



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:20 AM EDT

PDB ID : 8VR2 / pdb_00008vr2
Title : Crystal structure of the Pcryo_0617 oxidoreductase/decarboxylase from Psychrobacter cryohalolentis K5 in the presence of NAD and UDP
Authors : Bockhaus, N.J.; Thoden, J.B.; Holden, H.M.
Deposited on : 2024-01-20
Resolution : 1.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

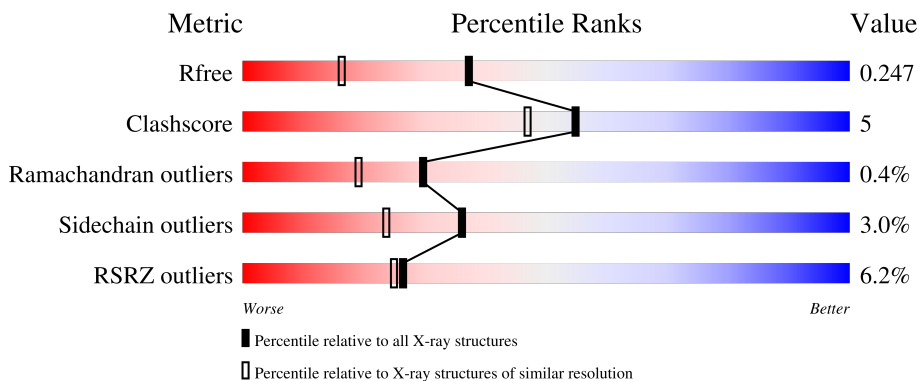
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	335	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">81% 10% • 9%</p>
1	B	335	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">87% 8% • •</p>
1	C	335	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">84% 9% • • 6%</p>
1	D	335	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center; margin-top: 5px;">85% 9% • 5%</p>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10507 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.

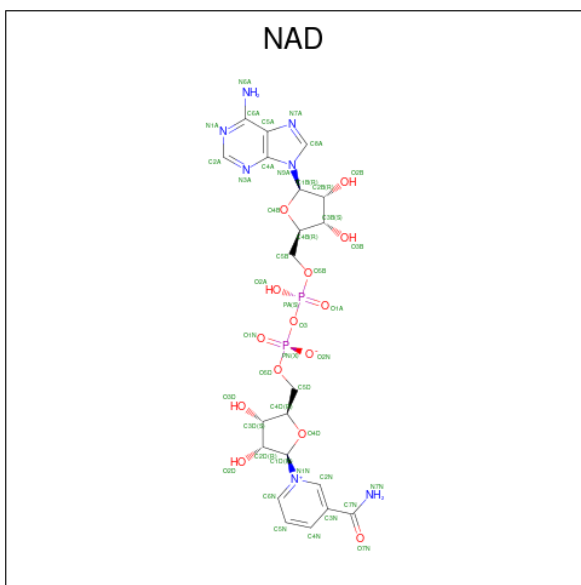
- Molecule 1 is a protein called NAD-dependent epimerase/dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2352	1488	407	448	9	0	0	0
1	B	321	2465	1560	426	468	11	0	2	0
1	C	316	2455	1556	425	465	9	0	4	0
1	D	318	2459	1554	421	475	9	0	5	0

There are 8 discrepancies between the modelled and reference sequences:

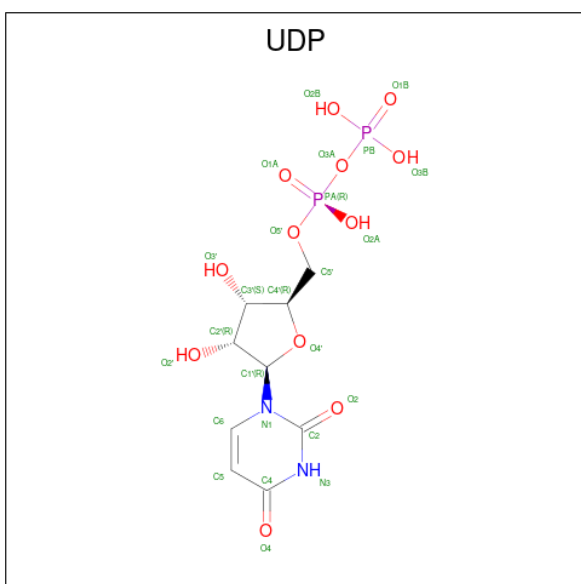
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q1QD53
A	0	HIS	-	expression tag	UNP Q1QD53
B	-1	GLY	-	expression tag	UNP Q1QD53
B	0	HIS	-	expression tag	UNP Q1QD53
C	-1	GLY	-	expression tag	UNP Q1QD53
C	0	HIS	-	expression tag	UNP Q1QD53
D	-1	GLY	-	expression tag	UNP Q1QD53
D	0	HIS	-	expression tag	UNP Q1QD53

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).

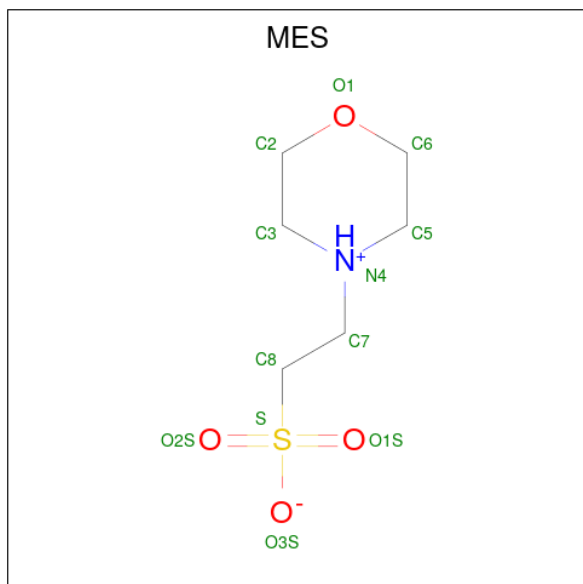


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

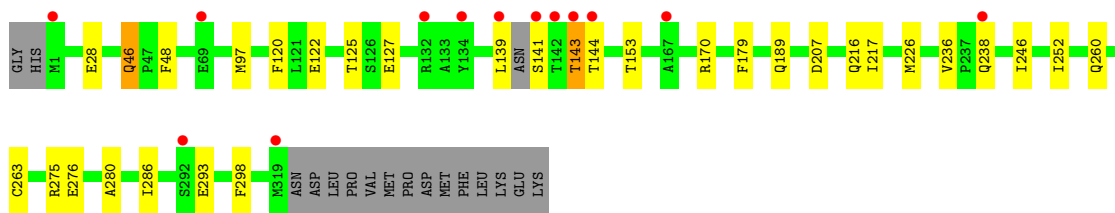
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total	O	0	0
			85	85		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	118	Total 118	O 118	0	0
6	C	153	Total 153	O 153	0	0
6	D	131	Total 131	O 131	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.58Å 114.85Å 206.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 1.80 48.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.95-1.80) 97.8 (48.95-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.196 , 0.241 0.203 , 0.247	Depositor DCC
R_{free} test set	6921 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10507	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MES, UDP, 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	0.58	0/2390	1.00	1/3233 (0.0%)
1	B	0.59	0/2511	1.00	2/3397 (0.1%)
1	C	0.61	0/2507	1.02	5/3391 (0.1%)
1	D	0.58	0/2512	1.01	1/3400 (0.0%)
All	All	0.59	0/9920	1.00	9/13421 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	PRO	N-CA-CB	7.11	110.72	103.25
1	D	207	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	236	VAL	CB-CA-C	6.05	116.57	110.94
1	C	228	ASP	CA-CB-CG	5.84	118.44	112.60
1	C	137	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	128	VAL	N-CA-CB	-5.47	103.63	110.47
1	A	28	GLU	CB-CG-CD	5.44	121.84	112.60
1	C	190	ILE	N-CA-C	-5.15	105.48	110.42
1	B	242	GLU	N-CA-CB	-5.10	102.94	111.20

There are no chirality outliers.

There are no planarity outliers.

