Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 10:13 AM EDT

PDB ID	:	4K9D
Title	:	X-ray crystal structure of a Glyceraldehyde 3-phosphate dehydrogenase from Brugia malayi bound to the co-factor NAD
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2013-04-19
Resolution	:	2.10 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 ⓘ) were used in the production of this report:

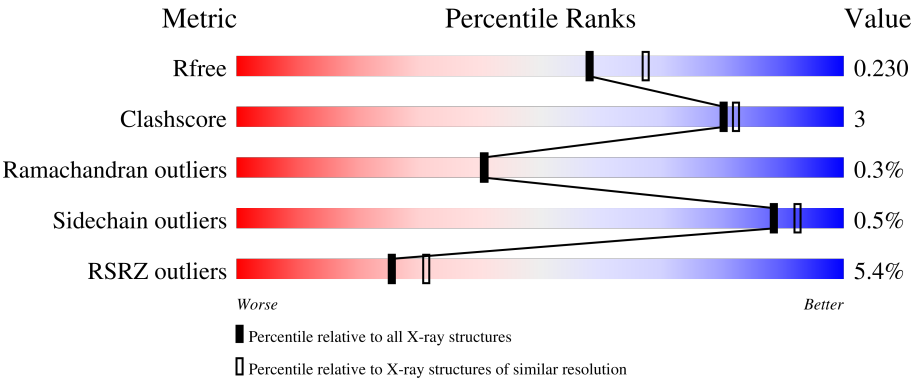
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	347	2% 89% 8% ·
1	B	347	% 91% 6% ·
1	C	347	2% 89% 7% ·
1	D	347	3% 91% 6% ·
1	E	347	11% 89% 7% ·

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Mol	Chain	Length	Quality of chain
1	F	347	2% 91% 6%
1	G	347	2% 91% 6%
1	H	347	19% 90% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20811 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	3	0
			2496	1569	427	488	12			
1	B	338	Total	C	N	O	S	0	6	0
			2536	1601	434	487	14			
1	C	337	Total	C	N	O	S	0	3	0
			2506	1580	427	486	13			
1	D	337	Total	C	N	O	S	0	0	0
			2463	1548	422	481	12			
1	E	335	Total	C	N	O	S	0	1	0
			2345	1469	402	462	12			
1	F	337	Total	C	N	O	S	0	1	0
			2499	1574	429	484	12			
1	G	337	Total	C	N	O	S	0	6	0
			2511	1583	429	486	13			
1	H	325	Total	C	N	O	S	0	0	0
			2170	1346	387	428	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A8Q3K8
A	-6	ALA	-	expression tag	UNP A8Q3K8
A	-5	HIS	-	expression tag	UNP A8Q3K8
A	-4	HIS	-	expression tag	UNP A8Q3K8
A	-3	HIS	-	expression tag	UNP A8Q3K8
A	-2	HIS	-	expression tag	UNP A8Q3K8
A	-1	HIS	-	expression tag	UNP A8Q3K8
A	0	HIS	-	expression tag	UNP A8Q3K8
B	-7	MET	-	expression tag	UNP A8Q3K8
B	-6	ALA	-	expression tag	UNP A8Q3K8
B	-5	HIS	-	expression tag	UNP A8Q3K8
B	-4	HIS	-	expression tag	UNP A8Q3K8
B	-3	HIS	-	expression tag	UNP A8Q3K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP A8Q3K8
B	-1	HIS	-	expression tag	UNP A8Q3K8
B	0	HIS	-	expression tag	UNP A8Q3K8
C	-7	MET	-	expression tag	UNP A8Q3K8
C	-6	ALA	-	expression tag	UNP A8Q3K8
C	-5	HIS	-	expression tag	UNP A8Q3K8
C	-4	HIS	-	expression tag	UNP A8Q3K8
C	-3	HIS	-	expression tag	UNP A8Q3K8
C	-2	HIS	-	expression tag	UNP A8Q3K8
C	-1	HIS	-	expression tag	UNP A8Q3K8
C	0	HIS	-	expression tag	UNP A8Q3K8
D	-7	MET	-	expression tag	UNP A8Q3K8
D	-6	ALA	-	expression tag	UNP A8Q3K8
D	-5	HIS	-	expression tag	UNP A8Q3K8
D	-4	HIS	-	expression tag	UNP A8Q3K8
D	-3	HIS	-	expression tag	UNP A8Q3K8
D	-2	HIS	-	expression tag	UNP A8Q3K8
D	-1	HIS	-	expression tag	UNP A8Q3K8
D	0	HIS	-	expression tag	UNP A8Q3K8
E	-7	MET	-	expression tag	UNP A8Q3K8
E	-6	ALA	-	expression tag	UNP A8Q3K8
E	-5	HIS	-	expression tag	UNP A8Q3K8
E	-4	HIS	-	expression tag	UNP A8Q3K8
E	-3	HIS	-	expression tag	UNP A8Q3K8
E	-2	HIS	-	expression tag	UNP A8Q3K8
E	-1	HIS	-	expression tag	UNP A8Q3K8
E	0	HIS	-	expression tag	UNP A8Q3K8
F	-7	MET	-	expression tag	UNP A8Q3K8
F	-6	ALA	-	expression tag	UNP A8Q3K8
F	-5	HIS	-	expression tag	UNP A8Q3K8
F	-4	HIS	-	expression tag	UNP A8Q3K8
F	-3	HIS	-	expression tag	UNP A8Q3K8
F	-2	HIS	-	expression tag	UNP A8Q3K8
F	-1	HIS	-	expression tag	UNP A8Q3K8
F	0	HIS	-	expression tag	UNP A8Q3K8
G	-7	MET	-	expression tag	UNP A8Q3K8
G	-6	ALA	-	expression tag	UNP A8Q3K8
G	-5	HIS	-	expression tag	UNP A8Q3K8
G	-4	HIS	-	expression tag	UNP A8Q3K8
G	-3	HIS	-	expression tag	UNP A8Q3K8
G	-2	HIS	-	expression tag	UNP A8Q3K8
G	-1	HIS	-	expression tag	UNP A8Q3K8

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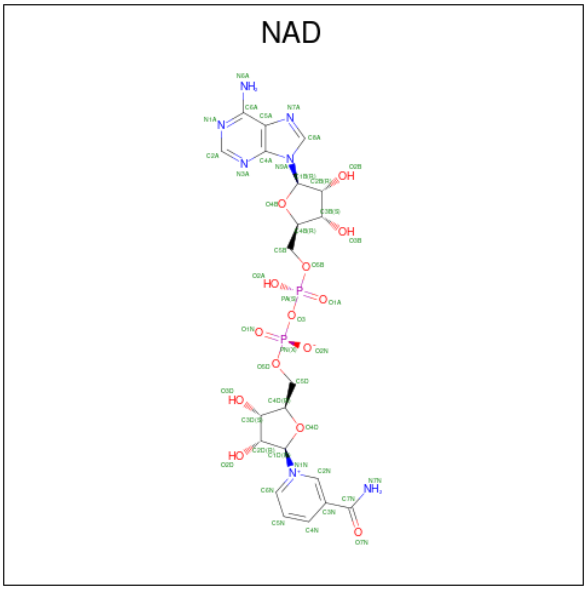
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A8Q3K8
H	-7	MET	-	expression tag	UNP A8Q3K8
H	-6	ALA	-	expression tag	UNP A8Q3K8
H	-5	HIS	-	expression tag	UNP A8Q3K8
H	-4	HIS	-	expression tag	UNP A8Q3K8
H	-3	HIS	-	expression tag	UNP A8Q3K8
H	-2	HIS	-	expression tag	UNP A8Q3K8
H	-1	HIS	-	expression tag	UNP A8Q3K8
H	0	HIS	-	expression tag	UNP A8Q3K8

- 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		

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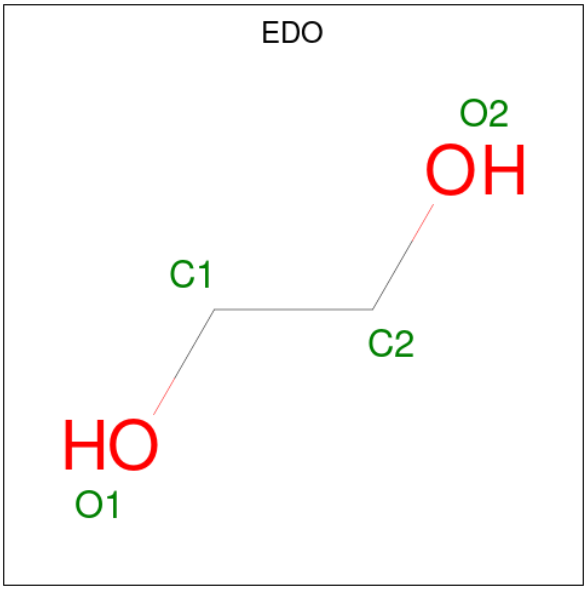
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C N O P 44 21 7 14 2	0	0
2	H	1	Total C N O P 44 21 7 14 2	0	0

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



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	128	Total O 128 128	0	0

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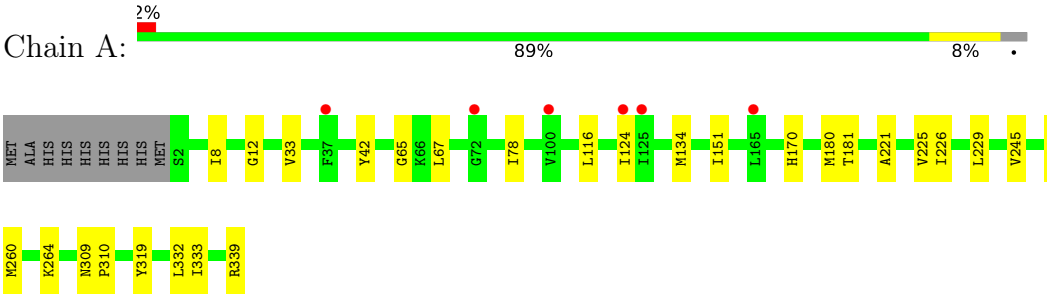
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	170	Total O 170 170	0	0
4	C	130	Total O 130 130	0	0
4	D	87	Total O 87 87	0	0
4	E	58	Total O 58 58	0	0
4	F	144	Total O 144 144	0	0
4	G	170	Total O 170 170	0	0
4	H	22	Total O 22 22	0	0

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.

