



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 08:45 PM EDT

PDB ID : 2ONP  
Title : Arg475Gln Mutant of Human Mitochondrial Aldehyde Dehydrogenase, complexed with NAD+  
Authors : Larson, H.N.; Hurley, T.D.  
Deposited on : 2007-01-24  
Resolution : 2.00 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](mailto: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.

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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	:	2.23.2
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)	:	2.23.2

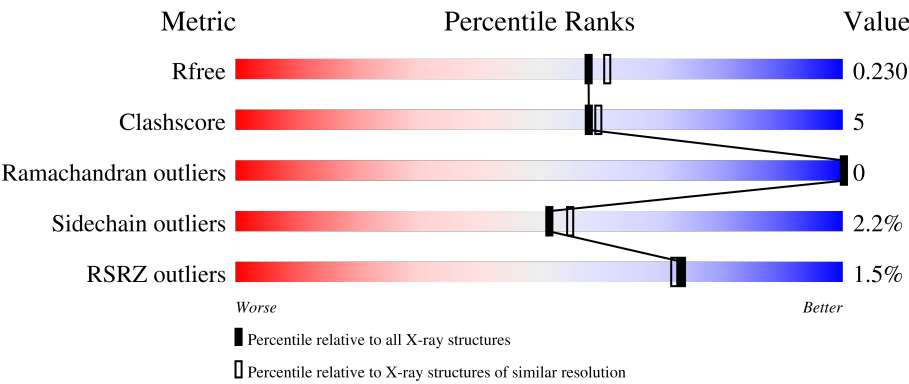
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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 <sub>free</sub>	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	<div><div>3%</div><div></div><div>86%</div><div>12%</div><div>..</div></div>
1	B	500	<div><div>2%</div><div></div><div>87%</div><div>11%</div><div>..</div></div>
1	C	500	<div><div></div><div></div><div>90%</div><div>8%</div><div>..</div></div>
1	D	500	<div><div>%</div><div></div><div>86%</div><div>12%</div><div>..</div></div>
1	E	500	<div><div>%</div><div></div><div>88%</div><div>10%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
1	F	500	 91% 7% ..
1	G	500	 2% 89% 9% ..
1	H	500	 3% 87% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	6952	-	-	-	X
5	EDO	E	6945	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33651 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	B	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	C	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	D	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	E	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	F	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	G	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	H	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	ARG	engineered mutation	UNP P05091
B	475	GLN	ARG	engineered mutation	UNP P05091
C	475	GLN	ARG	engineered mutation	UNP P05091
D	475	GLN	ARG	engineered mutation	UNP P05091
E	475	GLN	ARG	engineered mutation	UNP P05091
F	475	GLN	ARG	engineered mutation	UNP P05091
G	475	GLN	ARG	engineered mutation	UNP P05091
H	475	GLN	ARG	engineered mutation	UNP P05091

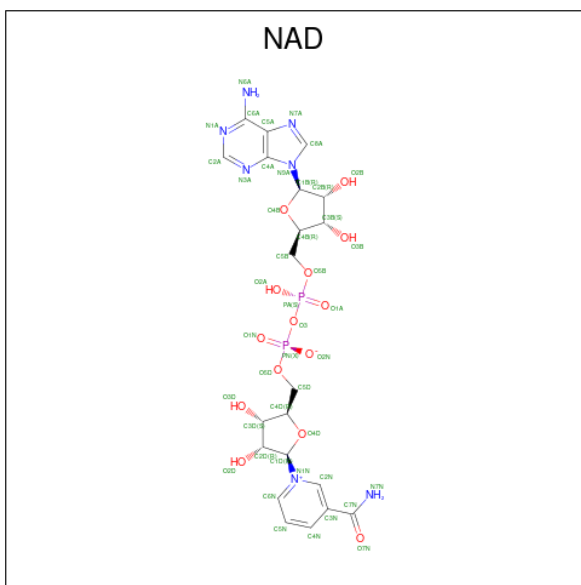
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	E	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0

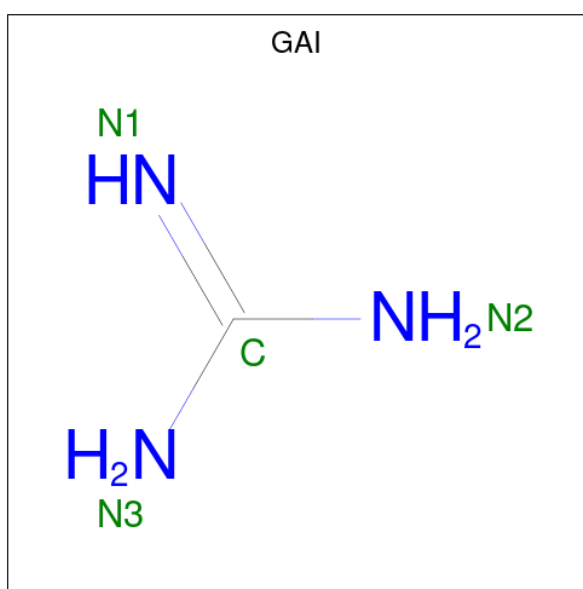
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GUANIDINE (three-letter code: GAI) (formula:  $\text{CH}_5\text{N}_3$ ).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total 4	C 1	N 3	0	0
6	C	1	Total 4	C 1	N 3	0	0
6	C	1	Total 4	C 1	N 3	0	0
6	C	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	D	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	E	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	F	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0
6	G	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0
6	H	1	Total 4	C 1	N 3	0	0

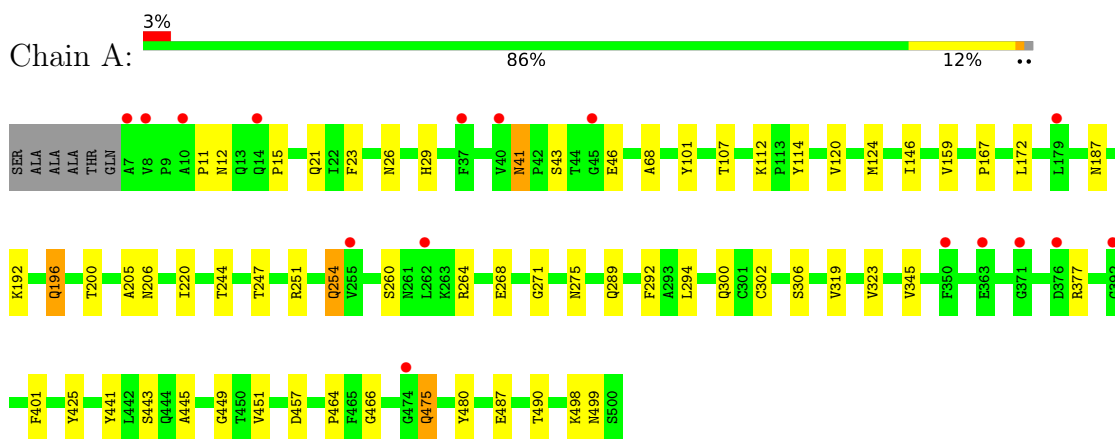
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	292	Total 292	O 292	0	0
7	B	317	Total 317	O 317	0	0
7	C	398	Total 398	O 398	0	0
7	D	333	Total 333	O 333	0	0
7	E	338	Total 338	O 338	0	0
7	F	410	Total 410	O 410	0	0
7	G	292	Total 292	O 292	0	0
7	H	267	Total 267	O 267	0	0

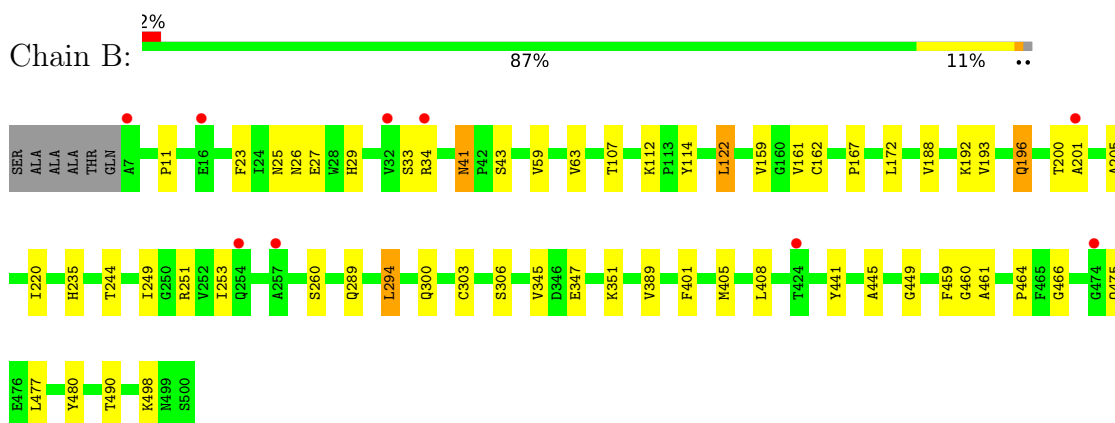
### 3 Residue-property plots [i](#)

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.

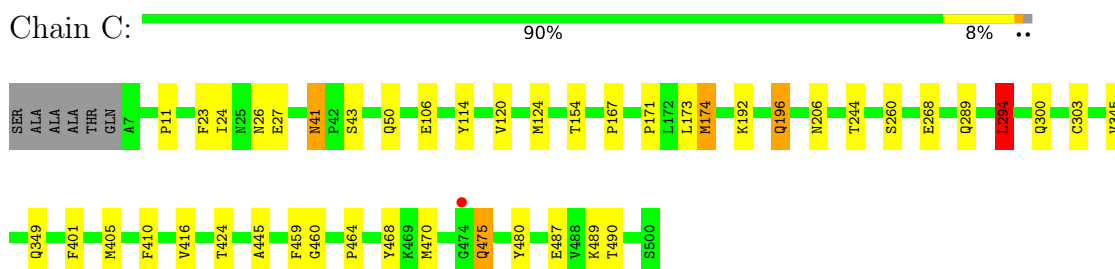
#### • Molecule 1: Aldehyde dehydrogenase



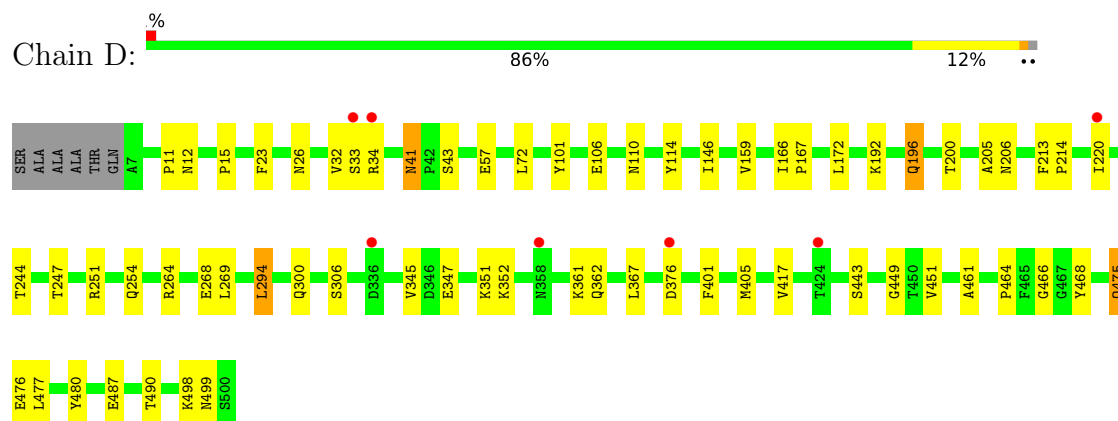
#### • Molecule 1: Aldehyde dehydrogenase



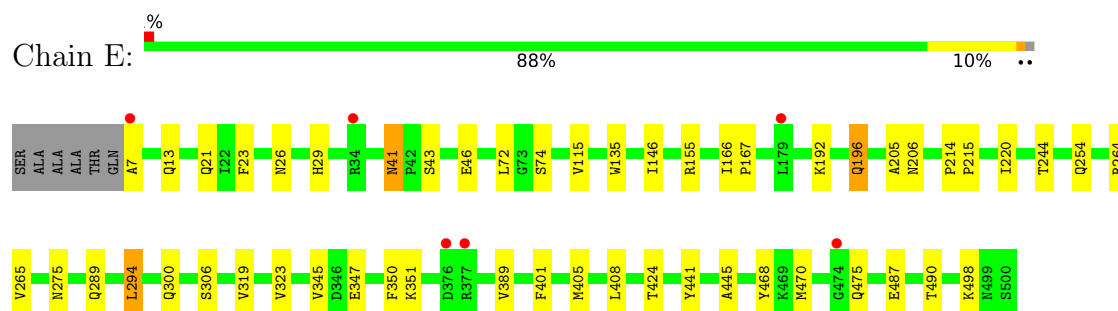
#### • Molecule 1: Aldehyde dehydrogenase



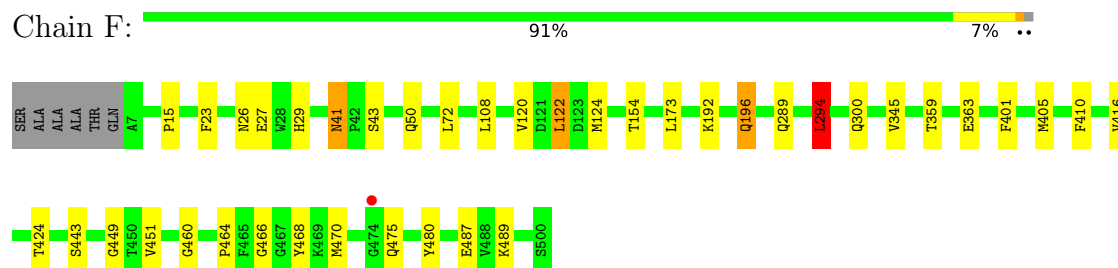
- Molecule 1: Aldehyde dehydrogenase



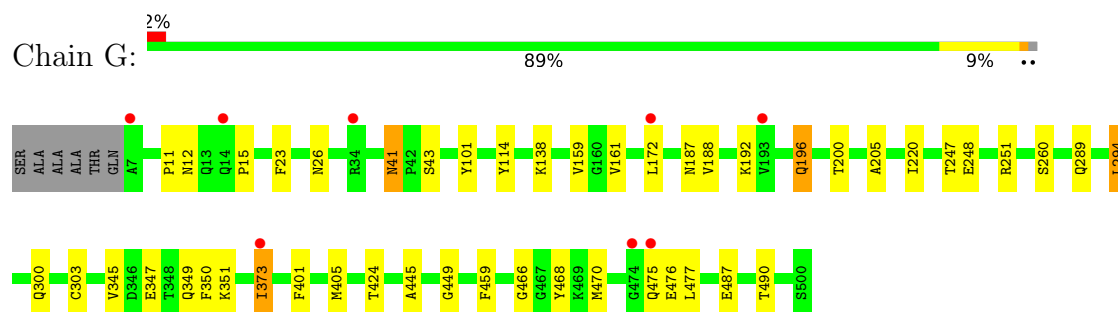
- Molecule 1: Aldehyde dehydrogenase



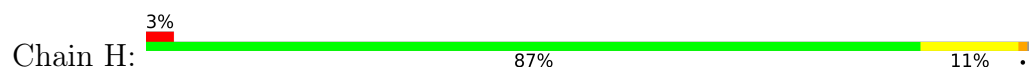
- Molecule 1: Aldehyde dehydrogenase

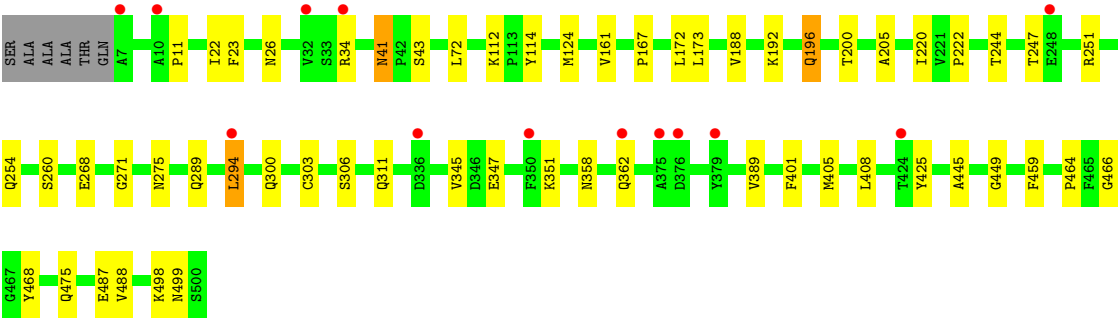


- Molecule 1: Aldehyde dehydrogenase



- Molecule 1: Aldehyde dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.85Å 150.84Å 177.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 2.00 29.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.97-2.00) 97.5 (29.97-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.26	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.204 , 0.240 0.195 , 0.230	Depositor DCC
$R_{free}$ test set	12705 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtrriage
Anisotropy	0.774	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	33651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0895e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	1/3880 (0.0%)	0.64	0/5265
1	B	0.50	0/3880	0.66	1/5265 (0.0%)
1	C	0.51	0/3880	0.67	1/5265 (0.0%)
1	D	0.48	0/3880	0.64	0/5265
1	E	0.47	0/3880	0.63	0/5265
1	F	0.48	0/3880	0.67	2/5265 (0.0%)
1	G	0.44	0/3880	0.63	0/5265
1	H	0.44	0/3880	0.62	0/5265
All	All	0.48	1/31040 (0.0%)	0.64	4/42120 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	487	GLU	CB-CG	-6.58	1.39	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	LEU	CA-CB-CG	-7.52	98.01	115.30
1	F	122	LEU	CA-CB-CG	-6.67	99.95	115.30
1	F	294	LEU	CA-CB-CG	-5.57	102.49	115.30
1	C	294	LEU	CA-CB-CG	-5.28	103.16	115.30

