



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2021 – 02:02 PM EST

PDB ID : 7KWS
Title : Cj1441 with NAD⁺ and UDP-glucose
Authors : Riegert, A.S.; Raushel, F.M.
Deposited on : 2020-12-02
Resolution : 2.09 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 : 2.16
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) : 2.16

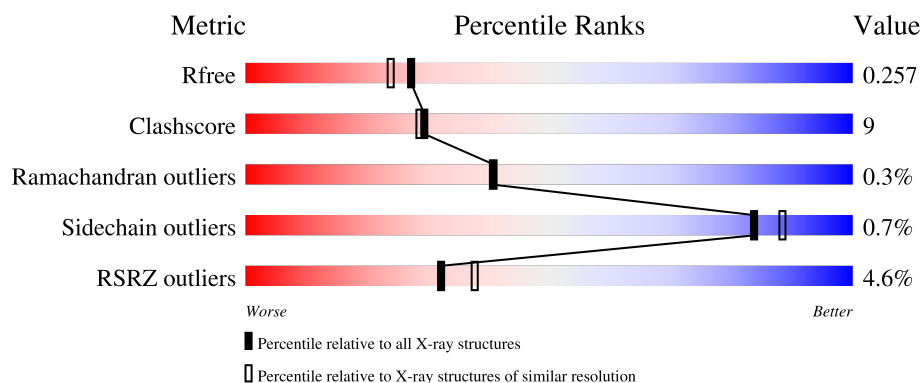
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	393	<div> <div>4%</div> <div>77%</div> <div>22%</div> <div>..</div> </div>
1	B	393	<div> <div>6%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>

2 Entry composition [i](#)

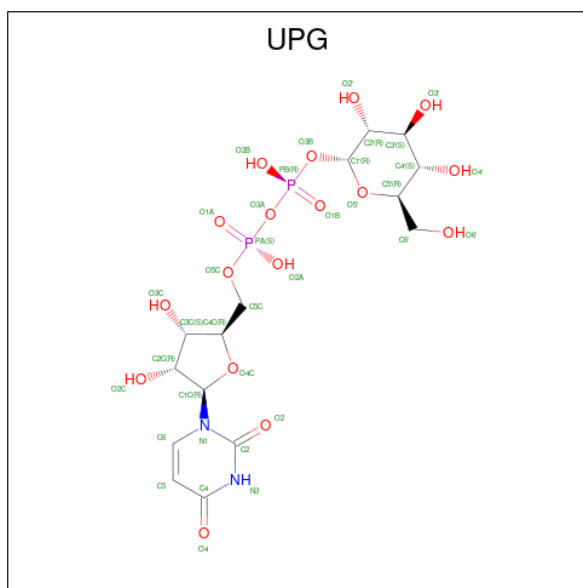
There are 4 unique types of molecules in this entry. The entry contains 6625 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3156	2041	516	593	6			
1	B	387	Total	C	N	O	S	0	0	0
			3129	2025	511	587	6			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

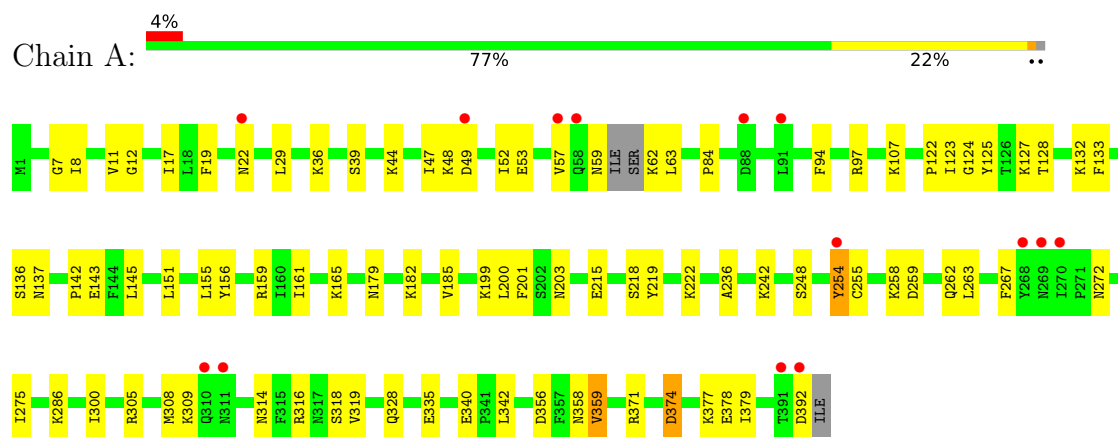
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	B	89	Total	O	0	0
			89	89		

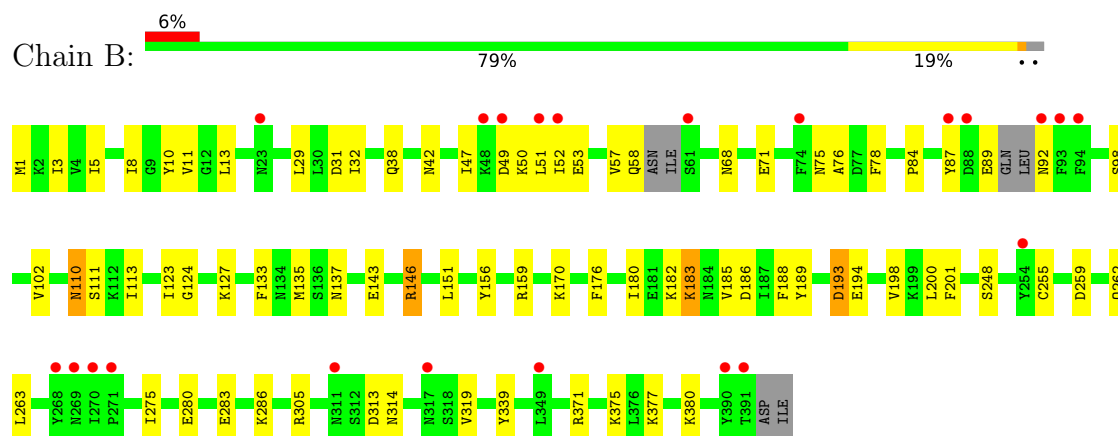
3 Residue-property plots

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-glucose 6-dehydrogenase



• Molecule 1: UDP-glucose 6-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.79Å 148.78Å 62.34Å 90.00° 107.52° 90.00°	Depositor
Resolution (Å)	46.44 – 2.09 46.44 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.6 (46.44-2.09) 96.6 (46.44-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.190 , 0.257 0.190 , 0.257	Depositor DCC
R_{free} test set	2004 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.3	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	0.96	EDS
Total number of atoms	6625	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: UPG, 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	0.44	1/3210 (0.0%)	0.60	1/4325 (0.0%)
1	B	0.40	0/3182	0.60	1/4285 (0.0%)
All	All	0.42	1/6392 (0.0%)	0.60	2/8610 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	VAL	CB-CG1	-5.66	1.41	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	ASP	CB-CG-OD1	-7.44	111.60	118.30
1	B	193	ASP	CB-CG-OD1	5.64	123.37	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	TYR	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	3156	0	3223	70	3
1	B	3129	0	3198	54	2
2	A	36	0	22	5	0
2	B	36	0	22	3	0
3	A	44	0	24	2	0
3	B	44	0	25	2	0
4	A	91	0	0	3	0
4	B	89	0	0	3	0
All	All	6625	0	6514	123	4

