



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:59 pm BST

PDB ID : 2QJO
Title : crystal structure of a bifunctional NMN adenylyltransferase/ADP ribose pyrophosphatase (NadM) complexed with ADPRP and NAD from *Synechocystis* sp.
Authors : Huang, N.; Sorci, L.; Zhang, X.; Brautigan, C.; Raffaelli, N.; Magni, G.; Grishin, N.V.; Osterman, A.; Zhang, H.
Deposited on : 2007-07-08
Resolution : 2.60 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

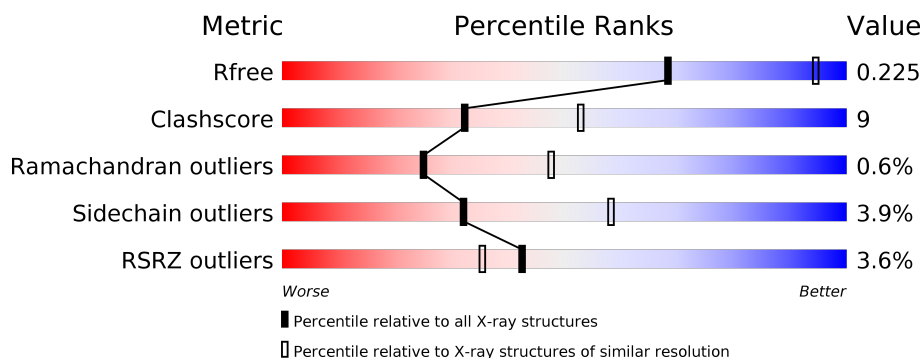
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	341	<div> <div>86%</div> <div>10% ..</div> </div>
1	B	341	<div> <div>2%</div> <div>85%</div> <div>12% ..</div> </div>
1	C	341	<div> <div>9%</div> <div>76%</div> <div>16% ...</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	POP	A	701	-	-	X	-
5	POP	B	702	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8648 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.

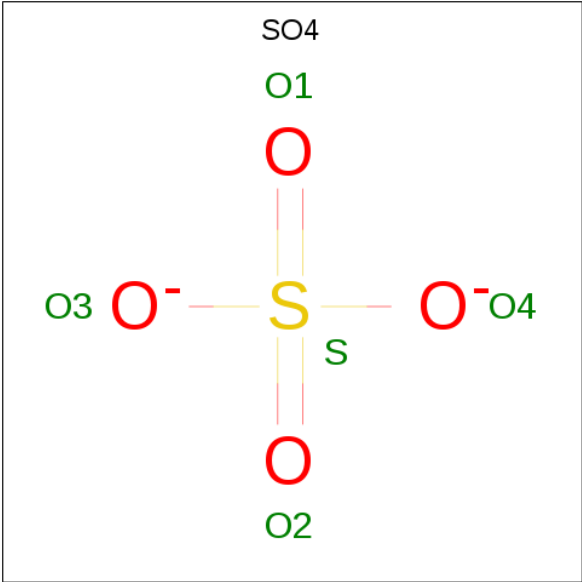
- Molecule 1 is a protein called Bifunctional NMN adenylyltransferase/Nudix hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2681	1735	461	477	8			
1	B	336	Total	C	N	O	S	0	2	0
			2722	1757	471	487	7			
1	C	327	Total	C	N	O	S	0	1	0
			2645	1713	454	471	7			

There are 6 discrepancies between the modelled and reference sequences:

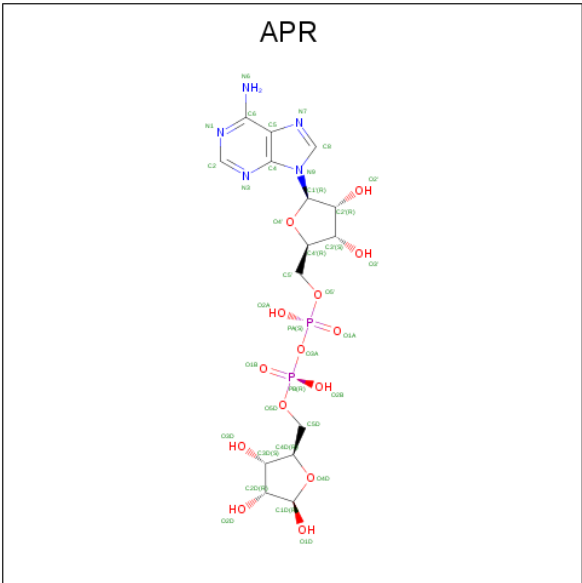
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	CLONING ARTIFACT	UNP Q55928
A	0	PRO	-	CLONING ARTIFACT	UNP Q55928
B	-1	ASP	-	CLONING ARTIFACT	UNP Q55928
B	0	PRO	-	CLONING ARTIFACT	UNP Q55928
C	-1	ASP	-	CLONING ARTIFACT	UNP Q55928
C	0	PRO	-	CLONING ARTIFACT	UNP Q55928

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



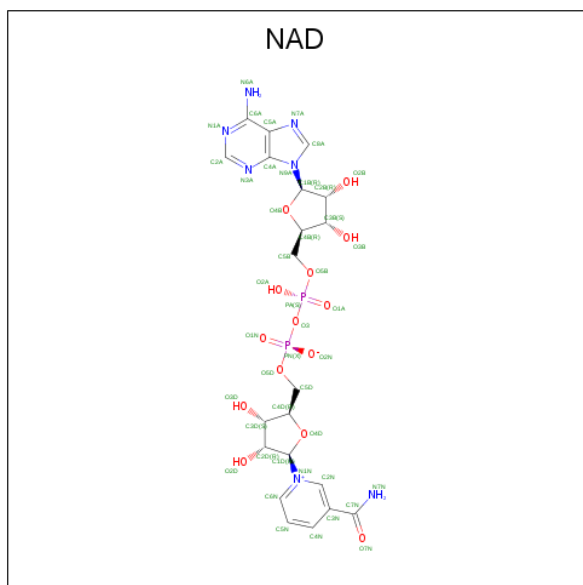
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

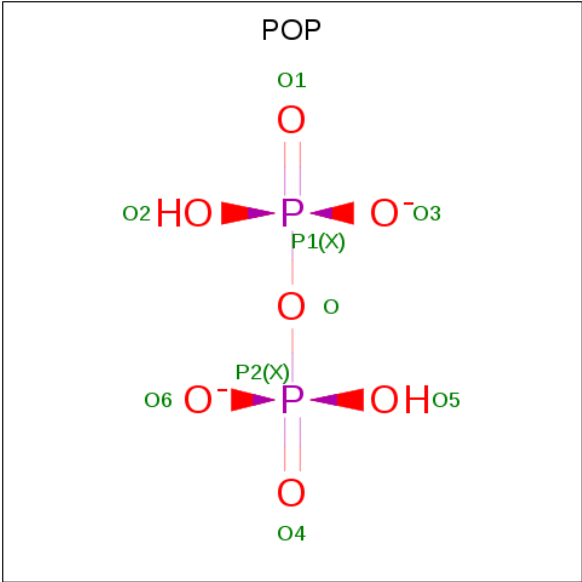
- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: C₁₅H₂₃N₅O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			9	7	2		
5	B	1	Total	O	P	0	0
			9	7	2		
5	C	1	Total	O	P	0	0
			9	7	2		


- Molecule 6 is water.

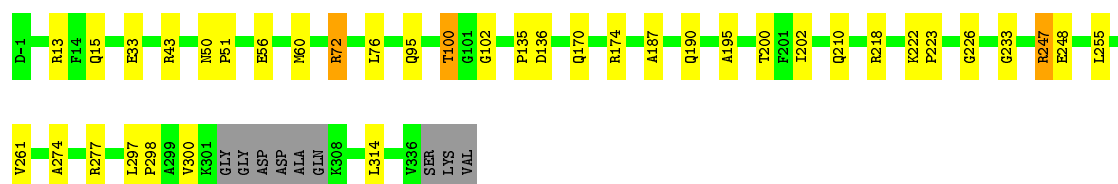
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	142	Total	O	0	0
			142	142		
6	C	46	Total	O	0	0
			46	46		

3 Residue-property plots [i](#)


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.

