



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:06 PM UTC

PDB ID : 1XNG / pdb_00001xng
Title : Crystal Structure of NH₃-dependent NAD⁺ synthetase from *Helicobacter pylori*
Authors : Kang, G.B.; Kim, Y.S.; Im, Y.J.; Rho, S.H.; Lee, J.H.; Eom, S.H.
Deposited on : 2004-10-05
Resolution : 1.70 Å(reported)

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

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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)
Xtriage (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

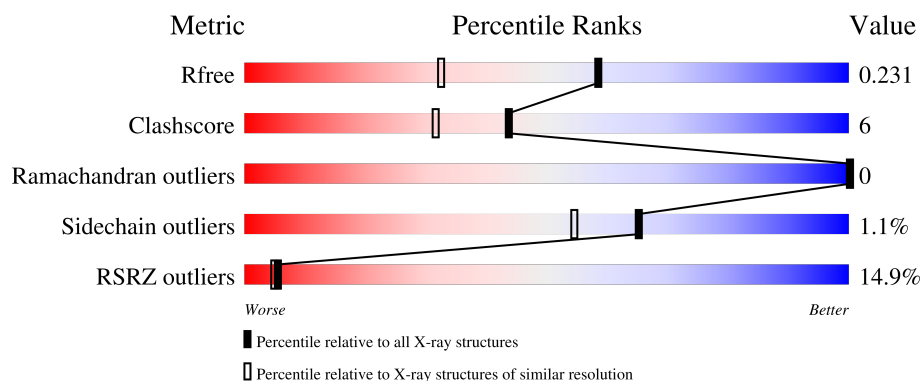
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	268	18% 82% 12% • 5%
1	B	268	11% 83% 15% •

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
3	DND	A	301	X	-	-	-
3	DND	B	302	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4457 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 NH(3)-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1989	1284	324	372	9			
1	B	262	Total	C	N	O	S	0	0	0
			2067	1335	339	384	9			

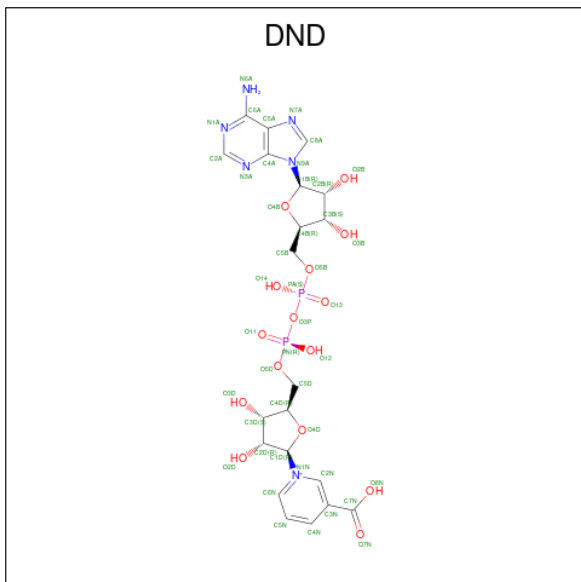
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	LEU	-	cloning artifact	UNP O25096
A	262	GLU	-	cloning artifact	UNP O25096
A	263	HIS	-	cloning artifact	UNP O25096
A	264	HIS	-	cloning artifact	UNP O25096
A	265	HIS	-	cloning artifact	UNP O25096
A	266	HIS	-	cloning artifact	UNP O25096
A	267	HIS	-	cloning artifact	UNP O25096
A	268	HIS	-	cloning artifact	UNP O25096
B	261	LEU	-	cloning artifact	UNP O25096
B	262	GLU	-	cloning artifact	UNP O25096
B	263	HIS	-	cloning artifact	UNP O25096
B	264	HIS	-	cloning artifact	UNP O25096
B	265	HIS	-	cloning artifact	UNP O25096
B	266	HIS	-	cloning artifact	UNP O25096
B	267	HIS	-	cloning artifact	UNP O25096
B	268	HIS	-	cloning artifact	UNP O25096

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

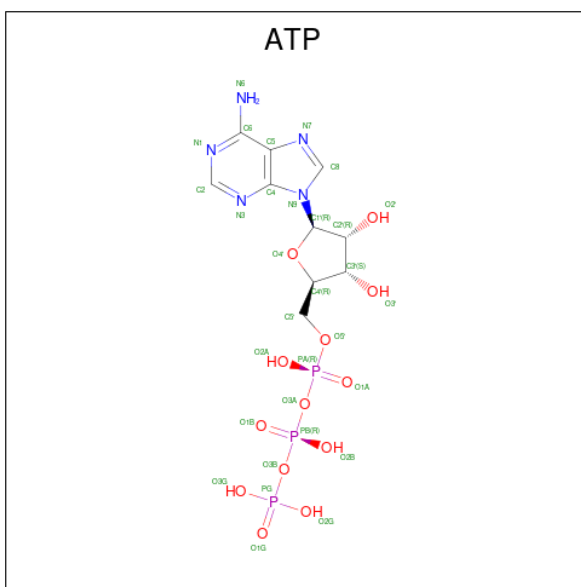
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is NICOTINIC ACID ADENINE DINUCLEOTIDE (CCD ID: DND) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_6\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 6	O 15	P 2	0	0
3	B	1	Total 44	C 21	N 6	O 15	P 2	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	134	Total	O	0	0
			134	134		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 63.40Å 125.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.35 – 1.70 41.35 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.35-1.70) 97.9 (41.35-1.70)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.21 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.257 0.234 , 0.231	Depositor DCC
R_{free} test set	6086 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l 0.031 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4457	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: ATP, DND, MG

