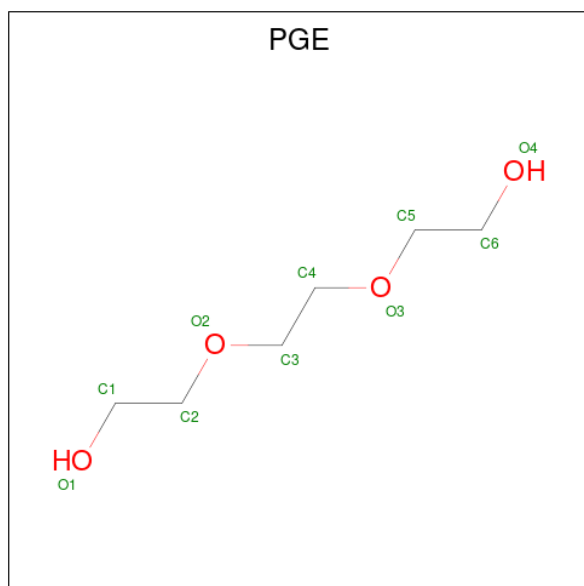
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		

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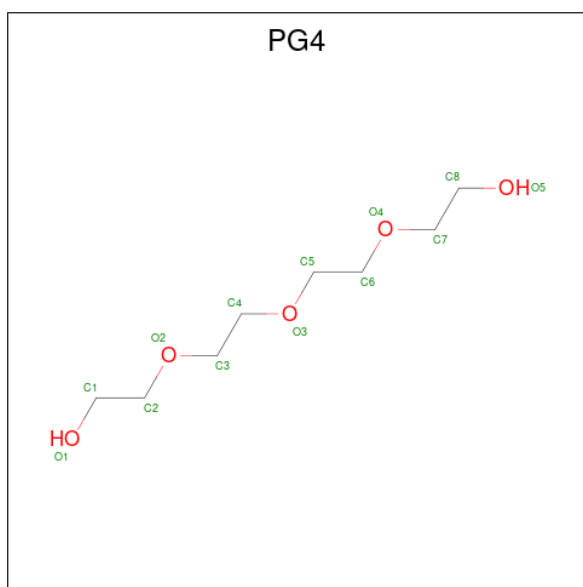
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Ca	0	0
			1	1		
7	F	1	Total	Ca	0	0
			1	1		
7	G	1	Total	Ca	0	0
			1	1		
7	H	1	Total	Ca	0	0
			1	1		
7	I	1	Total	Ca	0	0
			1	1		
7	J	1	Total	Ca	0	0
			1	1		
7	K	1	Total	Ca	0	0
			1	1		
7	L	1	Total	Ca	0	0
			1	1		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	F	1	Total	Na	0	0
			1	1		
10	G	1	Total	Na	0	0
			1	1		
10	I	1	Total	Na	0	0
			1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	133	Total	O	0	0
			133	133		
11	B	183	Total	O	0	0
			183	183		
11	C	135	Total	O	0	0
			135	135		
11	D	134	Total	O	0	0
			134	134		
11	E	97	Total	O	0	0
			97	97		

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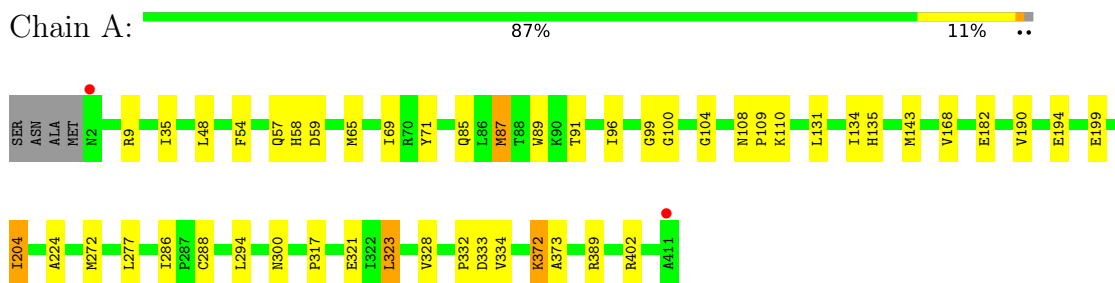
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	F	81	Total 81	O 81	0	0
11	G	85	Total 85	O 85	0	0
11	H	81	Total 81	O 81	0	0
11	I	82	Total 82	O 82	0	0
11	J	73	Total 73	O 73	0	0
11	K	62	Total 62	O 62	0	0
11	L	62	Total 62	O 62	0	0

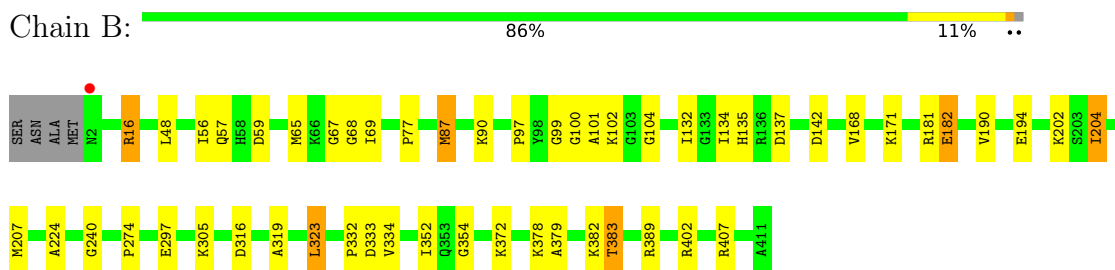
3 Residue-property plots [i](#)

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.

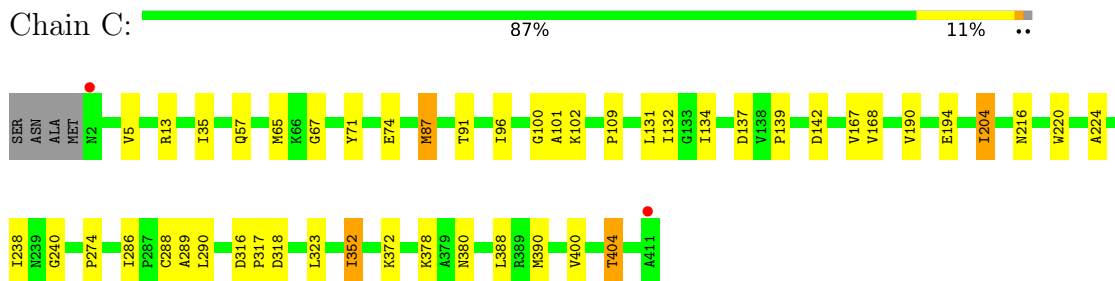
- Molecule 1: Glutamate dehydrogenase



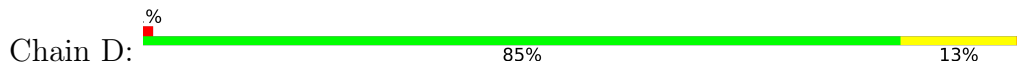
- Molecule 1: Glutamate dehydrogenase

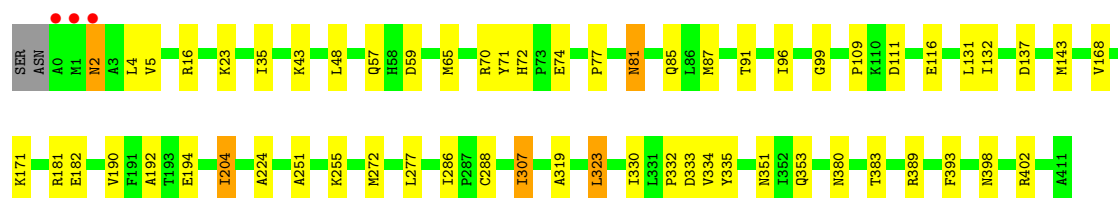


- Molecule 1: Glutamate dehydrogenase

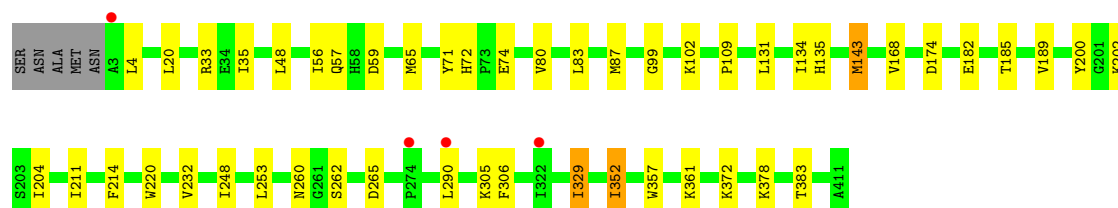
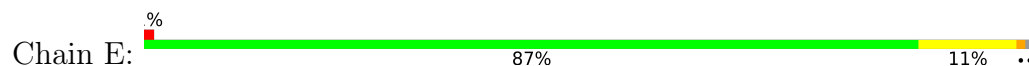


- Molecule 1: Glutamate dehydrogenase

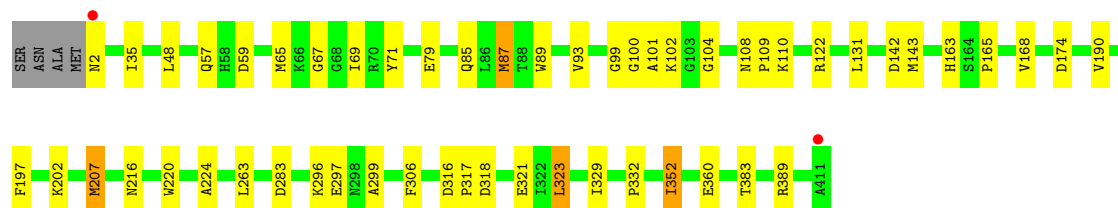
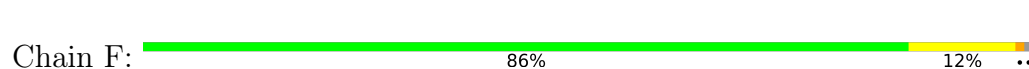




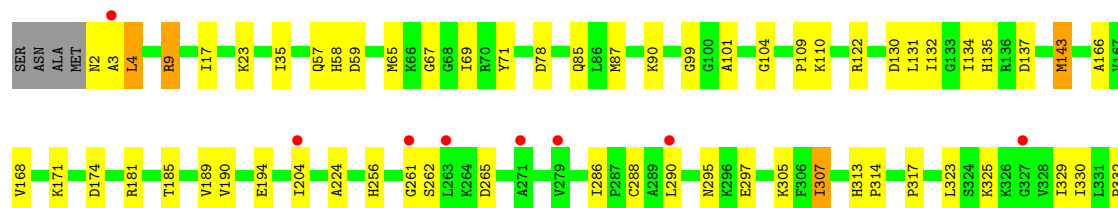
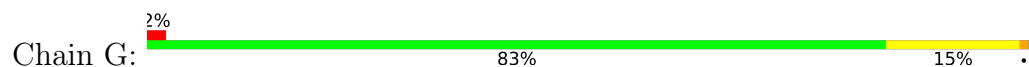
- Molecule 1: Glutamate dehydrogenase



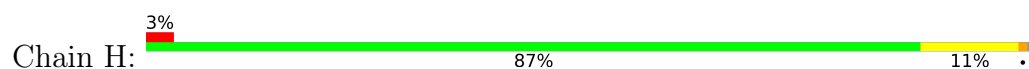
- Molecule 1: Glutamate dehydrogenase

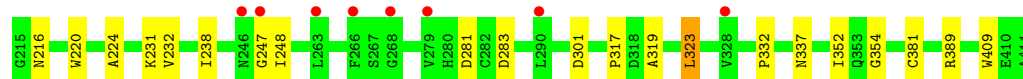


- Molecule 1: Glutamate dehydrogenase

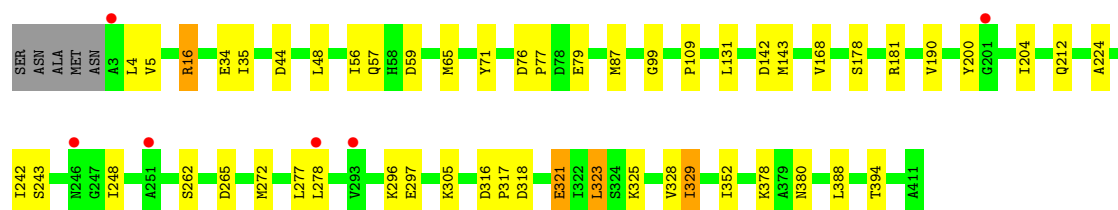
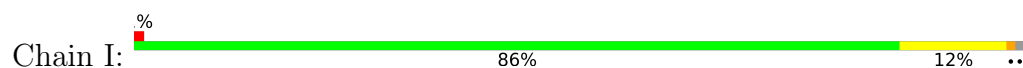


- Molecule 1: Glutamate dehydrogenase

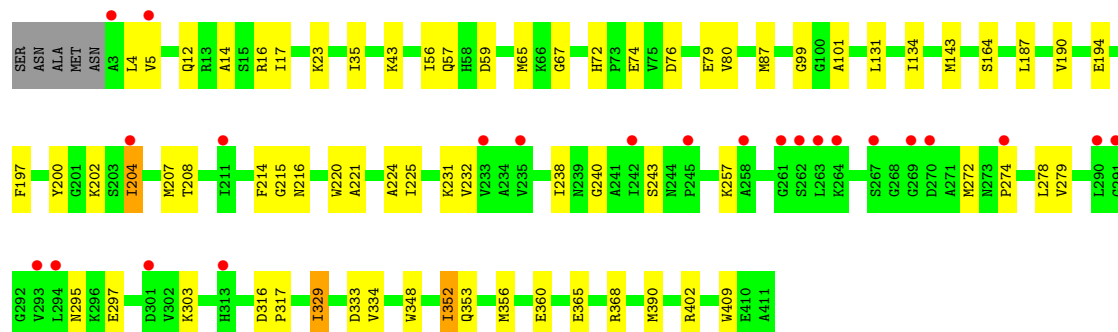
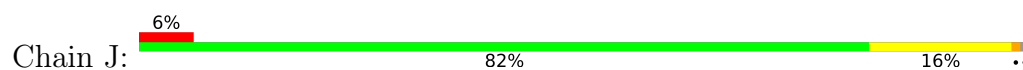




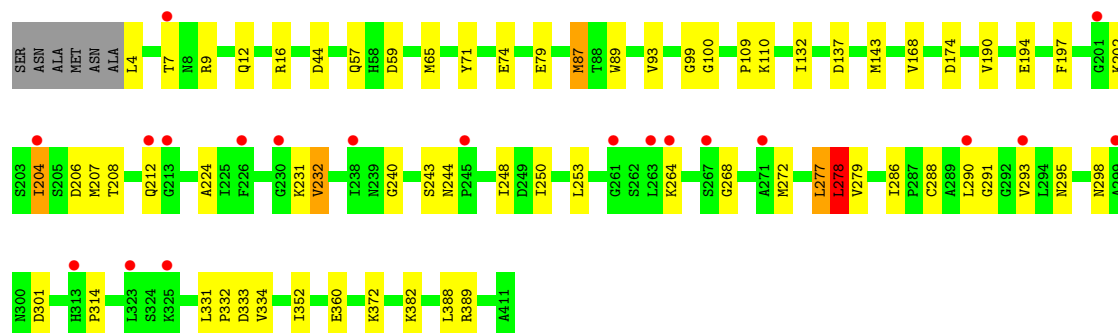
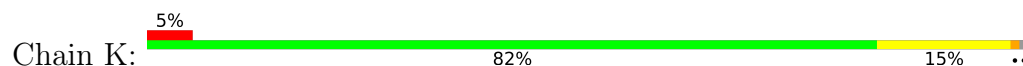
- Molecule 1: Glutamate dehydrogenase



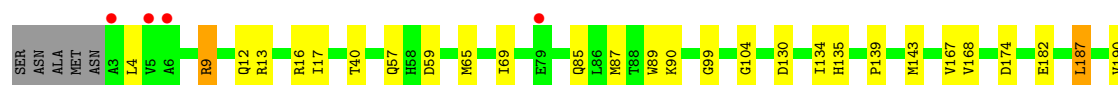
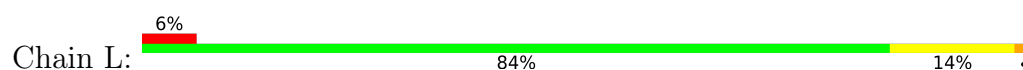
- Molecule 1: Glutamate dehydrogenase

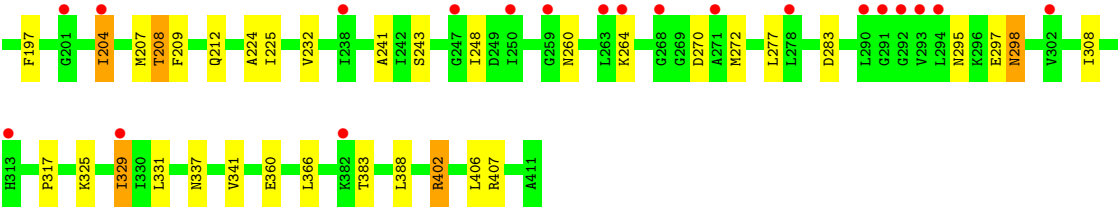


- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.81Å 109.86Å 156.37Å 79.00° 78.48° 72.22°	Depositor
Resolution (Å)	65.69 – 2.30 65.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	84.0 (65.69-2.30) 84.4 (65.69-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.169 , 0.188 0.170 , 0.191	Depositor DCC
R_{free} test set	1152 reflections (0.42%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39595	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1H40, TRS, CA, PGE, PG4, NA, NAD, PEG, EDO

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	0.40	0/3197	0.58	0/4328
1	B	0.43	0/3188	0.60	0/4316
1	C	0.39	0/3188	0.59	0/4316
1	D	0.42	0/3201	0.59	0/4333
1	E	0.36	0/3180	0.57	0/4305
1	F	0.37	0/3188	0.56	0/4316
1	G	0.35	0/3197	0.53	0/4328
1	H	0.33	0/3199	0.53	0/4330
1	I	0.35	0/3180	0.53	0/4305
1	J	0.35	0/3180	0.55	0/4305
1	K	0.33	0/3175	0.55	0/4298
1	L	0.34	0/3180	0.52	0/4305
All	All	0.37	0/38253	0.56	0/51785

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3135	0	3117	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3126	0	3110	36	0
1	C	3126	0	3110	30	0
1	D	3139	0	3127	32	0
1	E	3118	0	3104	29	0
1	F	3126	0	3110	31	0
1	G	3135	0	3117	39	0
1	H	3137	0	3122	27	0
1	I	3118	0	3104	28	0
1	J	3118	0	3104	42	0
1	K	3113	0	3099	40	0
1	L	3118	0	3104	37	0
2	A	14	0	0	0	0
2	B	14	0	0	1	0
2	C	14	0	0	0	0
2	D	14	0	0	1	0
2	H	14	0	0	0	0
2	K	14	0	0	0	0
3	A	20	0	30	3	0
3	B	16	0	24	4	0
3	C	8	0	12	2	0
3	D	4	0	6	1	0
3	E	4	0	6	0	0
3	F	8	0	12	1	0
3	G	12	0	18	1	0
3	H	4	0	6	0	0
3	I	20	0	30	5	0
3	J	4	0	6	0	0
3	K	12	0	18	1	0
3	L	4	0	6	0	0
4	A	7	0	10	1	0
4	C	14	0	20	2	0
4	D	7	0	10	0	0
4	E	7	0	10	1	0
4	F	7	0	10	2	0
4	G	7	0	10	0	0
4	H	7	0	10	1	0
5	A	44	0	26	0	0
5	B	44	0	26	0	0
5	C	44	0	26	3	0
5	D	44	0	26	1	0
5	E	44	0	26	0	0
5	F	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	44	0	26	0	0
5	H	44	0	26	2	0
5	I	44	0	26	0	0
5	J	44	0	26	2	0
5	K	44	0	26	0	0
5	L	44	0	26	0	0
6	A	8	0	12	0	0
6	D	8	0	12	0	0
6	G	8	0	12	0	0
6	H	8	0	12	1	0
6	I	8	0	12	2	0
6	K	8	0	12	1	0
6	L	8	0	12	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
8	B	10	0	14	3	0
9	B	13	0	18	2	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	I	1	0	0	0	0
11	A	133	0	0	4	0
11	B	183	0	0	3	0
11	C	135	0	0	0	0
11	D	134	0	0	1	0
11	E	97	0	0	1	0
11	F	81	0	0	0	0
11	G	85	0	0	1	0
11	H	81	0	0	2	0
11	I	82	0	0	0	0
11	J	73	0	0	3	0
11	K	62	0	0	0	0
11	L	62	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	39595	0	38010	385	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 5.

