



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 03:53 am BST

PDB ID : 1HZJ
Title : HUMAN UDP-GALACTOSE 4-EPIMERASE: ACCOMMODATION OF UD
P-N-ACETYLGLUCOSAMINE WITHIN THE ACTIVE SITE
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Deposited on : 2001-01-25
Resolution : 1.50 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 : 2.11
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) : 2.11

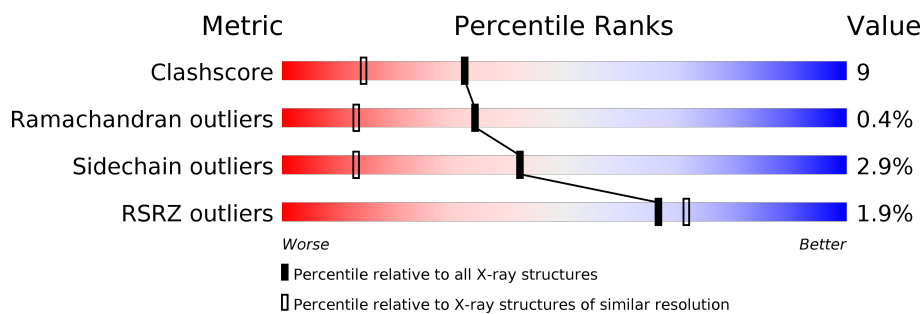
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 $\leq 5\%$. 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	348	 80% 16% . .
1	B	348	 65% 28% 5% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6484 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-GALACTOSE 4-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	5	0
			2689	1704	468	502	15			
1	B	345	Total	C	N	O	S	0	6	0
			2690	1703	468	503	16			

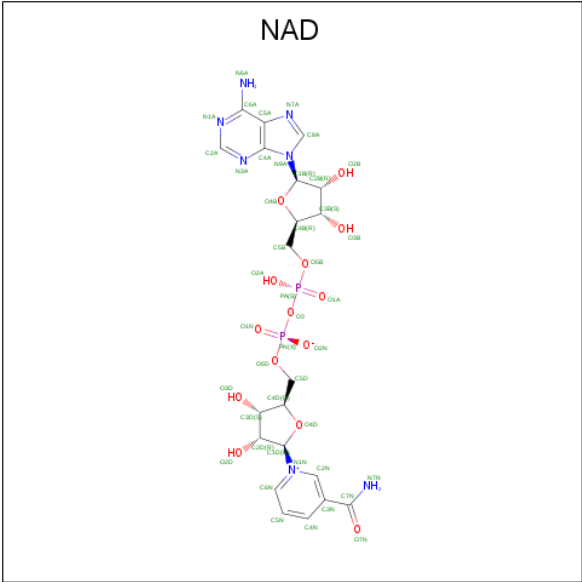
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	2	Total	Cl	0	0
			2	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

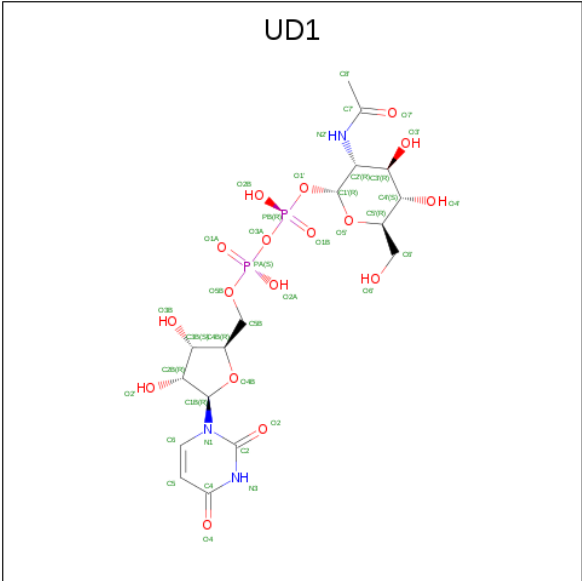
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: C₁₇H₂₇N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			43	19	4	18	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

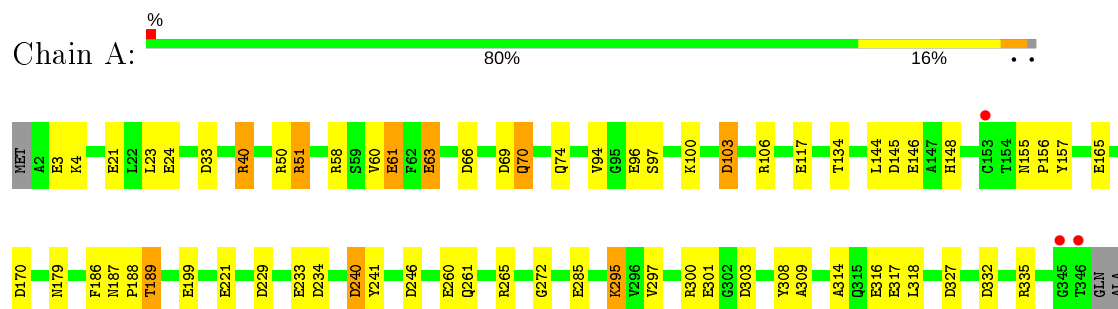
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	579	Total	O	0	0
			579	579		
6	B	352	Total	O	0	0
			352	352		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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-GALACTOSE 4-EPIMERASE



• Molecule 1: UDP-GALACTOSE 4-EPIMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.40 Å 88.90 Å 118.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 29.86 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-1.50) 97.0 (29.86-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 1.50 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.184 , 0.227 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 81.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6484	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UD1, NAD, CL