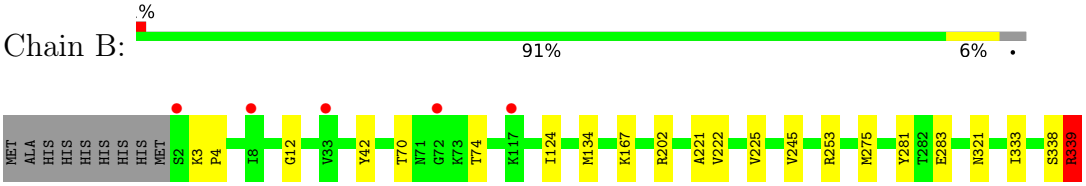
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain A:



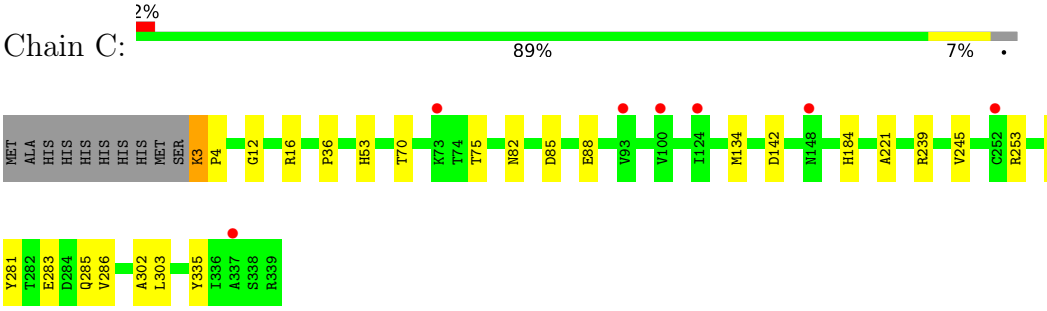
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain B:



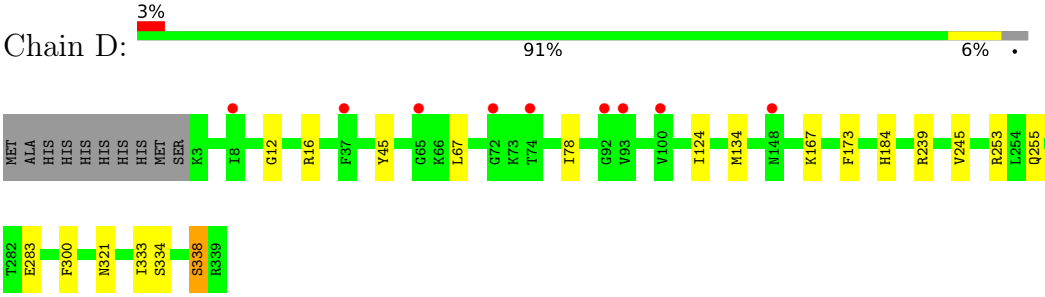
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain C:



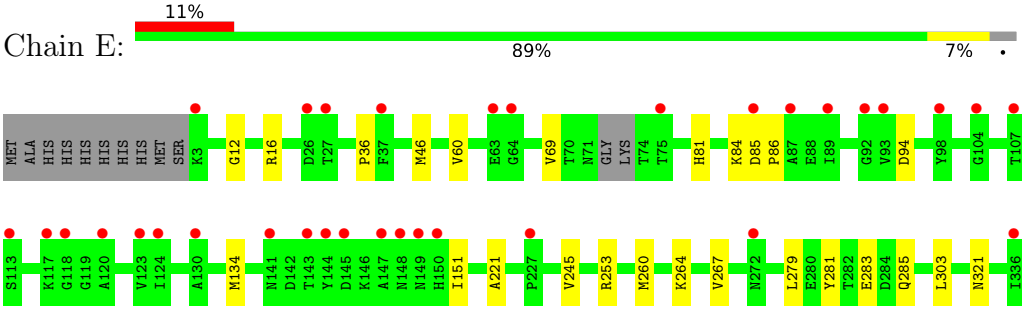
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain D:



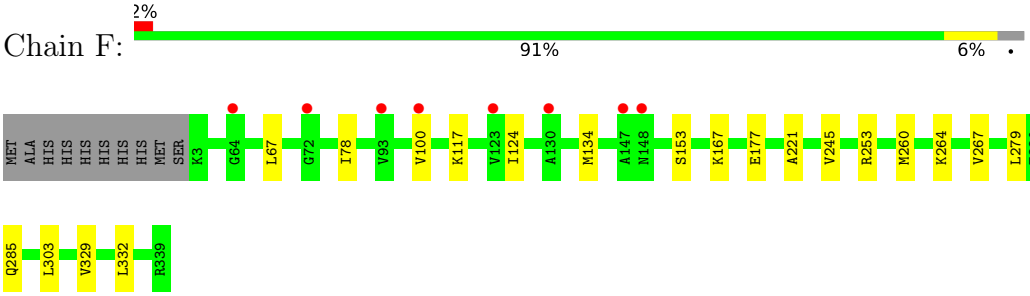
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain E:



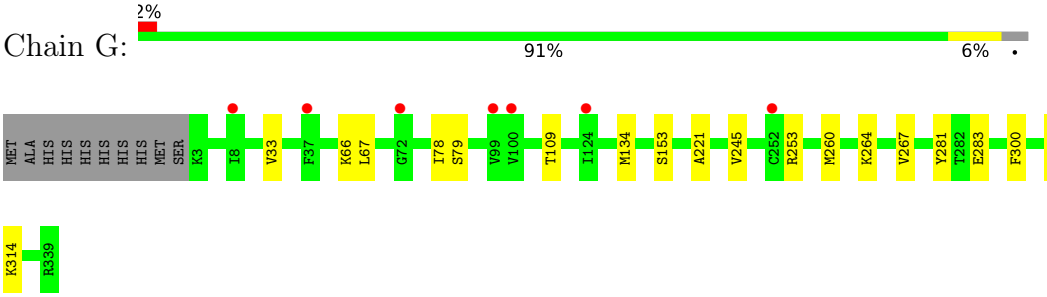
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain F:



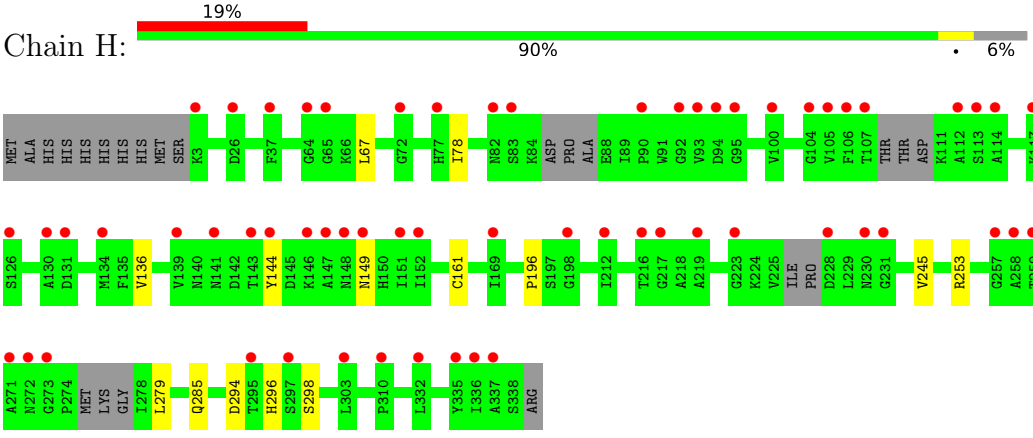
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain G:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.76Å 176.99Å 94.25Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	19.87 – 2.10 19.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.87-2.10) 97.4 (19.87-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.09Å)	Xtriage
Refinement program	PHENIX dev_1255	Depositor
R, R_{free}	0.184 , 0.230 0.185 , 0.230	Depositor DCC
R_{free} test set	8004 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20811	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: EDO, 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	0.40	0/2554	0.56	0/3484
1	B	0.46	0/2603	0.60	1/3539 (0.0%)
1	C	0.42	0/2564	0.57	0/3491
1	D	0.37	0/2512	0.56	0/3429
1	E	0.35	0/2394	0.53	0/3280
1	F	0.44	0/2551	0.59	0/3472
1	G	0.44	0/2578	0.57	0/3512
1	H	0.31	0/2206	0.53	0/3024
All	All	0.40	0/19962	0.57	1/27231 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	339	ARG	NE-CZ-NH1	5.88	123.24	120.30

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	2496	0	2419	15	0
1	B	2536	0	2524	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2506	0	2460	19	0
1	D	2463	0	2365	14	0
1	E	2345	0	2112	13	0
1	F	2499	0	2456	16	0
1	G	2511	0	2466	12	0
1	H	2170	0	1844	8	0
2	A	44	0	26	1	0
2	B	44	0	26	2	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
2	E	44	0	26	1	0
2	F	44	0	26	0	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
3	C	4	0	6	1	0
3	F	4	0	6	0	0
3	G	4	0	6	0	0
4	A	128	0	0	0	0
4	B	170	0	0	0	0
4	C	130	0	0	2	0
4	D	87	0	0	1	0
4	E	58	0	0	0	0
4	F	144	0	0	1	0
4	G	170	0	0	0	0
4	H	22	0	0	0	0
All	All	20811	0	18890	103	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 3.

