



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 01:16 PM BST

PDB ID : 4PZD  
Title : Crystal structure of (S)-3-hydroxybutyryl-CoA dehydrogenase PaaH1 in complex with NAD<sup>+</sup>  
Authors : Kim, J.; Chang, J.H.; Kim, K.J.  
Deposited on : 2014-03-29  
Resolution : 2.61 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 : 2.13  
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) : 2.13

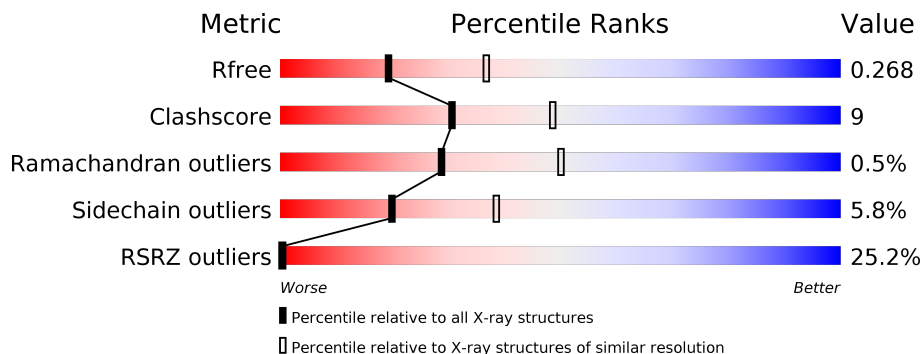
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 on 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	284	
1	B	284	
1	C	284	
1	D	284	
1	E	284	
1	F	284	

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Mol	Chain	Length	Quality of chain
1	G	284	
1	H	284	
1	I	284	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	C	301	-	-	-	X
2	NAD	E	301	-	-	-	X
2	NAD	G	301	-	-	-	X
2	NAD	I	301	-	-	-	X

## 2 Entry composition [i](#)

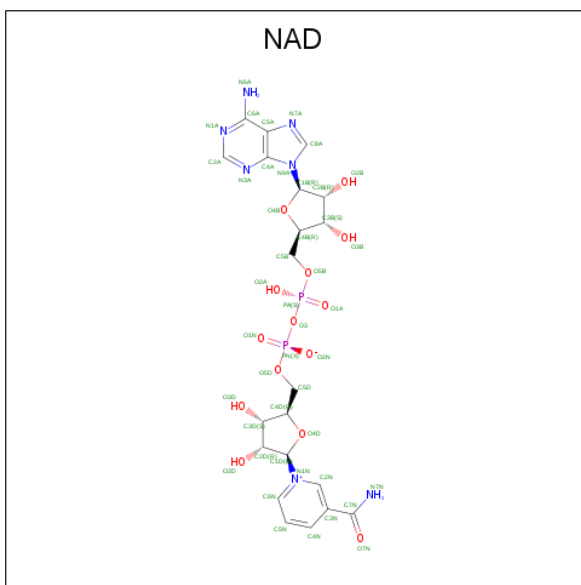
There are 3 unique types of molecules in this entry. The entry contains 19415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-Hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	2102	1331	355	400	16	0	0	0
1	B	283	2102	1331	355	400	16	0	0	0
1	C	283	2102	1331	355	400	16	0	0	0
1	D	283	2102	1331	355	400	16	0	0	0
1	E	283	2102	1331	355	400	16	0	0	0
1	F	283	2102	1331	355	400	16	0	0	0
1	G	283	2102	1331	355	400	16	0	0	0
1	H	283	2102	1331	355	400	16	0	0	0
1	I	283	2102	1331	355	400	16	0	0	0

- 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	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	I	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	10	Total	O	0	0
			10	10		
3	C	17	Total	O	0	0
			17	17		

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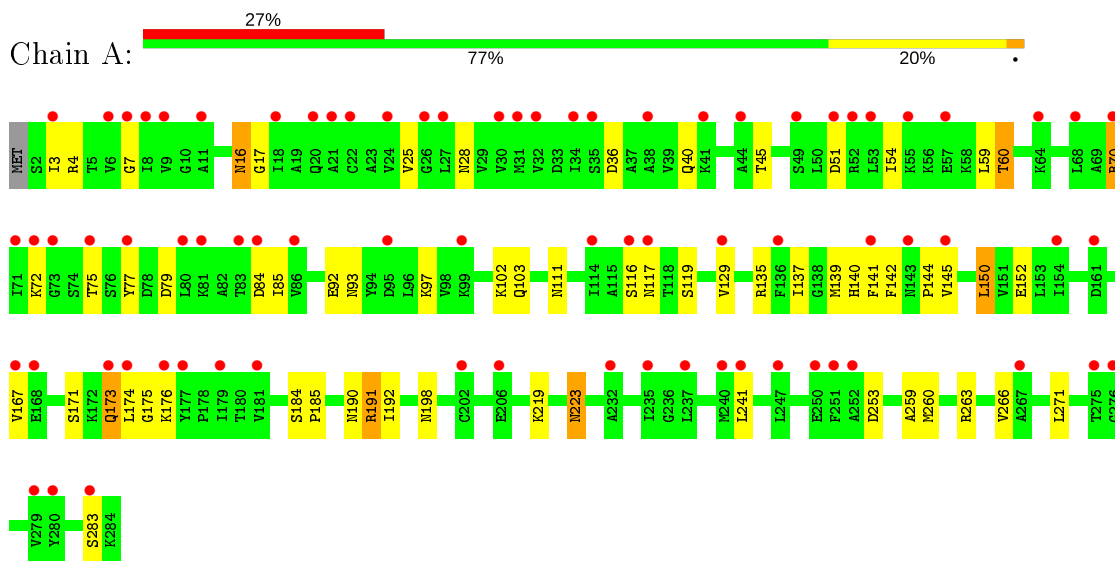
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	D	6	Total O 6 6	0	0
3	E	14	Total O 14 14	0	0
3	F	17	Total O 17 17	0	0
3	G	7	Total O 7 7	0	0
3	H	9	Total O 9 9	0	0
3	I	11	Total O 11 11	0	0

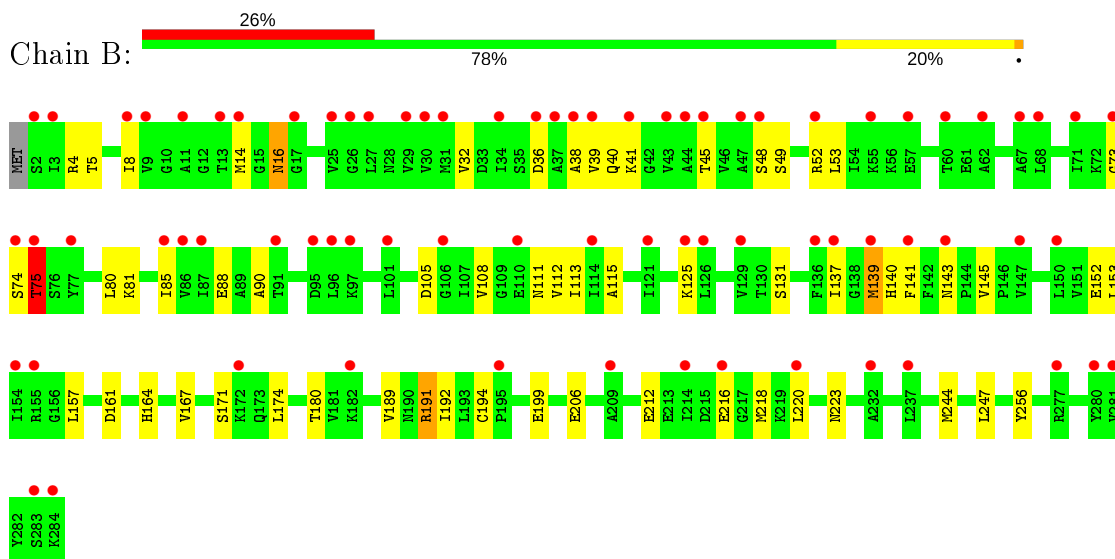
### 3 Residue-property plots [i](#)

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.

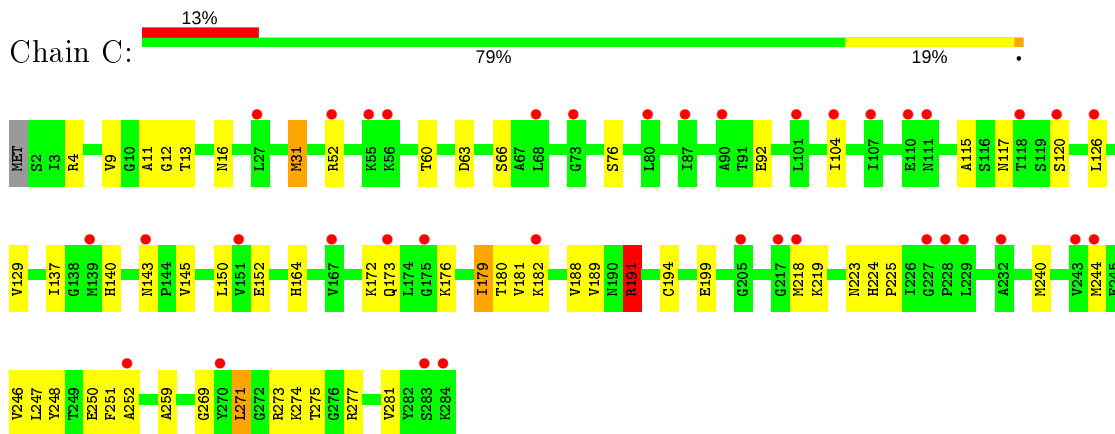
- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase



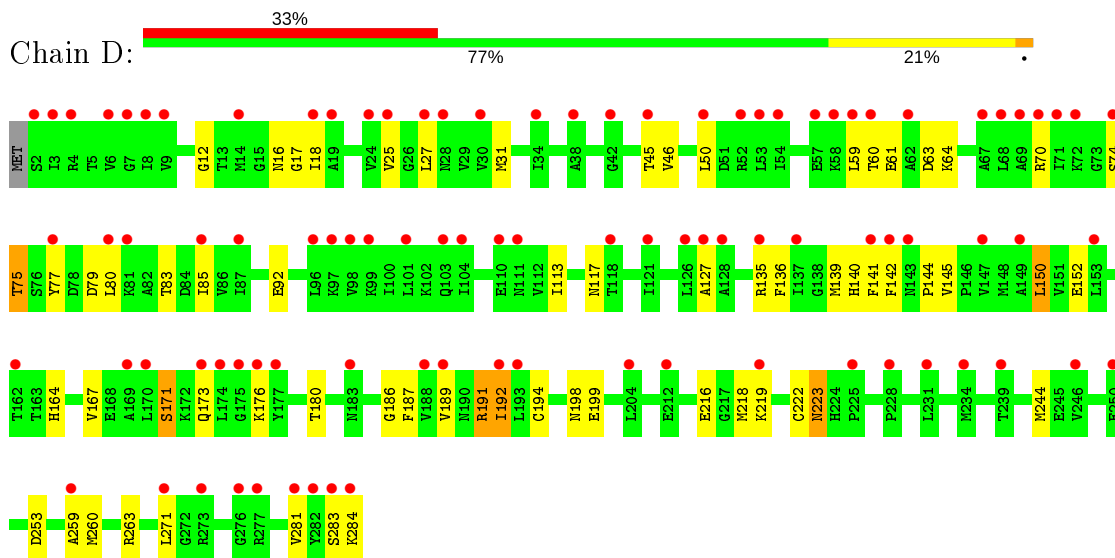
- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase



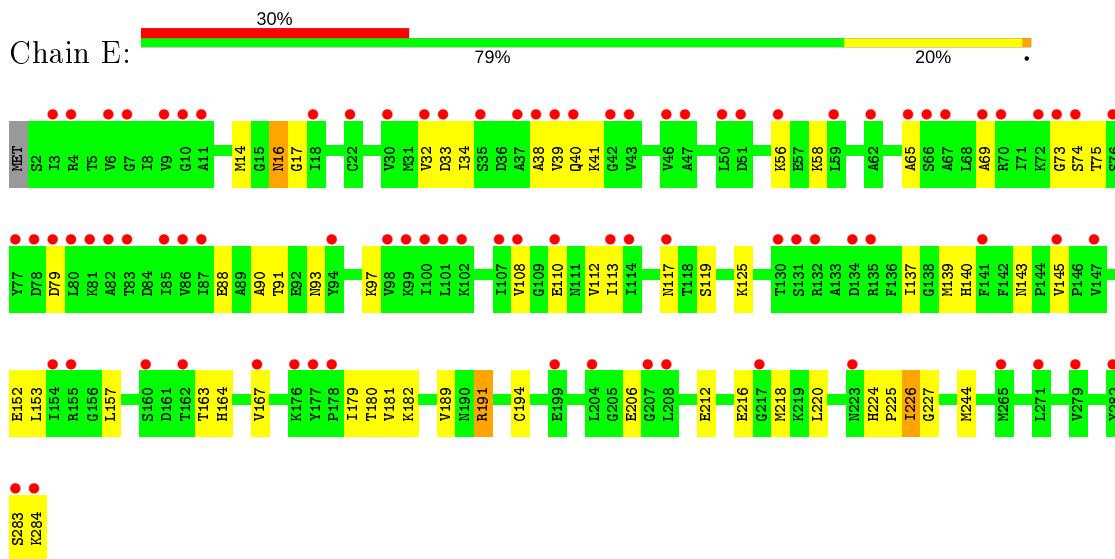
- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase



• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

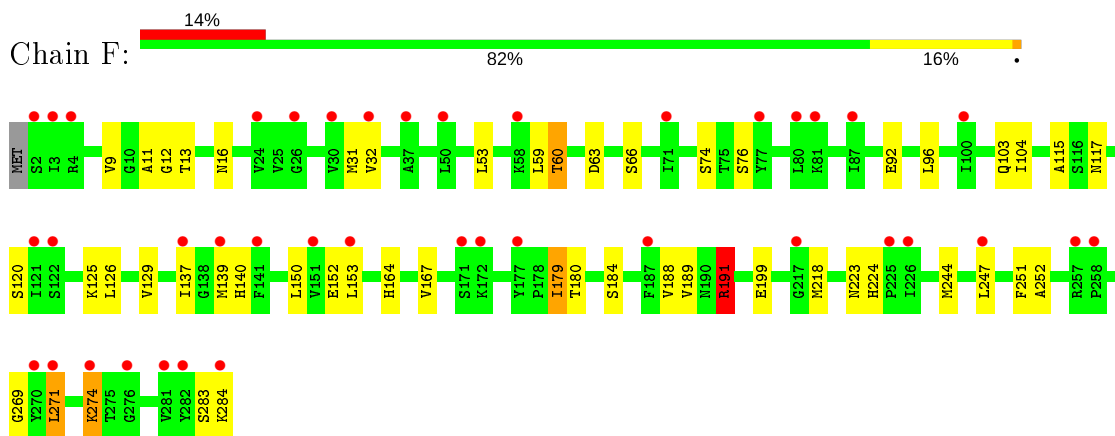


• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

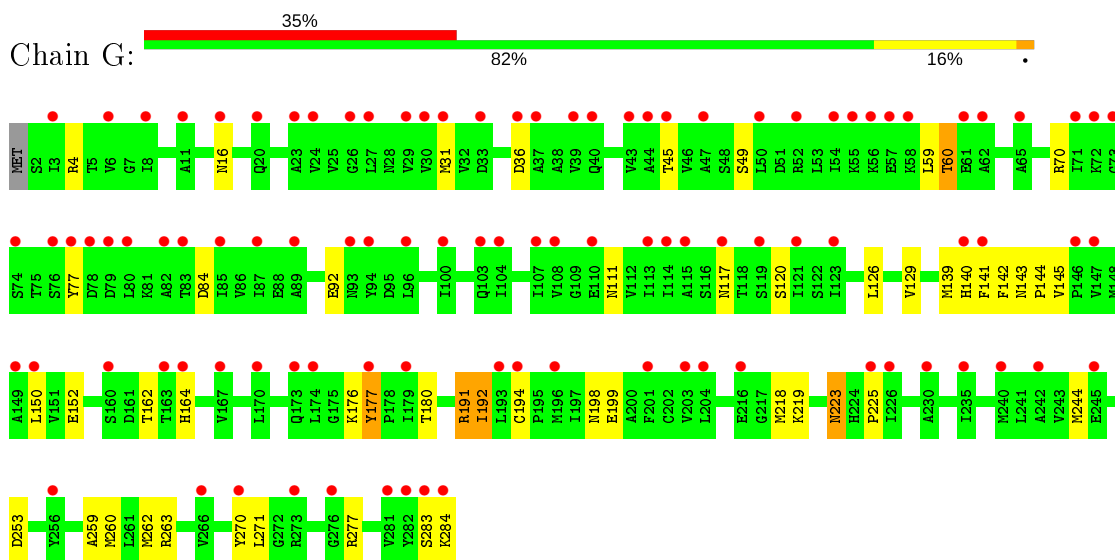


• Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase

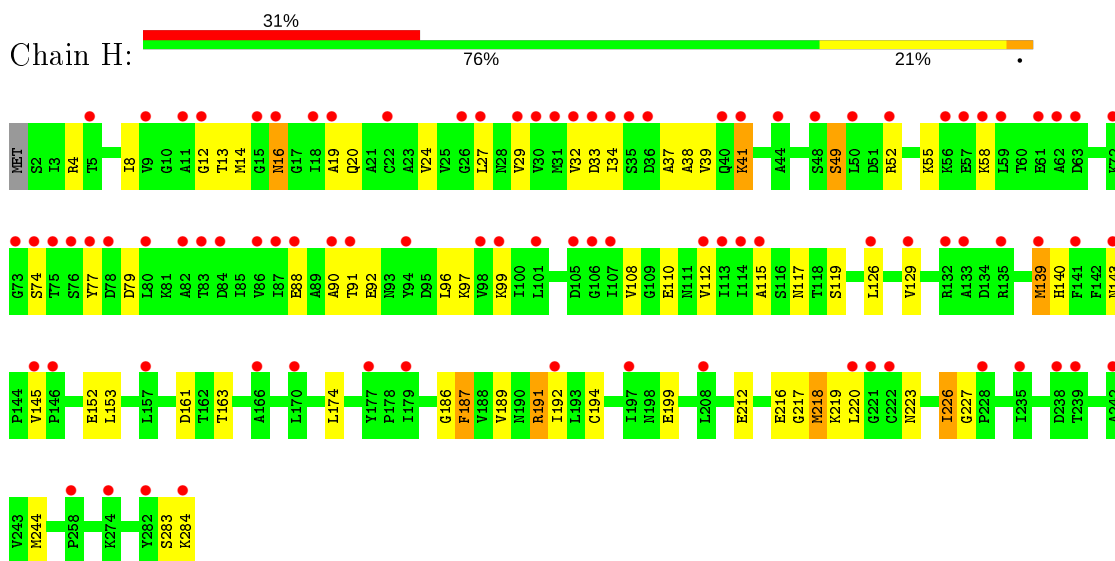




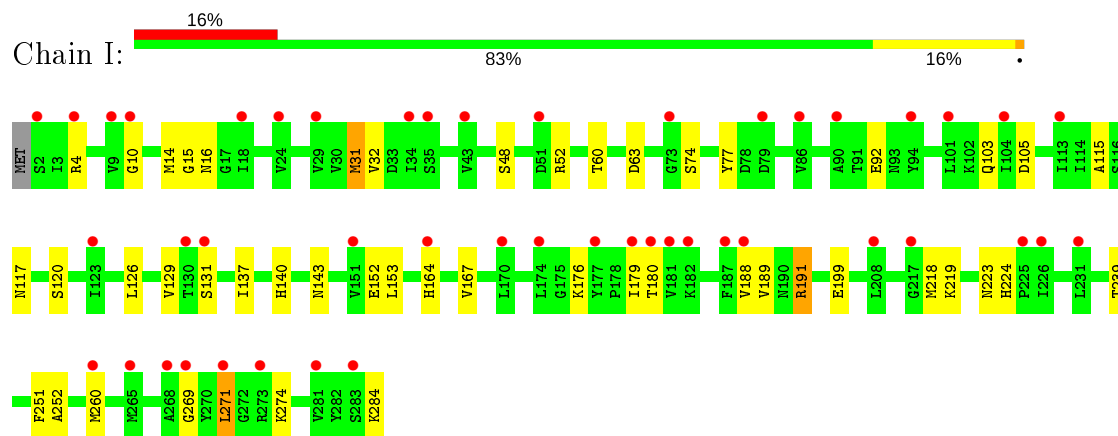
- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase



- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase



- Molecule 1: 3-Hydroxyacyl-CoA dehydrogenase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.08Å 135.59Å 97.44Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 32.85 – 2.61	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.61) 98.6 (32.85-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.02 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.199 , 0.269 0.199 , 0.268	Depositor DCC
$R_{free}$ test set	4557 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.013 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.439 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.437 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.013 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
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	0.59	0/2128	0.81	3/2879 (0.1%)
1	B	0.60	0/2128	0.78	2/2879 (0.1%)
1	C	0.67	0/2128	0.79	1/2879 (0.0%)
1	D	0.59	0/2128	0.82	4/2879 (0.1%)
1	E	0.58	0/2128	0.78	0/2879
1	F	0.68	0/2128	0.85	4/2879 (0.1%)
1	G	0.60	0/2128	0.81	4/2879 (0.1%)
1	H	0.59	0/2128	0.77	2/2879 (0.1%)
1	I	0.68	0/2128	0.82	1/2879 (0.0%)
All	All	0.62	0/19152	0.81	21/25911 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	G	0	1
All	All	0	5

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	THR	CB-CA-C	8.98	135.84	111.60
1	A	253	ASP	CB-CG-OD1	8.57	126.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	184	SER	CB-CA-C	7.86	125.03	110.10
1	G	253	ASP	CB-CG-OD1	7.56	125.10	118.30
1	F	191	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	F	191	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	G	191	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	191	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	D	253	ASP	CB-CG-OD1	6.65	124.28	118.30
1	H	187	PHE	N-CA-C	-6.06	94.63	111.00
1	B	75	THR	C-N-CA	5.71	135.98	121.70
1	F	191	ARG	CG-CD-NE	-5.70	99.83	111.80
1	A	253	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	I	31	MET	CG-SD-CE	-5.33	91.68	100.20
1	G	191	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	31	MET	CG-SD-CE	-5.25	91.81	100.20
1	H	218	MET	CG-SD-CE	-5.21	91.86	100.20
1	D	253	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	191	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	G	253	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	D	191	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	PHE	Peptide
1	B	75	THR	Peptide
1	C	191	ARG	Sidechain
1	D	142	PHE	Peptide
1	G	142	PHE	Peptide

## 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	2102	0	2187	32	0
1	B	2102	0	2187	42	0
1	C	2102	0	2187	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2102	0	2187	51	0
1	E	2102	0	2187	42	0
1	F	2102	0	2187	38	0
1	G	2102	0	2187	41	0
1	H	2102	0	2187	54	0
1	I	2102	0	2187	43	0
2	A	44	0	26	3	0
2	B	44	0	26	0	0
2	C	44	0	26	4	0
2	D	44	0	26	6	0
2	E	44	0	26	2	0
2	F	44	0	26	4	0
2	G	44	0	26	5	0
2	H	44	0	26	5	0
2	I	44	0	26	7	0
3	A	10	0	0	4	0
3	B	10	0	0	3	0
3	C	17	0	0	6	0
3	D	6	0	0	3	0
3	E	14	0	0	5	0
3	F	17	0	0	1	0
3	G	7	0	0	1	0
3	H	9	0	0	6	0
3	I	11	0	0	6	0
All	All	19415	0	19917	360	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 9.

