



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2020 – 12:14 PM JST

PDB ID : 7CGV  
Title : Full consensus L-threonine 3-dehydrogenase, FcTDH-IIYM (NAD<sup>+</sup> bound form)  
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Deposited on : 2020-07-02  
Resolution : 2.38 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 : 2.14.6  
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) : 2.14.6

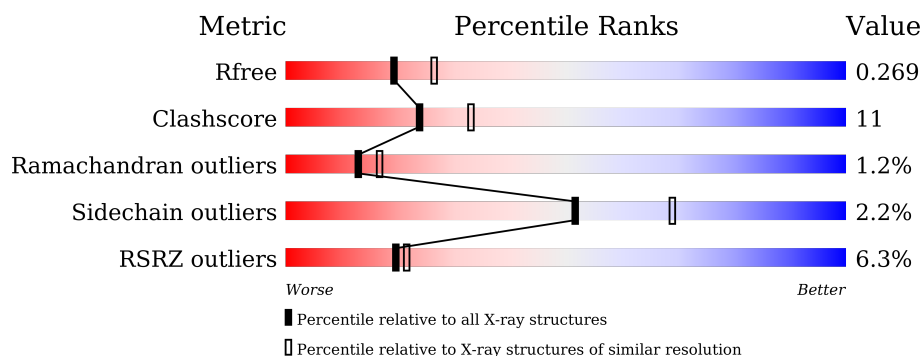
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	339	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	339	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	339	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	339	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition ⓘ

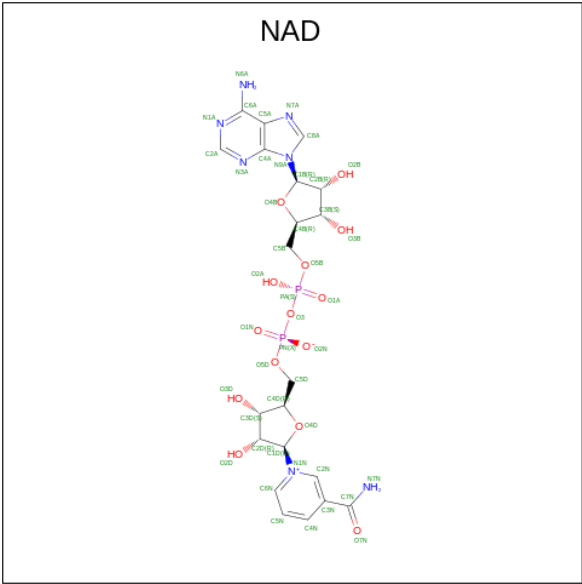
There are 3 unique types of molecules in this entry. The entry contains 10053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Artificial L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2446	1569	404	462	11			
1	B	303	Total	C	N	O	S	0	0	0
			2398	1541	395	451	11			
1	C	310	Total	C	N	O	S	0	0	0
			2446	1569	404	462	11			
1	D	303	Total	C	N	O	S	0	0	0
			2392	1536	395	450	11			

- Molecule 2 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>) (labeled as "Ligand of Interest" by author).



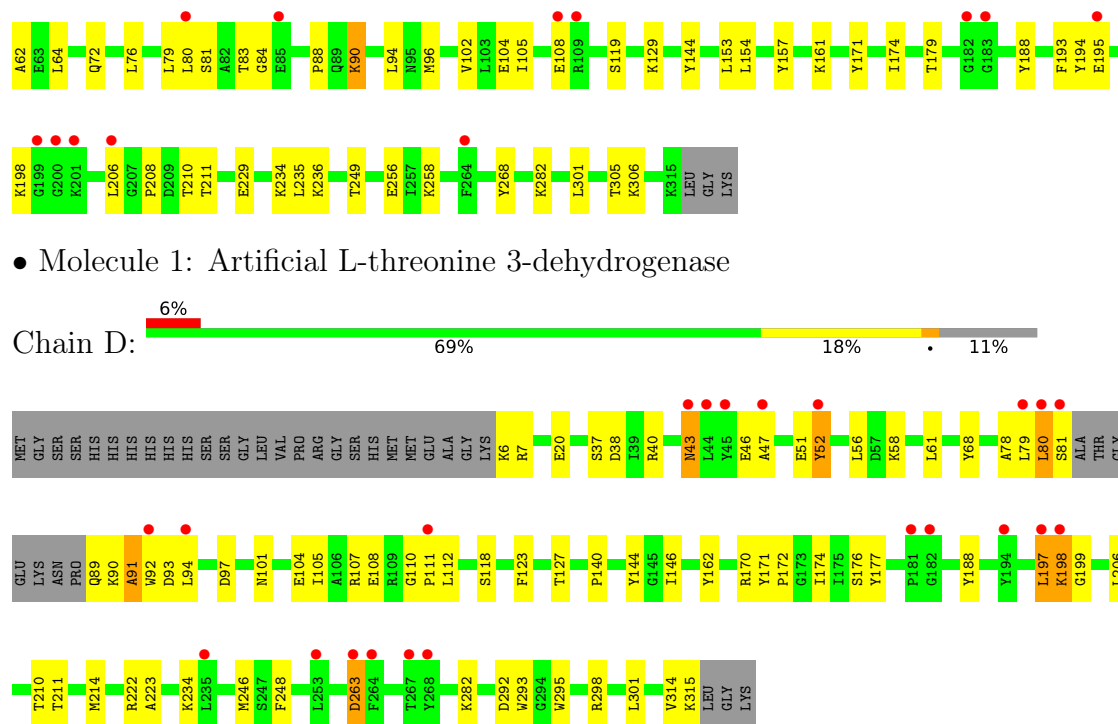
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	49	Total	O	0	0
			49	49		
3	C	59	Total	O	0	0
			59	59		
3	D	32	Total	O	0	0
			32	32		





● Molecule 1: Artificial L-threonine 3-dehydrogenase

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.58Å 77.51Å 76.83Å 71.01° 75.13° 74.88°	Depositor
Resolution (Å)	36.41 – 2.38 41.52 – 2.38	Depositor EDS
% Data completeness (in resolution range)	96.2 (36.41-2.38) 96.2 (41.52-2.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.39Å)	Xtriage
Refinement program	REFMAC 1.17.1 _3660	Depositor
R, $R_{free}$	0.212 , 0.263 0.222 , 0.269	Depositor DCC
$R_{free}$ test set	2256 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10053	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.01% 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

### 5.1 Standard geometry

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	0.45	0/2507	0.65	1/3405 (0.0%)
1	B	0.45	0/2457	0.66	1/3336 (0.0%)
1	C	0.47	1/2507 (0.0%)	0.65	1/3405 (0.0%)
1	D	0.71	3/2450 (0.1%)	0.69	3/3325 (0.1%)
All	All	0.53	4/9921 (0.0%)	0.67	6/13471 (0.0%)

