W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2024 – 06:57 PM EST

PDB ID	:	4GMG
Title	:	NADP+ bound structure of a Thiazolinyl Imine Reductase from Yersinia enterocolitica (Irp3)
Authors	:	Lamb, A.L.; Meneely, K.M.
Deposited on	:	2012-08-15
Resolution	:	2.31 Å(reported)

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

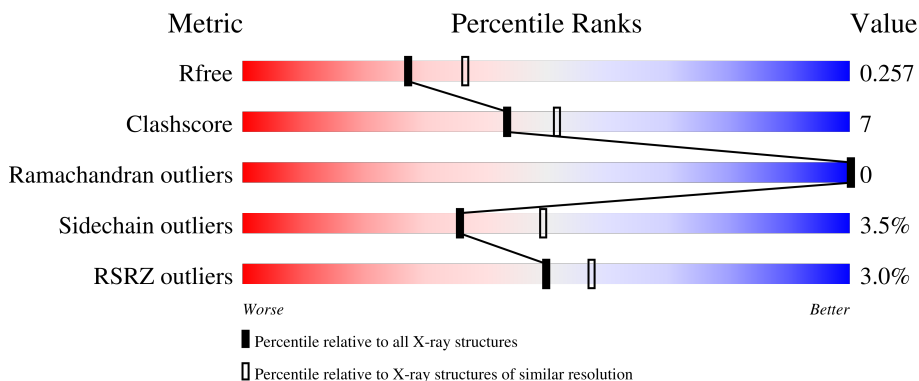|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.31 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		7
Ramachandran outliers		0
Sidechain outliers		3.5%
RSRZ outliers		3.0%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	385	3% 76% 16% • 7%
1	B	385	2% 71% 16% • 10%
1	C	385	2% 70% 15% • 13%
1	D	385	4% 74% 14% • 11%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11156 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 Yersiniabactin biosynthetic protein YbtU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2806	1784	511	495	16			
1	B	345	Total	C	N	O	S	0	0	0
			2715	1728	493	479	15			
1	C	336	Total	C	N	O	S	0	0	0
			2636	1679	476	466	15			
1	D	343	Total	C	N	O	S	0	0	0
			2699	1719	489	476	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A1JTG0
A	-18	GLY	-	expression tag	UNP A1JTG0
A	-17	SER	-	expression tag	UNP A1JTG0
A	-16	SER	-	expression tag	UNP A1JTG0
A	-15	HIS	-	expression tag	UNP A1JTG0
A	-14	HIS	-	expression tag	UNP A1JTG0
A	-13	HIS	-	expression tag	UNP A1JTG0
A	-12	HIS	-	expression tag	UNP A1JTG0
A	-11	HIS	-	expression tag	UNP A1JTG0
A	-10	HIS	-	expression tag	UNP A1JTG0
A	-9	SER	-	expression tag	UNP A1JTG0
A	-8	SER	-	expression tag	UNP A1JTG0
A	-7	GLY	-	expression tag	UNP A1JTG0
A	-6	LEU	-	expression tag	UNP A1JTG0
A	-5	VAL	-	expression tag	UNP A1JTG0
A	-4	PRO	-	expression tag	UNP A1JTG0
A	-3	ARG	-	expression tag	UNP A1JTG0
A	-2	GLY	-	expression tag	UNP A1JTG0
A	-1	SER	-	expression tag	UNP A1JTG0
A	0	HIS	-	expression tag	UNP A1JTG0
B	-19	MET	-	expression tag	UNP A1JTG0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A1JTG0
B	-17	SER	-	expression tag	UNP A1JTG0
B	-16	SER	-	expression tag	UNP A1JTG0
B	-15	HIS	-	expression tag	UNP A1JTG0
B	-14	HIS	-	expression tag	UNP A1JTG0
B	-13	HIS	-	expression tag	UNP A1JTG0
B	-12	HIS	-	expression tag	UNP A1JTG0
B	-11	HIS	-	expression tag	UNP A1JTG0
B	-10	HIS	-	expression tag	UNP A1JTG0
B	-9	SER	-	expression tag	UNP A1JTG0
B	-8	SER	-	expression tag	UNP A1JTG0
B	-7	GLY	-	expression tag	UNP A1JTG0
B	-6	LEU	-	expression tag	UNP A1JTG0
B	-5	VAL	-	expression tag	UNP A1JTG0
B	-4	PRO	-	expression tag	UNP A1JTG0
B	-3	ARG	-	expression tag	UNP A1JTG0
B	-2	GLY	-	expression tag	UNP A1JTG0
B	-1	SER	-	expression tag	UNP A1JTG0
B	0	HIS	-	expression tag	UNP A1JTG0
C	-19	MET	-	expression tag	UNP A1JTG0
C	-18	GLY	-	expression tag	UNP A1JTG0
C	-17	SER	-	expression tag	UNP A1JTG0
C	-16	SER	-	expression tag	UNP A1JTG0
C	-15	HIS	-	expression tag	UNP A1JTG0
C	-14	HIS	-	expression tag	UNP A1JTG0
C	-13	HIS	-	expression tag	UNP A1JTG0
C	-12	HIS	-	expression tag	UNP A1JTG0
C	-11	HIS	-	expression tag	UNP A1JTG0
C	-10	HIS	-	expression tag	UNP A1JTG0
C	-9	SER	-	expression tag	UNP A1JTG0
C	-8	SER	-	expression tag	UNP A1JTG0
C	-7	GLY	-	expression tag	UNP A1JTG0
C	-6	LEU	-	expression tag	UNP A1JTG0
C	-5	VAL	-	expression tag	UNP A1JTG0
C	-4	PRO	-	expression tag	UNP A1JTG0
C	-3	ARG	-	expression tag	UNP A1JTG0
C	-2	GLY	-	expression tag	UNP A1JTG0
C	-1	SER	-	expression tag	UNP A1JTG0
C	0	HIS	-	expression tag	UNP A1JTG0
D	-19	MET	-	expression tag	UNP A1JTG0
D	-18	GLY	-	expression tag	UNP A1JTG0
D	-17	SER	-	expression tag	UNP A1JTG0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A1JTG0
D	-15	HIS	-	expression tag	UNP A1JTG0
D	-14	HIS	-	expression tag	UNP A1JTG0
D	-13	HIS	-	expression tag	UNP A1JTG0
D	-12	HIS	-	expression tag	UNP A1JTG0
D	-11	HIS	-	expression tag	UNP A1JTG0
D	-10	HIS	-	expression tag	UNP A1JTG0
D	-9	SER	-	expression tag	UNP A1JTG0
D	-8	SER	-	expression tag	UNP A1JTG0
D	-7	GLY	-	expression tag	UNP A1JTG0
D	-6	LEU	-	expression tag	UNP A1JTG0
D	-5	VAL	-	expression tag	UNP A1JTG0
D	-4	PRO	-	expression tag	UNP A1JTG0
D	-3	ARG	-	expression tag	UNP A1JTG0
D	-2	GLY	-	expression tag	UNP A1JTG0
D	-1	SER	-	expression tag	UNP A1JTG0
D	0	HIS	-	expression tag	UNP A1JTG0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	29	Total	O	0	0
			29	29		
3	B	34	Total	O	0	0
			34	34		
3	C	23	Total	O	0	0
			23	23		
3	D	22	Total	O	0	0
			22	22		