All (103) 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:B:339:ARG:HG2	1:B:339:ARG:HH11	1.41	0.85
1:D:67:LEU:HB3	1:D:78:ILE:HB	1.65	0.79
1:B:253:ARG:HD2	1:C:253:ARG:HD2	1.73	0.70
1:F:253:ARG:HD2	1:G:253:ARG:HD2	1.74	0.68
1:D:253:ARG:HD2	1:E:253:ARG:HD2	1.74	0.68
1:E:81:HIS:NE2	1:E:94:ASP:OD2	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:HG2	1:B:339:ARG:NH1	2.13	0.63
1:A:253:ARG:HD2	1:H:253:ARG:HD2	1.82	0.61
1:H:67:LEU:HB3	1:H:78:ILE:HB	1.81	0.61
1:F:124:ILE:HD13	1:F:329:VAL:HG13	1.83	0.60
1:B:338:SER:OG	1:B:339:ARG:NH1	2.30	0.60
1:E:134:MET:HE1	1:E:221:ALA:HB1	1.82	0.59
1:A:260:MET:HG3	1:A:264:LYS:HE3	1.86	0.58
1:C:3:LYS:HD2	1:C:4:PRO:HD2	1.85	0.58
1:G:66:LYS:HD2	1:G:79:SER:HA	1.86	0.57
1:C:281:TYR:OH	1:C:283:GLU:OE2	2.19	0.57
1:A:65:GLY:HA3	1:F:117:LYS:HA	1.87	0.57
1:C:85:ASP:HB3	1:C:88:GLU:HG2	1.86	0.56
1:D:167:LYS:NZ	4:D:635:HOH:O	2.38	0.56
1:A:309:ASN:HB2	1:A:310:PRO:HD2	1.89	0.55
1:G:260:MET:HG3	1:G:264:LYS:HE3	1.89	0.55
1:E:260:MET:HG3	1:E:264:LYS:HE3	1.89	0.54
1:E:36:PRO:HG3	1:E:84:LYS:HA	1.88	0.54
1:G:134[A]:MET:HG2	1:G:153:SER:HB3	1.89	0.53
1:E:285:GLN:NE2	1:E:303:LEU:HD23	2.24	0.53
1:F:167:LYS:NZ	4:F:626:HOH:O	2.41	0.53
1:F:253:ARG:CD	1:G:253:ARG:HD2	2.39	0.53
1:H:161:CYS:HA	1:H:298:SER:HB2	1.91	0.53
1:A:67:LEU:HB3	1:A:78:ILE:HB	1.92	0.52
1:E:60:VAL:HG23	1:E:69:VAL:HG22	1.92	0.51
1:D:334:SER:O	1:D:338:SER:OG	2.28	0.51
1:C:281:TYR:CE1	1:C:283:GLU:HG3	2.46	0.50
1:D:321:ASN:O	2:D:500:NAD:H4N	2.10	0.50
1:F:281:TYR:CE1	1:F:283:GLU:HG3	2.46	0.50
1:F:134:MET:HE1	1:F:221:ALA:HB1	1.93	0.50
1:A:124:ILE:HD13	1:A:332:LEU:HD23	1.94	0.49
1:B:12:GLY:HA3	2:B:401:NAD:O5B	2.12	0.49
1:C:36:PRO:HA	1:C:82:ASN:HB3	1.94	0.49
1:B:222:VAL:HA	1:B:225[A]:VAL:HG22	1.95	0.49
1:G:267:VAL:HG11	1:G:300:PHE:CG	2.48	0.49
1:B:134:MET:HE1	1:B:221:ALA:HB1	1.96	0.48
1:F:285:GLN:NE2	1:F:303:LEU:HD23	2.29	0.47
1:H:294:ASP:OD1	1:H:296:HIS:ND1	2.34	0.47
1:D:124:ILE:HD12	1:D:333:ILE:HG13	1.96	0.47
1:C:184:HIS:HB3	1:C:239[A]:ARG:HD3	1.96	0.47
1:G:67:LEU:HB3	1:G:78:ILE:HB	1.96	0.47
1:C:134[A]:MET:HE1	1:C:221:ALA:HB1	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:TYR:CE1	1:D:283:GLU:HG3	2.50	0.47
1:F:260:MET:HG3	1:F:264:LYS:HE3	1.98	0.46
1:B:339:ARG:HH11	1:B:339:ARG:CG	2.22	0.46
1:C:70:THR:HG22	1:C:75:THR:HG23	1.98	0.46
1:D:45:TYR:CE1	1:H:285:GLN:HB2	2.51	0.45
1:D:134:MET:HB3	1:D:134:MET:HE3	1.75	0.45
1:C:142:ASP:HA	1:C:335:TYR:OH	2.16	0.45
1:A:134:MET:HE1	1:A:221:ALA:HB1	1.99	0.45
1:B:167:LYS:HD3	1:B:275[A]:MET:HE3	1.99	0.45
1:A:124:ILE:HD12	1:A:333:ILE:HG13	1.99	0.44
1:C:239[B]:ARG:NH2	4:C:625:HOH:O	2.50	0.44
1:B:253:ARG:HD2	1:C:253:ARG:CD	2.45	0.44
1:F:100:VAL:HA	1:F:124:ILE:HG23	1.99	0.44
1:B:202:ARG:HD3	1:C:286:VAL:O	2.18	0.44
1:E:267:VAL:HG13	1:E:279:LEU:HD21	1.98	0.44
1:G:281:TYR:CE1	1:G:283:GLU:HG3	2.53	0.44
1:F:177:GLU:HB2	1:G:308:LEU:CD2	2.47	0.44
1:C:285:GLN:NE2	1:C:303:LEU:HD23	2.33	0.44
1:D:173:PHE:O	1:D:255:GLN:HB3	2.18	0.44
1:F:267:VAL:HG13	1:F:279:LEU:HD21	1.99	0.44
1:G:33[A]:VAL:HG23	1:G:78:ILE:HG21	1.99	0.43
1:E:281:TYR:CE1	1:E:283:GLU:HG3	2.53	0.43
1:A:225:VAL:HG23	1:A:226:ILE:HG13	2.01	0.43
2:C:401:NAD:N1A	4:C:587:HOH:O	2.37	0.43
1:D:267:VAL:HG11	1:D:300:PHE:CG	2.54	0.43
1:F:67:LEU:HB3	1:F:78:ILE:HB	2.01	0.43
1:C:134[A]:MET:HE3	1:C:134[A]:MET:HB3	1.81	0.42
1:E:12:GLY:O	1:E:16:ARG:HG3	2.18	0.42
1:E:321:ASN:O	2:E:500:NAD:H4N	2.18	0.42
1:F:134:MET:HG2	1:F:153:SER:HB3	2.02	0.42
1:C:260:MET:HG3	1:C:264:LYS:HE3	2.00	0.42
1:A:116:LEU:HD11	1:A:151:ILE:HD11	2.01	0.42
1:B:281:TYR:CE1	1:B:283:GLU:HG3	2.55	0.42
1:C:53:HIS:HB3	3:C:402:EDO:H22	2.01	0.42
1:H:279:LEU:HA	1:H:298:SER:O	2.19	0.42
1:E:46:MET:HE3	1:H:196:PRO:HA	2.01	0.42
1:G:134[A]:MET:HE1	1:G:221:ALA:HB1	2.02	0.42
1:A:180:MET:HG2	1:A:181:THR:N	2.35	0.41
1:B:70:THR:OG1	1:B:74:THR:O	2.28	0.41
1:B:124:ILE:HD12	1:B:333:ILE:HG13	2.01	0.41
1:A:12:GLY:HA3	2:A:401:NAD:O5B	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:ILE:HG13	1:G:314:LYS:HB3	2.02	0.41
1:H:144:TYR:CE1	1:H:149:ASN:HB2	2.55	0.41
1:C:264:LYS:HE2	1:C:302:ALA:HB1	2.03	0.41
1:D:12:GLY:HA3	2:D:500:NAD:O5B	2.21	0.41
1:F:124:ILE:CD1	1:F:332:LEU:HD23	2.50	0.41
1:F:124:ILE:HD12	1:F:332:LEU:HD23	2.02	0.41
1:A:8:ILE:HB	1:A:33[B]:VAL:HG12	2.03	0.41
1:A:170:HIS:ND1	1:A:229:LEU:HD21	2.35	0.41
1:D:184:HIS:HB3	1:D:239:ARG:HD3	2.02	0.40
1:B:321:ASN:O	2:B:401:NAD:H4N	2.21	0.40
1:B:3:LYS:HA	1:B:4:PRO:HD3	1.96	0.40
1:D:12:GLY:O	1:D:16:ARG:HG3	2.22	0.40
1:E:85:ASP:HA	1:E:86:PRO:HD2	1.87	0.40
1:A:248:VAL:HG23	1:A:319:TYR:CE1	2.56	0.40
1:C:12:GLY:O	1:C:16:ARG:HG3	2.21	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	339/347 (98%)	326 (96%)	12 (4%)	1 (0%)	41	41
1	B	342/347 (99%)	331 (97%)	10 (3%)	1 (0%)	41	41
1	C	338/347 (97%)	326 (96%)	11 (3%)	1 (0%)	41	41
1	D	335/347 (96%)	323 (96%)	11 (3%)	1 (0%)	41	41
1	E	332/347 (96%)	320 (96%)	11 (3%)	1 (0%)	41	41
1	F	336/347 (97%)	323 (96%)	12 (4%)	1 (0%)	41	41
1	G	341/347 (98%)	329 (96%)	11 (3%)	1 (0%)	41	41
1	H	315/347 (91%)	302 (96%)	12 (4%)	1 (0%)	41	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2678/2776 (96%)	2580 (96%)	90 (3%)	8 (0%)	41 41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	VAL
1	B	245	VAL
1	C	245	VAL
1	D	245	VAL
1	F	245	VAL
1	G	245	VAL
1	H	245	VAL
1	E	245	VAL

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	263/282 (93%)	261 (99%)	2 (1%)	81 86
1	B	273/282 (97%)	271 (99%)	2 (1%)	84 88
1	C	266/282 (94%)	265 (100%)	1 (0%)	91 94
1	D	255/282 (90%)	254 (100%)	1 (0%)	91 94
1	E	220/282 (78%)	219 (100%)	1 (0%)	88 92
1	F	265/282 (94%)	265 (100%)	0	100 100
1	G	267/282 (95%)	266 (100%)	1 (0%)	91 94
1	H	182/282 (64%)	181 (100%)	1 (0%)	88 92
All	All	1991/2256 (88%)	1982 (100%)	9 (0%)	88 92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	TYR
1	A	339	ARG

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Mol	Chain	Res	Type
1	B	42	TYR
1	B	339	ARG
1	C	3	LYS
1	D	338	SER
1	E	151	ILE
1	G	109	THR
1	H	136	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	82	ASN
1	D	82	ASN
1	F	76	HIS
1	F	148	ASN
1	H	170	HIS

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

14 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	$\#\|Z\|>2$
2	NAD	H	500	-	42,48,48	0.89	2 (4%)	50,73,73	1.21	3 (6%)
2	NAD	E	500	-	42,48,48	0.87	2 (4%)	50,73,73	1.24	4 (8%)
2	NAD	B	401	-	42,48,48	0.92	4 (9%)	50,73,73	1.17	4 (8%)
2	NAD	C	401	-	42,48,48	0.82	1 (2%)	50,73,73	1.16	4 (8%)
2	NAD	F	401	-	42,48,48	0.91	3 (7%)	50,73,73	1.09	2 (4%)
2	NAD	D	500	-	42,48,48	0.85	1 (2%)	50,73,73	1.23	3 (6%)
3	EDO	F	402	-	3,3,3	0.67	0	2,2,2	0.14	0
3	EDO	G	402	-	3,3,3	0.53	0	2,2,2	0.17	0
3	EDO	C	402	-	3,3,3	0.46	0	2,2,2	0.37	0
3	EDO	A	402	-	3,3,3	0.56	0	2,2,2	0.31	0
2	NAD	G	401	-	42,48,48	0.91	3 (7%)	50,73,73	1.32	7 (14%)
2	NAD	A	401	-	42,48,48	0.84	3 (7%)	50,73,73	1.18	5 (10%)
3	EDO	B	402	-	3,3,3	0.52	0	2,2,2	0.36	0
3	EDO	A	403	-	3,3,3	0.53	0	2,2,2	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	H	500	-	-	12/26/62/62	0/5/5/5
2	NAD	E	500	-	-	15/26/62/62	0/5/5/5
2	NAD	B	401	-	-	6/26/62/62	0/5/5/5
2	NAD	C	401	-	-	8/26/62/62	0/5/5/5
2	NAD	F	401	-	-	9/26/62/62	0/5/5/5
2	NAD	D	500	-	-	6/26/62/62	0/5/5/5
3	EDO	F	402	-	-	1/1/1/1	-
3	EDO	G	402	-	-	0/1/1/1	-
3	EDO	C	402	-	-	0/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
2	NAD	G	401	-	-	11/26/62/62	0/5/5/5
2	NAD	A	401	-	-	7/26/62/62	0/5/5/5
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	A	403	-	-	0/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	NAD	C5A-C4A	2.63	1.47	1.40
2	D	500	NAD	C5A-C4A	2.59	1.47	1.40
2	E	500	NAD	C5A-C4A	2.55	1.47	1.40
2	F	401	NAD	C5A-C4A	2.52	1.47	1.40
2	B	401	NAD	C5A-C4A	2.50	1.47	1.40
2	C	401	NAD	C5A-C4A	2.50	1.47	1.40
2	B	401	NAD	O4D-C1D	2.40	1.44	1.41
2	G	401	NAD	C5A-C4A	2.39	1.47	1.40
2	F	401	NAD	C2A-N3A	2.35	1.35	1.32
2	B	401	NAD	O4B-C1B	2.34	1.44	1.41
2	F	401	NAD	O4D-C1D	2.33	1.44	1.41
2	G	401	NAD	O4D-C1D	2.29	1.44	1.41
2	A	401	NAD	C5A-C4A	2.21	1.46	1.40
2	E	500	NAD	C2A-N3A	2.17	1.35	1.32
2	A	401	NAD	O4D-C1D	2.16	1.44	1.41
2	H	500	NAD	O4B-C1B	2.10	1.44	1.41
2	G	401	NAD	C2A-N3A	2.10	1.35	1.32
2	B	401	NAD	C2A-N3A	2.09	1.35	1.32
2	A	401	NAD	C2A-N3A	2.04	1.35	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	NAD	N3A-C2A-N1A	-4.17	122.16	128.68
2	E	500	NAD	PN-O3-PA	-3.91	119.40	132.83
2	H	500	NAD	PN-O3-PA	-3.86	119.57	132.83
2	B	401	NAD	N3A-C2A-N1A	-3.58	123.08	128.68
2	G	401	NAD	N3A-C2A-N1A	-3.35	123.44	128.68
2	G	401	NAD	PN-O3-PA	-3.35	121.33	132.83
2	C	401	NAD	N3A-C2A-N1A	-3.25	123.60	128.68
2	B	401	NAD	PN-O3-PA	-3.17	121.94	132.83
2	C	401	NAD	PN-O3-PA	-3.14	122.05	132.83
2	H	500	NAD	N3A-C2A-N1A	-3.13	123.79	128.68
2	D	500	NAD	C4A-C5A-N7A	-3.11	106.16	109.40
2	G	401	NAD	C4A-C5A-N7A	-3.10	106.17	109.40
2	D	500	NAD	PN-O3-PA	-3.04	122.38	132.83
2	E	500	NAD	N3A-C2A-N1A	-2.94	124.08	128.68
2	D	500	NAD	N3A-C2A-N1A	-2.90	124.14	128.68
2	F	401	NAD	N3A-C2A-N1A	-2.80	124.31	128.68
2	H	500	NAD	C4A-C5A-N7A	-2.75	106.53	109.40
2	E	500	NAD	C4A-C5A-N7A	-2.68	106.61	109.40
2	C	401	NAD	C4A-C5A-N7A	-2.64	106.65	109.40
2	F	401	NAD	C4A-C5A-N7A	-2.49	106.80	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	NAD	C1B-N9A-C4A	-2.43	122.37	126.64
2	A	401	NAD	C4A-C5A-N7A	-2.38	106.92	109.40
2	E	500	NAD	C3D-C2D-C1D	2.32	104.47	100.98
2	G	401	NAD	C3N-C7N-N7N	2.31	120.53	117.75
2	A	401	NAD	C2A-N1A-C6A	2.28	122.65	118.75
2	C	401	NAD	O4B-C1B-C2B	-2.25	103.63	106.93
2	G	401	NAD	C2A-N1A-C6A	2.20	122.52	118.75
2	A	401	NAD	O2A-PA-O1A	2.18	123.02	112.24
2	G	401	NAD	O2A-PA-O1A	2.16	122.94	112.24
2	B	401	NAD	C2A-N1A-C6A	2.12	122.39	118.75
2	B	401	NAD	O2A-PA-O1A	2.04	122.30	112.24
2	A	401	NAD	C1B-N9A-C4A	-2.03	123.08	126.64