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	3
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	52	TYR	CD1-CE1	-21.00	1.07	1.39
1	D	52	TYR	CD2-CE2	-15.97	1.15	1.39
1	C	52	TYR	CB-CG	-5.23	1.43	1.51
1	D	52	TYR	CZ-OH	5.00	1.46	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	TYR	CB-CG-CD1	-9.84	115.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	TYR	CA-CB-CG	-8.36	97.51	113.40
1	C	52	TYR	CA-CB-CG	-7.37	99.40	113.40
1	D	197	LEU	CA-CB-CG	6.83	131.01	115.30
1	B	300	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	44	LEU	CB-CG-CD1	-5.28	102.02	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	ASN	Peptide
1	A	79	LEU	Peptide
1	A	87	ASN	Peptide
1	B	78	ALA	Peptide
1	C	43	ASN	Peptide
1	D	198	LYS	Peptide
1	D	46	GLU	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	2446	0	2436	53	1
1	B	2398	0	2392	65	0
1	C	2446	0	2436	56	0
1	D	2392	0	2379	49	1
2	A	44	0	26	3	0
2	B	44	0	26	3	0
2	C	44	0	26	8	0
2	D	44	0	26	3	0
3	A	55	0	0	2	0
3	B	49	0	0	5	0
3	C	59	0	0	6	0
3	D	32	0	0	9	0
All	All	10053	0	9747	217	1