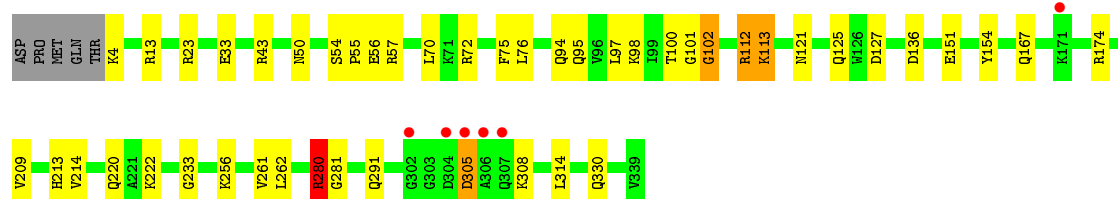
- Molecule 1: Bifunctional NMN adenylyltransferase/Nudix hydrolase

Chain A: 




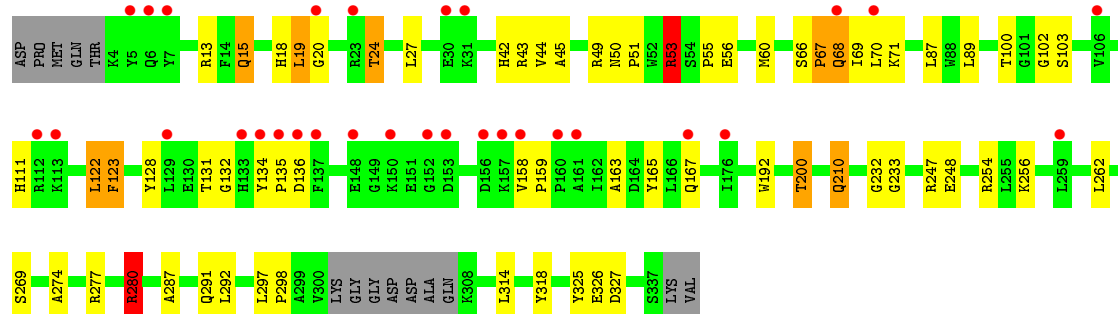
- Molecule 1: Bifunctional NMN adenylyltransferase/Nudix hydrolase

Chain B: 



- Molecule 1: Bifunctional NMN adenylyltransferase/Nudix hydrolase

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.54 Å 201.54 Å 98.69 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.48 – 2.60 43.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.48-2.60) 98.5 (43.46-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.228 0.192 , 0.225	Depositor DCC
R_{free} test set	3549 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8648	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: APR, SO4, NAD, POP

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	0.78	0/2754	0.75	2/3742 (0.1%)
1	B	0.76	0/2795	0.75	2/3796 (0.1%)
1	C	0.57	0/2720	0.70	2/3696 (0.1%)
All	All	0.71	0/8269	0.74	6/11234 (0.1%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	281	GLY	N-CA-C	6.64	129.71	113.10
1	C	280	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	A	72	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	A	247	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	280	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	PRO	Peptide
1	B	280	ARG	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	2681	0	2664	35	0
1	B	2722	0	2698	35	0
1	C	2645	0	2624	79	0
2	A	15	0	0	0	0
2	B	5	0	0	1	0
3	A	36	0	21	1	0
3	B	36	0	21	1	0
3	C	36	0	21	1	0
4	A	44	0	26	0	0
4	B	44	0	26	1	0
4	C	44	0	26	0	0
5	A	9	0	0	5	0
5	B	9	0	0	5	0
5	C	9	0	0	3	0
6	A	125	0	0	4	1
6	B	142	0	0	5	3
6	C	46	0	0	2	0
All	All	8648	0	8127	144	3