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	3796	0	3740	43	0
1	B	3796	0	3740	42	0
1	C	3796	0	3740	33	0
1	D	3796	0	3740	45	0
1	E	3796	0	3740	44	0
1	F	3796	0	3740	26	0
1	G	3796	0	3740	40	0
1	H	3796	0	3740	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	44	0	26	0	0
4	B	44	0	26	0	0
4	C	44	0	26	0	0
4	D	44	0	26	0	0
4	E	44	0	26	0	0
4	F	44	0	26	0	0
4	G	44	0	26	0	0
4	H	44	0	26	0	0
5	A	20	0	30	5	0
5	B	20	0	30	4	0
5	C	24	0	36	2	0
5	D	12	0	18	1	0
5	E	24	0	36	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	24	0	36	1	0
5	G	16	0	24	3	0
5	H	16	0	24	2	0
6	A	16	0	19	0	0
6	B	12	0	15	0	0
6	C	16	0	19	1	0
6	D	16	0	20	0	0
6	E	16	0	18	1	0
6	F	12	0	15	0	0
6	G	12	0	14	0	0
6	H	12	0	14	0	0
7	A	292	0	0	2	0
7	B	317	0	0	3	0
7	C	398	0	0	3	0
7	D	333	0	0	3	0
7	E	338	0	0	4	0
7	F	410	0	0	1	0
7	G	292	0	0	2	0
7	H	267	0	0	4	0
All	All	33651	0	30496	292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (292) 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:H:196:GLN:HE21	1:H:196:GLN:H	1.02	0.98
1:D:475:GLN:NE2	1:D:480:TYR:HB3	1.84	0.93
1:G:196:GLN:H	1:G:196:GLN:HE21	1.16	0.92
1:D:475:GLN:HE21	1:D:480:TYR:HB3	1.34	0.92
1:F:196:GLN:H	1:F:196:GLN:HE21	1.24	0.84
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.59	0.82
1:C:196:GLN:HE21	1:C:196:GLN:H	1.28	0.81
1:H:311:GLN:HG3	7:H:2748:HOH:O	1.82	0.78
1:D:300:GLN:HE22	1:D:345:VAL:H	1.33	0.76
1:G:347:GLU:HG2	1:G:351:LYS:HE2	1.67	0.76
1:G:300:GLN:HE22	1:G:345:VAL:H	1.34	0.76
1:H:445:ALA:HB2	5:H:6948:EDO:H11	1.68	0.76
1:B:196:GLN:H	1:B:196:GLN:HE21	1.33	0.74
1:C:475:GLN:HE21	1:C:480:TYR:HB3	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:GLN:H	1:H:196:GLN:NE2	1.83	0.73
1:E:347:GLU:HG2	1:E:351:LYS:HE2	1.69	0.73
1:H:294:LEU:HD22	1:H:405:MET:HB2	1.70	0.73
1:H:300:GLN:HE22	1:H:345:VAL:H	1.35	0.72
1:E:300:GLN:HE22	1:E:345:VAL:H	1.37	0.71
1:A:300:GLN:HE22	1:A:345:VAL:H	1.39	0.70
1:C:300:GLN:HE22	1:C:345:VAL:H	1.38	0.70
1:F:300:GLN:HE22	1:F:345:VAL:H	1.40	0.68
1:G:445:ALA:HB2	5:G:6947:EDO:H11	1.75	0.68
1:H:41:ASN:HD22	1:H:43:SER:H	1.40	0.67
1:B:300:GLN:HE22	1:B:345:VAL:H	1.42	0.67
1:D:196:GLN:H	1:D:196:GLN:HE21	1.43	0.67
1:A:475:GLN:HG3	1:A:480:TYR:HB3	1.76	0.66
1:H:196:GLN:HE21	1:H:196:GLN:N	1.84	0.65
1:F:294:LEU:HD22	1:F:405:MET:HB2	1.77	0.65
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.79	0.63
1:D:294:LEU:HD22	1:D:405:MET:HB2	1.80	0.63
1:G:196:GLN:H	1:G:196:GLN:NE2	1.94	0.63
1:H:358:ASN:O	1:H:362:GLN:HG2	1.99	0.62
1:H:41:ASN:ND2	1:H:43:SER:H	1.96	0.62
1:E:441:TYR:CE1	5:E:6945:EDO:H22	2.35	0.62
1:B:445:ALA:HB2	5:B:6942:EDO:H11	1.83	0.61
1:D:41:ASN:C	1:D:41:ASN:HD22	2.03	0.61
1:E:196:GLN:H	1:E:196:GLN:HE21	1.47	0.61
1:A:196:GLN:H	1:A:196:GLN:HE21	1.48	0.61
1:E:487:GLU:HG3	1:F:468:TYR:CE1	2.36	0.61
1:A:41:ASN:C	1:A:41:ASN:HD22	2.03	0.61
1:G:251:ARG:NH2	1:H:260:SER:O	2.34	0.60
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.83	0.60
1:F:41:ASN:C	1:F:41:ASN:HD22	2.04	0.60
1:G:172:LEU:HD21	1:G:200:THR:HB	1.82	0.60
1:B:172:LEU:HD21	1:B:200:THR:HB	1.83	0.59
1:F:289:GLN:NE2	7:F:3289:HOH:O	2.33	0.59
1:F:475:GLN:OE1	1:F:480:TYR:HB3	2.03	0.59
1:G:41:ASN:C	1:G:41:ASN:HD22	2.04	0.59
1:B:196:GLN:H	1:B:196:GLN:NE2	1.98	0.59
1:A:260:SER:O	1:B:251:ARG:NH2	2.34	0.59
1:B:294:LEU:HD22	1:B:405:MET:HB2	1.84	0.59
1:B:347:GLU:HG3	5:B:6962:EDO:H12	1.84	0.59
1:B:41:ASN:C	1:B:41:ASN:HD22	2.06	0.59
1:C:445:ALA:HB2	5:C:6943:EDO:H11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:THR:CG2	1:C:470:MET:SD	2.92	0.58
1:E:155:ARG:HD2	5:E:6905:EDO:H22	1.85	0.58
1:F:41:ASN:ND2	1:F:43:SER:H	2.01	0.58
1:D:41:ASN:ND2	1:D:43:SER:H	2.02	0.57
1:D:475:GLN:HE21	1:D:480:TYR:CB	2.14	0.57
1:E:74:SER:HA	5:E:6955:EDO:H22	1.85	0.57
1:E:264:ARG:HD2	6:E:6835:GAI:N1	2.20	0.57
1:B:41:ASN:HD22	1:B:43:SER:H	1.53	0.57
1:B:347:GLU:HG2	1:B:351:LYS:HE2	1.87	0.56
1:H:41:ASN:HD22	1:H:41:ASN:C	2.08	0.56
1:A:41:ASN:ND2	1:A:43:SER:H	2.03	0.56
1:C:41:ASN:C	1:C:41:ASN:HD22	2.08	0.56
1:C:487:GLU:HG3	1:D:468:TYR:CE1	2.41	0.56
1:E:41:ASN:HB2	5:E:6915:EDO:H11	1.87	0.56
1:E:72:LEU:HD21	5:F:6946:EDO:H11	1.86	0.56
1:E:347:GLU:O	1:E:351:LYS:HG2	2.05	0.56
1:C:475:GLN:NE2	1:C:480:TYR:HB3	2.18	0.55
1:A:445:ALA:HB2	5:A:6941:EDO:H11	1.88	0.55
1:A:196:GLN:H	1:A:196:GLN:NE2	2.04	0.55
1:G:196:GLN:HE21	1:G:196:GLN:N	1.97	0.55
1:A:475:GLN:HG3	1:A:480:TYR:CB	2.36	0.55
1:C:260:SER:O	1:D:251:ARG:NH2	2.40	0.55
1:E:424:THR:CG2	1:E:470:MET:SD	2.95	0.55
1:E:468:TYR:CE1	1:F:487:GLU:HG3	2.42	0.55
1:G:101:TYR:CG	5:G:6927:EDO:H11	2.42	0.55
1:E:46:GLU:HB2	5:E:6915:EDO:H21	1.88	0.54
1:F:196:GLN:H	1:F:196:GLN:NE2	1.99	0.54
1:B:41:ASN:ND2	1:B:43:SER:H	2.05	0.54
1:E:289:GLN:NE2	7:E:3288:HOH:O	2.39	0.54
1:D:172:LEU:HD21	1:D:200:THR:HB	1.89	0.54
1:D:294:LEU:HD12	1:D:306:SER:HA	1.90	0.54
1:G:468:TYR:CE1	1:H:487:GLU:HG3	2.43	0.53
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.90	0.53
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.43	0.53
1:A:498:LYS:HG2	1:A:499:ASN:N	2.24	0.53
1:A:251:ARG:NH2	1:B:260:SER:O	2.41	0.53
1:F:424:THR:CG2	1:F:470:MET:SD	2.96	0.53
1:G:475:GLN:HE21	1:H:488:VAL:HG21	1.74	0.53
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.45	0.52
1:A:302:CYS:SG	7:A:3143:HOH:O	2.58	0.52
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.43	0.52
1:B:289:GLN:NE2	7:B:3301:HOH:O	2.29	0.52
1:G:349:GLN:HG3	7:G:3432:HOH:O	2.09	0.52
1:B:205:ALA:HB2	1:B:220:ILE:HD12	1.92	0.52
1:G:487:GLU:HG3	1:H:468:TYR:CE1	2.45	0.52
1:A:247:THR:O	1:A:251:ARG:HG3	2.09	0.52
1:H:172:LEU:HD21	1:H:200:THR:HB	1.92	0.52
1:D:347:GLU:O	1:D:351:LYS:HG2	2.10	0.52
1:H:205:ALA:HB2	1:H:220:ILE:HD12	1.92	0.52
1:C:468:TYR:CE1	1:D:487:GLU:HG3	2.45	0.51
1:A:441:TYR:CD1	5:A:6941:EDO:H12	2.45	0.51
1:C:41:ASN:ND2	1:C:43:SER:H	2.09	0.51
1:E:41:ASN:ND2	1:E:43:SER:H	2.08	0.51
1:G:289:GLN:NE2	7:G:3261:HOH:O	2.34	0.51
1:H:449:GLY:HA3	1:H:466:GLY:O	2.10	0.51
1:E:41:ASN:CB	5:E:6915:EDO:H11	2.41	0.51
1:G:260:SER:O	1:H:251:ARG:NH2	2.43	0.51
1:G:41:ASN:ND2	1:G:43:SER:H	2.08	0.51
1:D:205:ALA:HB2	1:D:220:ILE:HD12	1.92	0.50
1:G:294:LEU:HD22	1:G:405:MET:CB	2.38	0.50
1:D:196:GLN:H	1:D:196:GLN:NE2	2.08	0.50
1:A:41:ASN:HD22	1:A:43:SER:H	1.60	0.50
1:G:424:THR:CG2	1:G:470:MET:SD	3.00	0.50
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.94	0.49
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.48	0.49
1:F:124:MET:HE3	1:F:173:LEU:HD22	1.93	0.49
1:F:41:ASN:HD22	1:F:43:SER:H	1.60	0.49
1:B:33:SER:O	1:B:34:ARG:HB2	2.11	0.49
5:E:6945:EDO:H11	1:F:72:LEU:HD21	1.95	0.49
1:D:167:PRO:HD3	1:D:244:THR:HB	1.95	0.49
1:F:15:PRO:HD2	1:F:108:LEU:HD22	1.93	0.49
1:E:350:PHE:CE2	5:E:6965:EDO:H12	2.46	0.49
1:D:41:ASN:HD22	1:D:43:SER:H	1.61	0.48
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.48	0.48
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.48	0.48
5:C:6943:EDO:H11	1:D:72:LEU:HD21	1.94	0.48
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.96	0.48
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.48	0.48
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.48	0.48
1:A:172:LEU:HD21	1:A:200:THR:HB	1.96	0.48
1:G:449:GLY:HA3	1:G:466:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:ASN:C	1:E:41:ASN:HD22	2.17	0.48
1:B:449:GLY:HA3	1:B:466:GLY:O	2.13	0.48
1:E:115:VAL:HG23	7:E:1458:HOH:O	2.13	0.48
1:E:167:PRO:HD3	1:E:244:THR:HB	1.96	0.48
1:B:475:GLN:OE1	1:B:480:TYR:HB3	2.14	0.48
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.96	0.47
1:C:196:GLN:H	1:C:196:GLN:NE2	2.04	0.47
1:D:294:LEU:HD13	7:D:1077:HOH:O	2.14	0.47
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.49	0.47
1:A:289:GLN:NE2	7:A:3151:HOH:O	2.37	0.47
1:A:490:THR:OG1	1:B:464:PRO:HG2	2.15	0.47
1:B:441:TYR:CD1	5:B:6942:EDO:H12	2.50	0.47
1:H:167:PRO:HD3	1:H:244:THR:HB	1.96	0.47
1:E:490:THR:OG1	1:F:464:PRO:HG2	2.15	0.47
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.50	0.47
1:A:449:GLY:HA3	1:A:466:GLY:O	2.14	0.47
1:B:27:GLU:HB2	1:B:29:HIS:CE1	2.49	0.47
1:H:389:VAL:HB	1:H:408:LEU:HG	1.97	0.47
1:E:21:GLN:HB3	1:E:29:HIS:O	2.14	0.47
1:C:174:MET:HE3	1:C:174:MET:HA	1.97	0.47
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.15	0.46
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.50	0.46
1:C:349:GLN:HB3	7:C:2406:HOH:O	2.14	0.46
1:D:268:GLU:HB3	7:D:1339:HOH:O	2.15	0.46
1:H:294:LEU:HD13	7:H:1076:HOH:O	2.15	0.46
1:E:146:ILE:HG13	1:F:460:GLY:HA3	1.97	0.46
1:G:350:PHE:HZ	1:G:373:ILE:CG2	2.28	0.46
1:D:352:LYS:HD3	7:D:1766:HOH:O	2.14	0.46
1:H:112:LYS:HB2	7:H:1922:HOH:O	2.16	0.46
1:D:247:THR:HA	1:D:269:LEU:HD13	1.97	0.46
1:A:46:GLU:HB2	5:A:6911:EDO:H21	1.97	0.46
1:B:59:VAL:O	1:B:63:VAL:HG23	2.15	0.46
1:D:361:LYS:HD3	1:D:367:LEU:HD22	1.98	0.46
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.17	0.45
1:C:464:PRO:HG2	1:D:490:THR:OG1	2.16	0.45
1:C:124:MET:HE3	1:C:173:LEU:CD2	2.46	0.45
1:B:161:VAL:HA	1:B:188:VAL:HG23	1.99	0.45
1:E:441:TYR:CD1	5:E:6945:EDO:H12	2.52	0.45
1:C:24:ILE:O	1:C:27:GLU:HG2	2.17	0.45
1:D:294:LEU:HD13	1:D:405:MET:HA	1.99	0.45
1:H:445:ALA:HB2	5:H:6948:EDO:C1	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:289:GLN:NE2	7:H:3279:HOH:O	2.48	0.45
1:C:268:GLU:HB3	7:C:1687:HOH:O	2.17	0.44
1:B:167:PRO:HD3	1:B:244:THR:HB	1.99	0.44
1:E:445:ALA:HB2	5:E:6945:EDO:H11	2.00	0.44
1:G:303:CYS:SG	1:G:459:PHE:HZ	2.41	0.44
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.17	0.44
1:B:193:VAL:HG11	1:B:201:ALA:CB	2.47	0.44
1:B:347:GLU:HG3	5:B:6962:EDO:C1	2.47	0.44
1:C:424:THR:HG22	1:C:470:MET:HB2	1.99	0.44
1:E:389:VAL:HB	1:E:408:LEU:HG	2.00	0.44
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.52	0.44
1:C:120:VAL:O	1:C:124:MET:HG3	2.18	0.44
1:D:461:ALA:HA	1:D:477:LEU:HD22	2.00	0.44
1:C:124:MET:HE3	1:C:173:LEU:HD22	1.98	0.44
1:D:498:LYS:HG2	1:D:499:ASN:N	2.33	0.44
1:F:196:GLN:HE21	1:F:196:GLN:N	2.04	0.44
1:E:13:GLN:NE2	7:E:3330:HOH:O	2.50	0.44
1:E:254:GLN:NE2	1:E:265:VAL:HG11	2.32	0.44
1:H:294:LEU:HD12	1:H:306:SER:HA	1.99	0.43
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.19	0.43
1:A:101:TYR:CD2	5:A:6921:EDO:H11	2.52	0.43
1:C:460:GLY:HA3	1:D:146:ILE:HG13	2.00	0.43
6:C:6834:GAI:N1	1:D:264:ARG:HD2	2.33	0.43
1:E:350:PHE:HE2	5:E:6965:EDO:H12	1.83	0.43
1:G:41:ASN:HD22	1:G:43:SER:H	1.65	0.43
1:A:21:GLN:HB3	1:A:29:HIS:O	2.18	0.43
1:B:461:ALA:HA	1:B:477:LEU:HD22	2.00	0.43
1:E:196:GLN:H	1:E:196:GLN:NE2	2.15	0.43
1:F:410:PHE:CD1	1:F:416:VAL:HB	2.52	0.43
1:A:120:VAL:O	1:A:124:MET:HG3	2.18	0.43
1:D:33:SER:O	1:D:34:ARG:HB2	2.19	0.43
1:F:154:THR:HA	1:F:489:LYS:O	2.19	0.43
1:A:146:ILE:HG13	1:B:460:GLY:HA3	2.00	0.43
1:H:41:ASN:HD21	1:H:43:SER:HB2	1.84	0.43
1:D:449:GLY:HA3	1:D:466:GLY:O	2.18	0.43
1:C:289:GLN:NE2	7:C:3194:HOH:O	2.40	0.43
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.53	0.43
1:F:27:GLU:HB2	1:F:29:HIS:CE1	2.54	0.43
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.53	0.42
1:E:74:SER:N	5:E:6955:EDO:H12	2.33	0.42
1:E:498:LYS:HE2	1:E:498:LYS:HB3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:VAL:HG12	1:F:124:MET:HE1	2.00	0.42
1:H:498:LYS:HG2	1:H:499:ASN:N	2.34	0.42
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.54	0.42
1:H:347:GLU:HG2	1:H:351:LYS:HE3	2.01	0.42
1:B:249:ILE:O	1:B:253:ILE:HG12	2.19	0.42
1:B:27:GLU:HG3	7:B:1707:HOH:O	2.19	0.42
1:C:106:GLU:OE2	1:C:171:PRO:HB2	2.19	0.42
1:G:350:PHE:CZ	1:G:373:ILE:CG2	3.02	0.42
1:A:443:SER:HA	1:A:451:VAL:HG11	2.01	0.42
1:B:63:VAL:HG11	1:B:235:HIS:CE1	2.54	0.42
1:G:12:ASN:O	1:G:15:PRO:HD3	2.18	0.42
1:E:214:PRO:HA	1:E:215:PRO:HD3	1.94	0.42
1:E:294:LEU:HD12	1:E:306:SER:HA	2.02	0.42
1:H:124:MET:HE3	1:H:173:LEU:CD2	2.50	0.42
1:D:166:ILE:HB	1:D:167:PRO:HD2	2.01	0.42
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.43	0.42
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.55	0.41
1:B:172:LEU:CD2	1:B:200:THR:HB	2.50	0.41
1:B:303:CYS:SG	1:B:459:PHE:HZ	2.43	0.41
1:C:154:THR:HA	1:C:489:LYS:O	2.20	0.41
1:D:12:ASN:O	1:D:15:PRO:HD3	2.20	0.41
1:E:166:ILE:HB	1:E:167:PRO:HD2	2.02	0.41
1:H:22:ILE:HG12	1:H:222:PRO:HD2	2.02	0.41
1:C:167:PRO:HD3	1:C:244:THR:HB	2.01	0.41
1:E:205:ALA:HB2	1:E:220:ILE:HD12	2.02	0.41
1:H:161:VAL:HA	1:H:188:VAL:HG23	2.03	0.41
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.56	0.41
1:A:475:GLN:CG	1:A:480:TYR:HB3	2.48	0.41
1:C:303:CYS:SG	1:C:459:PHE:HZ	2.43	0.41
1:D:32:VAL:HG11	1:D:57:GLU:OE2	2.20	0.41
1:D:498:LYS:HE2	1:D:498:LYS:HB3	1.91	0.41
1:D:106:GLU:O	1:D:110:ASN:HB3	2.21	0.41
1:A:244:THR:HG23	1:A:268:GLU:HG3	2.03	0.41
1:A:319:VAL:O	1:A:323:VAL:HG23	2.20	0.41
1:A:498:LYS:HE2	1:A:498:LYS:HB3	1.86	0.41
1:D:11:PRO:HB3	1:D:114:TYR:CE2	2.55	0.41
1:F:449:GLY:HA3	1:F:466:GLY:O	2.20	0.41
1:A:292:PHE:HE1	1:A:457:ASP:HB2	1.85	0.41
1:C:410:PHE:CD1	1:C:416:VAL:HB	2.55	0.41
1:A:107:THR:HG23	1:A:112:LYS:O	2.20	0.41
1:A:294:LEU:HD23	1:A:306:SER:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:VAL:HB	1:B:408:LEU:HG	2.01	0.41
1:D:101:TYR:CB	5:D:6924:EDO:H11	2.50	0.41
1:E:319:VAL:O	1:E:323:VAL:HG23	2.21	0.41
1:F:443:SER:HA	1:F:451:VAL:HG11	2.03	0.41
1:G:159:VAL:HG12	1:G:187:ASN:OD1	2.21	0.41
1:H:247:THR:O	1:H:251:ARG:HG3	2.21	0.41
1:A:254:GLN:HE21	1:A:254:GLN:HB2	1.64	0.41
1:B:294:LEU:HD12	1:B:306:SER:HA	2.02	0.41
1:C:196:GLN:HE21	1:C:196:GLN:N	2.06	0.41
1:D:213:PHE:HA	1:D:214:PRO:HD3	1.95	0.41
1:D:476:GLU:O	1:D:477:LEU:HB2	2.21	0.41
1:E:7:ALA:HA	7:E:2509:HOH:O	2.21	0.41
1:E:347:GLU:CG	1:E:351:LYS:HE2	2.46	0.41
1:G:475:GLN:NE2	1:H:488:VAL:CG2	2.84	0.41
1:A:167:PRO:HD3	1:A:244:THR:HB	2.02	0.40
5:G:6947:EDO:H11	1:H:72:LEU:HD21	2.03	0.40
1:A:12:ASN:O	1:A:15:PRO:HD3	2.21	0.40
1:A:68:ALA:HB1	5:A:6951:EDO:H21	2.03	0.40
1:D:443:SER:HA	1:D:451:VAL:HG11	2.04	0.40
1:F:359:THR:O	1:F:363:GLU:HG2	2.22	0.40
1:G:247:THR:O	1:G:251:ARG:HG3	2.20	0.40
1:G:350:PHE:HZ	1:G:373:ILE:HG21	1.87	0.40
1:G:475:GLN:HE21	1:H:488:VAL:CG2	2.34	0.40
1:E:155:ARG:HH11	5:E:6905:EDO:H22	1.86	0.40
1:G:41:ASN:C	1:G:41:ASN:ND2	2.74	0.40
1:B:25:ASN:O	1:B:27:GLU:HG2	2.21	0.40
1:B:107:THR:HG23	1:B:112:LYS:O	2.21	0.40
1:B:159:VAL:HG13	1:B:162:CYS:SG	2.62	0.40
1:B:294:LEU:HD13	7:B:1013:HOH:O	2.21	0.40
1:G:475:GLN:NE2	1:H:488:VAL:HG21	2.37	0.40
1:G:476:GLU:O	1:G:477:LEU:HB2	2.21	0.40
1:H:34:ARG:HD3	1:H:34:ARG:HA	1.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	B	492/500 (98%)	477 (97%)	15 (3%)	0	100	100
1	C	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	D	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
1	E	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	F	492/500 (98%)	478 (97%)	14 (3%)	0	100	100
1	G	492/500 (98%)	473 (96%)	19 (4%)	0	100	100
1	H	492/500 (98%)	477 (97%)	15 (3%)	0	100	100
All	All	3936/4000 (98%)	3812 (97%)	124 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/402 (99%)	389 (98%)	10 (2%)	47	49
1	B	399/402 (99%)	392 (98%)	7 (2%)	59	63
1	C	399/402 (99%)	390 (98%)	9 (2%)	50	53
1	D	399/402 (99%)	387 (97%)	12 (3%)	41	41
1	E	399/402 (99%)	391 (98%)	8 (2%)	55	58
1	F	399/402 (99%)	392 (98%)	7 (2%)	59	63
1	G	399/402 (99%)	392 (98%)	7 (2%)	59	63
1	H	399/402 (99%)	390 (98%)	9 (2%)	50	53
All	All	3192/3216 (99%)	3123 (98%)	69 (2%)	52	55