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 11.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:CD1	1:C:90:LYS:HE2	1.63	1.26
1:A:87:ASN:ND2	1:A:88:PRO:O	1.86	1.09
1:C:79:LEU:HD11	1:C:90:LYS:CE	1.84	1.07
1:C:96:MET:SD	3:C:557:HOH:O	2.20	1.00
1:B:203:GLU:OE2	3:B:501:HOH:O	1.84	0.95
1:B:44:LEU:O	1:B:45:TYR:CD2	2.25	0.90
1:C:79:LEU:CD1	1:C:90:LYS:CE	2.46	0.89
1:C:79:LEU:HD11	1:C:90:LYS:HE2	0.88	0.86
1:D:91:ALA:O	1:D:93:ASP:N	2.09	0.86
1:B:258:LYS:HE3	1:B:262:PRO:O	1.74	0.86
1:D:20:GLU:OE1	3:D:501:HOH:O	1.92	0.86
1:D:6:LYS:O	1:D:7:ARG:HG2	1.80	0.81
1:C:16:GLN:OE1	3:C:502:HOH:O	2.01	0.78
1:D:52:TYR:CE1	3:D:508:HOH:O	2.36	0.78
1:C:306:LYS:NZ	3:C:504:HOH:O	2.22	0.73
1:B:285:ASP:OD2	3:B:503:HOH:O	2.07	0.73
1:A:15:GLY:HA3	2:A:401:NAD:O2A	1.89	0.72
1:B:46:GLU:HB2	1:B:47:ALA:HA	1.69	0.72
1:D:246:MET:O	3:D:503:HOH:O	2.07	0.72
1:C:108:GLU:OE2	3:C:503:HOH:O	2.07	0.72
2:C:401:NAD:O1N	3:C:502:HOH:O	2.07	0.71
1:D:61:LEU:HD23	1:D:105:ILE:HG13	1.73	0.70
1:D:40:ARG:NH2	3:D:504:HOH:O	2.25	0.69
1:C:50:PHE:HE2	1:C:52:TYR:CZ	2.11	0.69
1:D:89:GLN:NE2	3:D:506:HOH:O	2.24	0.69
1:C:83:THR:N	1:C:84:GLY:HA3	2.08	0.68
2:A:401:NAD:H4B	2:A:401:NAD:O2A	1.92	0.68
1:B:246:MET:HE3	1:B:248:PHE:HE2	1.59	0.67
1:A:7:ARG:H	1:A:71:THR:HG22	1.59	0.67
1:B:78:ALA:HB2	2:B:401:NAD:H3D	1.77	0.67
1:A:58:LYS:HE3	1:B:89:GLN:HE22	1.58	0.66
1:C:56:LEU:HD21	1:C:94:LEU:HA	1.77	0.65
1:A:194:TYR:CD2	1:A:314:VAL:HG13	2.31	0.65
1:B:246:MET:HE3	1:B:248:PHE:CE2	2.31	0.65
1:C:50:PHE:CE2	1:C:52:TYR:CZ	2.85	0.65
1:D:79:LEU:HB3	1:D:80:LEU:HG	1.79	0.65
1:B:89:GLN:N	3:B:507:HOH:O	2.30	0.65
1:A:175:ILE:HG21	1:A:304:MET:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:HD13	1:C:90:LYS:HD2	1.80	0.64
1:A:211:THR:HG23	1:A:282:LYS:HD2	1.80	0.64
1:B:246:MET:CE	1:B:248:PHE:HE2	2.09	0.64
1:D:211:THR:HG23	1:D:282:LYS:HG2	1.80	0.64
1:C:41:PRO:HA	1:C:52:TYR:OH	1.99	0.63
1:D:104:GLU:OE1	1:D:107:ARG:NH2	2.32	0.63
1:A:194:TYR:HD2	1:A:314:VAL:HG13	1.61	0.63
1:A:134:GLN:NE2	3:A:501:HOH:O	1.90	0.63
1:B:108:GLU:O	1:B:109:ARG:HD3	2.00	0.62
1:B:211:THR:HG21	1:B:282:LYS:HD3	1.82	0.62
1:A:85:GLU:HB2	3:A:521:HOH:O	1.99	0.61
1:C:79:LEU:CD1	1:C:90:LYS:CD	2.79	0.61
1:D:234:LYS:HG2	1:D:292:ASP:O	2.01	0.61
1:A:175:ILE:HG21	1:A:304:MET:CE	2.32	0.60
1:A:26:ARG:HG2	1:A:31:ALA:HA	1.84	0.60
1:C:54:ASP:OD1	2:C:401:NAD:N6A	2.34	0.60
1:A:211:THR:CG2	1:A:282:LYS:HD2	2.32	0.60
1:A:146:ILE:HG21	1:B:154:LEU:CD1	2.32	0.60
1:C:79:LEU:HD13	1:C:90:LYS:CD	2.32	0.59
1:B:119:SER:HB2	2:B:401:NAD:H6N	1.84	0.59
1:D:37:SER:HA	1:D:51:GLU:O	2.03	0.59
1:B:46:GLU:HB2	1:B:47:ALA:CA	2.32	0.59
1:B:304:MET:CE	1:B:308:MET:HG3	2.33	0.58
1:D:52:TYR:C	1:D:52:TYR:CD2	2.76	0.58
1:D:177:TYR:N	3:D:502:HOH:O	2.00	0.58
1:D:144:TYR:OH	2:D:401:NAD:H2D	2.03	0.58
1:B:301:LEU:O	1:B:305:THR:HG23	2.03	0.58
1:C:64:LEU:HD23	1:C:64:LEU:O	2.05	0.57
1:B:80:LEU:HA	1:B:144:TYR:CD1	2.40	0.57
1:B:80:LEU:HA	1:B:144:TYR:CE1	2.40	0.56
1:A:208:PRO:HB3	1:A:268:TYR:CZ	2.40	0.56
1:B:56:LEU:HD21	1:B:94:LEU:HA	1.86	0.56
1:D:91:ALA:C	1:D:93:ASP:H	2.07	0.56
1:A:118:SER:HA	1:A:148:LYS:HD2	1.87	0.56
1:D:314:VAL:HA	1:D:315:LYS:C	2.25	0.56
1:B:197:LEU:HD12	1:B:312:LEU:HD23	1.87	0.55
1:D:43:ASN:OD1	3:D:504:HOH:O	2.18	0.55
1:B:90:LYS:H	1:B:90:LYS:HD3	1.72	0.55
1:B:46:GLU:HB2	1:B:48:GLY:N	2.22	0.55
1:C:28:ARG:NH2	1:C:229:GLU:HG2	2.21	0.54
1:A:104:GLU:HG3	1:B:89:GLN:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:GLU:HG2	1:C:47:ALA:H	1.72	0.54
1:B:258:LYS:CE	1:B:262:PRO:O	2.54	0.54
1:C:29:TYR:OH	1:C:229:GLU:OE1	2.25	0.54
1:C:43:ASN:O	1:C:44:LEU:HD12	2.08	0.54
1:C:79:LEU:HD13	1:C:90:LYS:CE	2.36	0.54
1:A:26:ARG:CZ	1:A:48:GLY:HA3	2.38	0.53
1:B:304:MET:HE3	1:B:308:MET:HG3	1.89	0.53
1:A:146:ILE:HG21	1:B:154:LEU:HD12	1.91	0.53
1:C:50:PHE:HE2	1:C:52:TYR:CE1	2.27	0.53
1:A:63:GLU:HA	1:A:66:LYS:HE3	1.90	0.53
1:B:46:GLU:OE2	1:B:47:ALA:HA	2.08	0.53
1:B:46:GLU:HB2	1:B:48:GLY:H	1.74	0.53
1:B:258:LYS:HG3	1:B:262:PRO:HA	1.91	0.52
1:C:154:LEU:CD1	1:D:146:ILE:HG21	2.40	0.52
1:A:234:LYS:O	1:A:236:LYS:N	2.42	0.52
1:D:110:GLY:O	1:D:112:LEU:N	2.42	0.52
1:D:52:TYR:N	1:D:52:TYR:CD1	2.67	0.52
1:A:107:ARG:HD3	1:A:162:TYR:CG	2.45	0.51
1:D:123:PHE:CD1	1:D:127:THR:HG21	2.46	0.51
1:B:78:ALA:O	1:B:79:LEU:HG	2.10	0.51
1:C:211:THR:HG21	1:C:282:LYS:HD3	1.92	0.51
1:A:7:ARG:H	1:A:71:THR:CG2	2.22	0.51
1:B:195:GLU:HB3	1:B:201:LYS:O	2.10	0.50
1:A:304:MET:CE	1:A:308:MET:HG3	2.42	0.50
1:B:175:ILE:HG21	1:B:304:MET:HE3	1.92	0.50
1:A:239:SER:OG	1:A:240:SER:N	2.43	0.50
1:C:8:ILE:HG12	1:C:72:GLN:HB2	1.94	0.50
1:A:65:VAL:HG13	1:A:70:ILE:HB	1.93	0.50
1:B:198:LYS:HB3	1:B:314:VAL:HG11	1.94	0.50
1:C:193:PHE:HE2	1:C:305:THR:HG1	1.58	0.49