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	C2D-C1D-N1N-C2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	O4D-C1D-N1N-C2N
2	B	401	NAD	O4D-C1D-N1N-C6N
2	B	401	NAD	C2D-C1D-N1N-C2N
2	B	401	NAD	C2D-C1D-N1N-C6N
2	C	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	C5D-O5D-PN-O1N
2	C	401	NAD	O4D-C1D-N1N-C2N
2	C	401	NAD	O4D-C1D-N1N-C6N
2	C	401	NAD	C2D-C1D-N1N-C2N
2	C	401	NAD	C2D-C1D-N1N-C6N
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	C5B-O5B-PA-O1A
2	E	500	NAD	C5D-O5D-PN-O2N
2	E	500	NAD	O4D-C1D-N1N-C2N
2	E	500	NAD	O4D-C1D-N1N-C6N
2	E	500	NAD	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
2	E	500	NAD	C2D-C1D-N1N-C6N
2	F	401	NAD	C5B-O5B-PA-O1A
2	F	401	NAD	O4B-C4B-C5B-O5B
2	F	401	NAD	O4D-C1D-N1N-C2N
2	F	401	NAD	O4D-C1D-N1N-C6N
2	F	401	NAD	C2D-C1D-N1N-C2N
2	F	401	NAD	C2D-C1D-N1N-C6N
2	G	401	NAD	C5B-O5B-PA-O1A
2	G	401	NAD	O4B-C4B-C5B-O5B
2	G	401	NAD	C5D-O5D-PN-O1N
2	G	401	NAD	O4D-C1D-N1N-C2N
2	G	401	NAD	O4D-C1D-N1N-C6N
2	G	401	NAD	C2D-C1D-N1N-C2N
2	G	401	NAD	C2D-C1D-N1N-C6N
2	H	500	NAD	C5B-O5B-PA-O1A
2	H	500	NAD	C5D-O5D-PN-O2N
2	H	500	NAD	O4D-C1D-N1N-C2N
2	H	500	NAD	O4D-C1D-N1N-C6N
2	H	500	NAD	C2D-C1D-N1N-C2N
2	H	500	NAD	C2D-C1D-N1N-C6N
2	B	401	NAD	O4B-C4B-C5B-O5B
2	C	401	NAD	C3B-C4B-C5B-O5B
2	D	500	NAD	O4B-C4B-C5B-O5B
2	E	500	NAD	O4B-C4B-C5B-O5B
2	E	500	NAD	C3B-C4B-C5B-O5B
2	H	500	NAD	O4B-C4B-C5B-O5B
2	H	500	NAD	C3B-C4B-C5B-O5B
2	F	401	NAD	C3B-C4B-C5B-O5B
2	G	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	D	500	NAD	C3B-C4B-C5B-O5B
2	E	500	NAD	O4D-C4D-C5D-O5D
2	C	401	NAD	C5D-O5D-PN-O3
2	E	500	NAD	C5B-O5B-PA-O3
2	E	500	NAD	C5D-O5D-PN-O3
2	G	401	NAD	C5B-O5B-PA-O3
2	H	500	NAD	C5B-O5B-PA-O3
2	H	500	NAD	C5D-O5D-PN-O3
2	E	500	NAD	C5B-O5B-PA-O2A
2	G	401	NAD	C5B-O5B-PA-O2A
2	H	500	NAD	C5B-O5B-PA-O2A
2	H	500	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	E	500	NAD	C3D-C4D-C5D-O5D
3	F	402	EDO	O1-C1-C2-O2
2	E	500	NAD	PN-O3-PA-O2A
2	B	401	NAD	C3B-C4B-C5B-O5B
2	F	401	NAD	C5B-O5B-PA-O3
2	G	401	NAD	C5D-O5D-PN-O3
2	E	500	NAD	C5D-O5D-PN-O1N
2	F	401	NAD	C5B-O5B-PA-O2A

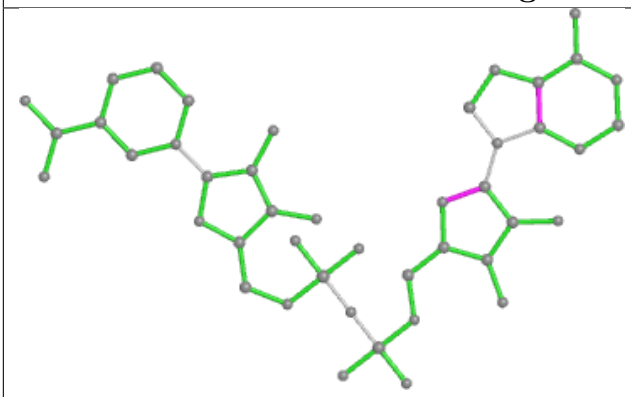
There are no ring outliers.

6 monomers are involved in 8 short contacts:

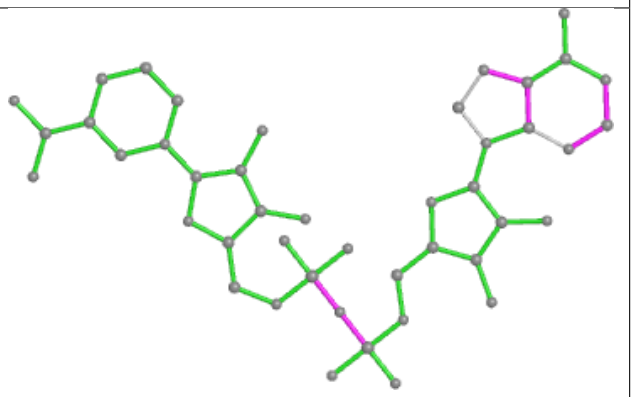
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	NAD	1	0
2	B	401	NAD	2	0
2	C	401	NAD	1	0
2	D	500	NAD	2	0
3	C	402	EDO	1	0
2	A	401	NAD	1	0

