



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:16 PM EDT

PDB ID : 3B6J / pdb_00003b6j
Title : WrbA from Escherichia coli, NADH complex
Authors : Andrade, S.L.A.; Patridge, E.V.; Ferry, J.G.; Einsle, O.
Deposited on : 2007-10-29
Resolution : 2.05 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

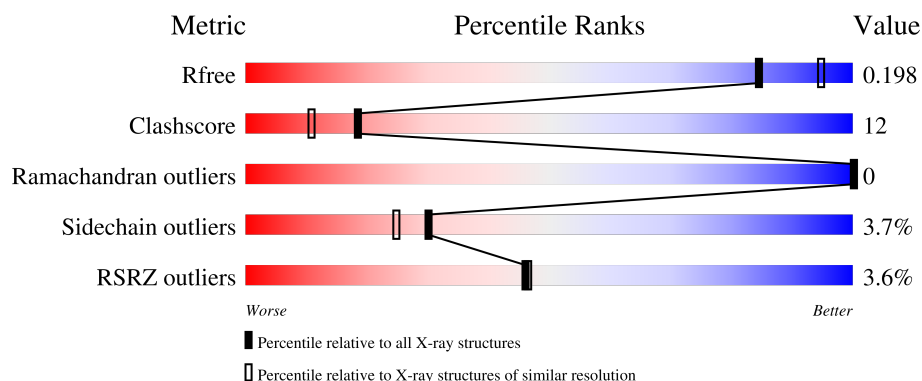
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	198	7% 84% 14% ...
1	B	198	86% 11% ..

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
4	15P	A	202	-	X	-	-
4	15P	B	203	-	X	-	-

2 Entry composition [i](#)

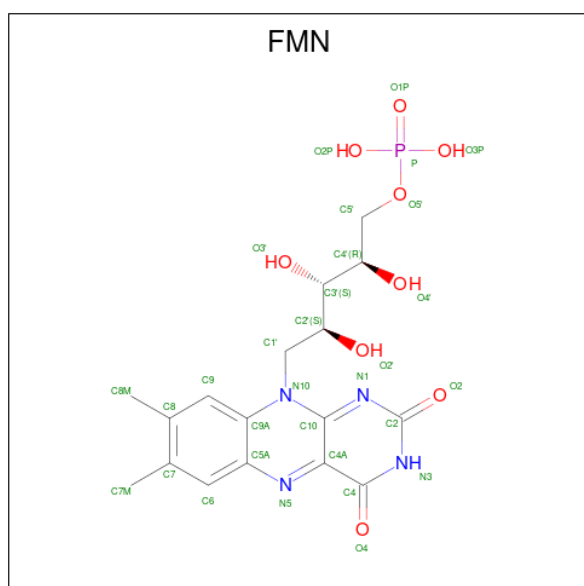
There are 6 unique types of molecules in this entry. The entry contains 3609 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Flavoprotein wrbA.

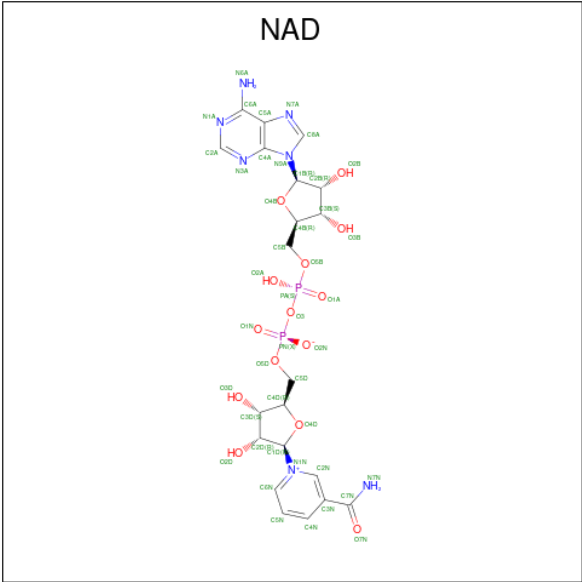
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	11	0
			1512	960	252	293	7			
1	B	197	Total	C	N	O	S	0	3	0
			1472	928	248	289	7			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



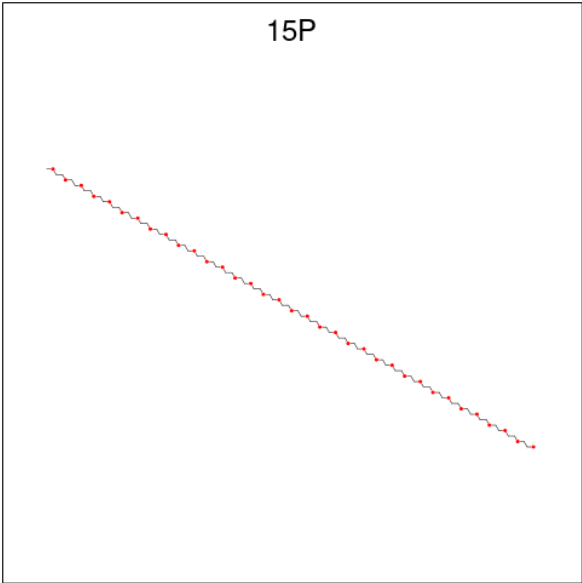
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: 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		

- Molecule 4 is POLYETHYLENE GLYCOL (N=34) (CCD ID: 15P) (formula: C₆₉H₁₄₀O₃₅).



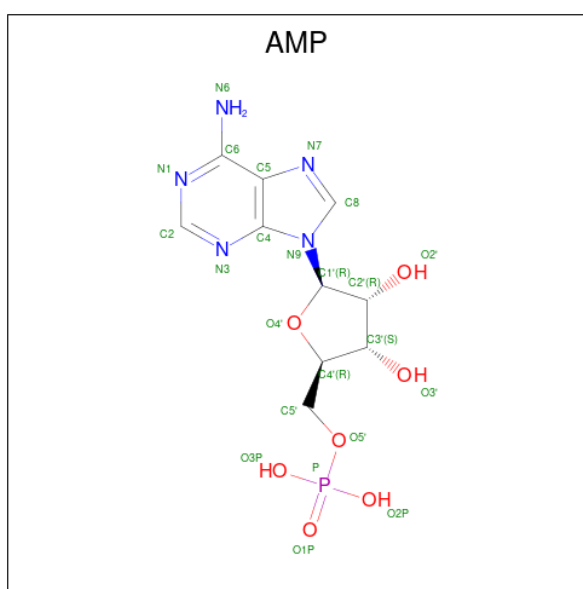
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	7	4		
4	A	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	13	7		
4	B	1	Total	C	O	0	0
			11	7	4		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			20	13	7		

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

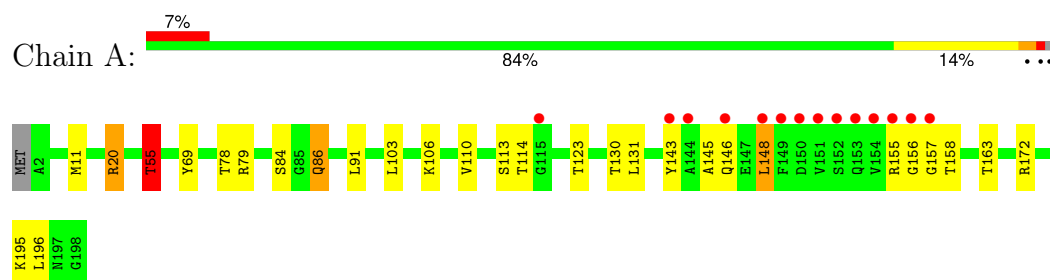
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	174	Total	O	0	0
			174	174		
6	B	187	Total	O	0	0
			187	187		

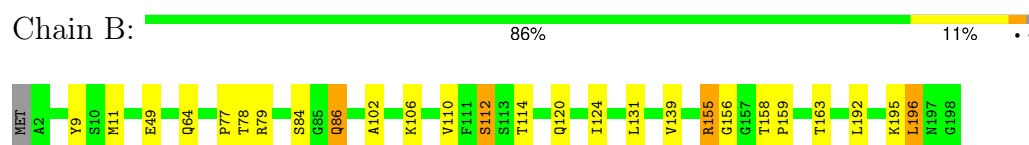
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Flavoprotein wrbA



• Molecule 1: Flavoprotein wrbA



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.20Å 94.20Å 173.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 2.05 49.32 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.32-2.05) 96.7 (49.32-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.168 , 0.199 0.167 , 0.198	Depositor DCC
R_{free} test set	2441 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3609	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 15P, AMP, FMN, 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	1.01	2/1575 (0.1%)	0.96	0/2134
1	B	1.01	1/1508 (0.1%)	0.98	2/2045 (0.1%)
All	All	1.01	3/3083 (0.1%)	0.97	2/4179 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	VAL	CA-CB	6.58	1.60	1.54
1	A	55	THR	CA-CB	6.15	1.62	1.53
1	A	110	VAL	CA-CB	5.07	1.62	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112[A]	SER	N-CA-C	5.08	116.53	108.96
1	B	112[B]	SER	N-CA-C	5.08	116.53	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1512	0	1524	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1472	0	1449	31	0
2	A	31	0	19	3	0
2	B	31	0	19	3	0
3	A	44	0	26	2	0
3	B	44	0	26	1	0
4	A	47	0	57	11	0
4	B	44	0	53	13	0
5	B	23	0	12	0	0
6	A	174	0	0	11	1
6	B	187	0	0	6	1
All	All	3609	0	3185	77	1

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 12.