1:C:26:ARG:HG2	1:C:31:ALA:HA	1.94	0.49
1:C:195:GLU:OE1	1:C:198:LYS:HE3	2.12	0.49
1:B:258:LYS:HD2	1:B:264:PHE:O	2.13	0.48
1:C:44:LEU:C	1:C:46:GLU:H	2.17	0.48
1:D:206:LEU:HD13	1:D:210:THR:HG21	1.95	0.48
1:D:223:ALA:HB2	1:D:295:TRP:CZ3	2.48	0.48
1:D:198:LYS:HG2	1:D:199:GLY:H	1.78	0.48
1:A:315:LYS:HE2	1:A:315:LYS:HB2	1.59	0.48
1:D:104:GLU:O	1:D:108:GLU:HG3	2.14	0.48
1:A:21:LEU:HD21	1:A:74:TYR:CD2	2.48	0.48
1:D:171:TYR:CG	1:D:174:ILE:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD21	2:A:401:NAD:H52N	1.96	0.48
1:B:37:SER:HA	1:B:51:GLU:O	2.13	0.48
1:C:80:LEU:HD21	2:C:401:NAD:H2D	1.96	0.48
1:B:211:THR:CG2	1:B:282:LYS:HD3	2.42	0.48
1:B:286:ASP:OD1	1:B:290:ARG:HD2	2.14	0.47
1:D:107:ARG:HG3	1:D:162:TYR:HB3	1.95	0.47
1:B:44:LEU:O	1:B:45:TYR:CG	2.66	0.47
1:A:100:LEU:HG	1:B:89:GLN:HG3	1.95	0.47
1:B:194:TYR:O	1:B:198:LYS:HG2	2.13	0.47
1:A:44:LEU:HD22	1:A:45:TYR:HB2	1.97	0.47
1:B:26:ARG:HG2	1:B:31:ALA:HA	1.97	0.47
1:C:234:LYS:O	1:C:236:LYS:N	2.48	0.46
1:A:258:LYS:HE2	1:A:264:PHE:O	2.15	0.46
1:A:312:LEU:HG	1:A:314:VAL:HG22	1.97	0.46
1:A:56:LEU:HD21	1:A:94:LEU:HA	1.97	0.46
1:B:115:PHE:CZ	1:B:224:THR:HG23	2.51	0.46
1:B:80:LEU:HD21	2:B:401:NAD:H2D	1.97	0.46
1:B:46:GLU:CB	1:B:47:ALA:HA	2.42	0.46
1:B:93:ASP:OD2	3:B:504:HOH:O	2.21	0.46
1:A:304:MET:HE2	1:A:308:MET:HG3	1.98	0.45
1:C:12:GLY:HA2	2:C:401:NAD:H1B	1.97	0.45
1:D:80:LEU:HA	1:D:81:SER:HA	1.41	0.45
1:C:171:TYR:CG	1:C:174:ILE:HD11	2.51	0.45
1:D:78:ALA:HB2	2:D:401:NAD:O3D	2.16	0.45
1:C:194:TYR:O	1:C:198:LYS:HG2	2.16	0.45
1:C:50:PHE:CE2	1:C:52:TYR:CE1	3.05	0.45
1:D:101:ASN:O	1:D:105:ILE:HG12	2.16	0.45
1:A:37:SER:HA	1:A:51:GLU:O	2.17	0.45
1:A:118:SER:HB3	1:A:170:ARG:HG2	1.99	0.45
1:A:208:PRO:HB3	1:A:268:TYR:CE2	2.52	0.45
1:C:157:TYR:CZ	1:C:161:LYS:HD2	2.52	0.45
1:C:80:LEU:CD2	2:C:401:NAD:H2D	2.47	0.45
1:D:176:SER:HB2	3:D:502:HOH:O	2.16	0.45
1:D:93:ASP:O	1:D:97:ASP:HB2	2.17	0.45
1:A:39:ILE:O	1:A:40:ARG:CB	2.65	0.44
1:B:175:ILE:HG21	1:B:304:MET:CE	2.47	0.44
1:C:104:GLU:HG3	1:D:90:LYS:HD3	1.99	0.44
1:C:19:SER:OG	1:C:179:THR:HG21	2.17	0.44
1:A:26:ARG:HG3	1:A:34:VAL:HB	2.00	0.44
1:D:222:ARG:NH2	1:D:298:ARG:HG3	2.33	0.44
1:C:81:SER:HA	1:C:144:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ASP:O	1:D:52:TYR:HA	2.17	0.44
1:A:84:GLY:O	1:A:88:PRO:HD3	2.18	0.44
1:C:53:LEU:HD22	1:C:64:LEU:HD13	1.98	0.44
1:C:62:ALA:HB2	1:C:105:ILE:HD11	1.99	0.44
1:A:96:MET:O	1:A:100:LEU:HD23	2.18	0.44
1:A:153:LEU:HD13	1:B:140:PRO:HD2	1.99	0.43
1:B:89:GLN:N	3:B:514:HOH:O	2.50	0.43
1:D:248:PHE:CD2	1:D:301:LEU:HD13	2.53	0.43
1:C:208:PRO:HB3	1:C:268:TYR:CZ	2.53	0.43
1:A:223:ALA:HB2	1:A:295:TRP:CZ3	2.54	0.43
1:A:194:TYR:CZ	1:A:312:LEU:HD11	2.54	0.42
1:B:43:ASN:HA	1:B:44:LEU:C	2.39	0.42
1:C:153:LEU:HD13	1:D:140:PRO:HD2	2.01	0.42
1:B:171:TYR:CG	1:B:174:ILE:HD11	2.54	0.42
1:C:206:LEU:HD13	1:C:210:THR:HG21	2.01	0.42
1:D:52:TYR:O	1:D:52:TYR:CD2	2.72	0.42
1:A:211:THR:HB	1:A:249:THR:HG22	2.00	0.42
1:B:188:TYR:CZ	1:B:250:PRO:HG3	2.54	0.42
1:A:14:ASN:ND2	1:A:40:ARG:O	2.53	0.42
1:B:112:LEU:HA	1:B:112:LEU:HD23	1.87	0.42
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.78	0.42
1:A:115:PHE:CZ	1:A:224:THR:HG23	2.55	0.42
1:D:56:LEU:HD21	1:D:94:LEU:HA	2.01	0.42
1:C:102:VAL:O	1:C:105:ILE:HG22	2.19	0.42
1:C:129:LYS:NZ	3:C:501:HOH:O	1.94	0.42
1:C:171:TYR:HB2	2:C:401:NAD:C5N	2.50	0.42
1:D:118:SER:HB3	1:D:170:ARG:HG2	2.02	0.42
1:A:188:TYR:CD2	1:A:206:LEU:HD12	2.55	0.42
1:B:191:GLU:HB3	1:B:202:TYR:CE1	2.54	0.41
1:B:43:ASN:HA	1:B:44:LEU:O	2.20	0.41
1:C:76:LEU:O	2:C:401:NAD:H52N	2.20	0.41
1:D:293:TRP:CZ3	1:D:295:TRP:HB2	2.54	0.41
1:A:194:TYR:O	1:A:198:LYS:HG2	2.20	0.41
1:D:263:ASP:N	1:D:263:ASP:OD1	2.51	0.41
1:B:16:GLN:HG3	1:B:179:THR:OG1	2.20	0.41
1:B:8:ILE:HG12	1:B:72:GLN:HB2	2.02	0.41
1:B:90:LYS:HA	1:B:93:ASP:OD1	2.20	0.41
1:C:90:LYS:C	1:C:90:LYS:HD3	2.41	0.41
1:B:17:ILE:HD13	1:B:171:TYR:CE2	2.56	0.41
1:B:123:PHE:CD1	1:B:127:THR:HG21	2.56	0.41
1:A:123:PHE:CD1	1:A:127:THR:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:O	1:A:146:ILE:HG13	2.21	0.41
1:C:256:GLU:HG2	1:C:305:THR:HG21	2.03	0.41
2:D:401:NAD:O2N	3:D:505:HOH:O	2.22	0.41
1:D:7:ARG:CD	1:D:68:TYR:O	2.69	0.41
1:C:301:LEU:O	1:C:305:THR:HG22	2.20	0.41
1:D:58:LYS:HG2	1:D:105:ILE:HD11	2.02	0.41
1:C:211:THR:HB	1:C:249:THR:HG22	2.02	0.40
1:D:198:LYS:CG	1:D:199:GLY:H	2.34	0.40
1:A:233:GLU:CD	1:A:233:GLU:H	2.25	0.40
1:B:115:PHE:HB2	1:B:228:MET:SD	2.62	0.40
1:B:256:GLU:OE1	1:B:259:LYS:HE3	2.21	0.40
1:D:214:MET:HG3	1:D:248:PHE:CZ	2.57	0.40
1:B:29:TYR:O	1:B:33:ASN:ND2	2.42	0.40
1:C:119:SER:HB2	2:C:401:NAD:H5N	2.02	0.40
1:D:172:PRO:O	1:D:174:ILE:HG13	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:O	1:D:52:TYR:OH[1_446]	1.75	0.45