3 Residue-property plots ⓘ

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: Yersiniabactin biosynthetic protein YbtU

- Molecule 1: Yersiniabactin biosynthetic protein YbtU

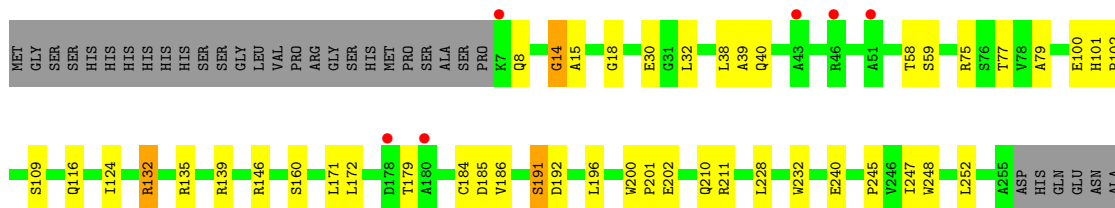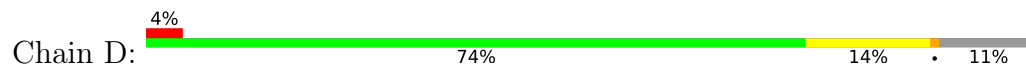
- Molecule 1: Yersiniabactin biosynthetic protein YbtU

HIS GLN GLU ASN ALA HIS SER LEU TYR ARG ARG PRO GLU I270 L271 R272 R287 E291 E296 W300 H303 S307 E312 Q319 Q323 S327 Q331 D351 Y357 ASN ASP ASP LYS GLU ALA LEU

• Molecule 1: Yersiniabactin biosynthetic protein YbtU

Chain D:

4%

74% 14% • 11%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET PRO SER ALA SER PRO K7 Q8 G14 A15 G18 E30 G31 L32 L38 A39 Q40 A43 R46 A51 T58 S59 R75 S76 T77 V78 A79 E100 H101 P102

S109 Q116 I124 R132 R135 R139 R146 S160 L171 L172 D178 T179 A180 C184 D185 V186 S191 D192 L196 W200 P201 E202 Q210 R211 L228 W232 E240 P245 V246 I247 W248 L252 A255 ASP HIS GLN GLU ASN ALA

HIS SER L264 Y265 R266 R267 P268 E269 I270 L271 E296 W300 H303 Q304 G311 E312 Q323 W330 R335 K336 I342 Y357 ASN ASP ASP LYS GLU ALA LEU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.42Å 93.82Å 181.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.89 – 2.31 39.89 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.89-2.31) 99.5 (39.89-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.197 , 0.260 0.196 , 0.257	Depositor DCC
R_{free} test set	3214 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 35.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11156	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5938e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAP

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	0.92	4/2885 (0.1%)	0.92	3/3933 (0.1%)
1	B	0.89	4/2790 (0.1%)	0.91	4/3803 (0.1%)
1	C	0.94	6/2708 (0.2%)	0.94	7/3692 (0.2%)
1	D	0.84	3/2773 (0.1%)	0.88	1/3780 (0.0%)
All	All	0.90	17/11156 (0.2%)	0.91	15/15208 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	1
All	All	0	4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	TRP	CD2-CE2	6.57	1.49	1.41
1	C	123	TRP	CD2-CE2	6.46	1.49	1.41
1	C	200	TRP	CD2-CE2	6.44	1.49	1.41
1	D	232	TRP	CD2-CE2	6.27	1.48	1.41
1	C	248	TRP	CD2-CE2	6.26	1.48	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	ARG	NE-CZ-NH1	8.46	124.53	120.30

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	LEU	CA-CB-CG	-7.78	97.42	115.30
1	C	135	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	103	LEU	CA-CB-CG	6.45	130.14	115.30
1	B	81	GLY	N-CA-C	5.94	127.95	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	VAL	Peptide
1	B	13	VAL	Peptide
1	B	14	GLY	Peptide
1	D	14	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2806	0	2785	41	1
1	B	2715	0	2691	40	0
1	C	2636	0	2615	34	1
1	D	2699	0	2679	39	0
2	A	48	0	25	3	0
2	B	48	0	25	4	0
2	C	48	0	25	4	0
2	D	48	0	25	4	0
3	A	29	0	0	0	0
3	B	34	0	0	1	0
3	C	23	0	0	0	0
3	D	22	0	0	1	0
All	All	11156	0	10870	146	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 7.

The worst 5 of 146 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:151:THR:HG21	1:C:202:GLU:OE1	1.36	1.23
1:C:151:THR:CG2	1:C:202:GLU:OE1	1.94	1.15
1:A:40:GLN:O	2:A:401:NAP:O1X	1.77	1.00
1:D:171:LEU:HD13	1:D:228:LEU:HD23	1.49	0.95
1:A:124:ILE:H	1:A:323:GLN:HE22	1.14	0.93

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)
1:A:339:ASN:OD1	1:C:27:GLN:NE2[1_655]	2.17	0.03

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	354/385 (92%)	341 (96%)	13 (4%)	0	100	100
1	B	341/385 (89%)	329 (96%)	12 (4%)	0	100	100
1	C	332/385 (86%)	321 (97%)	11 (3%)	0	100	100
1	D	339/385 (88%)	329 (97%)	10 (3%)	0	100	100
All	All	1366/1540 (89%)	1320 (97%)	46 (3%)	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	302/325 (93%)	293 (97%)	9 (3%)	41	56
1	B	291/325 (90%)	277 (95%)	14 (5%)	25	35
1	C	283/325 (87%)	273 (96%)	10 (4%)	36	49
1	D	289/325 (89%)	281 (97%)	8 (3%)	43	59
All	All	1165/1300 (90%)	1124 (96%)	41 (4%)	36	49

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	272	ARG
1	D	116	GLN
1	C	287	ARG
1	C	351	ASP
1	D	139	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	303	HIS
1	D	339	ASN
1	B	323	GLN
1	B	350	HIS
1	C	303	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	NAP	A	401	-	45,52,52	1.87	11 (24%)	56,80,80	1.29	5 (8%)
2	NAP	D	401	-	45,52,52	1.74	11 (24%)	56,80,80	1.19	6 (10%)
2	NAP	B	401	-	45,52,52	1.05	4 (8%)	56,80,80	1.68	10 (17%)
2	NAP	C	401	-	45,52,52	1.74	12 (26%)	56,80,80	1.18	5 (8%)

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	NAP	A	401	-	-	8/31/67/67	0/5/5/5
2	NAP	D	401	-	-	11/31/67/67	0/5/5/5
2	NAP	B	401	-	-	8/31/67/67	0/5/5/5
2	NAP	C	401	-	-	14/31/67/67	0/5/5/5

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	C2D-C1D	-4.03	1.47	1.53
2	D	401	NAP	C2N-N1N	-3.91	1.30	1.35
2	C	401	NAP	PN-O1N	-3.75	1.37	1.50
2	A	401	NAP	PA-O2A	-3.56	1.38	1.55
2	D	401	NAP	P2B-O2X	-3.36	1.41	1.54

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAP	C5D-C4D-C3D	-4.66	97.70	115.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	NAP	C4A-C5A-N7A	-4.32	104.89	109.40
2	B	401	NAP	C5A-C6A-N6A	4.32	126.91	120.35
2	A	401	NAP	N3A-C2A-N1A	-4.27	122.01	128.68
2	B	401	NAP	N3A-C2A-N1A	-4.17	122.17	128.68

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	PA-O3-PN-O5D
2	B	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	C5B-O5B-PA-O1A
2	C	401	NAP	PN-O3-PA-O5B

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	3	0
2	D	401	NAP	4	0
2	B	401	NAP	4	0
2	C	401	NAP	4	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 then 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 NAP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 401

