



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:34 pm BST

PDB ID : 2ZJ1
Title : Crystal structure of Mycobacterium tuberculosis S-adenosyl-L-homocysteine hydrolase in ternary complex with NAD and 3'-keto-aristeromycin
Authors : Reddy, M.C.M.; Gokulan, K.; Shetty, N.D.; Owen, J.L.; Ioerger, T.R.; Sacchettini, J.C.
Deposited on : 2008-02-29
Resolution : 2.01 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

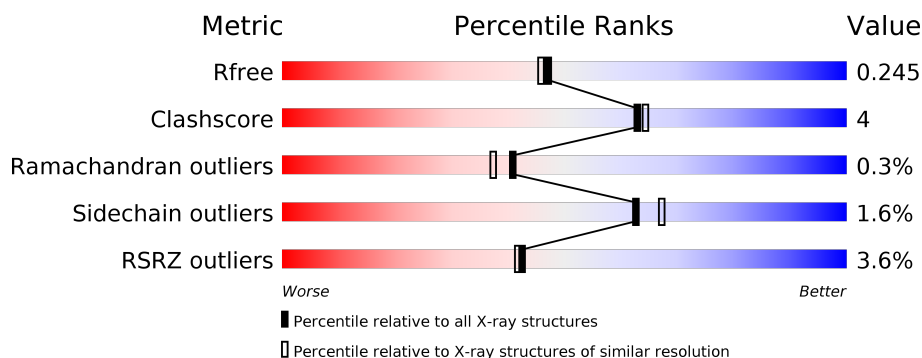
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	495	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>•</div> </div>
1	B	495	<div> <div>%</div> <div>89%</div> <div>8%</div> <div>••</div> </div>
1	C	495	<div> <div>7%</div> <div>85%</div> <div>11%</div> <div>••</div> </div>
1	D	495	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>•</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ARJ	A	500	X	-	-	-
2	ARJ	B	500	X	-	-	-
2	ARJ	C	500	X	-	-	-
2	ARJ	D	500	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16088 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.

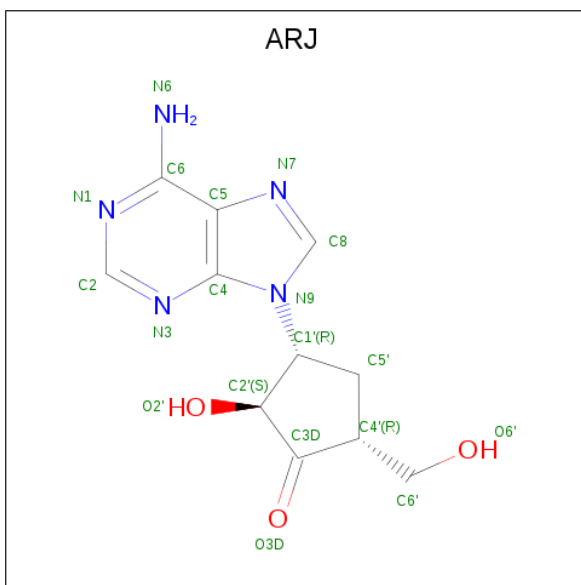
- Molecule 1 is a protein called Adenosylhomocysteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	B	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	C	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			
1	D	485	Total	C	N	O	S	0	0	0
			3748	2364	643	724	17			

There are 4 discrepancies between the modelled and reference sequences:

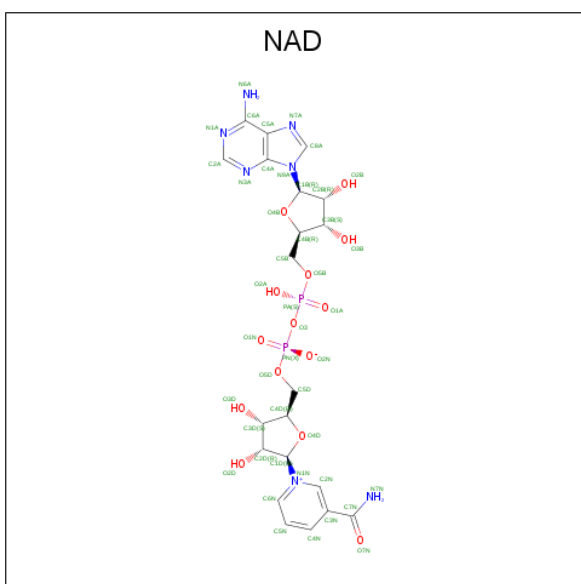
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP P60176
B	1	MET	-	EXPRESSION TAG	UNP P60176
C	1	MET	-	EXPRESSION TAG	UNP P60176
D	1	MET	-	EXPRESSION TAG	UNP P60176

- Molecule 2 is (2S,3R,5R)-3-(6-amino-9H-purin-9-yl)-2-hydroxy-5-(hydroxymethyl)cyclopent anone (three-letter code: ARJ) (formula: C₁₁H₁₃N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 19	C 11	N 5	O 3	0	0
2	B	1	Total 19	C 11	N 5	O 3	0	0
2	C	1	Total 19	C 11	N 5	O 3	0	0
2	D	1	Total 19	C 11	N 5	O 3	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

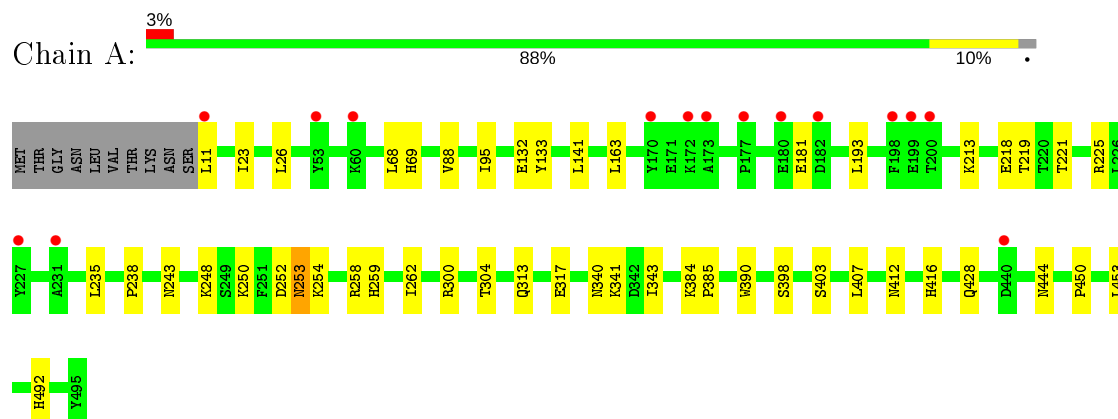
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	236	Total	O	0	0
			236	236		
4	C	193	Total	O	0	0
			193	193		
4	D	220	Total	O	0	0
			220	220		

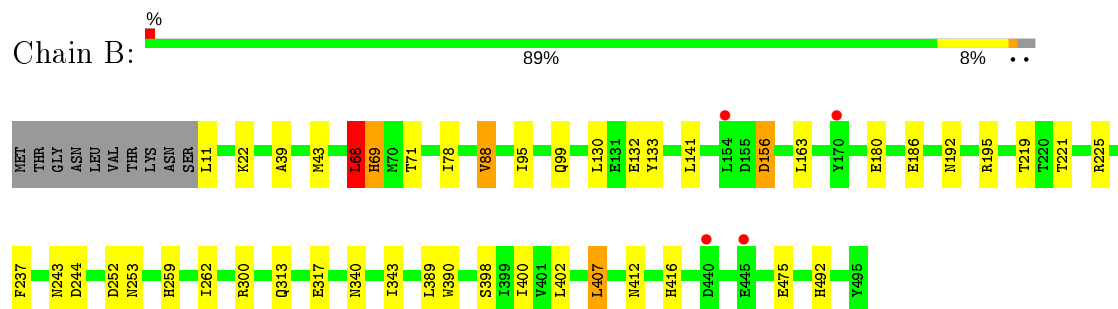
3 Residue-property plots [i](#)

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.

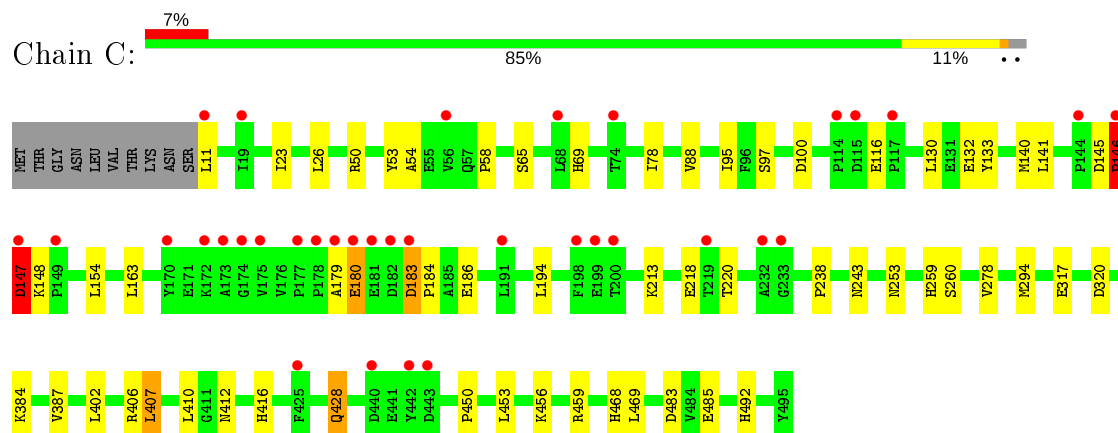
• Molecule 1: Adenosylhomocysteinase



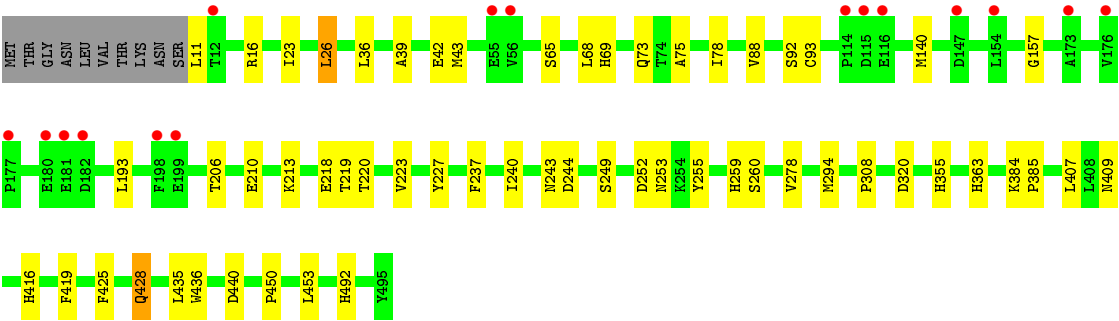
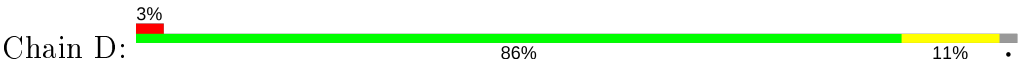
• Molecule 1: Adenosylhomocysteinase