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	0.37	0/2028	0.81	2/2742 (0.1%)
1	B	0.35	0/2110	0.77	1/2850 (0.0%)
All	All	0.36	0/4138	0.79	3/5592 (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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	64	MET	CA-C-N	5.23	124.68	119.24
1	A	64	MET	C-N-CA	5.23	124.68	119.24
1	B	34	GLY	N-CA-C	-5.18	107.97	115.27

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	TYR	Sidechain

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	1989	0	2007	25	0
1	B	2067	0	2095	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	44	0	23	0	0
3	B	44	0	23	0	0
4	A	31	0	12	1	0
4	B	31	0	12	0	0
5	A	115	0	0	1	0
5	B	134	0	0	0	0
All	All	4457	0	4172	51	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 6.

All (51) 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:32:LEU:HD12	1:A:71:ALA:HB1	1.62	0.81
1:B:70:ASP:HB3	1:B:177:ILE:HD11	1.61	0.80
1:A:186:LEU:H	1:A:190:GLN:NE2	1.85	0.74
1:A:196:LEU:HD23	1:A:240:ARG:HH12	1.63	0.62
1:B:186:LEU:H	1:B:190:GLN:NE2	2.00	0.60
1:A:88:ALA:N	1:A:89:PRO:HD2	2.17	0.60
1:A:120:ASP:OD1	1:B:105:ARG:HD2	2.03	0.59
1:B:250:LEU:HB3	1:B:251:PRO:HD2	1.86	0.57
1:B:88:ALA:N	1:B:89:PRO:HD2	2.20	0.57
1:A:250:LEU:HG	1:B:250:LEU:HD21	1.88	0.54
1:A:5:TYR:HB2	1:A:170:ARG:HG2	1.90	0.54
1:B:168:ALA:HB1	1:B:173:ILE:HD12	1.90	0.53
1:A:32:LEU:HD12	1:A:71:ALA:CB	2.37	0.51
1:B:130:ILE:HD12	1:B:153:ILE:HD11	1.92	0.51
1:B:204:ASP:N	1:B:205:PRO:HD2	2.26	0.49
1:A:77:LYS:HD2	1:A:78:PHE:CE1	2.47	0.49
1:A:252:ALA:HB3	1:B:153:ILE:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLY:O	1:B:177:ILE:HD12	2.11	0.48
1:B:62:VAL:HG23	1:B:188:VAL:HG23	1.93	0.48
1:A:186:LEU:HB2	1:A:190:GLN:HE22	1.78	0.48
1:A:202:VAL:HG12	1:A:233:LEU:HD11	1.95	0.48
1:B:62:VAL:CG2	1:B:188:VAL:HG23	2.44	0.47
1:B:160:PHE:CE1	1:B:208:LYS:HG2	2.50	0.46
1:A:57:LEU:HD12	1:A:57:LEU:N	2.30	0.46
1:A:186:LEU:H	1:A:190:GLN:HE22	1.60	0.46
1:A:253:ILE:CD1	1:B:154:ASN:HB3	2.46	0.45
1:A:204:ASP:N	1:A:205:PRO:HD2	2.31	0.45
1:B:184:ALA:HB3	1:B:190:GLN:NE2	2.31	0.45
1:B:204:ASP:O	1:B:208:LYS:HG3	2.16	0.45
1:B:3:LYS:O	1:B:7:LYS:HG3	2.16	0.45
1:B:62:VAL:HG21	1:B:187:PHE:HA	1.99	0.44
1:B:101:ALA:HA	1:B:105:ARG:NH2	2.33	0.43
1:B:57:LEU:HD12	1:B:57:LEU:N	2.33	0.43
1:B:261:LEU:H	1:B:264:HIS:CD2	2.35	0.43
1:B:58:MET:HE1	1:B:118:LEU:HG	1.99	0.43
1:B:70:ASP:HB3	1:B:177:ILE:CD1	2.42	0.43
1:A:30:TYR:HE1	1:A:32:LEU:HD23	1.83	0.43
1:A:238:THR:O	1:A:242:GLN:HG3	2.19	0.43
1:A:93:ILE:HD11	1:B:93:ILE:HD11	2.00	0.43
1:B:6:GLN:O	1:B:10:VAL:HG23	2.19	0.43
1:B:41:VAL:HG21	1:B:132:THR:HG22	2.00	0.42
1:A:122:SER:HB2	1:A:127:SER:O	2.20	0.42
1:A:77:LYS:O	1:A:77:LYS:HD3	2.21	0.41
1:A:250:LEU:HG	1:B:250:LEU:CD2	2.50	0.41
1:B:186:LEU:H	1:B:190:GLN:HE21	1.68	0.41
1:A:56:LEU:HD22	1:A:58:MET:HG3	2.02	0.41
1:B:168:ALA:CB	1:B:173:ILE:HD12	2.50	0.41
1:B:122:SER:HB2	1:B:127:SER:O	2.20	0.41
1:A:181:PRO:HA	1:A:182:PRO:HD3	1.97	0.40
4:A:303:ATP:H5'1	5:A:356:HOH:O	2.20	0.40
1:A:230:ASP:HB3	1:A:233:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/268 (94%)	249 (98%)	4 (2%)	0	100	100
1	B	260/268 (97%)	254 (98%)	6 (2%)	0	100	100
All	All	513/536 (96%)	503 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	216/236 (92%)	213 (99%)	3 (1%)	59	46
1	B	227/236 (96%)	225 (99%)	2 (1%)	70	62
All	All	443/472 (94%)	438 (99%)	5 (1%)	65	54