## 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	308/339 (91%)	289 (94%)	15 (5%)	4 (1%)	12	15
1	B	299/339 (88%)	282 (94%)	15 (5%)	2 (1%)	22	30
1	C	308/339 (91%)	290 (94%)	14 (4%)	4 (1%)	12	15
1	D	299/339 (88%)	279 (93%)	16 (5%)	4 (1%)	12	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1214/1356 (90%)	1140 (94%)	60 (5%)	14 (1%)	13 17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	B	46	GLU
1	D	47	ALA
1	D	92	TRP
1	A	235	LEU
1	C	45	TYR
1	A	47	ALA
1	C	46	GLU
1	C	235	LEU
1	D	91	ALA
1	A	239	SER
1	C	88	PRO
1	D	111	PRO
1	B	111	PRO

### 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	259/283 (92%)	249 (96%)	10 (4%)	32 48
1	B	254/283 (90%)	250 (98%)	4 (2%)	62 78
1	C	259/283 (92%)	255 (98%)	4 (2%)	65 79
1	D	254/283 (90%)	249 (98%)	5 (2%)	55 72
All	All	1026/1132 (91%)	1003 (98%)	23 (2%)	52 69

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASN

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Mol	Chain	Res	Type
1	A	45	TYR
1	A	86	LYS
1	A	109	ARG
1	A	113	LYS
1	A	188	TYR
1	A	251	GLU
1	A	265	GLU
1	A	304	MET
1	A	315	LYS
1	B	46	GLU
1	B	63	GLU
1	B	90	LYS
1	B	304	MET
1	C	32	ASP
1	C	90	LYS
1	C	188	TYR
1	C	258	LYS
1	D	43	ASN
1	D	80	LEU
1	D	188	TYR
1	D	197	LEU
1	D	263	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	B	89	GLN
1	C	159	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	D	401	-	42,48,48	0.88	2 (4%)	50,73,73	0.99	4 (8%)
2	NAD	C	401	-	42,48,48	0.71	1 (2%)	50,73,73	1.09	3 (6%)
2	NAD	B	401	-	42,48,48	0.72	1 (2%)	50,73,73	1.01	5 (10%)
2	NAD	A	401	-	42,48,48	0.96	1 (2%)	50,73,73	1.48	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	D	401	-	-	7/26/62/62	0/5/5/5
2	NAD	C	401	-	-	3/26/62/62	0/5/5/5
2	NAD	B	401	-	-	3/26/62/62	0/5/5/5
2	NAD	A	401	-	-	8/26/62/62	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C2N-N1N	4.40	1.40	1.35
2	D	401	NAD	C2N-N1N	3.79	1.39	1.35
2	B	401	NAD	C2N-N1N	2.93	1.38	1.35
2	C	401	NAD	C2N-N1N	2.73	1.38	1.35
2	D	401	NAD	O4D-C1D	2.53	1.44	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	C6N-N1N-C2N	-3.91	118.41	121.97
2	A	401	NAD	C2D-C3D-C4D	-3.86	95.15	102.64
2	C	401	NAD	O4D-C1D-C2D	-3.58	101.69	106.93
2	B	401	NAD	O4D-C1D-C2D	-3.24	102.19	106.93
2	A	401	NAD	C3D-C2D-C1D	-3.21	96.15	100.98
2	A	401	NAD	O4D-C1D-C2D	-2.94	102.63	106.93
2	D	401	NAD	O4B-C1B-C2B	-2.90	102.69	106.93
2	A	401	NAD	PN-O3-PA	-2.84	123.08	132.83
2	B	401	NAD	C6N-N1N-C2N	-2.71	119.50	121.97
2	C	401	NAD	O4B-C1B-C2B	-2.66	103.04	106.93
2	A	401	NAD	O2D-C2D-C3D	-2.54	103.61	111.82
2	D	401	NAD	C6N-N1N-C2N	-2.50	119.70	121.97
2	C	401	NAD	C6N-N1N-C2N	-2.46	119.73	121.97
2	D	401	NAD	C5A-C6A-N6A	2.31	123.86	120.35
2	A	401	NAD	C5A-C6A-N6A	2.25	123.77	120.35
2	B	401	NAD	O4B-C1B-C2B	-2.21	103.70	106.93
2	B	401	NAD	C5A-C6A-N6A	2.20	123.70	120.35
2	B	401	NAD	PN-O3-PA	-2.13	125.53	132.83
2	D	401	NAD	PN-O3-PA	-2.01	125.94	132.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	NAD	C5B-O5B-PA-O2A
2	D	401	NAD	C5B-O5B-PA-O3
2	A	401	NAD	C4B-C5B-O5B-PA
2	A	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C5D-O5D-PN-O1N
2	A	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	C3D-C4D-C5D-O5D
2	D	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	C3B-C4B-C5B-O5B
2	C	401	NAD	O4D-C4D-C5D-O5D
2	D	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	C5D-O5D-PN-O2N
2	D	401	NAD	PN-O3-PA-O2A
2	B	401	NAD	PN-O3-PA-O1A
2	C	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	O4B-C4B-C5B-O5B
2	D	401	NAD	PN-O3-PA-O1A

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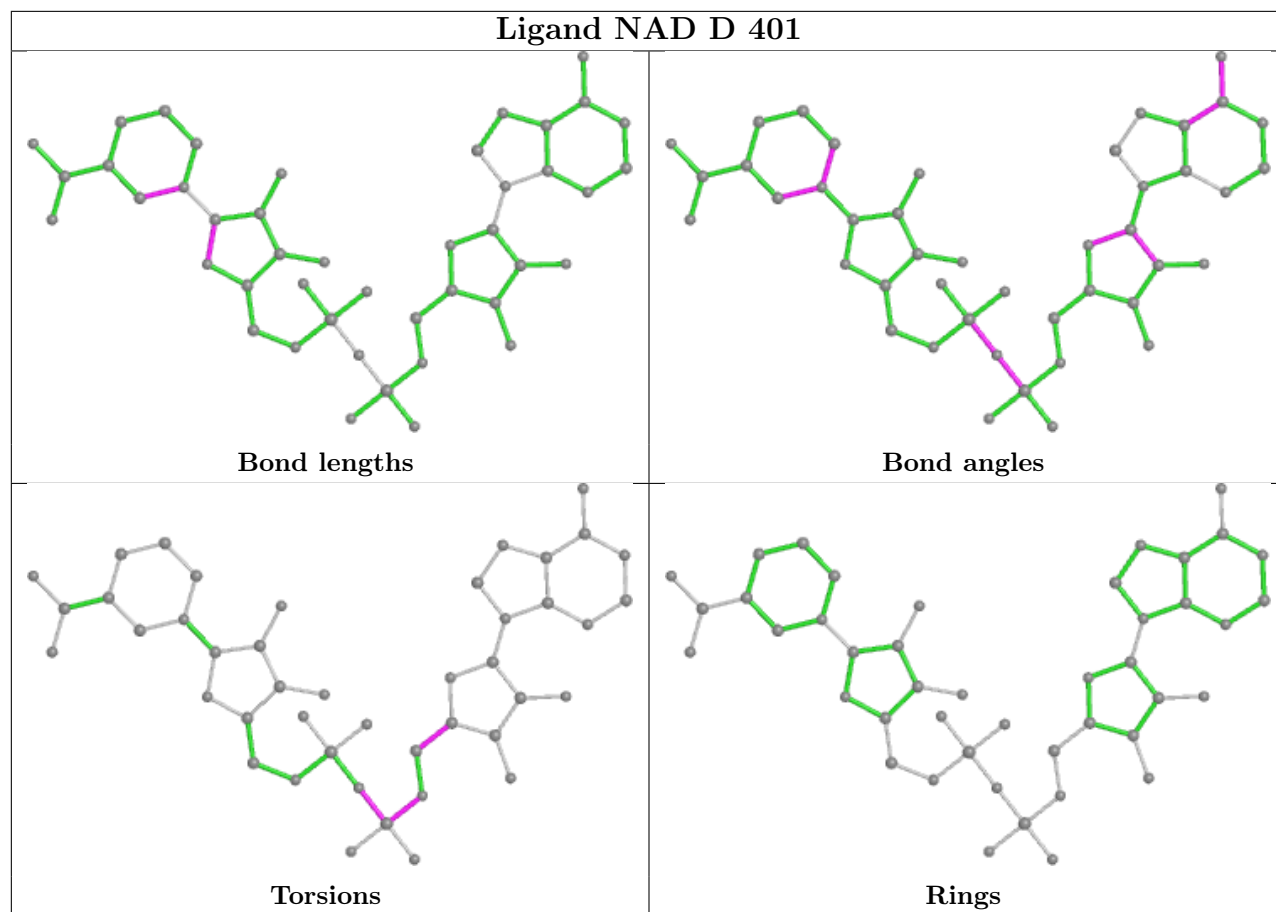
Mol	Chain	Res	Type	Atoms
2	B	401	NAD	PN-O3-PA-O2A
2	A	401	NAD	PA-O3-PN-O2N
2	C	401	NAD	C3D-C4D-C5D-O5D
2	B	401	NAD	O4B-C4B-C5B-O5B

