Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:16 PM BST

PDB ID	:	6H0P
Title	:	The structure of C100A mutant of Arabidopsis thaliana UDP-apiose/UDP-xylose synthase in complex with NADH and UDP-D-glucuronic acid
Authors	:	Savino, S.; Mattevi, A.
Deposited on	:	2018-07-10
Resolution	:	3.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

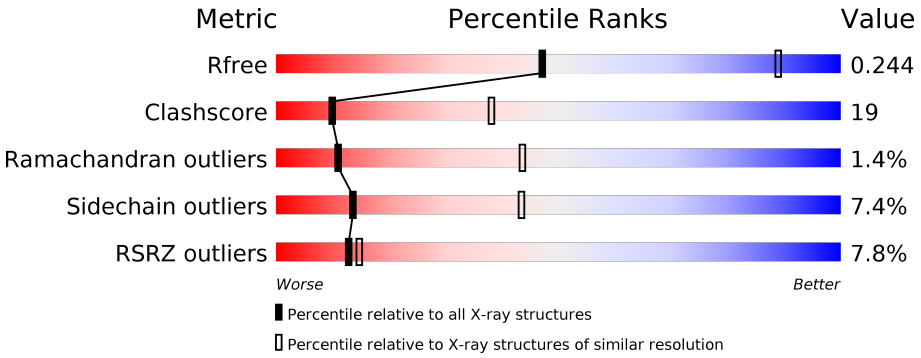
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.47 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	389	6% 67% 26%
1	B	389	9% 69% 21% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5869 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.

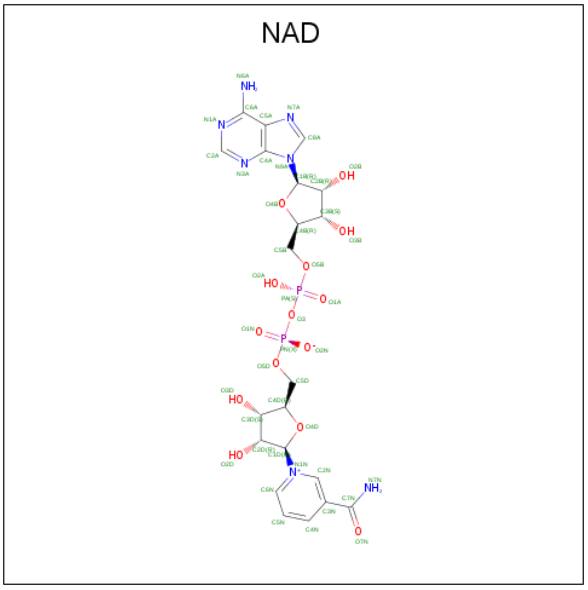
- Molecule 1 is a protein called UDP-D-apiose/UDP-D-xylose synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2892	1844	488	546	14			
1	B	367	Total	C	N	O	S	0	0	0
			2833	1808	478	534	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ALA	CYS	engineered mutation	UNP Q9ZUY6
B	100	ALA	CYS	engineered mutation	UNP Q9ZUY6

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

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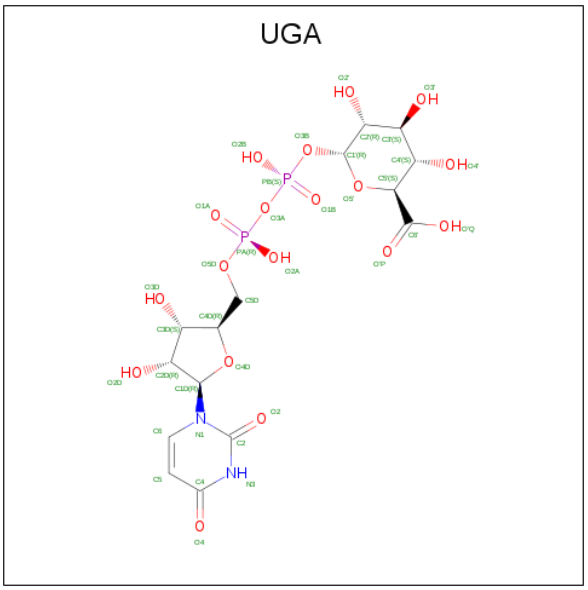
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula: $C_{15}H_{22}N_2O_{18}P_2$).



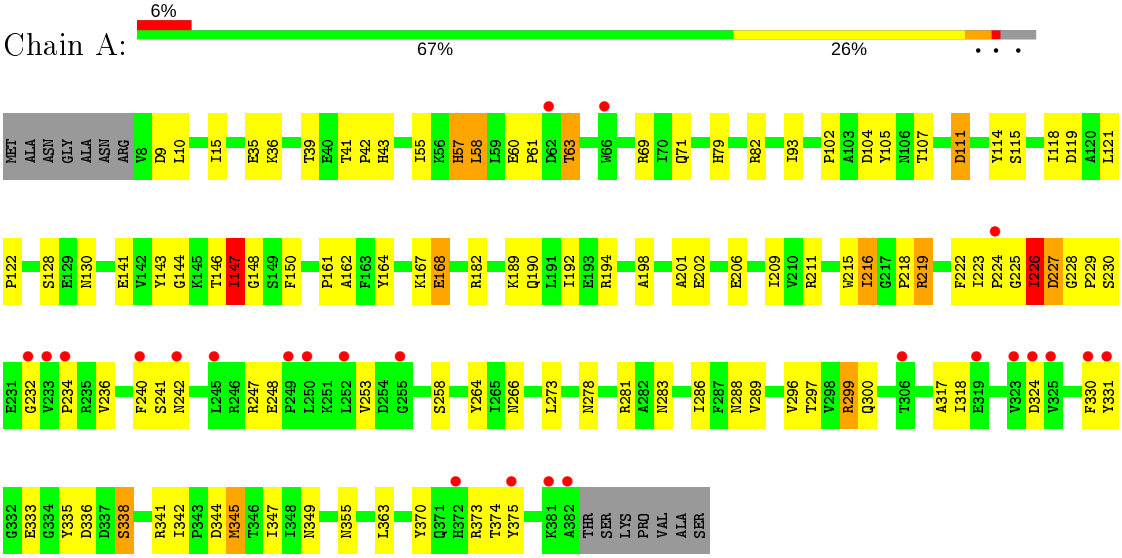
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

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.

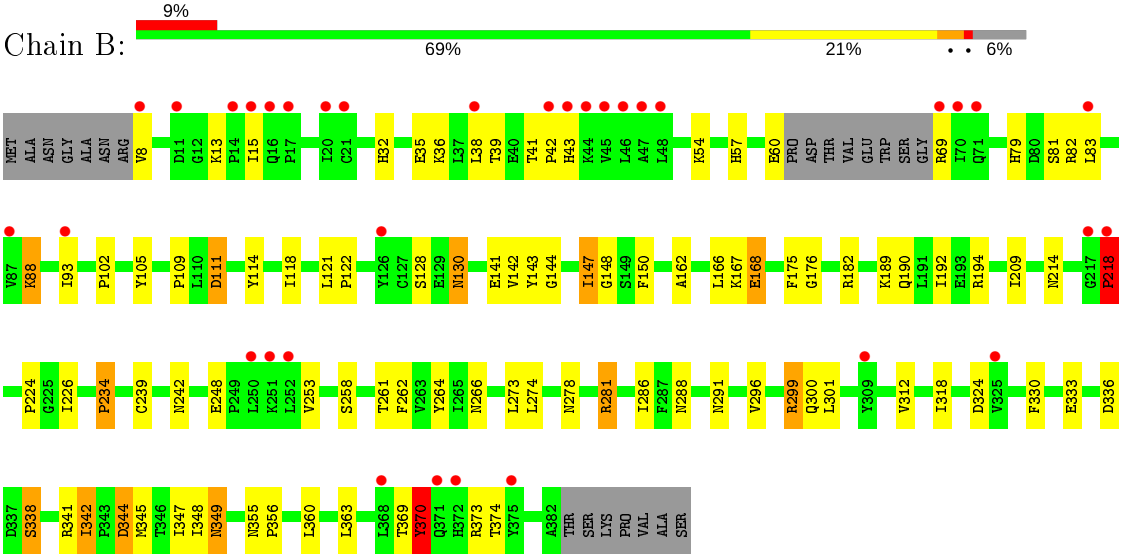
- Molecule 1: UDP-D-apiose/UDP-D-xylose synthase 1