All (360) 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:32:VAL:HG13	1:B:75:THR:O	1.56	1.04
1:F:244:MET:HE2	1:F:247:LEU:HD12	1.41	1.02
1:B:14:MET:SD	1:B:143:ASN:ND2	2.36	0.98
1:E:14:MET:SD	1:E:143:ASN:ND2	2.43	0.90
1:H:14:MET:SD	1:H:143:ASN:ND2	2.46	0.89
1:B:32:VAL:CG1	1:B:75:THR:O	2.23	0.86
1:F:244:MET:CE	1:F:247:LEU:HD12	2.05	0.85
1:C:244:MET:HE2	1:C:247:LEU:HD12	1.59	0.84
1:D:198:ASN:HD21	1:D:259:ALA:H	1.23	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:CYS:HB3	1:E:244:MET:CE	2.10	0.81
1:I:16:ASN:HA	1:I:31:MET:HE3	1.64	0.80
1:C:92:GLU:HG2	2:C:301:NAD:O2D	1.82	0.80
1:H:37:ALA:HB1	3:H:409:HOH:O	1.82	0.79
1:I:52:ARG:HD3	3:I:407:HOH:O	1.84	0.77
1:C:16:ASN:HA	1:C:31:MET:HE3	1.68	0.76
1:B:191:ARG:NH1	1:C:199:GLU:OE2	2.20	0.75
1:A:198:ASN:HD21	1:A:259:ALA:H	1.36	0.74
1:A:92:GLU:HG2	2:A:301:NAD:H2D	1.69	0.74
1:H:39:VAL:HG21	1:H:74:SER:O	1.88	0.74
1:E:191:ARG:NH1	1:F:199:GLU:OE2	2.22	0.73
1:H:108:VAL:HG11	1:H:112:VAL:HG11	1.71	0.72
1:I:152:GLU:HA	1:I:179:ILE:HG22	1.71	0.72
1:E:16:ASN:C	1:E:16:ASN:HD22	1.92	0.72
1:G:117:ASN:HD21	1:G:141:PHE:H	1.37	0.72
1:H:194:CYS:HB3	1:H:244:MET:HE3	1.72	0.72
1:G:198:ASN:HD21	1:G:259:ALA:H	1.36	0.71
1:H:88:GLU:OE1	1:H:97:LYS:NZ	2.22	0.71
1:H:192:ILE:HD12	1:I:218:MET:HE3	1.71	0.71
1:H:8:ILE:HG22	1:H:8:ILE:O	1.90	0.70
1:D:199:GLU:HB3	1:G:192:ILE:HG22	1.74	0.70
1:B:39:VAL:HG21	1:B:74:SER:O	1.91	0.70
1:A:145:VAL:O	1:A:176:LYS:NZ	2.26	0.69
1:H:34:ILE:HG22	3:H:408:HOH:O	1.91	0.69
1:I:60:THR:HG23	1:I:63:ASP:H	1.56	0.69
1:B:194:CYS:HB3	1:B:244:MET:HE3	1.76	0.68
1:I:143:ASN:HB2	3:I:408:HOH:O	1.92	0.68
1:I:117:ASN:HD21	2:I:301:NAD:H6N	1.59	0.67
1:H:79:ASP:HB2	3:H:406:HOH:O	1.94	0.67
1:A:117:ASN:HD21	1:A:141:PHE:H	1.42	0.66
1:A:92:GLU:HG2	2:A:301:NAD:C2D	2.24	0.66
1:D:260:MET:CE	3:D:403:HOH:O	2.43	0.66
1:H:38:ALA:HA	1:H:41:LYS:HE3	1.77	0.66
1:C:52:ARG:HD3	3:C:413:HOH:O	1.94	0.66
1:D:194:CYS:HB3	1:D:244:MET:HE3	1.78	0.65
1:H:191:ARG:NH1	1:I:199:GLU:OE2	2.30	0.65
1:E:108:VAL:HG11	1:E:112:VAL:HG11	1.79	0.65
1:D:117:ASN:HA	1:D:139:MET:O	1.97	0.65
1:C:244:MET:CE	1:C:247:LEU:HD12	2.27	0.63
1:D:199:GLU:CG	1:G:192:ILE:HG22	2.28	0.63
1:G:145:VAL:O	1:G:176:LYS:NZ	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:ASN:CB	3:I:408:HOH:O	2.45	0.62
1:B:192:ILE:HD12	1:C:218:MET:HE3	1.81	0.62
1:B:108:VAL:HG11	1:B:112:VAL:HG11	1.81	0.62
1:B:191:ARG:HD3	3:B:404:HOH:O	1.98	0.62
1:D:218:MET:CE	1:D:222:CYS:SG	2.87	0.62
1:I:117:ASN:ND2	2:I:301:NAD:H1D	2.14	0.61
1:A:4:ARG:N	1:A:84:ASP:OD2	2.34	0.61
1:A:260:MET:HE1	3:A:402:HOH:O	1.99	0.61
1:F:16:ASN:HA	1:F:31:MET:HE3	1.81	0.61
1:F:92:GLU:HG2	2:F:301:NAD:O2D	2.01	0.61
1:C:117:ASN:HD21	2:C:301:NAD:H6N	1.66	0.61
1:B:38:ALA:HA	1:B:41:LYS:HG2	1.82	0.60
1:D:117:ASN:HD21	1:D:141:PHE:H	1.48	0.60
1:H:194:CYS:HB3	1:H:244:MET:CE	2.32	0.60
1:F:92:GLU:HG2	2:F:301:NAD:C2D	2.32	0.60
1:A:260:MET:CE	3:A:402:HOH:O	2.50	0.60
1:E:194:CYS:HB3	1:E:244:MET:HE1	1.84	0.60
1:C:143:ASN:HA	3:C:404:HOH:O	2.02	0.59
1:D:18:ILE:HD13	1:D:145:VAL:HG11	1.84	0.59
1:E:39:VAL:HG21	1:E:74:SER:O	2.02	0.59
1:D:189:VAL:HA	1:G:218:MET:CE	2.33	0.59
1:F:76:SER:HB3	3:F:413:HOH:O	2.03	0.59
1:H:199:GLU:OE2	1:I:191:ARG:NH1	2.34	0.58
1:C:251:PHE:O	1:C:252:ALA:HB3	2.02	0.58
1:I:219:LYS:O	1:I:223:ASN:HA	2.04	0.58
1:G:140:HIS:HB3	1:G:152:GLU:HB2	1.85	0.58
1:D:199:GLU:CB	1:G:192:ILE:HG22	2.33	0.58
1:E:73:GLY:HA3	3:E:408:HOH:O	2.04	0.58
1:B:32:VAL:HG13	1:B:75:THR:C	2.23	0.57
1:B:88:GLU:OE2	1:B:90:ALA:N	2.38	0.57
1:I:251:PHE:O	1:I:252:ALA:HB3	2.03	0.57
1:A:77:TYR:HB3	3:A:410:HOH:O	2.04	0.57
1:D:164:HIS:HE1	1:D:180:THR:OG1	1.88	0.57
1:E:140:HIS:HB3	1:E:152:GLU:HB2	1.87	0.57
1:C:60:THR:HG21	3:C:407:HOH:O	2.04	0.56
1:H:189:VAL:HA	1:I:218:MET:CE	2.35	0.56
1:B:113:ILE:HD11	3:B:406:HOH:O	2.05	0.56
1:E:79:ASP:HB2	3:E:413:HOH:O	2.05	0.56
1:I:199:GLU:HA	1:I:199:GLU:OE1	2.05	0.56
1:B:140:HIS:HB3	1:B:152:GLU:HB2	1.88	0.56
1:D:59:LEU:HB3	1:D:60:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LYS:HE2	3:D:406:HOH:O	2.06	0.56
1:F:152:GLU:HA	1:F:179:ILE:HG23	1.86	0.56
1:H:38:ALA:HA	1:H:41:LYS:CE	2.36	0.56
1:G:194:CYS:O	1:G:244:MET:HE3	2.06	0.56
1:B:218:MET:CE	1:C:189:VAL:HA	2.37	0.55
1:C:126:LEU:O	1:C:129:VAL:HG22	2.06	0.55
1:C:164:HIS:HE1	1:C:180:THR:OG1	1.88	0.55
1:B:223:ASN:HB2	1:C:225:PRO:HG3	1.89	0.55
1:F:251:PHE:O	1:F:252:ALA:HB3	2.05	0.55
1:G:77:TYR:OH	2:G:301:NAD:N1A	2.39	0.55
1:E:16:ASN:HD22	1:E:17:GLY:N	2.03	0.55
1:C:269:GLY:C	1:C:271:LEU:HD13	2.26	0.55
1:E:194:CYS:HB3	1:E:244:MET:HE3	1.87	0.55
1:I:92:GLU:HG2	2:I:301:NAD:C2D	2.36	0.55
1:D:216:GLU:OE1	1:G:177:TYR:CE1	2.59	0.55
1:D:218:MET:CE	1:D:218:MET:HA	2.37	0.55
1:D:189:VAL:HA	1:G:218:MET:HE1	1.89	0.54
1:C:92:GLU:HG2	2:C:301:NAD:C2D	2.37	0.54
1:D:218:MET:HA	1:D:218:MET:HE3	1.89	0.54
1:E:113:ILE:HG12	1:E:163:THR:HG23	1.89	0.54
1:E:189:VAL:HA	1:F:218:MET:CE	2.37	0.54
1:I:117:ASN:HD21	2:I:301:NAD:C6N	2.19	0.54
1:H:115:ALA:HB1	1:H:139:MET:HE3	1.87	0.54
1:H:186:GLY:O	1:H:187:PHE:C	2.46	0.54
1:I:164:HIS:HE1	1:I:180:THR:OG1	1.89	0.54
1:C:143:ASN:CA	3:C:404:HOH:O	2.56	0.54
1:E:117:ASN:HA	1:E:139:MET:O	2.08	0.54
1:C:60:THR:HG23	1:C:63:ASP:H	1.73	0.54
1:F:150:LEU:HD11	1:F:179:ILE:CG2	2.38	0.54
1:E:206:GLU:OE1	1:F:191:ARG:NH2	2.40	0.53
1:C:244:MET:HE2	1:C:244:MET:HA	1.91	0.53
1:E:16:ASN:C	1:E:16:ASN:ND2	2.62	0.53
1:F:9:VAL:HG21	1:F:104:ILE:HD11	1.89	0.53
1:B:8:ILE:O	1:B:8:ILE:HG22	2.08	0.53
1:C:273:ARG:O	1:C:275:THR:N	2.42	0.53
1:E:137:ILE:HG21	1:E:167:VAL:HG21	1.91	0.53
1:B:194:CYS:HB3	1:B:244:MET:CE	2.38	0.52
1:D:283:SER:O	1:D:284:LYS:HB2	2.09	0.52
1:I:92:GLU:HG2	2:I:301:NAD:H2D	1.90	0.52
1:B:199:GLU:OE2	1:C:191:ARG:NH1	2.42	0.52
1:F:140:HIS:HB3	1:F:152:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:MET:CE	1:A:263:ARG:HE	2.22	0.52
1:G:194:CYS:HB3	1:G:244:MET:CE	2.40	0.52
1:B:139:MET:HG2	1:B:141:PHE:CE1	2.44	0.52
1:F:244:MET:HA	1:F:244:MET:CE	2.40	0.52
1:I:92:GLU:CG	2:I:301:NAD:H2D	2.40	0.52
1:E:38:ALA:HA	1:E:41:LYS:HG2	1.91	0.51
1:E:75:THR:CG2	3:E:405:HOH:O	2.59	0.51
1:I:269:GLY:C	1:I:271:LEU:HD13	2.31	0.51
1:D:167:VAL:O	1:D:171:SER:OG	2.28	0.51
1:G:164:HIS:HE1	1:G:180:THR:OG1	1.92	0.51
1:D:25:VAL:O	1:D:25:VAL:HG12	2.10	0.51
1:F:126:LEU:O	1:F:129:VAL:HG22	2.11	0.51
1:G:120:SER:HA	3:G:407:HOH:O	2.11	0.51
1:C:143:ASN:CB	3:C:404:HOH:O	2.59	0.51
1:I:16:ASN:HB3	1:I:31:MET:HE1	1.93	0.51
1:E:189:VAL:HA	1:F:218:MET:HE2	1.92	0.50
1:G:143:ASN:ND2	2:G:301:NAD:O7N	2.43	0.50
1:I:176:LYS:HE2	3:I:404:HOH:O	2.10	0.50
1:G:194:CYS:C	1:G:244:MET:CE	2.80	0.50
1:H:32:VAL:HG12	1:H:33:ASP:N	2.25	0.50
1:D:216:GLU:OE1	1:G:177:TYR:CD1	2.65	0.50
1:E:88:GLU:OE2	1:E:90:ALA:N	2.42	0.50
1:B:189:VAL:HA	1:C:218:MET:CE	2.42	0.50
1:G:194:CYS:HB3	1:G:244:MET:HE1	1.93	0.50
1:G:283:SER:O	1:G:284:LYS:CB	2.60	0.50
1:C:115:ALA:HA	1:C:137:ILE:O	2.11	0.50
1:D:164:HIS:CE1	1:D:180:THR:OG1	2.65	0.50
1:B:192:ILE:HB	1:C:218:MET:HE1	1.94	0.50
1:E:33:ASP:OD1	1:E:34:ILE:N	2.43	0.49
1:F:269:GLY:C	1:F:271:LEU:HD13	2.32	0.49
1:H:88:GLU:OE2	1:H:90:ALA:N	2.43	0.49
1:I:77:TYR:CD2	1:I:103:GLN:HG2	2.47	0.49
1:H:117:ASN:HA	1:H:139:MET:O	2.13	0.49
1:I:140:HIS:HB3	1:I:152:GLU:HB3	1.94	0.49
1:E:218:MET:CE	1:F:189:VAL:HA	2.42	0.49
1:D:223:ASN:HB3	1:G:225:PRO:HG3	1.95	0.49
1:E:32:VAL:HG12	1:E:33:ASP:N	2.28	0.49
1:F:92:GLU:HG2	2:F:301:NAD:H2D	1.94	0.49
1:I:60:THR:HG22	1:I:63:ASP:OD2	2.12	0.49
1:H:117:ASN:OD1	2:H:301:NAD:H1D	2.13	0.49
1:H:189:VAL:HA	1:I:218:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:HIS:HE1	1:F:180:THR:OG1	1.96	0.48
1:I:14:MET:HE3	1:I:143:ASN:HB3	1.94	0.48
1:E:73:GLY:CA	3:E:408:HOH:O	2.60	0.48
1:G:117:ASN:HA	1:G:139:MET:O	2.14	0.48
1:G:283:SER:O	1:G:284:LYS:HB2	2.14	0.48
1:E:283:SER:HA	1:E:284:LYS:HB3	1.95	0.48
1:F:53:LEU:CB	1:F:59:LEU:HD12	2.43	0.48
1:G:59:LEU:HA	1:G:60:THR:HG23	1.95	0.48
1:C:277:ARG:NH1	1:C:281:VAL:HG22	2.28	0.48
1:E:212:GLU:O	1:E:216:GLU:HG2	2.14	0.48
1:A:51:ASP:HA	1:A:54:ILE:HD12	1.95	0.48
1:B:85:ILE:HG13	1:B:113:ILE:O	2.14	0.48
1:E:117:ASN:OD1	2:E:301:NAD:H1D	2.13	0.48
1:A:59:LEU:HA	1:A:60:THR:HG23	1.95	0.48
1:D:16:ASN:HB3	1:D:46:VAL:HG23	1.96	0.48
1:H:126:LEU:O	1:H:129:VAL:HG22	2.14	0.47
1:A:7:GLY:N	1:A:85:ILE:O	2.43	0.47
1:E:226:ILE:HG13	1:E:227:GLY:N	2.29	0.47
1:E:164:HIS:HE1	1:E:180:THR:OG1	1.96	0.47
1:I:115:ALA:HA	1:I:137:ILE:O	2.14	0.47
1:D:260:MET:CE	1:D:263:ARG:HE	2.27	0.47
1:B:191:ARG:NH1	1:B:256:TYR:OH	2.47	0.47
1:C:11:ALA:HA	1:C:31:MET:CE	2.45	0.47
1:D:12:GLY:HA3	2:D:301:NAD:O5B	2.15	0.47
1:D:59:LEU:CB	1:D:60:THR:HG23	2.44	0.47
1:C:60:THR:HG22	1:C:63:ASP:CG	2.35	0.47
1:C:150:LEU:HD11	1:C:179:ILE:HG21	1.96	0.47
1:C:194:CYS:HA	1:C:240:MET:HE1	1.97	0.47
1:I:176:LYS:CE	3:I:404:HOH:O	2.63	0.47
1:C:248:TYR:O	1:C:252:ALA:N	2.48	0.46
1:D:218:MET:HE3	1:D:222:CYS:SG	2.55	0.46
1:C:60:THR:HG22	1:C:63:ASP:OD2	2.14	0.46
1:F:150:LEU:HD11	1:F:179:ILE:HG21	1.98	0.46
1:G:117:ASN:OD1	2:G:301:NAD:H1D	2.15	0.46
1:H:8:ILE:O	1:H:8:ILE:CG2	2.60	0.46
1:B:105:ASP:OD1	1:B:131:SER:OG	2.29	0.46
1:D:260:MET:HE1	1:D:263:ARG:HE	1.80	0.46
1:F:16:ASN:HA	1:F:31:MET:CE	2.44	0.46
1:I:152:GLU:OE2	1:I:188:VAL:HB	2.16	0.46
1:D:260:MET:HE1	3:D:403:HOH:O	2.11	0.46
1:F:115:ALA:HA	1:F:137:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:ARG:O	1:H:27:LEU:HD23	2.16	0.46
1:A:117:ASN:HA	1:A:139:MET:O	2.16	0.46
1:A:219:LYS:O	1:A:223:ASN:HA	2.16	0.46
1:H:283:SER:HA	1:H:284:LYS:C	2.36	0.46
1:G:92:GLU:HG2	2:G:301:NAD:C2D	2.46	0.46
1:H:226:ILE:HG13	1:H:227:GLY:N	2.30	0.46
1:B:189:VAL:HA	1:C:218:MET:HE2	1.97	0.45
1:G:194:CYS:CB	1:G:244:MET:HE1	2.46	0.45
1:H:20:GLN:O	1:H:24:VAL:HG23	2.16	0.45
1:D:92:GLU:HG2	2:D:301:NAD:C2D	2.46	0.45
1:E:225:PRO:HG3	1:F:223:ASN:HB3	1.98	0.45
1:C:246:VAL:O	1:C:250:GLU:HB2	2.17	0.45
1:H:218:MET:CE	1:I:189:VAL:HA	2.46	0.45
1:H:189:VAL:HA	1:I:218:MET:HE2	1.97	0.45
1:D:92:GLU:HG2	2:D:301:NAD:H2D	1.98	0.45
1:C:145:VAL:O	1:C:176:LYS:NZ	2.49	0.45
1:F:152:GLU:OE2	1:F:188:VAL:HB	2.16	0.45
1:C:140:HIS:HB3	1:C:152:GLU:HB3	1.99	0.45
1:D:127:ALA:HB2	1:D:136:PHE:CD1	2.50	0.45
1:B:16:ASN:C	1:B:16:ASN:HD22	2.19	0.45
1:B:244:MET:HE2	1:B:247:LEU:HD12	1.99	0.45
1:D:27:LEU:HD21	1:D:173:GLN:NE2	2.32	0.45
1:D:117:ASN:OD1	2:D:301:NAD:H6N	2.17	0.45
1:G:4:ARG:N	1:G:84:ASP:OD2	2.48	0.45
1:C:16:ASN:HB3	1:C:31:MET:HE1	1.97	0.44
1:D:281:VAL:CG1	1:E:58:LYS:HD2	2.48	0.44
1:G:270:TYR:CD1	1:G:277:ARG:HD3	2.51	0.44
1:H:37:ALA:C	3:H:409:HOH:O	2.54	0.44
1:H:49:SER:O	1:H:52:ARG:N	2.51	0.44
1:H:216:GLU:O	1:H:217:GLY:C	2.56	0.44
1:I:105:ASP:OD2	1:I:131:SER:N	2.42	0.44
1:C:172:LYS:O	1:C:173:GLN:C	2.53	0.44
1:H:219:LYS:O	1:H:223:ASN:HA	2.18	0.44
1:A:260:MET:HE1	1:A:263:ARG:HE	1.83	0.44
1:D:186:GLY:O	1:D:187:PHE:C	2.55	0.44
1:E:194:CYS:CB	1:E:244:MET:HE1	2.45	0.44
1:G:219:LYS:O	1:G:223:ASN:HA	2.16	0.44
1:H:108:VAL:HG11	1:H:112:VAL:CG1	2.45	0.44
1:B:75:THR:CG2	3:B:408:HOH:O	2.66	0.44
1:C:152:GLU:OE2	1:C:188:VAL:HB	2.17	0.44
1:F:103:GLN:HB2	1:F:103:GLN:HE21	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASN:O	1:A:17:GLY:C	2.55	0.44
1:D:140:HIS:HB3	1:D:152:GLU:HB2	2.00	0.44
1:G:117:ASN:OD1	2:G:301:NAD:H6N	2.18	0.44
1:H:212:GLU:O	1:H:216:GLU:HG2	2.18	0.44
1:C:164:HIS:CE1	1:C:180:THR:OG1	2.69	0.44
1:B:218:MET:HE2	1:C:189:VAL:HA	2.00	0.44
1:H:91:THR:O	1:H:97:LYS:HD2	2.18	0.44
1:B:137:ILE:HG21	1:B:167:VAL:HG21	1.99	0.43
1:A:102:LYS:HE3	1:A:129:VAL:HB	2.00	0.43
1:G:117:ASN:ND2	1:G:141:PHE:H	2.11	0.43
1:A:140:HIS:HD2	1:A:152:GLU:OE1	2.00	0.43
1:H:92:GLU:HG2	2:H:301:NAD:C2D	2.48	0.43
1:C:259:ALA:HB1	3:C:411:HOH:O	2.18	0.43
1:F:153:LEU:HD22	1:F:167:VAL:HG12	2.01	0.43
1:B:206:GLU:OE1	1:C:191:ARG:NH2	2.52	0.43
1:D:85:ILE:HG13	1:D:113:ILE:O	2.18	0.43
1:H:96:LEU:O	1:H:99:LYS:N	2.52	0.43
1:D:140:HIS:CE1	2:D:301:NAD:H5N	2.54	0.43
1:E:181:VAL:HG12	1:E:182:LYS:O	2.18	0.43
1:F:11:ALA:HA	1:F:31:MET:CE	2.49	0.43
1:H:13:THR:N	2:H:301:NAD:O2A	2.50	0.43
1:I:153:LEU:HD22	1:I:167:VAL:HG12	2.00	0.43
1:G:198:ASN:HD22	1:G:262:MET:CE	2.32	0.43
1:H:115:ALA:CB	1:H:139:MET:HE3	2.49	0.43
1:H:140:HIS:HB3	1:H:152:GLU:HB2	2.00	0.43
1:A:103:GLN:NE2	3:A:410:HOH:O	2.51	0.42
1:C:9:VAL:HG21	1:C:104:ILE:HD11	2.01	0.42
1:D:63:ASP:O	1:D:64:LYS:C	2.56	0.42
1:E:157:LEU:HA	1:E:157:LEU:HD23	1.91	0.42
1:F:139:MET:CE	1:F:167:VAL:HG13	2.49	0.42
1:F:60:THR:HG22	1:F:63:ASP:CG	2.38	0.42
1:H:16:ASN:C	1:H:16:ASN:HD22	2.23	0.42
1:H:77:TYR:OH	2:H:301:NAD:N1A	2.53	0.42
1:I:32:VAL:HA	1:I:74:SER:O	2.19	0.42
1:H:12:GLY:O	1:H:13:THR:C	2.58	0.42
1:D:17:GLY:HA3	1:D:145:VAL:HB	2.02	0.42
1:H:41:LYS:HD3	3:H:409:HOH:O	2.18	0.42
1:D:80:LEU:O	1:D:83:THR:OG1	2.36	0.42
1:E:65:ALA:O	1:E:69:ALA:N	2.47	0.42
1:B:164:HIS:HE1	1:B:180:THR:OG1	2.02	0.42
1:B:218:MET:HE1	1:C:189:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:MET:HE1	1:D:222:CYS:SG	2.59	0.42
1:I:260:MET:CE	3:I:405:HOH:O	2.68	0.42
1:A:173:GLN:O	1:A:175:GLY:N	2.53	0.42
1:B:191:ARG:O	1:B:191:ARG:HG3	2.19	0.42
1:C:150:LEU:HD11	1:C:179:ILE:CG2	2.49	0.42
1:G:194:CYS:C	1:G:244:MET:HE1	2.40	0.42
1:B:192:ILE:HD12	1:C:218:MET:CE	2.48	0.42
1:B:212:GLU:O	1:B:216:GLU:HG2	2.20	0.42
1:B:244:MET:CE	1:B:247:LEU:HD12	2.49	0.42
1:H:187:PHE:O	1:H:191:ARG:HB3	2.19	0.42
1:H:19:ALA:HB1	1:H:29:VAL:HG11	2.02	0.42
1:H:34:ILE:CG2	3:H:408:HOH:O	2.60	0.42
1:D:145:VAL:O	1:D:176:LYS:NZ	2.41	0.41
1:E:113:ILE:HD11	3:E:410:HOH:O	2.20	0.41
1:H:91:THR:HA	2:H:301:NAD:O3D	2.19	0.41
1:C:12:GLY:O	1:C:13:THR:C	2.58	0.41
1:H:39:VAL:CG2	1:H:74:SER:O	2.65	0.41
1:A:190:ASN:HD22	1:A:190:ASN:HA	1.65	0.41
1:A:92:GLU:N	2:A:301:NAD:O3D	2.53	0.41
1:C:181:VAL:HG12	1:C:182:LYS:O	2.20	0.41
1:H:119:SER:HA	1:H:140:HIS:CE1	2.55	0.41
1:D:77:TYR:OH	2:D:301:NAD:N1A	2.53	0.41
1:H:218:MET:HE1	1:I:189:VAL:HA	2.01	0.41
1:E:93:ASN:O	1:E:97:LYS:HB2	2.20	0.41
1:A:241:LEU:HD23	1:A:266:VAL:HG11	2.02	0.41
1:A:260:MET:HE2	1:A:263:ARG:HE	1.86	0.41
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.88	0.41
1:C:244:MET:HA	1:C:244:MET:CE	2.51	0.41
1:F:32:VAL:HA	1:F:74:SER:O	2.21	0.41
1:D:192:ILE:HG22	1:G:199:GLU:CG	2.51	0.41
1:I:10:GLY:O	1:I:15:GLY:HA3	2.21	0.41
1:B:115:ALA:HB1	1:B:139:MET:HE3	2.02	0.41
1:C:219:LYS:O	1:C:223:ASN:HA	2.21	0.41
1:E:179:ILE:HD13	1:E:179:ILE:HA	1.91	0.41
1:I:126:LEU:O	1:I:129:VAL:HG22	2.21	0.41
1:F:59:LEU:HD22	1:F:63:ASP:CB	2.51	0.41
1:I:103:GLN:HE21	1:I:103:GLN:HB2	1.67	0.41
1:I:179:ILE:HG21	1:I:179:ILE:HD13	1.73	0.41
1:A:198:ASN:ND2	1:A:259:ALA:H	2.11	0.41
1:A:3:ILE:O	1:A:3:ILE:HG22	2.20	0.41
1:G:126:LEU:O	1:G:129:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:VAL:HG12	1:G:145:VAL:O	2.21	0.41
1:G:260:MET:CE	1:G:263:ARG:HE	2.33	0.41
1:A:28:ASN:ND2	1:A:70:ARG:HG3	2.36	0.40
1:B:167:VAL:O	1:B:171:SER:OG	2.36	0.40
1:B:244:MET:HA	1:B:244:MET:HE2	2.03	0.40
1:D:150:LEU:O	1:D:150:LEU:HD13	2.21	0.40
1:E:191:ARG:HH11	1:E:191:ARG:CG	2.34	0.40
1:C:117:ASN:ND2	2:C:301:NAD:H1D	2.36	0.40
1:F:11:ALA:HA	1:F:31:MET:HE2	2.03	0.40
1:F:283:SER:O	1:F:284:LYS:HB2	2.20	0.40
1:F:117:ASN:ND2	2:F:301:NAD:H1D	2.37	0.40
1:G:164:HIS:CE1	1:G:180:THR:OG1	2.73	0.40
1:D:74:SER:OG	1:D:75:THR:N	2.55	0.40
1:A:150:LEU:O	1:A:150:LEU:HD13	2.21	0.40
1:A:137:ILE:HG21	1:A:167:VAL:HG21	2.03	0.40
1:A:184:SER:O	1:A:185:PRO:C	2.60	0.40
1:A:93:ASN:O	1:A:97:LYS:HB2	2.21	0.40
1:F:12:GLY:O	1:F:13:THR:C	2.59	0.40
1:D:74:SER:CB	1:D:79:ASP:OD2	2.70	0.40
1:E:91:THR:HA	2:E:301:NAD:O3D	2.22	0.40
1:G:194:CYS:C	1:G:244:MET:HE3	2.40	0.40
1:G:59:LEU:HB3	1:G:60:THR:HG23	2.04	0.40
1:I:117:ASN:HD21	2:I:301:NAD:H1D	1.84	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	281/284 (99%)	257 (92%)	22 (8%)	2 (1%)	22 41
1	B	281/284 (99%)	249 (89%)	29 (10%)	3 (1%)	14 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	281/284 (99%)	264 (94%)	15 (5%)	2 (1%)	22	41
1	D	281/284 (99%)	256 (91%)	24 (8%)	1 (0%)	34	55
1	E	281/284 (99%)	259 (92%)	22 (8%)	0	100	100
1	F	281/284 (99%)	272 (97%)	7 (2%)	2 (1%)	22	41
1	G	281/284 (99%)	259 (92%)	21 (8%)	1 (0%)	34	55
1	H	281/284 (99%)	253 (90%)	28 (10%)	0	100	100
1	I	281/284 (99%)	264 (94%)	15 (5%)	2 (1%)	22	41
All	All	2529/2556 (99%)	2333 (92%)	183 (7%)	13 (0%)	29	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	274	LYS
1	C	120	SER
1	F	274	LYS
1	I	274	LYS
1	A	174	LEU
1	B	80	LEU
1	F	120	SER
1	A	144	PRO
1	B	81	LYS
1	B	73	GLY
1	D	144	PRO
1	I	120	SER
1	G	144	PRO

