Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 05:02 AM EDT

PDB ID	:	4IYM
Title	:	Crystal structure of putative methylmalonate-semialdehyde dehydrogenase from Sinorhizobium meliloti 1021 complexed with NAD, target 011934
Authors	:	Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Lafluer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2013-01-28
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (1)) were used in the production of this report:

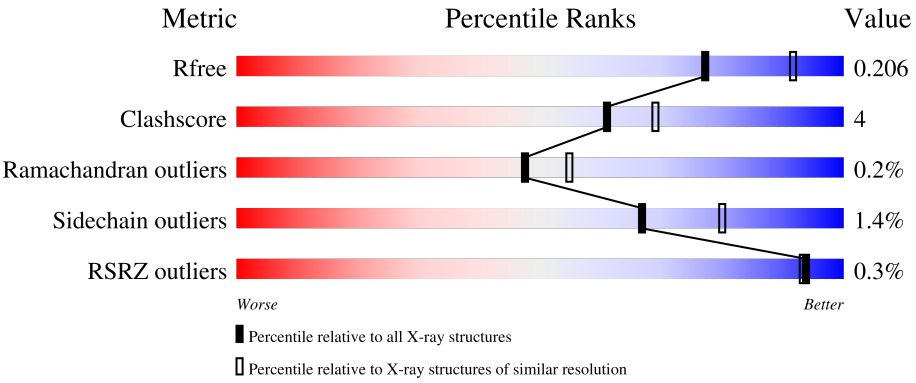
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	521	85% 8% 6%
1	B	521	87% 6% 6%
1	C	521	86% 7% • 6%

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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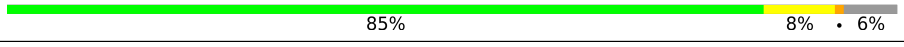
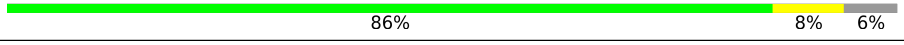
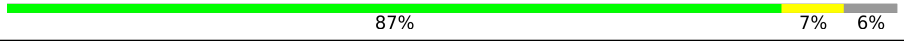
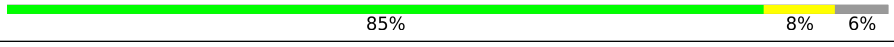
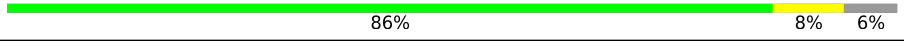
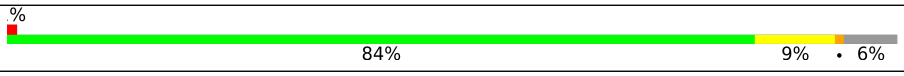
Mol	Chain	Length	Quality of chain
1	D	521	
1	E	521	
1	F	521	
1	G	521	
1	H	521	
1	I	521	
1	J	521	
1	K	521	
1	L	521	
1	M	521	
1	N	521	
1	O	521	
1	P	521	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 64517 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 Methylmalonate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	Se	0	3	0
			3696	2337	641	694	5	19			
1	B	488	Total	C	N	O	S	Se	0	3	0
			3702	2339	646	693	5	19			
1	C	491	Total	C	N	O	S	Se	0	3	0
			3722	2352	647	698	5	20			
1	D	488	Total	C	N	O	S	Se	0	4	0
			3704	2341	644	696	5	18			
1	E	490	Total	C	N	O	S	Se	0	2	0
			3703	2340	642	697	5	19			
1	F	488	Total	C	N	O	S	Se	0	3	0
			3699	2339	643	693	5	19			
1	G	488	Total	C	N	O	S	Se	0	2	0
			3694	2335	643	693	5	18			
1	H	489	Total	C	N	O	S	Se	0	1	0
			3693	2332	644	694	5	18			
1	I	489	Total	C	N	O	S	Se	0	2	0
			3701	2337	647	694	5	18			
1	J	488	Total	C	N	O	S	Se	0	1	0
			3689	2330	643	693	5	18			
1	K	488	Total	C	N	O	S	Se	0	5	0
			3710	2346	646	694	5	19			
1	L	489	Total	C	N	O	S	Se	0	2	0
			3695	2334	641	696	5	19			
1	M	489	Total	C	N	O	S	Se	0	1	0
			3690	2331	641	694	5	19			
1	N	488	Total	C	N	O	S	Se	0	0	0
			3681	2325	640	693	5	18			
1	O	489	Total	C	N	O	S	Se	0	4	0
			3716	2348	647	696	5	20			
1	P	489	Total	C	N	O	S	Se	0	1	0
			3690	2331	641	694	5	19			

There are 368 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MSE	-	expression tag	UNP Q92RW4
A	-23	HIS	-	expression tag	UNP Q92RW4
A	-22	HIS	-	expression tag	UNP Q92RW4
A	-21	HIS	-	expression tag	UNP Q92RW4
A	-20	HIS	-	expression tag	UNP Q92RW4
A	-19	HIS	-	expression tag	UNP Q92RW4
A	-18	HIS	-	expression tag	UNP Q92RW4
A	-17	SER	-	expression tag	UNP Q92RW4
A	-16	SER	-	expression tag	UNP Q92RW4
A	-15	GLY	-	expression tag	UNP Q92RW4
A	-14	VAL	-	expression tag	UNP Q92RW4
A	-13	ASP	-	expression tag	UNP Q92RW4
A	-12	LEU	-	expression tag	UNP Q92RW4
A	-11	GLY	-	expression tag	UNP Q92RW4
A	-10	THR	-	expression tag	UNP Q92RW4
A	-9	GLU	-	expression tag	UNP Q92RW4
A	-8	ASN	-	expression tag	UNP Q92RW4
A	-7	LEU	-	expression tag	UNP Q92RW4
A	-6	TYR	-	expression tag	UNP Q92RW4
A	-5	PHE	-	expression tag	UNP Q92RW4
A	-4	GLN	-	expression tag	UNP Q92RW4
A	-3	SER	-	expression tag	UNP Q92RW4
A	-2	MSE	-	expression tag	UNP Q92RW4
B	-24	MSE	-	expression tag	UNP Q92RW4
B	-23	HIS	-	expression tag	UNP Q92RW4
B	-22	HIS	-	expression tag	UNP Q92RW4
B	-21	HIS	-	expression tag	UNP Q92RW4
B	-20	HIS	-	expression tag	UNP Q92RW4
B	-19	HIS	-	expression tag	UNP Q92RW4
B	-18	HIS	-	expression tag	UNP Q92RW4
B	-17	SER	-	expression tag	UNP Q92RW4
B	-16	SER	-	expression tag	UNP Q92RW4
B	-15	GLY	-	expression tag	UNP Q92RW4
B	-14	VAL	-	expression tag	UNP Q92RW4
B	-13	ASP	-	expression tag	UNP Q92RW4
B	-12	LEU	-	expression tag	UNP Q92RW4
B	-11	GLY	-	expression tag	UNP Q92RW4
B	-10	THR	-	expression tag	UNP Q92RW4
B	-9	GLU	-	expression tag	UNP Q92RW4
B	-8	ASN	-	expression tag	UNP Q92RW4
B	-7	LEU	-	expression tag	UNP Q92RW4
B	-6	TYR	-	expression tag	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	PHE	-	expression tag	UNP Q92RW4
B	-4	GLN	-	expression tag	UNP Q92RW4
B	-3	SER	-	expression tag	UNP Q92RW4
B	-2	MSE	-	expression tag	UNP Q92RW4
C	-24	MSE	-	expression tag	UNP Q92RW4
C	-23	HIS	-	expression tag	UNP Q92RW4
C	-22	HIS	-	expression tag	UNP Q92RW4
C	-21	HIS	-	expression tag	UNP Q92RW4
C	-20	HIS	-	expression tag	UNP Q92RW4
C	-19	HIS	-	expression tag	UNP Q92RW4
C	-18	HIS	-	expression tag	UNP Q92RW4
C	-17	SER	-	expression tag	UNP Q92RW4
C	-16	SER	-	expression tag	UNP Q92RW4
C	-15	GLY	-	expression tag	UNP Q92RW4
C	-14	VAL	-	expression tag	UNP Q92RW4
C	-13	ASP	-	expression tag	UNP Q92RW4
C	-12	LEU	-	expression tag	UNP Q92RW4
C	-11	GLY	-	expression tag	UNP Q92RW4
C	-10	THR	-	expression tag	UNP Q92RW4
C	-9	GLU	-	expression tag	UNP Q92RW4
C	-8	ASN	-	expression tag	UNP Q92RW4
C	-7	LEU	-	expression tag	UNP Q92RW4
C	-6	TYR	-	expression tag	UNP Q92RW4
C	-5	PHE	-	expression tag	UNP Q92RW4
C	-4	GLN	-	expression tag	UNP Q92RW4
C	-3	SER	-	expression tag	UNP Q92RW4
C	-2	MSE	-	expression tag	UNP Q92RW4
D	-24	MSE	-	expression tag	UNP Q92RW4
D	-23	HIS	-	expression tag	UNP Q92RW4
D	-22	HIS	-	expression tag	UNP Q92RW4
D	-21	HIS	-	expression tag	UNP Q92RW4
D	-20	HIS	-	expression tag	UNP Q92RW4
D	-19	HIS	-	expression tag	UNP Q92RW4
D	-18	HIS	-	expression tag	UNP Q92RW4
D	-17	SER	-	expression tag	UNP Q92RW4
D	-16	SER	-	expression tag	UNP Q92RW4
D	-15	GLY	-	expression tag	UNP Q92RW4
D	-14	VAL	-	expression tag	UNP Q92RW4
D	-13	ASP	-	expression tag	UNP Q92RW4
D	-12	LEU	-	expression tag	UNP Q92RW4
D	-11	GLY	-	expression tag	UNP Q92RW4
D	-10	THR	-	expression tag	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLU	-	expression tag	UNP Q92RW4
D	-8	ASN	-	expression tag	UNP Q92RW4
D	-7	LEU	-	expression tag	UNP Q92RW4
D	-6	TYR	-	expression tag	UNP Q92RW4
D	-5	PHE	-	expression tag	UNP Q92RW4
D	-4	GLN	-	expression tag	UNP Q92RW4
D	-3	SER	-	expression tag	UNP Q92RW4
D	-2	MSE	-	expression tag	UNP Q92RW4
E	-24	MSE	-	expression tag	UNP Q92RW4
E	-23	HIS	-	expression tag	UNP Q92RW4
E	-22	HIS	-	expression tag	UNP Q92RW4
E	-21	HIS	-	expression tag	UNP Q92RW4
E	-20	HIS	-	expression tag	UNP Q92RW4
E	-19	HIS	-	expression tag	UNP Q92RW4
E	-18	HIS	-	expression tag	UNP Q92RW4
E	-17	SER	-	expression tag	UNP Q92RW4
E	-16	SER	-	expression tag	UNP Q92RW4
E	-15	GLY	-	expression tag	UNP Q92RW4
E	-14	VAL	-	expression tag	UNP Q92RW4
E	-13	ASP	-	expression tag	UNP Q92RW4
E	-12	LEU	-	expression tag	UNP Q92RW4
E	-11	GLY	-	expression tag	UNP Q92RW4
E	-10	THR	-	expression tag	UNP Q92RW4
E	-9	GLU	-	expression tag	UNP Q92RW4
E	-8	ASN	-	expression tag	UNP Q92RW4
E	-7	LEU	-	expression tag	UNP Q92RW4
E	-6	TYR	-	expression tag	UNP Q92RW4
E	-5	PHE	-	expression tag	UNP Q92RW4
E	-4	GLN	-	expression tag	UNP Q92RW4
E	-3	SER	-	expression tag	UNP Q92RW4
E	-2	MSE	-	expression tag	UNP Q92RW4
F	-24	MSE	-	expression tag	UNP Q92RW4
F	-23	HIS	-	expression tag	UNP Q92RW4
F	-22	HIS	-	expression tag	UNP Q92RW4
F	-21	HIS	-	expression tag	UNP Q92RW4
F	-20	HIS	-	expression tag	UNP Q92RW4
F	-19	HIS	-	expression tag	UNP Q92RW4
F	-18	HIS	-	expression tag	UNP Q92RW4
F	-17	SER	-	expression tag	UNP Q92RW4
F	-16	SER	-	expression tag	UNP Q92RW4
F	-15	GLY	-	expression tag	UNP Q92RW4
F	-14	VAL	-	expression tag	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	ASP	-	expression tag	UNP Q92RW4
F	-12	LEU	-	expression tag	UNP Q92RW4
F	-11	GLY	-	expression tag	UNP Q92RW4
F	-10	THR	-	expression tag	UNP Q92RW4
F	-9	GLU	-	expression tag	UNP Q92RW4
F	-8	ASN	-	expression tag	UNP Q92RW4
F	-7	LEU	-	expression tag	UNP Q92RW4
F	-6	TYR	-	expression tag	UNP Q92RW4
F	-5	PHE	-	expression tag	UNP Q92RW4
F	-4	GLN	-	expression tag	UNP Q92RW4
F	-3	SER	-	expression tag	UNP Q92RW4
F	-2	MSE	-	expression tag	UNP Q92RW4
G	-24	MSE	-	expression tag	UNP Q92RW4
G	-23	HIS	-	expression tag	UNP Q92RW4
G	-22	HIS	-	expression tag	UNP Q92RW4
G	-21	HIS	-	expression tag	UNP Q92RW4
G	-20	HIS	-	expression tag	UNP Q92RW4
G	-19	HIS	-	expression tag	UNP Q92RW4
G	-18	HIS	-	expression tag	UNP Q92RW4
G	-17	SER	-	expression tag	UNP Q92RW4
G	-16	SER	-	expression tag	UNP Q92RW4
G	-15	GLY	-	expression tag	UNP Q92RW4
G	-14	VAL	-	expression tag	UNP Q92RW4
G	-13	ASP	-	expression tag	UNP Q92RW4
G	-12	LEU	-	expression tag	UNP Q92RW4
G	-11	GLY	-	expression tag	UNP Q92RW4
G	-10	THR	-	expression tag	UNP Q92RW4
G	-9	GLU	-	expression tag	UNP Q92RW4
G	-8	ASN	-	expression tag	UNP Q92RW4
G	-7	LEU	-	expression tag	UNP Q92RW4
G	-6	TYR	-	expression tag	UNP Q92RW4
G	-5	PHE	-	expression tag	UNP Q92RW4
G	-4	GLN	-	expression tag	UNP Q92RW4
G	-3	SER	-	expression tag	UNP Q92RW4
G	-2	MSE	-	expression tag	UNP Q92RW4
H	-24	MSE	-	expression tag	UNP Q92RW4
H	-23	HIS	-	expression tag	UNP Q92RW4
H	-22	HIS	-	expression tag	UNP Q92RW4
H	-21	HIS	-	expression tag	UNP Q92RW4
H	-20	HIS	-	expression tag	UNP Q92RW4
H	-19	HIS	-	expression tag	UNP Q92RW4
H	-18	HIS	-	expression tag	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	SER	-	expression tag	UNP Q92RW4
H	-16	SER	-	expression tag	UNP Q92RW4
H	-15	GLY	-	expression tag	UNP Q92RW4
H	-14	VAL	-	expression tag	UNP Q92RW4
H	-13	ASP	-	expression tag	UNP Q92RW4
H	-12	LEU	-	expression tag	UNP Q92RW4
H	-11	GLY	-	expression tag	UNP Q92RW4
H	-10	THR	-	expression tag	UNP Q92RW4
H	-9	GLU	-	expression tag	UNP Q92RW4
H	-8	ASN	-	expression tag	UNP Q92RW4
H	-7	LEU	-	expression tag	UNP Q92RW4
H	-6	TYR	-	expression tag	UNP Q92RW4
H	-5	PHE	-	expression tag	UNP Q92RW4
H	-4	GLN	-	expression tag	UNP Q92RW4
H	-3	SER	-	expression tag	UNP Q92RW4
H	-2	MSE	-	expression tag	UNP Q92RW4
I	-24	MSE	-	expression tag	UNP Q92RW4
I	-23	HIS	-	expression tag	UNP Q92RW4
I	-22	HIS	-	expression tag	UNP Q92RW4
I	-21	HIS	-	expression tag	UNP Q92RW4
I	-20	HIS	-	expression tag	UNP Q92RW4
I	-19	HIS	-	expression tag	UNP Q92RW4
I	-18	HIS	-	expression tag	UNP Q92RW4
I	-17	SER	-	expression tag	UNP Q92RW4
I	-16	SER	-	expression tag	UNP Q92RW4
I	-15	GLY	-	expression tag	UNP Q92RW4
I	-14	VAL	-	expression tag	UNP Q92RW4
I	-13	ASP	-	expression tag	UNP Q92RW4
I	-12	LEU	-	expression tag	UNP Q92RW4
I	-11	GLY	-	expression tag	UNP Q92RW4
I	-10	THR	-	expression tag	UNP Q92RW4
I	-9	GLU	-	expression tag	UNP Q92RW4
I	-8	ASN	-	expression tag	UNP Q92RW4
I	-7	LEU	-	expression tag	UNP Q92RW4
I	-6	TYR	-	expression tag	UNP Q92RW4
I	-5	PHE	-	expression tag	UNP Q92RW4
I	-4	GLN	-	expression tag	UNP Q92RW4
I	-3	SER	-	expression tag	UNP Q92RW4
I	-2	MSE	-	expression tag	UNP Q92RW4
J	-24	MSE	-	expression tag	UNP Q92RW4
J	-23	HIS	-	expression tag	UNP Q92RW4
J	-22	HIS	-	expression tag	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-21	HIS	-	expression tag	UNP Q92RW4
J	-20	HIS	-	expression tag	UNP Q92RW4
J	-19	HIS	-	expression tag	UNP Q92RW4
J	-18	HIS	-	expression tag	UNP Q92RW4
J	-17	SER	-	expression tag	UNP Q92RW4
J	-16	SER	-	expression tag	UNP Q92RW4
J	-15	GLY	-	expression tag	UNP Q92RW4
J	-14	VAL	-	expression tag	UNP Q92RW4
J	-13	ASP	-	expression tag	UNP Q92RW4
J	-12	LEU	-	expression tag	UNP Q92RW4
J	-11	GLY	-	expression tag	UNP Q92RW4
J	-10	THR	-	expression tag	UNP Q92RW4
J	-9	GLU	-	expression tag	UNP Q92RW4
J	-8	ASN	-	expression tag	UNP Q92RW4
J	-7	LEU	-	expression tag	UNP Q92RW4
J	-6	TYR	-	expression tag	UNP Q92RW4
J	-5	PHE	-	expression tag	UNP Q92RW4
J	-4	GLN	-	expression tag	UNP Q92RW4
J	-3	SER	-	expression tag	UNP Q92RW4
J	-2	MSE	-	expression tag	UNP Q92RW4
K	-24	MSE	-	expression tag	UNP Q92RW4
K	-23	HIS	-	expression tag	UNP Q92RW4
K	-22	HIS	-	expression tag	UNP Q92RW4
K	-21	HIS	-	expression tag	UNP Q92RW4
K	-20	HIS	-	expression tag	UNP Q92RW4
K	-19	HIS	-	expression tag	UNP Q92RW4
K	-18	HIS	-	expression tag	UNP Q92RW4
K	-17	SER	-	expression tag	UNP Q92RW4
K	-16	SER	-	expression tag	UNP Q92RW4
K	-15	GLY	-	expression tag	UNP Q92RW4
K	-14	VAL	-	expression tag	UNP Q92RW4
K	-13	ASP	-	expression tag	UNP Q92RW4
K	-12	LEU	-	expression tag	UNP Q92RW4
K	-11	GLY	-	expression tag	UNP Q92RW4
K	-10	THR	-	expression tag	UNP Q92RW4
K	-9	GLU	-	expression tag	UNP Q92RW4
K	-8	ASN	-	expression tag	UNP Q92RW4
K	-7	LEU	-	expression tag	UNP Q92RW4
K	-6	TYR	-	expression tag	UNP Q92RW4
K	-5	PHE	-	expression tag	UNP Q92RW4
K	-4	GLN	-	expression tag	UNP Q92RW4
K	-3	SER	-	expression tag	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	MSE	-	expression tag	UNP Q92RW4
L	-24	MSE	-	expression tag	UNP Q92RW4
L	-23	HIS	-	expression tag	UNP Q92RW4
L	-22	HIS	-	expression tag	UNP Q92RW4
L	-21	HIS	-	expression tag	UNP Q92RW4
L	-20	HIS	-	expression tag	UNP Q92RW4
L	-19	HIS	-	expression tag	UNP Q92RW4
L	-18	HIS	-	expression tag	UNP Q92RW4
L	-17	SER	-	expression tag	UNP Q92RW4
L	-16	SER	-	expression tag	UNP Q92RW4
L	-15	GLY	-	expression tag	UNP Q92RW4
L	-14	VAL	-	expression tag	UNP Q92RW4
L	-13	ASP	-	expression tag	UNP Q92RW4
L	-12	LEU	-	expression tag	UNP Q92RW4
L	-11	GLY	-	expression tag	UNP Q92RW4
L	-10	THR	-	expression tag	UNP Q92RW4
L	-9	GLU	-	expression tag	UNP Q92RW4
L	-8	ASN	-	expression tag	UNP Q92RW4
L	-7	LEU	-	expression tag	UNP Q92RW4
L	-6	TYR	-	expression tag	UNP Q92RW4
L	-5	PHE	-	expression tag	UNP Q92RW4
L	-4	GLN	-	expression tag	UNP Q92RW4
L	-3	SER	-	expression tag	UNP Q92RW4
L	-2	MSE	-	expression tag	UNP Q92RW4
M	-24	MSE	-	expression tag	UNP Q92RW4
M	-23	HIS	-	expression tag	UNP Q92RW4
M	-22	HIS	-	expression tag	UNP Q92RW4
M	-21	HIS	-	expression tag	UNP Q92RW4
M	-20	HIS	-	expression tag	UNP Q92RW4
M	-19	HIS	-	expression tag	UNP Q92RW4
M	-18	HIS	-	expression tag	UNP Q92RW4
M	-17	SER	-	expression tag	UNP Q92RW4
M	-16	SER	-	expression tag	UNP Q92RW4
M	-15	GLY	-	expression tag	UNP Q92RW4
M	-14	VAL	-	expression tag	UNP Q92RW4
M	-13	ASP	-	expression tag	UNP Q92RW4
M	-12	LEU	-	expression tag	UNP Q92RW4
M	-11	GLY	-	expression tag	UNP Q92RW4
M	-10	THR	-	expression tag	UNP Q92RW4
M	-9	GLU	-	expression tag	UNP Q92RW4
M	-8	ASN	-	expression tag	UNP Q92RW4
M	-7	LEU	-	expression tag	UNP Q92RW4

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-6	TYR	-	expression tag	UNP Q92RW4
M	-5	PHE	-	expression tag	UNP Q92RW4
M	-4	GLN	-	expression tag	UNP Q92RW4
M	-3	SER	-	expression tag	UNP Q92RW4
M	-2	MSE	-	expression tag	UNP Q92RW4
N	-24	MSE	-	expression tag	UNP Q92RW4
N	-23	HIS	-	expression tag	UNP Q92RW4
N	-22	HIS	-	expression tag	UNP Q92RW4
N	-21	HIS	-	expression tag	UNP Q92RW4
N	-20	HIS	-	expression tag	UNP Q92RW4
N	-19	HIS	-	expression tag	UNP Q92RW4
N	-18	HIS	-	expression tag	UNP Q92RW4
N	-17	SER	-	expression tag	UNP Q92RW4
N	-16	SER	-	expression tag	UNP Q92RW4
N	-15	GLY	-	expression tag	UNP Q92RW4
N	-14	VAL	-	expression tag	UNP Q92RW4
N	-13	ASP	-	expression tag	UNP Q92RW4
N	-12	LEU	-	expression tag	UNP Q92RW4
N	-11	GLY	-	expression tag	UNP Q92RW4
N	-10	THR	-	expression tag	UNP Q92RW4
N	-9	GLU	-	expression tag	UNP Q92RW4
N	-8	ASN	-	expression tag	UNP Q92RW4
N	-7	LEU	-	expression tag	UNP Q92RW4
N	-6	TYR	-	expression tag	UNP Q92RW4
N	-5	PHE	-	expression tag	UNP Q92RW4
N	-4	GLN	-	expression tag	UNP Q92RW4
N	-3	SER	-	expression tag	UNP Q92RW4
N	-2	MSE	-	expression tag	UNP Q92RW4
O	-24	MSE	-	expression tag	UNP Q92RW4
O	-23	HIS	-	expression tag	UNP Q92RW4
O	-22	HIS	-	expression tag	UNP Q92RW4
O	-21	HIS	-	expression tag	UNP Q92RW4
O	-20	HIS	-	expression tag	UNP Q92RW4
O	-19	HIS	-	expression tag	UNP Q92RW4
O	-18	HIS	-	expression tag	UNP Q92RW4
O	-17	SER	-	expression tag	UNP Q92RW4
O	-16	SER	-	expression tag	UNP Q92RW4
O	-15	GLY	-	expression tag	UNP Q92RW4
O	-14	VAL	-	expression tag	UNP Q92RW4
O	-13	ASP	-	expression tag	UNP Q92RW4
O	-12	LEU	-	expression tag	UNP Q92RW4
O	-11	GLY	-	expression tag	UNP Q92RW4

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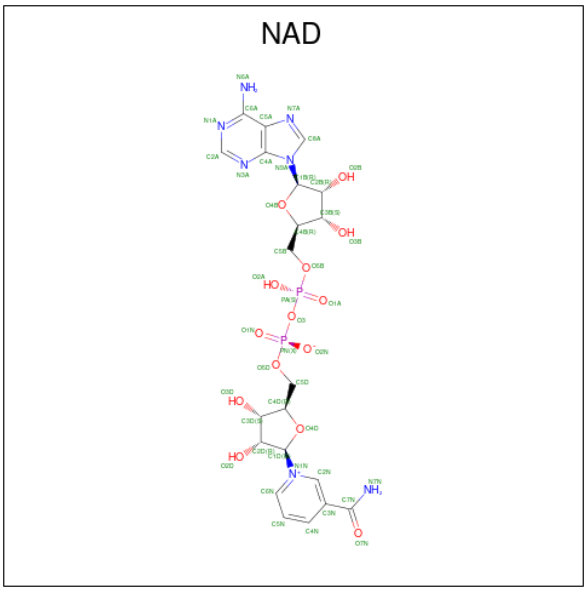
Chain	Residue	Modelled	Actual	Comment	Reference
O	-10	THR	-	expression tag	UNP Q92RW4
O	-9	GLU	-	expression tag	UNP Q92RW4
O	-8	ASN	-	expression tag	UNP Q92RW4
O	-7	LEU	-	expression tag	UNP Q92RW4
O	-6	TYR	-	expression tag	UNP Q92RW4
O	-5	PHE	-	expression tag	UNP Q92RW4
O	-4	GLN	-	expression tag	UNP Q92RW4
O	-3	SER	-	expression tag	UNP Q92RW4
O	-2	MSE	-	expression tag	UNP Q92RW4
P	-24	MSE	-	expression tag	UNP Q92RW4
P	-23	HIS	-	expression tag	UNP Q92RW4
P	-22	HIS	-	expression tag	UNP Q92RW4
P	-21	HIS	-	expression tag	UNP Q92RW4
P	-20	HIS	-	expression tag	UNP Q92RW4
P	-19	HIS	-	expression tag	UNP Q92RW4
P	-18	HIS	-	expression tag	UNP Q92RW4
P	-17	SER	-	expression tag	UNP Q92RW4
P	-16	SER	-	expression tag	UNP Q92RW4
P	-15	GLY	-	expression tag	UNP Q92RW4
P	-14	VAL	-	expression tag	UNP Q92RW4
P	-13	ASP	-	expression tag	UNP Q92RW4
P	-12	LEU	-	expression tag	UNP Q92RW4
P	-11	GLY	-	expression tag	UNP Q92RW4
P	-10	THR	-	expression tag	UNP Q92RW4
P	-9	GLU	-	expression tag	UNP Q92RW4
P	-8	ASN	-	expression tag	UNP Q92RW4
P	-7	LEU	-	expression tag	UNP Q92RW4
P	-6	TYR	-	expression tag	UNP Q92RW4
P	-5	PHE	-	expression tag	UNP Q92RW4
P	-4	GLN	-	expression tag	UNP Q92RW4
P	-3	SER	-	expression tag	UNP Q92RW4
P	-2	MSE	-	expression tag	UNP Q92RW4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	J	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	K	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	L	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	M	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	N	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	P	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	333	Total	O	0	0
			333	333		
4	B	307	Total	O	0	0
			307	307		
4	C	288	Total	O	0	0
			288	288		
4	D	223	Total	O	0	0
			223	223		
4	E	340	Total	O	0	0
			340	340		
4	F	312	Total	O	0	0
			312	312		
4	G	278	Total	O	0	0
			278	278		
4	H	260	Total	O	0	0
			260	260		
4	I	287	Total	O	0	0
			287	287		
4	J	281	Total	O	0	0
			281	281		

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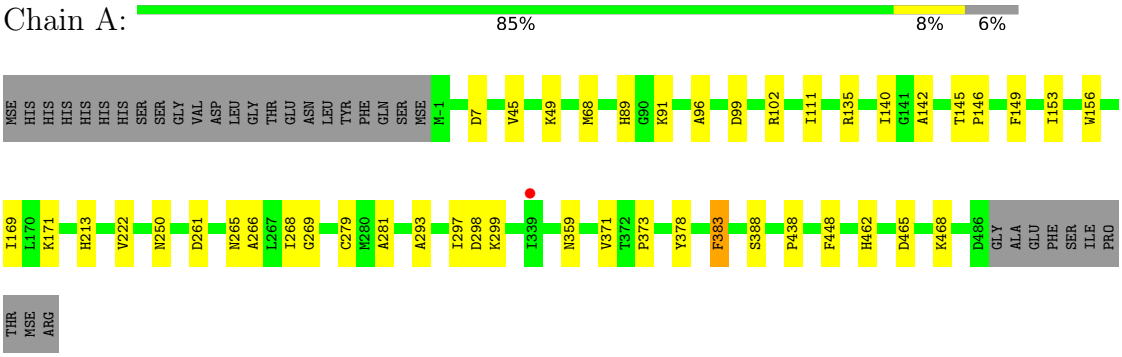
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	363	Total O 363 363	0	0
4	L	264	Total O 264 264	0	0
4	M	225	Total O 225 225	0	0
4	N	249	Total O 249 249	0	0
4	O	338	Total O 338 338	0	0
4	P	274	Total O 274 274	0	0

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.