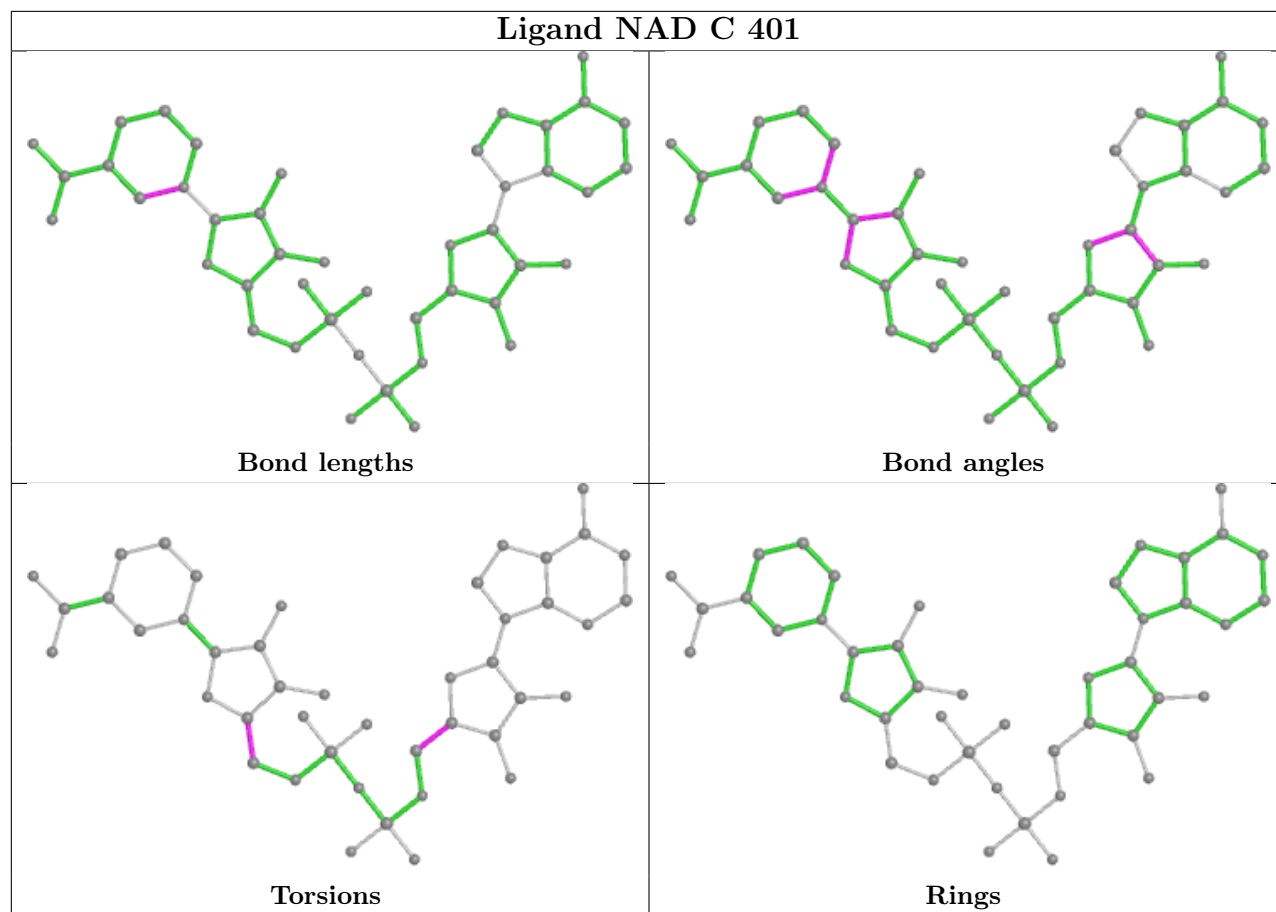
There are no ring outliers.

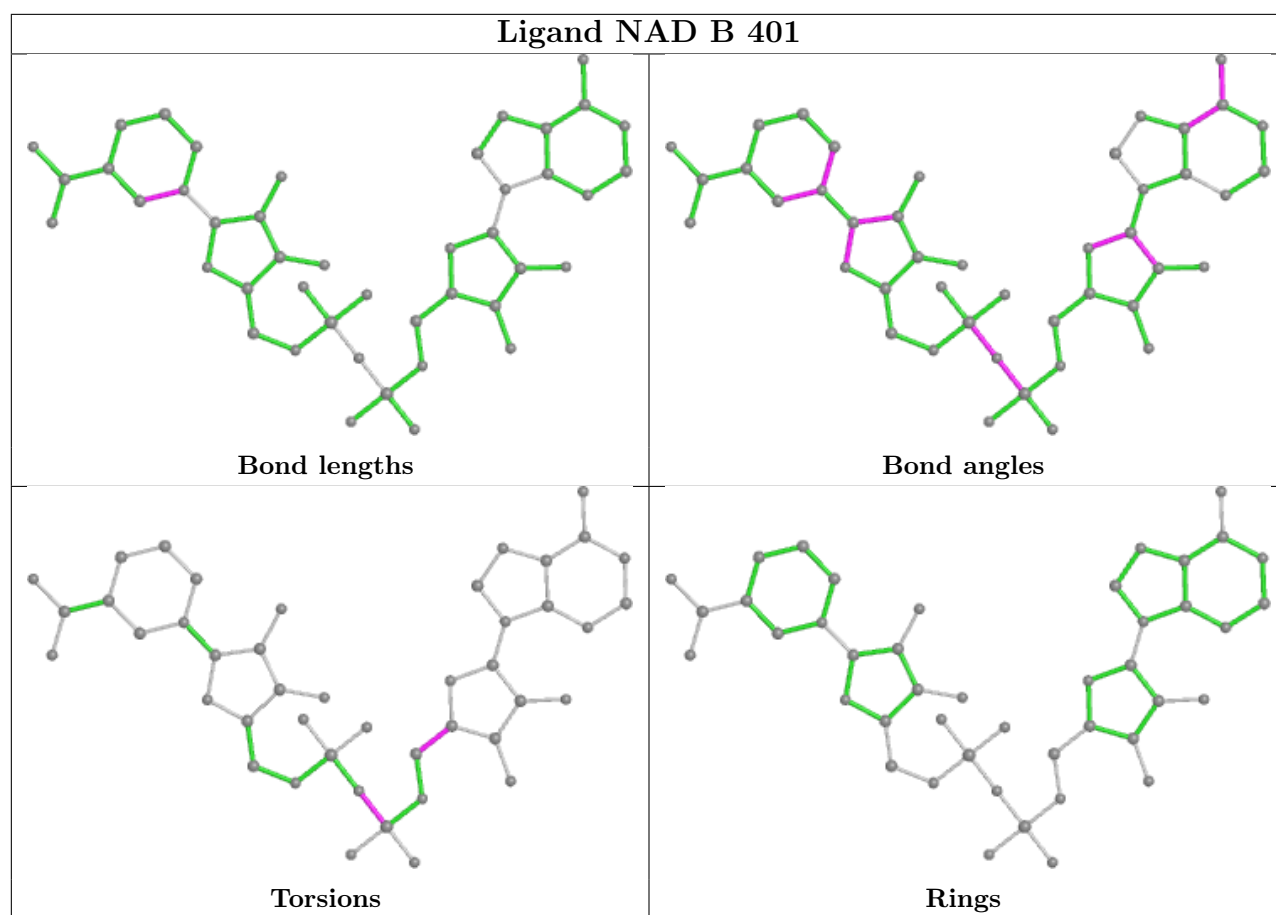
4 monomers are involved in 17 short contacts:

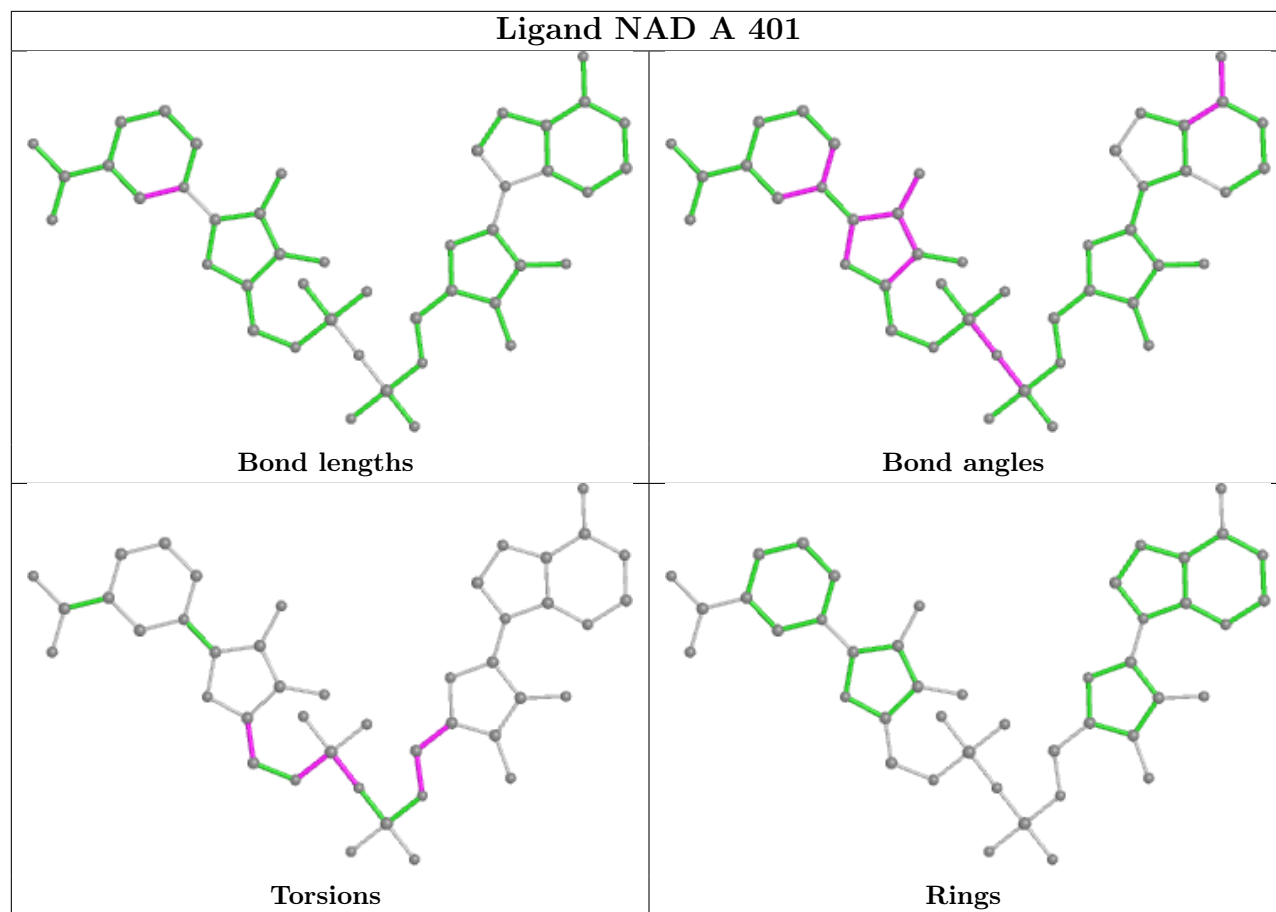
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NAD	3	0
2	C	401	NAD	8	0
2	B	401	NAD	3	0
2	A	401	NAD	3	0

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	310/339 (91%)	0.43	23 (7%)	14 16	26, 43, 82, 110	0
1	B	303/339 (89%)	0.39	16 (5%)	26 29	29, 44, 77, 116	0
1	C	310/339 (91%)	0.44	16 (5%)	27 30	31, 45, 87, 121	0
1	D	303/339 (89%)	0.54	22 (7%)	15 16	30, 50, 80, 125	0
All	All	1226/1356 (90%)	0.45	77 (6%)	20 21	26, 45, 82, 125	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	45	TYR	7.2
1	C	183	GLY	7.0
1	B	79	LEU	7.0
1	C	201	LYS	6.6
1	B	80	LEU	6.5
1	D	81	SER	5.3
1	A	85	GLU	4.8
1	A	80	LEU	4.8
1	A	45	TYR	4.4
1	D	197	LEU	4.3
1	D	92	TRP	4.0
1	C	85	GLU	3.9
1	D	45	TYR	3.8
1	A	314	VAL	3.5
1	A	233	GLU	3.5
1	C	52	TYR	3.5
1	D	52	TYR	3.5
1	A	181	PRO	3.4
1	A	84	GLY	3.3
1	C	195	GLU	3.3
1	B	81	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	94	LEU	3.2
1	A	201	LYS	3.2
1	B	181	PRO	3.2
1	B	44	LEU	3.1
1	C	44	LEU	3.1
1	C	264	PHE	3.1
1	D	79	LEU	3.1
1	C	199	GLY	3.1
1	D	253	LEU	3.1
1	A	82	ALA	3.0
1	B	109	ARG	3.0
1	A	83	THR	3.0
1	B	45	TYR	2.9
1	C	200	GLY	2.9
1	D	44	LEU	2.9
1	A	47	ALA	2.9
1	A	272	VAL	2.8
1	D	80	LEU	2.8
1	B	111	PRO	2.7
1	D	263	ASP	2.7
1	D	111	PRO	2.7
1	D	198	LYS	2.7
1	C	47	ALA	2.7
1	B	94	LEU	2.7
1	D	194	TYR	2.6
1	A	88	PRO	2.6
1	A	262	PRO	2.6
1	D	43	ASN	2.6
1	B	233	GLU	2.6
1	D	267	THR	2.5
1	A	183	GLY	2.5
1	B	91	ALA	2.5
1	A	180	PRO	2.5
1	B	52	TYR	2.4
1	D	235	LEU	2.4
1	A	29	TYR	2.4
1	A	202	TYR	2.4
1	A	231	PRO	2.4
1	C	109	ARG	2.3
1	A	39	ILE	2.3
1	A	89	GLN	2.3
1	C	108	GLU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	182	GLY	2.3
1	C	182	GLY	2.3
1	D	268	TYR	2.3
1	D	47	ALA	2.3
1	B	194	TYR	2.3
1	D	182	GLY	2.3
1	B	276	ILE	2.3
1	B	182	GLY	2.2
1	C	206	LEU	2.2
1	B	199	GLY	2.1
1	D	181	PRO	2.1
1	D	264	PHE	2.1
1	A	198	LYS	2.0
1	C	80	LEU	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](#)