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 (144) 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:68:GLN:HA	1:C:68:GLN:OE1	1.64	0.97
1:C:18:HIS:CE1	1:C:20:GLY:HA3	2.02	0.94
1:C:19:LEU:CD2	1:C:159:PRO:HD3	1.99	0.92
1:C:19:LEU:CD2	1:C:159:PRO:CD	2.56	0.84
1:C:19:LEU:HD23	1:C:159:PRO:HD3	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:GLN:CG	1:C:51:PRO:HD2	2.12	0.79
1:C:18:HIS:ND1	1:C:20:GLY:N	2.31	0.78
1:C:122:LEU:HD13	1:C:122:LEU:H	1.48	0.77
1:A:15:GLN:HG3	1:A:51:PRO:HD2	1.68	0.76
1:C:15:GLN:HG2	1:C:51:PRO:HD2	1.68	0.76
1:A:13:ARG:HH22	5:A:701:POP:P1	2.10	0.75
1:C:277:ARG:O	1:C:326:GLU:HG2	1.88	0.74
1:C:18:HIS:HE1	1:C:20:GLY:HA3	1.52	0.73
1:C:18:HIS:CE1	1:C:20:GLY:CA	2.71	0.73
1:C:19:LEU:HD22	1:C:159:PRO:HD3	1.69	0.73
1:A:33:GLU:O	1:A:72:ARG:HD2	1.89	0.73
1:A:200:THR:O	1:C:200:THR:HG22	1.90	0.72
1:A:13:ARG:NH2	5:A:701:POP:P1	2.63	0.72
1:B:76:LEU:HD13	1:B:95:GLN:HB3	1.73	0.71
1:B:13:ARG:HH22	5:B:702:POP:P2	2.13	0.71
1:C:89:LEU:HD21	1:C:122:LEU:HD23	1.71	0.71
1:C:53:ARG:HB3	1:C:55:PRO:HD2	1.71	0.71
1:C:67:PRO:O	1:C:68:GLN:C	2.30	0.69
1:C:123:PHE:N	1:C:123:PHE:CD2	2.60	0.69
1:B:113:LYS:HE2	5:B:702:POP:O2	1.92	0.69
1:A:56:GLU:O	1:A:60:MET:HG3	1.93	0.68
1:C:19:LEU:CD2	1:C:159:PRO:N	2.56	0.68
1:C:19:LEU:HD22	1:C:159:PRO:CD	2.22	0.68
1:B:13:ARG:HD2	1:B:50:ASN:OD1	1.93	0.67
1:A:100:THR:HG22	1:A:102:GLY:H	1.58	0.67
1:B:97:LEU:HA	1:B:100:THR:HG22	1.77	0.67
1:C:15:GLN:HG2	1:C:51:PRO:CD	2.25	0.65
1:C:135:PRO:HA	1:C:136:ASP:HB3	1.78	0.65
1:C:13:ARG:HH22	5:C:703:POP:P2	2.20	0.65
1:C:66:SER:OG	1:C:69:ILE:HD12	1.95	0.65
1:C:60:MET:HG2	1:C:165:TYR:CD2	2.31	0.65
1:B:100:THR:HG21	6:B:761:HOH:O	1.99	0.63
1:A:202:ILE:HG13	1:C:200:THR:HG23	1.79	0.63
1:C:19:LEU:HD23	1:C:158:VAL:HA	1.82	0.62
1:A:202:ILE:HG13	1:C:200:THR:CG2	2.30	0.62
1:B:233:GLY:HA2	3:B:502:APR:H5R1	1.82	0.62
1:A:13:ARG:HD2	1:A:50:ASN:OD1	1.99	0.61
1:C:18:HIS:ND1	1:C:20:GLY:CA	2.64	0.60
1:C:19:LEU:HD23	1:C:159:PRO:CD	2.27	0.60
1:C:247:ARG:NH2	1:C:248:GLU:OE1	2.34	0.60
1:B:13:ARG:NH2	5:B:702:POP:P2	2.74	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ARG:NH2	1:A:248:GLU:OE1	2.35	0.60
1:B:314:LEU:N	1:B:314:LEU:HD12	2.16	0.60
1:A:210:GLN:HB3	1:A:297:LEU:CD2	2.32	0.59
1:B:222:LYS:HG2	6:B:718:HOH:O	2.02	0.58
1:C:291:GLN:HG3	6:C:741:HOH:O	2.03	0.57
1:B:121:ASN:C	1:B:121:ASN:OD1	2.43	0.56
1:C:15:GLN:HG3	1:C:51:PRO:HD2	1.87	0.56
1:A:15:GLN:HG3	1:A:51:PRO:CD	2.35	0.54
1:B:314:LEU:H	1:B:314:LEU:HD12	1.73	0.54
1:C:280:ARG:NH2	3:C:503:APR:O4D	2.41	0.53
1:C:19:LEU:HD23	1:C:158:VAL:CA	2.39	0.53
1:B:209:VAL:HA	1:B:213:HIS:O	2.09	0.52
1:C:13:ARG:HD2	1:C:50:ASN:OD1	2.10	0.52
1:C:18:HIS:C	1:C:20:GLY:H	2.10	0.52
1:C:274:ALA:O	1:C:277:ARG:HG2	2.10	0.52
1:B:13:ARG:NH2	5:B:702:POP:O4	2.42	0.52
1:C:123:PHE:HD2	1:C:123:PHE:H	1.55	0.52
6:A:711:HOH:O	1:C:200:THR:HG21	2.11	0.51
1:A:15:GLN:HG2	1:A:50:ASN:HA	1.92	0.51
1:C:210:GLN:HG3	1:C:292:LEU:HB2	1.93	0.51
1:A:13:ARG:NH2	5:A:701:POP:O1	2.44	0.51
1:A:233:GLY:HA2	3:A:501:APR:H5R1	1.93	0.51
1:B:151:GLU:HA	1:B:154:TYR:CE1	2.45	0.51
1:B:56:GLU:OE1	1:B:174:ARG:NH2	2.44	0.50
1:B:33:GLU:O	1:B:72:ARG:HD2	2.11	0.50
1:C:135:PRO:HA	1:C:136:ASP:CB	2.35	0.50
1:C:325:TYR:CZ	1:C:326:GLU:OE2	2.64	0.50
1:B:4:LYS:HE2	6:B:810:HOH:O	2.11	0.50
1:A:15:GLN:CG	1:A:51:PRO:HD2	2.41	0.49
1:C:100:THR:C	1:C:102:GLY:H	2.16	0.49
1:A:297:LEU:HD12	1:B:94:GLN:CG	2.42	0.49
1:C:18:HIS:ND1	1:C:20:GLY:HA3	2.26	0.49
1:C:325:TYR:OH	1:C:326:GLU:OE2	2.30	0.49
1:B:112:ARG:HH21	1:B:121:ASN:HB3	1.77	0.49
1:C:18:HIS:C	1:C:20:GLY:N	2.61	0.48
1:B:121:ASN:OD1	1:B:121:ASN:O	2.30	0.48
1:B:75:PHE:O	1:B:76:LEU:HD23	2.14	0.48
1:C:19:LEU:HD22	1:C:159:PRO:HG3	1.96	0.48
1:C:134:TYR:O	1:C:136:ASP:HA	2.14	0.47
1:C:68:GLN:OE1	1:C:68:GLN:CA	2.46	0.47
1:C:87:LEU:O	1:C:87:LEU:HD23	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD21	1:C:159:PRO:N	2.29	0.47
1:A:187:ALA:O	1:A:190:GLN:HB3	2.15	0.47
1:A:233:GLY:N	1:A:248:GLU:HG2	2.29	0.47
1:C:233:GLY:HA3	1:C:248:GLU:CD	2.35	0.47
1:C:122:LEU:CD1	1:C:122:LEU:H	2.22	0.46
1:C:13:ARG:NH2	5:C:703:POP:O4	2.48	0.46
1:C:15:GLN:HB2	1:C:15:GLN:HE21	1.52	0.46
1:C:13:ARG:NH2	5:C:703:POP:P2	2.88	0.46
1:C:19:LEU:HD22	1:C:159:PRO:CG	2.46	0.46
1:C:232:GLY:C	1:C:248:GLU:HG2	2.37	0.45
1:C:297:LEU:HA	1:C:297:LEU:HD23	1.84	0.45
1:C:233:GLY:N	1:C:248:GLU:HG2	2.32	0.45
1:B:100:THR:O	1:B:102:GLY:N	2.45	0.44
1:C:111:HIS:HA	1:C:128:TYR:OH	2.17	0.44
1:B:314:LEU:H	1:B:314:LEU:CD1	2.30	0.44
1:A:274:ALA:O	1:A:277:ARG:HG2	2.17	0.44
1:A:56:GLU:OE1	1:A:174:ARG:NH2	2.43	0.44
1:A:255:LEU:HA	1:A:300:VAL:HG12	1.98	0.44
1:C:326:GLU:HB3	1:C:327:ASP:H	1.46	0.44
1:B:220:GLN:HG3	6:B:794:HOH:O	2.17	0.44
1:A:60:MET:HE2	6:A:730:HOH:O	2.17	0.44
1:B:54:SER:HB3	1:B:57:ARG:HH21	1.83	0.43
1:C:19:LEU:HD23	1:C:158:VAL:C	2.39	0.43
1:A:95:GLN:HG2	6:A:792:HOH:O	2.18	0.43
1:B:54:SER:N	1:B:55:PRO:CD	2.81	0.43
1:C:66:SER:HG	1:C:69:ILE:HD12	1.80	0.43
1:A:13:ARG:NH2	5:A:701:POP:O3	2.51	0.43
1:C:19:LEU:CD2	1:C:158:VAL:C	2.87	0.43
1:B:70:LEU:HA	1:B:70:LEU:HD23	1.84	0.43
1:A:43:ARG:NH1	6:A:805:HOH:O	2.52	0.43
1:A:222:LYS:HB3	1:A:223:PRO:HA	2.01	0.43
1:C:277:ARG:O	1:C:326:GLU:CG	2.62	0.42
1:B:13:ARG:HG3	4:B:602:NAD:H3D	2.02	0.42
1:C:24:THR:HG22	1:C:131:THR:HG21	2.01	0.42
1:B:291:GLN:HG2	6:B:727:HOH:O	2.18	0.42
1:C:163:ALA:O	1:C:167:GLN:HG2	2.19	0.42
1:A:76:LEU:HD13	1:A:95:GLN:HB3	2.02	0.42
1:C:100:THR:HG23	1:C:103:SER:HB3	2.02	0.42
1:A:195:ALA:HB1	1:C:192:TRP:CZ3	2.55	0.42
1:C:56:GLU:O	1:C:60:MET:HG3	2.20	0.42
1:C:44:VAL:HG12	1:C:45:ALA:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LYS:HE2	6:C:733:HOH:O	2.20	0.41
1:C:297:LEU:HA	1:C:298:PRO:HD3	1.87	0.41
1:A:314:LEU:HA	1:A:314:LEU:HD12	1.89	0.41
1:B:113:LYS:CE	5:B:702:POP:O2	2.65	0.41
1:C:325:TYR:O	1:C:326:GLU:C	2.59	0.41
1:A:13:ARG:NH2	5:A:701:POP:O2	2.54	0.41
1:B:43:ARG:NH1	2:B:401:SO4:O1	2.41	0.41
1:C:314:LEU:O	1:C:318:TYR:HD1	2.04	0.41
1:A:297:LEU:HA	1:A:298:PRO:HD3	1.95	0.41
1:B:56:GLU:CD	1:B:174:ARG:HH22	2.22	0.41
1:A:210:GLN:HB3	1:A:297:LEU:HD21	2.02	0.41
1:A:218:ARG:NH1	1:A:226:GLY:O	2.54	0.41
1:C:269:SER:HA	1:C:287:ALA:O	2.21	0.40
1:B:209:VAL:HG22	1:B:214:VAL:HG22	2.04	0.40
1:B:305:ASP:O	1:B:308:LYS:HG2	2.21	0.40
1:C:42:HIS:CE1	1:C:43:ARG:HG2	2.56	0.40

All (3) 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)
6:A:813:HOH:O	6:B:774:HOH:O[2_564]	1.95	0.25
6:B:757:HOH:O	6:B:838:HOH:O[5_555]	2.13	0.07
6:B:714:HOH:O	6:B:805:HOH:O[5_555]	2.14	0.06

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	328/341 (96%)	320 (98%)	8 (2%)	0	100	100
1	B	336/341 (98%)	318 (95%)	15 (4%)	3 (1%)	17	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	324/341 (95%)	301 (93%)	20 (6%)	3 (1%)	17	35
All	All	988/1023 (97%)	939 (95%)	43 (4%)	6 (1%)	25	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	305	ASP
1	C	70	LEU
1	B	102	GLY
1	B	101	GLY
1	C	53	ARG
1	C	132	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	281/287 (98%)	277 (99%)	4 (1%)	67	85
1	B	284/287 (99%)	271 (95%)	13 (5%)	27	51
1	C	277/287 (96%)	261 (94%)	16 (6%)	20	40
All	All	842/861 (98%)	809 (96%)	33 (4%)	32	58