### 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	227/228 (100%)	205 (90%)	22 (10%)	8	15
1	B	227/228 (100%)	208 (92%)	19 (8%)	11	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	227/228 (100%)	220 (97%)	7 (3%)	40	65
1	D	227/228 (100%)	214 (94%)	13 (6%)	20	39
1	E	227/228 (100%)	215 (95%)	12 (5%)	22	43
1	F	227/228 (100%)	218 (96%)	9 (4%)	31	55
1	G	227/228 (100%)	212 (93%)	15 (7%)	16	32
1	H	227/228 (100%)	212 (93%)	15 (7%)	16	32
1	I	227/228 (100%)	220 (97%)	7 (3%)	40	65
All	All	2043/2052 (100%)	1924 (94%)	119 (6%)	20	38

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	25	VAL
1	A	36	ASP
1	A	40	GLN
1	A	45	THR
1	A	60	THR
1	A	70	ARG
1	A	72	LYS
1	A	75	THR
1	A	79	ASP
1	A	111	ASN
1	A	116	SER
1	A	119	SER
1	A	135	ARG
1	A	150	LEU
1	A	171	SER
1	A	173	GLN
1	A	191	ARG
1	A	192	ILE
1	A	223	ASN
1	A	271	LEU
1	A	283	SER
1	B	4	ARG
1	B	5	THR
1	B	16	ASN
1	B	36	ASP
1	B	40	GLN
1	B	45	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	48	SER
1	B	49	SER
1	B	52	ARG
1	B	53	LEU
1	B	111	ASN
1	B	125	LYS
1	B	139	MET
1	B	145	VAL
1	B	153	LEU
1	B	161	ASP
1	B	174	LEU
1	B	191	ARG
1	B	220	LEU
1	C	4	ARG
1	C	66	SER
1	C	76	SER
1	C	179	ILE
1	C	191	ARG
1	C	224	HIS
1	C	271	LEU
1	D	31	MET
1	D	45	THR
1	D	50	LEU
1	D	61	GLU
1	D	70	ARG
1	D	75	THR
1	D	135	ARG
1	D	150	LEU
1	D	171	SER
1	D	191	ARG
1	D	192	ILE
1	D	223	ASN
1	D	271	LEU
1	E	16	ASN
1	E	40	GLN
1	E	56	LYS
1	E	110	GLU
1	E	119	SER
1	E	125	LYS
1	E	145	VAL
1	E	153	LEU
1	E	191	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	220	LEU
1	E	224	HIS
1	E	226	ILE
1	F	60	THR
1	F	66	SER
1	F	96	LEU
1	F	125	LYS
1	F	179	ILE
1	F	191	ARG
1	F	224	HIS
1	F	271	LEU
1	F	274	LYS
1	G	16	ASN
1	G	31	MET
1	G	36	ASP
1	G	45	THR
1	G	49	SER
1	G	60	THR
1	G	70	ARG
1	G	111	ASN
1	G	150	LEU
1	G	162	THR
1	G	177	TYR
1	G	191	ARG
1	G	192	ILE
1	G	223	ASN
1	G	271	LEU
1	H	16	ASN
1	H	41	LYS
1	H	49	SER
1	H	55	LYS
1	H	58	LYS
1	H	110	GLU
1	H	139	MET
1	H	145	VAL
1	H	153	LEU
1	H	161	ASP
1	H	163	THR
1	H	174	LEU
1	H	191	ARG
1	H	220	LEU
1	H	226	ILE

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Mol	Chain	Res	Type
1	I	4	ARG
1	I	48	SER
1	I	191	ARG
1	I	224	HIS
1	I	239	THR
1	I	271	LEU
1	I	284	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	117	ASN
1	A	140	HIS
1	A	164	HIS
1	A	190	ASN
1	A	198	ASN
1	B	16	ASN
1	B	164	HIS
1	B	173	GLN
1	B	190	ASN
1	C	40	GLN
1	C	103	GLN
1	C	117	ASN
1	C	164	HIS
1	D	16	ASN
1	D	28	ASN
1	D	140	HIS
1	D	164	HIS
1	D	190	ASN
1	D	198	ASN
1	D	223	ASN
1	E	16	ASN
1	E	164	HIS
1	E	190	ASN
1	F	40	GLN
1	F	103	GLN
1	F	164	HIS
1	G	28	ASN
1	G	140	HIS
1	G	164	HIS
1	G	190	ASN

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Mol	Chain	Res	Type
1	G	198	ASN
1	G	223	ASN
1	H	16	ASN
1	H	111	ASN
1	H	164	HIS
1	H	173	GLN
1	H	190	ASN
1	H	223	ASN
1	I	40	GLN
1	I	103	GLN
1	I	117	ASN
1	I	164	HIS

### 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](#)

9 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	I	301	-	42,48,48	1.17	5 (11%)	50,73,73	1.62	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAD	F	301	-	42,48,48	1.13	4 (9%)	50,73,73	1.53	8 (16%)
2	NAD	B	301	-	42,48,48	1.09	5 (11%)	50,73,73	1.46	7 (14%)
2	NAD	H	301	-	42,48,48	1.07	5 (11%)	50,73,73	1.37	8 (16%)
2	NAD	D	301	-	42,48,48	0.97	5 (11%)	50,73,73	1.37	7 (14%)
2	NAD	E	301	-	42,48,48	1.10	4 (9%)	50,73,73	1.35	5 (10%)
2	NAD	G	301	-	42,48,48	0.95	3 (7%)	50,73,73	1.36	6 (12%)
2	NAD	A	301	-	42,48,48	1.10	4 (9%)	50,73,73	1.33	6 (12%)
2	NAD	C	301	-	42,48,48	1.22	4 (9%)	50,73,73	1.57	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
2	NAD	I	301	-	-	7/26/62/62	0/5/5/5
2	NAD	F	301	-	-	9/26/62/62	0/5/5/5
2	NAD	B	301	-	-	11/26/62/62	0/5/5/5
2	NAD	H	301	-	-	10/26/62/62	0/5/5/5
2	NAD	D	301	-	-	9/26/62/62	0/5/5/5
2	NAD	E	301	-	-	4/26/62/62	0/5/5/5
2	NAD	G	301	-	-	8/26/62/62	0/5/5/5
2	NAD	A	301	-	-	11/26/62/62	0/5/5/5
2	NAD	C	301	-	-	12/26/62/62	0/5/5/5

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	NAD	O4D-C1D	3.46	1.45	1.41
2	I	301	NAD	O4D-C1D	3.16	1.45	1.41
2	F	301	NAD	O4D-C1D	3.14	1.45	1.41
2	E	301	NAD	O4D-C1D	3.05	1.45	1.41
2	C	301	NAD	C5A-C4A	3.05	1.49	1.40
2	B	301	NAD	O4D-C1D	3.01	1.45	1.41
2	F	301	NAD	C5A-C4A	2.98	1.48	1.40
2	I	301	NAD	C5A-C4A	2.97	1.48	1.40
2	C	301	NAD	C2A-N3A	2.93	1.36	1.32
2	H	301	NAD	O4D-C1D	2.83	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NAD	C2A-N3A	2.79	1.36	1.32
2	F	301	NAD	C2A-N3A	2.78	1.36	1.32
2	B	301	NAD	C5A-C4A	2.78	1.48	1.40
2	E	301	NAD	C2A-N3A	2.76	1.36	1.32
2	I	301	NAD	O4B-C1B	2.75	1.44	1.41
2	E	301	NAD	C5A-C4A	2.73	1.48	1.40
2	D	301	NAD	O4D-C1D	2.71	1.44	1.41
2	A	301	NAD	C2A-N3A	2.68	1.36	1.32
2	C	301	NAD	O4B-C1B	2.67	1.44	1.41
2	H	301	NAD	C5A-C4A	2.66	1.48	1.40
2	A	301	NAD	O4D-C1D	2.59	1.44	1.41
2	A	301	NAD	O4B-C1B	2.57	1.44	1.41
2	A	301	NAD	C5A-C4A	2.56	1.47	1.40
2	G	301	NAD	O4D-C1D	2.53	1.44	1.41
2	G	301	NAD	O4B-C1B	2.49	1.44	1.41
2	H	301	NAD	O4B-C1B	2.47	1.44	1.41
2	I	301	NAD	C2A-N3A	2.47	1.36	1.32
2	I	301	NAD	C2D-C1D	-2.43	1.50	1.53
2	G	301	NAD	C5A-C4A	2.41	1.47	1.40
2	H	301	NAD	C2A-N3A	2.40	1.36	1.32
2	E	301	NAD	O4B-C1B	2.34	1.44	1.41
2	D	301	NAD	C5A-C4A	2.32	1.47	1.40
2	B	301	NAD	O4B-C1B	2.21	1.44	1.41
2	D	301	NAD	O4B-C1B	2.19	1.44	1.41
2	D	301	NAD	C2A-N3A	2.10	1.35	1.32
2	F	301	NAD	C2D-C1D	-2.07	1.50	1.53
2	B	301	NAD	C6A-C5A	2.06	1.50	1.43
2	D	301	NAD	C6A-C5A	2.03	1.50	1.43
2	H	301	NAD	C2D-C1D	-2.02	1.50	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	301	NAD	C6N-N1N-C2N	-4.54	117.83	121.97
2	G	301	NAD	N3A-C2A-N1A	-4.41	121.78	128.68
2	B	301	NAD	C4A-C5A-N7A	-4.22	105.00	109.40
2	I	301	NAD	N3A-C2A-N1A	-4.22	122.09	128.68
2	C	301	NAD	N3A-C2A-N1A	-4.12	122.24	128.68
2	B	301	NAD	C3N-C7N-N7N	4.10	122.67	117.75
2	D	301	NAD	N3A-C2A-N1A	-4.08	122.30	128.68
2	C	301	NAD	C6N-N1N-C2N	-3.97	118.35	121.97
2	E	301	NAD	C4A-C5A-N7A	-3.94	105.30	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAD	N3A-C2A-N1A	-3.93	122.53	128.68
2	H	301	NAD	C4A-C5A-N7A	-3.92	105.31	109.40
2	I	301	NAD	O4D-C1D-C2D	-3.84	101.32	106.93
2	A	301	NAD	N3A-C2A-N1A	-3.73	122.85	128.68
2	F	301	NAD	C6N-N1N-C2N	-3.66	118.63	121.97
2	C	301	NAD	O4D-C1D-C2D	-3.56	101.72	106.93
2	D	301	NAD	C4A-C5A-N7A	-3.51	105.74	109.40
2	D	301	NAD	C6N-N1N-C2N	-3.40	118.87	121.97
2	H	301	NAD	N3A-C2A-N1A	-3.36	123.43	128.68
2	E	301	NAD	C6N-N1N-C2N	-3.36	118.92	121.97
2	F	301	NAD	O4D-C1D-C2D	-3.25	102.17	106.93
2	G	301	NAD	C1B-N9A-C4A	-3.12	121.16	126.64
2	I	301	NAD	C4A-C5A-N7A	-3.11	106.16	109.40
2	E	301	NAD	N3A-C2A-N1A	-3.10	123.84	128.68
2	A	301	NAD	C4A-C5A-N7A	-3.07	106.20	109.40
2	A	301	NAD	C6N-N1N-C2N	-3.06	119.18	121.97
2	B	301	NAD	N3A-C2A-N1A	-3.04	123.93	128.68
2	G	301	NAD	C4A-C5A-N7A	-2.94	106.33	109.40
2	H	301	NAD	C3N-C7N-N7N	2.86	121.18	117.75
2	C	301	NAD	C3D-C2D-C1D	2.80	105.19	100.98
2	B	301	NAD	C6N-N1N-C2N	-2.73	119.48	121.97
2	G	301	NAD	C3D-C2D-C1D	2.65	104.97	100.98
2	A	301	NAD	C3D-C2D-C1D	2.65	104.96	100.98
2	G	301	NAD	C6N-N1N-C2N	-2.60	119.61	121.97
2	E	301	NAD	C3N-C7N-N7N	2.59	120.86	117.75
2	C	301	NAD	C3N-C7N-N7N	2.57	120.83	117.75
2	C	301	NAD	C4A-C5A-N7A	-2.55	106.74	109.40
2	F	301	NAD	PN-O3-PA	-2.55	124.07	132.83
2	I	301	NAD	C2A-N1A-C6A	2.54	123.10	118.75
2	H	301	NAD	C6N-N1N-C2N	-2.54	119.66	121.97
2	B	301	NAD	O7N-C7N-C3N	-2.52	116.62	119.63
2	F	301	NAD	O4B-C4B-C3B	2.39	109.85	105.11
2	D	301	NAD	C1B-N9A-C4A	-2.39	122.44	126.64
2	F	301	NAD	C2A-N1A-C6A	2.39	122.84	118.75
2	B	301	NAD	C3D-C2D-C1D	2.38	104.57	100.98
2	C	301	NAD	O7N-C7N-N7N	-2.37	119.21	122.58
2	D	301	NAD	C3D-C2D-C1D	2.35	104.51	100.98
2	B	301	NAD	C3B-C2B-C1B	2.26	104.38	100.98
2	H	301	NAD	C3D-C2D-C1D	2.25	104.36	100.98
2	D	301	NAD	C5N-C4N-C3N	-2.20	117.74	120.34
2	A	301	NAD	C1B-N9A-C4A	-2.18	122.81	126.64
2	A	301	NAD	O4D-C1D-C2D	-2.17	103.75	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NAD	C2D-C3D-C4D	-2.17	98.43	102.64
2	H	301	NAD	PN-O3-PA	-2.16	125.41	132.83
2	E	301	NAD	PN-O3-PA	-2.15	125.43	132.83
2	F	301	NAD	C4A-C5A-N7A	-2.10	107.21	109.40
2	H	301	NAD	C1B-N9A-C4A	-2.05	123.04	126.64
2	H	301	NAD	O4B-C1B-C2B	-2.05	103.94	106.93
2	D	301	NAD	O4D-C4D-C3D	-2.02	101.12	105.11
2	G	301	NAD	C2A-N1A-C6A	2.01	122.20	118.75

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	301	NAD	O4D-C1D-N1N-C2N
2	F	301	NAD	O4D-C1D-N1N-C2N
2	F	301	NAD	C2N-C3N-C7N-O7N
2	F	301	NAD	C2N-C3N-C7N-N7N
2	B	301	NAD	C5B-O5B-PA-O1A
2	B	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	O4D-C1D-N1N-C2N
2	B	301	NAD	O4D-C1D-N1N-C6N
2	H	301	NAD	C5B-O5B-PA-O1A
2	H	301	NAD	C5D-O5D-PN-O2N
2	H	301	NAD	O4D-C1D-N1N-C2N
2	E	301	NAD	O4D-C1D-N1N-C2N
2	G	301	NAD	C5B-O5B-PA-O1A
2	G	301	NAD	O4D-C1D-N1N-C2N
2	A	301	NAD	C5B-O5B-PA-O1A
2	A	301	NAD	C5B-O5B-PA-O3
2	A	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	O4B-C4B-C5B-O5B
2	C	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	O4D-C1D-N1N-C2N
2	C	301	NAD	O4D-C1D-N1N-C6N
2	C	301	NAD	C2D-C1D-N1N-C2N
2	C	301	NAD	C2D-C1D-N1N-C6N
2	F	301	NAD	C4N-C3N-C7N-O7N
2	F	301	NAD	C4N-C3N-C7N-N7N
2	I	301	NAD	C2N-C3N-C7N-O7N
2	I	301	NAD	C2N-C3N-C7N-N7N
2	D	301	NAD	C2N-C3N-C7N-O7N
2	D	301	NAD	C2N-C3N-C7N-N7N

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Mol	Chain	Res	Type	Atoms
2	I	301	NAD	C4N-C3N-C7N-O7N
2	I	301	NAD	C4N-C3N-C7N-N7N
2	D	301	NAD	C4N-C3N-C7N-O7N
2	F	301	NAD	O4B-C4B-C5B-O5B
2	F	301	NAD	C3B-C4B-C5B-O5B
2	B	301	NAD	O4B-C4B-C5B-O5B
2	B	301	NAD	C3B-C4B-C5B-O5B
2	H	301	NAD	O4B-C4B-C5B-O5B
2	H	301	NAD	C3B-C4B-C5B-O5B
2	D	301	NAD	O4B-C4B-C5B-O5B
2	E	301	NAD	O4B-C4B-C5B-O5B
2	E	301	NAD	C3B-C4B-C5B-O5B
2	D	301	NAD	C4N-C3N-C7N-N7N
2	I	301	NAD	O4B-C4B-C5B-O5B
2	D	301	NAD	C3B-C4B-C5B-O5B
2	C	301	NAD	C3B-C4B-C5B-O5B
2	A	301	NAD	C4N-C3N-C7N-O7N
2	A	301	NAD	C4N-C3N-C7N-N7N
2	A	301	NAD	C2N-C3N-C7N-O7N
2	A	301	NAD	C2N-C3N-C7N-N7N
2	G	301	NAD	C2N-C3N-C7N-O7N
2	G	301	NAD	C4N-C3N-C7N-O7N
2	G	301	NAD	C4N-C3N-C7N-N7N
2	F	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5B-O5B-PA-O3
2	B	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	C5B-O5B-PA-O3
2	H	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O3
2	G	301	NAD	C5B-O5B-PA-O3
2	A	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	O4D-C4D-C5D-O5D
2	C	301	NAD	C3D-C4D-C5D-O5D
2	B	301	NAD	C5B-O5B-PA-O2A
2	B	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	C5D-O5D-PN-O1N
2	G	301	NAD	C2N-C3N-C7N-N7N
2	H	301	NAD	PA-O3-PN-O2N
2	I	301	NAD	C3B-C4B-C5B-O5B
2	D	301	NAD	O4D-C4D-C5D-O5D