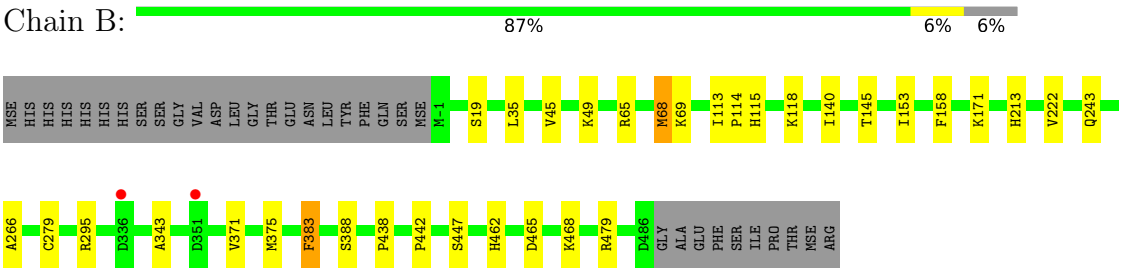
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain A:



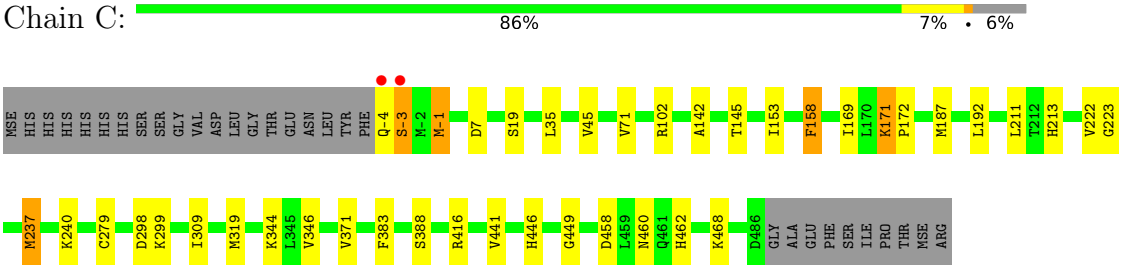
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain B:



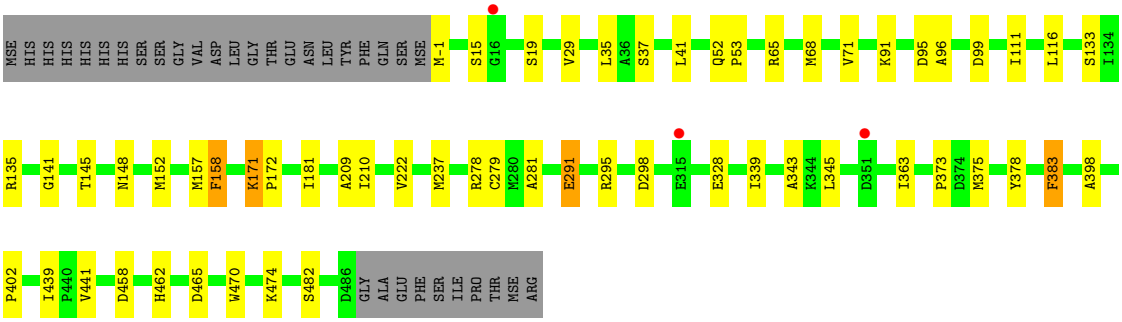
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain C:



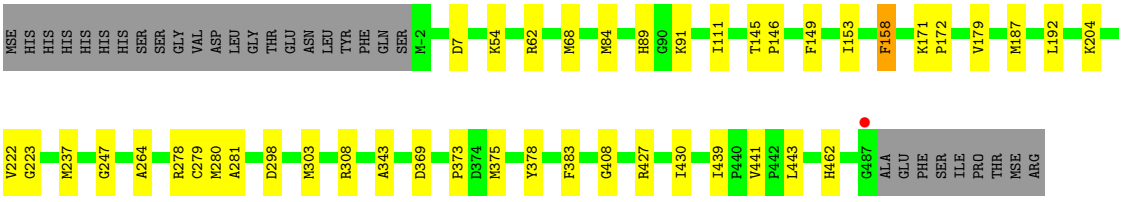
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain D:



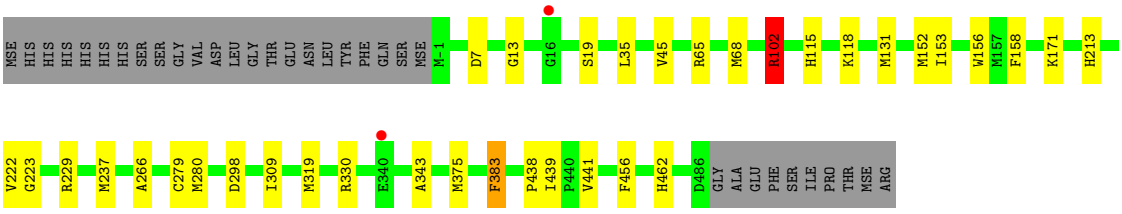
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain E:



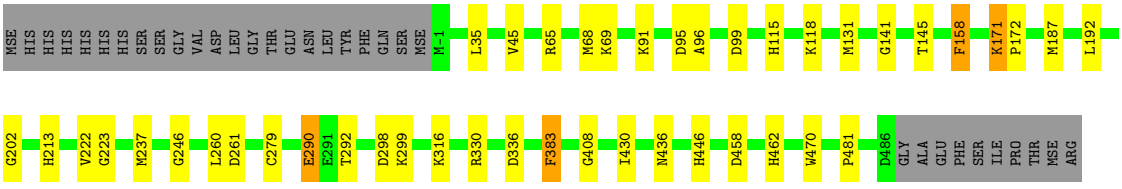
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain F:



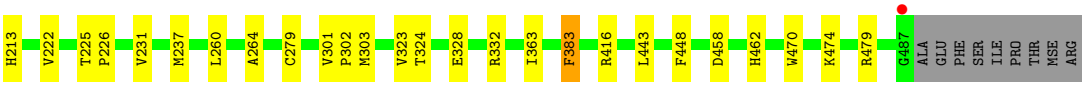
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain G:



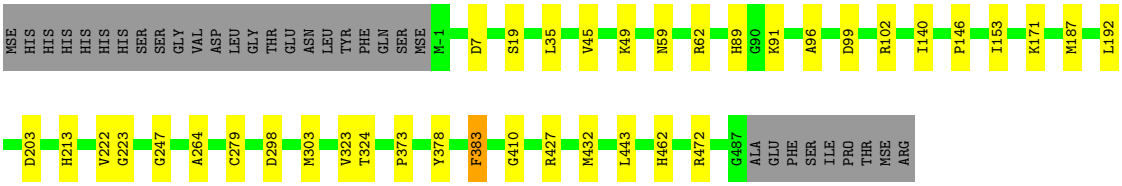
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain H:



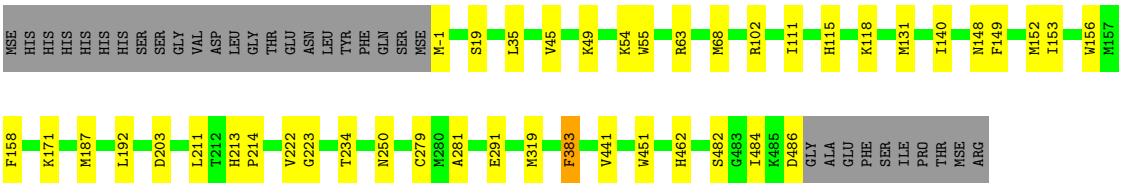
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain I:



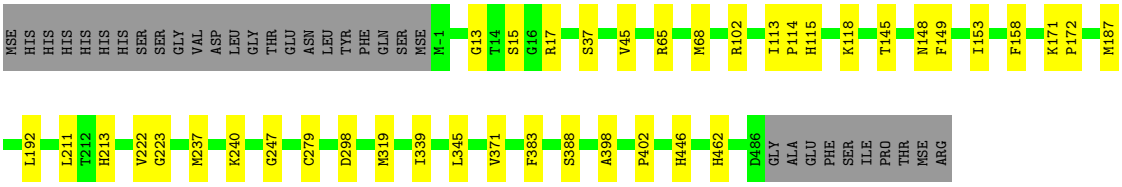
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain J:



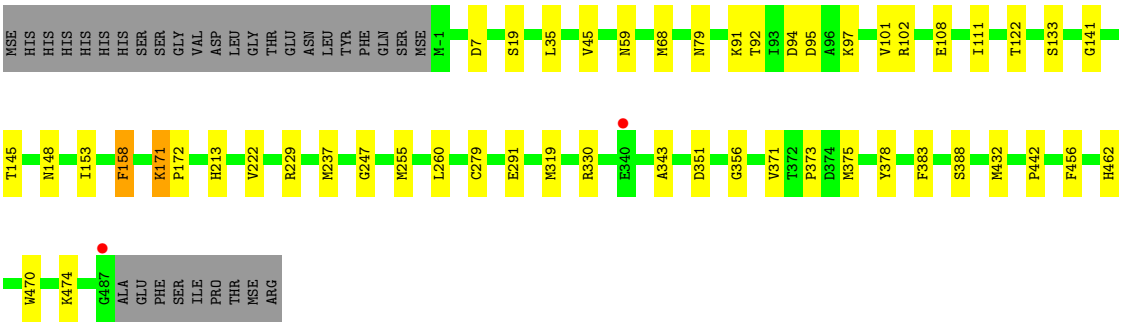
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain K:



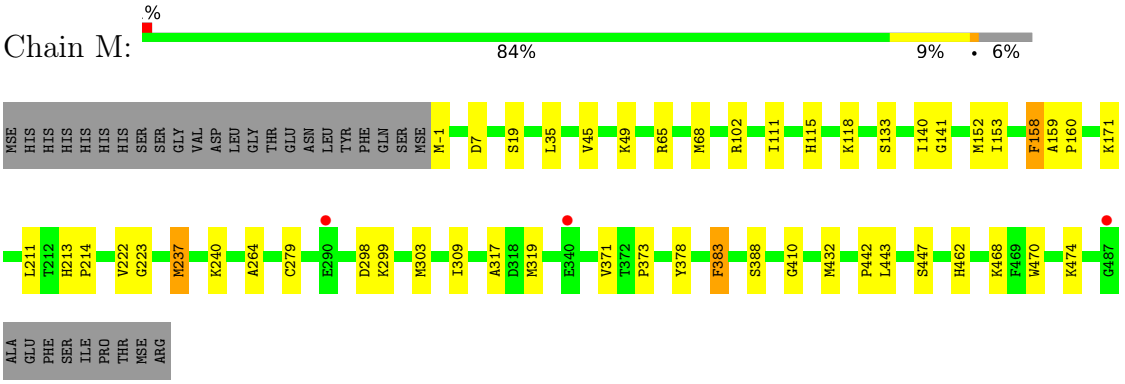
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain L:



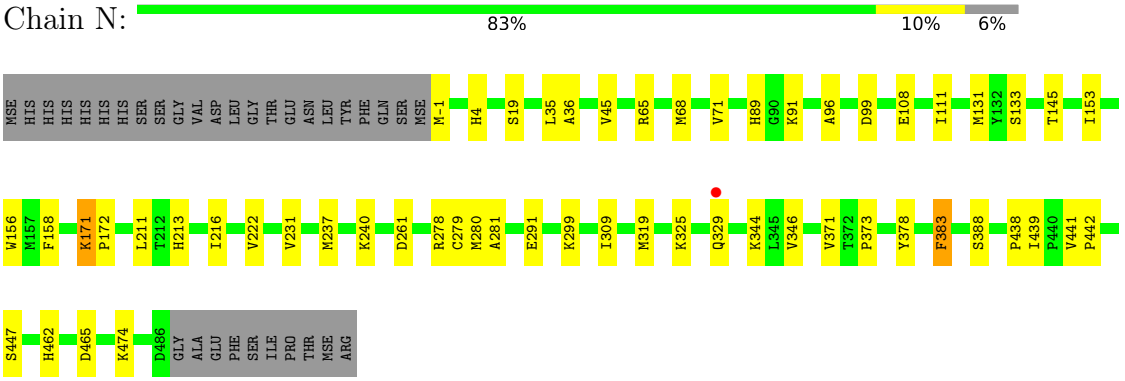
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain M:



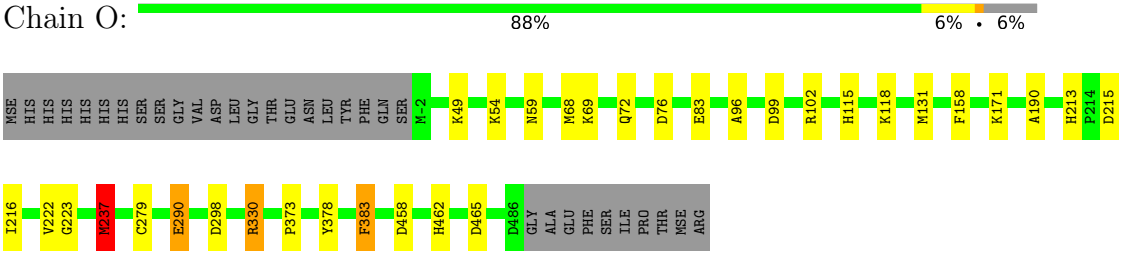
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain N:



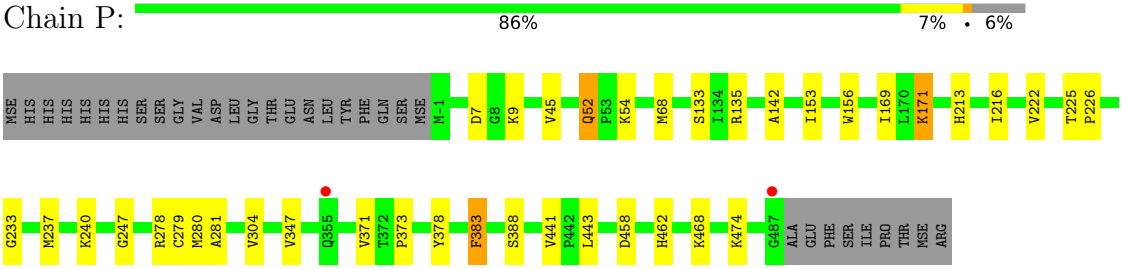
• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain O:



• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

Chain P:



• Molecule 1: Methylmalonate-semialdehyde dehydrogenase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	159.47Å 170.91Å 170.47Å 90.00° 106.33° 90.00°	Depositor
Resolution (Å)	19.99 – 2.20 46.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.99-2.20) 99.6 (46.75-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.165 , 0.209 0.164 , 0.206	Depositor DCC
R_{free} test set	22061 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	64517	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8047e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.51	0/3766	0.61	0/5076
1	B	0.48	0/3772	0.66	6/5081 (0.1%)
1	C	0.45	0/3790	0.65	6/5102 (0.1%)
1	D	0.41	0/3777	0.60	0/5091
1	E	0.51	0/3769	0.64	1/5078 (0.0%)
1	F	0.50	0/3769	0.62	1/5078 (0.0%)
1	G	0.43	0/3761	0.62	1/5068 (0.0%)
1	H	0.42	0/3757	0.58	0/5062
1	I	0.43	0/3768	0.60	0/5076
1	J	0.42	0/3753	0.61	2/5057 (0.0%)
1	K	0.49	0/3786	0.66	5/5100 (0.1%)
1	L	0.42	0/3762	0.65	6/5069 (0.1%)
1	M	0.41	0/3754	0.58	0/5058
1	N	0.41	0/3742	0.59	0/5043
1	O	0.48	2/3788 (0.1%)	0.71	13/5100 (0.3%)
1	P	0.43	0/3754	0.60	0/5058
All	All	0.45	2/60268 (0.0%)	0.63	41/81197 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	330[A]	ARG	N-CA	5.00	1.56	1.46
1	O	330[B]	ARG	N-CA	5.00	1.56	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	94[A]	ASP	CA-C-O	8.26	137.45	120.10
1	L	94[B]	ASP	CA-C-O	8.26	137.45	120.10
1	J	319	MSE	N-CA-CB	-8.18	95.87	110.60
1	O	237	MSE	CG-SE-CE	8.13	116.78	98.90
1	B	68[A]	MSE	CA-C-O	8.04	136.97	120.10
1	B	68[B]	MSE	CA-C-O	8.04	136.97	120.10
1	K	102[A]	ARG	CA-C-O	7.42	135.68	120.10
1	K	102[B]	ARG	CA-C-O	7.42	135.68	120.10
1	O	290[A]	GLU	CA-C-O	7.37	135.58	120.10
1	O	290[B]	GLU	CA-C-O	7.37	135.58	120.10
1	C	237[A]	MSE	CA-C-O	7.37	135.58	120.10
1	C	237[B]	MSE	CA-C-O	7.37	135.58	120.10
1	J	319	MSE	CG-SE-CE	7.26	114.88	98.90
1	B	68[A]	MSE	CA-C-N	-6.90	102.02	117.20
1	B	68[B]	MSE	CA-C-N	-6.90	102.02	117.20
1	L	94[A]	ASP	CA-C-N	-6.45	103.01	117.20
1	L	94[B]	ASP	CA-C-N	-6.45	103.01	117.20
1	O	68[A]	MSE	CA-C-O	6.26	133.25	120.10
1	O	68[B]	MSE	CA-C-O	6.26	133.25	120.10
1	B	68[A]	MSE	N-CA-C	6.21	127.78	111.00
1	B	68[B]	MSE	N-CA-C	6.21	127.78	111.00
1	O	68[A]	MSE	CA-C-N	-6.18	103.59	117.20
1	O	68[B]	MSE	CA-C-N	-6.18	103.59	117.20
1	K	102[A]	ARG	CA-C-N	-6.09	104.02	116.20
1	K	102[B]	ARG	CA-C-N	-6.09	104.02	116.20
1	G	237	MSE	CG-SE-CE	6.00	112.10	98.90
1	C	237[A]	MSE	CA-C-N	-5.90	104.23	117.20
1	C	237[B]	MSE	CA-C-N	-5.90	104.23	117.20
1	C	237[A]	MSE	N-CA-C	5.82	126.72	111.00
1	C	237[B]	MSE	N-CA-C	5.82	126.72	111.00
1	K	319	MSE	N-CA-CB	-5.72	100.30	110.60
1	O	290[A]	GLU	CA-C-N	-5.70	104.66	117.20
1	O	290[B]	GLU	CA-C-N	-5.70	104.66	117.20
1	L	94[A]	ASP	N-CA-C	5.63	126.20	111.00
1	L	94[B]	ASP	N-CA-C	5.63	126.20	111.00
1	O	68[A]	MSE	N-CA-C	5.62	126.17	111.00
1	O	68[B]	MSE	N-CA-C	5.62	126.17	111.00
1	F	102	ARG	CG-CD-NE	5.41	123.16	111.80
1	O	290[A]	GLU	N-CA-C	5.19	125.00	111.00
1	O	290[B]	GLU	N-CA-C	5.19	125.00	111.00
1	E	369	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	330[A]	ARG	Mainchain
1	O	330[B]	ARG	Mainchain

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	3696	0	3678	36	0
1	B	3702	0	3687	27	0
1	C	3722	0	3707	34	0
1	D	3704	0	3686	47	0
1	E	3703	0	3679	34	0
1	F	3699	0	3685	34	0
1	G	3694	0	3676	34	0
1	H	3693	0	3668	37	0
1	I	3701	0	3681	31	0
1	J	3689	0	3665	37	0
1	K	3710	0	3705	30	0
1	L	3695	0	3668	35	0
1	M	3690	0	3666	38	0
1	N	3681	0	3652	37	0
1	O	3716	0	3702	28	0
1	P	3690	0	3664	35	0
2	A	44	0	26	11	0
2	B	44	0	26	10	0
2	C	44	0	26	12	0
2	D	44	0	26	11	0
2	E	44	0	26	9	0
2	F	44	0	26	12	0
2	G	44	0	26	10	0
2	H	44	0	26	10	0
2	I	44	0	26	11	0
2	J	44	0	26	12	0
2	K	44	0	26	11	0
2	L	44	0	26	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	44	0	26	9	0
2	N	44	0	26	10	0
2	O	44	0	26	11	0
2	P	44	0	26	11	0
3	A	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	O	1	0	0	0	0
4	A	333	0	0	5	0
4	B	307	0	0	4	0
4	C	288	0	0	3	0
4	D	223	0	0	4	0
4	E	340	0	0	5	0
4	F	312	0	0	4	0
4	G	278	0	0	4	0
4	H	260	0	0	3	0
4	I	287	0	0	5	0
4	J	281	0	0	6	0
4	K	363	0	0	2	0
4	L	264	0	0	6	0
4	M	225	0	0	3	0
4	N	249	0	0	4	0
4	O	338	0	0	5	0
4	P	274	0	0	5	0
All	All	64517	0	59285	534	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 4.