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	192	LYS
1	A	196	GLN
1	A	206	ASN
1	A	254	GLN
1	A	264	ARG
1	A	275	ASN
1	A	377	ARG
1	A	401	PHE
1	A	475	GLN
1	B	41	ASN
1	B	122	LEU
1	B	192	LYS
1	B	196	GLN
1	B	294	LEU
1	B	401	PHE
1	B	498	LYS
1	C	41	ASN
1	C	50	GLN
1	C	174	MET
1	C	192	LYS
1	C	196	GLN
1	C	206	ASN
1	C	294	LEU
1	C	401	PHE
1	C	475	GLN
1	D	41	ASN
1	D	159	VAL
1	D	192	LYS
1	D	196	GLN
1	D	206	ASN
1	D	254	GLN
1	D	294	LEU
1	D	362	GLN
1	D	376	ASP
1	D	401	PHE
1	D	417	VAL
1	D	475	GLN
1	E	41	ASN
1	E	192	LYS
1	E	196	GLN
1	E	206	ASN
1	E	275	ASN

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Mol	Chain	Res	Type
1	E	294	LEU
1	E	401	PHE
1	E	475	GLN
1	F	41	ASN
1	F	50	GLN
1	F	122	LEU
1	F	192	LYS
1	F	196	GLN
1	F	294	LEU
1	F	401	PHE
1	G	41	ASN
1	G	192	LYS
1	G	196	GLN
1	G	248	GLU
1	G	294	LEU
1	G	373	ILE
1	G	401	PHE
1	H	41	ASN
1	H	192	LYS
1	H	196	GLN
1	H	254	GLN
1	H	268	GLU
1	H	275	ASN
1	H	294	LEU
1	H	401	PHE
1	H	475	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	41	ASN
1	A	175	GLN
1	A	196	GLN
1	A	254	GLN
1	A	275	ASN
1	A	300	GLN
1	A	475	GLN
1	B	26	ASN
1	B	29	HIS
1	B	41	ASN
1	B	50	GLN

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Mol	Chain	Res	Type
1	B	175	GLN
1	B	196	GLN
1	B	275	ASN
1	B	300	GLN
1	B	349	GLN
1	C	14	GLN
1	C	26	ASN
1	C	41	ASN
1	C	50	GLN
1	C	175	GLN
1	C	196	GLN
1	C	254	GLN
1	C	300	GLN
1	C	475	GLN
1	D	13	GLN
1	D	26	ASN
1	D	41	ASN
1	D	50	GLN
1	D	175	GLN
1	D	196	GLN
1	D	254	GLN
1	D	289	GLN
1	D	300	GLN
1	D	475	GLN
1	E	13	GLN
1	E	26	ASN
1	E	41	ASN
1	E	175	GLN
1	E	196	GLN
1	E	254	GLN
1	E	275	ASN
1	E	289	GLN
1	E	300	GLN
1	E	475	GLN
1	F	14	GLN
1	F	26	ASN
1	F	29	HIS
1	F	41	ASN
1	F	50	GLN
1	F	175	GLN
1	F	196	GLN
1	F	254	GLN

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Mol	Chain	Res	Type
1	F	275	ASN
1	F	300	GLN
1	G	13	GLN
1	G	26	ASN
1	G	41	ASN
1	G	175	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	H	26	ASN
1	H	41	ASN
1	H	175	GLN
1	H	196	GLN
1	H	275	ASN
1	H	300	GLN