All (77) 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:B:195:LYS:HZ2	4:B:205:15P:H18	1.19	1.03
1:A:20[B]:ARG:HG3	1:A:20[B]:ARG:HH11	1.17	1.03
4:B:203:15P:H14	6:B:381:HOH:O	1.68	0.92
4:A:202:15P:H26	6:A:351:HOH:O	1.70	0.92
1:B:86:GLN:H	1:B:86:GLN:HE21	1.19	0.91
1:A:20[B]:ARG:HG3	1:A:20[B]:ARG:NH1	1.79	0.86
1:B:195:LYS:NZ	4:B:205:15P:H16	1.96	0.80
1:B:195:LYS:HZ2	4:B:205:15P:H16	1.47	0.80
1:A:86:GLN:HE21	1:A:86:GLN:H	1.31	0.79
1:A:195:LYS:HE3	4:A:204:15P:H23	1.66	0.78
1:A:20[B]:ARG:HH11	1:A:20[B]:ARG:CG	1.98	0.77
1:A:78[B]:THR:CG2	1:A:114:THR:HG22	2.16	0.75
1:A:195:LYS:HZ2	4:A:204:15P:H19	1.51	0.74
1:A:78[A]:THR:CG2	1:A:114:THR:HG22	2.19	0.71
1:A:11[B]:MET:HE1	6:A:259:HOH:O	1.94	0.67
1:A:78[A]:THR:HG21	1:A:114:THR:HG22	1.76	0.67
1:A:195:LYS:NZ	4:A:204:15P:H19	2.10	0.67
1:B:195:LYS:NZ	4:B:205:15P:H18	2.05	0.66
1:B:11[B]:MET:CE	6:B:257:HOH:O	2.44	0.65
1:B:86:GLN:H	1:B:86:GLN:NE2	1.90	0.65
4:A:204:15P:H29	1:B:196:LEU:HD22	1.77	0.64
1:B:11[B]:MET:HE3	6:B:271:HOH:O	1.97	0.64
1:A:11[B]:MET:HE3	6:A:258:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11[B]:MET:CE	6:A:259:HOH:O	2.45	0.64
1:A:78[B]:THR:HG21	1:A:114:THR:HG22	1.80	0.63
1:A:86:GLN:H	1:A:86:GLN:NE2	1.98	0.62
1:A:69:TYR:O	1:A:106:LYS:HE3	2.00	0.62
1:A:146[B]:GLN:H	1:A:146[B]:GLN:CD	2.06	0.62
1:A:155:ARG:HD2	1:A:156:GLY:O	2.01	0.61
1:B:192:LEU:HD13	4:B:205:15P:H26	1.83	0.60
1:B:155:ARG:HB3	6:B:249:HOH:O	2.02	0.59
1:B:11[B]:MET:HE1	6:B:257:HOH:O	2.04	0.58
1:B:11[B]:MET:HE2	6:B:257:HOH:O	2.04	0.57
1:A:183:ARG:NH1	6:A:380:HOH:O	2.38	0.56
1:B:112[A]:SER:O	1:B:163:THR:HA	2.05	0.56
1:A:172:ARG:HD2	6:A:239:HOH:O	2.05	0.55
3:A:201:NAD:H4N	6:A:358:HOH:O	2.06	0.55
1:B:195:LYS:NZ	4:B:205:15P:H102	2.22	0.54
1:A:78[B]:THR:HG23	1:A:113:SER:O	2.06	0.54
1:A:78[B]:THR:HG23	1:A:114:THR:HG22	1.89	0.53
1:A:158:THR:HA	6:A:308:HOH:O	2.09	0.52
2:A:200:FMN:N3	4:A:202:15P:H11	2.25	0.51
3:B:201:NAD:O2A	4:B:203:15P:H26	2.09	0.51
1:B:195:LYS:HZ3	4:B:205:15P:H102	1.76	0.51
1:B:78:THR:CG2	1:B:114:THR:HG22	2.40	0.51
1:A:78[B]:THR:HG21	1:A:114:THR:CG2	2.40	0.50
1:A:195:LYS:NZ	4:A:204:15P:H16	2.27	0.50
1:A:78[B]:THR:HB	1:A:123:THR:OG1	2.12	0.49
2:B:200:FMN:C4	4:B:203:15P:H11	2.42	0.48
1:A:195:LYS:HE2	4:A:204:15P:H111	1.97	0.47
1:B:158:THR:HB	1:B:159:PRO:HD2	1.96	0.47
1:B:195:LYS:HZ3	4:B:205:15P:C10	2.26	0.47
2:A:200:FMN:C4	4:A:202:15P:H11	2.44	0.47
1:A:157:GLY:H	1:A:163:THR:HG1	1.59	0.46
1:B:102:ALA:O	1:B:106:LYS:HE2	2.16	0.46
1:B:195:LYS:HZ1	4:B:205:15P:H16	1.79	0.46
1:B:9:TYR:O	1:B:77:PRO:HD3	2.16	0.46
1:A:145:ALA:HB3	1:A:148:LEU:HD22	1.99	0.44
1:B:78:THR:HG21	1:B:114:THR:HG22	1.99	0.44
1:A:11[B]:MET:HE2	6:A:259:HOH:O	2.17	0.43
1:B:120:GLN:NE2	1:B:163:THR:OG1	2.51	0.43
1:B:155:ARG:HD2	1:B:156:GLY:O	2.18	0.43
2:B:200:FMN:N3	4:B:203:15P:H11	2.33	0.43
1:A:103:LEU:HA	1:A:106:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:HG22	6:A:349:HOH:O	2.18	0.43
1:A:196:LEU:HD21	1:B:196:LEU:HG	2.01	0.42
1:A:79:ARG:HG3	1:A:84:SER:HA	2.01	0.42
1:A:143:TYR:HA	1:A:148:LEU:HD23	2.00	0.42
1:B:64:GLN:NE2	1:B:64:GLN:H	2.17	0.42
3:A:201:NAD:PA	4:A:202:15P:H25	2.60	0.41
1:B:110:VAL:HB	1:B:124:ILE:HG23	2.02	0.41
1:B:114:THR:HB	2:B:200:FMN:O2	2.21	0.41
1:A:114:THR:HB	2:A:200:FMN:O2	2.21	0.41
1:B:79:ARG:HG3	1:B:84:SER:HA	2.03	0.41
4:A:202:15P:C6	6:A:351:HOH:O	2.48	0.40
1:A:91:LEU:HD13	1:A:130:THR:HG21	2.03	0.40
1:B:86:GLN:HE21	1:B:86:GLN:N	2.00	0.40

All (1) 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:302:HOH:O	6:B:241:HOH:O[7_555]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/198 (104%)	205 (100%)	1 (0%)	0	100	100
1	B	198/198 (100%)	195 (98%)	3 (2%)	0	100	100
All	All	404/396 (102%)	400 (99%)	4 (1%)	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	159/149 (107%)	151 (95%)	8 (5%)	22	15
1	B	151/149 (101%)	146 (97%)	5 (3%)	33	28
All	All	310/298 (104%)	297 (96%)	13 (4%)	30	20

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20[A]	ARG
1	A	20[B]	ARG
1	A	55	THR
1	A	86	GLN
1	A	131	LEU
1	A	148	LEU
1	A	192[A]	LEU
1	A	192[B]	LEU
1	B	49	GLU
1	B	86	GLN
1	B	131	LEU
1	B	155	ARG
1	B	196	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	B	56	GLN
1	B	64	GLN
1	B	86	GLN
1	B	120	GLN
1	B	146	GLN
1	B	173	GLN

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 ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAD	A	201	-	46,48,48	1.90	7 (15%)	64,73,73	1.76	13 (20%)
4	15P	A	204	-	19,19,103	1.25	3 (15%)	18,18,102	0.94	2 (11%)
2	FMN	B	200	-	33,33,33	1.15	2 (6%)	48,50,50	1.47	9 (18%)
4	15P	B	205	-	19,19,103	1.22	2 (10%)	18,18,102	1.38	2 (11%)
4	15P	A	203	-	15,15,103	0.58	0	14,14,102	0.25	0
4	15P	A	202	-	10,10,103	1.76	3 (30%)	9,9,102	2.34	7 (77%)
4	15P	B	204	-	12,12,103	0.46	0	11,11,102	0.61	0
3	NAD	B	201	-	46,48,48	1.91	5 (10%)	64,73,73	1.77	13 (20%)
4	15P	B	203	-	10,10,103	1.82	3 (30%)	9,9,102	3.33	7 (77%)
5	AMP	B	202	-	25,25,25	1.61	3 (12%)	37,38,38	2.27	11 (29%)
2	FMN	A	200	-	33,33,33	1.07	2 (6%)	48,50,50	1.43	6 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	A	201	-	-	6/30/62/62	0/5/5/5
4	15P	A	204	-	-	12/17/17/101	-
2	FMN	B	200	-	-	0/18/18/18	0/3/3/3
4	15P	B	205	-	-	11/17/17/101	-
4	15P	A	203	-	-	3/13/13/101	-
4	15P	A	202	-	-	5/8/8/101	-
4	15P	B	204	-	-	5/10/10/101	-
3	NAD	B	201	-	-	12/30/62/62	0/5/5/5
4	15P	B	203	-	-	4/8/8/101	-
5	AMP	B	202	-	-	2/10/26/26	0/3/3/3
2	FMN	A	200	-	-	0/18/18/18	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	NAD	O7N-C7N	10.02	1.42	1.24
3	A	201	NAD	O7N-C7N	9.76	1.42	1.24
5	B	202	AMP	C5-C4	5.08	1.48	1.39
3	B	201	NAD	C2A-N1A	3.91	1.40	1.33
3	A	201	NAD	PN-O3	3.80	1.63	1.59
5	B	202	AMP	C5-C6	3.69	1.51	1.41
2	B	200	FMN	C4A-N5	3.60	1.38	1.30
4	B	205	15P	OXT-C1	-3.42	1.24	1.42
2	A	200	FMN	C4A-N5	3.34	1.38	1.30
3	B	201	NAD	C2A-N3A	3.31	1.39	1.33
4	A	204	15P	O1-C2	3.14	1.55	1.42
2	B	200	FMN	C10-N1	3.03	1.39	1.33
4	B	203	15P	C4-C3	-2.96	1.34	1.49
3	A	201	NAD	C8A-N7A	2.86	1.37	1.31
4	A	202	15P	C4-C3	-2.86	1.34	1.49
4	B	203	15P	C6-C5	-2.79	1.35	1.49
4	A	202	15P	C6-C5	-2.75	1.35	1.49
3	A	201	NAD	C2A-N3A	2.72	1.38	1.33
3	B	201	NAD	C8A-N7A	2.68	1.36	1.31
3	A	201	NAD	C2A-N1A	2.61	1.38	1.33
4	A	202	15P	C2-C1	-2.57	1.35	1.49
4	B	203	15P	C2-C1	-2.50	1.36	1.49
5	B	202	AMP	C8-N7	2.34	1.36	1.31
4	B	205	15P	C2-C1	-2.33	1.37	1.49
2	A	200	FMN	C10-N1	2.19	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	NAD	O4D-C1D	2.19	1.43	1.40
3	A	201	NAD	C2N-N1N	2.13	1.37	1.35
4	A	204	15P	O1-C3	2.09	1.51	1.42
4	A	204	15P	C2-C1	-2.06	1.38	1.49
3	A	201	NAD	O4D-C1D	2.03	1.43	1.40