Bond lengths

Bond angles

Torsions

Rings
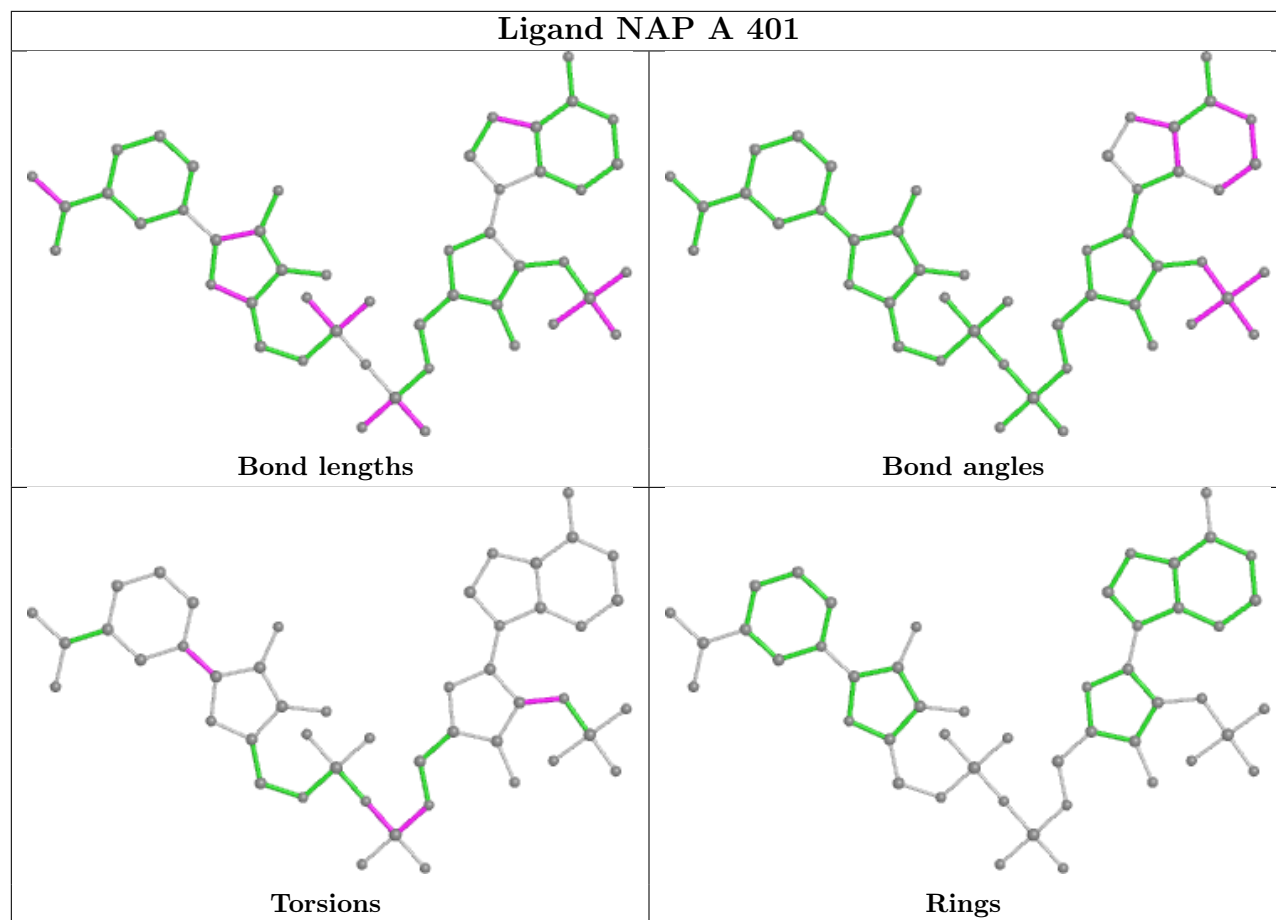