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	THR
1	A	136	ASP
1	A	170	GLN
1	A	261	VAL
1	B	23	ARG
1	B	98	LYS
1	B	112	ARG
1	B	113	LYS
1	B	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	127	ASP
1	B	136	ASP
1	B	167	GLN
1	B	256	LYS
1	B	261	VAL
1	B	262	LEU
1	B	280	ARG
1	B	330	GLN
1	C	15	GLN
1	C	19	LEU
1	C	24	THR
1	C	27	LEU
1	C	49	ARG
1	C	53	ARG
1	C	67	PRO
1	C	68	GLN
1	C	122	LEU
1	C	123	PHE
1	C	200	THR
1	C	210	GLN
1	C	254	ARG
1	C	256	LYS
1	C	262	LEU
1	C	280	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	B	93	GLN
1	B	167	GLN
1	B	220	GLN
1	C	133	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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$
4	NAD	C	603	-	42,48,48	1.85	3 (7%)	50,73,73	1.20	2 (4%)
2	SO4	A	402	-	4,4,4	0.11	0	6,6,6	0.20	0
2	SO4	A	403	-	4,4,4	0.18	0	6,6,6	0.64	0
4	NAD	B	602	-	42,48,48	1.75	4 (9%)	50,73,73	1.16	3 (6%)
5	POP	C	703	-	6,8,8	0.74	0	13,13,13	1.20	3 (23%)
2	SO4	A	404	-	4,4,4	0.19	0	6,6,6	0.53	0
4	NAD	A	601	-	42,48,48	1.82	5 (11%)	50,73,73	1.41	5 (10%)
3	APR	A	501	-	34,39,39	0.89	2 (5%)	40,60,60	1.09	2 (5%)
5	POP	B	702	-	6,8,8	0.92	0	13,13,13	1.76	3 (23%)
3	APR	C	503	-	34,39,39	0.83	1 (2%)	40,60,60	1.26	6 (15%)
5	POP	A	701	-	6,8,8	0.71	0	13,13,13	1.49	3 (23%)
2	SO4	B	401	-	4,4,4	0.25	0	6,6,6	0.56	0
3	APR	B	502	-	34,39,39	0.86	1 (2%)	40,60,60	1.27	4 (10%)

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	C	603	-	-	5/26/62/62	0/5/5/5
3	APR	A	501	-	-	5/18/54/54	0/4/4/4
4	NAD	B	602	-	-	4/26/62/62	0/5/5/5
5	POP	C	703	-	-	0/6/6/6	-
4	NAD	A	601	-	-	2/26/62/62	0/5/5/5
5	POP	B	702	-	-	2/6/6/6	-
3	APR	C	503	-	-	4/18/54/54	0/4/4/4
5	POP	A	701	-	-	3/6/6/6	-
3	APR	B	502	-	-	6/18/54/54	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	NAD	O7N-C7N	9.68	1.42	1.24
4	B	602	NAD	O7N-C7N	8.87	1.41	1.24
4	A	601	NAD	O7N-C7N	8.58	1.40	1.24
4	A	601	NAD	C2A-N3A	4.36	1.39	1.32
4	C	603	NAD	C2A-N3A	4.27	1.39	1.32
4	B	602	NAD	C2A-N3A	4.07	1.38	1.32
4	C	603	NAD	C2A-N1A	2.90	1.39	1.33
4	A	601	NAD	C2A-N1A	2.88	1.39	1.33
4	A	601	NAD	C2N-N1N	2.57	1.38	1.35
3	A	501	APR	C5-C4	2.43	1.47	1.40
3	B	502	APR	C5-C4	2.39	1.47	1.40
4	A	601	NAD	PA-O2A	-2.31	1.44	1.55
4	B	602	NAD	C2A-N1A	2.26	1.38	1.33
3	C	503	APR	C5-C4	2.26	1.46	1.40
3	A	501	APR	O4'-C1'	2.21	1.44	1.41
4	B	602	NAD	PA-O2A	-2.01	1.45	1.55

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	NAD	N3A-C2A-N1A	-6.17	119.03	128.68
4	B	602	NAD	N3A-C2A-N1A	-5.31	120.38	128.68
4	A	601	NAD	N3A-C2A-N1A	-5.25	120.47	128.68
4	A	601	NAD	C3N-C7N-N7N	4.36	122.98	117.75
5	B	702	POP	O3-P1-O	4.03	118.14	104.64
3	B	502	APR	N3-C2-N1	-3.97	122.47	128.68
3	C	503	APR	PB-O3A-PA	-3.16	121.98	132.83
3	A	501	APR	N3-C2-N1	-3.04	123.92	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	POP	O6-P2-O	2.88	114.31	104.64
3	C	503	APR	N3-C2-N1	-2.85	124.22	128.68
4	C	603	NAD	C1B-N9A-C4A	-2.78	121.75	126.64
5	A	701	POP	O3-P1-O	2.73	113.81	104.64
5	B	702	POP	O6-P2-O	2.61	113.40	104.64
4	A	601	NAD	O3D-C3D-C4D	-2.58	103.58	111.05
3	B	502	APR	C3'-C2'-C1'	2.57	104.85	100.98
3	A	501	APR	PB-O3A-PA	-2.47	124.36	132.83
3	B	502	APR	C2-N1-C6	2.45	122.94	118.75
3	C	503	APR	O3D-C3D-C4D	-2.45	103.97	111.05
3	C	503	APR	O1D-C1D-O4D	-2.42	108.04	111.13
5	B	702	POP	O6-P2-O4	-2.38	101.35	110.68
4	B	602	NAD	C3N-C7N-N7N	2.23	120.43	117.75
3	C	503	APR	N6-C6-N1	2.22	123.17	118.57
4	B	602	NAD	C4A-C5A-N7A	-2.16	107.15	109.40
4	A	601	NAD	O7N-C7N-C3N	-2.15	117.06	119.63
5	C	703	POP	O5-P2-O	2.13	111.78	104.64
5	A	701	POP	O5-P2-O	2.12	111.75	104.64
3	C	503	APR	C3'-C2'-C1'	2.08	104.10	100.98
5	C	703	POP	O6-P2-O	2.07	111.59	104.64
3	B	502	APR	C4-C5-N7	-2.06	107.25	109.40
5	C	703	POP	O3-P1-O	2.06	111.54	104.64
4	A	601	NAD	O4D-C1D-C2D	-2.05	103.92	106.93

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	603	NAD	O4D-C4D-C5D-O5D
3	A	501	APR	C5'-O5'-PA-O3A
4	B	602	NAD	O4D-C4D-C5D-O5D
4	A	601	NAD	C5D-O5D-PN-O1N
5	B	702	POP	P1-O-P2-O6
3	C	503	APR	C5'-O5'-PA-O1A
3	C	503	APR	C5'-O5'-PA-O2A
3	C	503	APR	C5'-O5'-PA-O3A
5	A	701	POP	P2-O-P1-O3
3	B	502	APR	C5'-O5'-PA-O3A
4	C	603	NAD	C3D-C4D-C5D-O5D
4	B	602	NAD	C3D-C4D-C5D-O5D
3	B	502	APR	C3'-C4'-C5'-O5'
4	C	603	NAD	PN-O3-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	701	POP	P2-O-P1-O2
3	A	501	APR	C5'-O5'-PA-O1A
3	A	501	APR	C5'-O5'-PA-O2A
3	B	502	APR	C5'-O5'-PA-O1A
3	A	501	APR	C3'-C4'-C5'-O5'
4	B	602	NAD	PN-O3-PA-O2A
3	B	502	APR	C4D-C5D-O5D-PB
5	A	701	POP	P2-O-P1-O1
4	B	602	NAD	PN-O3-PA-O1A
3	B	502	APR	O4'-C4'-C5'-O5'
5	B	702	POP	P1-O-P2-O5
3	C	503	APR	C4D-C5D-O5D-PB
4	A	601	NAD	O4D-C4D-C5D-O5D
4	C	603	NAD	PN-O3-PA-O2A
4	C	603	NAD	C5B-O5B-PA-O1A
3	B	502	APR	C5'-O5'-PA-O2A
3	A	501	APR	C4D-C5D-O5D-PB

