wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2024 – 08:19 pm BST

PDB ID	:	8S3B
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

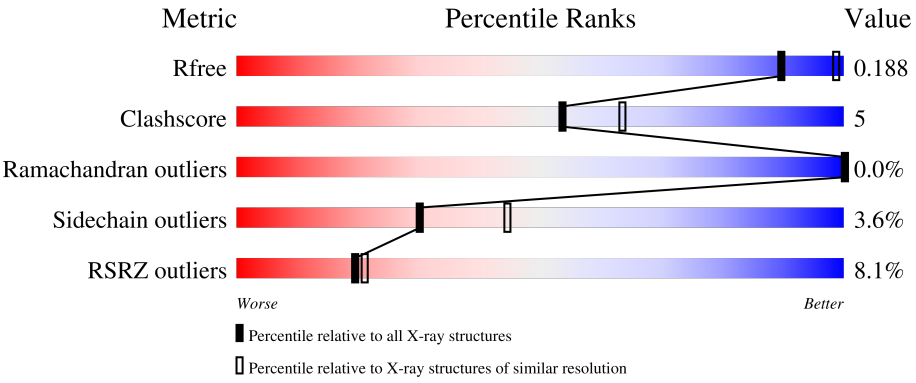
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	414	87% 10%
1	B	414	87% 11%
1	C	414	88% 9%
1	D	414	87% 12%
1	E	414	8% 87% 11%

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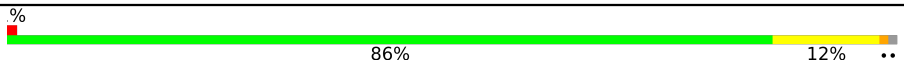
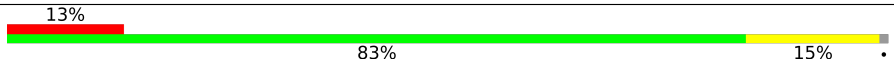
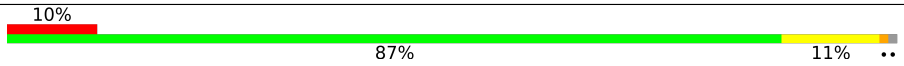
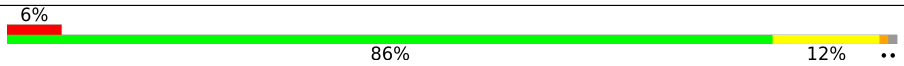
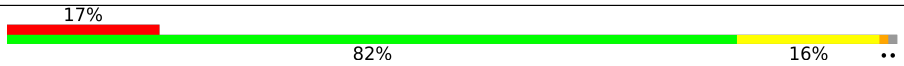
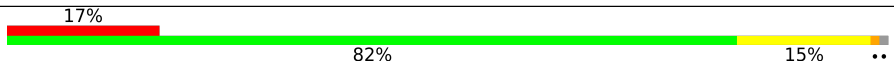
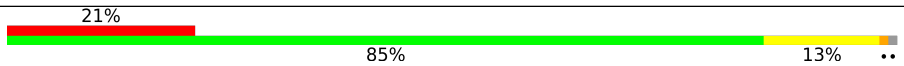
Mol	Chain	Length	Quality of chain
1	F	414	
1	G	414	
1	H	414	
1	I	414	
1	J	414	
1	K	414	
1	L	414	

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	A1H40	K	501	-	X	-	-

2 Entry composition (i)

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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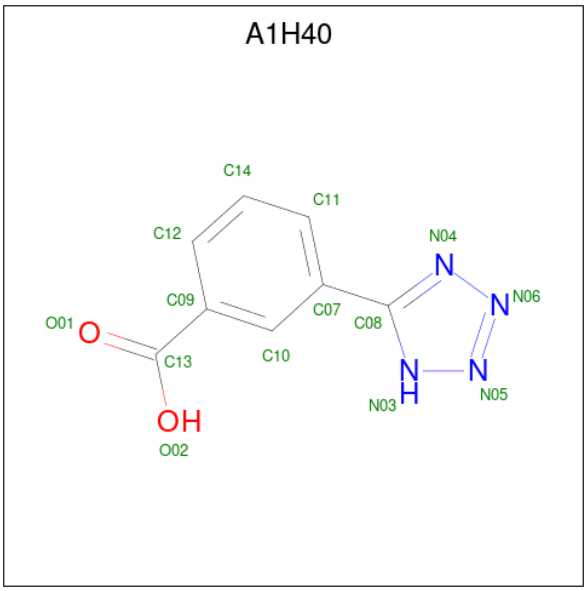
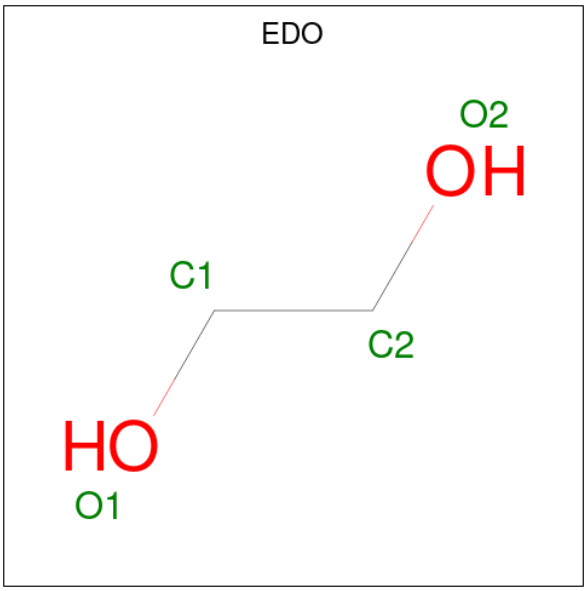
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP G7JYL4
C	-2	SER	-	expression tag	UNP G7JYL4
C	-1	ASN	-	expression tag	UNP G7JYL4
C	0	ALA	-	expression tag	UNP G7JYL4
D	-2	SER	-	expression tag	UNP G7JYL4
D	-1	ASN	-	expression tag	UNP G7JYL4
D	0	ALA	-	expression tag	UNP G7JYL4
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 (three-letter code: A1H40) (formula: $C_8H_6N_4O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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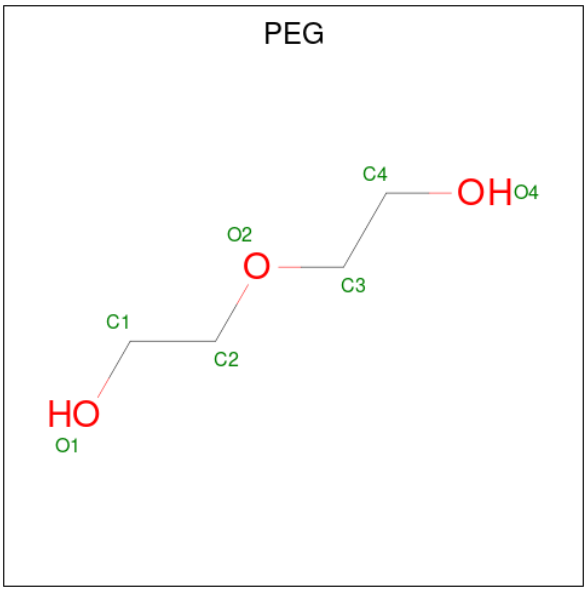
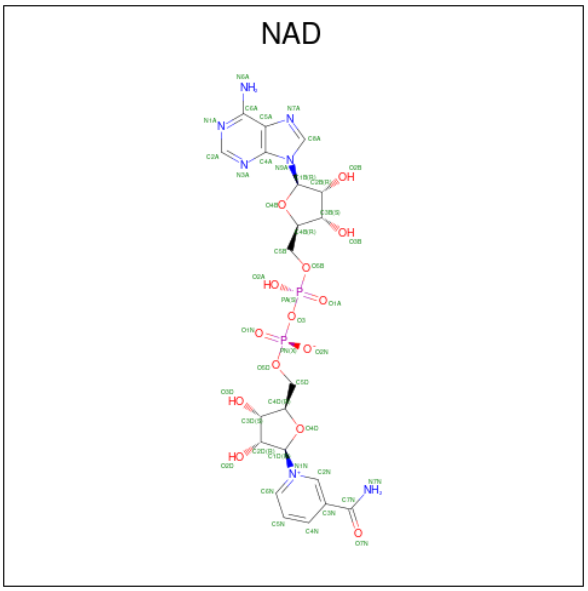
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



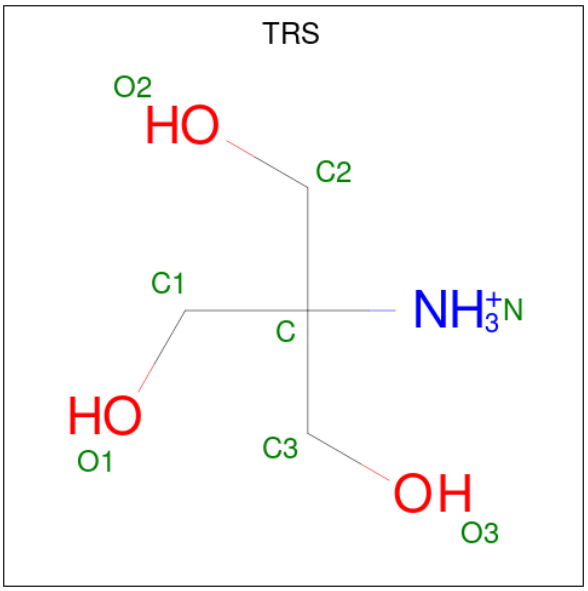
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	F	1	Total C O 7 4 3	0	0
4	G	1	Total C O 7 4 3	0	0
4	H	1	Total C O 7 4 3	0	0

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

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

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

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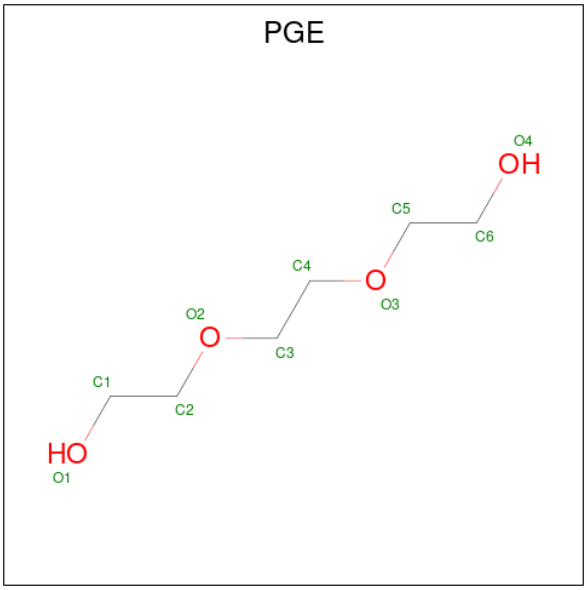
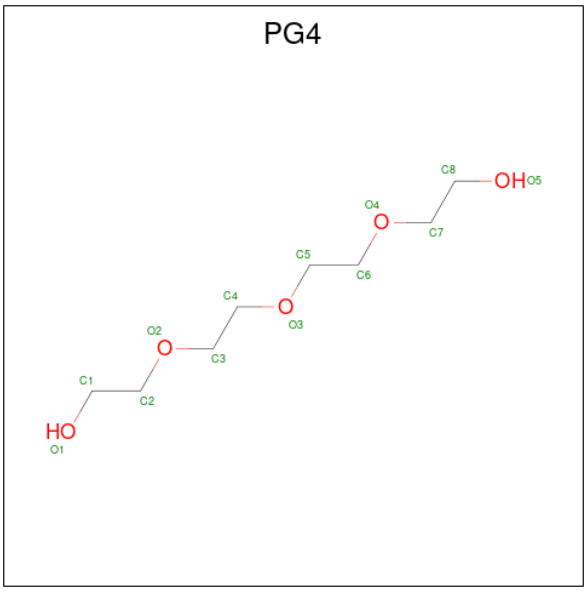
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total Ca 1 1	0	0
7	F	1	Total Ca 1 1	0	0
7	G	1	Total Ca 1 1	0	0
7	H	1	Total Ca 1 1	0	0
7	I	1	Total Ca 1 1	0	0
7	J	1	Total Ca 1 1	0	0
7	K	1	Total Ca 1 1	0	0
7	L	1	Total Ca 1 1	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 11 is water.

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

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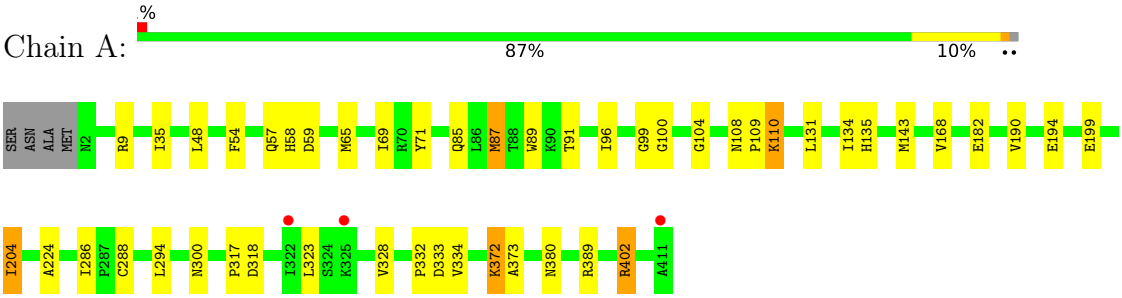
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	81	Total O 81 81	0	0
11	G	85	Total O 85 85	0	0
11	H	81	Total O 81 81	0	0
11	I	82	Total O 82 82	0	0
11	J	73	Total O 73 73	0	0
11	K	62	Total O 62 62	0	0
11	L	62	Total O 62 62	0	0

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.

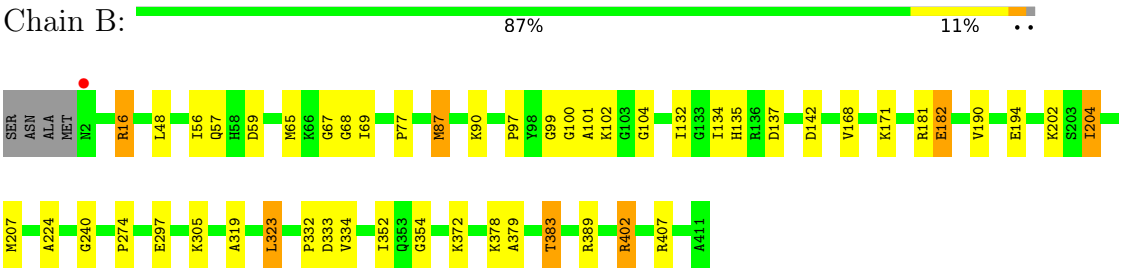
• Molecule 1: Glutamate dehydrogenase

Chain A:



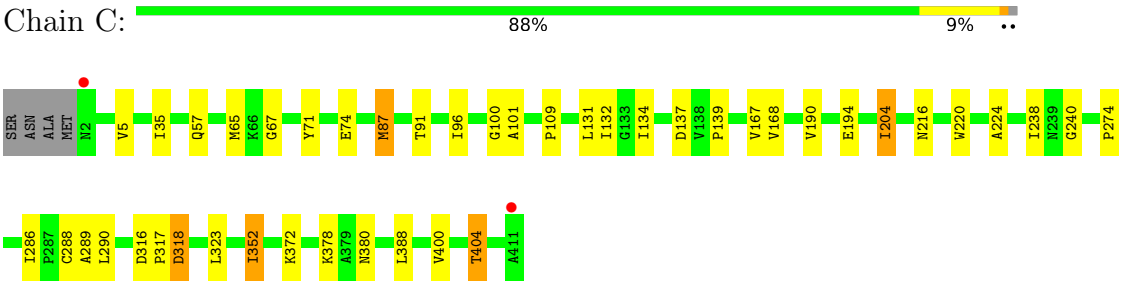
• Molecule 1: Glutamate dehydrogenase

Chain B:



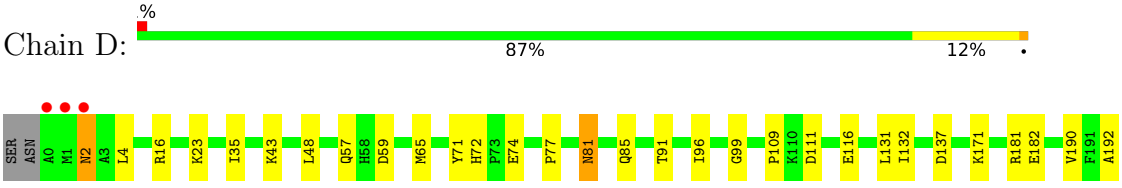
• Molecule 1: Glutamate dehydrogenase

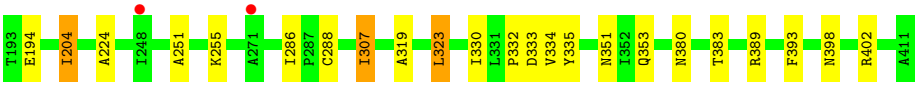
Chain C:



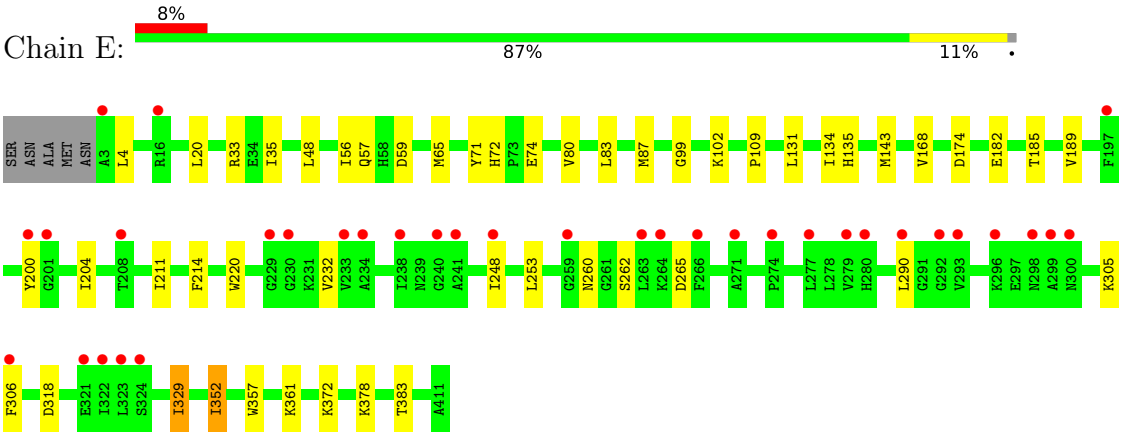
• Molecule 1: Glutamate dehydrogenase

Chain D:

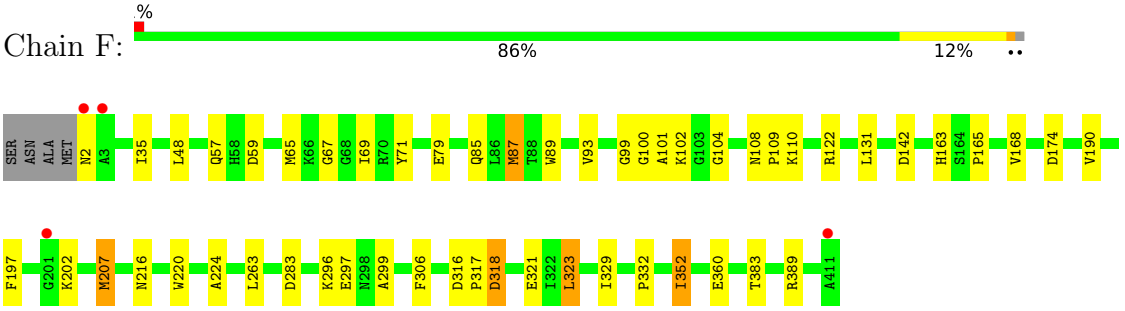




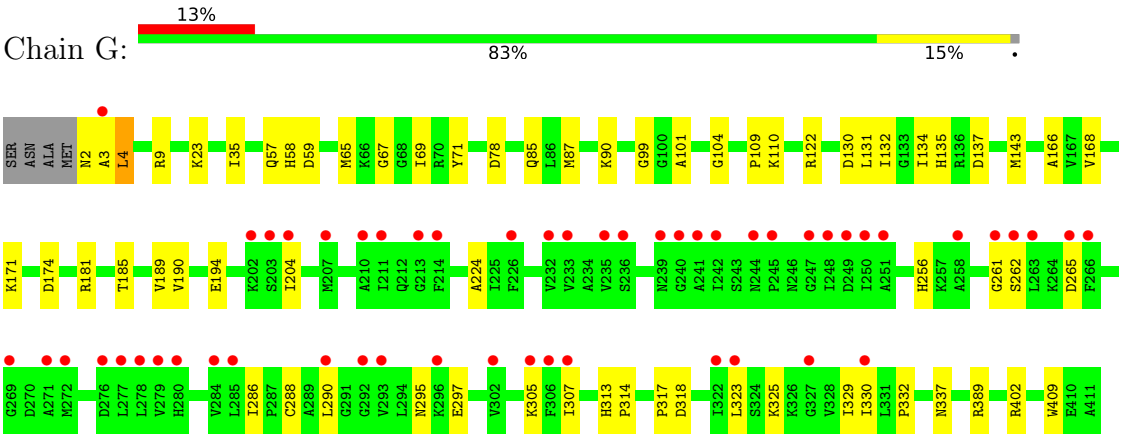
• Molecule 1: Glutamate dehydrogenase



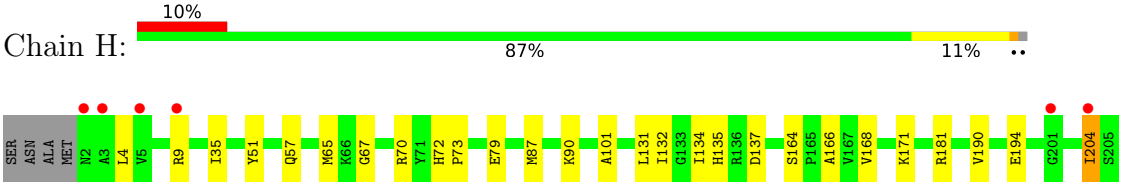
• Molecule 1: Glutamate dehydrogenase

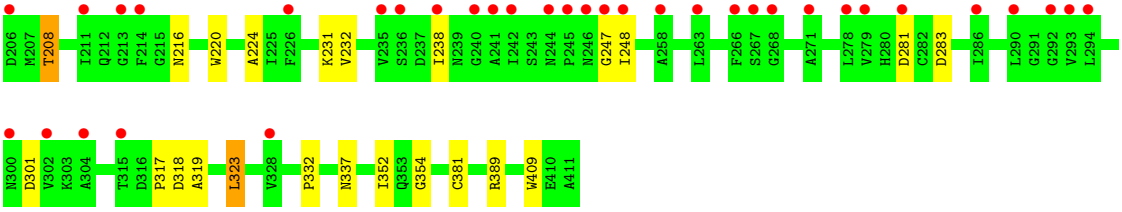


• Molecule 1: Glutamate dehydrogenase

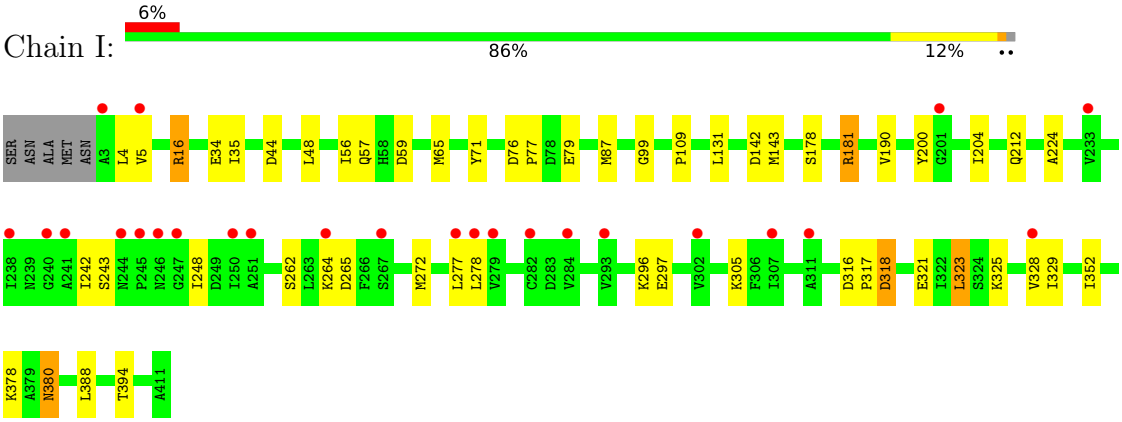


• Molecule 1: Glutamate dehydrogenase

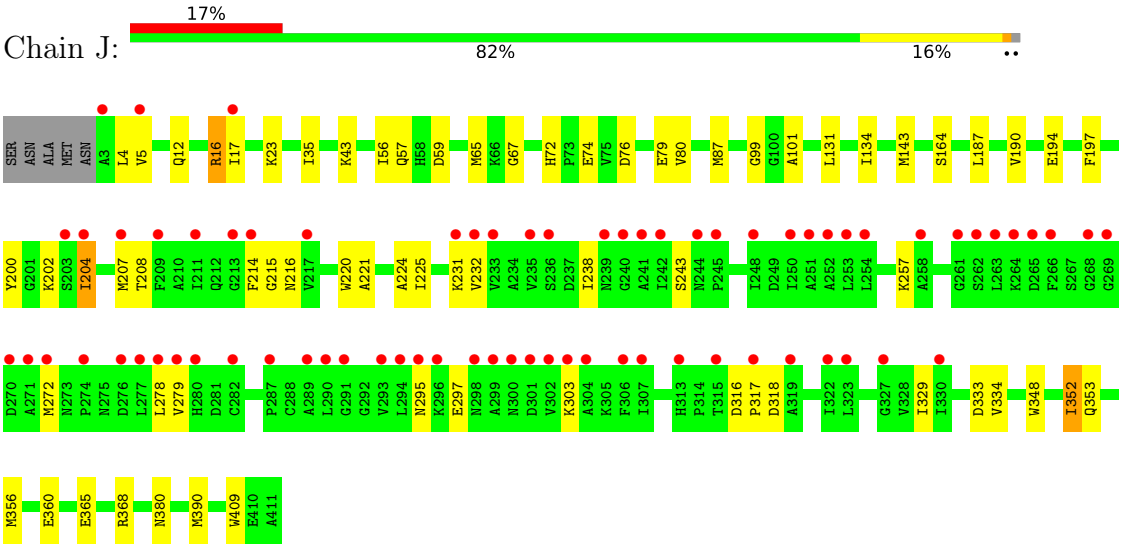




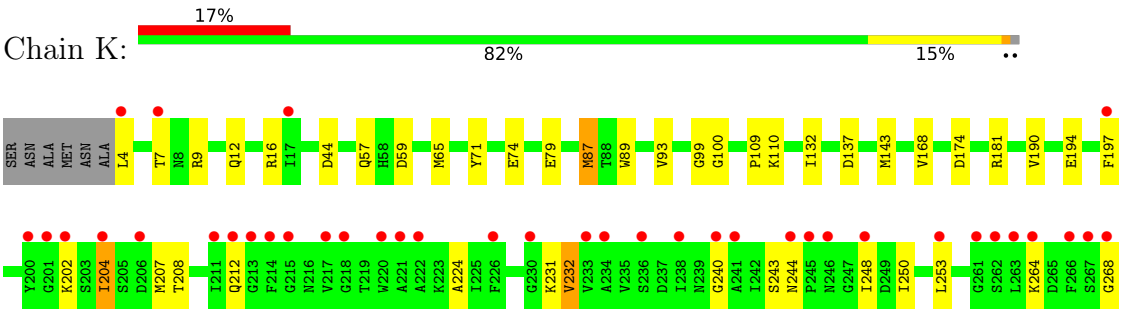
• Molecule 1: Glutamate dehydrogenase

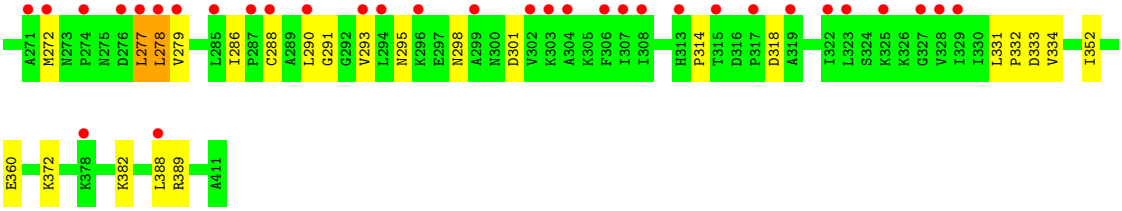


• Molecule 1: Glutamate dehydrogenase

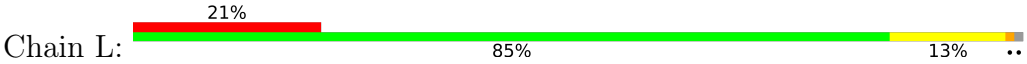


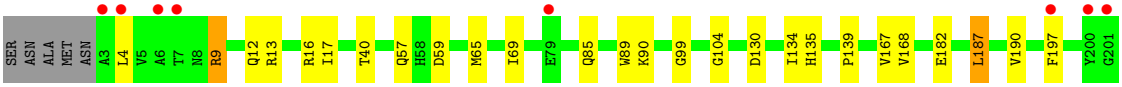
• Molecule 1: Glutamate dehydrogenase

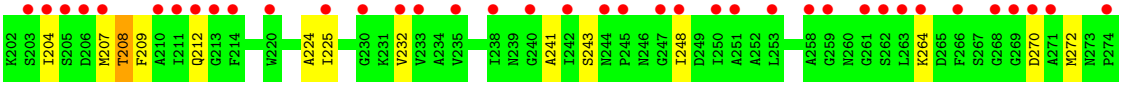


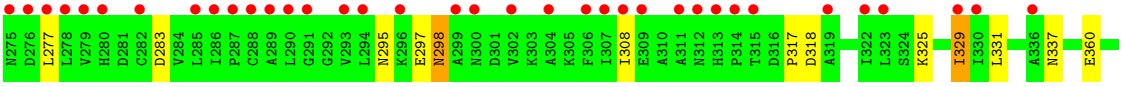


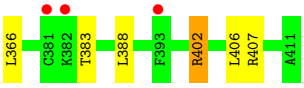
• Molecule 1: Glutamate dehydrogenase











4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.10 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.169 , 0.188 0.169 , 0.188	Depositor DCC
R_{free} test set	271616 reflections (0.50%)	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)	0.36 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.45	0/3197	0.59	0/4328
1	B	0.47	0/3188	0.61	0/4316
1	C	0.44	0/3188	0.60	0/4316
1	D	0.47	0/3201	0.60	0/4333
1	E	0.42	0/3180	0.59	0/4305
1	F	0.42	0/3188	0.58	0/4316
1	G	0.41	0/3197	0.56	0/4328
1	H	0.40	0/3199	0.56	0/4330
1	I	0.41	0/3180	0.56	0/4305
1	J	0.41	0/3180	0.56	0/4305
1	K	0.40	0/3175	0.56	0/4298
1	L	0.40	0/3180	0.55	0/4305
All	All	0.43	0/38253	0.58	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

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	27	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	27	0
1	D	3139	0	3127	29	0
1	E	3118	0	3104	26	0
1	F	3126	0	3110	29	0
1	G	3135	0	3117	37	0
1	H	3137	0	3122	27	0
1	I	3118	0	3104	27	0
1	J	3118	0	3104	40	0
1	K	3113	0	3099	38	0
1	L	3118	0	3104	33	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	0	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	1	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	2	0
9	B	13	0	18	4	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	0	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	364	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 364 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: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
1:G:204:ILE:HD12	1:G:204:ILE:H	1.53	0.73

There are no symmetry-related clashes.

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	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%)	44	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 (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	330/332 (99%)	319 (97%)	11 (3%)	33	48
1	B	329/332 (99%)	319 (97%)	10 (3%)	36	52
1	C	329/332 (99%)	318 (97%)	11 (3%)	33	48
1	D	330/332 (99%)	319 (97%)	11 (3%)	33	48
1	E	328/332 (99%)	315 (96%)	13 (4%)	27	40
1	F	329/332 (99%)	318 (97%)	11 (3%)	33	48
1	G	330/332 (99%)	320 (97%)	10 (3%)	36	52
1	H	330/332 (99%)	319 (97%)	11 (3%)	33	48
1	I	328/332 (99%)	315 (96%)	13 (4%)	27	40
1	J	328/332 (99%)	316 (96%)	12 (4%)	29	43
1	K	328/332 (99%)	312 (95%)	16 (5%)	21	31
1	L	328/332 (99%)	316 (96%)	12 (4%)	29	43
All	All	3947/3984 (99%)	3806 (96%)	141 (4%)	30	44

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	9	ARG
1	K	110	LYS
1	L	9	ARG
1	E	204	ILE
1	E	168	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	72	HIS
1	L	298	ASN
1	G	72	HIS
1	G	380	ASN
1	H	216	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\|>2$
4	PEG	E	801	-	6,6,6	0.22	0	5,5,5	0.24	0
4	PEG	C	502	-	6,6,6	0.27	0	5,5,5	0.19	0
6	TRS	I	902	10	7,7,7	0.53	0	9,9,9	0.97	0
3	EDO	B	503	-	3,3,3	0.31	0	2,2,2	1.24	0
5	NAD	B	508	-	42,48,48	0.71	1 (2%)	50,73,73	0.87	2 (4%)
3	EDO	I	904	-	3,3,3	0.52	0	2,2,2	0.35	0
2	A1H40	A	601	-	15,15,15	1.40	3 (20%)	20,20,20	3.09	11 (55%)
2	A1H40	H	501	-	15,15,15	1.39	3 (20%)	20,20,20	2.19	9 (45%)
3	EDO	F	604	-	3,3,3	0.51	0	2,2,2	0.64	0
3	EDO	C	503	-	3,3,3	0.43	0	2,2,2	0.57	0
3	EDO	E	802	-	3,3,3	0.43	0	2,2,2	1.06	0
4	PEG	C	504	-	6,6,6	0.21	0	5,5,5	0.17	0
3	EDO	D	603	-	3,3,3	0.58	0	2,2,2	0.55	0
3	EDO	K	506	-	3,3,3	0.47	0	2,2,2	0.80	0
2	A1H40	D	602	-	15,15,15	1.49	3 (20%)	20,20,20	2.92	9 (45%)
3	EDO	I	901	-	3,3,3	0.57	0	2,2,2	0.09	0
3	EDO	A	607	-	3,3,3	0.40	0	2,2,2	1.14	0
3	EDO	L	702	-	3,3,3	0.54	0	2,2,2	0.84	0
5	NAD	K	505	-	42,48,48	0.66	1 (2%)	50,73,73	0.80	2 (4%)
9	PG4	B	506	-	12,12,12	0.29	0	11,11,11	0.15	0
3	EDO	F	602	-	3,3,3	0.56	0	2,2,2	0.96	0
3	EDO	G	705	-	3,3,3	0.42	0	2,2,2	1.14	0
3	EDO	I	903	-	3,3,3	0.69	0	2,2,2	0.23	0
3	EDO	I	906	-	3,3,3	0.41	0	2,2,2	1.29	0
5	NAD	H	505	-	42,48,48	0.60	0	50,73,73	0.82	3 (6%)
3	EDO	G	702	-	3,3,3	0.49	0	2,2,2	0.38	0
5	NAD	I	907	-	42,48,48	0.63	0	50,73,73	0.79	2 (4%)
5	NAD	J	602	-	42,48,48	0.62	0	50,73,73	0.80	2 (4%)
3	EDO	J	601	-	3,3,3	0.40	0	2,2,2	1.02	0
5	NAD	C	506	-	42,48,48	0.61	0	50,73,73	0.79	2 (4%)
4	PEG	H	504	-	6,6,6	0.19	0	5,5,5	0.19	0
8	PGE	B	504	-	9,9,9	0.39	0	8,8,8	0.34	0
4	PEG	F	601	-	6,6,6	0.15	0	5,5,5	0.15	0
5	NAD	D	605	-	42,48,48	0.68	1 (2%)	50,73,73	0.81	2 (4%)
3	EDO	A	606	-	3,3,3	0.65	0	2,2,2	0.35	0
3	EDO	C	505	-	3,3,3	0.52	0	2,2,2	0.90	0
2	A1H40	C	501	-	15,15,15	1.29	2 (13%)	20,20,20	2.49	7 (35%)
3	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.67	0
5	NAD	G	706	-	42,48,48	0.59	0	50,73,73	0.79	2 (4%)
5	NAD	L	703	-	42,48,48	0.61	0	50,73,73	0.82	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	TRS	D	601	-	7,7,7	0.65	0	9,9,9	1.42	2 (22%)
2	A1H40	K	501	-	15,15,15	1.33	3 (20%)	20,20,20	2.18	9 (45%)
6	TRS	K	504	10	7,7,7	0.60	0	9,9,9	1.17	0
3	EDO	B	507	-	3,3,3	0.60	0	2,2,2	0.45	0
3	EDO	A	604	-	3,3,3	0.48	0	2,2,2	0.40	0
3	EDO	G	703	10	3,3,3	0.44	0	2,2,2	0.69	0
3	EDO	H	502	-	3,3,3	0.46	0	2,2,2	1.15	0
5	NAD	E	803	-	42,48,48	0.59	0	50,73,73	0.80	2 (4%)
6	TRS	H	503	-	7,7,7	0.35	0	9,9,9	0.98	1 (11%)
5	NAD	F	603	-	42,48,48	0.63	0	50,73,73	0.80	1 (2%)
4	PEG	A	605	-	6,6,6	0.21	0	5,5,5	0.18	0
6	TRS	A	609	-	7,7,7	0.56	0	9,9,9	1.22	1 (11%)
3	EDO	K	503	-	3,3,3	0.47	0	2,2,2	0.71	0
4	PEG	D	604	-	6,6,6	0.20	0	5,5,5	0.15	0
3	EDO	A	602	-	3,3,3	0.54	0	2,2,2	1.04	0
2	A1H40	B	501	-	15,15,15	1.44	3 (20%)	20,20,20	1.75	5 (25%)
5	NAD	A	608	-	42,48,48	0.59	0	50,73,73	0.84	2 (4%)
3	EDO	K	502	-	3,3,3	0.41	0	2,2,2	1.21	0
6	TRS	L	701	-	7,7,7	0.28	0	9,9,9	0.66	0
3	EDO	B	502	-	3,3,3	0.48	0	2,2,2	0.18	0
6	TRS	G	701	-	7,7,7	0.54	0	9,9,9	0.73	0
4	PEG	G	704	-	6,6,6	0.15	0	5,5,5	0.11	0
3	EDO	I	905	-	3,3,3	0.37	0	2,2,2	0.76	0
3	EDO	A	603	-	3,3,3	0.55	0	2,2,2	0.14	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
4	PEG	E	801	-	-	0/4/4/4	-
4	PEG	C	502	-	-	0/4/4/4	-
6	TRS	I	902	10	-	6/9/9/9	-
3	EDO	B	503	-	-	1/1/1/1	-
5	NAD	B	508	-	-	1/26/62/62	0/5/5/5
3	EDO	I	904	-	-	1/1/1/1	-
2	A1H40	A	601	-	-	7/8/8/8	0/2/2/2
2	A1H40	H	501	-	-	4/8/8/8	0/2/2/2
3	EDO	F	604	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	503	-	-	0/1/1/1	-
3	EDO	E	802	-	-	0/1/1/1	-
4	PEG	C	504	-	-	1/4/4/4	-
3	EDO	D	603	-	-	0/1/1/1	-
3	EDO	K	506	-	-	1/1/1/1	-
2	A1H40	D	602	-	-	4/8/8/8	0/2/2/2
3	EDO	I	901	-	-	0/1/1/1	-
3	EDO	A	607	-	-	0/1/1/1	-
3	EDO	L	702	-	-	1/1/1/1	-
5	NAD	K	505	-	-	1/26/62/62	0/5/5/5
9	PG4	B	506	-	-	5/10/10/10	-
3	EDO	F	602	-	-	1/1/1/1	-
3	EDO	G	705	-	-	1/1/1/1	-
3	EDO	I	903	-	-	1/1/1/1	-
3	EDO	I	906	-	-	1/1/1/1	-
5	NAD	H	505	-	-	1/26/62/62	0/5/5/5
3	EDO	G	702	-	-	0/1/1/1	-
5	NAD	I	907	-	-	1/26/62/62	0/5/5/5
5	NAD	J	602	-	-	1/26/62/62	0/5/5/5
3	EDO	J	601	-	-	1/1/1/1	-
5	NAD	C	506	-	-	1/26/62/62	0/5/5/5
4	PEG	H	504	-	-	0/4/4/4	-
8	PGE	B	504	-	-	5/7/7/7	-
4	PEG	F	601	-	-	0/4/4/4	-
5	NAD	D	605	-	-	1/26/62/62	0/5/5/5
3	EDO	A	606	-	-	1/1/1/1	-
3	EDO	C	505	-	-	0/1/1/1	-
2	A1H40	C	501	-	-	4/8/8/8	0/2/2/2
3	EDO	B	505	-	-	0/1/1/1	-
5	NAD	G	706	-	-	1/26/62/62	0/5/5/5
5	NAD	L	703	-	-	1/26/62/62	0/5/5/5
6	TRS	D	601	-	-	1/9/9/9	-
2	A1H40	K	501	-	-	8/8/8/8	0/2/2/2
6	TRS	K	504	10	-	9/9/9/9	-
3	EDO	B	507	-	-	1/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	G	703	10	-	1/1/1/1	-
3	EDO	H	502	-	-	1/1/1/1	-
5	NAD	E	803	-	-	1/26/62/62	0/5/5/5
6	TRS	H	503	-	-	1/9/9/9	-
5	NAD	F	603	-	-	1/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	605	-	-	0/4/4/4	-
6	TRS	A	609	-	-	1/9/9/9	-
3	EDO	K	503	-	-	1/1/1/1	-
4	PEG	D	604	-	-	0/4/4/4	-
3	EDO	A	602	-	-	1/1/1/1	-
2	A1H40	B	501	-	-	4/8/8/8	0/2/2/2
5	NAD	A	608	-	-	1/26/62/62	0/5/5/5
3	EDO	K	502	-	-	1/1/1/1	-
6	TRS	L	701	-	-	9/9/9/9	-
3	EDO	B	502	-	-	0/1/1/1	-
6	TRS	G	701	-	-	3/9/9/9	-
4	PEG	G	704	-	-	1/4/4/4	-
3	EDO	I	905	-	-	1/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	A1H40	C08-N04	3.06	1.37	1.33
2	B	501	A1H40	C08-N04	3.03	1.37	1.33
2	B	501	A1H40	C09-C13	2.91	1.55	1.49
2	H	501	A1H40	C08-N04	2.87	1.37	1.33
2	D	602	A1H40	C09-C13	2.76	1.55	1.49

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	A1H40	C10-C07-C08	-8.23	107.95	120.05
2	D	602	A1H40	C10-C07-C08	-7.53	108.97	120.05
2	C	501	A1H40	C10-C07-C08	-6.61	110.33	120.05
2	A	601	A1H40	C11-C07-C08	4.74	128.84	120.79
2	K	501	A1H40	C10-C07-C08	-4.73	113.09	120.05

There are no chirality outliers.

5 of 102 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.

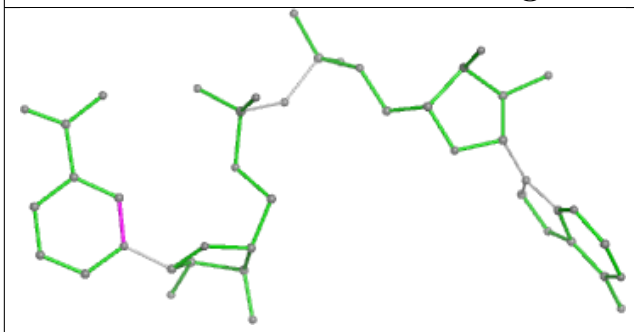
29 monomers are involved in 43 short contacts:

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

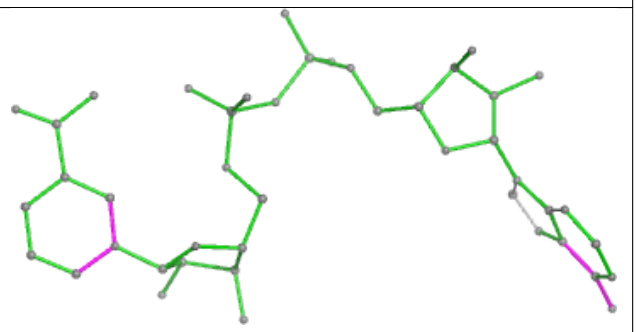
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