Chain A:



- Molecule 1: UDP-D-apiose/UDP-D-xylose synthase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.56Å 144.56Å 130.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.44 – 3.47 48.44 – 3.47	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.44-3.47) 99.9 (48.44-3.47)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.196 , 0.239 0.203 , 0.244	Depositor DCC
R_{free} test set	1073 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	122.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 100.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5869	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UGA, 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	0.68	0/2960	0.95	1/4039 (0.0%)
1	B	0.66	0/2897	1.00	2/3947 (0.1%)
All	All	0.67	0/5857	0.97	3/7986 (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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	370	TYR	CB-CG-CD1	6.05	124.63	121.00
1	A	331	TYR	CB-CG-CD2	5.47	124.28	121.00
1	B	218	PRO	N-CA-CB	-5.45	96.61	102.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	ARG	Sidechain
1	A	373	ARG	Sidechain
1	B	299	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	373	ARG	Sidechain

5.2 Too-close contacts (i)

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	2892	0	2780	131	0
1	B	2833	0	2742	97	0
2	A	35	0	19	0	0
2	B	35	0	19	0	0
3	A	37	0	19	1	0
3	B	37	0	18	3	0
All	All	5869	0	5597	219	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 19.

All (219) 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:A:218:PRO:HB3	1:A:370:TYR:CD2	1.44	1.53
1:A:55:ILE:O	1:A:58:LEU:CD1	1.72	1.37
1:B:224:PRO:HD2	1:B:242:ASN:ND2	1.51	1.25
1:A:55:ILE:O	1:A:58:LEU:HD12	1.10	1.23
1:A:55:ILE:HA	1:A:58:LEU:HD11	1.22	1.14
1:A:55:ILE:CA	1:A:58:LEU:HD11	1.77	1.14
1:A:218:PRO:HB3	1:A:370:TYR:CE2	1.83	1.14
1:A:224:PRO:HD2	1:A:242:ASN:HD22	1.13	1.07
1:B:141:GLU:OE2	1:B:182:ARG:NH2	1.86	1.07
1:A:215:TRP:C	1:A:216:ILE:HD13	1.78	1.04
1:A:55:ILE:C	1:A:58:LEU:CD1	2.26	1.03
1:A:218:PRO:CB	1:A:370:TYR:CD2	2.40	1.03
1:B:224:PRO:CD	1:B:242:ASN:HD22	1.72	1.01
1:A:224:PRO:HD2	1:A:242:ASN:ND2	1.74	1.01
1:B:54:LYS:O	1:B:57:HIS:NE2	1.93	1.00
1:A:297:THR:H	1:A:300:GLN:NE2	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:CD	1:A:182:ARG:HH22	1.69	0.96
1:A:218:PRO:CB	1:A:370:TYR:HD2	1.77	0.96
1:A:55:ILE:CA	1:A:58:LEU:CD1	2.43	0.96
1:A:253:VAL:HG22	1:A:330:PHE:HD2	1.30	0.95
1:A:190:GLN:HE21	1:A:194:ARG:HE	1.15	0.94
1:B:345:MET:O	1:B:349:ASN:HB2	1.68	0.93
1:B:224:PRO:HD2	1:B:242:ASN:HD22	0.78	0.93
1:A:55:ILE:C	1:A:58:LEU:HD12	1.88	0.92
1:A:202:GLU:OE2	1:B:109:PRO:CD	2.19	0.90
1:A:60:GLU:HA	1:A:63:THR:O	1.71	0.89
1:A:345:MET:O	1:A:349:ASN:HB2	1.72	0.88
1:B:190:GLN:HE21	1:B:194:ARG:HE	1.21	0.86
1:A:55:ILE:HB	1:A:58:LEU:HD13	1.55	0.86
1:A:253:VAL:CG2	1:A:330:PHE:HD2	1.90	0.84
1:A:57:HIS:CD2	1:A:58:LEU:HG	2.14	0.81
1:A:58:LEU:HD12	1:A:58:LEU:H	1.44	0.81
1:A:202:GLU:OE2	1:B:109:PRO:HD2	1.81	0.80
1:B:253:VAL:HG22	1:B:330:PHE:HD2	1.47	0.80
1:A:218:PRO:CB	1:A:370:TYR:CE2	2.61	0.79
1:B:281:ARG:HH11	1:B:281:ARG:HG2	1.45	0.79
1:A:215:TRP:O	1:A:216:ILE:CD1	2.33	0.76
1:B:141:GLU:O	1:B:144:GLY:N	2.18	0.75
1:A:55:ILE:O	1:A:58:LEU:HD13	1.82	0.74
1:A:36:LYS:NZ	1:A:266:ASN:ND2	2.37	0.73
1:A:57:HIS:HD2	1:A:58:LEU:CD1	2.01	0.73
1:A:222:PHE:CE1	1:A:229:PRO:HD2	2.23	0.73
1:A:224:PRO:CD	1:A:242:ASN:HD22	1.98	0.72
1:A:215:TRP:C	1:A:216:ILE:CD1	2.54	0.72
1:A:218:PRO:HB3	1:A:370:TYR:HD2	0.93	0.72
1:B:43:HIS:O	1:B:69:ARG:NH1	2.22	0.72
1:B:344:ASP:C	1:B:344:ASP:OD1	2.28	0.71
1:A:253:VAL:HG22	1:A:330:PHE:CD2	2.21	0.70
1:A:60:GLU:CA	1:A:63:THR:O	2.41	0.69
1:A:190:GLN:NE2	1:A:194:ARG:HE	1.88	0.69
1:B:370:TYR:O	1:B:370:TYR:CD1	2.45	0.69
1:B:141:GLU:HG3	1:B:341:ARG:NH2	2.08	0.69
1:A:215:TRP:O	1:A:216:ILE:HD13	1.93	0.68
1:A:226:ILE:HD13	1:A:226:ILE:N	2.07	0.68
1:A:58:LEU:N	1:A:58:LEU:HD12	2.07	0.68
1:B:88:LYS:HG3	1:B:130:ASN:OD1	1.94	0.68
1:A:198:ALA:O	1:A:201:ALA:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:HE21	1:A:194:ARG:NE	1.91	0.67
1:A:55:ILE:HB	1:A:58:LEU:CD1	2.25	0.66
1:B:209:ILE:HB	1:B:286:ILE:HG12	1.77	0.66
1:A:209:ILE:HB	1:A:286:ILE:HG12	1.79	0.65
1:A:215:TRP:O	1:A:216:ILE:HD12	1.97	0.65
1:A:55:ILE:CB	1:A:58:LEU:CD1	2.74	0.65
1:A:297:THR:H	1:A:300:GLN:HE21	1.43	0.65
1:A:141:GLU:OE1	1:A:182:ARG:NH2	2.29	0.65
1:A:36:LYS:NZ	1:A:266:ASN:HD21	1.94	0.64
1:B:190:GLN:NE2	1:B:194:ARG:HE	1.94	0.64
1:A:253:VAL:CG2	1:A:330:PHE:CD2	2.78	0.64
1:A:216:ILE:N	1:A:216:ILE:HD13	2.12	0.64
1:A:202:GLU:OE2	1:B:109:PRO:CG	2.46	0.64
1:B:253:VAL:CG2	1:B:330:PHE:HD2	2.09	0.64
1:B:36:LYS:NZ	1:B:266:ASN:ND2	2.45	0.64
1:B:288:ASN:HD22	1:B:344:ASP:H	1.46	0.63
1:A:202:GLU:OE2	1:B:109:PRO:HG2	1.98	0.63
1:B:190:GLN:HE21	1:B:194:ARG:NE	1.95	0.63
1:B:167:LYS:HE2	1:B:347:ILE:HD11	1.79	0.62
1:B:182:ARG:HD2	1:B:336:ASP:O	2.00	0.62
1:A:57:HIS:CD2	1:A:58:LEU:CG	2.83	0.61
1:A:370:TYR:CD1	1:A:370:TYR:O	2.53	0.61
1:A:202:GLU:OE2	1:B:109:PRO:N	2.34	0.60
1:B:144:GLY:O	1:B:338:SER:OG	2.18	0.60
1:A:43:HIS:O	1:A:69:ARG:NH1	2.34	0.60
1:A:167:LYS:HG3	1:A:344:ASP:OD2	2.01	0.60
1:A:150:PHE:CD1	1:B:147:ILE:HD11	2.36	0.60
1:A:225:GLY:N	1:A:229:PRO:O	2.31	0.60
1:A:57:HIS:CD2	1:A:58:LEU:CD1	2.84	0.60
1:A:167:LYS:HE2	1:A:347:ILE:HD11	1.85	0.59
1:B:130:ASN:N	1:B:130:ASN:HD22	2.00	0.59
1:B:36:LYS:NZ	1:B:266:ASN:HD21	1.99	0.59
1:A:36:LYS:HZ1	1:A:266:ASN:ND2	2.00	0.58
1:A:297:THR:N	1:A:300:GLN:NE2	2.43	0.58
1:B:347:ILE:H	1:B:347:ILE:HD12	1.69	0.58
1:B:370:TYR:O	1:B:370:TYR:HD1	1.86	0.57
1:B:342:ILE:HG22	1:B:342:ILE:O	2.04	0.57
1:B:57:HIS:CD2	1:B:57:HIS:H	2.20	0.57
1:A:227:ASP:OD2	1:A:375:TYR:CE1	2.57	0.57