### 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](#)

Of 91 ligands modelled in this entry, 16 are monoatomic - leaving 75 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	E	6925	-	3,3,3	0.39	0	2,2,2	0.42	0
5	EDO	F	6946	-	3,3,3	0.64	0	2,2,2	0.32	0
5	EDO	E	6945	-	3,3,3	0.84	0	2,2,2	0.06	0
5	EDO	B	6952	-	3,3,3	0.58	0	2,2,2	0.28	0
5	EDO	H	6948	-	3,3,3	0.49	0	2,2,2	0.31	0
6	GAI	H	6818	-	3,3,3	1.45	1 (33%)	3,3,3	0.99	0
6	GAI	B	6802	-	3,3,3	1.44	1 (33%)	3,3,3	1.02	0
5	EDO	F	6926	-	3,3,3	0.55	0	2,2,2	0.32	0
4	NAD	G	507	2	42,48,48	1.84	7 (16%)	50,73,73	1.48	9 (18%)
6	GAI	F	6816	-	3,3,3	1.35	1 (33%)	3,3,3	1.00	0
4	NAD	F	506	2	42,48,48	2.05	8 (19%)	50,73,73	1.58	9 (18%)
5	EDO	E	6965	-	3,3,3	0.52	0	2,2,2	0.35	0
5	EDO	F	6916	-	3,3,3	0.45	0	2,2,2	0.39	0
6	GAI	E	6836	-	3,3,3	1.24	1 (33%)	3,3,3	1.17	0
5	EDO	C	6913	-	3,3,3	0.55	0	2,2,2	0.36	0
6	GAI	E	6805	-	3,3,3	1.39	1 (33%)	3,3,3	1.24	0
6	GAI	D	6824	-	3,3,3	1.53	1 (33%)	3,3,3	1.07	0
6	GAI	A	6801	-	3,3,3	1.13	0	3,3,3	1.11	0
6	GAI	A	6821	-	3,3,3	1.62	1 (33%)	3,3,3	1.08	0
6	GAI	G	6838	-	3,3,3	1.47	1 (33%)	3,3,3	0.93	0
5	EDO	G	6947	-	3,3,3	0.65	0	2,2,2	0.25	0
6	GAI	F	6826	-	3,3,3	1.44	1 (33%)	3,3,3	1.07	0
5	EDO	F	6906	-	3,3,3	0.61	0	2,2,2	0.24	0
5	EDO	H	6908	-	3,3,3	0.57	0	2,2,2	0.41	0
5	EDO	B	6962	-	3,3,3	0.57	0	2,2,2	0.22	0
5	EDO	H	6928	-	3,3,3	0.37	0	2,2,2	0.45	0
6	GAI	C	6803	-	3,3,3	1.03	0	3,3,3	1.07	0
5	EDO	B	6942	-	3,3,3	0.52	0	2,2,2	0.37	0
6	GAI	B	6831	-	3,3,3	1.83	1 (33%)	3,3,3	1.09	0
4	NAD	C	503	2	42,48,48	2.07	10 (23%)	50,73,73	1.76	12 (24%)
4	NAD	H	508	2	42,48,48	2.05	8 (19%)	50,73,73	1.71	11 (22%)
5	EDO	D	6914	-	3,3,3	0.58	0	2,2,2	0.30	0
6	GAI	A	6832	-	3,3,3	1.38	1 (33%)	3,3,3	1.01	0
5	EDO	B	6912	-	3,3,3	0.56	0	2,2,2	0.29	0
6	GAI	D	6804	-	3,3,3	1.75	1 (33%)	3,3,3	0.98	0
5	EDO	A	6951	-	3,3,3	0.59	0	2,2,2	0.28	0
5	EDO	G	6927	-	3,3,3	0.40	0	2,2,2	0.39	0
5	EDO	H	6918	-	3,3,3	0.57	0	2,2,2	0.27	0
4	NAD	D	504	2	42,48,48	2.11	11 (26%)	50,73,73	1.65	13 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GAI	A	6811	-	3,3,3	1.44	1 (33%)	3,3,3	1.03	0
5	EDO	G	6917	-	3,3,3	0.52	0	2,2,2	0.33	0
5	EDO	D	6924	-	3,3,3	0.44	0	2,2,2	0.37	0
6	GAI	C	6823	-	3,3,3	1.46	1 (33%)	3,3,3	0.99	0
6	GAI	D	6814	-	3,3,3	1.70	1 (33%)	3,3,3	1.08	0
6	GAI	E	6835	-	3,3,3	1.31	0	3,3,3	1.21	0
6	GAI	G	6807	-	3,3,3	1.39	1 (33%)	3,3,3	1.20	0
6	GAI	G	6817	-	3,3,3	1.29	1 (33%)	3,3,3	1.00	0
6	GAI	C	6834	-	3,3,3	1.83	1 (33%)	3,3,3	1.10	0
6	GAI	H	6837	-	3,3,3	1.24	1 (33%)	3,3,3	1.03	0
5	EDO	C	6903	-	3,3,3	0.48	0	2,2,2	0.26	0
5	EDO	G	6907	-	3,3,3	0.46	0	2,2,2	0.36	0
6	GAI	F	6806	-	3,3,3	1.38	1 (33%)	3,3,3	1.08	0
5	EDO	C	6923	-	3,3,3	0.35	0	2,2,2	0.45	0
5	EDO	F	6956	-	3,3,3	0.53	0	2,2,2	0.33	0
6	GAI	E	6815	-	3,3,3	1.59	1 (33%)	3,3,3	1.06	0
6	GAI	H	6808	-	3,3,3	1.48	1 (33%)	3,3,3	1.16	0
5	EDO	A	6921	-	3,3,3	0.43	0	2,2,2	0.36	0
5	EDO	A	6941	-	3,3,3	0.66	0	2,2,2	0.24	0
5	EDO	C	6943	-	3,3,3	0.59	0	2,2,2	0.30	0
5	EDO	E	6915	-	3,3,3	0.46	0	2,2,2	0.26	0
5	EDO	C	6963	-	3,3,3	0.48	0	2,2,2	0.41	0
5	EDO	E	6905	-	3,3,3	0.46	0	2,2,2	0.44	0
5	EDO	C	6953	-	3,3,3	0.65	0	2,2,2	0.30	0
4	NAD	A	501	2	42,48,48	2.27	7 (16%)	50,73,73	1.43	8 (16%)
5	EDO	F	6966	-	3,3,3	0.68	0	2,2,2	0.33	0
5	EDO	B	6902	-	3,3,3	0.55	0	2,2,2	0.29	0
6	GAI	C	6813	-	3,3,3	1.47	1 (33%)	3,3,3	1.05	0
5	EDO	E	6955	-	3,3,3	0.53	0	2,2,2	0.28	0
4	NAD	E	505	2	42,48,48	2.12	8 (19%)	50,73,73	1.55	11 (22%)
6	GAI	B	6812	-	3,3,3	1.54	1 (33%)	3,3,3	1.02	0
6	GAI	D	6833	-	3,3,3	1.45	1 (33%)	3,3,3	1.06	0
5	EDO	A	6911	-	3,3,3	0.63	0	2,2,2	0.23	0
5	EDO	D	6904	-	3,3,3	0.54	0	2,2,2	0.35	0
5	EDO	A	6901	-	3,3,3	0.58	0	2,2,2	0.32	0
4	NAD	B	502	2	42,48,48	2.11	9 (21%)	50,73,73	1.36	7 (14%)

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
5	EDO	E	6925	-	-	0/1/1/1	-
5	EDO	F	6946	-	-	1/1/1/1	-
5	EDO	E	6945	-	-	1/1/1/1	-
5	EDO	B	6952	-	-	0/1/1/1	-
5	EDO	H	6948	-	-	0/1/1/1	-
5	EDO	F	6926	-	-	1/1/1/1	-
4	NAD	G	507	2	-	0/26/62/62	0/5/5/5
4	NAD	F	506	2	-	0/26/62/62	0/5/5/5
5	EDO	E	6965	-	-	0/1/1/1	-
5	EDO	F	6916	-	-	0/1/1/1	-
5	EDO	C	6913	-	-	0/1/1/1	-
5	EDO	G	6947	-	-	0/1/1/1	-
5	EDO	F	6906	-	-	0/1/1/1	-
5	EDO	H	6908	-	-	0/1/1/1	-
5	EDO	B	6962	-	-	1/1/1/1	-
5	EDO	H	6928	-	-	0/1/1/1	-
5	EDO	B	6942	-	-	0/1/1/1	-
4	NAD	C	503	2	-	0/26/62/62	0/5/5/5
4	NAD	H	508	2	-	4/26/62/62	0/5/5/5
5	EDO	D	6914	-	-	0/1/1/1	-
5	EDO	B	6912	-	-	0/1/1/1	-
5	EDO	A	6951	-	-	0/1/1/1	-
5	EDO	G	6927	-	-	0/1/1/1	-
5	EDO	H	6918	-	-	0/1/1/1	-
4	NAD	D	504	2	-	5/26/62/62	0/5/5/5
5	EDO	G	6917	-	-	0/1/1/1	-
5	EDO	D	6924	-	-	0/1/1/1	-
5	EDO	C	6903	-	-	0/1/1/1	-
5	EDO	G	6907	-	-	0/1/1/1	-
5	EDO	C	6923	-	-	0/1/1/1	-
5	EDO	F	6956	-	-	1/1/1/1	-
5	EDO	A	6921	-	-	0/1/1/1	-
5	EDO	A	6941	-	-	0/1/1/1	-
5	EDO	C	6943	-	-	0/1/1/1	-
5	EDO	E	6915	-	-	0/1/1/1	-
5	EDO	C	6963	-	-	0/1/1/1	-
5	EDO	E	6905	-	-	0/1/1/1	-
5	EDO	C	6953	-	-	0/1/1/1	-
4	NAD	A	501	2	-	6/26/62/62	0/5/5/5
5	EDO	F	6966	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	6902	-	-	0/1/1/1	-
5	EDO	E	6955	-	-	0/1/1/1	-
4	NAD	E	505	2	-	5/26/62/62	0/5/5/5
5	EDO	A	6911	-	-	0/1/1/1	-
5	EDO	D	6904	-	-	1/1/1/1	-
5	EDO	A	6901	-	-	1/1/1/1	-
4	NAD	B	502	2	-	1/26/62/62	0/5/5/5

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAD	C3N-C7N	-10.83	1.34	1.50
4	D	504	NAD	C3N-C7N	-9.62	1.36	1.50
4	E	505	NAD	C3N-C7N	-9.56	1.36	1.50
4	C	503	NAD	C3N-C7N	-9.22	1.36	1.50
4	B	502	NAD	C3N-C7N	-9.20	1.36	1.50
4	H	508	NAD	C3N-C7N	-9.17	1.36	1.50
4	F	506	NAD	C3N-C7N	-9.15	1.36	1.50
4	G	507	NAD	C3N-C7N	-7.78	1.38	1.50
4	B	502	NAD	C2A-N3A	5.79	1.41	1.32
4	E	505	NAD	C2A-N3A	5.30	1.40	1.32
4	C	503	NAD	C2A-N3A	5.25	1.40	1.32
4	H	508	NAD	C2A-N3A	5.10	1.40	1.32
4	F	506	NAD	C2A-N3A	5.02	1.40	1.32
4	G	507	NAD	C2A-N3A	4.45	1.39	1.32
4	A	501	NAD	C2A-N3A	4.20	1.38	1.32
4	D	504	NAD	C8A-N7A	4.04	1.41	1.34
4	A	501	NAD	O4D-C1D	3.36	1.45	1.41
4	D	504	NAD	C2N-C3N	-3.32	1.33	1.39
4	A	501	NAD	C2N-C3N	-3.31	1.33	1.39
4	C	503	NAD	C2A-N1A	3.30	1.40	1.33
4	G	507	NAD	C2A-N1A	3.28	1.40	1.33
4	G	507	NAD	C8A-N7A	3.22	1.40	1.34
6	B	6831	GAI	C-N1	3.16	1.37	1.30
4	B	502	NAD	C2A-N1A	3.11	1.39	1.33
4	D	504	NAD	C2A-N1A	3.09	1.39	1.33
6	C	6834	GAI	C-N1	3.06	1.37	1.30
4	E	505	NAD	C4N-C3N	-3.05	1.34	1.39
4	A	501	NAD	C2A-N1A	3.02	1.39	1.33
6	D	6804	GAI	C-N1	2.96	1.36	1.30
4	B	502	NAD	C8A-N7A	2.95	1.40	1.34
4	D	504	NAD	C2A-N3A	2.94	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	506	NAD	C2A-N1A	2.94	1.39	1.33
4	H	508	NAD	C2A-N1A	2.93	1.39	1.33
4	F	506	NAD	C4N-C3N	-2.93	1.34	1.39
4	A	501	NAD	C8A-N7A	2.86	1.39	1.34
6	D	6814	GAI	C-N1	2.85	1.36	1.30
6	A	6821	GAI	C-N1	2.77	1.36	1.30
4	H	508	NAD	C5N-C4N	-2.74	1.33	1.38
4	B	502	NAD	C4A-N3A	2.74	1.39	1.35
6	E	6815	GAI	C-N1	2.73	1.36	1.30
4	D	504	NAD	C5N-C4N	-2.72	1.33	1.38
4	E	505	NAD	C2N-C3N	-2.68	1.34	1.39
4	E	505	NAD	C2A-N1A	2.67	1.38	1.33
4	H	508	NAD	O4D-C1D	2.65	1.44	1.41
6	D	6824	GAI	C-N1	2.62	1.36	1.30
4	C	503	NAD	C8A-N7A	2.62	1.39	1.34
6	B	6812	GAI	C-N1	2.60	1.36	1.30
4	C	503	NAD	C2D-C1D	2.57	1.57	1.53
4	A	501	NAD	O4B-C1B	2.56	1.44	1.41
6	C	6813	GAI	C-N1	2.53	1.36	1.30
6	G	6838	GAI	C-N1	2.52	1.36	1.30
6	D	6833	GAI	C-N1	2.50	1.35	1.30
6	H	6818	GAI	C-N1	2.50	1.35	1.30
4	E	505	NAD	C8A-N7A	2.50	1.39	1.34
6	A	6811	GAI	C-N1	2.49	1.35	1.30
4	F	506	NAD	C8A-N7A	2.47	1.39	1.34
6	C	6823	GAI	C-N1	2.47	1.35	1.30
6	B	6802	GAI	C-N1	2.46	1.35	1.30
4	F	506	NAD	C2D-C1D	2.45	1.57	1.53
6	H	6808	GAI	C-N1	2.43	1.35	1.30
4	G	507	NAD	C4A-N3A	2.42	1.39	1.35
4	B	502	NAD	C4N-C3N	-2.42	1.35	1.39
6	F	6826	GAI	C-N1	2.42	1.35	1.30
4	D	504	NAD	C2N-N1N	-2.41	1.32	1.35
4	F	506	NAD	C2N-C3N	-2.40	1.35	1.39
6	G	6807	GAI	C-N1	2.37	1.35	1.30
6	E	6805	GAI	C-N1	2.33	1.35	1.30
4	H	508	NAD	C2N-C3N	-2.32	1.35	1.39
6	F	6806	GAI	C-N1	2.31	1.35	1.30
4	F	506	NAD	PN-O2N	-2.26	1.44	1.55
6	F	6816	GAI	C-N1	2.26	1.35	1.30
4	D	504	NAD	C4N-C3N	-2.25	1.35	1.39
4	H	508	NAD	C8A-N7A	2.23	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6832	GAI	C-N1	2.21	1.35	1.30
4	C	503	NAD	PN-O2N	-2.20	1.45	1.55
4	D	504	NAD	O4D-C1D	2.19	1.44	1.41
4	C	503	NAD	C4N-C3N	-2.19	1.35	1.39
6	G	6817	GAI	C-N1	2.18	1.35	1.30
6	H	6837	GAI	C-N1	2.13	1.35	1.30
4	D	504	NAD	C2D-C1D	2.13	1.57	1.53
6	E	6836	GAI	C-N1	2.12	1.35	1.30
4	B	502	NAD	O4B-C1B	2.11	1.44	1.41
4	C	503	NAD	O4D-C1D	2.09	1.44	1.41
4	E	505	NAD	C2D-C1D	2.08	1.56	1.53
4	B	502	NAD	C5N-C4N	-2.08	1.34	1.38
4	G	507	NAD	C4N-C3N	-2.08	1.35	1.39
4	E	505	NAD	O4D-C1D	2.07	1.44	1.41
4	G	507	NAD	O4B-C1B	2.07	1.44	1.41
4	H	508	NAD	C4N-C3N	-2.06	1.35	1.39
4	C	503	NAD	PN-O5D	2.04	1.67	1.59
4	D	504	NAD	PA-O2A	-2.03	1.45	1.55
4	C	503	NAD	C2N-C3N	-2.02	1.35	1.39
4	B	502	NAD	C2N-C3N	-2.00	1.35	1.39