• Molecule 1: Adenosylhomocysteinase



● Molecule 1: Adenosylhomocysteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.85Å 111.85Å 100.40Å 90.00° 96.49° 90.00°	Depositor
Resolution (Å)	34.59 – 2.01 34.59 – 2.01	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.59-2.01) 98.9 (34.59-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.247 0.189 , 0.245	Depositor DCC
R_{free} test set	6853 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16088	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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: ARJ, 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	0.73	0/3824	0.73	1/5186 (0.0%)
1	B	0.77	0/3824	0.73	3/5186 (0.1%)
1	C	0.70	0/3824	0.71	4/5186 (0.1%)
1	D	0.74	0/3824	0.70	1/5186 (0.0%)
All	All	0.73	0/15296	0.72	9/20744 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	68	LEU	CA-CB-CG	5.84	128.74	115.30
1	C	407	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	258	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	146	PRO	N-CA-C	5.34	126.00	112.10
1	B	156	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	146	PRO	C-N-CA	5.28	134.89	121.70
1	C	100	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	407	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3748	0	3693	24	0
1	B	3748	0	3693	30	0
1	C	3748	0	3693	48	0
1	D	3748	0	3693	36	0
2	A	19	0	10	0	0
2	B	19	0	10	2	0
2	C	19	0	10	0	0
2	D	19	0	10	0	0
3	A	44	0	26	0	0
3	B	44	0	26	0	0
3	C	44	0	26	0	0
3	D	44	0	26	0	0
4	A	195	0	0	2	0
4	B	236	0	0	3	0
4	C	193	0	0	8	0
4	D	220	0	0	3	0
All	All	16088	0	14916	131	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 4.

All (131) 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:483:ASP:HB3	1:C:485:GLU:OE2	1.49	1.10
1:C:145:ASP:OD2	1:C:147:ASP:HB3	1.54	1.06
1:B:130:LEU:HD22	1:B:186:GLU:HG3	1.61	0.81
1:C:146:PRO:HB2	1:C:147:ASP:HB2	1.63	0.81
1:B:68:LEU:HD22	1:B:156:ASP:HB2	1.69	0.74
1:C:146:PRO:CB	1:C:147:ASP:HB2	2.18	0.73
1:A:262:ILE:HD11	4:A:663:HOH:O	1.89	0.71
1:D:39:ALA:HB1	1:D:43:MET:CE	2.21	0.70
1:B:262:ILE:HD11	4:B:713:HOH:O	1.91	0.69
1:D:39:ALA:HB1	1:D:43:MET:HE3	1.71	0.69
1:B:243:ASN:HD21	1:B:253:ASN:HD21	1.42	0.66
1:C:243:ASN:HD21	1:C:253:ASN:HD21	1.43	0.65
1:C:146:PRO:CA	1:C:147:ASP:HB2	2.27	0.64
4:A:587:HOH:O	1:C:259:HIS:HE1	1.80	0.64
1:A:11:LEU:HD11	1:A:132:GLU:HG2	1.81	0.63
1:C:492:HIS:HE1	1:D:244:ASP:OD2	1.82	0.63
1:D:43:MET:HE2	1:D:73:GLN:HG3	1.81	0.63
1:C:260:SER:OG	1:C:416:HIS:HD2	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:SER:HB3	1:D:140:MET:SD	2.42	0.60
1:B:313:GLN:O	1:B:317:GLU:HG2	2.03	0.59
1:C:145:ASP:OD2	1:C:147:ASP:CB	2.43	0.57
1:B:11:LEU:HD11	1:B:132:GLU:HG2	1.85	0.57
1:A:259:HIS:HE1	4:C:727:HOH:O	1.86	0.57
1:B:141:LEU:HD12	1:B:163:LEU:HD23	1.86	0.56
4:B:718:HOH:O	1:D:259:HIS:HE1	1.88	0.56
1:D:243:ASN:HD21	1:D:253:ASN:HD21	1.52	0.56
1:A:252:ASP:OD1	1:A:416:HIS:CE1	2.59	0.56
1:A:252:ASP:OD1	1:A:416:HIS:HE1	1.89	0.55
1:B:11:LEU:HD22	1:B:22:LYS:HE2	1.89	0.55
1:C:450:PRO:HD2	1:C:453:LEU:HD12	1.88	0.55
1:C:78:ILE:HG23	1:C:88:VAL:HG21	1.88	0.54
1:B:141:LEU:CD1	1:B:163:LEU:HD23	2.37	0.54
1:B:95:ILE:HG22	1:B:133:TYR:HB2	1.89	0.54
1:C:23:ILE:HD11	1:C:26:LEU:HD13	1.90	0.54
1:C:468:HIS:HB3	4:C:744:HOH:O	2.07	0.54
1:C:492:HIS:HD2	4:C:783:HOH:O	1.91	0.54
1:D:492:HIS:HD2	4:D:948:HOH:O	1.91	0.54
1:A:218:GLU:O	1:A:248:LYS:HE3	2.08	0.53
1:C:218:GLU:HG2	1:C:428:GLN:HE22	1.74	0.53
1:C:213:LYS:O	1:C:238:PRO:HD2	2.08	0.53
1:B:390:TRP:O	1:B:398:SER:HA	2.09	0.53
1:C:278:VAL:HG11	1:C:294:MET:HG3	1.90	0.53
1:C:163:LEU:HD12	1:C:194:LEU:HD21	1.92	0.52
1:C:145:ASP:HB3	1:C:148:LYS:HB2	1.93	0.51
1:D:213:LYS:HG3	1:D:436:TRP:HZ3	1.75	0.51
1:A:492:HIS:HE1	1:B:244:ASP:OD2	1.94	0.50
1:A:141:LEU:HD12	1:A:163:LEU:HD23	1.92	0.50
1:D:355:HIS:HE1	4:D:892:HOH:O	1.95	0.50
1:C:183:ASP:HB2	1:C:184:PRO:CD	2.43	0.49
1:B:389:LEU:HD13	1:B:400:ILE:HG13	1.95	0.49
1:B:69:HIS:CD2	2:B:500:ARJ:H5A'	2.48	0.48
1:C:459:ARG:NH2	4:C:748:HOH:O	2.45	0.48
1:B:252:ASP:OD1	1:B:416:HIS:HE1	1.97	0.48
1:D:213:LYS:HG3	1:D:436:TRP:CZ3	2.47	0.48
1:D:78:ILE:HG23	1:D:88:VAL:HG21	1.95	0.48
1:C:163:LEU:CD1	1:C:194:LEU:HD21	2.43	0.48
1:D:260:SER:OG	1:D:416:HIS:HD2	1.97	0.48
1:B:402:LEU:HB3	1:B:412:ASN:HD21	1.79	0.48
1:C:65:SER:HB3	1:C:140:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:GLU:CG	1:C:428:GLN:HE22	2.26	0.47
1:B:300:ARG:HD2	1:C:320:ASP:OD1	2.14	0.47
1:C:53:TYR:CD1	1:C:58:PRO:HG3	2.49	0.47
1:C:95:ILE:HG22	1:C:133:TYR:HB2	1.96	0.47
1:B:259:HIS:HE1	4:B:712:HOH:O	1.98	0.47
1:D:260:SER:HB2	1:D:409:ASN:HB2	1.96	0.47
1:A:300:ARG:HD2	1:D:320:ASP:OD1	2.14	0.47
1:A:313:GLN:O	1:A:317:GLU:HG2	2.14	0.47
1:A:340:ASN:HB3	1:A:343:ILE:HD11	1.97	0.47
1:C:146:PRO:N	1:C:147:ASP:HB2	2.30	0.47
1:D:193:LEU:HD23	1:D:193:LEU:C	2.36	0.47
1:B:402:LEU:HB3	1:B:412:ASN:ND2	2.30	0.46
1:A:221:THR:O	1:A:225:ARG:HG3	2.16	0.46
1:D:39:ALA:HB1	1:D:43:MET:HE1	1.96	0.46
1:D:219:THR:O	1:D:223:VAL:HG23	2.16	0.46
1:B:252:ASP:OD1	1:B:416:HIS:CE1	2.69	0.46
1:C:485:GLU:CD	1:C:485:GLU:H	2.19	0.46
1:D:23:ILE:HD11	1:D:26:LEU:HD13	1.98	0.46
1:B:39:ALA:O	1:B:43:MET:HG3	2.15	0.46
1:B:492:HIS:CD2	1:B:492:HIS:H	2.35	0.45
1:A:243:ASN:HD21	1:A:253:ASN:HD21	1.63	0.45
1:C:317:GLU:OE2	1:D:255:TYR:OH	2.30	0.45
1:C:384:LYS:HE3	1:C:387:VAL:HG21	1.98	0.45
1:B:71:THR:HG22	1:B:99:GLN:NE2	2.31	0.45
1:C:492:HIS:CD2	4:C:783:HOH:O	2.67	0.45
1:A:23:ILE:HD11	1:A:26:LEU:HD13	1.98	0.45
1:A:68:LEU:O	1:A:69:HIS:C	2.55	0.45
1:C:141:LEU:HD12	1:C:163:LEU:HD23	1.99	0.45
1:C:406:ARG:NE	4:C:732:HOH:O	2.46	0.44
1:D:206:THR:O	1:D:210:GLU:HG3	2.17	0.44
1:B:313:GLN:O	1:B:317:GLU:CG	2.65	0.44
1:D:218:GLU:HG3	1:D:428:GLN:NE2	2.31	0.44
1:A:213:LYS:O	1:A:238:PRO:HD2	2.17	0.44
1:C:130:LEU:HD22	1:C:186:GLU:HG3	1.99	0.44
1:D:384:LYS:HB2	1:D:385:PRO:CD	2.47	0.44
1:A:95:ILE:HG22	1:A:133:TYR:HB2	2.00	0.44
1:B:192:ASN:OD1	1:B:195:ARG:NH1	2.51	0.44
1:C:469:LEU:HD11	1:D:308:PRO:HB3	2.00	0.44
1:D:69:HIS:CE1	1:D:93:CYS:SG	3.10	0.44
1:A:403:SER:OG	1:A:412:ASN:ND2	2.50	0.44
1:B:78:ILE:HG23	1:B:88:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:O	1:B:225:ARG:HG3	2.18	0.43
1:A:341:LYS:HE3	1:B:475:GLU:HG2	2.00	0.43
1:C:179:ALA:O	1:C:180:GLU:CB	2.66	0.43
1:D:157:GLY:HA3	1:D:363:HIS:NE2	2.33	0.43
1:B:252:ASP:OD2	2:B:500:ARJ:O2'	2.36	0.43
1:D:450:PRO:HD2	1:D:453:LEU:HD12	2.00	0.43
1:D:42:GLU:O	1:D:419:PHE:HA	2.20	0.42
1:C:456:LYS:NZ	4:C:776:HOH:O	2.48	0.42
1:A:235:LEU:O	1:A:444:ASN:HB3	2.19	0.42
1:A:450:PRO:HD2	1:A:453:LEU:HD12	2.01	0.42
1:B:340:ASN:HB3	1:B:343:ILE:HD11	2.01	0.42
1:C:50:ARG:O	1:C:54:ALA:HB2	2.20	0.42
1:A:390:TRP:O	1:A:398:SER:HA	2.20	0.42
1:D:278:VAL:HG11	1:D:294:MET:HG3	2.02	0.42
1:A:250:LYS:NZ	1:A:254:LYS:NZ	2.68	0.41
1:C:146:PRO:HB2	1:C:147:ASP:CB	2.44	0.41
1:C:218:GLU:CG	1:C:428:GLN:NE2	2.83	0.41
1:A:384:LYS:HB2	1:A:385:PRO:HD2	2.03	0.41
1:C:154:LEU:HD11	1:C:428:GLN:HG2	2.02	0.41
1:D:240:ILE:HD12	1:D:435:LEU:HG	2.02	0.41
1:C:406:ARG:NH2	4:C:732:HOH:O	2.51	0.41
1:C:97:SER:HB2	1:C:410:LEU:HB3	2.02	0.41
1:C:11:LEU:HD11	1:C:132:GLU:HG2	2.03	0.41
1:C:402:LEU:HB3	1:C:412:ASN:ND2	2.36	0.41
1:D:227:TYR:HD2	4:D:941:HOH:O	2.03	0.41
1:D:243:ASN:O	1:D:249:SER:HB3	2.21	0.41
1:D:69:HIS:HA	1:D:92:SER:OG	2.21	0.41
1:C:116:GLU:HG3	1:C:116:GLU:O	2.21	0.41
1:D:68:LEU:HD21	1:D:425:PHE:CE1	2.56	0.41
1:D:218:GLU:HG3	1:D:428:GLN:HE22	1.86	0.40
1:D:36:LEU:HD21	1:D:75:ALA:HB1	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	483/495 (98%)	473 (98%)	10 (2%)	0	100	100
1	B	483/495 (98%)	472 (98%)	10 (2%)	1 (0%)	47	44
1	C	483/495 (98%)	465 (96%)	13 (3%)	5 (1%)	15	9
1	D	483/495 (98%)	471 (98%)	12 (2%)	0	100	100
All	All	1932/1980 (98%)	1881 (97%)	45 (2%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	147	ASP
1	B	69	HIS
1	C	180	GLU
1	C	69	HIS
1	C	183	ASP
1	C	146	PRO