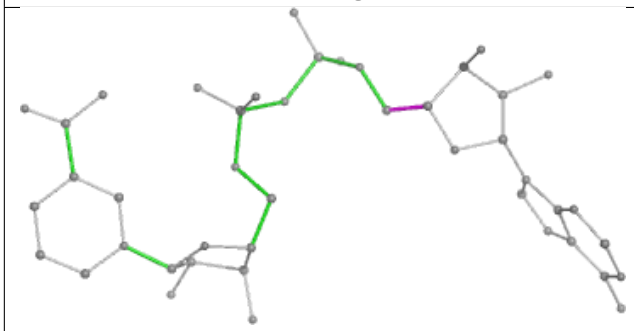
Ligand NAD B 508



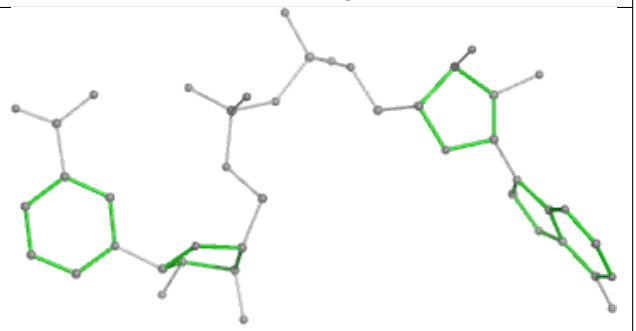
Bond lengths



Bond angles

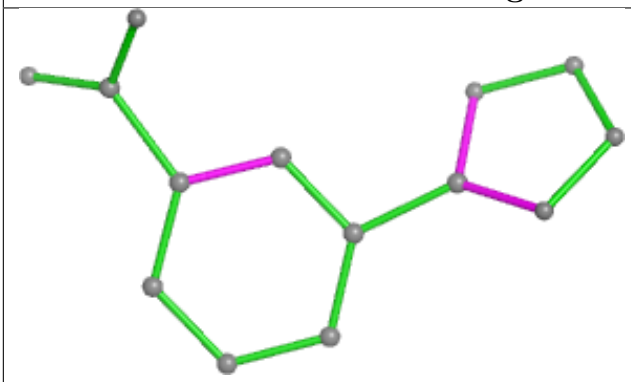


Torsions

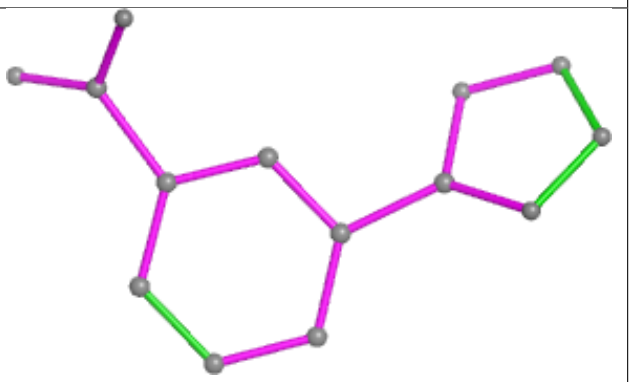


Rings

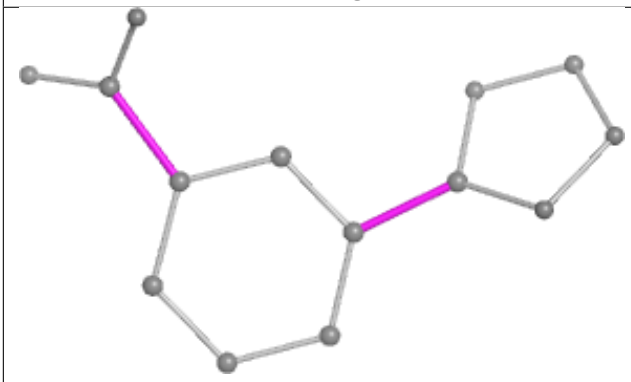
Ligand A1H40 A 601



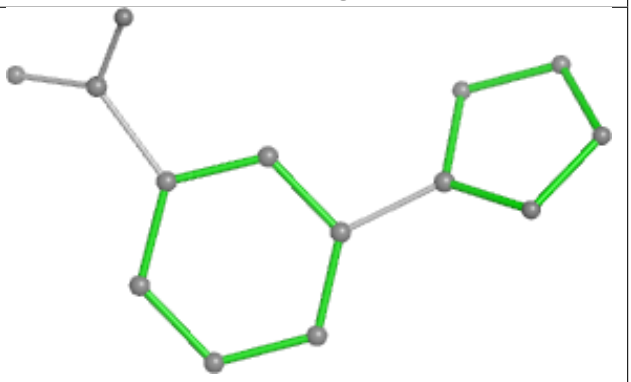
Bond lengths



Bond angles

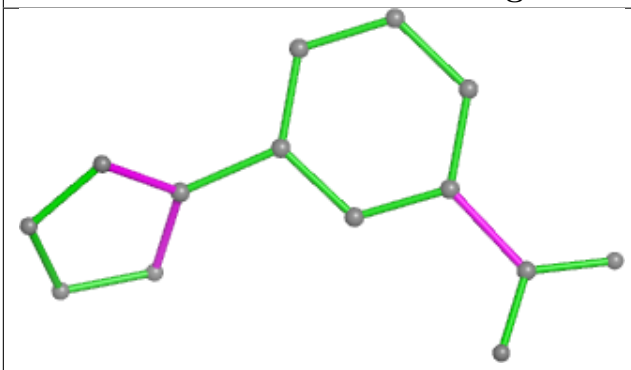


Torsions

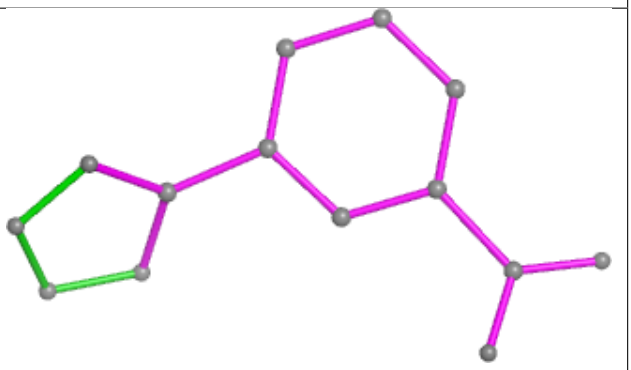


Rings

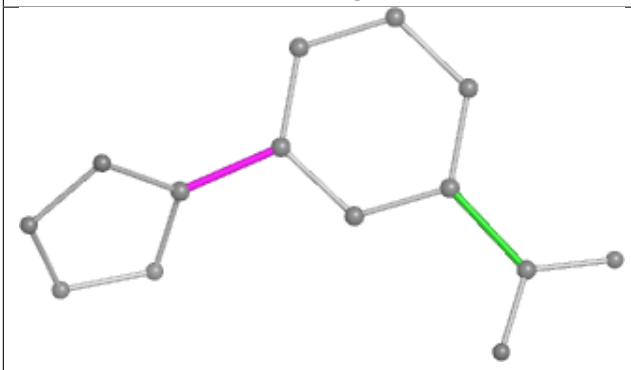
Ligand A1H40 H 501



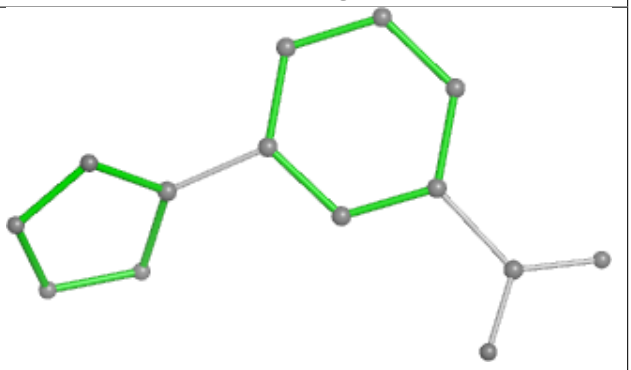
Bond lengths



Bond angles

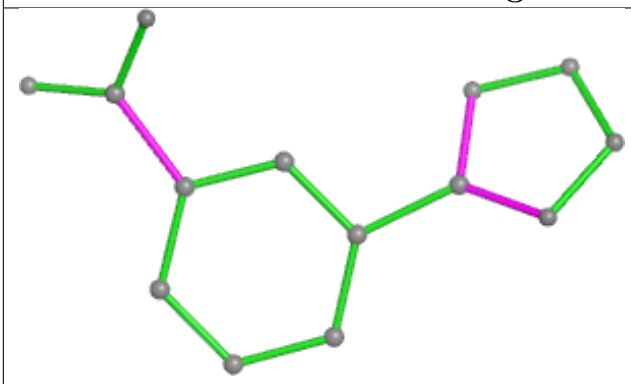


Torsions



Rings

Ligand A1H40 D 602



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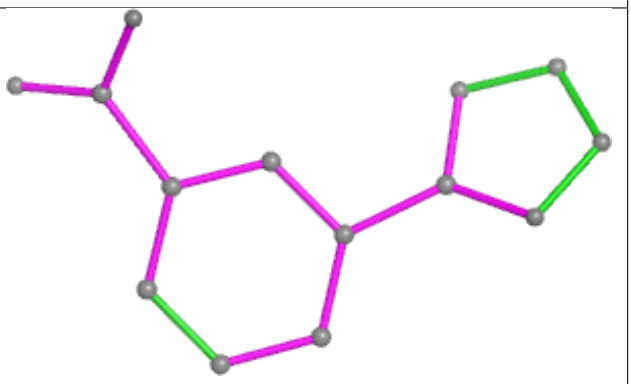
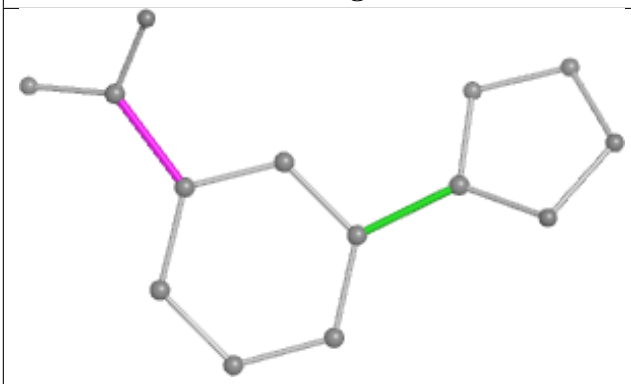
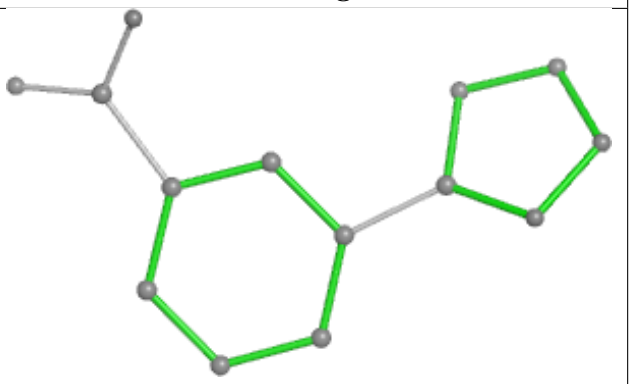


Bond angles

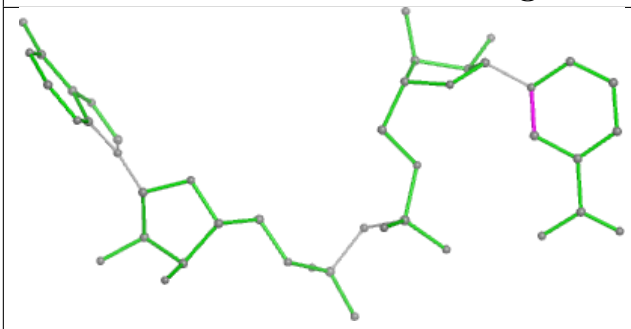


Torsions

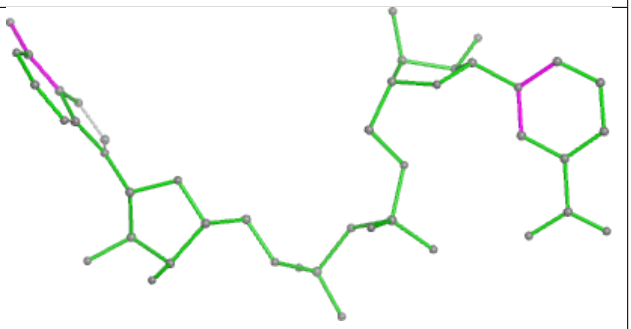


Rings

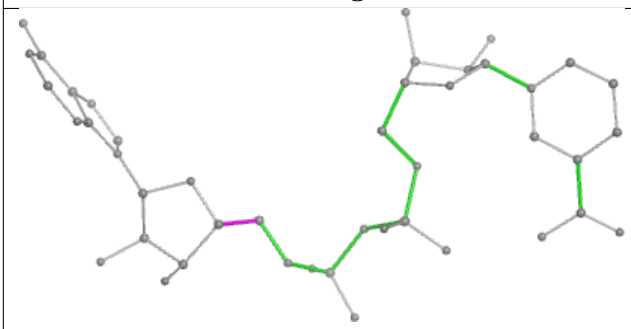
Ligand NAD K 505



Bond lengths



Bond angles



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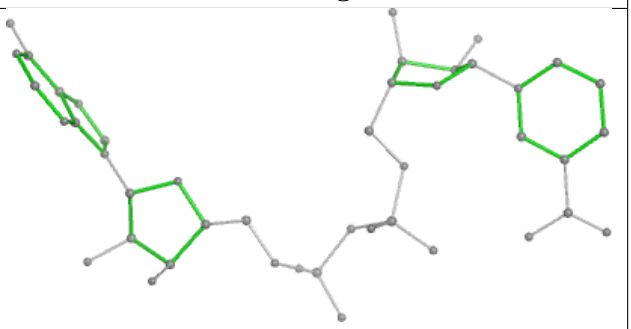
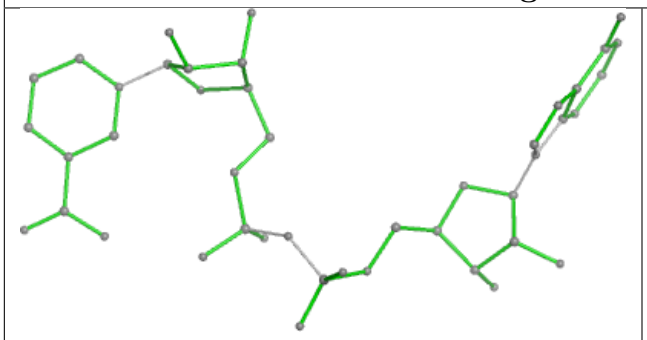


Rings

Ligand NAD H 505



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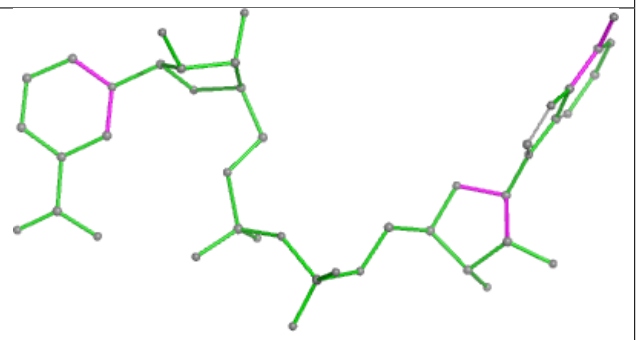
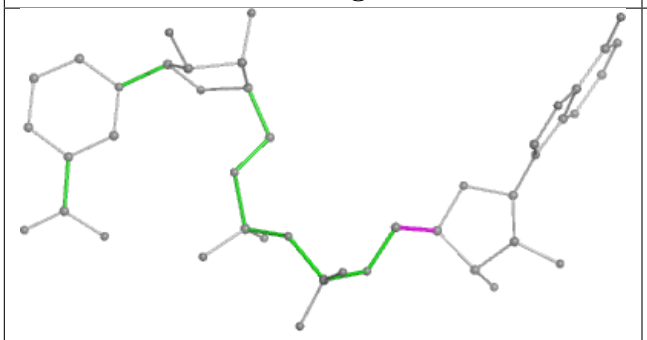
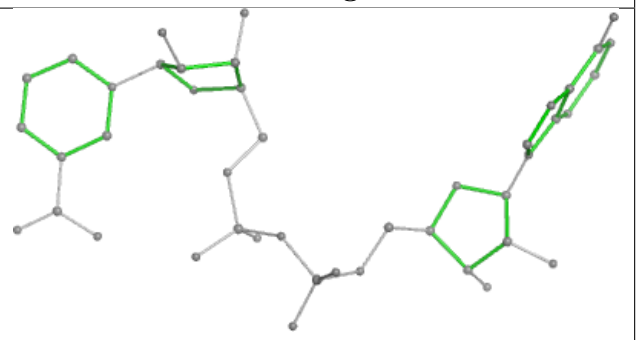


Bond angles

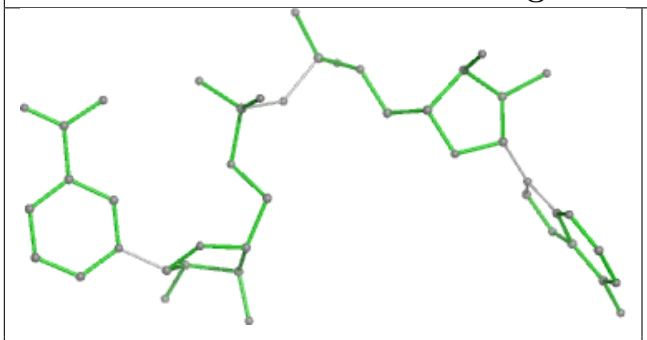


Torsions



Rings

Ligand NAD I 907



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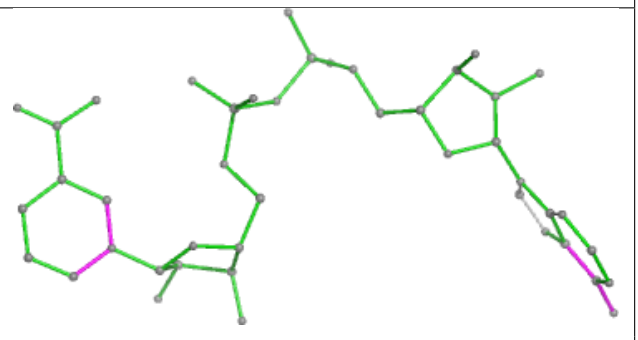

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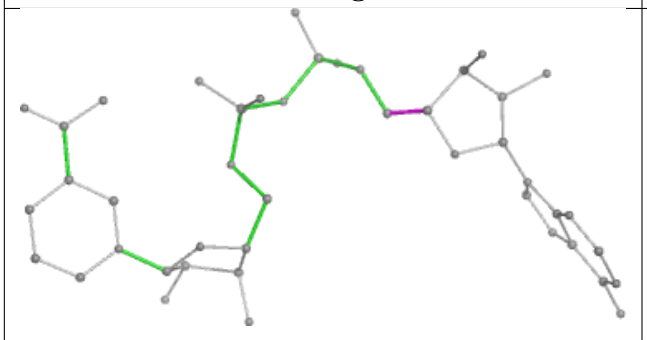

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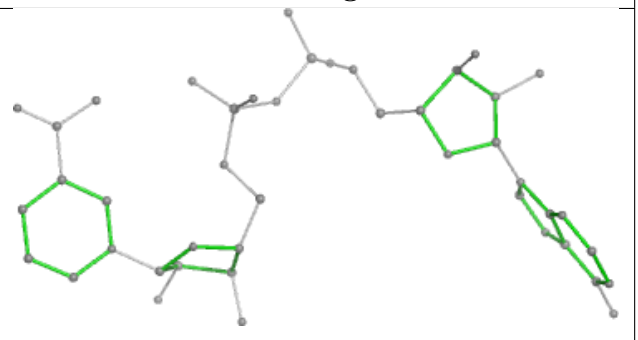
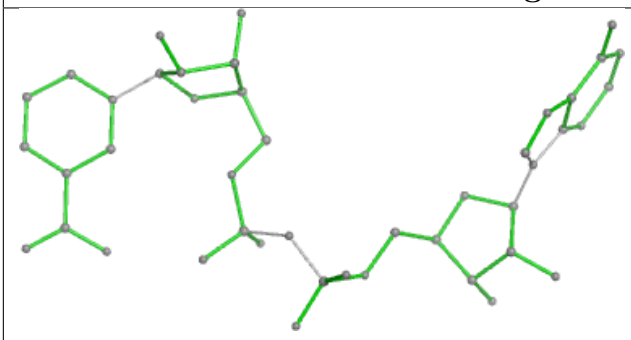


Rings

Ligand NAD J 602



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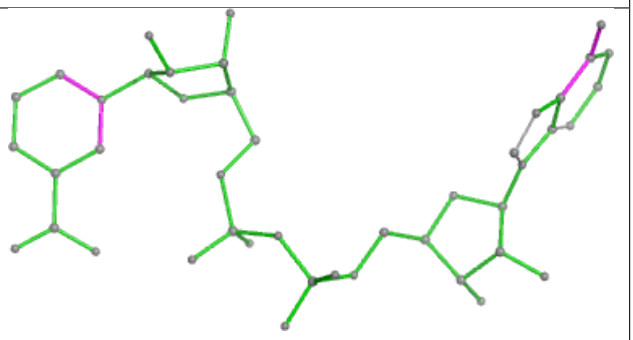
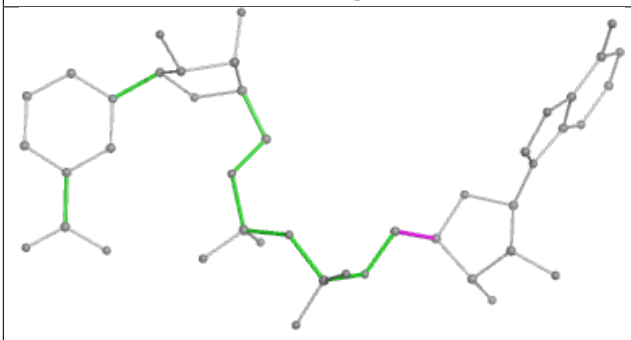
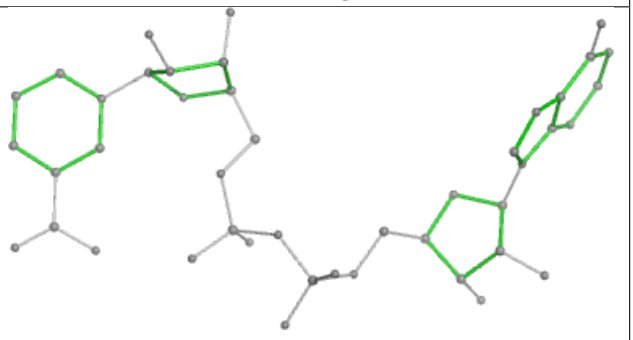