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	NAD	N3A-C2A-N1A	-7.24	117.62	128.58
5	B	202	AMP	C5-C4-N3	-6.49	117.78	126.72
3	B	201	NAD	N3A-C2A-N1A	-5.18	120.75	128.58
5	B	202	AMP	N3-C4-N9	5.12	135.88	127.17
4	B	203	15P	O1-C2-C1	4.98	132.05	110.11
4	B	203	15P	O1-C3-C4	4.76	132.03	110.35
3	B	201	NAD	N9A-C8A-N7A	-4.72	107.24	113.94
3	A	201	NAD	N9A-C8A-N7A	-4.64	107.36	113.94
5	B	202	AMP	C2-N3-C4	4.58	123.01	111.83
4	B	203	15P	O2-C5-C6	4.51	130.89	110.35
4	B	205	15P	OXT-C1-C2	4.26	136.90	111.82
3	B	201	NAD	C5A-N7A-C8A	4.20	110.06	103.45
3	A	201	NAD	C5A-C4A-N3A	-4.13	121.03	126.72
5	B	202	AMP	C4-C5-N7	-4.01	106.00	110.58
5	B	202	AMP	N3-C2-N1	-3.97	122.56	128.58
3	A	201	NAD	C2A-N3A-C4A	3.95	121.48	111.83
2	A	200	FMN	C4-N3-C2	-3.74	119.00	125.64
4	B	203	15P	O2-C4-C3	3.72	127.31	110.35
2	B	200	FMN	C9A-C5A-N5	-3.72	118.51	122.45
3	B	201	NAD	C5A-C4A-N3A	-3.70	121.62	126.72
2	B	200	FMN	O2P-P-O5'	3.54	115.91	106.67
3	A	201	NAD	C5A-N7A-C8A	3.42	108.82	103.45
3	B	201	NAD	C4A-C5A-N7A	-3.40	106.69	110.58
4	A	202	15P	O2-C5-C6	3.38	125.75	110.35
2	A	200	FMN	C4A-C10-N10	3.36	121.29	116.48
3	A	201	NAD	C4A-N9A-C8A	3.19	109.09	105.74
2	B	200	FMN	C4A-C4-N3	3.15	121.26	113.25
2	A	200	FMN	C4-C4A-N5	3.04	122.41	118.21
2	A	200	FMN	C4A-C4-N3	3.00	120.89	113.25
5	B	202	AMP	C5-N7-C8	2.96	108.11	103.45
3	B	201	NAD	C4A-N9A-C8A	2.96	108.85	105.74
3	A	201	NAD	N3A-C4A-N9A	2.96	132.20	127.17
4	A	204	15P	OXT-C1-C2	2.93	129.06	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	200	FMN	C10-C4A-N5	-2.91	118.86	124.81
2	B	200	FMN	C5A-C9A-N10	2.89	120.58	117.97
3	B	201	NAD	C2A-N3A-C4A	2.88	118.87	111.83
2	B	200	FMN	O4-C4-C4A	-2.87	118.96	126.53
5	B	202	AMP	C4-N9-C8	2.81	108.69	105.74
3	B	201	NAD	PA-O5B-C5B	2.80	137.42	121.35
4	B	203	15P	OXT-C1-C2	2.80	128.32	111.82
5	B	202	AMP	C2'-C1'-N9	2.79	120.24	113.30
2	B	200	FMN	C4-N3-C2	-2.78	120.70	125.64
3	A	201	NAD	O2A-PA-O3	2.69	114.54	107.27
5	B	202	AMP	C6-C5-N7	2.67	137.24	132.09
4	A	202	15P	C3-O1-C2	2.64	124.83	113.26
3	A	201	NAD	O5B-PA-O1A	2.62	119.34	108.94
4	A	202	15P	OXT-C1-C2	2.51	126.59	111.82
4	A	202	15P	O1-C2-C1	2.45	120.92	110.11
3	B	201	NAD	N3A-C4A-N9A	2.38	131.22	127.17
5	B	202	AMP	C2'-C3'-C4'	2.38	107.21	102.61
4	B	205	15P	C3-O1-C2	2.36	123.59	113.26
3	A	201	NAD	C4A-C5A-N7A	-2.29	107.96	110.58
3	B	201	NAD	O4D-C4D-C5D	2.29	116.68	109.33
3	B	201	NAD	O2A-PA-O3	2.28	113.43	107.27
2	B	200	FMN	O3P-P-O5'	2.24	112.51	106.67
4	A	202	15P	O1-C3-C4	2.21	120.42	110.35
2	B	200	FMN	C4'-C3'-C2'	-2.20	109.91	113.57
4	B	203	15P	O3-C6-C5	2.17	126.90	111.00
5	B	202	AMP	N9-C8-N7	-2.17	110.86	113.94
3	A	201	NAD	O4B-C1B-N9A	2.09	112.11	108.09
3	B	201	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
3	A	201	NAD	C2A-N1A-C6A	2.09	122.16	118.73
4	B	203	15P	C5-O2-C4	2.08	122.37	113.26
2	B	200	FMN	C4-C4A-N5	2.07	121.07	118.21
3	A	201	NAD	C4A-N9A-C1B	-2.07	121.79	126.63
3	B	201	NAD	C2N-C3N-C4N	2.05	120.64	118.26
4	A	202	15P	C5-O2-C4	2.05	122.21	113.26
4	A	202	15P	O2-C4-C3	2.05	119.67	110.35
2	A	200	FMN	O3P-P-O2P	2.04	115.47	107.80
4	A	204	15P	O1-C2-C1	2.00	118.94	110.11

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	NAD	O4D-C4D-C5D-O5D
3	B	201	NAD	PN-O3-PA-O5B
3	B	201	NAD	PA-O3-PN-O5D
3	B	201	NAD	C5D-O5D-PN-O3
3	B	201	NAD	C5D-O5D-PN-O1N
3	B	201	NAD	O4D-C4D-C5D-O5D
4	B	203	15P	C6-C5-O2-C4
4	A	202	15P	OXT-C1-C2-O1
3	B	201	NAD	O4B-C4B-C5B-O5B
3	B	201	NAD	C3B-C4B-C5B-O5B
3	B	201	NAD	C3D-C4D-C5D-O5D
4	A	204	15P	O2-C5-C6-O3
4	A	204	15P	O5-C11-C12-O6
4	A	204	15P	O3-C7-C8-O4
4	B	203	15P	OXT-C1-C2-O1
4	B	205	15P	O3-C7-C8-O4
3	A	201	NAD	C3D-C4D-C5D-O5D
4	A	202	15P	O2-C5-C6-O3
4	B	205	15P	C8-C7-O3-C6
4	B	204	15P	O3-C7-C8-O4
4	B	203	15P	O2-C5-C6-O3
4	B	203	15P	O1-C3-C4-O2
4	A	203	15P	O2-C5-C6-O3
4	B	205	15P	OXT-C1-C2-O1
4	B	205	15P	O1-C3-C4-O2
4	A	204	15P	C1-C2-O1-C3
3	A	201	NAD	PN-O3-PA-O1A
4	A	204	15P	O5-C10-C9-O4
4	B	205	15P	O5-C10-C9-O4
4	A	203	15P	O3-C7-C8-O4
4	A	204	15P	C11-C12-O6-C13
4	B	204	15P	OXT-C1-C2-O1
3	A	201	NAD	PN-O3-PA-O5B
4	B	205	15P	C11-C12-O6-C13
4	B	204	15P	C8-C7-O3-C6
4	A	204	15P	C4-C3-O1-C2
4	A	202	15P	C3-C4-O2-C5
4	A	204	15P	OXT-C1-C2-O1
4	B	204	15P	O1-C3-C4-O2
4	B	205	15P	O2-C5-C6-O3
3	A	201	NAD	C5B-O5B-PA-O2A
3	A	201	NAD	C5D-O5D-PN-O1N
3	B	201	NAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	B	201	NAD	C5B-O5B-PA-O3
3	B	201	NAD	C5D-O5D-PN-O2N
4	A	204	15P	C7-C8-O4-C9
4	A	204	15P	C8-C7-O3-C6
4	A	204	15P	C6-C5-O2-C4
4	A	204	15P	C10-C9-O4-C8
4	B	205	15P	C10-C9-O4-C8
4	B	204	15P	C6-C5-O2-C4
5	B	202	AMP	O4'-C1'-N9-C4
4	B	205	15P	C1-C2-O1-C3
3	B	201	NAD	C4D-C5D-O5D-PN
4	B	205	15P	C6-C5-O2-C4
5	B	202	AMP	O4'-C1'-N9-C8
4	A	202	15P	O1-C3-C4-O2
4	A	203	15P	C10-C9-O4-C8
4	B	205	15P	O5-C11-C12-O6
4	A	202	15P	C5-C6-O3-C7