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

Mol	Chain	Res	Type
1	A	56	LEU
1	A	76	GLU
1	A	170	ARG
1	B	56	LEU
1	B	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	67	ASN
1	A	73	ASN
1	A	190	GLN
1	B	21	GLN
1	B	54	HIS
1	B	67	ASN
1	B	97	HIS
1	B	190	GLN
1	B	244	ASN
1	B	264	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	A	303	2	32,33,33	1.14	4 (12%)	48,52,52	1.89	10 (20%)
3	DND	A	301	-	46,48,48	1.80	9 (19%)	64,73,73	2.93	23 (35%)
4	ATP	B	304	2	32,33,33	1.13	2 (6%)	48,52,52	1.93	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DND	B	302	-	46,48,48	1.72	8 (17%)	64,73,73	2.85	26 (40%)

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	ATP	A	303	2	-	8/22/38/38	0/3/3/3
3	DND	A	301	-	1/1/11/11	6/30/62/62	0/5/5/5
4	ATP	B	304	2	-	8/22/38/38	0/3/3/3
3	DND	B	302	-	1/1/11/11	6/30/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	DND	C2N-N1N	6.71	1.42	1.35
3	B	302	DND	C2N-N1N	6.07	1.41	1.35
3	B	302	DND	PN-O3P	-4.43	1.54	1.59
3	A	301	DND	PN-O3P	-4.12	1.55	1.59
3	A	301	DND	C2N-C3N	3.46	1.44	1.39
3	B	302	DND	C2N-C3N	3.39	1.44	1.39
3	A	301	DND	C6N-N1N	3.17	1.42	1.35
3	B	302	DND	C6N-N1N	3.14	1.42	1.35
3	A	301	DND	O4D-C1D	2.85	1.44	1.40
3	A	301	DND	C4N-C3N	2.52	1.43	1.39
4	A	303	ATP	C2-N1	2.44	1.38	1.33
3	A	301	DND	PA-O3P	2.44	1.62	1.59
3	B	302	DND	C4N-C3N	2.42	1.43	1.39
4	B	304	ATP	C2-N1	2.41	1.38	1.33
4	B	304	ATP	C2-N3	2.38	1.38	1.33
4	A	303	ATP	C2-N3	2.30	1.38	1.33
3	B	302	DND	C3B-C4B	-2.27	1.47	1.53
3	A	301	DND	C3B-C4B	-2.23	1.47	1.53
3	B	302	DND	PA-O3P	2.11	1.61	1.59
3	A	301	DND	C5A-N7A	-2.08	1.35	1.39
3	B	302	DND	O4D-C1D	2.06	1.43	1.40
4	A	303	ATP	C4-N3	2.05	1.38	1.34
4	A	303	ATP	C1'-N9	2.04	1.52	1.46