1:A:182:ARG:HD2	1:A:336:ASP:O	2.05	0.57
1:A:36:LYS:CE	1:A:266:ASN:HD22	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:PRO:HD2	1:B:239:CYS:SG	2.45	0.57
1:A:55:ILE:CB	1:A:58:LEU:HD13	2.30	0.57
1:A:299:ARG:NH2	1:A:324:ASP:OD1	2.38	0.57
1:A:10:LEU:H	1:A:278:ASN:HD21	1.50	0.56
1:B:168:GLU:OE2	1:B:288:ASN:N	2.31	0.56
1:B:349:ASN:HD21	1:B:355:ASN:HD21	1.52	0.56
1:B:182:ARG:CD	1:B:336:ASP:O	2.53	0.56
1:A:35:GLU:O	1:A:39:THR:HG23	2.06	0.55
1:A:281:ARG:HG2	1:A:281:ARG:HH11	1.71	0.55
1:B:114:TYR:CE2	1:B:118:ILE:HD12	2.41	0.55
1:B:41:THR:HB	1:B:42:PRO:HD2	1.89	0.55
1:A:182:ARG:CD	1:A:336:ASP:O	2.55	0.54
1:A:57:HIS:HD2	1:A:58:LEU:HD11	1.72	0.54
1:B:121:LEU:HB2	1:B:122:PRO:HD3	1.90	0.53
1:A:57:HIS:CD2	1:A:58:LEU:HD11	2.43	0.53
1:B:370:TYR:CE1	1:B:374:THR:OG1	2.62	0.53
1:A:216:ILE:CD1	1:A:216:ILE:N	2.72	0.52
1:A:141:GLU:HG3	1:A:341:ARG:NH2	2.25	0.52
1:A:35:GLU:OE1	1:A:219:ARG:NH1	2.42	0.52
1:A:370:TYR:HE1	1:A:374:THR:HG1	1.56	0.52
1:A:55:ILE:CB	1:A:58:LEU:HD11	2.37	0.52
1:B:141:GLU:CG	1:B:341:ARG:NH2	2.73	0.51
1:A:223:ILE:N	1:A:227:ASP:OD1	2.43	0.51
1:B:370:TYR:HE1	1:B:374:THR:OG1	1.92	0.51
1:B:281:ARG:HG2	1:B:281:ARG:NH1	2.20	0.51
1:A:60:GLU:O	1:A:63:THR:O	2.28	0.51
1:A:297:THR:N	1:A:300:GLN:HE21	2.07	0.50
1:A:60:GLU:N	1:A:61:PRO:HD2	2.25	0.50
1:A:102:PRO:HA	1:A:105:TYR:CE2	2.47	0.50
1:B:182:ARG:HH21	1:B:182:ARG:HG2	1.76	0.50
1:B:253:VAL:HG22	1:B:330:PHE:CD2	2.37	0.50
1:B:264:TYR:CD1	1:B:363:LEU:HB2	2.47	0.50
1:A:41:THR:HG21	1:A:273:LEU:HD11	1.94	0.50
1:A:240:PHE:O	1:A:241:SER:C	2.49	0.49
1:A:206:GLU:HG2	1:A:283:ASN:ND2	2.27	0.49
1:B:182:ARG:NH1	3:B:402:UGA:O2B	2.45	0.49
1:A:206:GLU:HG2	1:A:283:ASN:HD22	1.76	0.49
1:A:114:TYR:CE2	1:A:118:ILE:HD12	2.48	0.49
1:B:262:PHE:CZ	1:B:301:LEU:HD22	2.47	0.49
1:B:57:HIS:CD2	1:B:57:HIS:N	2.81	0.48
1:B:36:LYS:CE	1:B:266:ASN:HD22	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PRO:HB3	1:B:370:TYR:CE2	2.48	0.48
1:A:335:TYR:HH	3:A:402:UGA:HOA3	1.60	0.48
1:B:299:ARG:NH2	1:B:324:ASP:OD1	2.46	0.48
1:B:370:TYR:C	1:B:370:TYR:CD1	2.86	0.48
1:A:121:LEU:HB2	1:A:122:PRO:HD3	1.94	0.48
1:A:147:ILE:HD11	1:B:150:PHE:CD1	2.48	0.48
1:A:247:ARG:NH2	1:A:317:ALA:O	2.47	0.47
1:A:161:PRO:HA	1:A:164:TYR:CZ	2.49	0.47
1:B:102:PRO:HA	1:B:105:TYR:CE2	2.50	0.47
1:B:347:ILE:N	1:B:347:ILE:HD12	2.29	0.47
1:A:147:ILE:CG2	1:A:148:GLY:N	2.78	0.47
1:A:182:ARG:HG2	1:A:182:ARG:HH21	1.80	0.47
1:A:347:ILE:HD12	1:A:347:ILE:H	1.80	0.46
1:A:36:LYS:CE	1:A:266:ASN:ND2	2.77	0.46
1:B:312:VAL:HG13	1:B:369:THR:HG22	1.97	0.46
1:A:227:ASP:OD2	1:A:375:TYR:HE1	1.98	0.46
1:B:274:LEU:O	1:B:278:ASN:HB2	2.15	0.46
1:A:229:PRO:HG2	1:A:232:GLY:HA3	1.97	0.46
1:B:35:GLU:O	1:B:39:THR:HG23	2.16	0.46
1:B:38:LEU:HA	1:B:69:ARG:NH2	2.30	0.46
1:A:161:PRO:HA	1:A:164:TYR:CE2	2.51	0.46
1:A:218:PRO:CB	1:A:370:TYR:HE2	2.23	0.46
1:B:121:LEU:N	1:B:122:PRO:CD	2.78	0.46
1:B:189:LYS:O	1:B:192:ILE:HG22	2.16	0.46
1:A:36:LYS:HZ3	1:A:266:ASN:HD21	1.62	0.46
1:B:41:THR:HG21	1:B:273:LEU:HD11	1.98	0.46
1:A:189:LYS:O	1:A:192:ILE:HG22	2.16	0.45
1:A:222:PHE:CD1	1:A:228:GLY:HA3	2.51	0.45
1:A:146:THR:O	1:A:147:ILE:C	2.55	0.45
1:A:264:TYR:CD1	1:A:363:LEU:HB2	2.52	0.45
1:A:296:VAL:HB	1:A:300:GLN:HE21	1.82	0.45
1:A:190:GLN:HE22	1:B:175:PHE:HD2	1.64	0.45
1:A:141:GLU:CD	1:A:182:ARG:NH2	2.53	0.45
1:B:261:THR:OG1	1:B:261:THR:O	2.28	0.45
1:A:370:TYR:CD1	1:A:370:TYR:C	2.91	0.44
1:B:114:TYR:CD2	1:B:118:ILE:HD12	2.53	0.44
1:B:147:ILE:CG2	1:B:148:GLY:N	2.81	0.44
1:B:36:LYS:HZ3	1:B:266:ASN:HD21	1.61	0.44
1:A:41:THR:HB	1:A:42:PRO:HD2	2.00	0.44
1:B:291:ASN:HA	1:B:356:PRO:HG3	2.00	0.44
1:B:114:TYR:HA	1:B:118:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLY:C	1:A:226:ILE:HD13	2.38	0.43
1:A:143:TYR:CZ	1:A:211:ARG:NH1	2.86	0.43
1:B:253:VAL:HG23	3:B:402:UGA:C2	2.48	0.43
1:B:370:TYR:HE1	1:B:374:THR:HG1	1.55	0.43
1:B:345:MET:HA	1:B:348:ILE:HG22	2.00	0.43
1:A:115:SER:HA	1:A:119:ASP:OD2	2.18	0.43
1:A:111:ASP:N	1:A:111:ASP:OD1	2.48	0.43
1:B:349:ASN:HD21	1:B:355:ASN:ND2	2.15	0.43
1:B:36:LYS:HZ1	1:B:266:ASN:ND2	2.14	0.42
1:B:60:GLU:HA	1:B:60:GLU:OE2	2.19	0.42
1:B:344:ASP:O	1:B:345:MET:CB	2.64	0.42
1:A:227:ASP:OD2	1:A:375:TYR:CZ	2.73	0.42
1:A:227:ASP:OD2	1:A:375:TYR:OH	2.32	0.42
1:B:253:VAL:CG2	1:B:330:PHE:CD2	2.97	0.42
1:B:344:ASP:C	1:B:345:MET:HG2	2.40	0.42
1:A:296:VAL:HB	1:A:300:GLN:HB2	2.00	0.42
1:B:130:ASN:N	1:B:130:ASN:ND2	2.67	0.42
1:A:144:GLY:O	1:A:338:SER:OG	2.34	0.42
1:B:36:LYS:CE	1:B:266:ASN:ND2	2.83	0.42
1:A:215:TRP:CZ2	1:A:289:VAL:HG11	2.55	0.41
1:A:226:ILE:HB	1:A:227:ASP:H	1.62	0.41
1:B:218:PRO:HB3	1:B:370:TYR:CD2	2.55	0.41
1:A:141:GLU:CG	1:A:341:ARG:NH2	2.83	0.41
1:B:143:TYR:CD1	1:B:166:LEU:HB3	2.55	0.41
1:A:168:GLU:OE2	1:A:288:ASN:N	2.39	0.41
1:B:141:GLU:O	1:B:142:VAL:C	2.59	0.41
1:A:349:ASN:HD21	1:A:355:ASN:HD21	1.67	0.41
1:B:111:ASP:OD1	1:B:111:ASP:N	2.54	0.41
1:B:296:VAL:HB	1:B:300:GLN:HB2	2.02	0.41
1:B:57:HIS:H	1:B:57:HIS:HD2	1.66	0.41
1:A:347:ILE:HD12	1:A:347:ILE:N	2.35	0.41
1:B:32:HIS:CE1	1:B:218:PRO:HB2	2.56	0.41
1:B:214:ASN:HA	3:B:402:UGA:O'P	2.21	0.40
1:B:81:SER:O	1:B:83:LEU:N	2.54	0.40
1:A:104:ASP:HA	1:A:107:THR:OG1	2.21	0.40
1:A:194:ARG:NH2	1:B:176:GLY:O	2.53	0.40
1:A:9:ASP:HB2	1:A:278:ASN:HD21	1.85	0.40
1:B:360:LEU:O	1:B:363:LEU:HG	2.22	0.40
1:B:8:VAL:HG23	1:B:13:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	373/389 (96%)	340 (91%)	27 (7%)	6 (2%)	9 41
1	B	363/389 (93%)	331 (91%)	28 (8%)	4 (1%)	14 50
All	All	736/778 (95%)	671 (91%)	55 (8%)	10 (1%)	11 43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	VAL
1	A	147	ILE
1	B	82	ARG
1	A	82	ARG
1	A	162	ALA
1	A	226	ILE
1	B	218	PRO
1	A	234	PRO
1	B	234	PRO
1	B	162	ALA