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	503	NAD	O4B-C1B-C2B	-5.63	98.70	106.93
4	H	508	NAD	N3A-C2A-N1A	-4.79	121.19	128.68
4	D	504	NAD	PN-O3-PA	-4.61	117.00	132.83
4	C	503	NAD	O7N-C7N-N7N	-4.47	116.23	122.58
4	A	501	NAD	N3A-C2A-N1A	-4.29	121.97	128.68
4	F	506	NAD	O7N-C7N-C3N	4.24	124.70	119.63
4	G	507	NAD	O7N-C7N-N7N	-4.07	116.79	122.58
4	F	506	NAD	N3A-C2A-N1A	-4.07	122.32	128.68
4	E	505	NAD	O7N-C7N-N7N	-4.05	116.83	122.58
4	B	502	NAD	O4D-C4D-C3D	-3.95	97.30	105.11
4	G	507	NAD	O4B-C1B-C2B	-3.86	101.28	106.93
4	E	505	NAD	N3A-C2A-N1A	-3.78	122.76	128.68
4	H	508	NAD	C6N-C5N-C4N	-3.71	114.05	119.44
4	A	501	NAD	O7N-C7N-C3N	-3.69	115.22	119.63
4	C	503	NAD	O7N-C7N-C3N	3.62	123.96	119.63
4	H	508	NAD	O7N-C7N-N7N	-3.57	117.50	122.58
4	D	504	NAD	O7N-C7N-N7N	-3.53	117.56	122.58
4	F	506	NAD	O4B-C1B-C2B	-3.52	101.79	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	NAD	C5A-C6A-N6A	3.48	125.64	120.35
4	F	506	NAD	O7N-C7N-N7N	-3.35	117.81	122.58
4	C	503	NAD	O4D-C4D-C3D	-3.26	98.66	105.11
4	B	502	NAD	C3N-C7N-N7N	3.26	121.66	117.75
4	F	506	NAD	O4D-C4D-C3D	-3.24	98.71	105.11
4	C	503	NAD	C2B-C3B-C4B	-3.20	96.42	102.64
4	D	504	NAD	C6N-C5N-C4N	-3.19	114.80	119.44
4	B	502	NAD	N3A-C2A-N1A	-3.13	123.78	128.68
4	C	503	NAD	C6N-C5N-C4N	-3.13	114.89	119.44
4	E	505	NAD	C2D-C3D-C4D	-3.13	96.57	102.64
4	B	502	NAD	O7N-C7N-N7N	-3.10	118.18	122.58
4	E	505	NAD	C5N-C4N-C3N	3.06	123.97	120.34
4	E	505	NAD	O4D-C4D-C3D	-3.04	99.10	105.11
4	G	507	NAD	C5N-C4N-C3N	3.03	123.93	120.34
4	G	507	NAD	N3A-C2A-N1A	-3.01	123.98	128.68
4	D	504	NAD	C5N-C4N-C3N	3.00	123.89	120.34
4	D	504	NAD	N3A-C2A-N1A	-2.92	124.11	128.68
4	A	501	NAD	O7N-C7N-N7N	2.90	126.70	122.58
4	E	505	NAD	O7N-C7N-C3N	2.86	123.05	119.63
4	C	503	NAD	N3A-C2A-N1A	-2.82	124.27	128.68
4	G	507	NAD	C3N-C7N-N7N	2.80	121.11	117.75
4	B	502	NAD	C3D-C2D-C1D	-2.78	96.79	100.98
4	E	505	NAD	O4B-C1B-C2B	-2.70	102.98	106.93
4	H	508	NAD	PN-O3-PA	-2.68	123.63	132.83
4	H	508	NAD	C5N-C4N-C3N	2.68	123.51	120.34
4	F	506	NAD	C6N-C5N-C4N	-2.66	115.58	119.44
4	H	508	NAD	C3N-C2N-N1N	-2.65	117.84	120.43
4	E	505	NAD	C5A-C6A-N6A	2.63	124.35	120.35
4	H	508	NAD	O4D-C4D-C3D	-2.63	99.91	105.11
4	F	506	NAD	C2B-C3B-C4B	-2.60	97.58	102.64
4	A	501	NAD	C6N-C5N-C4N	-2.57	115.71	119.44
4	H	508	NAD	C2B-C3B-C4B	-2.56	97.68	102.64
4	H	508	NAD	O7N-C7N-C3N	2.53	122.65	119.63
4	A	501	NAD	C3D-C2D-C1D	-2.46	97.27	100.98
4	F	506	NAD	C5N-C4N-C3N	2.46	123.26	120.34
4	A	501	NAD	C5N-C4N-C3N	2.43	123.22	120.34
4	E	505	NAD	C6N-C5N-C4N	-2.40	115.95	119.44
4	A	501	NAD	O4B-C1B-C2B	-2.36	103.47	106.93
4	E	505	NAD	PN-O3-PA	-2.35	124.75	132.83
4	G	507	NAD	C2B-C3B-C4B	-2.32	98.13	102.64
4	E	505	NAD	C2B-C3B-C4B	-2.29	98.20	102.64
4	D	504	NAD	O4D-C4D-C3D	-2.28	100.61	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	NAD	C3N-C2N-N1N	-2.27	118.21	120.43
4	H	508	NAD	C5N-C6N-N1N	2.25	123.63	120.40
4	D	504	NAD	C5A-C6A-N1A	-2.25	115.25	120.35
4	F	506	NAD	O4D-C1D-C2D	-2.22	103.69	106.93
4	C	503	NAD	C3N-C2N-N1N	-2.21	118.27	120.43
4	B	502	NAD	O4B-C4B-C3B	2.20	109.48	105.11
4	G	507	NAD	C5A-C6A-N6A	2.19	123.69	120.35
4	D	504	NAD	O7N-C7N-C3N	2.17	122.23	119.63
4	B	502	NAD	C5N-C4N-C3N	2.17	122.91	120.34
4	C	503	NAD	C2N-C3N-C4N	2.17	120.71	118.26
4	A	501	NAD	C2B-C3B-C4B	-2.16	98.45	102.64
4	H	508	NAD	C2N-C3N-C4N	2.15	120.70	118.26
4	C	503	NAD	C5N-C4N-C3N	2.15	122.89	120.34
4	D	504	NAD	O4B-C1B-C2B	-2.14	103.80	106.93
4	C	503	NAD	PN-O3-PA	-2.14	125.49	132.83
4	C	503	NAD	C3B-C2B-C1B	2.12	104.17	100.98
4	G	507	NAD	O7N-C7N-C3N	2.06	122.10	119.63
4	D	504	NAD	C2B-C3B-C4B	-2.05	98.65	102.64
4	G	507	NAD	O5D-C5D-C4D	2.02	115.96	108.99
4	D	504	NAD	C3N-C7N-N7N	2.02	120.17	117.75

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	508	NAD	C4N-C3N-C7N-N7N
4	H	508	NAD	C4N-C3N-C7N-O7N
4	A	501	NAD	C2N-C3N-C7N-O7N
4	H	508	NAD	C2N-C3N-C7N-O7N
4	H	508	NAD	C2N-C3N-C7N-N7N
4	D	504	NAD	PN-O3-PA-O1A
4	A	501	NAD	C4N-C3N-C7N-O7N
4	A	501	NAD	C4N-C3N-C7N-N7N
4	A	501	NAD	C5B-O5B-PA-O3
4	E	505	NAD	PN-O3-PA-O1A
4	A	501	NAD	C5B-O5B-PA-O2A
4	D	504	NAD	C5B-O5B-PA-O2A
4	A	501	NAD	C2N-C3N-C7N-N7N
4	D	504	NAD	C4N-C3N-C7N-N7N
4	E	505	NAD	C4N-C3N-C7N-N7N
4	B	502	NAD	PN-O3-PA-O1A
4	E	505	NAD	C4N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
5	B	6962	EDO	O1-C1-C2-O2
5	D	6904	EDO	O1-C1-C2-O2
5	E	6945	EDO	O1-C1-C2-O2
5	F	6926	EDO	O1-C1-C2-O2
5	F	6956	EDO	O1-C1-C2-O2
4	E	505	NAD	C5D-O5D-PN-O3
4	D	504	NAD	PN-O3-PA-O2A
4	E	505	NAD	PN-O3-PA-O2A
5	A	6901	EDO	O1-C1-C2-O2
5	F	6946	EDO	O1-C1-C2-O2
4	D	504	NAD	C4N-C3N-C7N-O7N

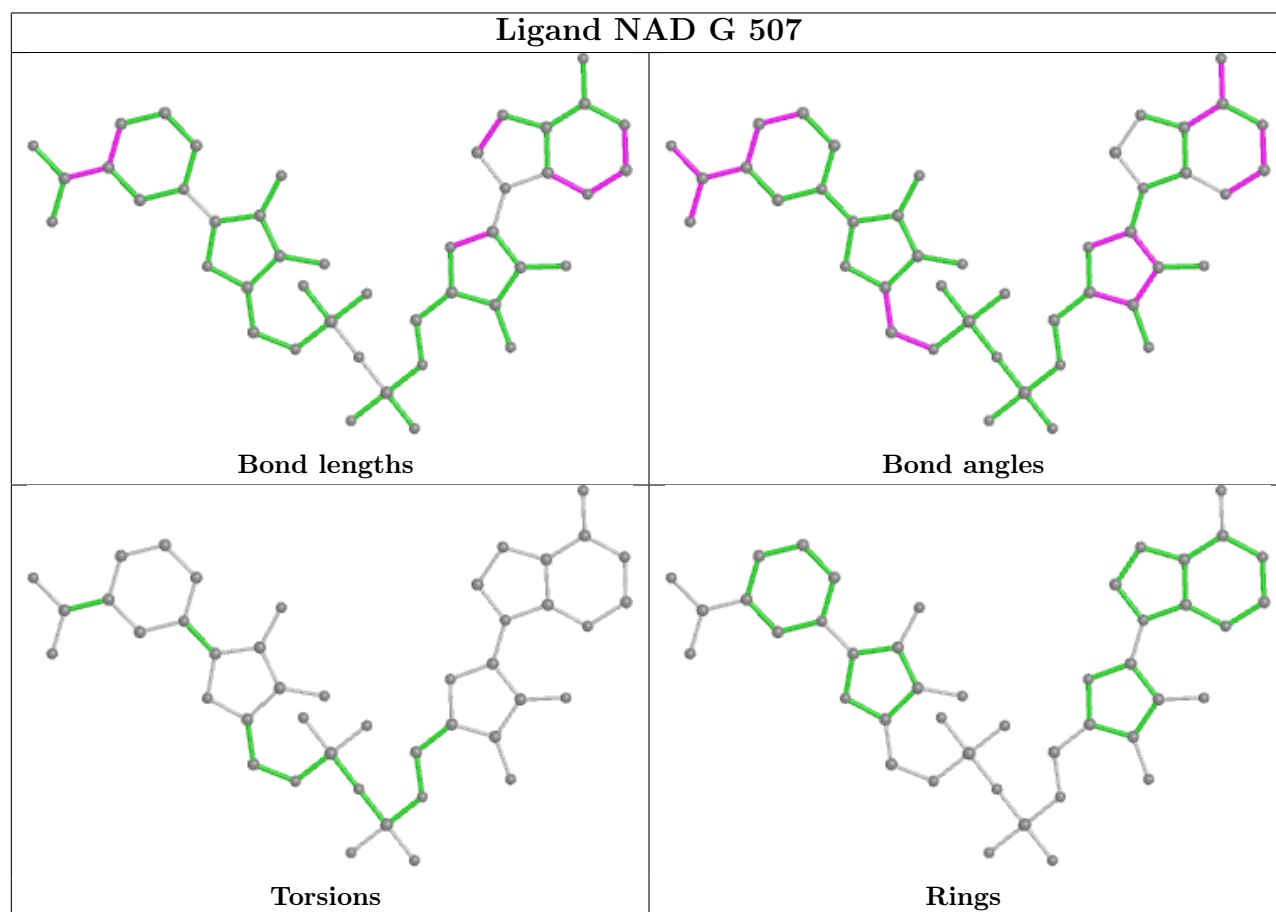
There are no ring outliers.

19 monomers are involved in 33 short contacts:

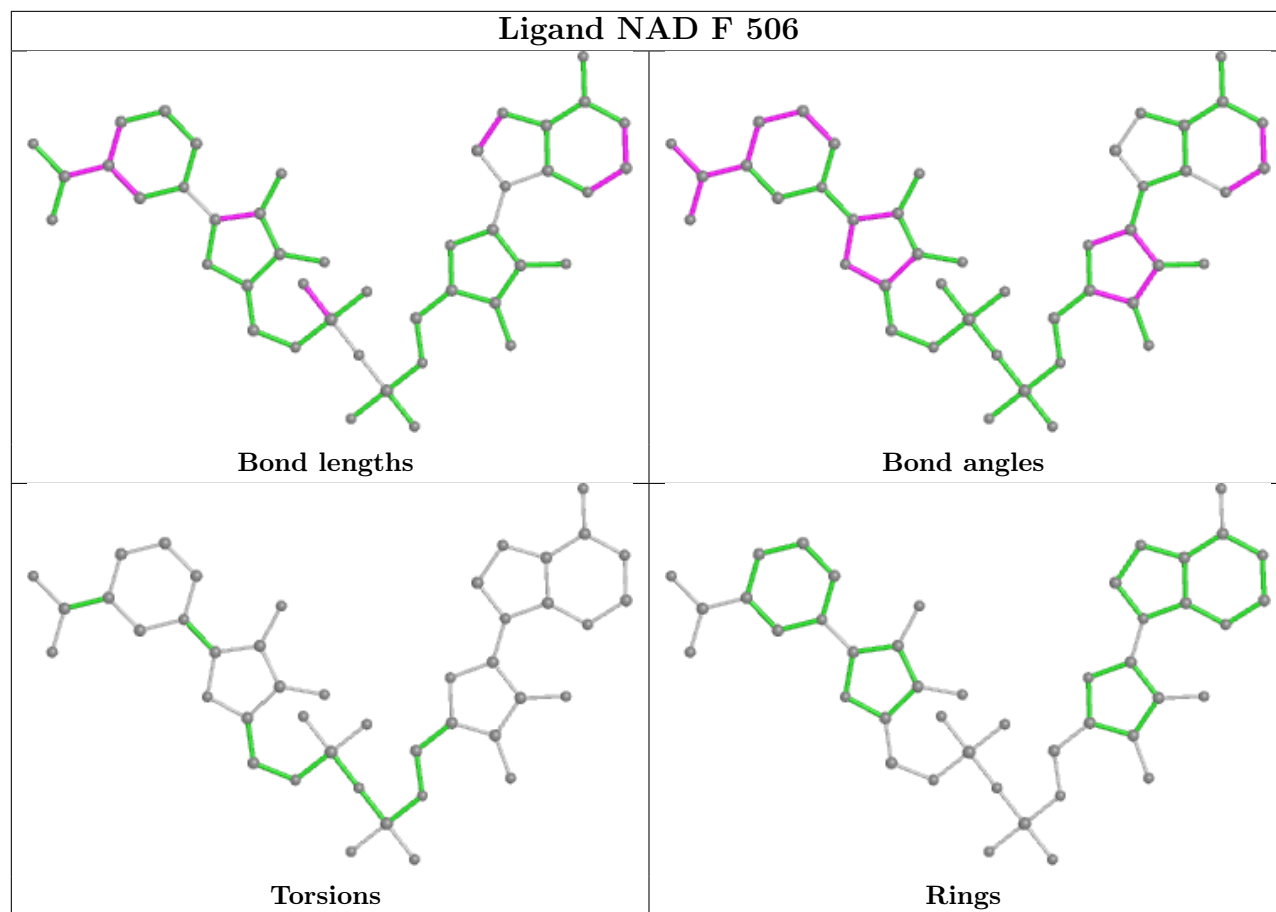
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	6946	EDO	1	0
5	E	6945	EDO	4	0
5	H	6948	EDO	2	0
5	E	6965	EDO	2	0
5	G	6947	EDO	2	0
5	B	6962	EDO	2	0
5	B	6942	EDO	2	0
5	A	6951	EDO	1	0
5	G	6927	EDO	1	0
5	D	6924	EDO	1	0
6	E	6835	GAI	1	0
6	C	6834	GAI	1	0
5	A	6921	EDO	1	0
5	A	6941	EDO	2	0
5	C	6943	EDO	2	0
5	E	6915	EDO	3	0
5	E	6905	EDO	2	0
5	E	6955	EDO	2	0
5	A	6911	EDO	1	0