Bond angles

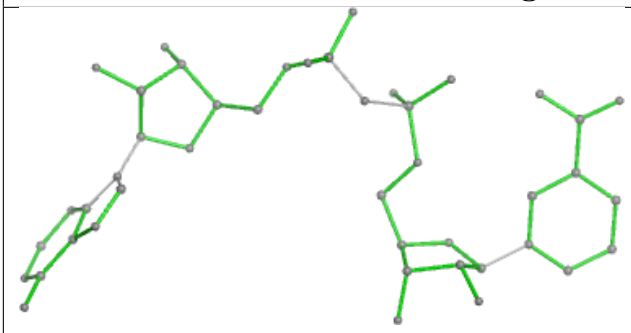


Torsions

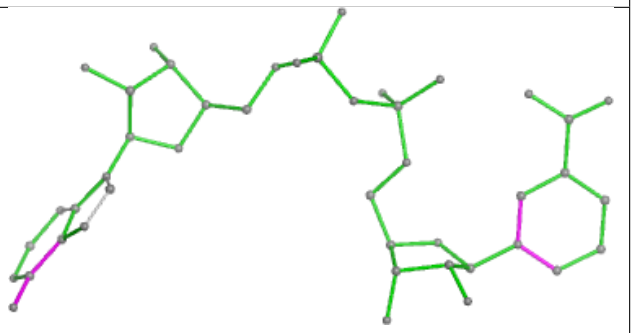


Rings

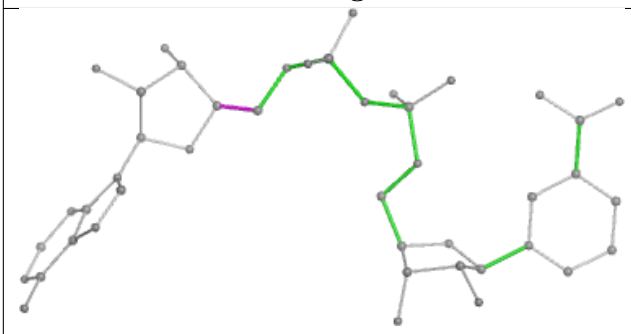
Ligand NAD C 506



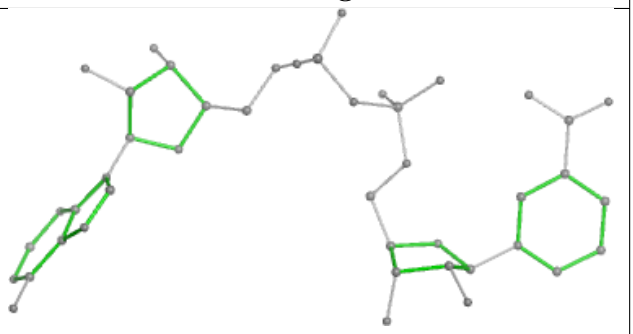
Bond lengths



Bond angles

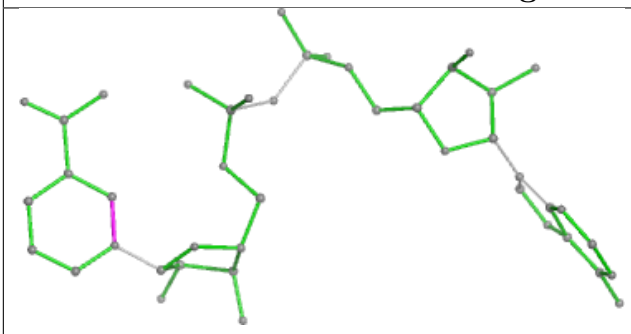


Torsions

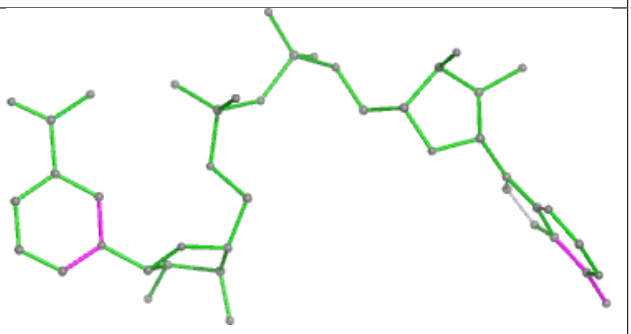


Rings

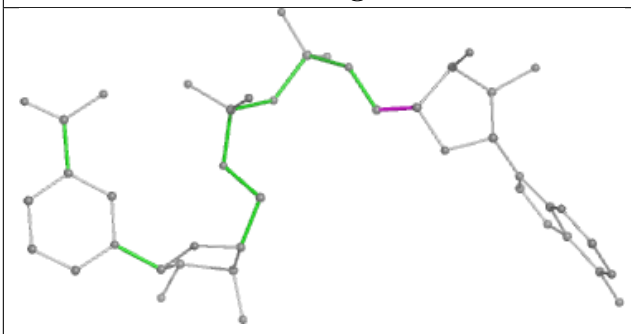
Ligand NAD D 605



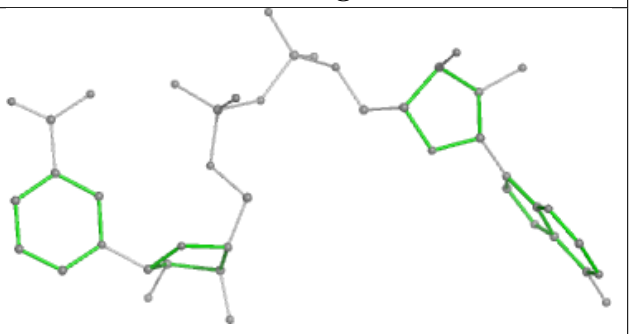
Bond lengths



Bond angles

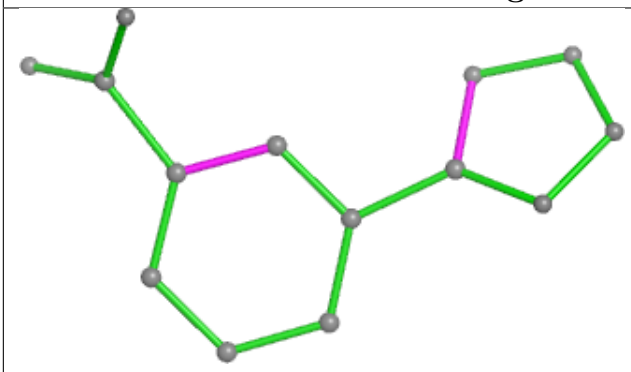


Torsions

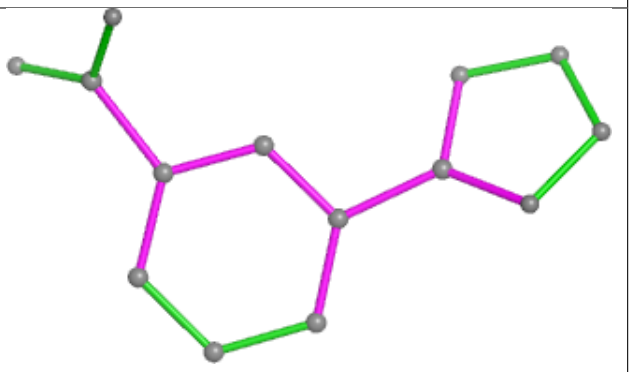


Rings

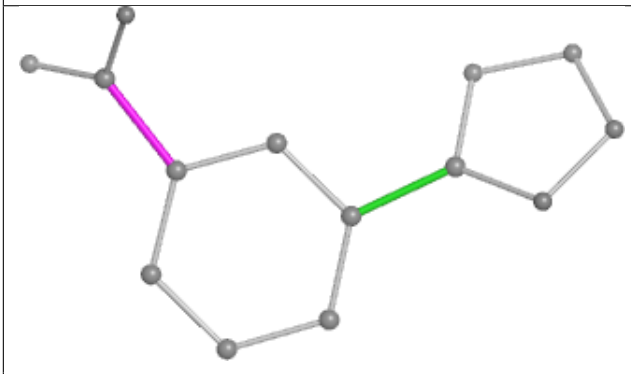
Ligand A1H40 C 501



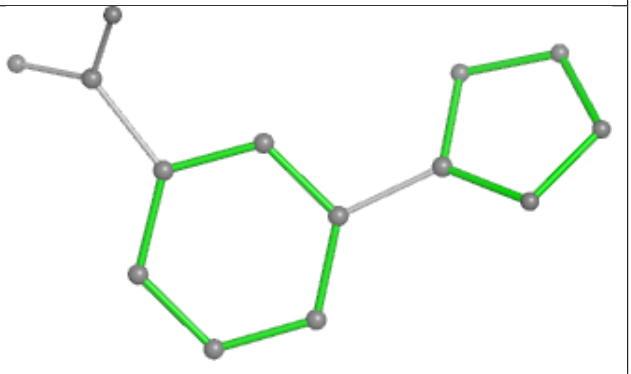
Bond lengths



Bond angles

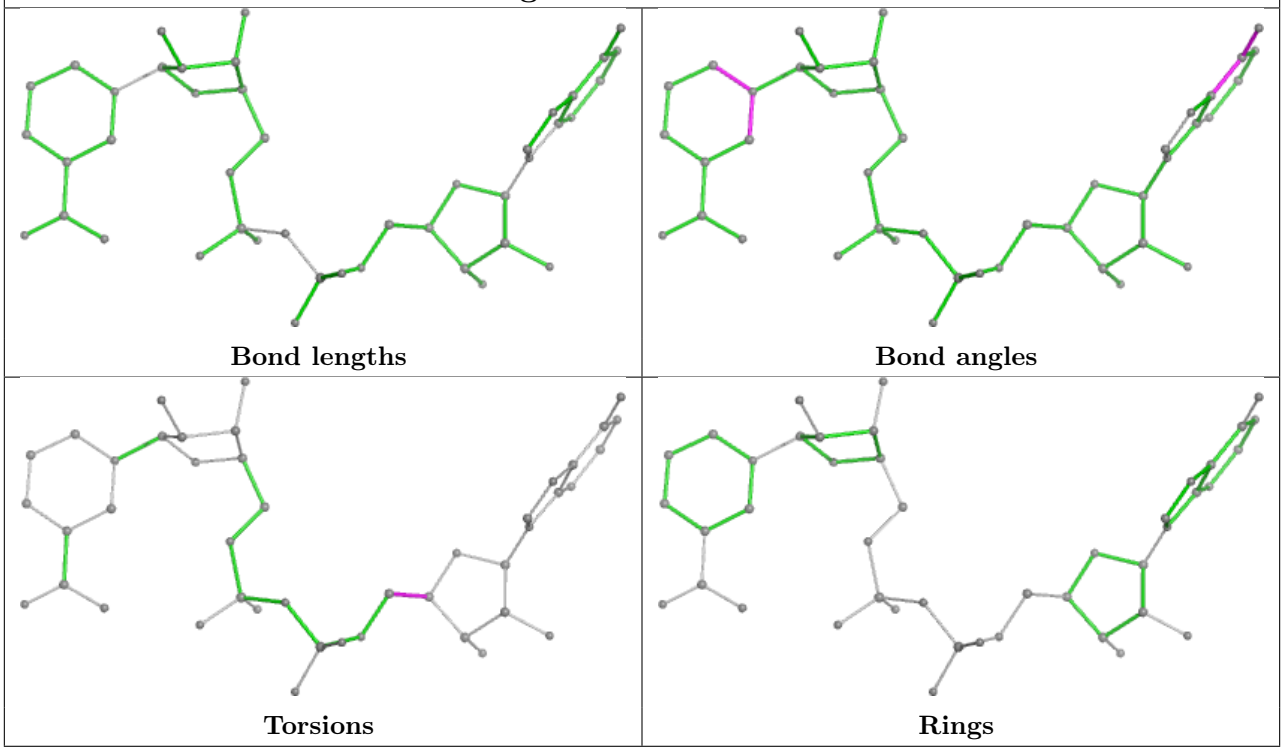


Torsions

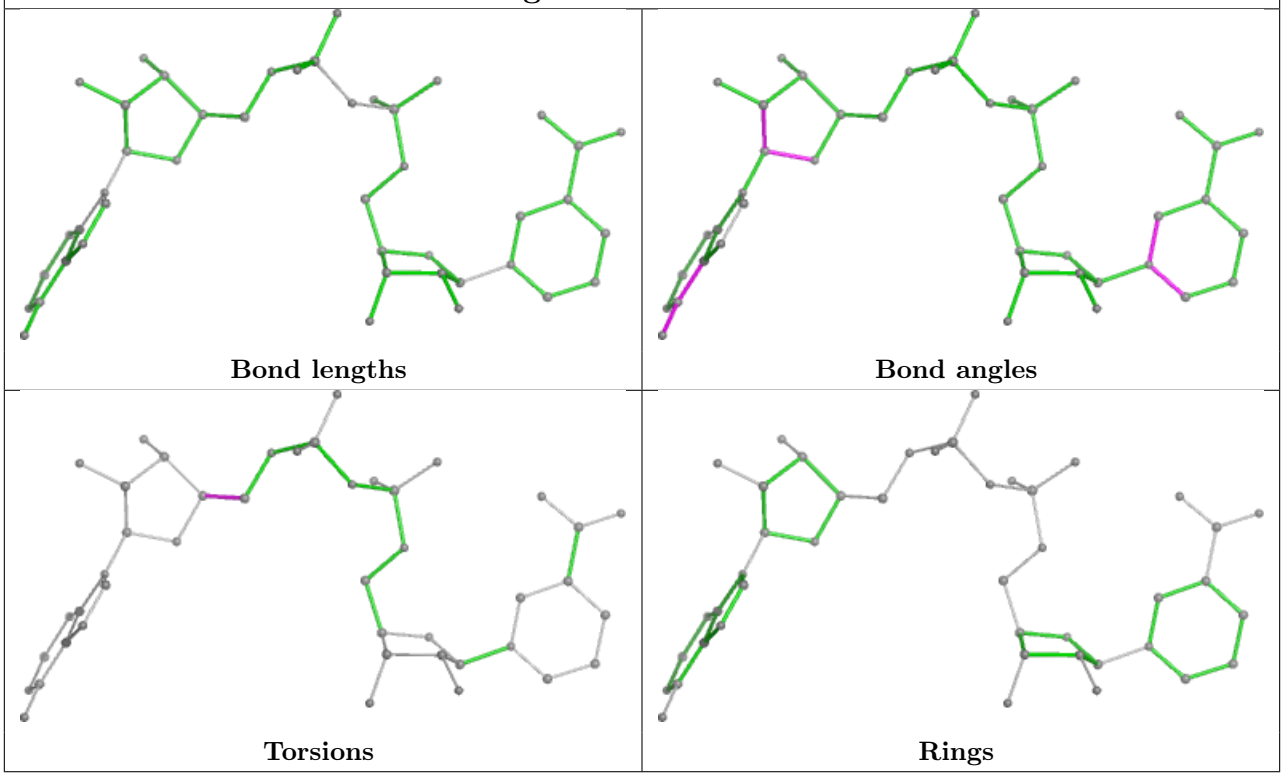


Rings

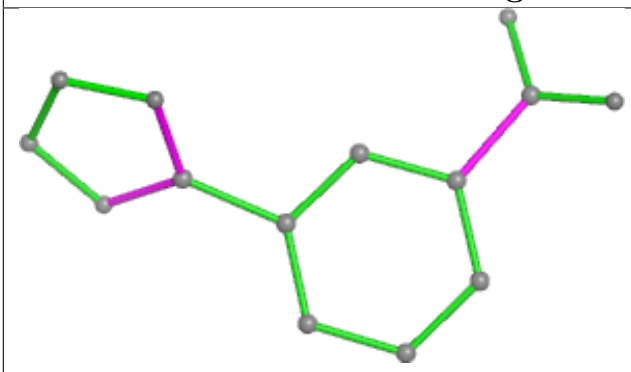
Ligand NAD G 706



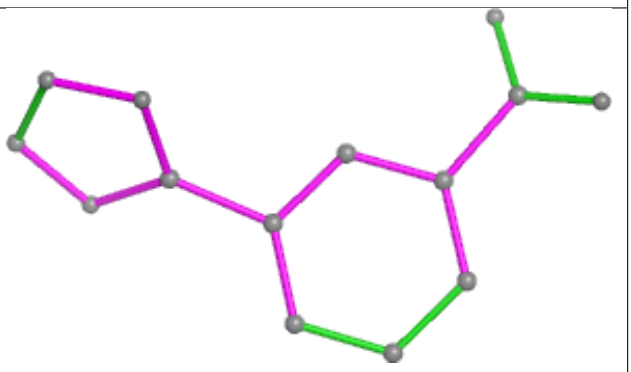
Ligand NAD L 703



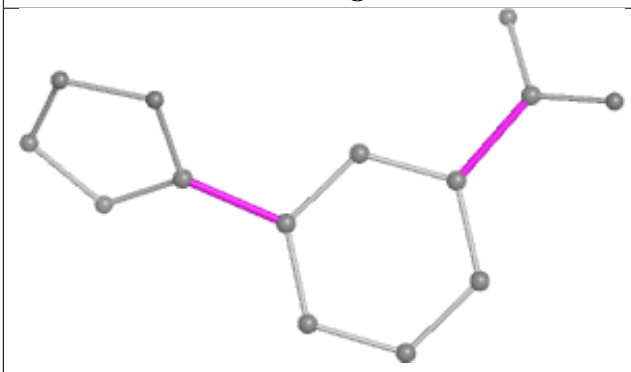
Ligand A1H40 K 501



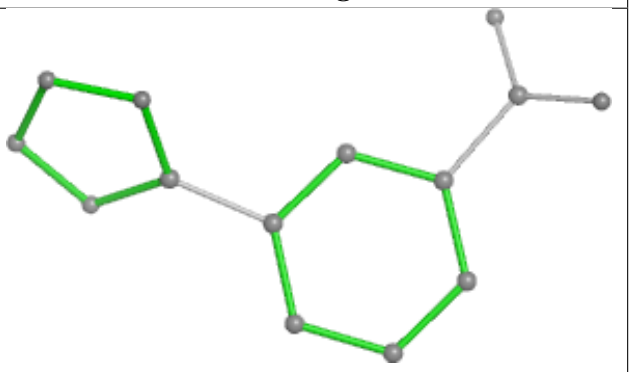
Bond lengths



Bond angles

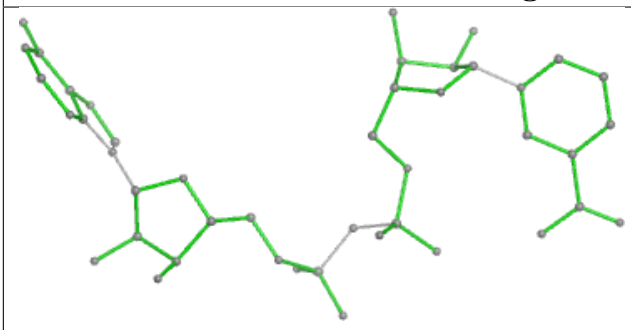


Torsions

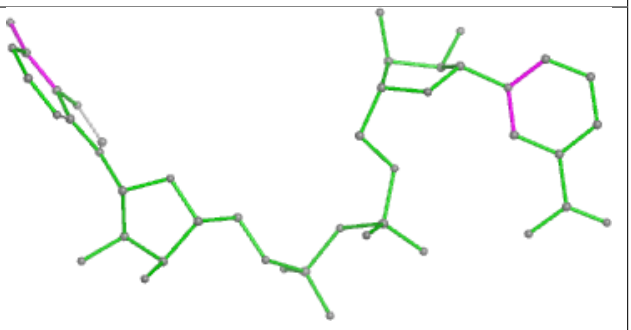


Rings

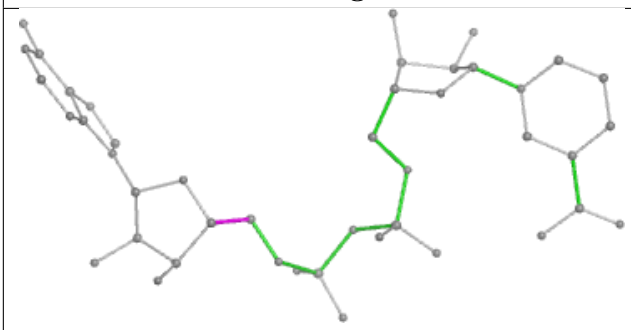
Ligand NAD E 803



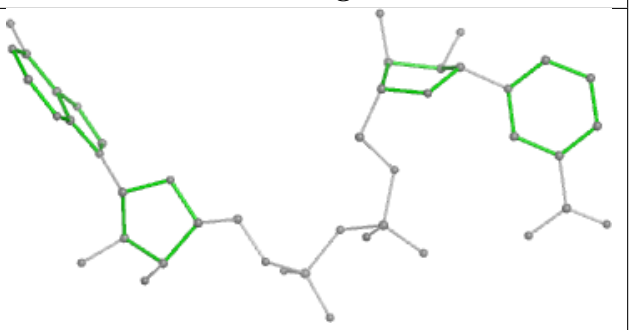
Bond lengths



Bond angles

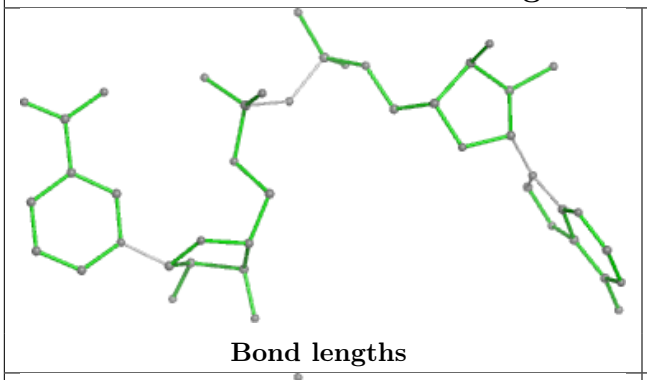


Torsions

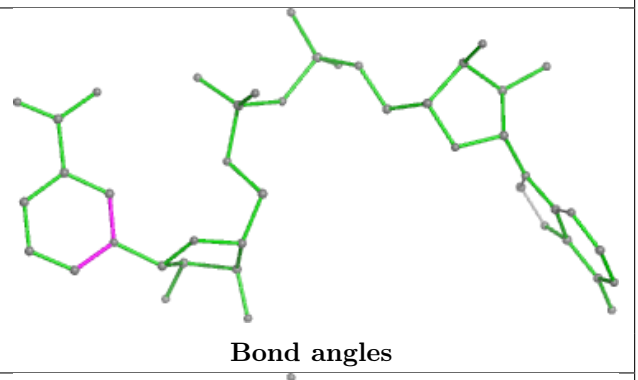


Rings

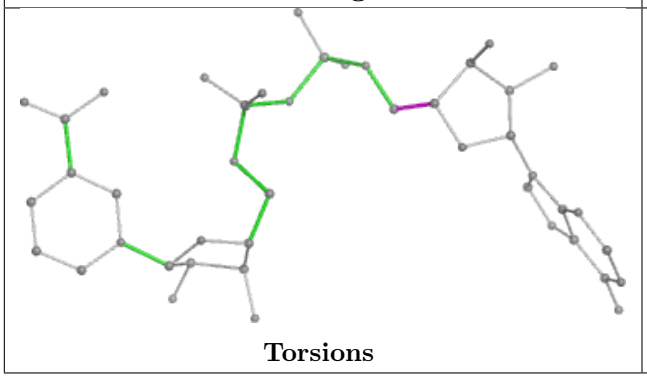
Ligand NAD F 603



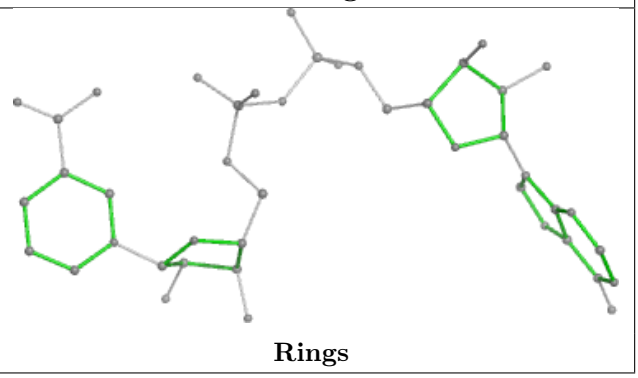
Bond lengths



Bond angles

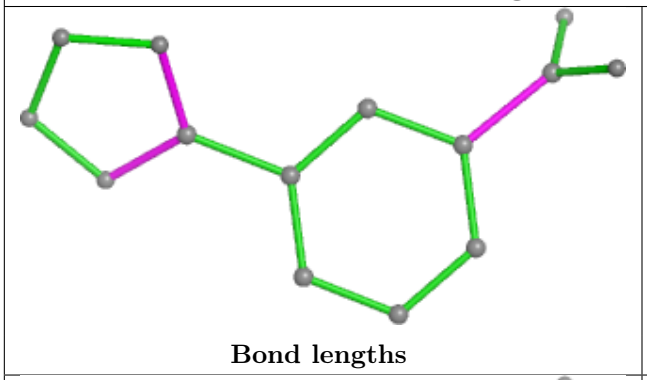


Torsions

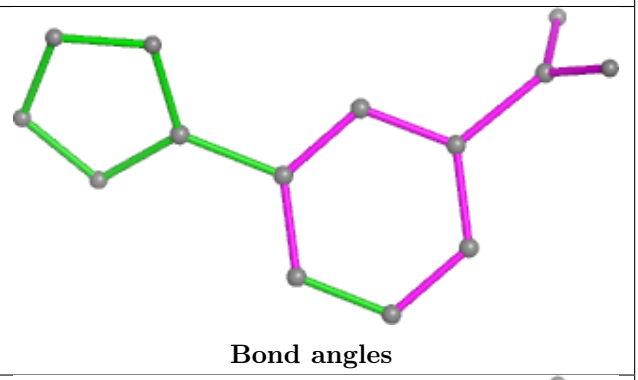


Rings

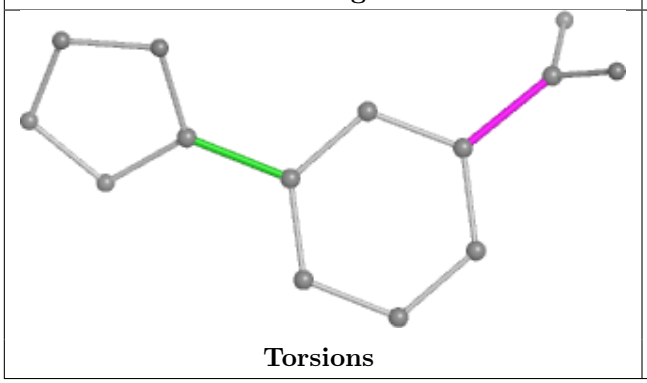
Ligand A1H40 B 501



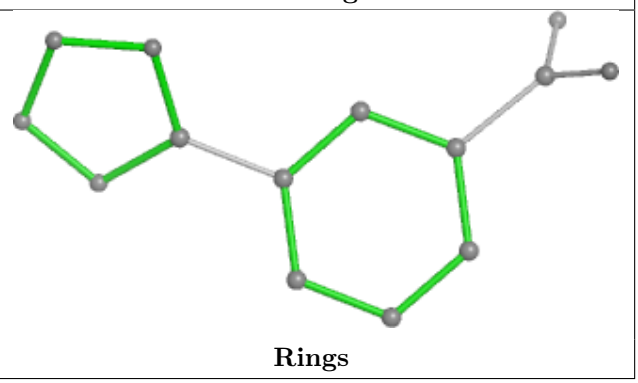
Bond lengths



Bond angles

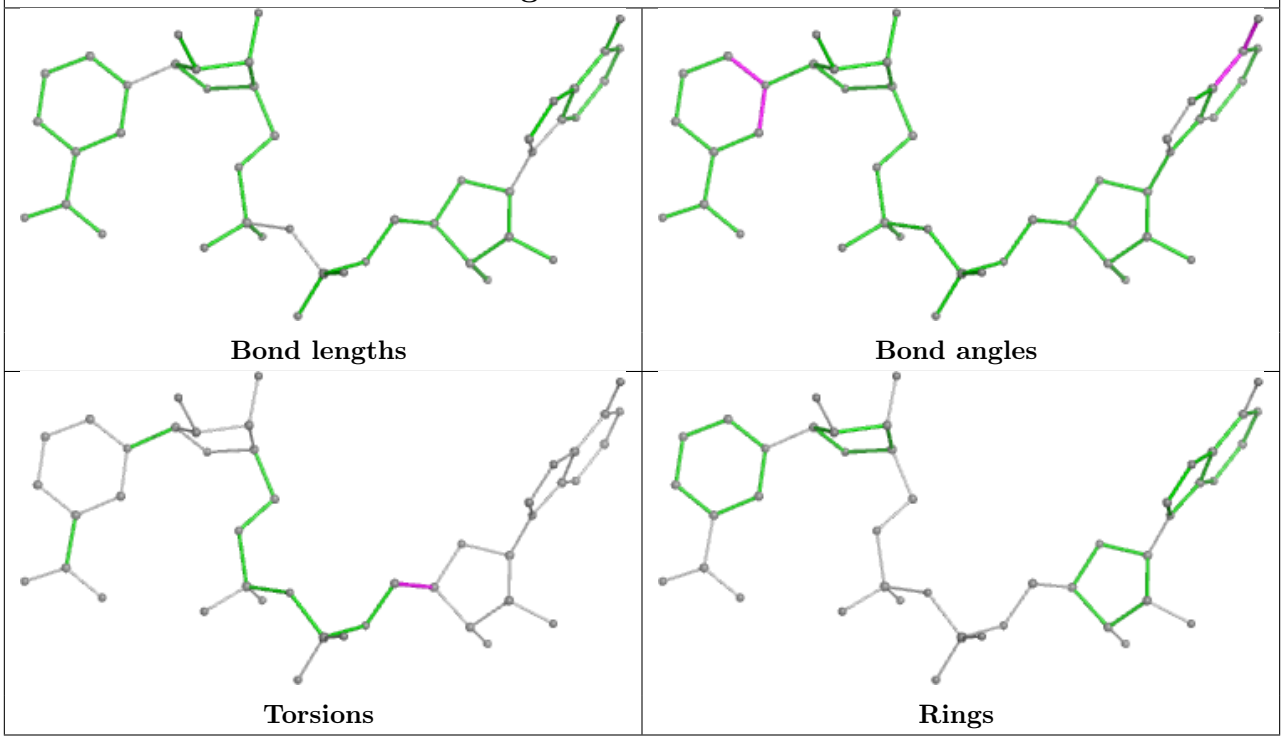


Torsions



Rings

Ligand NAD A 608



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	410/414 (99%)	-0.10	3 (0%) 84 84	15, 35, 64, 80	1 (0%)
1	B	410/414 (99%)	-0.48	1 (0%) 92 92	21, 30, 46, 87	0
1	C	410/414 (99%)	-0.22	2 (0%) 87 88	23, 35, 58, 96	0
1	D	412/414 (99%)	-0.09	5 (1%) 76 76	20, 34, 70, 96	0
1	E	409/414 (98%)	0.33	35 (8%) 18 19	21, 44, 97, 122	0
1	F	410/414 (99%)	0.09	4 (0%) 79 79	25, 41, 69, 92	0
1	G	410/414 (99%)	0.52	53 (12%) 9 10	17, 46, 102, 119	1 (0%)
1	H	410/414 (99%)	0.51	41 (10%) 14 15	19, 46, 100, 120	1 (0%)
1	I	409/414 (98%)	0.39	25 (6%) 28 30	24, 46, 97, 144	0
1	J	409/414 (98%)	0.64	72 (17%) 4 6	24, 49, 106, 126	0
1	K	408/414 (98%)	0.71	72 (17%) 4 6	26, 55, 117, 132	0
1	L	409/414 (98%)	0.80	85 (20%) 3 4	28, 53, 117, 147	0
All	All	4916/4968 (98%)	0.26	398 (8%) 19 21	15, 40, 100, 147	3 (0%)

The worst 5 of 398 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	3	ALA	5.5
1	J	241	ALA	5.1
1	H	268	GLY	5.1
1	D	0	ALA	5.0
1	J	242	ILE	5.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1H40	K	501	14/14	0.71	0.19	39,47,55,56	14
6	TRS	G	701	8/8	0.71	0.19	47,48,51,53	0
6	TRS	K	504	8/8	0.71	0.19	32,42,47,51	0
2	A1H40	H	501	14/14	0.74	0.22	36,43,46,48	14
2	A1H40	A	601	14/14	0.74	0.20	26,32,37,38	14
2	A1H40	B	501	14/14	0.76	0.20	30,35,39,41	14
5	NAD	L	703	44/44	0.76	0.15	71,87,99,102	0
2	A1H40	C	501	14/14	0.78	0.20	31,36,40,41	14
6	TRS	D	601	8/8	0.79	0.17	39,46,53,53	0
4	PEG	C	502	7/7	0.80	0.15	50,55,57,61	0
2	A1H40	D	602	14/14	0.80	0.15	23,32,35,36	14
6	TRS	A	609	8/8	0.80	0.16	35,40,44,52	0
4	PEG	H	504	7/7	0.81	0.17	60,62,64,65	0
3	EDO	B	507	4/4	0.82	0.17	44,44,46,51	0
4	PEG	A	605	7/7	0.82	0.17	51,56,62,63	0
3	EDO	A	604	4/4	0.82	0.14	58,58,58,64	0