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

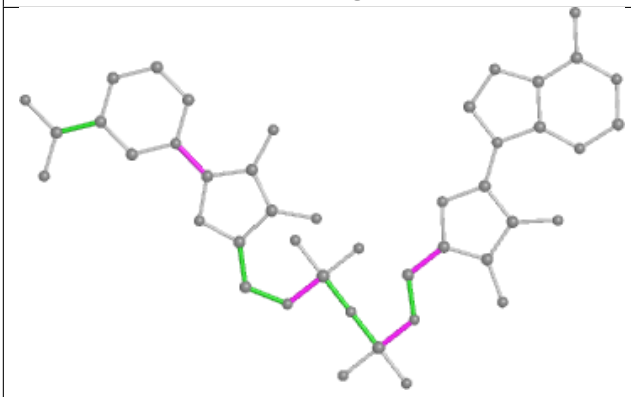
Ligand NAD H 500



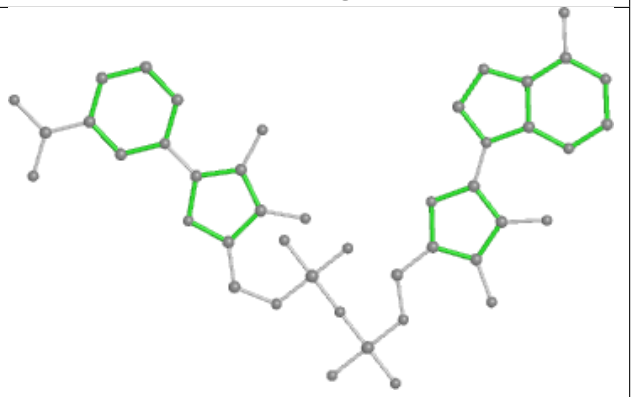
Bond lengths



Bond angles

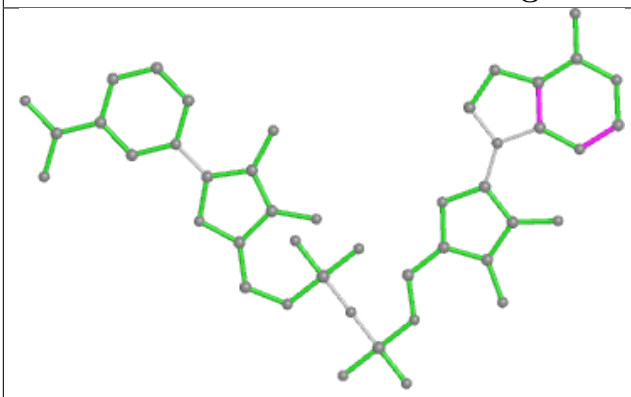


Torsions

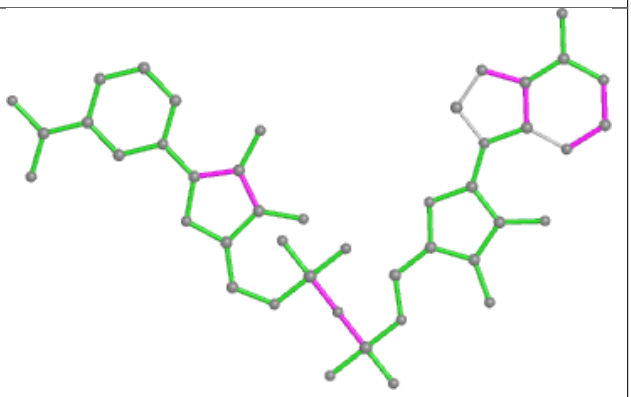


Rings

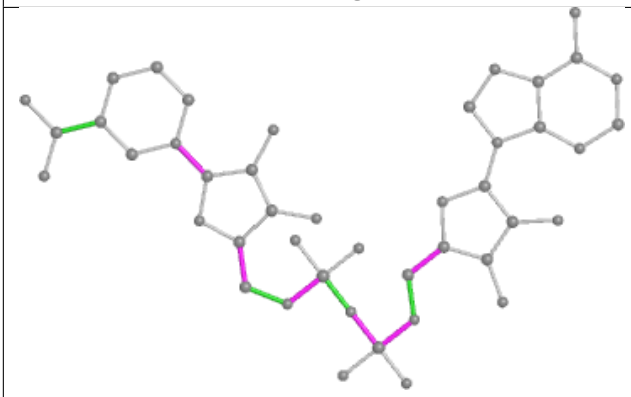
Ligand NAD E 500



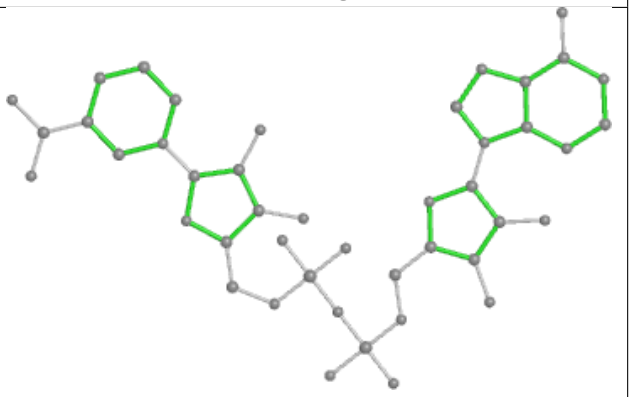
Bond lengths



Bond angles

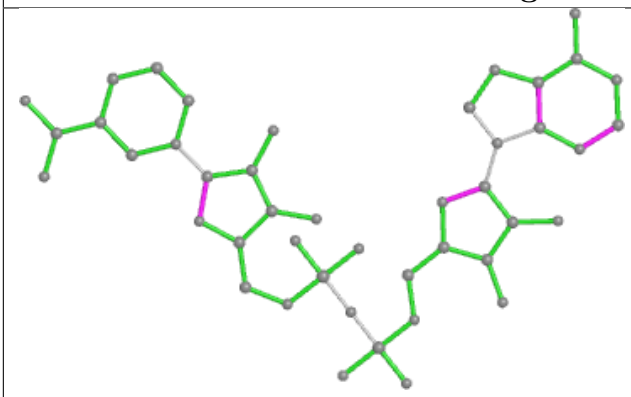


Torsions

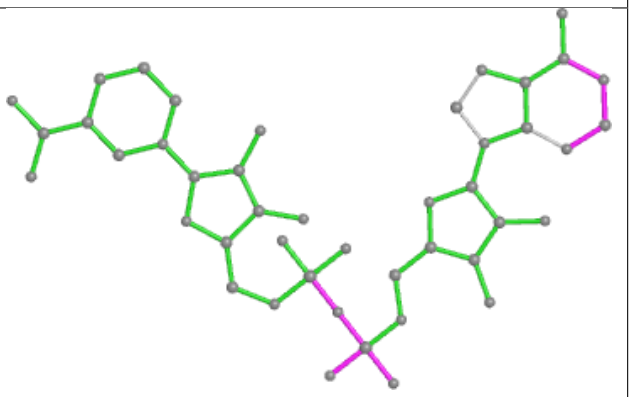


Rings

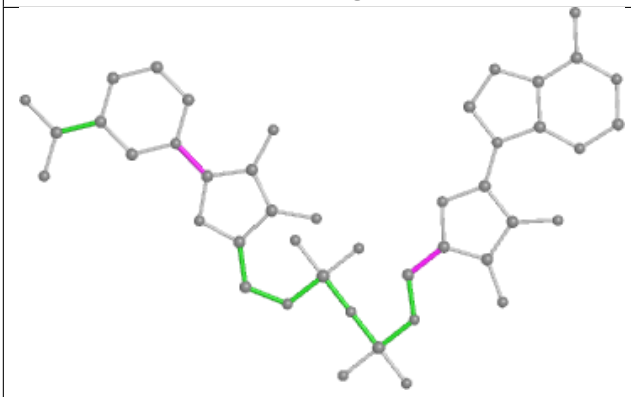
Ligand NAD B 401



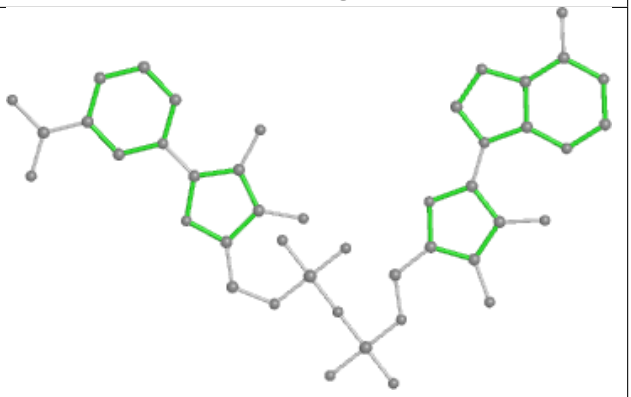
Bond lengths



Bond angles

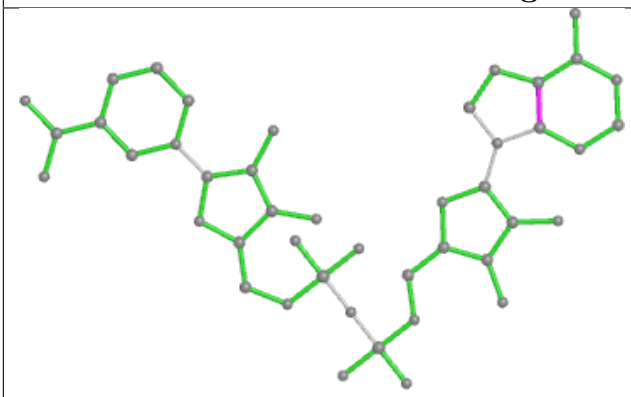


Torsions

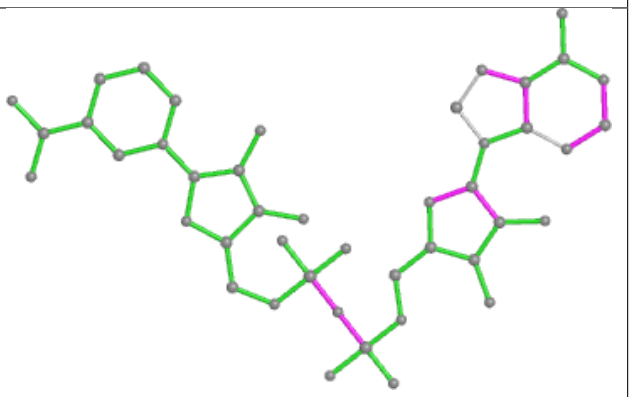


Rings

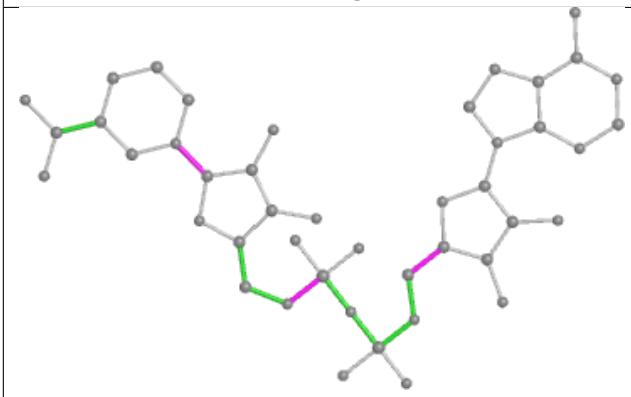
Ligand NAD C 401



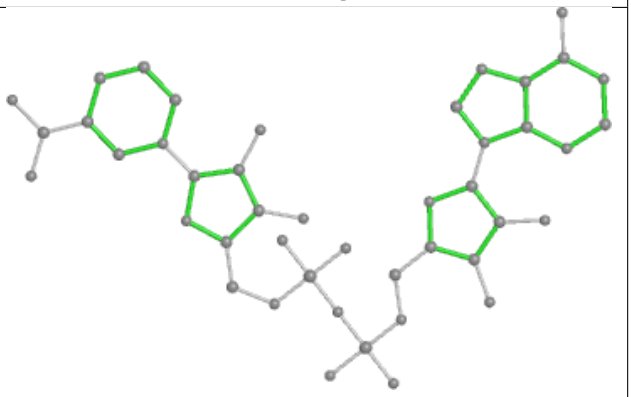
Bond lengths



Bond angles

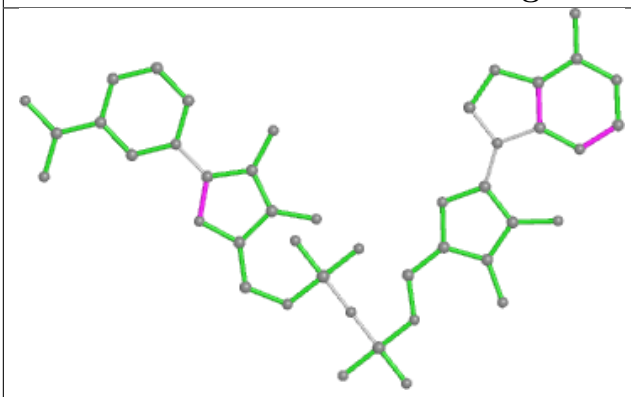


Torsions

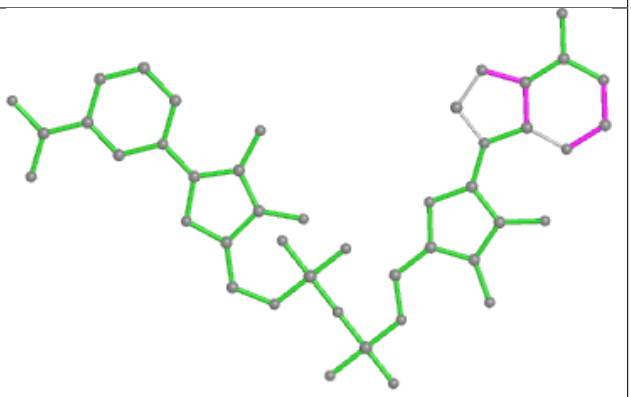


Rings

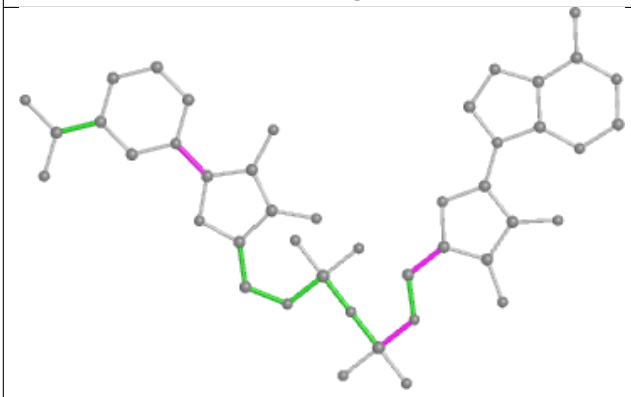
Ligand NAD F 401



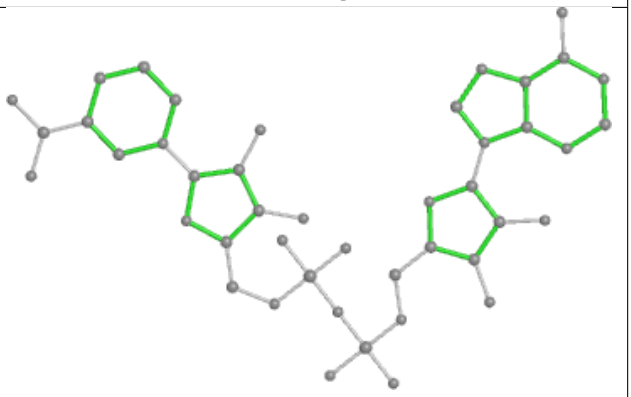
Bond lengths



Bond angles

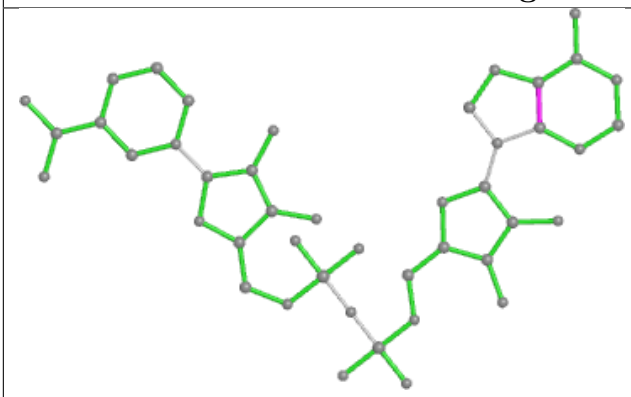


Torsions

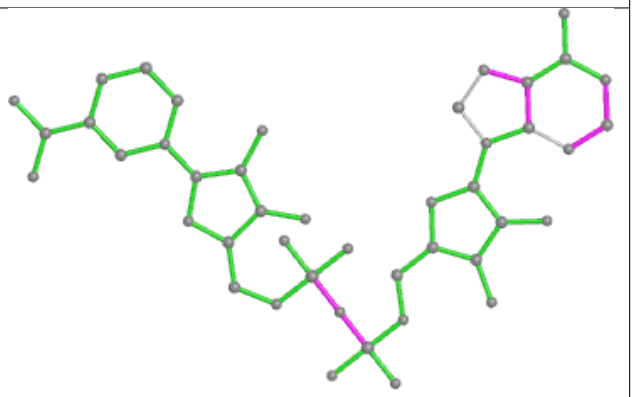


Rings

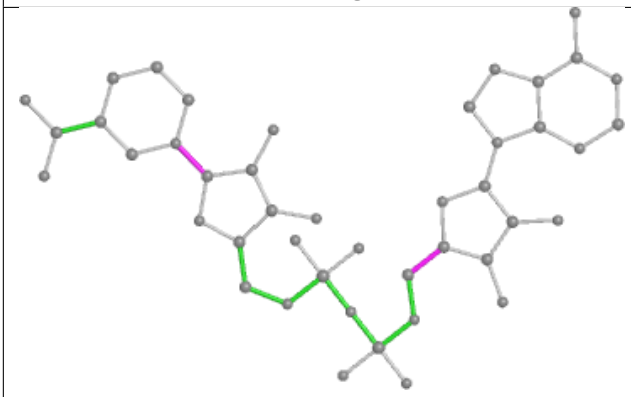
Ligand NAD D 500



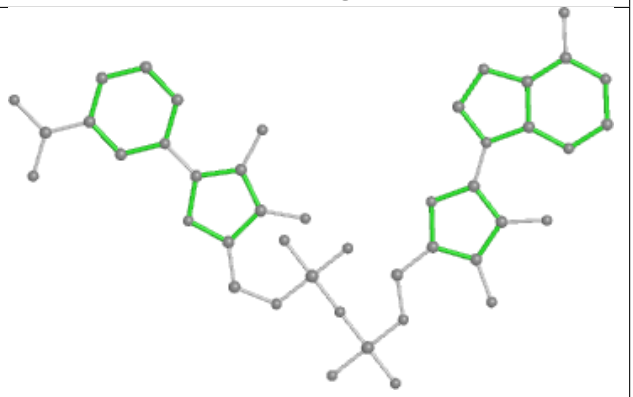
Bond lengths



Bond angles

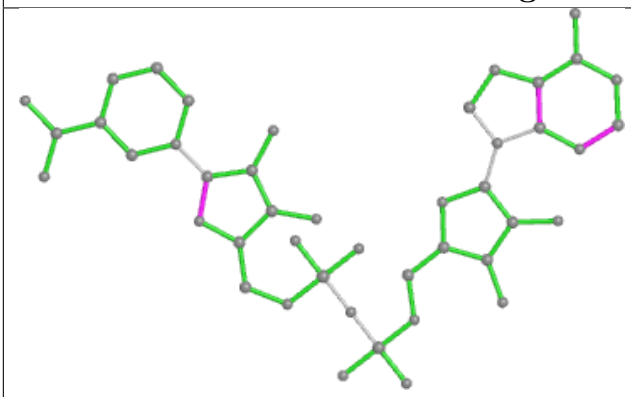


Torsions

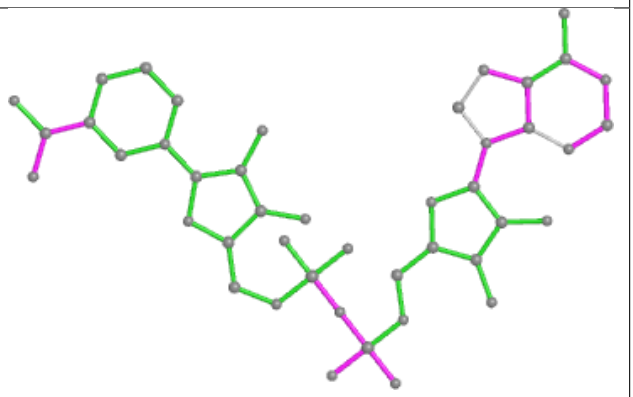


Rings

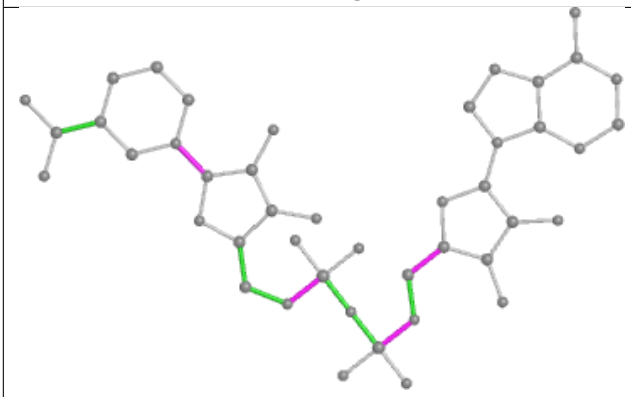
Ligand NAD G 401



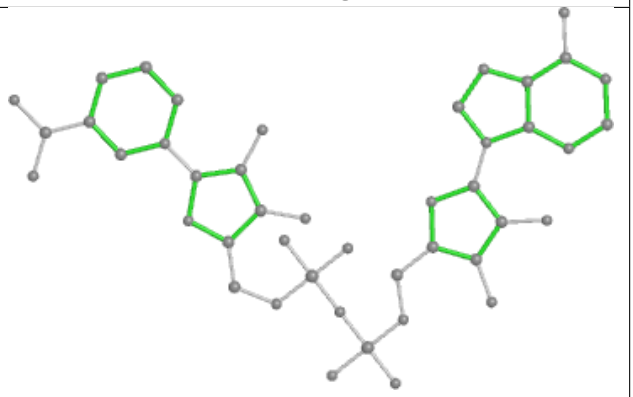
Bond lengths



Bond angles

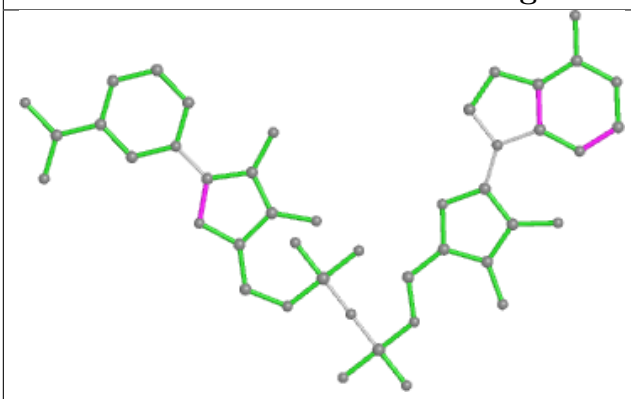


Torsions

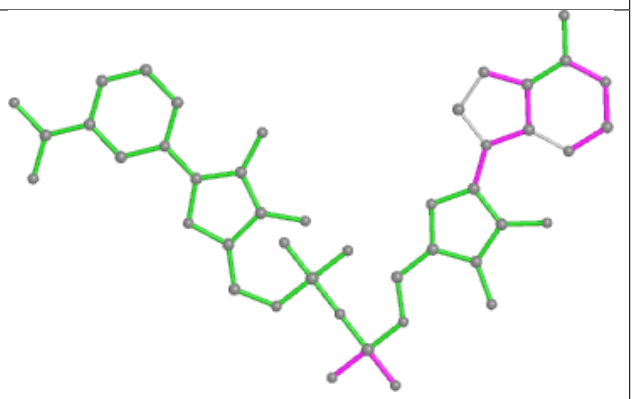


Rings

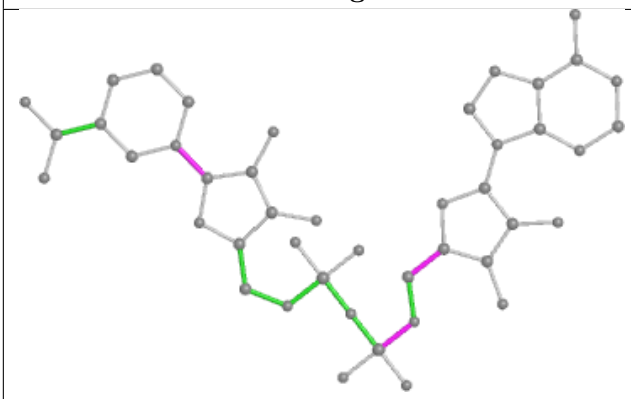
Ligand NAD A 401



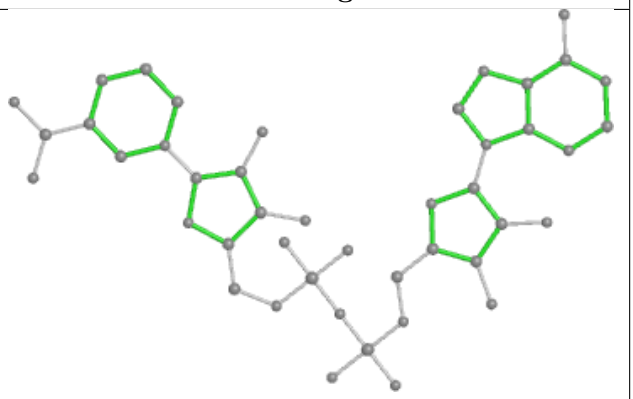
Bond lengths



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	338/347 (97%)	0.00	6 (1%) 68 72	20, 35, 57, 73	0