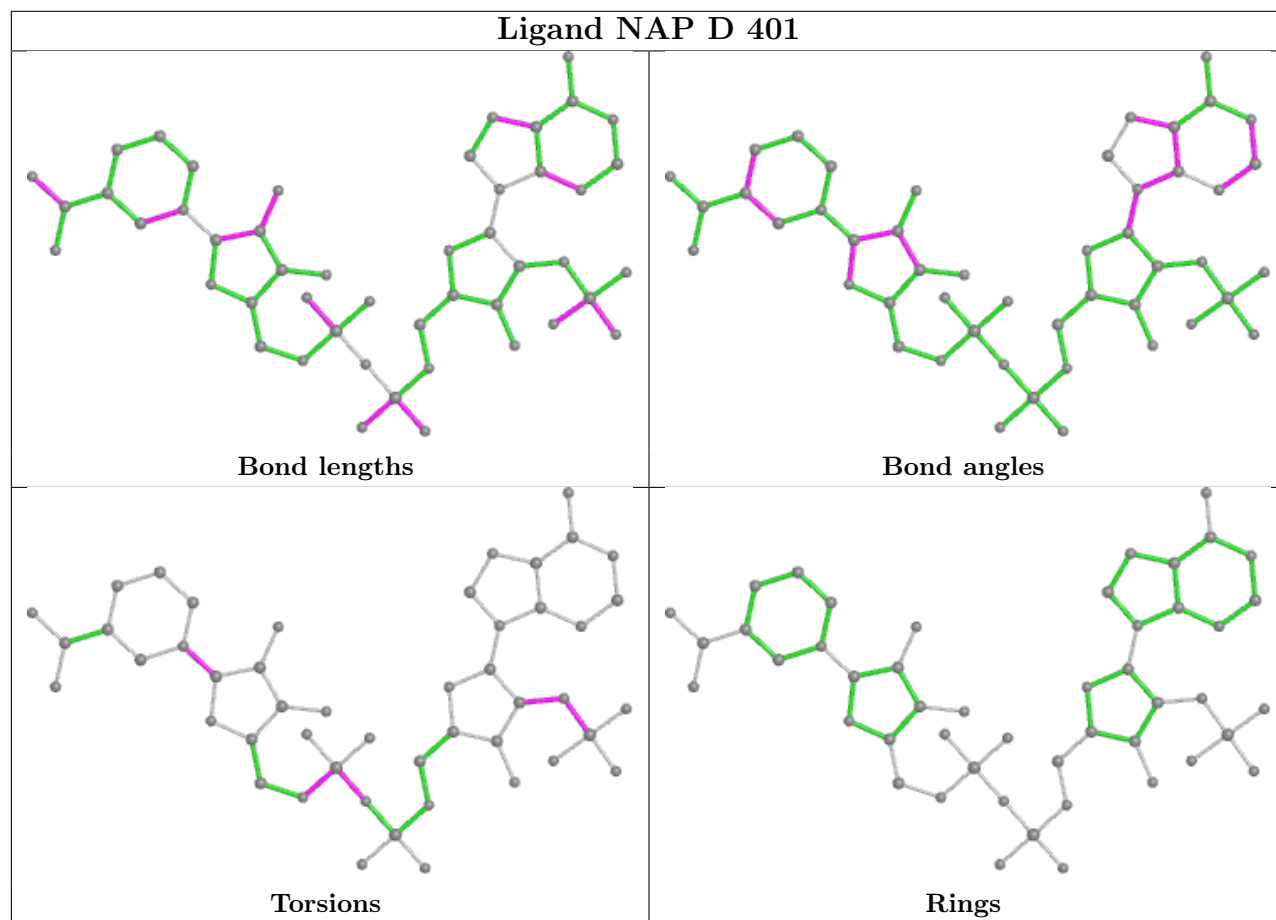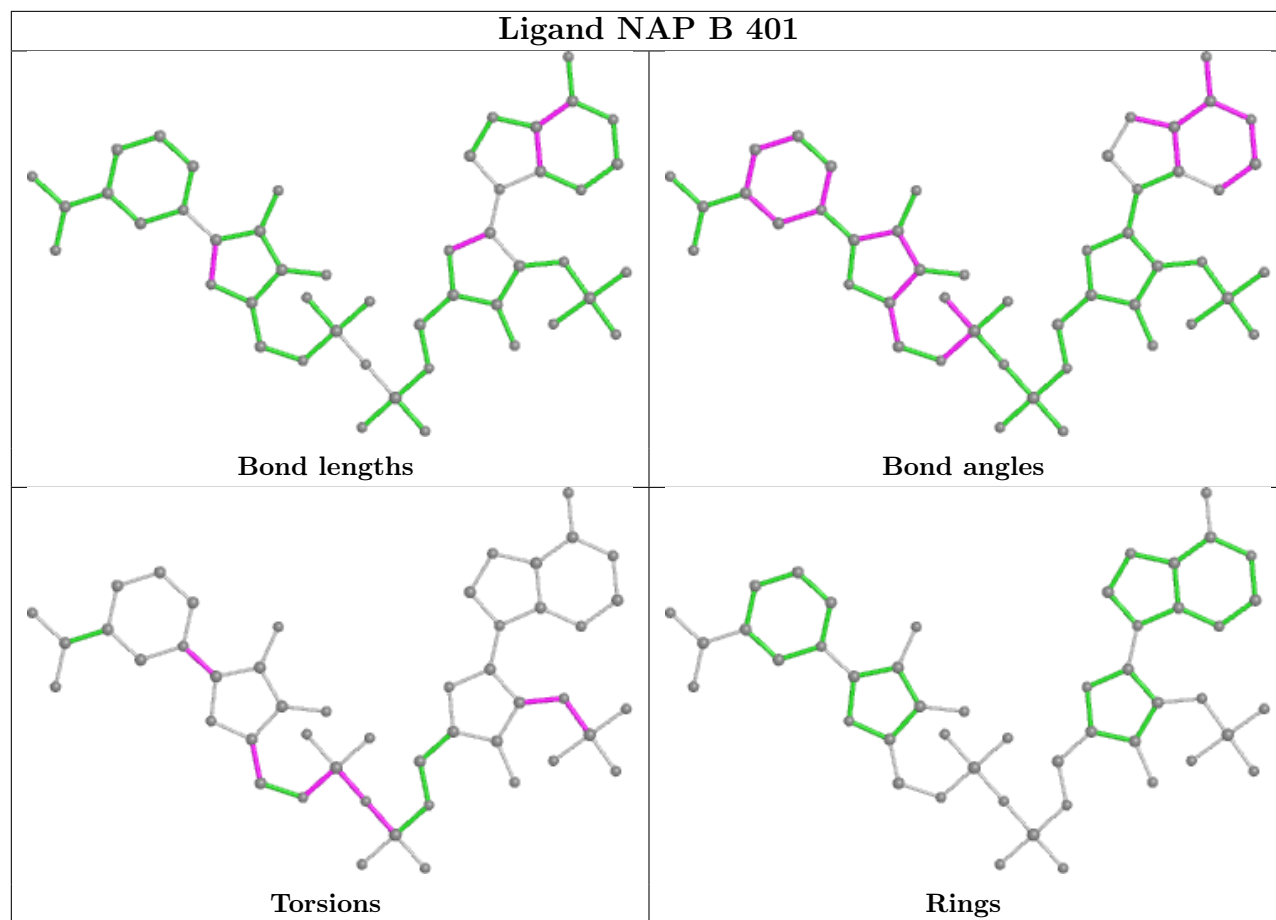