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	306/337 (91%)	282 (92%)	24 (8%)	12 41
1	B	301/337 (89%)	280 (93%)	21 (7%)	15 46
All	All	607/674 (90%)	562 (93%)	45 (7%)	13 43

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	57	HIS
1	A	58	LEU
1	A	63	THR
1	A	71	GLN
1	A	79	HIS
1	A	93	ILE
1	A	111	ASP
1	A	128	SER
1	A	130	ASN
1	A	147	ILE
1	A	168	GLU
1	A	216	ILE
1	A	219	ARG
1	A	226	ILE
1	A	227	ASP
1	A	230	SER
1	A	248	GLU
1	A	258	SER
1	A	318	ILE
1	A	333	GLU
1	A	338	SER
1	A	342	ILE
1	A	345	MET
1	B	15	ILE
1	B	79	HIS
1	B	88	LYS
1	B	93	ILE
1	B	111	ASP
1	B	128	SER
1	B	130	ASN
1	B	147	ILE
1	B	168	GLU
1	B	218	PRO
1	B	226	ILE
1	B	248	GLU
1	B	258	SER
1	B	281	ARG
1	B	318	ILE
1	B	333	GLU
1	B	338	SER
1	B	342	ILE

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Mol	Chain	Res	Type
1	B	344	ASP
1	B	349	ASN
1	B	370	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	57	HIS
1	A	130	ASN
1	A	190	GLN
1	A	203	ASN
1	A	242	ASN
1	A	243	ASN
1	A	266	ASN
1	A	278	ASN
1	A	285	HIS
1	A	294	ASN
1	A	300	GLN
1	A	349	ASN
1	A	355	ASN
1	A	372	HIS
1	B	79	HIS
1	B	190	GLN
1	B	203	ASN
1	B	242	ASN
1	B	266	ASN
1	B	288	ASN
1	B	355	ASN
1	B	372	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)

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	A	401	-	33,38,48	1.08	1 (3%)	37,58,73	2.33	9 (24%)
2	NAD	B	401	-	33,38,48	1.15	2 (6%)	37,58,73	2.49	11 (29%)
3	UGA	B	402	-	33,39,39	2.08	5 (15%)	46,60,60	2.28	14 (30%)
3	UGA	A	402	-	33,39,39	2.19	7 (21%)	46,60,60	2.17	13 (28%)