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	395/404 (98%)	387 (98%)	8 (2%)	55	58
1	B	395/404 (98%)	389 (98%)	6 (2%)	65	69
1	C	395/404 (98%)	391 (99%)	4 (1%)	76	81
1	D	395/404 (98%)	387 (98%)	8 (2%)	55	58
All	All	1580/1616 (98%)	1554 (98%)	26 (2%)	62	67

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	181	GLU

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	219	THR
1	A	253	ASN
1	A	304	THR
1	A	407	LEU
1	A	428	GLN
1	B	68	LEU
1	B	88	VAL
1	B	180	GLU
1	B	219	THR
1	B	237	PHE
1	B	407	LEU
1	C	147	ASP
1	C	220	THR
1	C	407	LEU
1	C	428	GLN
1	D	11	LEU
1	D	16	ARG
1	D	26	LEU
1	D	220	THR
1	D	237	PHE
1	D	407	LEU
1	D	428	GLN
1	D	440	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	243	ASN
1	A	259	HIS
1	A	310	ASN
1	A	412	ASN
1	A	416	HIS
1	A	492	HIS
1	B	57	GLN
1	B	243	ASN
1	B	259	HIS
1	B	310	ASN
1	B	355	HIS
1	B	412	ASN
1	B	416	HIS

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Mol	Chain	Res	Type
1	B	492	HIS
1	C	57	GLN
1	C	243	ASN
1	C	259	HIS
1	C	310	ASN
1	C	355	HIS
1	C	412	ASN
1	C	416	HIS
1	C	428	GLN
1	C	492	HIS
1	D	57	GLN
1	D	243	ASN
1	D	259	HIS
1	D	310	ASN
1	D	355	HIS
1	D	412	ASN
1	D	416	HIS
1	D	427	ASN
1	D	428	GLN
1	D	492	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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
2	ARJ	C	500	-	16,21,21	2.94	2 (12%)	12,31,31	2.59	4 (33%)
2	ARJ	A	500	-	16,21,21	3.00	2 (12%)	12,31,31	2.73	4 (33%)
2	ARJ	B	500	-	16,21,21	2.96	2 (12%)	12,31,31	2.46	4 (33%)
3	NAD	A	550	-	42,48,48	1.39	5 (11%)	50,73,73	1.82	11 (22%)
2	ARJ	D	500	-	16,21,21	2.95	3 (18%)	12,31,31	2.51	3 (25%)
3	NAD	B	550	-	42,48,48	1.56	6 (14%)	50,73,73	1.77	11 (22%)
3	NAD	D	550	-	42,48,48	1.54	6 (14%)	50,73,73	1.75	7 (14%)
3	NAD	C	550	-	42,48,48	1.48	4 (9%)	50,73,73	1.53	11 (22%)

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	ARJ	C	500	-	2/2/4/4	1/2/22/22	0/3/3/3
2	ARJ	A	500	-	2/2/4/4	1/2/22/22	0/3/3/3
2	ARJ	B	500	-	2/2/4/4	1/2/22/22	0/3/3/3
3	NAD	A	550	-	-	5/26/62/62	0/5/5/5
2	ARJ	D	500	-	2/2/4/4	1/2/22/22	0/3/3/3
3	NAD	B	550	-	-	5/26/62/62	0/5/5/5
3	NAD	D	550	-	-	5/26/62/62	0/5/5/5
3	NAD	C	550	-	-	5/26/62/62	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	ARJ	C4'-C3D	-10.56	1.34	1.51
2	B	500	ARJ	C4'-C3D	-10.15	1.34	1.51
2	D	500	ARJ	C4'-C3D	-9.76	1.35	1.51
2	C	500	ARJ	C4'-C3D	-9.64	1.35	1.51
3	C	550	NAD	O7N-C7N	5.99	1.35	1.24
2	D	500	ARJ	O2'-C2'	-5.17	1.31	1.42
2	C	500	ARJ	O2'-C2'	-5.13	1.31	1.42
3	B	550	NAD	O4D-C1D	4.91	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	550	NAD	O4D-C1D	4.85	1.47	1.41
3	D	550	NAD	O7N-C7N	4.70	1.33	1.24
2	B	500	ARJ	O2'-C2'	-4.64	1.32	1.42
2	A	500	ARJ	O2'-C2'	-4.63	1.32	1.42
3	A	550	NAD	O7N-C7N	4.52	1.32	1.24
3	B	550	NAD	O7N-C7N	4.18	1.32	1.24
3	B	550	NAD	C7N-N7N	-3.98	1.25	1.33
3	A	550	NAD	O4D-C1D	3.50	1.46	1.41
3	C	550	NAD	O4D-C1D	3.39	1.45	1.41
3	A	550	NAD	C7N-N7N	-3.33	1.26	1.33
3	D	550	NAD	C3N-C7N	3.32	1.55	1.50
3	C	550	NAD	C5A-C4A	3.32	1.49	1.40
3	A	550	NAD	C5A-C4A	2.92	1.48	1.40
3	B	550	NAD	O3B-C3B	2.75	1.49	1.43
3	B	550	NAD	C5A-C4A	2.64	1.47	1.40
3	D	550	NAD	O3D-C3D	2.61	1.49	1.43
3	D	550	NAD	C5A-C4A	2.53	1.47	1.40
3	B	550	NAD	O2B-C2B	2.39	1.48	1.43
2	D	500	ARJ	O3D-C3D	2.22	1.25	1.21
3	A	550	NAD	O2B-C2B	2.16	1.48	1.43
3	C	550	NAD	C4A-N3A	2.08	1.38	1.35
3	D	550	NAD	C2A-N3A	2.04	1.35	1.32