The worst 5 of 385 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:GLU:HG3	1:G:204:ILE:HD11	1.59	0.82
1:J:17:ILE:HD12	1:J:390:MET:HE2	1.63	0.80
1:D:334:VAL:HG21	1:D:393:PHE:CE2	2.21	0.75
1:J:134:ILE:HD11	1:J:164:SER:HB3	1.69	0.74
1:J:76:ASP:HB3	1:J:79:GLU:HG3	1.70	0.74

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	409/414 (99%)	396 (97%)	13 (3%)	0	100	100
1	B	408/414 (99%)	397 (97%)	11 (3%)	0	100	100
1	C	408/414 (99%)	396 (97%)	12 (3%)	0	100	100
1	D	410/414 (99%)	400 (98%)	10 (2%)	0	100	100
1	E	407/414 (98%)	395 (97%)	12 (3%)	0	100	100
1	F	408/414 (99%)	398 (98%)	10 (2%)	0	100	100
1	G	409/414 (99%)	399 (98%)	10 (2%)	0	100	100
1	H	409/414 (99%)	394 (96%)	15 (4%)	0	100	100
1	I	407/414 (98%)	395 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	407/414 (98%)	393 (97%)	14 (3%)	0	100	100
1	K	406/414 (98%)	393 (97%)	12 (3%)	1 (0%)	43	55
1	L	407/414 (98%)	392 (96%)	15 (4%)	0	100	100
All	All	4895/4968 (98%)	4748 (97%)	146 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	278	LEU

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	330/332 (99%)	321 (97%)	9 (3%)	39	58
1	B	329/332 (99%)	319 (97%)	10 (3%)	36	53
1	C	329/332 (99%)	319 (97%)	10 (3%)	36	53
1	D	330/332 (99%)	317 (96%)	13 (4%)	28	43
1	E	328/332 (99%)	316 (96%)	12 (4%)	30	45
1	F	329/332 (99%)	319 (97%)	10 (3%)	36	53
1	G	330/332 (99%)	318 (96%)	12 (4%)	31	47
1	H	330/332 (99%)	320 (97%)	10 (3%)	36	53
1	I	328/332 (99%)	316 (96%)	12 (4%)	30	45
1	J	328/332 (99%)	318 (97%)	10 (3%)	36	53
1	K	328/332 (99%)	313 (95%)	15 (5%)	24	36
1	L	328/332 (99%)	315 (96%)	13 (4%)	28	42
All	All	3947/3984 (99%)	3811 (97%)	136 (3%)	32	49

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	143	MET
1	K	277	LEU
1	L	298	ASN
1	E	260	ASN
1	E	204	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	298	ASN
1	L	298	ASN
1	I	312	ASN
1	K	212	GLN
1	E	72	HIS

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](#)

Of 79 ligands modelled in this entry, 15 are monoatomic - leaving 64 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	A1H40	A	601	-	15,15,15	1.41	2 (13%)	20,20,20	2.78	8 (40%)
3	EDO	A	602	-	3,3,3	0.52	0	2,2,2	1.05	0
3	EDO	K	506	-	3,3,3	0.45	0	2,2,2	0.82	0
2	A1H40	K	501	-	15,15,15	1.38	3 (20%)	20,20,20	1.76	4 (20%)
3	EDO	A	607	-	3,3,3	0.38	0	2,2,2	1.14	0
3	EDO	I	905	-	3,3,3	0.34	0	2,2,2	0.78	0
5	NAD	F	603	-	46,48,48	0.52	0	64,73,73	0.63	1 (1%)
4	PEG	C	502	-	6,6,6	0.27	0	5,5,5	0.19	0
4	PEG	H	504	-	6,6,6	0.20	0	5,5,5	0.18	0
5	NAD	H	505	-	46,48,48	0.56	0	64,73,73	0.64	1 (1%)
4	PEG	D	604	-	6,6,6	0.20	0	5,5,5	0.15	0
5	NAD	G	706	-	46,48,48	0.50	0	64,73,73	0.58	1 (1%)
5	NAD	J	602	-	46,48,48	0.55	1 (2%)	64,73,73	0.63	1 (1%)
2	A1H40	H	501	-	15,15,15	1.38	3 (20%)	20,20,20	2.05	7 (35%)
6	TRS	A	609	-	7,7,7	0.66	0	9,9,9	1.38	2 (22%)
3	EDO	C	503	-	3,3,3	0.40	0	2,2,2	0.60	0
3	EDO	I	906	-	3,3,3	0.41	0	2,2,2	1.27	0
8	PGE	B	504	-	9,9,9	0.40	0	8,8,8	0.34	0
3	EDO	C	505	-	3,3,3	0.50	0	2,2,2	0.90	0
3	EDO	I	901	-	3,3,3	0.54	0	2,2,2	0.12	0
4	PEG	E	801	-	6,6,6	0.22	0	5,5,5	0.23	0
3	EDO	B	505	-	3,3,3	0.44	0	2,2,2	0.70	0
6	TRS	H	503	-	7,7,7	0.36	0	9,9,9	1.10	1 (11%)
5	NAD	I	907	-	46,48,48	0.55	0	64,73,73	0.60	1 (1%)
3	EDO	G	705	-	3,3,3	0.42	0	2,2,2	1.14	0
5	NAD	A	608	-	46,48,48	0.47	0	64,73,73	0.63	1 (1%)
5	NAD	C	506	-	46,48,48	0.51	0	64,73,73	0.59	1 (1%)
3	EDO	G	703	10	3,3,3	0.42	0	2,2,2	0.72	0
3	EDO	A	606	-	3,3,3	0.60	0	2,2,2	0.39	0
3	EDO	I	904	-	3,3,3	0.49	0	2,2,2	0.39	0
4	PEG	A	605	-	6,6,6	0.22	0	5,5,5	0.18	0
5	NAD	L	703	-	46,48,48	0.55	0	64,73,73	0.61	1 (1%)
6	TRS	G	701	-	7,7,7	0.62	0	9,9,9	0.86	0
2	A1H40	C	501	-	15,15,15	1.32	3 (20%)	20,20,20	2.27	6 (30%)
3	EDO	E	802	-	3,3,3	0.42	0	2,2,2	1.06	0
3	EDO	J	601	-	3,3,3	0.39	0	2,2,2	1.03	0
3	EDO	A	603	-	3,3,3	0.52	0	2,2,2	0.19	0
3	EDO	D	603	-	3,3,3	0.57	0	2,2,2	0.57	0
9	PG4	B	506	-	12,12,12	0.29	0	11,11,11	0.15	0
3	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TRS	K	504	10	7,7,7	0.69	0	9,9,9	1.35	0
6	TRS	L	701	-	7,7,7	0.30	0	9,9,9	0.75	0
3	EDO	A	604	-	3,3,3	0.45	0	2,2,2	0.44	0
3	EDO	K	503	-	3,3,3	0.44	0	2,2,2	0.73	0
4	PEG	C	504	-	6,6,6	0.21	0	5,5,5	0.16	0
6	TRS	I	902	10	7,7,7	0.63	0	9,9,9	1.11	0
2	A1H40	B	501	-	15,15,15	1.39	3 (20%)	20,20,20	1.74	4 (20%)
3	EDO	F	604	-	3,3,3	0.49	0	2,2,2	0.67	0
3	EDO	L	702	-	3,3,3	0.51	0	2,2,2	0.85	0
3	EDO	F	602	-	3,3,3	0.54	0	2,2,2	0.97	0
2	A1H40	D	602	-	15,15,15	1.49	3 (20%)	20,20,20	2.77	9 (45%)
5	NAD	B	508	-	46,48,48	0.68	1 (2%)	64,73,73	0.68	1 (1%)
5	NAD	E	803	-	46,48,48	0.48	0	64,73,73	0.61	1 (1%)
3	EDO	H	502	-	3,3,3	0.44	0	2,2,2	1.14	0
5	NAD	D	605	-	46,48,48	0.66	1 (2%)	64,73,73	0.62	1 (1%)
3	EDO	K	502	-	3,3,3	0.40	0	2,2,2	1.20	0
4	PEG	G	704	-	6,6,6	0.15	0	5,5,5	0.11	0
3	EDO	B	503	-	3,3,3	0.29	0	2,2,2	1.23	0
3	EDO	I	903	-	3,3,3	0.66	0	2,2,2	0.19	0
3	EDO	B	507	-	3,3,3	0.57	0	2,2,2	0.48	0
6	TRS	D	601	-	7,7,7	0.74	0	9,9,9	1.66	2 (22%)
3	EDO	G	702	-	3,3,3	0.47	0	2,2,2	0.42	0
5	NAD	K	505	-	46,48,48	0.61	1 (2%)	64,73,73	0.61	1 (1%)
4	PEG	F	601	-	6,6,6	0.16	0	5,5,5	0.15	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
2	A1H40	A	601	-	-	8/8/8/8	0/2/2/2
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	K	506	-	-	1/1/1/1	-
2	A1H40	K	501	-	-	8/8/8/8	0/2/2/2
3	EDO	A	607	-	-	0/1/1/1	-
3	EDO	I	905	-	-	1/1/1/1	-
5	NAD	F	603	-	-	1/30/62/62	0/5/5/5
4	PEG	C	502	-	-	0/4/4/4	-
4	PEG	H	504	-	-	0/4/4/4	-
5	NAD	H	505	-	-	1/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	D	604	-	-	0/4/4/4	-
5	NAD	G	706	-	-	1/30/62/62	0/5/5/5
5	NAD	J	602	-	-	1/30/62/62	0/5/5/5
2	A1H40	H	501	-	-	4/8/8/8	0/2/2/2
6	TRS	A	609	-	-	2/9/9/9	-
3	EDO	C	503	-	-	0/1/1/1	-
3	EDO	I	906	-	-	1/1/1/1	-
8	PGE	B	504	-	-	5/7/7/7	-
3	EDO	C	505	-	-	0/1/1/1	-
3	EDO	I	901	-	-	0/1/1/1	-
4	PEG	E	801	-	-	0/4/4/4	-
3	EDO	B	505	-	-	0/1/1/1	-
6	TRS	H	503	-	-	1/9/9/9	-
5	NAD	I	907	-	-	1/30/62/62	0/5/5/5
3	EDO	G	705	-	-	1/1/1/1	-
5	NAD	A	608	-	-	0/30/62/62	0/5/5/5
5	NAD	C	506	-	-	0/30/62/62	0/5/5/5
3	EDO	G	703	10	-	1/1/1/1	-
3	EDO	A	606	-	-	1/1/1/1	-
3	EDO	I	904	-	-	1/1/1/1	-
4	PEG	A	605	-	-	0/4/4/4	-
5	NAD	L	703	-	-	2/30/62/62	0/5/5/5
6	TRS	G	701	-	-	3/9/9/9	-
2	A1H40	C	501	-	-	6/8/8/8	0/2/2/2
3	EDO	E	802	-	-	0/1/1/1	-
3	EDO	J	601	-	-	1/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
3	EDO	D	603	-	-	0/1/1/1	-
9	PG4	B	506	-	-	5/10/10/10	-
3	EDO	B	502	-	-	0/1/1/1	-
6	TRS	K	504	10	-	9/9/9/9	-
6	TRS	L	701	-	-	9/9/9/9	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	K	503	-	-	1/1/1/1	-
4	PEG	C	504	-	-	1/4/4/4	-
6	TRS	I	902	10	-	8/9/9/9	-
2	A1H40	B	501	-	-	4/8/8/8	0/2/2/2
3	EDO	F	604	-	-	0/1/1/1	-
3	EDO	L	702	-	-	1/1/1/1	-
3	EDO	F	602	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1H40	D	602	-	-	5/8/8/8	0/2/2/2
5	NAD	B	508	-	-	0/30/62/62	0/5/5/5
5	NAD	E	803	-	-	1/30/62/62	0/5/5/5
3	EDO	H	502	-	-	1/1/1/1	-
5	NAD	D	605	-	-	1/30/62/62	0/5/5/5
3	EDO	K	502	-	-	1/1/1/1	-
4	PEG	G	704	-	-	1/4/4/4	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	I	903	-	-	1/1/1/1	-
3	EDO	B	507	-	-	1/1/1/1	-
6	TRS	D	601	-	-	3/9/9/9	-
3	EDO	G	702	-	-	0/1/1/1	-
5	NAD	K	505	-	-	1/30/62/62	0/5/5/5
4	PEG	F	601	-	-	0/4/4/4	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1H40	C09-C13	2.90	1.55	1.49
2	K	501	A1H40	C07-C08	2.87	1.52	1.47
2	D	602	A1H40	C09-C13	2.75	1.55	1.49
2	A	601	A1H40	C10-C09	-2.68	1.35	1.39
5	D	605	NAD	C2N-N1N	2.65	1.37	1.35

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1H40	C10-C07-C08	-7.00	107.95	120.26
2	D	602	A1H40	C10-C07-C08	-6.42	108.97	120.26
2	C	501	A1H40	C10-C07-C08	-5.64	110.33	120.26
2	D	602	A1H40	C12-C09-C13	4.66	129.59	120.37
2	A	601	A1H40	C11-C07-C08	4.50	128.84	120.83

There are no chirality outliers.

5 of 109 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	609	TRS	N-C-C3-O3
6	I	902	TRS	C2-C-C1-O1
6	I	902	TRS	C3-C-C1-O1
6	I	902	TRS	N-C-C1-O1

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Mol	Chain	Res	Type	Atoms
6	I	902	TRS	C2-C-C3-O3

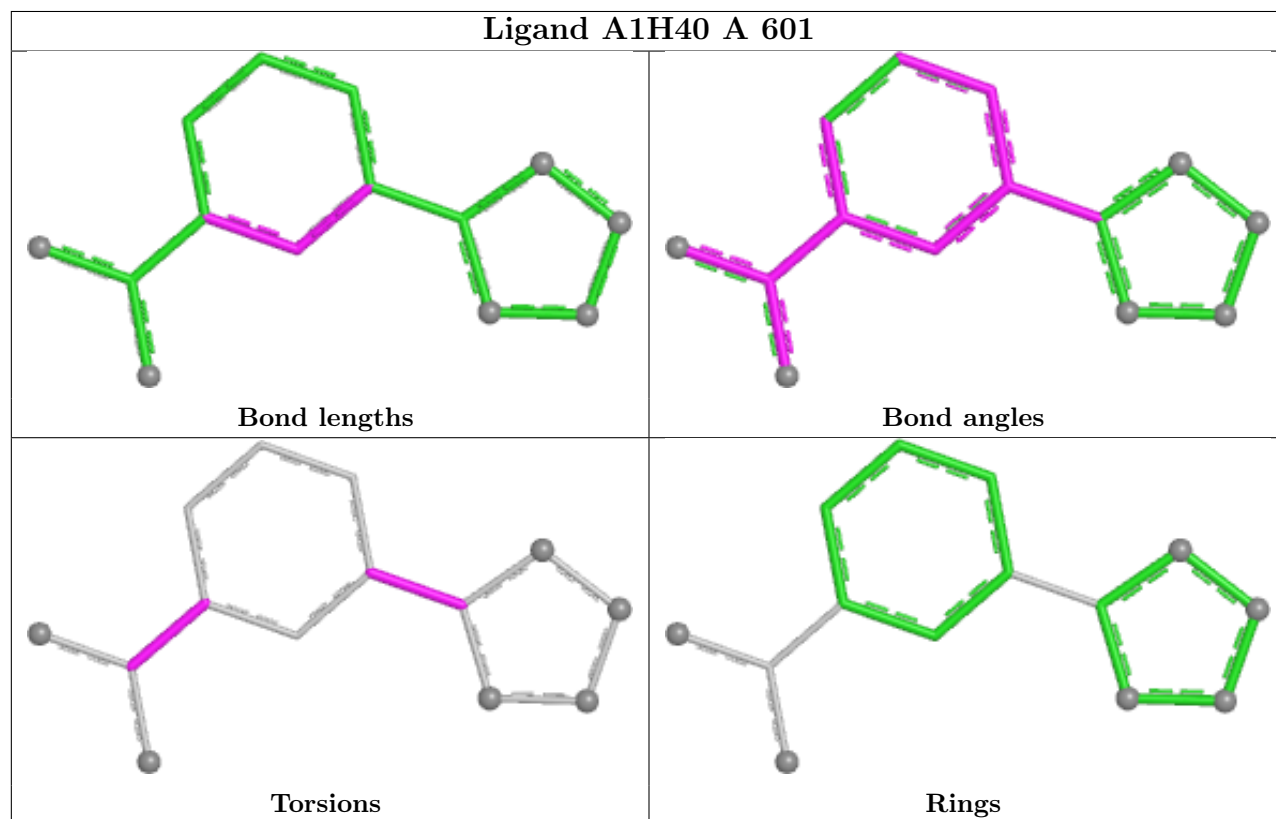
There are no ring outliers.

30 monomers are involved in 44 short contacts:

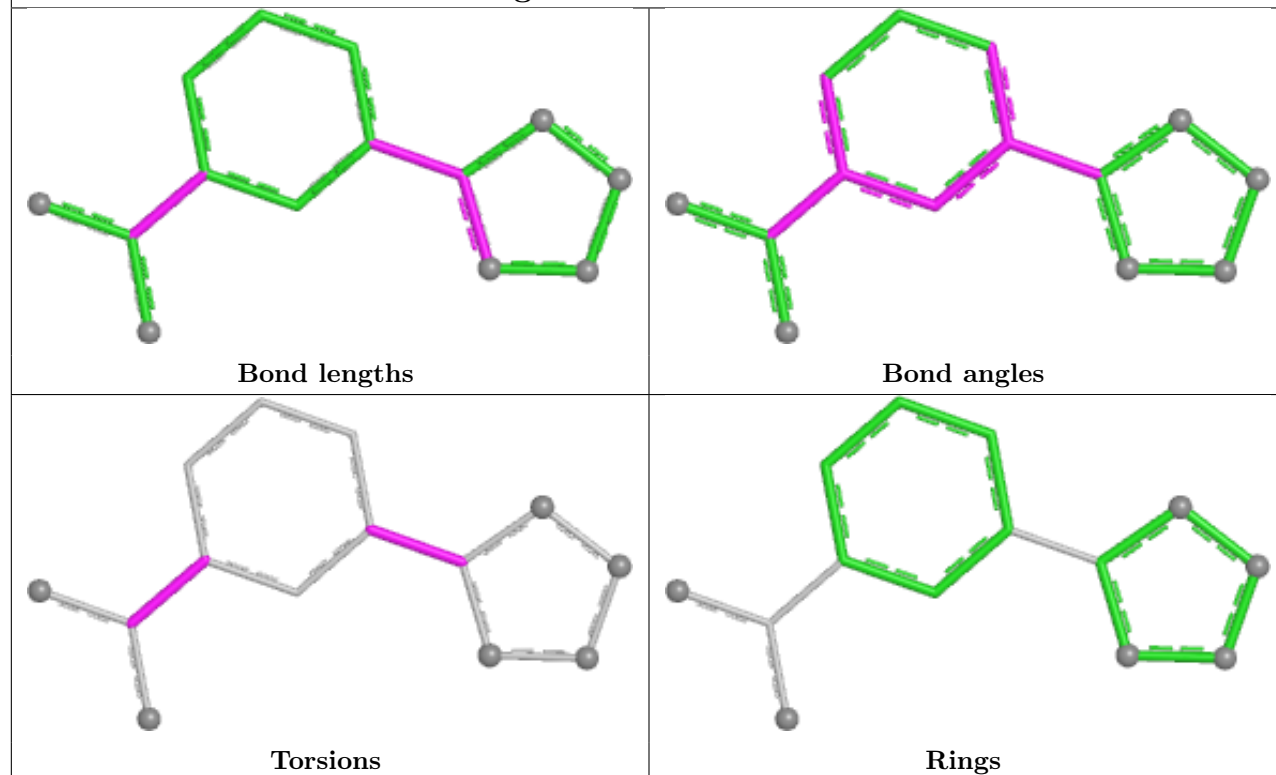
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	506	EDO	1	0
3	A	607	EDO	1	0
3	I	905	EDO	1	0
4	C	502	PEG	2	0
4	H	504	PEG	1	0
5	H	505	NAD	2	0
5	J	602	NAD	2	0
3	C	503	EDO	1	0
8	B	504	PGE	3	0
3	C	505	EDO	1	0
3	I	901	EDO	1	0
4	E	801	PEG	1	0
3	B	505	EDO	2	0
6	H	503	TRS	1	0
5	C	506	NAD	3	0
3	A	606	EDO	1	0
3	I	904	EDO	3	0
4	A	605	PEG	1	0
3	A	603	EDO	1	0
3	D	603	EDO	1	0
9	B	506	PG4	2	0
3	B	502	EDO	2	0
6	K	504	TRS	1	0
6	I	902	TRS	2	0
2	B	501	A1H40	1	0
3	F	604	EDO	1	0
2	D	602	A1H40	1	0
5	D	605	NAD	1	0
3	G	702	EDO	1	0
4	F	601	PEG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

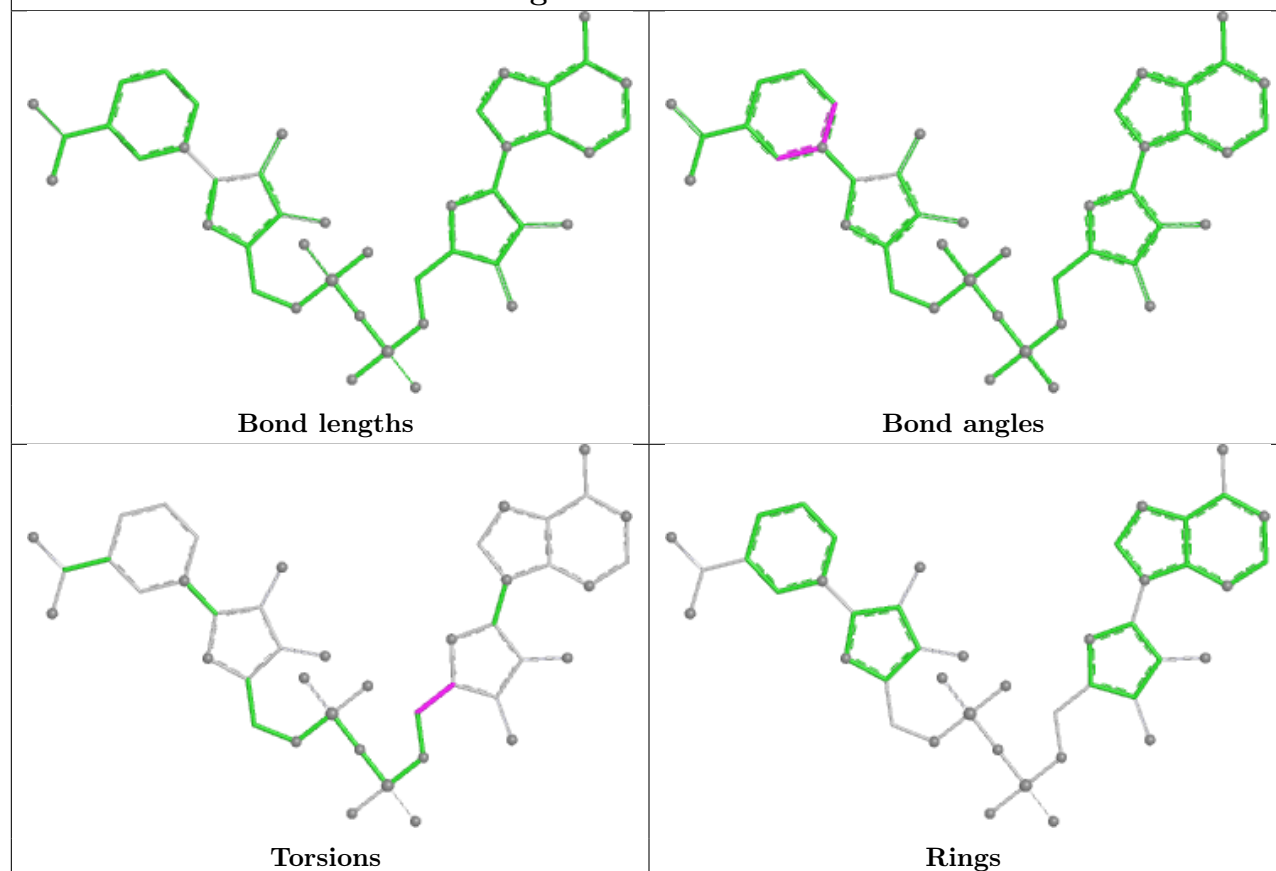
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