All (534) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:GLU:OE1	1:D:295:ARG:HD2	1.46	1.16
1:O:237:MSE:HE3	1:P:233:GLY:HA3	1.45	0.97
1:L:279:CYS:SG	2:L:500:NAD:C3N	2.59	0.90
1:P:279:CYS:SG	2:P:500:NAD:C4N	2.60	0.90
1:P:279:CYS:SG	2:P:500:NAD:C3N	2.60	0.89
1:L:279:CYS:SG	2:L:500:NAD:C4N	2.60	0.89
1:D:279:CYS:SG	2:D:500:NAD:C3N	2.60	0.89
1:C:102:ARG:NH2	1:C:441:VAL:HG11	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:CYS:SG	2:E:500:NAD:C4N	2.63	0.86
1:C:279:CYS:SG	2:C:500:NAD:C3N	2.64	0.86
1:B:279:CYS:SG	2:B:500:NAD:C4N	2.64	0.85
1:O:279:CYS:SG	2:O:501:NAD:C3N	2.64	0.85
1:D:41:LEU:HD11	1:D:210:ILE:HG13	1.59	0.84
1:K:279:CYS:SG	2:K:500:NAD:C3N	2.65	0.84
1:E:279:CYS:SG	2:E:500:NAD:C3N	2.65	0.84
1:J:279:CYS:SG	2:J:500:NAD:C3N	2.67	0.82
1:M:279:CYS:SG	2:M:500:NAD:C3N	2.68	0.82
1:O:279:CYS:SG	2:O:501:NAD:C4N	2.68	0.82
1:G:279:CYS:SG	2:G:501:NAD:C3N	2.68	0.81
1:K:279:CYS:HB3	2:K:500:NAD:C2N	2.09	0.81
1:A:279:CYS:SG	2:A:501:NAD:C3N	2.68	0.81
1:D:279:CYS:SG	2:D:500:NAD:C4N	2.68	0.81
1:D:291:GLU:OE1	1:D:295:ARG:CD	2.28	0.81
1:D:222:VAL:CG1	2:D:500:NAD:H5N	2.11	0.80
1:C:279:CYS:SG	2:C:500:NAD:C4N	2.70	0.79
1:A:279:CYS:SG	2:A:501:NAD:C4N	2.70	0.79
1:M:279:CYS:SG	2:M:500:NAD:C4N	2.71	0.79
1:H:264:ALA:HB1	1:H:303:MSE:HE1	1.65	0.79
1:J:279:CYS:SG	2:J:500:NAD:C7N	2.71	0.78
1:A:222:VAL:HG13	2:A:501:NAD:C5N	2.14	0.78
1:G:279:CYS:SG	2:G:501:NAD:C7N	2.73	0.77
1:E:222:VAL:HG13	2:E:500:NAD:C5N	2.14	0.77
1:F:279:CYS:SG	2:F:501:NAD:C3N	2.73	0.77
1:D:52:GLN:HG3	1:D:53:PRO:HD3	1.68	0.76
1:L:356:GLY:HA3	4:L:861:HOH:O	1.84	0.76
1:M:222:VAL:HG13	2:M:500:NAD:C5N	2.15	0.76
1:L:222:VAL:HG13	2:L:500:NAD:C5N	2.15	0.76
1:K:222:VAL:HG13	2:K:500:NAD:C5N	2.16	0.76
1:N:279:CYS:SG	2:N:500:NAD:C3N	2.74	0.76
1:O:279:CYS:HB3	2:O:501:NAD:C2N	2.16	0.76
1:K:279:CYS:SG	2:K:500:NAD:C4N	2.75	0.75
1:H:279:CYS:SG	2:H:500:NAD:C4N	2.75	0.75
1:H:279:CYS:SG	2:H:500:NAD:C3N	2.75	0.74
1:H:222:VAL:HG13	2:H:500:NAD:H5N	1.68	0.74
1:G:279:CYS:SG	2:G:501:NAD:C4N	2.76	0.73
1:D:222:VAL:CG1	2:D:500:NAD:C5N	2.65	0.73
1:D:222:VAL:HG13	2:D:500:NAD:H5N	1.68	0.73
1:C:19:SER:HB2	1:C:35:LEU:HD21	1.71	0.73
1:P:279:CYS:HB3	2:P:500:NAD:C2N	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:472:ARG:HG3	1:J:451:TRP:CZ2	2.25	0.71
1:L:222:VAL:HG13	2:L:500:NAD:H5N	1.72	0.71
1:O:279:CYS:SG	2:O:501:NAD:C7N	2.80	0.70
1:I:222:VAL:HG13	2:I:501:NAD:C5N	2.21	0.70
1:J:222:VAL:HG13	2:J:500:NAD:C5N	2.22	0.70
1:F:279:CYS:SG	2:F:501:NAD:C4N	2.80	0.70
1:B:279:CYS:SG	2:B:500:NAD:C3N	2.80	0.69
1:I:279:CYS:SG	2:I:501:NAD:C3N	2.81	0.69
1:N:279:CYS:SG	2:N:500:NAD:C4N	2.80	0.69
1:M:264:ALA:HB1	1:M:303:MSE:HE1	1.75	0.69
1:K:13:GLY:HA3	4:K:821:HOH:O	1.91	0.68
1:H:222:VAL:HG13	2:H:500:NAD:C5N	2.22	0.68
1:H:222:VAL:CG1	2:H:500:NAD:C5N	2.71	0.68
1:O:222:VAL:HG13	2:O:501:NAD:H5N	1.76	0.68
1:D:52:GLN:NE2	4:D:664:HOH:O	2.21	0.68
1:J:222:VAL:HG13	2:J:500:NAD:H5N	1.75	0.68
1:M:222:VAL:HG13	2:M:500:NAD:H5N	1.75	0.68
1:C:-4:GLN:OE1	1:C:-1:MSE:HE1	1.92	0.68
1:K:446:HIS:HD2	4:L:656:HOH:O	1.76	0.68
1:I:279:CYS:SG	2:I:501:NAD:C4N	2.82	0.68
1:J:222:VAL:CG1	2:J:500:NAD:C5N	2.72	0.68
1:J:55:TRP:CZ2	1:J:63:ARG:HG2	2.29	0.67
1:J:279:CYS:SG	2:J:500:NAD:C4N	2.83	0.67
1:C:222:VAL:HG13	2:C:500:NAD:C5N	2.24	0.67
1:K:222:VAL:HG13	2:K:500:NAD:H5N	1.75	0.66
1:N:279:CYS:SG	2:N:500:NAD:C7N	2.84	0.66
1:P:279:CYS:SG	2:P:500:NAD:C7N	2.84	0.66
1:L:279:CYS:SG	2:L:500:NAD:C7N	2.84	0.66
1:I:187:MSE:HE3	1:I:192:LEU:HD22	1.78	0.66
1:J:279:CYS:HB3	2:J:500:NAD:C2N	2.26	0.65
1:E:439:ILE:HG22	1:E:441[A]:VAL:HG23	1.79	0.65
1:M:222:VAL:CG1	2:M:500:NAD:C5N	2.75	0.65
1:P:52:GLN:NE2	4:P:817:HOH:O	2.21	0.65
1:N:222:VAL:HG13	2:N:500:NAD:C5N	2.27	0.64
1:K:279:CYS:SG	2:K:500:NAD:C7N	2.85	0.64
1:O:222:VAL:HG13	2:O:501:NAD:C5N	2.27	0.64
1:C:279:CYS:SG	2:C:500:NAD:C7N	2.86	0.64
1:E:222:VAL:HG13	2:E:500:NAD:H5N	1.77	0.64
1:E:279:CYS:SG	2:E:500:NAD:C7N	2.86	0.64
1:D:19:SER:HB2	1:D:35:LEU:HD21	1.79	0.64
1:D:279:CYS:SG	2:D:500:NAD:C7N	2.85	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:SER:HB2	1:N:35:LEU:HD21	1.80	0.64
1:J:54:LYS:NZ	4:J:833:HOH:O	2.31	0.63
1:O:83:GLU:HB3	4:O:648:HOH:O	1.99	0.63
1:P:371:VAL:HG21	1:P:388:SER:HB3	1.80	0.63
1:L:222:VAL:CG1	2:L:500:NAD:C5N	2.76	0.63
1:D:222:VAL:HG12	2:D:500:NAD:C5N	2.28	0.63
1:N:325:LYS:O	1:N:329:GLN:HG2	1.99	0.62
1:M:159:ALA:HB3	1:M:160:PRO:HD3	1.81	0.62
1:G:446:HIS:HD2	4:H:686:HOH:O	1.83	0.62
1:C:-4:GLN:HG2	4:C:771:HOH:O	2.00	0.62
1:C:279:CYS:HB3	2:C:500:NAD:C2N	2.30	0.62
1:G:279:CYS:HB3	2:G:501:NAD:C2N	2.30	0.61
1:N:261:ASP:OD1	1:N:299:LYS:HE3	2.00	0.61
1:H:237:MSE:HA	1:H:237:MSE:HE3	1.81	0.61
1:E:222:VAL:CG1	2:E:500:NAD:C5N	2.79	0.61
1:F:222:VAL:HG13	2:F:501:NAD:C5N	2.31	0.61
1:J:55:TRP:CH2	1:J:63:ARG:HG2	2.34	0.61
1:C:222:VAL:HG13	2:C:500:NAD:H5N	1.82	0.61
1:B:45:VAL:HG11	1:B:213:HIS:CE1	2.36	0.60
1:A:383:PHE:CZ	2:A:501:NAD:H2D	2.37	0.60
1:M:279:CYS:SG	2:M:500:NAD:C7N	2.89	0.60
1:O:102:ARG:NH2	4:O:830:HOH:O	2.33	0.60
1:O:222:VAL:CG1	2:O:501:NAD:C5N	2.80	0.60
1:M:102:ARG:HE	1:M:152:MSE:SE	2.35	0.60
1:G:261:ASP:OD1	1:G:299:LYS:HE3	2.01	0.60
1:K:148:ASN:ND2	2:K:500:NAD:O7N	2.32	0.60
1:N:45:VAL:HG11	1:N:213:HIS:CE1	2.37	0.60
1:F:279:CYS:SG	2:F:501:NAD:C7N	2.90	0.60
1:L:171:LYS:HD2	1:L:171:LYS:C	2.21	0.60
1:A:89:HIS:CE1	1:A:91:LYS:HD3	2.37	0.59
1:I:19:SER:HB2	1:I:35:LEU:HD21	1.84	0.59
1:D:279:CYS:HB3	2:D:500:NAD:C2N	2.31	0.59
1:G:383:PHE:CE1	2:G:501:NAD:H2D	2.37	0.59
1:I:222:VAL:HG13	2:I:501:NAD:H5N	1.82	0.59
1:O:279:CYS:HG	2:O:501:NAD:C4N	2.15	0.59
1:P:222:VAL:HG13	2:P:500:NAD:C5N	2.32	0.59
1:A:146:PRO:HB2	4:A:911:HOH:O	2.03	0.59
1:I:222:VAL:CG1	2:I:501:NAD:C5N	2.81	0.58
1:F:115:HIS:HD2	1:F:118:LYS:NZ	2.01	0.58
1:A:222:VAL:HG13	2:A:501:NAD:H5N	1.84	0.58
1:H:148:ASN:HD21	2:H:500:NAD:C7N	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:LYS:HG3	1:J:140:ILE:HD11	1.85	0.58
1:B:222:VAL:HG13	2:B:500:NAD:C5N	2.33	0.58
2:B:500:NAD:H5N	4:B:839:HOH:O	2.03	0.58
1:I:279:CYS:SG	2:I:501:NAD:C7N	2.91	0.58
1:K:222:VAL:CG1	2:K:500:NAD:C5N	2.82	0.58
1:M:279:CYS:HB3	2:M:500:NAD:C2N	2.34	0.58
1:N:222:VAL:HG13	2:N:500:NAD:H5N	1.84	0.58
1:K:115:HIS:HD2	1:K:118:LYS:NZ	2.02	0.58
1:N:439:ILE:HG22	1:N:441:VAL:HG23	1.86	0.58
1:C:279:CYS:HG	2:C:500:NAD:C4N	2.17	0.58
1:G:222:VAL:HG13	2:G:501:NAD:C5N	2.34	0.57
1:I:264:ALA:HB1	1:I:303:MSE:HE1	1.87	0.57
1:L:92:THR:HG22	4:L:844:HOH:O	2.04	0.57
1:N:222:VAL:CG1	2:N:500:NAD:C5N	2.82	0.57
1:F:279:CYS:HB3	2:F:501:NAD:C2N	2.34	0.57
1:J:102:ARG:NH2	4:J:743:HOH:O	2.36	0.57
1:L:19:SER:HB2	1:L:35:LEU:HD21	1.86	0.57
1:C:446:HIS:HD2	4:D:692:HOH:O	1.87	0.57
1:D:91:LYS:HD2	1:D:95:ASP:HB3	1.87	0.57
1:P:247:GLY:HA2	2:P:500:NAD:O2D	2.05	0.57
1:D:383:PHE:CE1	2:D:500:NAD:H2D	2.39	0.57
1:I:427:ARG:HD2	4:I:748:HOH:O	2.03	0.57
1:L:148:ASN:HD21	2:L:500:NAD:H2N	1.70	0.57
1:D:383:PHE:CZ	2:D:500:NAD:H2D	2.40	0.56
1:B:115:HIS:HD2	1:B:118:LYS:NZ	2.02	0.56
1:P:222:VAL:HG13	2:P:500:NAD:H5N	1.86	0.56
1:C:222:VAL:CG1	2:C:500:NAD:C5N	2.83	0.56
1:D:41:LEU:HD13	1:D:209:ALA:HB3	1.88	0.56
1:D:116:LEU:O	1:D:135:ARG:NH2	2.38	0.56
1:I:323:VAL:HG13	1:I:324:THR:HG23	1.86	0.56
1:D:148:ASN:ND2	2:D:500:NAD:O7N	2.39	0.56
1:N:279:CYS:HB3	2:N:500:NAD:C2N	2.36	0.56
1:K:237:MSE:HE2	1:L:237:MSE:HG3	1.86	0.56
1:O:383:PHE:CE1	2:O:501:NAD:H2D	2.41	0.56
1:P:222:VAL:CG1	2:P:500:NAD:C5N	2.83	0.56
1:G:45:VAL:HG11	1:G:213:HIS:CE1	2.41	0.56
1:H:279:CYS:HB3	2:H:500:NAD:C2N	2.34	0.56
1:H:328:GLU:O	1:H:332:ARG:HG3	2.06	0.56
1:B:279:CYS:HB3	2:B:500:NAD:C2N	2.36	0.56
1:I:472:ARG:HG3	1:J:451:TRP:CE2	2.40	0.56
1:P:54:LYS:HG2	4:P:709:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:299:LYS:O	1:M:303:MSE:HE2	2.05	0.56
1:O:237:MSE:HE2	4:O:793:HOH:O	2.05	0.55
1:D:15:SER:HB3	1:D:37:SER:HB3	1.88	0.55
1:O:69:LYS:HG2	1:O:190:ALA:HA	1.88	0.55
1:G:222:VAL:HG13	2:G:501:NAD:H5N	1.89	0.55
1:I:223:GLY:O	2:I:501:NAD:H1D	2.06	0.55
1:A:279:CYS:SG	2:A:501:NAD:C7N	2.95	0.55
1:A:383:PHE:CE1	2:A:501:NAD:H2D	2.41	0.54
1:C:187:MSE:HE3	1:C:192:LEU:HD22	1.88	0.54
1:J:115:HIS:HD2	1:J:118:LYS:NZ	2.04	0.54
1:A:279:CYS:HB3	2:A:501:NAD:C2N	2.37	0.54
1:F:222:VAL:HG13	2:F:501:NAD:H5N	1.89	0.54
1:L:91:LYS:HD3	1:L:95:ASP:HB3	1.89	0.54
1:D:439:ILE:HG22	1:D:441[A]:VAL:HG23	1.89	0.54
1:H:279:CYS:SG	2:H:500:NAD:C7N	2.96	0.54
1:N:171:LYS:HD2	1:N:171:LYS:C	2.28	0.54
1:P:171:LYS:HD2	1:P:171:LYS:C	2.27	0.54
1:D:41:LEU:HD13	1:D:209:ALA:CB	2.38	0.53
1:A:465:ASP:OD1	1:B:468:LYS:HE2	2.08	0.53
1:E:427:ARG:HD2	4:E:799:HOH:O	2.07	0.53
1:L:279:CYS:HB3	2:L:500:NAD:C2N	2.38	0.53
1:J:19:SER:HB2	1:J:35:LEU:HD21	1.91	0.53
1:M:65:ARG:HA	1:M:68:MSE:HE3	1.91	0.53
1:K:115:HIS:HD2	1:K:118:LYS:HZ1	1.57	0.53
1:C:171:LYS:CE	1:C:172:PRO:O	2.57	0.52
1:F:222:VAL:CG1	2:F:501:NAD:C5N	2.87	0.52
2:N:500:NAD:H5N	4:N:785:HOH:O	2.09	0.52
1:K:247:GLY:HA2	2:K:500:NAD:O2D	2.09	0.52
1:D:65:ARG:HA	1:D:68:MSE:HE3	1.91	0.52
1:G:222:VAL:CG1	2:G:501:NAD:C5N	2.88	0.52
1:M:309:ILE:HG12	1:M:319:MSE:HE2	1.90	0.52
1:C:45:VAL:HG11	1:C:213:HIS:CE1	2.45	0.52
1:K:45:VAL:HG11	1:K:213:HIS:CE1	2.45	0.52
1:N:237:MSE:HE3	1:N:237:MSE:HA	1.92	0.52
1:C:171:LYS:NZ	2:C:500:NAD:O2B	2.43	0.52
1:C:211:LEU:O	1:C:240:LYS:HE2	2.10	0.52
1:C:468:LYS:HE3	1:D:465:ASP:OD1	2.09	0.52
1:G:330:ARG:HD3	4:G:807:HOH:O	2.10	0.52
1:B:266:ALA:HB1	1:B:438:PRO:HB3	1.90	0.52
1:N:211:LEU:HD21	1:N:231:VAL:HG13	1.91	0.52
1:E:62:ARG:HG2	4:E:837:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:62:ARG:HD2	4:I:785:HOH:O	2.09	0.51
1:P:45:VAL:HG11	1:P:213:HIS:CE1	2.45	0.51
1:A:102:ARG:HD2	4:A:708:HOH:O	2.10	0.51
1:G:260:LEU:HD21	1:G:292:THR:HG23	1.92	0.51
2:C:500:NAD:C5N	4:C:656:HOH:O	2.58	0.51
1:L:371:VAL:HG21	1:L:388:SER:HB3	1.92	0.51
1:N:89:HIS:CE1	1:N:91:LYS:HD3	2.46	0.51
1:H:148:ASN:ND2	2:H:500:NAD:O7N	2.43	0.51
1:I:49:LYS:HG3	1:I:140:ILE:HD11	1.93	0.51
1:I:102:ARG:NH2	4:I:880:HOH:O	2.43	0.50
1:M:237:MSE:HA	1:M:237:MSE:HE3	1.94	0.50
1:N:153:ILE:O	1:N:156:TRP:HB2	2.11	0.50
1:J:115:HIS:HD2	1:J:118:LYS:HZ1	1.60	0.50
2:A:501:NAD:C5N	4:A:861:HOH:O	2.59	0.50
1:J:149:PHE:HB2	1:J:153:ILE:HD12	1.93	0.50
1:E:89:HIS:CE1	1:E:91:LYS:HD3	2.46	0.50
1:F:383:PHE:CE1	2:F:501:NAD:H2D	2.46	0.50
1:E:237:MSE:HG3	1:F:237:MSE:HE2	1.93	0.50
1:M:317:ALA:HB3	4:M:824:HOH:O	2.12	0.50
1:B:383:PHE:CE1	2:B:500:NAD:H2D	2.47	0.50
1:L:343:ALA:HB2	1:L:375:MSE:SE	2.62	0.50
1:A:222:VAL:CG1	2:A:501:NAD:C5N	2.88	0.50
1:D:181:ILE:HG13	4:D:620:HOH:O	2.12	0.50
1:E:264:ALA:HB1	1:E:303:MSE:HE1	1.92	0.50
1:M:115:HIS:HE1	4:M:738:HOH:O	1.94	0.50
1:M:383:PHE:CE1	2:M:500:NAD:H2D	2.47	0.50
1:E:278:ARG:HB2	1:E:281:ALA:HB2	1.94	0.50
1:G:115:HIS:HD2	1:G:118:LYS:NZ	2.10	0.50
1:K:211:LEU:O	1:K:240:LYS:HE2	2.12	0.50
1:L:108:GLU:HA	1:L:111:ILE:HD12	1.93	0.50
1:L:247:GLY:HA2	2:L:500:NAD:O2D	2.11	0.50
1:C:158:PHE:CD1	1:C:158:PHE:C	2.86	0.49
1:K:223:GLY:O	2:K:500:NAD:H1D	2.12	0.49
1:H:328:GLU:HG3	1:H:363:ILE:HD11	1.93	0.49
1:A:371:VAL:HG21	1:A:388:SER:HB3	1.94	0.49
1:F:45:VAL:HG11	1:F:213:HIS:CE1	2.47	0.49
1:M:115:HIS:HD2	1:M:118:LYS:NZ	2.10	0.49
1:A:261:ASP:OD1	1:A:299:LYS:HE3	2.11	0.49
1:E:145:THR:HG22	1:E:153:ILE:HG22	1.93	0.49
1:M:141:GLY:HA3	1:M:470:TRP:HZ3	1.77	0.49
1:N:344:LYS:HD2	1:N:346:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:237:MSE:CE	1:P:233:GLY:HA3	2.30	0.49
2:C:500:NAD:H5N	4:C:656:HOH:O	2.12	0.49
1:I:45:VAL:HG11	1:I:213:HIS:CE1	2.47	0.49
1:N:309:ILE:HG12	1:N:319:MSE:HE2	1.94	0.49
1:N:280:MSE:HG3	1:N:441:VAL:HG22	1.95	0.49
1:D:-1:MSE:HE1	1:D:29:VAL:O	2.13	0.49
1:L:79:ASN:HD22	1:L:97:LYS:HE2	1.78	0.49
1:E:408:GLY:HA2	1:E:430:ILE:HG12	1.95	0.48
1:E:247:GLY:HA2	2:E:500:NAD:O2D	2.14	0.48
1:F:102:ARG:HG2	1:F:102:ARG:HH11	1.77	0.48
1:I:279:CYS:HB3	2:I:501:NAD:C2N	2.43	0.48
1:E:149:PHE:HB2	1:E:153:ILE:HD12	1.94	0.48
1:F:102:ARG:CZ	1:F:152:MSE:SE	3.11	0.48
1:O:115:HIS:HD2	1:O:118:LYS:NZ	2.11	0.48
1:E:308:ARG:HD2	4:E:823:HOH:O	2.14	0.48
1:J:223:GLY:O	2:J:500:NAD:H6N	2.14	0.48
1:N:65:ARG:HA	1:N:68:MSE:HE3	1.96	0.48
1:K:446:HIS:HE1	1:L:122:THR:OG1	1.95	0.48
1:O:373:PRO:HA	1:O:378:TYR:CD2	2.49	0.48
1:F:153:ILE:O	1:F:156:TRP:HB2	2.14	0.48
1:N:216:ILE:O	1:N:240:LYS:HE3	2.14	0.48
1:E:237:MSE:CG	1:F:237:MSE:HE2	2.44	0.48
1:D:171:LYS:HD2	1:D:171:LYS:C	2.35	0.47
1:M:211:LEU:O	1:M:240:LYS:HE2	2.14	0.47
1:P:373:PRO:HA	1:P:378:TYR:CD2	2.49	0.47
1:D:343:ALA:HB2	1:D:375:MSE:SE	2.65	0.47
1:F:266:ALA:HB1	1:F:438:PRO:HB3	1.97	0.47
1:H:323:VAL:HG13	1:H:324:THR:HG23	1.96	0.47
1:K:149:PHE:HB2	1:K:153:ILE:HD12	1.96	0.47
1:F:102:ARG:HB3	1:F:152:MSE:SE	2.65	0.47
1:P:216:ILE:O	1:P:240:LYS:HE3	2.14	0.47
1:A:468:LYS:HE2	1:B:465:ASP:OD1	2.14	0.47
1:G:408:GLY:HA2	1:G:430:ILE:HG12	1.95	0.47
2:G:501:NAD:C5N	4:G:829:HOH:O	2.62	0.47
1:N:96:ALA:O	1:N:99:ASP:HB3	2.14	0.47
1:P:279:CYS:HG	2:P:500:NAD:C4N	2.26	0.47
1:B:343:ALA:HB2	1:B:375:MSE:SE	2.64	0.47
1:B:479:ARG:HD3	4:B:806:HOH:O	2.15	0.47
1:D:157:MSE:CE	1:D:222:VAL:HG23	2.44	0.47
1:E:223:GLY:O	2:E:500:NAD:H1D	2.15	0.47
2:F:501:NAD:C5N	4:F:848:HOH:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:MSE:HG3	1:H:111:ILE:HD13	1.97	0.47
1:O:96:ALA:O	1:O:99:ASP:HB3	2.15	0.47
2:B:500:NAD:C5N	4:B:839:HOH:O	2.62	0.47
1:K:187:MSE:HE3	1:K:192:LEU:HD22	1.97	0.47
2:A:501:NAD:H5N	4:A:861:HOH:O	2.13	0.47
1:N:4:HIS:CE1	1:N:36:ALA:HB2	2.50	0.47
1:P:142:ALA:HA	1:P:169:ILE:O	2.15	0.47
1:B:49:LYS:HG3	1:B:140:ILE:HD11	1.97	0.46
1:C:309:ILE:HG12	1:C:319:MSE:HE2	1.96	0.46
1:C:416[B]:ARG:NH1	1:D:482:SER:O	2.44	0.46
1:H:225:THR:HB	1:H:226:PRO:HD3	1.97	0.46
1:G:458:ASP:OD1	1:H:458:ASP:OD1	2.33	0.46
1:J:211:LEU:HD13	1:J:234:THR:HB	1.98	0.46
1:A:293:ALA:O	1:A:297:ILE:HG12	2.15	0.46
1:D:157:MSE:HE3	1:D:222:VAL:HG23	1.98	0.46
1:M:141:GLY:HA3	1:M:470:TRP:CZ3	2.50	0.46
2:N:500:NAD:C5N	4:N:785:HOH:O	2.64	0.46
1:H:149:PHE:HB2	1:H:153:ILE:HD12	1.98	0.46
1:B:19:SER:HB2	1:B:35:LEU:HD21	1.97	0.46
1:E:204:LYS:HE2	4:E:833:HOH:O	2.15	0.46
1:H:301:VAL:HB	1:H:302:PRO:HD3	1.98	0.46
1:J:187:MSE:HE3	1:J:192:LEU:HD22	1.97	0.46
1:L:373:PRO:HA	1:L:378:TYR:CD2	2.50	0.46
1:E:279:CYS:HB3	2:E:500:NAD:C2N	2.46	0.46
1:D:133:SER:HA	1:D:474:LYS:O	2.15	0.46
1:K:398:ALA:O	1:K:402:PRO:HD2	2.16	0.46
1:A:373:PRO:HA	1:A:378:TYR:CD2	2.51	0.46
1:B:222:VAL:CG1	2:B:500:NAD:C5N	2.93	0.46
1:F:68[B]:MSE:HB3	1:F:68[B]:MSE:HE2	1.75	0.46
1:G:223:GLY:O	1:G:246:GLY:HA2	2.16	0.46
1:A:265:ASN:O	1:A:268:ILE:HG22	2.16	0.45
1:A:268:ILE:HG23	1:A:269:GLY:N	2.31	0.45
1:B:383:PHE:CZ	2:B:500:NAD:H2D	2.51	0.45
1:L:145:THR:OG1	1:L:172:PRO:HA	2.16	0.45
1:H:211:LEU:HD21	1:H:231:VAL:HG13	1.98	0.45
1:O:223:GLY:O	2:O:501:NAD:H1D	2.16	0.45
1:D:96:ALA:O	1:D:99:ASP:HB3	2.17	0.45
1:A:49:LYS:HG3	1:A:140:ILE:HD11	1.98	0.45
1:J:45:VAL:HG11	1:J:213:HIS:CE1	2.52	0.45
1:L:45:VAL:HG11	1:L:213:HIS:CE1	2.51	0.45
1:N:442:PRO:HG2	1:N:447:SER:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:THR:HG22	1:C:153:ILE:HG22	1.99	0.45
1:E:237:MSE:HE2	1:F:237:MSE:HG3	1.97	0.45
1:G:187:MSE:HE3	1:G:192:LEU:HD22	1.98	0.45
1:I:373:PRO:HA	1:I:378:TYR:CD2	2.52	0.45
1:A:146:PRO:HG3	1:A:222:VAL:HG12	1.99	0.45
1:F:330[B]:ARG:NE	4:F:825:HOH:O	2.50	0.45
1:P:225:THR:HB	1:P:226:PRO:HD3	1.98	0.45
1:M:410:GLY:HA2	1:M:432:MSE:O	2.17	0.45
1:K:145:THR:OG1	1:K:172:PRO:HA	2.17	0.45
1:P:383:PHE:CE1	2:P:500:NAD:H2D	2.51	0.45
1:A:68[A]:MSE:HG3	1:A:111:ILE:HD13	1.99	0.44
1:H:141:GLY:HA3	1:H:470:TRP:HZ3	1.82	0.44
1:J:441:VAL:CG1	4:J:879:HOH:O	2.64	0.44
1:O:54:LYS:HB2	4:O:651:HOH:O	2.17	0.44
1:C:371:VAL:HG21	1:C:388:SER:HB3	1.98	0.44
1:J:203:ASP:HB2	4:J:808:HOH:O	2.16	0.44
1:J:383:PHE:CE1	2:J:500:NAD:H2D	2.53	0.44
1:P:9:LYS:HE2	4:P:791:HOH:O	2.17	0.44
1:C:102:ARG:HH22	1:C:441:VAL:HG11	1.76	0.44
1:I:247:GLY:HA2	2:I:501:NAD:O2D	2.17	0.44
1:M:68:MSE:HG3	1:M:111:ILE:HD13	1.99	0.44
1:G:141:GLY:HA3	1:G:470:TRP:HZ3	1.81	0.44
1:A:448:PHE:CD1	1:A:448:PHE:C	2.90	0.44
1:F:280:MSE:HG3	1:F:441:VAL:HG12	2.00	0.44
1:H:237:MSE:CE	4:H:676:HOH:O	2.65	0.44
1:K:15:SER:HB3	1:K:37:SER:HB3	1.99	0.44
1:L:158:PHE:CD1	1:L:158:PHE:C	2.90	0.44
1:A:135:ARG:HD3	4:A:812:HOH:O	2.18	0.44
1:B:371:VAL:HG21	1:B:388:SER:HB3	1.98	0.44
1:H:448:PHE:CD1	1:H:448:PHE:C	2.90	0.44
1:B:65:ARG:HA	1:B:68[A]:MSE:HE3	2.00	0.44
1:M:158:PHE:CD1	1:M:158:PHE:C	2.91	0.44
2:F:501:NAD:H5N	4:F:848:HOH:O	2.17	0.44
1:G:171:LYS:HD2	1:G:171:LYS:C	2.38	0.44
1:I:203:ASP:HB2	4:I:705:HOH:O	2.17	0.44
1:O:131:MSE:SE	1:P:443:LEU:H	2.50	0.44
1:P:153:ILE:HD13	1:P:222:VAL:HG11	2.00	0.44
1:B:279:CYS:SG	2:B:500:NAD:C7N	3.06	0.43
1:F:68[B]:MSE:HE1	1:H:71:VAL:HG11	2.00	0.43
1:I:383:PHE:CE1	2:I:501:NAD:H2D	2.53	0.43
1:H:133:SER:HA	1:H:474:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:MSE:HE2	1:J:111:ILE:HG23	1.99	0.43
1:J:148:ASN:ND2	2:J:500:NAD:O7N	2.45	0.43
1:K:371:VAL:HG21	1:K:388:SER:HB3	2.00	0.43
1:L:141:GLY:HA3	1:L:470:TRP:HZ3	1.83	0.43
1:M:153:ILE:HD13	1:M:222:VAL:HG11	2.01	0.43
1:M:373:PRO:HA	1:M:378:TYR:CD2	2.53	0.43
1:P:304:VAL:HG12	1:P:347:VAL:HG11	2.00	0.43
1:H:181:ILE:HG13	4:H:634:HOH:O	2.17	0.43
1:N:371:VAL:HG21	1:N:388:SER:HB3	2.00	0.43
1:N:438:PRO:HD2	4:N:655:HOH:O	2.18	0.43
1:O:213:HIS:HB3	1:O:216:ILE:HD12	2.00	0.43
1:D:145:THR:OG1	1:D:172:PRO:HA	2.18	0.43
1:K:279:CYS:SG	2:K:500:NAD:N7N	2.91	0.43
1:L:133:SER:HA	1:L:474:LYS:O	2.18	0.43
1:C:446:HIS:CD2	4:D:692:HOH:O	2.67	0.43
1:F:309:ILE:HG12	1:F:319:MSE:HE2	2.00	0.43
1:G:91:LYS:HD3	1:G:95:ASP:HB3	2.01	0.43
1:K:339:ILE:HD11	1:K:345:LEU:HD22	2.01	0.43
1:D:68:MSE:HG3	1:D:111:ILE:HD13	2.01	0.43
1:H:45:VAL:HG11	1:H:213:HIS:CE1	2.53	0.43
1:K:446:HIS:CD2	4:L:656:HOH:O	2.61	0.43
1:L:102:ARG:NH2	4:L:845:HOH:O	2.52	0.43
1:O:237:MSE:HG3	1:P:237:MSE:HE2	1.99	0.43
1:A:149:PHE:HB2	1:A:153:ILE:HD12	2.01	0.43
1:B:145:THR:HG22	1:B:153:ILE:HG22	2.01	0.43
1:D:398:ALA:O	1:D:402:PRO:HD2	2.19	0.43
1:G:446:HIS:HE1	1:H:122:THR:OG1	2.01	0.43
2:J:500:NAD:C5N	4:J:638:HOH:O	2.66	0.43
1:N:108:GLU:HA	1:N:111:ILE:HD12	2.00	0.43
1:P:280:MSE:HG3	1:P:441:VAL:HG22	2.00	0.43
1:A:153:ILE:O	1:A:156:TRP:HB2	2.18	0.43
1:B:113:ILE:N	1:B:114:PRO:CD	2.82	0.43
1:G:481:PRO:HG2	1:H:416:ARG:HG2	2.01	0.43
1:L:432:MSE:SE	1:L:442:PRO:HD3	2.69	0.43
1:O:131:MSE:HE1	1:P:443:LEU:HG	2.01	0.43
1:F:229:ARG:HG2	1:F:456:PHE:CZ	2.54	0.42
1:G:131:MSE:SE	1:H:443:LEU:H	2.52	0.42
1:O:49:LYS:NZ	1:O:215:ASP:OD2	2.52	0.42
1:A:68[B]:MSE:HE2	1:A:68[B]:MSE:HB3	1.83	0.42
1:E:158:PHE:CD1	1:E:158:PHE:C	2.93	0.42
1:I:223:GLY:O	2:I:501:NAD:H6N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:MSE:HG3	1:E:441[A]:VAL:HG22	2.01	0.42
1:H:141:GLY:HA3	1:H:470:TRP:CZ3	2.55	0.42
1:C:237[B]:MSE:HE1	1:D:237:MSE:HG3	2.02	0.42
1:G:141:GLY:HA3	1:G:470:TRP:CZ3	2.54	0.42
1:L:68[A]:MSE:HE2	1:L:68[A]:MSE:HB3	1.93	0.42
1:J:213:HIS:HA	1:J:214:PRO:HD3	1.90	0.42
1:M:223:GLY:O	2:M:500:NAD:H1D	2.20	0.42
1:H:383:PHE:CE1	2:H:500:NAD:H2D	2.54	0.42
1:L:330:ARG:HD3	4:L:798:HOH:O	2.18	0.42
1:M:45:VAL:HG11	1:M:213:HIS:CE1	2.54	0.42
1:M:213:HIS:HA	1:M:214:PRO:HD3	1.84	0.42
1:M:468:LYS:HE2	1:N:465:ASP:OD1	2.20	0.42
1:A:68[B]:MSE:HE1	1:C:71:VAL:HG11	2.00	0.42
1:F:19:SER:HB2	1:F:35:LEU:HD21	2.01	0.42
1:H:19:SER:HB2	1:H:35:LEU:HD21	2.00	0.42
1:J:49:LYS:HG3	1:J:140:ILE:CD1	2.48	0.42
1:A:268:ILE:CG2	1:A:269:GLY:N	2.83	0.42
1:B:243:GLN:HG3	1:B:243:GLN:O	2.19	0.42
1:G:96:ALA:O	1:G:99:ASP:HB3	2.20	0.42
1:L:97:LYS:O	1:L:101:VAL:HG23	2.19	0.42
1:M:19:SER:HB2	1:M:35:LEU:HD21	2.02	0.42
2:O:501:NAD:C5N	4:O:851:HOH:O	2.68	0.42
1:E:443:LEU:HG	1:F:131:MSE:HE1	2.01	0.42
1:G:290:GLU:HG2	4:G:722:HOH:O	2.20	0.42
1:I:89:HIS:ND1	1:I:91:LYS:HG2	2.35	0.42
1:N:71:VAL:HG11	1:P:68[A]:MSE:HE1	2.01	0.42
1:A:266:ALA:HB1	1:A:438:PRO:HB3	2.02	0.42
1:C:344:LYS:HD2	1:C:346:VAL:CG1	2.50	0.42
1:D:158:PHE:CD1	1:D:158:PHE:C	2.93	0.42
1:B:68[B]:MSE:HE1	1:D:71:VAL:HG11	2.01	0.41
1:D:141:GLY:HA3	1:D:470:TRP:CZ3	2.55	0.41
1:F:280:MSE:HE2	1:F:441:VAL:HG12	2.00	0.41
1:G:158:PHE:CD1	1:G:158:PHE:C	2.93	0.41
1:J:250:ASN:HB2	1:J:281:ALA:O	2.20	0.41
1:M:371:VAL:HG21	1:M:388:SER:HB3	2.02	0.41
1:N:373:PRO:HA	1:N:378:TYR:CD2	2.55	0.41
1:A:145:THR:HG22	1:A:153:ILE:HG22	2.02	0.41
1:I:443:LEU:HG	1:J:131:MSE:HE1	2.01	0.41
1:K:65:ARG:HA	1:K:68:MSE:HE3	2.03	0.41
1:O:72:GLN:NE2	1:O:76:ASP:OD1	2.53	0.41
1:P:135:ARG:HD3	4:P:714:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ASP:O	1:D:152:MSE:HB2	2.20	0.41
1:E:146:PRO:HG3	1:E:222:VAL:HG12	2.01	0.41
1:L:79:ASN:ND2	1:L:97:LYS:HE2	2.35	0.41
1:M:115:HIS:CE1	4:M:738:HOH:O	2.71	0.41
1:P:133:SER:HA	1:P:474:LYS:O	2.20	0.41
1:E:84:MSE:HG3	1:E:179:VAL:HG23	2.02	0.41
1:E:373:PRO:HA	1:E:378:TYR:CD2	2.54	0.41
1:F:383:PHE:CZ	2:F:501:NAD:H2D	2.55	0.41
1:G:436:ASN:HB2	1:H:479:ARG:O	2.20	0.41
1:I:96:ALA:O	1:I:99:ASP:HB3	2.20	0.41
1:K:17:ARG:HD3	4:K:896:HOH:O	2.20	0.41
1:C:449:GLY:HA3	1:C:460:ASN:ND2	2.36	0.41
1:E:343:ALA:HB2	1:E:375:MSE:SE	2.70	0.41
1:F:439:ILE:HG22	1:F:441:VAL:HG13	2.03	0.41
1:J:149:PHE:CG	1:J:152:MSE:HE2	2.55	0.41
1:M:443:LEU:HG	1:N:131:MSE:HE1	2.02	0.41
1:J:482:SER:OG	1:J:486:ASP:OD2	2.31	0.41
1:J:484:ILE:HD12	1:L:255:MSE:HE3	2.02	0.41
1:M:49:LYS:HG3	1:M:140:ILE:HD11	2.01	0.41
1:O:458:ASP:OD1	1:P:458:ASP:OD1	2.37	0.41
1:A:96:ALA:O	1:A:99:ASP:HB3	2.21	0.41
1:C:171:LYS:HE3	1:C:172:PRO:O	2.19	0.41
1:F:65:ARG:HA	1:F:68[A]:MSE:HE3	2.01	0.41
1:G:145:THR:OG1	1:G:172:PRO:HA	2.21	0.41
1:J:153:ILE:O	1:J:156:TRP:HB2	2.21	0.41
1:A:45:VAL:HG11	1:A:213:HIS:CE1	2.56	0.41
1:B:442:PRO:HG2	1:B:447:SER:O	2.21	0.41
1:E:187:MSE:HE3	1:E:192:LEU:HD22	2.03	0.41
1:J:223:GLY:O	2:J:500:NAD:H1D	2.20	0.41
1:N:-1:MSE:N	4:N:752:HOH:O	2.53	0.41
1:P:153:ILE:O	1:P:156:TRP:HB2	2.19	0.41
1:A:250:ASN:HB2	1:A:281:ALA:O	2.21	0.41
1:C:142:ALA:HA	1:C:169:ILE:O	2.21	0.41
1:C:223:GLY:O	2:C:500:NAD:H1D	2.20	0.41
1:D:373:PRO:HA	1:D:378:TYR:CD2	2.56	0.41
1:F:343:ALA:HB2	1:F:375:MSE:SE	2.70	0.41
1:O:465:ASP:OD1	1:P:468:LYS:HE2	2.21	0.41
1:P:278:ARG:HB2	1:P:281:ALA:HB2	2.02	0.41
2:P:500:NAD:C5N	4:P:815:HOH:O	2.68	0.41
1:B:69:LYS:HD2	1:B:69:LYS:HA	1.83	0.41
1:F:13:GLY:HA3	4:F:762:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:264:ALA:HB1	1:H:303:MSE:CE	2.44	0.41
1:D:278:ARG:HB2	1:D:281:ALA:HB2	2.03	0.40
1:G:65:ARG:HA	1:G:68:MSE:HE3	2.03	0.40
1:I:146:PRO:HB2	4:I:864:HOH:O	2.21	0.40
1:I:264:ALA:HB1	1:I:303:MSE:CE	2.49	0.40
1:K:113:ILE:CG2	1:K:114:PRO:HD3	2.52	0.40
1:M:-1[B]:MSE:HE3	1:M:-1[B]:MSE:HB3	1.95	0.40
1:M:133:SER:HA	1:M:474:LYS:O	2.21	0.40
1:F:223:GLY:O	2:F:501:NAD:H6N	2.22	0.40
1:G:279:CYS:HG	2:G:501:NAD:C4N	2.30	0.40
1:H:158:PHE:CD1	1:H:158:PHE:C	2.94	0.40
1:H:260:LEU:HD23	1:H:260:LEU:HA	1.77	0.40
1:J:441:VAL:HG13	4:J:879:HOH:O	2.21	0.40
1:L:229:ARG:HG2	1:L:456:PHE:CZ	2.55	0.40
1:N:145:THR:OG1	1:N:172:PRO:HA	2.21	0.40
1:B:295:ARG:HD3	4:B:888:HOH:O	2.21	0.40
1:D:339:ILE:HD11	1:D:345:LEU:HD22	2.02	0.40
1:E:145:THR:OG1	1:E:172:PRO:HA	2.21	0.40
1:F:115:HIS:HD2	1:F:118:LYS:HZ1	1.70	0.40
1:G:316:LYS:NZ	4:G:733:HOH:O	2.54	0.40
1:N:133:SER:HA	1:N:474:LYS:O	2.21	0.40
1:N:383:PHE:CE1	2:N:500:NAD:H2D	2.57	0.40
1:A:142:ALA:HA	1:A:169:ILE:O	2.21	0.40
1:B:115:HIS:HD2	1:B:118:LYS:HZ1	1.68	0.40
1:C:458:ASP:OD1	1:D:458:ASP:OD1	2.39	0.40
1:D:328:GLU:HG3	1:D:363:ILE:HD11	2.04	0.40
1:E:68:MSE:HG3	1:E:111:ILE:HD13	2.03	0.40
1:G:35:LEU:HA	1:G:202:GLY:HA2	2.03	0.40
1:N:278:ARG:HB2	1:N:281:ALA:HB2	2.02	0.40
1:E:54:LYS:HB2	4:E:731:HOH:O	2.22	0.40
1:I:153:ILE:HD13	1:I:222:VAL:HG11	2.02	0.40
1:I:410:GLY:HA2	1:I:432:MSE:O	2.21	0.40
1:L:145:THR:HG22	1:L:153:ILE:HG22	2.03	0.40
1:M:442:PRO:HG2	1:M:447:SER:O	2.22	0.40