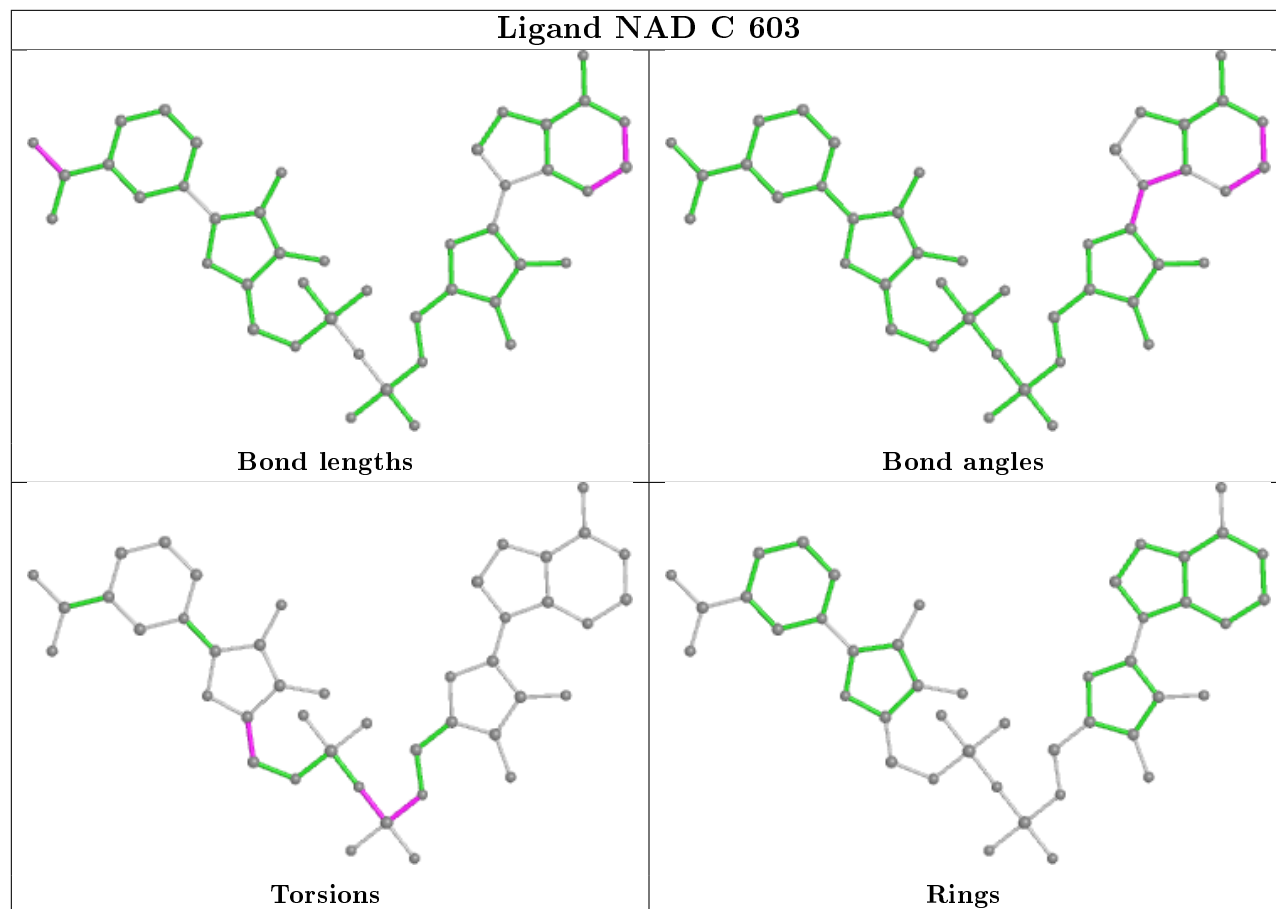
There are no ring outliers.

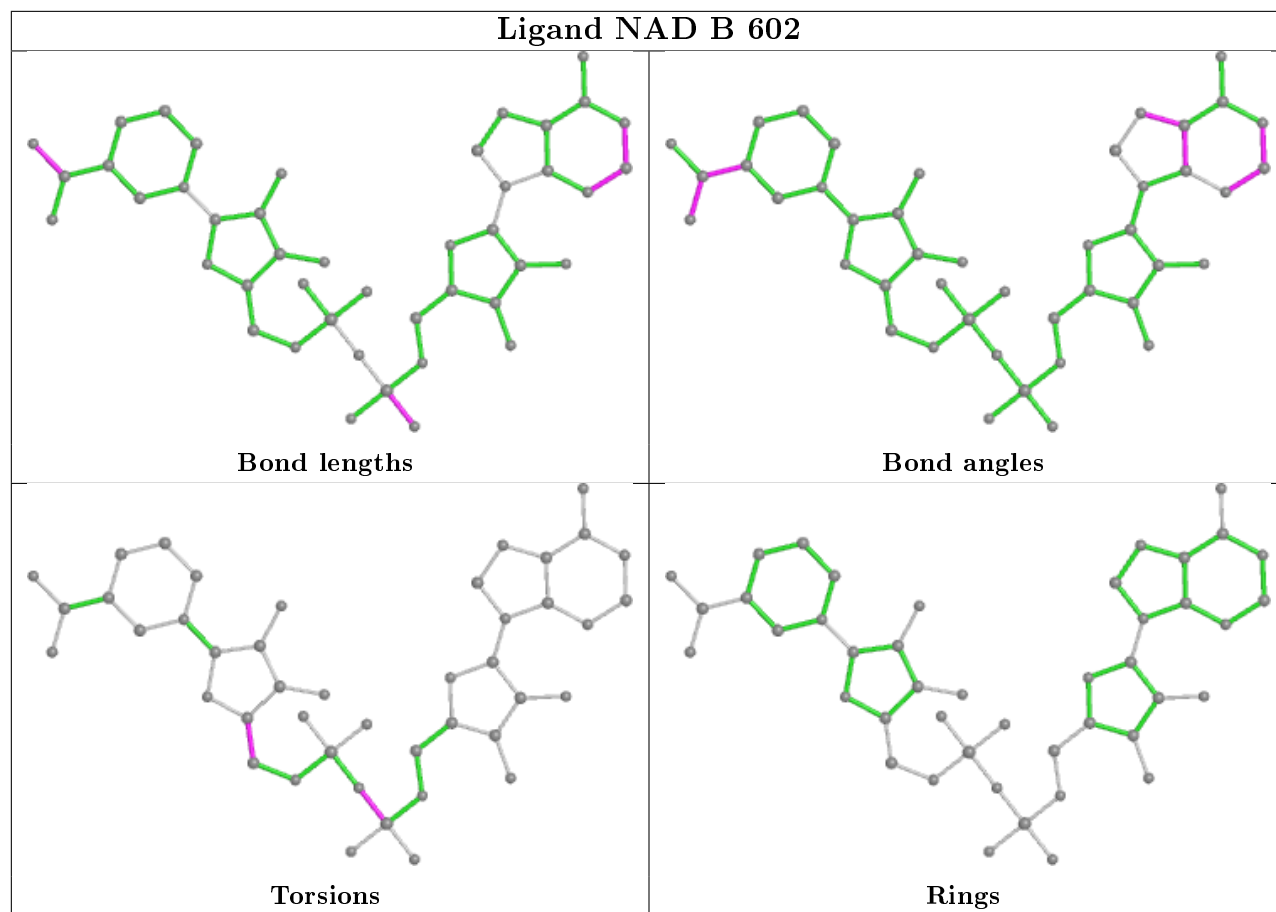
8 monomers are involved in 18 short contacts:

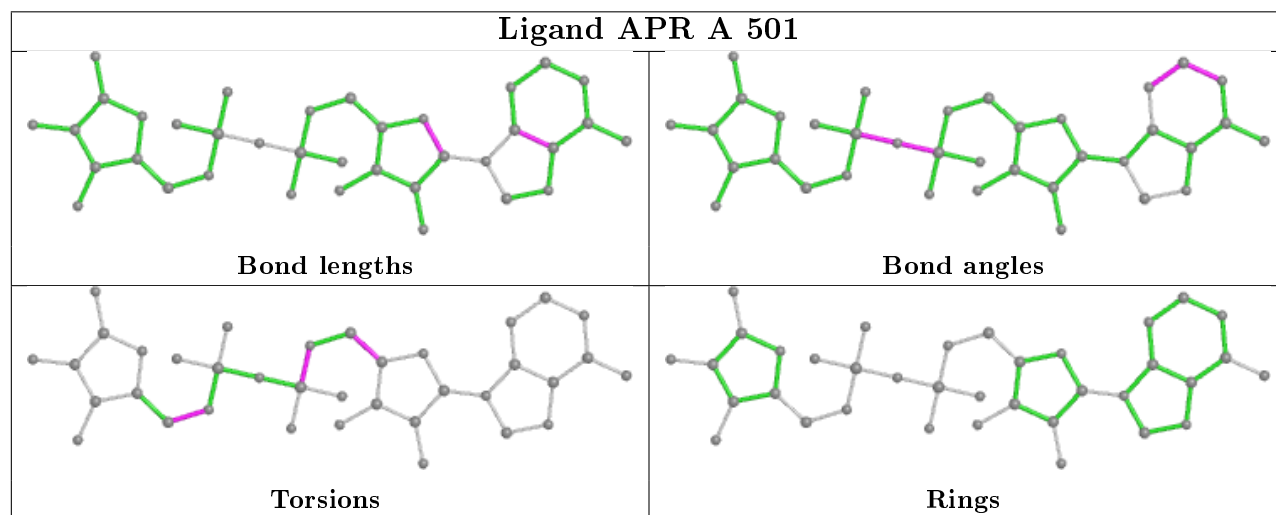
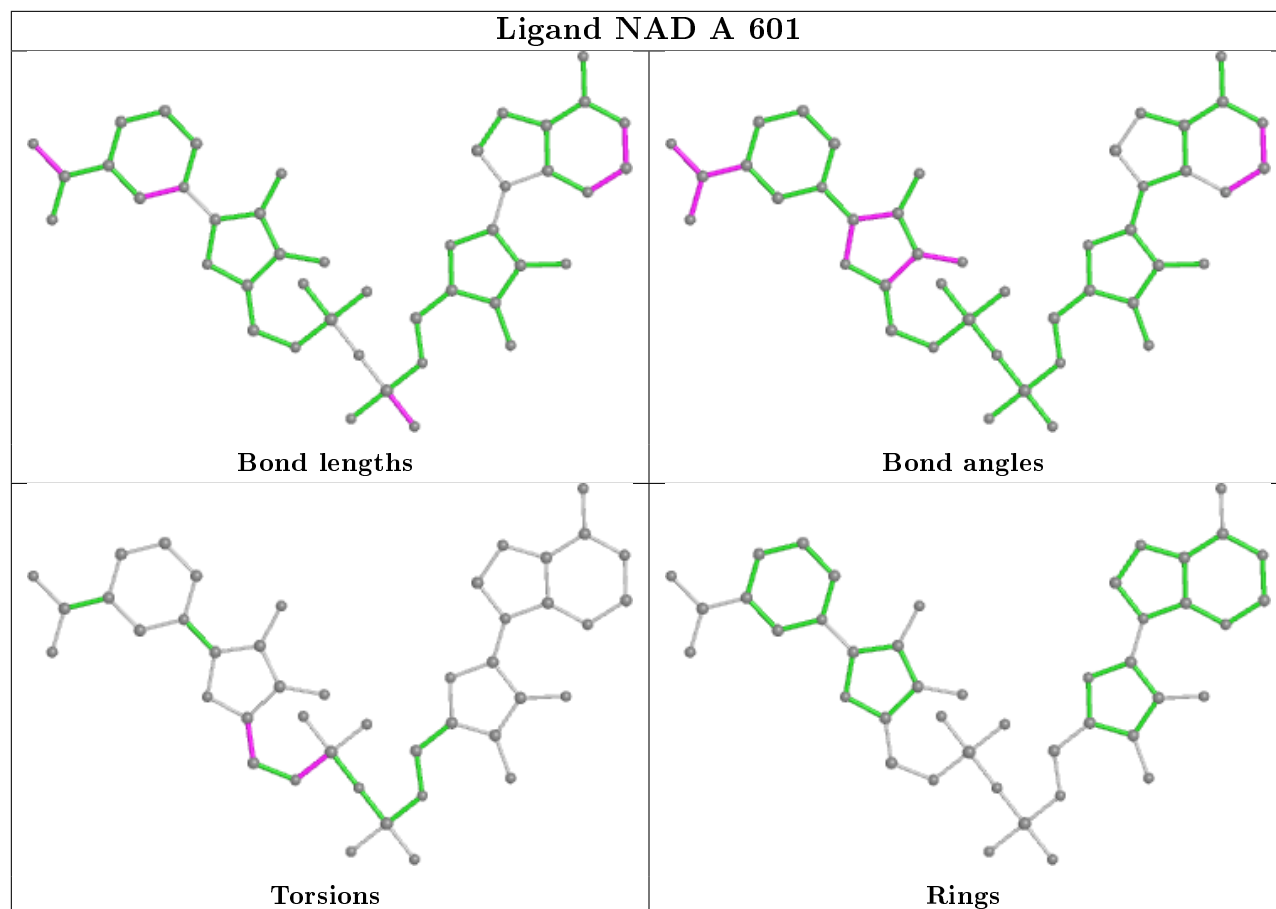
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	NAD	1	0
5	C	703	POP	3	0
3	A	501	APR	1	0
5	B	702	POP	5	0
3	C	503	APR	1	0
5	A	701	POP	5	0
2	B	401	SO4	1	0
3	B	502	APR	1	0

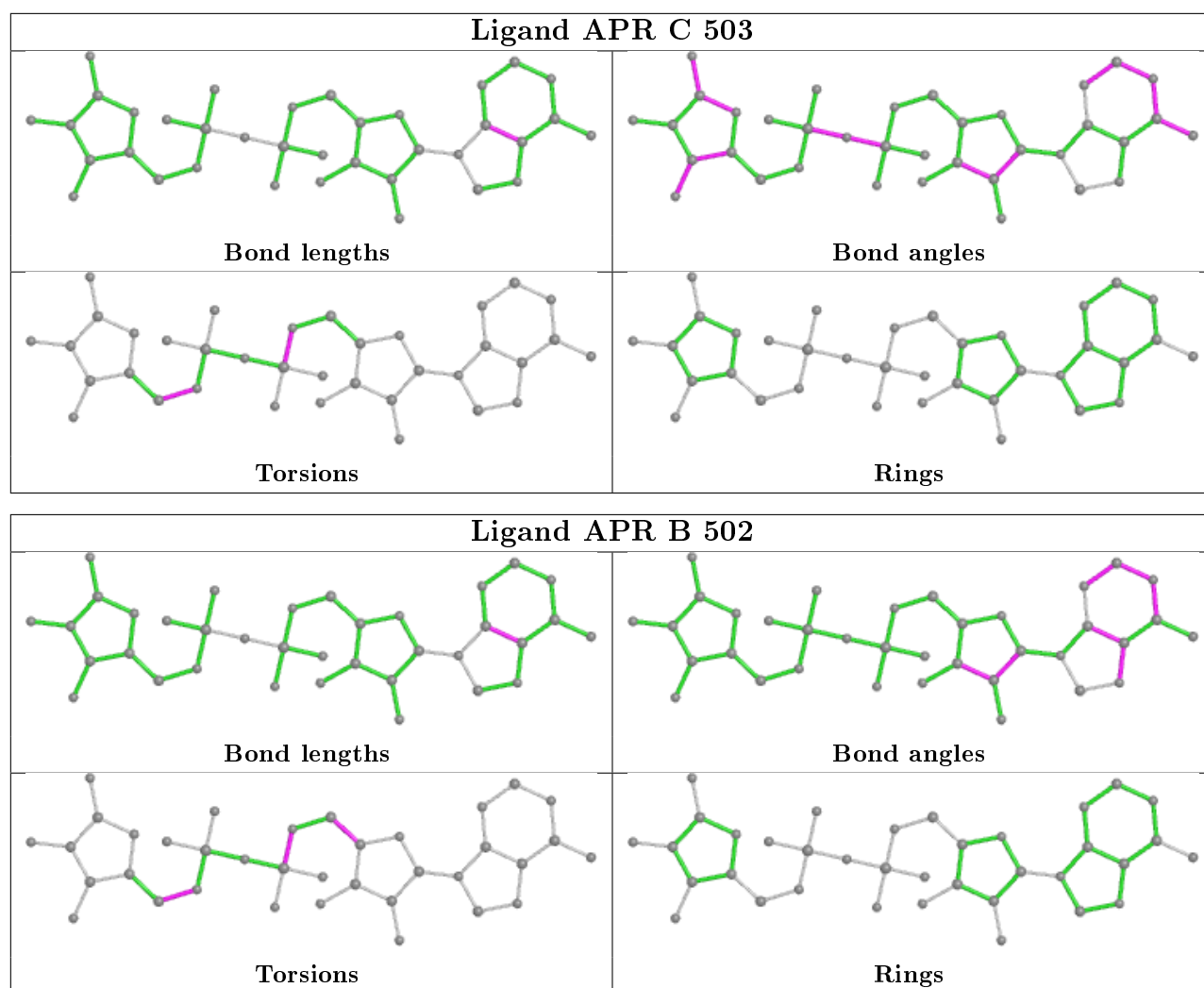
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	332/341 (97%)	-0.48	0 100 100	25, 37, 56, 75	0
1	B	336/341 (98%)	-0.30	6 (1%) 68 64	19, 38, 66, 88	0
1	C	327/341 (95%)	0.35	30 (9%) 9 6	32, 66, 107, 114	0
All	All	995/1023 (97%)	-0.15	36 (3%) 42 35	19, 43, 101, 114	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	ALA	6.4
1	C	135	PRO	4.9
1	C	153	ASP	4.3
1	B	305	ASP	4.0
1	C	106	VAL	3.9
1	C	137	PHE	3.8
1	C	68	GLN	3.8
1	B	302	GLY	3.4
1	C	161	ALA	3.4
1	C	5	TYR	3.0
1	C	129	LEU	2.9
1	C	136	ASP	2.8
1	C	6	GLN	2.7
1	C	160	PRO	2.6
1	B	304	ASP	2.6
1	C	113	LYS	2.6
1	C	134	TYR	2.5
1	C	70	LEU	2.5
1	C	30	GLU	2.5
1	C	156	ASP	2.5
1	C	176	ILE	2.5
1	C	20	GLY	2.5
1	B	307	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	259	LEU	2.4
1	C	152	GLY	2.4
1	C	23	ARG	2.3
1	C	157	LYS	2.3
1	C	31	LYS	2.3
1	C	148	GLU	2.2
1	C	150	LYS	2.2
1	C	7	TYR	2.1
1	C	112	ARG	2.1
1	B	171	LYS	2.1
1	C	158	VAL	2.1
1	C	167	GLN	2.1
1	C	133	HIS	2.1