5	NAD	J	602	44/44	0.83	0.14	68,76,90,93	0
4	PEG	F	601	7/7	0.83	0.16	69,71,75,75	0
5	NAD	K	505	44/44	0.84	0.13	67,82,94,97	0
3	EDO	I	901	4/4	0.84	0.16	52,54,56,56	0
6	TRS	H	503	8/8	0.84	0.15	49,53,57,58	0
4	PEG	G	704	7/7	0.84	0.15	63,65,69,71	0
6	TRS	I	902	8/8	0.85	0.15	29,36,42,47	0
5	NAD	H	505	44/44	0.86	0.12	59,72,83,85	0
3	EDO	A	602	4/4	0.86	0.13	43,43,43,49	0
3	EDO	K	506	4/4	0.86	0.16	42,42,45,47	0
4	PEG	E	801	7/7	0.86	0.14	63,64,68,69	0
5	NAD	G	706	44/44	0.86	0.13	60,71,83,85	0
6	TRS	L	701	8/8	0.86	0.12	48,50,56,56	0
3	EDO	A	606	4/4	0.87	0.13	29,30,31,39	0
3	EDO	G	703	4/4	0.87	0.14	46,49,50,51	0
3	EDO	K	503	4/4	0.88	0.12	36,42,44,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PG4	B	506	13/13	0.88	0.13	40,45,56,61	0
3	EDO	F	602	4/4	0.89	0.15	31,31,44,46	0
3	EDO	I	904	4/4	0.89	0.15	58,59,59,62	0
4	PEG	C	504	7/7	0.89	0.13	54,55,62,63	0
3	EDO	G	702	4/4	0.89	0.16	38,40,42,43	0
3	EDO	D	603	4/4	0.89	0.12	30,34,37,43	0
3	EDO	F	604	4/4	0.90	0.11	32,34,40,51	0
3	EDO	I	905	4/4	0.90	0.13	44,46,51,52	0
8	PGE	B	504	10/10	0.90	0.11	40,47,52,55	0
3	EDO	C	505	4/4	0.90	0.14	31,32,38,39	0
3	EDO	B	505	4/4	0.91	0.10	35,38,45,46	0
4	PEG	D	604	7/7	0.91	0.11	50,54,59,61	0
5	NAD	I	907	44/44	0.91	0.11	59,67,74,74	0
3	EDO	L	702	4/4	0.91	0.13	29,31,35,43	0
5	NAD	E	803	44/44	0.91	0.10	54,62,77,78	0
3	EDO	I	903	4/4	0.92	0.11	34,34,36,39	0
3	EDO	C	503	4/4	0.92	0.09	39,39,41,43	0
3	EDO	K	502	4/4	0.93	0.10	31,31,37,40	0
3	EDO	B	503	4/4	0.93	0.10	34,35,35,37	0
3	EDO	A	607	4/4	0.93	0.09	28,29,33,37	0
3	EDO	B	502	4/4	0.93	0.14	38,39,41,44	0
3	EDO	E	802	4/4	0.93	0.10	24,24,36,38	0
3	EDO	I	906	4/4	0.93	0.11	26,26,35,39	0
3	EDO	J	601	4/4	0.93	0.11	28,30,39,43	0
10	NA	F	605	1/1	0.93	0.17	34,34,34,34	0
10	NA	I	908	1/1	0.94	0.12	26,26,26,26	0
5	NAD	F	603	44/44	0.95	0.09	35,47,53,56	0
3	EDO	G	705	4/4	0.95	0.10	26,27,34,37	0
3	EDO	H	502	4/4	0.95	0.09	28,31,37,39	0
5	NAD	A	608	44/44	0.95	0.08	33,44,50,54	0
5	NAD	D	605	44/44	0.95	0.08	41,50,55,58	0
3	EDO	A	603	4/4	0.95	0.10	33,36,39,39	0
5	NAD	B	508	44/44	0.96	0.07	26,31,38,47	0
5	NAD	C	506	44/44	0.96	0.07	33,40,45,52	0
7	CA	E	804	1/1	0.98	0.03	30,30,30,30	0
10	NA	G	707	1/1	0.98	0.04	38,38,38,38	0
7	CA	H	506	1/1	0.98	0.04	29,29,29,29	0
7	CA	L	704	1/1	0.99	0.02	30,30,30,30	0
7	CA	F	606	1/1	0.99	0.02	31,31,31,31	0
7	CA	G	708	1/1	0.99	0.03	32,32,32,32	0
7	CA	C	507	1/1	0.99	0.02	26,26,26,26	0
7	CA	I	909	1/1	0.99	0.03	31,31,31,31	0

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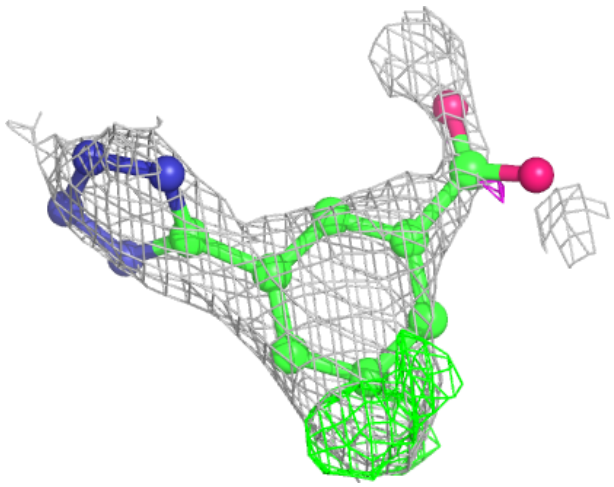
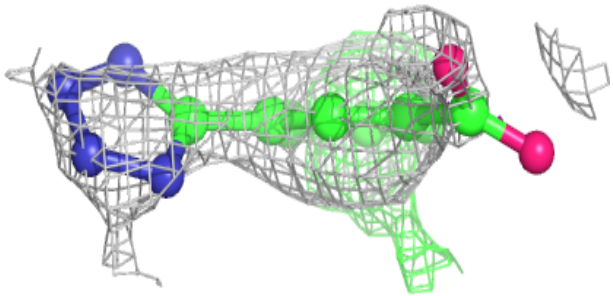
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	J	603	1/1	0.99	0.02	30,30,30,30	0
7	CA	D	606	1/1	1.00	0.01	18,18,18,18	0
7	CA	K	507	1/1	1.00	0.01	34,34,34,34	0
7	CA	B	509	1/1	1.00	0.02	25,25,25,25	0
7	CA	A	610	1/1	1.00	0.01	21,21,21,21	0

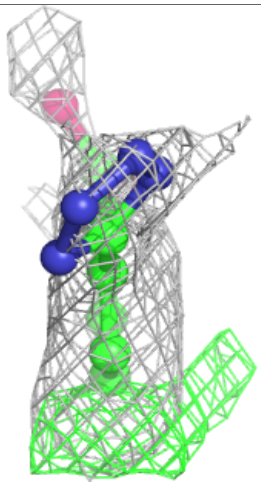
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H40 K 501:

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

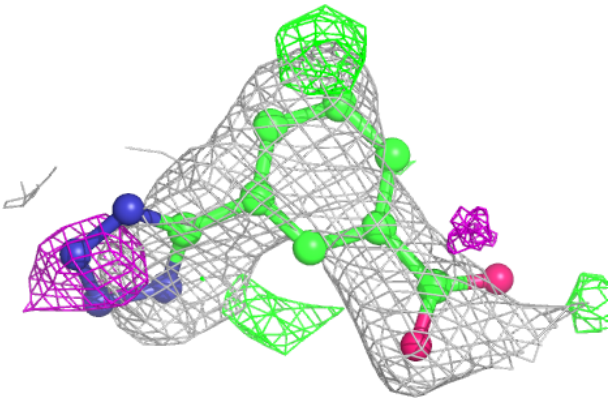


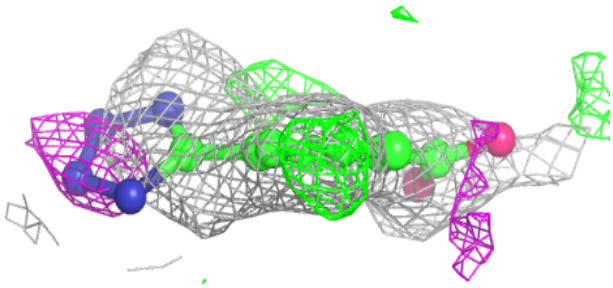


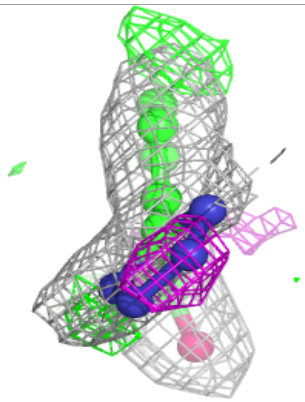


Electron density around A1H40 H 501:

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

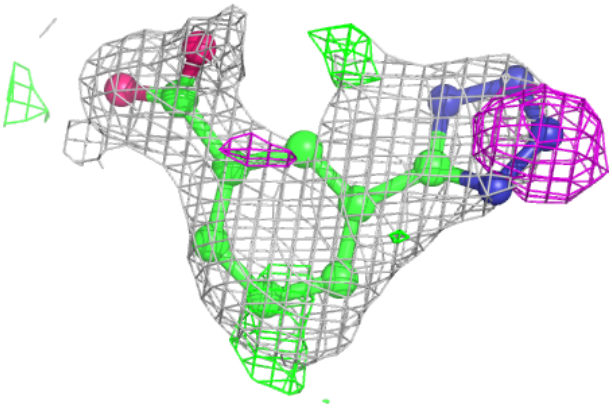


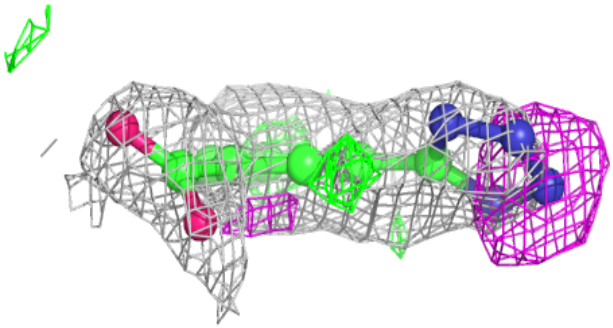


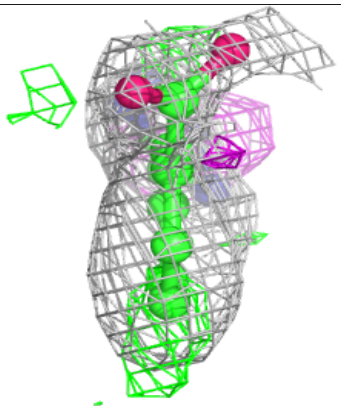


Electron density around A1H40 A 601:

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

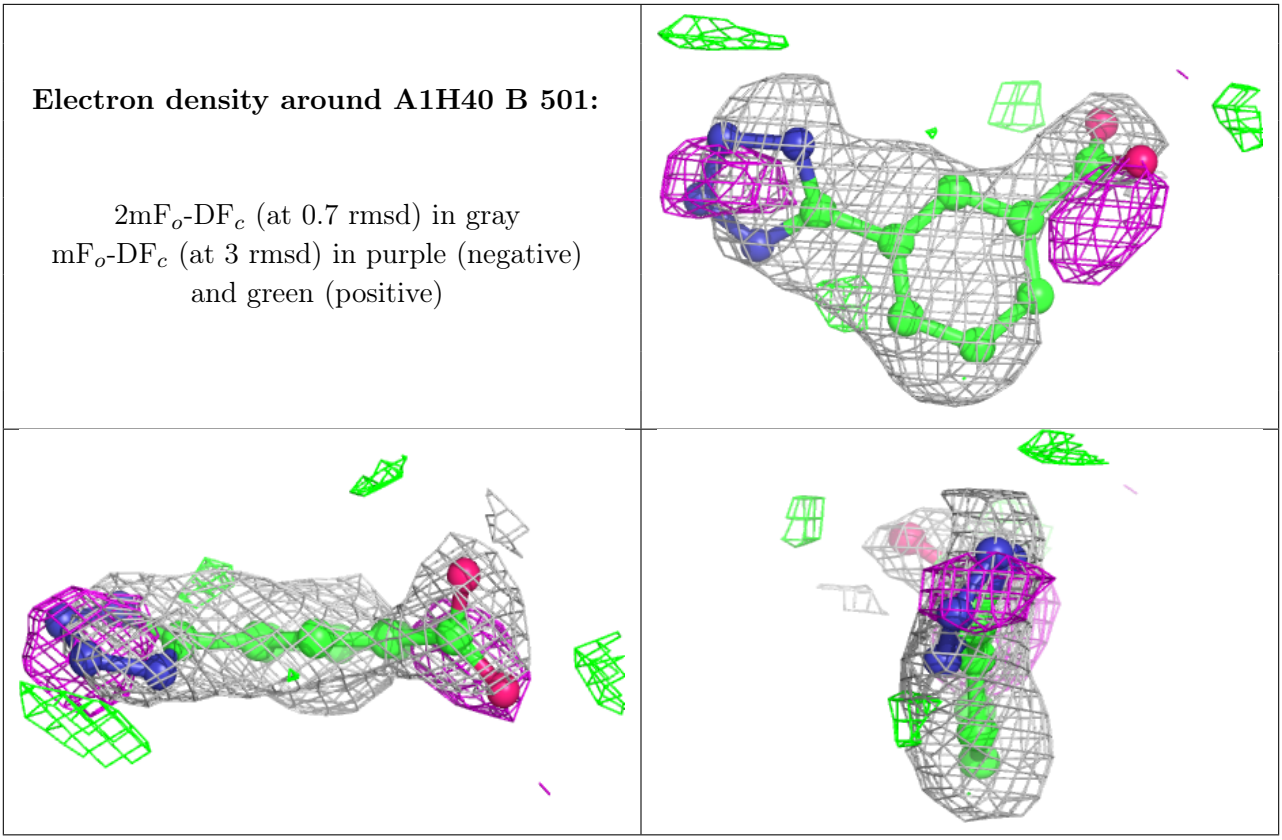






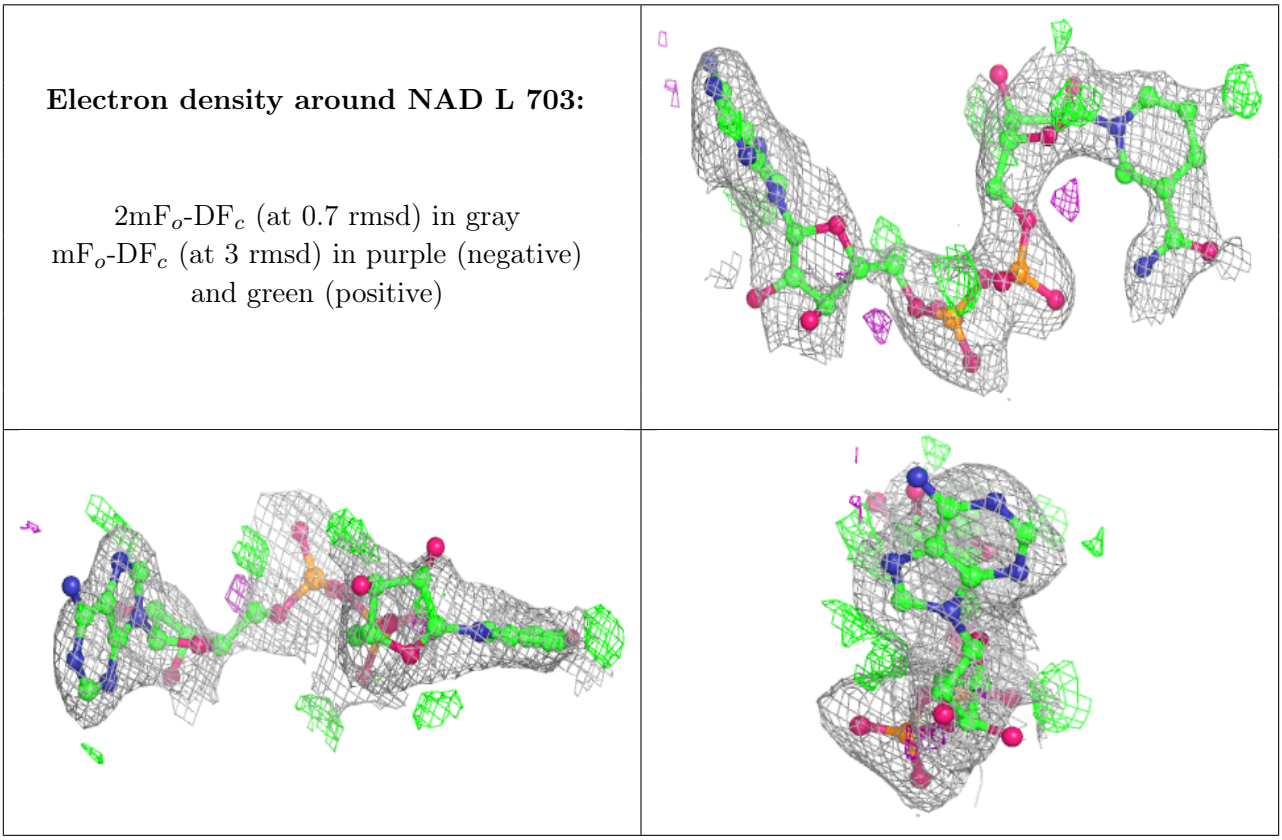
Electron density around A1H40 B 501:

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



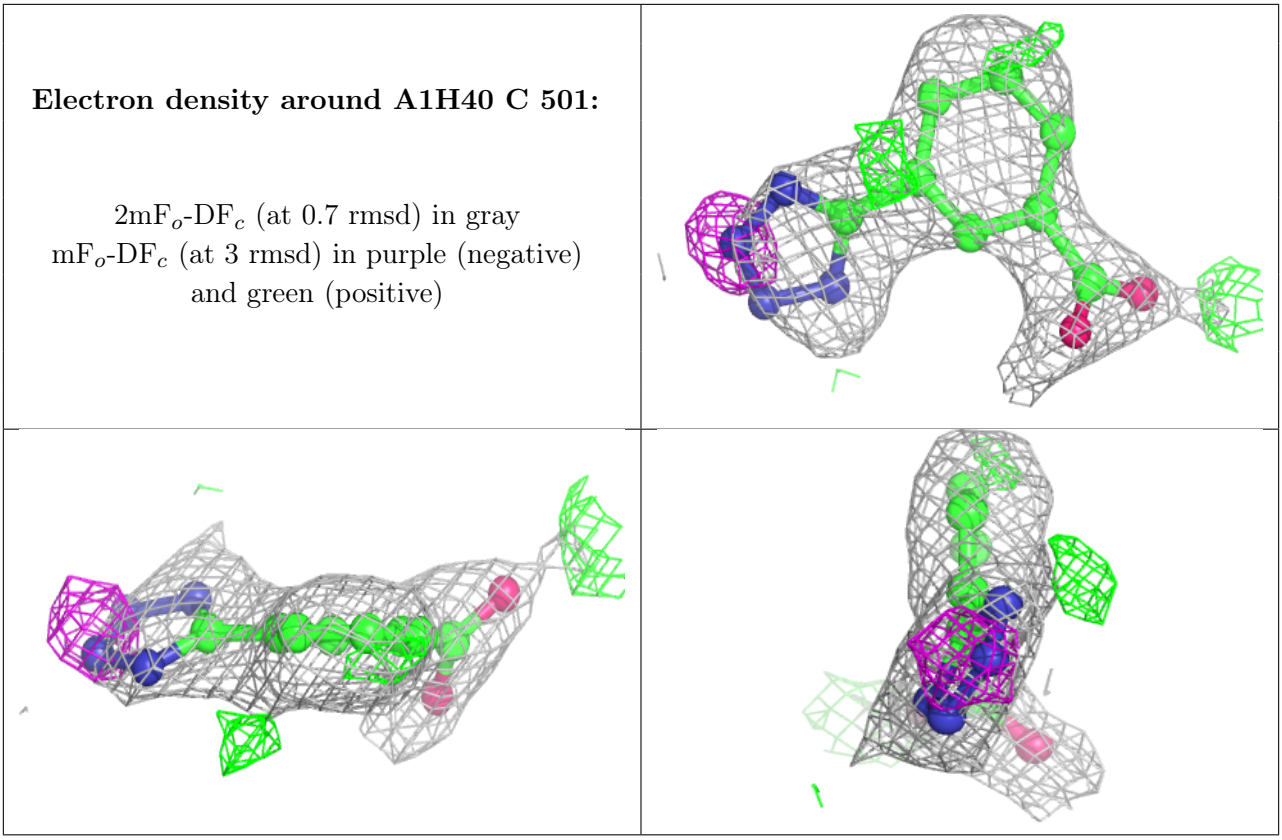
Electron density around NAD L 703:

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



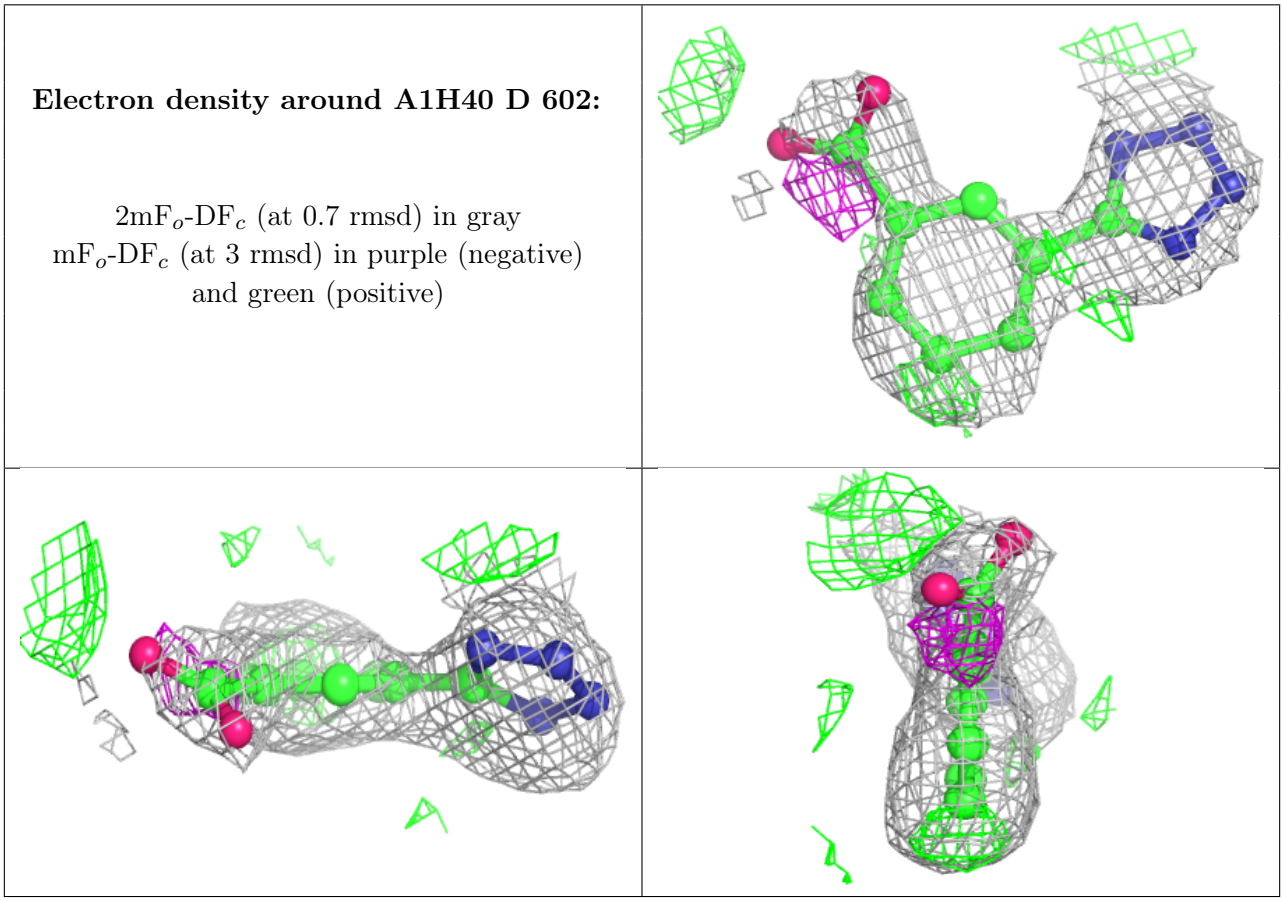
Electron density around A1H40 C 501:

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



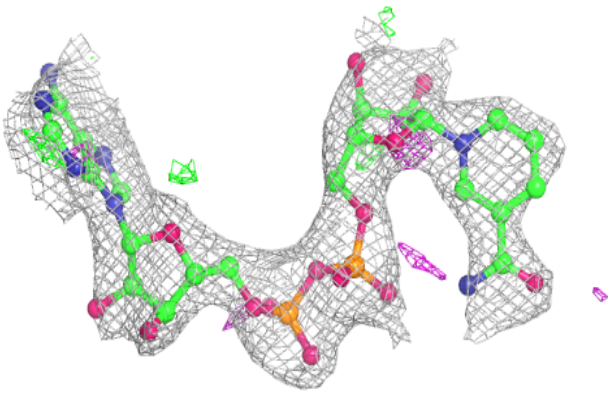
Electron density around A1H40 D 602:

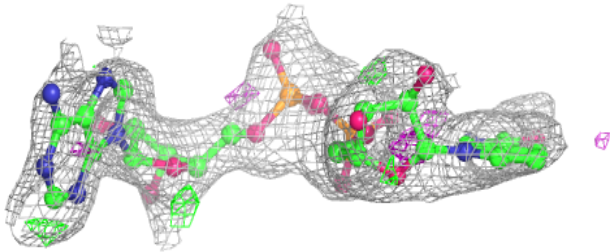
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

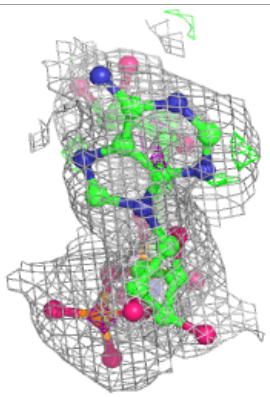


Electron density around NAD J 602:

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

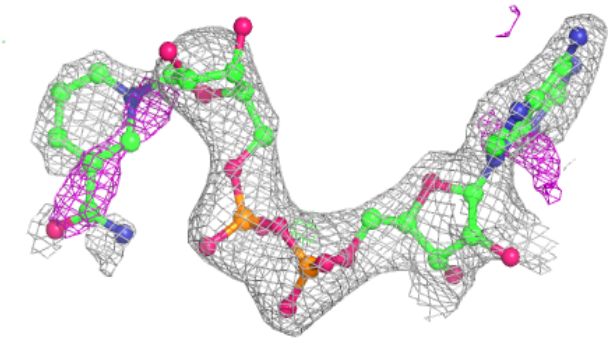


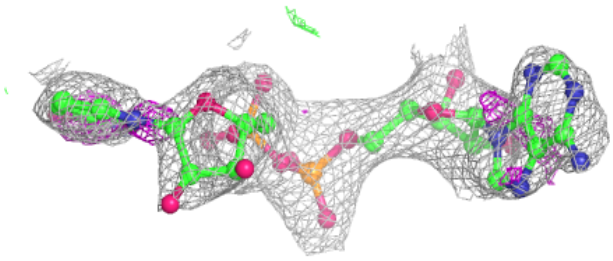


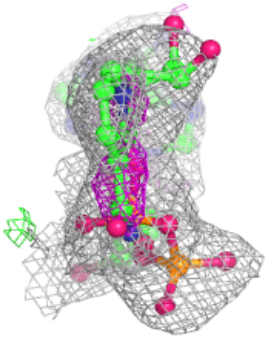


Electron density around NAD K 505:

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

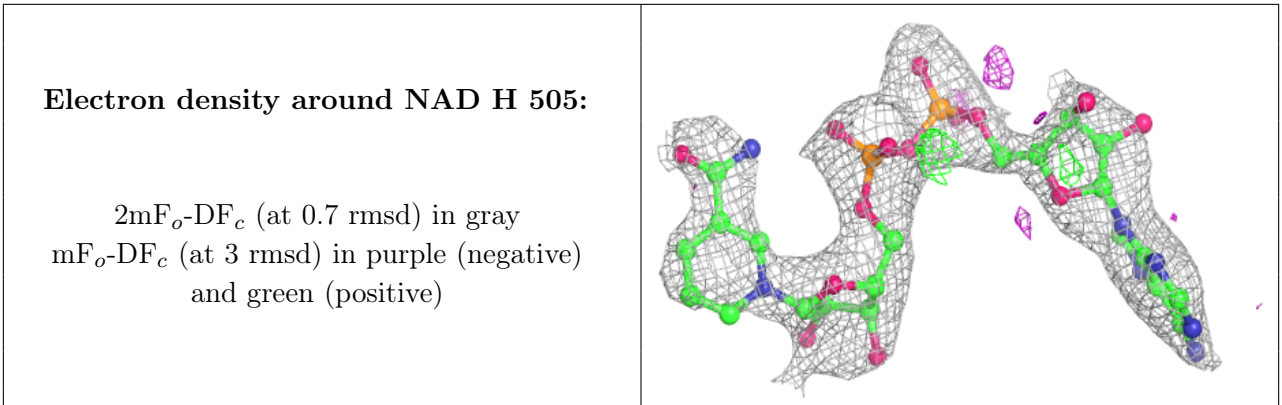






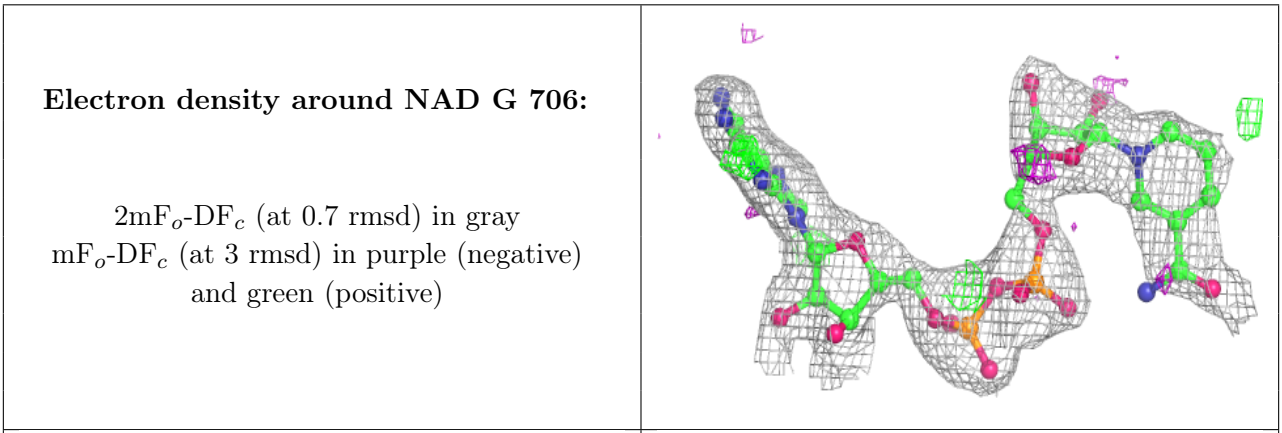
Electron density around NAD H 505:

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



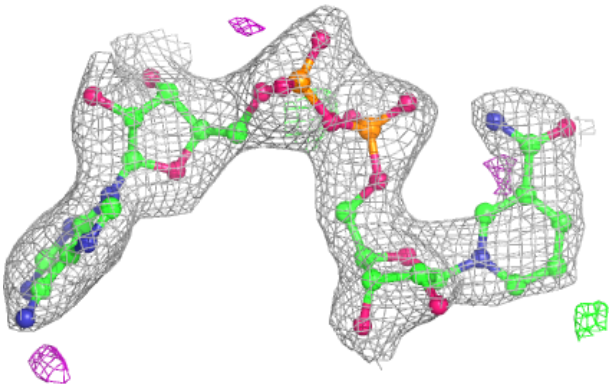
Electron density around NAD G 706:

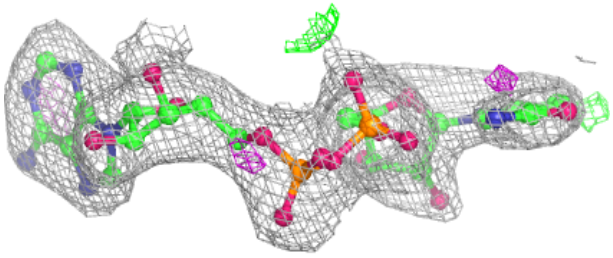
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

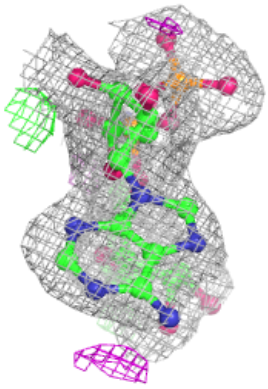


Electron density around NAD I 907:

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

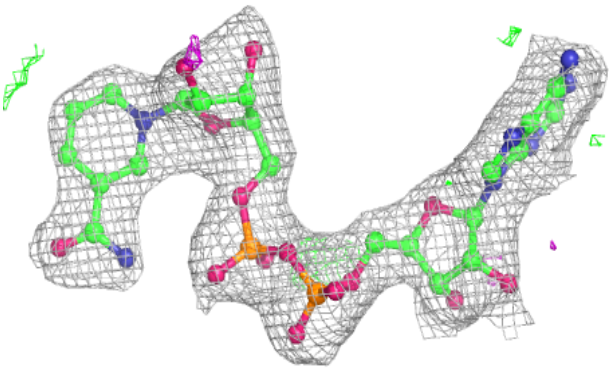


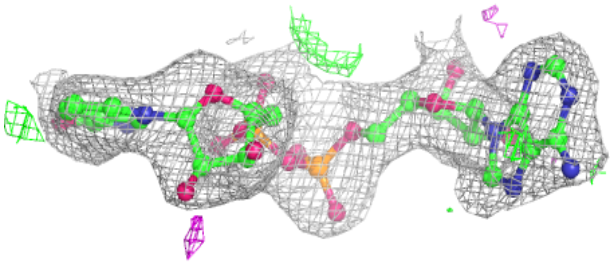


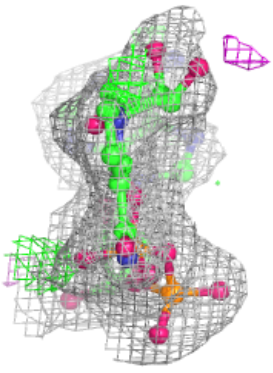


Electron density around NAD E 803:

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

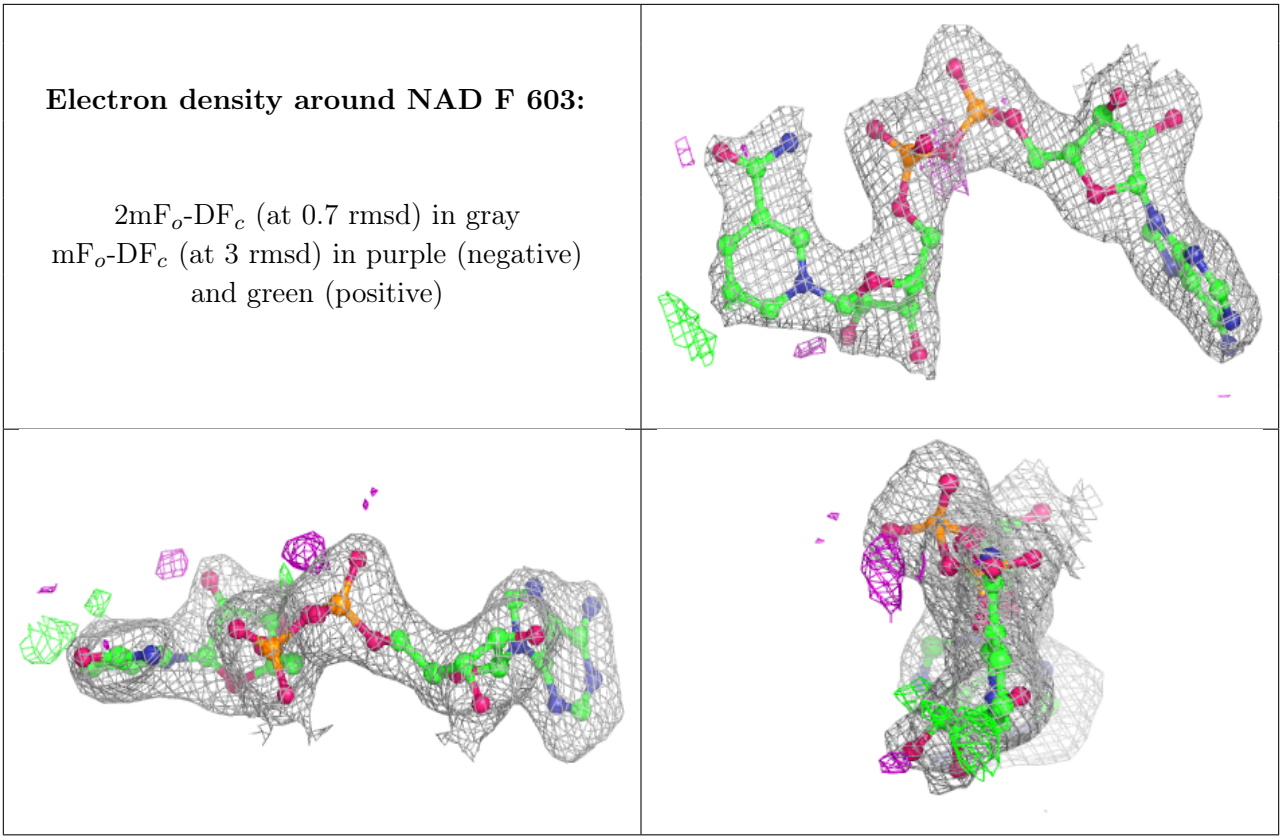






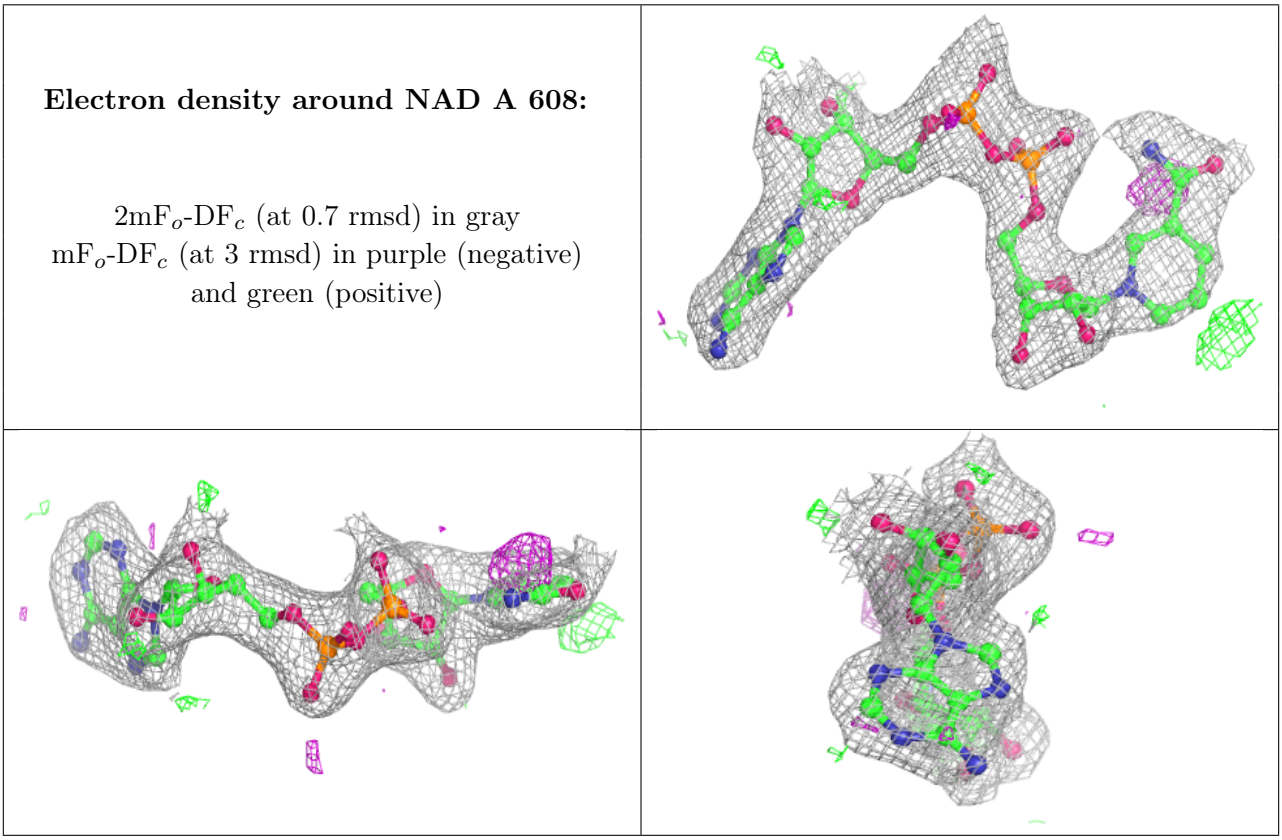
Electron density around NAD F 603:

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



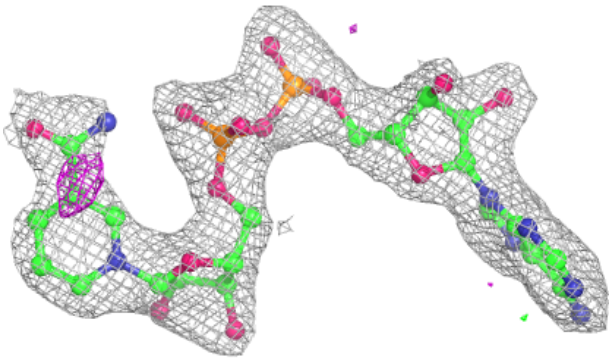
Electron density around NAD A 608:

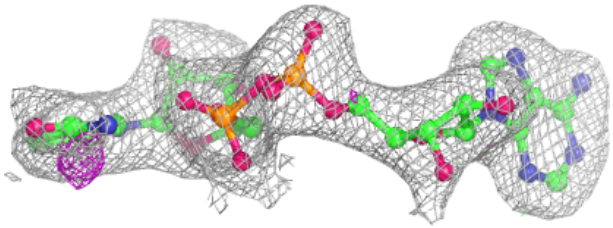
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

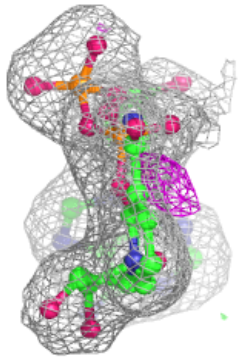


Electron density around NAD D 605:

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

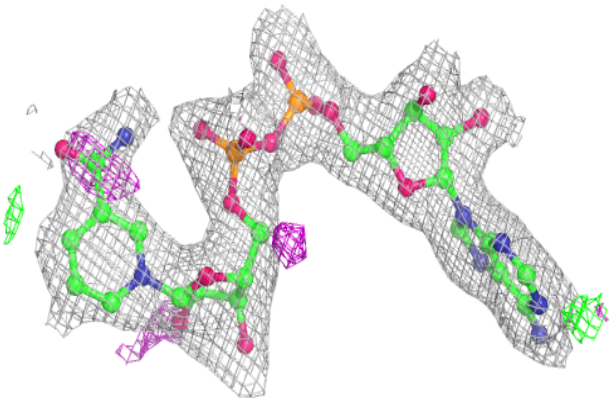


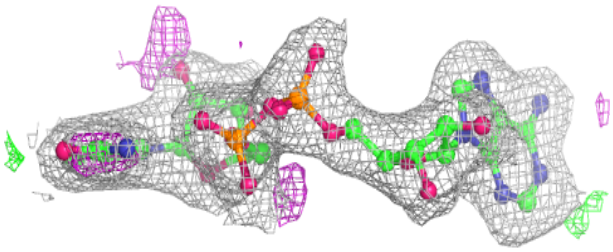


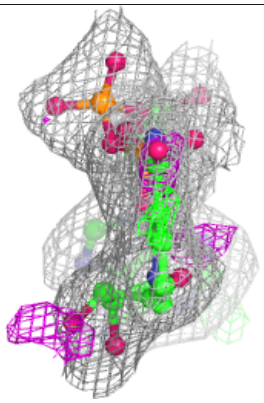


Electron density around NAD B 508:

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

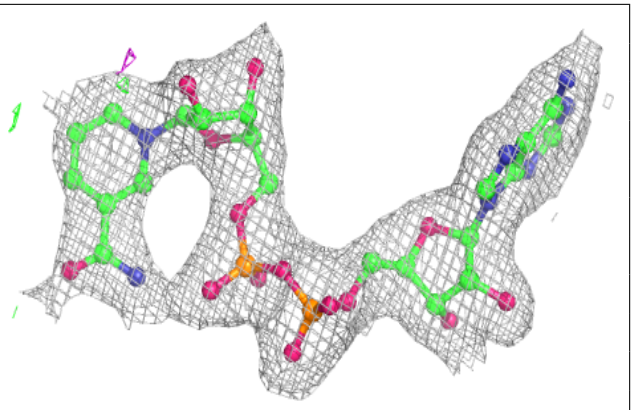


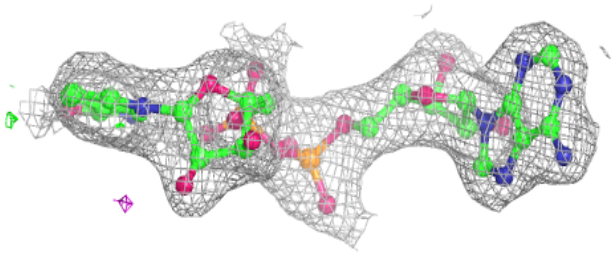




Electron density around NAD C 506:

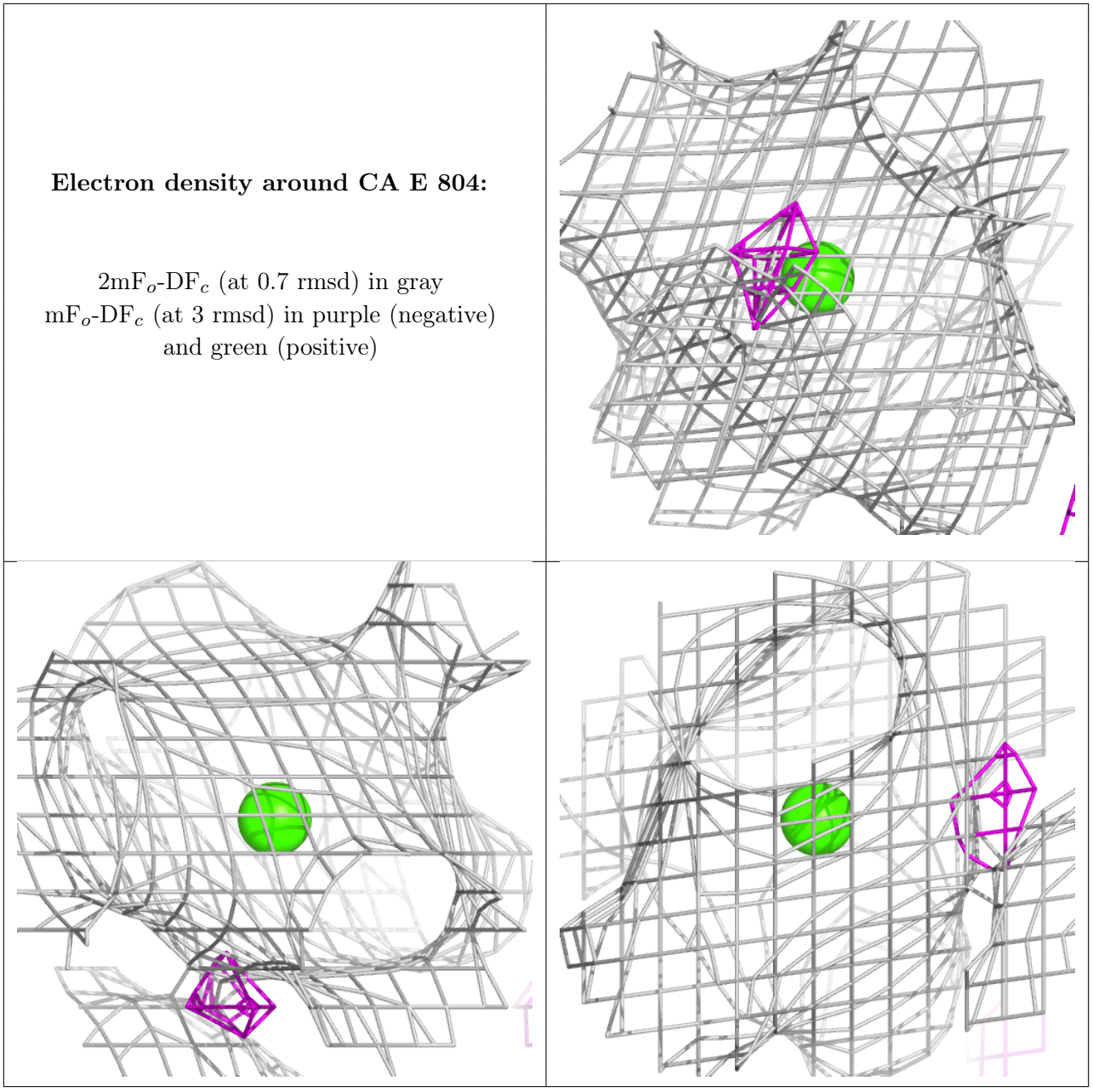
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





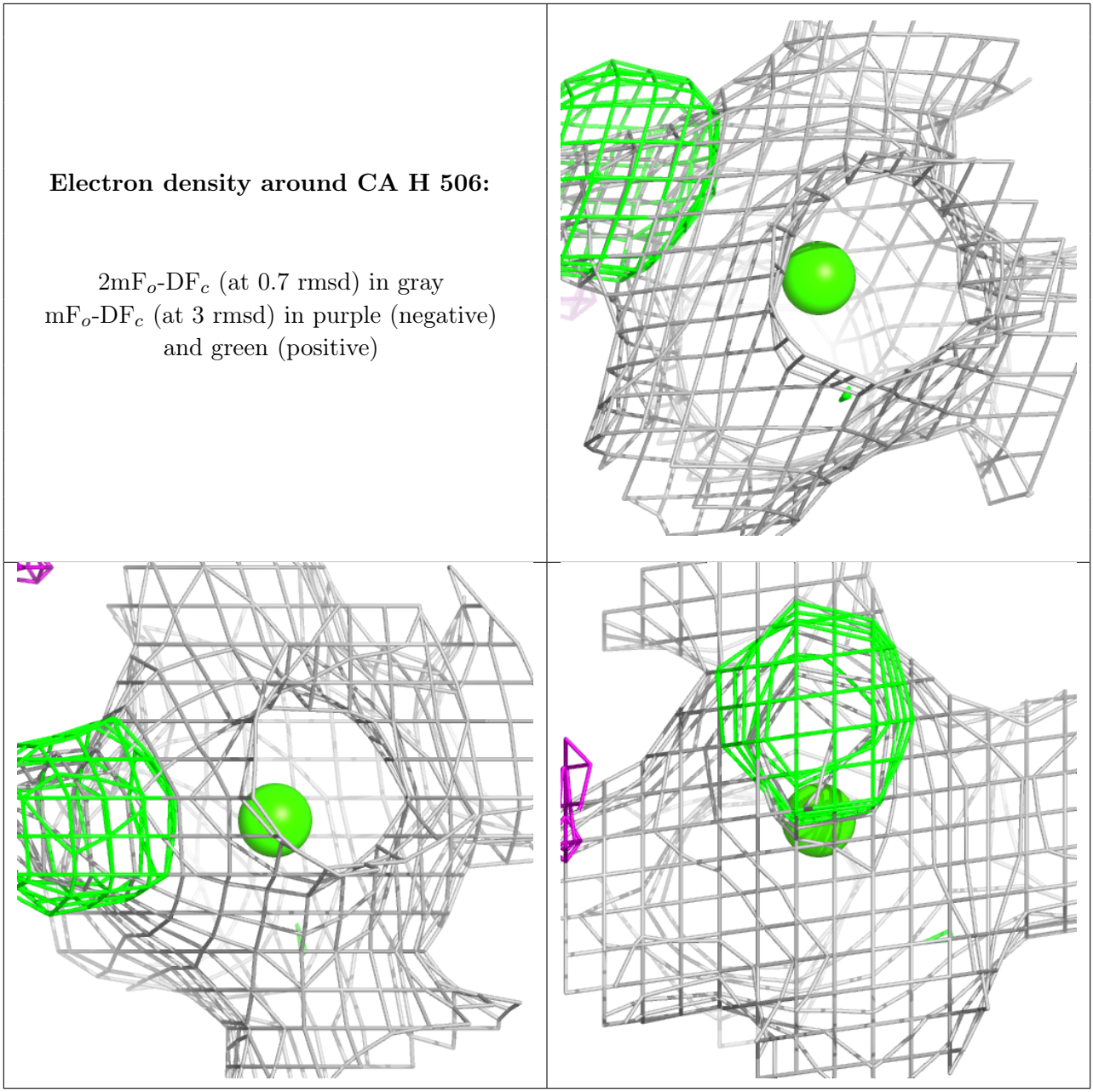
Electron density around CA E 804:

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



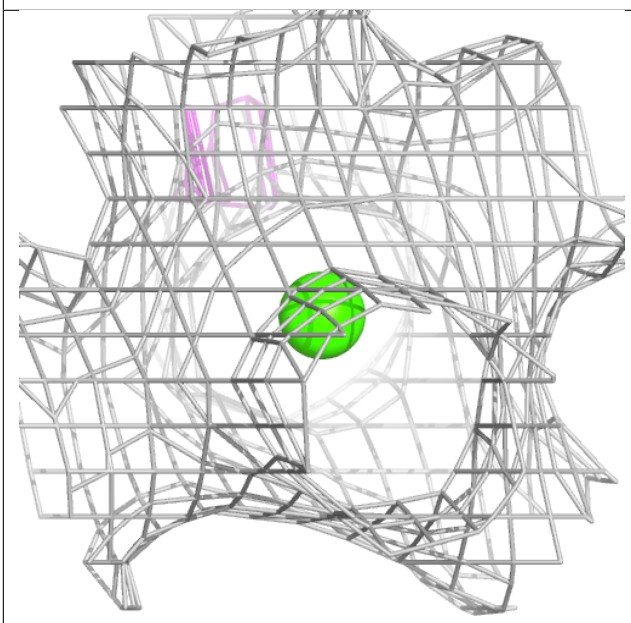
Electron density around CA H 506:

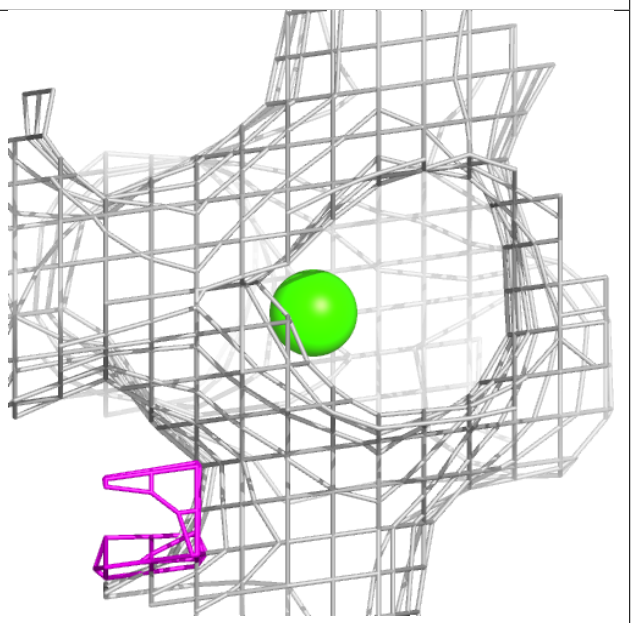
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CA L 704:

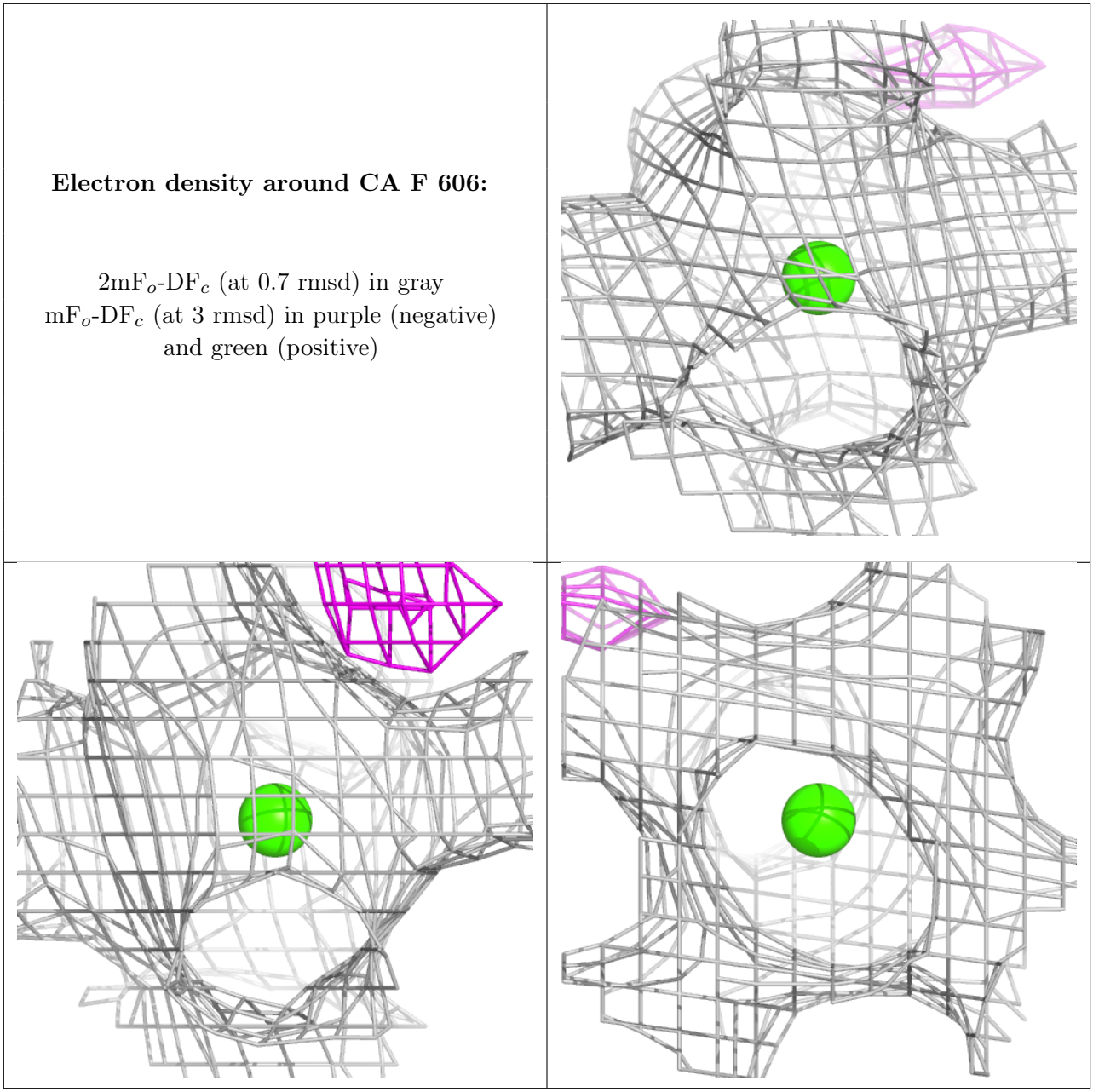
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





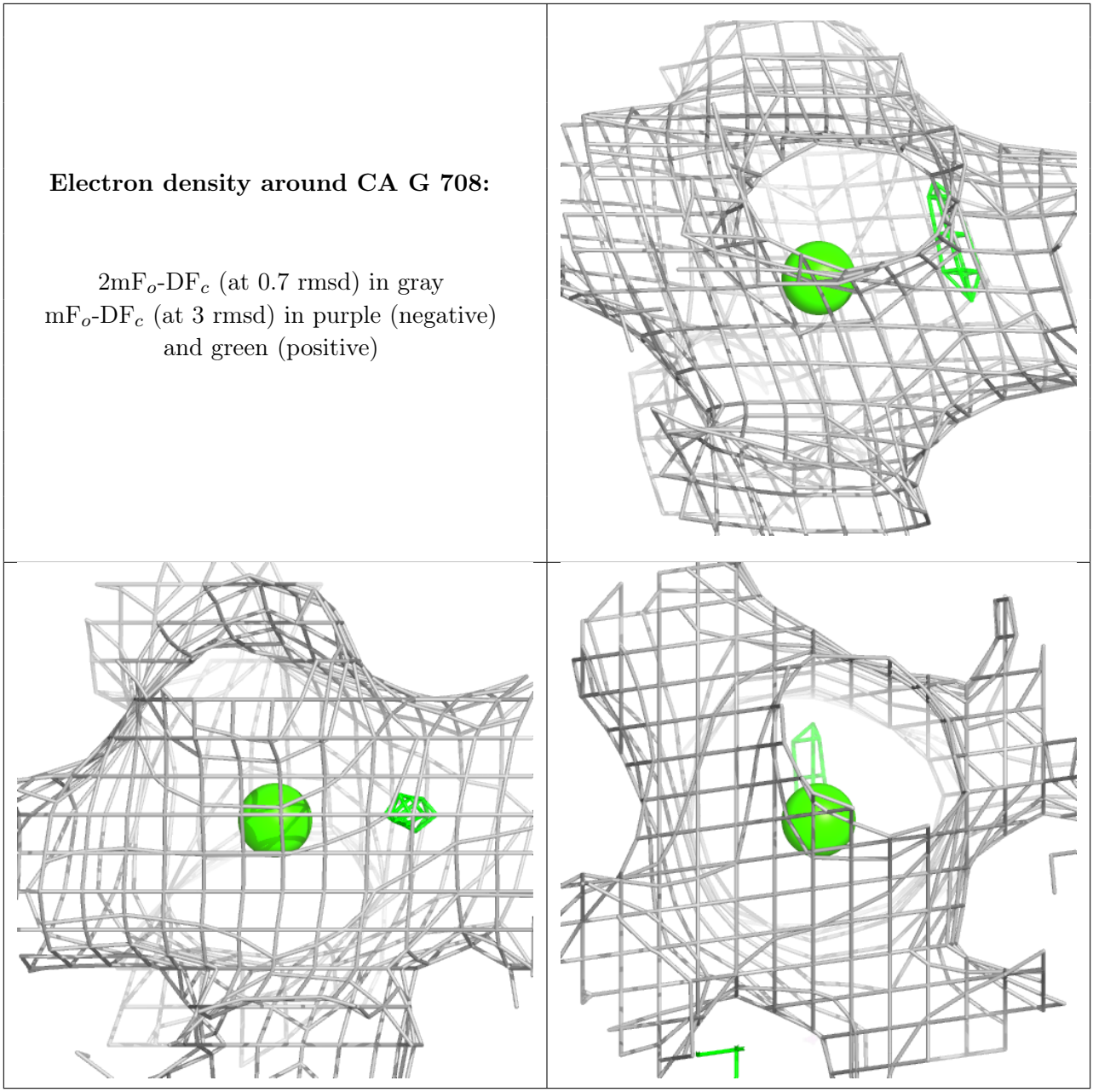
Electron density around CA F 606:

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



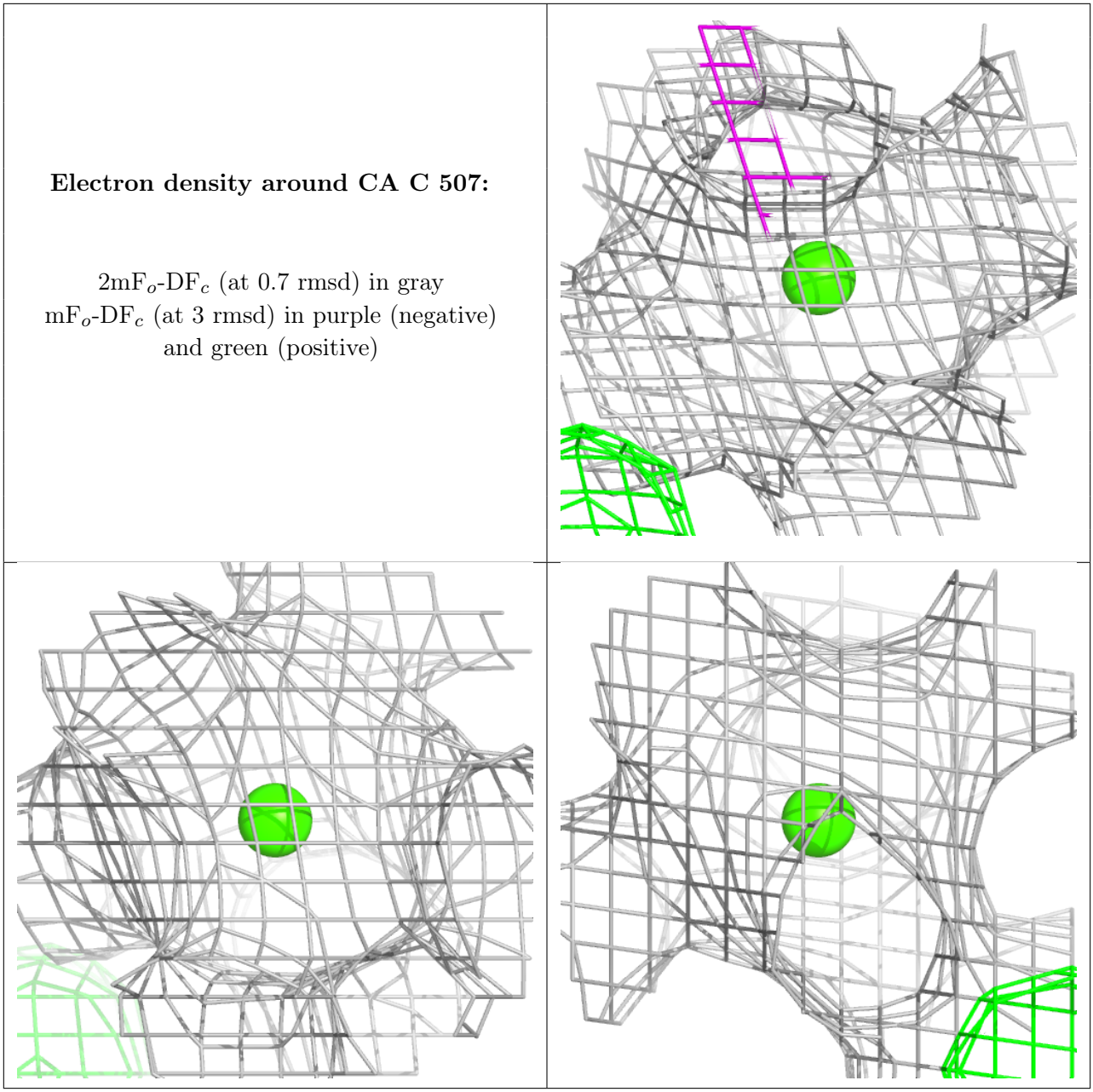
Electron density around CA G 708:

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



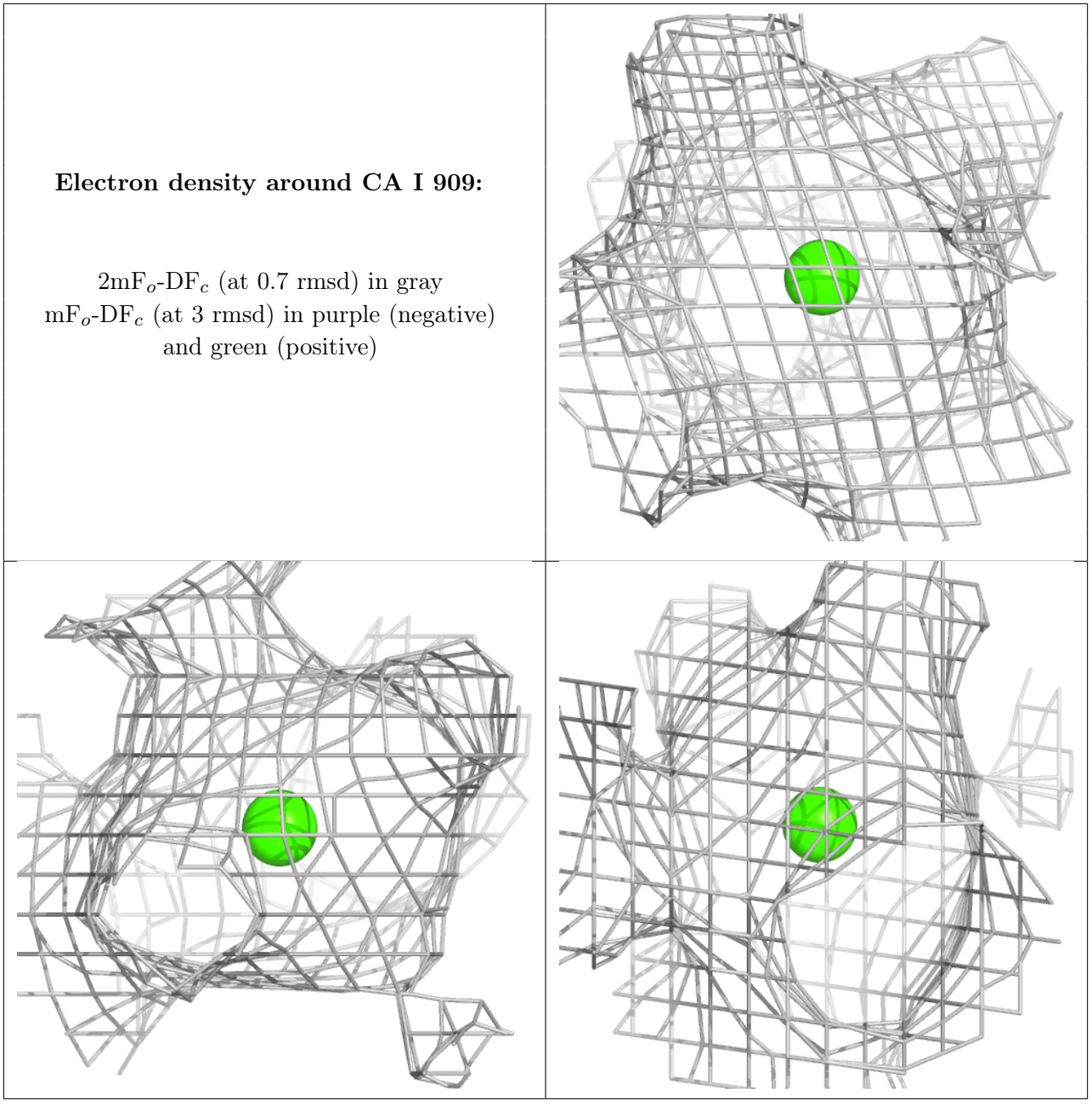
Electron density around CA C 507:

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



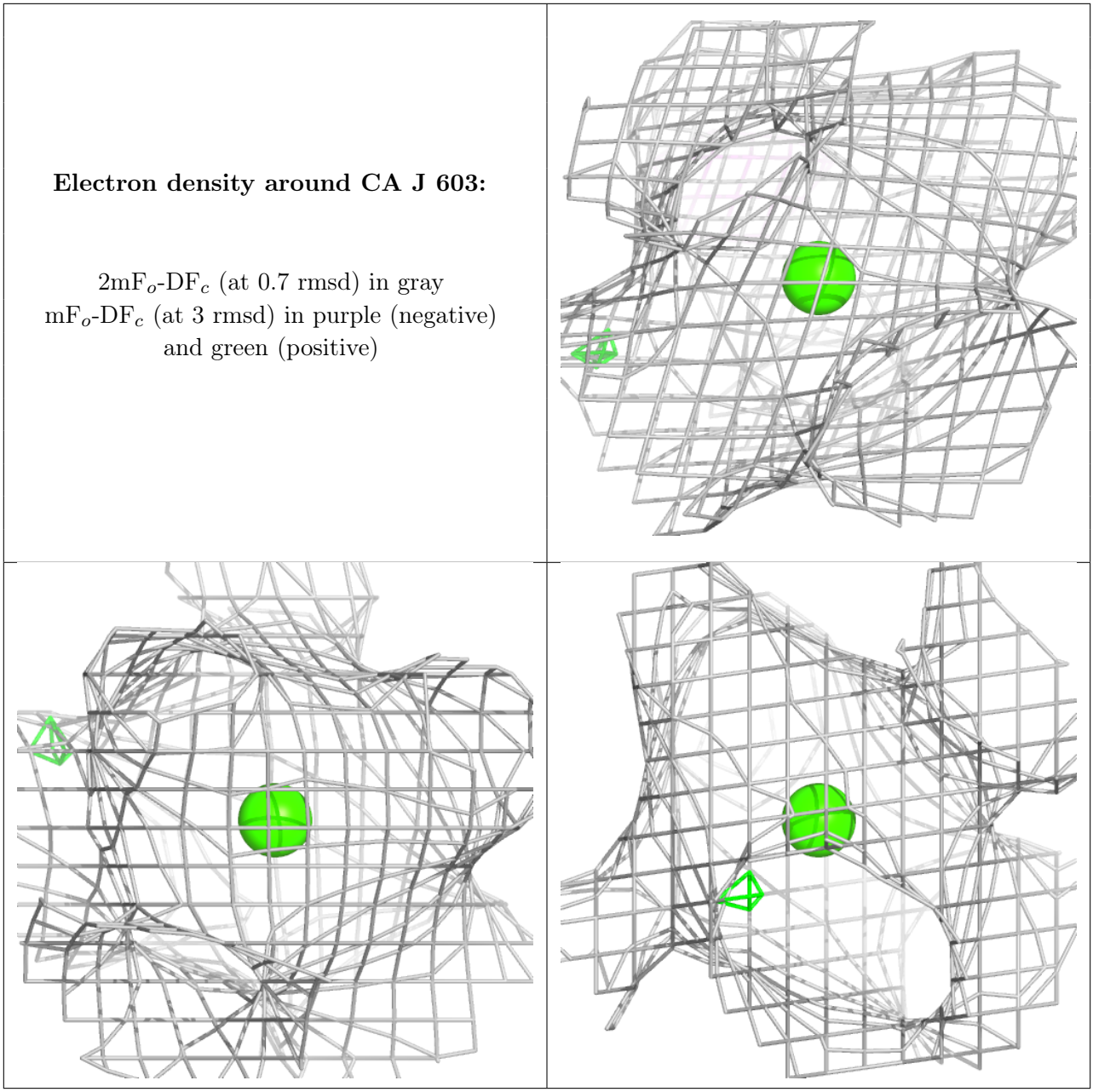
Electron density around CA I 909:

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



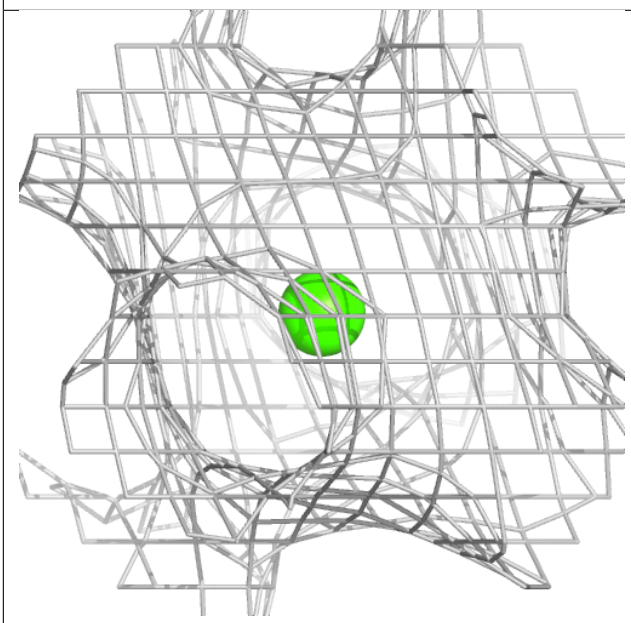
Electron density around CA J 603:

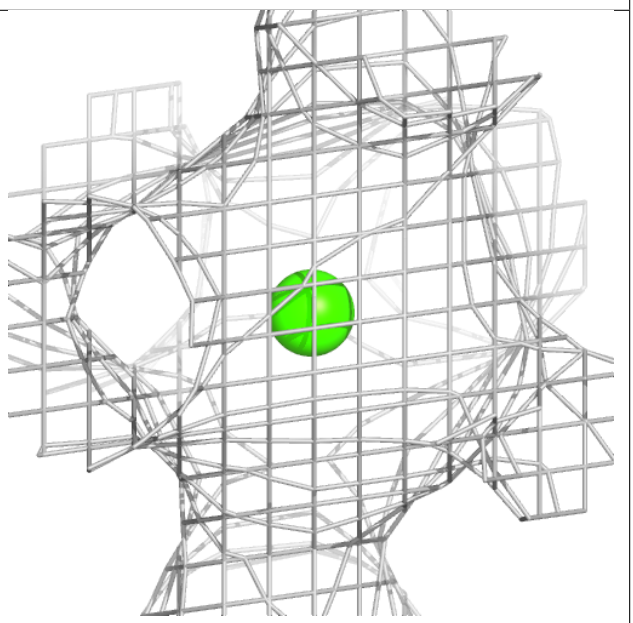
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CA D 606:

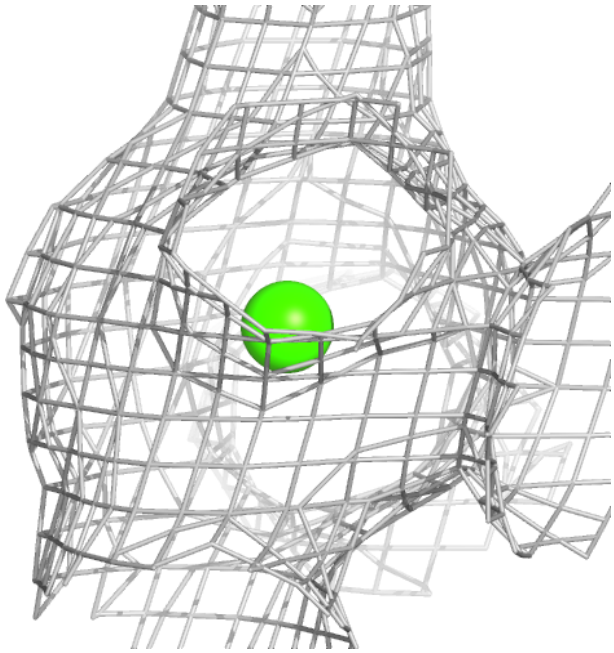
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

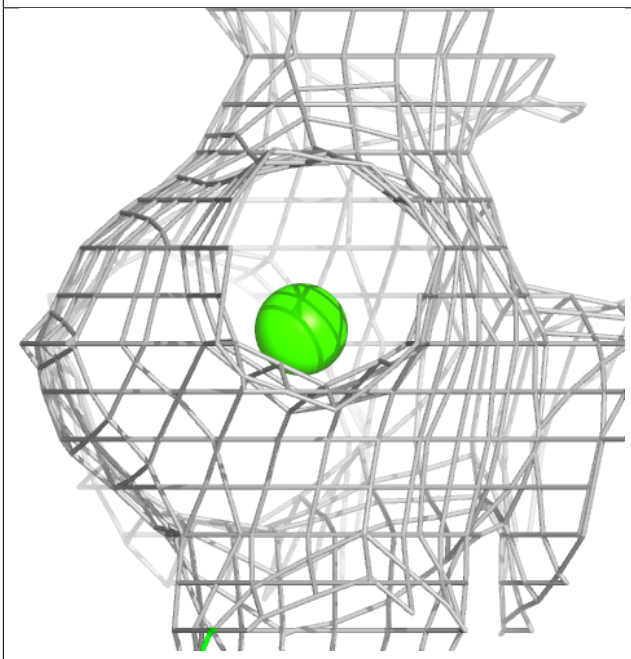


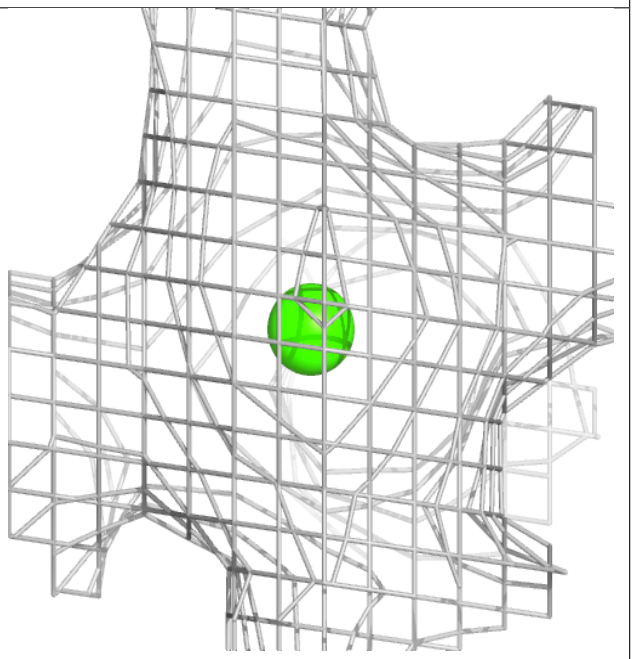


Electron density around CA K 507:

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

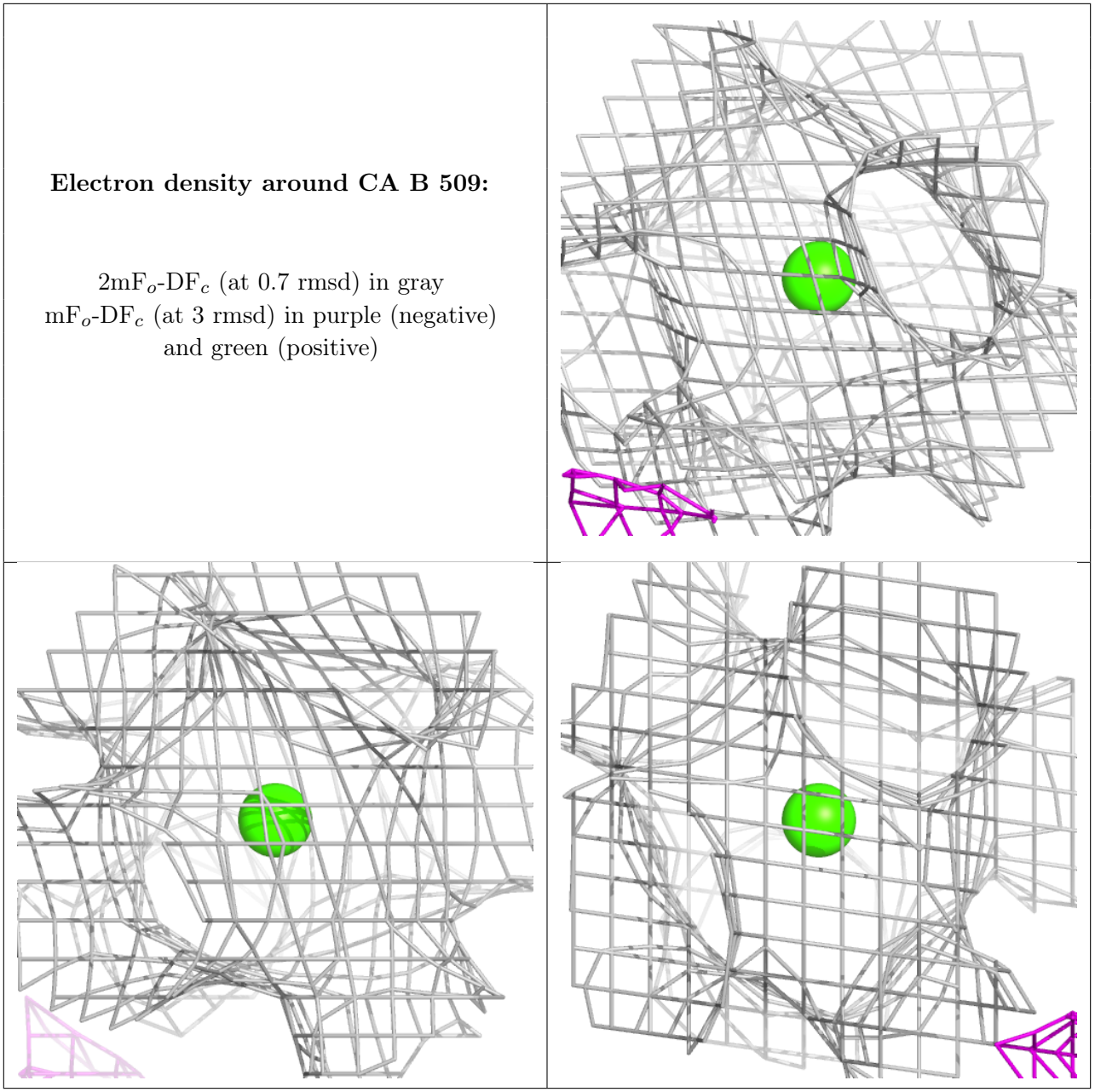






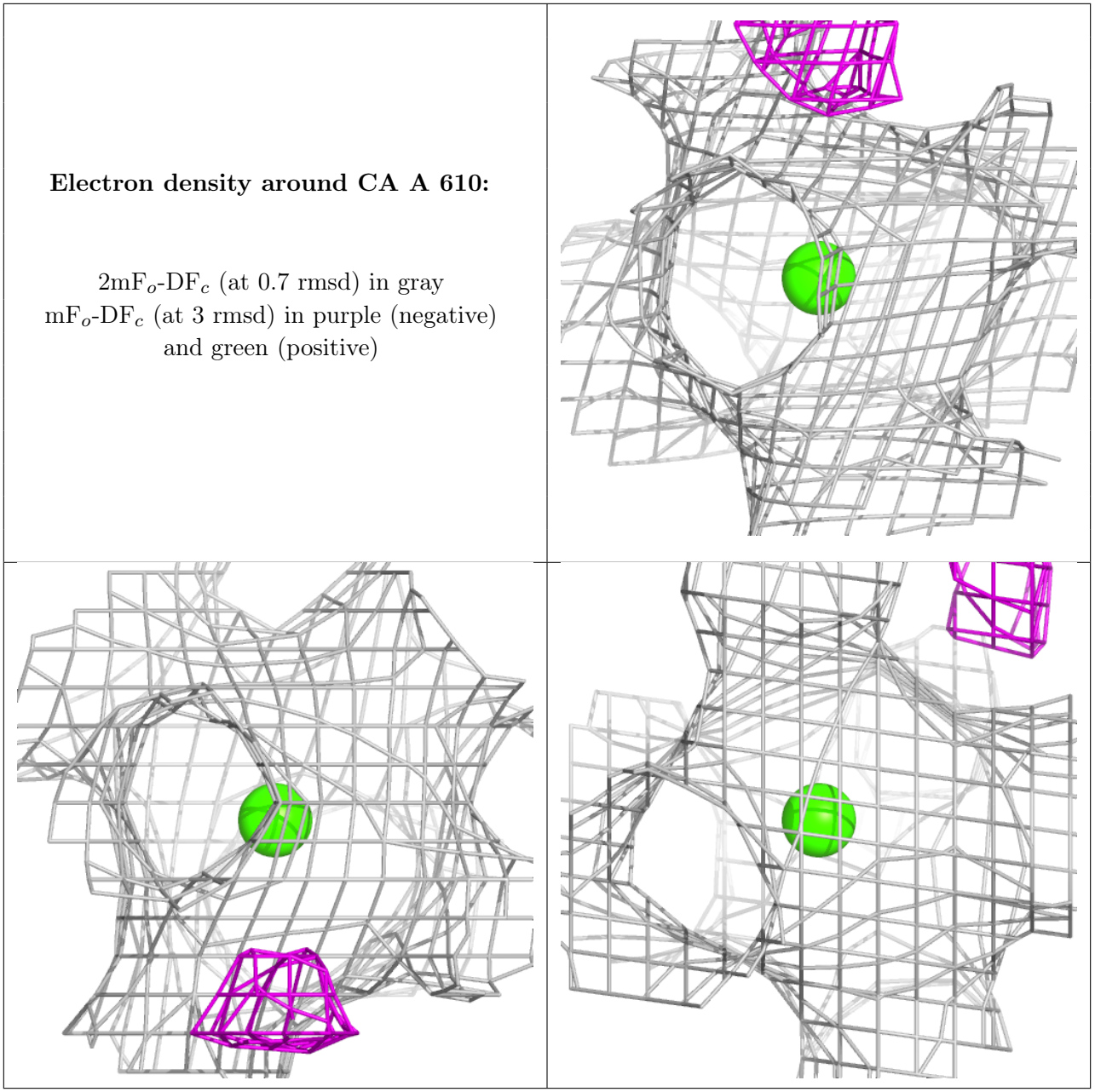
Electron density around CA B 509:

$2mF_o$-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 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 (i)

There are no such residues in this entry.