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 (i)

Oct 9, 2023 – 07:59 AM EDT

PDB ID	:	7TWZ
Title	:	Crystal Structure of NADP-linked putative oxidoreductase from Klebsiella pneumoniae
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2022-02-07
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

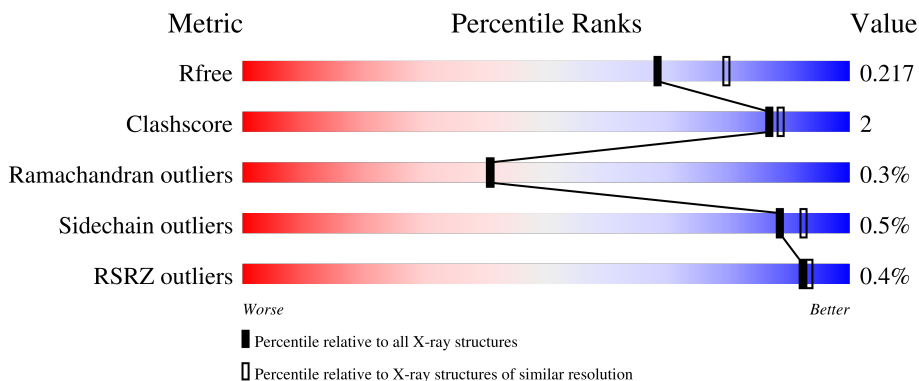|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 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.
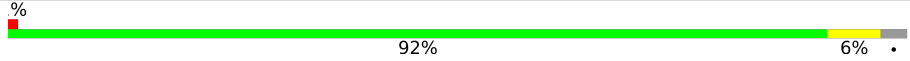
Metric	Percentile Ranks	Value
Rfree		0.217
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		0.5%
RSRZ outliers		0.4%

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	306	92% 5% ·
1	B	306	% 92% 5% ·
1	C	306	94% · ·
1	D	306	93% · ·
1	E	306	% 89% 8% ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	306	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15983 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 Putative oxidoreductase, NAD(P)-linked.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	5	0
			2396	1519	430	434	13			
1	B	298	Total	C	N	O	S	0	5	0
			2403	1525	433	432	13			
1	C	298	Total	C	N	O	S	0	5	0
			2399	1521	431	434	13			
1	D	298	Total	C	N	O	S	0	8	0
			2417	1535	436	433	13			
1	E	298	Total	C	N	O	S	0	4	0
			2389	1515	429	432	13			
1	F	298	Total	C	N	O	S	0	5	0
			2401	1522	435	432	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP A0A0H3GP70
A	-6	ALA	-	expression tag	UNP A0A0H3GP70
A	-5	HIS	-	expression tag	UNP A0A0H3GP70
A	-4	HIS	-	expression tag	UNP A0A0H3GP70
A	-3	HIS	-	expression tag	UNP A0A0H3GP70
A	-2	HIS	-	expression tag	UNP A0A0H3GP70
A	-1	HIS	-	expression tag	UNP A0A0H3GP70
A	0	HIS	-	expression tag	UNP A0A0H3GP70
B	-7	MET	-	initiating methionine	UNP A0A0H3GP70
B	-6	ALA	-	expression tag	UNP A0A0H3GP70
B	-5	HIS	-	expression tag	UNP A0A0H3GP70
B	-4	HIS	-	expression tag	UNP A0A0H3GP70
B	-3	HIS	-	expression tag	UNP A0A0H3GP70
B	-2	HIS	-	expression tag	UNP A0A0H3GP70
B	-1	HIS	-	expression tag	UNP A0A0H3GP70
B	0	HIS	-	expression tag	UNP A0A0H3GP70
C	-7	MET	-	initiating methionine	UNP A0A0H3GP70