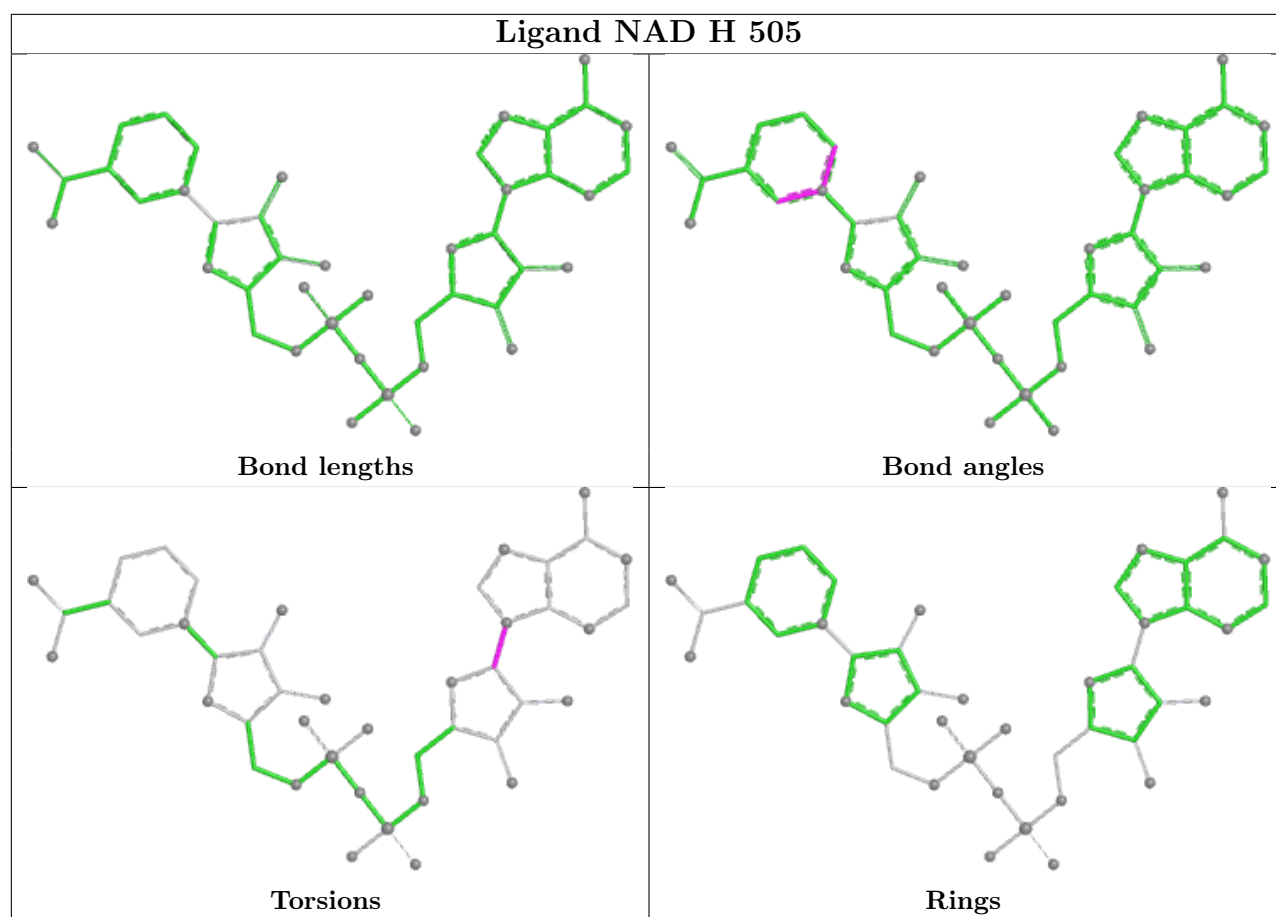


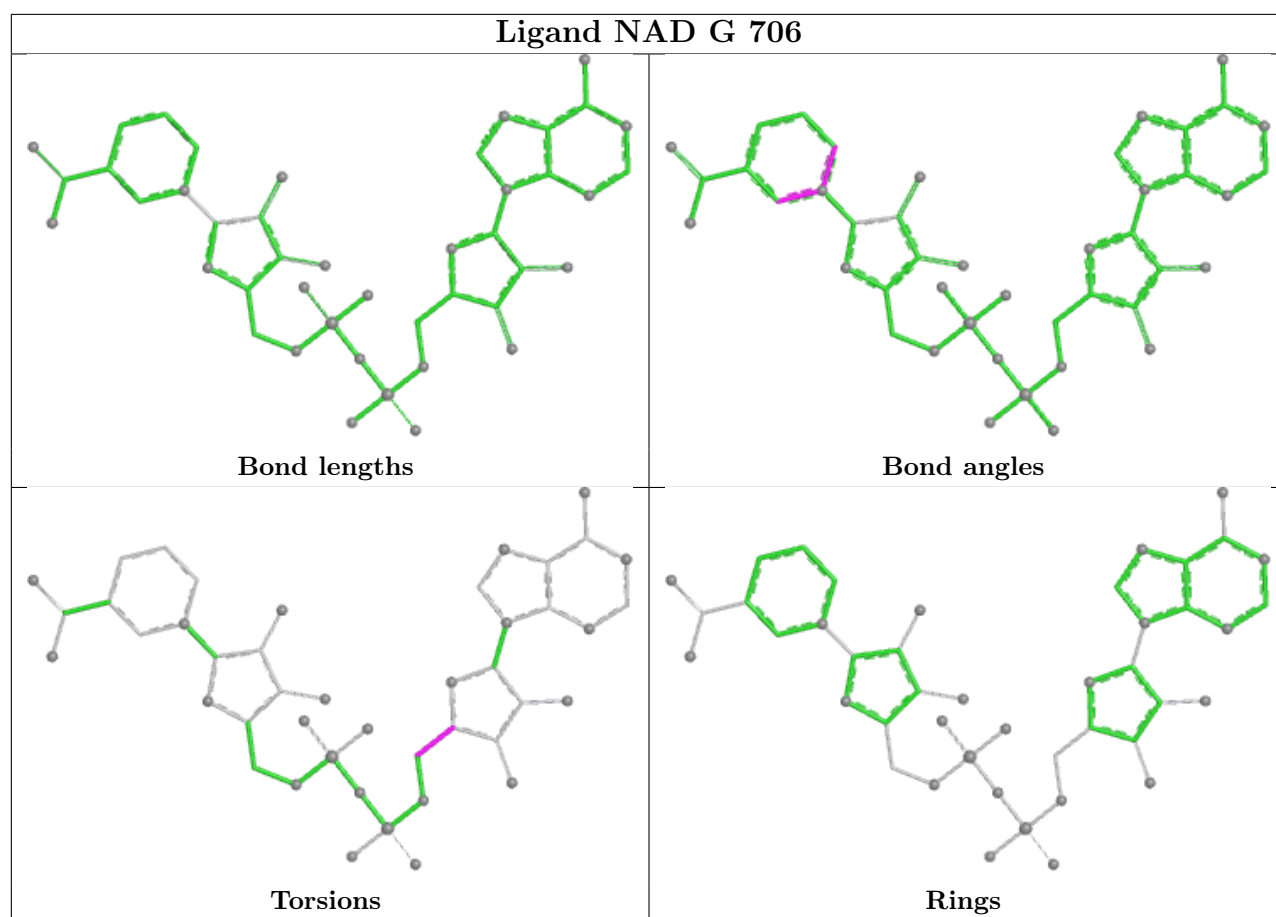
Ligand A1H40 K 501



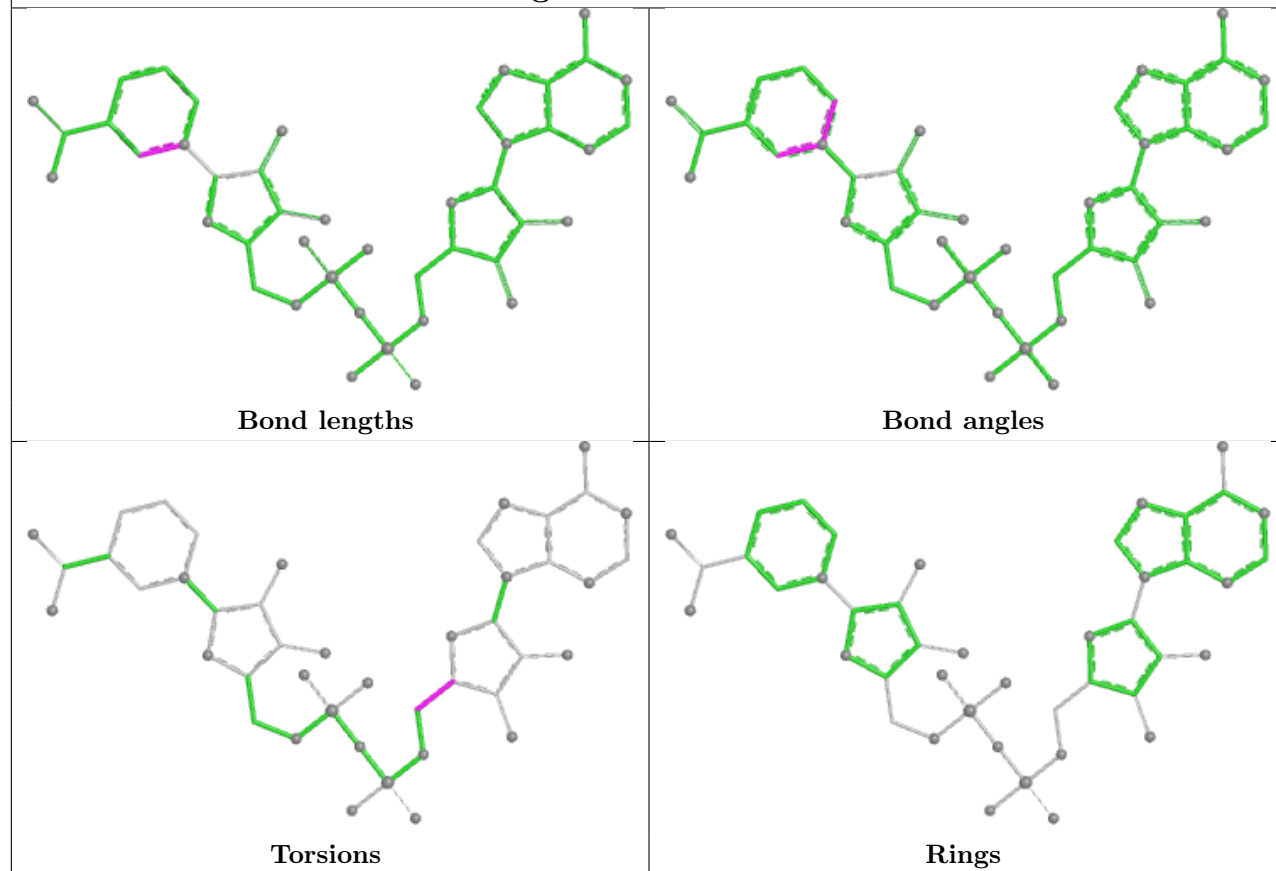
Ligand NAD F 603



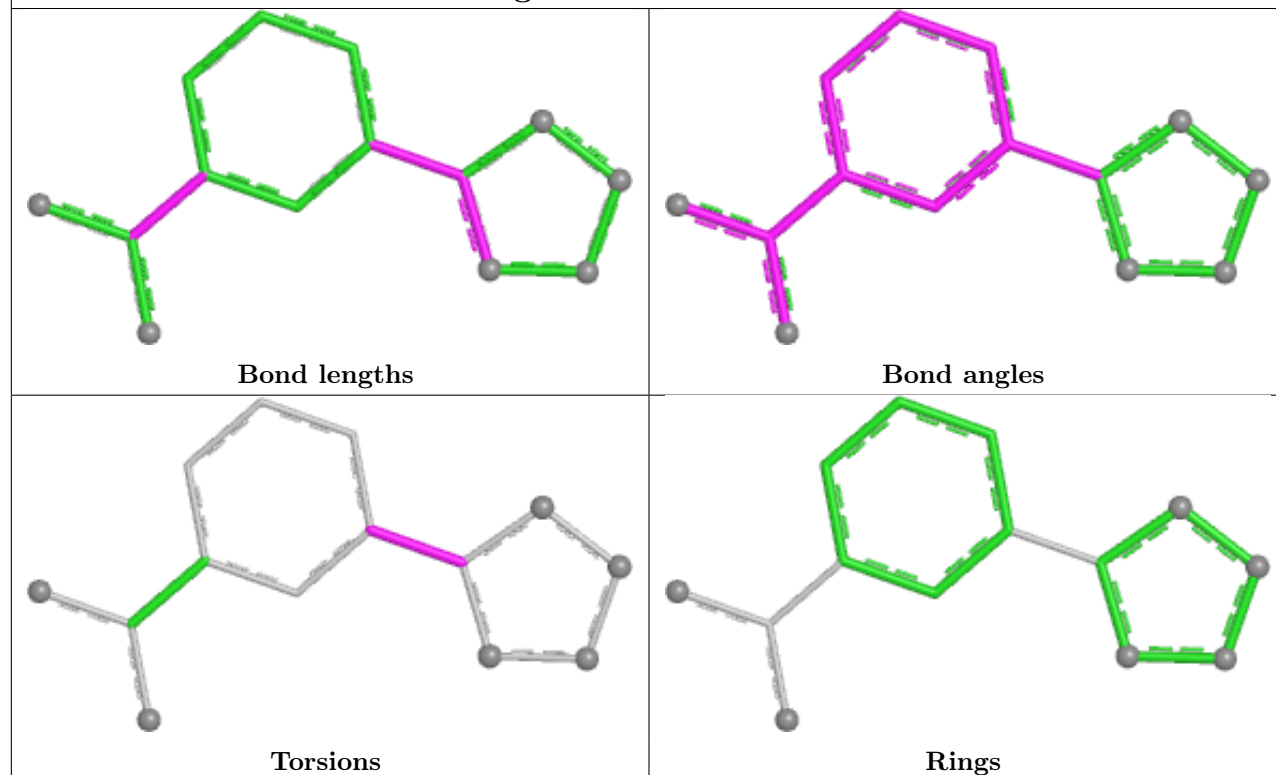


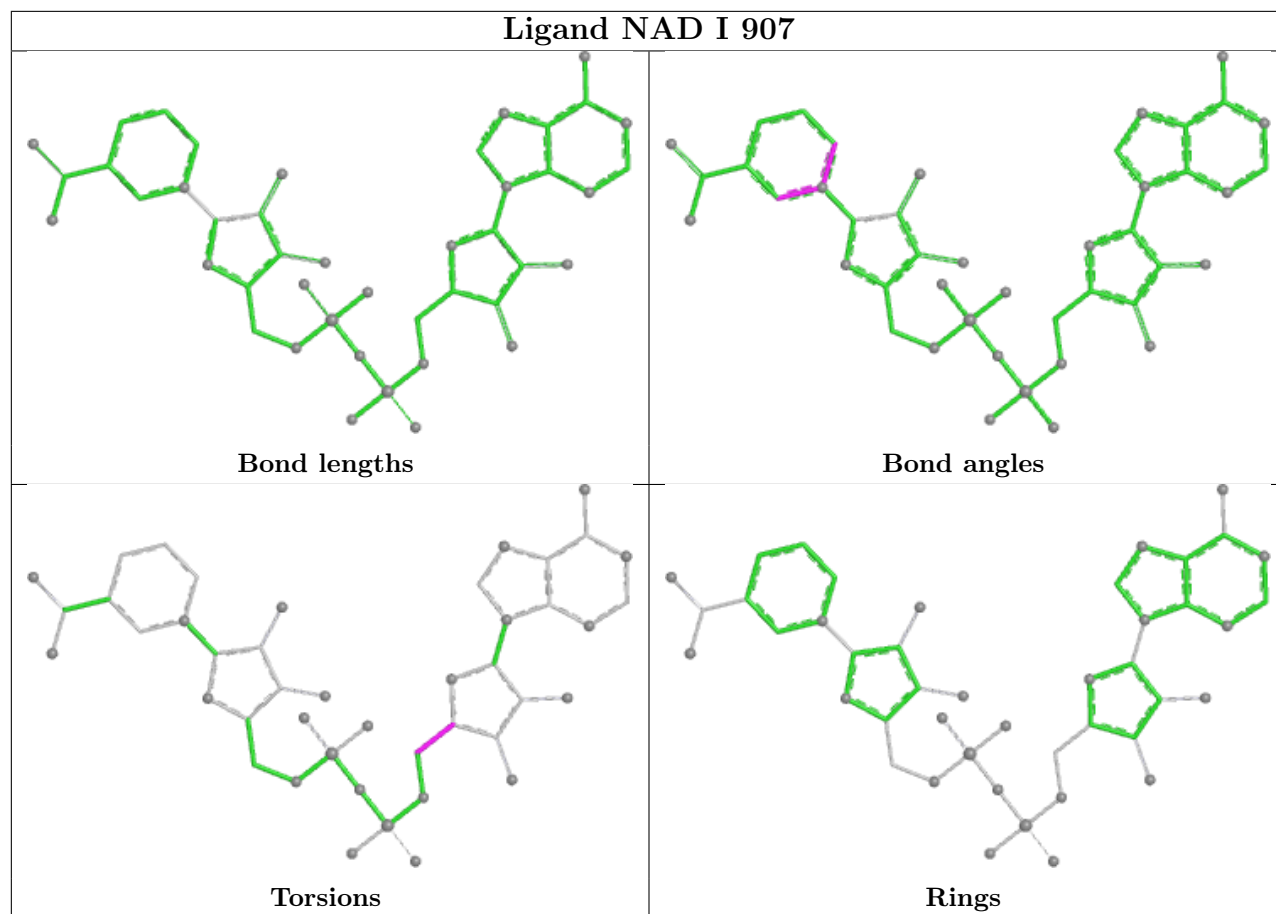


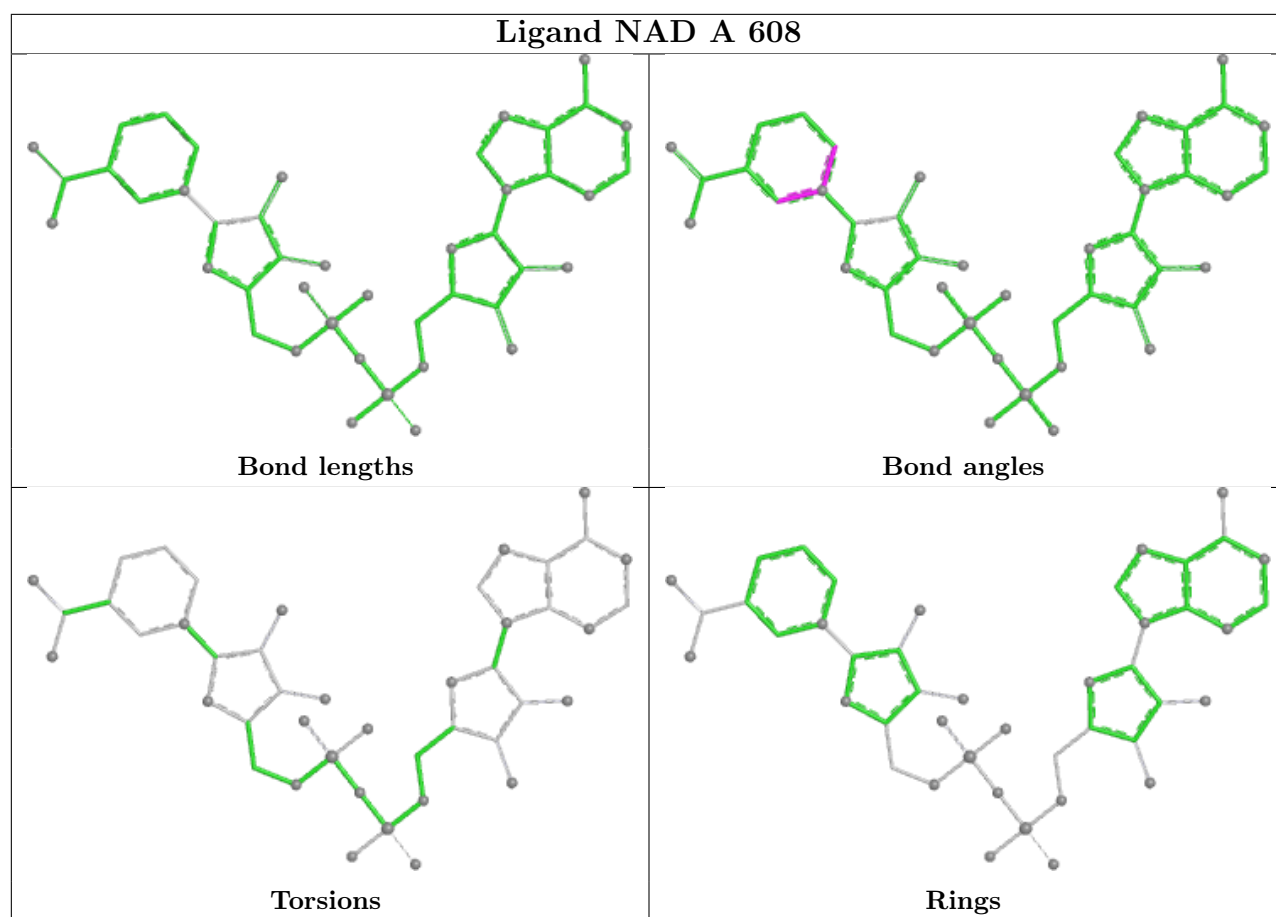
Ligand NAD J 602