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	DND	C4D-O4D-C1D	-12.36	98.61	109.92
3	B	302	DND	C4D-O4D-C1D	-10.98	99.87	109.92
3	B	302	DND	N1A-C2A-N3A	-6.04	119.44	128.58
3	A	301	DND	N1A-C2A-N3A	-5.90	119.66	128.58
4	B	304	ATP	N3-C2-N1	-5.67	120.00	128.58
4	A	303	ATP	N3-C2-N1	-5.62	120.07	128.58
3	A	301	DND	O3B-C3B-C4B	5.53	126.98	111.08
3	A	301	DND	O2D-C2D-C3D	5.22	128.53	111.82
3	B	302	DND	C5A-C4A-N3A	-5.14	119.64	126.72
3	B	302	DND	O3B-C3B-C4B	5.10	125.72	111.08
4	B	304	ATP	C5-N7-C8	5.02	111.33	103.45
3	A	301	DND	C5A-C4A-N3A	-4.99	119.85	126.72
4	A	303	ATP	C5-N7-C8	4.94	111.21	103.45
3	B	302	DND	C6N-N1N-C1D	-4.92	110.08	119.73
3	B	302	DND	O2D-C2D-C3D	4.91	127.55	111.82
3	A	301	DND	O3D-C3D-C4D	4.91	125.17	111.08
3	B	302	DND	O3D-C3D-C4D	4.90	125.17	111.08
3	B	302	DND	N3A-C4A-N9A	4.85	135.41	127.17
3	A	301	DND	N3A-C4A-N9A	4.71	135.17	127.17
4	B	304	ATP	N9-C8-N7	-4.65	107.34	113.94
4	B	304	ATP	C4-C5-N7	-4.62	105.30	110.58
3	A	301	DND	C6N-N1N-C1D	-4.57	110.76	119.73
4	A	303	ATP	N9-C8-N7	-4.50	107.55	113.94
4	A	303	ATP	C4-C5-N7	-4.45	105.49	110.58
3	B	302	DND	C2N-C3N-C4N	4.36	123.33	118.26
3	A	301	DND	C2N-C3N-C4N	3.99	122.90	118.26
3	A	301	DND	O3P-PA-O13	-3.96	98.78	110.70
3	A	301	DND	O2B-C2B-C1B	3.76	123.05	110.10
3	A	301	DND	C2A-N1A-C6A	3.62	124.68	118.73
3	B	302	DND	O3P-PA-O13	-3.60	99.87	110.70
3	B	302	DND	C2A-N1A-C6A	3.59	124.62	118.73
3	B	302	DND	O2B-C2B-C1B	3.58	122.42	110.10
3	B	302	DND	O8N-C7N-O7N	3.35	130.55	123.35
3	B	302	DND	C2A-N3A-C4A	3.34	119.98	111.83
3	A	301	DND	O8N-C7N-O7N	3.21	130.26	123.35
3	A	301	DND	C2A-N3A-C4A	3.18	119.59	111.83
3	A	301	DND	C6A-C5A-C4A	3.12	121.44	117.18
3	A	301	DND	C6A-C5A-N7A	-3.09	126.13	132.09
3	B	302	DND	C2N-N1N-C1D	3.08	125.94	119.13
3	A	301	DND	C2B-C1B-N9A	3.05	120.89	113.30
3	A	301	DND	C4B-O4B-C1B	-3.02	102.80	109.47
3	B	302	DND	C6A-C5A-N7A	-3.00	126.31	132.09
4	B	304	ATP	C6-C5-N7	2.95	137.77	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	DND	C2B-C1B-N9A	2.91	120.54	113.30
3	B	302	DND	C6A-C5A-C4A	2.90	121.14	117.18
4	B	304	ATP	C2-N3-C4	2.89	118.90	111.83
4	A	303	ATP	C2-N3-C4	2.89	118.89	111.83
3	A	301	DND	C4N-C3N-C7N	-2.86	114.72	120.37
4	A	303	ATP	C6-C5-N7	2.81	137.50	132.09
4	A	303	ATP	C5-C4-N3	-2.81	122.85	126.72
3	B	302	DND	C4N-C3N-C7N	-2.74	114.95	120.37
3	A	301	DND	C2N-N1N-C1D	2.74	125.17	119.13
3	B	302	DND	C4B-O4B-C1B	-2.67	103.56	109.47
3	B	302	DND	O4D-C4D-C3D	-2.65	99.90	105.15
4	B	304	ATP	C5-C4-N3	-2.64	123.09	126.72
3	A	301	DND	C6N-N1N-C2N	2.57	124.07	121.88
3	B	302	DND	C5D-C4D-C3D	2.56	124.42	115.21
3	B	302	DND	C6N-N1N-C2N	2.46	123.97	121.88
3	A	301	DND	O5D-C5D-C4D	-2.44	100.68	108.99
4	A	303	ATP	C4-N9-C8	2.38	108.24	105.74
3	B	302	DND	O4B-C1B-N9A	-2.34	103.60	108.09
4	B	304	ATP	C4-N9-C8	2.33	108.19	105.74
3	A	301	DND	O4B-C1B-N9A	-2.31	103.65	108.09
4	B	304	ATP	O2B-PB-O3A	2.26	113.38	107.27
4	B	304	ATP	O2'-C2'-C3'	2.23	118.98	111.82
4	A	303	ATP	O2G-PG-O3B	2.20	112.02	104.64
3	B	302	DND	O3D-C3D-C2D	-2.14	104.95	111.82
3	B	302	DND	O4B-C4B-C3B	2.11	109.34	105.15
4	A	303	ATP	O2'-C2'-C3'	2.04	118.36	111.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	301	DND	C1D
3	B	302	DND	C1D

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	DND	O4D-C1D-N1N-C6N
3	A	301	DND	O4D-C1D-N1N-C2N
3	B	302	DND	O4D-C1D-N1N-C6N
3	B	302	DND	O4D-C1D-N1N-C2N
4	A	303	ATP	C5'-O5'-PA-O1A
4	A	303	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	A	303	ATP	C5'-O5'-PA-O3A
4	B	304	ATP	C5'-O5'-PA-O2A
4	B	304	ATP	C5'-O5'-PA-O3A
4	A	303	ATP	O4'-C4'-C5'-O5'
4	A	303	ATP	C3'-C4'-C5'-O5'
3	A	301	DND	PA-O3P-PN-O12
3	B	302	DND	PA-O3P-PN-O12
4	A	303	ATP	PA-O3A-PB-O2B
4	B	304	ATP	PA-O3A-PB-O2B
3	B	302	DND	C4D-C5D-O5D-PN
3	B	302	DND	C4B-C5B-O5B-PA
4	B	304	ATP	C5'-O5'-PA-O1A
4	B	304	ATP	PB-O3A-PA-O1A
3	A	301	DND	C4D-C5D-O5D-PN
3	A	301	DND	C4B-C5B-O5B-PA
4	B	304	ATP	O4'-C4'-C5'-O5'
4	A	303	ATP	PA-O3A-PB-O1B
4	B	304	ATP	PB-O3A-PA-O2A
3	A	301	DND	O4D-C4D-C5D-O5D
4	A	303	ATP	C4'-C5'-O5'-PA
4	B	304	ATP	PA-O3A-PB-O1B
3	B	302	DND	O4D-C4D-C5D-O5D