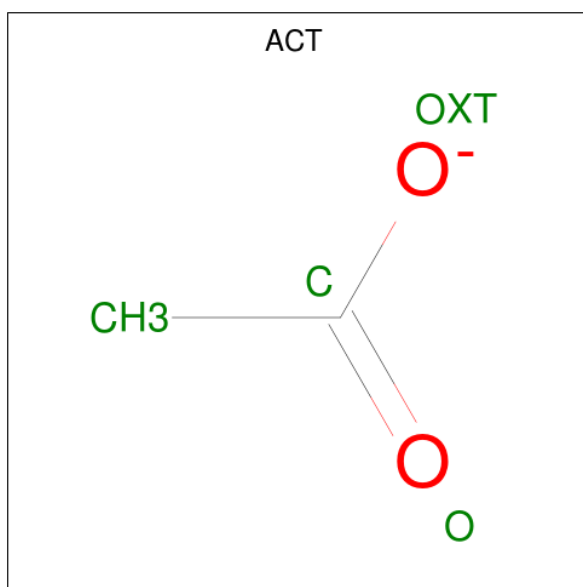*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ALA	-	expression tag	UNP A0A0H3GP70
C	-5	HIS	-	expression tag	UNP A0A0H3GP70
C	-4	HIS	-	expression tag	UNP A0A0H3GP70
C	-3	HIS	-	expression tag	UNP A0A0H3GP70
C	-2	HIS	-	expression tag	UNP A0A0H3GP70
C	-1	HIS	-	expression tag	UNP A0A0H3GP70
C	0	HIS	-	expression tag	UNP A0A0H3GP70
D	-7	MET	-	initiating methionine	UNP A0A0H3GP70
D	-6	ALA	-	expression tag	UNP A0A0H3GP70
D	-5	HIS	-	expression tag	UNP A0A0H3GP70
D	-4	HIS	-	expression tag	UNP A0A0H3GP70
D	-3	HIS	-	expression tag	UNP A0A0H3GP70
D	-2	HIS	-	expression tag	UNP A0A0H3GP70
D	-1	HIS	-	expression tag	UNP A0A0H3GP70
D	0	HIS	-	expression tag	UNP A0A0H3GP70
E	-7	MET	-	initiating methionine	UNP A0A0H3GP70
E	-6	ALA	-	expression tag	UNP A0A0H3GP70
E	-5	HIS	-	expression tag	UNP A0A0H3GP70
E	-4	HIS	-	expression tag	UNP A0A0H3GP70
E	-3	HIS	-	expression tag	UNP A0A0H3GP70
E	-2	HIS	-	expression tag	UNP A0A0H3GP70
E	-1	HIS	-	expression tag	UNP A0A0H3GP70
E	0	HIS	-	expression tag	UNP A0A0H3GP70
F	-7	MET	-	initiating methionine	UNP A0A0H3GP70
F	-6	ALA	-	expression tag	UNP A0A0H3GP70
F	-5	HIS	-	expression tag	UNP A0A0H3GP70
F	-4	HIS	-	expression tag	UNP A0A0H3GP70
F	-3	HIS	-	expression tag	UNP A0A0H3GP70
F	-2	HIS	-	expression tag	UNP A0A0H3GP70
F	-1	HIS	-	expression tag	UNP A0A0H3GP70
F	0	HIS	-	expression tag	UNP A0A0H3GP70

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).
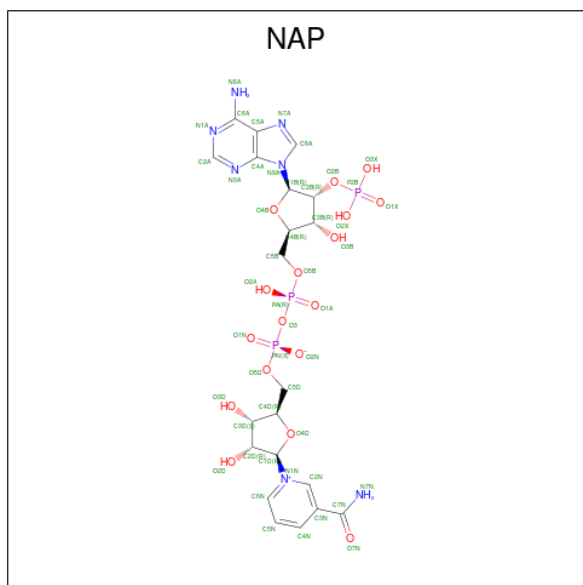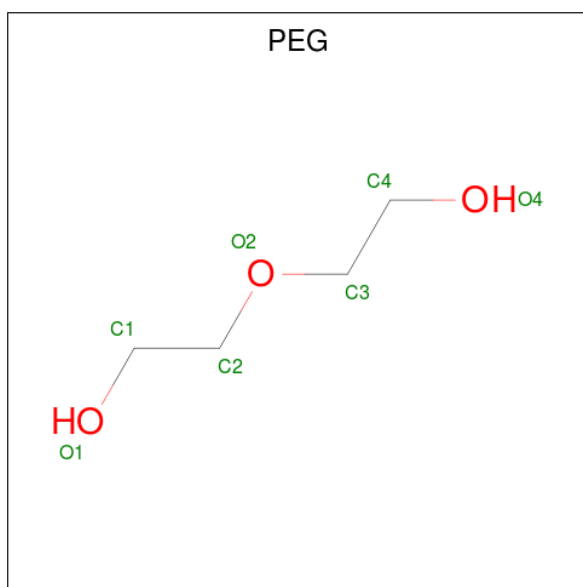
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O^-