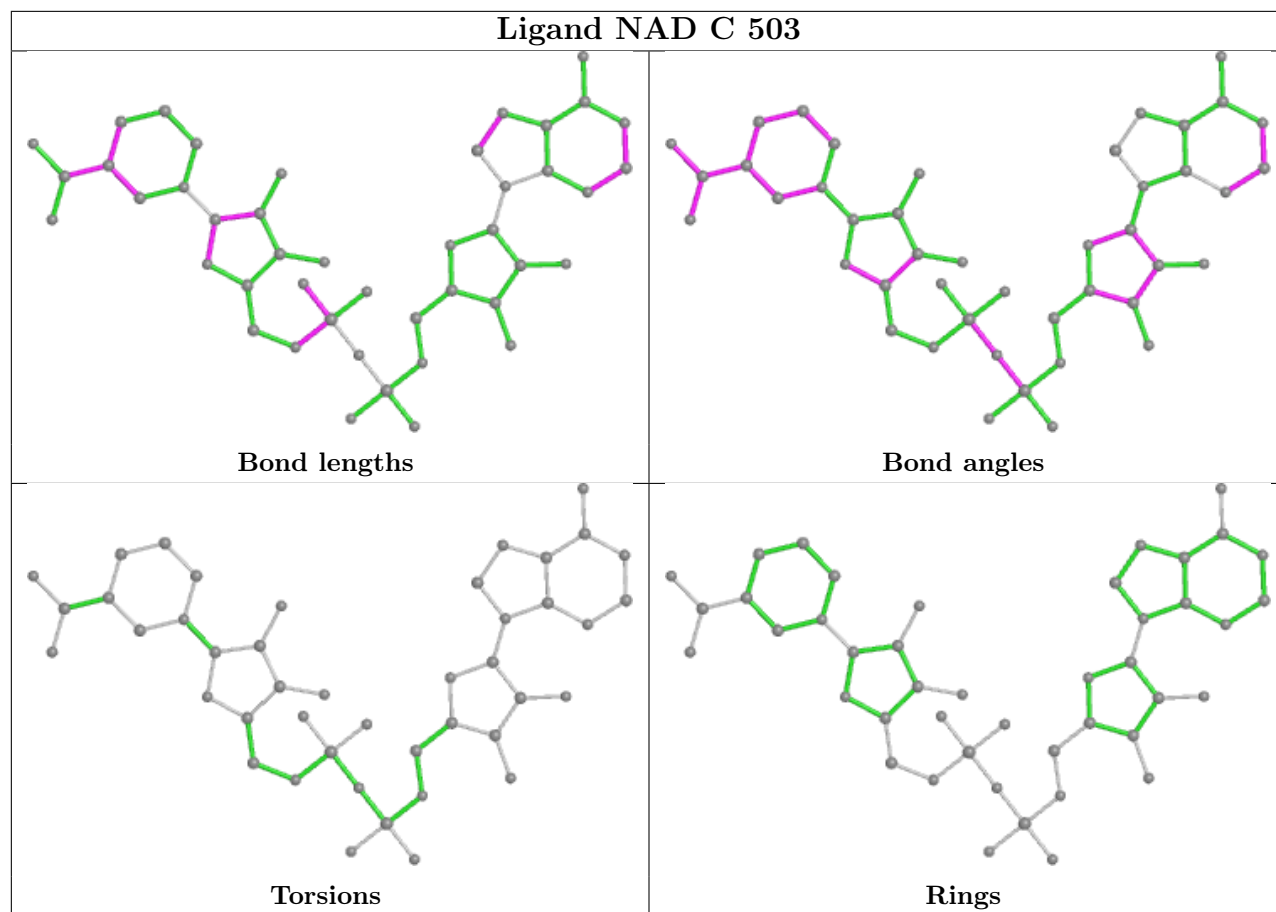
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

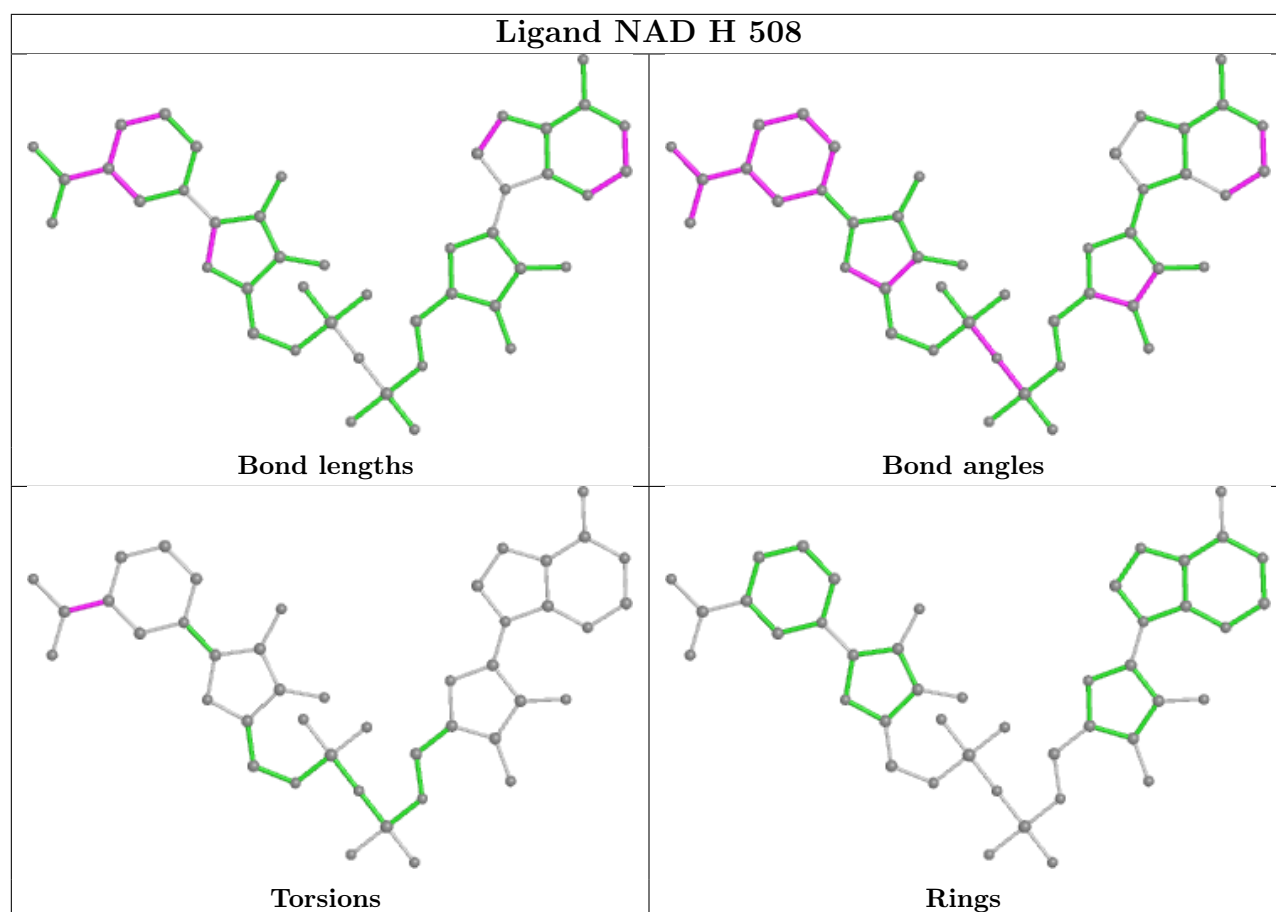
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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