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	550	NAD	C3N-C7N-N7N	6.63	125.70	117.75
2	C	500	ARJ	C5'-C4'-C3D	6.34	112.43	102.33
3	A	550	NAD	N3A-C2A-N1A	-6.10	119.14	128.68
2	D	500	ARJ	C5'-C4'-C3D	6.07	111.99	102.33
2	A	500	ARJ	C5'-C4'-C3D	5.56	111.19	102.33
2	A	500	ARJ	N3-C2-N1	-5.37	120.29	128.68
3	B	550	NAD	O4D-C1D-C2D	-5.10	99.47	106.93
2	B	500	ARJ	N3-C2-N1	-5.03	120.81	128.68
2	B	500	ARJ	C5'-C4'-C3D	5.02	110.32	102.33
2	D	500	ARJ	N3-C2-N1	-4.65	121.41	128.68
3	D	550	NAD	O7N-C7N-N7N	-4.38	116.35	122.58
3	B	550	NAD	C5A-C6A-N6A	4.37	126.99	120.35
3	D	550	NAD	N3A-C2A-N1A	-4.35	121.87	128.68
3	A	550	NAD	O4D-C1D-C2D	-4.28	100.67	106.93
2	C	500	ARJ	N3-C2-N1	-4.09	122.29	128.68
3	C	550	NAD	O4D-C1D-C2D	-3.81	101.36	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	550	NAD	O3D-C3D-C4D	-3.57	100.72	111.05
3	A	550	NAD	C5N-C4N-C3N	-3.51	116.19	120.34
3	A	550	NAD	C6N-N1N-C2N	-3.42	118.86	121.97
3	B	550	NAD	C3N-C7N-N7N	3.36	121.79	117.75
3	C	550	NAD	N3A-C2A-N1A	-3.36	123.42	128.68
2	A	500	ARJ	C5'-C1'-N9	-3.33	108.93	113.39
3	B	550	NAD	C2A-N1A-C6A	3.27	124.34	118.75
3	B	550	NAD	N3A-C2A-N1A	-3.21	123.66	128.68
3	A	550	NAD	C2A-N1A-C6A	3.18	124.20	118.75
3	C	550	NAD	C3N-C2N-N1N	3.17	123.52	120.43
3	B	550	NAD	C6N-N1N-C2N	-3.06	119.19	121.97
3	C	550	NAD	O4B-C1B-C2B	-2.99	102.56	106.93
2	C	500	ARJ	C5'-C1'-N9	-2.97	109.42	113.39
3	A	550	NAD	C3N-C7N-N7N	2.93	121.27	117.75
3	A	550	NAD	C1B-N9A-C4A	-2.91	121.52	126.64
3	D	550	NAD	O4D-C1D-C2D	-2.91	102.68	106.93
3	A	550	NAD	C3N-C2N-N1N	2.91	123.27	120.43
3	C	550	NAD	C2A-N1A-C6A	2.90	123.71	118.75
2	B	500	ARJ	C2-N1-C6	2.86	123.64	118.75
3	D	550	NAD	C3N-C2N-N1N	2.72	123.08	120.43
3	D	550	NAD	C4A-C5A-N7A	-2.62	106.67	109.40
3	D	550	NAD	C2A-N1A-C6A	2.61	123.22	118.75
2	A	500	ARJ	N6-C6-N1	2.57	123.91	118.57
3	B	550	NAD	C3D-C2D-C1D	2.46	104.68	100.98
3	B	550	NAD	O7N-C7N-N7N	-2.45	119.10	122.58
3	A	550	NAD	PN-O3-PA	-2.37	124.70	132.83
2	D	500	ARJ	C5'-C1'-N9	-2.36	110.23	113.39
3	C	550	NAD	O3D-C3D-C4D	-2.31	104.38	111.05
3	C	550	NAD	PN-O3-PA	-2.28	125.00	132.83
3	B	550	NAD	C1B-N9A-C4A	-2.25	122.68	126.64
2	B	500	ARJ	N6-C6-N1	2.25	123.25	118.57
2	C	500	ARJ	C2-N1-C6	2.22	122.55	118.75
3	A	550	NAD	O7N-C7N-N7N	-2.19	119.47	122.58
3	A	550	NAD	C3D-C2D-C1D	2.18	104.26	100.98
3	C	550	NAD	O7N-C7N-N7N	-2.16	119.51	122.58
3	C	550	NAD	O2A-PA-O1A	2.15	122.88	112.24
3	C	550	NAD	C3N-C7N-N7N	2.07	120.23	117.75
3	C	550	NAD	C5N-C4N-C3N	-2.06	117.91	120.34
3	B	550	NAD	C5N-C6N-N1N	2.03	123.32	120.40

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	500	ARJ	C2'
2	C	500	ARJ	C4'
2	A	500	ARJ	C2'
2	A	500	ARJ	C4'
2	B	500	ARJ	C2'
2	B	500	ARJ	C4'
2	D	500	ARJ	C2'
2	D	500	ARJ	C4'

All (24) torsion outliers are listed below:

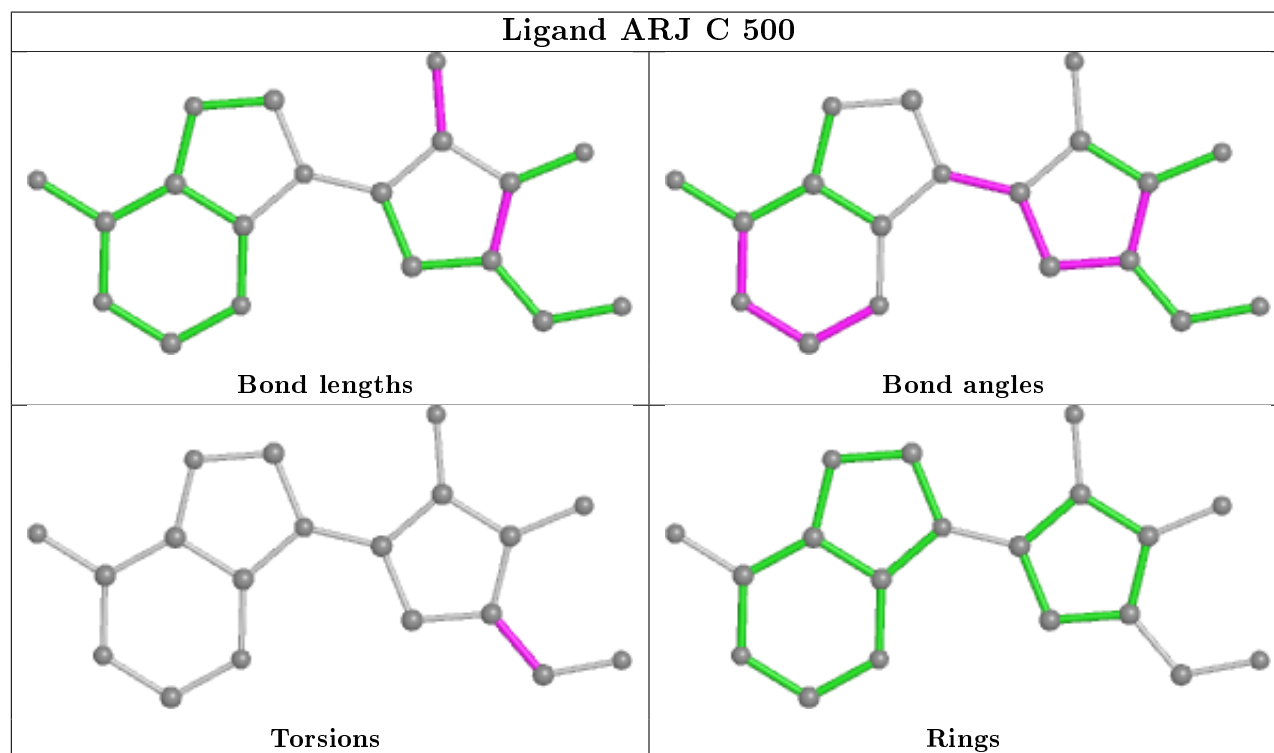
Mol	Chain	Res	Type	Atoms
2	C	500	ARJ	C3D-C4'-C6'-O6'
2	A	500	ARJ	C3D-C4'-C6'-O6'
2	B	500	ARJ	C3D-C4'-C6'-O6'
3	A	550	NAD	O4D-C1D-N1N-C2N
3	A	550	NAD	O4D-C1D-N1N-C6N
3	A	550	NAD	C2D-C1D-N1N-C2N
3	A	550	NAD	C2D-C1D-N1N-C6N
2	D	500	ARJ	C3D-C4'-C6'-O6'
3	B	550	NAD	O4D-C1D-N1N-C2N
3	B	550	NAD	O4D-C1D-N1N-C6N
3	B	550	NAD	C2D-C1D-N1N-C2N
3	B	550	NAD	C2D-C1D-N1N-C6N
3	D	550	NAD	O4D-C1D-N1N-C2N
3	D	550	NAD	O4D-C1D-N1N-C6N
3	D	550	NAD	C2D-C1D-N1N-C2N
3	D	550	NAD	C2D-C1D-N1N-C6N
3	C	550	NAD	O4D-C1D-N1N-C2N
3	C	550	NAD	O4D-C1D-N1N-C6N
3	C	550	NAD	C2D-C1D-N1N-C2N
3	C	550	NAD	C2D-C1D-N1N-C6N
3	A	550	NAD	O4B-C4B-C5B-O5B
3	D	550	NAD	O4B-C4B-C5B-O5B
3	C	550	NAD	O4B-C4B-C5B-O5B
3	B	550	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