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	489/521 (94%)	475 (97%)	13 (3%)	1 (0%)	47	55
1	B	489/521 (94%)	476 (97%)	12 (2%)	1 (0%)	47	55
1	C	492/521 (94%)	478 (97%)	12 (2%)	2 (0%)	34	37
1	D	490/521 (94%)	477 (97%)	12 (2%)	1 (0%)	47	55
1	E	490/521 (94%)	478 (98%)	11 (2%)	1 (0%)	47	55
1	F	489/521 (94%)	475 (97%)	13 (3%)	1 (0%)	47	55
1	G	488/521 (94%)	472 (97%)	15 (3%)	1 (0%)	47	55
1	H	488/521 (94%)	475 (97%)	12 (2%)	1 (0%)	47	55
1	I	489/521 (94%)	474 (97%)	14 (3%)	1 (0%)	47	55
1	J	487/521 (94%)	472 (97%)	14 (3%)	1 (0%)	47	55
1	K	490/521 (94%)	477 (97%)	12 (2%)	1 (0%)	47	55
1	L	489/521 (94%)	475 (97%)	13 (3%)	1 (0%)	47	55
1	M	487/521 (94%)	472 (97%)	14 (3%)	1 (0%)	47	55
1	N	486/521 (93%)	471 (97%)	14 (3%)	1 (0%)	47	55
1	O	491/521 (94%)	478 (97%)	12 (2%)	1 (0%)	47	55
1	P	488/521 (94%)	474 (97%)	13 (3%)	1 (0%)	47	55
All	All	7822/8336 (94%)	7599 (97%)	206 (3%)	17 (0%)	47	55

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-3	SER
1	J	462	HIS
1	L	462	HIS
1	M	462	HIS
1	F	462	HIS
1	G	462	HIS

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Mol	Chain	Res	Type
1	H	462	HIS
1	I	462	HIS
1	K	462	HIS
1	N	462	HIS
1	P	462	HIS
1	B	462	HIS
1	C	462	HIS
1	D	462	HIS
1	E	462	HIS
1	O	462	HIS
1	A	462	HIS

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	386/391 (99%)	381 (99%)	5 (1%)	69	81
1	B	386/391 (99%)	383 (99%)	3 (1%)	81	90
1	C	389/391 (100%)	381 (98%)	8 (2%)	53	67
1	D	387/391 (99%)	382 (99%)	5 (1%)	69	81
1	E	386/391 (99%)	381 (99%)	5 (1%)	69	81
1	F	386/391 (99%)	380 (98%)	6 (2%)	62	76
1	G	385/391 (98%)	378 (98%)	7 (2%)	59	72
1	H	384/391 (98%)	380 (99%)	4 (1%)	76	86
1	I	385/391 (98%)	380 (99%)	5 (1%)	69	81
1	J	384/391 (98%)	379 (99%)	5 (1%)	69	81
1	K	388/391 (99%)	384 (99%)	4 (1%)	76	86
1	L	385/391 (98%)	376 (98%)	9 (2%)	50	63
1	M	384/391 (98%)	378 (98%)	6 (2%)	62	76
1	N	383/391 (98%)	379 (99%)	4 (1%)	76	86
1	O	388/391 (99%)	380 (98%)	8 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	384/391 (98%)	380 (99%)	4 (1%)	76 86
All	All	6170/6256 (99%)	6082 (99%)	88 (1%)	67 80

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	171	LYS
1	A	298	ASP
1	A	359	ASN
1	A	383	PHE
1	B	158	PHE
1	B	171	LYS
1	B	383	PHE
1	C	-3	SER
1	C	-1	MSE
1	C	7	ASP
1	C	158	PHE
1	C	171	LYS
1	C	298	ASP
1	C	299	LYS
1	C	383	PHE
1	D	158	PHE
1	D	171	LYS
1	D	291	GLU
1	D	298	ASP
1	D	383	PHE
1	E	7	ASP
1	E	158	PHE
1	E	171	LYS
1	E	298	ASP
1	E	383	PHE
1	F	7	ASP
1	F	102	ARG
1	F	158	PHE
1	F	171	LYS
1	F	298	ASP
1	F	383	PHE
1	G	69	LYS
1	G	158	PHE
1	G	171	LYS
1	G	290	GLU

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Mol	Chain	Res	Type
1	G	298	ASP
1	G	336	ASP
1	G	383	PHE
1	H	95	ASP
1	H	158	PHE
1	H	171	LYS
1	H	383	PHE
1	I	7	ASP
1	I	59	ASN
1	I	171	LYS
1	I	298	ASP
1	I	383	PHE
1	J	-1	MSE
1	J	158	PHE
1	J	171	LYS
1	J	291	GLU
1	J	383	PHE
1	K	158	PHE
1	K	171	LYS
1	K	298	ASP
1	K	383	PHE
1	L	7	ASP
1	L	59	ASN
1	L	158	PHE
1	L	171	LYS
1	L	260	LEU
1	L	291	GLU
1	L	319	MSE
1	L	351	ASP
1	L	383	PHE
1	M	7	ASP
1	M	158	PHE
1	M	171	LYS
1	M	237	MSE
1	M	298	ASP
1	M	383	PHE
1	N	158	PHE
1	N	171	LYS
1	N	291	GLU
1	N	383	PHE
1	O	59	ASN
1	O	158	PHE

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Mol	Chain	Res	Type
1	O	171	LYS
1	O	237	MSE
1	O	290[A]	GLU
1	O	290[B]	GLU
1	O	298	ASP
1	O	383	PHE
1	P	7	ASP
1	P	52	GLN
1	P	171	LYS
1	P	383	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	79	ASN
1	B	115	HIS
1	C	446	HIS
1	C	460	ASN
1	D	79	ASN
1	D	460	ASN
1	F	115	HIS
1	G	115	HIS
1	G	243	GLN
1	G	446	HIS
1	G	460	ASN
1	H	79	ASN
1	H	243	GLN
1	H	460	ASN
1	J	115	HIS
1	K	115	HIS
1	K	446	HIS
1	K	460	ASN
1	L	79	ASN
1	L	243	GLN
1	L	460	ASN
1	M	115	HIS
1	O	115	HIS
1	O	243	GLN
1	O	460	ASN
1	P	460	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAD	E	500	-	42,48,48	0.89	1 (2%)	50,73,73	1.12	3 (6%)
2	NAD	D	500	-	42,48,48	0.93	1 (2%)	50,73,73	1.28	5 (10%)
2	NAD	C	500	-	42,48,48	0.89	1 (2%)	50,73,73	1.14	2 (4%)
2	NAD	K	500	-	42,48,48	0.90	1 (2%)	50,73,73	1.23	4 (8%)
2	NAD	N	500	-	42,48,48	0.83	2 (4%)	50,73,73	1.22	4 (8%)
2	NAD	B	500	-	42,48,48	0.89	2 (4%)	50,73,73	1.15	4 (8%)
2	NAD	H	500	-	42,48,48	0.91	1 (2%)	50,73,73	1.20	4 (8%)
2	NAD	O	501	-	42,48,48	0.85	1 (2%)	50,73,73	1.24	4 (8%)
2	NAD	G	501	-	42,48,48	0.91	3 (7%)	50,73,73	1.17	4 (8%)
2	NAD	L	500	-	42,48,48	0.89	2 (4%)	50,73,73	1.19	5 (10%)
2	NAD	I	501	-	42,48,48	0.86	2 (4%)	50,73,73	1.20	3 (6%)
2	NAD	A	501	-	42,48,48	0.90	3 (7%)	50,73,73	1.10	3 (6%)
2	NAD	M	500	-	42,48,48	0.92	2 (4%)	50,73,73	1.13	4 (8%)
2	NAD	J	500	-	42,48,48	0.87	2 (4%)	50,73,73	1.25	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAD	P	500	-	42,48,48	0.90	2 (4%)	50,73,73	1.32	4 (8%)
2	NAD	F	501	-	42,48,48	0.89	2 (4%)	50,73,73	1.17	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	E	500	-	-	2/26/62/62	0/5/5/5
2	NAD	D	500	-	-	5/26/62/62	0/5/5/5
2	NAD	C	500	-	-	2/26/62/62	0/5/5/5
2	NAD	K	500	-	-	4/26/62/62	0/5/5/5
2	NAD	N	500	-	-	3/26/62/62	0/5/5/5
2	NAD	B	500	-	-	2/26/62/62	0/5/5/5
2	NAD	H	500	-	-	3/26/62/62	0/5/5/5
2	NAD	O	501	-	-	4/26/62/62	0/5/5/5
2	NAD	G	501	-	-	3/26/62/62	0/5/5/5
2	NAD	L	500	-	-	2/26/62/62	0/5/5/5
2	NAD	I	501	-	-	5/26/62/62	0/5/5/5
2	NAD	A	501	-	-	4/26/62/62	0/5/5/5
2	NAD	M	500	-	-	4/26/62/62	0/5/5/5
2	NAD	J	500	-	-	5/26/62/62	0/5/5/5
2	NAD	P	500	-	-	3/26/62/62	0/5/5/5
2	NAD	F	501	-	-	3/26/62/62	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	500	NAD	C5A-C4A	2.60	1.47	1.40
2	B	500	NAD	C5A-C4A	2.57	1.47	1.40
2	F	501	NAD	C5A-C4A	2.53	1.47	1.40
2	C	500	NAD	C5A-C4A	2.48	1.47	1.40
2	M	500	NAD	C5A-C4A	2.48	1.47	1.40
2	H	500	NAD	O4D-C1D	2.46	1.44	1.41
2	E	500	NAD	C5A-C4A	2.41	1.47	1.40
2	J	500	NAD	C5A-C4A	2.39	1.47	1.40
2	I	501	NAD	C5A-C4A	2.39	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAD	C2A-N3A	2.38	1.35	1.32
2	D	500	NAD	C5A-C4A	2.37	1.47	1.40
2	A	501	NAD	C5A-C4A	2.36	1.47	1.40
2	F	501	NAD	O4D-C1D	2.31	1.44	1.41
2	P	500	NAD	C5A-C4A	2.30	1.47	1.40
2	I	501	NAD	C2A-N3A	2.28	1.35	1.32
2	L	500	NAD	C5A-C4A	2.28	1.47	1.40
2	A	501	NAD	O4B-C1B	2.27	1.44	1.41
2	O	501	NAD	C5A-C4A	2.27	1.46	1.40
2	G	501	NAD	O4D-C1D	2.23	1.44	1.41
2	N	500	NAD	C5A-C4A	2.22	1.46	1.40
2	G	501	NAD	C5A-C4A	2.12	1.46	1.40
2	G	501	NAD	C2A-N3A	2.12	1.35	1.32
2	B	500	NAD	C2A-N3A	2.07	1.35	1.32
2	P	500	NAD	O4D-C1D	2.07	1.44	1.41
2	L	500	NAD	C2A-N3A	2.03	1.35	1.32
2	N	500	NAD	O4B-C1B	2.02	1.43	1.41
2	J	500	NAD	C2A-N3A	2.01	1.35	1.32
2	M	500	NAD	O4B-C1B	2.01	1.43	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	NAD	N3A-C2A-N1A	-4.39	121.81	128.68
2	H	500	NAD	N3A-C2A-N1A	-4.05	122.35	128.68
2	J	500	NAD	N3A-C2A-N1A	-3.89	122.60	128.68
2	P	500	NAD	N3A-C2A-N1A	-3.86	122.65	128.68
2	F	501	NAD	N3A-C2A-N1A	-3.74	122.83	128.68
2	K	500	NAD	N3A-C2A-N1A	-3.69	122.91	128.68
2	N	500	NAD	N3A-C2A-N1A	-3.64	122.98	128.68
2	L	500	NAD	N3A-C2A-N1A	-3.63	123.01	128.68
2	E	500	NAD	N3A-C2A-N1A	-3.60	123.06	128.68
2	B	500	NAD	N3A-C2A-N1A	-3.58	123.09	128.68
2	A	501	NAD	N3A-C2A-N1A	-3.45	123.29	128.68
2	O	501	NAD	N3A-C2A-N1A	-3.32	123.50	128.68
2	C	500	NAD	N3A-C2A-N1A	-3.27	123.56	128.68
2	G	501	NAD	N3A-C2A-N1A	-3.23	123.62	128.68
2	I	501	NAD	N3A-C2A-N1A	-3.23	123.63	128.68
2	P	500	NAD	C4A-C5A-N7A	-3.13	106.14	109.40
2	P	500	NAD	C2N-N1N-C1D	3.11	126.06	119.14
2	I	501	NAD	C2N-N1N-C1D	3.05	125.92	119.14
2	O	501	NAD	C4A-C5A-N7A	-2.93	106.34	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	NAD	C1B-N9A-C4A	-2.91	121.53	126.64
2	M	500	NAD	N3A-C2A-N1A	-2.89	124.17	128.68
2	C	500	NAD	C2N-N1N-C1D	2.86	125.51	119.14
2	D	500	NAD	C2N-N1N-C1D	2.82	125.41	119.14
2	L	500	NAD	C2N-N1N-C1D	2.80	125.37	119.14
2	G	501	NAD	C2N-N1N-C1D	2.73	125.22	119.14
2	G	501	NAD	C4A-C5A-N7A	-2.71	106.57	109.40
2	M	500	NAD	PN-O3-PA	-2.68	123.63	132.83
2	I	501	NAD	C4A-C5A-N7A	-2.68	106.61	109.40
2	F	501	NAD	C2A-N1A-C6A	2.67	123.31	118.75
2	B	500	NAD	C4A-C5A-N7A	-2.59	106.69	109.40
2	E	500	NAD	C4A-C5A-N7A	-2.59	106.70	109.40
2	H	500	NAD	C2N-N1N-C1D	2.59	124.90	119.14
2	D	500	NAD	C4A-C5A-N7A	-2.58	106.71	109.40
2	K	500	NAD	C2A-N1A-C6A	2.57	123.15	118.75
2	N	500	NAD	C2N-N1N-C1D	2.53	124.77	119.14
2	B	500	NAD	O4D-C1D-C2D	-2.53	103.23	106.93
2	E	500	NAD	C2N-N1N-C1D	2.52	124.76	119.14
2	O	501	NAD	C2N-N1N-C1D	2.52	124.75	119.14
2	L	500	NAD	C4A-C5A-N7A	-2.50	106.79	109.40
2	F	501	NAD	C1B-N9A-C4A	-2.46	122.32	126.64
2	K	500	NAD	C6N-N1N-C2N	-2.45	119.74	121.97
2	N	500	NAD	C4A-C5A-N7A	-2.41	106.89	109.40
2	K	500	NAD	C2N-N1N-C1D	2.37	124.41	119.14
2	D	500	NAD	C2A-N1A-C6A	2.34	122.76	118.75
2	J	500	NAD	PN-O3-PA	-2.34	124.80	132.83
2	M	500	NAD	C4A-C5A-N7A	-2.34	106.96	109.40
2	J	500	NAD	C2A-N1A-C6A	2.32	122.72	118.75
2	F	501	NAD	C4A-C5A-N7A	-2.30	107.00	109.40
2	O	501	NAD	C2A-N1A-C6A	2.30	122.68	118.75
2	M	500	NAD	C2N-N1N-C1D	2.27	124.20	119.14
2	B	500	NAD	C2N-N1N-C1D	2.26	124.18	119.14
2	G	501	NAD	C1B-N9A-C4A	-2.24	122.70	126.64
2	A	501	NAD	C2N-N1N-C1D	2.20	124.04	119.14
2	P	500	NAD	C2A-N1A-C6A	2.19	122.49	118.75
2	N	500	NAD	C2A-N1A-C6A	2.17	122.46	118.75
2	J	500	NAD	C6N-N1N-C2N	-2.14	120.02	121.97
2	L	500	NAD	C3B-C2B-C1B	2.13	104.19	100.98
2	A	501	NAD	C4A-C5A-N7A	-2.12	107.19	109.40
2	H	500	NAD	C4A-C5A-N7A	-2.09	107.22	109.40
2	L	500	NAD	C3D-C2D-C1D	2.07	104.10	100.98
2	J	500	NAD	C2N-N1N-C1D	2.07	123.74	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	500	NAD	C2A-N1A-C6A	2.05	122.27	118.75