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	2352	0	2356	27	0
1	B	2465	0	2447	25	0
1	C	2455	0	2460	35	0
1	D	2459	0	2457	18	0
2	A	44	0	26	1	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	25	0	11	1	0
3	B	25	0	11	0	0
3	C	25	0	11	0	0
3	D	25	0	11	0	0
4	D	1	0	0	0	0
5	D	12	0	13	0	0
6	A	85	0	0	2	0
6	B	118	0	0	4	0
6	C	153	0	0	5	0
6	D	131	0	0	1	0
All	All	10507	0	9881	95	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 5.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264[A]:ARG:HD3	1:D:260:GLN:OE1	1.63	0.99
1:C:306:GLU:OE1	1:C:310:ARG:NH2	2.02	0.91
1:C:264[B]:ARG:HH11	1:C:264[B]:ARG:HG3	1.35	0.90
1:B:101:MET:SD	1:C:101:MET:HE3	2.14	0.87
1:A:128:VAL:CG1	1:A:159:LEU:HD13	2.08	0.84
1:C:253:THR:HG22	6:C:596:HOH:O	1.77	0.83
1:D:122[A]:GLU:OE1	6:D:501:HOH:O	2.02	0.76
1:A:188:GLY:O	1:A:189:GLN:HB2	1.86	0.76
1:C:264[B]:ARG:HH11	1:C:264[B]:ARG:CG	2.00	0.74
1:B:97[A]:MET:HE3	1:B:101:MET:CE	2.21	0.71
1:A:97:MET:HE3	1:A:153:THR:HG23	1.72	0.71
1:C:135:ARG:HB2	1:C:138:GLU:HB3	1.73	0.70
1:A:236:VAL:CG1	1:A:238:GLN:OE1	2.41	0.68
1:B:135:ARG:HD3	1:C:132:ARG:CZ	2.23	0.68
1:A:128:VAL:HG11	1:A:159:LEU:HD13	1.76	0.68
1:A:128:VAL:HG13	1:A:159:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLU:OE2	6:B:502:HOH:O	2.15	0.65
1:A:122:GLU:OE1	6:A:501:HOH:O	2.14	0.65
1:C:122:GLU:OE1	6:C:502:HOH:O	2.14	0.64
1:B:122:GLU:OE1	6:B:503:HOH:O	2.15	0.64
1:D:46[A]:GLN:HG2	1:D:48:PHE:CZ	2.34	0.63
1:B:101:MET:SD	1:C:101:MET:CE	2.88	0.62
1:C:134:TYR:CZ	1:C:282:ILE:HG13	2.36	0.60
1:B:306:GLU:OE1	1:B:310:ARG:CZ	2.50	0.60
1:A:83:ILE:CD1	1:A:95:ARG:HG2	2.33	0.59
1:B:288:ASN:HD21	1:B:290:ASP:CG	2.11	0.58
1:A:188:GLY:O	1:A:189:GLN:CB	2.51	0.58
1:B:101:MET:CG	1:C:101:MET:CE	2.82	0.57
1:C:318:ASN:HD22	1:C:318:ASN:N	2.03	0.57
1:C:236:VAL:HG13	1:C:238:GLN:OE1	2.06	0.56
1:C:253:THR:CG2	6:C:596:HOH:O	2.44	0.56
1:B:101:MET:HG3	1:C:101:MET:CE	2.37	0.55
1:A:236:VAL:HG12	1:A:238:GLN:OE1	2.07	0.54
1:D:125:THR:OG1	1:D:127:GLU:OE1	2.20	0.54
1:C:128:VAL:HG22	1:C:159:LEU:HB2	1.89	0.54
1:A:93:PRO:HA	1:A:153:THR:HG21	1.90	0.54
1:B:97[A]:MET:HE3	1:B:101:MET:HE3	1.90	0.54
1:B:97[A]:MET:CE	1:B:101:MET:CE	2.87	0.53
1:B:293:GLU:OE2	1:B:299:LYS:HD2	2.10	0.52
1:C:264[B]:ARG:CG	1:C:264[B]:ARG:NH1	2.71	0.52
1:B:306:GLU:OE1	1:B:310:ARG:NH2	2.43	0.52
1:A:218:ARG:NH2	3:A:402:UDP:H5'2	2.26	0.51
1:A:218:ARG:HH11	1:A:255:ILE:HD11	1.75	0.51
1:D:217:ILE:HG22	1:D:286:ILE:HD11	1.93	0.51
1:D:46[B]:GLN:HA	1:D:46[B]:GLN:OE1	2.10	0.49
1:B:97[A]:MET:CE	1:B:101:MET:HE1	2.43	0.49
1:A:305:GLU:HG3	6:A:560:HOH:O	2.11	0.49
1:B:25:ARG:HH21	1:B:25:ARG:HG2	1.78	0.48
1:B:253:THR:OG1	6:B:501:HOH:O	2.04	0.48
1:C:2:ILE:HG23	1:C:7:LYS:HZ2	1.79	0.47
1:A:43:LEU:HD21	1:A:54:LEU:HD21	1.97	0.47
1:C:253:THR:HG23	1:C:254:THR:O	2.15	0.47
1:A:236:VAL:HG13	1:A:238:GLN:OE1	2.13	0.47
1:A:83:ILE:HG23	1:A:88:ASN:HB3	1.97	0.47
1:B:28:GLU:HB2	6:B:571:HOH:O	2.15	0.46
1:A:98:THR:HG23	1:A:102:ILE:HD12	1.96	0.46
1:A:189:GLN:HG2	1:A:191:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:ILE:N	1:C:286:ILE:CD1	2.79	0.45
1:D:236:VAL:HG12	1:D:238:GLN:OE1	2.16	0.45
1:C:226:MET:HE3	1:C:226:MET:HB3	1.87	0.45
1:D:46[A]:GLN:HG2	1:D:48:PHE:CE1	2.51	0.45
1:C:253:THR:OG1	6:C:501:HOH:O	2.12	0.44
1:A:245:ASN:ND2	1:A:287:PRO:HB2	2.33	0.44
1:D:97:MET:HE3	1:D:153:THR:HG23	2.00	0.44
1:A:2:ILE:O	1:A:235:SER:HB2	2.17	0.44
1:B:97[B]:MET:HE3	1:B:153:THR:HG23	1.99	0.44
1:C:130:GLY:HA3	1:C:284:LEU:HD22	2.00	0.44
1:D:144:THR:O	1:D:280:ALA:O	2.36	0.43
1:C:216:GLN:HG2	1:C:255:ILE:HG12	2.01	0.43
1:D:141:SER:CB	1:D:143:THR:HB	2.49	0.43
1:B:164:LEU:HD11	1:C:101:MET:HE1	2.00	0.43
1:A:83:ILE:HD11	1:A:95:ARG:HG2	2.01	0.43
1:C:7:LYS:NZ	6:C:504:HOH:O	2.29	0.43
1:B:25:ARG:HG2	1:B:25:ARG:NH2	2.33	0.42
1:B:97[A]:MET:HE3	1:B:101:MET:HE1	1.99	0.42
1:C:264[B]:ARG:CZ	1:D:263:CYS:HB3	2.49	0.42
1:C:40:ARG:HG2	1:C:41:ASN:N	2.35	0.42
1:C:132:ARG:HH21	1:C:132:ARG:HG3	1.85	0.42
1:A:22:LEU:CD2	1:A:78:ILE:HD13	2.50	0.41
1:C:124:SER:HB3	1:C:180:ARG:HG2	2.02	0.41
1:D:293:GLU:HA	1:D:298:PHE:O	2.21	0.41
1:D:179:PHE:CE1	1:D:246:ILE:HG13	2.56	0.41
1:C:98:THR:HG23	1:C:102[A]:ILE:HD12	2.03	0.41
1:D:252:ILE:HG23	1:D:286:ILE:HD13	2.02	0.41
1:D:275:ARG:HG3	1:D:276:GLU:N	2.35	0.41
1:A:182:PHE:CD2	1:A:219:ALA:HB1	2.56	0.41
1:B:135:ARG:HH11	1:C:132:ARG:HD3	1.85	0.41
1:A:2:ILE:HB	1:A:235:SER:HA	2.02	0.41
1:B:184:VAL:HA	1:B:221:CYS:O	2.21	0.40
1:D:226:MET:C	1:D:226:MET:SD	3.05	0.40
1:A:124:SER:O	2:A:401:NAD:H6N	2.21	0.40
1:A:179:PHE:CZ	1:A:246:ILE:HG13	2.57	0.40
1:B:101:MET:HG3	1:C:101:MET:HE1	2.02	0.40
1:D:120:PHE:CE2	1:D:122[B]:GLU:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/335 (90%)	293 (97%)	8 (3%)	1 (0%)	36	25
1	B	319/335 (95%)	308 (97%)	7 (2%)	4 (1%)	9	3
1	C	316/335 (94%)	312 (99%)	4 (1%)	0	100	100
1	D	319/335 (95%)	315 (99%)	4 (1%)	0	100	100
All	All	1256/1340 (94%)	1228 (98%)	23 (2%)	5 (0%)	30	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	B	321	ASP
1	B	323	PRO
1	B	322	LEU
1	B	190	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/274 (90%)	241 (98%)	6 (2%)	43	31
1	B	256/274 (93%)	247 (96%)	9 (4%)	32	19
1	C	258/274 (94%)	250 (97%)	8 (3%)	35	23
1	D	260/274 (95%)	252 (97%)	8 (3%)	35	23
All	All	1021/1096 (93%)	990 (97%)	31 (3%)	36	24