C

CH3

O

O

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

C4
OH O4
O2
O
C3
C1
C2
HO
O1

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 4	O 3	0	0
4	A	1	Total 7	C 4	O 3	0	0
4	B	1	Total 7	C 4	O 3	0	0
4	F	1	Total 7	C 4	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	240	Total 244	O 244	0	4
5	B	233	Total 235	O 235	0	2
5	C	229	Total 230	O 230	0	1
5	D	206	Total 207	O 207	0	1
5	E	154	Total 154	O 154	0	0
5	F	163	Total 164	O 164	0	1

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

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: Putative oxidoreductase, NAD(P)-linked

Chain A:

- Molecule 1: Putative oxidoreductase, NAD(P)-linked

Chain B:
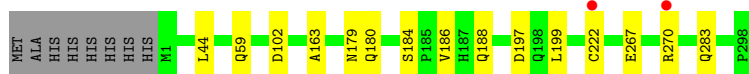
- Molecule 1: Putative oxidoreductase, NAD(P)-linked

Chain C:

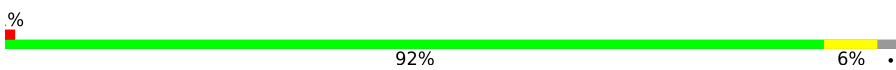- Molecule 1: Putative oxidoreductase, NAD(P)-linked

Chain D:

- Molecule 1: Putative oxidoreductase, NAD(P)-linked

Chain E:

F286 P298

• Molecule 1: Putative oxidoreductase, NAD(P)-linked

Chain F:

%

92% 6% •

MET ALA HIS HIS HIS HIS HIS HIS M1 V2 Q3 M29 L34 V35 S36 E39 Q40 L68 L74 H98 E111 K151 Q180 V181 E182 Q188 Q198 W209 C222 I266 R289 P298

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	83.15Å 89.10Å 89.71Å 119.63° 90.13° 92.13°	Depositor
Resolution (Å)	44.92 – 2.10 44.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.8 (44.92-2.10) 92.1 (44.92-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.10Å)	Xtriage
Refinement program	PHENIX 4438	Depositor
R, R_{free}	0.183 , 0.217 0.183 , 0.217	Depositor DCC
R_{free} test set	1873 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.1	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.036 for h,k+l,-k 0.036 for h,-l,k+l 0.048 for h,l,-k-l 0.048 for h,-k-l,k 0.040 for h,-k,-l 0.043 for -h,k,-k-l 0.359 for -h,-k-l,l 0.075 for -h,l,k 0.044 for -h,-l,-k 0.039 for -h,-k,k+l 0.036 for -h,k+l,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15983	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 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ACT, 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	0.40	0/2465	0.62	1/3342 (0.0%)
1	B	0.36	0/2472	0.62	0/3350
1	C	0.37	0/2468	0.61	0/3346
1	D	0.37	0/2495	0.61	0/3381
1	E	0.35	0/2455	0.59	0/3329
1	F	0.34	0/2470	0.61	0/3348
All	All	0.37	0/14825	0.61	1/20096 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	193	ASP	CB-CG-OD1	5.53	123.28	118.30

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	2396	0	2397	10	0
1	B	2403	0	2411	12	0
1	C	2399	0	2400	7	0
1	D	2417	0	2433	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2389	0	2380	16	0
1	F	2401	0	2399	12	0
2	A	48	0	23	1	0
2	B	48	0	24	1	0
2	C	48	0	23	1	0
2	D	48	0	25	1	0
2	E	48	0	23	0	0
2	F	48	0	23	1	0
3	A	8	0	6	0	0
3	B	8	0	6	0	0
3	C	8	0	6	1	0
3	E	4	0	3	0	0
4	A	14	0	20	5	0
4	B	7	0	10	1	0
4	F	7	0	10	2	0
5	A	244	0	0	5	0
5	B	235	0	0	5	0
5	C	230	0	0	0	0
5	D	207	0	0	4	0
5	E	154	0	0	1	0
5	F	164	0	0	2	0
All	All	15983	0	14622	61	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 2.

The worst 5 of 61 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:NH1	1:A:95:THR:O	2.23	0.70
1:A:57:ASP:OD2	5:A:501:HOH:O	2.08	0.70
1:D:277:LYS:NZ	5:D:501:HOH:O	2.25	0.69
1:A:115:ARG:NH1	5:A:502:HOH:O	2.27	0.65
1:F:3:GLN:OE1	5:F:501:HOH:O	2.14	0.65

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	301/306 (98%)	299 (99%)	1 (0%)	1 (0%)	41	41
1	B	301/306 (98%)	300 (100%)	0	1 (0%)	41	41
1	C	301/306 (98%)	300 (100%)	0	1 (0%)	41	41
1	D	304/306 (99%)	302 (99%)	1 (0%)	1 (0%)	41	41
1	E	300/306 (98%)	296 (99%)	3 (1%)	1 (0%)	41	41
1	F	301/306 (98%)	298 (99%)	2 (1%)	1 (0%)	41	41
All	All	1808/1836 (98%)	1795 (99%)	7 (0%)	6 (0%)	41	41