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	0.94	15/2766 (0.5%)	1.22	32/3741 (0.9%)
1	B	0.92	17/2771 (0.6%)	1.33	36/3749 (1.0%)
All	All	0.93	32/5537 (0.6%)	1.28	68/7490 (0.9%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	GLU	CD-OE2	9.05	1.35	1.25
1	A	285	GLU	CD-OE2	7.93	1.34	1.25
1	B	96	GLU	CD-OE2	7.26	1.33	1.25
1	A	61	GLU	CD-OE2	6.99	1.33	1.25
1	B	199	GLU	CD-OE2	6.92	1.33	1.25
1	A	21	GLU	CD-OE2	6.38	1.32	1.25
1	B	63	GLU	CD-OE2	6.25	1.32	1.25
1	B	146	GLU	CD-OE2	6.19	1.32	1.25
1	B	331	GLU	CD-OE2	6.17	1.32	1.25
1	B	221	GLU	CD-OE2	6.04	1.32	1.25
1	A	233	GLU	CD-OE2	6.03	1.32	1.25
1	B	64	GLU	CD-OE2	6.03	1.32	1.25
1	A	199	GLU	CD-OE2	5.93	1.32	1.25
1	B	301	GLU	CD-OE2	5.84	1.32	1.25
1	B	233	GLU	CD-OE2	5.80	1.32	1.25
1	B	316	GLU	CD-OE2	5.71	1.31	1.25
1	A	146	GLU	CD-OE2	5.68	1.31	1.25
1	B	317	GLU	CD-OE2	5.68	1.31	1.25
1	B	260	GLU	CD-OE2	5.67	1.31	1.25
1	A	165	GLU	CD-OE2	5.62	1.31	1.25
1	B	61	GLU	CD-OE2	5.60	1.31	1.25
1	B	166	GLU	CD-OE2	5.49	1.31	1.25
1	A	117	GLU	CD-OE2	5.47	1.31	1.25
1	A	24	GLU	CD-OE2	5.46	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	GLU	CD-OE2	5.45	1.31	1.25
1	A	221	GLU	CD-OE2	5.44	1.31	1.25
1	B	285	GLU	CD-OE2	5.37	1.31	1.25
1	B	54	GLU	CD-OE2	5.28	1.31	1.25
1	A	301	GLU	CD-OE2	5.28	1.31	1.25
1	B	165	GLU	CD-OE2	5.26	1.31	1.25
1	A	260	GLU	CD-OE2	5.16	1.31	1.25
1	A	317	GLU	CD-OE2	5.01	1.31	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	GLU	O-C-N	-11.48	104.34	122.70
1	B	335	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	B	145	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	300	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	69	ASP	CB-CG-OD2	-8.15	110.97	118.30
1	B	66	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	58	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	B	316	GLU	CA-C-O	7.58	136.02	120.10
1	B	170	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	B	256	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	299	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	327	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	B	66	ASP	CB-CG-OD1	7.34	124.90	118.30
1	A	335	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	234	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	B	69	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	303	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	246	ASP	CB-CG-OD1	6.75	124.37	118.30
1	B	231	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	145	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	B	106	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	200	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	332	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	327	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	303	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	69	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	75	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	58	ARG	CD-NE-CZ	6.37	132.51	123.60
1	A	103	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	51	ARG	NE-CZ-NH2	-6.32	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	70	GLN	N-CA-CB	-6.28	99.30	110.60
1	B	170	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	103	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	303	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	239	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	234	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	69	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	332	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	332	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	58	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	300	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	170	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	240	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	332	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	145	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	170	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	50	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	265	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	33	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	50	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	66	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	246	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	231	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	303	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	219	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	265	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	327	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	186	PHE	CB-CA-C	5.21	120.83	110.40
1	A	33	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	63[A]	GLU	N-CA-CB	5.15	119.86	110.60
1	A	63[B]	GLU	N-CA-CB	5.15	119.86	110.60
1	A	40	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	229[A]	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	229[B]	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	229	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	335	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	246	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2689	0	2650	23	0
1	B	2690	0	2644	71	0
2	A	2	0	0	1	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
4	A	44	0	26	1	0
4	B	44	0	26	4	0
5	A	43	0	10	0	0
5	B	39	0	25	3	0
6	A	579	0	0	6	0
6	B	352	0	0	11	0
All	All	6484	0	5381	97	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 (97) 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:65:MET:HE2	1:B:72:ALA:HB1	1.42	0.98
1:B:83:MET:HE1	1:B:259:LYS:HE2	1.57	0.84
1:B:316:GLU:HA	6:B:1743:HOH:O	1.80	0.81
1:B:125:LYS:HD3	1:B:178:TRP:NE1	2.00	0.76
1:B:2:ALA:N	1:B:81[B]:SER:HB2	2.03	0.73
1:B:2:ALA:N	1:B:81[A]:SER:HB2	2.03	0.73
4:B:900:NAD:C4N	5:B:901:UD1:H4'	2.18	0.73
1:B:291:LYS:HD3	1:B:291:LYS:H	1.53	0.73
1:B:210:PRO:O	1:B:214:GLN:HG3	1.91	0.70
4:B:900:NAD:O7N	5:B:901:UD1:H2'	1.92	0.70
1:B:140:GLN:NE2	1:B:149:PRO:HG2	2.07	0.69
1:B:316:GLU:O	6:B:1743:HOH:O	2.11	0.69
1:B:83:MET:HE1	1:B:259:LYS:CE	2.22	0.68
1:A:106:ARG:HD3	1:B:117:GLU:OE1	1.96	0.66
1:B:126:ASN:HB3	1:B:258:LEU:HD13	1.78	0.65
1:A:134[B]:THR:HG21	6:A:1775:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:H	1:B:291:LYS:CD	2.10	0.63
1:B:316:GLU:C	6:B:1743:HOH:O	2.36	0.63
1:B:178:TRP:O	1:B:263:GLY:HA2	2.00	0.62
1:B:22:LEU:HD23	1:B:252:ILE:CD1	2.29	0.61
1:B:315:GLN:HG2	1:B:321:THR:CG2	2.30	0.61
1:B:315:GLN:HG2	1:B:321:THR:HG22	1.83	0.61
1:A:70:GLN:HB3	6:A:1983:HOH:O	2.01	0.61
1:B:272:GLY:HA2	1:B:309:ALA:O	2.02	0.60
1:B:316:GLU:CA	6:B:1743:HOH:O	2.42	0.60
1:B:140:GLN:HE22	1:B:149:PRO:HG2	1.67	0.59
1:B:125:LYS:HD3	1:B:178:TRP:CD1	2.38	0.58
1:B:55:LEU:HD11	1:B:196[B]:CYS:SG	2.43	0.58
1:B:105:TYR:O	1:B:109:LEU:HB2	2.07	0.55
1:B:67:ILE:HD12	1:B:111:GLY:HA3	1.90	0.54
1:B:35:PHE:CZ	1:B:40:ARG:HG2	2.43	0.54
1:B:119:MET:HB3	1:B:124:VAL:O	2.10	0.52
1:B:271:THR:O	6:B:1965:HOH:O	2.18	0.51
1:A:179:ASN:HD21	1:A:261:GLN:NE2	2.08	0.51
1:A:314:ALA:O	1:A:318:LEU:HB2	2.10	0.51
1:B:186:PHE:O	1:B:188:PRO:HD3	2.10	0.50
1:B:92:LYS:HA	1:B:157:TYR:CE2	2.47	0.50
1:B:110[A]:THR:HG21	6:B:1459:HOH:O	2.12	0.50
1:A:240:ASP:HB2	1:A:308:TYR:HA	1.95	0.49
1:B:165:GLU:O	1:B:169:ARG:HG3	2.12	0.48
1:B:83:MET:HE1	1:B:259:LYS:NZ	2.28	0.48
1:B:223:LEU:HG	1:B:224:ASN:N	2.27	0.48
1:B:291:LYS:N	1:B:291:LYS:CD	2.76	0.48
1:A:63[B]:GLU:OE2	6:A:1767:HOH:O	2.20	0.48
1:B:153:CYS:HB2	1:B:159:LYS:HG3	1.96	0.48
1:B:319:GLY:HA3	6:B:2031:HOH:O	2.13	0.48
1:B:10:GLY:HA3	1:B:31:VAL:HG13	1.97	0.47
1:B:70:GLN:O	1:B:74:GLN:HG3	2.14	0.47
1:B:240:ASP:HB2	1:B:308:TYR:HA	1.96	0.47
1:B:186:PHE:CE2	1:B:309:ALA:HB2	2.50	0.47
1:A:186:PHE:O	1:A:188:PRO:HD3	2.15	0.46
1:A:155:ASN:OD1	1:A:157:TYR:HB3	2.16	0.46
1:B:190:GLY:H	1:B:333:LEU:HD12	1.80	0.46
4:B:900:NAD:O1N	4:B:900:NAD:N7N	2.48	0.46
1:B:35:PHE:CE2	1:B:40:ARG:HA	2.51	0.45
1:A:189:THR:HG21	1:A:241:TYR:HD1	1.82	0.45
1:B:71:GLY:O	1:B:75:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HE2	2:A:952:CL:CL	2.55	0.44
1:B:188:PRO:HB3	1:B:247:LEU:CD1	2.48	0.44
1:B:39:PHE:HE1	6:B:1644:HOH:O	2.01	0.44
1:B:83:MET:CE	1:B:259:LYS:NZ	2.81	0.44
1:A:94:VAL:HG13	1:A:155:ASN:CG	2.39	0.43
1:A:97:SER:O	1:A:156:PRO:HG2	2.18	0.43
1:B:139:PRO:HG2	1:B:306:ALA:O	2.18	0.43
1:A:144:LEU:HD23	1:A:148:HIS:CD2	2.53	0.43
1:A:61:GLU:HG2	6:A:1506:HOH:O	2.19	0.43
1:A:295:LYS:HD3	1:A:297:VAL:CG1	2.49	0.43
1:B:213:SER:OG	1:B:337:GLN:OE1	2.35	0.43
1:B:204:ILE:HG23	1:B:211:TYR:HE1	1.84	0.43
1:B:138:ASN:ND2	6:B:1297:HOH:O	2.47	0.43
1:A:100:LYS:HE3	1:A:103:ASP:OD1	2.19	0.43
1:B:8:THR:O	1:B:88:PHE:HB2	2.18	0.43
1:A:23:LEU:HD11	1:A:60:VAL:HG22	2.00	0.42
1:B:96:GLU:HG3	1:B:100:LYS:HD3	2.00	0.42
1:B:233:GLU:HG2	1:B:233:GLU:O	2.15	0.42
1:B:67:ILE:HD12	1:B:111:GLY:CA	2.49	0.42
1:B:315:GLN:O	1:B:319:GLY:HA2	2.20	0.42
1:A:100:LYS:HB3	1:A:100:LYS:HE3	1.87	0.42
1:A:316:GLU:HG2	6:A:1815:HOH:O	2.19	0.42
1:A:51:ARG:HD3	6:A:1500:HOH:O	2.19	0.42
1:B:185:TYR:HB2	4:B:900:NAD:C5N	2.50	0.41
1:A:272:GLY:HA2	1:A:309:ALA:O	2.20	0.41
1:B:50:ARG:HH11	1:B:50:ARG:HG2	1.85	0.41
1:B:44:SER:HB2	6:B:1911:HOH:O	2.20	0.41
1:B:207:ASN:OD1	1:B:210:PRO:HG2	2.20	0.41
1:B:207:ASN:HB3	5:B:901:UD1:H8'2	2.02	0.41
1:B:312:SER:O	1:B:315:GLN:HB3	2.20	0.41
1:B:3:GLU:HG2	1:B:4:LYS:N	2.35	0.41
1:B:277:VAL:O	1:B:281:VAL:HG23	2.21	0.40
1:B:240:ASP:HB2	1:B:308:TYR:CB	2.50	0.40
1:A:187:ASN:O	1:A:189:THR:HG23	2.21	0.40
1:B:301:GLU:HB2	6:B:1207:HOH:O	2.21	0.40
1:B:184:ARG:CZ	1:B:266:ILE:HG21	2.52	0.40
1:B:3:GLU:HG2	1:B:4:LYS:H	1.85	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	348/348 (100%)	339 (97%)	8 (2%)	1 (0%)	41	18
1	B	349/348 (100%)	336 (96%)	11 (3%)	2 (1%)	25	7
All	All	697/696 (100%)	675 (97%)	19 (3%)	3 (0%)	34	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	ASP
1	A	40	ARG
1	B	41	GLY