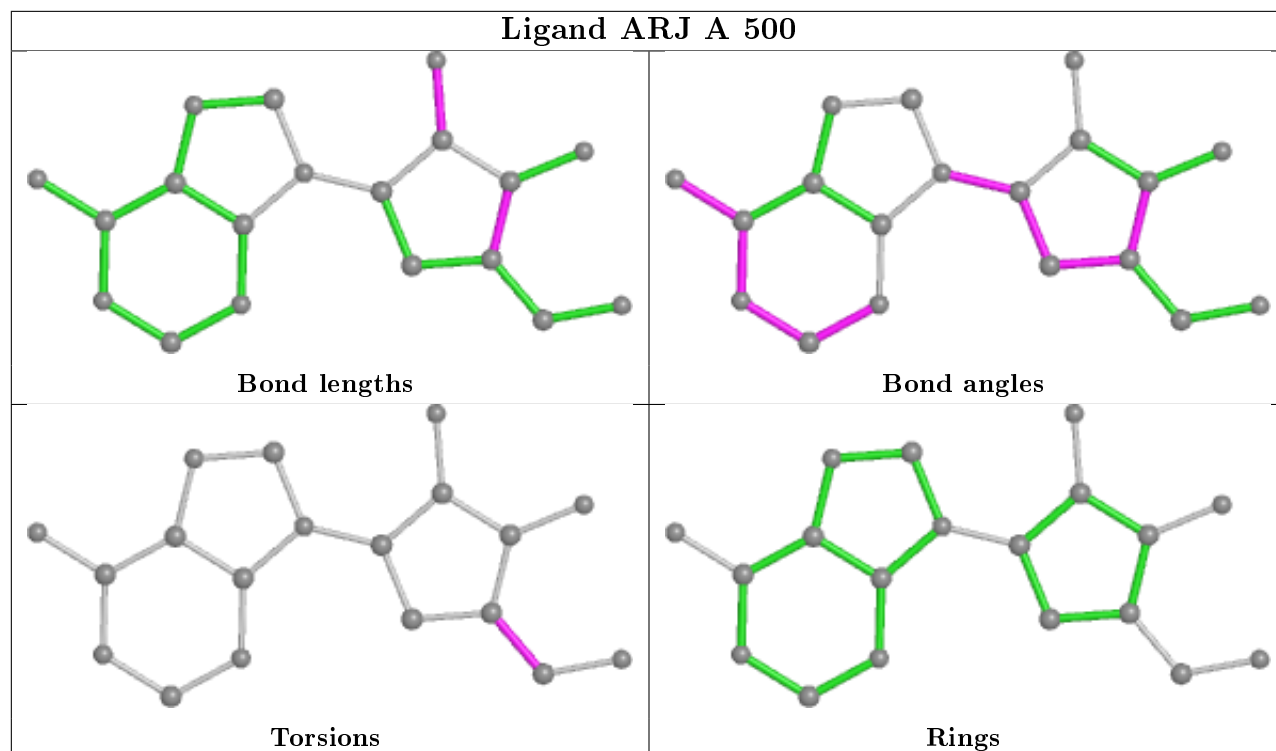
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	ARJ	2	0

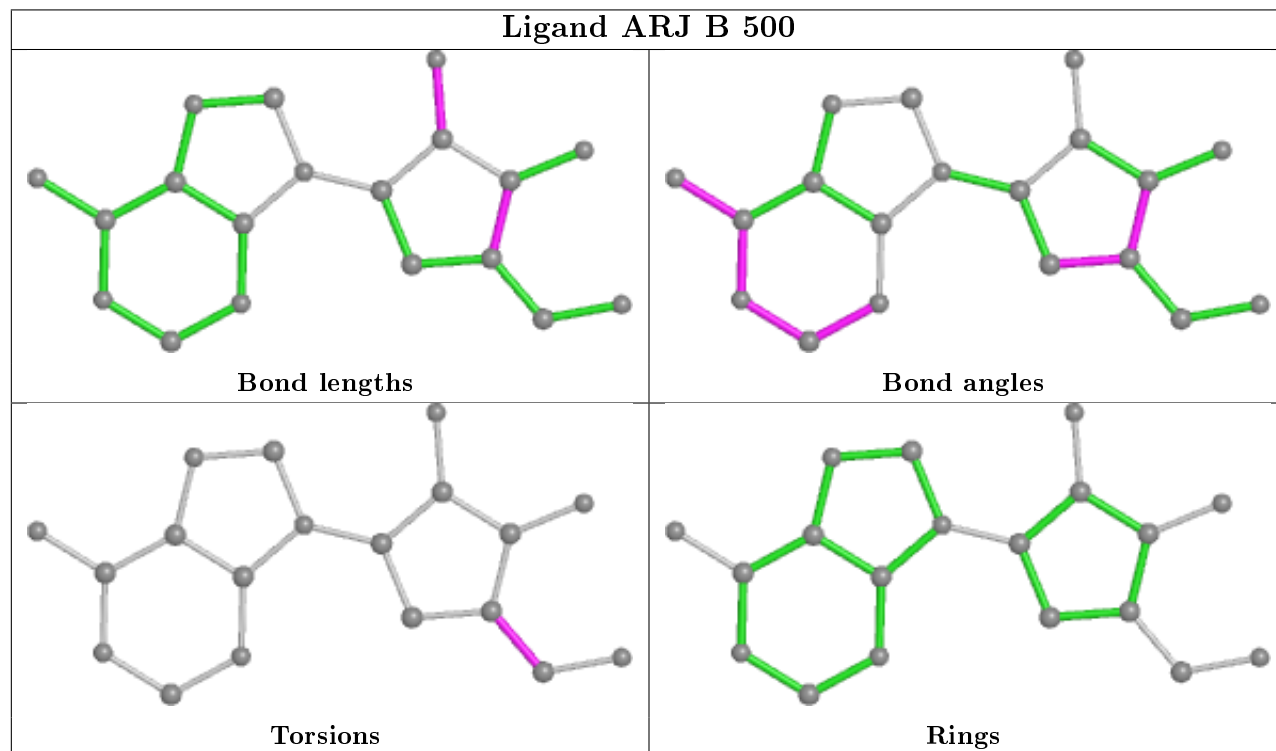
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

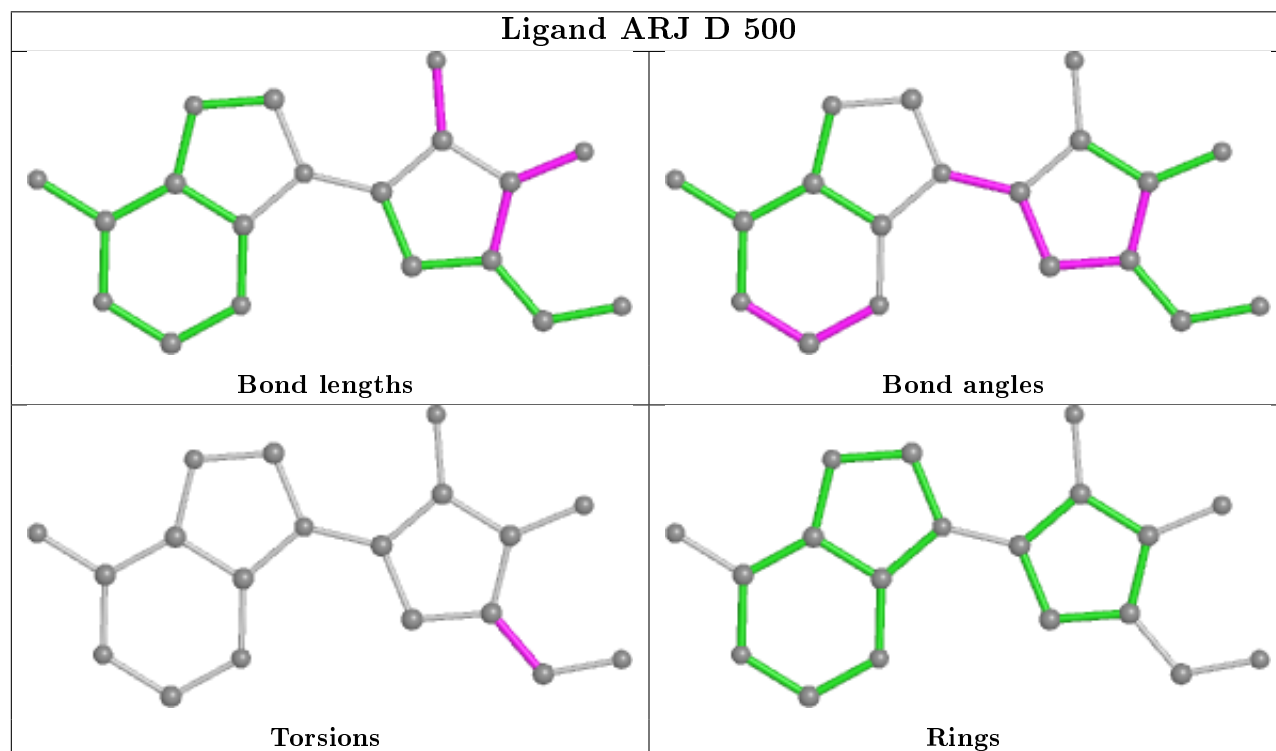
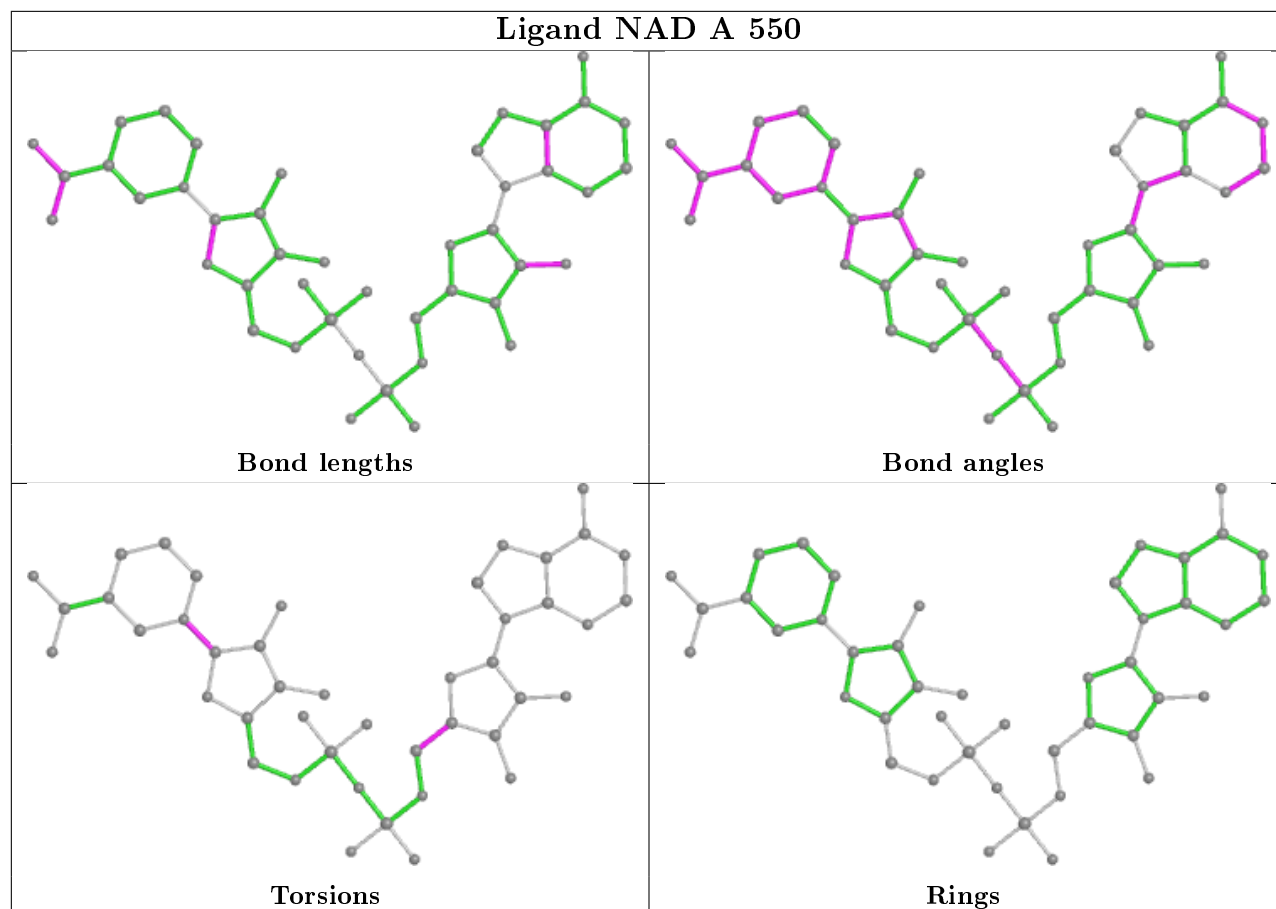