1	B	338/347 (97%)	-0.21	5 (1%) 73 77	14, 26, 47, 73	0
1	C	337/347 (97%)	-0.03	7 (2%) 63 68	14, 33, 60, 71	0
1	D	337/347 (97%)	0.12	9 (2%) 54 60	19, 39, 68, 84	0
1	E	335/347 (96%)	0.55	38 (11%) 5 6	23, 51, 85, 97	0
1	F	337/347 (97%)	-0.06	8 (2%) 59 64	16, 31, 55, 85	0
1	G	337/347 (97%)	-0.12	7 (2%) 63 68	14, 31, 51, 69	0
1	H	325/347 (93%)	1.13	65 (20%) 1 1	26, 65, 91, 113	0
All	All	2684/2776 (96%)	0.17	145 (5%) 25 31	14, 37, 78, 113	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	147	ALA	7.1
1	H	72	GLY	6.3
1	H	113	SER	6.2
1	H	37	PHE	5.9
1	H	130	ALA	5.6
1	H	104	GLY	5.4
1	E	87	ALA	5.0
1	H	295	THR	4.9
1	H	223	GLY	4.9
1	H	271	ALA	4.8
1	E	130	ALA	4.7
1	C	93	VAL	4.7
1	H	337	ALA	4.6
1	H	106	PHE	4.5
1	H	332	LEU	4.4
1	E	118	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	143	THR	4.2
1	G	72	GLY	4.1
1	H	65	GLY	4.0
1	H	117	LYS	4.0
1	B	2	SER	4.0
1	H	93	VAL	4.0
1	B	72	GLY	4.0
1	H	124	ILE	3.9
1	E	3	LYS	3.9
1	H	265	ALA	3.6
1	E	108	THR	3.5
1	E	148	ASN	3.5
1	H	149	ASN	3.5
1	D	100	VAL	3.5
1	H	257	GLY	3.5
1	H	216	THR	3.4
1	D	72	GLY	3.4
1	H	112	ALA	3.4
1	E	124	ILE	3.3
1	E	123	VAL	3.3
1	H	272	ASN	3.3
1	H	92	GLY	3.3
1	H	144	TYR	3.3
1	H	151	ILE	3.3
1	E	26	ASP	3.2
1	E	93	VAL	3.2
1	E	147	ALA	3.2
1	H	335	TYR	3.2
1	H	231	GLY	3.1
1	H	148	ASN	3.1
1	H	139	VAL	3.1
1	E	37	PHE	3.1
1	H	105	VAL	3.1
1	F	72	GLY	3.0
1	G	99	VAL	3.0
1	A	72	GLY	2.9
1	H	217	GLY	2.9
1	D	37	PHE	2.9
1	H	131	ASP	2.9
1	C	124[A]	ILE	2.9
1	H	134	MET	2.9
1	H	152	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	83	SER	2.9
1	E	339	ARG	2.9
1	E	338	SER	2.9
1	H	26	ASP	2.8
1	H	228	ASP	2.8
1	H	107	THR	2.8
1	H	82	ASN	2.8
1	D	92	GLY	2.8
1	H	100	VAL	2.8
1	E	107	THR	2.8
1	E	117	LYS	2.8
1	E	143	THR	2.8
1	H	90	PRO	2.8
1	H	64	GLY	2.8
1	H	198	GLY	2.7
1	G	252	CYS	2.7
1	H	114	ALA	2.7
1	D	8	ILE	2.7
1	D	93	VAL	2.6
1	H	95	GLY	2.6
1	E	64	GLY	2.6
1	H	297	SER	2.6
1	E	120	ALA	2.6
1	F	100	VAL	2.5
1	H	77	HIS	2.5
1	H	258	ALA	2.5