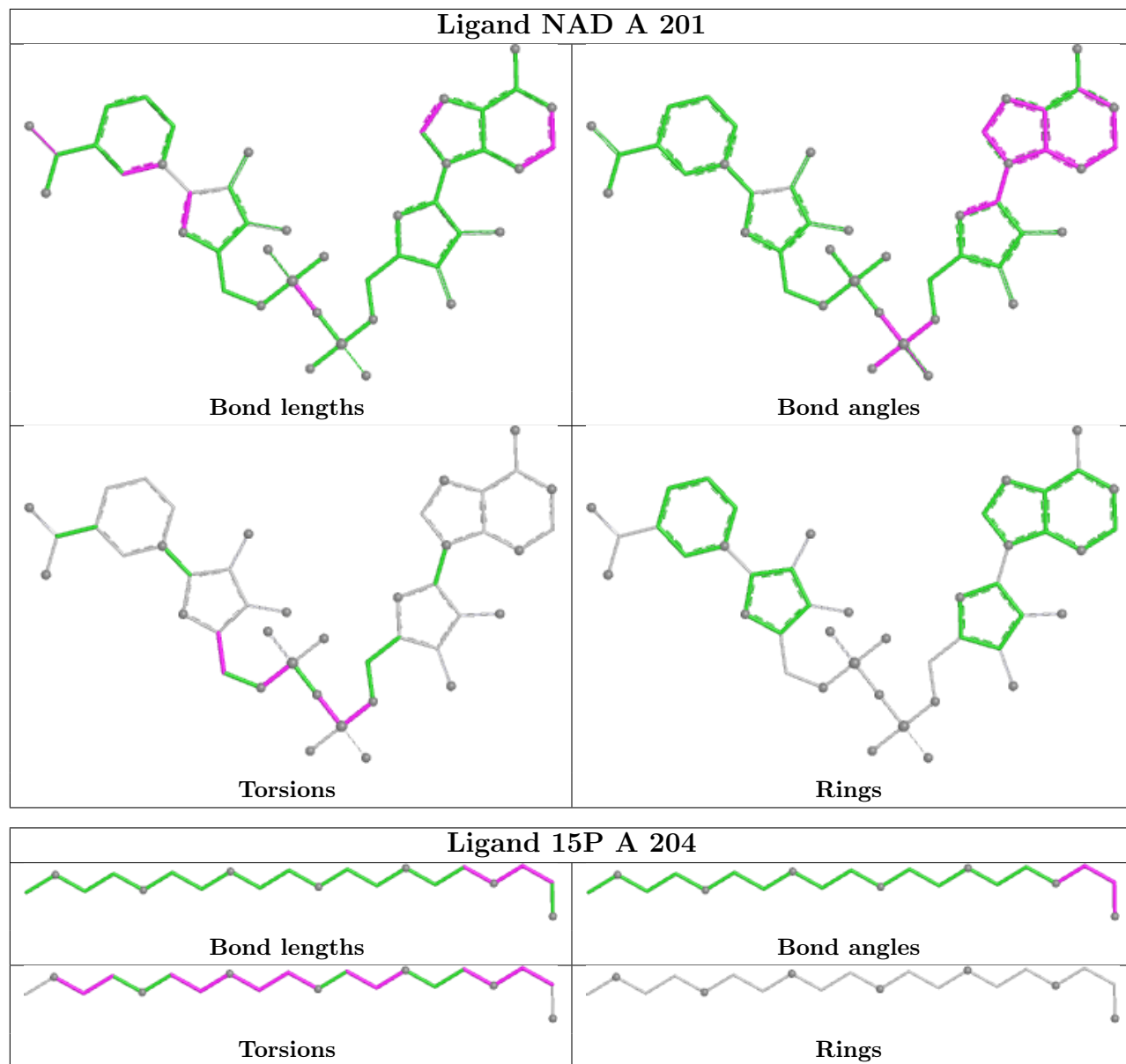
There are no ring outliers.

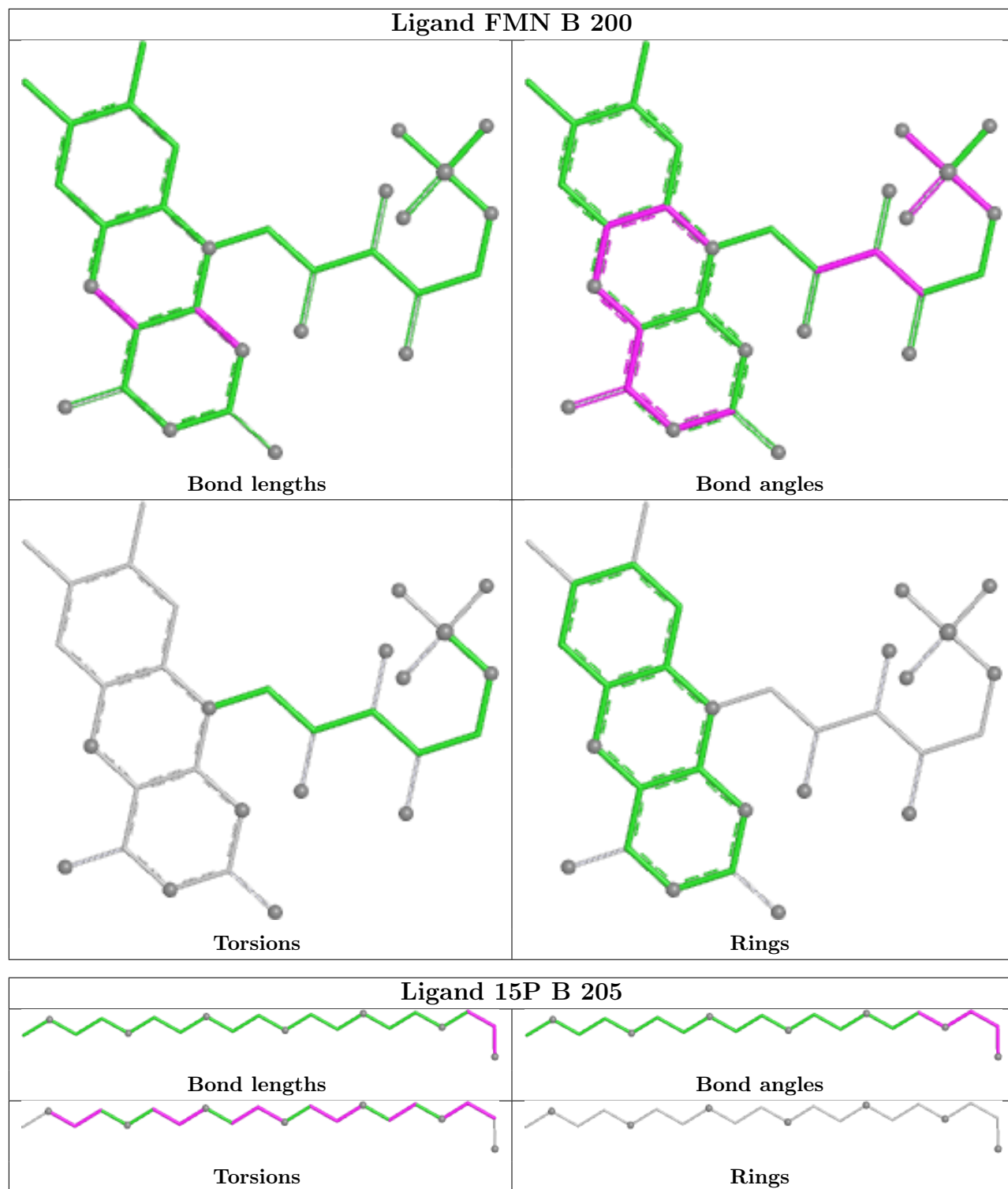
8 monomers are involved in 27 short contacts:

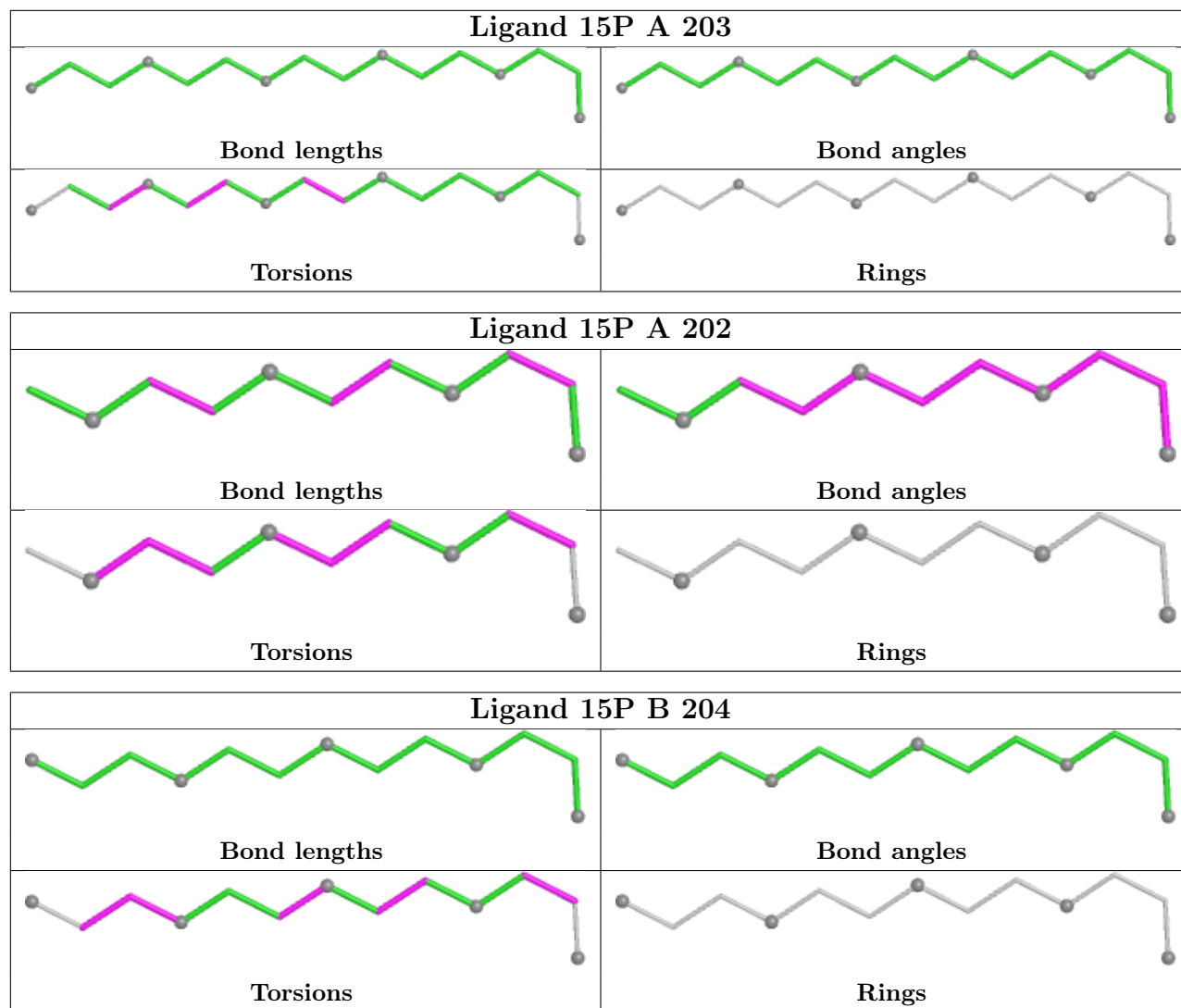
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	NAD	2	0
4	A	204	15P	6	0
2	B	200	FMN	3	0
4	B	205	15P	9	0
4	A	202	15P	5	0
3	B	201	NAD	1	0
4	B	203	15P	4	0
2	A	200	FMN	3	0

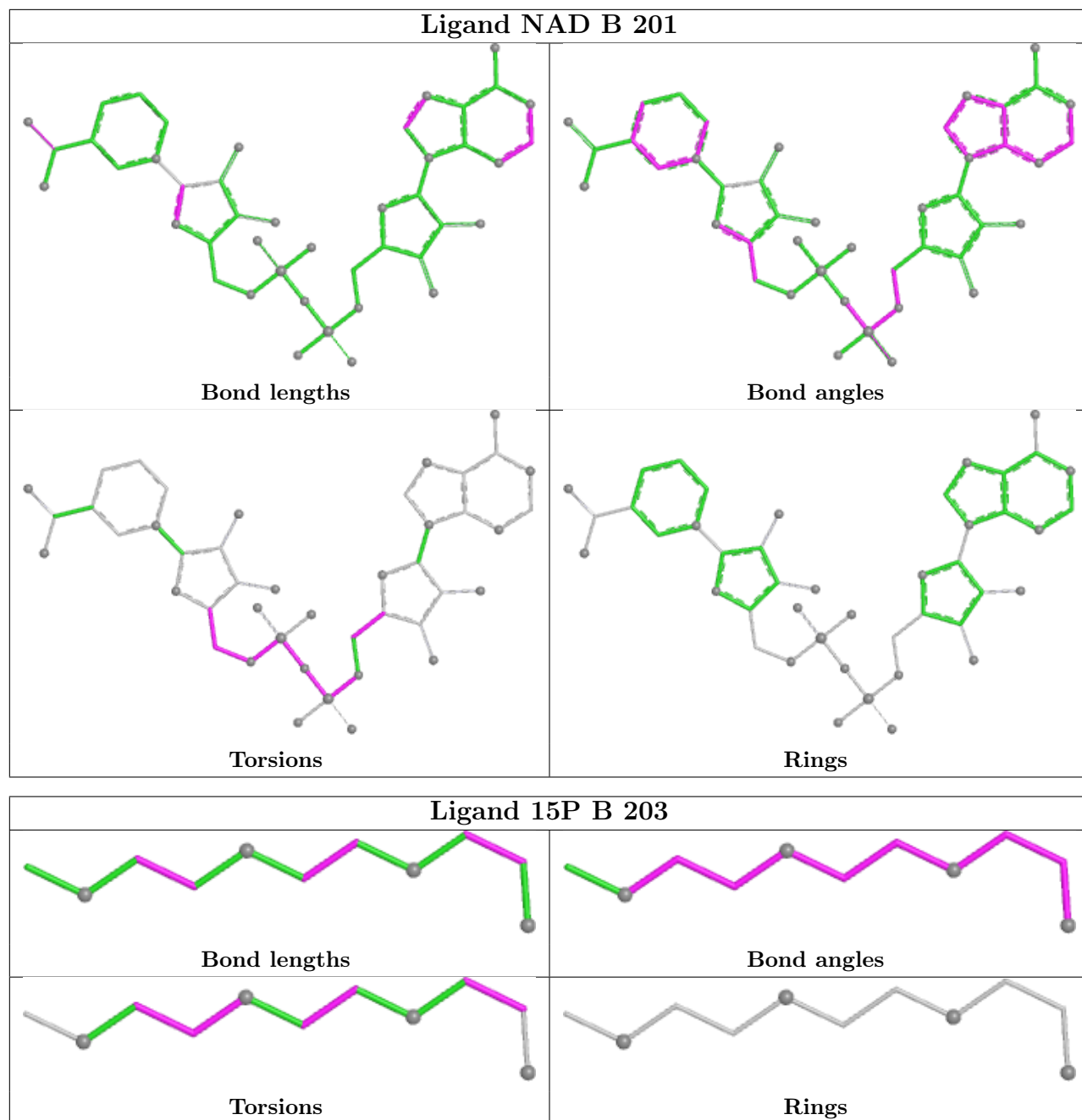
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

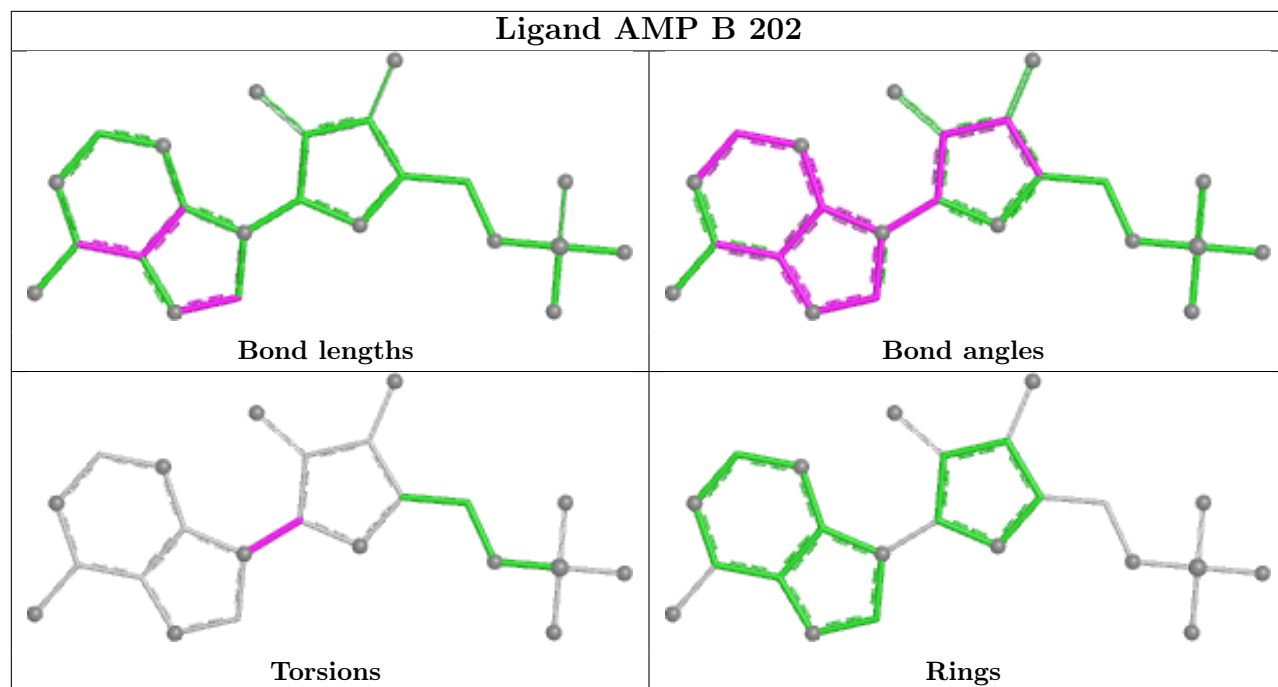
equivalents in the CSD to analyse the geometry.