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 (123) 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:203:ASN:HD21	2:A:401:UPG:H6'1	1.47	0.78
1:B:8:ILE:HD12	1:B:31:ASP:HB2	1.66	0.78
1:A:199:LYS:HZ1	2:A:401:UPG:H6'2	1.47	0.78
1:B:1:MET:HE3	1:B:3:ILE:HD11	1.66	0.78
1:B:377:LYS:HA	1:B:380:LYS:HG3	1.67	0.77
1:B:49:ASP:HB2	1:B:313:ASP:HB2	1.68	0.76
1:B:50:LYS:NZ	1:B:53:GLU:HA	2.01	0.75
1:B:286:LYS:HE2	1:B:319:VAL:HG23	1.67	0.74
1:B:8:ILE:HG13	1:B:29:LEU:HD22	1.69	0.73
1:A:156:TYR:HA	1:A:182:LYS:HB2	1.70	0.73
1:A:49:ASP:HB3	1:A:52:ILE:HB	1.70	0.72
1:B:50:LYS:HZ1	1:B:53:GLU:HA	1.56	0.71
1:B:111:SER:O	1:B:137:ASN:ND2	2.19	0.70
1:A:199:LYS:NZ	2:A:401:UPG:H6'2	2.10	0.67
1:B:52:ILE:HB	1:B:151:LEU:HD23	1.76	0.67
1:B:5:ILE:HB	1:B:29:LEU:HD23	1.77	0.66
1:B:255:CYS:HB2	2:B:401:UPG:H6'2	1.78	0.66
1:A:309:LYS:CE	1:A:392:ASP:HA	2.28	0.63
1:A:203:ASN:HD21	2:A:401:UPG:C6'	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:NH2	1:A:342:LEU:HD23	2.15	0.61
1:B:8:ILE:CD1	1:B:31:ASP:HB2	2.31	0.61
1:A:84:PRO:HG3	3:A:402:NAD:H52A	1.82	0.60
1:B:156:TYR:HA	1:B:182:LYS:HB2	1.84	0.60
1:B:182:LYS:HG2	1:B:185:VAL:HG22	1.85	0.59
1:A:47:ILE:HG22	1:A:48:LYS:H	1.68	0.59
1:A:300:ILE:HD12	1:A:335:GLU:OE2	2.03	0.58
1:A:309:LYS:HE3	1:A:392:ASP:HA	1.85	0.58
1:A:374:ASP:O	1:A:377:LYS:HG2	2.04	0.58
1:A:151:LEU:HD23	1:A:155:LEU:HG	1.87	0.57
2:B:401:UPG:H6'1	3:B:402:NAD:C4N	2.35	0.57
1:A:8:ILE:HG12	1:A:29:LEU:HD22	1.87	0.56
1:B:38:GLN:NE2	1:B:42:ASN:HD21	2.03	0.56
1:A:286:LYS:HE2	1:A:319:VAL:HG23	1.88	0.56
1:A:203:ASN:ND2	1:A:259:ASP:OD2	2.38	0.55
1:A:11:VAL:HG13	1:A:143:GLU:HG2	1.88	0.55
1:A:218:SER:O	1:A:222:LYS:HG3	2.07	0.54
1:A:248:SER:HB3	1:A:371:ARG:HH12	1.72	0.54
1:A:52:ILE:HG12	1:A:151:LEU:HD12	1.89	0.53
1:A:94:PHE:HB2	1:A:262:GLN:OE1	2.09	0.53
1:A:137:ASN:N	1:A:137:ASN:OD1	2.39	0.53
1:A:254:TYR:CE2	1:A:258:LYS:HE2	2.44	0.53
1:A:124:GLY:O	1:A:128:THR:HG23	2.09	0.52
1:B:11:VAL:HG13	1:B:143:GLU:HG2	1.92	0.52
1:B:186:ASP:HB3	1:B:188:PHE:CE1	2.46	0.51
1:A:84:PRO:HG3	3:A:402:NAD:C5B	2.40	0.51
1:A:272:ASN:ND2	1:B:280:GLU:OE2	2.32	0.51
1:B:110:ASN:OD1	1:B:110:ASN:C	2.48	0.51
1:B:47:ILE:HG13	1:B:47:ILE:O	2.11	0.51
1:A:305:ARG:HH22	1:A:342:LEU:HD23	1.76	0.50
1:B:146:ARG:NH1	4:B:505:HOH:O	2.41	0.50
1:B:248:SER:HB3	1:B:371:ARG:HH12	1.76	0.50
1:B:76:ALA:HB3	1:B:113:ILE:HD13	1.94	0.50
1:B:123:ILE:HG13	1:B:200:LEU:HD12	1.92	0.50
1:B:57:VAL:HG23	1:B:58:GLN:HG2	1.94	0.50
1:B:194:GLU:O	1:B:198:VAL:HG23	2.12	0.49
1:A:63:LEU:HD23	1:A:63:LEU:H	1.76	0.49
1:A:11:VAL:HA	1:A:145:LEU:HD21	1.93	0.49
1:B:3:ILE:HD13	1:B:78:PHE:HB2	1.95	0.49
1:B:133:PHE:HB3	1:B:135:MET:HG3	1.94	0.48