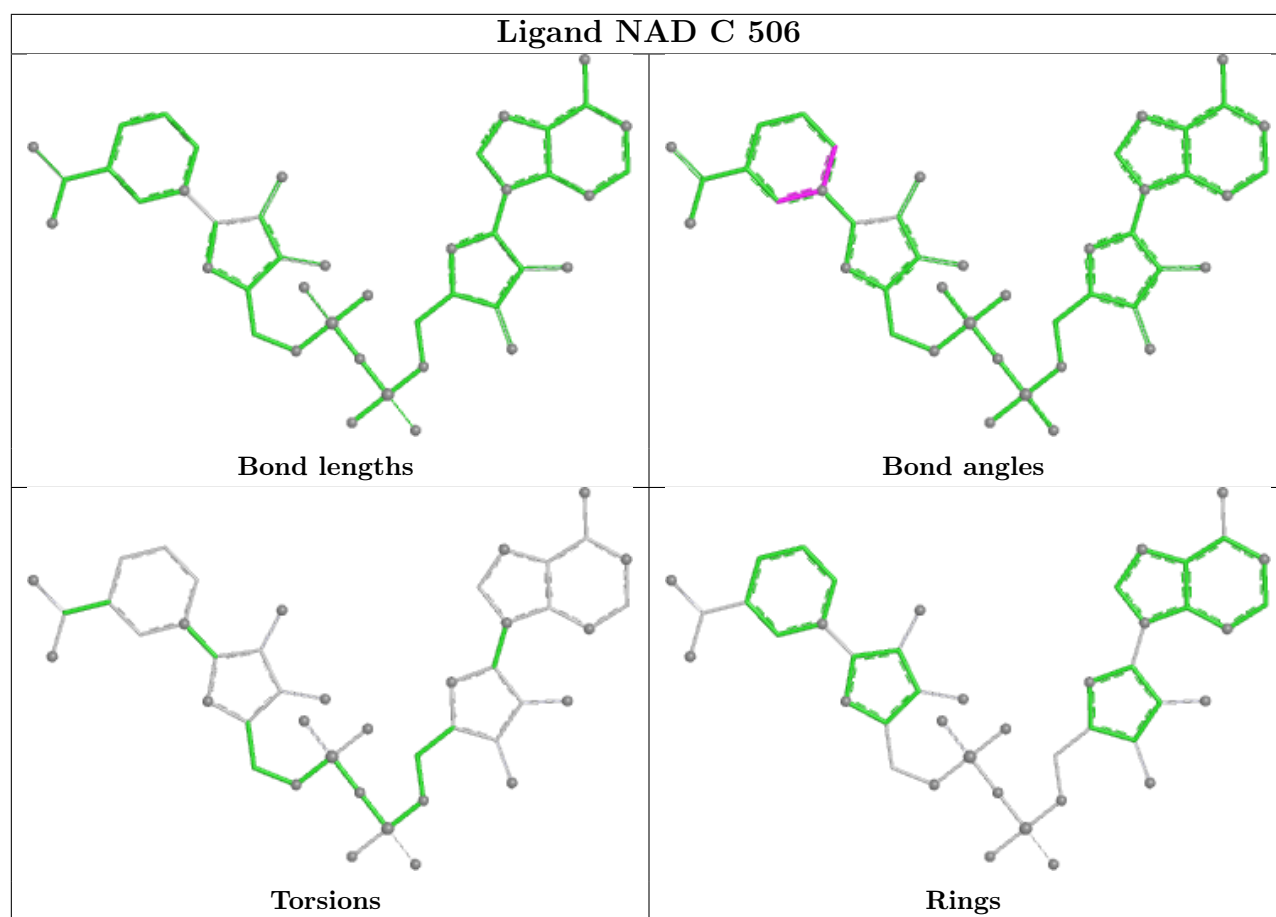


Ligand A1H40 H 501

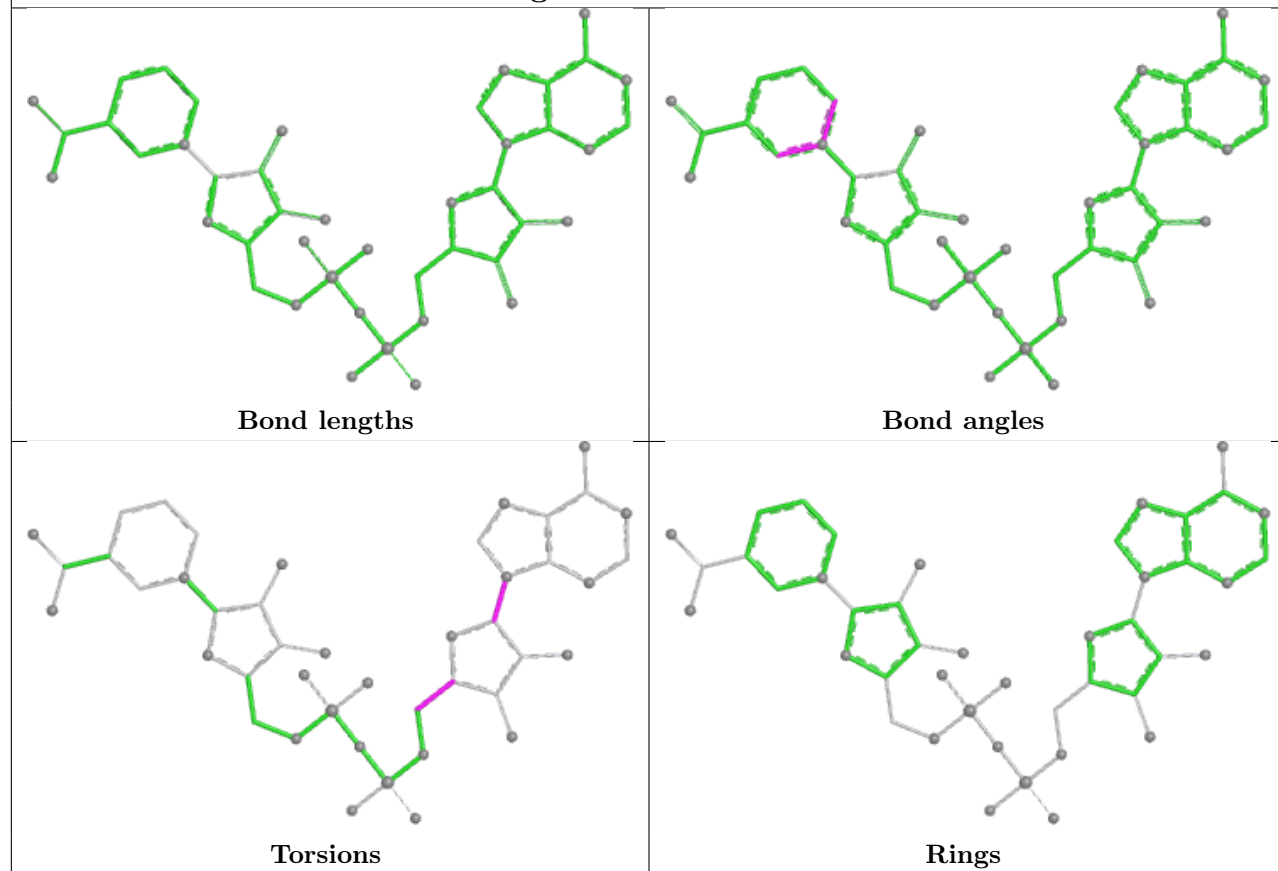




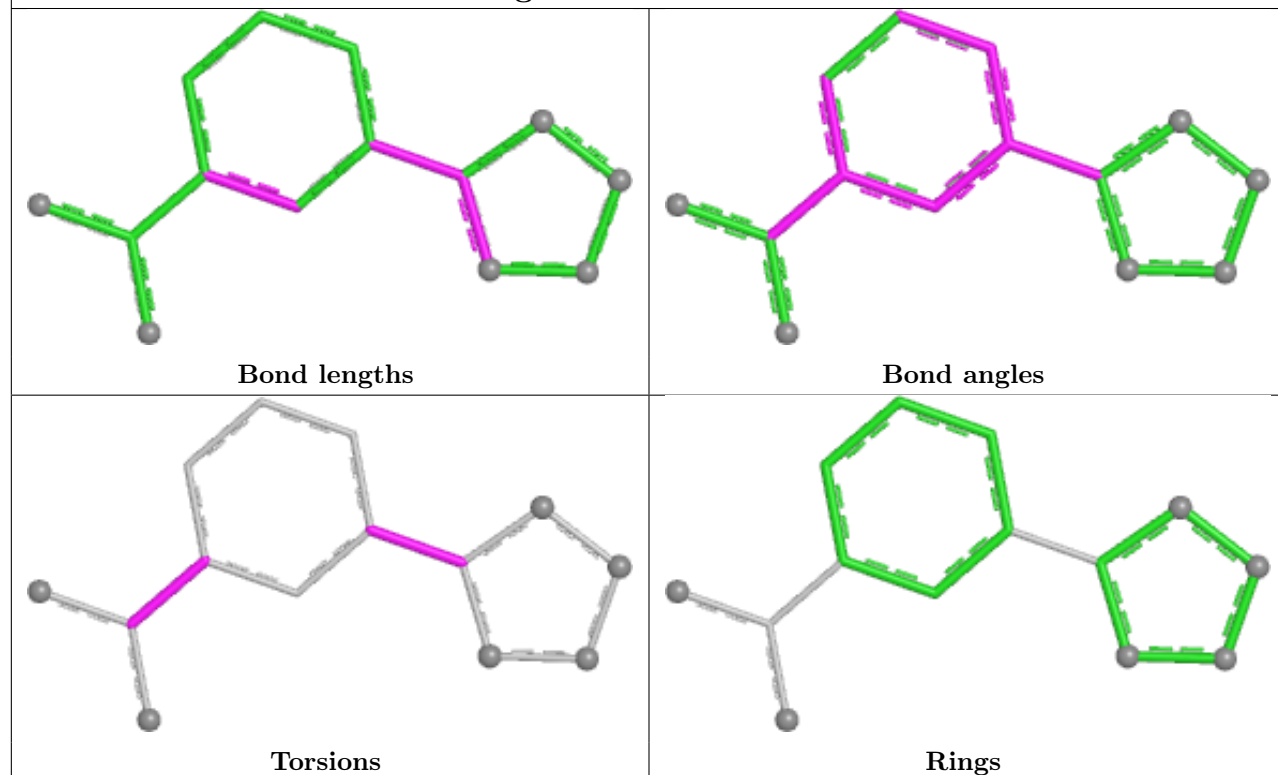




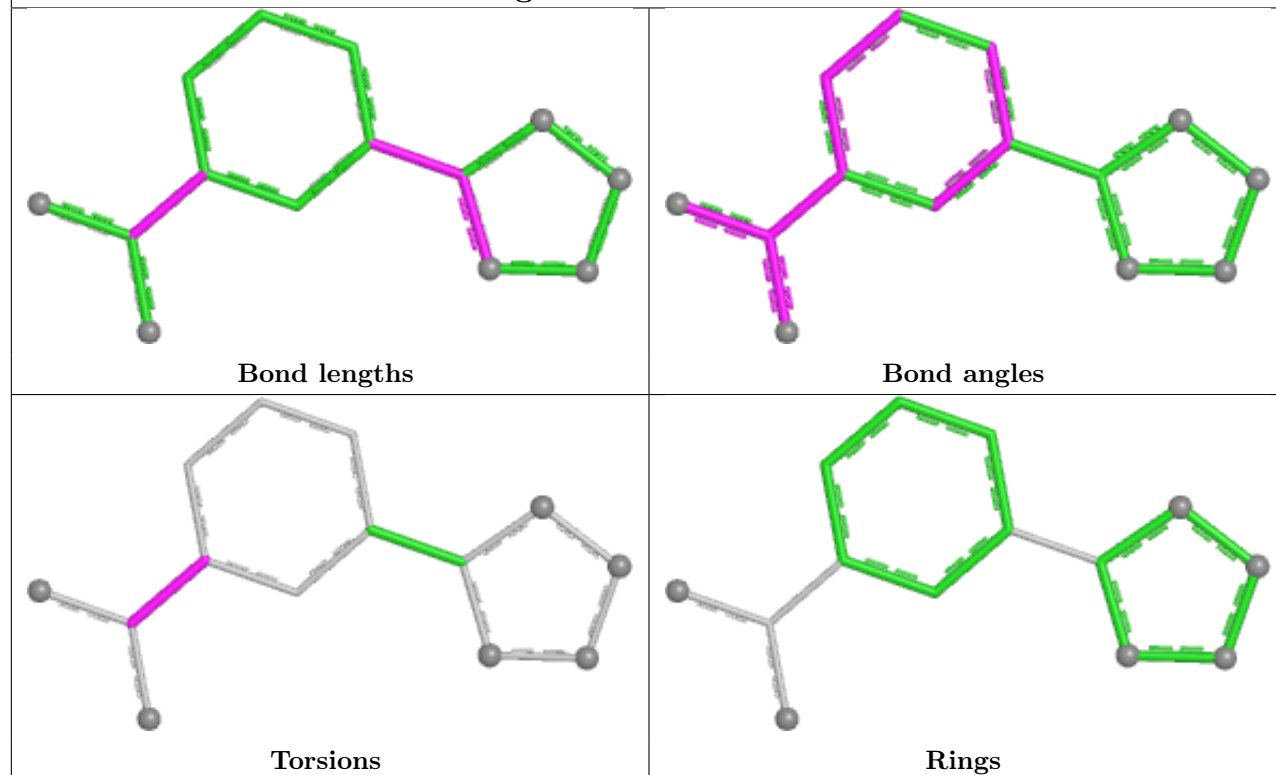
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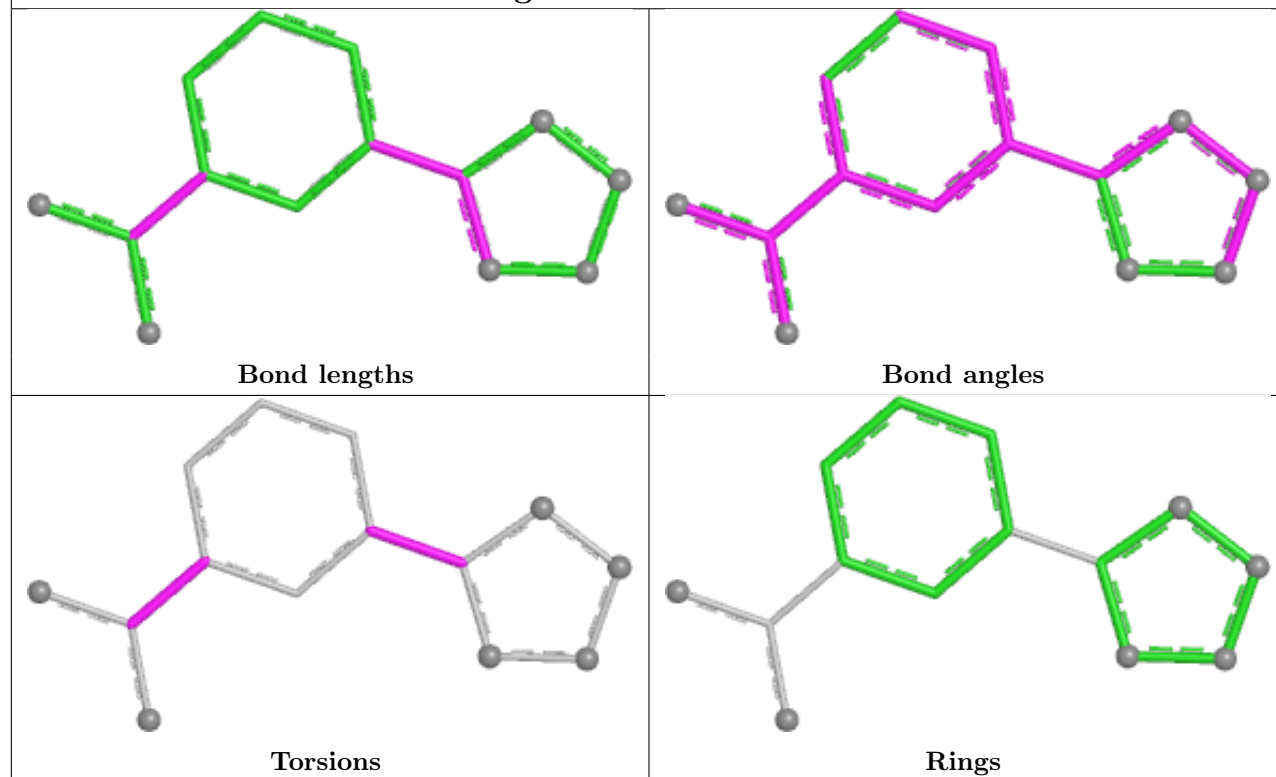
Ligand A1H40 C 501