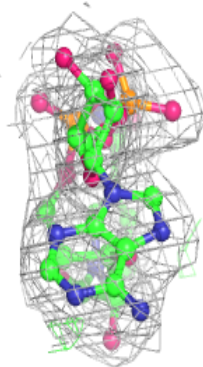
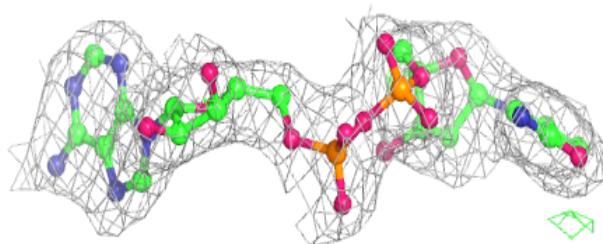
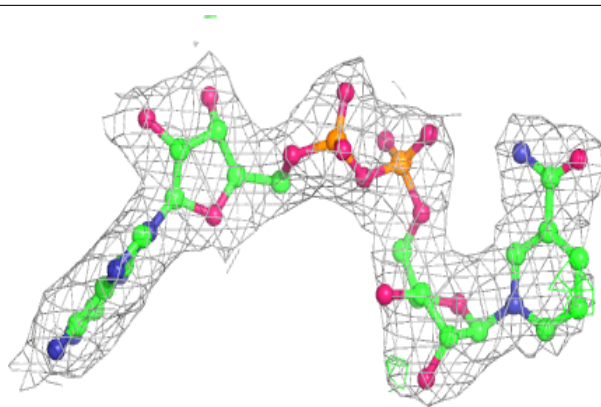
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	D	401	44/44	0.95	0.12	31,49,56,60	0
2	NAD	C	401	44/44	0.95	0.15	31,39,48,54	0
2	NAD	A	401	44/44	0.95	0.17	32,39,51,62	0
2	NAD	B	401	44/44	0.97	0.12	36,44,55,59	0

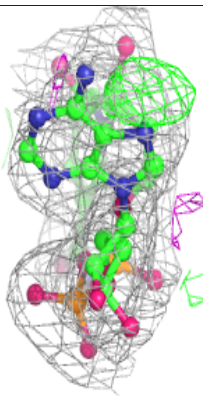
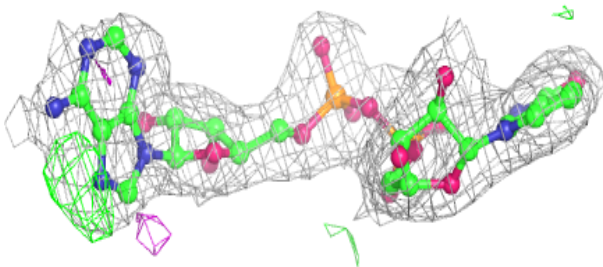
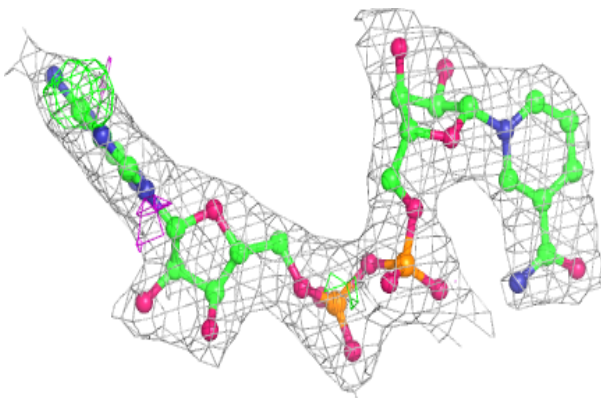
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAD D 401:**

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

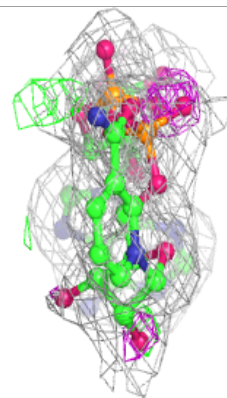
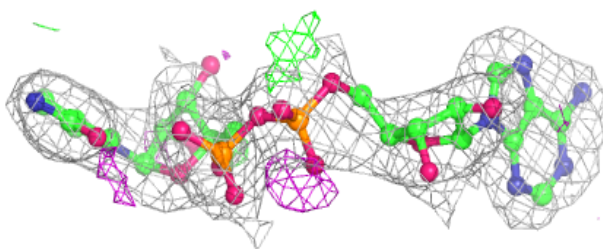
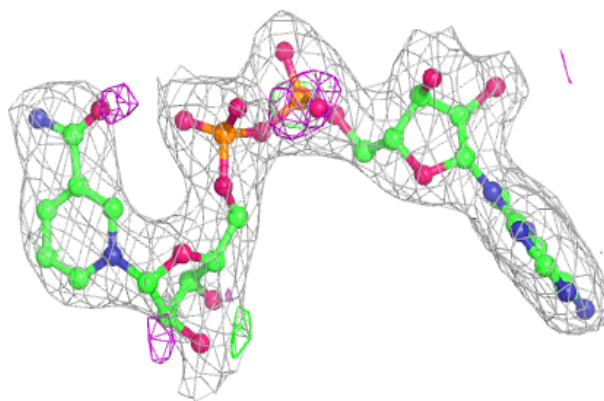
**Electron density around NAD C 401:**

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

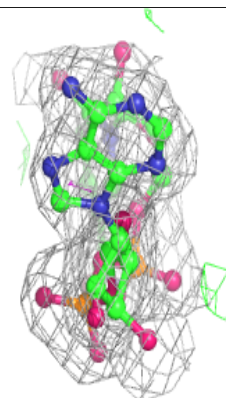
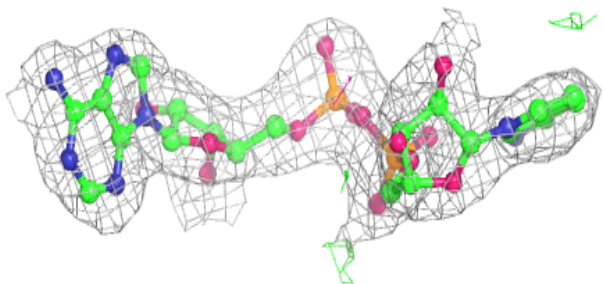
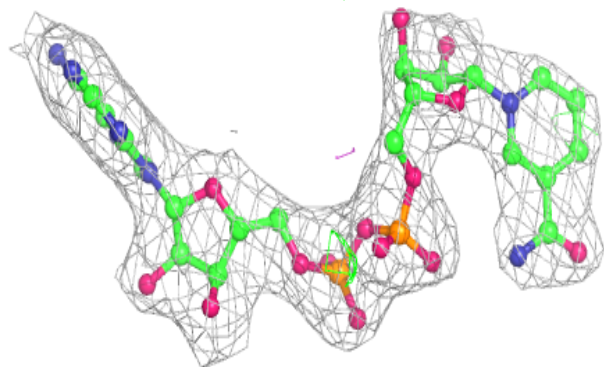


**Electron density around NAD A 401:**

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

**Electron density around NAD B 401:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.