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	44	LYS
1	A	97	MET
1	A	128	VAL
1	A	264	ARG
1	A	284	LEU
1	B	25	ARG
1	B	128	VAL
1	B	136	VAL
1	B	159	LEU
1	B	192	GLU
1	B	216	GLN
1	B	276	GLU
1	B	294	GLU
1	B	319	MET
1	C	128	VAL
1	C	138	GLU
1	C	140	ASN
1	C	189	GLN
1	C	236	VAL
1	C	282	ILE
1	C	286	ILE
1	C	318	ASN
1	D	28	GLU
1	D	46[A]	GLN
1	D	46[B]	GLN
1	D	139	LEU
1	D	143	THR
1	D	170	ARG
1	D	189	GLN
1	D	216	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	88	ASN
1	B	58	GLN
1	B	118	GLN
1	B	183	ASN
1	C	58	GLN

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Mol	Chain	Res	Type
1	C	118	GLN
1	C	166	HIS
1	C	189	GLN
1	C	318	ASN
1	D	58	GLN
1	D	267	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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
2	NAD	D	401	-	46,48,48	0.68	1 (2%)	64,73,73	0.69	0
3	UDP	A	402	-	25,26,26	0.66	1 (4%)	38,40,40	0.78	0
2	NAD	C	401	-	46,48,48	0.70	1 (2%)	64,73,73	0.75	0
3	UDP	B	402	-	25,26,26	0.73	1 (4%)	38,40,40	0.69	1 (2%)
3	UDP	D	402	-	25,26,26	0.54	0	38,40,40	0.60	0
3	UDP	C	402	-	25,26,26	0.66	1 (4%)	38,40,40	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	401	-	46,48,48	0.69	1 (2%)	64,73,73	0.79	3 (4%)
5	MES	D	404	-	12,12,12	0.90	0	15,16,16	0.63	0
2	NAD	A	401	-	46,48,48	0.73	1 (2%)	64,73,73	0.77	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	401	-	-	0/30/62/62	0/5/5/5
3	UDP	A	402	-	-	2/16/32/32	0/2/2/2
2	NAD	C	401	-	-	1/30/62/62	0/5/5/5
3	UDP	B	402	-	-	1/16/32/32	0/2/2/2
3	UDP	D	402	-	-	1/16/32/32	0/2/2/2
3	UDP	C	402	-	-	2/16/32/32	0/2/2/2
2	NAD	B	401	-	-	4/30/62/62	0/5/5/5
5	MES	D	404	-	-	6/6/14/14	0/1/1/1
2	NAD	A	401	-	-	1/30/62/62	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C2N-N1N	3.51	1.38	1.35
2	B	401	NAD	C2N-N1N	3.31	1.38	1.35
2	D	401	NAD	C2N-N1N	2.98	1.38	1.35
2	C	401	NAD	C2N-N1N	2.71	1.38	1.35
3	A	402	UDP	PA-O3A	2.24	1.61	1.59
3	B	402	UDP	PA-O3A	2.17	1.61	1.59
3	C	402	UDP	PA-O3A	2.11	1.61	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAD	C6N-N1N-C2N	-2.72	119.56	121.88
2	B	401	NAD	O2N-PN-O1N	2.70	125.00	112.44
2	A	401	NAD	C6N-N1N-C2N	-2.59	119.68	121.88
2	B	401	NAD	O3-PN-O1N	-2.50	103.18	110.70
3	B	402	UDP	O3A-PA-O1A	-2.42	103.42	110.70

There are no chirality outliers.

All (18) torsion outliers are listed below:

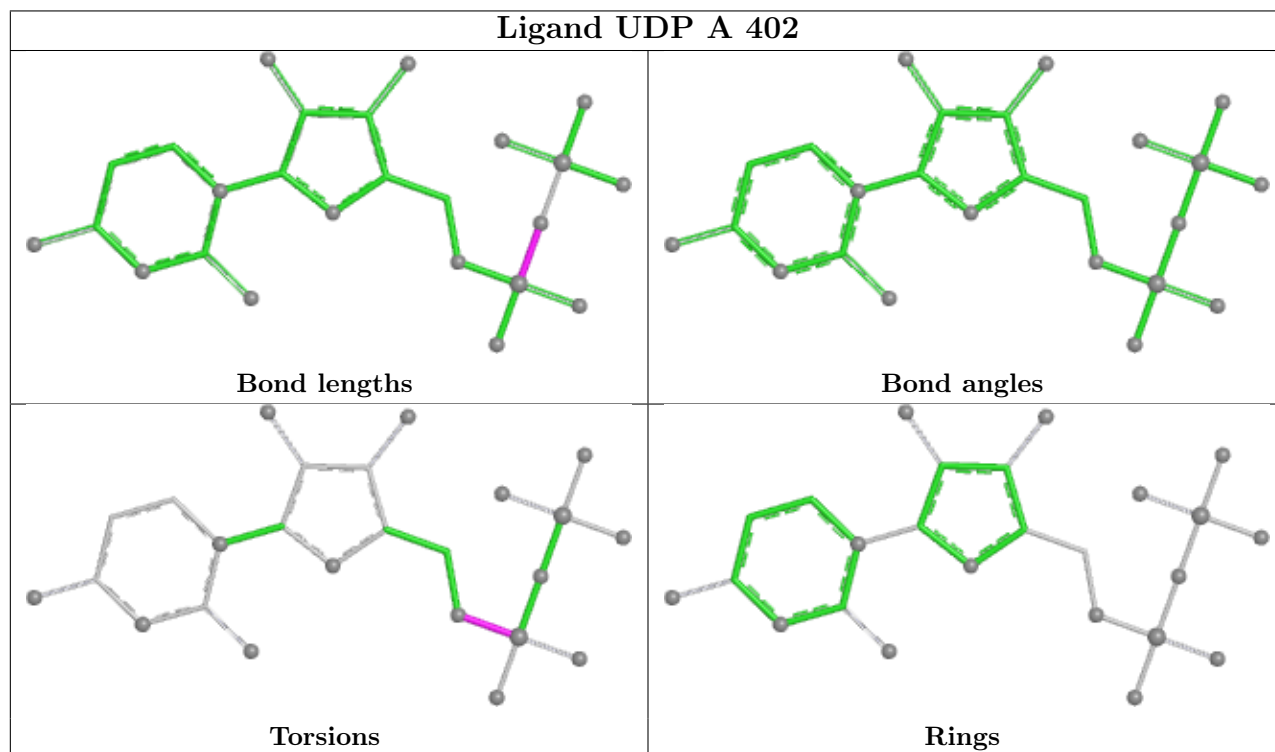
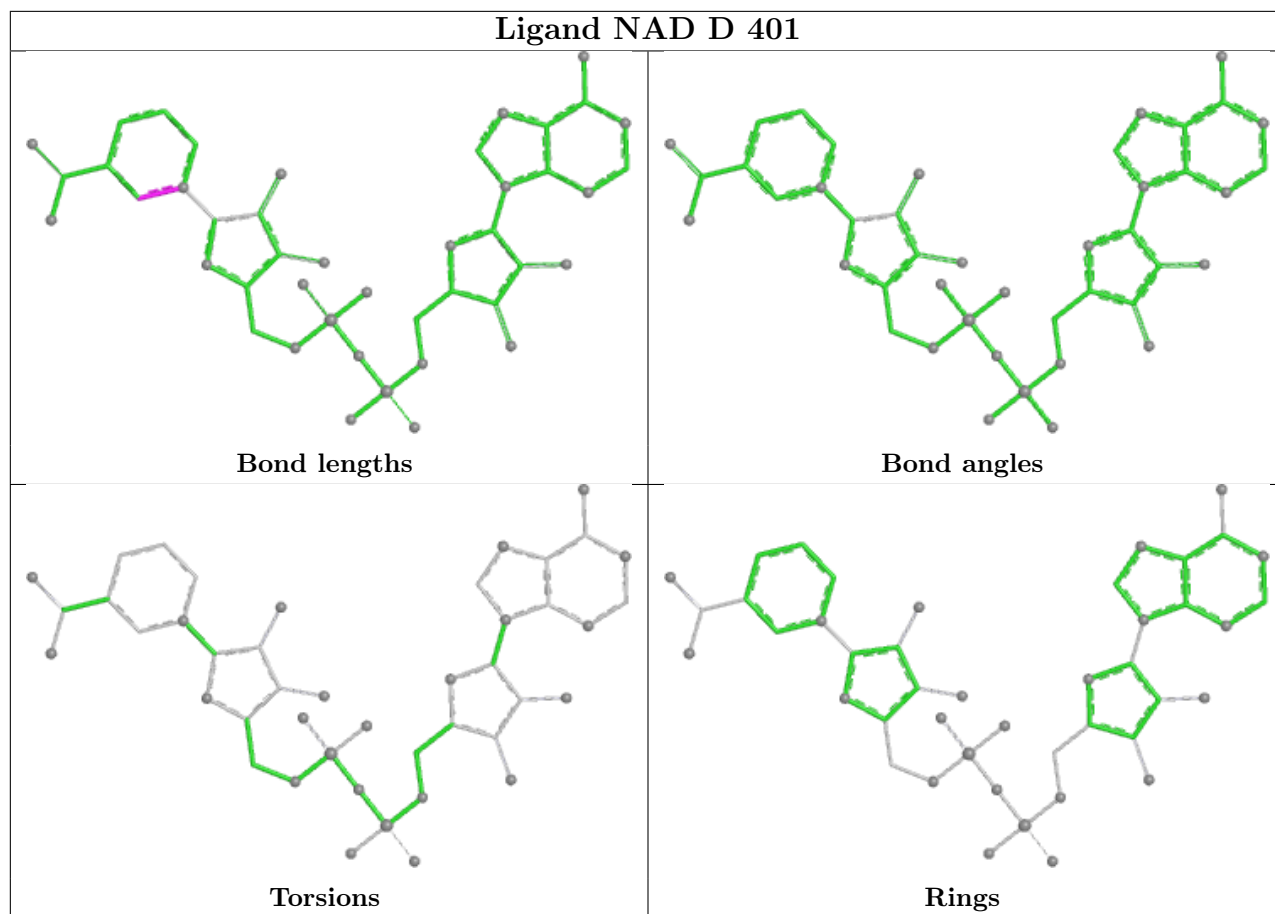
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	B	401	NAD	C5D-O5D-PN-O2N
3	A	402	UDP	C5'-O5'-PA-O3A
5	D	404	MES	C8-C7-N4-C5
3	B	402	UDP	PB-O3A-PA-O5'
3	C	402	UDP	PB-O3A-PA-O5'
3	D	402	UDP	PB-O3A-PA-O5'
5	D	404	MES	C7-C8-S-O3S
5	D	404	MES	C7-C8-S-O1S
5	D	404	MES	N4-C7-C8-S
2	B	401	NAD	C5D-O5D-PN-O3
3	A	402	UDP	C5'-O5'-PA-O1A
5	D	404	MES	C8-C7-N4-C3
3	C	402	UDP	PB-O3A-PA-O1A
5	D	404	MES	C7-C8-S-O2S
2	B	401	NAD	PA-O3-PN-O1N
2	C	401	NAD	O4B-C4B-C5B-O5B
2	B	401	NAD	O4B-C4B-C5B-O5B