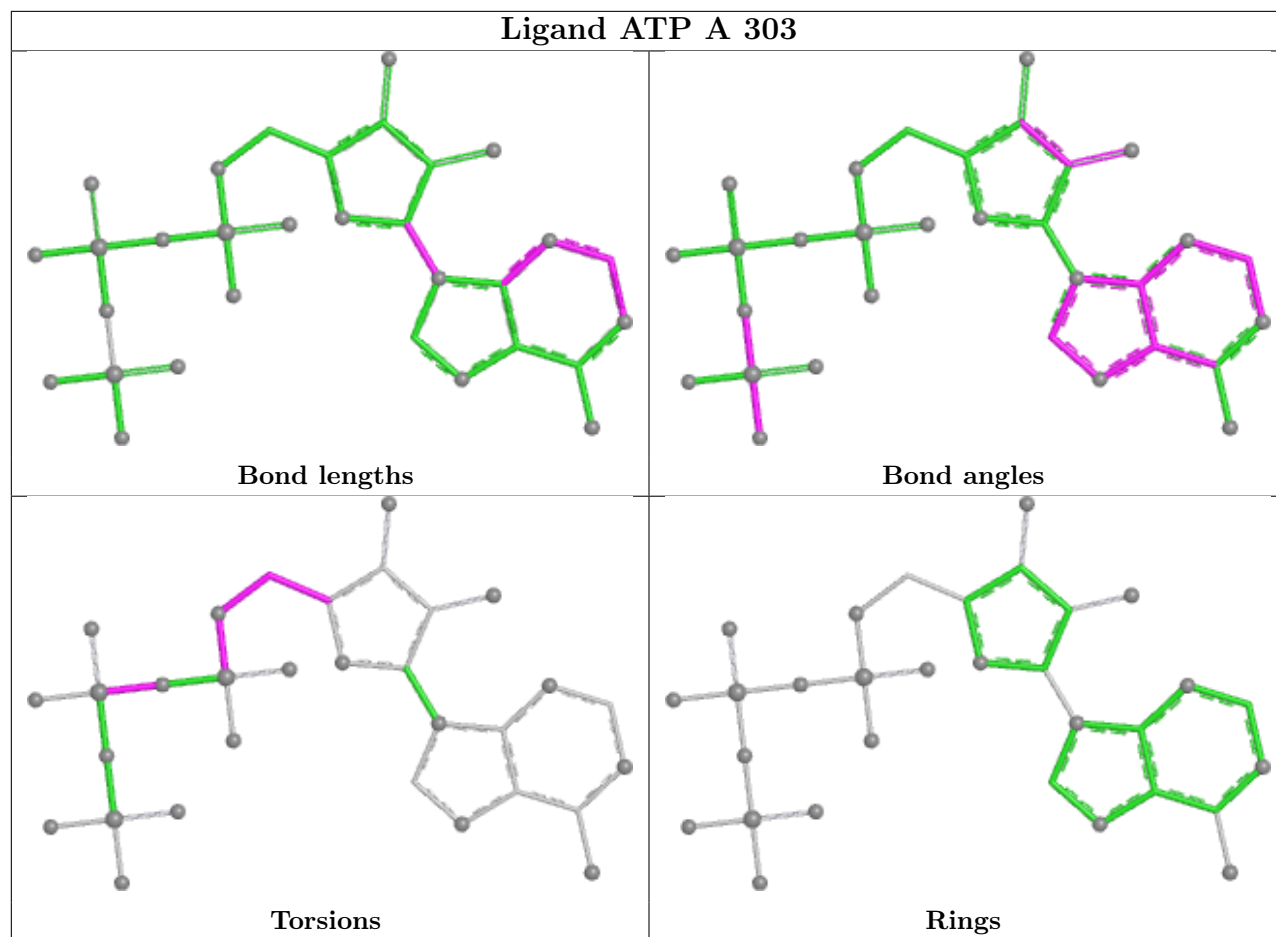
There are no ring outliers.

1 monomer is involved in 1 short contact:

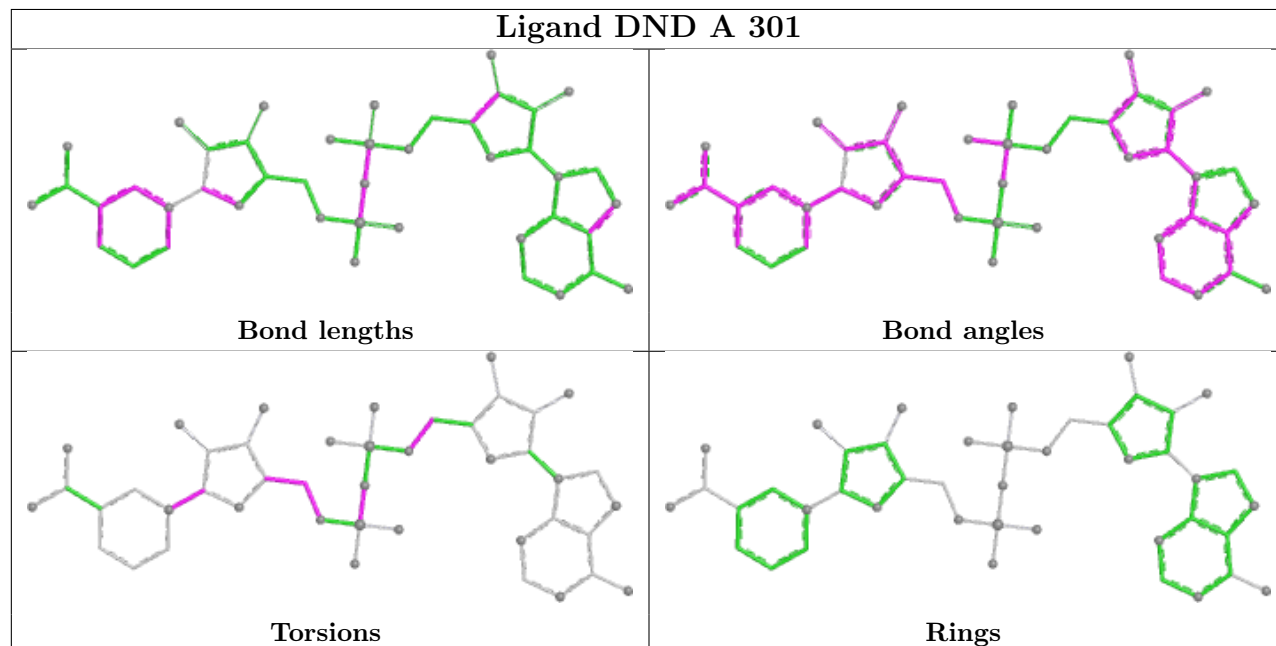
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	ATP	1	0

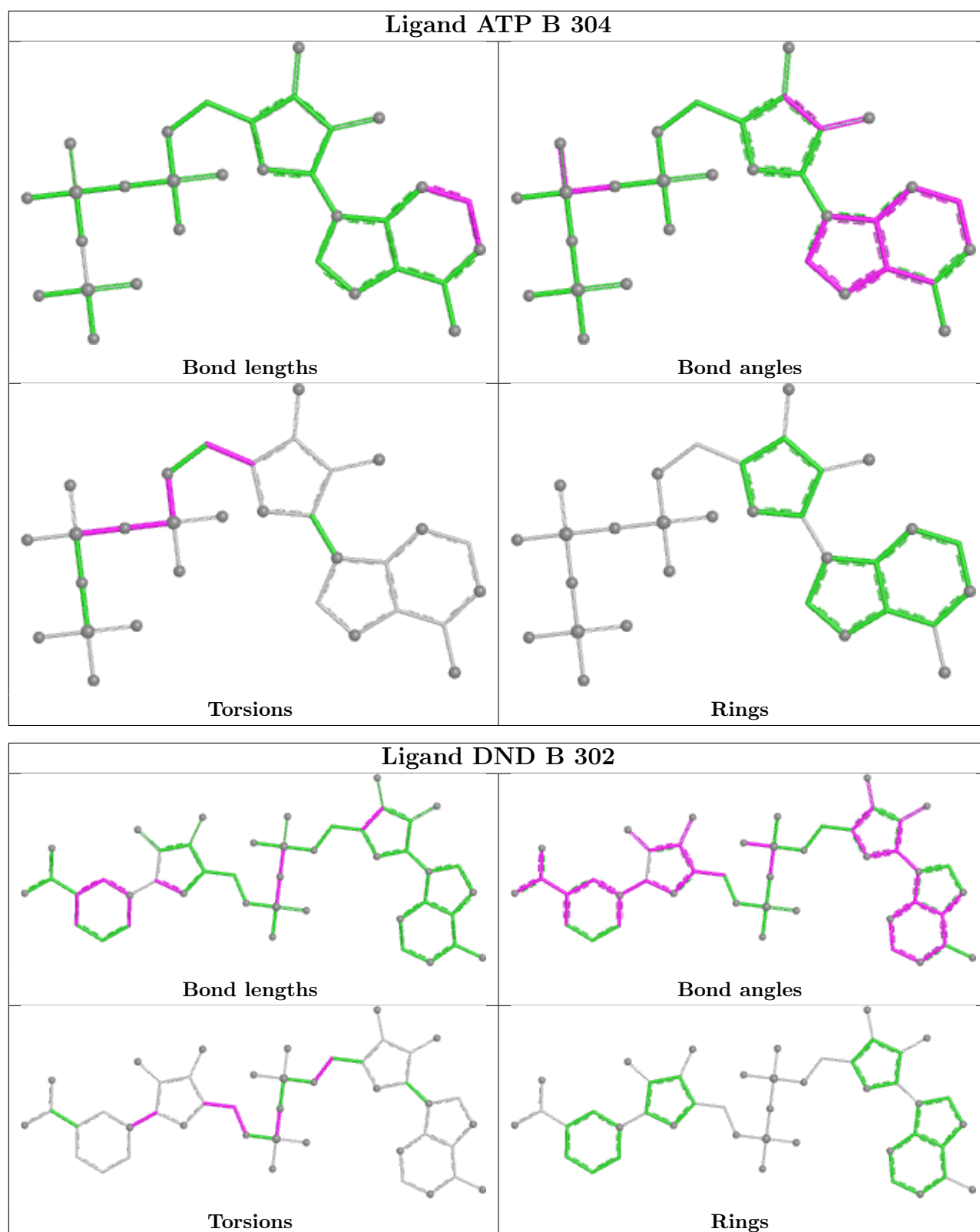
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ATP A 303