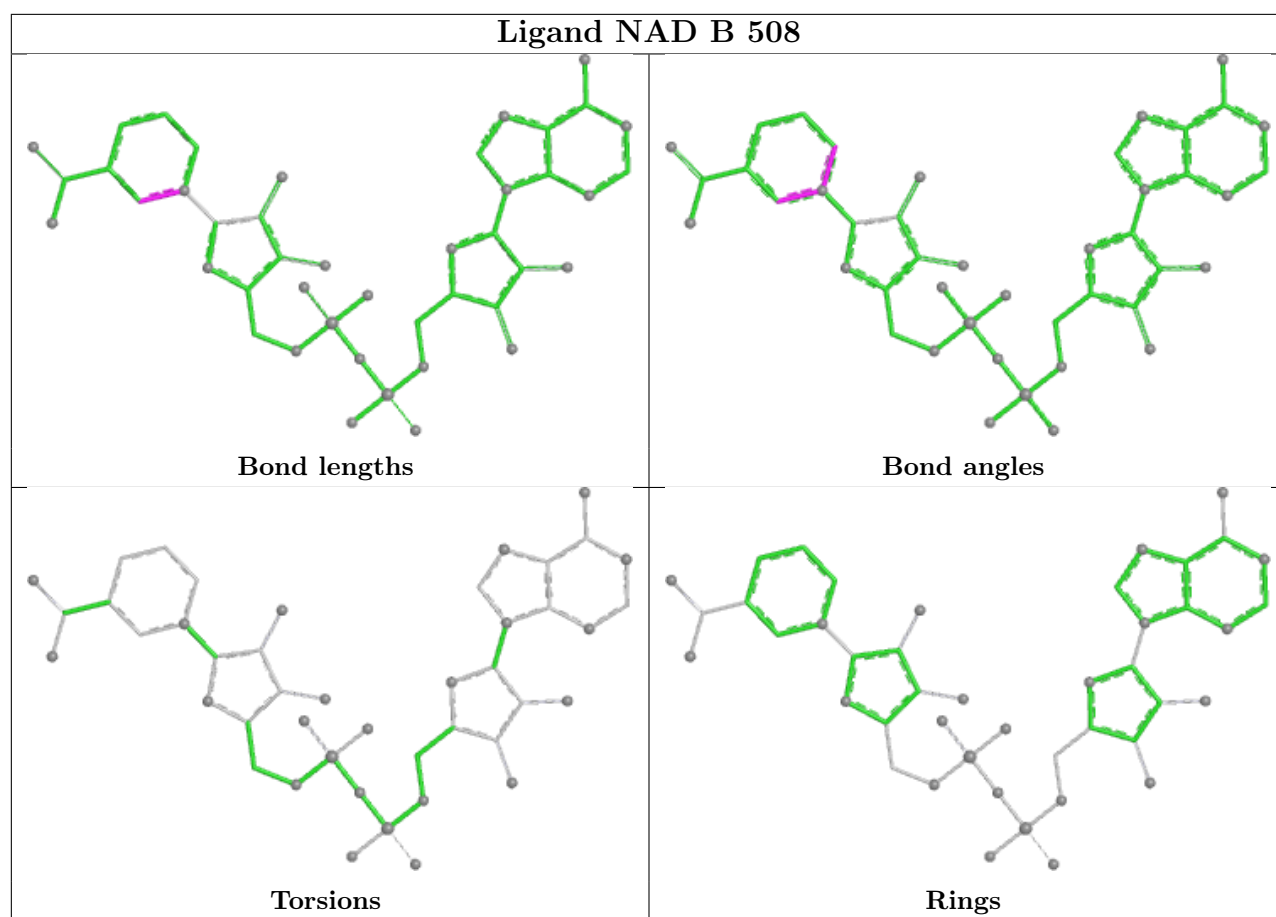


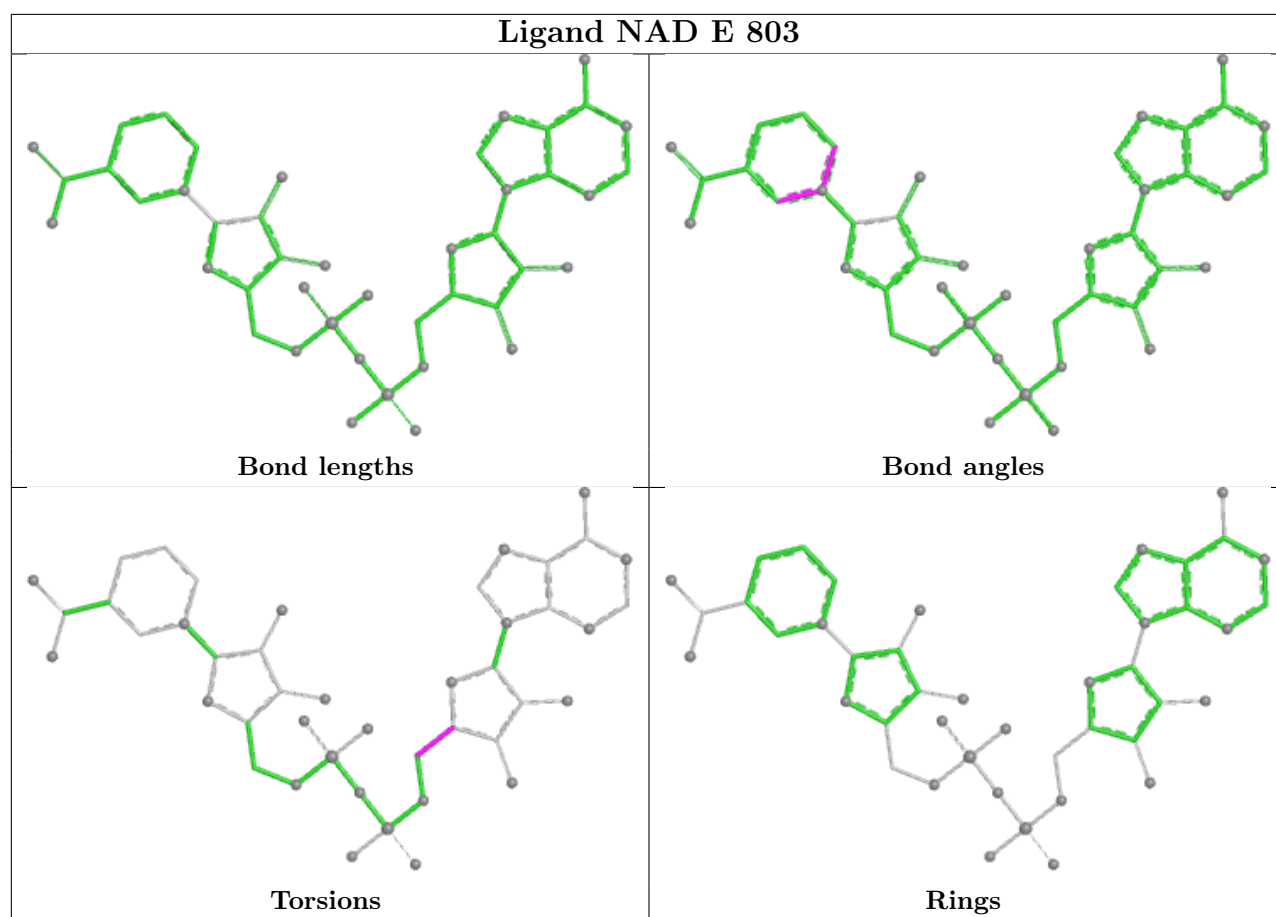
Ligand A1H40 B 501

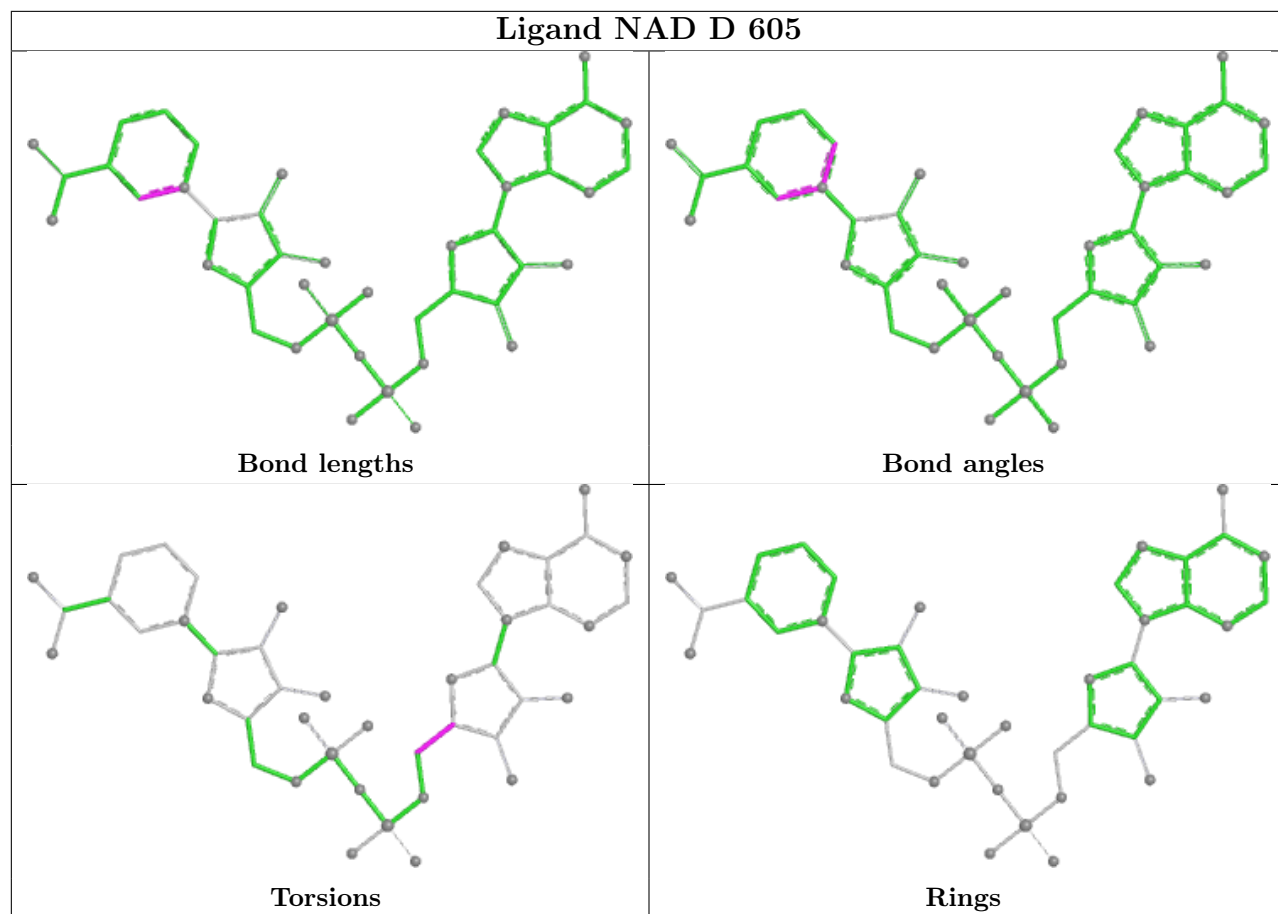


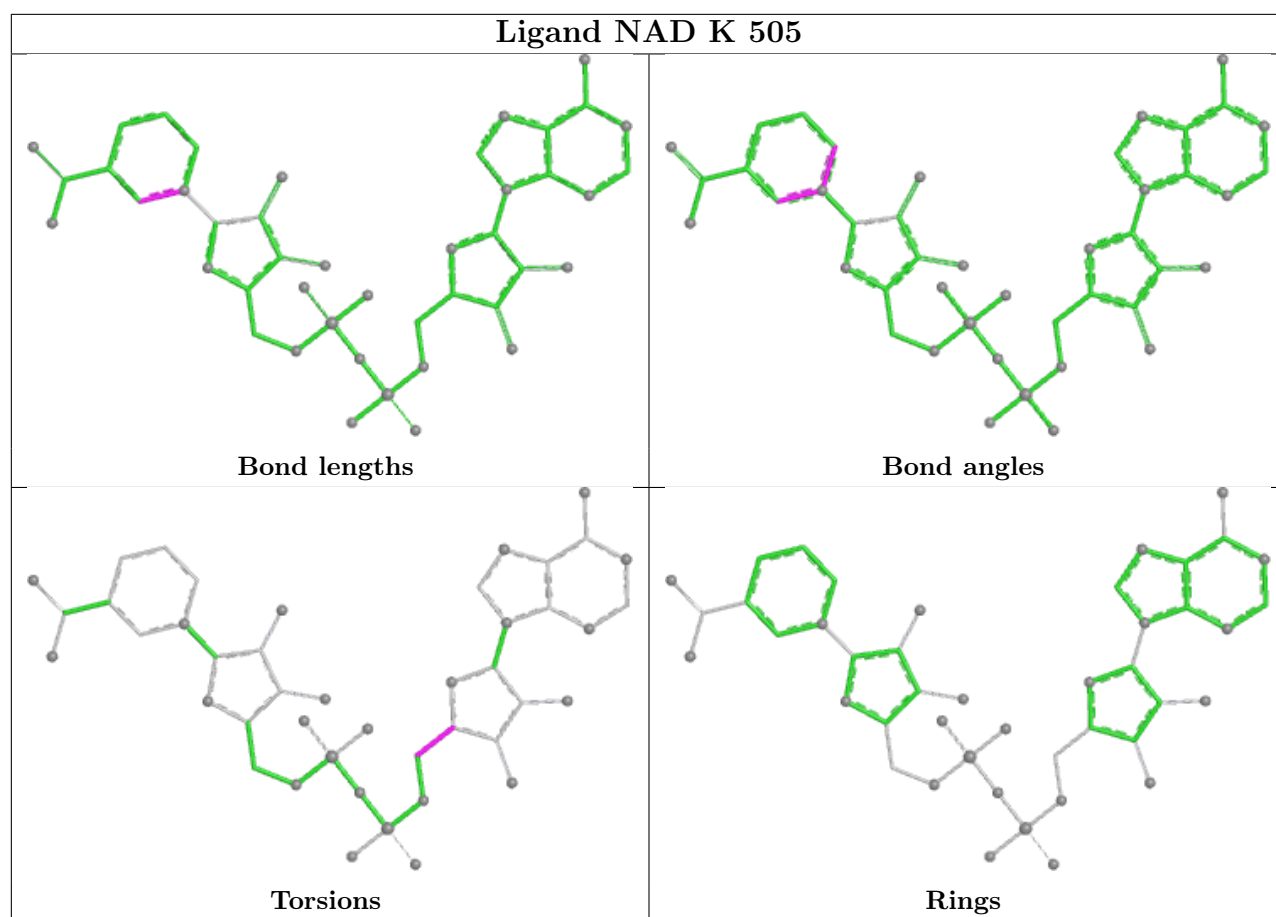
Ligand A1H40 D 602











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 [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	410/414 (99%)	-0.38	2 (0%) 87 87	15, 35, 64, 80	1 (0%)
1	B	410/414 (99%)	-0.57	1 (0%) 91 91	21, 30, 46, 87	0
1	C	410/414 (99%)	-0.41	2 (0%) 87 87	23, 35, 58, 96	0
1	D	412/414 (99%)	-0.33	3 (0%) 84 85	20, 34, 70, 96	0
1	E	409/414 (98%)	-0.07	4 (0%) 79 80	21, 44, 97, 122	0
1	F	410/414 (99%)	-0.28	2 (0%) 87 87	25, 41, 69, 92	0
1	G	410/414 (99%)	0.00	8 (1%) 65 66	17, 46, 102, 119	1 (0%)
1	H	410/414 (99%)	0.10	11 (2%) 56 58	19, 46, 100, 120	1 (0%)
1	I	409/414 (98%)	0.05	6 (1%) 72 73	24, 46, 97, 144	0
1	J	409/414 (98%)	0.21	23 (5%) 30 32	24, 49, 106, 126	0
1	K	408/414 (98%)	0.30	20 (4%) 35 36	26, 55, 117, 132	0
1	L	409/414 (98%)	0.36	24 (5%) 28 30	28, 53, 117, 147	0
All	All	4916/4968 (98%)	-0.09	106 (2%) 62 64	15, 40, 100, 147	3 (0%)

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	ALA	5.3
1	L	3	ALA	5.2
1	J	3	ALA	4.7
1	A	411	ALA	4.4
1	J	242	ILE	4.3

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	A1H40	K	501	14/14	0.71	0.19	39,47,55,56	14
6	TRS	K	504	8/8	0.71	0.20	32,42,47,51	0
2	A1H40	A	601	14/14	0.76	0.19	26,32,37,38	14
6	TRS	G	701	8/8	0.76	0.17	47,48,51,53	0
2	A1H40	B	501	14/14	0.76	0.20	30,35,39,41	14
2	A1H40	H	501	14/14	0.77	0.19	36,43,46,48	14
2	A1H40	C	501	14/14	0.78	0.19	31,36,40,41	14
2	A1H40	D	602	14/14	0.78	0.16	23,32,35,36	14
5	NAD	L	703	44/44	0.79	0.15	71,87,99,102	0
6	TRS	A	609	8/8	0.79	0.16	35,40,44,52	0
3	EDO	A	604	4/4	0.80	0.15	58,58,58,64	0
6	TRS	D	601	8/8	0.80	0.16	39,46,53,53	0
3	EDO	B	507	4/4	0.83	0.16	44,44,46,51	0
5	NAD	J	602	44/44	0.84	0.13	68,76,90,93	0
6	TRS	H	503	8/8	0.84	0.15	49,53,57,58	0
4	PEG	F	601	7/7	0.84	0.15	69,71,75,75	0
4	PEG	H	504	7/7	0.85	0.16	60,62,64,65	0
3	EDO	I	901	4/4	0.85	0.15	52,54,56,56	0
6	TRS	I	902	8/8	0.85	0.15	29,36,42,47	0
5	NAD	K	505	44/44	0.85	0.13	67,82,94,97	0
4	PEG	E	801	7/7	0.86	0.15	63,64,68,69	0
3	EDO	A	602	4/4	0.86	0.13	43,43,43,49	0
4	PEG	A	605	7/7	0.86	0.14	51,56,62,63	0
5	NAD	H	505	44/44	0.87	0.11	59,72,83,85	0
3	EDO	K	503	4/4	0.87	0.12	36,42,44,49	0
3	EDO	G	703	4/4	0.87	0.14	46,49,50,51	0
4	PEG	G	704	7/7	0.87	0.14	63,65,69,71	0
4	PEG	C	502	7/7	0.87	0.12	50,55,57,61	0
3	EDO	K	506	4/4	0.88	0.14	42,42,45,47	0
5	NAD	G	706	44/44	0.88	0.12	60,71,83,85	0
6	TRS	L	701	8/8	0.89	0.12	48,50,56,56	0
9	PG4	B	506	13/13	0.89	0.13	40,45,56,61	0

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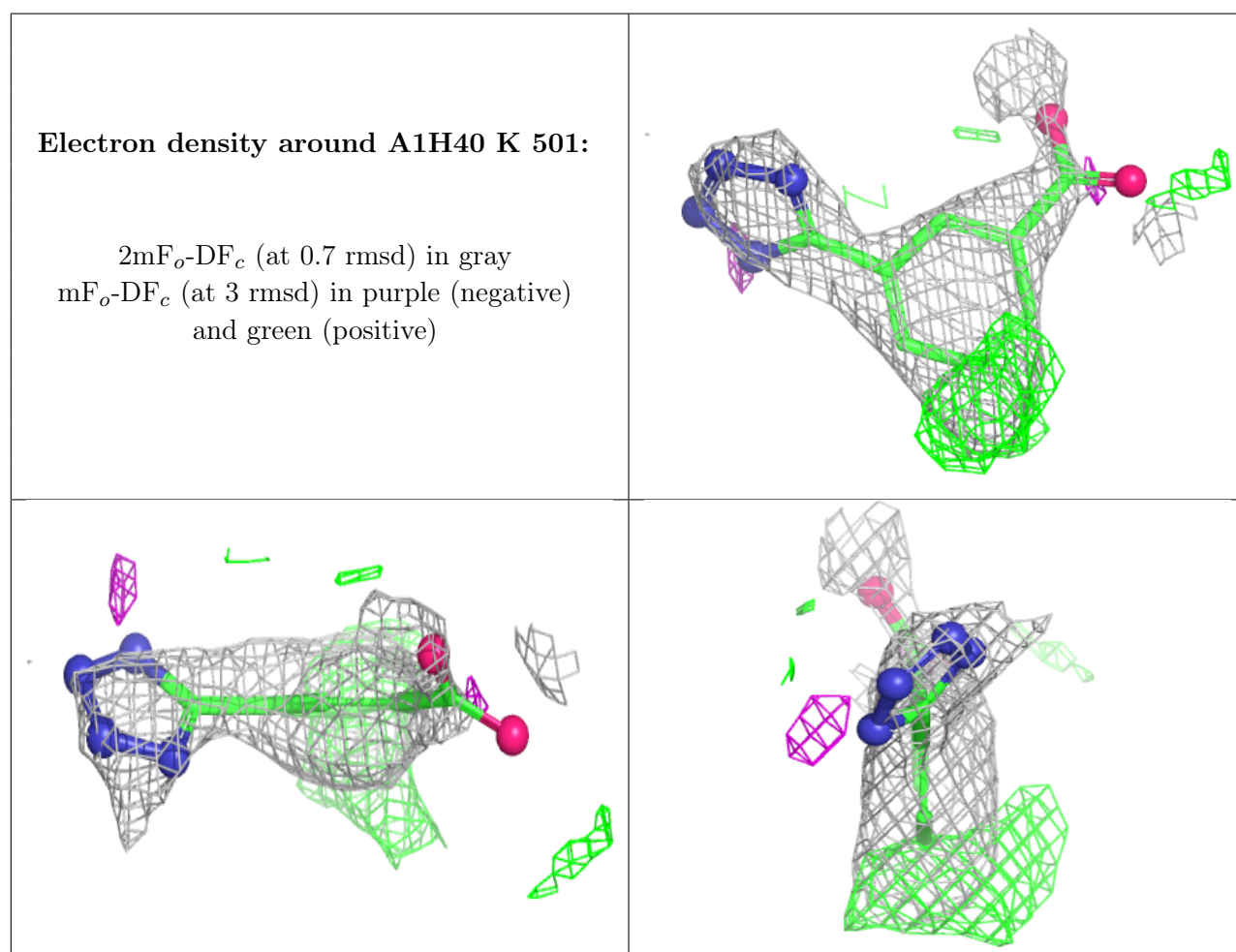
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	C	504	7/7	0.90	0.13	54,55,62,63	0
3	EDO	I	905	4/4	0.90	0.13	44,46,51,52	0
3	EDO	F	602	4/4	0.90	0.14	31,31,44,46	0
3	EDO	F	604	4/4	0.90	0.10	32,34,40,51	0
3	EDO	A	606	4/4	0.90	0.12	29,30,31,39	0
3	EDO	D	603	4/4	0.90	0.12	30,34,37,43	0
3	EDO	I	904	4/4	0.91	0.12	58,59,59,62	0
5	NAD	E	803	44/44	0.91	0.10	54,62,77,78	0
3	EDO	C	505	4/4	0.91	0.12	31,32,38,39	0
3	EDO	I	903	4/4	0.92	0.10	34,34,36,39	0
3	EDO	B	505	4/4	0.92	0.09	35,38,45,46	0
4	PEG	D	604	7/7	0.92	0.10	50,54,59,61	0
5	NAD	I	907	44/44	0.93	0.10	59,67,74,74	0
3	EDO	I	906	4/4	0.93	0.11	26,26,35,39	0
3	EDO	G	702	4/4	0.93	0.14	38,40,42,43	0
3	EDO	B	503	4/4	0.93	0.09	34,35,35,37	0
3	EDO	L	702	4/4	0.93	0.11	29,31,35,43	0
8	PGE	B	504	10/10	0.93	0.10	40,47,52,55	0
3	EDO	E	802	4/4	0.93	0.10	24,24,36,38	0
3	EDO	K	502	4/4	0.94	0.09	31,31,37,40	0
3	EDO	A	603	4/4	0.94	0.11	33,36,39,39	0
3	EDO	A	607	4/4	0.94	0.08	28,29,33,37	0
3	EDO	B	502	4/4	0.94	0.13	38,39,41,44	0
5	NAD	F	603	44/44	0.95	0.08	35,47,53,56	0
3	EDO	J	601	4/4	0.95	0.10	28,30,39,43	0
5	NAD	D	605	44/44	0.95	0.08	41,50,55,58	0
3	EDO	G	705	4/4	0.95	0.10	26,27,34,37	0
5	NAD	A	608	44/44	0.96	0.08	33,44,50,54	0
5	NAD	C	506	44/44	0.96	0.07	33,40,45,52	0
3	EDO	C	503	4/4	0.96	0.07	39,39,41,43	0
3	EDO	H	502	4/4	0.96	0.08	28,31,37,39	0
10	NA	F	605	1/1	0.96	0.15	34,34,34,34	0
10	NA	I	908	1/1	0.96	0.11	26,26,26,26	0
5	NAD	B	508	44/44	0.97	0.06	26,31,38,47	0
10	NA	G	707	1/1	0.98	0.03	38,38,38,38	0
7	CA	E	804	1/1	0.98	0.02	30,30,30,30	0
7	CA	H	506	1/1	0.99	0.03	29,29,29,29	0
7	CA	I	909	1/1	0.99	0.02	31,31,31,31	0
7	CA	J	603	1/1	0.99	0.02	30,30,30,30	0
7	CA	G	708	1/1	0.99	0.03	32,32,32,32	0
7	CA	K	507	1/1	1.00	0.01	34,34,34,34	0
7	CA	L	704	1/1	1.00	0.01	30,30,30,30	0

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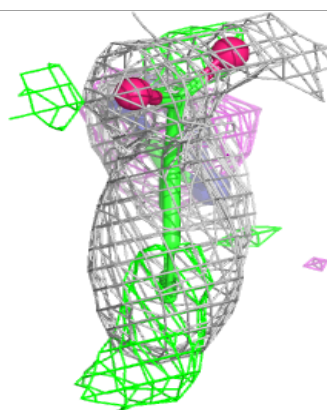
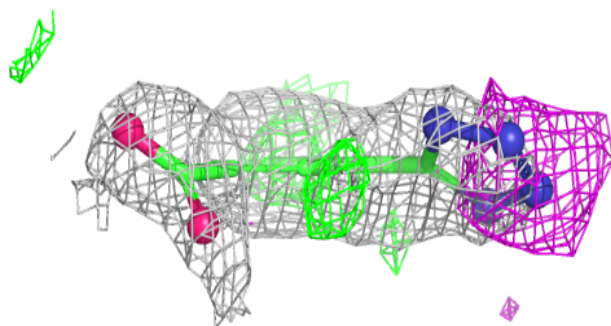
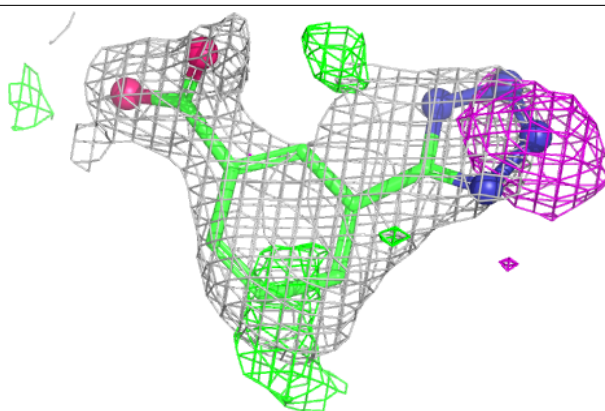
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CA	F	606	1/1	1.00	0.01	31,31,31,31	0
7	CA	B	509	1/1	1.00	0.01	25,25,25,25	0
7	CA	C	507	1/1	1.00	0.01	26,26,26,26	0
7	CA	D	606	1/1	1.00	0.01	18,18,18,18	0
7	CA	A	610	1/1	1.00	0.01	21,21,21,21	0

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

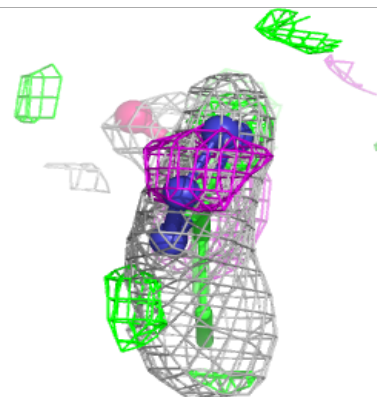
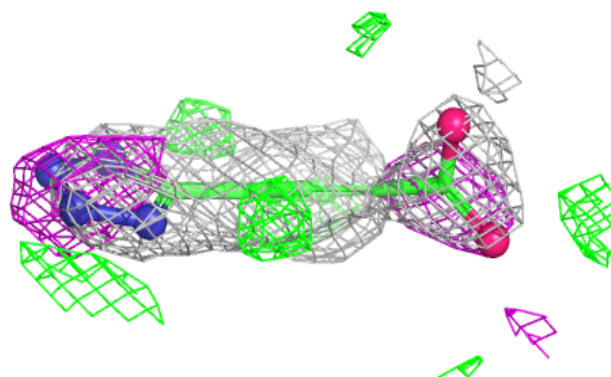
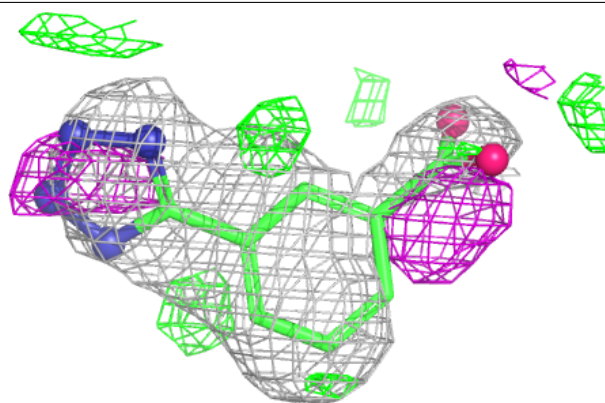