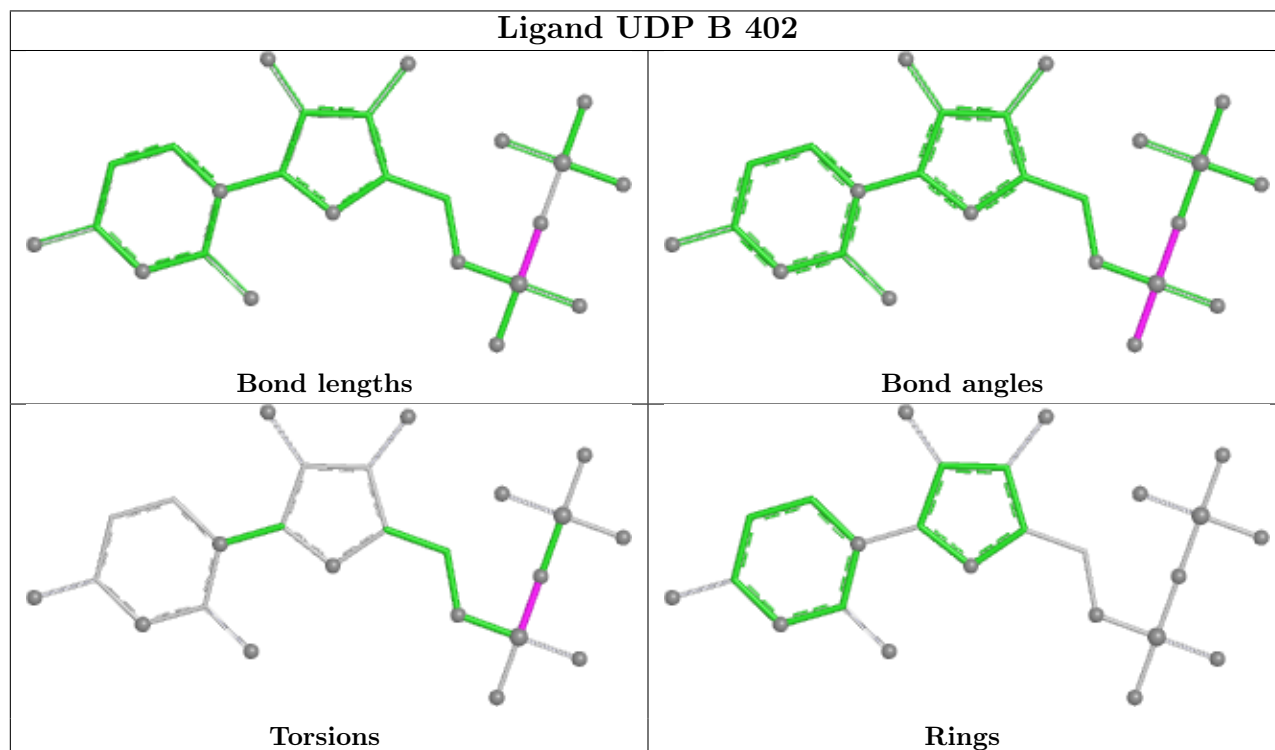
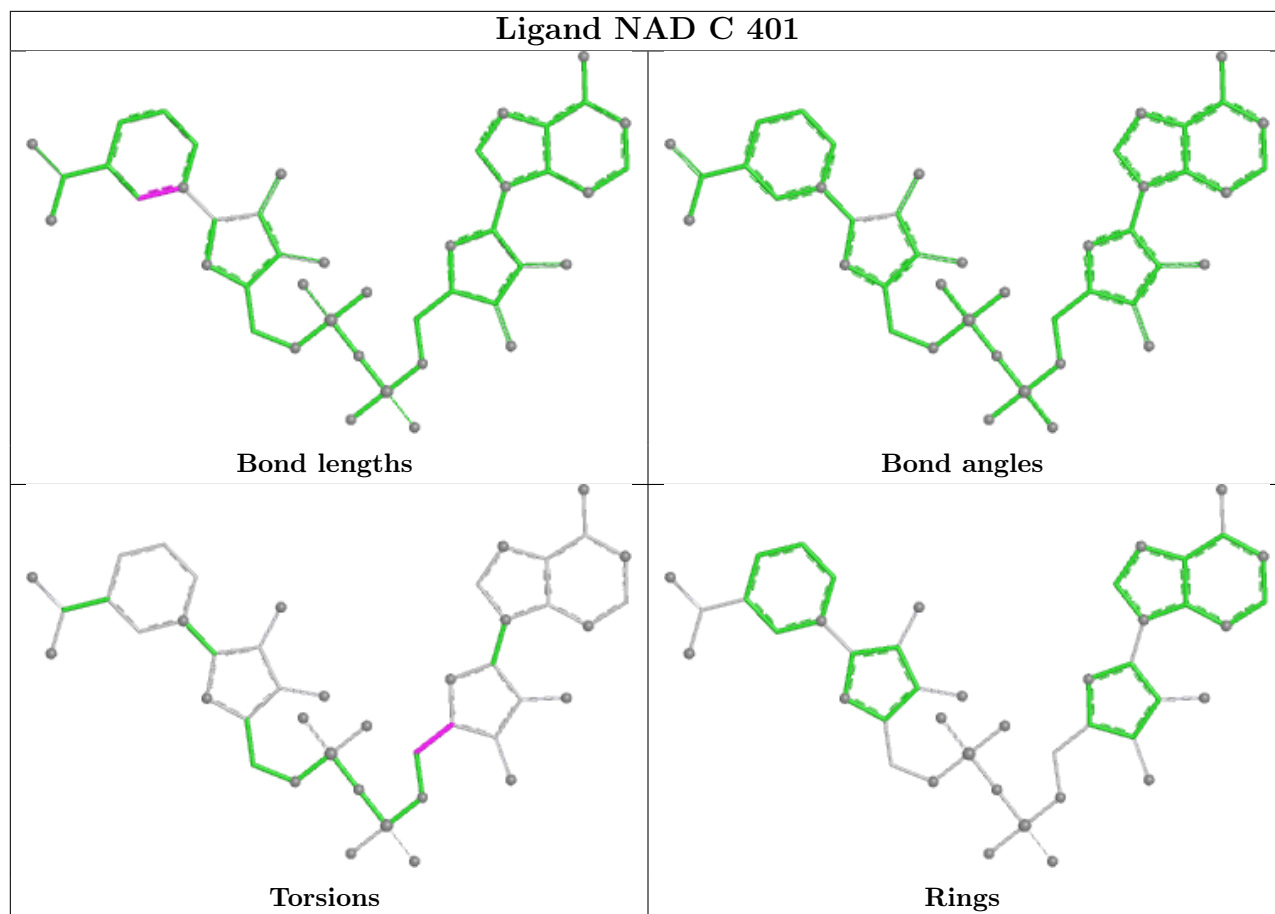
There are no ring outliers.