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	283/282 (100%)	280 (99%)	3 (1%)	73	53
1	B	284/282 (101%)	271 (95%)	13 (5%)	27	5
All	All	567/564 (100%)	551 (97%)	16 (3%)	42	14

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	189	THR
1	A	295	LYS

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Mol	Chain	Res	Type
1	B	40	ARG
1	B	44	SER
1	B	58	ARG
1	B	59	SER
1	B	63	GLU
1	B	92	LYS
1	B	138	ASN
1	B	173	GLN
1	B	213	SER
1	B	233	GLU
1	B	291	LYS
1	B	315	GLN
1	B	333	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	114	GLN
1	A	138	ASN
1	A	261	GLN
1	A	339	GLN
1	B	74	GLN
1	B	114	GLN
1	B	140	GLN
1	B	173	GLN
1	B	339	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAD	B	900	-	42,48,48	1.35	7 (16%)	50,73,73	2.15	13 (26%)
5	UD1	A	401[B]	-	34,41,41	1.23	3 (8%)	45,62,62	1.33	4 (8%)
4	NAD	A	400	-	42,48,48	1.20	4 (9%)	50,73,73	1.93	10 (20%)
5	UD1	A	401[A]	-	34,41,41	1.21	3 (8%)	45,62,62	1.36	5 (11%)
5	UD1	B	901	-	34,41,41	1.09	3 (8%)	45,62,62	1.26	6 (13%)