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	B	500	NAD	O4D-C1D-N1N-C2N
2	C	500	NAD	O4D-C1D-N1N-C2N
2	D	500	NAD	O4D-C1D-N1N-C2N
2	D	500	NAD	O4D-C1D-N1N-C6N
2	D	500	NAD	C2D-C1D-N1N-C2N
2	D	500	NAD	C2D-C1D-N1N-C6N
2	E	500	NAD	O4D-C1D-N1N-C2N
2	F	501	NAD	O4D-C1D-N1N-C2N
2	F	501	NAD	O4D-C1D-N1N-C6N
2	G	501	NAD	O4D-C1D-N1N-C2N
2	G	501	NAD	O4D-C1D-N1N-C6N
2	H	500	NAD	O4D-C1D-N1N-C2N
2	H	500	NAD	O4D-C1D-N1N-C6N
2	I	501	NAD	O4D-C1D-N1N-C2N
2	I	501	NAD	O4D-C1D-N1N-C6N
2	J	500	NAD	O4D-C1D-N1N-C2N
2	J	500	NAD	O4D-C1D-N1N-C6N
2	K	500	NAD	O4D-C1D-N1N-C2N
2	K	500	NAD	O4D-C1D-N1N-C6N
2	L	500	NAD	O4D-C1D-N1N-C2N
2	M	500	NAD	O4D-C1D-N1N-C2N
2	N	500	NAD	O4D-C1D-N1N-C2N
2	O	501	NAD	O4D-C1D-N1N-C2N
2	O	501	NAD	O4D-C1D-N1N-C6N
2	P	500	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	C4D-C5D-O5D-PN
2	C	500	NAD	C4D-C5D-O5D-PN
2	F	501	NAD	C4D-C5D-O5D-PN
2	I	501	NAD	C4D-C5D-O5D-PN
2	J	500	NAD	C4D-C5D-O5D-PN
2	K	500	NAD	C4D-C5D-O5D-PN
2	B	500	NAD	C4D-C5D-O5D-PN
2	D	500	NAD	C4D-C5D-O5D-PN
2	G	501	NAD	C4D-C5D-O5D-PN

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Mol	Chain	Res	Type	Atoms
2	H	500	NAD	C4D-C5D-O5D-PN
2	N	500	NAD	C4D-C5D-O5D-PN
2	P	500	NAD	C4D-C5D-O5D-PN
2	E	500	NAD	C4D-C5D-O5D-PN
2	M	500	NAD	C4D-C5D-O5D-PN
2	O	501	NAD	C4D-C5D-O5D-PN
2	I	501	NAD	O4D-C4D-C5D-O5D
2	I	501	NAD	C3D-C4D-C5D-O5D
2	M	500	NAD	O4D-C4D-C5D-O5D
2	M	500	NAD	C3D-C4D-C5D-O5D
2	J	500	NAD	C3D-C4D-C5D-O5D
2	L	500	NAD	C4D-C5D-O5D-PN
2	J	500	NAD	O4D-C4D-C5D-O5D
2	K	500	NAD	C2D-C1D-N1N-C6N
2	A	501	NAD	C3D-C4D-C5D-O5D
2	N	500	NAD	C3D-C4D-C5D-O5D
2	P	500	NAD	C5B-O5B-PA-O1A
2	O	501	NAD	C3D-C4D-C5D-O5D

There are no ring outliers.

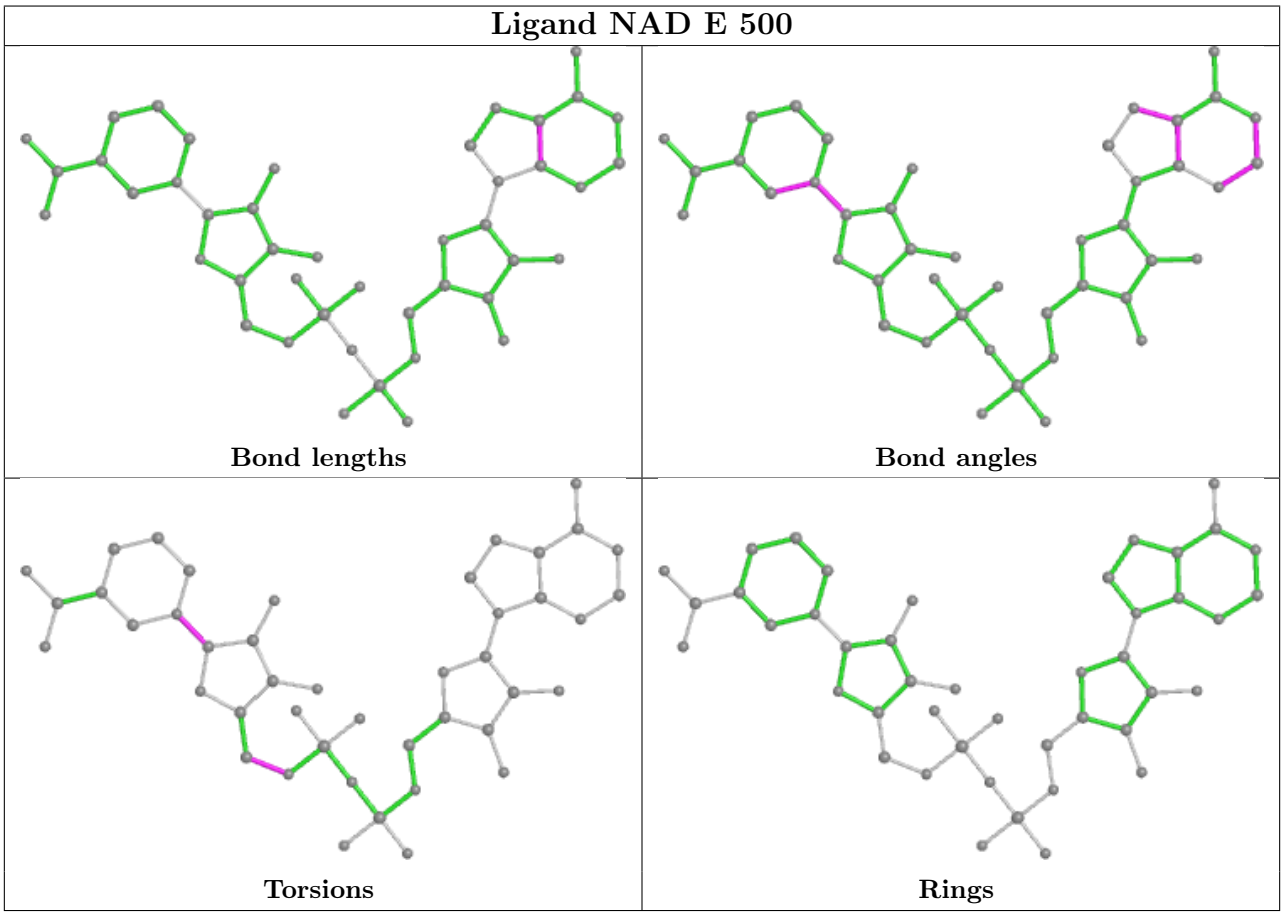
16 monomers are involved in 169 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	NAD	9	0
2	D	500	NAD	11	0
2	C	500	NAD	12	0
2	K	500	NAD	11	0
2	N	500	NAD	10	0
2	B	500	NAD	10	0
2	H	500	NAD	10	0
2	O	501	NAD	11	0
2	G	501	NAD	10	0
2	L	500	NAD	9	0
2	I	501	NAD	11	0
2	A	501	NAD	11	0
2	M	500	NAD	9	0
2	J	500	NAD	12	0
2	P	500	NAD	11	0
2	F	501	NAD	12	0

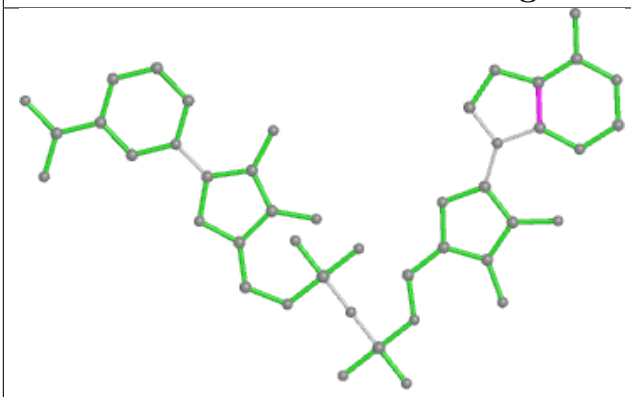
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

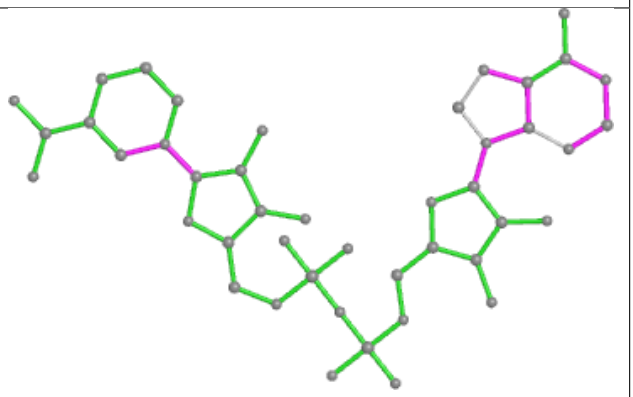
Ligand NAD E 500



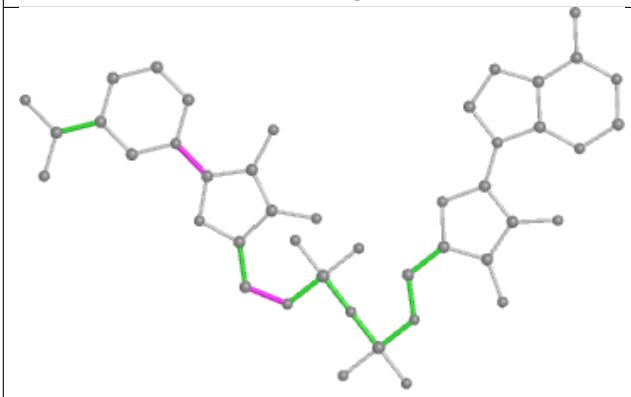
Ligand NAD D 500



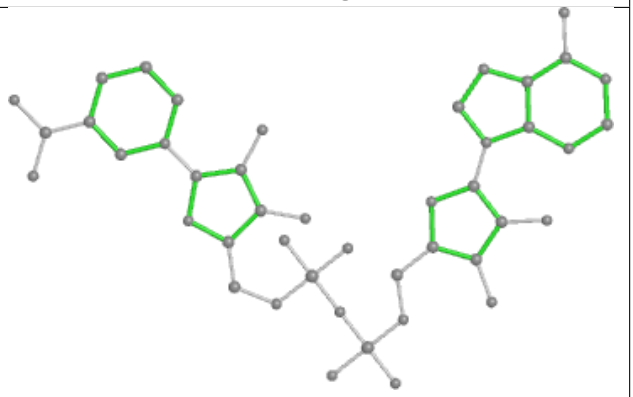
Bond lengths



Bond angles

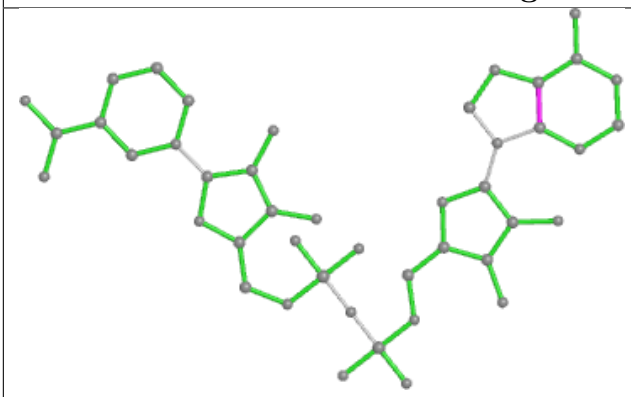


Torsions



Rings

Ligand NAD C 500



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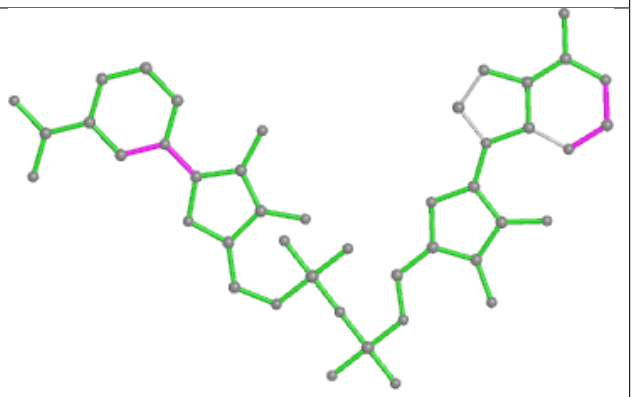
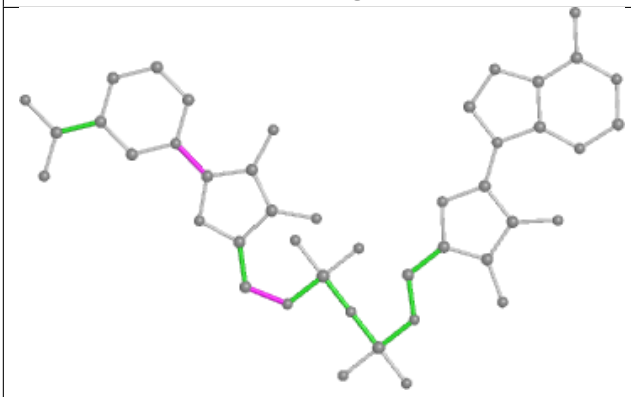


Bond angles



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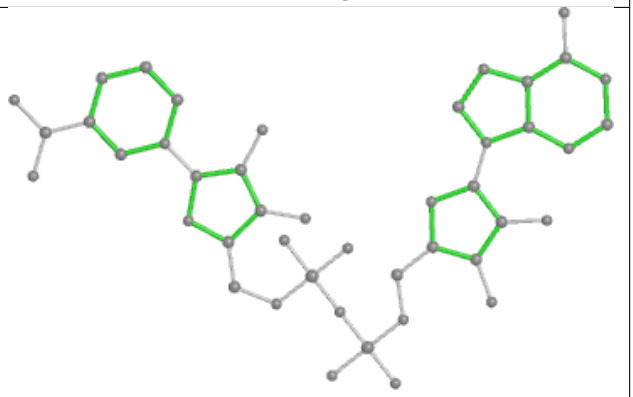
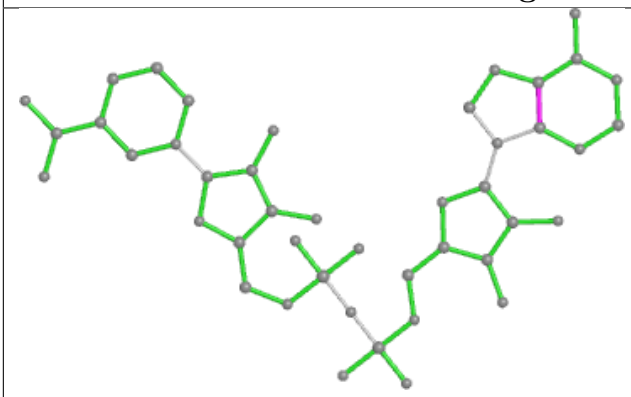
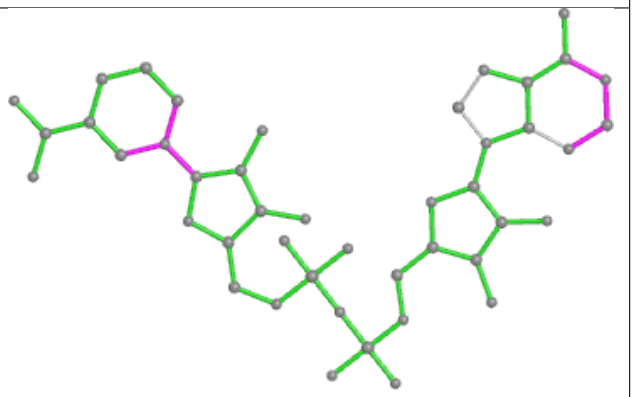


Rings

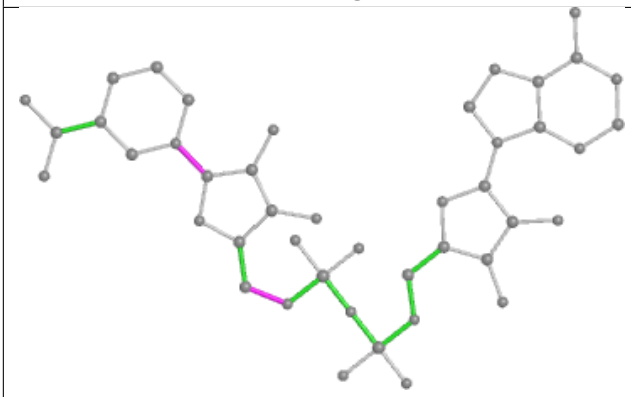
Ligand NAD K 500



Bond lengths



Bond angles



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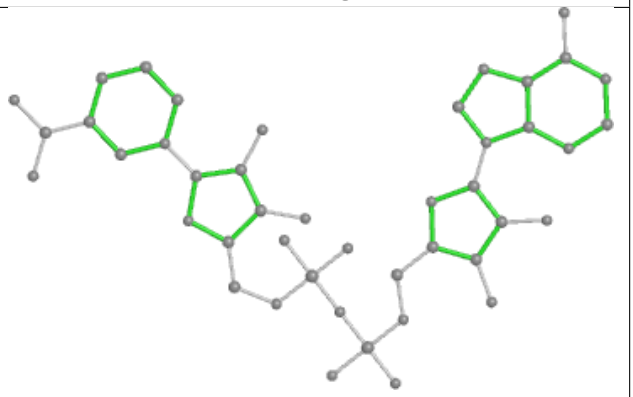
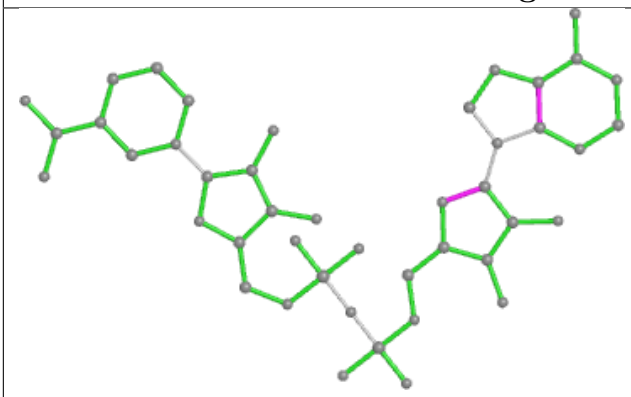
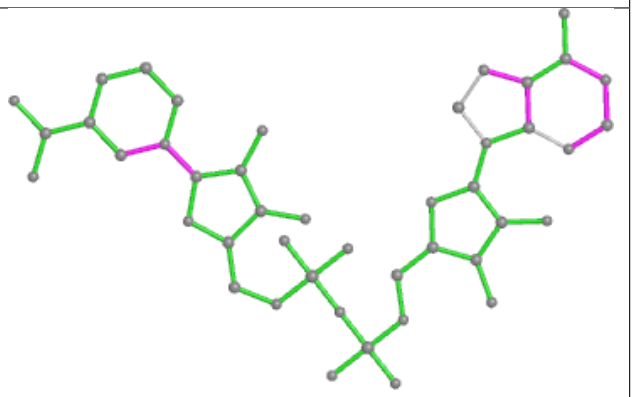


Rings

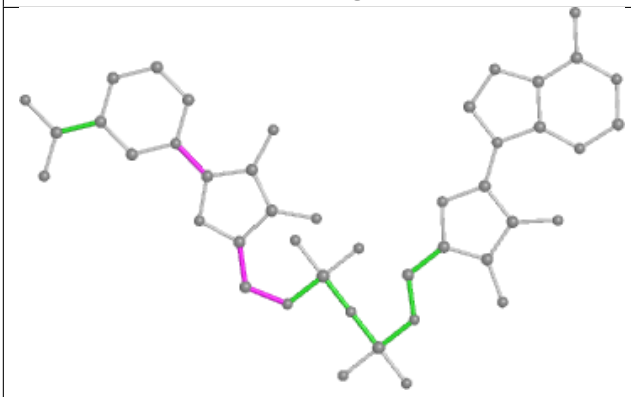
Ligand NAD N 500



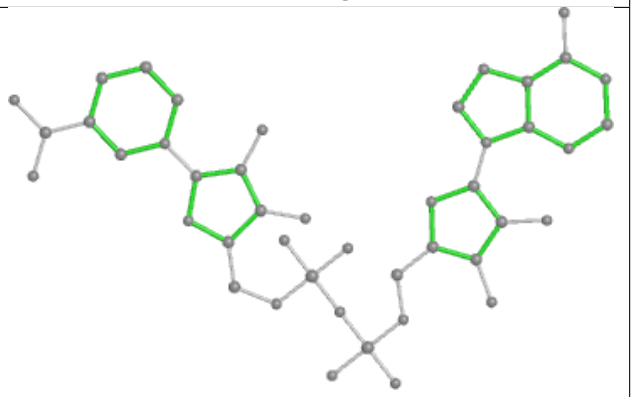
Bond lengths



Bond angles

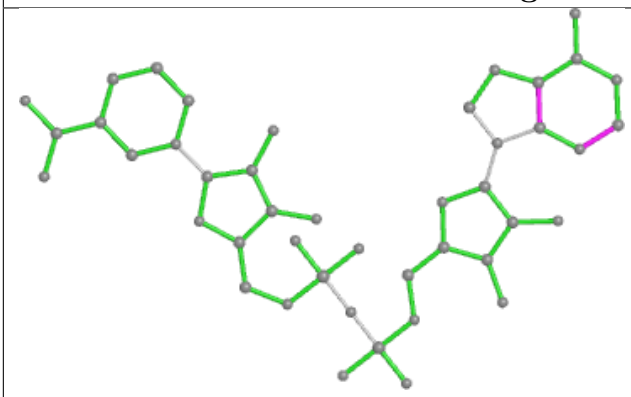


Torsions

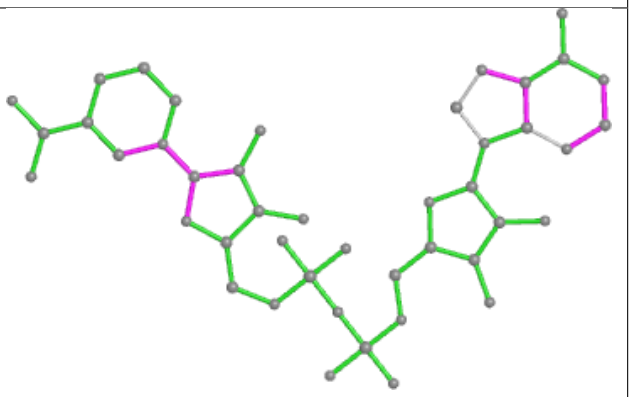


Rings

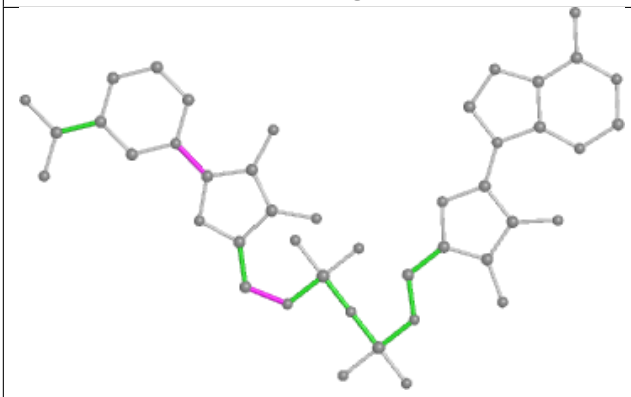
Ligand NAD B 500



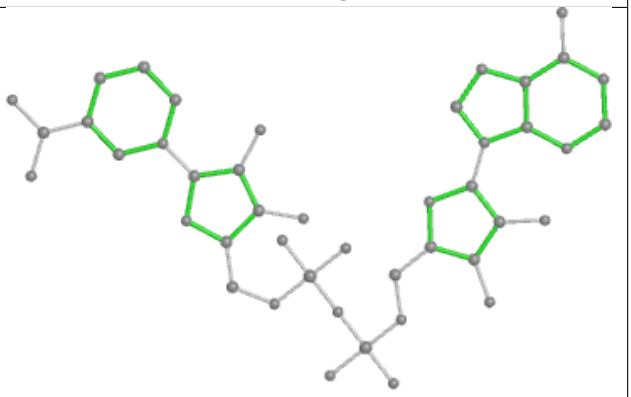
Bond lengths



Bond angles

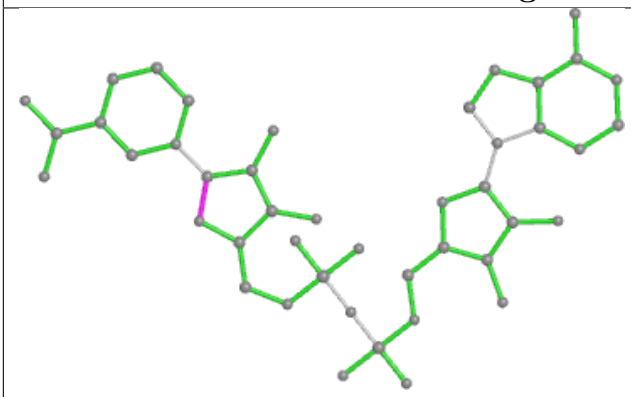


Torsions

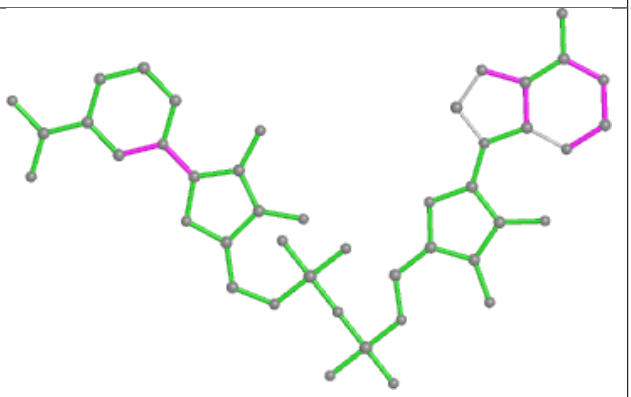


Rings

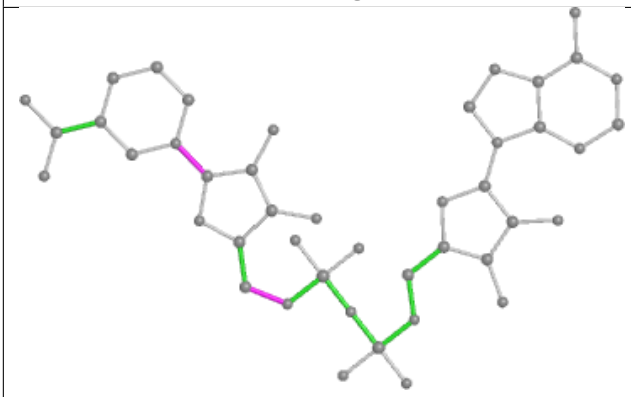
Ligand NAD H 500



Bond lengths



Bond angles



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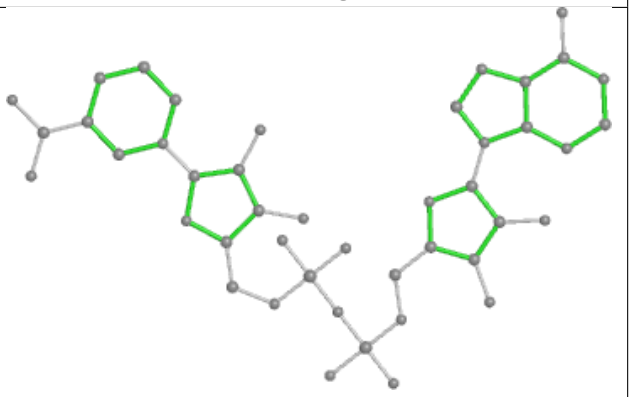