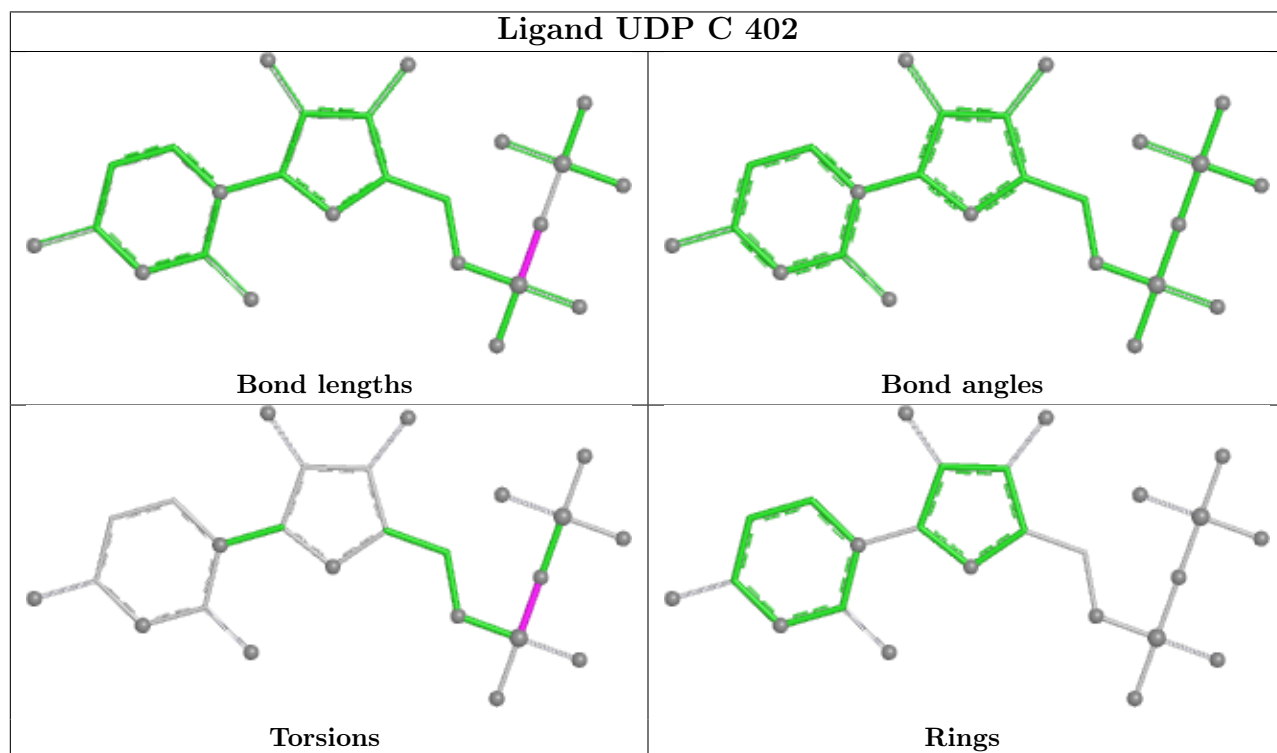
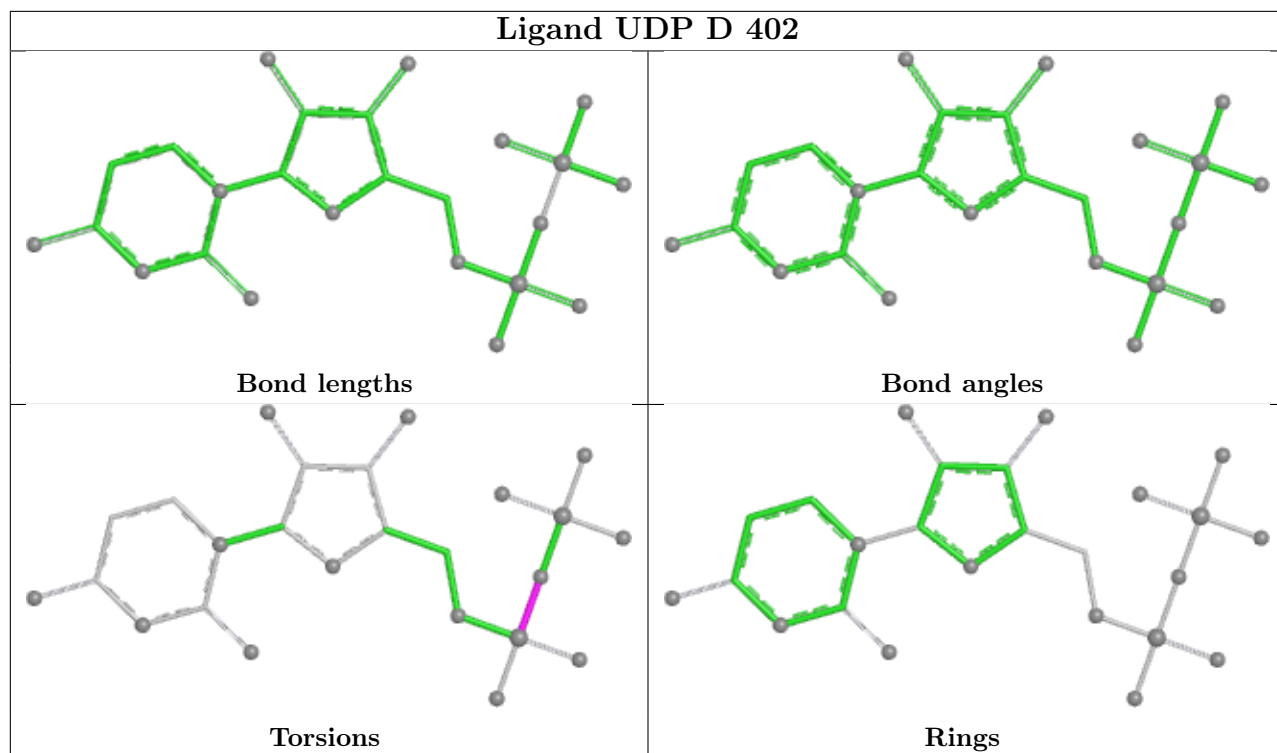
2 monomers are involved in 2 short contacts:

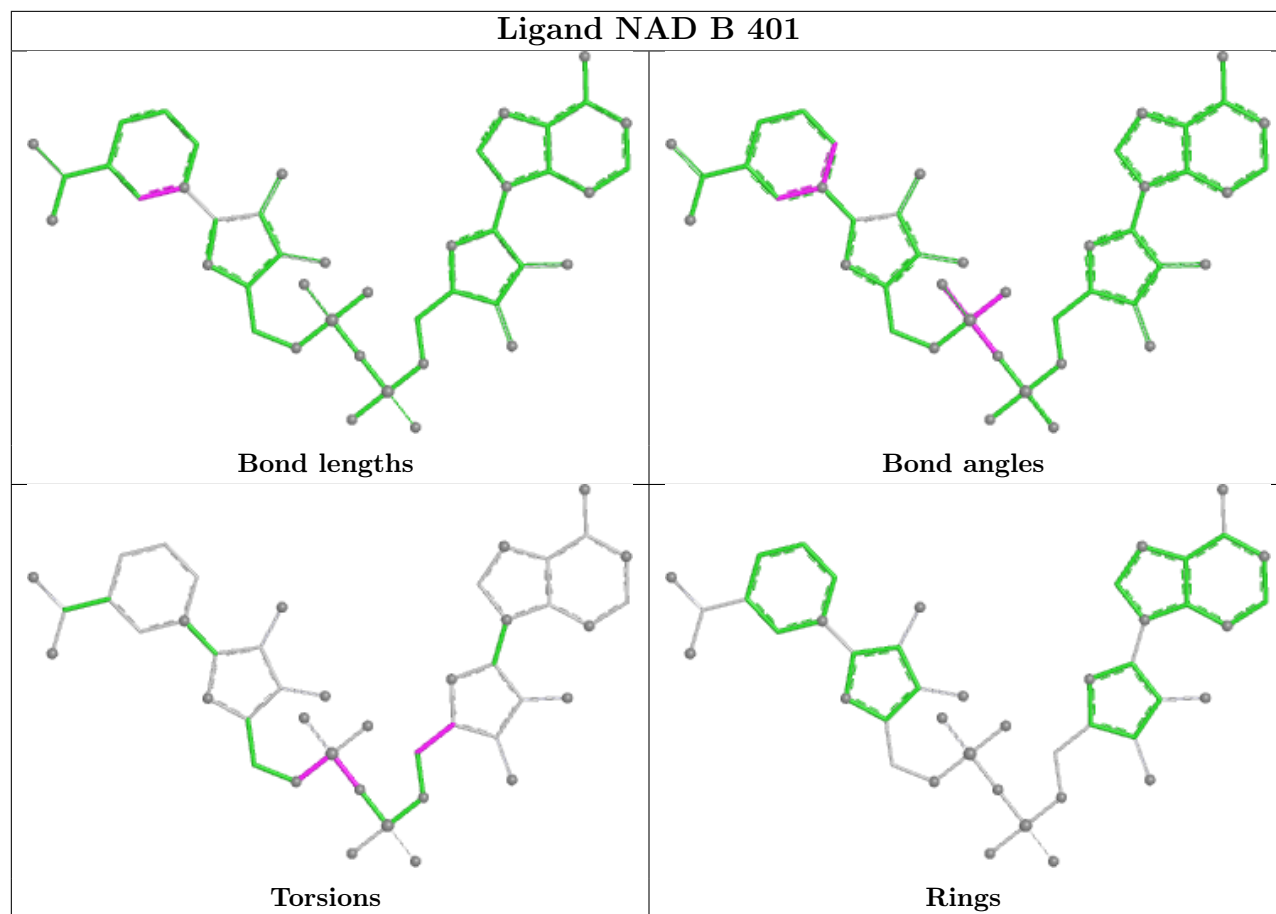
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	UDP	1	0
2	A	401	NAD	1	0

