Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 02:03 PM EDT

PDB ID	:	5JXW
Title	:	2.25 Angstrom Crystal Structure of S-adenosylhomocysteinase from Cryptosporidium parvum in Complex with Neplanocin-A and NAD
Authors	:	Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Dubrovska, I.; Bishop, B.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2016-05-13
Resolution	:	2.25 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 ⓘ 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:

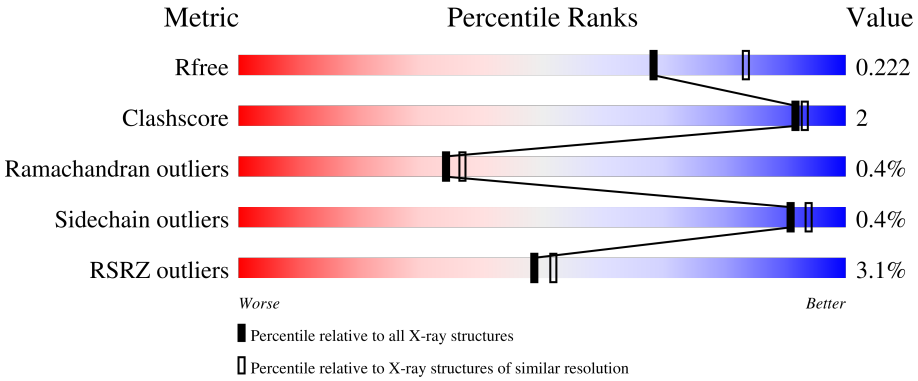
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	498	2% 93% 5%
1	B	498	4% 91% 6%
1	C	498	3% 93%
1	D	498	3% 95%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16584 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.

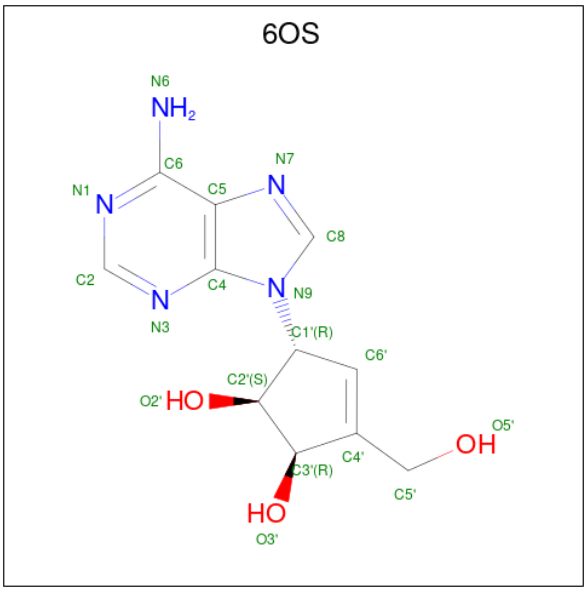
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	7	0
			3896	2475	649	742	30			
1	B	486	Total	C	N	O	S	0	2	0
			3855	2452	642	732	29			
1	C	486	Total	C	N	O	S	0	2	0
			3852	2446	644	734	28			
1	D	491	Total	C	N	O	S	0	1	0
			3884	2468	648	739	29			

There are 12 discrepancies between the modelled and reference sequences:

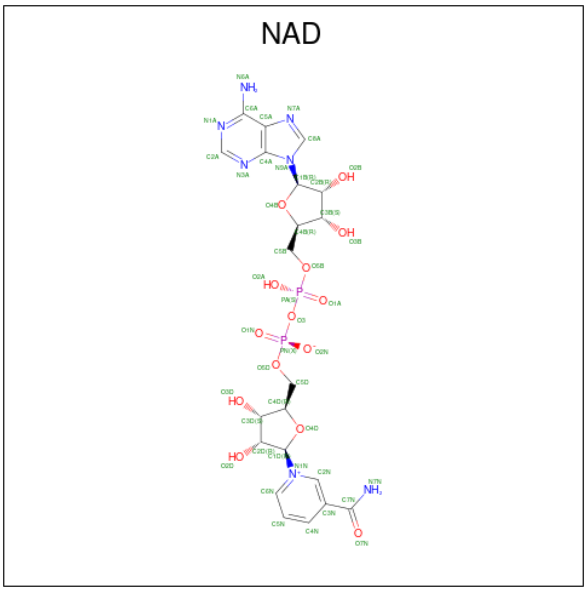
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5CPH1
A	-1	ASN	-	expression tag	UNP Q5CPH1
A	0	ALA	-	expression tag	UNP Q5CPH1
B	-2	SER	-	expression tag	UNP Q5CPH1
B	-1	ASN	-	expression tag	UNP Q5CPH1
B	0	ALA	-	expression tag	UNP Q5CPH1
C	-2	SER	-	expression tag	UNP Q5CPH1
C	-1	ASN	-	expression tag	UNP Q5CPH1
C	0	ALA	-	expression tag	UNP Q5CPH1
D	-2	SER	-	expression tag	UNP Q5CPH1
D	-1	ASN	-	expression tag	UNP Q5CPH1
D	0	ALA	-	expression tag	UNP Q5CPH1

- Molecule 2 is Neplanocin-A (three-letter code: 6OS) (formula: $C_{11}H_{13}N_5O_3$).



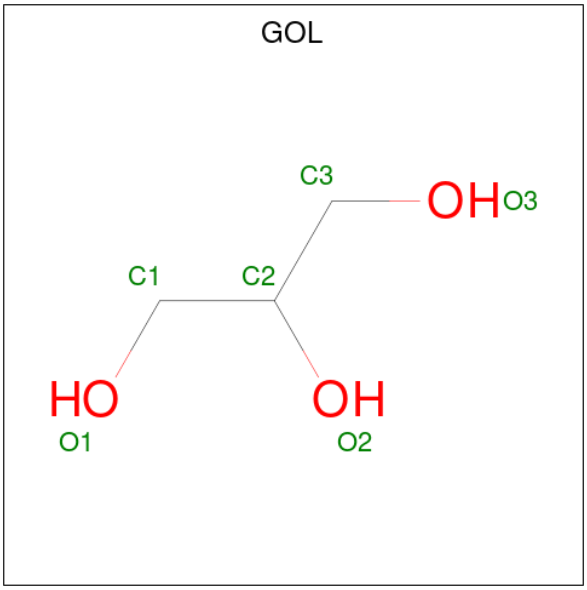
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 19 11 5 3	0	0
2	B	1	Total C N O 19 11 5 3	0	0
2	C	1	Total C N O 19 11 5 3	0	0
2	D	1	Total C N O 19 11 5 3	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



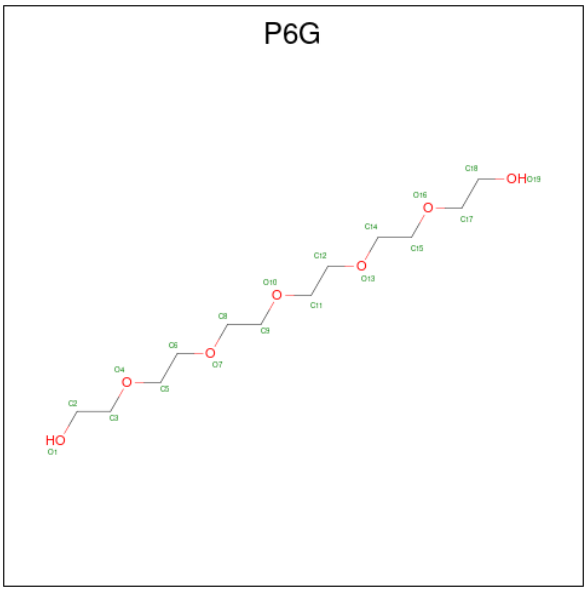
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



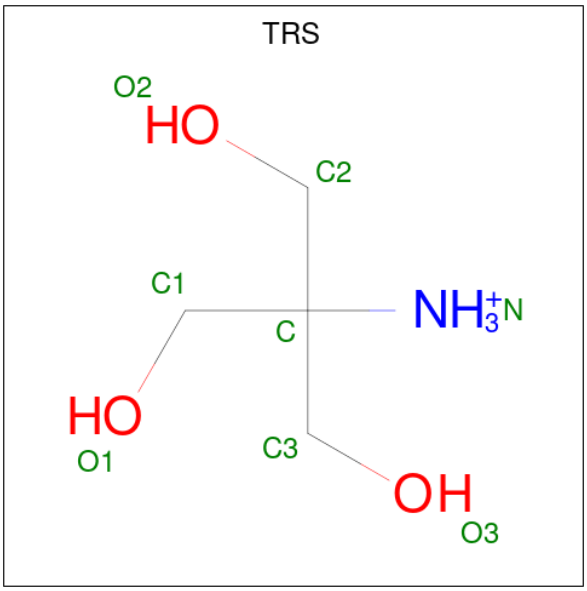
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 19 12 7	0	0
5	D	1	Total C O 19 12 7	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 8 4 1 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O 8 4 1 3	0	0
6	D	1	Total C N O 8 4 1 3	0	0

- Molecule 7 is water.

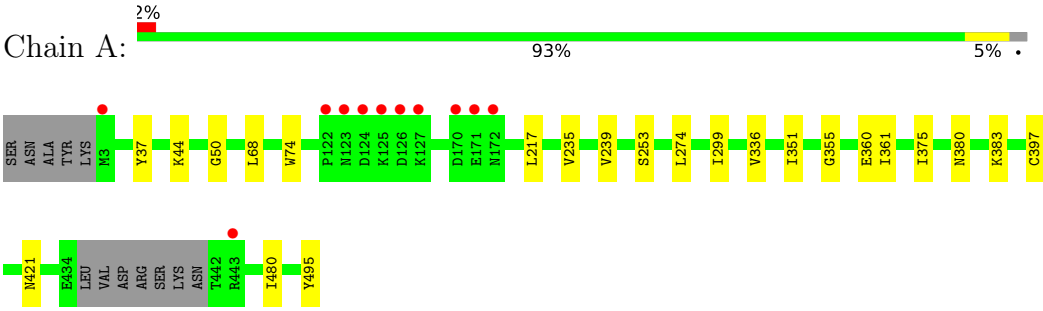
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	209	Total O 209 209	0	0
7	B	174	Total O 176 176	0	2
7	C	150	Total O 152 152	0	2
7	D	221	Total O 222 222	0	1

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.