1:A:47:ILE:HG22	1:A:48:LYS:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ASN:N	1:B:137:ASN:OD1	2.40	0.48
1:B:13:LEU:HD23	1:B:47:ILE:HG12	1.95	0.48
1:A:165:LYS:NZ	4:A:506:HOH:O	2.47	0.48
1:A:19:PHE:HA	1:A:179:ASN:HD22	1.79	0.47
1:A:378:GLU:O	1:A:379:ILE:HD13	2.14	0.47
1:A:305:ARG:NH2	1:A:340:GLU:OE2	2.47	0.47
1:B:180:ILE:HD12	1:B:185:VAL:HG21	1.96	0.47
1:A:201:PHE:CD1	1:A:263:LEU:HD21	2.49	0.47
1:A:142:PRO:HB3	1:A:199:LYS:HB2	1.97	0.47
1:A:328:GLN:HG2	4:A:582:HOH:O	2.15	0.47
1:B:259:ASP:O	1:B:262:GLN:HB3	2.13	0.47
1:B:127:LYS:NZ	4:B:507:HOH:O	2.47	0.47
1:A:308:MET:CE	1:A:318:SER:HA	2.45	0.47
1:A:59:ASN:O	1:A:62:LYS:HD3	2.14	0.47
1:B:183:LYS:HA	4:B:556:HOH:O	2.13	0.47
1:A:22:ASN:OD1	1:A:179:ASN:ND2	2.47	0.47
1:A:203:ASN:ND2	2:A:401:UPG:H6'1	2.23	0.47
1:A:142:PRO:HD2	1:A:161:ILE:HB	1.96	0.46
1:A:182:LYS:HG2	1:A:185:VAL:HB	1.97	0.46
1:B:110:ASN:O	1:B:113:ILE:HG13	2.15	0.46
1:B:201:PHE:CD1	1:B:263:LEU:HD21	2.50	0.46
1:B:89:GLU:HA	1:B:92:ASN:N	2.30	0.46
1:A:356:ASP:HB3	1:A:359:VAL:CG1	2.45	0.46
1:B:180:ILE:CD1	1:B:185:VAL:HG21	2.46	0.45
1:B:31:ASP:OD1	1:B:32:ILE:N	2.50	0.45
1:A:309:LYS:NZ	1:A:392:ASP:HA	2.32	0.45
1:B:176:PHE:O	1:B:180:ILE:HG23	2.16	0.45
1:A:248:SER:HB3	1:A:371:ARG:NH1	2.30	0.45
1:A:39:SER:OG	1:A:44:LYS:O	2.35	0.45
1:A:123:ILE:HG13	1:A:200:LEU:HD12	1.99	0.44
1:A:236:ALA:HA	1:A:242:LYS:HE2	2.00	0.44
1:A:254:TYR:HD1	1:A:316:ARG:NH1	2.16	0.44
1:A:36:LYS:NZ	4:A:513:HOH:O	2.51	0.44
1:B:68:ASN:OD1	1:B:71:GLU:N	2.41	0.44
1:A:254:TYR:HB3	1:A:255:CYS:SG	2.57	0.44
1:A:128:THR:O	1:A:132:LYS:HG2	2.17	0.44
1:A:314:ASN:OD1	1:A:316:ARG:HG2	2.18	0.44
1:B:170:LYS:HD3	1:B:189:TYR:CE1	2.53	0.43
1:B:50:LYS:O	1:B:53:GLU:HB2	2.19	0.43
1:B:84:PRO:HG3	3:B:402:NAD:H51A	2.00	0.43
1:A:122:PRO:HD2	1:A:125:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:CYS:CB	2:B:401:UPG:H6'2	2.47	0.43
1:A:29:LEU:HD12	1:A:63:LEU:HD12	2.01	0.43
1:B:8:ILE:HG12	1:B:29:LEU:HD13	1.99	0.43
1:A:7:GLY:O	1:A:12:GLY:HA3	2.19	0.43
1:A:17:ILE:CG2	1:A:151:LEU:HD11	2.49	0.43
1:B:248:SER:HB3	1:B:371:ARG:NH1	2.33	0.43
1:A:356:ASP:HB3	1:A:359:VAL:HG12	2.00	0.42
1:B:87:TYR:OH	1:B:92:ASN:OD1	2.37	0.42
1:B:98:SER:O	1:B:102:VAL:HG23	2.19	0.42
1:A:127:LYS:HB3	1:A:127:LYS:HE2	1.74	0.41
1:A:219:TYR:HA	1:A:222:LYS:HE2	2.02	0.41
1:A:309:LYS:HD2	1:A:309:LYS:HA	1.62	0.41
1:B:339:TYR:OH	1:B:375:LYS:NZ	2.46	0.41
1:A:107:LYS:HE3	1:A:133:PHE:O	2.21	0.41
1:B:124:GLY:HA2	1:B:193:ASP:OD1	2.20	0.41
1:A:215:GLU:OE2	1:B:275:ILE:HG12	2.20	0.40
1:A:309:LYS:CD	1:A:371:ARG:HG3	2.51	0.40
1:B:10:TYR:OH	1:B:314:ASN:ND2	2.55	0.40
1:A:19:PHE:HA	1:A:179:ASN:ND2	2.35	0.40
1:A:52:ILE:HG12	1:A:151:LEU:CD1	2.50	0.40
1:A:267:PHE:CE2	1:A:275:ILE:HG13	2.56	0.40
1:A:49:ASP:N	1:A:53:GLU:OE2	2.55	0.40