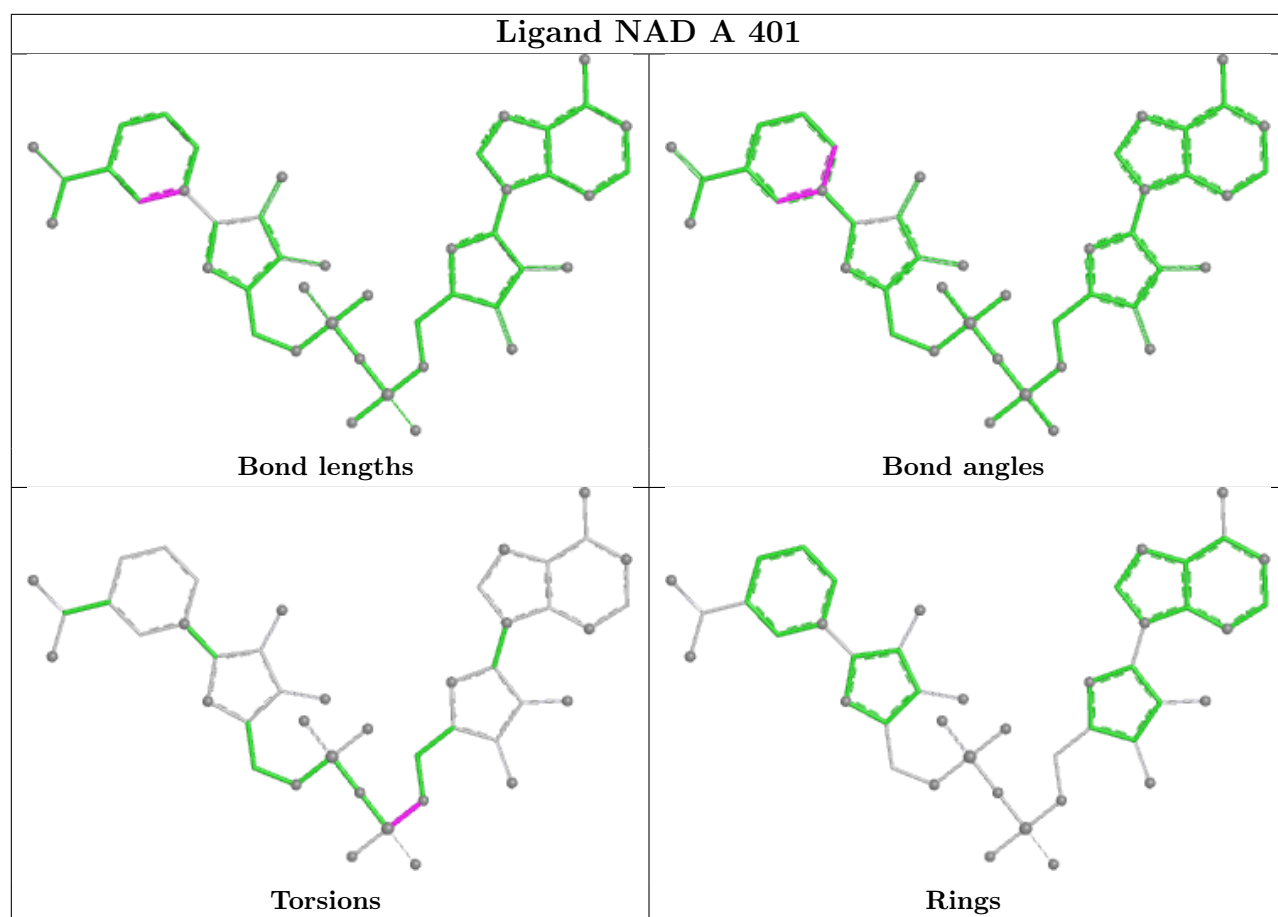
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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	306/335 (91%)	0.64	31 (10%) 12 11	27, 38, 64, 95	0
1	B	321/335 (95%)	0.46	19 (5%) 28 27	18, 37, 69, 92	2 (0%)
1	C	316/335 (94%)	0.24	15 (4%) 36 35	17, 31, 57, 97	4 (1%)
1	D	318/335 (94%)	0.37	13 (4%) 41 41	19, 35, 60, 96	5 (1%)
All	All	1261/1340 (94%)	0.42	78 (6%) 26 25	17, 35, 63, 97	11 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	ILE	7.9
1	B	136	VAL	6.1
1	A	84	ALA	5.6
1	B	190	ILE	5.5
1	A	85	GLY	5.2
1	B	323	PRO	5.1
1	B	138	GLU	4.9
1	C	136	VAL	4.9
1	B	324	VAL	4.8
1	A	89	THR	4.7
1	C	144	THR	4.7
1	A	280	ALA	4.5
1	C	140	ASN	4.4
1	A	130	GLY	4.3
1	C	137	ASP	4.3
1	D	143	THR	4.2
1	D	142	THR	4.2
1	A	190	ILE	4.2
1	B	322	LEU	4.1
1	D	141	SER	4.0
1	C	188	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	132	ARG	3.7
1	C	189	GLN	3.7
1	C	134	TYR	3.7
1	B	325	MET	3.6
1	C	133	ALA	3.6
1	D	1	MET	3.6
1	B	191	GLY	3.5
1	A	150	ALA	3.5
1	A	253	THR	3.4
1	A	284	LEU	3.3
1	A	148	GLY	3.3
1	B	132	ARG	3.3
1	B	135	ARG	3.3
1	A	144	THR	3.1
1	A	188	GLY	3.1
1	B	129[A]	PHE	3.1
1	A	146	ALA	3.1
1	D	144	THR	2.9
1	A	251	ALA	2.9
1	D	139	LEU	2.9
1	B	0	HIS	2.8
1	A	252	ILE	2.8
1	A	217	ILE	2.8
1	A	286	ILE	2.8
1	B	319	MET	2.8
1	A	285	ARG	2.7
1	B	137	ASP	2.7
1	C	139	LEU	2.7
1	D	292	SER	2.6
1	D	134	TYR	2.6
1	A	129	PHE	2.5
1	A	86	ILE	2.5
1	C	284	LEU	2.4
1	B	133	ALA	2.4
1	B	321	ASP	2.4
1	D	319	MET	2.4
1	B	144	THR	2.4
1	A	278	LEU	2.4
1	A	97	MET	2.4
1	B	49	ALA	2.3
1	D	132	ARG	2.3
1	A	128	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	189	GLN	2.3
1	A	39	GLU	2.2
1	C	192	GLU	2.2
1	B	278	LEU	2.2
1	A	81	ALA	2.2
1	C	278	LEU	2.2
1	A	0	HIS	2.1
1	D	69	GLU	2.1
1	A	282	ILE	2.1
1	A	281	ASP	2.1
1	D	167	ALA	2.1
1	A	40	ARG	2.1
1	A	91	LYS	2.0
1	D	238	GLN	2.0
1	C	129[A]	PHE	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 oligosaccharides 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.