Rings

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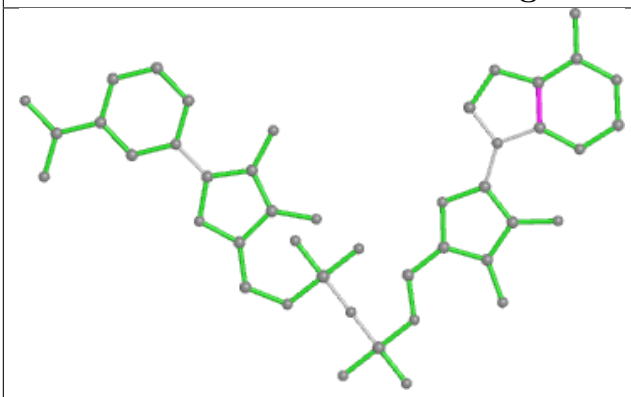

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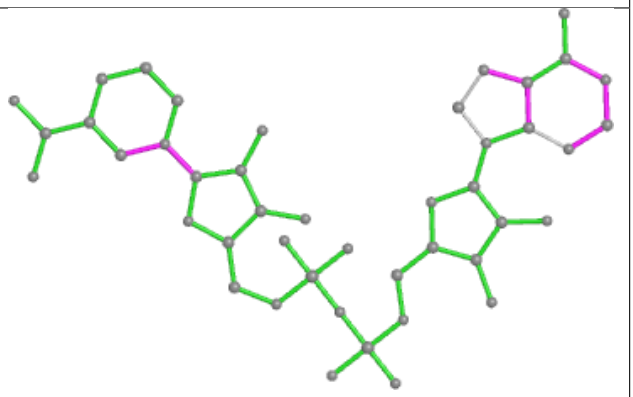
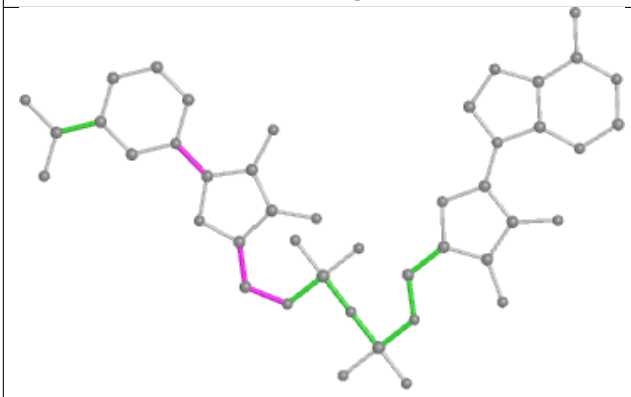
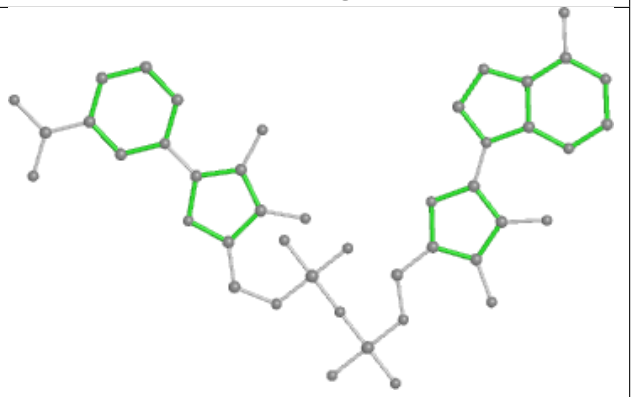


Bond angles

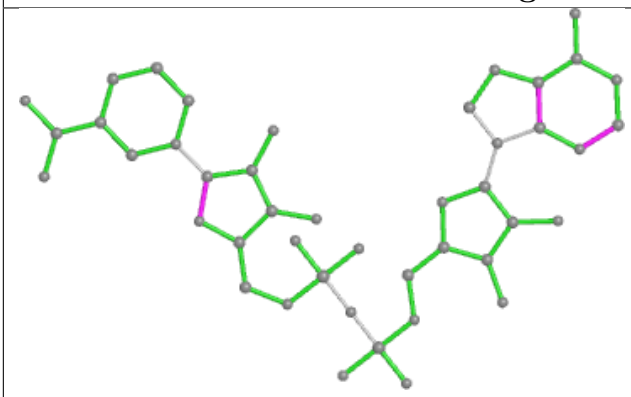


Torsions

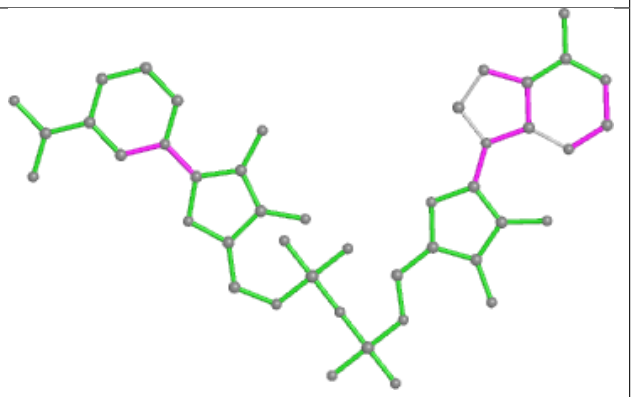


Rings

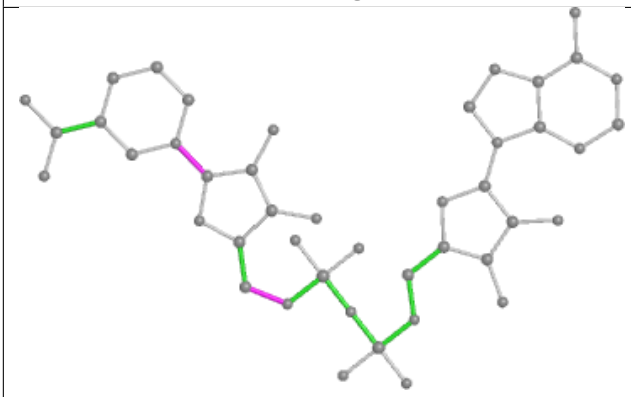
Ligand NAD G 501



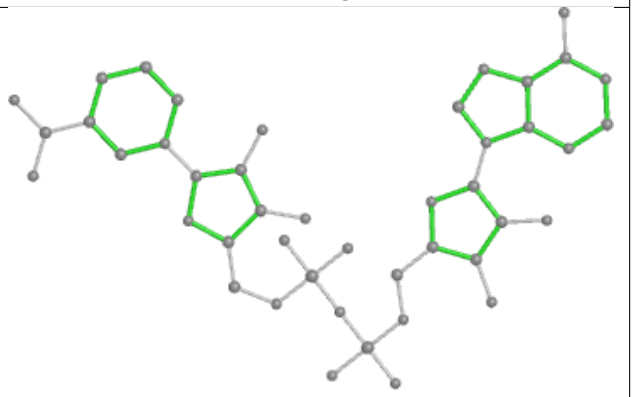
Bond lengths



Bond angles

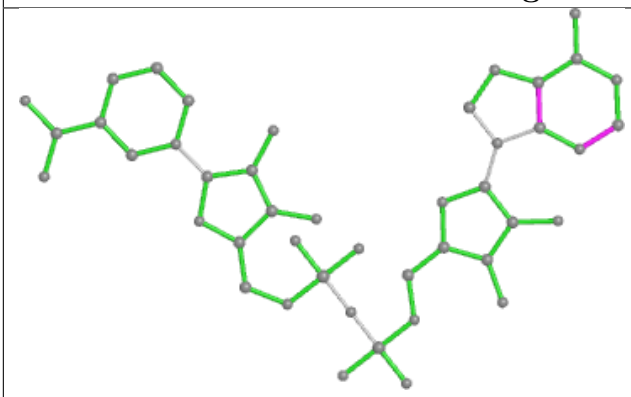


Torsions



Rings

Ligand NAD L 500



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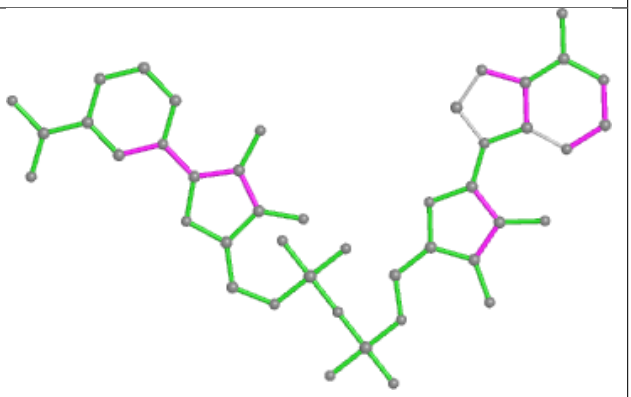
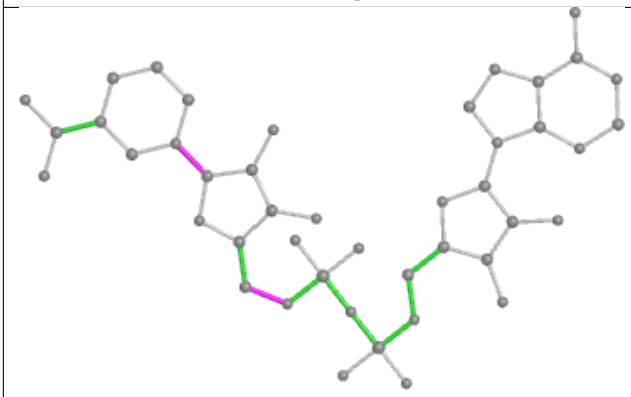
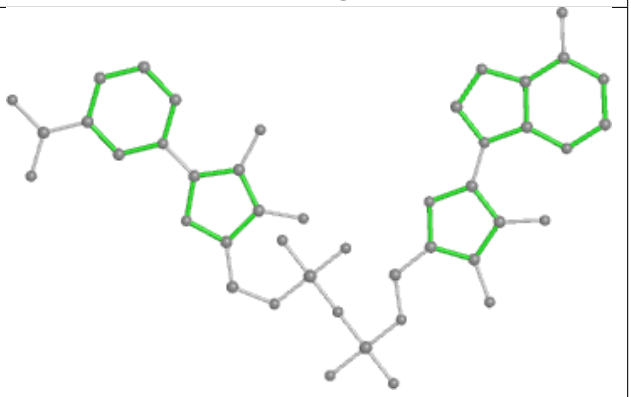


Bond angles

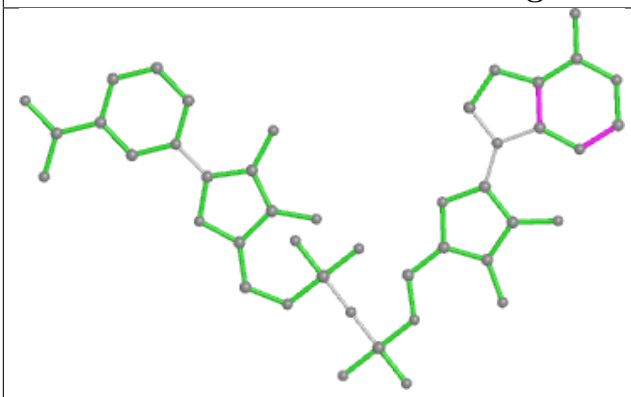


Torsions

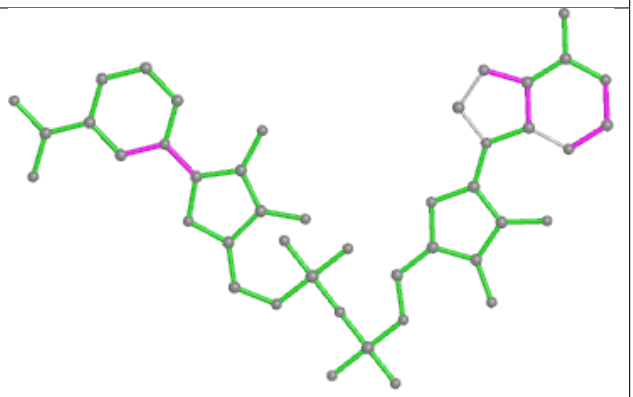


Rings

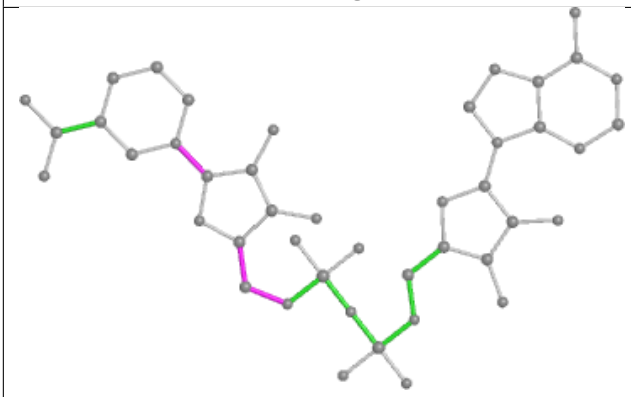
Ligand NAD I 501



Bond lengths



Bond angles



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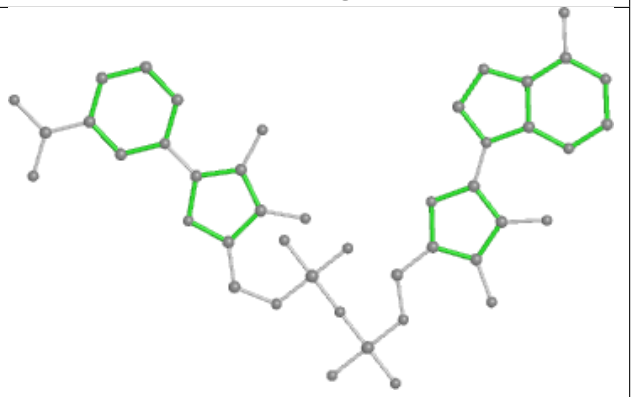
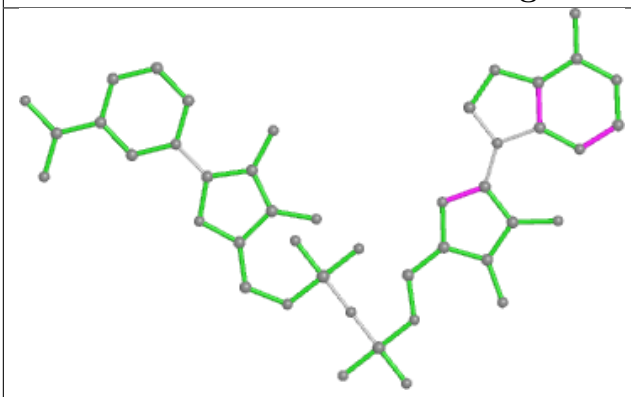


Rings

Ligand NAD A 501



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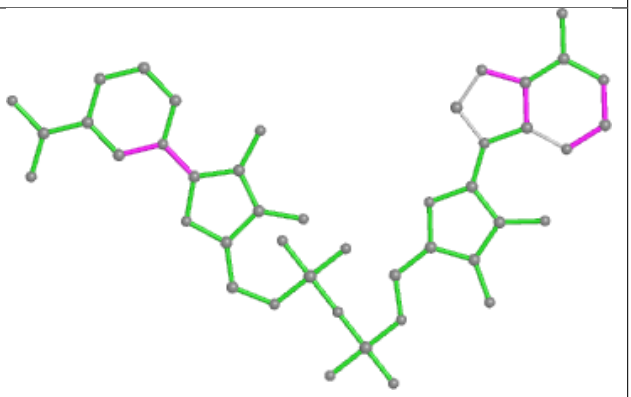
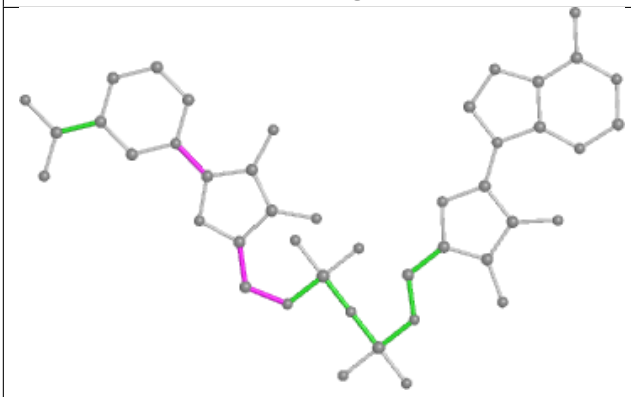


Bond angles



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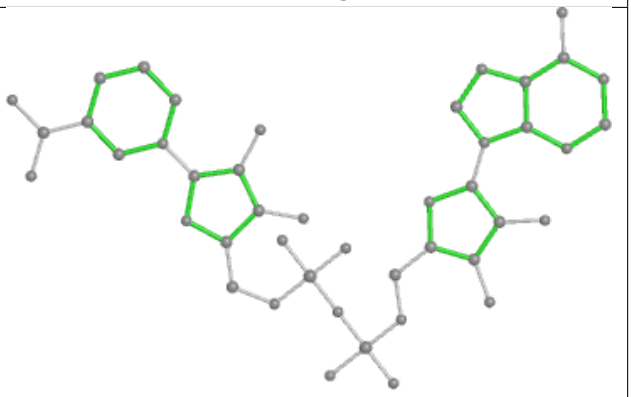
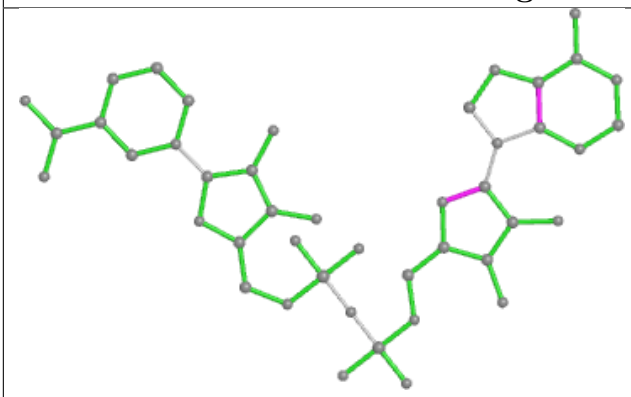


Rings

Ligand NAD M 500



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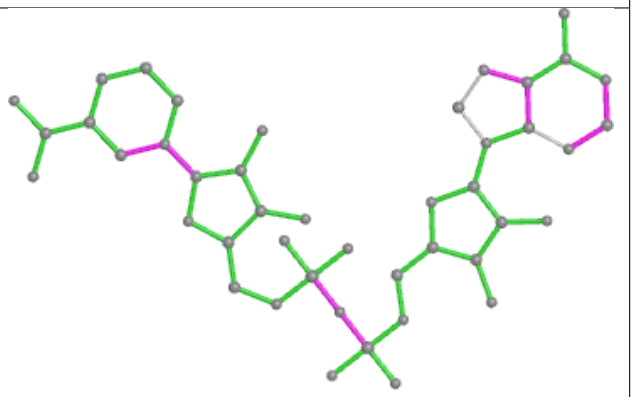
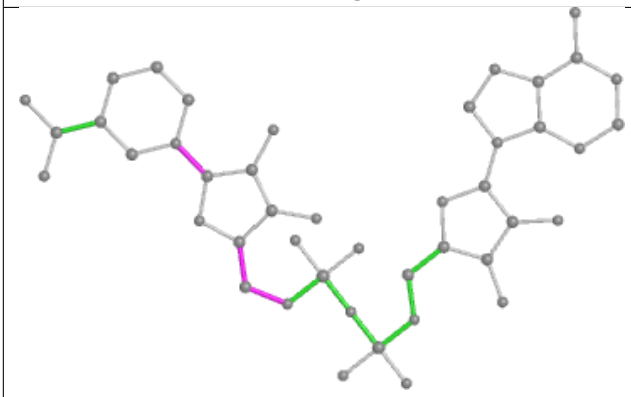
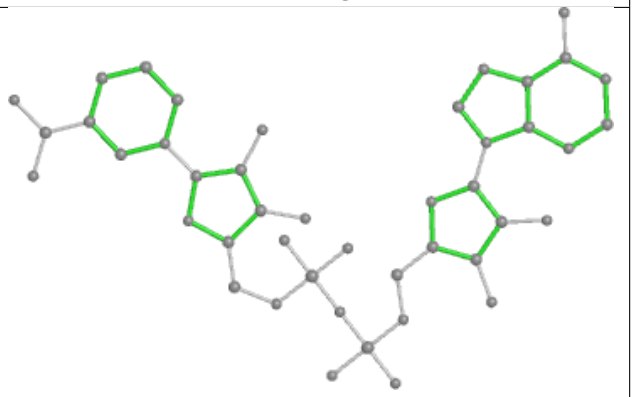


Bond angles



Torsions



Rings

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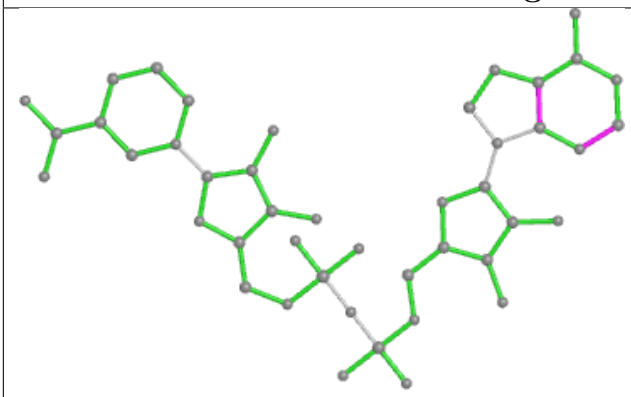
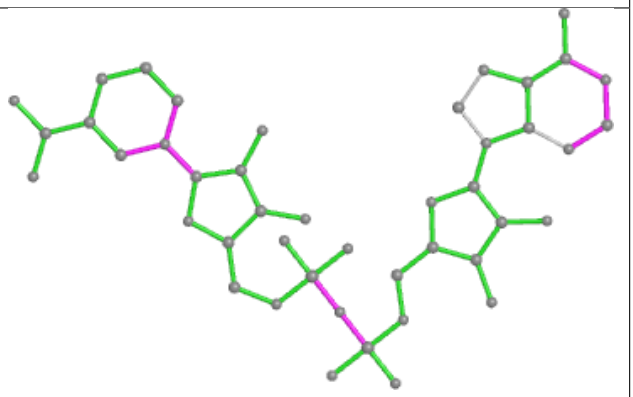
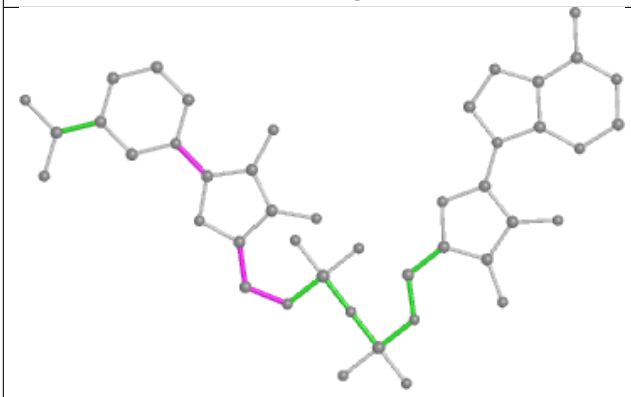


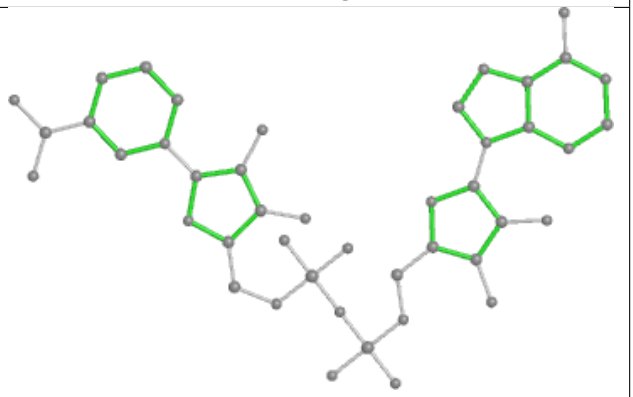
Bond lengths



Bond angles



Torsions



Rings

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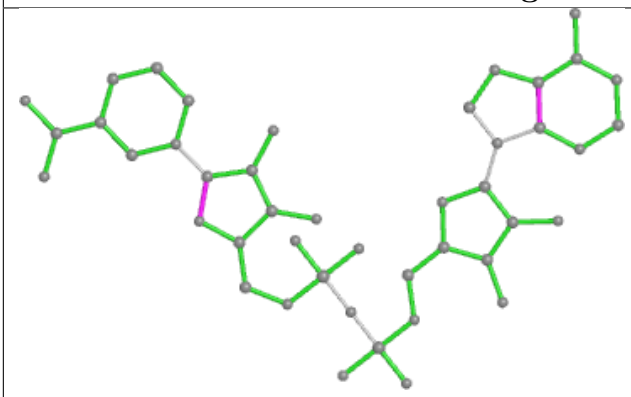
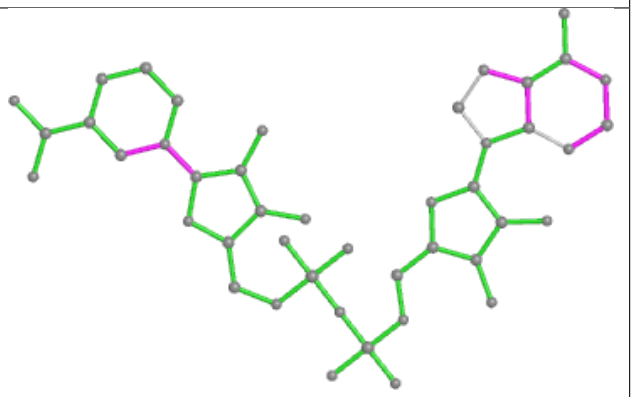
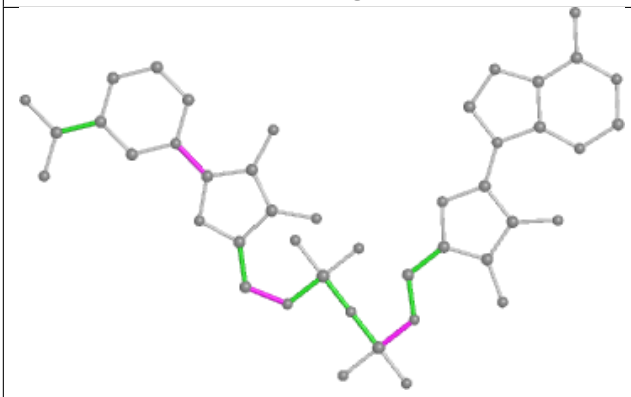