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
4	NAD	B	900	-	-	6/26/62/62	0/5/5/5
5	UD1	A	401[B]	-	-	8/24/63/63	0/3/3/3
4	NAD	A	400	-	-	6/26/62/62	0/5/5/5
5	UD1	A	401[A]	-	-	5/24/63/63	0/3/3/3
5	UD1	B	901	-	-	2/24/63/63	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401[A]	UD1	C4-N3	4.40	1.40	1.33
5	A	401[B]	UD1	C4-N3	4.40	1.40	1.33
5	B	901	UD1	C6-C5	-3.91	1.29	1.38
4	B	900	NAD	C4N-C3N	3.77	1.45	1.39
4	A	400	NAD	C3N-C7N	3.64	1.56	1.50
4	B	900	NAD	C2N-C3N	-3.57	1.33	1.39
4	A	400	NAD	C4N-C3N	3.33	1.45	1.39
5	A	401[A]	UD1	C6-C5	-3.30	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	401[B]	UD1	C6-C5	-3.30	1.30	1.38
4	A	400	NAD	C2A-N1A	2.89	1.39	1.33
4	B	900	NAD	C2A-N1A	2.59	1.38	1.33
4	B	900	NAD	C6N-N1N	2.55	1.41	1.35
4	B	900	NAD	C2N-N1N	-2.45	1.32	1.35
5	B	901	UD1	C4-N3	2.38	1.37	1.33
4	B	900	NAD	O4B-C1B	-2.25	1.37	1.41
4	A	400	NAD	C2N-N1N	2.18	1.37	1.35
5	A	401[A]	UD1	C2B-C1B	-2.18	1.50	1.53
5	A	401[B]	UD1	C2B-C1B	-2.18	1.50	1.53
5	B	901	UD1	PB-O1'	2.06	1.65	1.60
4	B	900	NAD	C5N-C4N	2.01	1.43	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	NAD	C6N-C5N-C4N	6.68	129.16	119.44
4	B	900	NAD	C6N-N1N-C2N	6.65	128.04	121.97
4	A	400	NAD	C5N-C4N-C3N	-6.44	112.72	120.34
4	B	900	NAD	C5N-C4N-C3N	-5.67	113.63	120.34
4	B	900	NAD	C5N-C6N-N1N	-5.17	112.98	120.40
4	B	900	NAD	C3N-C2N-N1N	-5.13	115.41	120.43
4	A	400	NAD	C5N-C6N-N1N	-5.03	113.19	120.40
5	A	401[A]	UD1	O3A-PB-O1'	4.69	111.93	102.48
5	A	401[B]	UD1	O3A-PB-O1'	4.69	111.93	102.48
4	B	900	NAD	O7N-C7N-C3N	4.66	125.21	119.63
5	B	901	UD1	C5-C4-N3	-4.30	113.85	123.31
5	A	401[A]	UD1	C5-C4-N3	-3.80	114.94	123.31
5	A	401[B]	UD1	C5-C4-N3	-3.80	114.94	123.31
4	B	900	NAD	C2N-N1N-C1D	-3.68	110.95	119.14
4	A	400	NAD	O4B-C1B-C2B	-3.31	102.08	106.93
4	B	900	NAD	C4N-C3N-C7N	3.25	129.74	121.04
4	A	400	NAD	C5A-C6A-N6A	3.07	125.02	120.35
4	B	900	NAD	C2N-C3N-C7N	-3.03	110.68	119.46
4	B	900	NAD	C3N-C7N-N7N	-2.92	114.24	117.75
5	B	901	UD1	C2'-N2'-C7'	-2.59	116.89	123.18
4	B	900	NAD	C5A-C6A-N1A	-2.46	114.77	120.35
5	A	401[A]	UD1	C2'-N2'-C7'	-2.46	117.20	123.18
4	A	400	NAD	C2N-C3N-C4N	2.44	121.02	118.26
5	A	401[A]	UD1	O5'-C1'-O1'	-2.30	108.36	111.36
5	A	401[B]	UD1	O5'-C1'-O1'	-2.30	108.36	111.36
4	B	900	NAD	C6N-C5N-C4N	2.27	122.74	119.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	901	UD1	O5'-C1'-O1'	-2.20	108.48	111.36
5	A	401[B]	UD1	C8'-C7'-N2'	2.18	119.80	116.10
4	B	900	NAD	N6A-C6A-N1A	2.17	123.08	118.57
5	B	901	UD1	C3'-C2'-N2'	-2.15	106.55	110.62
4	A	400	NAD	C3N-C7N-N7N	2.14	120.32	117.75
4	A	400	NAD	C4A-C5A-N7A	2.13	111.62	109.40
4	A	400	NAD	C6N-N1N-C2N	2.12	123.91	121.97
5	B	901	UD1	C8'-C7'-N2'	2.11	119.68	116.10
4	A	400	NAD	O7N-C7N-N7N	-2.10	119.60	122.58
5	A	401[A]	UD1	C8'-C7'-N2'	2.08	119.62	116.10
5	B	901	UD1	O5'-C5'-C4'	-2.08	105.92	109.69
4	B	900	NAD	C3D-C2D-C1D	-2.03	97.92	100.98

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	900	NAD	C5B-O5B-PA-O2A
4	B	900	NAD	O4D-C1D-N1N-C2N
5	A	401[A]	UD1	C1'-O1'-PB-O3A
5	A	401[A]	UD1	C2B-C1B-N1-C6
5	A	401[A]	UD1	O4B-C1B-N1-C6
5	A	401[B]	UD1	C3'-C2'-N2'-C7'
5	A	401[B]	UD1	C1'-O1'-PB-O3A
5	A	401[B]	UD1	C2B-C1B-N1-C6
5	A	401[B]	UD1	O4B-C1B-N1-C6
4	A	400	NAD	C5D-O5D-PN-O2N
4	A	400	NAD	O4D-C1D-N1N-C2N
5	B	901	UD1	C1'-O1'-PB-O3A
5	A	401[B]	UD1	O7'-C7'-N2'-C2'
5	A	401[B]	UD1	C8'-C7'-N2'-C2'
5	A	401[A]	UD1	PA-O3A-PB-O1B
5	A	401[B]	UD1	PA-O3A-PB-O1B
5	A	401[A]	UD1	C1'-O1'-PB-O2B
5	A	401[B]	UD1	C1'-O1'-PB-O2B
5	B	901	UD1	PB-O3A-PA-O5B
4	B	900	NAD	C5B-O5B-PA-O3
4	A	400	NAD	C5D-O5D-PN-O3
4	B	900	NAD	C5B-O5B-PA-O1A
4	B	900	NAD	PA-O3-PN-O2N
4	A	400	NAD	PA-O3-PN-O2N
4	B	900	NAD	O4B-C4B-C5B-O5B