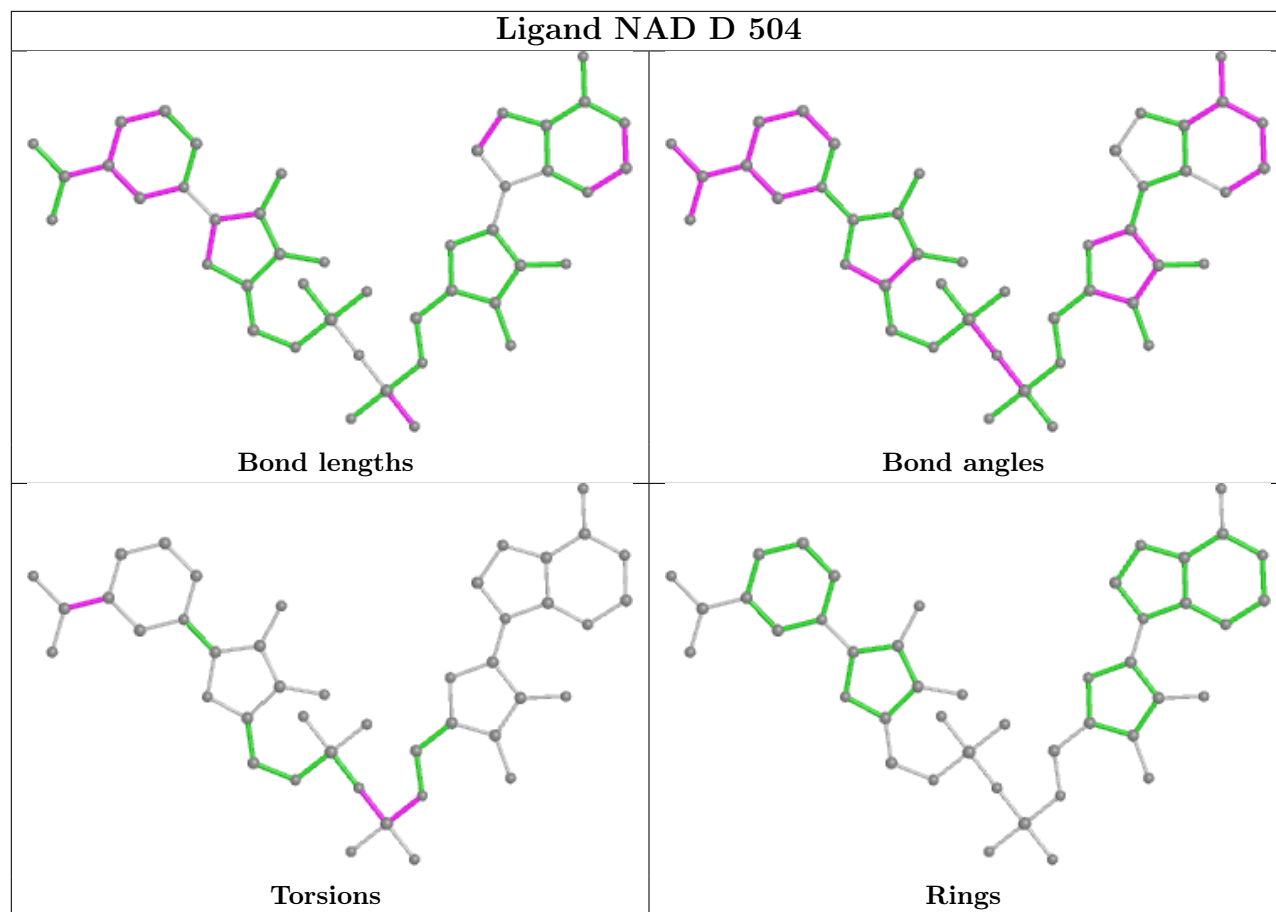


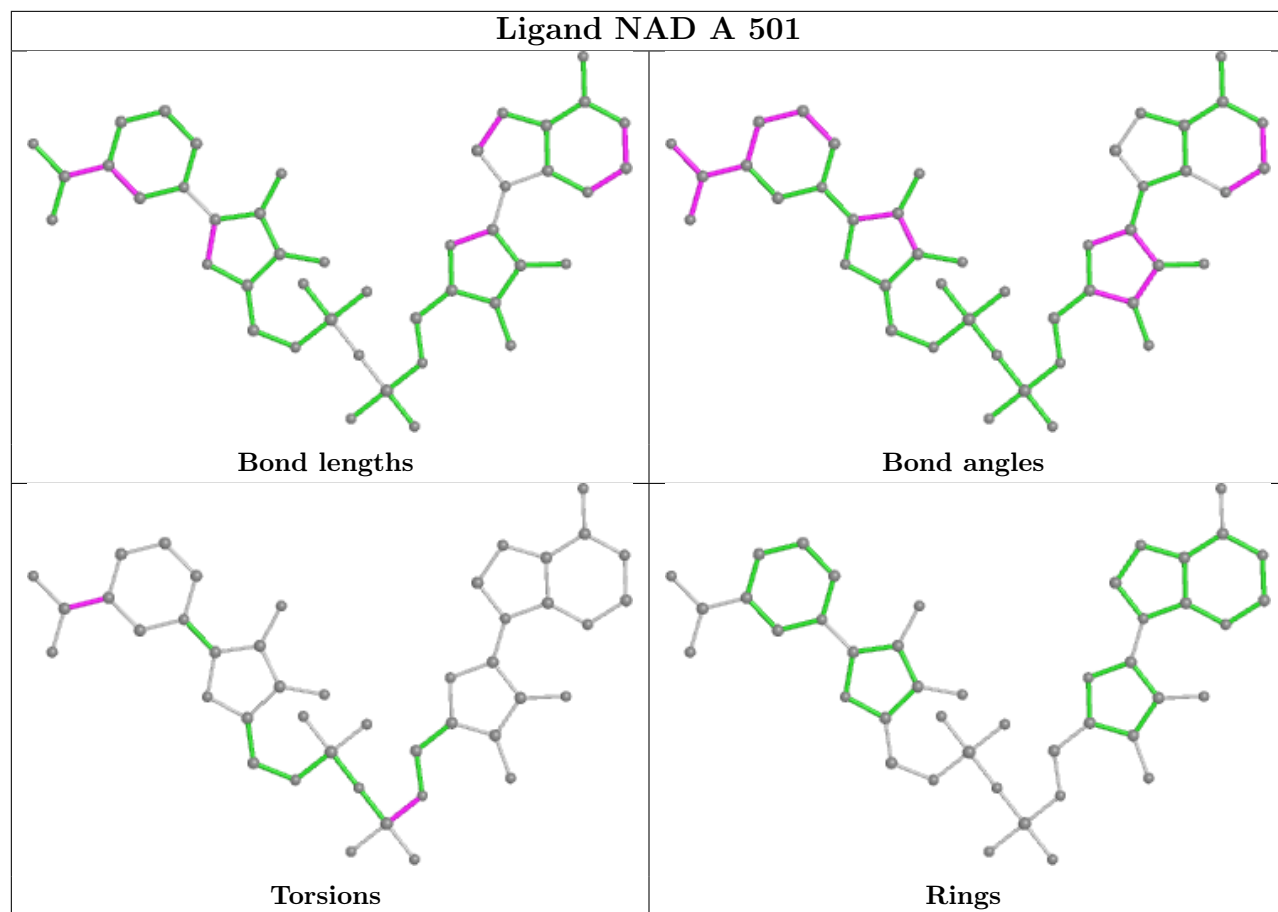


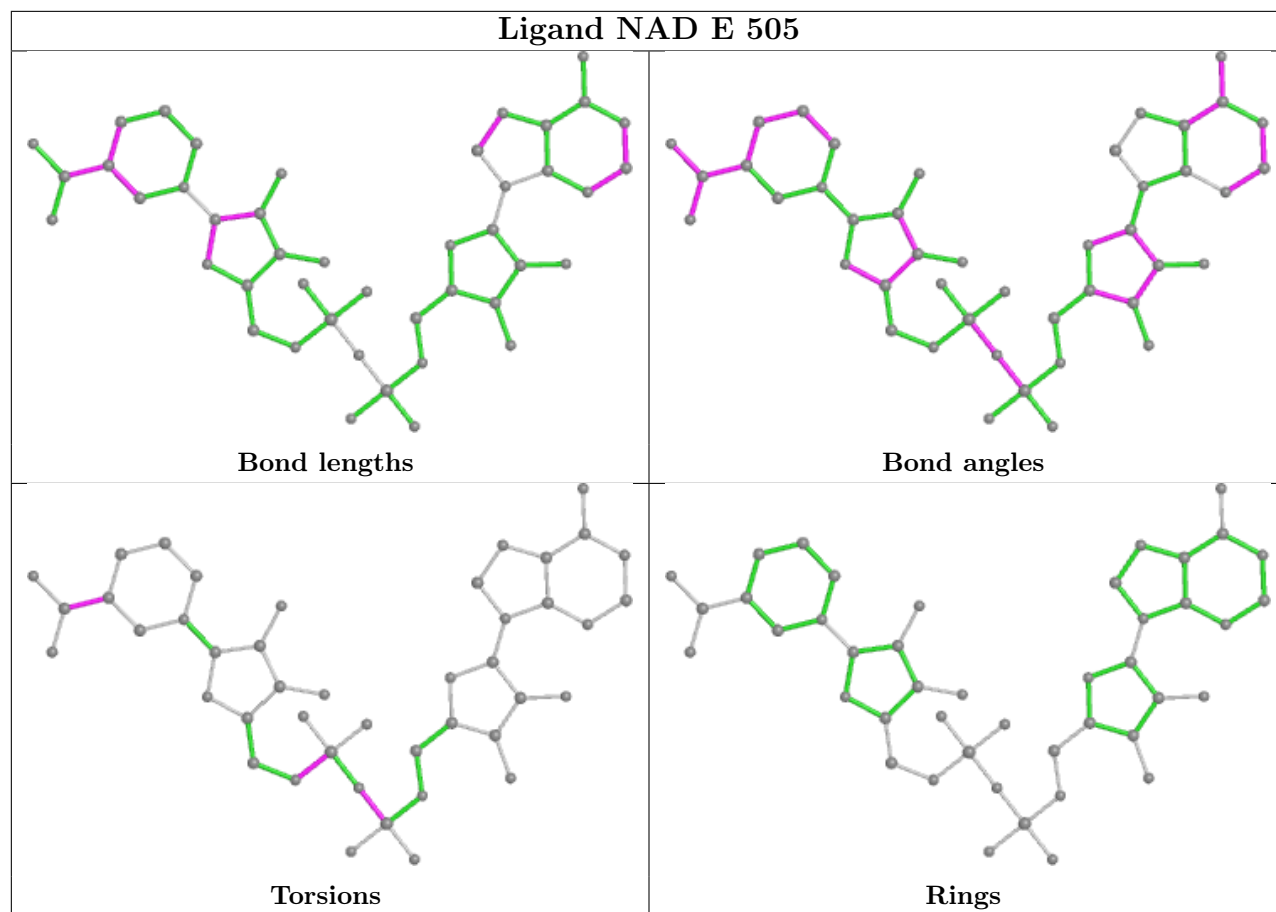


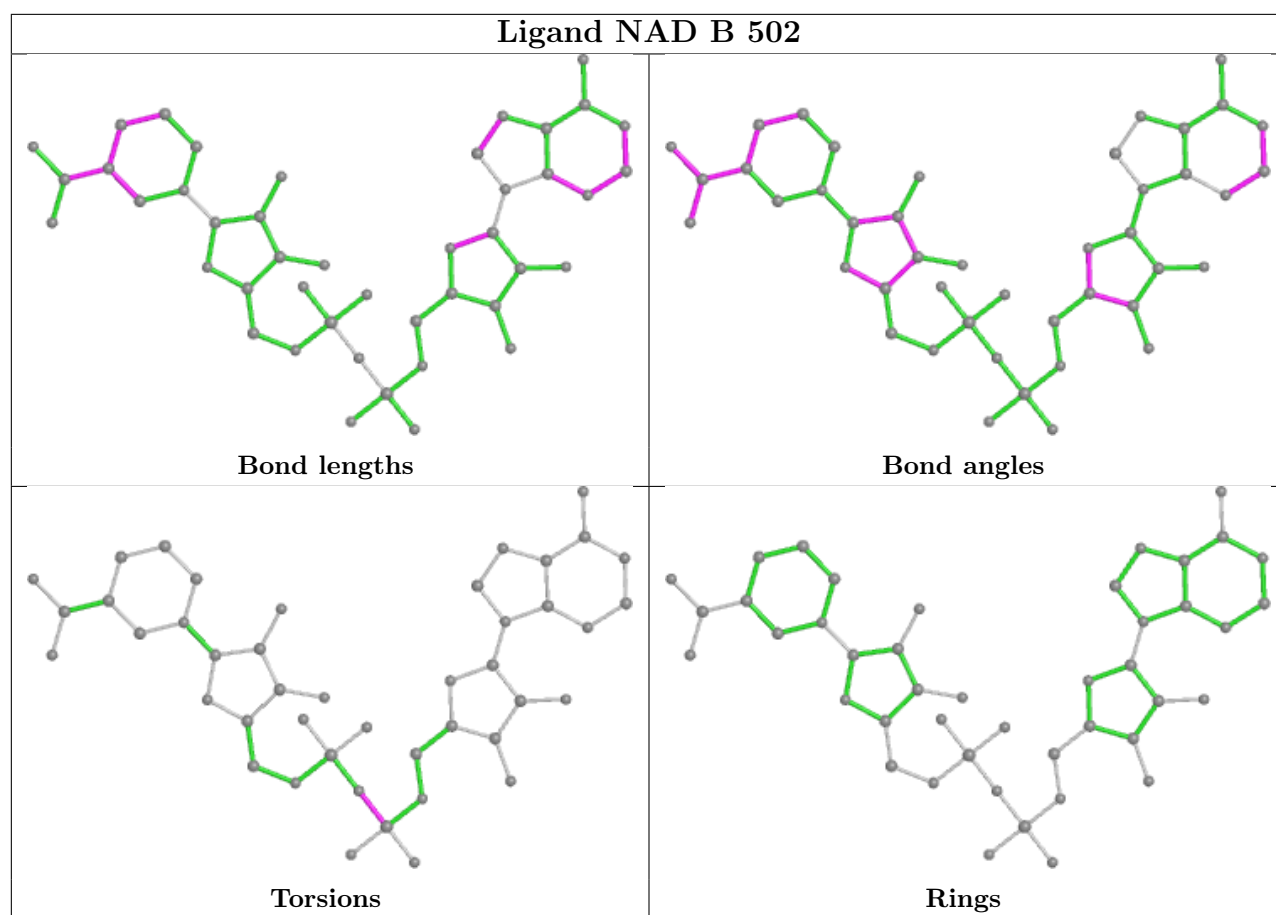












## 5.7 Other polymers [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	494/500 (98%)	0.22	16 (3%) 47 46	17, 32, 47, 62	0
1	B	494/500 (98%)	-0.00	9 (1%) 68 66	16, 28, 42, 61	0
1	C	494/500 (98%)	-0.38	1 (0%) 95 94	15, 22, 33, 54	0
1	D	494/500 (98%)	-0.03	7 (1%) 75 74	15, 30, 45, 60	0
1	E	494/500 (98%)	-0.23	6 (1%) 79 78	18, 28, 42, 59	0
1	F	494/500 (98%)	-0.39	1 (0%) 95 94	16, 22, 33, 55	0
1	G	494/500 (98%)	0.04	8 (1%) 72 70	21, 31, 45, 61	0
1	H	494/500 (98%)	0.29	13 (2%) 56 54	20, 35, 52, 72	0
All	All	3952/4000 (98%)	-0.06	61 (1%) 73 72	15, 28, 45, 72	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	376	ASP	7.2
1	A	474	GLY	6.0
1	A	7	ALA	4.5
1	H	7	ALA	4.0
1	D	376	ASP	3.9
1	G	7	ALA	3.9
1	B	7	ALA	3.6
1	G	474	GLY	3.5
1	G	14	GLN	3.4
1	E	7	ALA	3.2
1	E	376	ASP	3.2
1	D	358	ASN	3.2
1	E	377	ARG	3.1
1	B	32	VAL	3.1
1	A	262	LEU	3.0
1	B	257	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	363	GLU	3.0
1	H	424	THR	3.0
1	H	34	ARG	2.8
1	A	376	ASP	2.8
1	A	40	VAL	2.8
1	H	350	PHE	2.7
1	H	10	ALA	2.6
1	B	34	ARG	2.6
1	E	474	GLY	2.6
1	G	193	VAL	2.5
1	B	254	GLN	2.5
1	E	34	ARG	2.5
1	B	474	GLY	2.5
1	H	336	ASP	2.4
1	D	34	ARG	2.4
1	B	424	THR	2.4
1	B	16	GLU	2.4
1	H	248	GLU	2.3
1	A	392	GLY	2.3
1	D	424	THR	2.3
1	D	220	ILE	2.3
1	A	8	VAL	2.3
1	G	373	ILE	2.3
1	B	201	ALA	2.2
1	E	179	LEU	2.2
1	G	172	LEU	2.2
1	A	179	LEU	2.2
1	A	14	GLN	2.2
1	H	375	ALA	2.2
1	D	33	SER	2.2
1	F	474	GLY	2.2
1	A	45	GLY	2.2
1	A	371	GLY	2.2
1	A	350	PHE	2.2
1	G	475	GLN	2.1
1	G	34	ARG	2.1
1	D	336	ASP	2.1
1	A	10	ALA	2.1
1	A	37	PHE	2.1
1	A	255	VAL	2.1
1	H	32	VAL	2.1
1	H	379	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	362	GLN	2.0
1	H	294	LEU	2.0
1	C	474	GLY	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NA	H	708	1/1	0.60	0.24	55,55,55,55	0
5	EDO	D	6914	4/4	0.67	0.26	59,59,61,61	0
2	MG	E	605	1/1	0.69	0.11	50,50,50,50	0
5	EDO	B	6952	4/4	0.71	0.40	60,60,61,61	0
6	GAI	A	6821	4/4	0.71	0.35	55,56,56,56	0
5	EDO	A	6951	4/4	0.72	0.25	54,55,56,56	0
6	GAI	D	6824	4/4	0.72	0.34	65,66,66,67	0
5	EDO	H	6918	4/4	0.78	0.21	60,61,61,61	0
2	MG	H	608	1/1	0.79	0.10	59,59,59,59	0
5	EDO	E	6925	4/4	0.79	0.18	48,49,49,49	0
5	EDO	E	6965	4/4	0.79	0.36	69,70,70,71	0
6	GAI	G	6838	4/4	0.80	0.19	47,47,49,50	0
5	EDO	A	6941	4/4	0.81	0.26	38,43,44,44	0
6	GAI	B	6831	4/4	0.81	0.20	59,59,59,60	0
5	EDO	B	6962	4/4	0.81	0.32	71,71,72,72	0
3	NA	A	701	1/1	0.81	0.11	40,40,40,40	0
5	EDO	F	6956	4/4	0.83	0.23	49,51,52,52	0
5	EDO	E	6955	4/4	0.83	0.36	52,53,55,55	0
2	MG	G	607	1/1	0.83	0.15	59,59,59,59	0
5	EDO	A	6911	4/4	0.84	0.21	56,57,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	H	6928	4/4	0.84	0.22	66,66,66,68	0
5	EDO	F	6926	4/4	0.85	0.17	46,47,47,50	0
6	GAI	F	6826	4/4	0.85	0.16	44,44,44,45	0
6	GAI	G	6817	4/4	0.85	0.36	52,52,52,53	0
2	MG	D	604	1/1	0.85	0.17	52,52,52,52	0
5	EDO	F	6966	4/4	0.86	0.17	47,49,49,51	0
6	GAI	A	6811	4/4	0.86	0.27	56,57,57,58	0
6	GAI	H	6837	4/4	0.86	0.17	51,52,53,53	0
2	MG	A	601	1/1	0.87	0.10	49,49,49,49	0
2	MG	F	606	1/1	0.87	0.12	41,41,41,41	0
5	EDO	F	6946	4/4	0.87	0.32	29,37,39,39	0
6	GAI	C	6813	4/4	0.88	0.19	53,53,54,56	0
5	EDO	B	6902	4/4	0.88	0.17	38,42,42,42	0
5	EDO	C	6953	4/4	0.88	0.24	54,54,55,56	0
3	NA	G	707	1/1	0.88	0.12	35,35,35,35	0
6	GAI	B	6812	4/4	0.88	0.36	51,52,53,53	0
6	GAI	H	6818	4/4	0.88	0.37	57,57,57,57	0
5	EDO	D	6924	4/4	0.88	0.22	56,57,57,58	0
5	EDO	E	6945	4/4	0.89	0.24	34,40,40,41	0
6	GAI	D	6833	4/4	0.89	0.14	54,55,55,55	0
5	EDO	G	6927	4/4	0.89	0.19	54,54,54,54	0
5	EDO	G	6947	4/4	0.89	0.20	34,42,42,43	0
5	EDO	E	6905	4/4	0.89	0.17	37,39,40,40	0
5	EDO	C	6923	4/4	0.89	0.16	51,52,52,54	0
6	GAI	D	6814	4/4	0.89	0.13	43,44,45,45	0
2	MG	C	603	1/1	0.90	0.11	41,41,41,41	0
5	EDO	E	6915	4/4	0.90	0.14	42,44,45,47	0
5	EDO	G	6907	4/4	0.90	0.18	38,40,40,41	0
5	EDO	G	6917	4/4	0.90	0.21	50,51,52,53	0
5	EDO	F	6906	4/4	0.90	0.15	37,38,38,40	0
4	NAD	A	501	44/44	0.90	0.15	32,44,50,50	0
2	MG	B	602	1/1	0.90	0.08	47,47,47,47	0
6	GAI	F	6806	4/4	0.91	0.17	31,32,32,33	0
4	NAD	G	507	44/44	0.91	0.14	30,40,44,45	0
6	GAI	C	6834	4/4	0.91	0.15	42,42,43,45	0
4	NAD	H	508	44/44	0.91	0.13	35,46,50,51	0
5	EDO	B	6912	4/4	0.91	0.24	46,46,47,48	0
5	EDO	C	6943	4/4	0.91	0.29	30,36,37,37	0
5	EDO	H	6948	4/4	0.92	0.23	45,47,47,49	0
6	GAI	E	6836	4/4	0.92	0.16	37,39,40,41	0
6	GAI	C	6803	4/4	0.92	0.16	32,34,34,36	0
5	EDO	A	6901	4/4	0.92	0.13	33,36,36,36	0