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	A	401	-	-	7/18/51/62	0/4/4/5
2	NAD	B	401	-	-	5/18/51/62	0/4/4/5
3	UGA	B	402	-	-	3/21/61/61	0/3/3/3
3	UGA	A	402	-	-	4/21/61/61	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	UGA	C6-N1	-7.68	1.33	1.47
3	B	402	UGA	C6-N1	-7.11	1.34	1.47
3	A	402	UGA	C2-N1	5.26	1.43	1.35
3	B	402	UGA	C2-N1	5.24	1.43	1.35
3	A	402	UGA	C5-C4	-4.54	1.39	1.50
3	A	402	UGA	C6-C5	-4.41	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	UGA	C6-C5	-4.37	1.40	1.52
3	B	402	UGA	C5-C4	-4.07	1.40	1.50
2	A	401	NAD	C1D-C2D	3.86	1.58	1.51
2	B	401	NAD	C1D-C2D	3.33	1.57	1.51
3	A	402	UGA	C4-N3	-2.74	1.32	1.37
3	B	402	UGA	O4-C4	2.36	1.28	1.23
3	A	402	UGA	C1D-N1	2.23	1.50	1.46
2	B	401	NAD	C2D-C3D	-2.21	1.50	1.53
3	A	402	UGA	C2-N3	-2.05	1.34	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	NAD	O4D-C4D-C3D	8.93	112.61	104.70
2	A	401	NAD	O4D-C4D-C3D	7.56	111.39	104.70
3	B	402	UGA	O3A-PB-O3B	7.41	117.43	102.48
3	A	402	UGA	N3-C2-N1	7.04	124.09	116.65
3	B	402	UGA	N3-C2-N1	5.72	122.71	116.65
3	A	402	UGA	C4-N3-C2	-5.49	121.24	125.79
2	B	401	NAD	C1D-C2D-C3D	5.34	109.76	101.63
2	B	401	NAD	O2D-C2D-C3D	-5.29	101.25	111.27
3	B	402	UGA	C4-N3-C2	-4.96	121.68	125.79
2	A	401	NAD	N3A-C2A-N1A	-4.80	121.18	128.68
2	A	401	NAD	C1B-N9A-C4A	-4.63	118.50	126.64
2	A	401	NAD	O2D-C2D-C1D	4.62	124.75	110.97
3	A	402	UGA	C6'-C5'-C4'	-4.48	101.85	113.04
3	B	402	UGA	C1'-C2'-C3'	4.32	119.00	110.00
3	A	402	UGA	O3A-PB-O3B	4.27	111.10	102.48
3	A	402	UGA	O2-C2-N3	-4.00	114.05	121.50
2	A	401	NAD	C1D-C2D-C3D	3.99	107.71	101.63
3	B	402	UGA	O2-C2-N3	-3.95	114.15	121.50
2	B	401	NAD	C4A-C5A-N7A	-3.93	105.31	109.40
2	A	401	NAD	O2D-C2D-C3D	-3.53	104.57	111.27
2	B	401	NAD	O2N-PN-O1N	3.39	128.98	112.24
2	B	401	NAD	N3A-C2A-N1A	-3.37	123.41	128.68
3	A	402	UGA	C1'-C2'-C3'	3.29	116.85	110.00
2	A	401	NAD	C5D-C4D-C3D	-3.24	103.03	115.18
3	B	402	UGA	C2D-C3D-C4D	-3.15	96.53	102.64
3	B	402	UGA	O2'-C2'-C3'	-3.11	103.17	110.35
2	B	401	NAD	C5D-C4D-C3D	-3.05	103.73	115.18
2	B	401	NAD	O2D-C2D-C1D	3.05	120.07	110.97
3	B	402	UGA	O4'-C4'-C5'	3.04	115.86	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	UGA	C5-C6-N1	2.96	121.38	111.61
3	B	402	UGA	C5-C6-N1	2.85	121.00	111.61
3	B	402	UGA	O3'-C3'-C4'	-2.82	103.82	110.35
3	A	402	UGA	C1'-O5'-C5'	2.68	116.58	112.24
3	B	402	UGA	C6'-C5'-C4'	-2.57	106.61	113.04
3	A	402	UGA	O2D-C2D-C3D	-2.53	103.64	111.82
2	B	401	NAD	C1B-N9A-C4A	-2.47	122.31	126.64
3	B	402	UGA	C1'-O5'-C5'	2.46	116.23	112.24
3	A	402	UGA	O3'-C3'-C4'	-2.46	104.65	110.35
3	A	402	UGA	O5'-C5'-C4'	2.45	112.95	108.91
2	A	401	NAD	C2B-C3B-C4B	2.34	107.18	102.64
2	B	401	NAD	O2A-PA-O5B	2.32	118.53	107.75
3	B	402	UGA	O3D-C3D-C2D	2.31	119.30	111.82
3	A	402	UGA	C2D-C3D-C4D	-2.29	98.19	102.64
3	B	402	UGA	C3'-C4'-C5'	-2.28	104.34	109.02
2	A	401	NAD	O2N-PN-O1N	2.18	123.00	112.24
3	A	402	UGA	O5'-C1'-O3B	2.17	114.21	111.36
2	B	401	NAD	O5B-PA-O1A	-2.04	101.10	109.07

There are no chirality outliers.

All (19) torsion outliers are listed below:

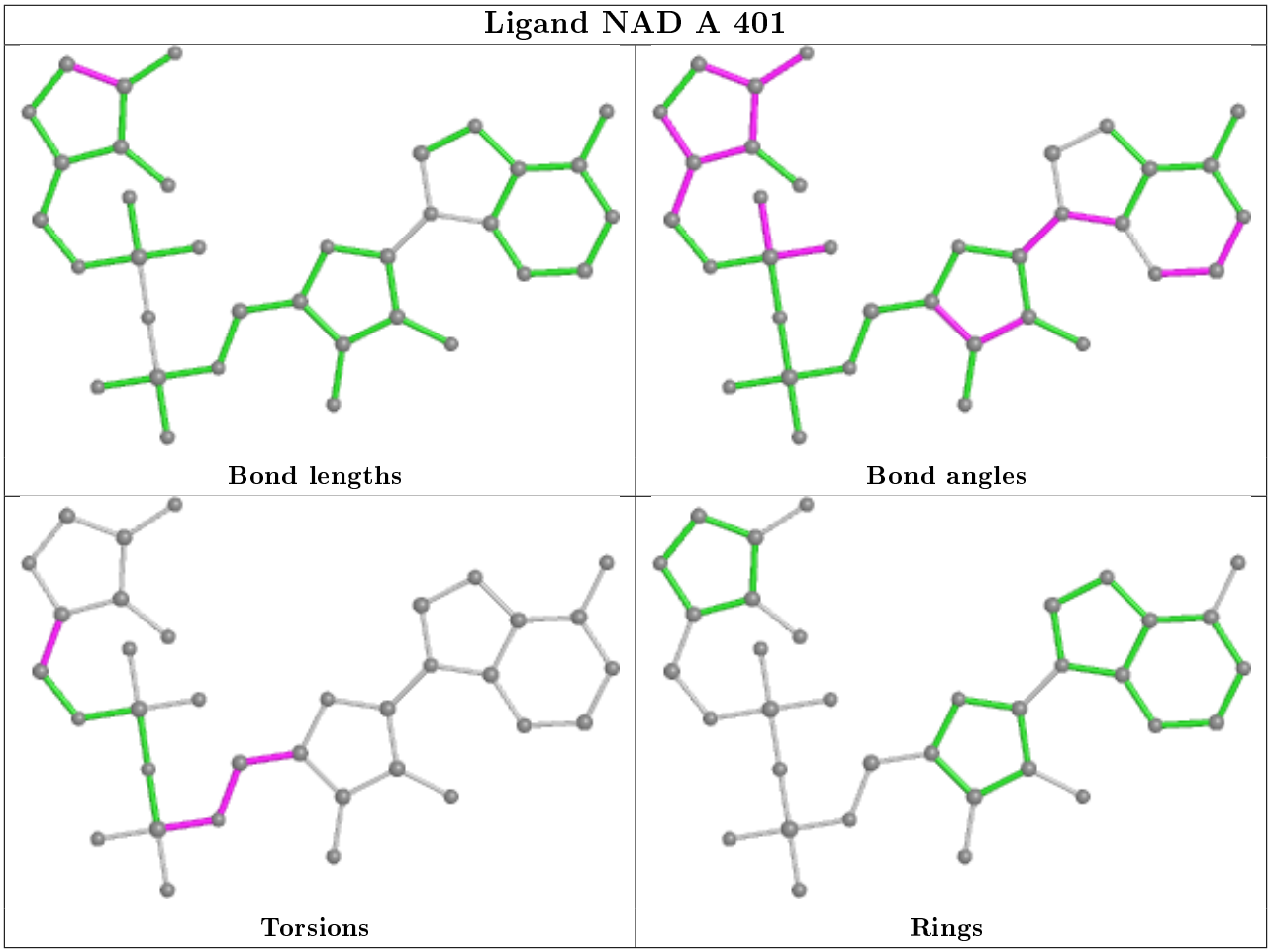
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
3	B	402	UGA	C5D-O5D-PA-O3A
3	A	402	UGA	C5D-O5D-PA-O3A
2	B	401	NAD	C3D-C4D-C5D-O5D
2	B	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	O4D-C4D-C5D-O5D
2	A	401	NAD	C3D-C4D-C5D-O5D
3	B	402	UGA	C5D-O5D-PA-O1A
3	B	402	UGA	C5D-O5D-PA-O2A
3	A	402	UGA	C5D-O5D-PA-O2A
2	B	401	NAD	C4B-C5B-O5B-PA
2	A	401	NAD	C4B-C5B-O5B-PA
2	A	401	NAD	C5B-O5B-PA-O3
2	B	401	NAD	C5B-O5B-PA-O3
2	A	401	NAD	O4B-C4B-C5B-O5B
3	A	402	UGA	PA-O3A-PB-O2B
2	A	401	NAD	C5B-O5B-PA-O2A
3	A	402	UGA	C5D-O5D-PA-O1A
2	B	401	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