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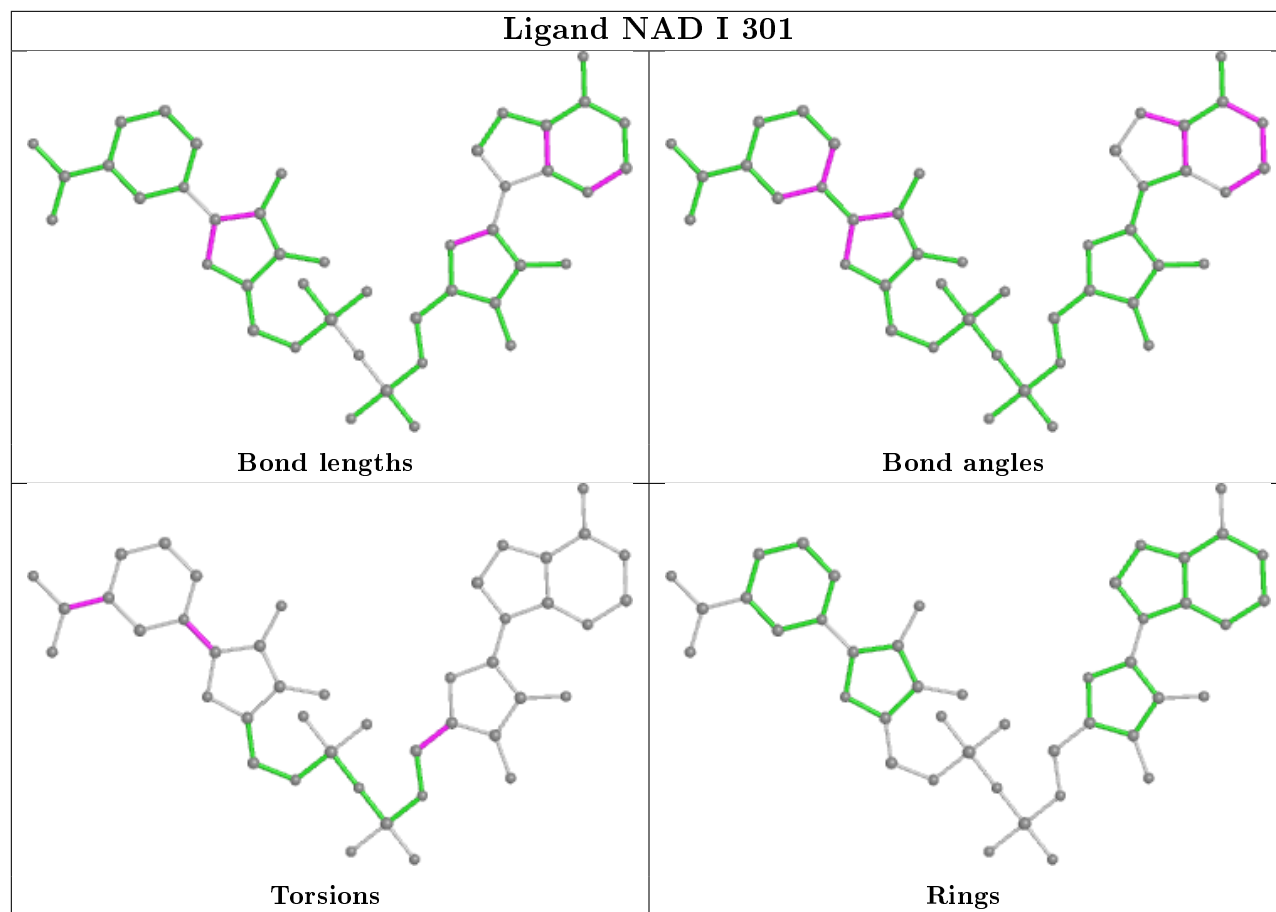
Mol	Chain	Res	Type	Atoms
2	G	301	NAD	O4B-C4B-C5B-O5B
2	B	301	NAD	PA-O3-PN-O1N
2	E	301	NAD	PA-O3-PN-O1N
2	A	301	NAD	PN-O3-PA-O2A
2	C	301	NAD	PA-O3-PN-O1N
2	F	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5B-O5B-PA-O2A
2	D	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	O4B-C4B-C5B-O5B

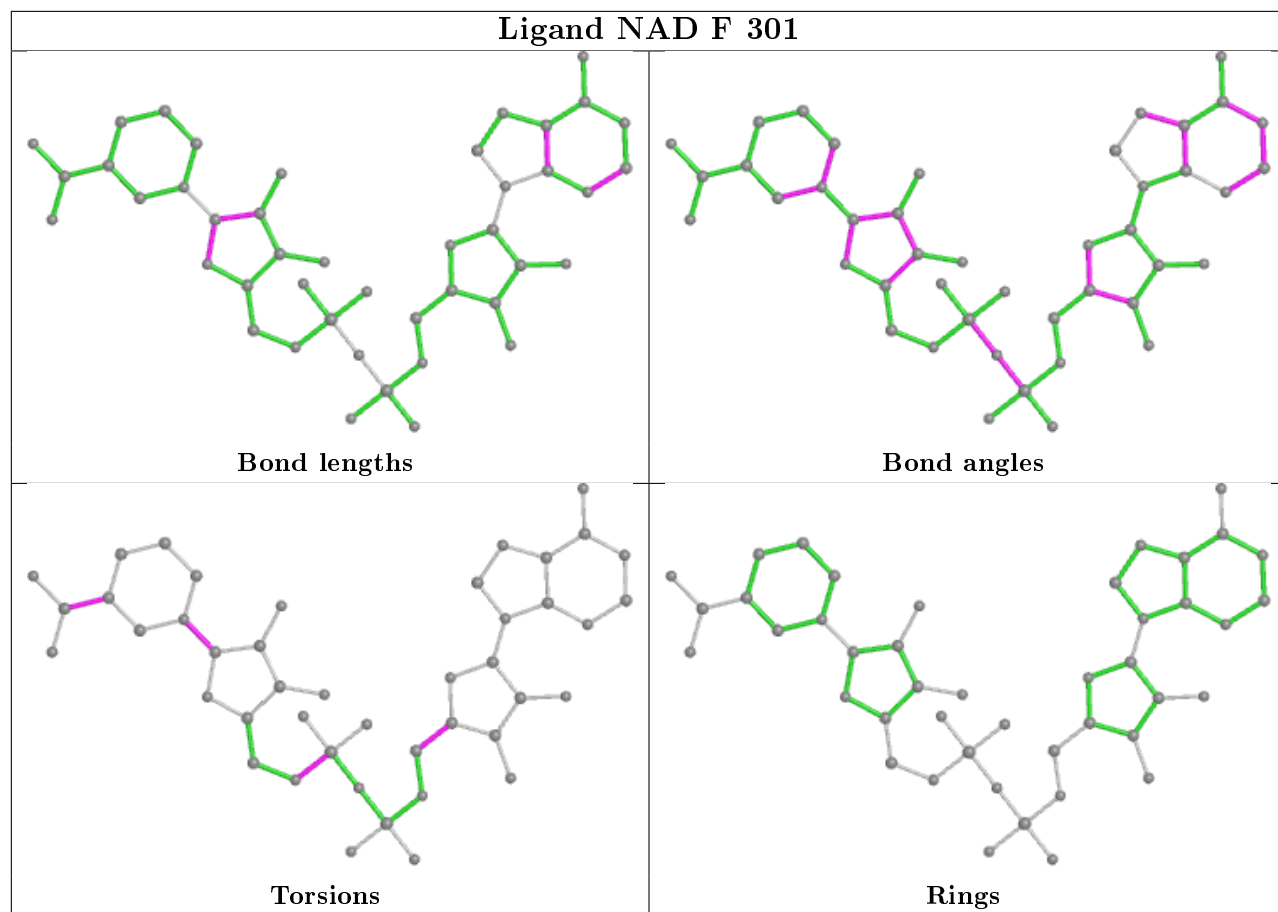
There are no ring outliers.

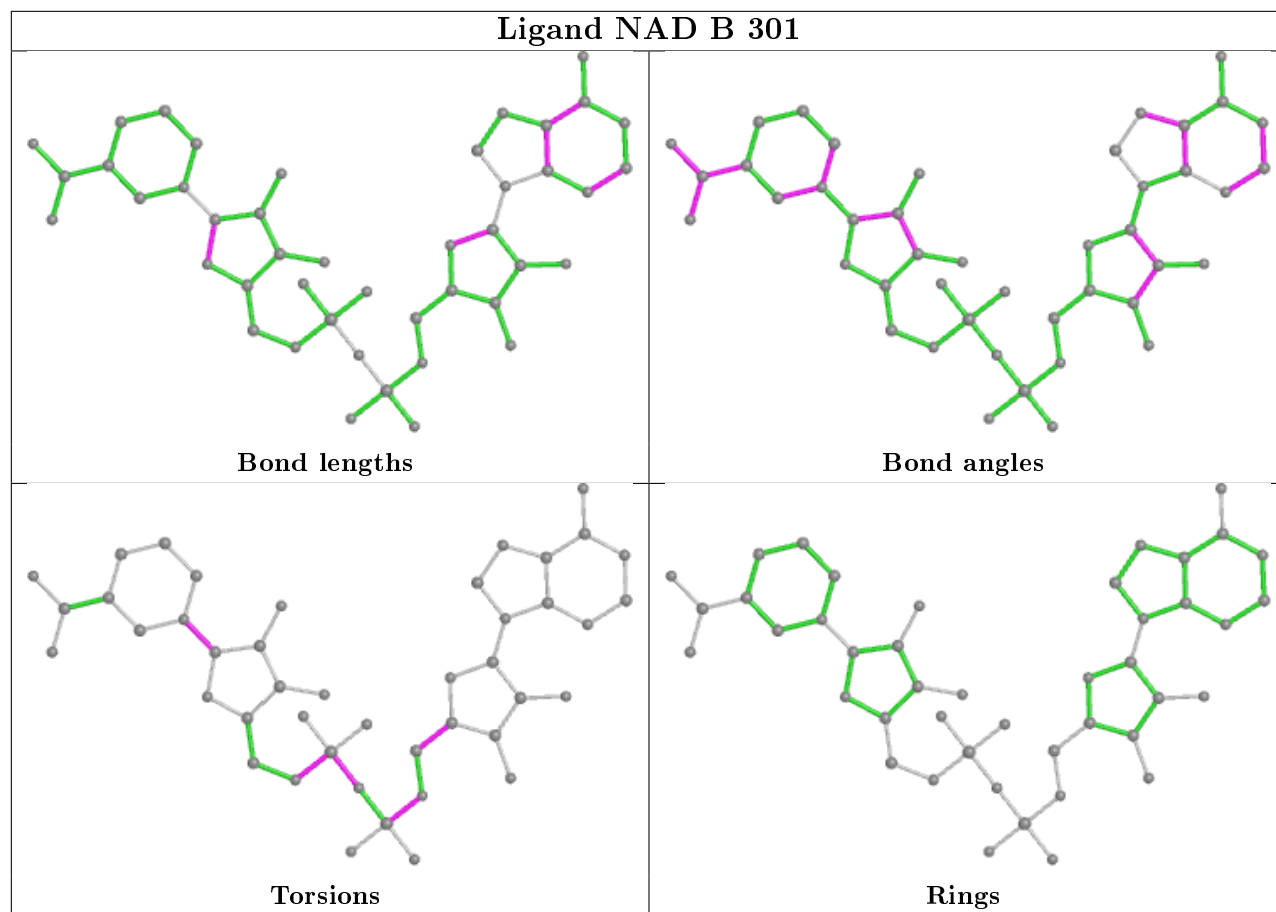
8 monomers are involved in 36 short contacts:

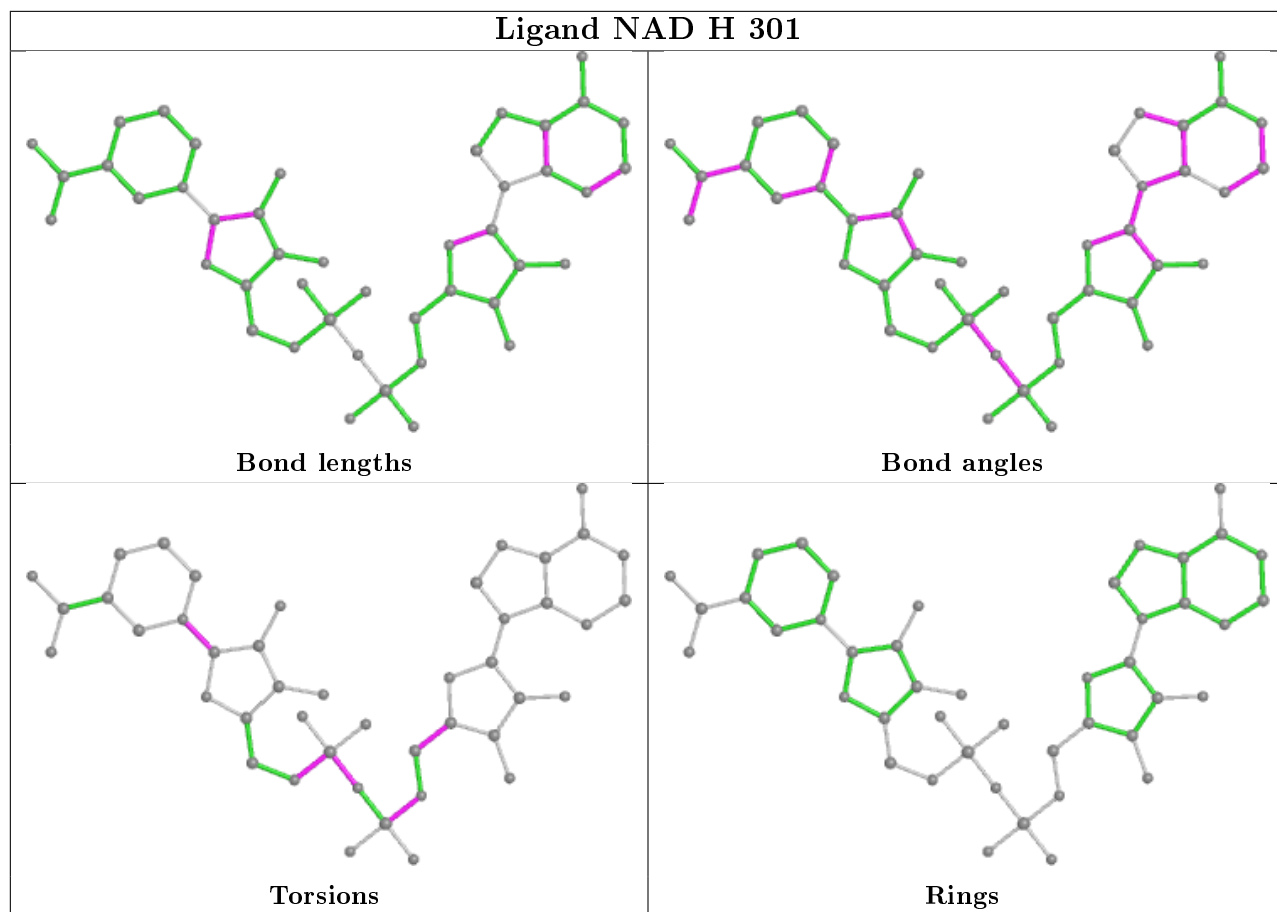
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	301	NAD	7	0
2	F	301	NAD	4	0
2	H	301	NAD	5	0
2	D	301	NAD	6	0
2	E	301	NAD	2	0
2	G	301	NAD	5	0
2	A	301	NAD	3	0
2	C	301	NAD	4	0

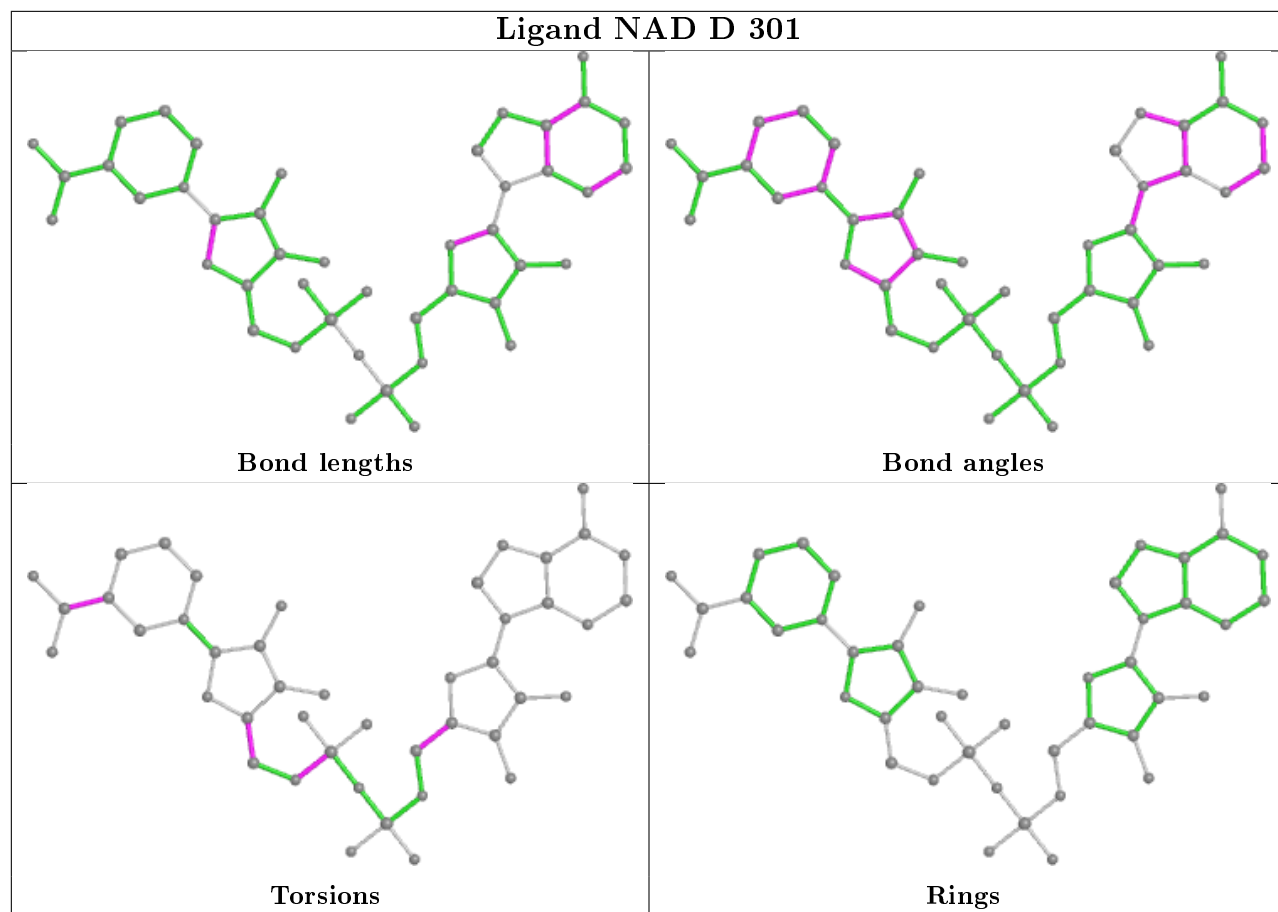
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