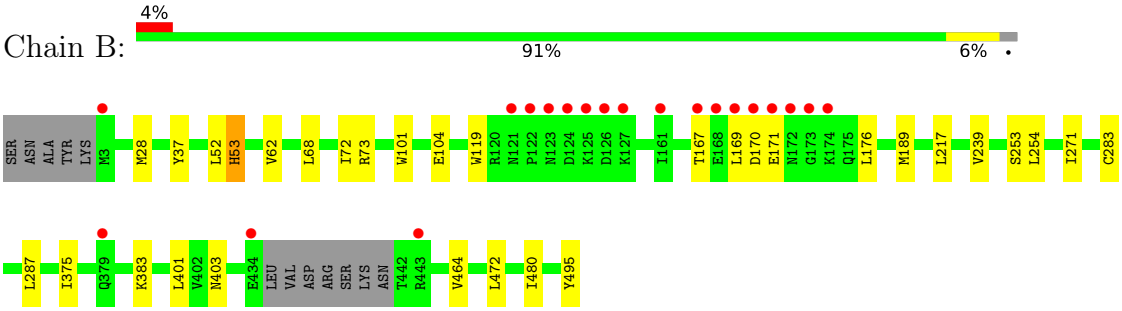
• Molecule 1: Adenosylhomocysteinase

Chain A:



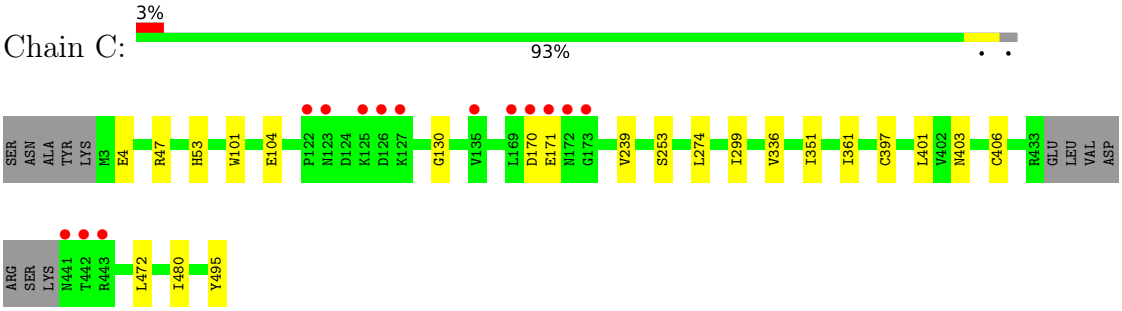
• Molecule 1: Adenosylhomocysteinase

Chain B:



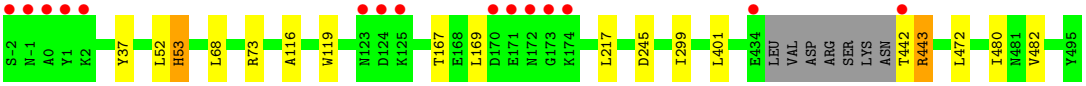
• Molecule 1: Adenosylhomocysteinase

Chain C:



• Molecule 1: Adenosylhomocysteinase

Chain D:


S-2
N-1
A0
Y1
K2
Y37
L52
H53
L68
R73
A116
W119
N123
D124
K125
T167
E168
L169
D170
E171
N172
G173
K174
L217
D245
I299
L401
E434
LEU
VAL
ASP
ARG
SER
LYS
ASN
T442
R443
L472
I480
N481
V482
Y495

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.89Å 136.49Å 107.81Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	29.93 – 2.25 29.93 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.93-2.25) 99.7 (29.93-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.173 , 0.221 0.177 , 0.222	Depositor DCC
R_{free} test set	4857 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16584	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, NAD, 6OS, P6G, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.45	0/3959	0.68	0/5336
1	B	0.43	0/3919	0.67	0/5284
1	C	0.42	0/3915	0.67	0/5280
1	D	0.47	0/3948	0.70	0/5323
All	All	0.44	0/15741	0.68	0/21223

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3896	0	3941	15	0
1	B	3855	0	3902	19	0
1	C	3852	0	3896	11	0
1	D	3884	0	3935	10	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	0	0
2	D	19	0	0	0	0
3	A	44	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
4	D	6	0	8	0	0
5	B	19	0	26	0	0
5	D	19	0	26	0	0
6	B	8	0	12	0	0
6	C	8	0	12	0	0
6	D	8	0	12	0	0
7	A	209	0	0	0	0
7	B	176	0	0	0	0
7	C	152	0	0	0	0
7	D	222	0	0	0	0
All	All	16584	0	15898	49	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 2.

All (49) 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:C:47:ARG:NH1	1:C:130:GLY:O	2.28	0.67
1:A:397:CYS:HG	1:A:406:CYS:HG	1.39	0.64
1:C:480:ILE:HA	1:D:217:LEU:HD21	1.81	0.60
1:D:73:ARG:HG2	1:D:119:TRP:CZ2	2.37	0.60
1:A:37:TYR:HB2	1:A:68:LEU:HD22	1.84	0.59
1:A:217:LEU:HD21	1:B:480:ILE:HA	1.86	0.57
1:B:73:ARG:HG2	1:B:119:TRP:CZ2	2.40	0.56
1:B:28[B]:MET:HG3	1:B:464:VAL:HG23	1.89	0.55
1:B:28[B]:MET:HG3	1:B:464:VAL:CG2	2.37	0.53
1:C:101:TRP:O	1:C:104:GLU:HG3	2.09	0.53
1:A:375:ILE:HD11	1:A:383:LYS:HE2	1.91	0.53
1:B:101:TRP:O	1:B:104:GLU:HG3	2.10	0.52
1:C:4[B]:GLU:HG2	1:C:4[B]:GLU:O	2.09	0.52
1:C:397:CYS:SG	1:C:406:CYS:SG	3.08	0.51
1:A:380:ASN:OD1	1:A:380:ASN:N	2.44	0.51
1:B:170:ASP:HB2	1:B:176:LEU:HD21	1.91	0.51
1:A:253:SER:HB2	1:A:403:ASN:HB2	1.94	0.48
1:B:239:VAL:HG21	1:B:495:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:VAL:HG21	1:C:495:TYR:CE1	2.50	0.47
1:A:37:TYR:CB	1:A:68:LEU:HD22	2.44	0.46
1:C:299:ILE:HD13	1:D:472:LEU:HD21	1.97	0.46
1:B:37:TYR:HB2	1:B:68:LEU:HD22	1.97	0.45
1:C:274:LEU:HD22	1:C:336:VAL:HG12	1.99	0.45
1:B:271:ILE:HG21	1:B:287:LEU:HD13	1.99	0.45
1:B:375:ILE:HD11	1:B:383:LYS:HE2	1.98	0.45
1:D:442:THR:O	1:D:443:ARG:CB	2.64	0.45
1:D:480:ILE:HG13	1:D:482:VAL:HG22	1.99	0.45
1:B:73:ARG:HD3	1:B:119:TRP:CE2	2.52	0.44
1:D:37:TYR:HB2	1:D:68:LEU:HD22	1.99	0.44
1:A:239:VAL:HG21	1:A:495:TYR:CE1	2.52	0.44
1:A:480:ILE:HA	1:B:217:LEU:HD21	1.99	0.44
1:B:37:TYR:CB	1:B:68:LEU:HD22	2.48	0.43
1:A:274:LEU:HD22	1:A:336:VAL:HG12	1.99	0.43
1:B:62:VAL:HG13	1:B:72:ILE:HG21	1.99	0.43
1:A:355:GLY:HA3	1:A:360:GLU:OE1	2.20	0.42
1:A:235:VAL:HG13	1:A:421:ASN:HB3	2.01	0.42
1:A:299:ILE:HD13	1:B:472:LEU:HD21	2.02	0.41
1:B:52:LEU:O	1:B:53:HIS:C	2.59	0.41
1:A:351:ILE:HG22	1:A:361:ILE:HD13	2.03	0.41
1:C:472:LEU:HD21	1:D:299:ILE:HD13	2.02	0.41
1:D:73:ARG:HG3	1:D:116:ALA:O	2.20	0.41
1:A:50:GLY:HA3	1:A:74:TRP:CE3	2.55	0.41
1:B:253:SER:HB2	1:B:403:ASN:HB2	2.01	0.41
1:B:254:LEU:HD22	1:B:283:CYS:SG	2.61	0.41
1:C:253:SER:HB2	1:C:403:ASN:HB2	2.03	0.41
1:D:52:LEU:O	1:D:53:HIS:C	2.58	0.41
1:B:167:THR:HG22	1:B:169:LEU:H	1.86	0.41
1:C:351:ILE:HG22	1:C:361:ILE:HD13	2.02	0.41
1:D:167:THR:HG22	1:D:169:LEU:H	1.86	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	489/498 (98%)	470 (96%)	19 (4%)	0	100	100
1	B	484/498 (97%)	469 (97%)	13 (3%)	2 (0%)	34	37
1	C	484/498 (97%)	466 (96%)	15 (3%)	3 (1%)	25	25
1	D	488/498 (98%)	469 (96%)	17 (4%)	2 (0%)	34	37
All	All	1945/1992 (98%)	1874 (96%)	64 (3%)	7 (0%)	34	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	GLU
1	D	443	ARG
1	B	53	HIS
1	C	53	HIS
1	C	170	ASP
1	C	171	GLU
1	D	53	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	431/435 (99%)	430 (100%)	1 (0%)	93	96
1	B	426/435 (98%)	424 (100%)	2 (0%)	88	92
1	C	426/435 (98%)	425 (100%)	1 (0%)	93	96
1	D	429/435 (99%)	427 (100%)	2 (0%)	88	92
All	All	1712/1740 (98%)	1706 (100%)	6 (0%)	91	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS

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Mol	Chain	Res	Type
1	B	189	MET
1	B	401	LEU
1	C	401	LEU
1	D	245	ASP
1	D	401	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	C	502	-	42,48,48	0.85	3 (7%)	50,73,73	1.22	6 (12%)
3	NAD	A	502	-	42,48,48	0.86	2 (4%)	50,73,73	1.23	5 (10%)
2	6OS	C	501	-	18,21,21	1.00	1 (5%)	11,31,31	1.68	3 (27%)
4	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.19	0
2	6OS	D	501	-	18,21,21	0.99	1 (5%)	11,31,31	1.70	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAD	B	502	-	42,48,48	0.86	2 (4%)	50,73,73	1.31	6 (12%)
4	GOL	D	505	-	5,5,5	0.23	0	5,5,5	0.22	0
3	NAD	D	502	-	42,48,48	0.87	2 (4%)	50,73,73	1.25	7 (14%)
2	6OS	A	501	-	18,21,21	1.03	1 (5%)	11,31,31	1.68	3 (27%)
6	TRS	B	504	-	7,7,7	0.28	0	9,9,9	0.20	0
2	6OS	B	501	-	18,21,21	0.95	1 (5%)	11,31,31	1.72	3 (27%)
4	GOL	B	505	-	5,5,5	0.29	0	5,5,5	0.18	0
6	TRS	C	503	-	7,7,7	0.33	0	9,9,9	0.22	0
5	P6G	D	503	-	18,18,18	0.55	0	17,17,17	0.40	0
6	TRS	D	504	-	7,7,7	0.27	0	9,9,9	0.15	0
5	P6G	B	503	-	18,18,18	0.54	0	17,17,17	0.40	0
4	GOL	A	503	-	5,5,5	0.29	0	5,5,5	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	502	-	-	5/26/62/62	0/5/5/5
3	NAD	A	502	-	-	5/26/62/62	0/5/5/5
2	6OS	C	501	-	-	2/2/22/22	0/3/3/3
4	GOL	A	504	-	-	2/4/4/4	-
2	6OS	D	501	-	-	2/2/22/22	0/3/3/3
3	NAD	B	502	-	-	5/26/62/62	0/5/5/5
4	GOL	D	505	-	-	1/4/4/4	-
3	NAD	D	502	-	-	5/26/62/62	0/5/5/5
2	6OS	A	501	-	-	2/2/22/22	0/3/3/3
6	TRS	B	504	-	-	5/9/9/9	-
2	6OS	B	501	-	-	2/2/22/22	0/3/3/3
4	GOL	B	505	-	-	1/4/4/4	-
6	TRS	C	503	-	-	1/9/9/9	-
5	P6G	D	503	-	-	10/16/16/16	-
6	TRS	D	504	-	-	6/9/9/9	-
5	P6G	B	503	-	-	8/16/16/16	-
4	GOL	A	503	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	NAD	O4D-C1D	2.44	1.44	1.41
3	C	502	NAD	O4D-C1D	2.39	1.44	1.41
2	D	501	6OS	C5-C4	2.27	1.46	1.40
3	D	502	NAD	O4D-C1D	2.25	1.44	1.41
3	B	502	NAD	C5A-C4A	2.25	1.46	1.40
2	A	501	6OS	C5-C4	2.23	1.46	1.40
3	B	502	NAD	O4D-C1D	2.23	1.44	1.41
2	C	501	6OS	C5-C4	2.22	1.46	1.40
2	B	501	6OS	C5-C4	2.20	1.46	1.40
3	C	502	NAD	C5A-C4A	2.16	1.46	1.40
3	D	502	NAD	C5A-C4A	2.13	1.46	1.40
3	A	502	NAD	C5A-C4A	2.07	1.46	1.40
3	C	502	NAD	C2A-N3A	2.04	1.35	1.32

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	NAD	N3A-C2A-N1A	-4.00	122.42	128.68
3	C	502	NAD	N3A-C2A-N1A	-3.93	122.53	128.68
3	D	502	NAD	N3A-C2A-N1A	-3.82	122.70	128.68
3	A	502	NAD	N3A-C2A-N1A	-3.73	122.86	128.68
2	D	501	6OS	N3-C2-N1	-3.63	123.00	128.68
2	B	501	6OS	N3-C2-N1	-3.52	123.17	128.68
2	A	501	6OS	N3-C2-N1	-3.43	123.32	128.68
2	C	501	6OS	N3-C2-N1	-3.38	123.39	128.68
3	B	502	NAD	PN-O3-PA	-3.20	121.85	132.83
3	C	502	NAD	PN-O3-PA	-3.03	122.41	132.83
3	D	502	NAD	PN-O3-PA	-3.02	122.48	132.83
2	C	501	6OS	C4-C5-N7	-2.89	106.38	109.40
3	B	502	NAD	C3N-C7N-N7N	2.83	121.15	117.75
3	A	502	NAD	PN-O3-PA	-2.83	123.12	132.83
3	A	502	NAD	C3N-C7N-N7N	2.81	121.12	117.75
3	B	502	NAD	C4A-C5A-N7A	-2.71	106.57	109.40
3	D	502	NAD	C3N-C7N-N7N	2.67	120.95	117.75
3	C	502	NAD	C4A-C5A-N7A	-2.64	106.65	109.40
3	B	502	NAD	C1B-N9A-C4A	-2.54	122.18	126.64
2	B	501	6OS	C4-C5-N7	-2.49	106.81	109.40
2	D	501	6OS	C4-C5-N7	-2.45	106.84	109.40
3	A	502	NAD	C4A-C5A-N7A	-2.42	106.87	109.40
3	C	502	NAD	C2N-N1N-C1D	-2.37	113.86	119.14
3	B	502	NAD	C2A-N1A-C6A	2.35	122.77	118.75
2	A	501	6OS	C4-C5-N7	-2.32	106.98	109.40
3	D	502	NAD	C4A-C5A-N7A	-2.27	107.03	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	6OS	C2-N1-C6	2.27	122.63	118.75
2	A	501	6OS	C2-N1-C6	2.17	122.47	118.75
3	C	502	NAD	C2A-N1A-C6A	2.15	122.43	118.75
3	C	502	NAD	C1B-N9A-C4A	-2.14	122.89	126.64
2	C	501	6OS	C2-N1-C6	2.10	122.34	118.75
3	D	502	NAD	C2A-N1A-C6A	2.05	122.25	118.75
3	D	502	NAD	C1B-N9A-C4A	-2.04	123.05	126.64
3	A	502	NAD	C2N-N1N-C1D	-2.03	114.61	119.14
3	D	502	NAD	C2N-N1N-C1D	-2.02	114.63	119.14
2	B	501	6OS	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	6OS	C3'-C4'-C5'-O5'
2	A	501	6OS	C6'-C4'-C5'-O5'
2	B	501	6OS	C3'-C4'-C5'-O5'
2	B	501	6OS	C6'-C4'-C5'-O5'
2	C	501	6OS	C3'-C4'-C5'-O5'
2	D	501	6OS	C3'-C4'-C5'-O5'
2	D	501	6OS	C6'-C4'-C5'-O5'
3	A	502	NAD	O4D-C1D-N1N-C2N
3	A	502	NAD	O4D-C1D-N1N-C6N
3	A	502	NAD	C2D-C1D-N1N-C2N
3	A	502	NAD	C2D-C1D-N1N-C6N
3	B	502	NAD	O4D-C1D-N1N-C2N
3	B	502	NAD	O4D-C1D-N1N-C6N
3	B	502	NAD	C2D-C1D-N1N-C2N
3	B	502	NAD	C2D-C1D-N1N-C6N
3	C	502	NAD	O4D-C1D-N1N-C2N
3	C	502	NAD	O4D-C1D-N1N-C6N
3	C	502	NAD	C2D-C1D-N1N-C2N
3	C	502	NAD	C2D-C1D-N1N-C6N
3	D	502	NAD	O4D-C1D-N1N-C2N
3	D	502	NAD	O4D-C1D-N1N-C6N
3	D	502	NAD	C2D-C1D-N1N-C2N
3	D	502	NAD	C2D-C1D-N1N-C6N
4	A	504	GOL	O1-C1-C2-C3
6	B	504	TRS	N-C-C3-O3
6	D	504	TRS	N-C-C1-O1
6	D	504	TRS	N-C-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	503	P6G	C5-C6-O7-C8
5	B	503	P6G	O16-C17-C18-O19
5	B	503	P6G	O13-C14-C15-O16
5	D	503	P6G	O10-C11-C12-O13
5	B	503	P6G	O4-C5-C6-O7
5	B	503	P6G	O7-C8-C9-O10
5	D	503	P6G	C18-C17-O16-C15
5	B	503	P6G	O1-C2-C3-O4
6	B	504	TRS	C1-C-C3-O3
6	D	504	TRS	C3-C-C1-O1
6	D	504	TRS	C2-C-C3-O3
5	D	503	P6G	O7-C8-C9-O10
4	A	504	GOL	O1-C1-C2-O2
3	C	502	NAD	O4B-C4B-C5B-O5B
6	B	504	TRS	C3-C-C2-O2
6	B	504	TRS	N-C-C2-O2
2	C	501	6OS	C6'-C4'-C5'-O5'
5	D	503	P6G	C9-C8-O7-C6
5	D	503	P6G	O1-C2-C3-O4
5	B	503	P6G	C15-C14-O13-C12
5	D	503	P6G	O4-C5-C6-O7
3	A	502	NAD	O4B-C4B-C5B-O5B
3	B	502	NAD	O4B-C4B-C5B-O5B
5	D	503	P6G	C14-C15-O16-C17
6	B	504	TRS	C2-C-C3-O3
6	C	503	TRS	C2-C-C3-O3
5	B	503	P6G	C8-C9-O10-C11
4	B	505	GOL	O1-C1-C2-O2
5	D	503	P6G	C11-C12-O13-C14
6	D	504	TRS	C2-C-C1-O1
6	D	504	TRS	C1-C-C3-O3
4	D	505	GOL	O1-C1-C2-C3
3	D	502	NAD	O4B-C4B-C5B-O5B
5	D	503	P6G	O16-C17-C18-O19
5	D	503	P6G	O13-C14-C15-O16

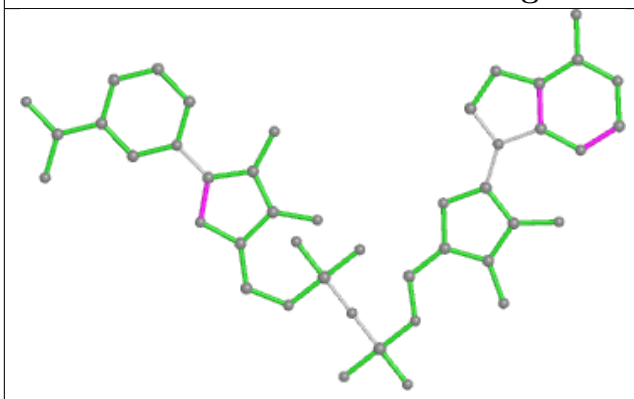
There are no ring outliers.

No monomer is involved in short contacts.