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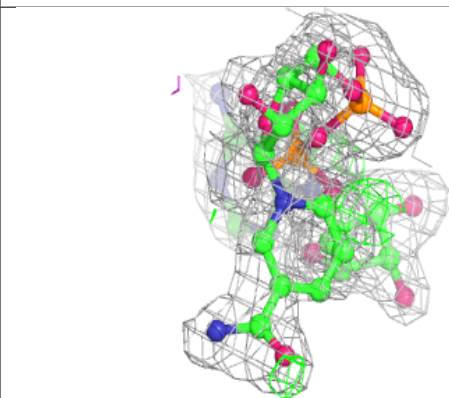
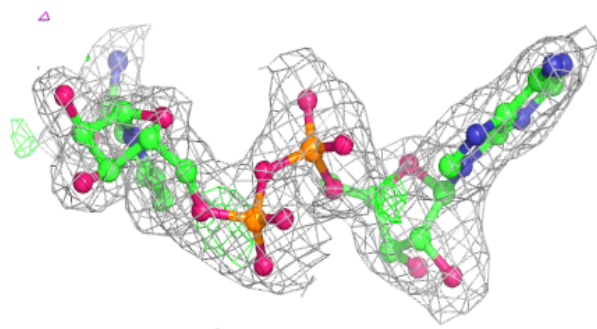
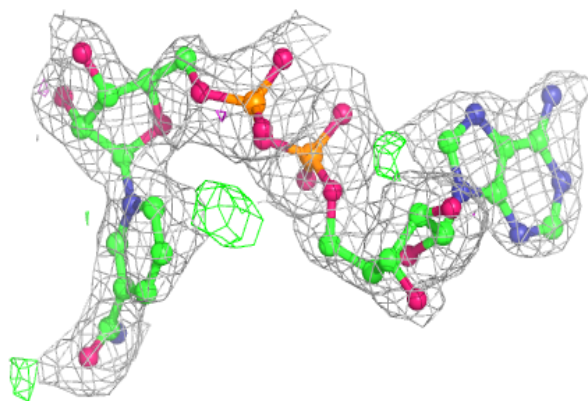
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	C	6963	4/4	0.93	0.11	35,35,36,38	0
4	NAD	B	502	44/44	0.93	0.12	35,41,44,47	0
4	NAD	D	504	44/44	0.93	0.12	24,36,42,43	0
5	EDO	C	6903	4/4	0.93	0.14	37,38,39,39	0
6	GAI	F	6816	4/4	0.93	0.19	50,50,50,51	0
3	NA	E	705	1/1	0.93	0.08	40,40,40,40	0
5	EDO	A	6921	4/4	0.93	0.13	53,53,54,54	0
6	GAI	C	6823	4/4	0.93	0.12	35,35,36,36	0
5	EDO	B	6942	4/4	0.93	0.18	36,39,40,40	0
6	GAI	A	6801	4/4	0.93	0.17	35,36,37,37	0
4	NAD	E	505	44/44	0.94	0.10	23,33,41,42	0
5	EDO	H	6908	4/4	0.94	0.14	36,37,38,38	0
6	GAI	A	6832	4/4	0.94	0.14	48,48,48,50	0
6	GAI	E	6815	4/4	0.94	0.11	45,46,46,46	0
6	GAI	B	6802	4/4	0.94	0.12	37,38,39,39	0
5	EDO	D	6904	4/4	0.94	0.12	30,35,35,35	0
5	EDO	F	6916	4/4	0.95	0.11	31,33,33,35	0
3	NA	C	703	1/1	0.95	0.15	24,24,24,24	0
3	NA	D	704	1/1	0.95	0.10	41,41,41,41	0
5	EDO	C	6913	4/4	0.96	0.12	27,29,30,31	0
6	GAI	E	6835	4/4	0.96	0.13	37,38,38,40	0
6	GAI	H	6808	4/4	0.96	0.14	30,32,32,32	0
3	NA	B	702	1/1	0.96	0.10	34,34,34,34	0
6	GAI	G	6807	4/4	0.96	0.13	41,41,42,43	0
4	NAD	C	503	44/44	0.97	0.09	16,26,30,32	0
4	NAD	F	506	44/44	0.97	0.09	16,25,30,31	0
6	GAI	D	6804	4/4	0.97	0.09	25,26,27,29	0
6	GAI	E	6805	4/4	0.98	0.10	27,27,28,29	0
3	NA	F	706	1/1	0.99	0.10	26,26,26,26	0

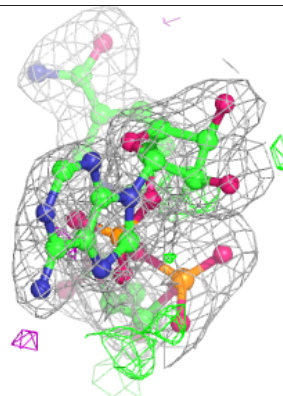
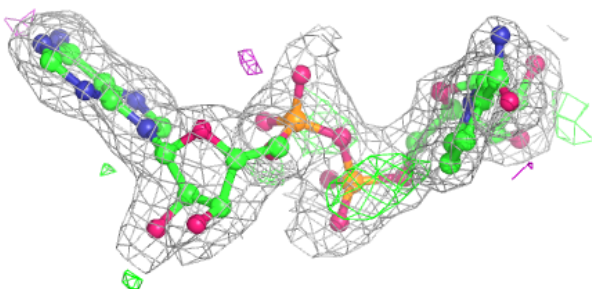
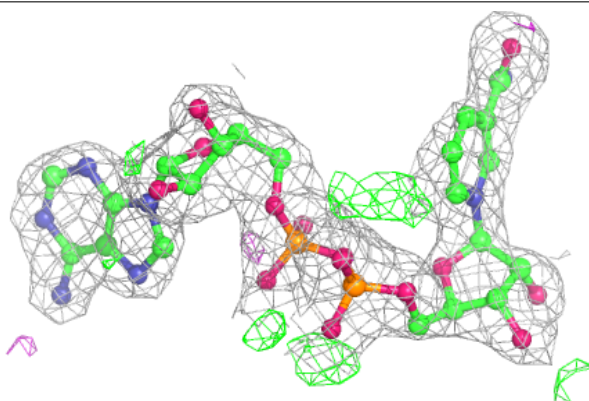
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD A 501:**

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

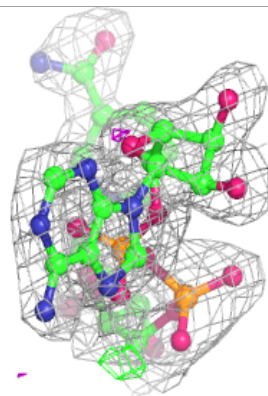
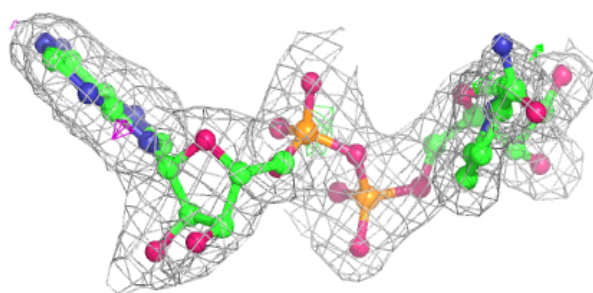
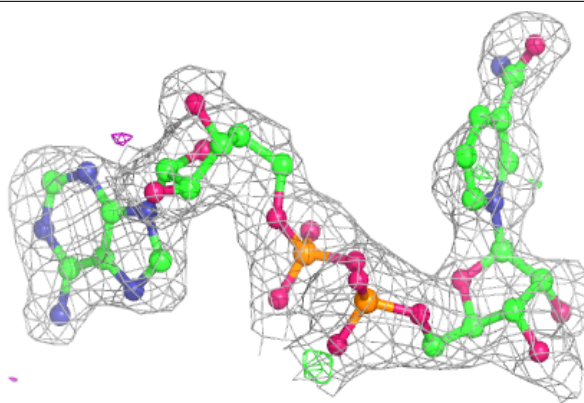
**Electron density around NAD G 507:**

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

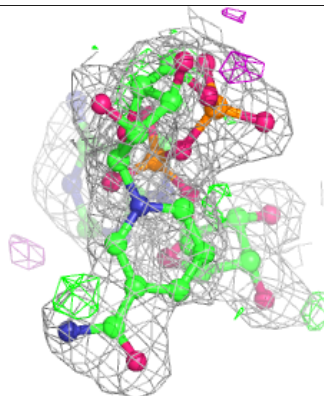
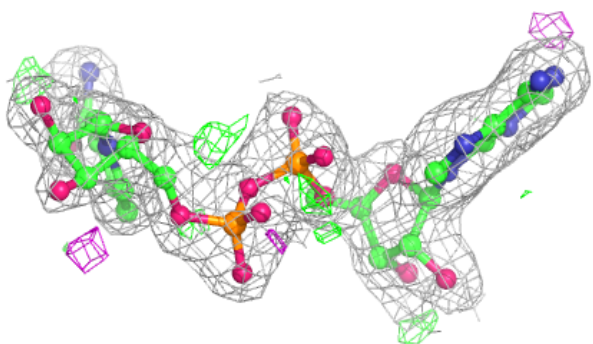
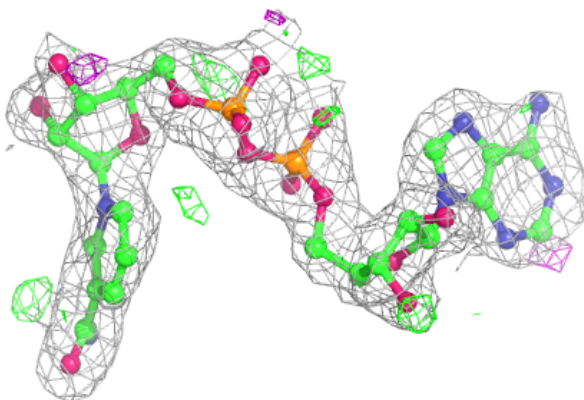


**Electron density around NAD H 508:**

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

**Electron density around NAD B 502:**

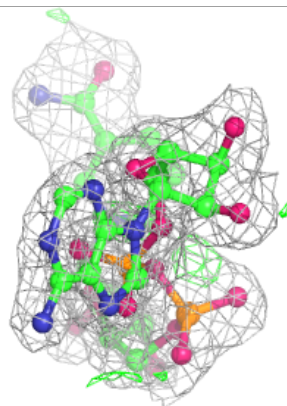
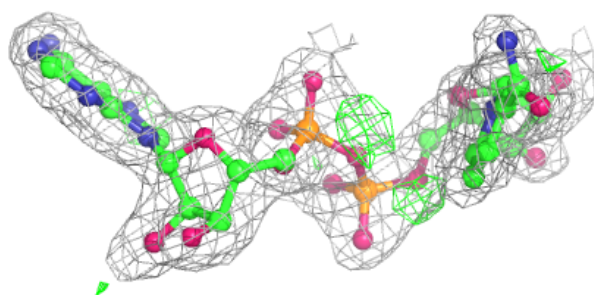
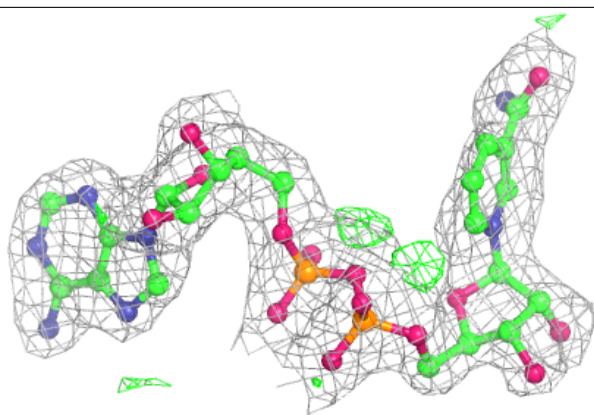
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



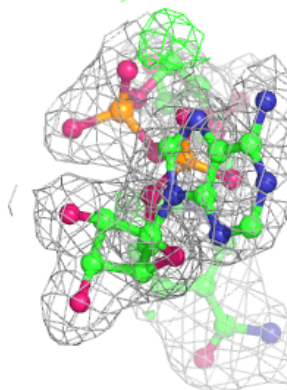
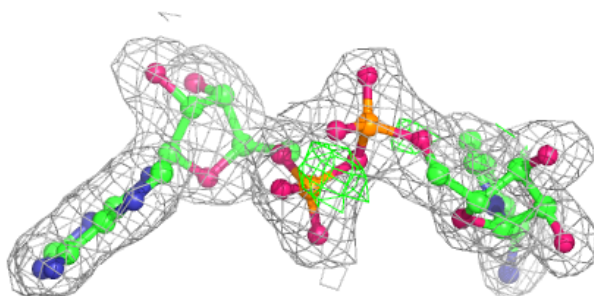
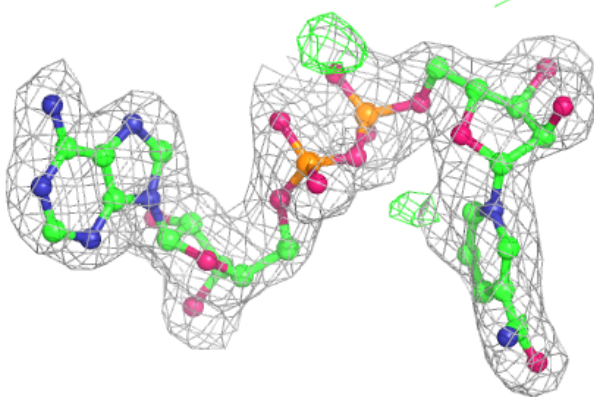


**Electron density around NAD D 504:**

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

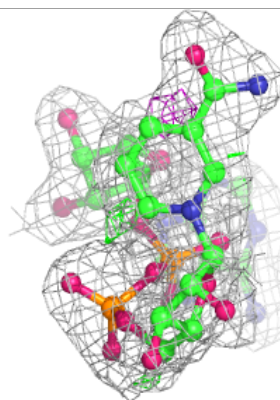
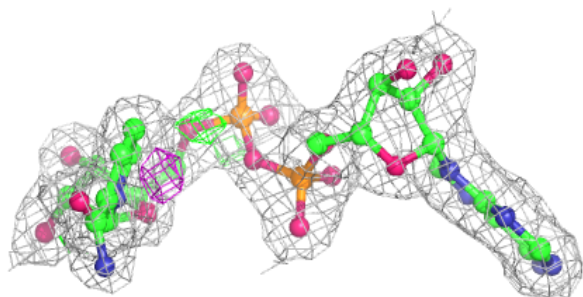
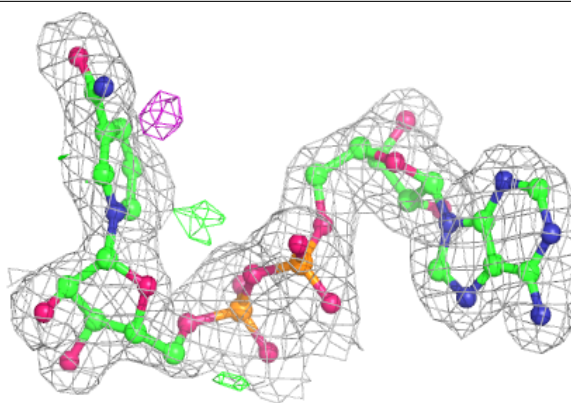
**Electron density around NAD E 505:**

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

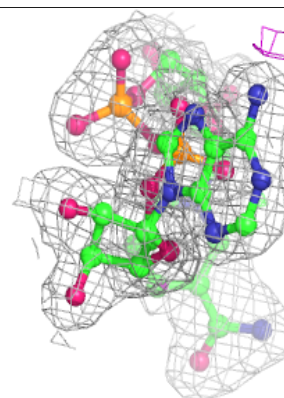
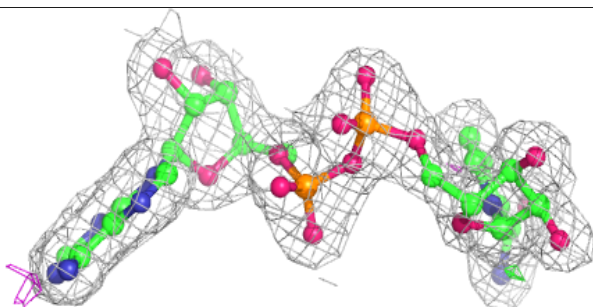
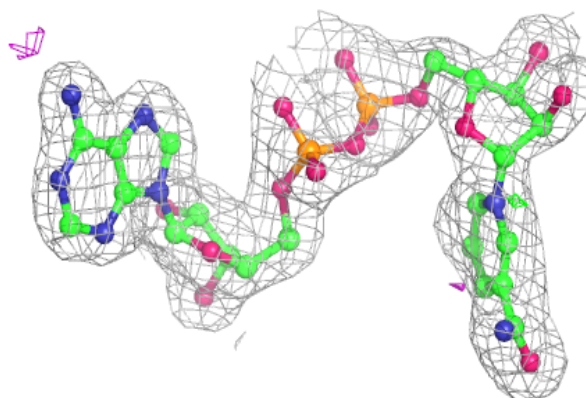


**Electron density around NAD C 503:**

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

**Electron density around NAD F 506:**

$2mF_o-DF_c$  (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.