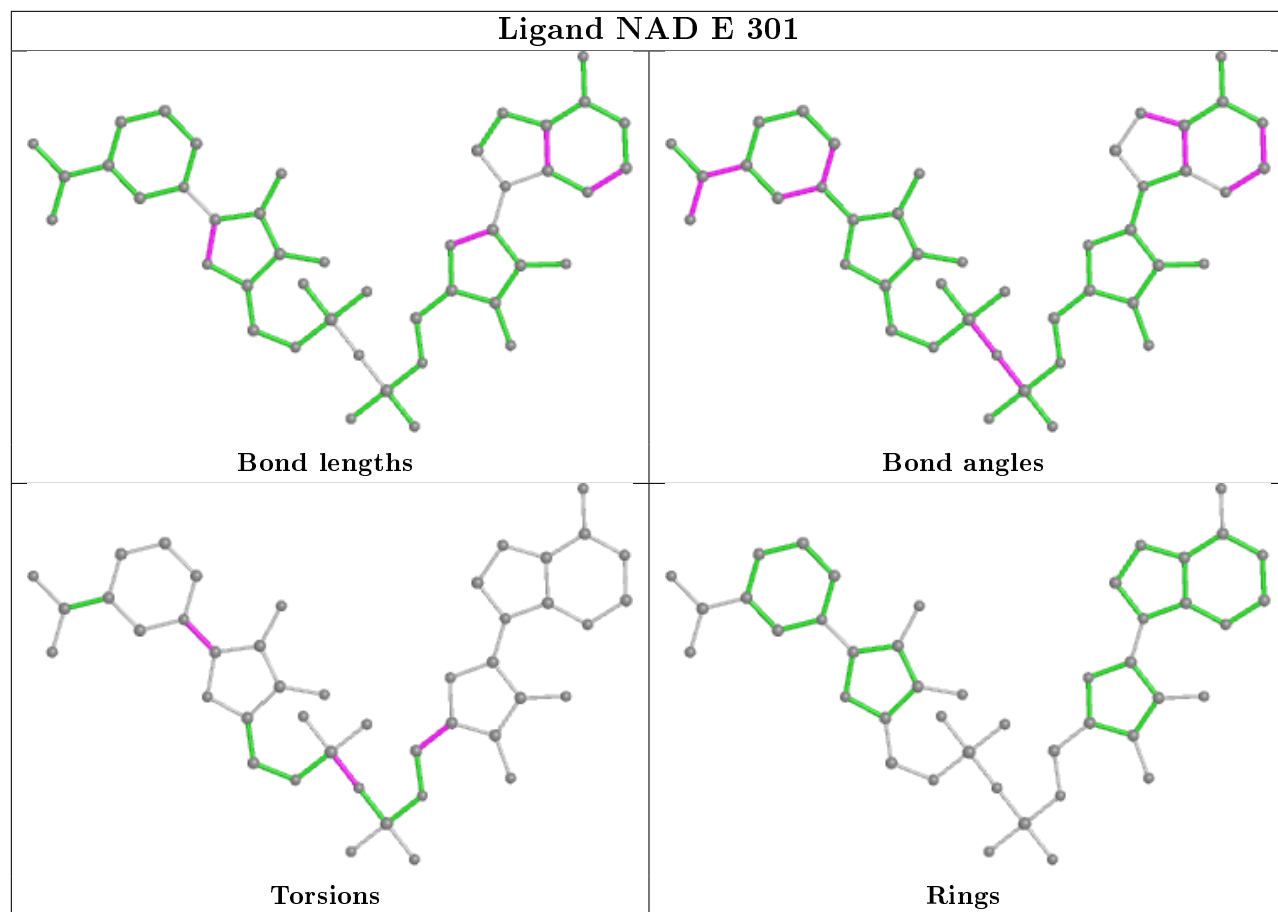


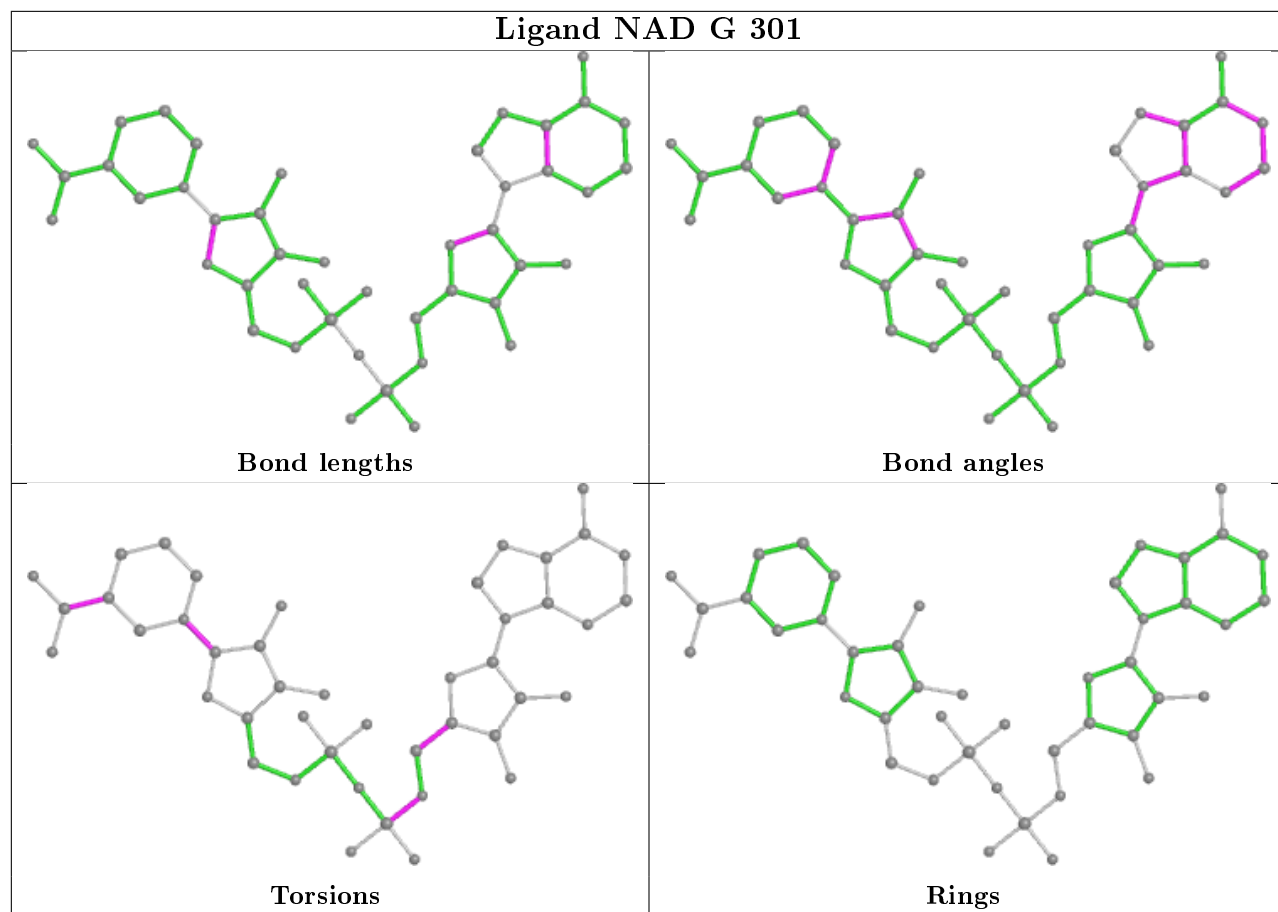


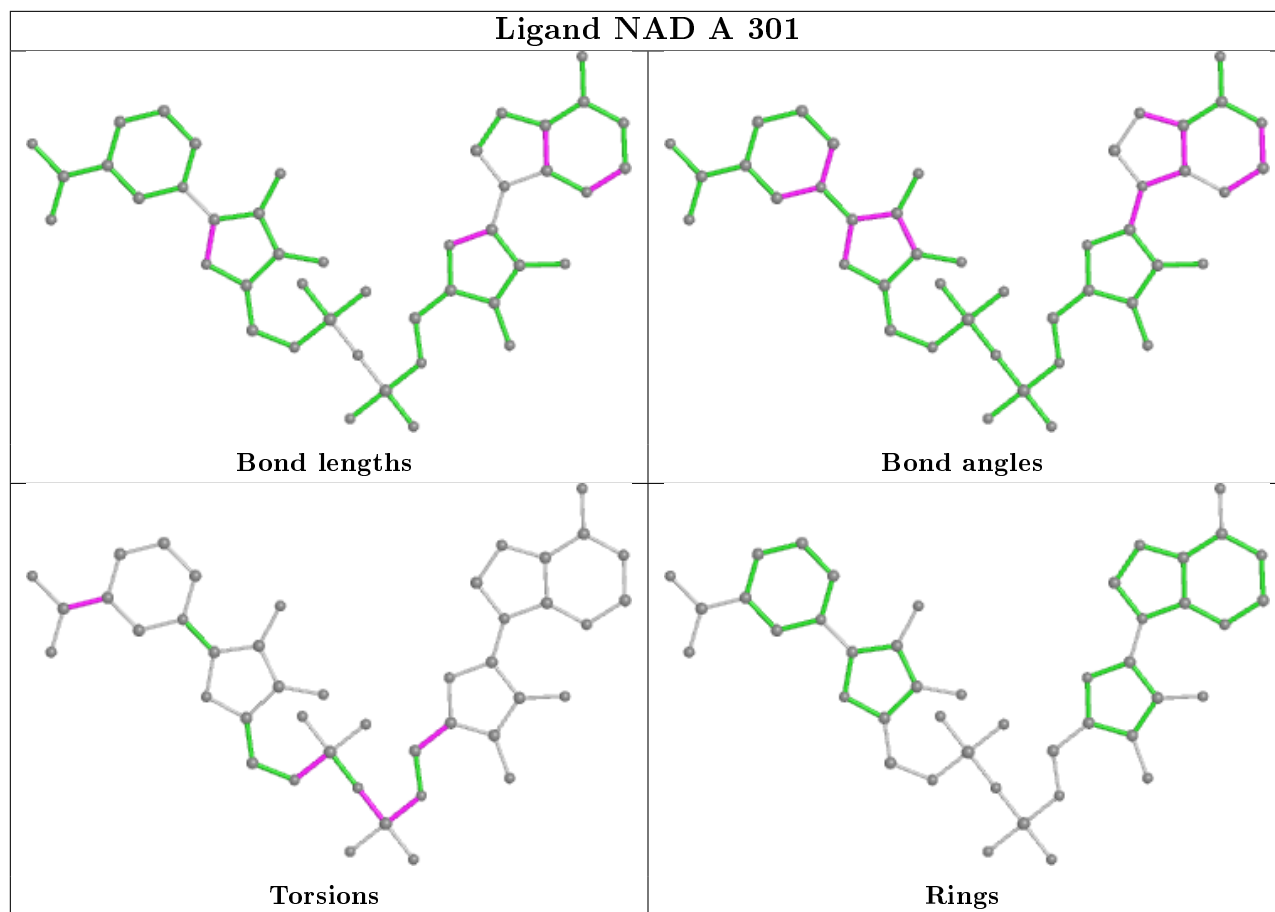


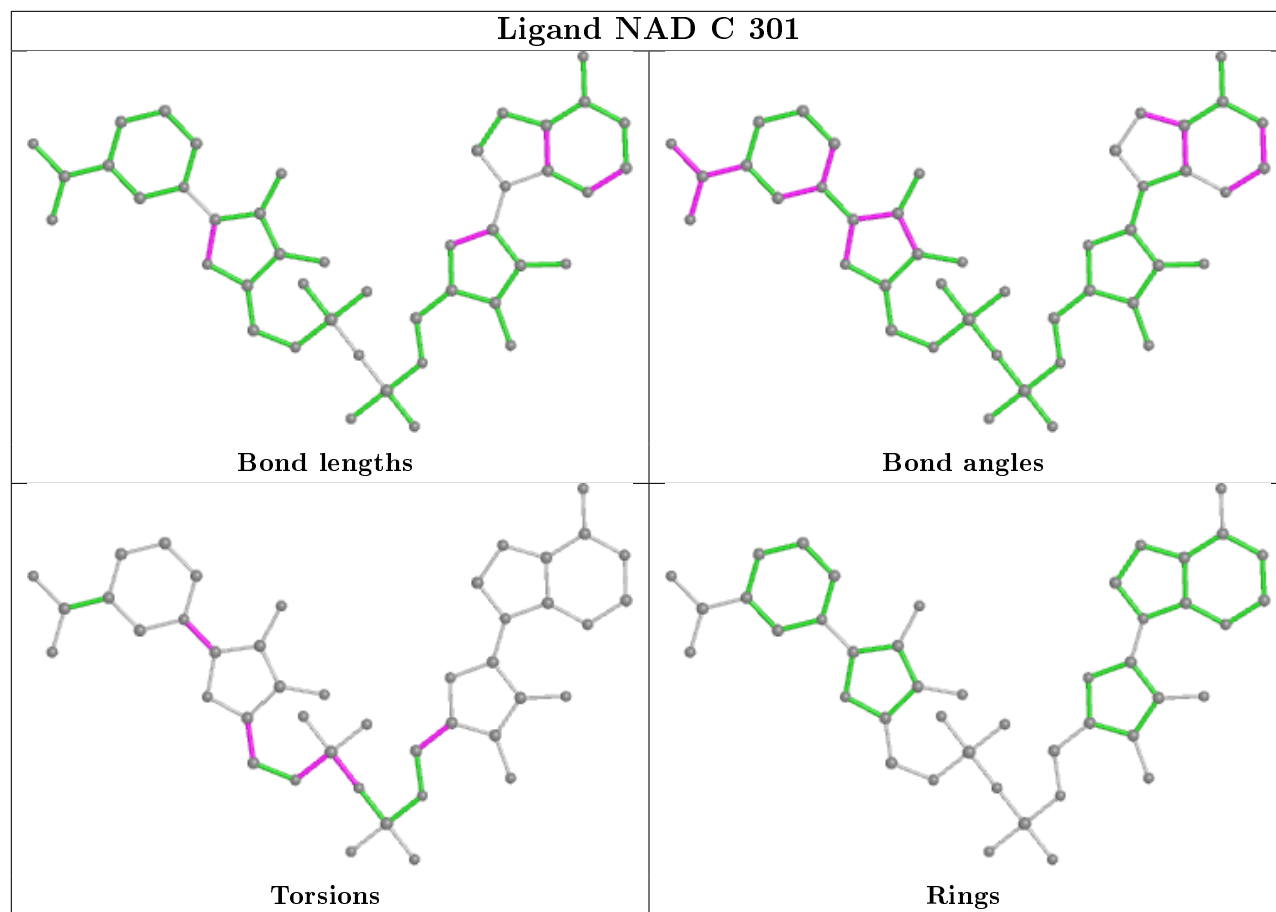












## 5.7 Other polymers [i](#)

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	283/284 (99%)	1.48	77 (27%) 0 0	43, 68, 108, 129	0
1	B	283/284 (99%)	1.61	75 (26%) 0 0	40, 74, 109, 127	0
1	C	283/284 (99%)	0.91	37 (13%) 3 2	42, 56, 73, 112	0
1	D	283/284 (99%)	1.69	94 (33%) 0 0	43, 66, 110, 129	0
1	E	283/284 (99%)	1.77	85 (30%) 0 0	41, 75, 112, 130	0
1	F	283/284 (99%)	1.03	40 (14%) 2 1	42, 55, 73, 122	0
1	G	283/284 (99%)	1.90	100 (35%) 0 0	43, 67, 109, 139	0
1	H	283/284 (99%)	1.75	89 (31%) 0 0	41, 75, 112, 131	0
1	I	283/284 (99%)	1.08	46 (16%) 1 1	42, 55, 72, 102	0
All	All	2547/2556 (99%)	1.47	643 (25%) 0 0	40, 62, 107, 139	0