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 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.

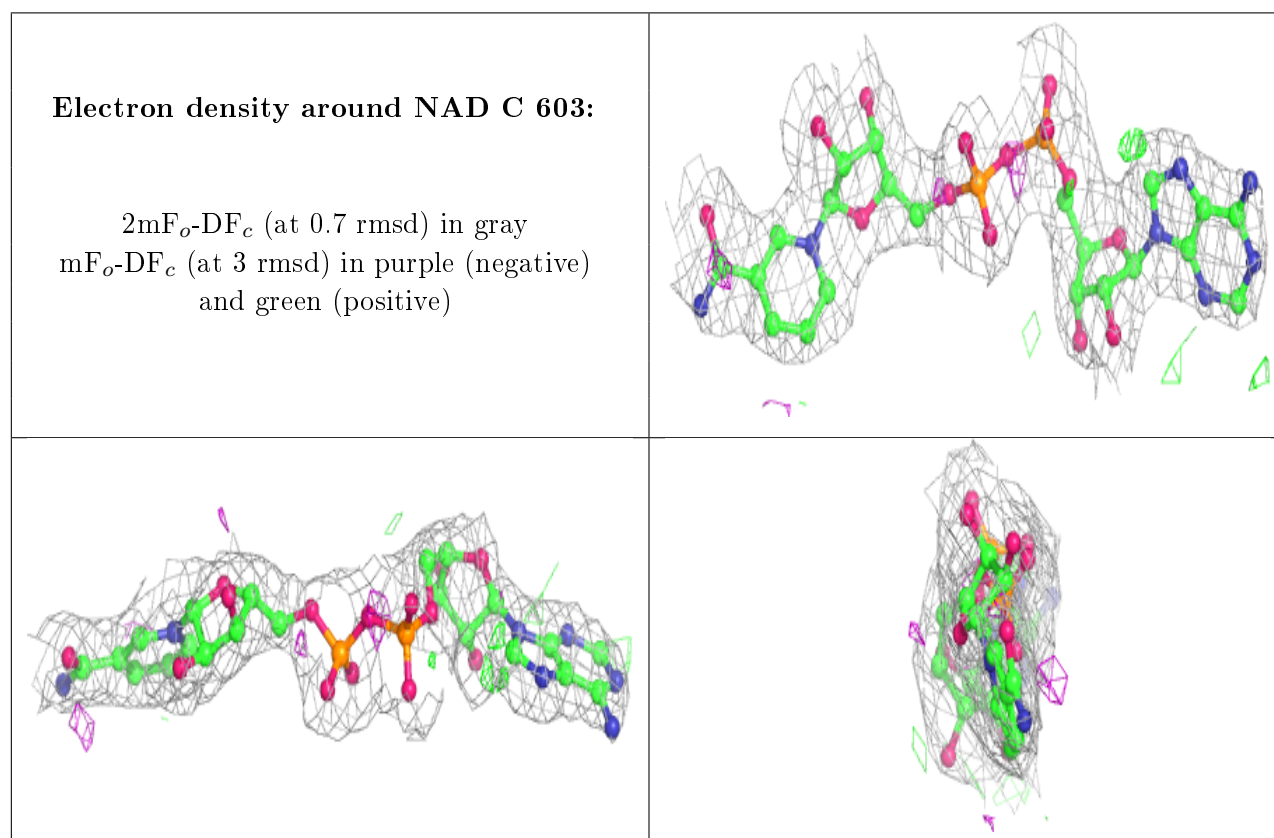
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	POP	C	703	9/9	0.74	0.18	107,108,109,109	0
4	NAD	C	603	44/44	0.86	0.19	59,73,85,85	0
5	POP	B	702	9/9	0.86	0.22	68,70,73,75	0
5	POP	A	701	9/9	0.91	0.16	74,75,76,76	0
2	SO4	A	402	5/5	0.93	0.13	93,93,93,94	0
2	SO4	B	401	5/5	0.96	0.11	81,81,82,82	0
4	NAD	B	602	44/44	0.98	0.12	31,39,44,46	0
3	APR	C	503	36/36	0.98	0.12	36,43,49,50	0
2	SO4	A	403	5/5	0.98	0.10	44,46,49,51	0
4	NAD	A	601	44/44	0.98	0.14	23,29,35,35	0

Continued on next page...

Continued from previous page...

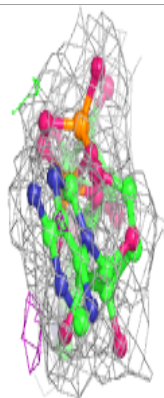
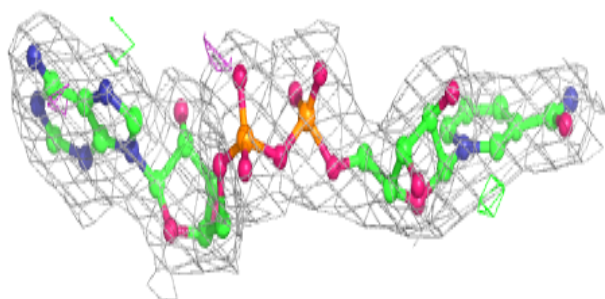
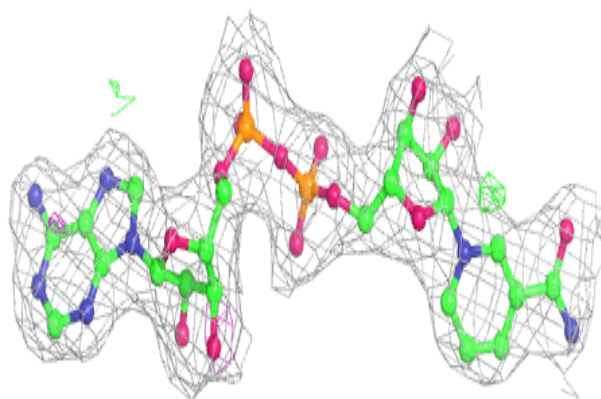
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	APR	B	502	36/36	0.98	0.12	23,29,38,42	0
3	APR	A	501	36/36	0.99	0.11	28,35,38,41	0
2	SO4	A	404	5/5	0.99	0.14	58,59,60,61	0