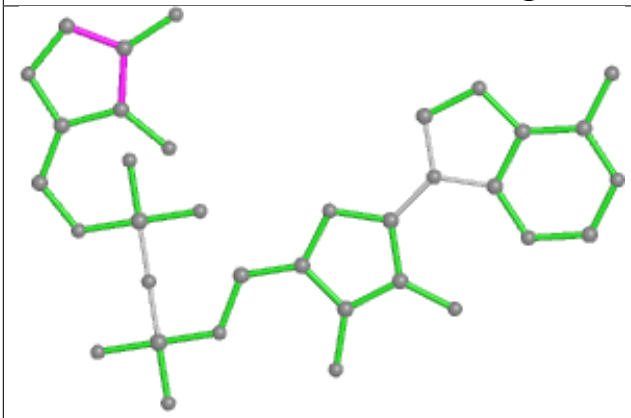
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	UGA	3	0
3	A	402	UGA	1	0

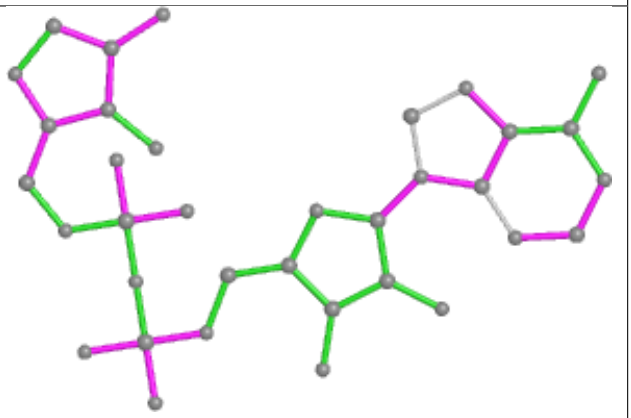
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