Ligand DND A 301





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	255/268 (95%)	1.06	47 (18%) 3 3	15, 25, 41, 74	0
1	B	262/268 (97%)	0.91	30 (11%) 9 9	16, 25, 39, 60	0
All	All	517/536 (96%)	0.99	77 (14%) 5 5	15, 25, 41, 74	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	LYS	6.2
1	A	5	TYR	5.5
1	A	4	ASP	5.1
1	B	5	TYR	4.7
1	A	257	PHE	4.6
1	A	187	PHE	4.4
1	A	233	LEU	4.2
1	B	6	GLN	4.2
1	A	6	GLN	4.1
1	B	215	GLN	3.9
1	A	232	ILE	3.7
1	B	214	PHE	3.7
1	A	248	LEU	3.5
1	B	76	GLU	3.4
1	A	230	ASP	3.4
1	B	62	VAL	3.3
1	A	216	THR	3.3
1	A	225	ALA	3.3
1	A	188	VAL	3.1
1	A	21	GLN	3.1
1	B	99	LYS	3.1
1	A	226	GLN	3.0
1	A	231	GLU	3.0
1	A	96	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	64	MET	3.0
1	B	64	MET	3.0
1	B	176	LYS	3.0
1	B	216	THR	3.0
1	B	14	ASP	2.9
1	A	99	LYS	2.9
1	A	26	LYS	2.9
1	A	202	VAL	2.9
1	A	100	ASP	2.9
1	A	236	ASN	2.7
1	A	227	LEU	2.7
1	A	126	ASP	2.7
1	A	186	LEU	2.7
1	B	175	LYS	2.7
1	B	89	PRO	2.6
1	A	162	THR	2.6
1	B	178	LEU	2.6
1	A	198	TYR	2.6
1	A	234	VAL	2.6
1	B	96	SER	2.6
1	B	65	PRO	2.6
1	A	240	ARG	2.5
1	B	165	TYR	2.5
1	B	3	LYS	2.5
1	B	173	ILE	2.5
1	B	4	ASP	2.4
1	A	229	TYR	2.4
1	A	63	SER	2.4
1	A	223	THR	2.4
1	B	100	ASP	2.4
1	B	7	LYS	2.4
1	A	256	ARG	2.4
1	B	51	GLU	2.4
1	A	93	ILE	2.3
1	A	214	PHE	2.3
1	B	153	ILE	2.3
1	A	184	ALA	2.3
1	A	189	GLY	2.3
1	B	72	LEU	2.2
1	B	189	GLY	2.2
1	A	199	PRO	2.2
1	A	194	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	235	LYS	2.2
1	A	95	SER	2.2
1	A	77	LYS	2.2
1	A	7	LYS	2.1
1	A	18	LYS	2.1
1	B	187	PHE	2.1
1	B	256	ARG	2.1
1	A	170	ARG	2.1
1	A	98	PHE	2.1
1	B	188	VAL	2.0
1	B	8	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

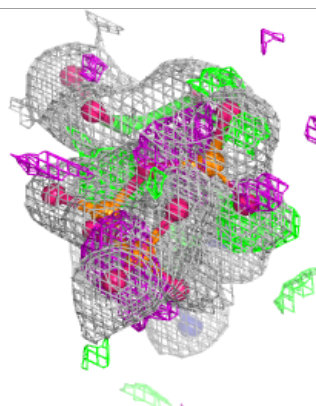
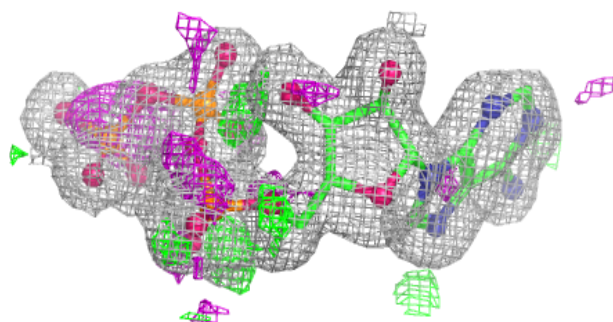
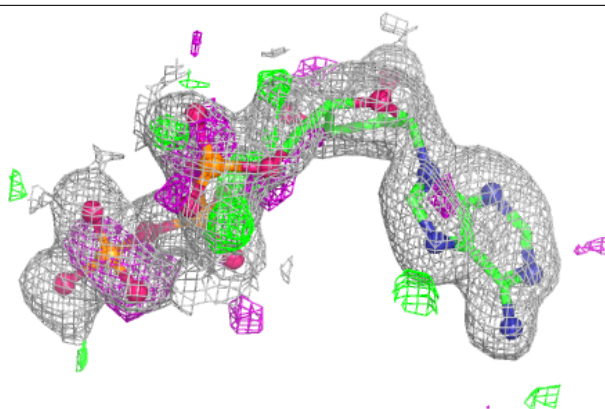
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	308	1/1	0.43	0.34	60,60,60,60	0
4	ATP	A	303	31/31	0.87	0.13	21,26,33,35	0
4	ATP	B	304	31/31	0.89	0.12	20,24,31,36	0
3	DND	A	301	44/44	0.92	0.12	19,24,38,42	0
2	MG	A	309	1/1	0.93	0.06	27,27,27,27	0
3	DND	B	302	44/44	0.95	0.09	13,20,26,35	0