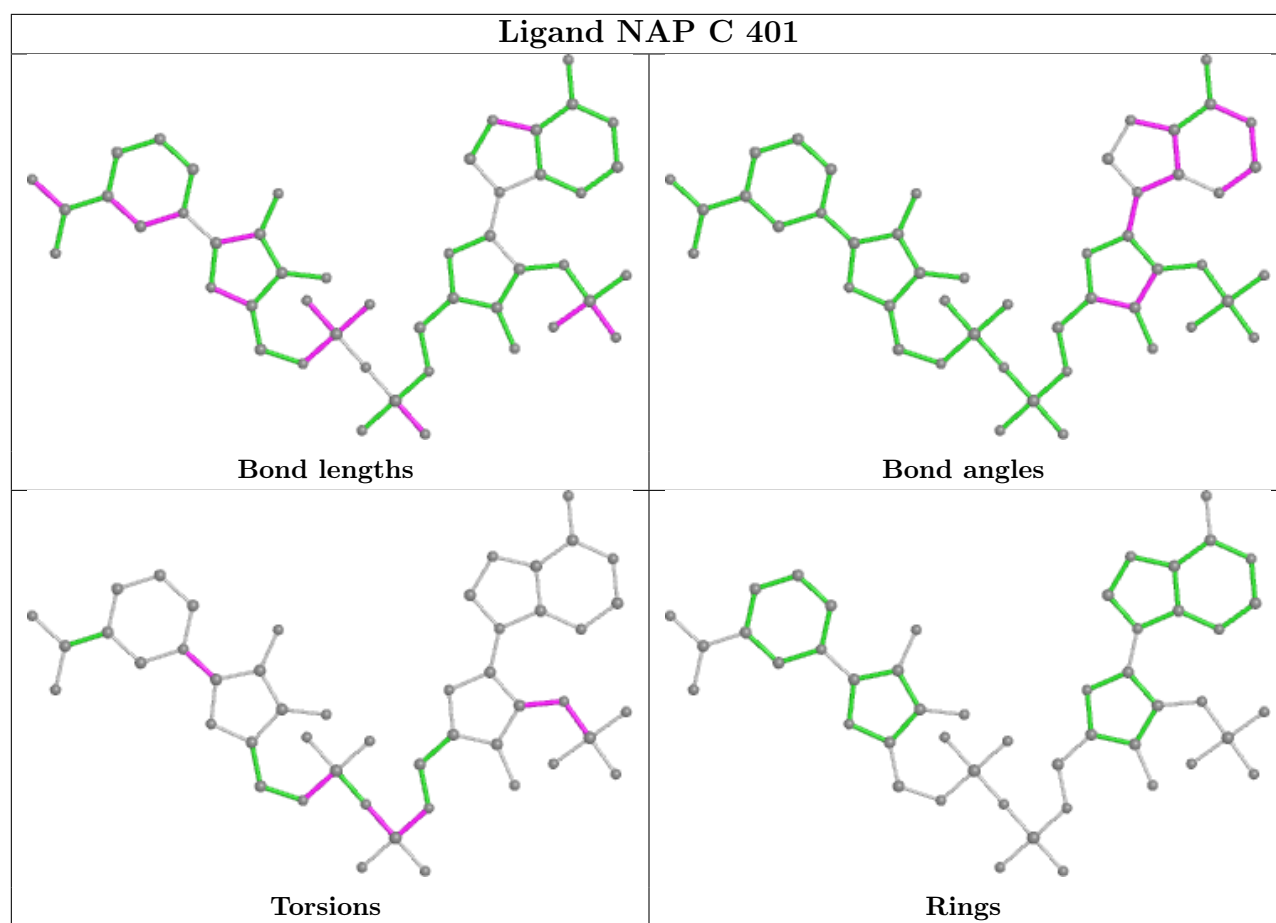
5.7 Other polymers ⓘ