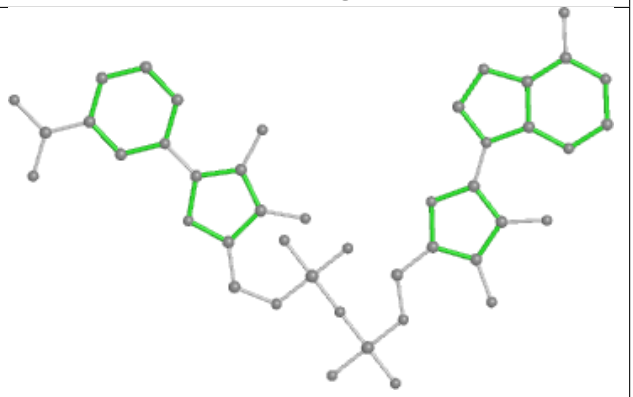
Bond lengths



Bond angles

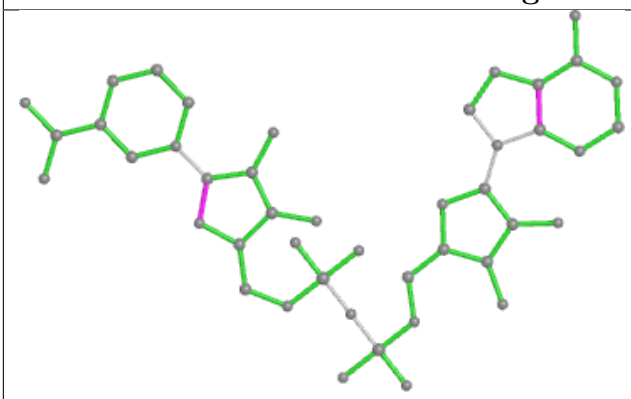


Torsions

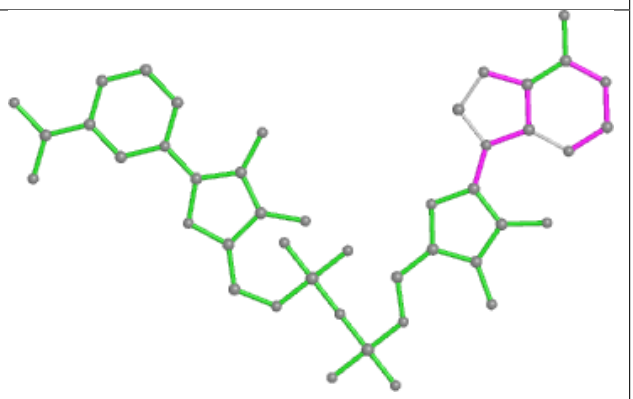


Rings

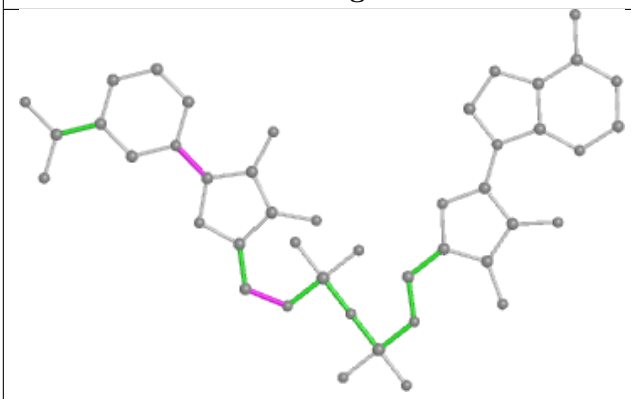
Ligand NAD F 501



Bond lengths



Bond angles



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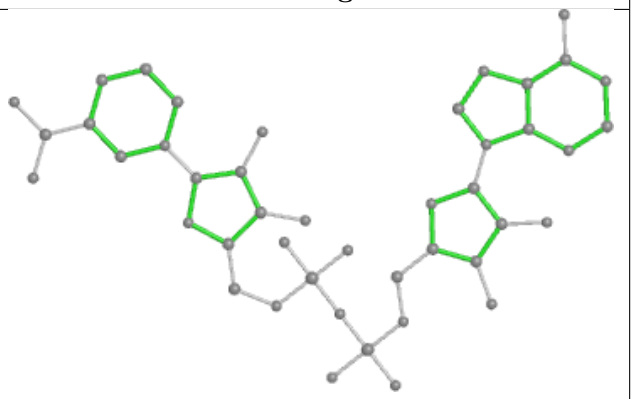

Rings

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	470/521 (90%)	-0.43	1 (0%) 95 94	14, 23, 37, 58	0
1	B	470/521 (90%)	-0.38	2 (0%) 92 91	14, 23, 39, 60	0
1	C	472/521 (90%)	-0.58	2 (0%) 92 91	14, 23, 41, 102	0
1	D	470/521 (90%)	-0.37	3 (0%) 89 88	16, 27, 49, 69	0
1	E	471/521 (90%)	-0.56	1 (0%) 95 94	13, 20, 36, 62	0
1	F	470/521 (90%)	-0.44	2 (0%) 92 91	15, 23, 40, 58	0
1	G	470/521 (90%)	-0.58	0 100 100	14, 23, 42, 62	0
1	H	471/521 (90%)	-0.45	2 (0%) 92 91	13, 25, 46, 68	0
1	I	471/521 (90%)	-0.48	0 100 100	14, 24, 41, 59	0
1	J	470/521 (90%)	-0.65	0 100 100	14, 24, 40, 54	0
1	K	470/521 (90%)	-0.64	0 100 100	11, 18, 34, 54	0
1	L	471/521 (90%)	-0.38	2 (0%) 92 91	13, 28, 51, 70	0
1	M	471/521 (90%)	-0.35	3 (0%) 89 88	15, 29, 48, 69	0
1	N	470/521 (90%)	-0.53	1 (0%) 95 94	15, 29, 47, 62	0
1	O	470/521 (90%)	-0.64	0 100 100	12, 20, 38, 65	0
1	P	471/521 (90%)	-0.44	2 (0%) 92 91	13, 27, 46, 65	0
All	All	7528/8336 (90%)	-0.49	21 (0%) 94 93	11, 24, 43, 102	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	487	GLY	4.9
1	C	-3	SER	4.5
1	C	-4	GLN	3.9
1	H	16	GLY	3.0
1	H	487	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	487	GLY	2.9
1	F	16	GLY	2.5
1	M	487	GLY	2.4
1	D	16	GLY	2.4
1	B	336	ASP	2.4
1	M	290	GLU	2.4
1	P	355	GLN	2.3
1	P	487	GLY	2.3
1	D	315	GLU	2.2
1	F	340	GLU	2.2
1	B	351	ASP	2.1
1	A	339	ILE	2.1
1	L	340	GLU	2.0
1	N	329	GLN	2.0
1	M	340	GLU	2.0
1	D	351	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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
3	MG	I	502	1/1	0.58	0.15	54,54,54,54	0
3	MG	G	502	1/1	0.82	0.28	57,57,57,57	0
3	MG	F	502	1/1	0.87	0.11	41,41,41,41	0
3	MG	A	502	1/1	0.92	0.05	47,47,47,47	0
3	MG	O	502	1/1	0.94	0.09	49,49,49,49	0
2	NAD	A	501	44/44	0.95	0.14	20,28,75,88	0
3	MG	A	503	1/1	0.95	0.10	49,49,49,49	0

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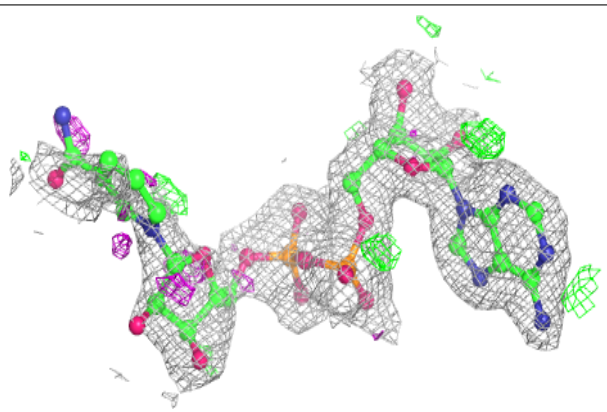
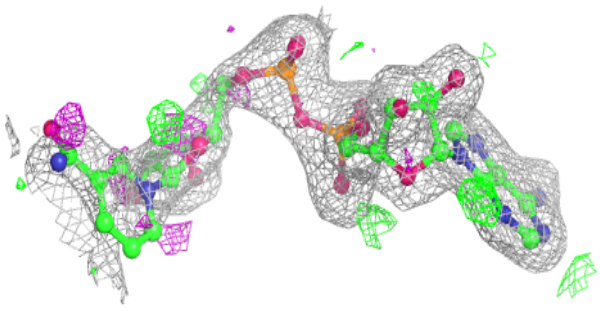
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	M	500	44/44	0.96	0.13	28,31,80,86	0
2	NAD	N	500	44/44	0.96	0.14	31,35,73,81	0
2	NAD	O	501	44/44	0.96	0.14	20,24,59,67	0
2	NAD	P	500	44/44	0.96	0.13	29,32,64,72	0
2	NAD	B	500	44/44	0.96	0.14	22,29,68,83	0
2	NAD	D	500	44/44	0.96	0.13	26,32,74,85	0
2	NAD	F	501	44/44	0.96	0.12	21,26,71,85	0
2	NAD	J	500	44/44	0.96	0.12	25,28,65,70	0
2	NAD	K	500	44/44	0.96	0.14	20,24,65,66	0
2	NAD	L	500	44/44	0.96	0.13	27,32,62,64	0
2	NAD	H	500	44/44	0.97	0.12	23,27,68,77	0
2	NAD	I	501	44/44	0.97	0.12	24,28,69,75	0
2	NAD	E	500	44/44	0.97	0.12	20,24,66,70	0
2	NAD	C	500	44/44	0.97	0.13	20,25,64,66	0
2	NAD	G	501	44/44	0.97	0.12	21,30,61,63	0

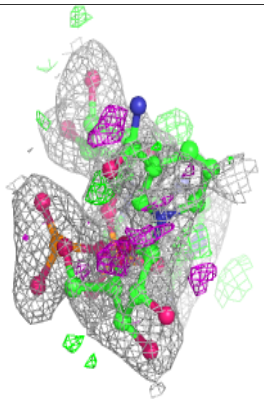
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 501:

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

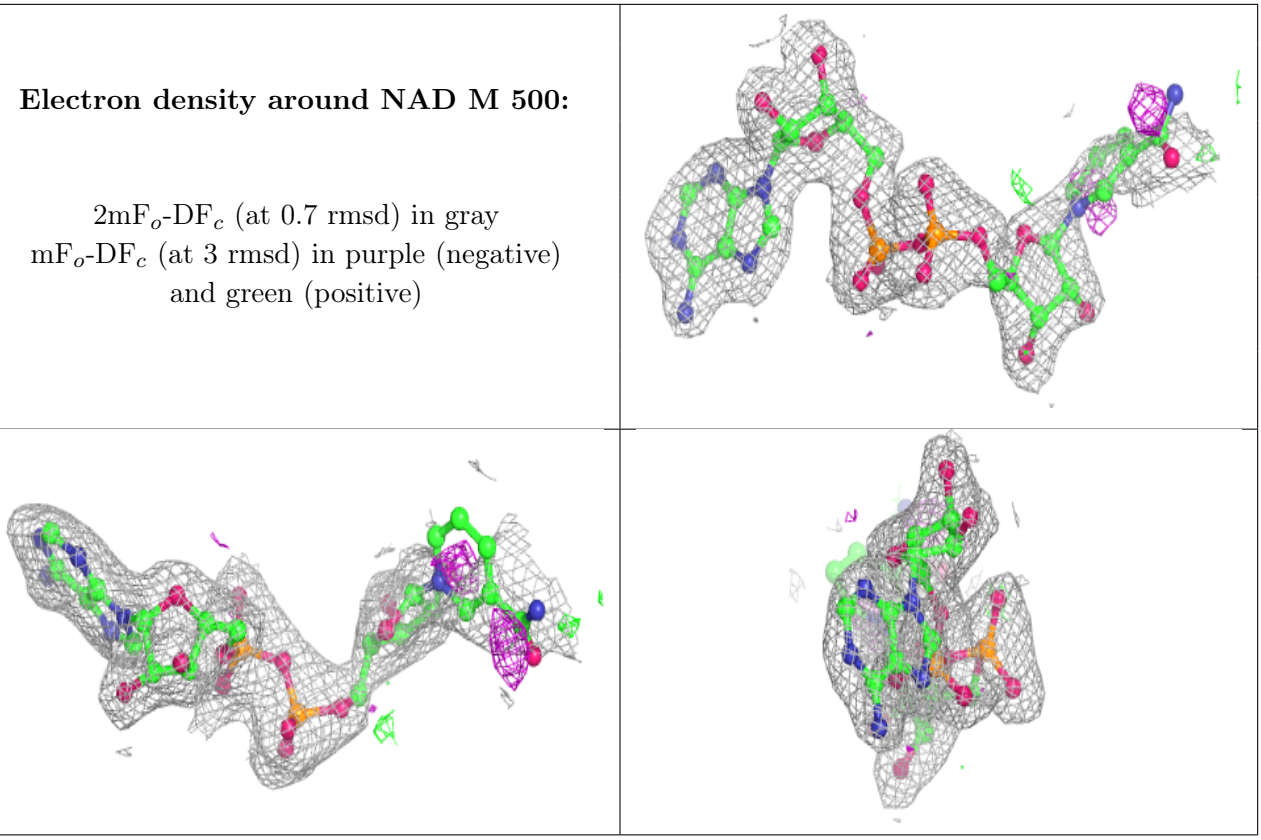






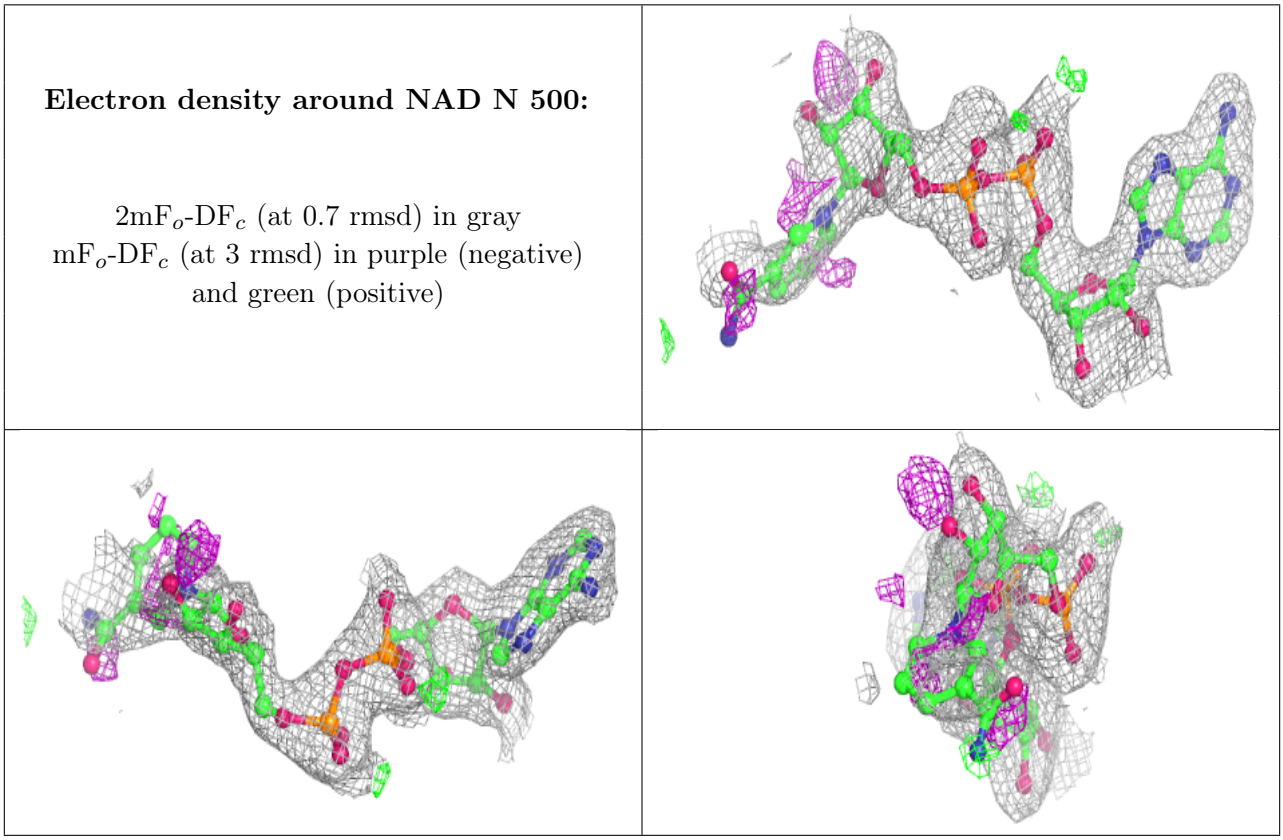
Electron density around NAD M 500:

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



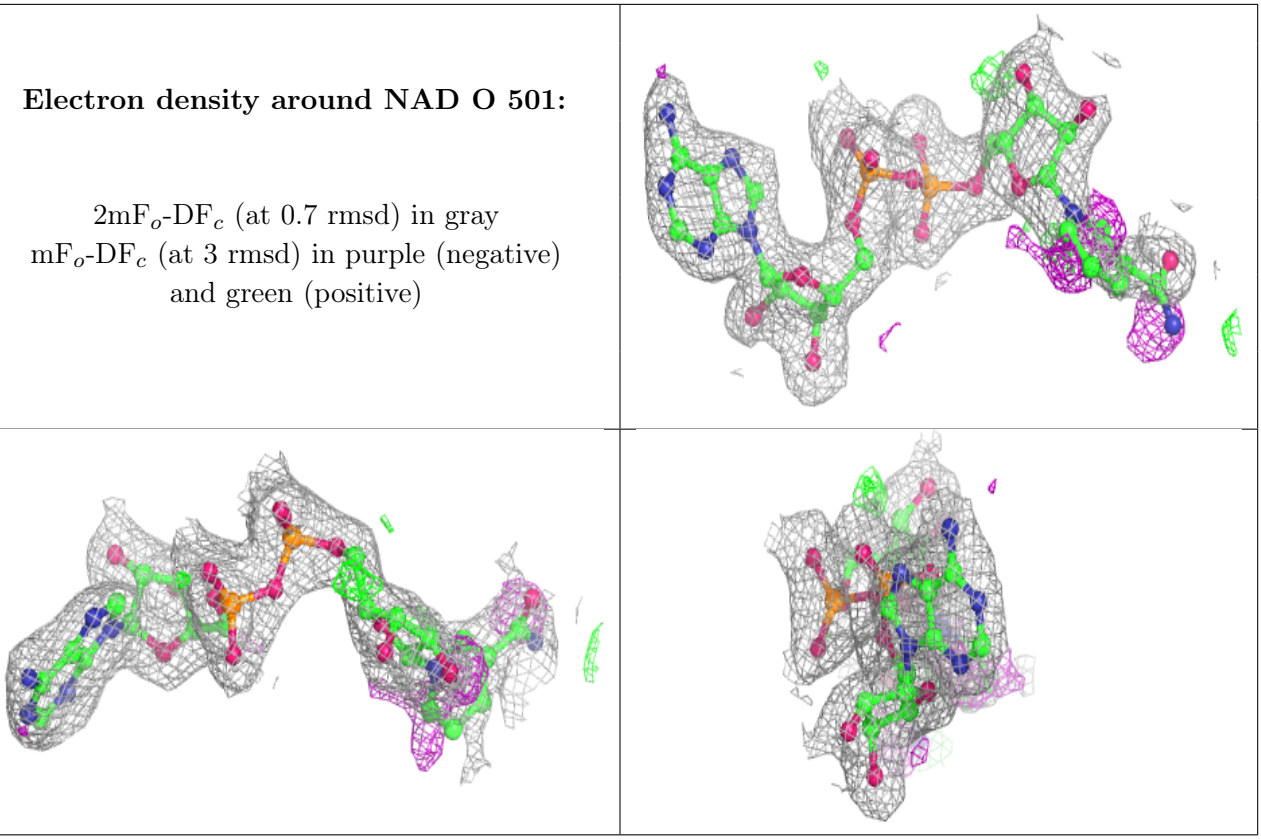
Electron density around NAD N 500:

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



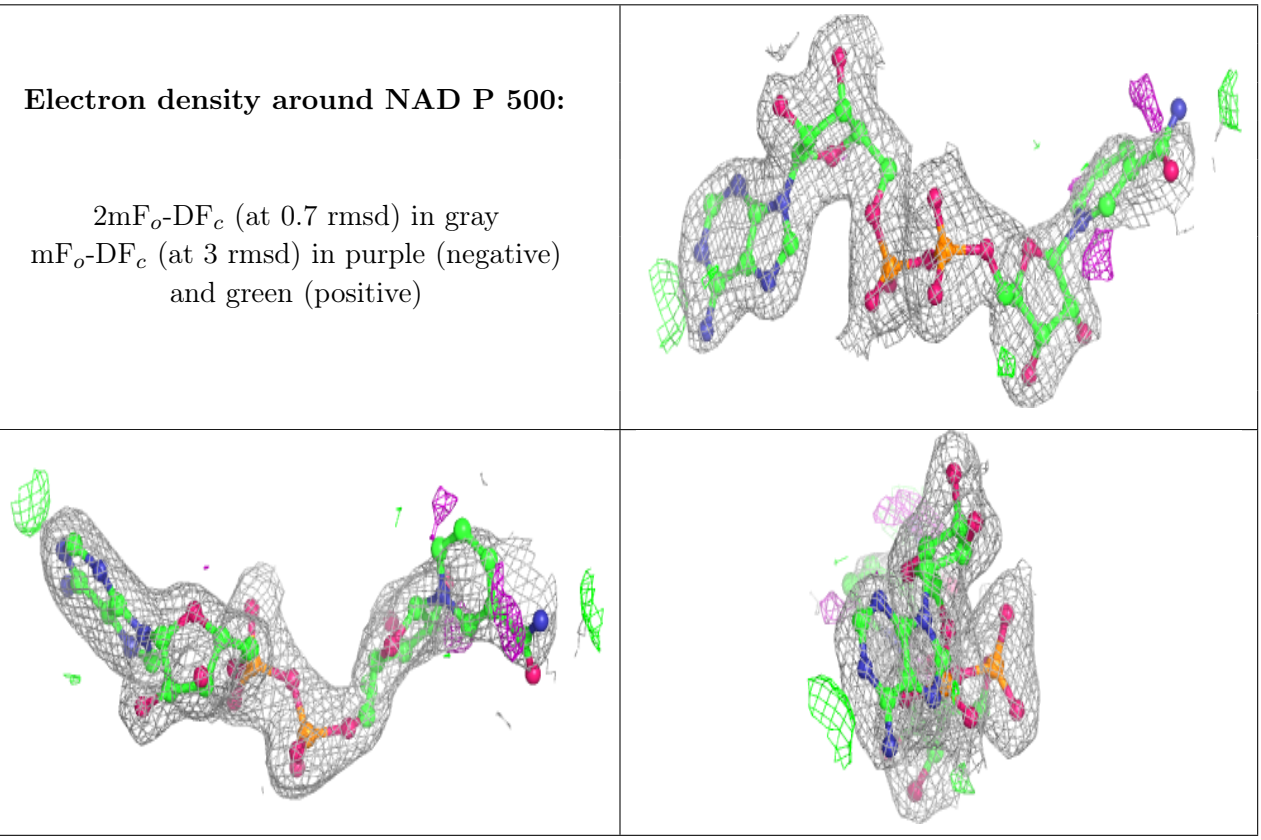
Electron density around NAD O 501:

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



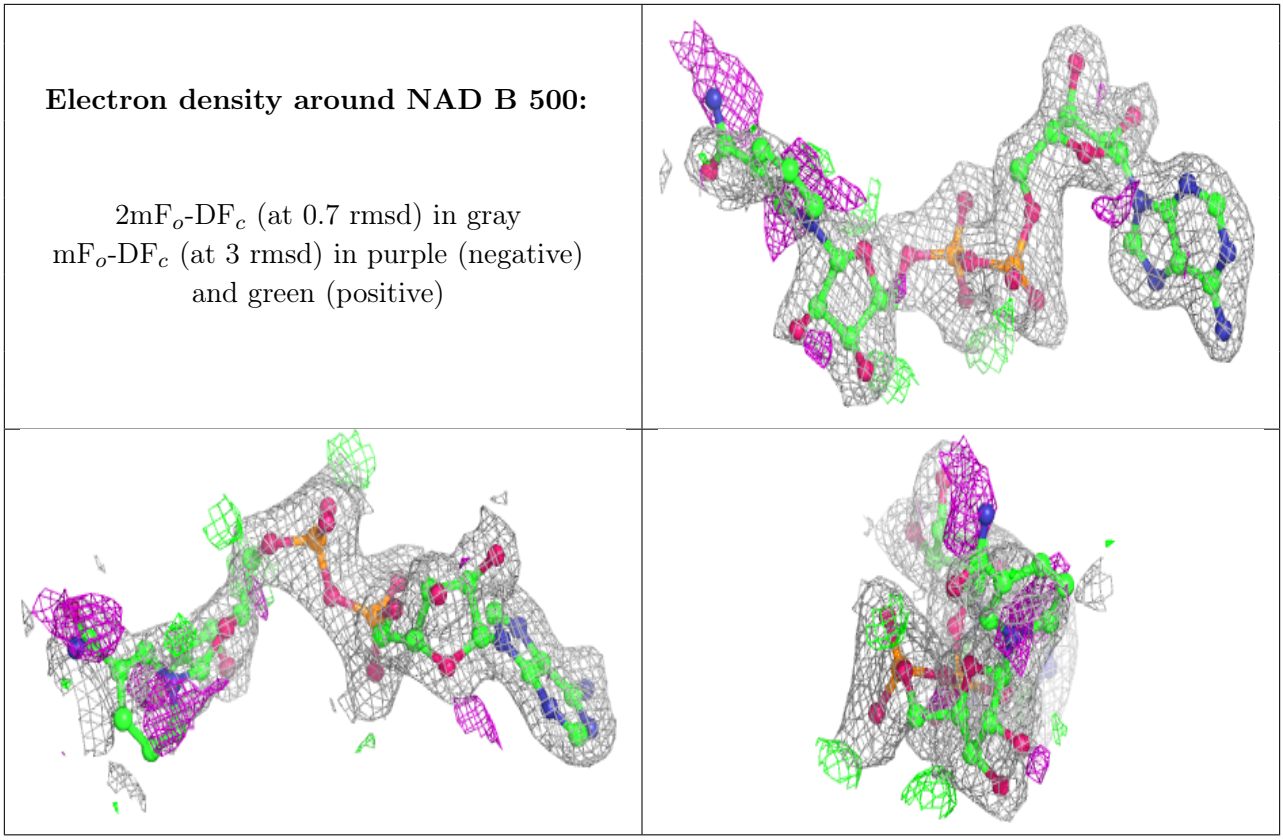
Electron density around NAD P 500:

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



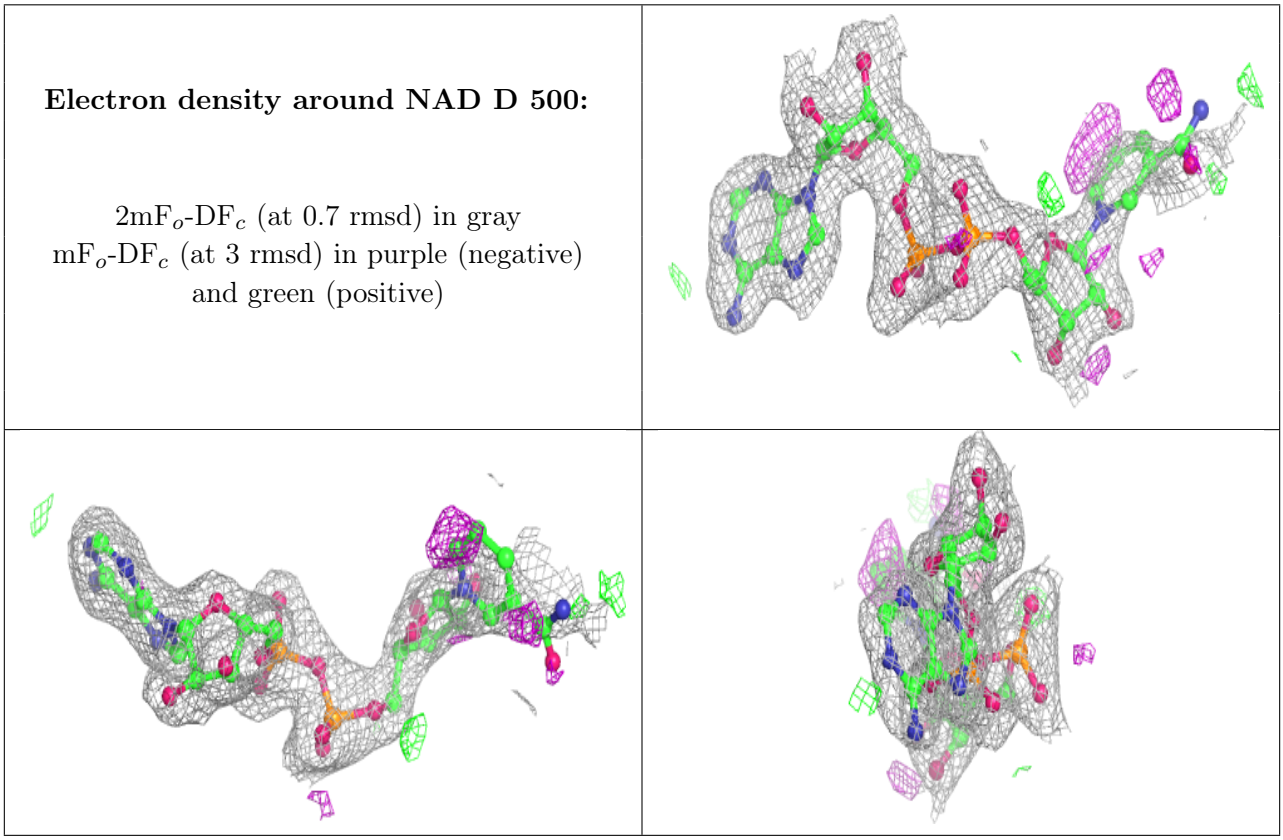
Electron density around NAD B 500:

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



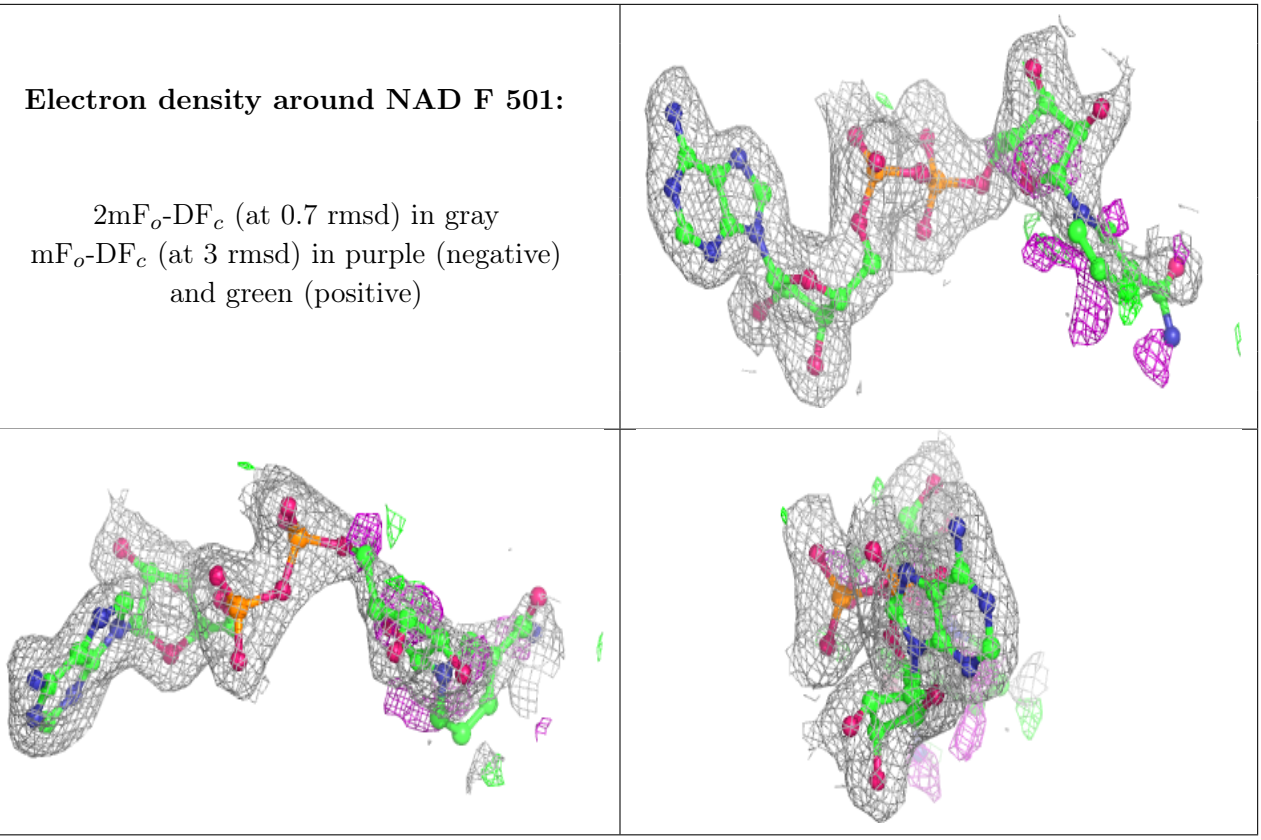
Electron density around NAD D 500:

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



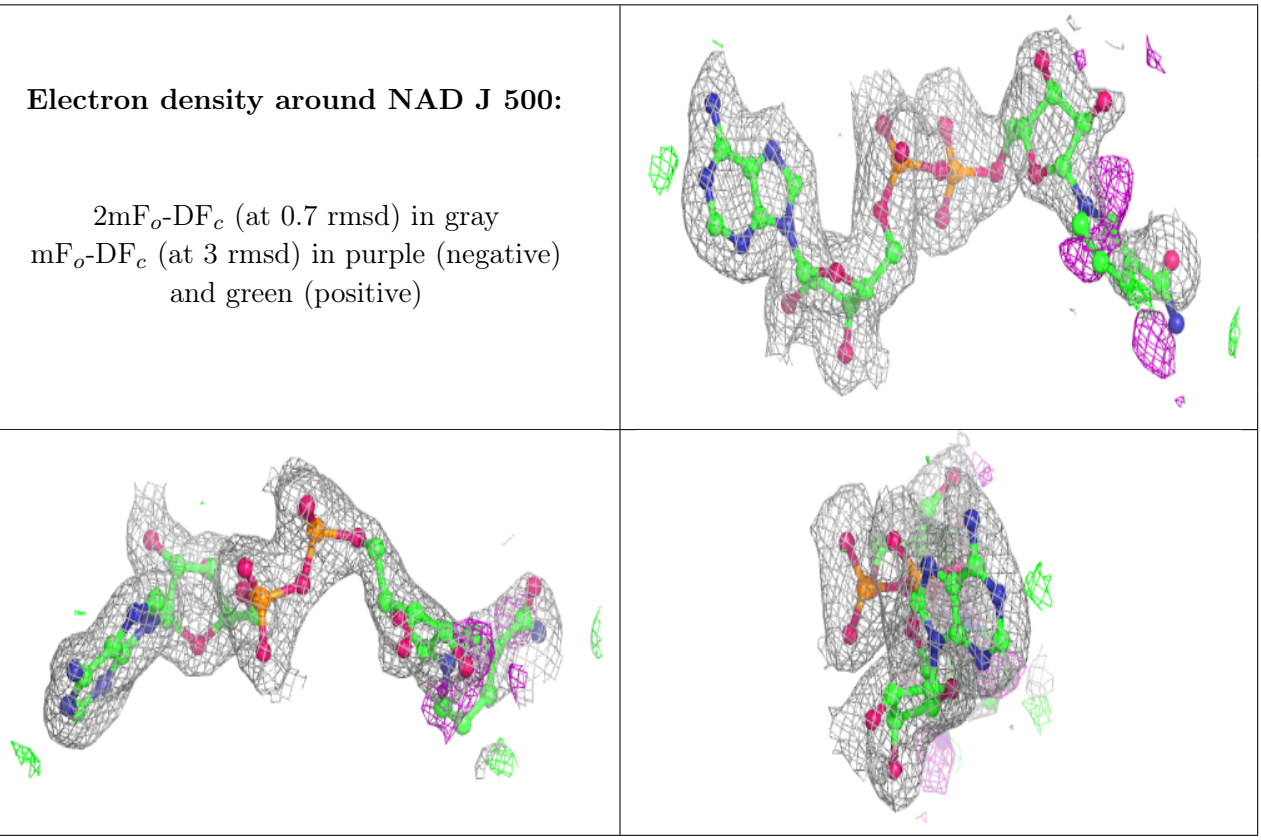
Electron density around NAD F 501:

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



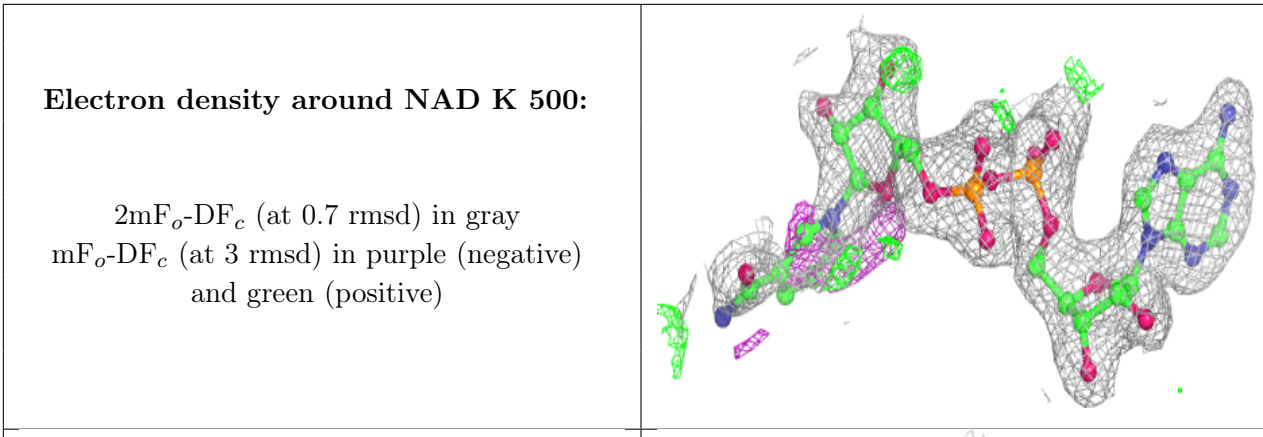
Electron density around NAD J 500:

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



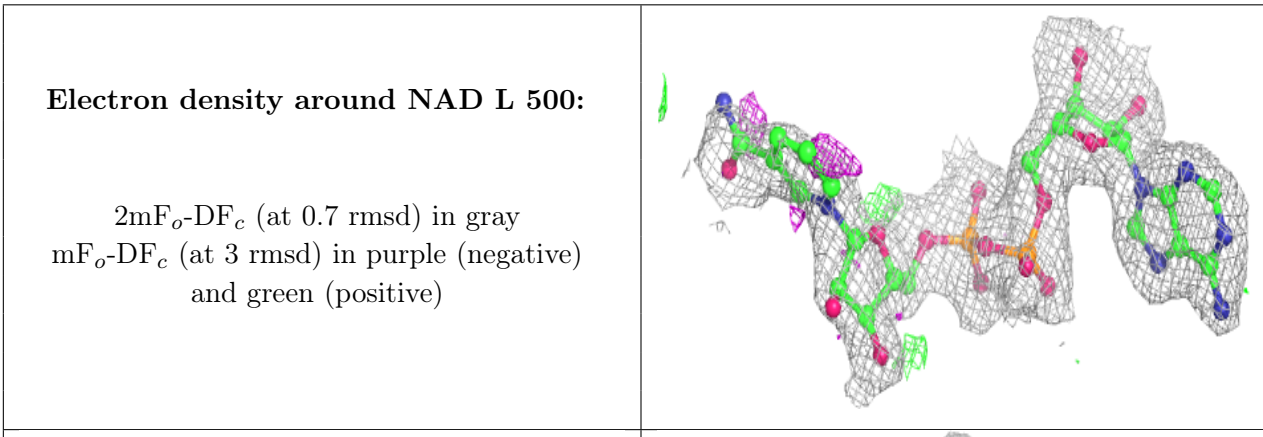
Electron density around NAD K 500:

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



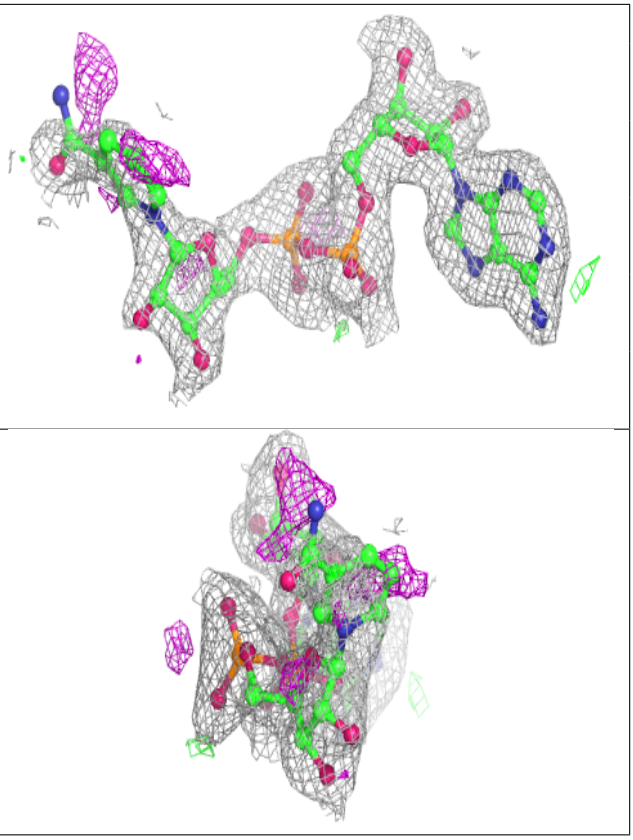
Electron density around NAD L 500:

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



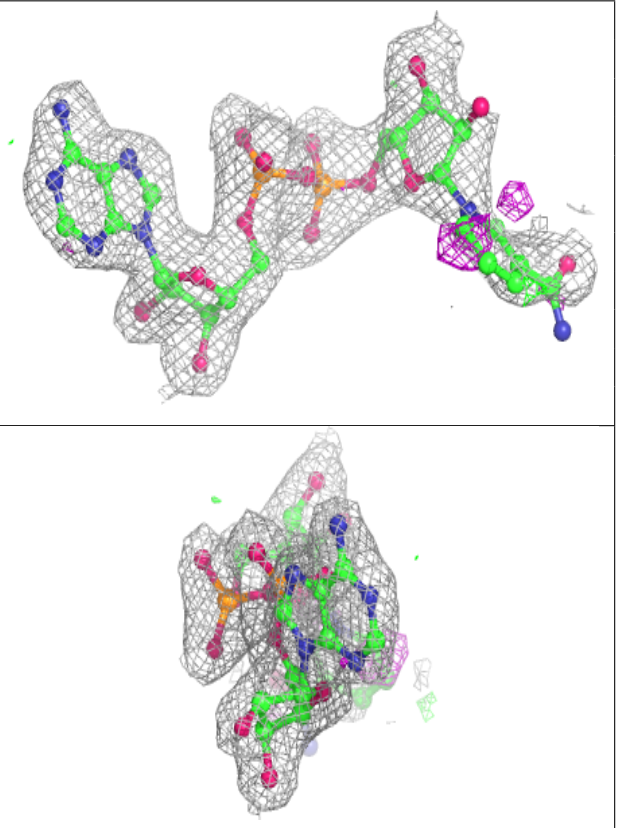
Electron density around NAD H 500:

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



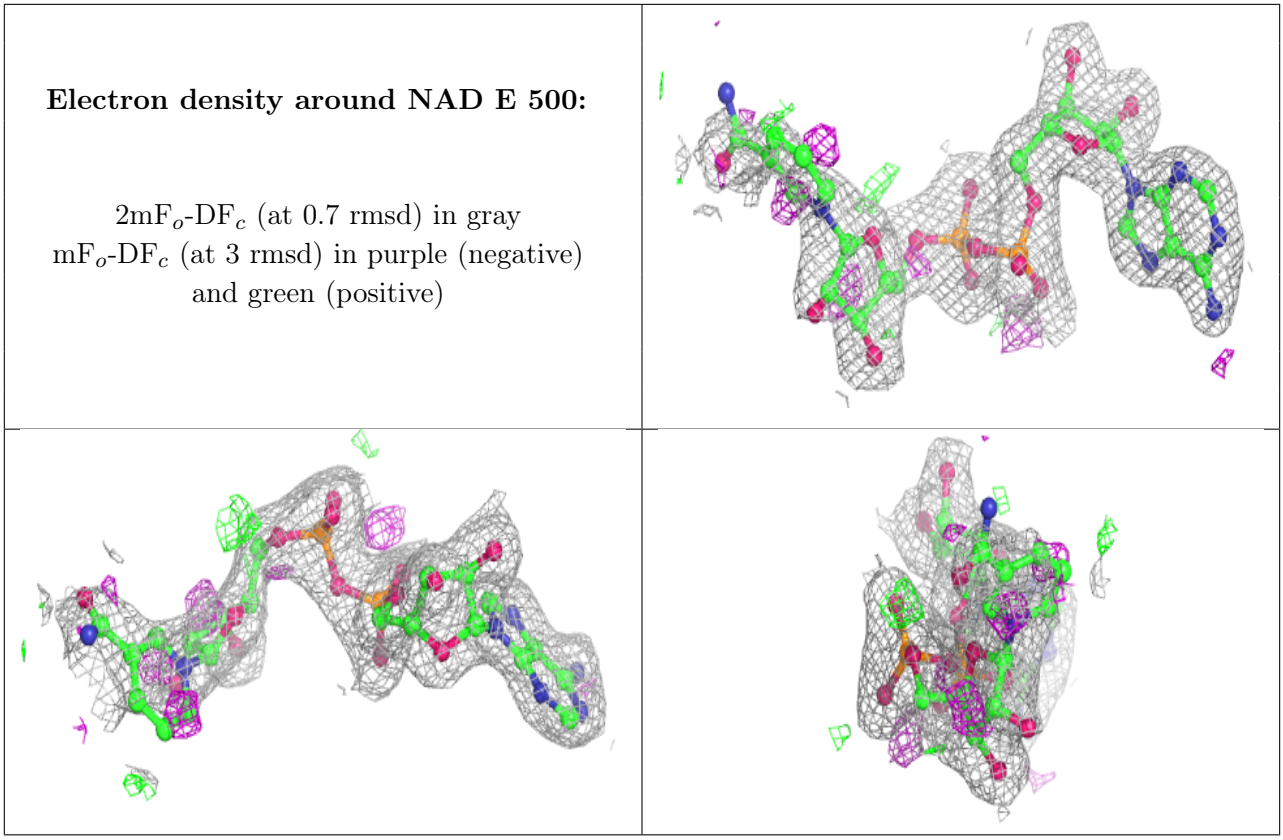
Electron density around NAD I 501:

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



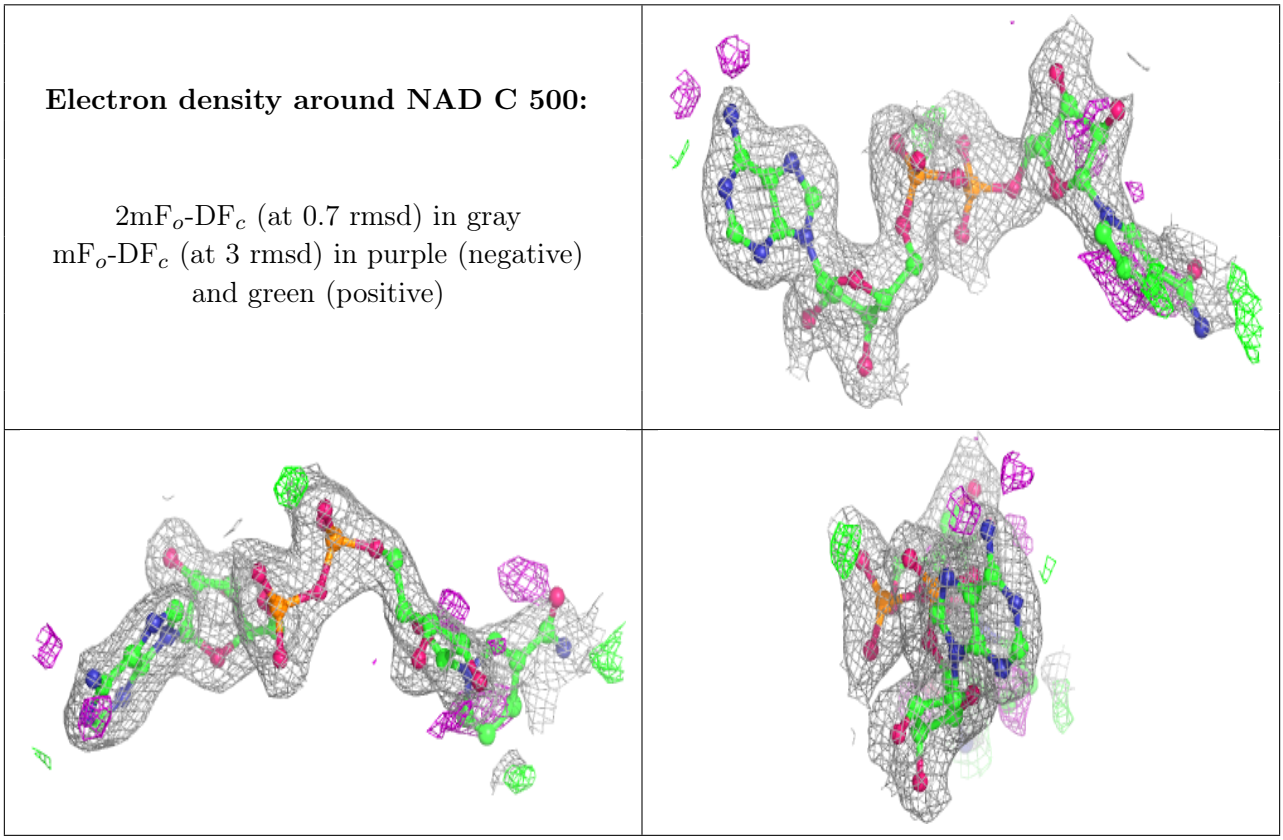
Electron density around NAD E 500:

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



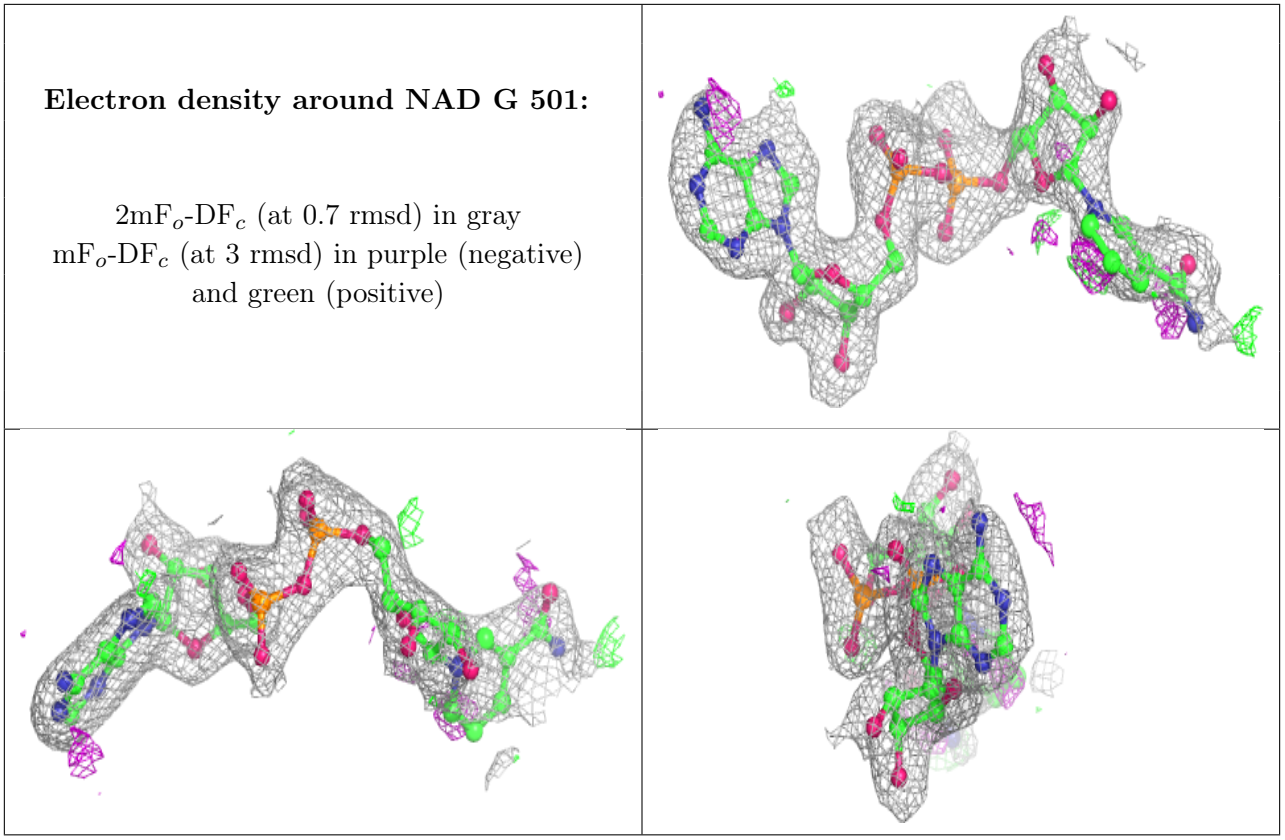
Electron density around NAD C 500:

$2mF_o$-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 501:

$2mF_o$-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.