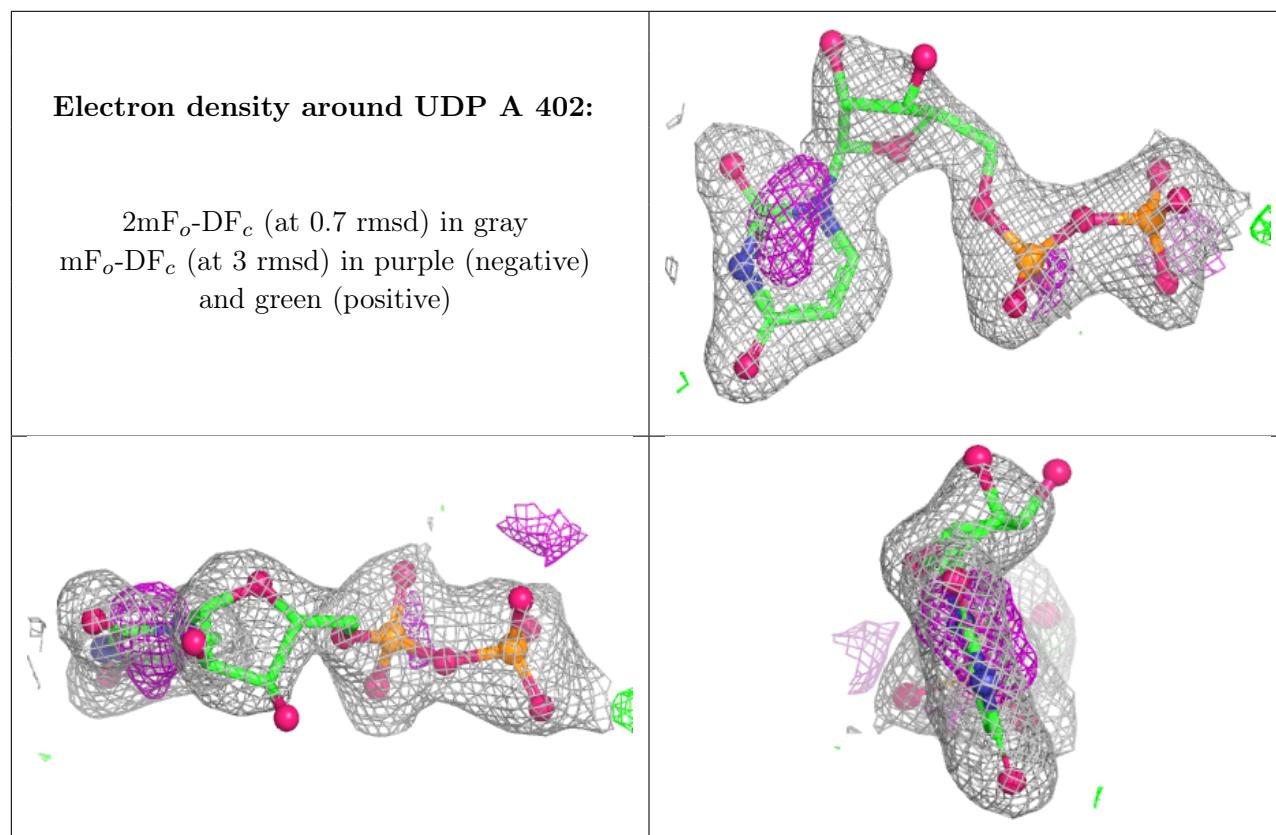
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MES	D	404	12/12	0.83	0.17	55,64,74,78	0
3	UDP	A	402	25/25	0.91	0.11	39,55,74,88	0
3	UDP	D	402	25/25	0.96	0.07	29,34,41,45	0
2	NAD	A	401	44/44	0.96	0.07	27,35,39,41	0
2	NAD	C	401	44/44	0.97	0.05	23,26,29,32	0
3	UDP	B	402	25/25	0.97	0.07	34,38,42,48	0
3	UDP	C	402	25/25	0.98	0.05	29,32,34,35	0
2	NAD	B	401	44/44	0.98	0.06	28,32,37,38	0

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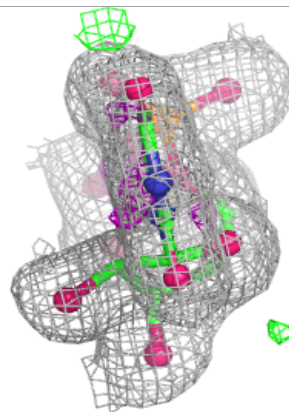
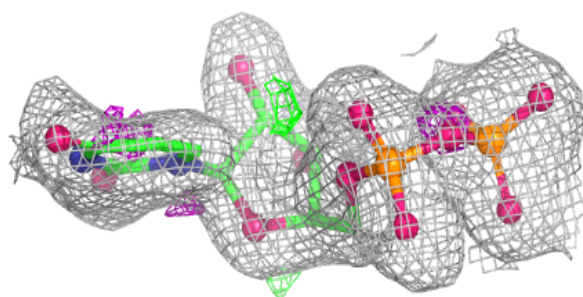
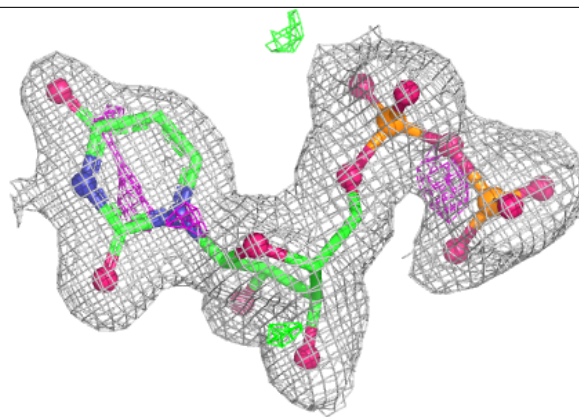
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NA	D	403	1/1	0.98	0.06	38,38,38,38	0
2	NAD	D	401	44/44	0.98	0.05	23,26,29,30	0

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.

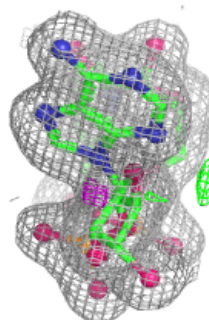
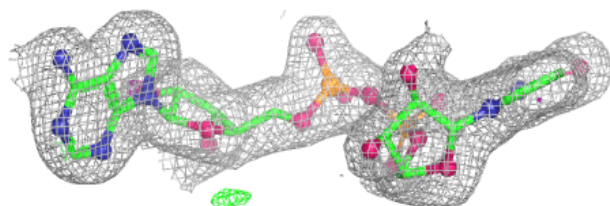
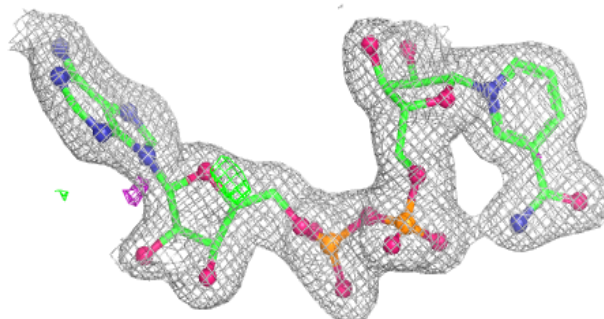


Electron density around UDP D 402:

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

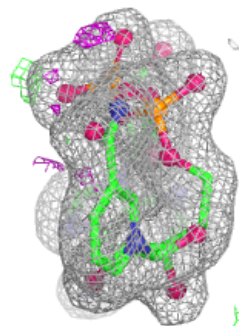
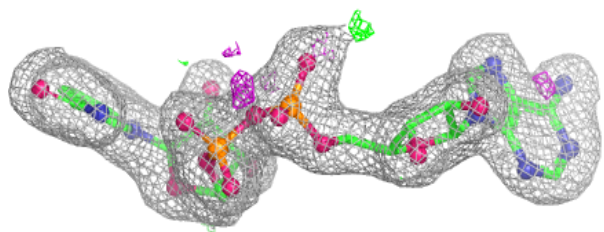
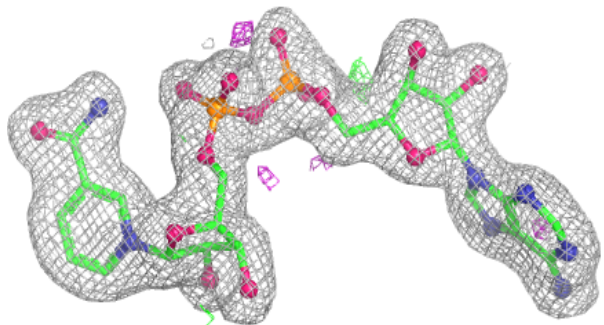
**Electron density around NAD A 401:**