All (643) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	69	ALA	18.0
1	B	2	SER	16.5
1	E	39	VAL	14.2
1	H	9	VAL	11.6
1	B	283	SER	11.5
1	H	15	GLY	11.3
1	D	59	LEU	11.0
1	H	30	VAL	10.9
1	E	72	LYS	10.8
1	G	82	ALA	10.5
1	H	78	ASP	10.0
1	H	34	ILE	10.0
1	E	32	VAL	9.6
1	G	11	ALA	9.0
1	B	13	THR	9.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	5	THR	9.0
1	E	85	ILE	8.8
1	G	27	LEU	8.8
1	B	3	ILE	8.6
1	G	73	GLY	8.5
1	G	54	ILE	8.5
1	I	281	VAL	8.4
1	G	40	GLN	8.4
1	E	82	ALA	8.2
1	D	192	ILE	8.2
1	H	76	SER	8.0
1	G	119	SER	7.8
1	A	174	LEU	7.8
1	E	6	VAL	7.8
1	B	14	MET	7.7
1	B	36	ASP	7.6
1	E	113	ILE	7.5
1	H	56	LYS	7.5
1	E	79	ASP	7.5
1	G	57	GLU	7.4
1	E	66	SER	7.4
1	A	176	LYS	7.4
1	D	70	ARG	7.4
1	G	284	LYS	7.4
1	H	86	VAL	7.3
1	G	47	ALA	7.2
1	E	160	SER	7.2
1	B	27	LEU	7.1
1	D	18	ILE	6.9
1	G	113	ILE	6.9
1	D	7	GLY	6.8
1	E	10	GLY	6.8
1	G	62	ALA	6.6
1	I	2	SER	6.6
1	D	284	LYS	6.6
1	G	24	VAL	6.4
1	I	123	ILE	6.4
1	D	149	ALA	6.4
1	D	137	ILE	6.4
1	B	281	VAL	6.2
1	E	207	GLY	6.2
1	B	31	MET	6.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	91	THR	6.1
1	E	107	ILE	6.1
1	D	14	MET	6.1
1	E	101	LEU	6.1
1	H	133	ALA	6.0
1	A	80	LEU	6.0
1	B	38	ALA	5.9
1	B	77	TYR	5.9
1	H	146	PRO	5.9
1	E	70	ARG	5.9
1	E	177	TYR	5.9
1	H	58	LYS	5.8
1	E	40	GLN	5.7
1	D	4	ARG	5.6
1	G	65	ALA	5.5
1	E	30	VAL	5.4
1	A	27	LEU	5.4
1	H	170	LEU	5.4
1	E	11	ALA	5.4
1	E	37	ALA	5.4
1	G	50	LEU	5.3
1	G	107	ILE	5.3
1	A	53	LEU	5.3
1	E	56	LYS	5.2
1	D	71	ILE	5.1
1	H	32	VAL	5.1
1	C	283	SER	5.0
1	D	231	LEU	5.0
1	E	43	VAL	5.0
1	G	61	GLU	5.0
1	F	226	ILE	5.0
1	B	106	GLY	5.0
1	A	86	VAL	4.9
1	B	110	GLU	4.9
1	D	58	LYS	4.9
1	D	25	VAL	4.9
1	I	9	VAL	4.9
1	E	38	ALA	4.9
1	G	16	ASN	4.9
1	H	41	LYS	4.8
1	I	269	GLY	4.8
1	B	147	VAL	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	172	LYS	4.8
1	H	35	SER	4.8
1	A	73	GLY	4.8
1	H	221	GLY	4.8
1	H	143	ASN	4.7
1	G	201	PHE	4.7
1	B	44	ALA	4.7
1	B	101	LEU	4.7
1	A	95	ASP	4.7
1	I	265	MET	4.7
1	G	76	SER	4.7
1	A	71	ILE	4.7
1	B	45	THR	4.6
1	A	279	VAL	4.6
1	D	85	ILE	4.6
1	I	131	SER	4.6
1	I	217	GLY	4.6
1	G	23	ALA	4.6
1	E	22	CYS	4.5
1	E	46	VAL	4.5
1	A	38	ALA	4.5
1	G	281	VAL	4.5
1	A	52	ARG	4.4
1	A	84	ASP	4.4
1	B	284	LYS	4.4
1	E	80	LEU	4.4
1	D	60	THR	4.4
1	E	59	LEU	4.4
1	A	34	ILE	4.4
1	B	67	ALA	4.4
1	A	68	LEU	4.4
1	E	35	SER	4.4
1	E	7	GLY	4.4
1	B	11	ALA	4.3
1	I	10	GLY	4.3
1	A	77	TYR	4.3
1	H	57	GLU	4.3
1	E	4	ARG	4.3
1	G	150	LEU	4.3
1	H	27	LEU	4.3
1	G	103	GLN	4.3
1	G	72	LYS	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	271	LEU	4.2
1	B	182	LYS	4.2
1	G	20	GLN	4.2
1	G	26	GLY	4.2
1	G	147	VAL	4.2
1	H	112	VAL	4.2
1	G	89	ALA	4.2
1	B	62	ALA	4.2
1	C	27	LEU	4.2
1	E	67	ALA	4.2
1	H	284	LYS	4.2
1	B	43	VAL	4.2
1	H	99	LYS	4.2
1	G	115	ALA	4.2
1	B	60	THR	4.2
1	D	162	THR	4.1
1	G	36	ASP	4.1
1	H	177	TYR	4.1
1	G	29	VAL	4.1
1	D	8	ILE	4.1
1	H	106	GLY	4.1
1	B	121	ILE	4.1
1	D	50	LEU	4.1
1	C	167	VAL	4.1
1	F	2	SER	4.1
1	E	47	ALA	4.1
1	H	48	SER	4.1
1	H	59	LEU	4.1
1	C	143	ASN	4.1
1	G	121	ILE	4.1
1	B	114	ILE	4.0
1	H	179	ILE	4.0
1	D	52	ARG	4.0
1	A	83	THR	4.0
1	B	26	GLY	4.0
1	H	88	GLU	4.0
1	D	28	ASN	4.0
1	H	135	ARG	4.0
1	H	84	ASP	4.0
1	D	3	ILE	4.0
1	E	145	VAL	3.9
1	G	87	ILE	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	50	LEU	3.9
1	B	214	ILE	3.9
1	H	90	ALA	3.9
1	G	146	PRO	3.9
1	H	145	VAL	3.9
1	E	132	ARG	3.9
1	H	141	PHE	3.9
1	E	62	ALA	3.8
1	E	176	LYS	3.8
1	B	139	MET	3.8
1	G	104	ILE	3.8
1	G	55	LYS	3.8
1	D	188	VAL	3.8
1	F	80	LEU	3.8
1	F	258	PRO	3.8
1	E	94	TYR	3.8
1	G	216	GLU	3.8
1	A	275	THR	3.8
1	C	244	MET	3.8
1	H	61	GLU	3.8
1	H	62	ALA	3.8
1	D	67	ALA	3.8
1	H	33	ASP	3.7
1	B	91	THR	3.7
1	B	209	ALA	3.7
1	D	193	LEU	3.7
1	G	96	LEU	3.7
1	C	218	MET	3.7
1	B	25	VAL	3.7
1	I	73	GLY	3.7
1	B	126	LEU	3.7
1	A	24	VAL	3.7
1	G	37	ALA	3.6
1	E	167	VAL	3.6
1	G	39	VAL	3.6
1	D	118	THR	3.6
1	A	232	ALA	3.6
1	H	19	ALA	3.6
1	D	24	VAL	3.6
1	A	81	LYS	3.6
1	A	35	SER	3.6
1	B	95	ASP	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	94	TYR	3.6
1	E	51	ASP	3.5
1	G	44	ALA	3.5
1	F	153	LEU	3.5
1	H	101	LEU	3.5
1	G	141	PHE	3.5
1	D	2	SER	3.5
1	G	170	LEU	3.5
1	G	194	CYS	3.5
1	B	39	VAL	3.5
1	A	237	LEU	3.5
1	G	240	MET	3.5
1	H	73	GLY	3.5
1	D	72	LYS	3.5
1	F	81	LYS	3.5
1	G	85	ILE	3.5
1	H	77	TYR	3.5
1	H	139	MET	3.5
1	H	29	VAL	3.5
1	G	203	VAL	3.5
1	B	34	ILE	3.5
1	E	271	LEU	3.5
1	H	40	GLN	3.5
1	G	52	ARG	3.5
1	I	208	LEU	3.5
1	C	252	ALA	3.4
1	C	87	ILE	3.4
1	C	205	GLY	3.4
1	C	52	ARG	3.4
1	G	167	VAL	3.4
1	C	139	MET	3.4
1	E	130	THR	3.4
1	B	41	LYS	3.4
1	B	52	ARG	3.4
1	I	51	ASP	3.4
1	G	100	ILE	3.4
1	D	6	VAL	3.3
1	A	51	ASP	3.3
1	E	3	ILE	3.3
1	D	42	GLY	3.3
1	D	80	LEU	3.3
1	G	164	HIS	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	77	TYR	3.3
1	E	81	LYS	3.3
1	F	71	ILE	3.3
1	H	114	ILE	3.3
1	G	276	GLY	3.3
1	H	220	LEU	3.3
1	A	177	TYR	3.3
1	D	69	ALA	3.3
1	F	30	VAL	3.2
1	D	87	ILE	3.2
1	A	31	MET	3.2
1	D	74	SER	3.2
1	I	177	TYR	3.2
1	D	126	LEU	3.2
1	F	172	LYS	3.2
1	D	77	TYR	3.2
1	E	117	ASN	3.2
1	B	30	VAL	3.2
1	B	85	ILE	3.2
1	F	257	ARG	3.2
1	E	102	LYS	3.2
1	E	110	GLU	3.2
1	C	90	ALA	3.2
1	H	63	ASP	3.2
1	H	126	LEU	3.2
1	B	73	GLY	3.2
1	D	259	ALA	3.2
1	F	4	ARG	3.2
1	F	187	PHE	3.1
1	H	238	ASP	3.1
1	A	55	LYS	3.1
1	G	114	ILE	3.1
1	G	33	ASP	3.1
1	G	79	ASP	3.1
1	A	129	VAL	3.1
1	D	57	GLU	3.1
1	H	98	VAL	3.1
1	C	228	PRO	3.1
1	G	282	TYR	3.1
1	A	251	PHE	3.1
1	H	75	THR	3.1
1	H	274	LYS	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	246	VAL	3.1
1	E	9	VAL	3.1
1	A	3	ILE	3.1
1	A	154	ILE	3.1
1	D	111	ASN	3.1
1	F	32	VAL	3.1
1	E	87	ILE	3.1
1	E	114	ILE	3.1
1	E	155	ARG	3.1
1	H	22	CYS	3.1
1	C	284	LYS	3.1
1	H	31	MET	3.0
1	D	81	LYS	3.0
1	G	196	MET	3.0
1	I	273	ARG	3.0
1	D	54	ILE	3.0
1	H	74	SER	3.0
1	A	11	ALA	3.0
1	G	8	ILE	3.0
1	E	33	ASP	3.0
1	E	74	SER	3.0
1	E	134	ASP	3.0
1	G	160	SER	3.0
1	D	174	LEU	3.0
1	G	80	LEU	3.0
1	D	128	ALA	3.0
1	D	34	ILE	3.0
1	A	41	LYS	3.0
1	C	182	LYS	3.0
1	G	6	VAL	3.0
1	F	274	LYS	3.0
1	I	180	THR	3.0
1	C	101	LEU	3.0
1	B	137	ILE	2.9
1	B	150	LEU	2.9
1	H	18	ILE	2.9
1	A	57	GLU	2.9
1	I	130	THR	2.9
1	F	151	VAL	2.9
1	B	154	ILE	2.9
1	B	277	ARG	2.9
1	C	56	LYS	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	277	ARG	2.9
1	I	24	VAL	2.9
1	D	175	GLY	2.9
1	F	247	LEU	2.9
1	D	282	TYR	2.9
1	D	142	PHE	2.9
1	C	80	LEU	2.9
1	B	17	GLY	2.9
1	H	166	ALA	2.9
1	A	116	SER	2.8
1	E	204	LEU	2.8
1	H	83	THR	2.8
1	C	243	VAL	2.8
1	E	265	MET	2.8
1	G	94	TYR	2.8
1	B	57	GLU	2.8
1	I	35	SER	2.8
1	D	27	LEU	2.8
1	G	117	ASN	2.8
1	A	18	ILE	2.8
1	B	8	ILE	2.8
1	E	135	ARG	2.8
1	E	65	ALA	2.8
1	E	283	SER	2.8
1	A	235	ILE	2.8
1	B	29	VAL	2.8
1	I	179	ILE	2.8
1	A	9	VAL	2.8
1	G	226	ILE	2.8
1	A	181	VAL	2.8
1	H	82	ALA	2.8
1	E	77	TYR	2.8
1	E	178	PRO	2.7
1	C	229	LEU	2.7
1	H	208	LEU	2.7
1	F	87	ILE	2.7
1	D	147	VAL	2.7
1	F	58	LYS	2.7
1	E	83	THR	2.7
1	A	145	VAL	2.7
1	D	62	ALA	2.7
1	D	127	ALA	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	76	SER	2.7
1	F	225	PRO	2.7
1	H	36	ASP	2.7
1	B	216	GLU	2.7
1	H	16	ASN	2.7
1	G	30	VAL	2.7
1	E	73	GLY	2.7
1	F	217	GLY	2.7
1	G	149	ALA	2.7
1	H	228	PRO	2.7
1	F	270	TYR	2.7
1	D	110	GLU	2.7
1	A	240	MET	2.7
1	A	49	SER	2.7
1	B	129	VAL	2.7
1	C	111	ASN	2.7
1	B	96	LEU	2.7
1	B	237	LEU	2.7
1	C	107	ILE	2.7
1	A	252	ALA	2.6
1	H	157	LEU	2.6
1	G	77	TYR	2.6
1	H	107	ILE	2.6
1	C	175	GLY	2.6
1	F	281	VAL	2.6
1	A	20	GLN	2.6
1	B	71	ILE	2.6
1	E	131	SER	2.6
1	H	12	GLY	2.6
1	B	37	ALA	2.6
1	G	140	HIS	2.6
1	E	18	ILE	2.6
1	B	55	LYS	2.6
1	B	143	ASN	2.6
1	D	143	ASN	2.6
1	I	29	VAL	2.6
1	D	68	LEU	2.6
1	C	227	GLY	2.6
1	D	177	TYR	2.6
1	G	242	ALA	2.6
1	I	268	ALA	2.6
1	D	53	LEU	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	153	LEU	2.6
1	I	101	LEU	2.6
1	B	136	PHE	2.6
1	G	273	ARG	2.6
1	I	226	ILE	2.6
1	A	44	ALA	2.6
1	G	179	ILE	2.6
1	B	47	ALA	2.6
1	D	38	ALA	2.6
1	G	177	TYR	2.6
1	A	173	GLN	2.5
1	H	50	LEU	2.5
1	H	80	LEU	2.5
1	I	188	VAL	2.5
1	B	48	SER	2.5
1	C	151	VAL	2.5
1	A	99	LYS	2.5
1	H	72	LYS	2.5
1	I	283	SER	2.5
1	A	117	ASN	2.5
1	I	225	PRO	2.5
1	H	115	ALA	2.5
1	D	96	LEU	2.5
1	D	141	PHE	2.5
1	D	121	ILE	2.5
1	I	79	ASP	2.5
1	B	155	ARG	2.5
1	A	247	LEU	2.5
1	B	86	VAL	2.5
1	G	245	GLU	2.5
1	H	258	PRO	2.5
1	E	154	ILE	2.5
1	A	250	GLU	2.5
1	D	212	GLU	2.5
1	D	169	ALA	2.5
1	A	168	GLU	2.5
1	A	6	VAL	2.5
1	E	282	TYR	2.5
1	D	271	LEU	2.4
1	D	281	VAL	2.4
1	I	86	VAL	2.4
1	D	19	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	34	ILE	2.4
1	I	113	ILE	2.4
1	I	187	PHE	2.4
1	A	276	GLY	2.4
1	F	100	ILE	2.4
1	H	52	ARG	2.4
1	E	99	LYS	2.4
1	G	230	ALA	2.4
1	I	260	MET	2.4
1	H	242	ALA	2.4
1	E	141	PHE	2.4
1	E	208	LEU	2.4
1	A	8	ILE	2.4
1	A	143	ASN	2.4
1	D	30	VAL	2.4
1	F	141	PHE	2.4
1	D	250	GLU	2.4
1	F	177	TYR	2.4
1	I	94	TYR	2.4
1	A	283	SER	2.4
1	C	118	THR	2.4
1	G	78	ASP	2.4
1	H	197	ILE	2.4
1	I	18	ILE	2.4
1	H	129	VAL	2.4
1	D	228	PRO	2.3
1	C	55	LYS	2.3
1	A	136	PHE	2.3
1	G	31	MET	2.3
1	D	176	LYS	2.3
1	E	284	LYS	2.3
1	A	7	GLY	2.3
1	A	30	VAL	2.3
1	B	74	SER	2.3
1	D	45	THR	2.3
1	D	239	THR	2.3
1	C	120	SER	2.3
1	F	50	LEU	2.3
1	G	256	TYR	2.3
1	I	170	LEU	2.3
1	B	87	ILE	2.3
1	H	235	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	225	PRO	2.3
1	E	217	GLY	2.3
1	I	231	LEU	2.3
1	H	282	TYR	2.3
1	A	141	PHE	2.3
1	B	9	VAL	2.3
1	F	26	GLY	2.3
1	C	173	GLN	2.3
1	I	90	ALA	2.3
1	I	104	ILE	2.3
1	D	98	VAL	2.3
1	E	86	VAL	2.3
1	A	72	LYS	2.3
1	G	56	LYS	2.3
1	A	21	ALA	2.3
1	B	195	PRO	2.2
1	G	93	ASN	2.2
1	G	283	SER	2.2
1	I	4	ARG	2.2
1	A	32	VAL	2.2
1	A	179	ILE	2.2
1	F	24	VAL	2.2
1	G	123	ILE	2.2
1	I	181	VAL	2.2
1	D	283	SER	2.2
1	F	122	SER	2.2
1	F	171	SER	2.2
1	C	68	LEU	2.2
1	D	135	ARG	2.2
1	F	282	TYR	2.2
1	D	276	GLY	2.2
1	D	173	GLN	2.2
1	E	100	ILE	2.2
1	F	121	ILE	2.2
1	B	68	LEU	2.2
1	B	75	THR	2.2
1	G	45	THR	2.2
1	E	42	GLY	2.2
1	H	87	ILE	2.2
1	A	202	CYS	2.2
1	D	219	LYS	2.2
1	B	220	LEU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	44	ALA	2.2
1	E	279	VAL	2.2
1	G	225	PRO	2.2
1	C	232	ALA	2.2
1	A	26	GLY	2.2
1	G	270	TYR	2.2
1	E	223	ASN	2.2
1	F	3	ILE	2.2
1	H	113	ILE	2.2
1	G	110	GLU	2.2
1	H	11	ALA	2.2
1	E	162	THR	2.2
1	D	104	ILE	2.2
1	I	151	VAL	2.2
1	I	164	HIS	2.2
1	I	174	LEU	2.2
1	A	161	ASP	2.2
1	A	267	ALA	2.2
1	B	232	ALA	2.2
1	H	26	GLY	2.2
1	E	108	VAL	2.1
1	G	74	SER	2.1
1	A	241	LEU	2.1
1	G	204	LEU	2.1
1	C	217	GLY	2.1
1	D	273	ARG	2.1
1	H	239	THR	2.1
1	A	167	VAL	2.1
1	G	235	ILE	2.1
1	G	266	VAL	2.1
1	G	193	LEU	2.1
1	A	75	THR	2.1
1	F	137	ILE	2.1
1	C	73	GLY	2.1
1	C	110	GLU	2.1
1	D	234	MET	2.1
1	D	103	GLN	2.1
1	D	183	ASN	2.1
1	A	70	ARG	2.1
1	C	104	ILE	2.1
1	D	99	LYS	2.1
1	I	182	LYS	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	64	LYS	2.1
1	A	22	CYS	2.1
1	C	126	LEU	2.1
1	E	98	VAL	2.1
1	F	276	GLY	2.1
1	G	3	ILE	2.1
1	D	101	LEU	2.1
1	D	189	VAL	2.1
1	D	204	LEU	2.1
1	G	43	VAL	2.1
1	B	280	TYR	2.1
1	H	222	CYS	2.1
1	G	173	GLN	2.1
1	B	97	LYS	2.1
1	D	9	VAL	2.1
1	G	108	VAL	2.1
1	E	199	GLU	2.1
1	G	58	LYS	2.0
1	I	271	LEU	2.0
1	I	43	VAL	2.0
1	H	132	ARG	2.0
1	F	139	MET	2.0
1	G	163	THR	2.0
1	B	125	LYS	2.0
1	B	141	PHE	2.0
1	D	97	LYS	2.0
1	G	71	ILE	2.0
1	H	192	ILE	2.0
1	C	270	TYR	2.0
1	F	37	ALA	2.0
1	F	284	LYS	2.0
1	D	170	LEU	2.0
1	A	114	ILE	2.0
1	A	206	GLU	2.0
1	A	280	TYR	2.0
1	E	78	ASP	2.0
1	H	105	ASP	2.0
1	G	83	THR	2.0
1	G	174	LEU	2.0
1	E	147	VAL	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](#)