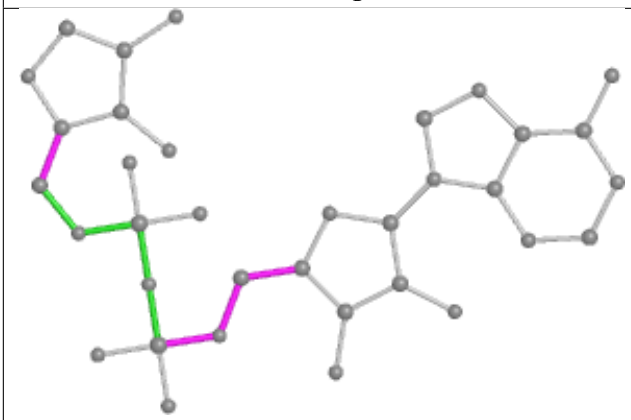
Ligand NAD B 401



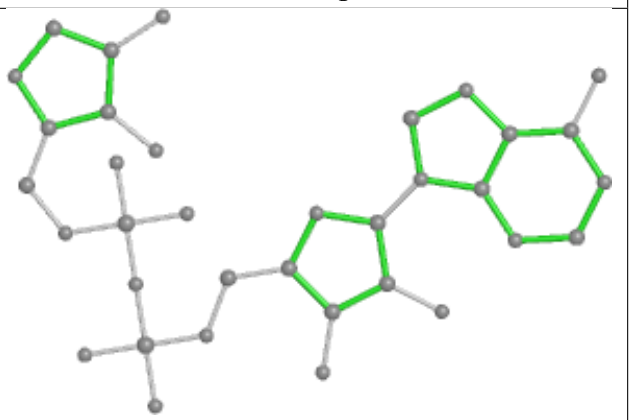
Bond lengths



Bond angles

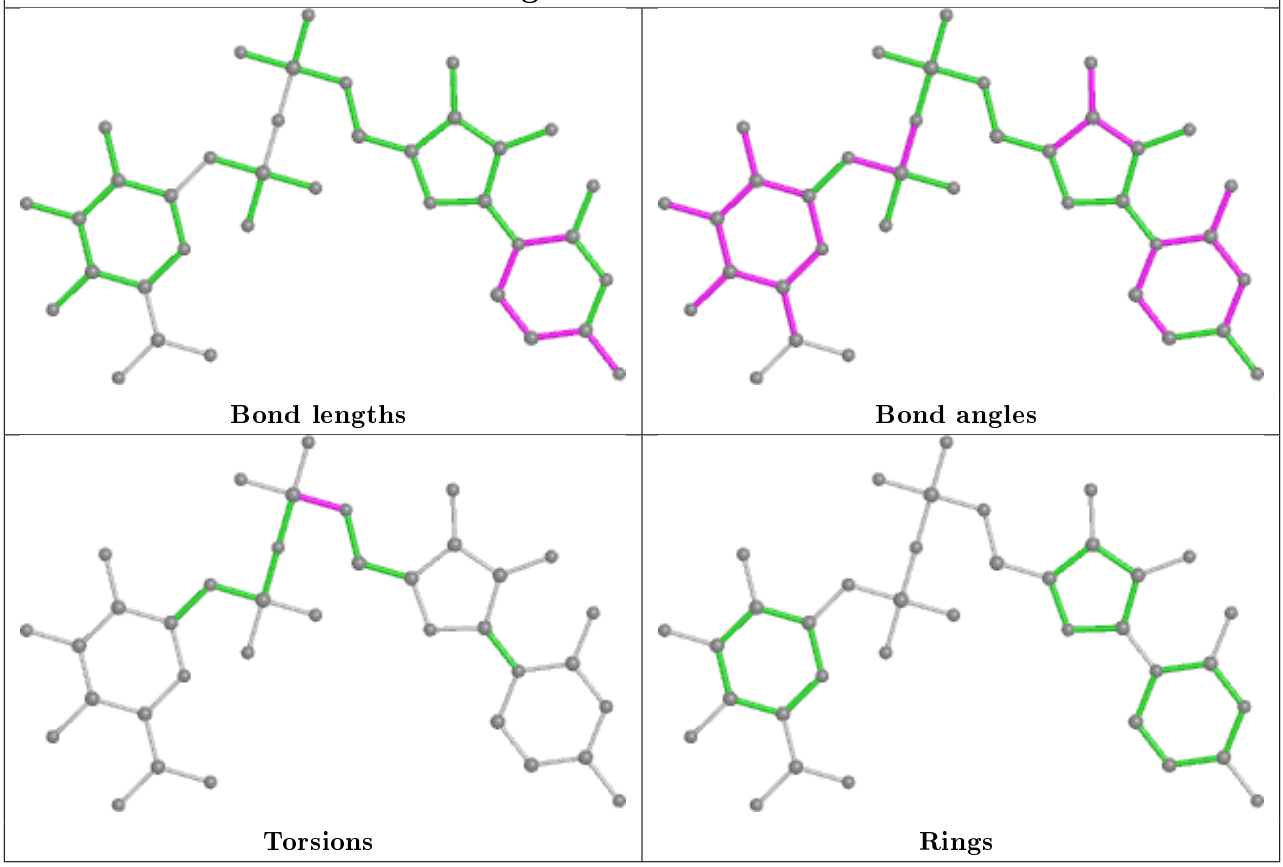


Torsions

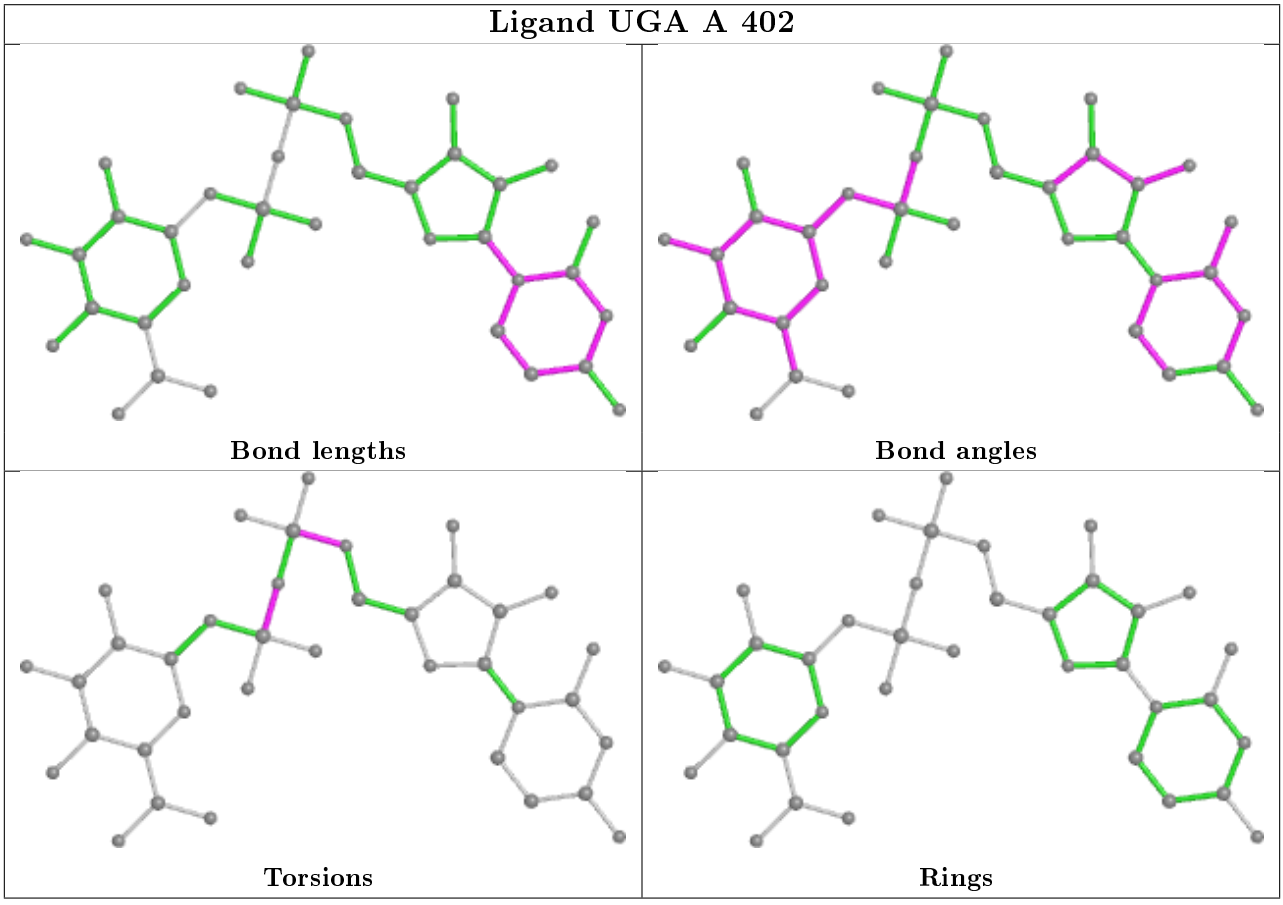


Rings

Ligand UGA B 402



Ligand UGA A 402



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	375/389 (96%)	0.36	24 (6%) 19 19	98, 124, 154, 183	0
1	B	367/389 (94%)	0.45	34 (9%) 8 10	87, 134, 169, 198	0
All	All	742/778 (95%)	0.41	58 (7%) 13 15	87, 130, 165, 198	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	ILE	4.3
1	B	44	LYS	4.3
1	B	21	CYS	4.2
1	B	42	PRO	4.1
1	B	14	PRO	4.0
1	B	46	LEU	4.0
1	B	45	VAL	3.7
1	B	70	ILE	3.6
1	B	47	ALA	3.6
1	A	375	TYR	3.5
1	B	69	ARG	3.4
1	B	20	ILE	3.2
1	A	224	PRO	3.2
1	B	17	PRO	3.1
1	A	233	VAL	3.1
1	A	323	VAL	3.1
1	A	250	LEU	3.0
1	B	43	HIS	3.0
1	A	252	LEU	3.0
1	A	330	PHE	2.9
1	B	309	TYR	2.8
1	B	375	TYR	2.8
1	B	71	GLN	2.7
1	A	325	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	240	PHE	2.6
1	A	381	LYS	2.5
1	A	319	GLU	2.5
1	B	250	LEU	2.5
1	B	48	LEU	2.4
1	A	324	ASP	2.4
1	A	66	TRP	2.3
1	B	251	LYS	2.3
1	B	217	GLY	2.3
1	B	218	PRO	2.3
1	A	306	THR	2.3
1	B	16	GLN	2.3
1	B	325	VAL	2.3
1	B	372	HIS	2.3
1	B	8	VAL	2.2
1	A	234	PRO	2.2
1	B	11	ASP	2.2
1	B	371	GLN	2.2
1	A	331	TYR	2.2
1	B	368	LEU	2.2
1	A	232	GLY	2.2
1	A	382	ALA	2.1
1	A	242	ASN	2.1
1	B	83	LEU	2.1
1	A	372	HIS	2.1
1	B	252	LEU	2.1
1	A	245	LEU	2.0
1	B	93	ILE	2.0
1	A	255	GLY	2.0
1	B	87	VAL	2.0
1	A	249	PRO	2.0
1	A	62	ASP	2.0
1	B	38	LEU	2.0
1	B	126	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

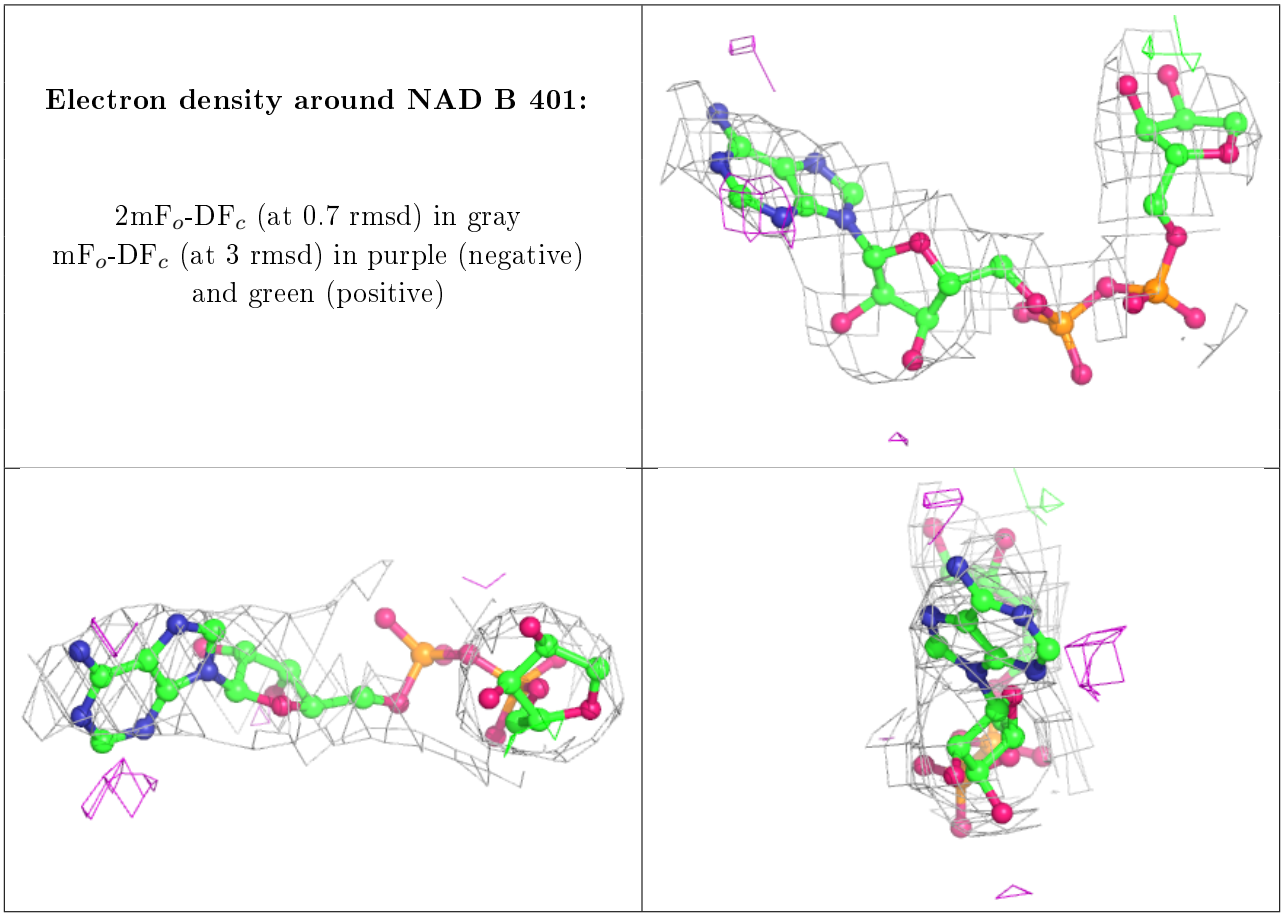
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	B	401	35/44	0.89	0.22	91,134,155,160	0
3	UGA	B	402	37/37	0.91	0.24	103,116,137,160	0
3	UGA	A	402	37/37	0.91	0.22	117,133,164,196	0
2	NAD	A	401	35/44	0.93	0.20	93,121,137,143	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.