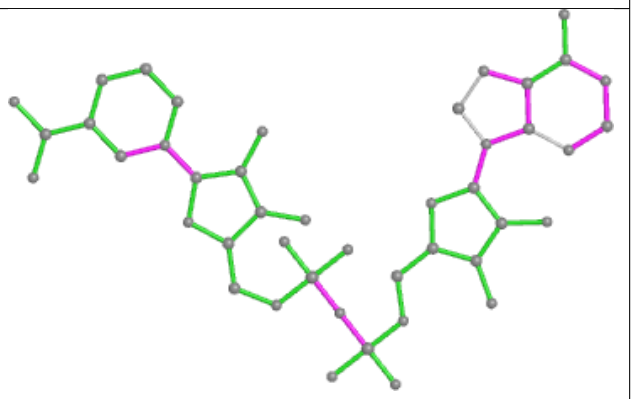
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

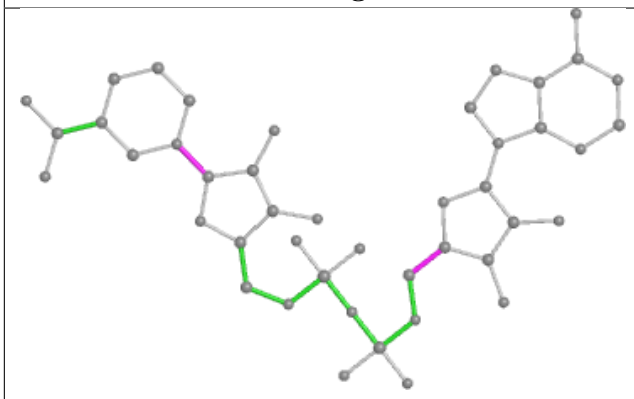
Ligand NAD C 502



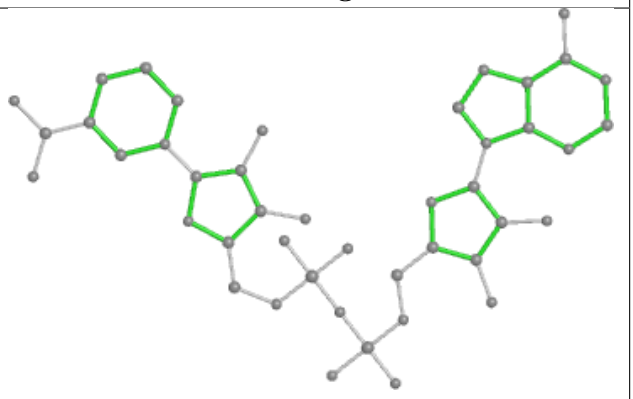
Bond lengths



Bond angles

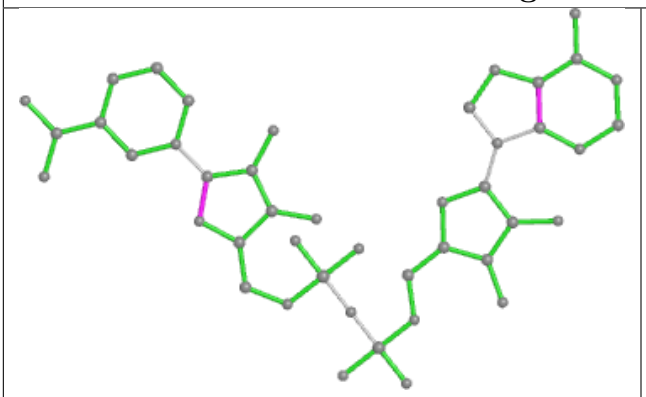


Torsions



Rings

Ligand NAD A 502



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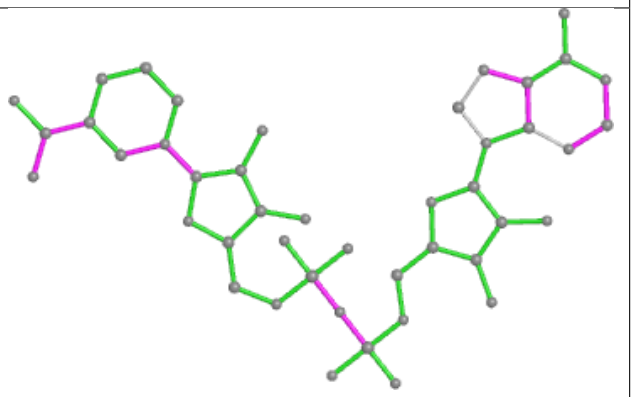

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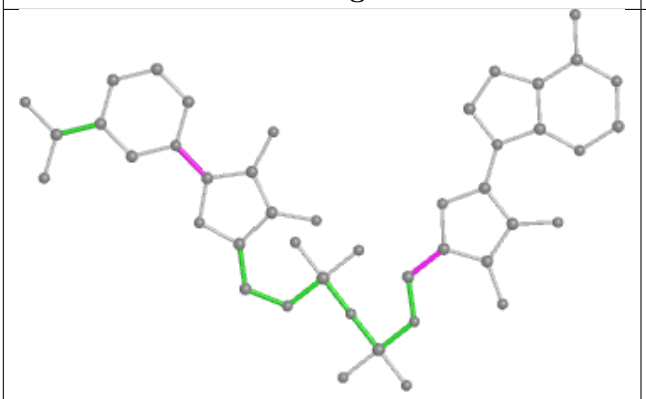

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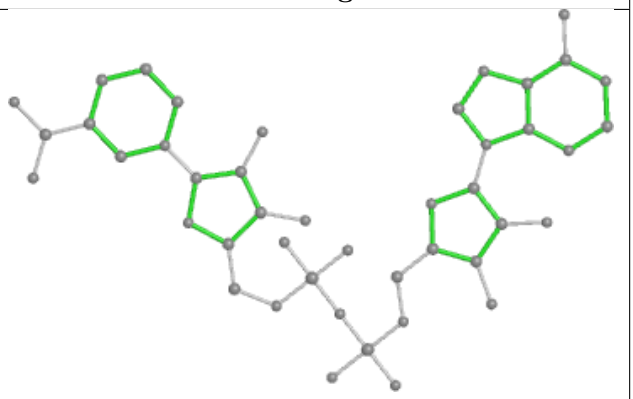
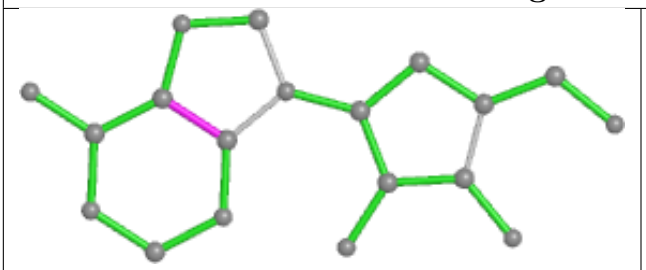


Rings

Ligand 6OS C 501



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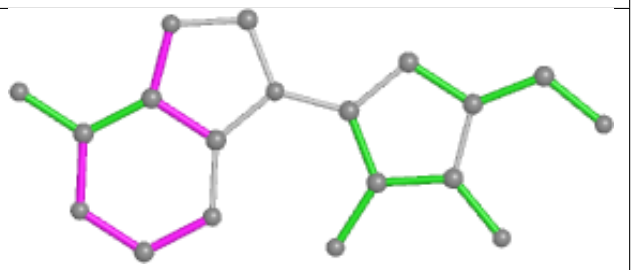

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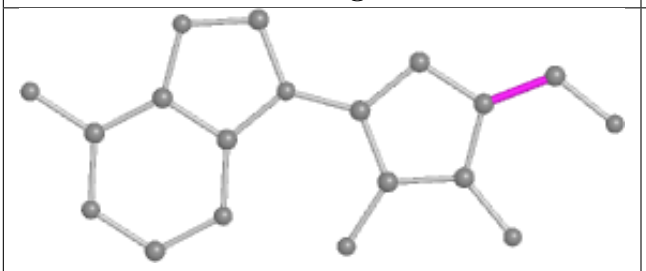

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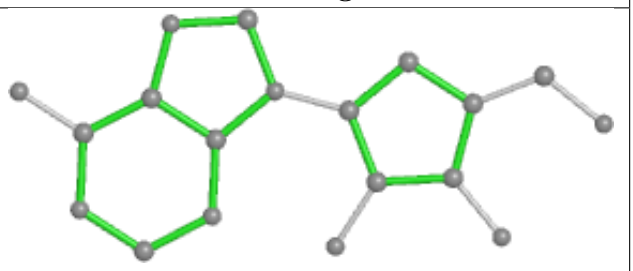
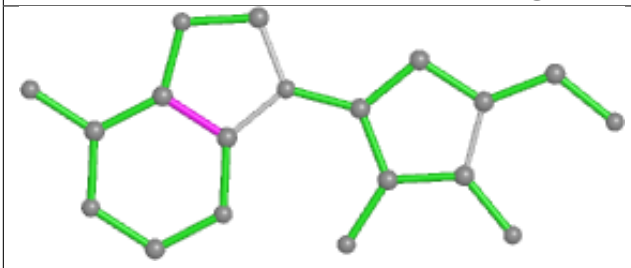


Rings

Ligand 6OS D 501



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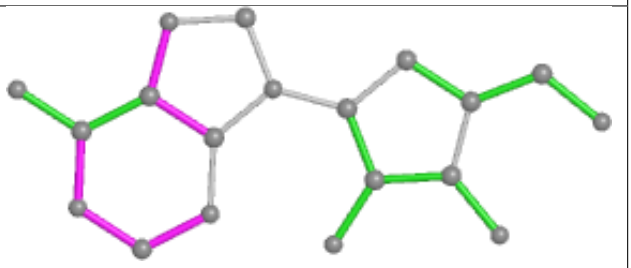
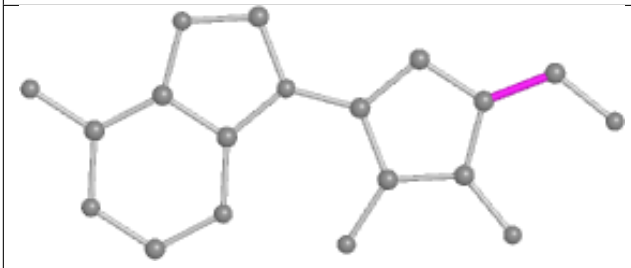


Bond angles



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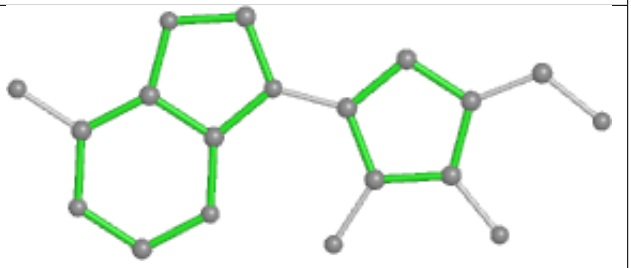
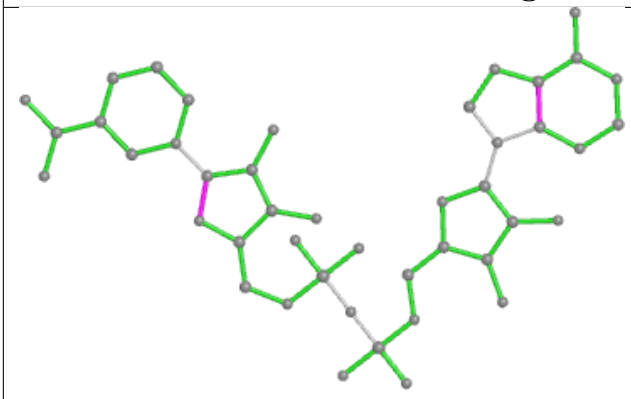
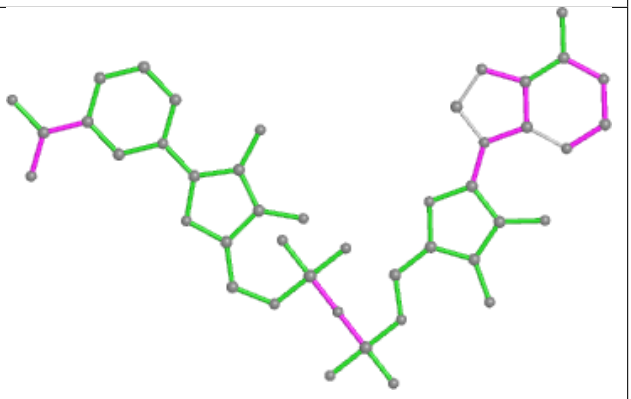