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

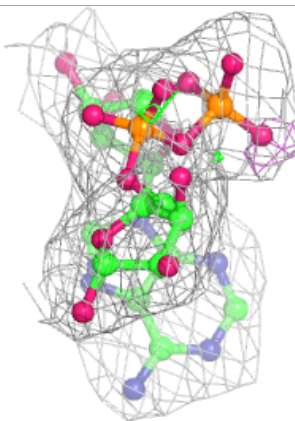
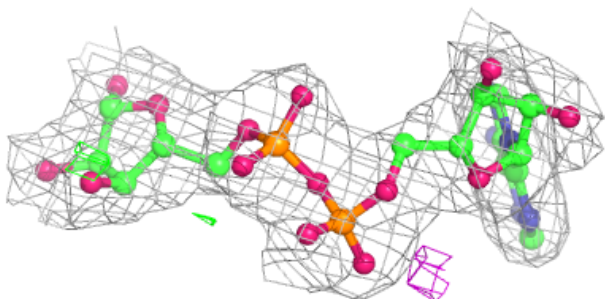
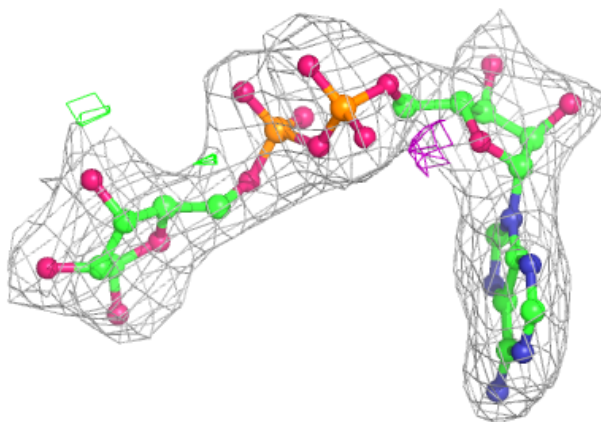


Electron density around NAD B 602:

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

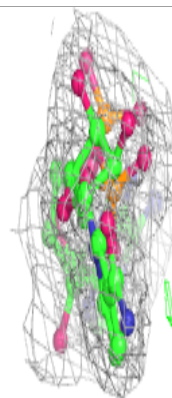
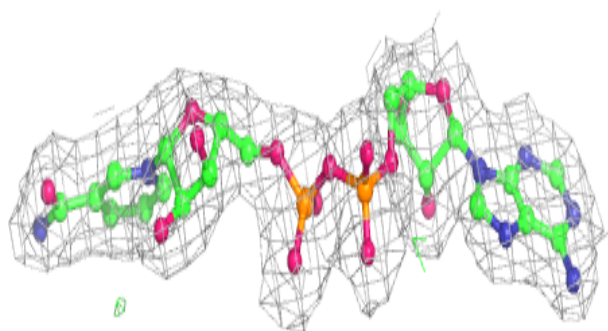
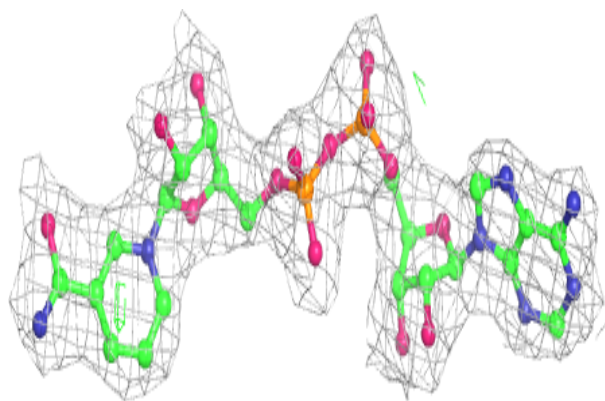
**Electron density around APR C 503:**

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

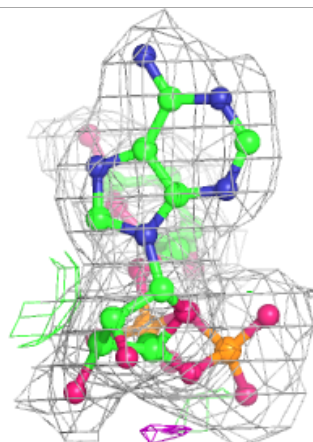
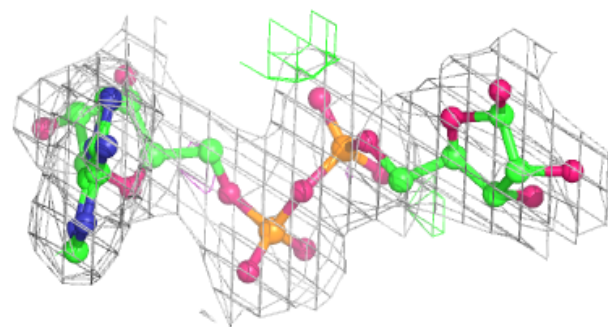
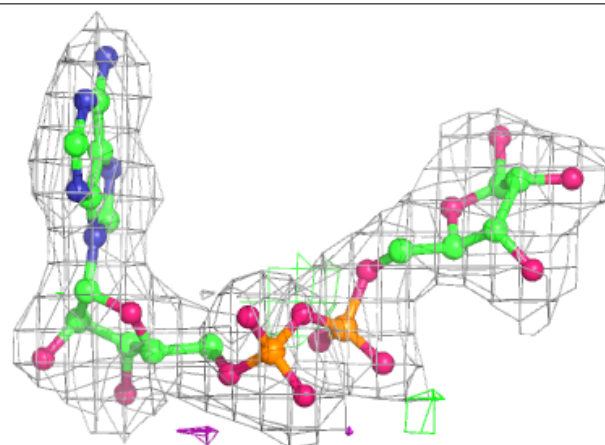


Electron density around NAD A 601:

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

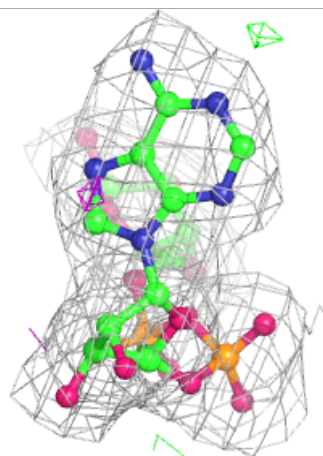
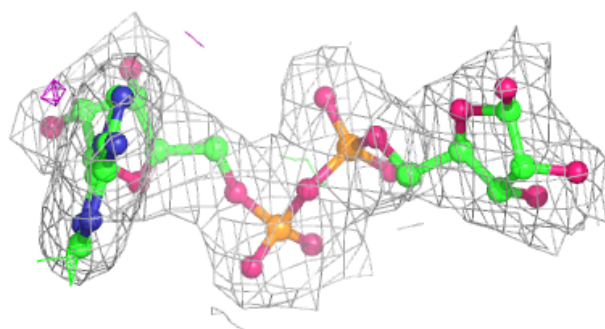
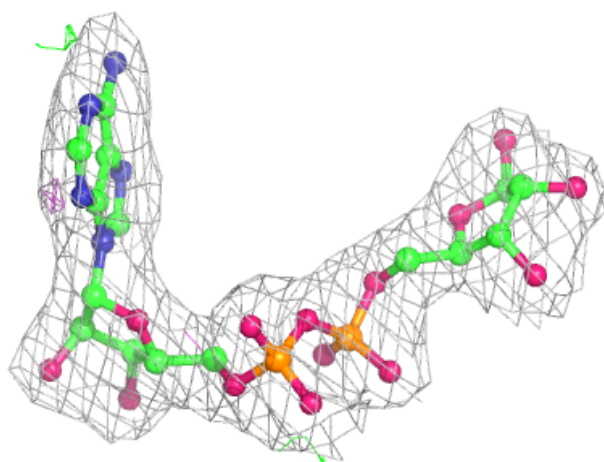
**Electron density around APR B 502:**

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



Electron density around APR A 501:

$2mF_o-DF_c$ (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.