All (4) 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:136:SER:OG	1:A:358:ASN:OD1[1_656]	2.01	0.19
1:A:44:LYS:NZ	1:B:75:ASN:O[2_454]	2.01	0.19
1:B:183:LYS:NZ	1:B:283:GLU:OE2[1_455]	2.13	0.07
1:A:57:VAL:O	1:A:97:ARG:NH1[1_455]	2.15	0.05

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	386/393 (98%)	371 (96%)	15 (4%)	0	100	100
1	B	381/393 (97%)	365 (96%)	14 (4%)	2 (0%)	29	26
All	All	767/786 (98%)	736 (96%)	29 (4%)	2 (0%)	41	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	LEU
1	B	305	ARG

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	355/359 (99%)	354 (100%)	1 (0%)	92	95
1	B	352/359 (98%)	348 (99%)	4 (1%)	73	79
All	All	707/718 (98%)	702 (99%)	5 (1%)	84	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ARG
1	B	110	ASN
1	B	146	ARG
1	B	159	ARG
1	B	183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN

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Mol	Chain	Res	Type
1	A	179	ASN
1	B	38	GLN
1	B	184	ASN

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
3	NAD	A	402	-	42,48,48	4.70	18 (42%)	50,73,73	1.44	6 (12%)
2	UPG	B	401	-	31,38,38	4.27	11 (35%)	41,58,58	1.34	5 (12%)
3	NAD	B	402	-	42,48,48	4.74	19 (45%)	50,73,73	1.55	8 (16%)
2	UPG	A	401	-	31,38,38	4.25	11 (35%)	41,58,58	1.72	6 (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
3	NAD	A	402	-	-	8/26/62/62	0/5/5/5
2	UPG	B	401	-	-	4/21/59/59	0/3/3/3
3	NAD	B	402	-	-	10/26/62/62	0/5/5/5
2	UPG	A	401	-	-	4/21/59/59	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAD	C2B-C1B	-16.20	1.29	1.53
3	A	402	NAD	C2B-C1B	-15.61	1.30	1.53
3	A	402	NAD	O4B-C1B	14.84	1.61	1.41
3	B	402	NAD	O4B-C1B	14.73	1.61	1.41
2	B	401	UPG	C2C-C1C	-12.71	1.34	1.53
2	A	401	UPG	C2C-C1C	-12.47	1.34	1.53
2	A	401	UPG	O4C-C1C	12.35	1.58	1.41
2	B	401	UPG	O4C-C1C	12.08	1.57	1.41
3	A	402	NAD	C2D-C3D	-10.53	1.24	1.53
3	B	402	NAD	C2D-C3D	-10.45	1.24	1.53
3	B	402	NAD	C7N-N7N	7.43	1.47	1.33
2	B	401	UPG	C4-N3	7.36	1.45	1.33
3	A	402	NAD	C7N-N7N	7.29	1.46	1.33
3	B	402	NAD	O4D-C1D	7.01	1.50	1.41
3	A	402	NAD	O4D-C1D	7.01	1.50	1.41
2	B	401	UPG	C6-N1	6.99	1.44	1.35
2	A	401	UPG	C4-N3	6.83	1.44	1.33
3	A	402	NAD	O4D-C4D	-6.39	1.30	1.45
2	A	401	UPG	C6-N1	6.34	1.43	1.35
2	B	401	UPG	C3C-C4C	-6.16	1.37	1.53
3	B	402	NAD	O4D-C4D	-6.03	1.31	1.45
3	A	402	NAD	O4B-C4B	-5.99	1.31	1.45
3	B	402	NAD	O4B-C4B	-5.98	1.31	1.45
2	A	401	UPG	C2-N3	5.77	1.49	1.38
2	A	401	UPG	C3C-C4C	-5.76	1.38	1.53
3	A	402	NAD	C2D-C1D	5.64	1.62	1.53
3	B	402	NAD	C2D-C1D	5.60	1.62	1.53
3	B	402	NAD	C3D-C4D	5.45	1.66	1.53
3	A	402	NAD	C3D-C4D	5.26	1.66	1.53
2	B	401	UPG	C2-N3	5.24	1.48	1.38
2	B	401	UPG	C6-C5	5.08	1.49	1.38
3	B	402	NAD	C3N-C7N	4.90	1.57	1.50
2	A	401	UPG	C6-C5	4.82	1.48	1.38
3	A	402	NAD	C3N-C7N	4.61	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	UPG	O4C-C4C	4.07	1.54	1.45
2	B	401	UPG	O4C-C4C	4.04	1.54	1.45
3	B	402	NAD	O2D-C2D	3.90	1.52	1.43
2	A	401	UPG	PB-O3B	3.87	1.70	1.60
2	A	401	UPG	O5'-C1'	3.62	1.51	1.41
2	A	401	UPG	C3C-C2C	3.54	1.63	1.53
3	A	402	NAD	O2D-C2D	3.46	1.51	1.43
3	B	402	NAD	C6A-N6A	3.43	1.46	1.34
3	A	402	NAD	C6A-N6A	3.42	1.46	1.34
2	B	401	UPG	PB-O3B	3.40	1.69	1.60
2	B	401	UPG	C3C-C2C	3.16	1.62	1.53
3	A	402	NAD	O2B-C2B	3.11	1.50	1.43
2	B	401	UPG	O5'-C1'	3.09	1.49	1.41
3	A	402	NAD	O7N-C7N	-2.81	1.18	1.24
3	A	402	NAD	O3B-C3B	-2.76	1.36	1.43
3	A	402	NAD	C5A-C4A	-2.72	1.33	1.40
3	B	402	NAD	O2B-C2B	2.70	1.49	1.43
3	B	402	NAD	O3B-C3B	-2.70	1.36	1.43
3	B	402	NAD	O3D-C3D	2.49	1.48	1.43
3	B	402	NAD	C5A-C4A	-2.46	1.34	1.40
3	B	402	NAD	O7N-C7N	-2.45	1.19	1.24
3	B	402	NAD	C2A-N3A	2.41	1.36	1.32
3	B	402	NAD	C2N-N1N	2.31	1.37	1.35
3	A	402	NAD	O3D-C3D	2.28	1.48	1.43
3	A	402	NAD	C2A-N3A	2.07	1.35	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	UPG	C6'-C5'-C4'	-6.05	98.84	113.00
2	A	401	UPG	O3A-PB-O3B	5.52	113.61	102.48
2	B	401	UPG	O5'-C1'-O3B	-5.42	104.28	111.36
3	B	402	NAD	N3A-C2A-N1A	-5.41	120.22	128.68
3	A	402	NAD	N3A-C2A-N1A	-5.38	120.28	128.68
3	B	402	NAD	C5A-C6A-N6A	3.85	126.20	120.35
3	B	402	NAD	C6N-N1N-C2N	-3.32	118.95	121.97
3	B	402	NAD	O7N-C7N-N7N	-3.16	118.09	122.58
3	A	402	NAD	C6N-N1N-C2N	-3.08	119.17	121.97
2	A	401	UPG	O5'-C5'-C4'	3.06	115.25	109.69
2	B	401	UPG	O3A-PB-O3B	2.89	108.31	102.48
3	A	402	NAD	C5A-C6A-N6A	2.81	124.63	120.35
3	A	402	NAD	C3D-C2D-C1D	2.74	105.10	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	UPG	C3'-C4'-C5'	2.65	114.97	110.24
3	B	402	NAD	PN-O3-PA	-2.58	123.97	132.83
3	A	402	NAD	O7N-C7N-N7N	-2.57	118.92	122.58
2	B	401	UPG	C1'-O5'-C5'	-2.40	108.97	113.69
3	A	402	NAD	C5B-C4B-C3B	-2.31	106.52	115.18
2	A	401	UPG	C2C-C3C-C4C	2.29	107.09	102.64
3	B	402	NAD	C2N-N1N-C1D	2.27	124.20	119.14
2	B	401	UPG	O4C-C1C-C2C	-2.23	103.67	106.93
3	B	402	NAD	N6A-C6A-N1A	-2.21	114.00	118.57
2	A	401	UPG	O4C-C1C-C2C	-2.11	103.85	106.93
2	B	401	UPG	O3C-C3C-C2C	-2.06	105.17	111.82
3	B	402	NAD	O7N-C7N-C3N	2.02	122.05	119.63