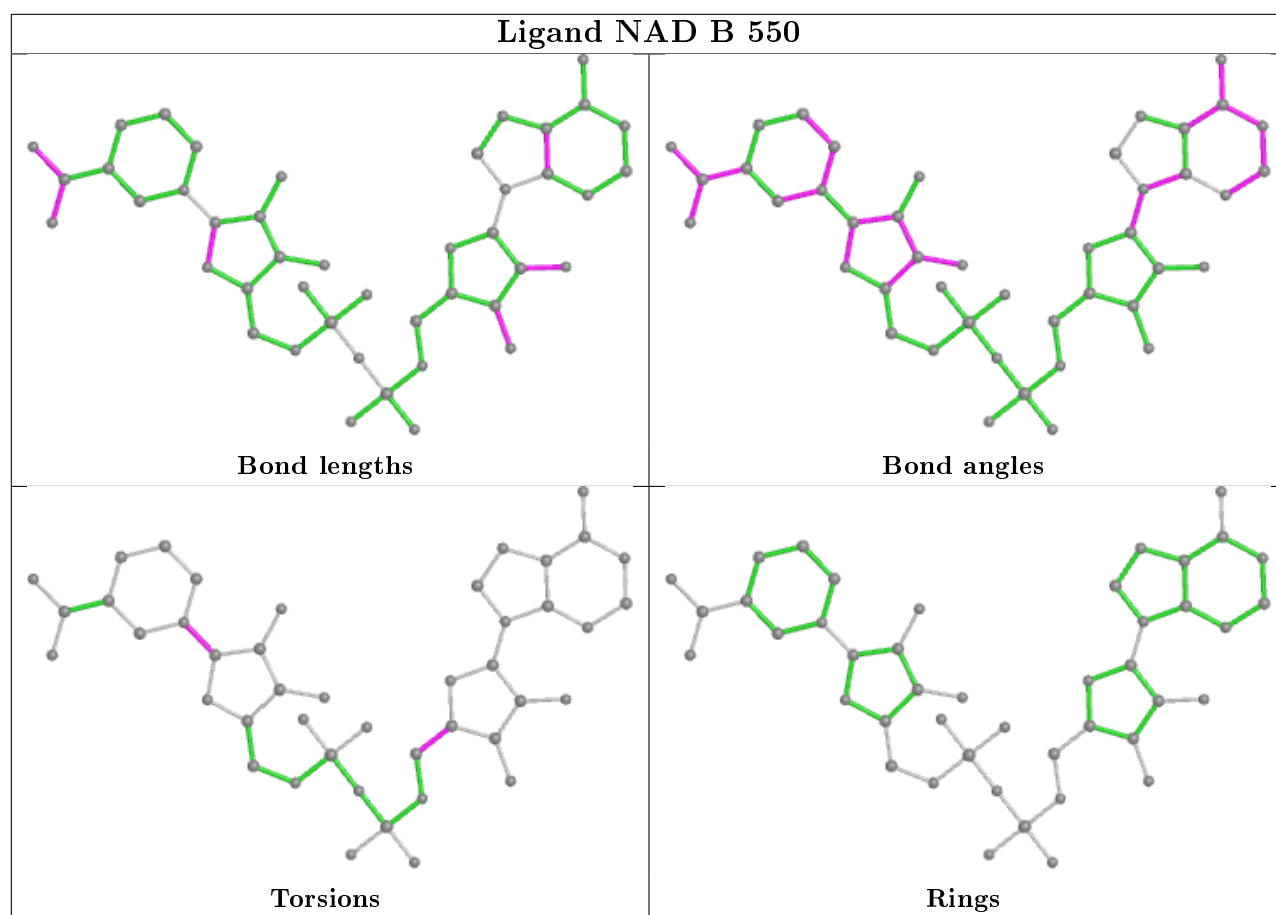
Ligand ARJ A 500

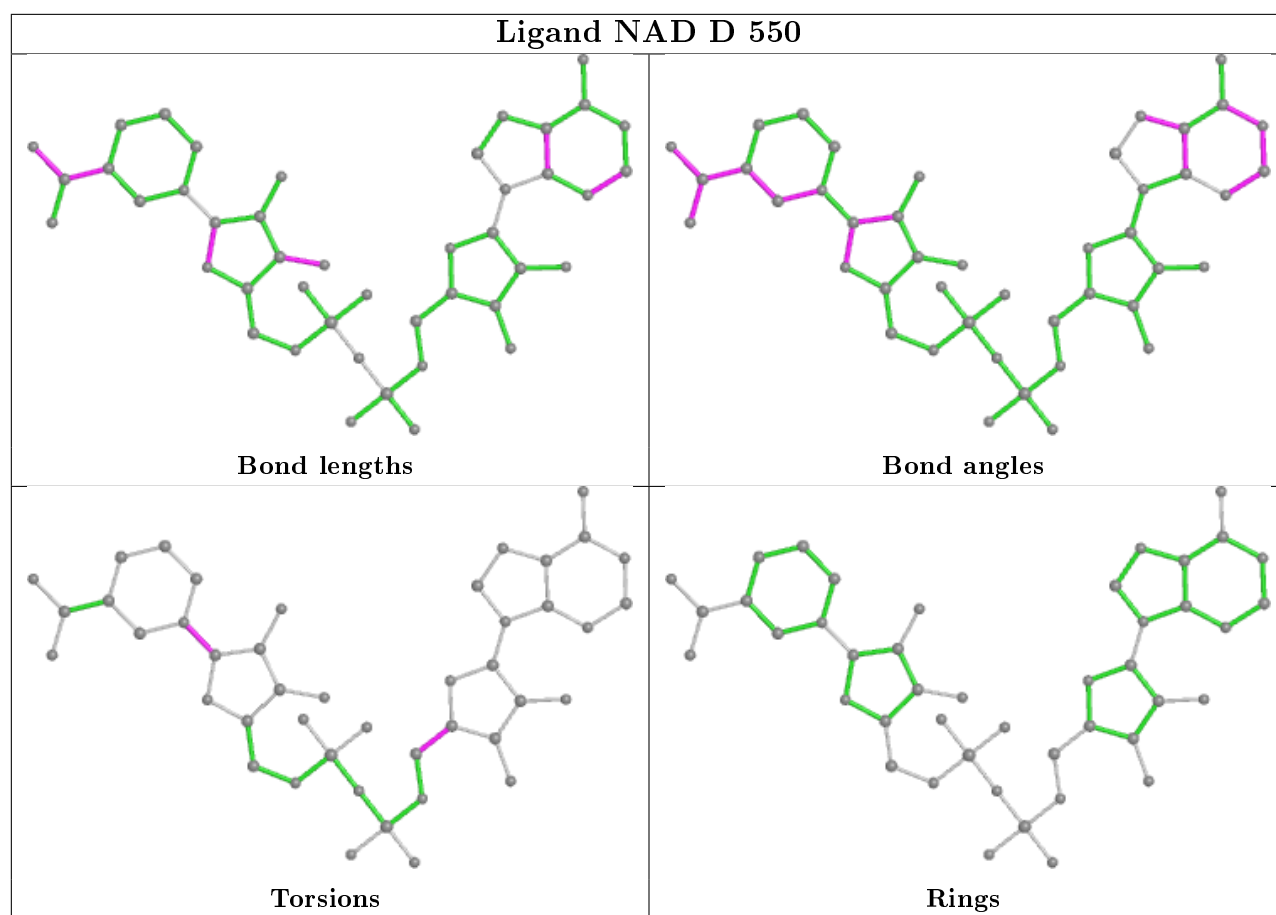


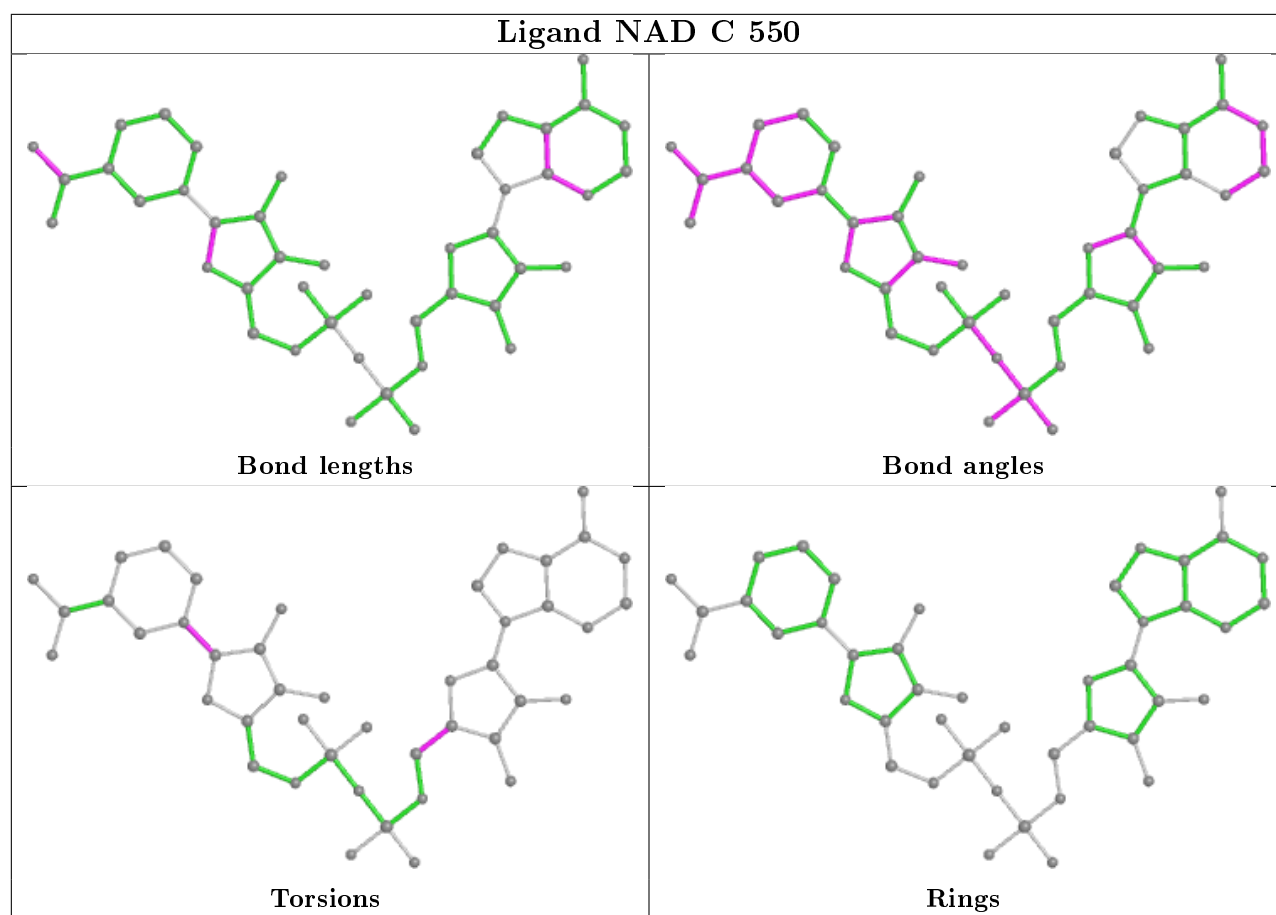
Ligand ARJ B 500











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	485/495 (97%)	-0.03	15 (3%) 49 48	14, 25, 44, 72	0
1	B	485/495 (97%)	-0.09	4 (0%) 86 85	12, 22, 41, 64	0
1	C	485/495 (97%)	0.27	35 (7%) 15 14	12, 28, 56, 101	0
1	D	485/495 (97%)	0.01	16 (3%) 46 45	12, 24, 47, 81	0
All	All	1940/1980 (97%)	0.04	70 (3%) 42 42	12, 24, 49, 101	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	181	GLU	7.3
1	D	182	ASP	5.7
1	A	440	ASP	5.2
1	D	181	GLU	4.7
1	C	180	GLU	4.6
1	C	179	ALA	4.6
1	C	56	VAL	4.5
1	C	177	PRO	4.4
1	C	440	ASP	4.4
1	C	144	PRO	3.8
1	C	182	ASP	3.8
1	C	175	VAL	3.7
1	C	174	GLY	3.6
1	C	114	PRO	3.5
1	C	68	LEU	3.5
1	D	56	VAL	3.5
1	C	198	PHE	3.4
1	D	198	PHE	3.4
1	C	442	TYR	3.1
1	A	177	PRO	3.1
1	D	147	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLU	3.0
1	A	200	THR	2.9
1	C	425	PHE	2.9
1	D	177	PRO	2.9
1	C	74	THR	2.9
1	C	219	THR	2.9
1	C	172	LYS	2.9
1	D	55	GLU	2.9
1	A	231	ALA	2.8
1	D	114	PRO	2.8
1	C	170	TYR	2.6
1	C	117	PRO	2.6
1	D	115	ASP	2.6
1	A	173	ALA	2.6
1	C	178	PRO	2.6
1	C	232	ALA	2.5
1	C	199	GLU	2.5
1	D	180	GLU	2.5
1	A	198	PHE	2.5
1	B	154	LEU	2.5