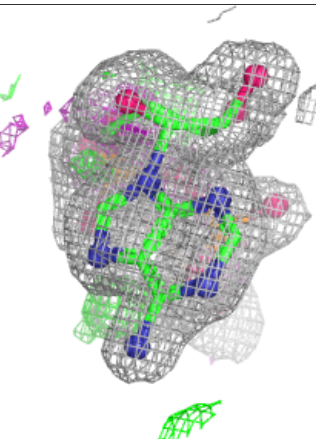
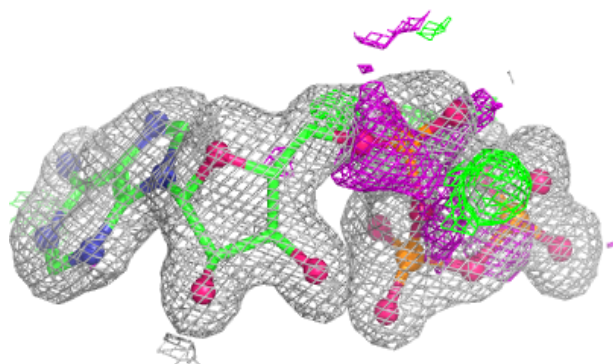
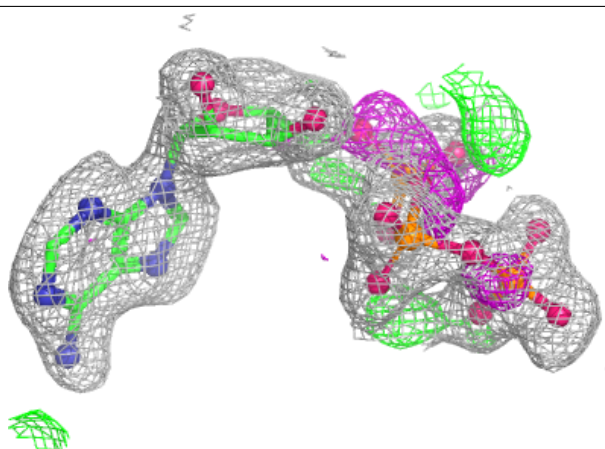
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 303:

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

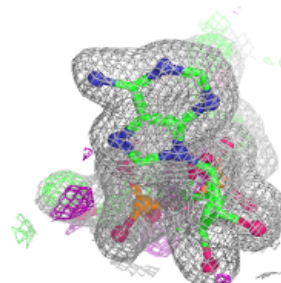
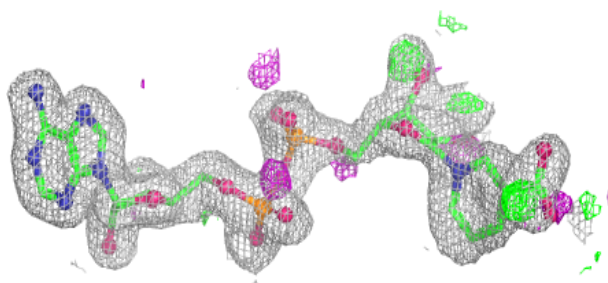
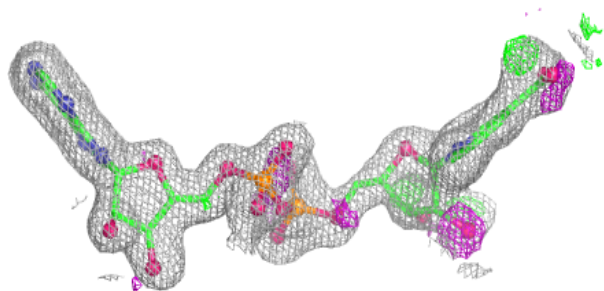
**Electron density around ATP B 304:**

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

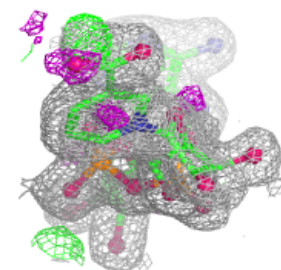
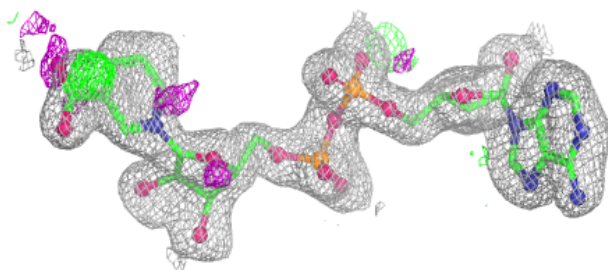
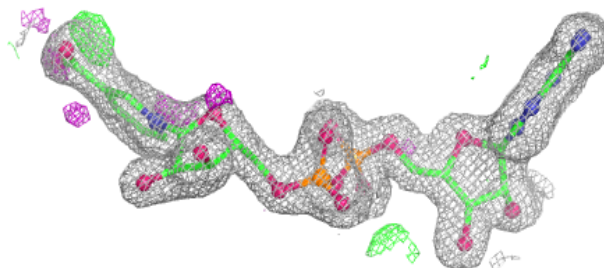


Electron density around DND A 301:

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

**Electron density around DND B 302:**

$2mF_o-DF_c$ (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.