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

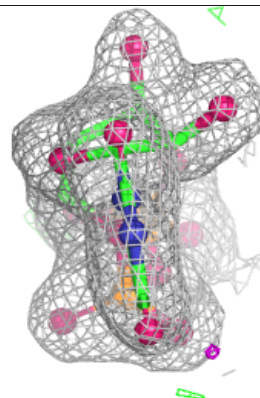
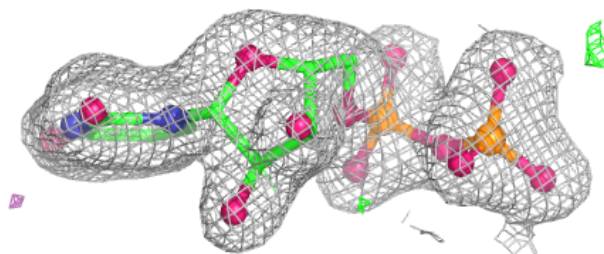
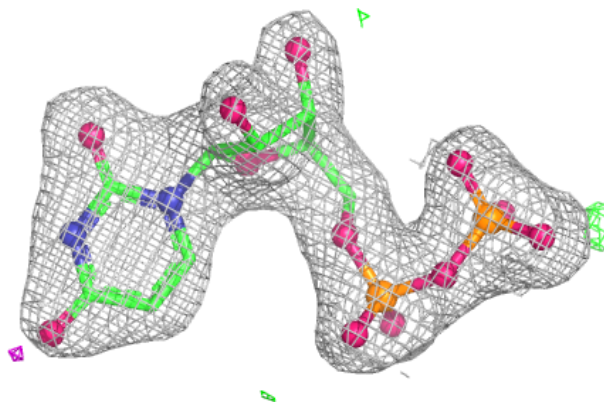


Electron density around NAD C 401:

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

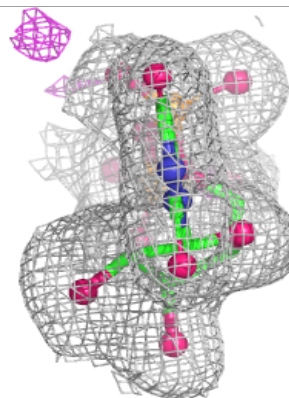
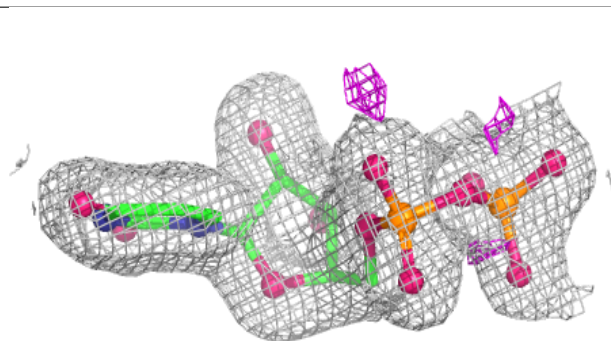
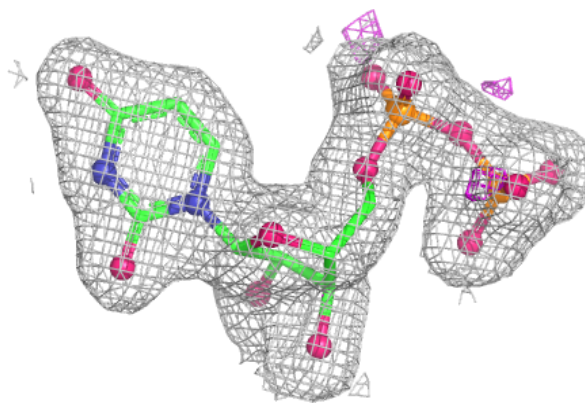
**Electron density around UDP B 402:**

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

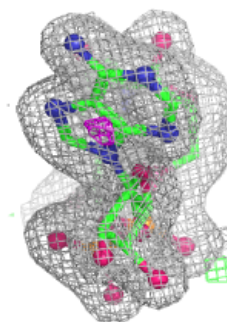
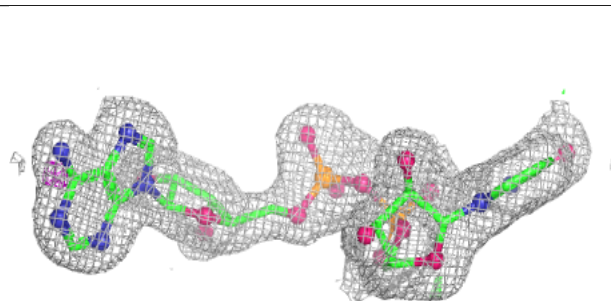
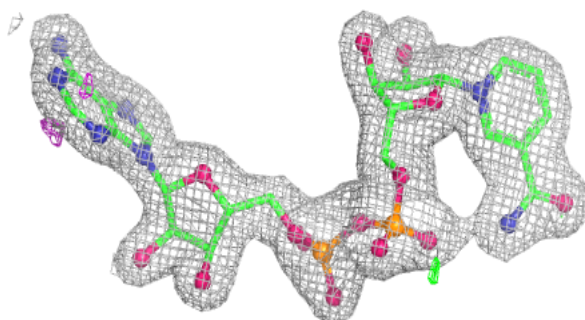


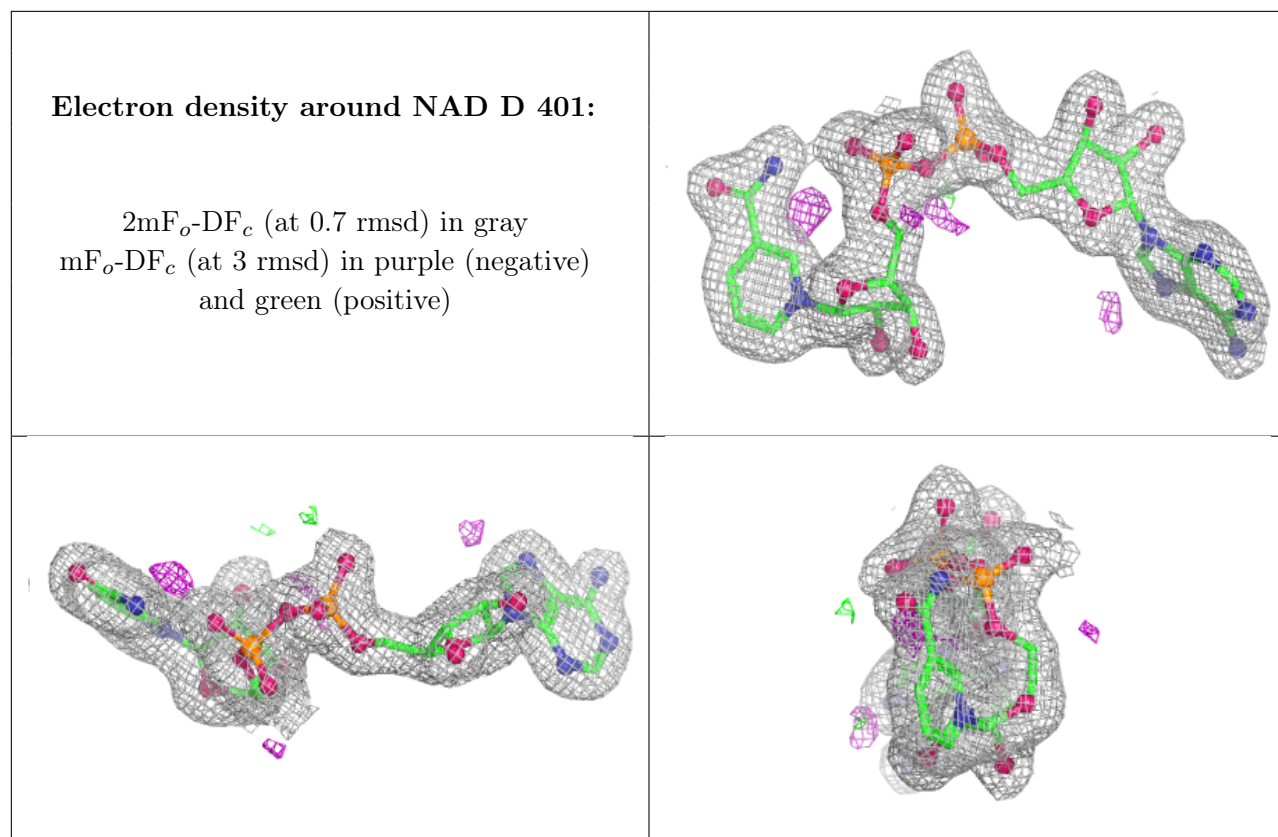
Electron density around UDP C 402:

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

**Electron density around NAD B 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.