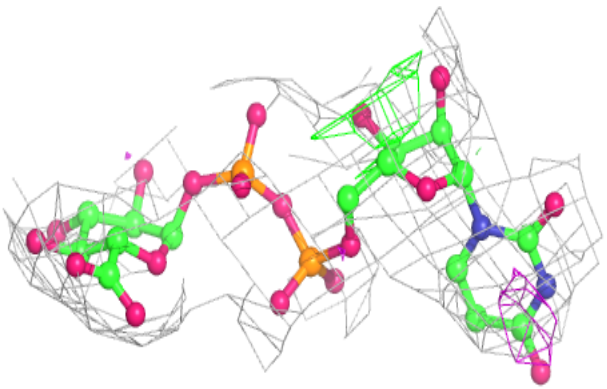
Electron density around NAD B 401:

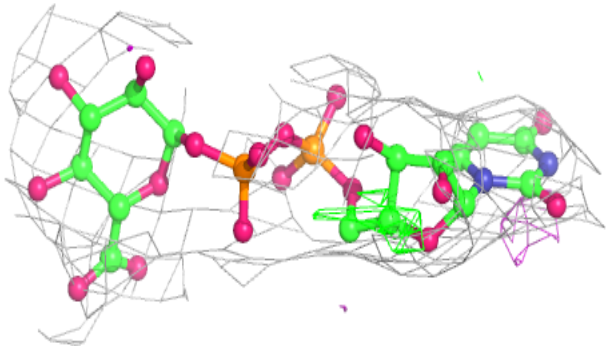
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

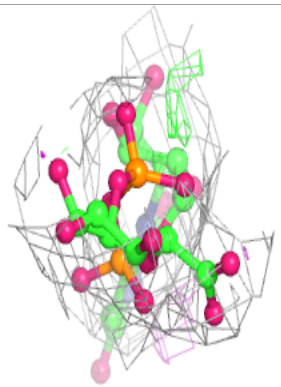


Electron density around UGA B 402:

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

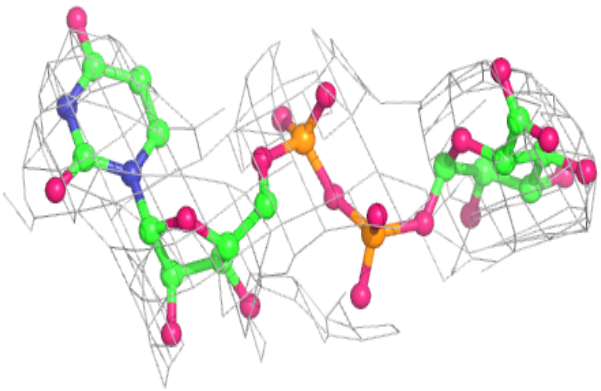


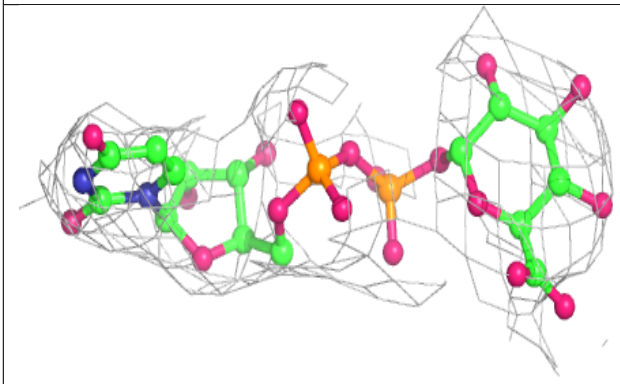


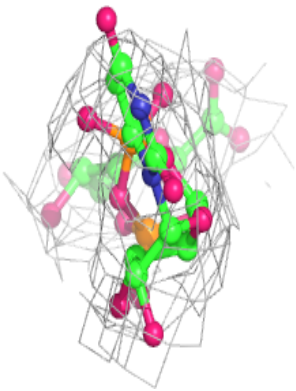


Electron density around UGA A 402:

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

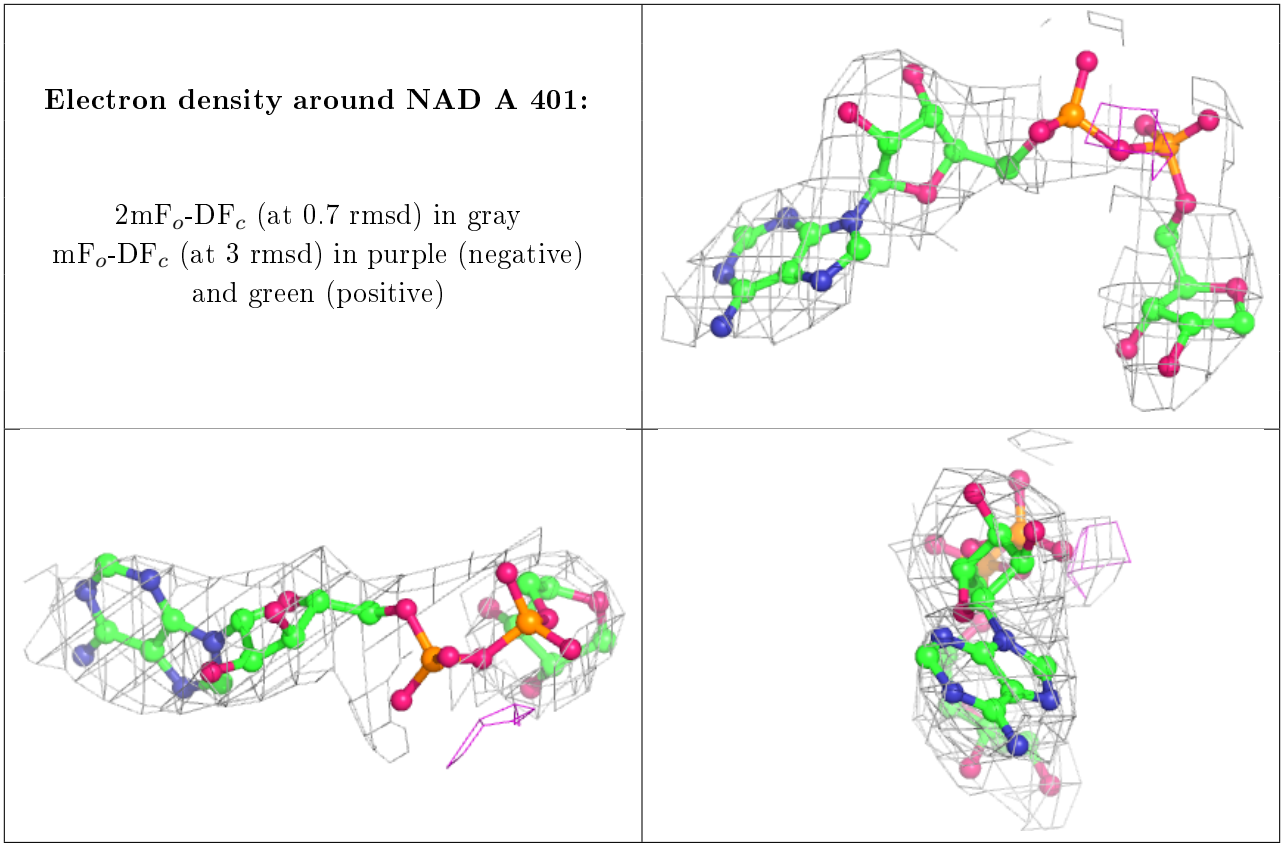






Electron density around NAD A 401:

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



6.5 Other polymers

There are no such residues in this entry.