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	358/385 (92%)	-0.10	12 (3%)	45	52	13, 24, 49, 98	0
1	B	345/385 (89%)	-0.04	8 (2%)	60	67	12, 25, 48, 67	0
1	C	336/385 (87%)	-0.14	7 (2%)	63	70	14, 26, 44, 67	0
1	D	343/385 (89%)	0.06	14 (4%)	37	44	13, 28, 52, 86	0
All	All	1382/1540 (89%)	-0.06	41 (2%)	50	57	12, 26, 49, 98	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	PRO	6.5
1	D	268	PRO	4.2
1	A	265	TYR	4.1
1	D	43	ALA	4.1
1	A	266	ARG	3.8

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

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

6.3 Carbohydrates ⓘ

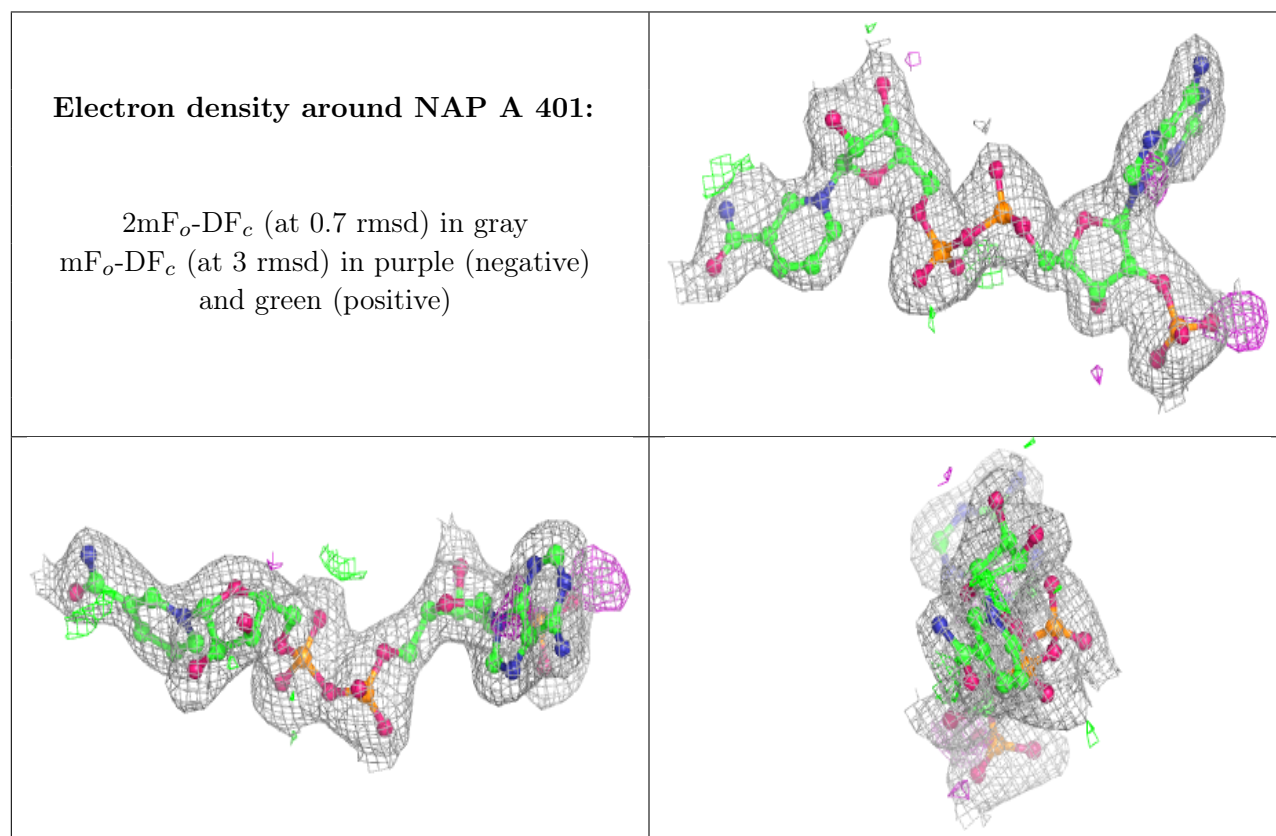There are no monosaccharides in this entry.