1	D	154	LEU	2.5
1	A	227	TYR	2.4
1	C	19	ILE	2.4
1	C	191	LEU	2.4
1	C	115	ASP	2.4
1	C	147	ASP	2.4
1	A	180	GLU	2.3
1	C	183	ASP	2.3
1	A	53	TYR	2.3
1	C	11	LEU	2.3
1	D	116	GLU	2.3
1	C	173	ALA	2.2
1	D	173	ALA	2.2
1	A	170	TYR	2.2
1	C	149	PRO	2.2
1	C	146	PRO	2.2
1	B	445	GLU	2.2
1	A	60	LYS	2.2
1	B	440	ASP	2.1
1	C	233	GLY	2.1
1	C	443	ASP	2.1
1	C	200	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	11	LEU	2.1
1	D	199	GLU	2.0
1	A	182	ASP	2.0
1	D	176	VAL	2.0
1	A	172	LYS	2.0
1	B	170	TYR	2.0
1	D	12	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

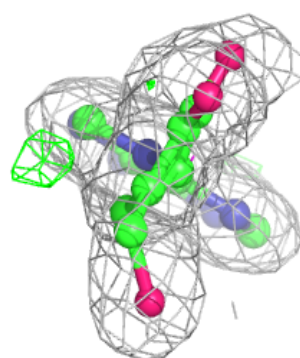
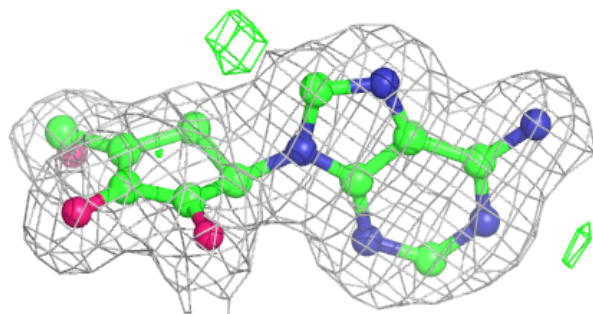
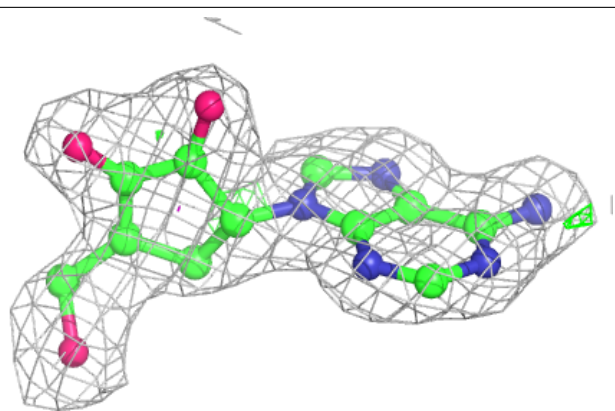
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ARJ	C	500	19/19	0.95	0.19	14,21,33,34	0
2	ARJ	A	500	19/19	0.95	0.15	13,20,31,31	0
2	ARJ	B	500	19/19	0.95	0.17	11,17,27,31	0
2	ARJ	D	500	19/19	0.95	0.16	14,19,29,32	0
3	NAD	C	550	44/44	0.95	0.11	12,19,23,24	0
3	NAD	D	550	44/44	0.96	0.10	12,17,21,23	0
3	NAD	A	550	44/44	0.96	0.10	15,20,23,26	0
3	NAD	B	550	44/44	0.97	0.09	9,17,19,23	0

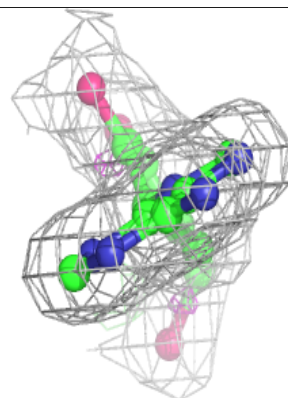
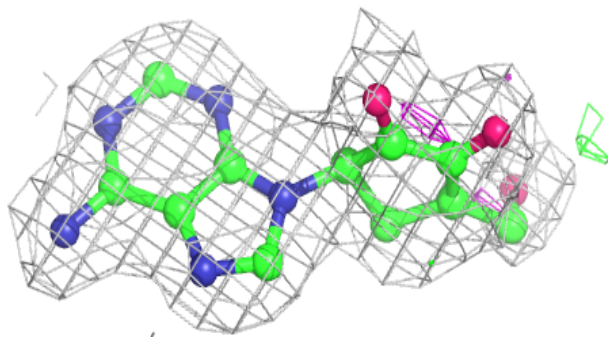
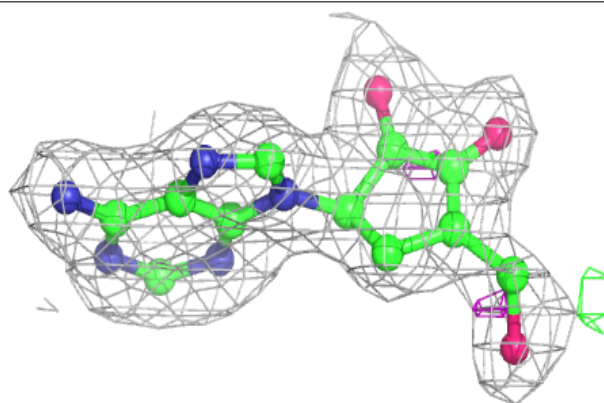
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ARJ C 500:

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

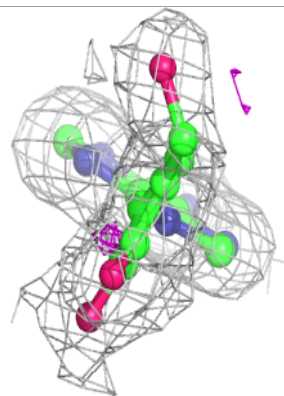
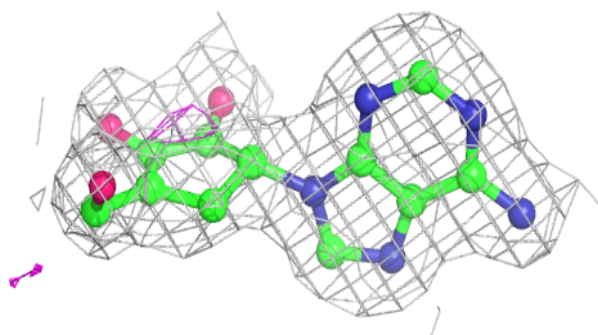
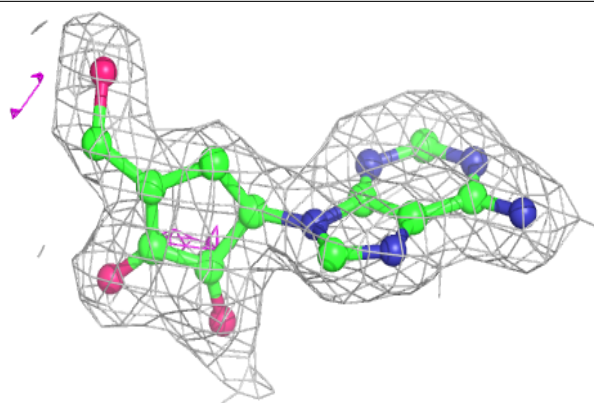
**Electron density around ARJ A 500:**

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

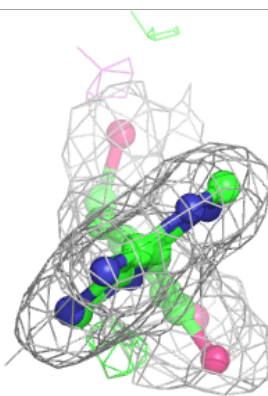
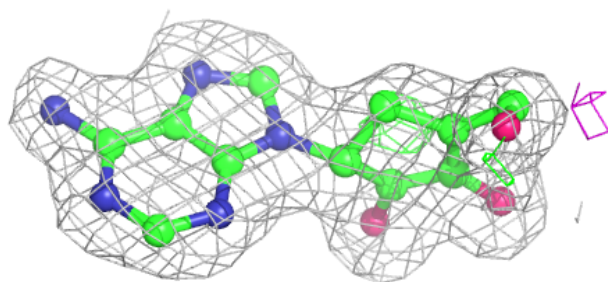
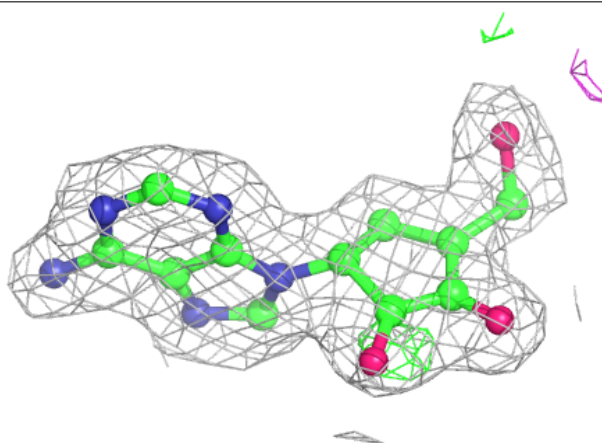


Electron density around ARJ B 500:

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

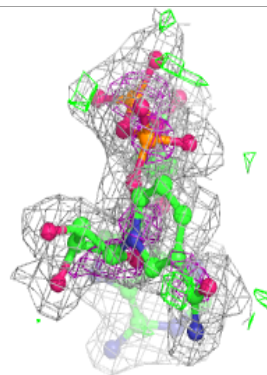
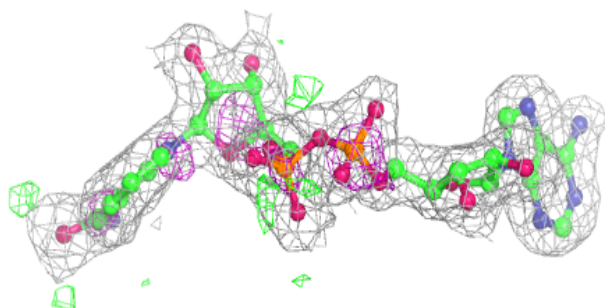
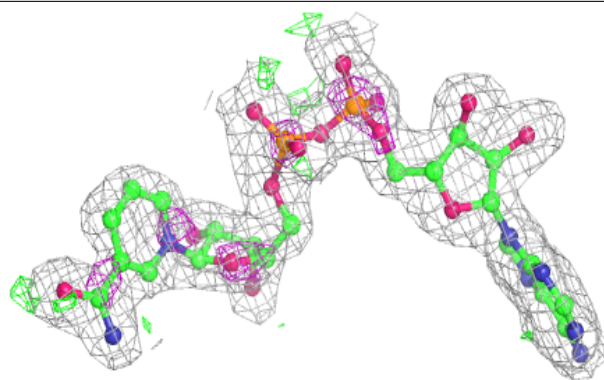
**Electron density around ARJ D 500:**

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

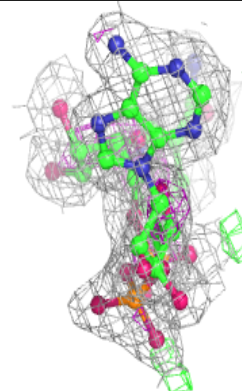
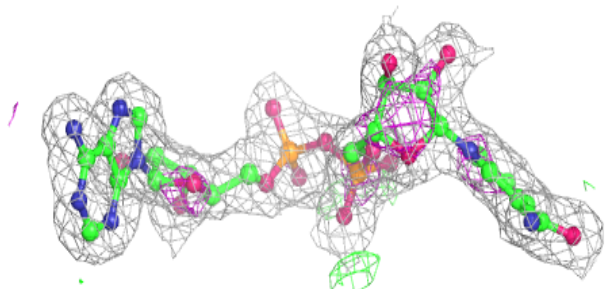
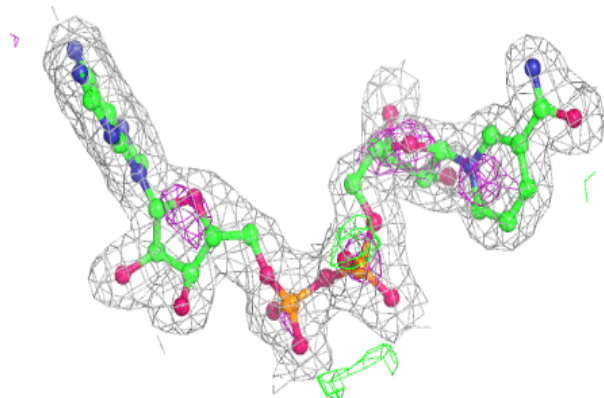


Electron density around NAD C 550:

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

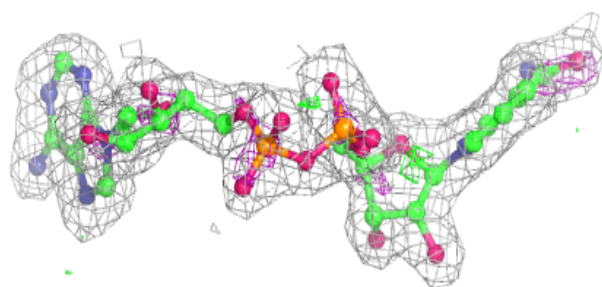
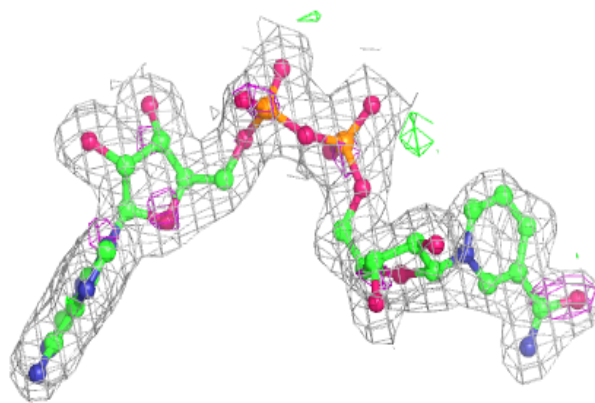
**Electron density around NAD D 550:**

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

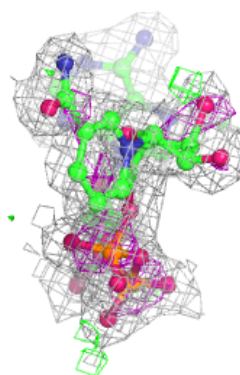
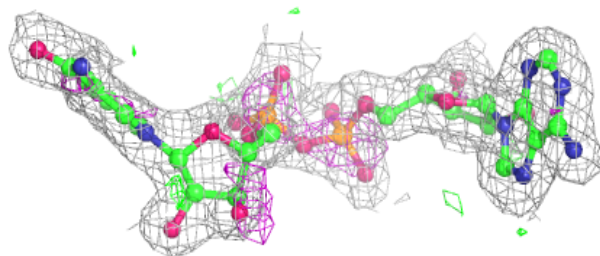
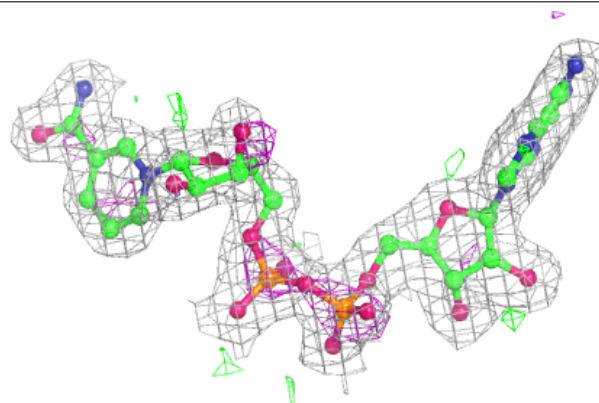


Electron density around NAD A 550:

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

**Electron density around NAD B 550:**

$2mF_o-DF_c$ (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.