Rings

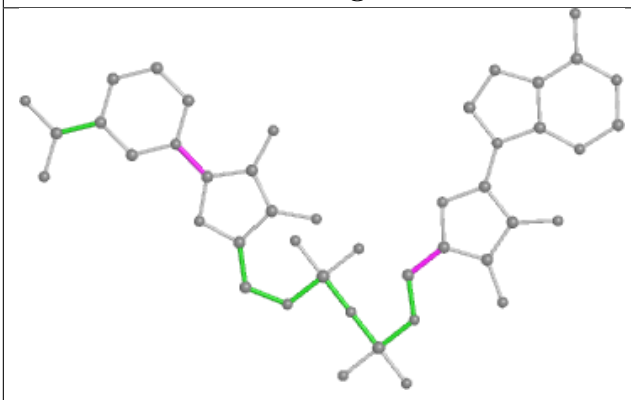
Ligand NAD B 502



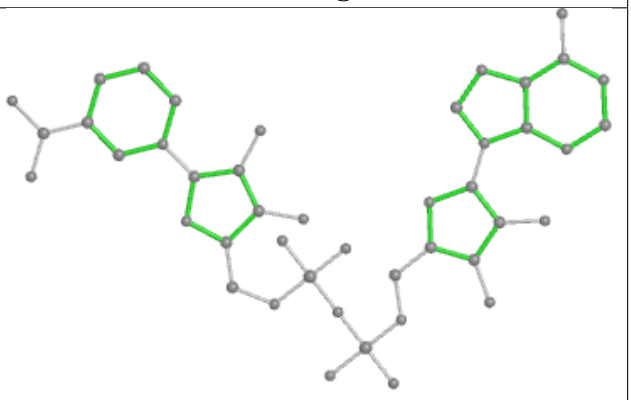
Bond lengths



Bond angles

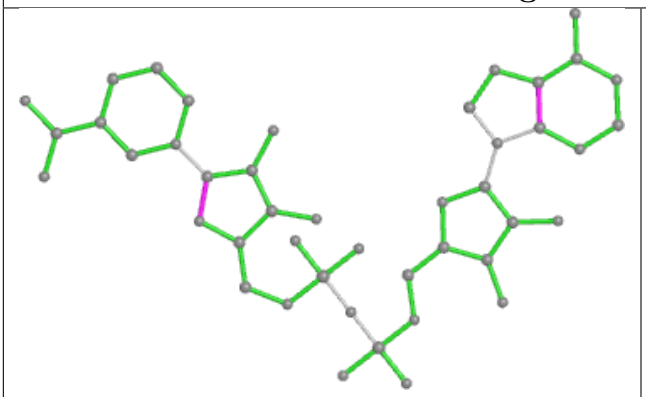


Torsions

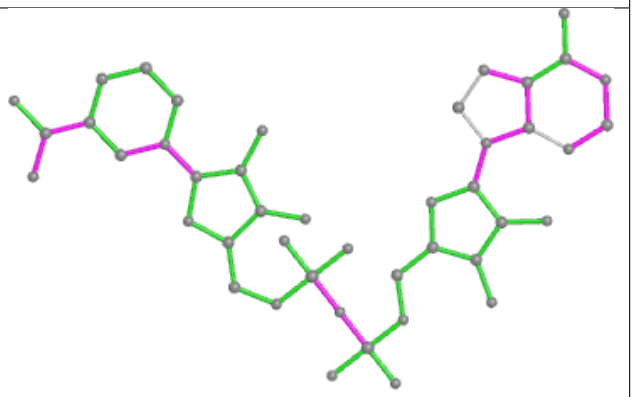


Rings

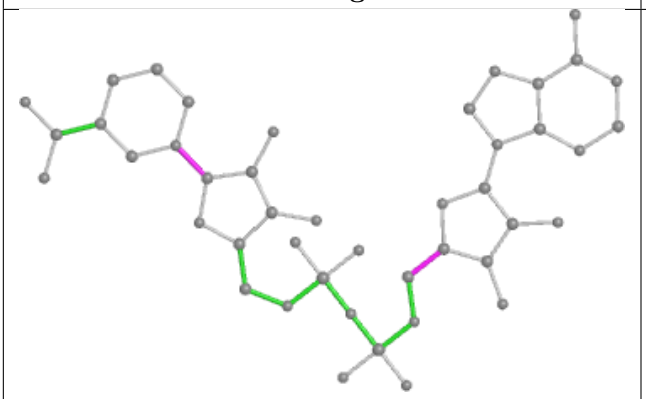
Ligand NAD D 502



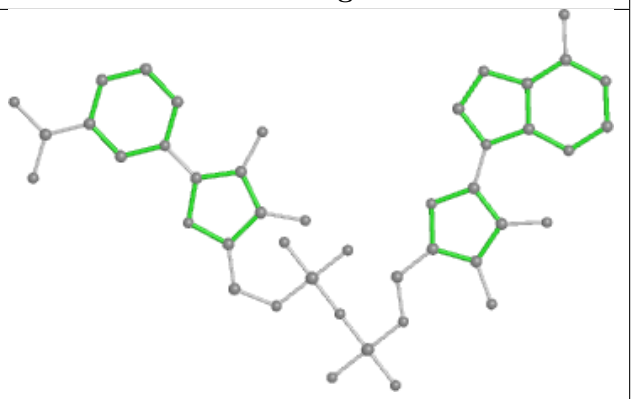
Bond lengths



Bond angles

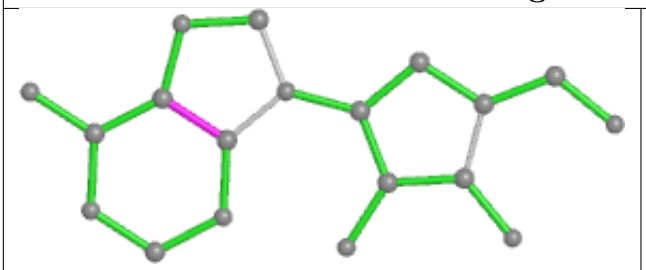


Torsions

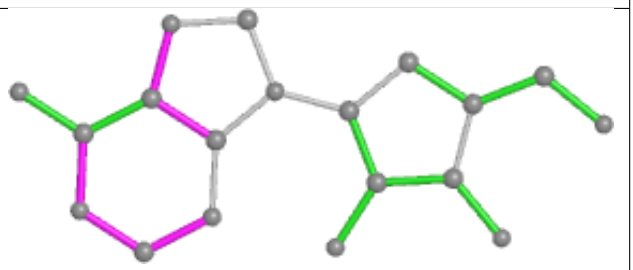


Rings

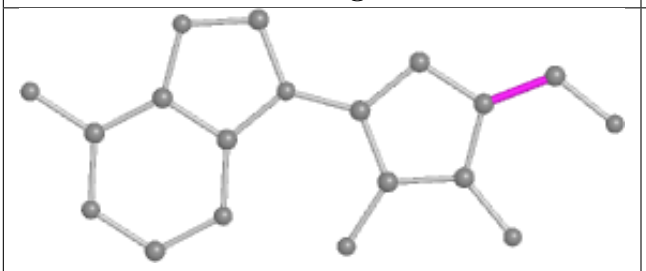
Ligand 6OS A 501



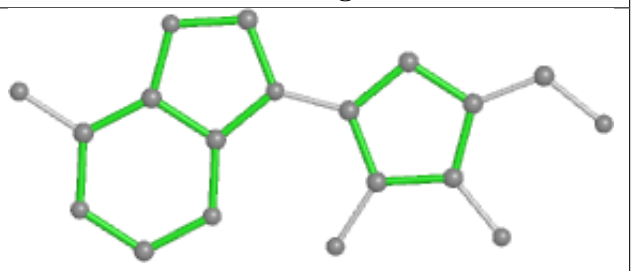
Bond lengths



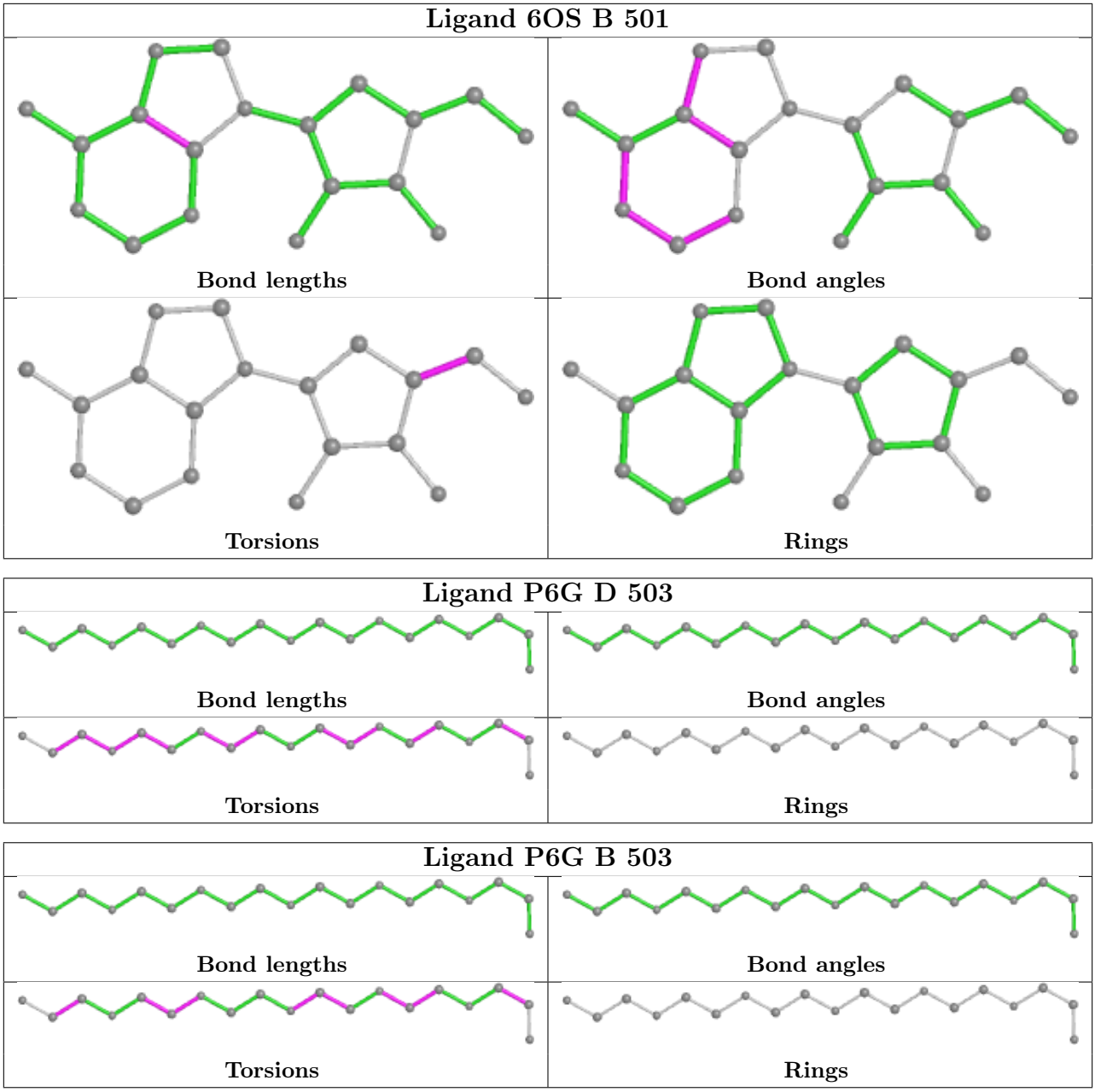
Bond angles



Torsions



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	486/498 (97%)	-0.36	11 (2%)	60	63	31, 40, 66, 133	0
1	B	486/498 (97%)	-0.18	20 (4%)	37	40	33, 47, 79, 140	0
1	C	486/498 (97%)	-0.13	14 (2%)	51	55	31, 50, 85, 129	0
1	D	491/498 (98%)	-0.34	15 (3%)	49	52	30, 40, 76, 123	0
All	All	1949/1992 (97%)	-0.25	60 (3%)	49	52	30, 44, 78, 140	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	MET	7.5
1	C	441	ASN	6.8
1	B	172	ASN	6.1
1	B	125	LYS	5.4
1	C	170	ASP	5.3
1	C	171	GLU	5.1
1	C	442	THR	5.0
1	D	171	GLU	5.0
1	B	434	GLU	4.7
1	D	434	GLU	4.6
1	C	126	ASP	4.5
1	B	122	PRO	4.4
1	B	124	ASP	4.4
1	B	121	ASN	4.3
1	A	123	ASN	4.2
1	B	173	GLY	4.2
1	C	123	ASN	4.1
1	B	126	ASP	4.1
1	C	122	PRO	4.1
1	A	126	ASP	4.1
1	C	172	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	-1	ASN	4.0
1	A	122	PRO	3.9
1	D	172	ASN	3.8
1	C	169	LEU	3.7
1	D	123	ASN	3.6
1	B	170	ASP	3.5
1	B	167	THR	3.5
1	B	123	ASN	3.4
1	A	3	MET	3.4
1	D	442	THR	3.4
1	B	171	GLU	3.4
1	C	443	ARG	3.4
1	D	124	ASP	3.3
1	C	127	LYS	3.3
1	A	125	LYS	3.2