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	NAD	C5B-O5B-PA-O1A
3	A	402	NAD	C3B-C4B-C5B-O5B
3	A	402	NAD	O4D-C1D-N1N-C2N
3	A	402	NAD	O4D-C1D-N1N-C6N
2	B	401	UPG	C2C-C1C-N1-C6
3	B	402	NAD	C5B-O5B-PA-O1A
3	B	402	NAD	C5D-O5D-PN-O3
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C6N
2	A	401	UPG	PA-O3A-PB-O3B
2	A	401	UPG	O5'-C5'-C6'-O6'
2	B	401	UPG	C4'-C5'-C6'-O6'
2	A	401	UPG	C4'-C5'-C6'-O6'
3	A	402	NAD	O4B-C4B-C5B-O5B
2	B	401	UPG	O5'-C5'-C6'-O6'
3	A	402	NAD	C5B-O5B-PA-O3
3	B	402	NAD	C5B-O5B-PA-O3
3	A	402	NAD	C5B-O5B-PA-O2A
3	B	402	NAD	C5D-O5D-PN-O2N
2	B	401	UPG	C1'-O3B-PB-O3A
2	A	401	UPG	C1'-O3B-PB-O3A
3	B	402	NAD	PN-O3-PA-O2A
3	B	402	NAD	O4B-C4B-C5B-O5B
3	A	402	NAD	C2D-C1D-N1N-C6N
3	B	402	NAD	C2D-C1D-N1N-C6N

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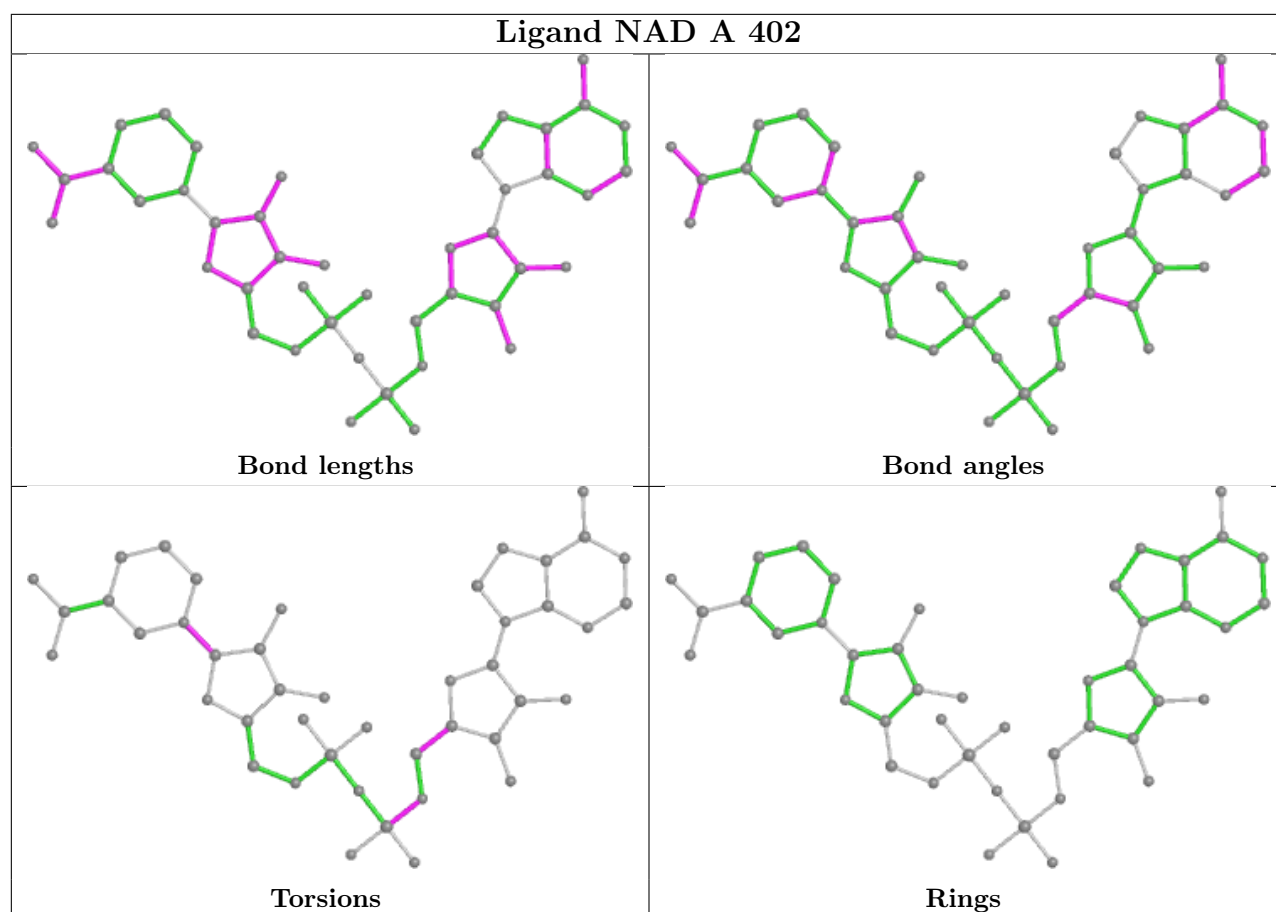
Mol	Chain	Res	Type	Atoms
3	B	402	NAD	C5D-O5D-PN-O1N