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(Å^2)	Q<0.9
2	NAP	A	401	48/48	0.94	0.12	24,28,52,54	0
2	NAP	B	401	48/48	0.95	0.10	29,35,43,45	0
2	NAP	D	401	48/48	0.95	0.10	25,35,42,52	0
2	NAP	C	401	48/48	0.96	0.10	26,31,49,50	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.
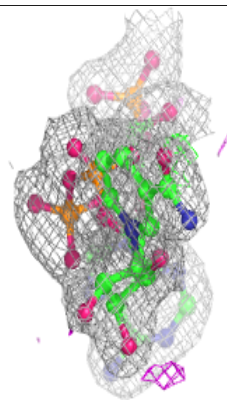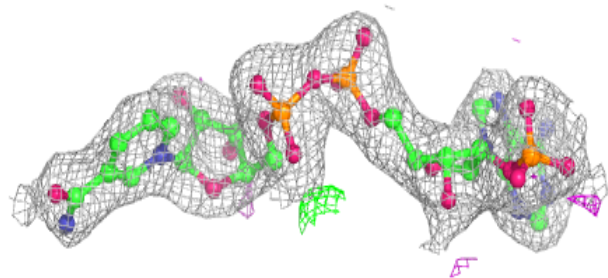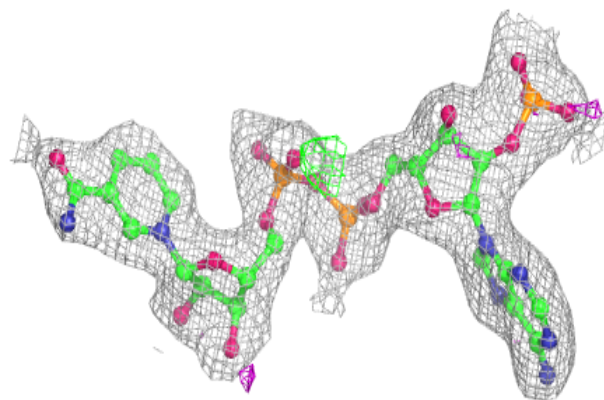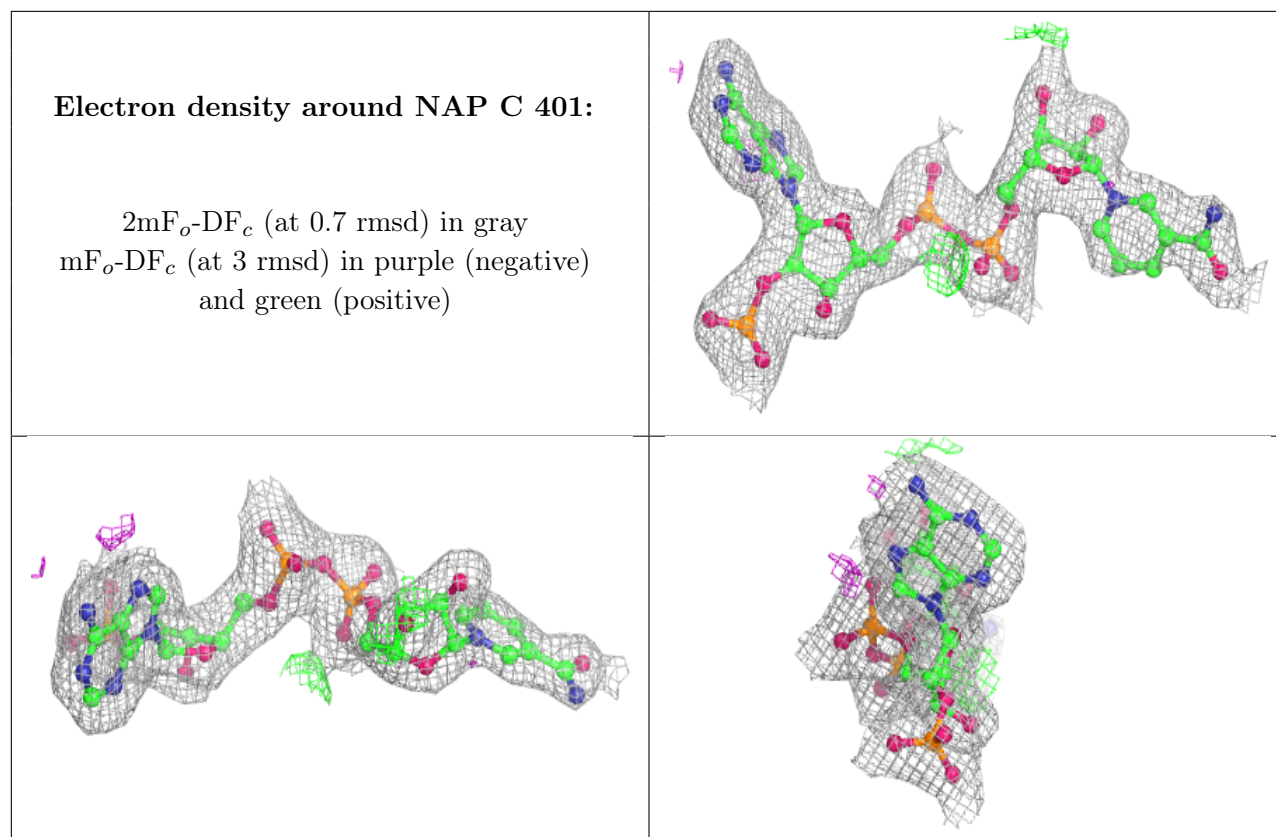
Electron density around NAP A 401:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

Electron density around NAP B 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
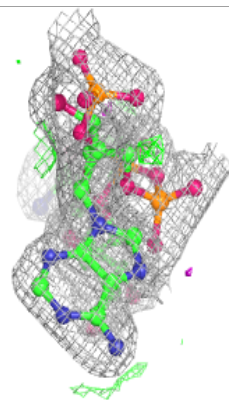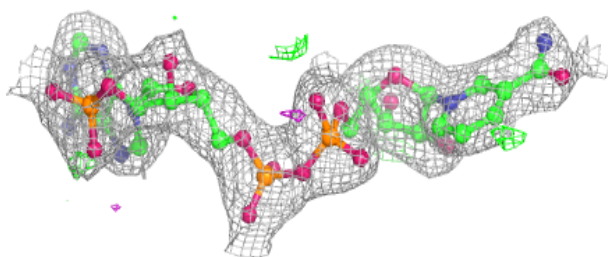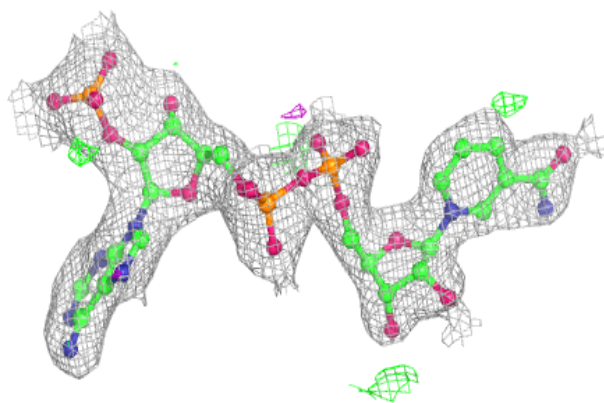
Electron density around NAP D 401:

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

Electron density around NAP C 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.