1	D	173	GLY	3.1
1	C	173	GLY	3.0
1	A	171	GLU	2.9
1	A	172	ASN	2.9
1	C	125	LYS	2.9
1	B	169	LEU	2.7
1	D	0	ALA	2.7
1	D	125	LYS	2.6
1	C	135	VAL	2.6
1	A	127	LYS	2.6
1	B	168	GLU	2.6
1	D	2	LYS	2.6
1	B	443	ARG	2.5
1	B	174	LYS	2.5
1	D	174	LYS	2.3
1	B	127	LYS	2.3
1	D	170	ASP	2.3
1	D	1	TYR	2.3
1	B	379	GLN	2.2
1	A	170	ASP	2.2
1	B	161	ILE	2.2
1	D	-2	SER	2.2
1	A	124	ASP	2.1
1	A	443	ARG	2.1

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)

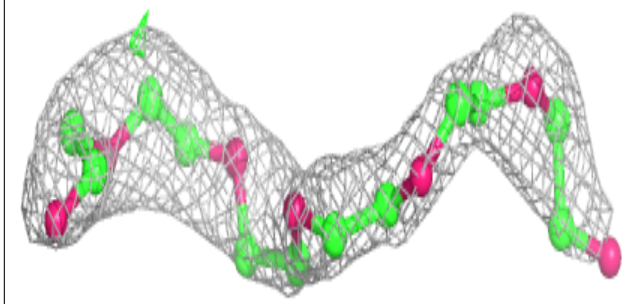
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

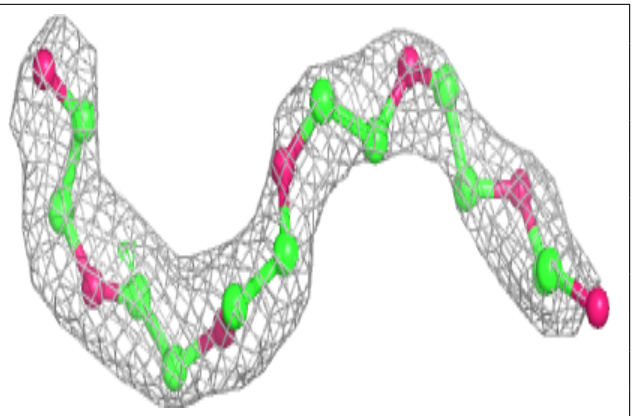
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	TRS	D	504	8/8	0.72	0.20	87,93,95,95	0
5	P6G	B	503	19/19	0.80	0.23	64,86,92,95	0
5	P6G	D	503	19/19	0.80	0.28	55,74,84,85	0
4	GOL	B	505	6/6	0.80	0.17	83,87,88,90	0
4	GOL	D	505	6/6	0.81	0.17	56,60,62,72	0
6	TRS	C	503	8/8	0.82	0.16	71,77,78,79	0
4	GOL	A	504	6/6	0.86	0.21	58,64,66,69	0
6	TRS	B	504	8/8	0.88	0.16	67,70,76,76	0
4	GOL	A	503	6/6	0.90	0.17	60,67,72,73	0
2	6OS	A	501	19/19	0.95	0.13	31,33,36,38	0
2	6OS	C	501	19/19	0.95	0.12	39,41,43,44	0
2	6OS	D	501	19/19	0.95	0.12	30,31,33,36	0
2	6OS	B	501	19/19	0.96	0.10	33,41,45,45	0
3	NAD	B	502	44/44	0.97	0.12	32,36,40,43	0
3	NAD	A	502	44/44	0.97	0.15	27,34,39,43	0
3	NAD	D	502	44/44	0.98	0.12	27,34,38,42	0
3	NAD	C	502	44/44	0.98	0.13	32,37,40,43	0

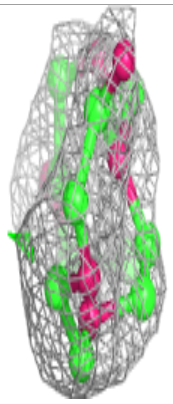
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G B 503:

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

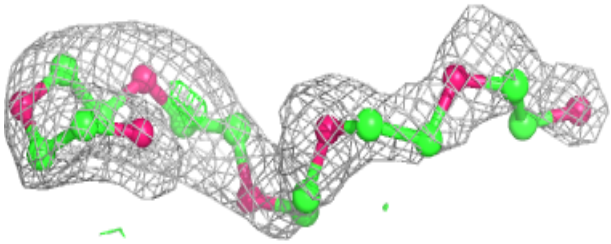


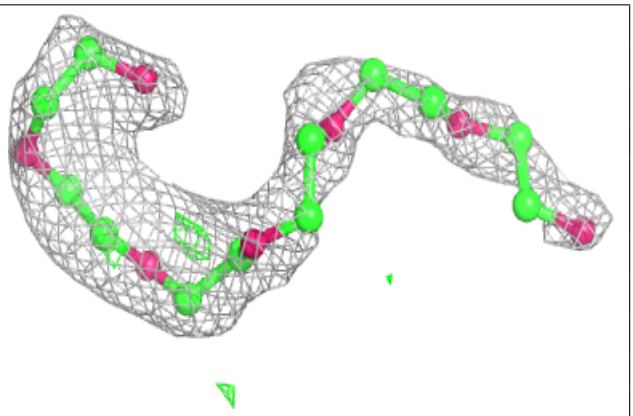


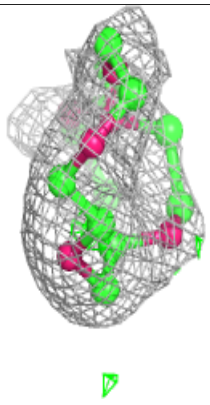


Electron density around P6G D 503:

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

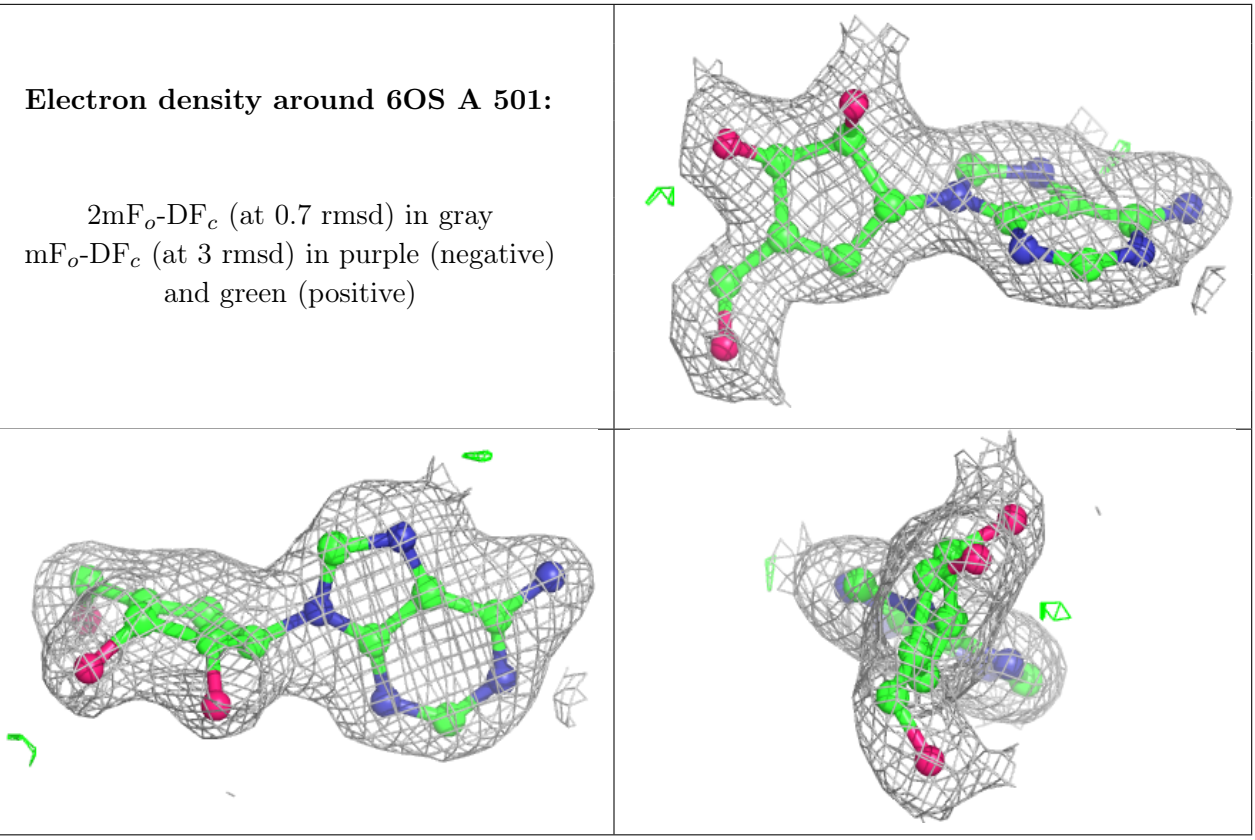






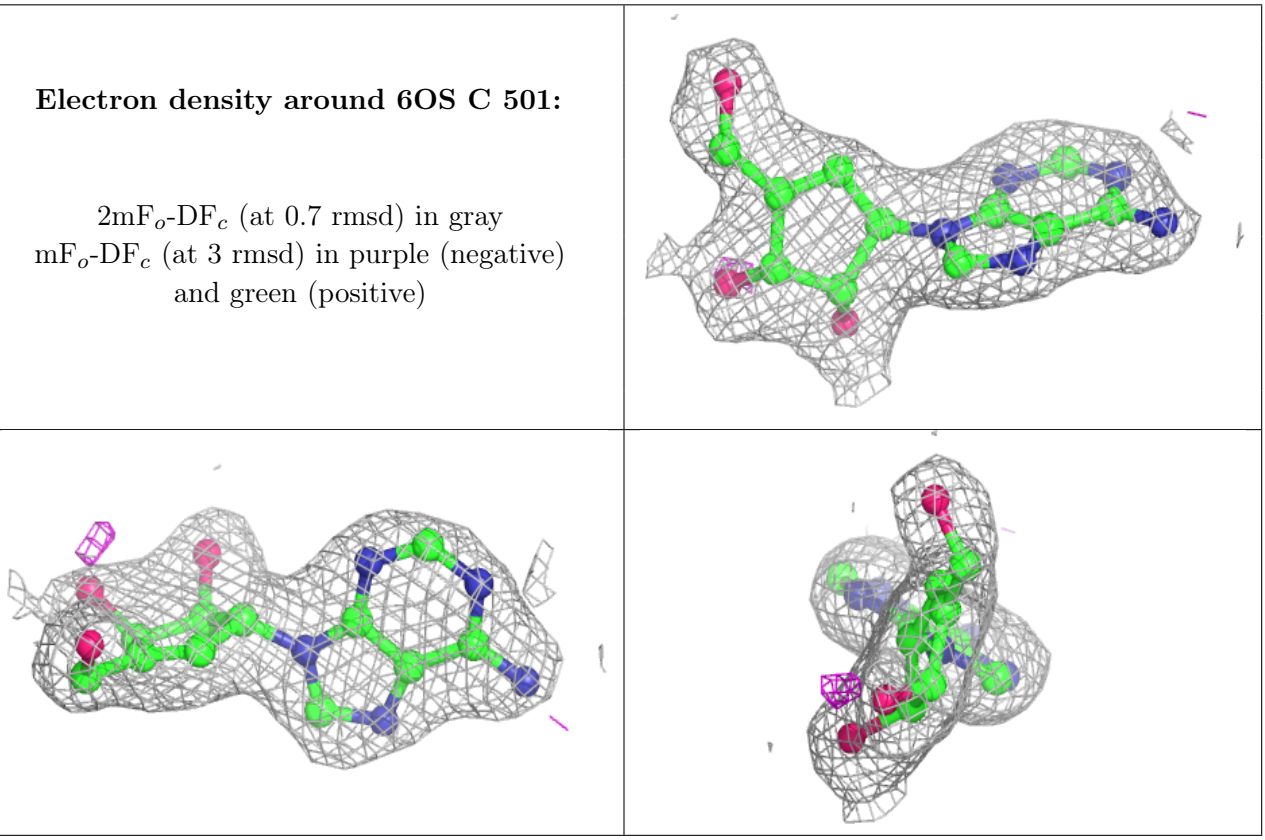
Electron density around 6OS A 501:

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



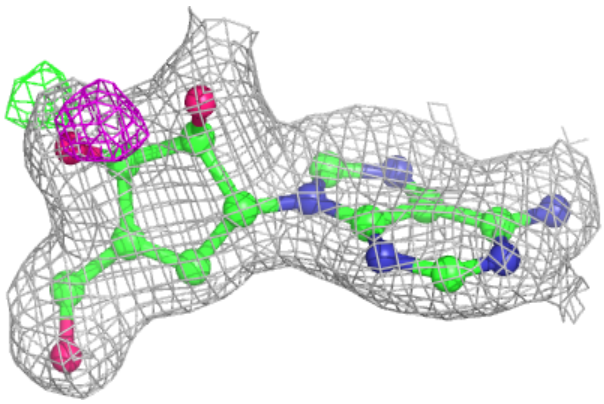
Electron density around 6OS C 501:

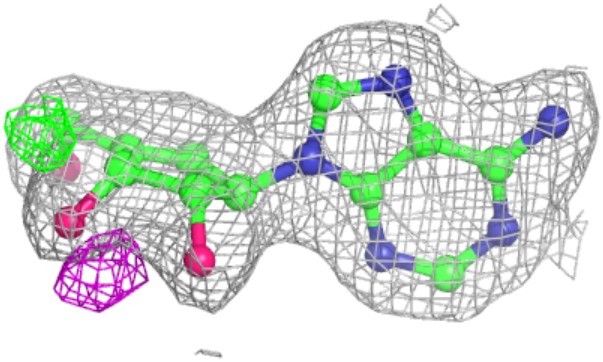
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

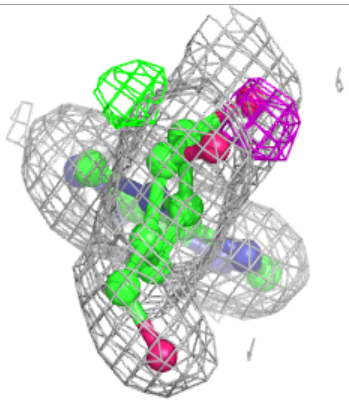


Electron density around 6OS D 501:

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

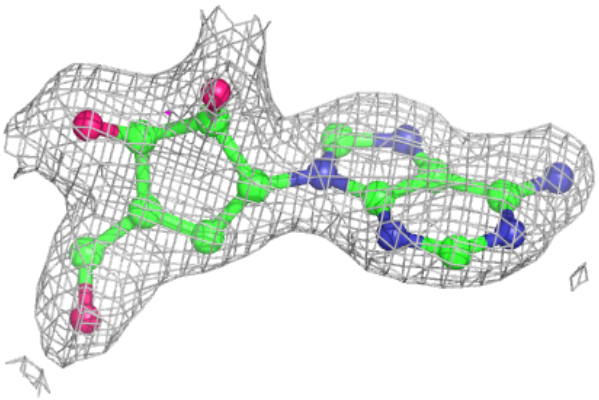


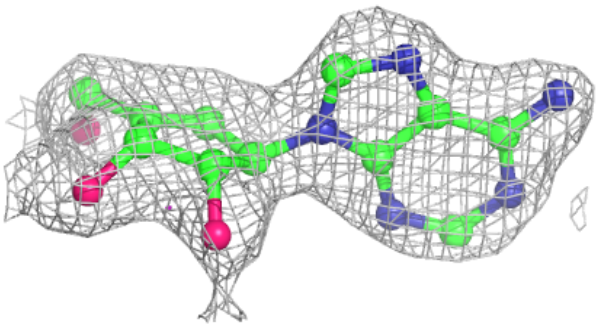


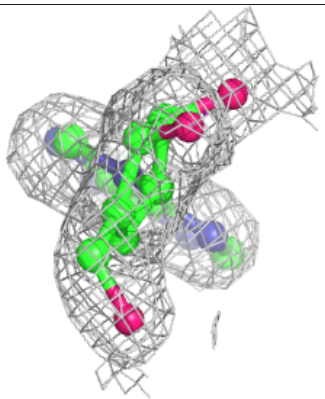


Electron density around 6OS B 501:

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

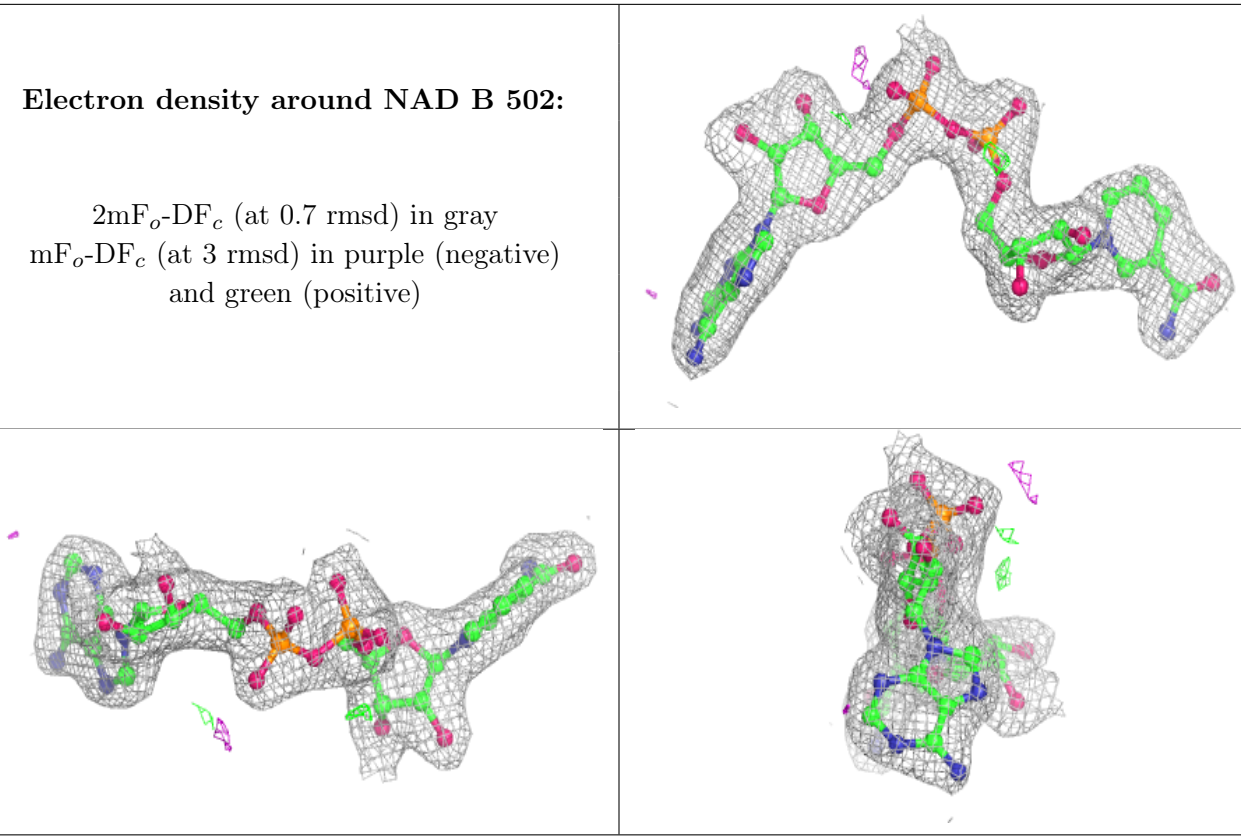






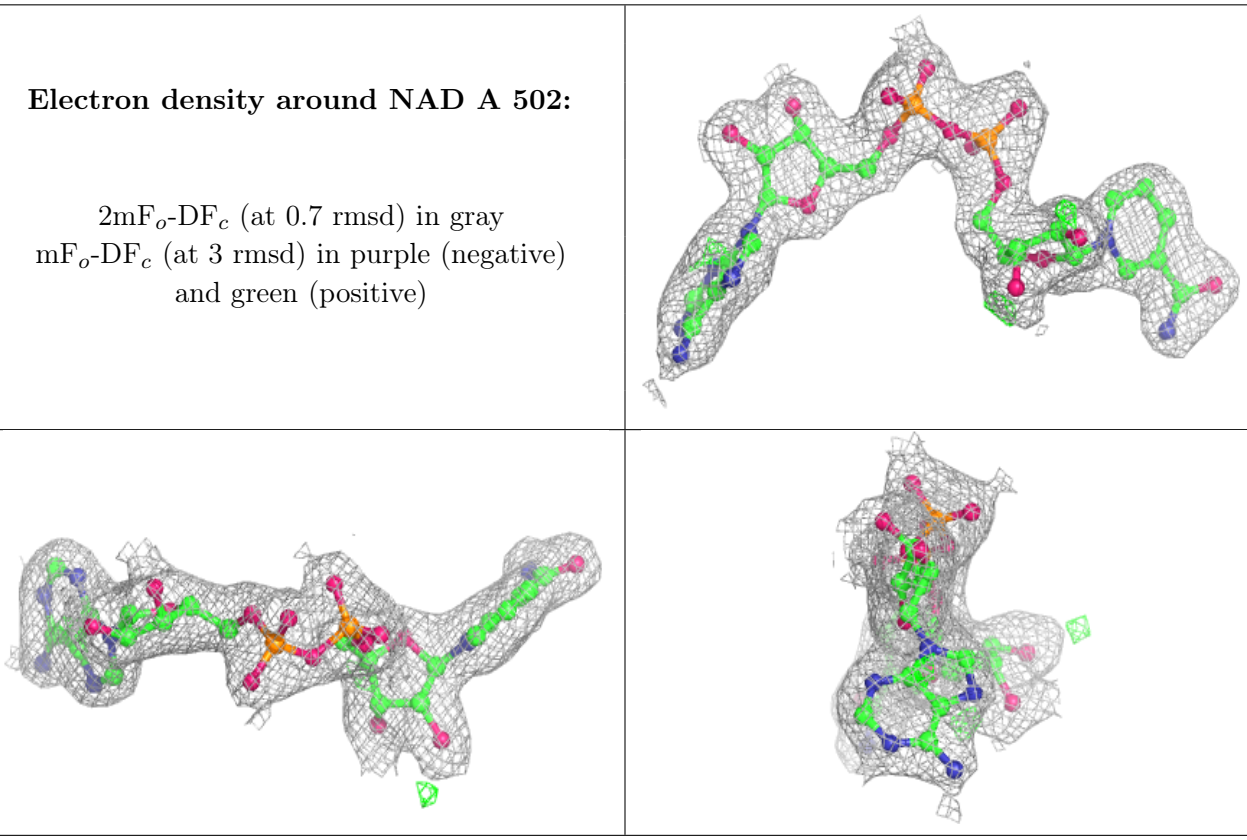
Electron density around NAD B 502:

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



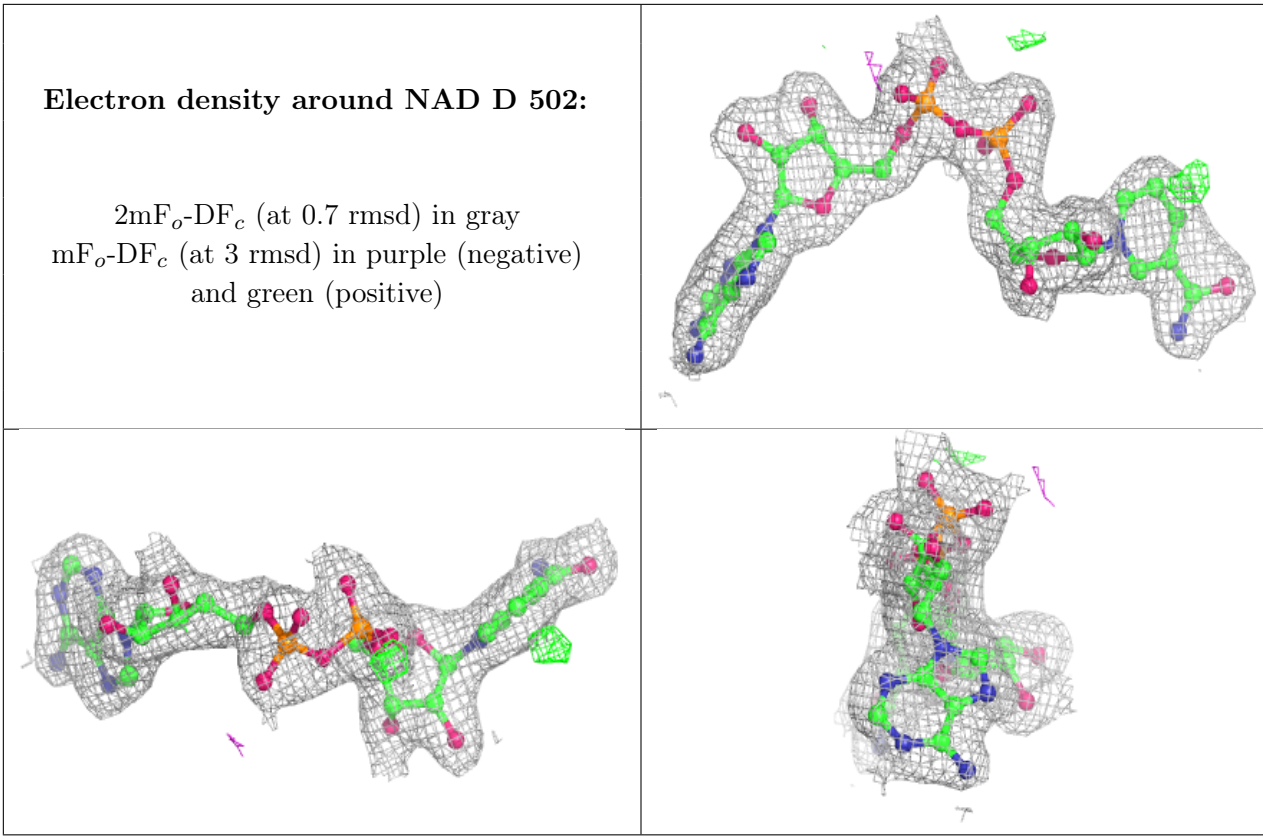
Electron density around NAD A 502:

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



Electron density around NAD D 502:

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



Electron density around NAD C 502:

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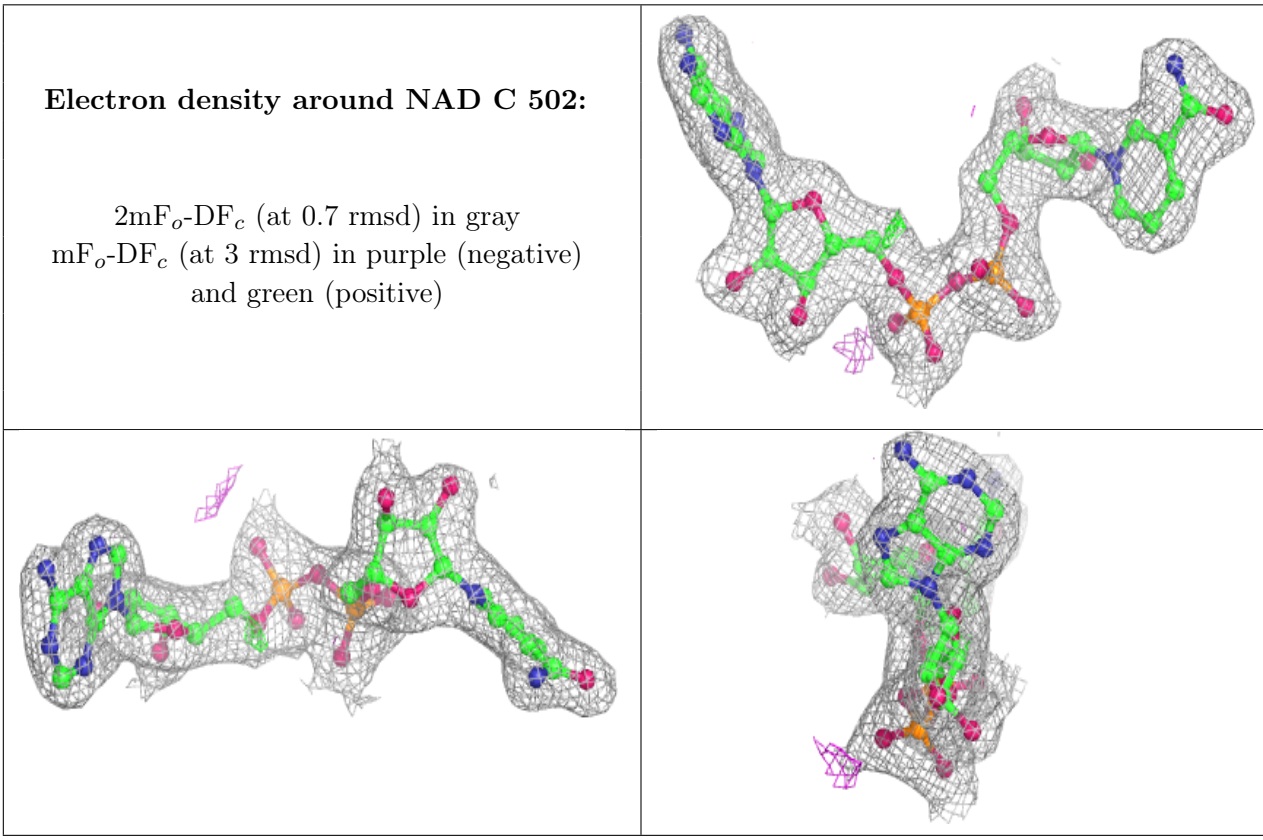
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.