Electron density around A1H40 A 601:

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

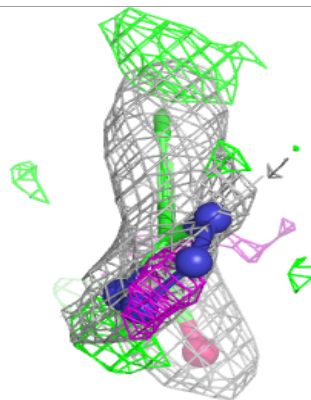
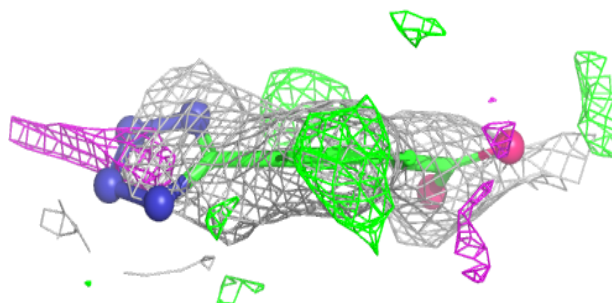
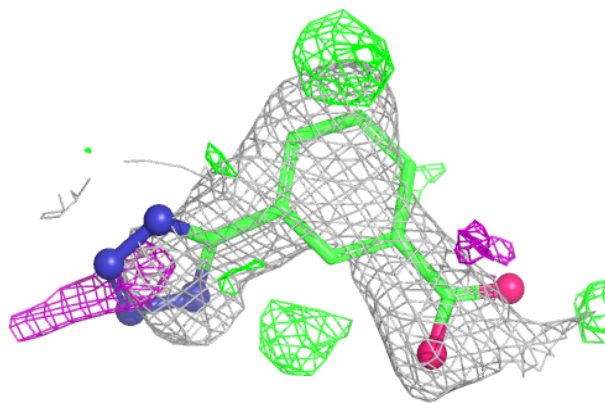
**Electron density around A1H40 B 501:**

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

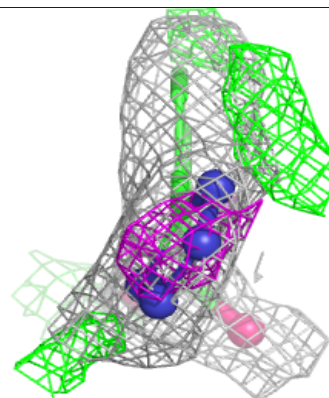
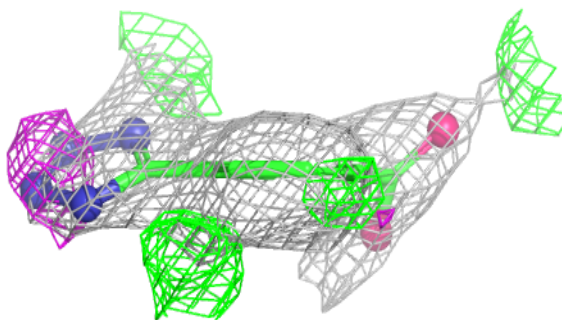
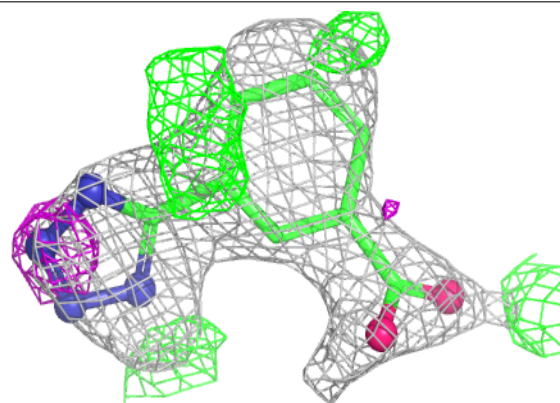


Electron density around A1H40 H 501:

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

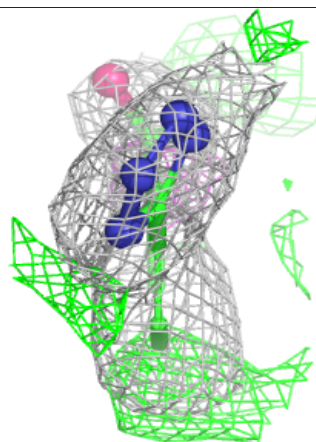
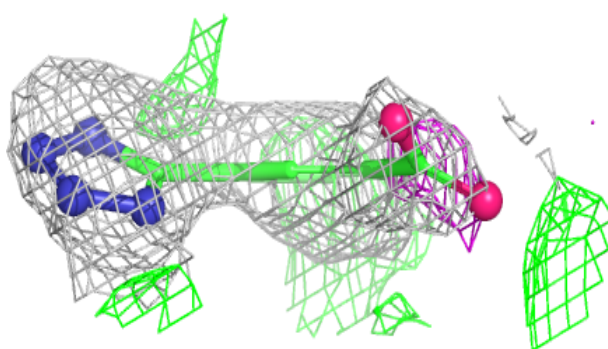
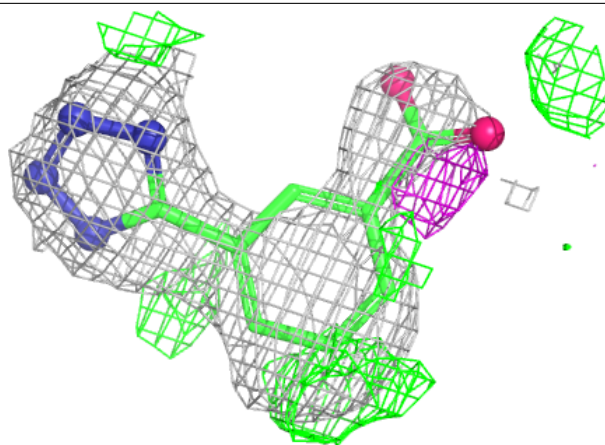
**Electron density around A1H40 C 501:**

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

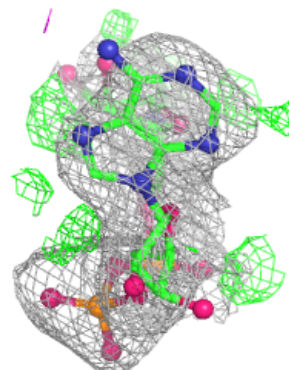
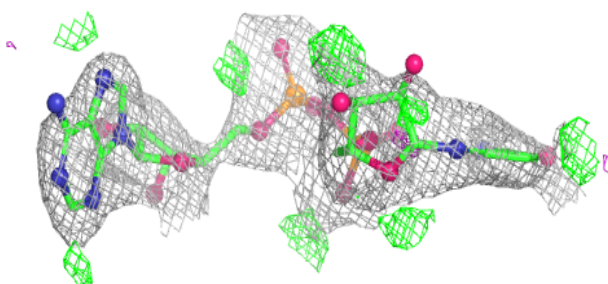
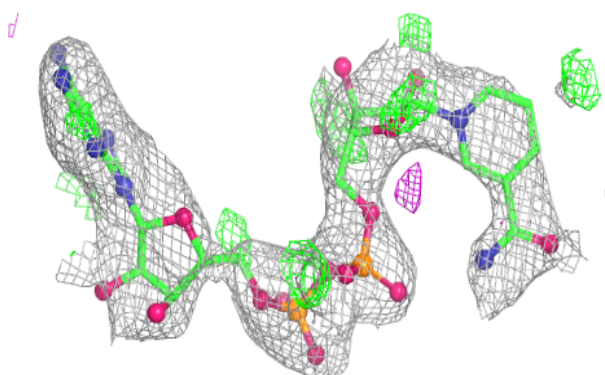


Electron density around A1H40 D 602:

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

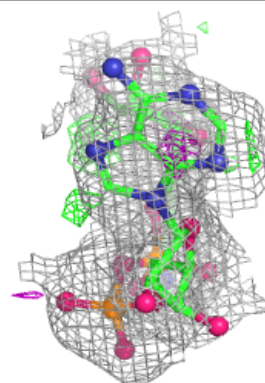
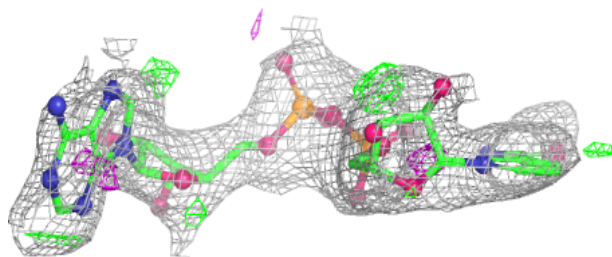
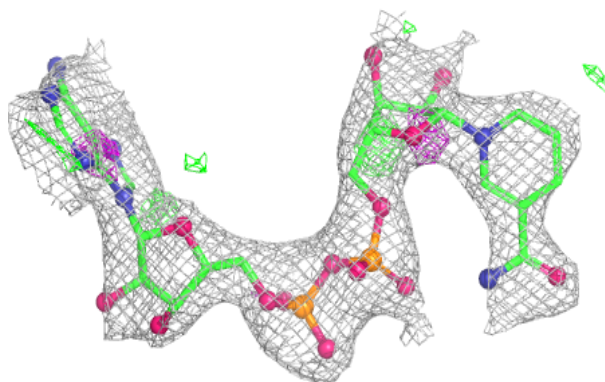
**Electron density around NAD L 703:**

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

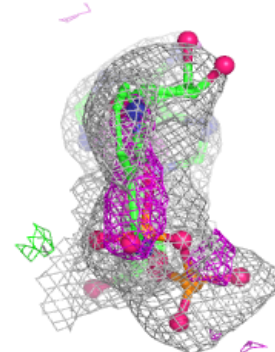
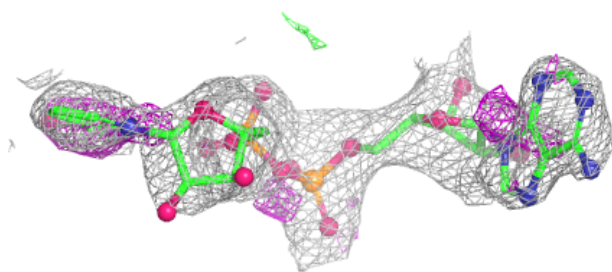
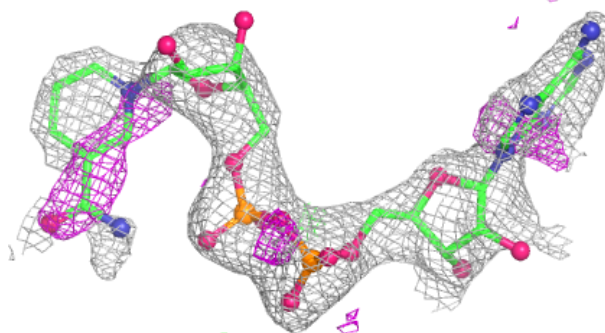


Electron density around NAD J 602:

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

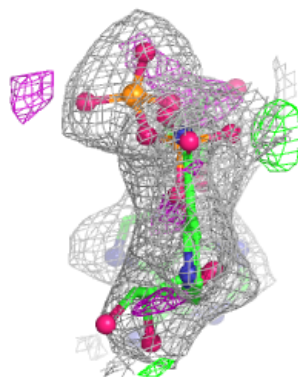
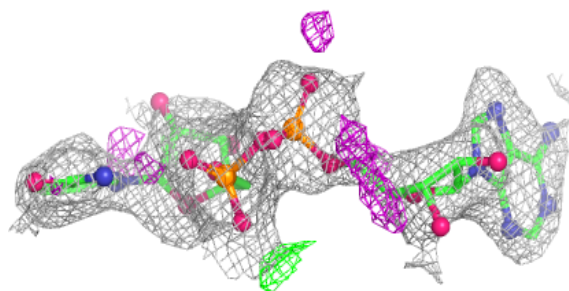
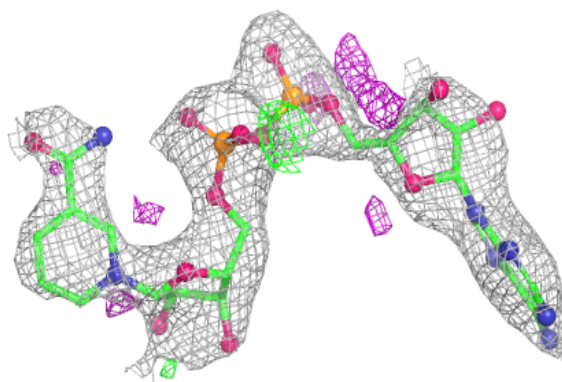
**Electron density around NAD K 505:**

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

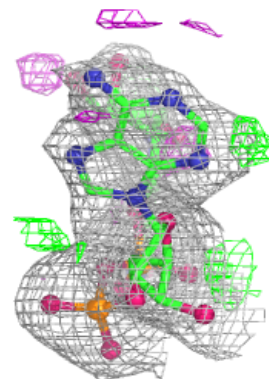
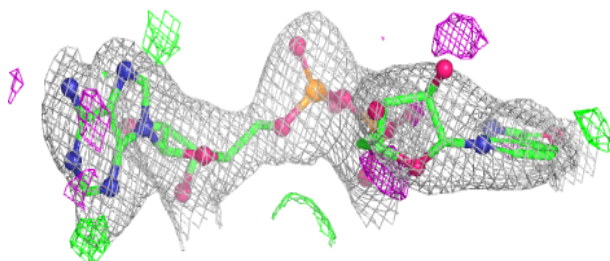
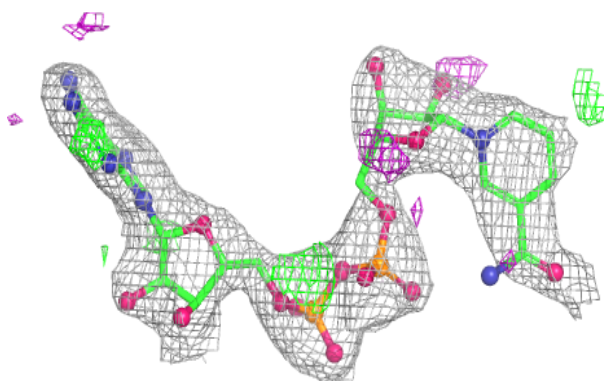


Electron density around NAD H 505:

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

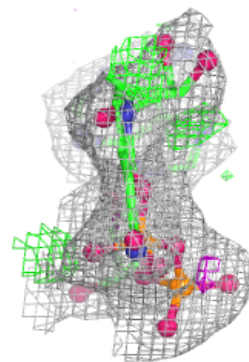
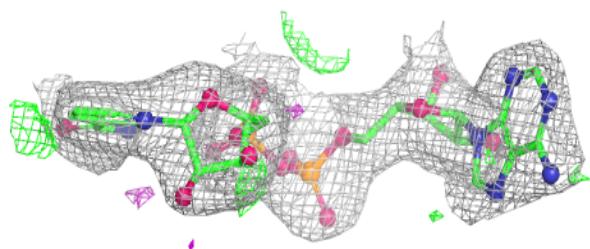
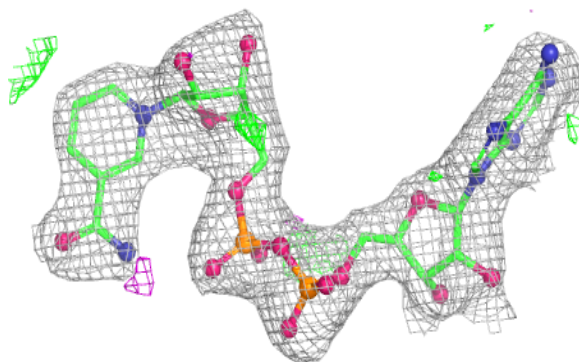
**Electron density around NAD G 706:**

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

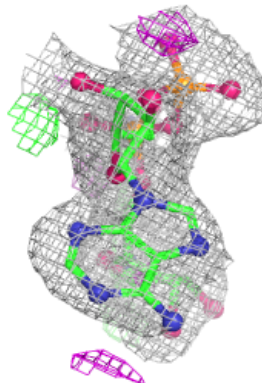
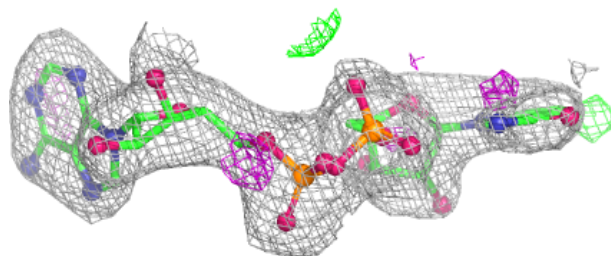
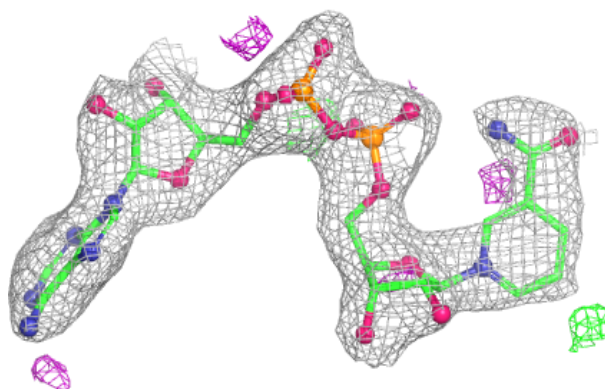


Electron density around NAD E 803:

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

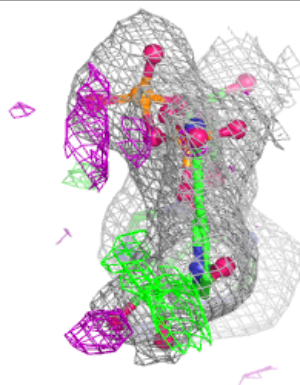
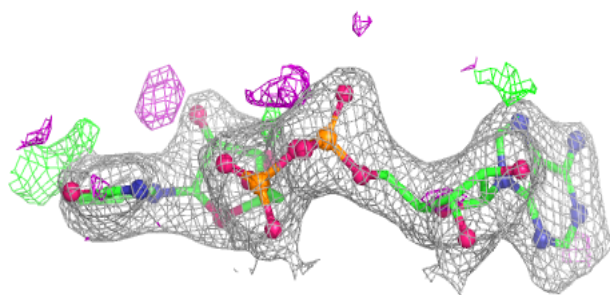
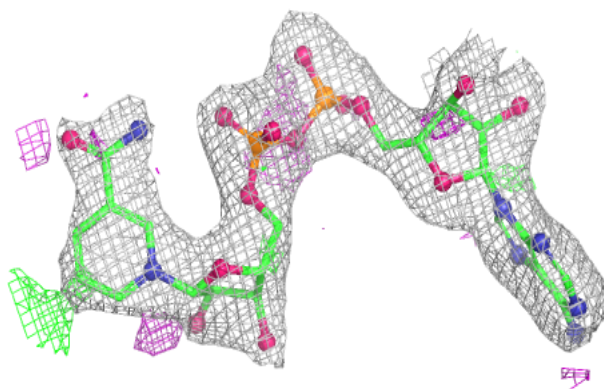
**Electron density around NAD I 907:**

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

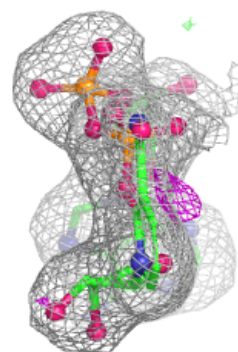
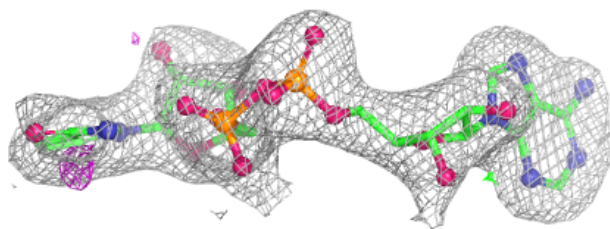
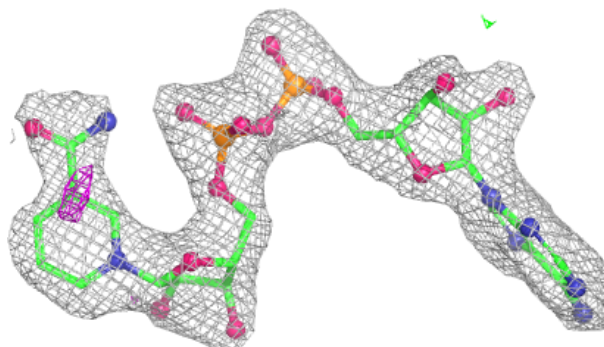


Electron density around NAD F 603:

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

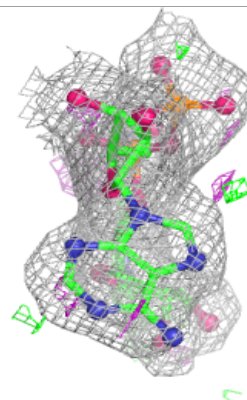
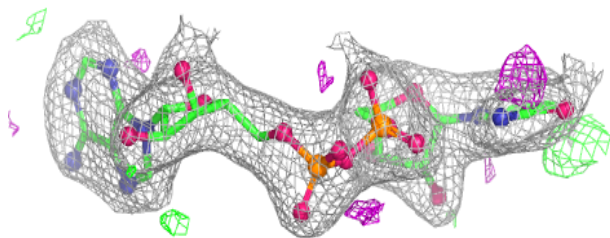
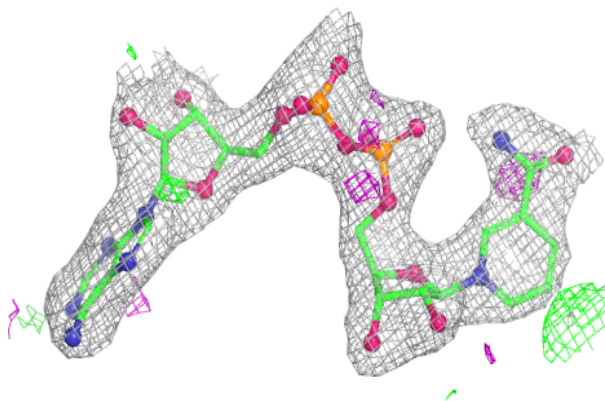
**Electron density around NAD D 605:**