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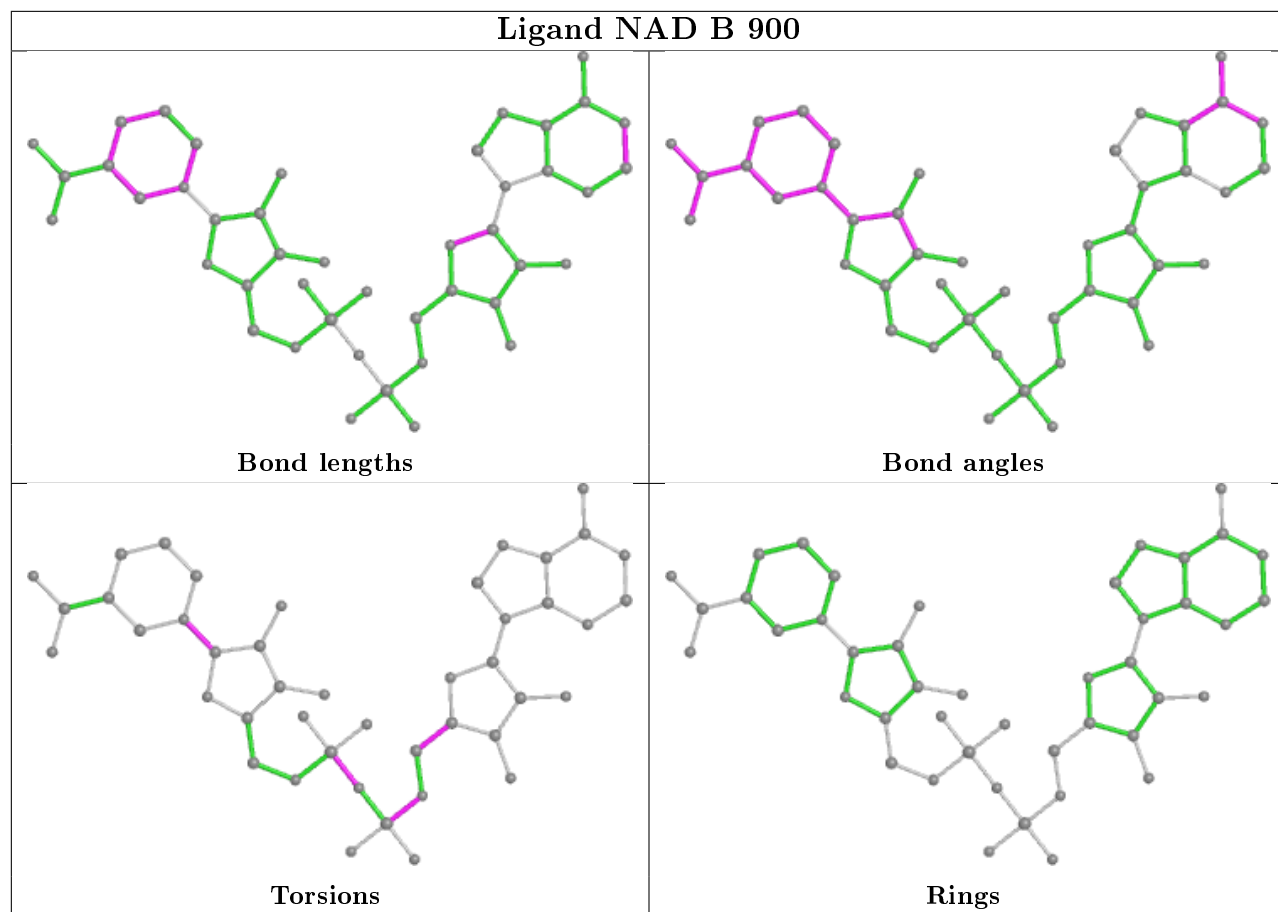
Mol	Chain	Res	Type	Atoms
4	A	400	NAD	O4B-C4B-C5B-O5B
4	A	400	NAD	C5D-O5D-PN-O1N

There are no ring outliers.

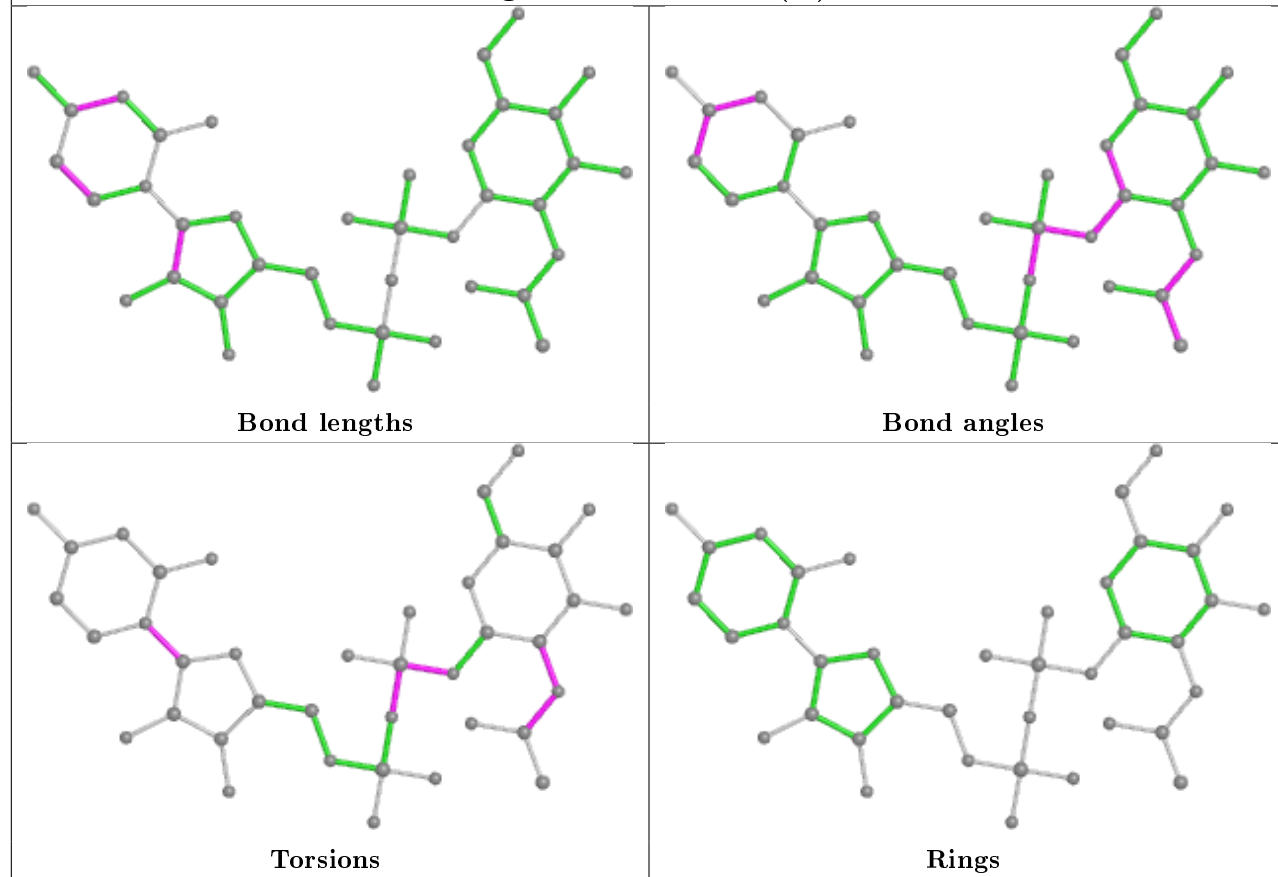
3 monomers are involved in 6 short contacts:

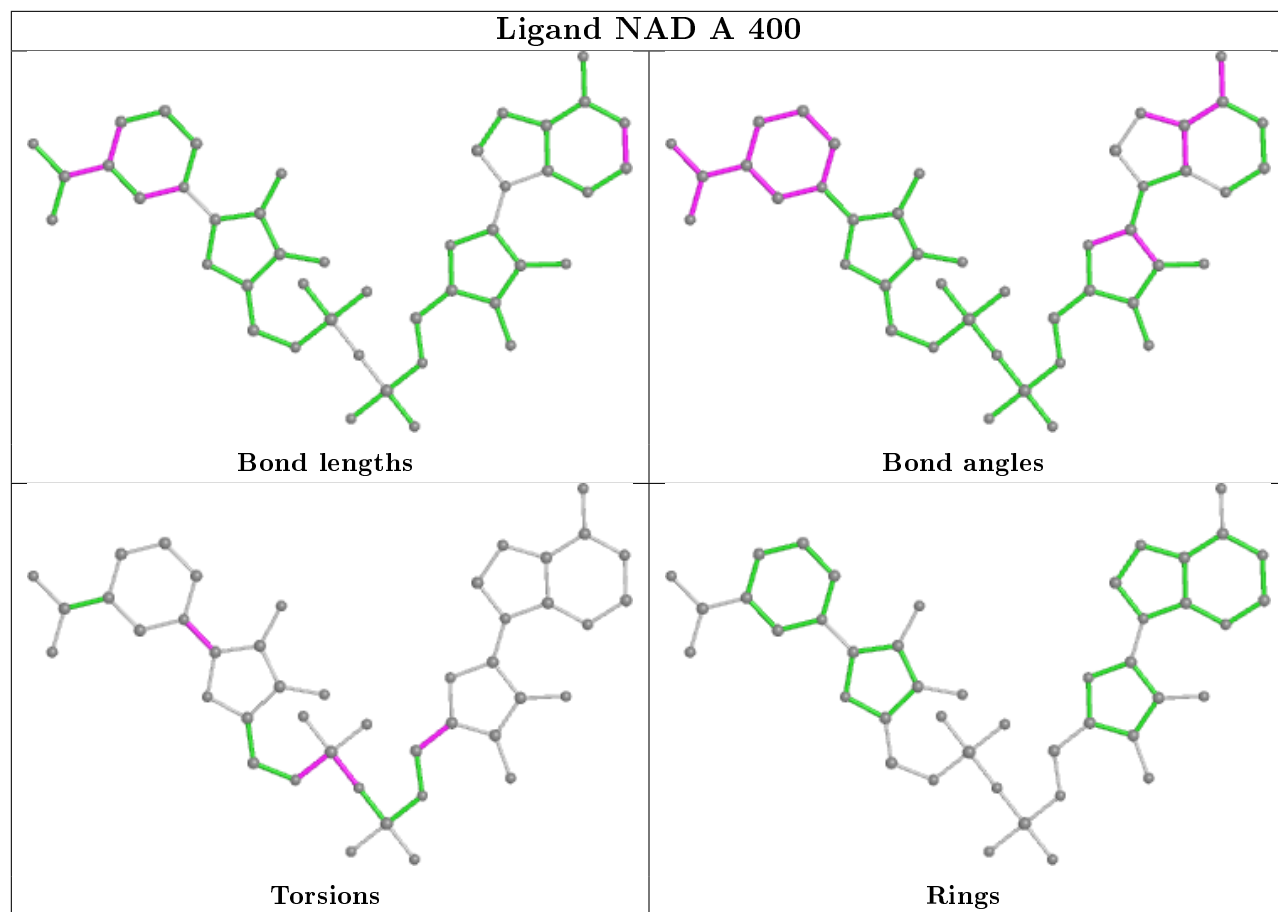
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	900	NAD	4	0
4	A	400	NAD	1	0
5	B	901	UD1	3	0

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.