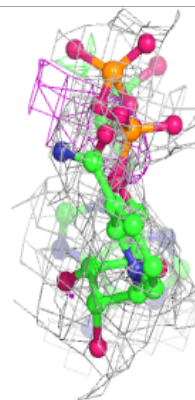
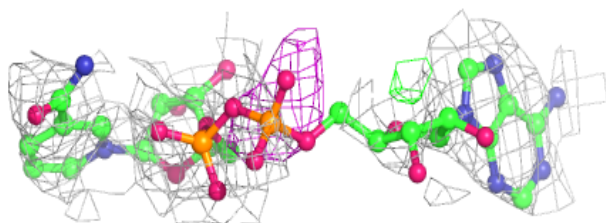
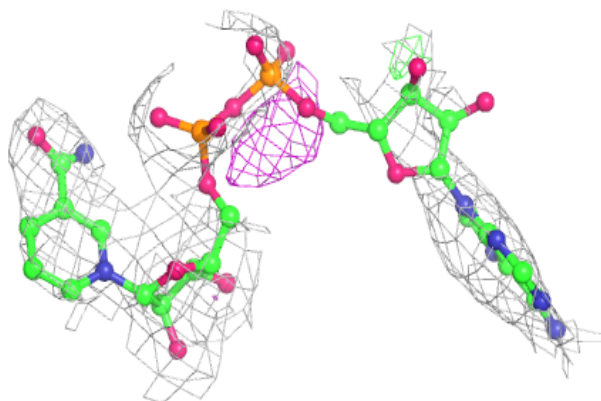
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	H	301	44/44	0.50	0.40	93,129,151,159	0
2	NAD	A	301	44/44	0.53	0.39	73,117,158,162	0
2	NAD	E	301	44/44	0.57	0.40	96,130,150,160	0
2	NAD	I	301	44/44	0.60	0.50	56,91,149,158	0
2	NAD	G	301	44/44	0.61	0.60	87,126,180,188	0
2	NAD	C	301	44/44	0.63	0.49	60,82,165,171	0
2	NAD	D	301	44/44	0.66	0.39	83,121,160,166	0
2	NAD	B	301	44/44	0.68	0.28	83,122,146,162	0
2	NAD	F	301	44/44	0.77	0.27	59,85,157,165	0

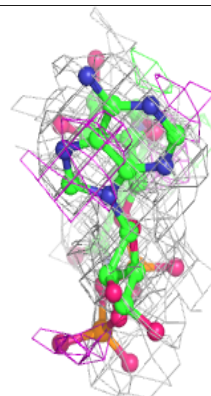
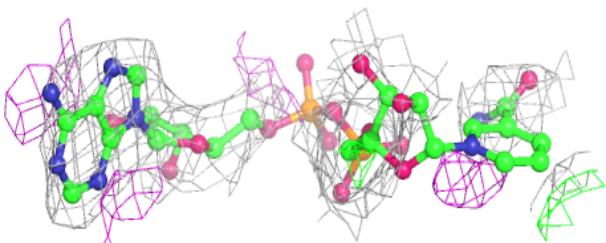
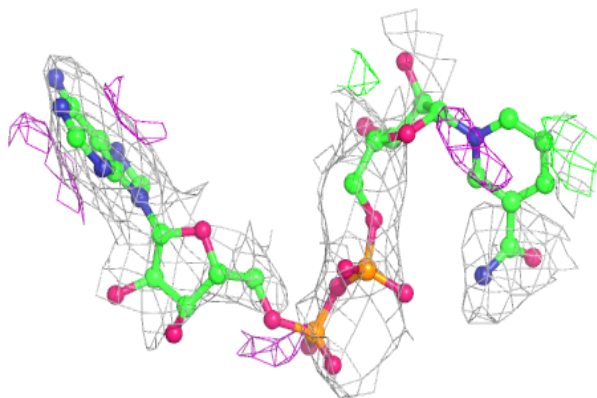
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD H 301:**

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

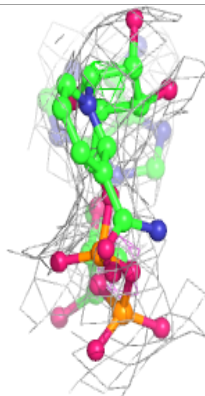
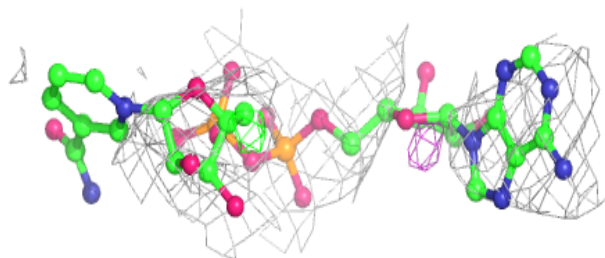
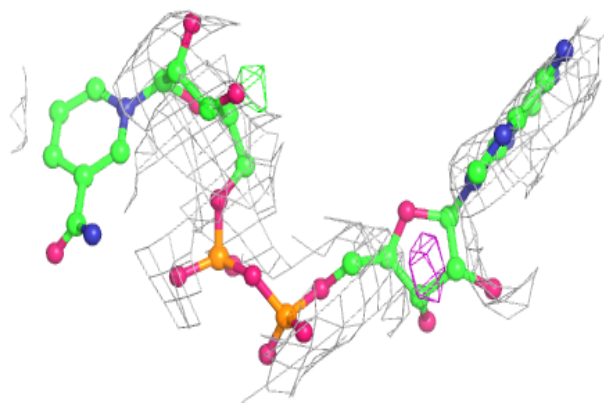
**Electron density around NAD A 301:**

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

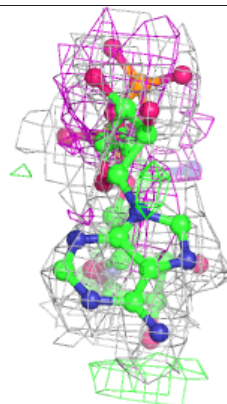
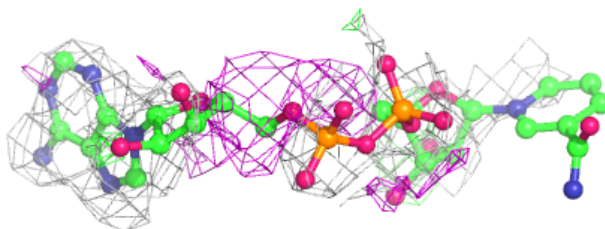
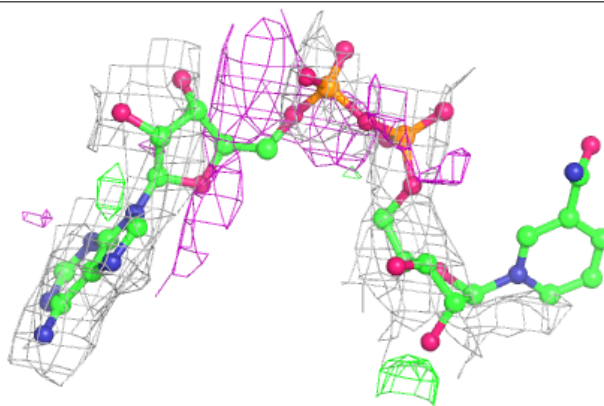


**Electron density around NAD E 301:**

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

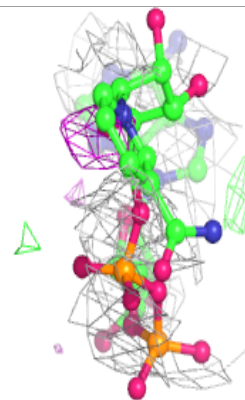
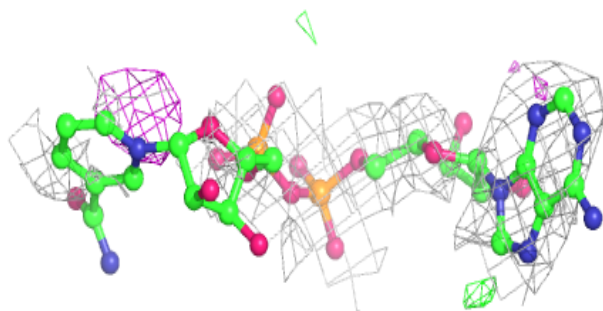
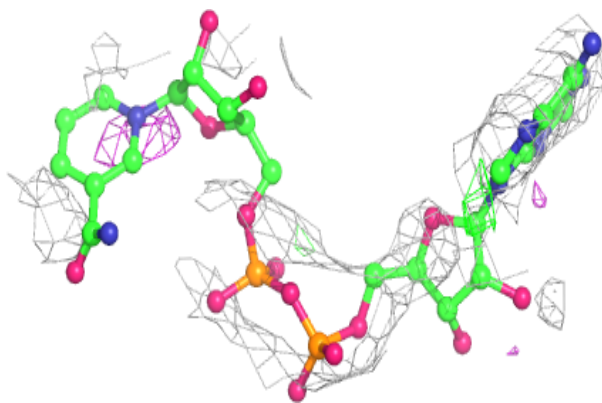
**Electron density around NAD I 301:**

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

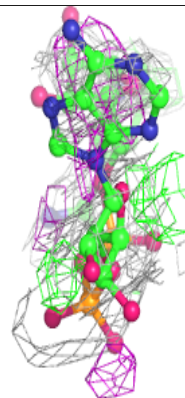
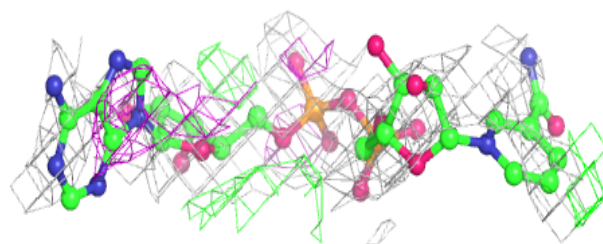
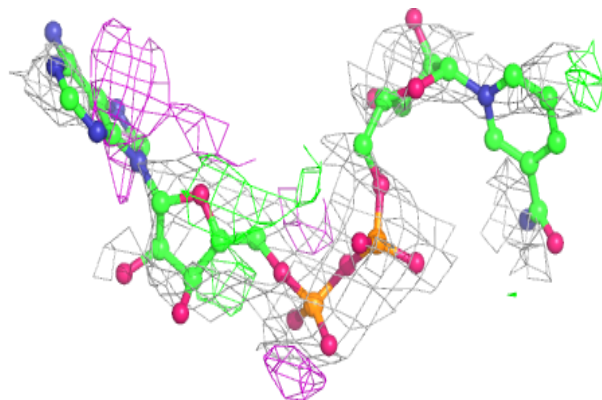


**Electron density around NAD G 301:**

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

**Electron density around NAD C 301:**

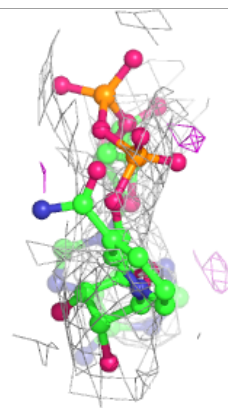
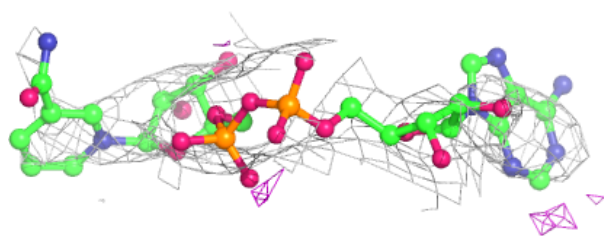
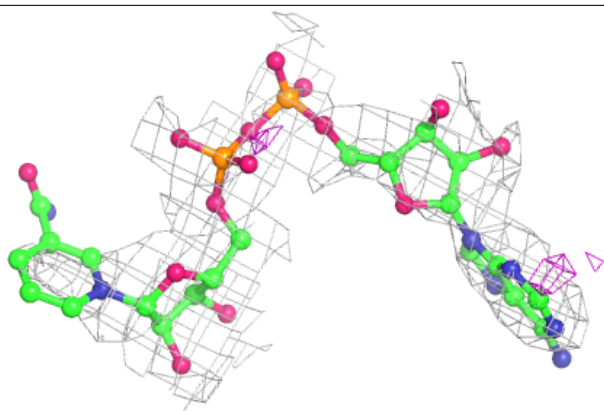
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



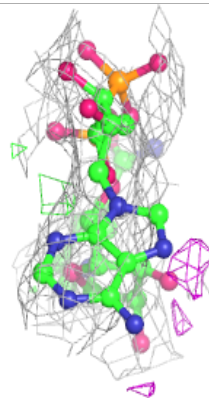
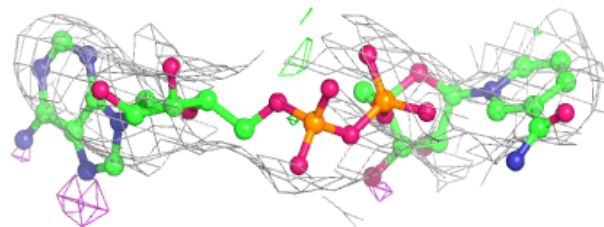
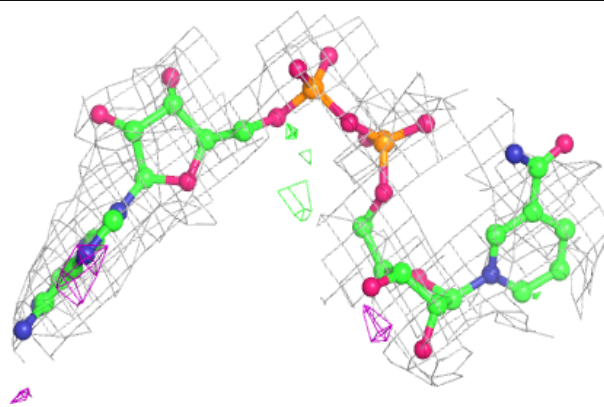


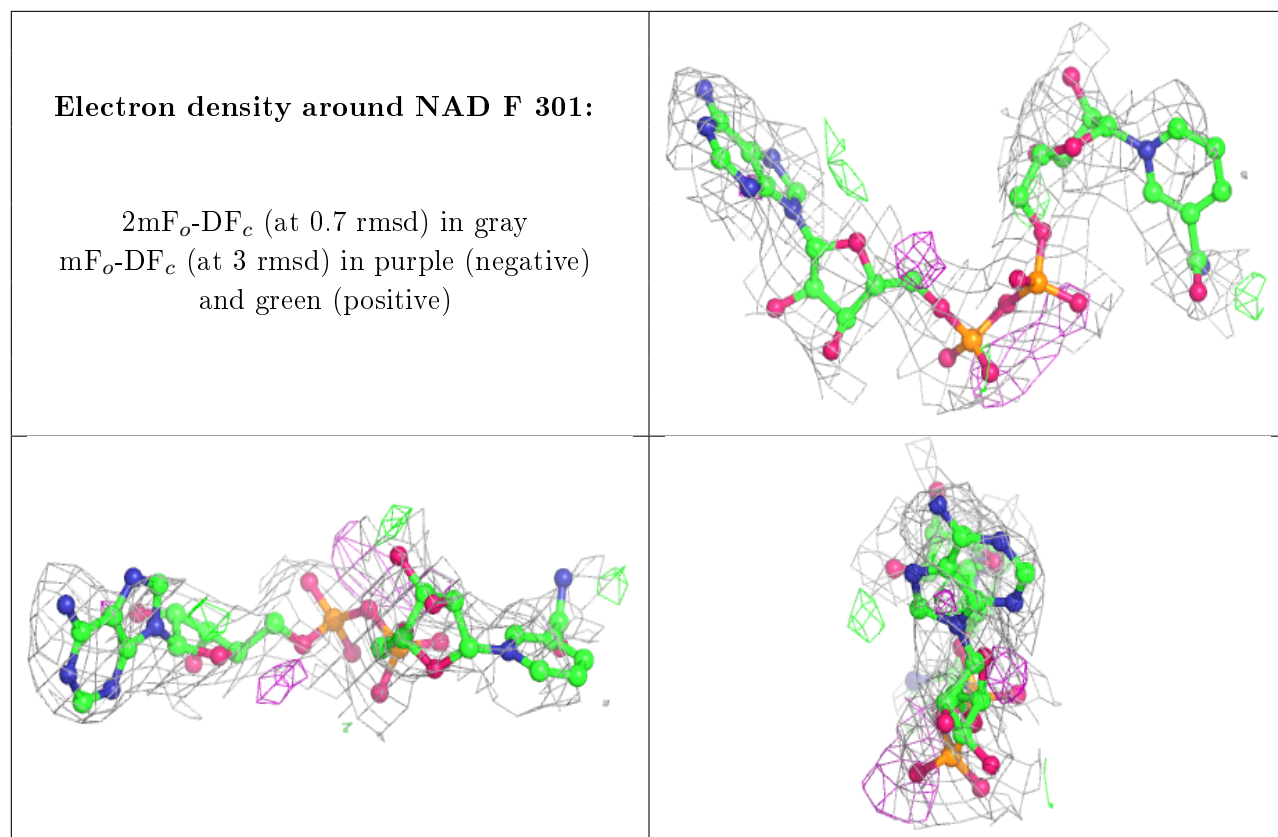
**Electron density around NAD D 301:**

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

**Electron density around NAD B 301:**

$2mF_o-DF_c$  (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.