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

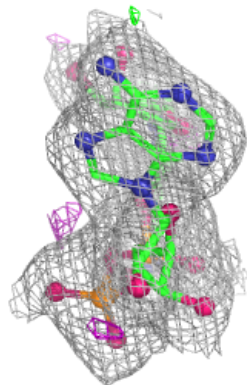
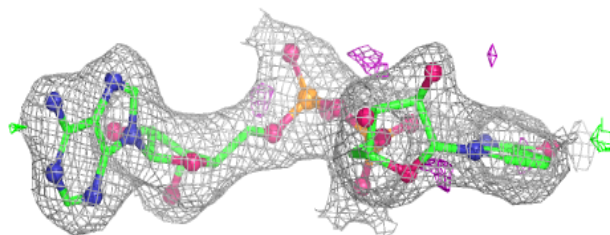
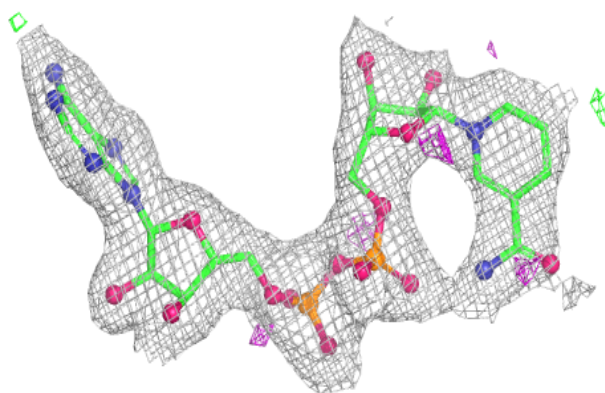


Electron density around NAD A 608:

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

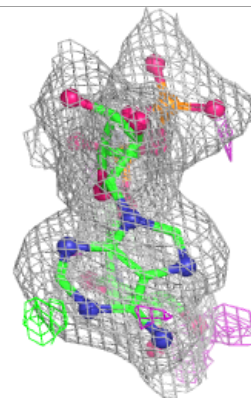
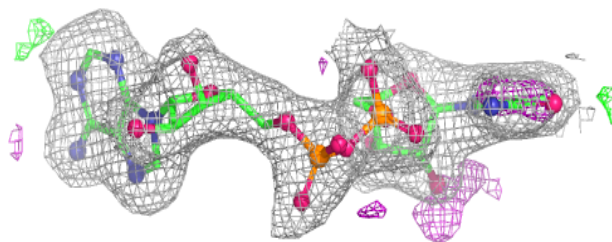
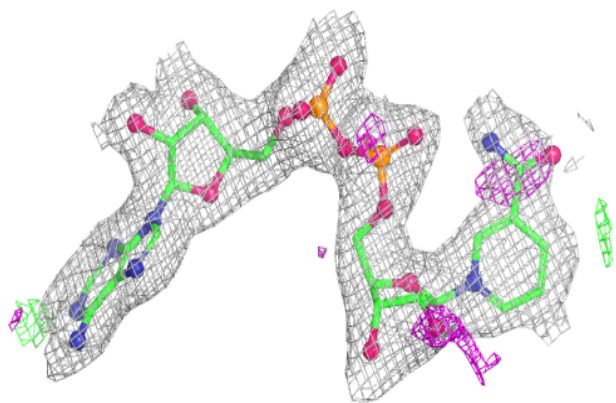
**Electron density around NAD C 506:**

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



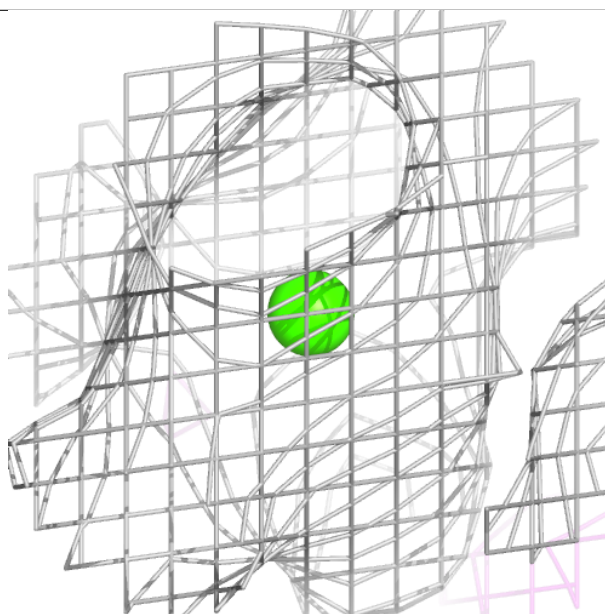
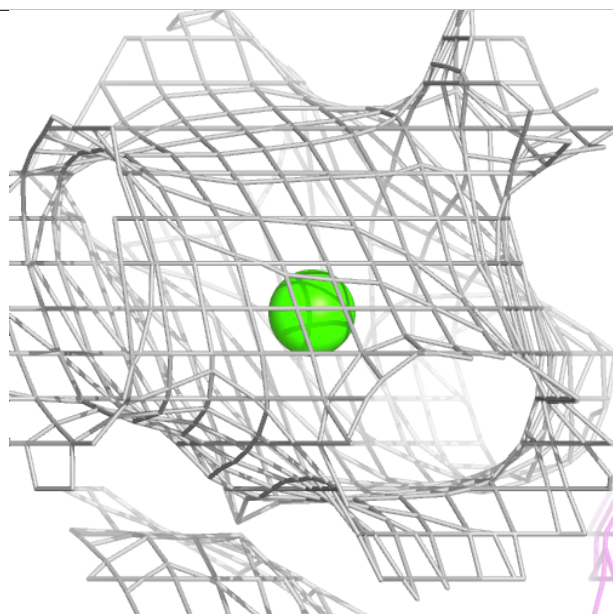
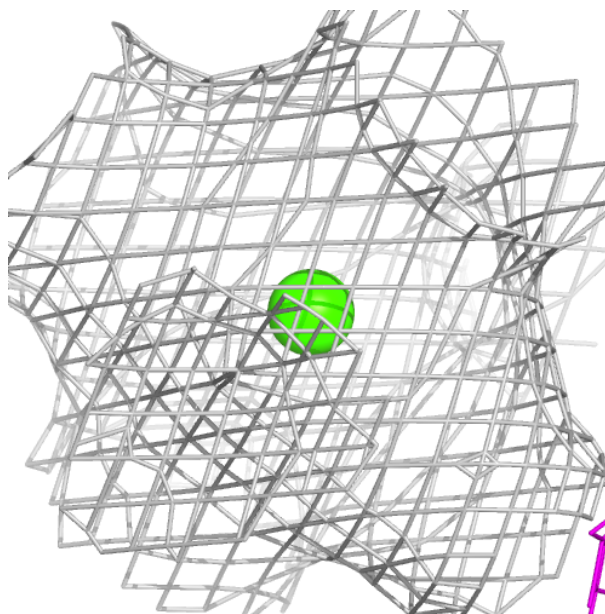
Electron density around NAD B 508:

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



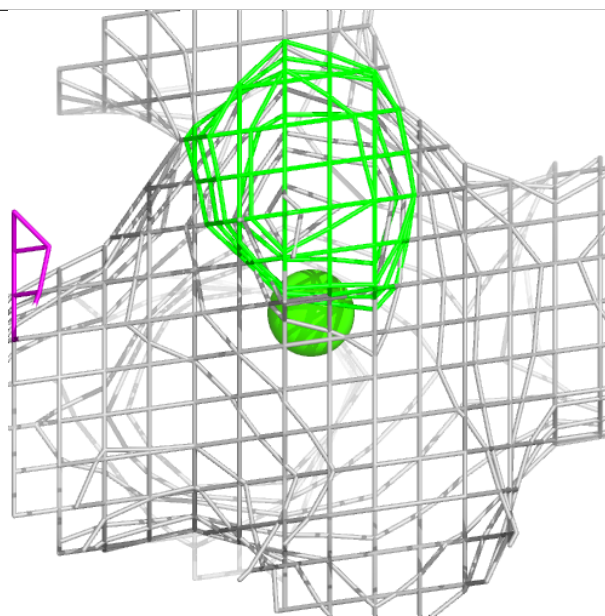
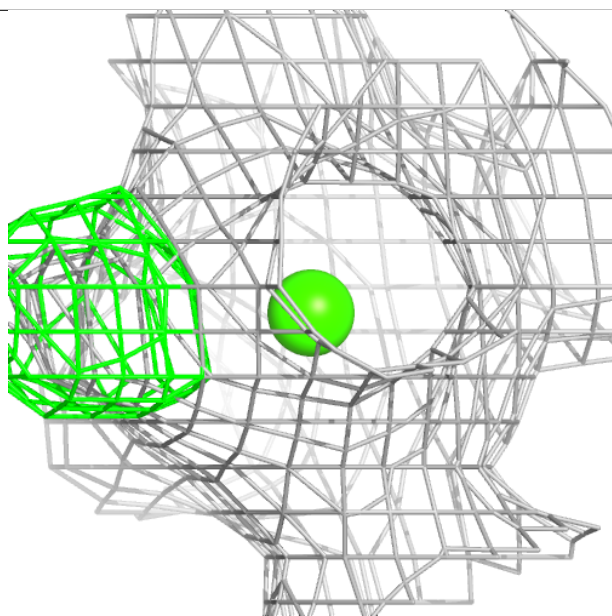
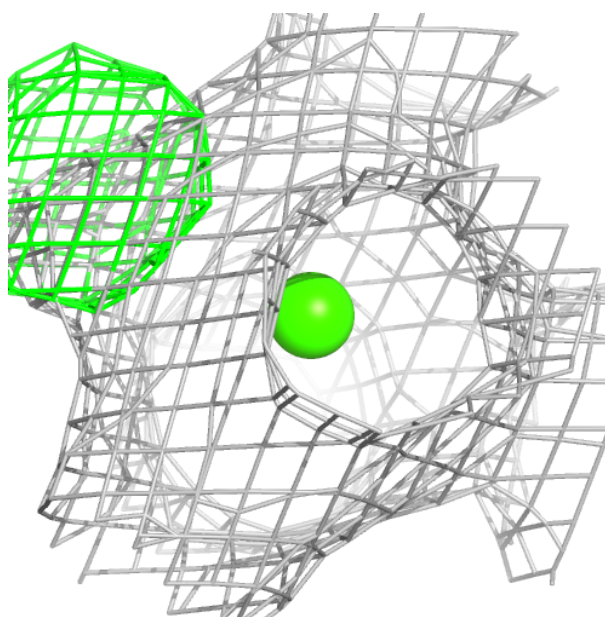
Electron density around CA E 804:

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



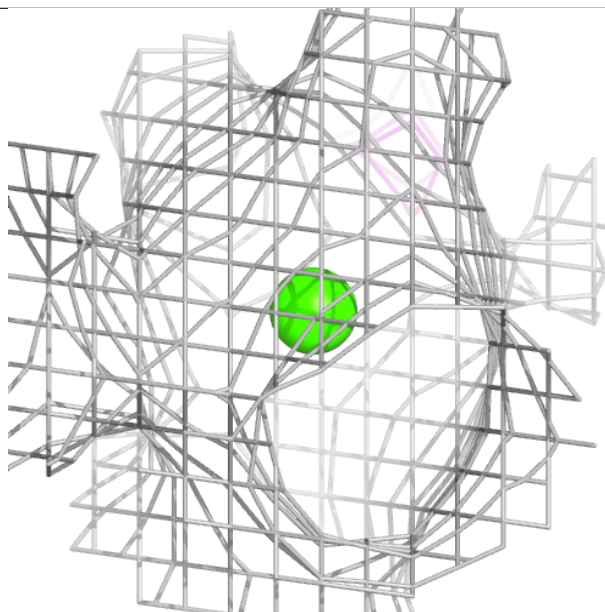
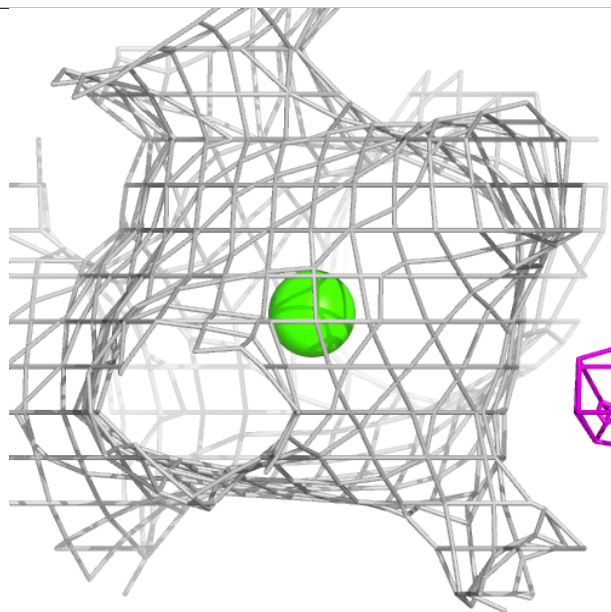
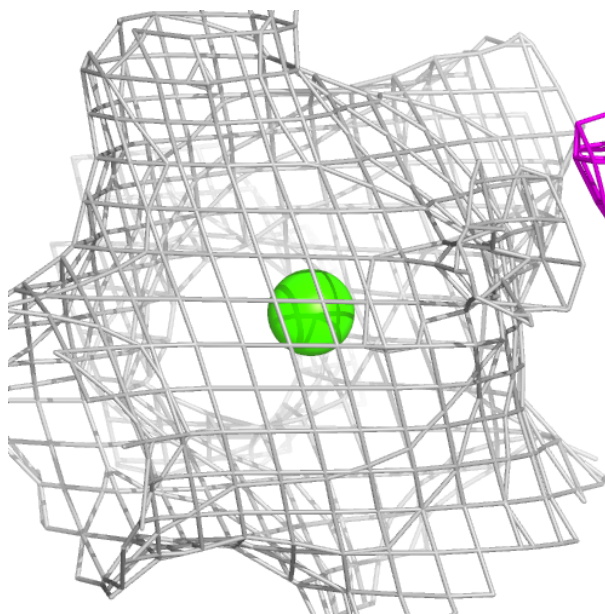
Electron density around CA H 506:

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



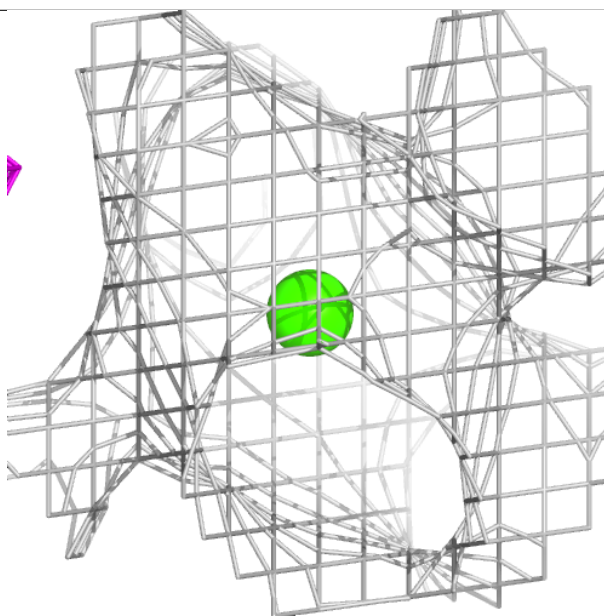
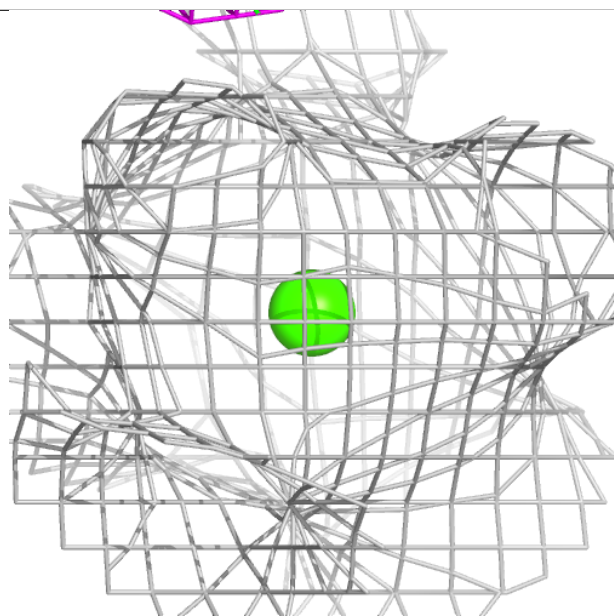
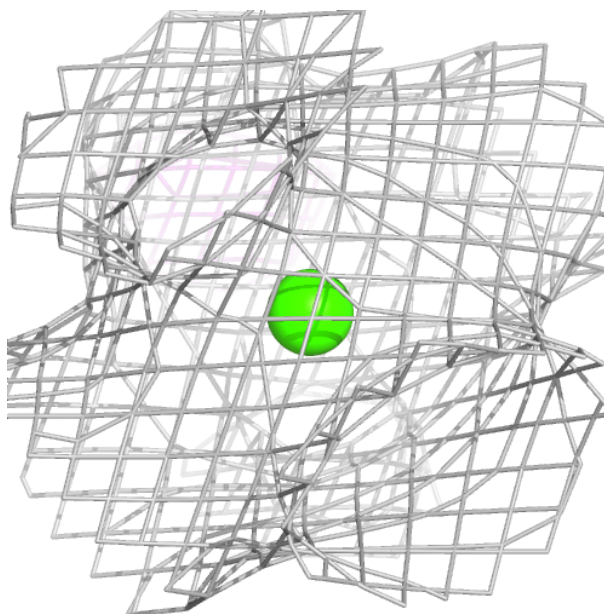
Electron density around CA I 909:

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



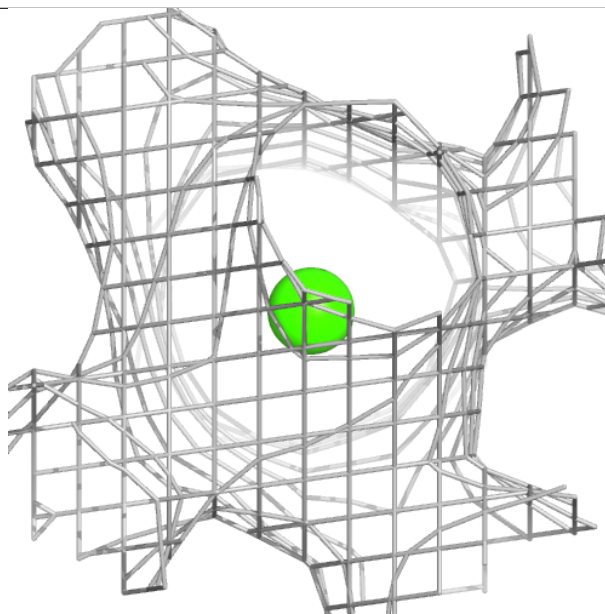
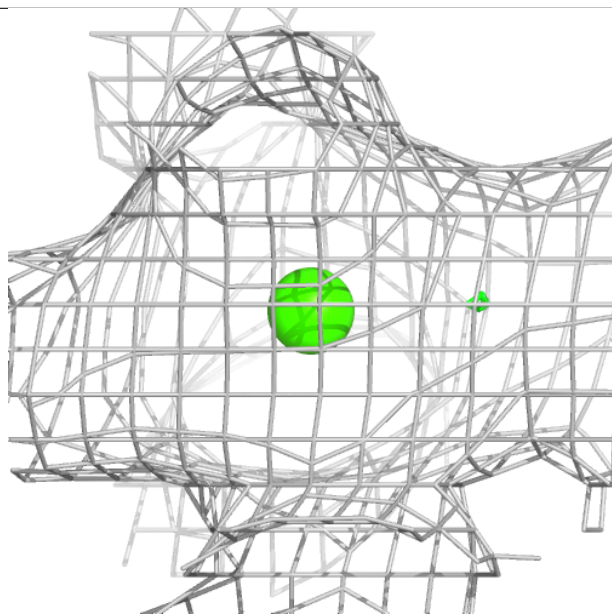
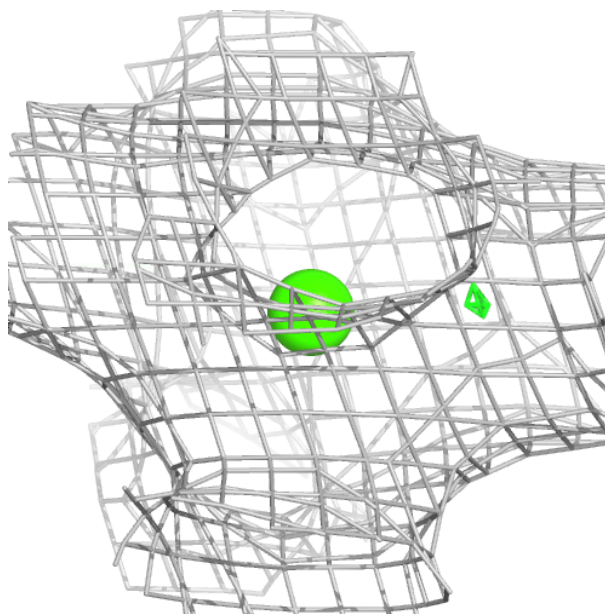
Electron density around CA J 603:

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



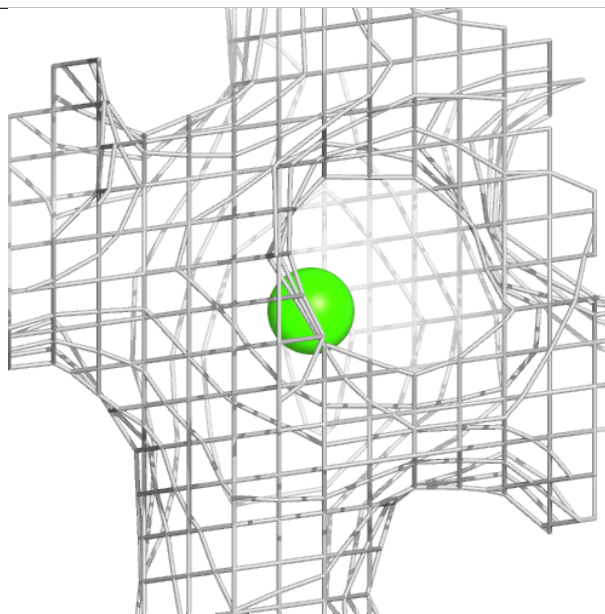
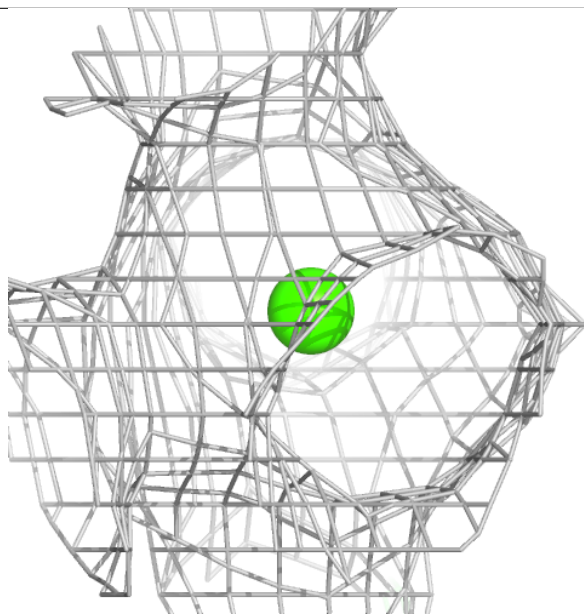
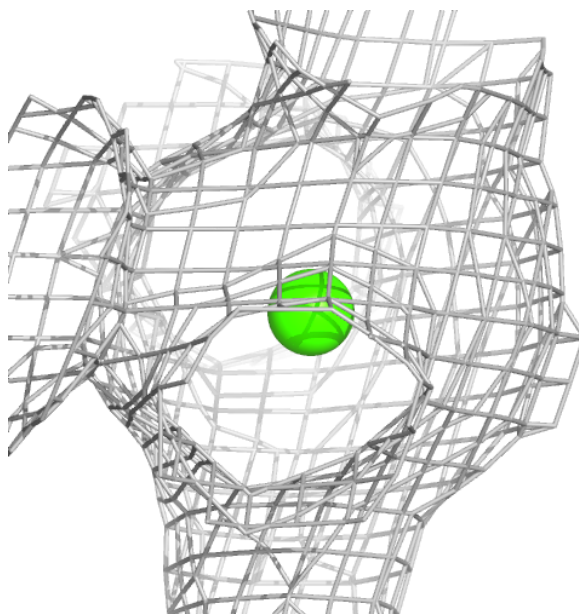
Electron density around CA G 708:

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



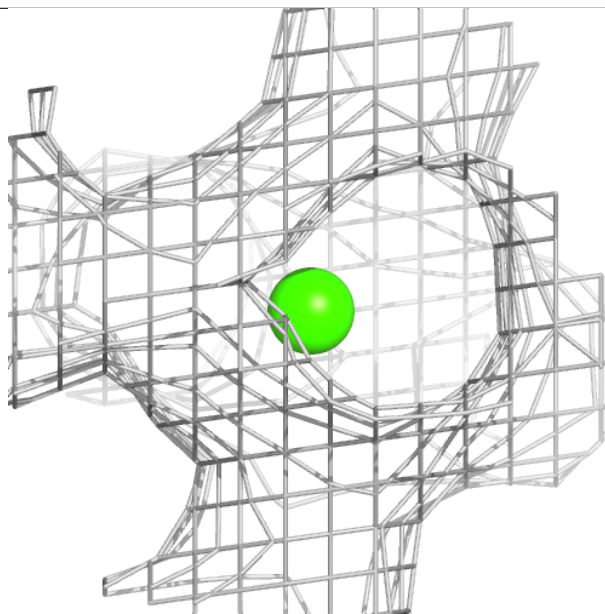
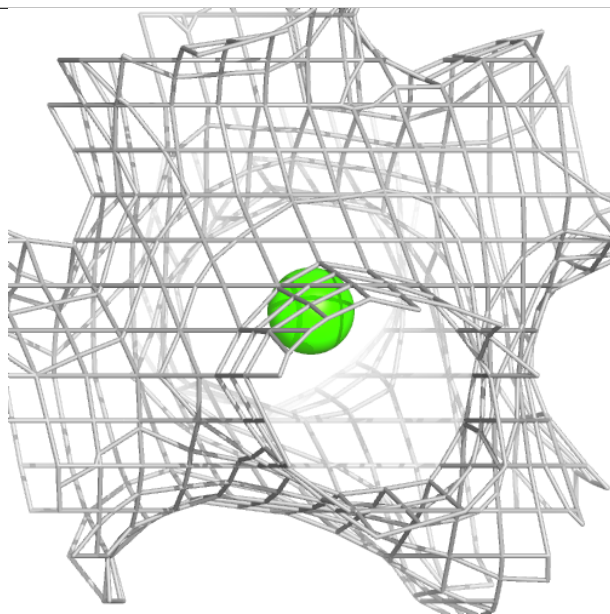
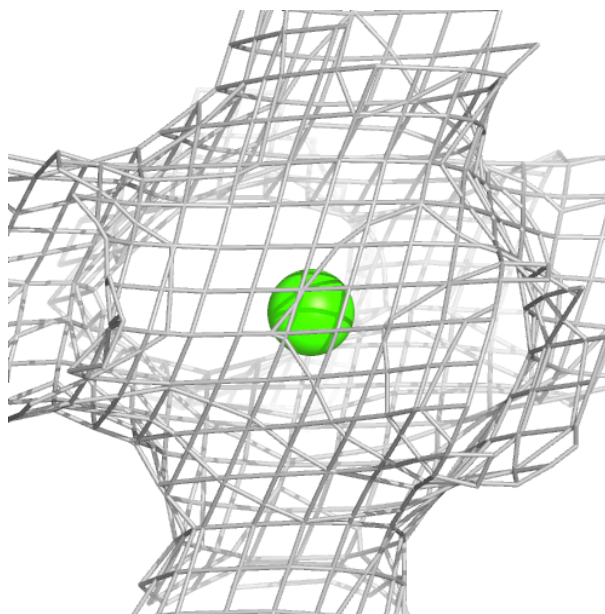
Electron density around CA K 507:

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



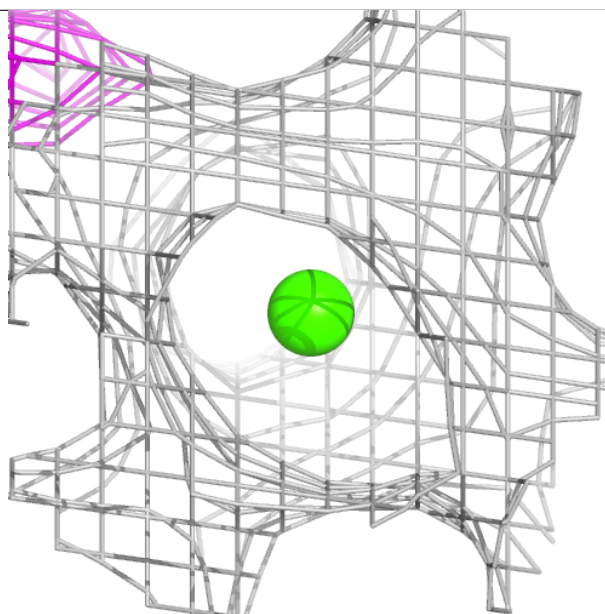
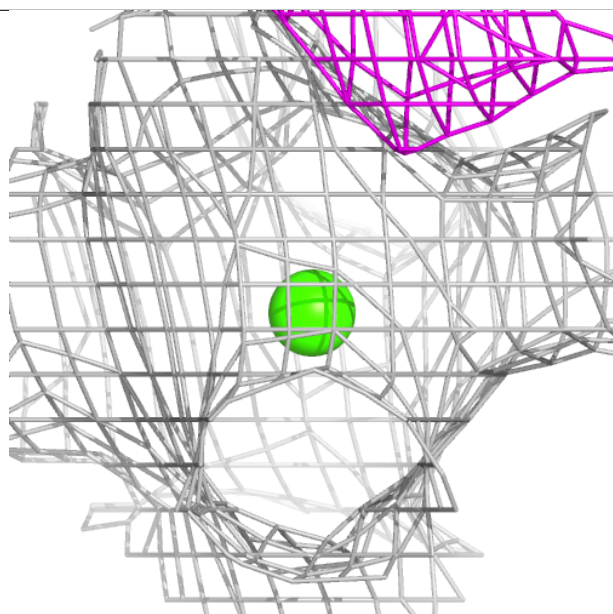
Electron density around CA L 704:

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



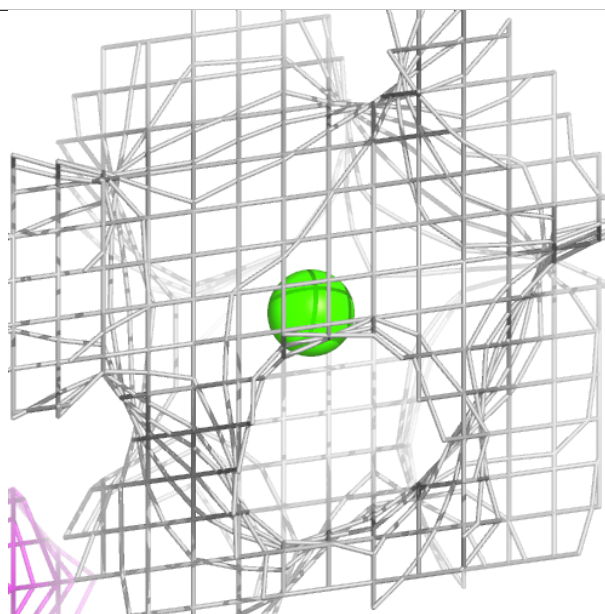
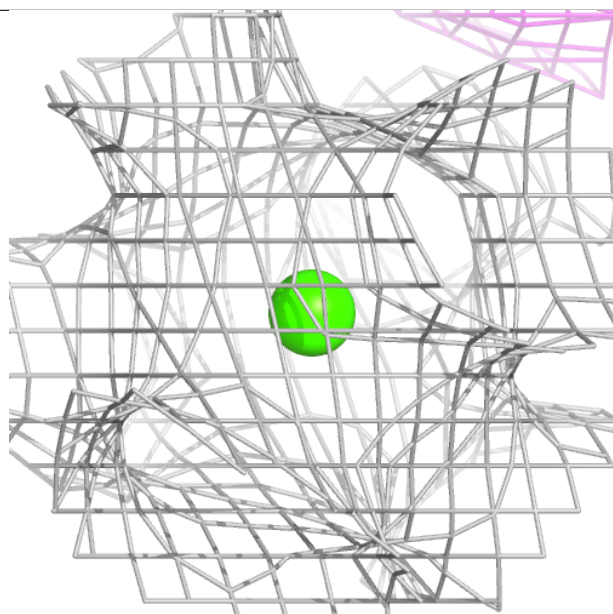
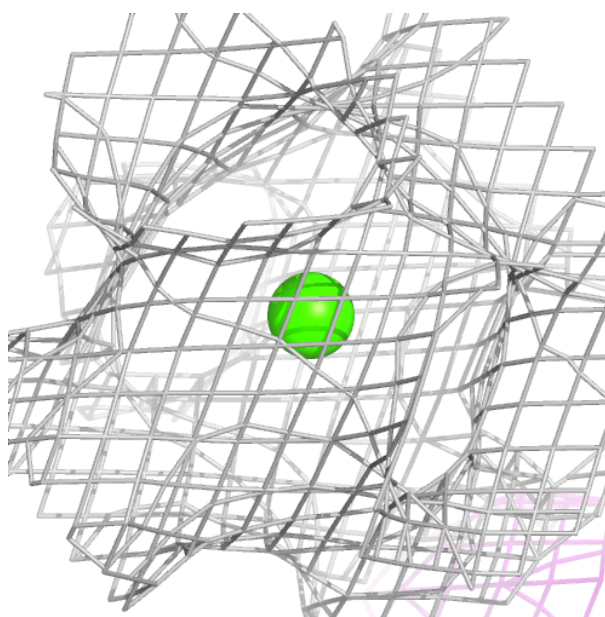
Electron density around CA F 606:

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



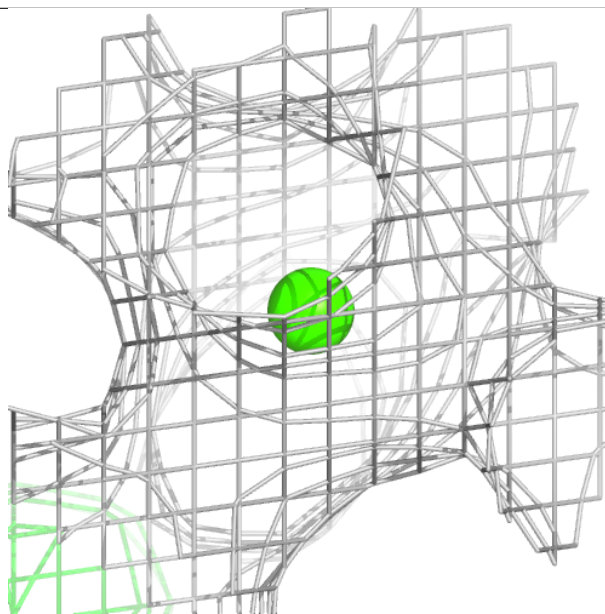
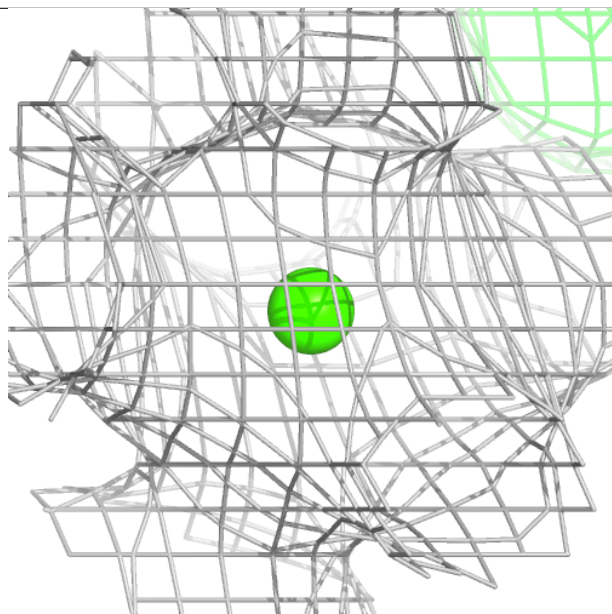
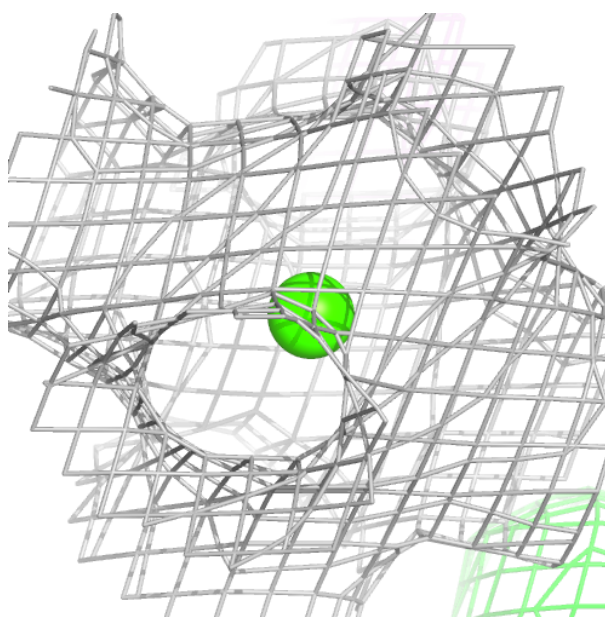
Electron density around CA B 509:

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



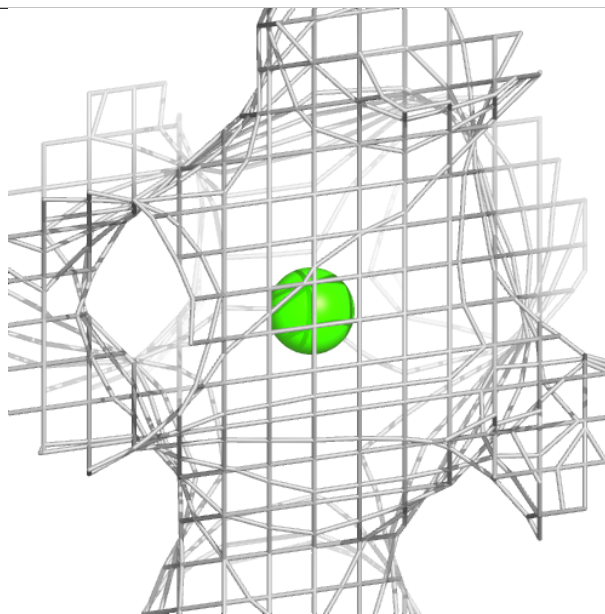
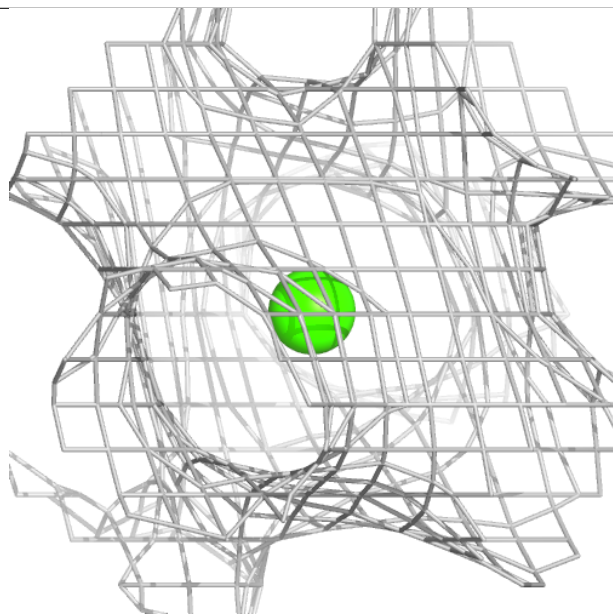
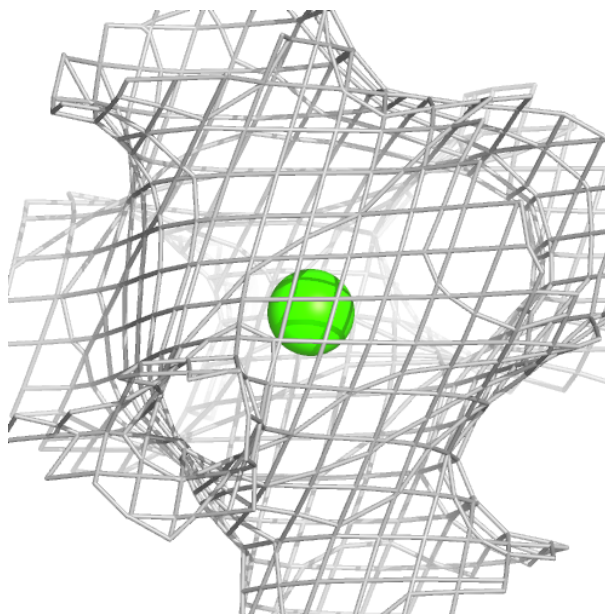
Electron density around CA C 507:

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



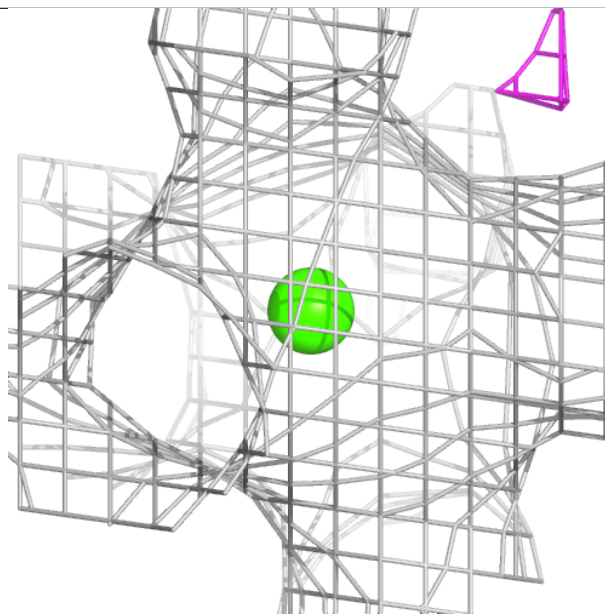
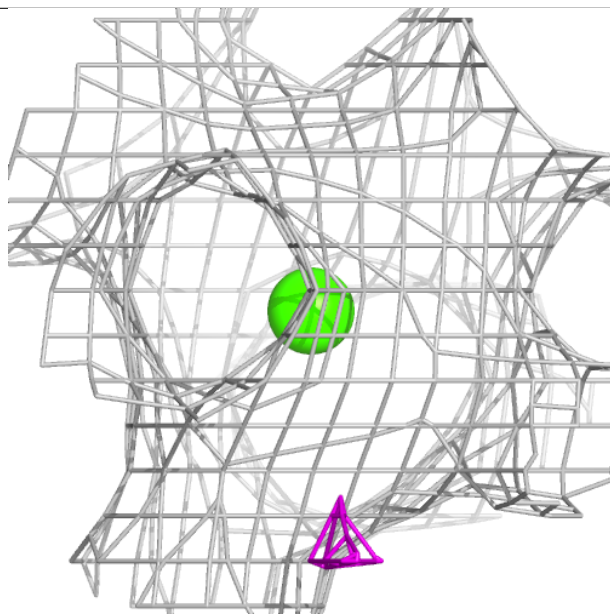
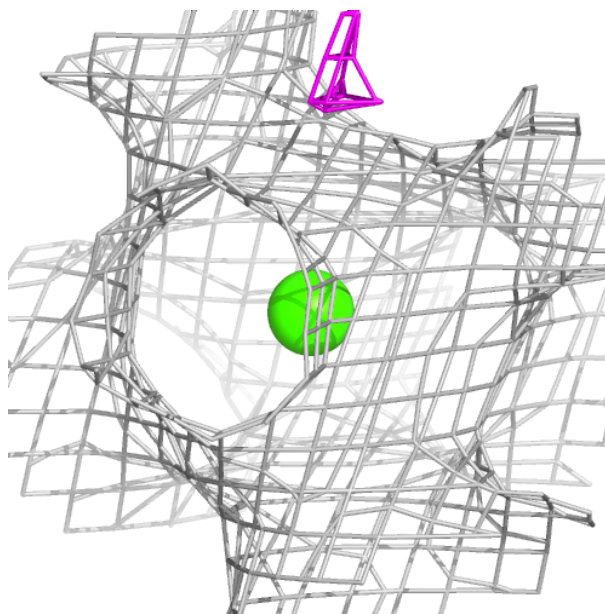
Electron density around CA D 606:

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



Electron density around CA A 610:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.