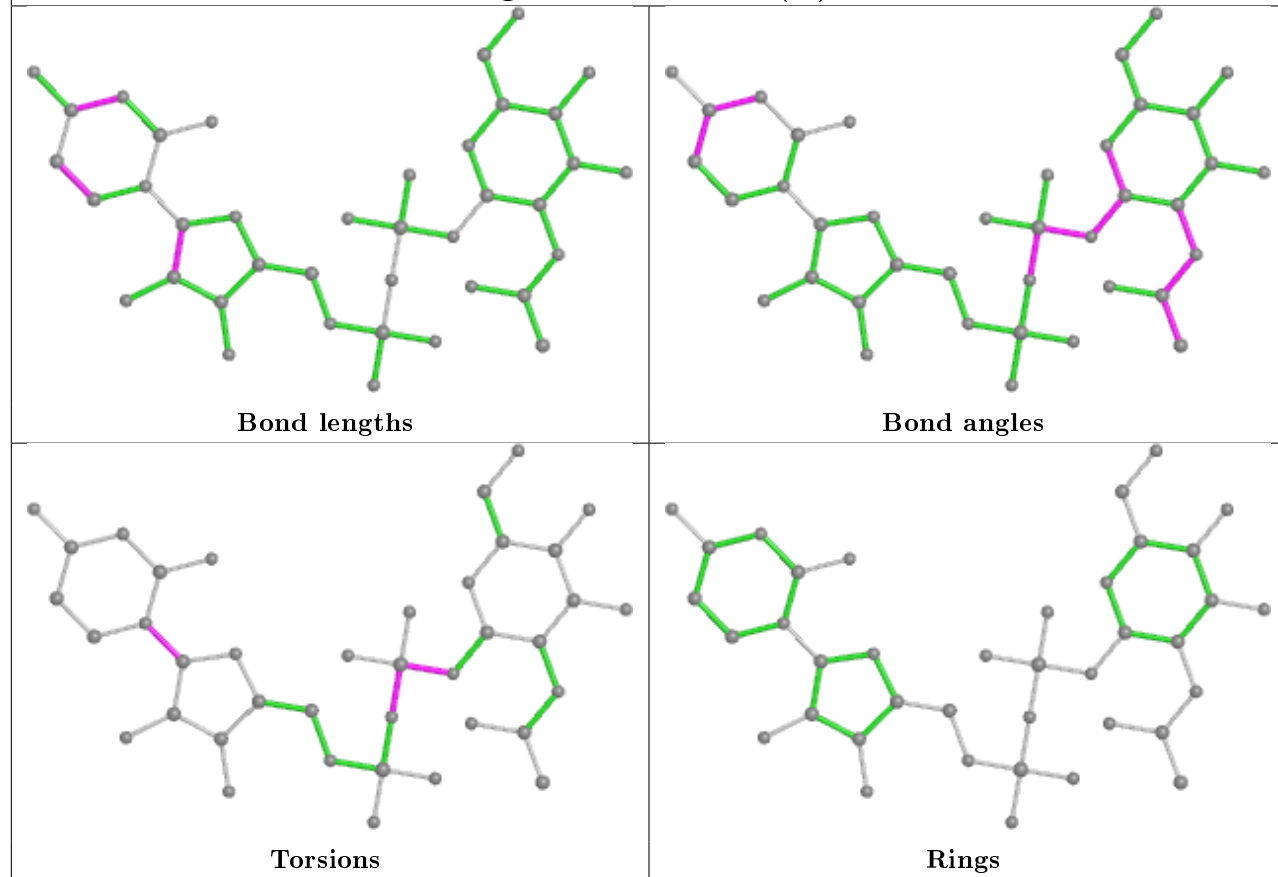


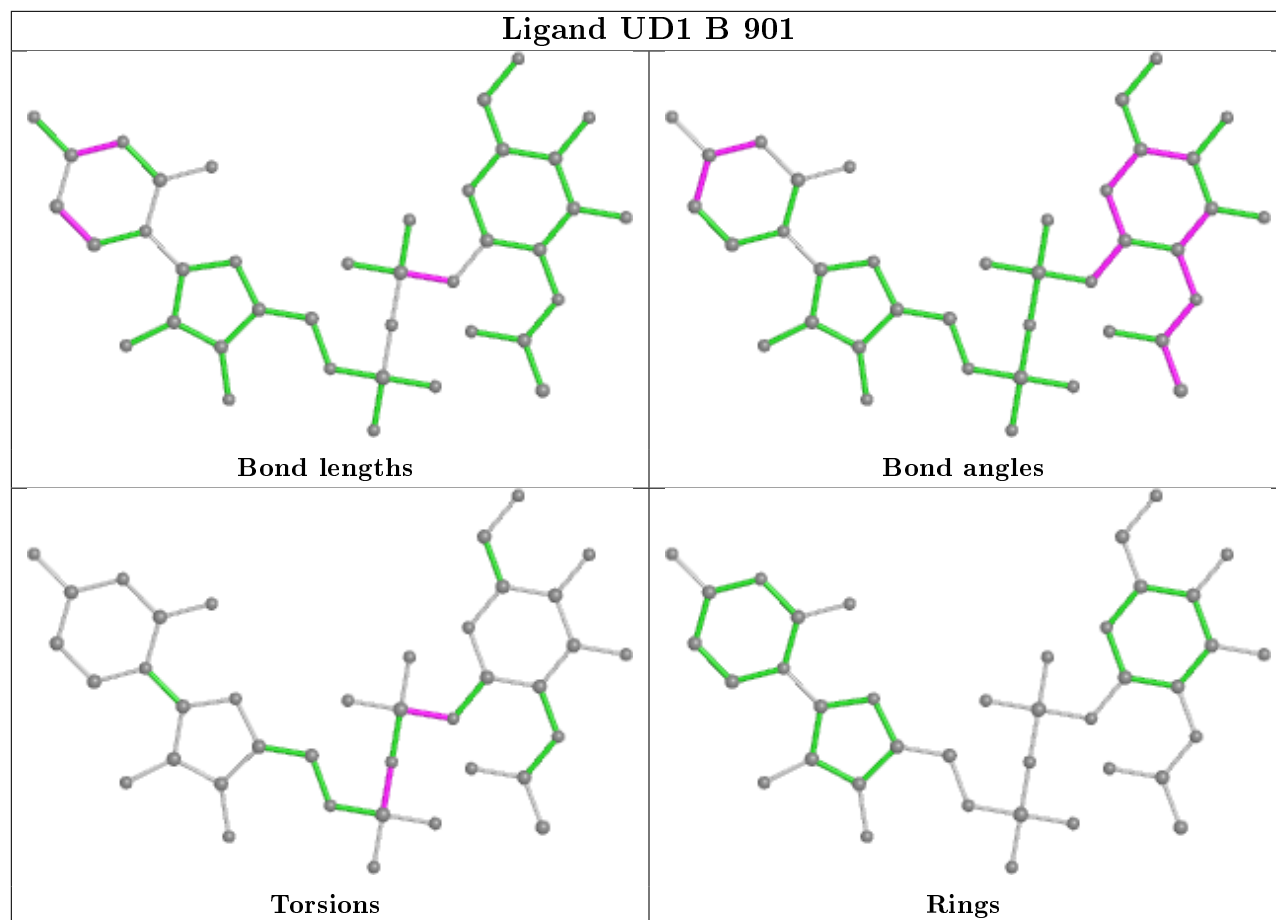
Ligand UD1 A 401 (B)





Ligand UD1 A 401 (A)





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, 95th 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	345/348 (99%)	-0.59	3 (0%) 84 87	7, 15, 35, 98	0
1	B	345/348 (99%)	-0.04	10 (2%) 51 56	13, 24, 57, 98	0
All	All	690/696 (99%)	-0.31	13 (1%) 66 71	7, 19, 51, 98	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	THR	10.0
1	B	39	PHE	6.2
1	B	346	THR	5.9
1	B	345	GLY	4.5
1	B	43	GLY	2.9
1	A	345	GLY	2.9
1	B	296	VAL	2.8
1	B	35	PHE	2.7
1	B	229[A]	ASP	2.2
1	B	38	ALA	2.1
1	A	153	CYS	2.1
1	B	2	ALA	2.1
1	B	44	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

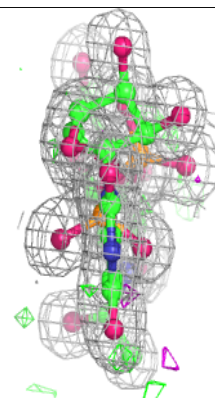
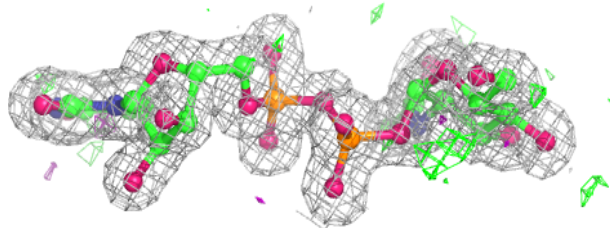
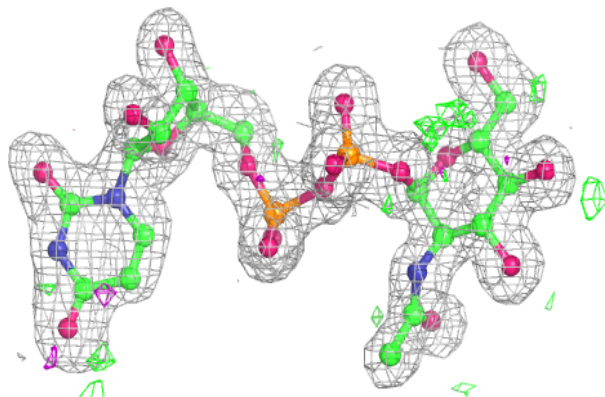
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	UD1	B	901	39/39	0.96	0.07	12,18,28,34	0
4	NAD	B	900	44/44	0.97	0.08	15,20,95,100	0
2	CL	A	952	1/1	0.98	0.06	24,24,24,24	0
3	MG	A	960	1/1	0.98	0.11	37,37,37,37	0
2	CL	A	950	1/1	0.98	0.11	25,25,25,25	0
2	CL	B	951	1/1	0.98	0.04	22,22,22,22	0
4	NAD	A	400	44/44	0.99	0.06	6,11,18,22	0
5	UD1	A	401[B]	39/39	0.99	0.07	8,18,99,100	4
5	UD1	A	401[A]	39/39	0.99	0.07	8,18,48,71	4

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.