1	D	65	GLY	2.5
1	F	147	ALA	2.5
1	H	273	GLY	2.5
1	E	27	THR	2.5
1	E	110	ASP	2.5
1	H	310	PRO	2.5
1	F	130	ALA	2.5
1	H	270	ALA	2.5
1	H	169	ILE	2.4
1	H	219	ALA	2.4
1	E	63	GLU	2.4
1	E	85	ASP	2.4
1	F	64	GLY	2.4
1	E	141	ASN	2.4
1	E	98	TYR	2.4
1	E	92	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	230	ASN	2.4
1	H	3	LYS	2.4
1	H	336	ILE	2.4
1	G	37	PHE	2.3
1	H	94	ASP	2.3
1	H	141	ASN	2.3
1	E	112	ALA	2.3
1	D	74	THR	2.3
1	B	8	ILE	2.3
1	C	148	ASN	2.2
1	A	37	PHE	2.2
1	B	117	LYS	2.2
1	D	148	ASN	2.2
1	E	104	GLY	2.2
1	H	126	SER	2.2
1	E	145	ASP	2.2
1	E	149	ASN	2.2
1	H	118	GLY	2.2
1	H	303	LEU	2.2
1	C	252	CYS	2.2
1	G	8	ILE	2.1
1	H	212	ILE	2.1
1	F	148	ASN	2.1
1	G	100	VAL	2.1
1	E	75	THR	2.1
1	E	227	PRO	2.1
1	A	124	ILE	2.1
1	G	124	ILE	2.1
1	E	144	TYR	2.1
1	F	93	VAL	2.1
1	E	89	ILE	2.1
1	E	113	SER	2.1
1	C	100	VAL	2.1
1	H	259	THR	2.1
1	E	336	ILE	2.1
1	C	73	LYS	2.1
1	A	165	LEU	2.0
1	C	337	ALA	2.0
1	E	150	HIS	2.0
1	F	123	VAL	2.0
1	A	125	ILE	2.0
1	A	100	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	272	ASN	2.0
1	B	33[A]	VAL	2.0
1	H	146	LYS	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)

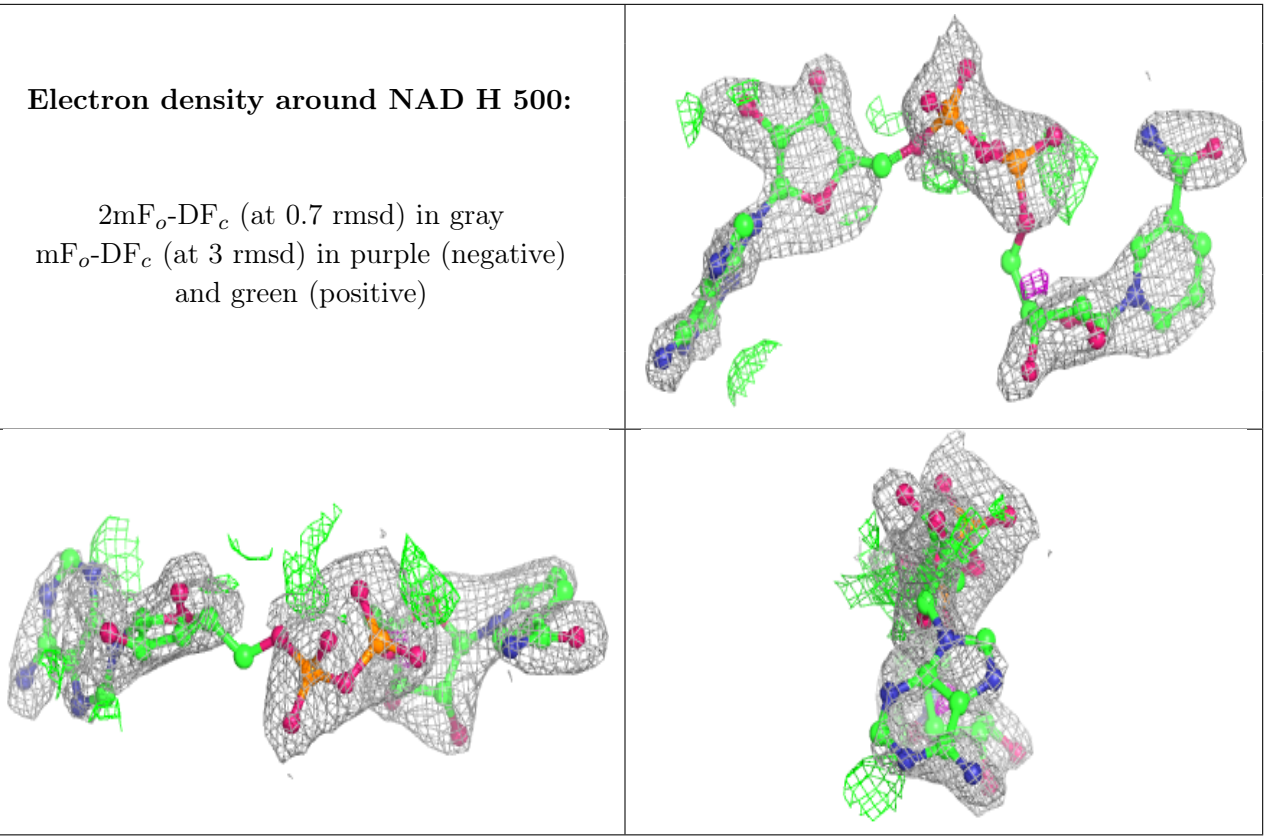
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	EDO	F	402	4/4	0.82	0.17	37,40,40,41	0
2	NAD	H	500	44/44	0.87	0.21	21,47,68,71	44
3	EDO	A	403	4/4	0.89	0.14	41,44,44,50	0
3	EDO	A	402	4/4	0.91	0.13	35,36,37,39	0
2	NAD	E	500	44/44	0.92	0.18	30,49,62,66	0
3	EDO	B	402	4/4	0.93	0.15	36,37,39,40	0
3	EDO	G	402	4/4	0.93	0.18	36,44,46,48	0
2	NAD	D	500	44/44	0.95	0.14	29,41,52,55	0
2	NAD	C	401	44/44	0.95	0.11	22,31,39,46	0
3	EDO	C	402	4/4	0.96	0.08	38,38,39,42	0
2	NAD	B	401	44/44	0.96	0.11	22,29,34,36	0
2	NAD	G	401	44/44	0.96	0.09	18,29,38,43	0
2	NAD	A	401	44/44	0.97	0.12	19,31,35,39	0
2	NAD	F	401	44/44	0.97	0.10	18,33,39,47	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.

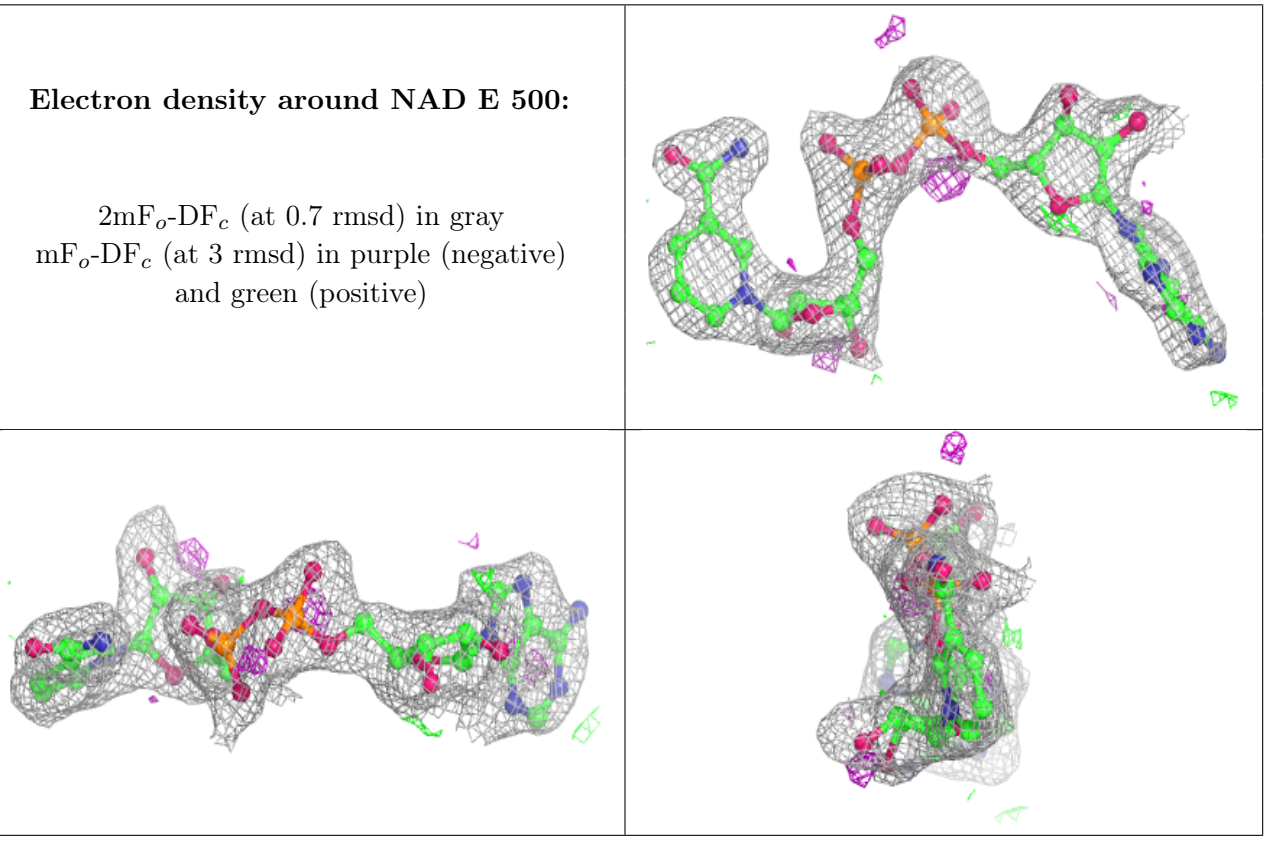
Electron density around NAD H 500:

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



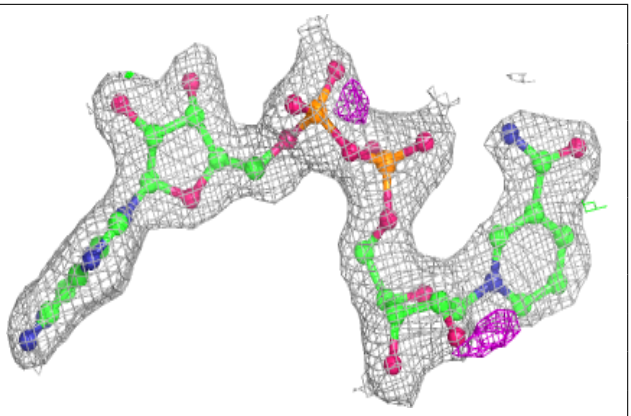
Electron density around NAD E 500:

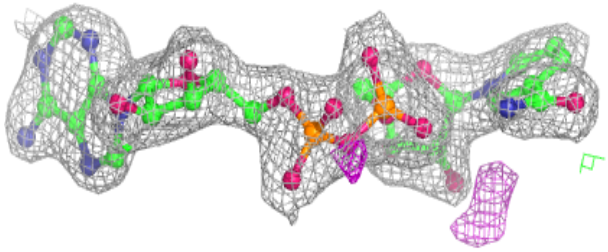
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

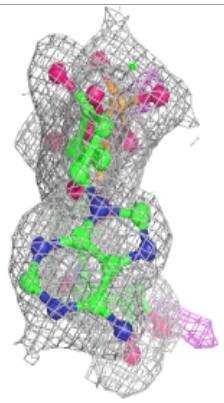


Electron density around NAD D 500:

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

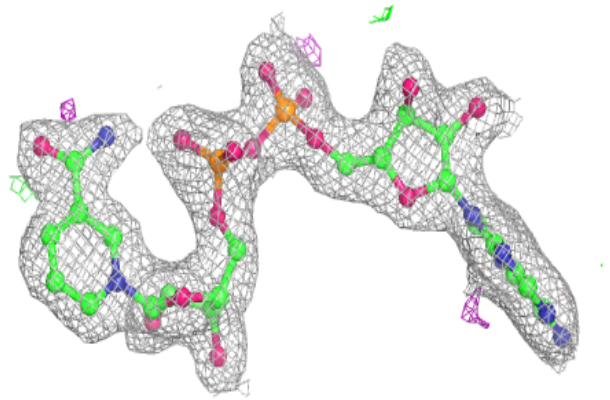


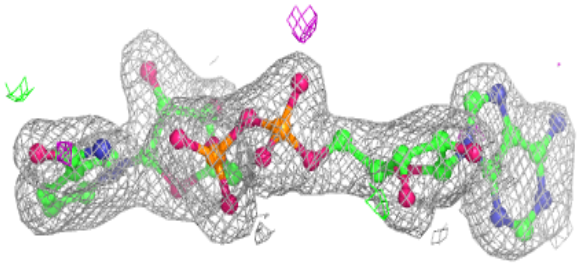


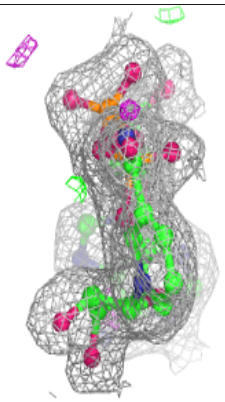


Electron density around NAD C 401:

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

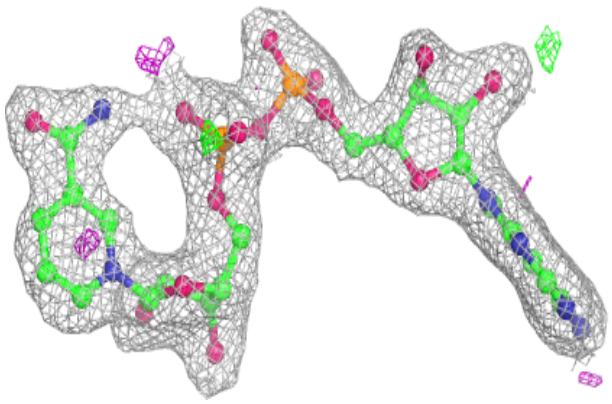


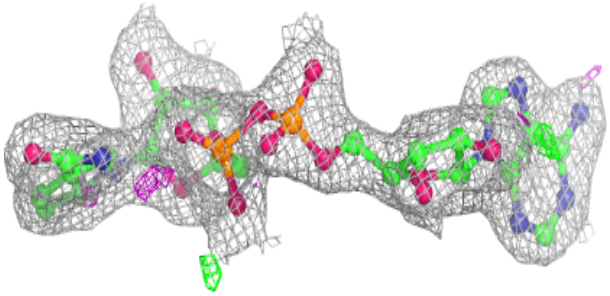


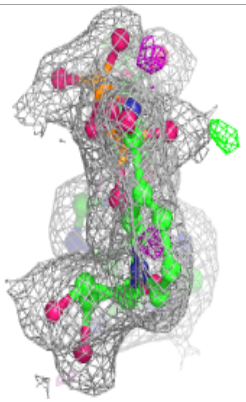


Electron density around NAD B 401:

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

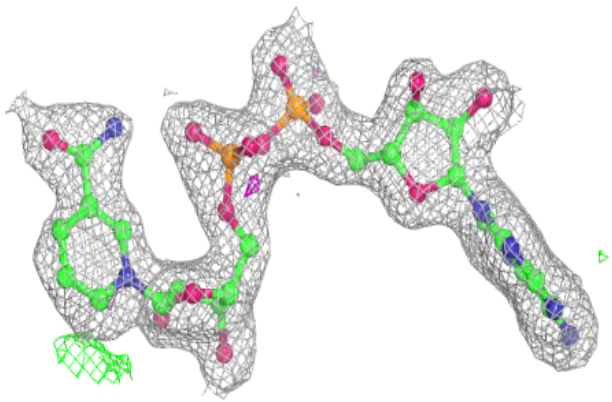


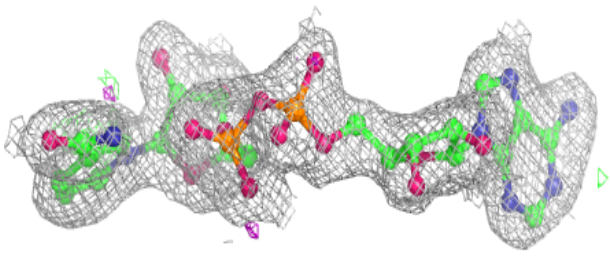


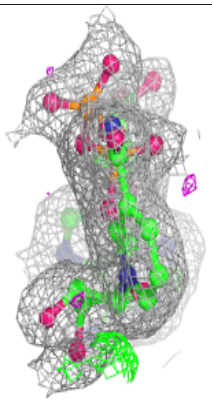


Electron density around NAD G 401:

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

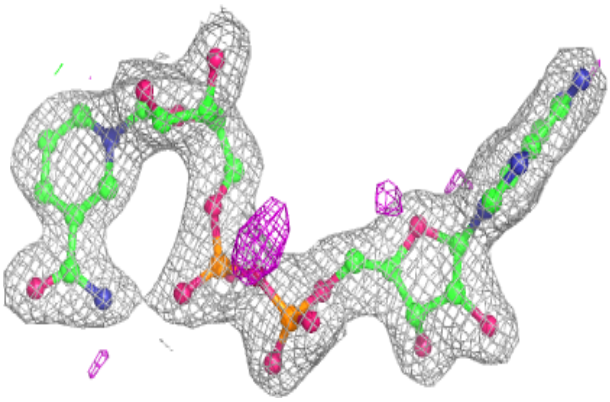


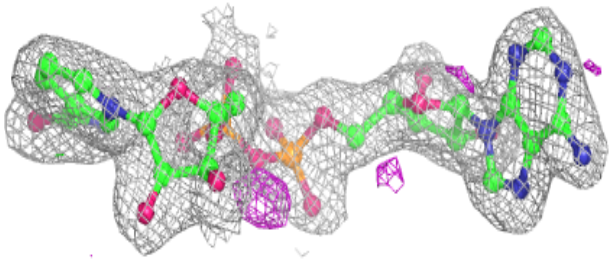


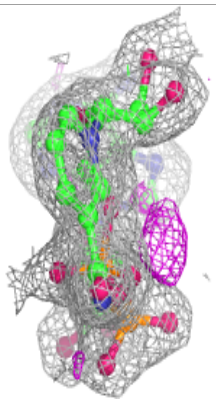


Electron density around NAD A 401:

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

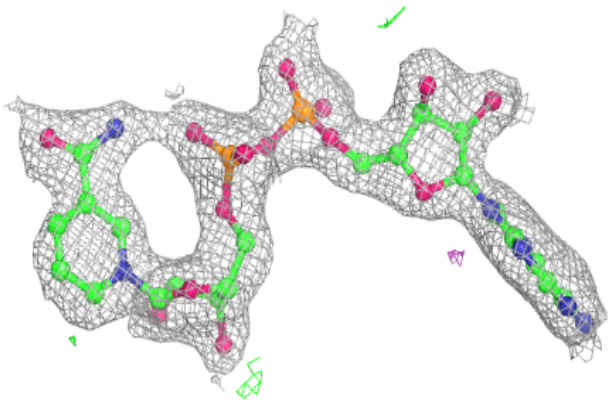


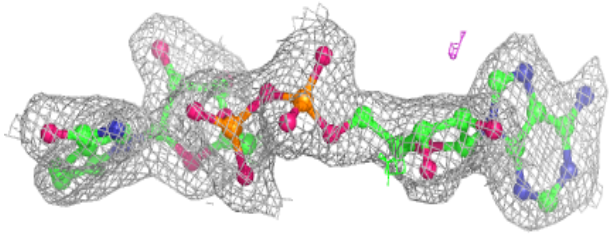


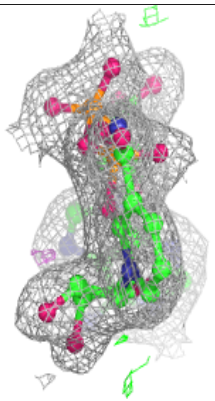


Electron density around NAD F 401:

$2mF_o$-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.