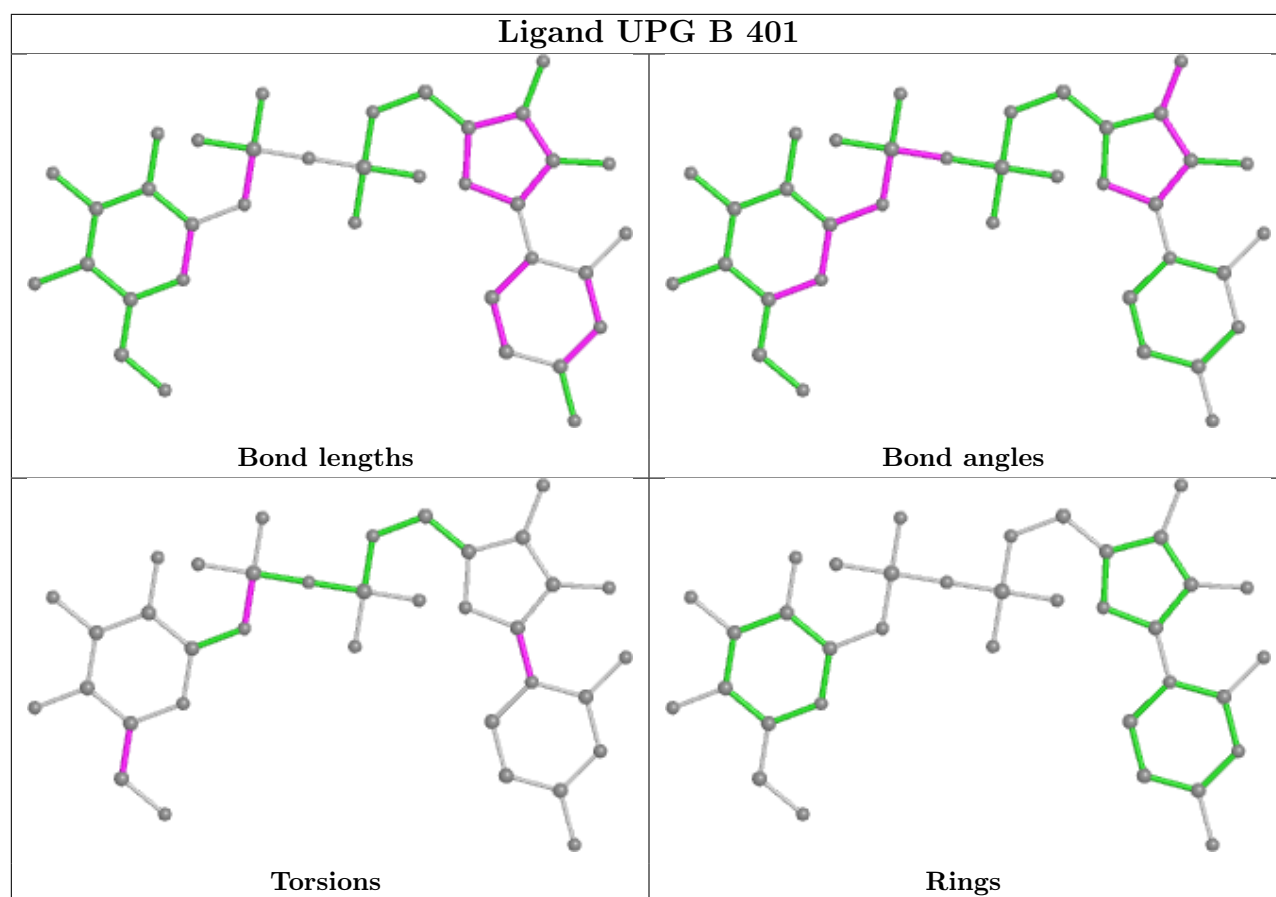
There are no ring outliers.

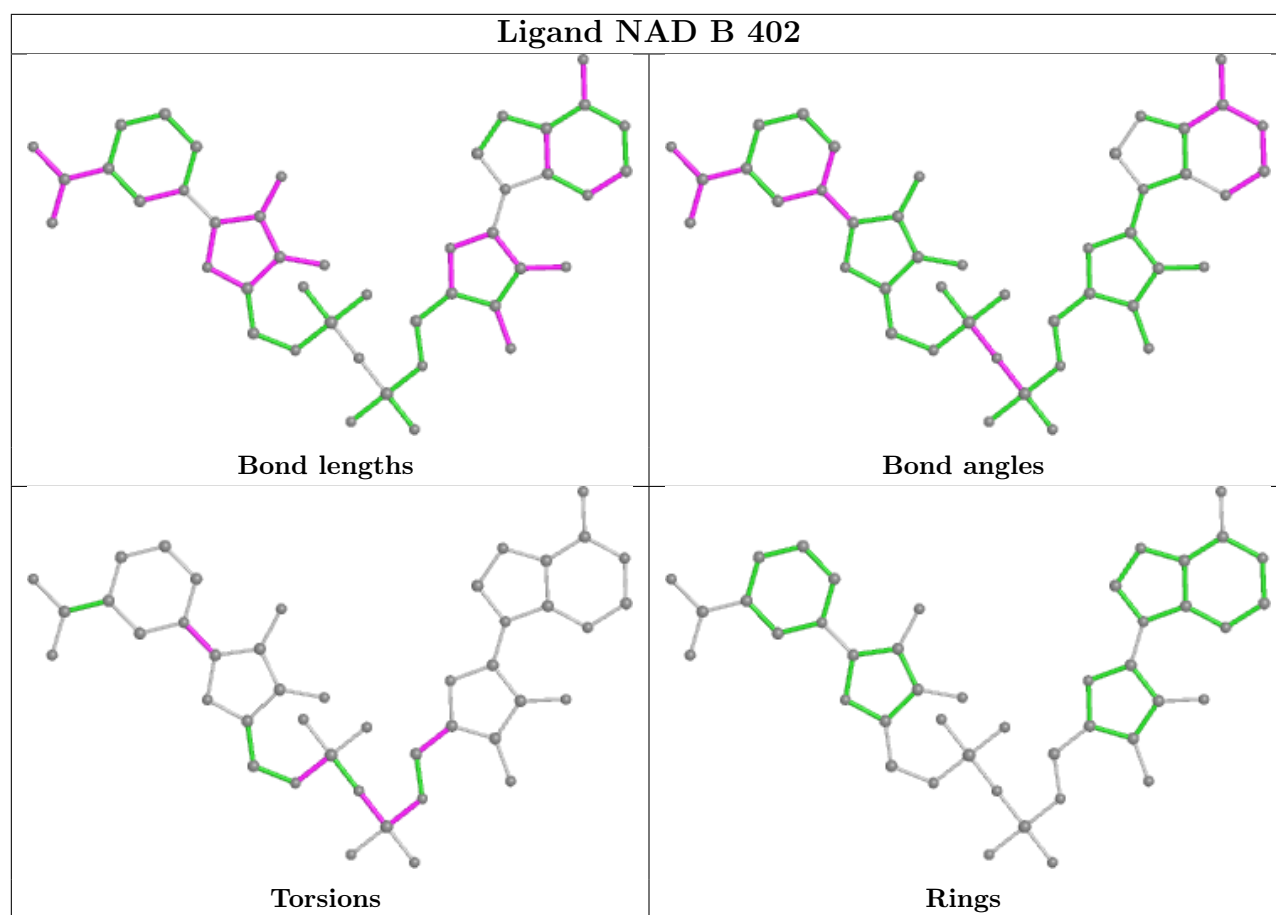
4 monomers are involved in 11 short contacts:

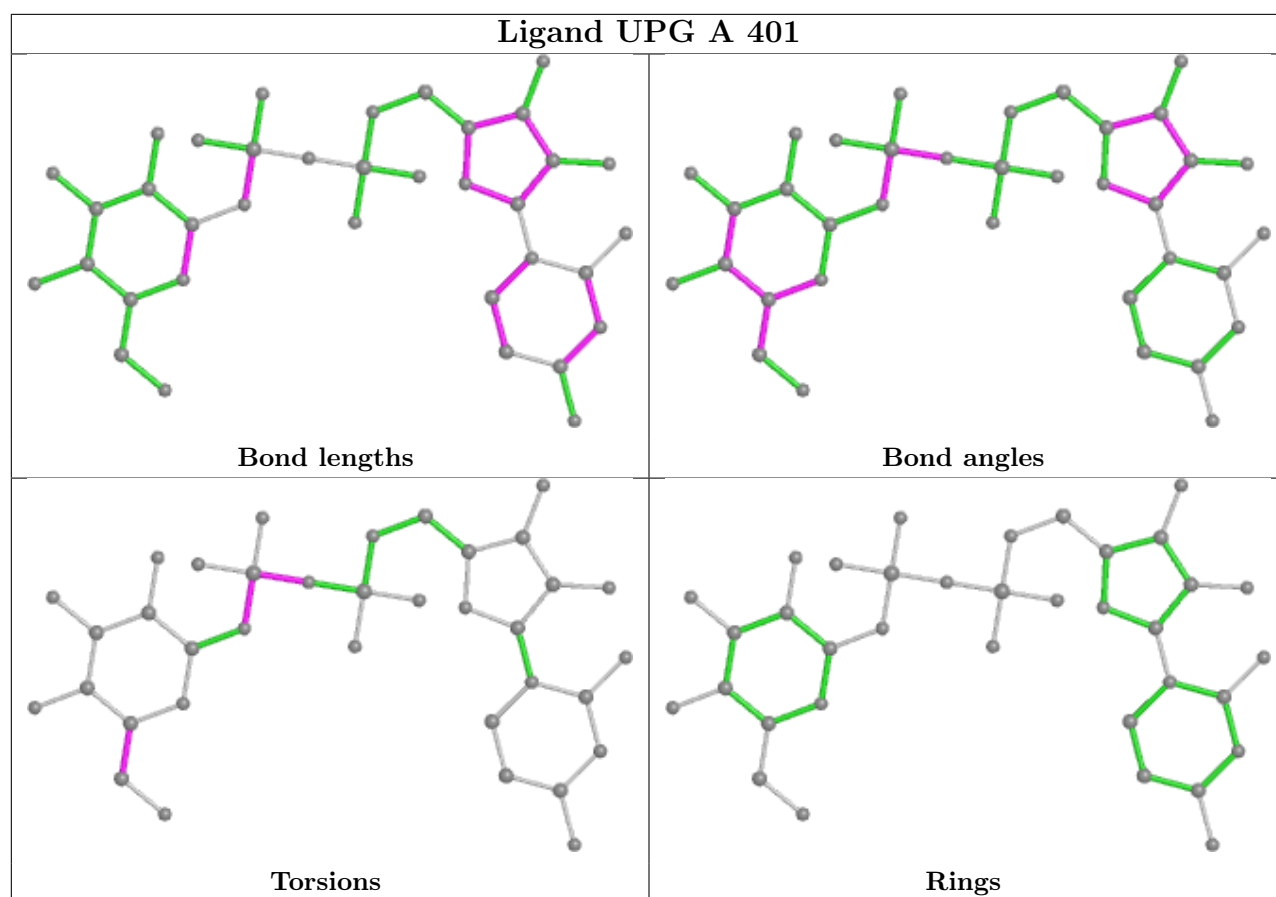
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	NAD	2	0
2	B	401	UPG	3	0
3	B	402	NAD	2	0
2	A	401	UPG	5	0

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, 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	390/393 (99%)	0.27	14 (3%) 42 49	29, 45, 76, 85	0
1	B	387/393 (98%)	0.30	22 (5%) 23 29	29, 46, 73, 87	0
All	All	777/786 (98%)	0.28	36 (4%) 32 38	29, 45, 75, 87	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	LEU	5.6
1	B	52	ILE	4.9
1	B	48	LYS	4.3
1	A	310	GLN	4.3
1	A	57	VAL	4.2
1	B	311	ASN	4.1
1	B	268	TYR	4.1
1	B	92	ASN	4.0
1	B	94	PHE	3.9
1	B	269	ASN	3.7
1	A	391	THR	3.7
1	B	391	THR	3.7
1	A	392	ASP	3.7
1	B	271	PRO	3.4
1	A	269	ASN	3.3
1	A	311	ASN	3.3
1	B	74	PHE	3.2
1	B	93	PHE	3.2
1	B	270	ILE	2.9
1	B	49	ASP	2.9
1	B	254	TYR	2.8
1	A	254	TYR	2.8
1	A	88	ASP	2.6
1	A	270	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	87	TYR	2.5
1	B	88	ASP	2.5
1	B	317	ASN	2.4
1	B	390	TYR	2.3
1	B	61	SER	2.2
1	A	22	ASN	2.2
1	A	268	TYR	2.2
1	A	58	GLN	2.1
1	B	349	LEU	2.1
1	A	49	ASP	2.1
1	B	23	ASN	2.0
1	A	91	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](#)