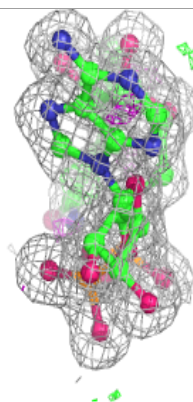
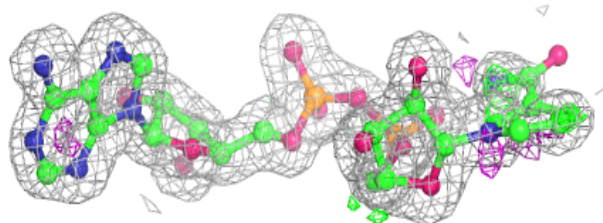
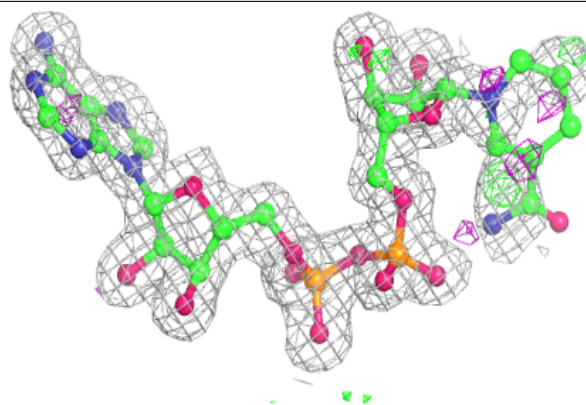
Electron density around UD1 B 901:

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

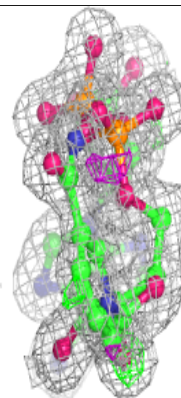
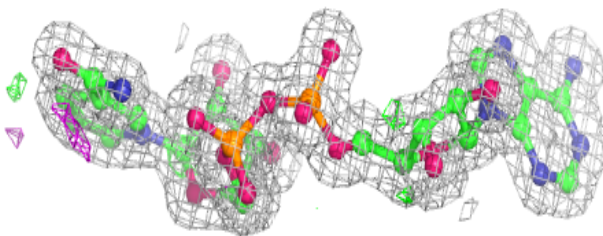
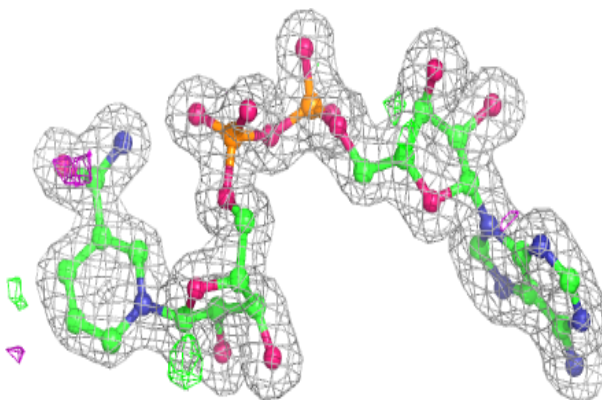


Electron density around NAD B 900:

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

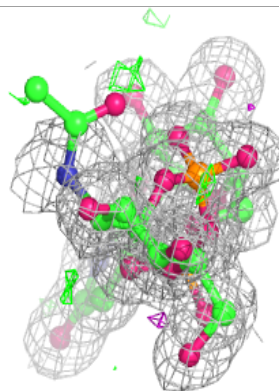
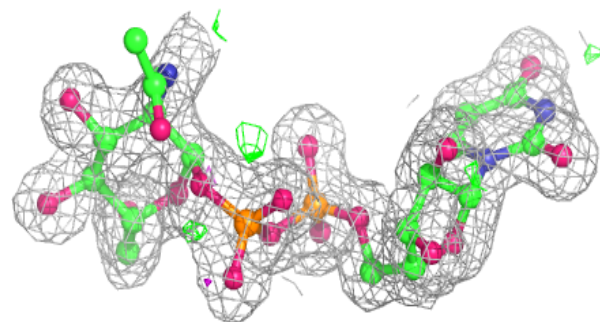
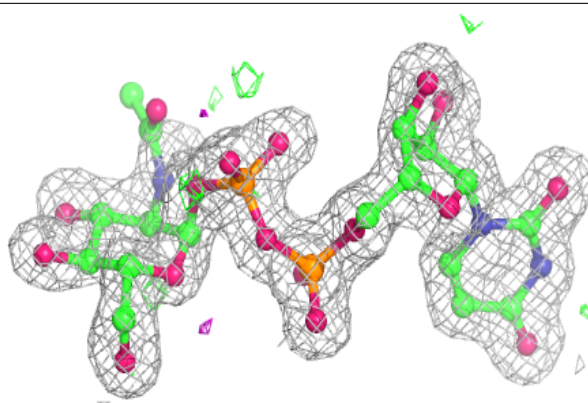
**Electron density around NAD A 400:**

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

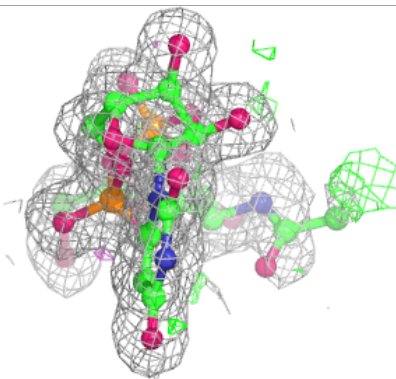
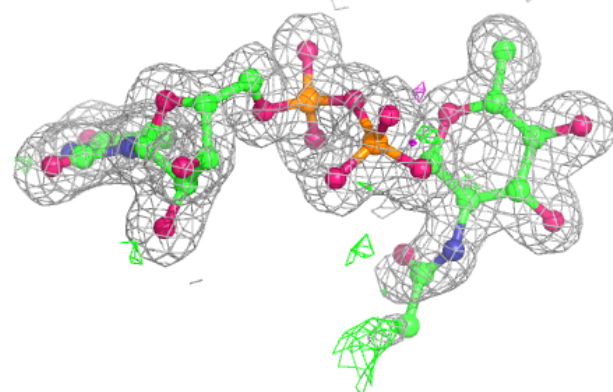
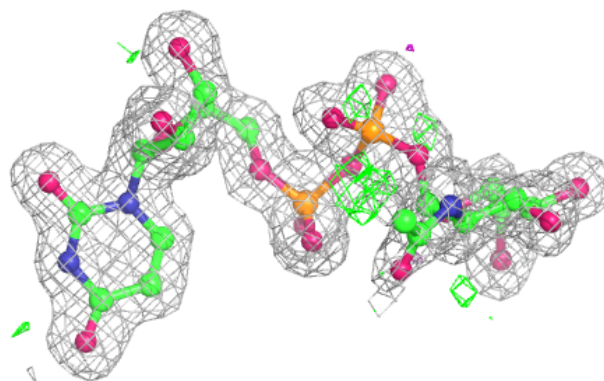


Electron density around UD1 A 401 (B):

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

**Electron density around UD1 A 401 (A):**

$2mF_o-DF_c$ (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.