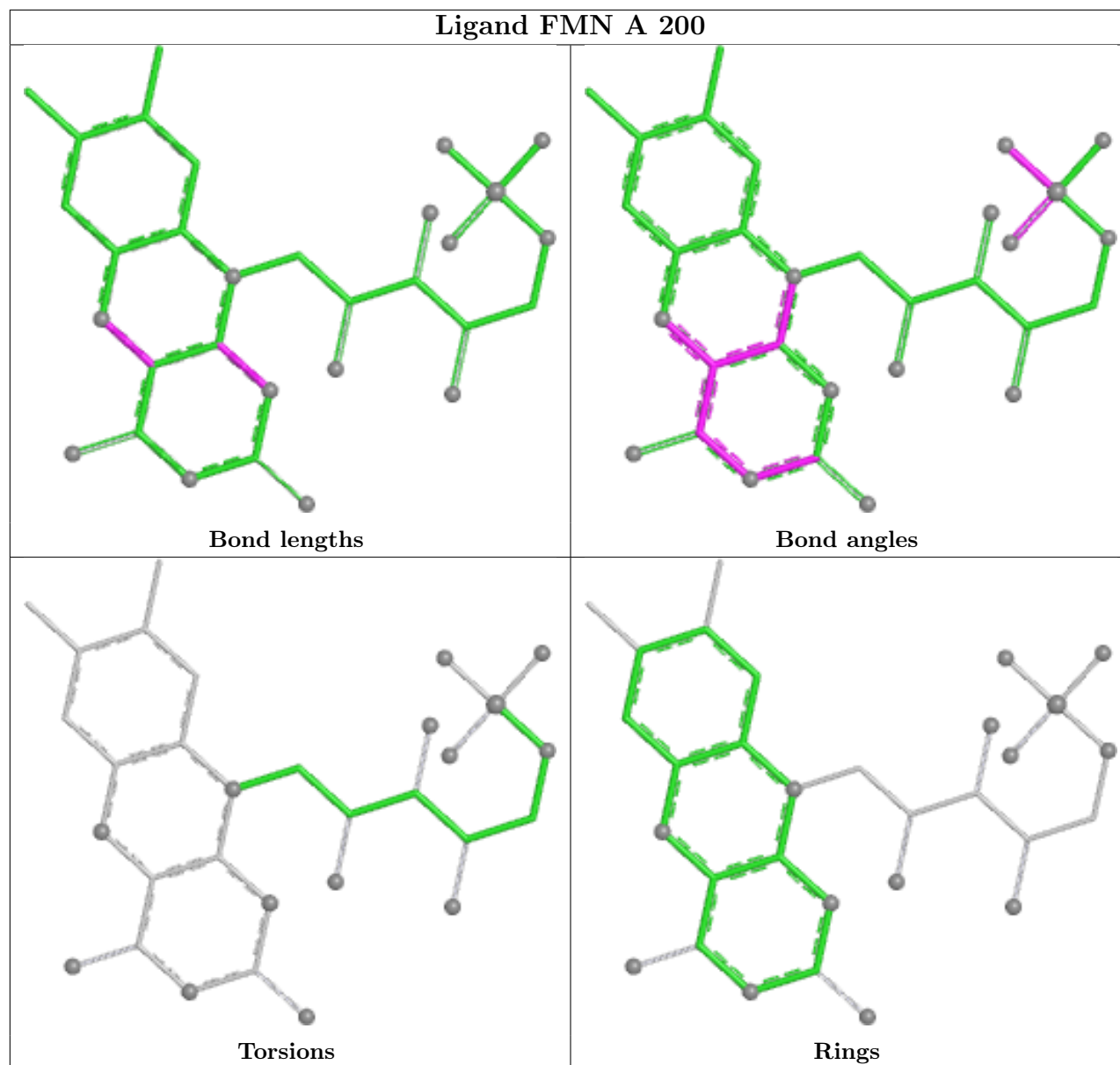












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	197/198 (99%)	-0.09	14 (7%)	22 22	15, 28, 48, 61	11 (5%)
1	B	197/198 (99%)	-0.39	0	100 100	13, 29, 43, 51	3 (1%)
All	All	394/396 (99%)	-0.24	14 (3%)	46 46	13, 28, 44, 61	14 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	144	ALA	6.7
1	A	154	VAL	4.8
1	A	149	PHE	4.2
1	A	148	LEU	4.0
1	A	156	GLY	3.8
1	A	153	GLN	3.2
1	A	152	SER	2.6
1	A	157	GLY	2.6
1	A	115	GLY	2.5
1	A	155	ARG	2.5
1	A	150	ASP	2.4
1	A	146[A]	GLN	2.3
1	A	143	TYR	2.3
1	A	151	VAL	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 oligosaccharides in this entry.

6.4 Ligands

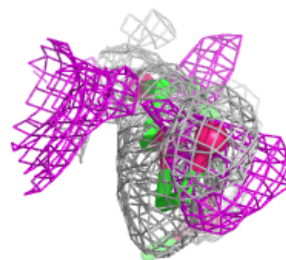
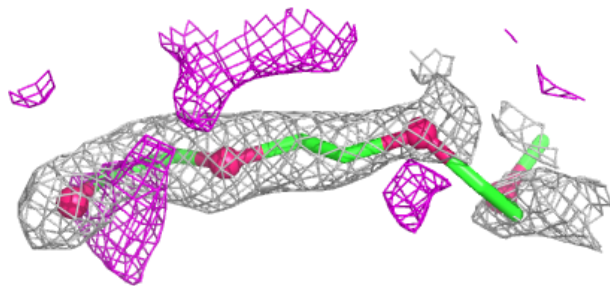
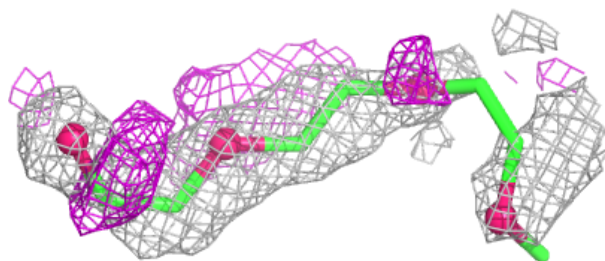
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	15P	A	202	11/104	0.82	0.23	51,59,73,73	0
5	AMP	B	202	23/23	0.84	0.16	61,66,74,75	0
4	15P	B	203	11/104	0.85	0.23	50,68,77,77	0
4	15P	A	204	20/104	0.85	0.20	57,65,75,78	0
4	15P	B	204	13/104	0.87	0.18	56,60,68,71	0
4	15P	B	205	20/104	0.92	0.13	35,46,61,62	0
4	15P	A	203	16/104	0.92	0.12	38,53,65,68	0
3	NAD	A	201	44/44	0.93	0.12	28,56,81,83	0
3	NAD	B	201	44/44	0.94	0.10	34,57,81,84	0
2	FMN	B	200	31/31	0.97	0.07	24,30,31,32	0
2	FMN	A	200	31/31	0.97	0.07	22,28,29,30	0

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

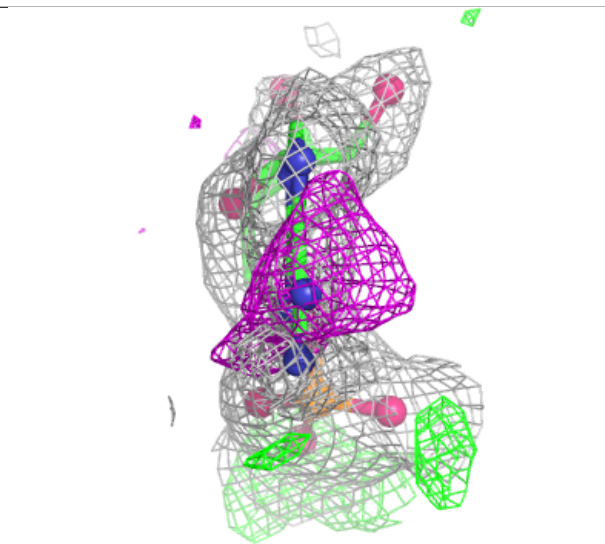
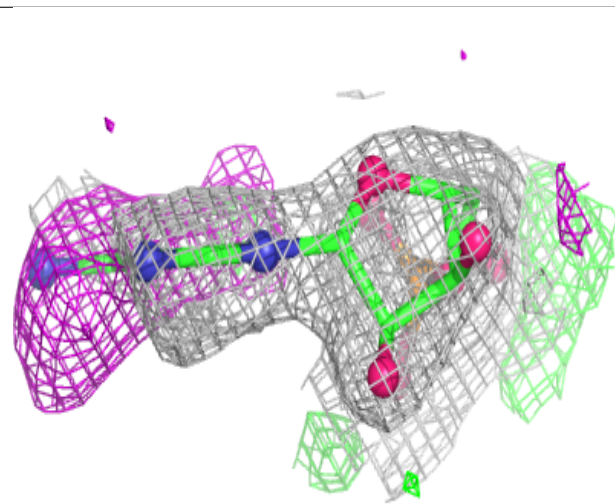
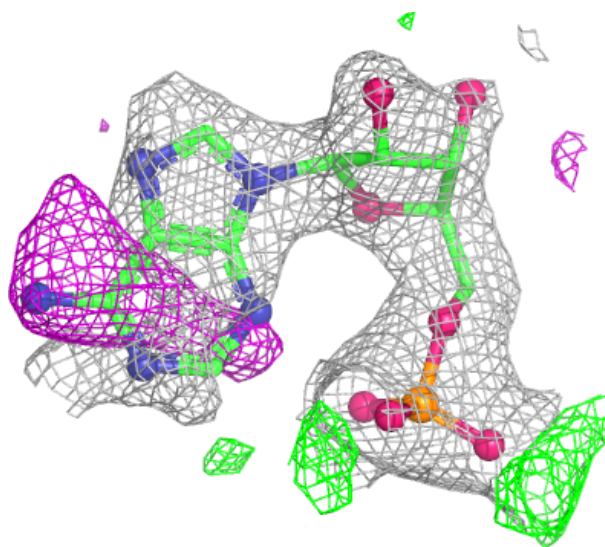
Electron density around 15P A 202:

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



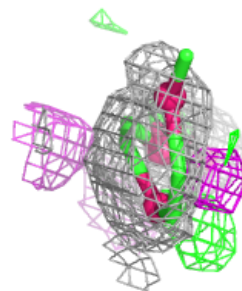
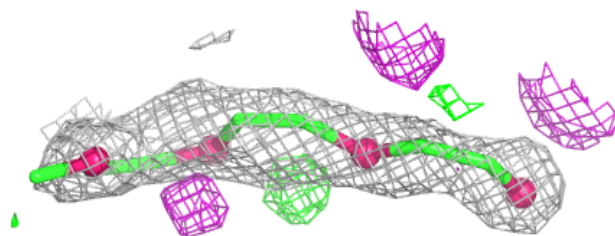
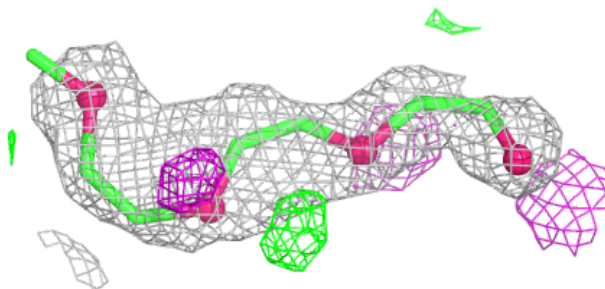
Electron density around AMP B 202:

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



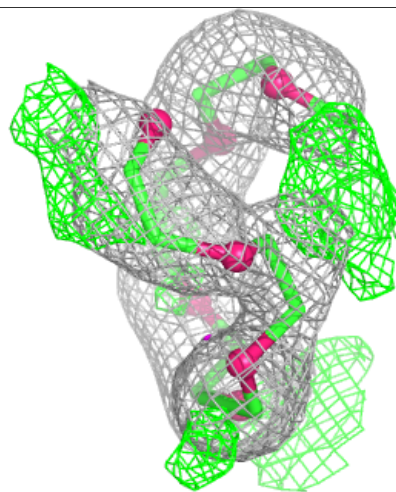
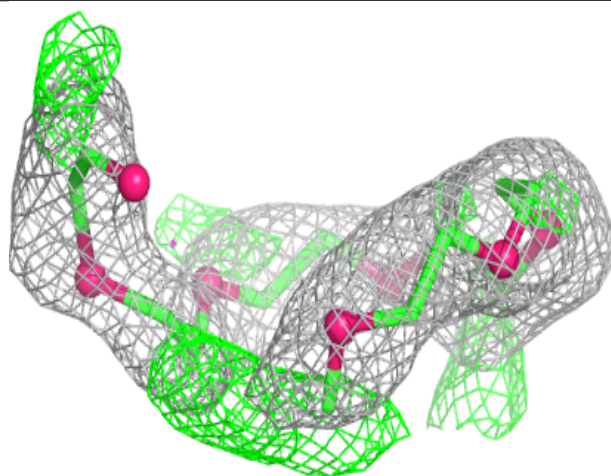
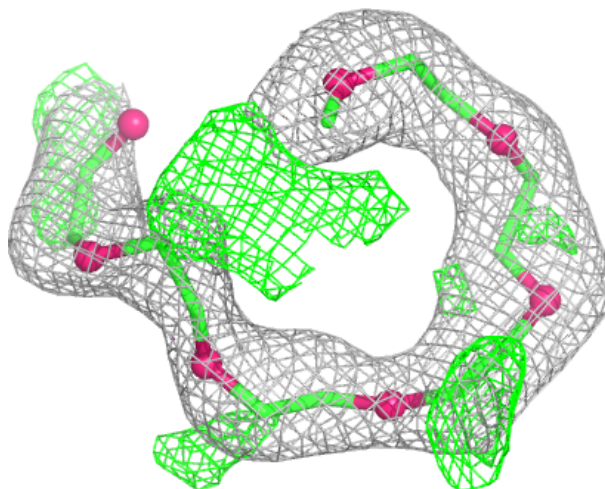
Electron density around 15P B 203:

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



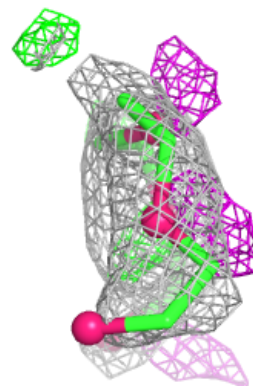
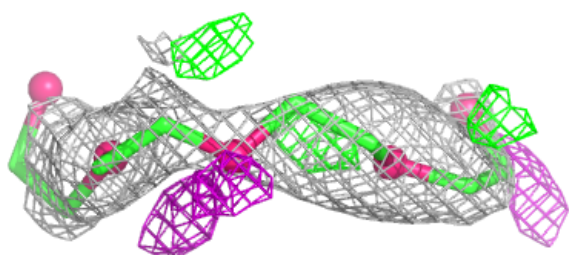
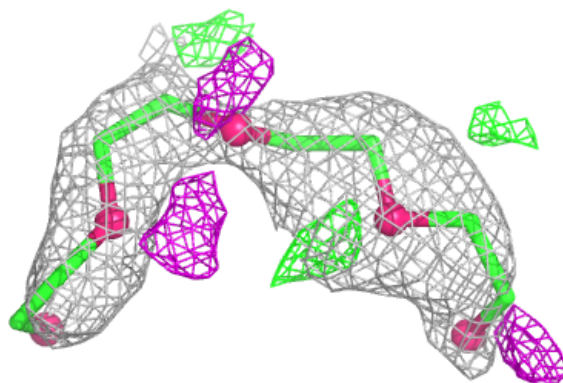
Electron density around 15P A 204:

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



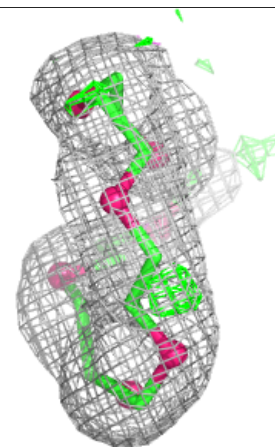
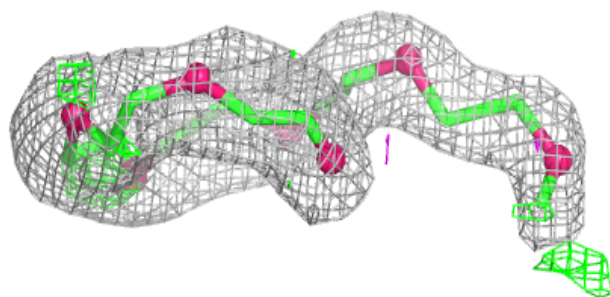
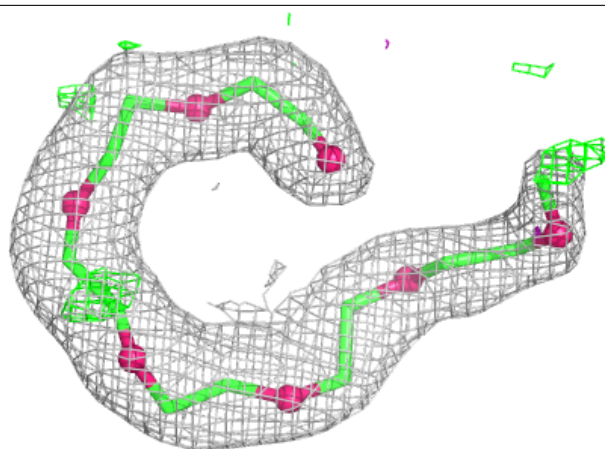
Electron density around 15P B 204:

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



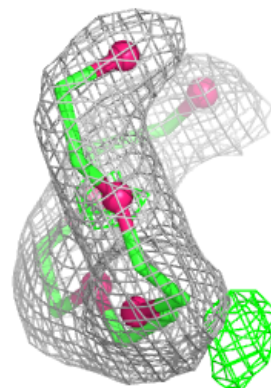
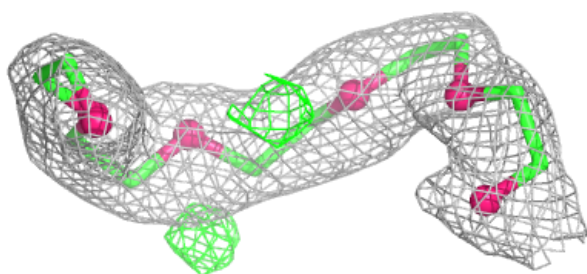
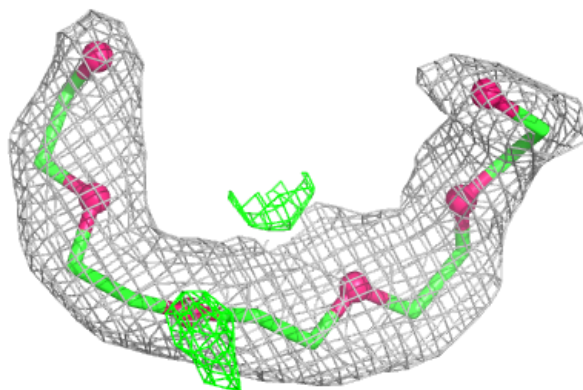
Electron density around 15P B 205:

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



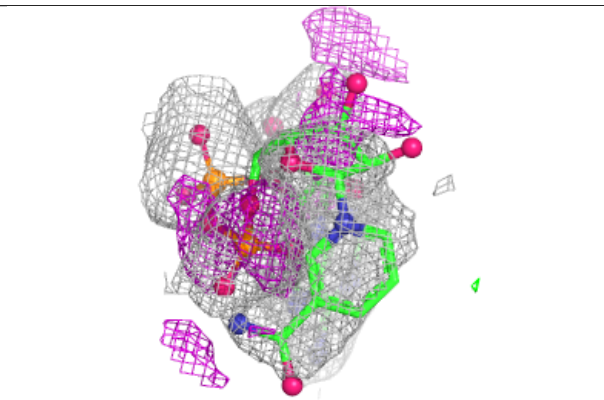
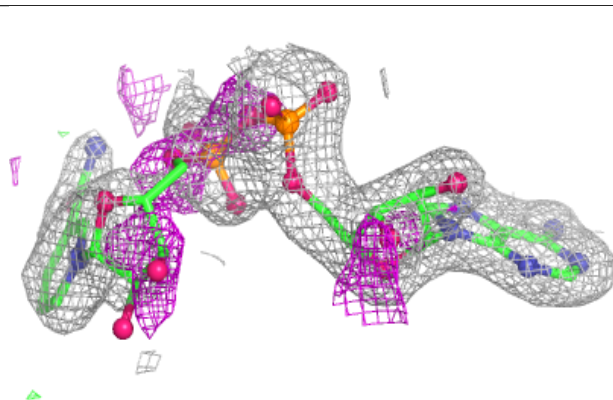
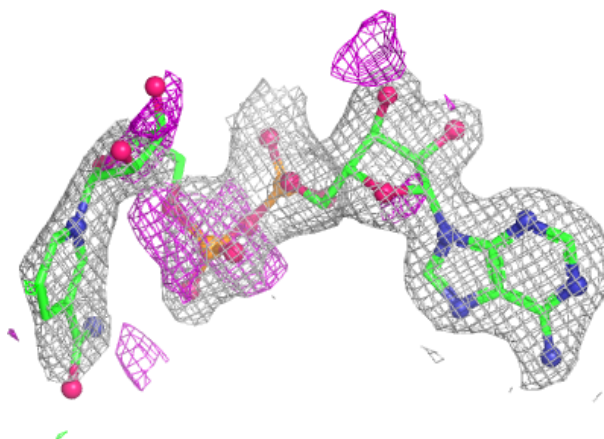
Electron density around 15P A 203:

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

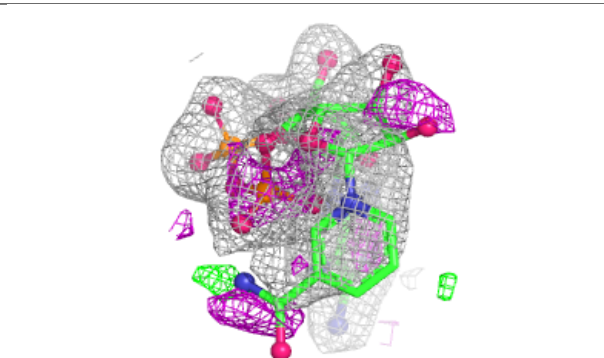
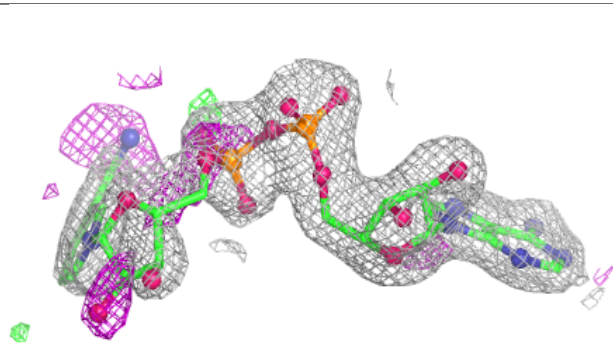
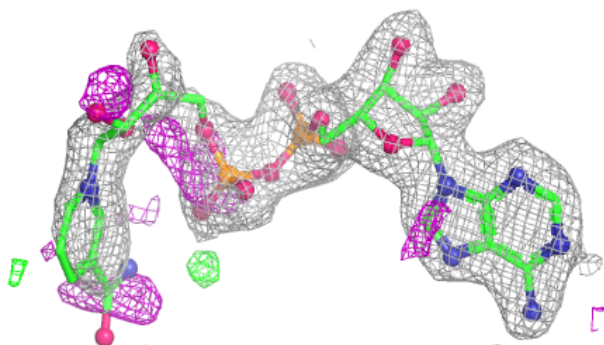


Electron density around NAD A 201:

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

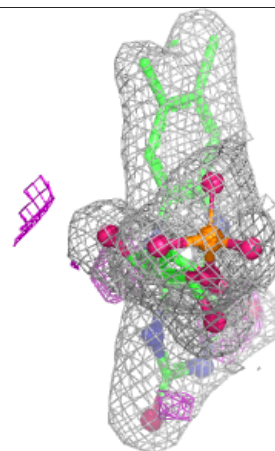
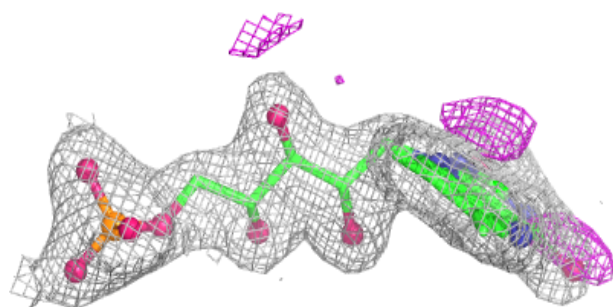
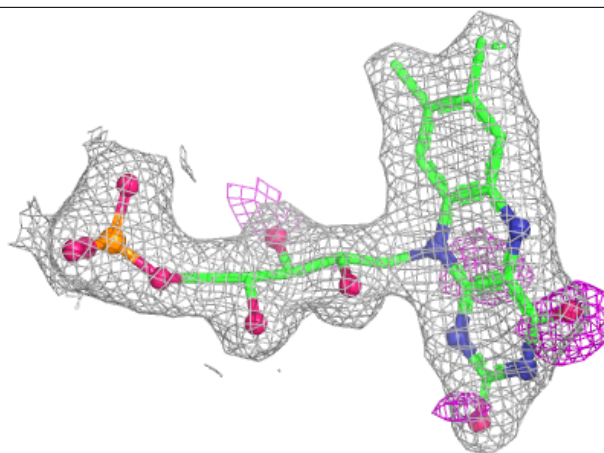
**Electron density around NAD B 201:**

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



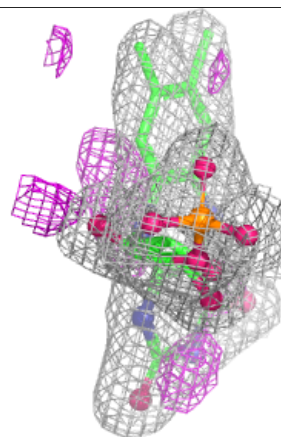
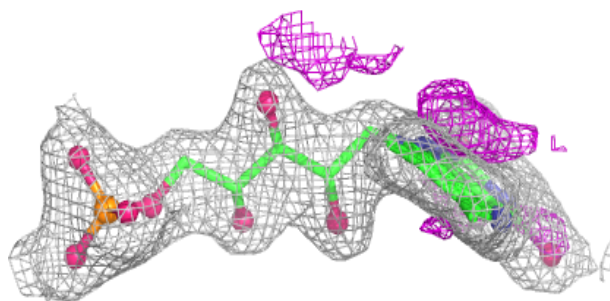
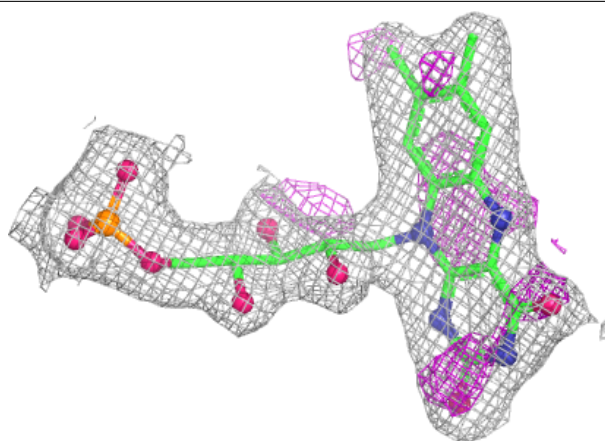
Electron density around FMN B 200:

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



Electron density around FMN A 200:

$2mF_o - DF_c$ (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.