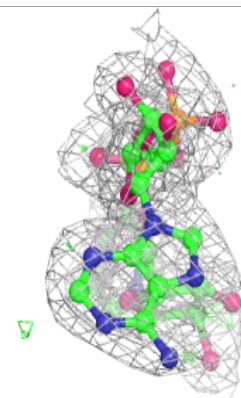
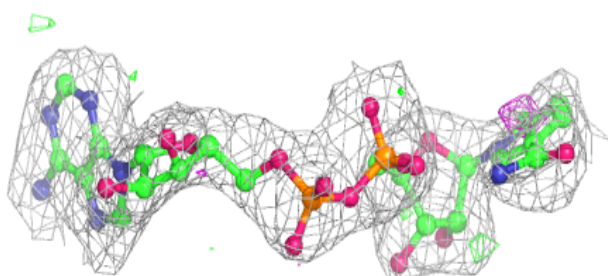
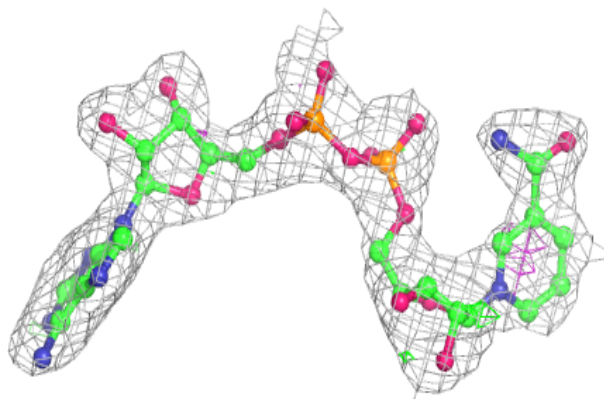
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAD	A	402	44/44	0.91	0.13	43,51,59,62	0
3	NAD	B	402	44/44	0.92	0.12	38,45,54,55	0
2	UPG	A	401	36/36	0.95	0.12	32,36,45,49	0
2	UPG	B	401	36/36	0.96	0.11	32,39,43,45	0

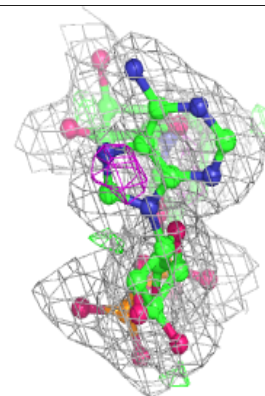
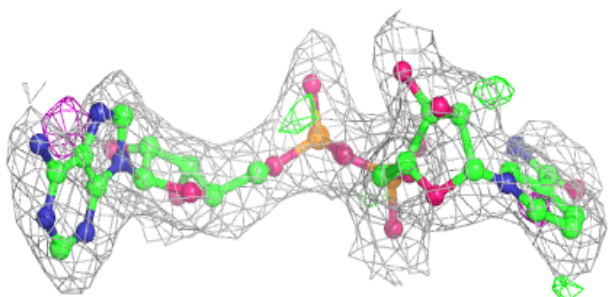
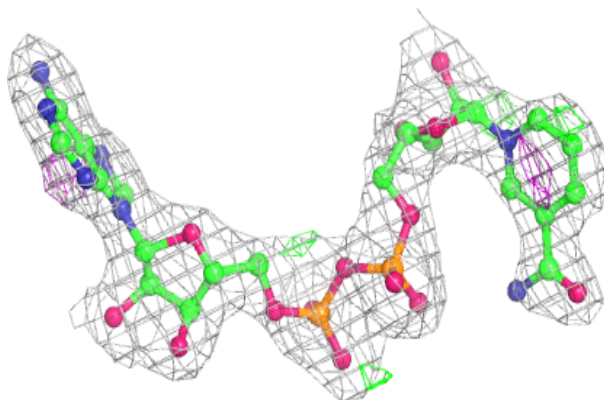
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD A 402:

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

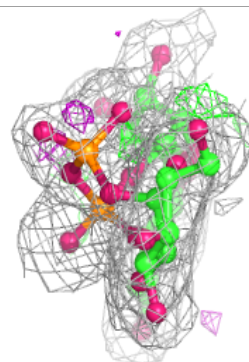
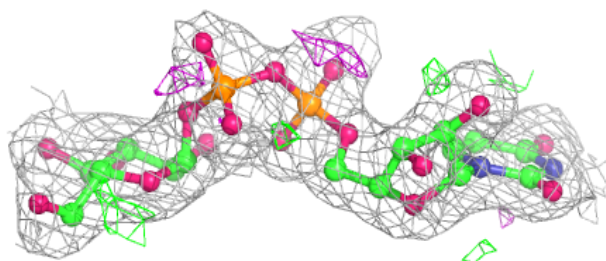
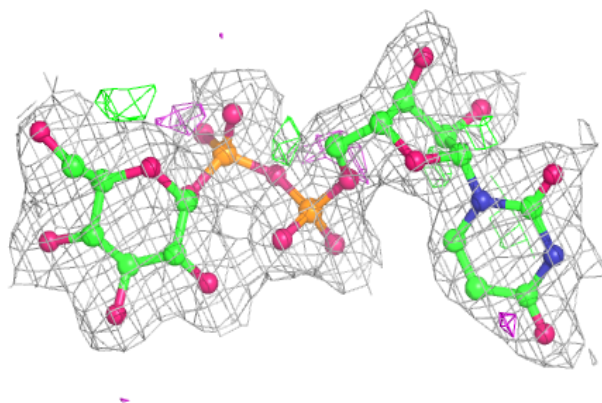
**Electron density around NAD B 402:**

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

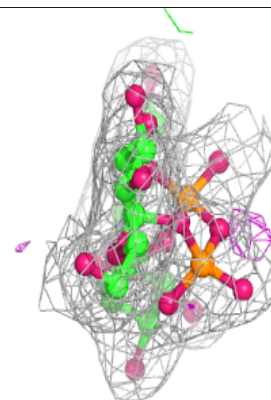
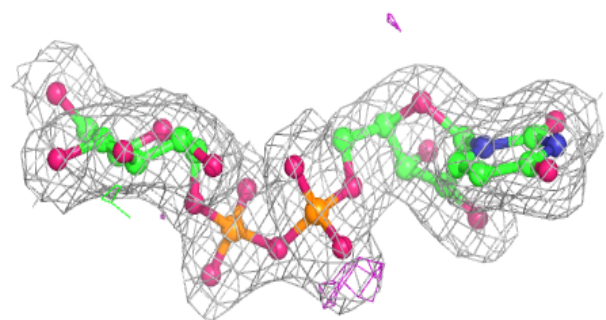
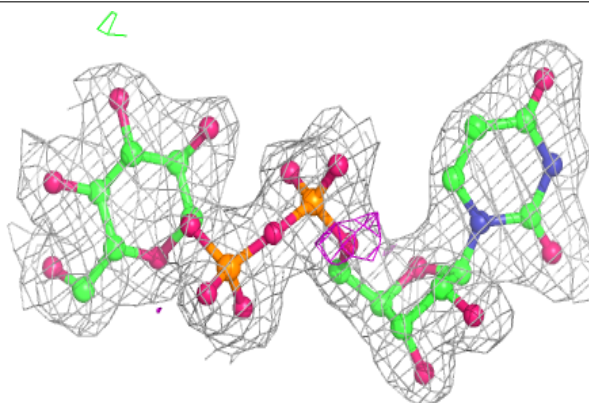


Electron density around UPG A 401:

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

**Electron density around UPG 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.