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	188	GLN
1	D	188	GLN
1	E	188	GLN
1	F	188	GLN
1	A	188	GLN

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	258/260 (99%)	255 (99%)	3 (1%)	71	77
1	B	258/260 (99%)	257 (100%)	1 (0%)	91	94
1	C	258/260 (99%)	257 (100%)	1 (0%)	91	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	260/260 (100%)	259 (100%)	1 (0%)	91	94
1	E	255/260 (98%)	254 (100%)	1 (0%)	91	94
1	F	256/260 (98%)	255 (100%)	1 (0%)	91	94
All	All	1545/1560 (99%)	1537 (100%)	8 (0%)	88	92

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	36	SER
1	E	184	SER
1	C	222	CYS
1	B	222	CYS
1	D	222	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	154	HIS
1	B	232	GLN
1	E	256	GLN
1	C	232	GLN
1	A	256	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	ACT	C	402	-	3,3,3	1.32	0	3,3,3	1.43	0
3	ACT	C	403	-	3,3,3	1.50	0	3,3,3	1.24	0
2	NAP	C	401	-	45,52,52	4.37	15 (33%)	56,80,80	1.78	10 (17%)
2	NAP	E	401	-	45,52,52	4.44	15 (33%)	56,80,80	1.62	8 (14%)
3	ACT	A	402	-	3,3,3	1.51	1 (33%)	3,3,3	1.36	0
4	PEG	B	404	-	6,6,6	0.26	0	5,5,5	0.26	0
2	NAP	F	401	-	45,52,52	4.46	16 (35%)	56,80,80	1.62	8 (14%)
3	ACT	B	402	-	3,3,3	1.36	1 (33%)	3,3,3	1.54	0
4	PEG	A	404	-	6,6,6	0.29	0	5,5,5	0.27	0
4	PEG	F	402	-	6,6,6	0.17	0	5,5,5	0.11	0
3	ACT	B	403	-	3,3,3	1.48	1 (33%)	3,3,3	1.40	0
4	PEG	A	403	-	6,6,6	0.18	0	5,5,5	0.15	0
2	NAP	A	401	-	45,52,52	4.37	15 (33%)	56,80,80	1.62	7 (12%)
2	NAP	B	401	-	45,52,52	4.49	15 (33%)	56,80,80	1.66	8 (14%)
3	ACT	E	402	-	3,3,3	1.30	0	3,3,3	1.35	0
3	ACT	A	405	-	3,3,3	1.39	0	3,3,3	1.54	0
2	NAP	D	401	-	45,52,52	4.30	15 (33%)	56,80,80	1.72	8 (14%)

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	C	401	-	-	3/31/67/67	0/5/5/5
2	NAP	E	401	-	-	4/31/67/67	0/5/5/5
4	PEG	F	402	-	-	1/4/4/4	-
4	PEG	B	404	-	-	0/4/4/4	-
2	NAP	F	401	-	-	4/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	403	-	-	1/4/4/4	-
2	NAP	A	401	-	-	5/31/67/67	0/5/5/5
2	NAP	B	401	-	-	5/31/67/67	0/5/5/5
4	PEG	A	404	-	-	4/4/4/4	-
2	NAP	D	401	-	-	4/31/67/67	0/5/5/5

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	O4B-C1B	15.88	1.63	1.41
2	F	401	NAP	O4D-C1D	15.34	1.62	1.41
2	F	401	NAP	O4B-C1B	15.31	1.62	1.41
2	E	401	NAP	O4B-C1B	15.26	1.62	1.41
2	C	401	NAP	O4D-C1D	15.25	1.62	1.41

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	NAP	N3A-C2A-N1A	-5.85	119.53	128.68
2	A	401	NAP	N3A-C2A-N1A	-5.59	119.94	128.68
2	F	401	NAP	N3A-C2A-N1A	-5.58	119.96	128.68
2	D	401	NAP	C5A-C6A-N6A	5.53	128.76	120.35
2	E	401	NAP	N3A-C2A-N1A	-5.50	120.08	128.68

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C6N
2	B	401	NAP	PN-O3-PA-O5B
2	B	401	NAP	C2B-O2B-P2B-O2X
2	B	401	NAP	O4D-C1D-N1N-C6N
2	C	401	NAP	PN-O3-PA-O5B

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	ACT	1	0
2	C	401	NAP	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	PEG	1	0
2	F	401	NAP	1	0
4	A	404	PEG	3	0
4	F	402	PEG	2	0
4	A	403	PEG	2	0
2	A	401	NAP	1	0
2	B	401	NAP	1	0
2	D	401	NAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP E 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 401

Bond lengths

Bond angles

Torsions

Rings
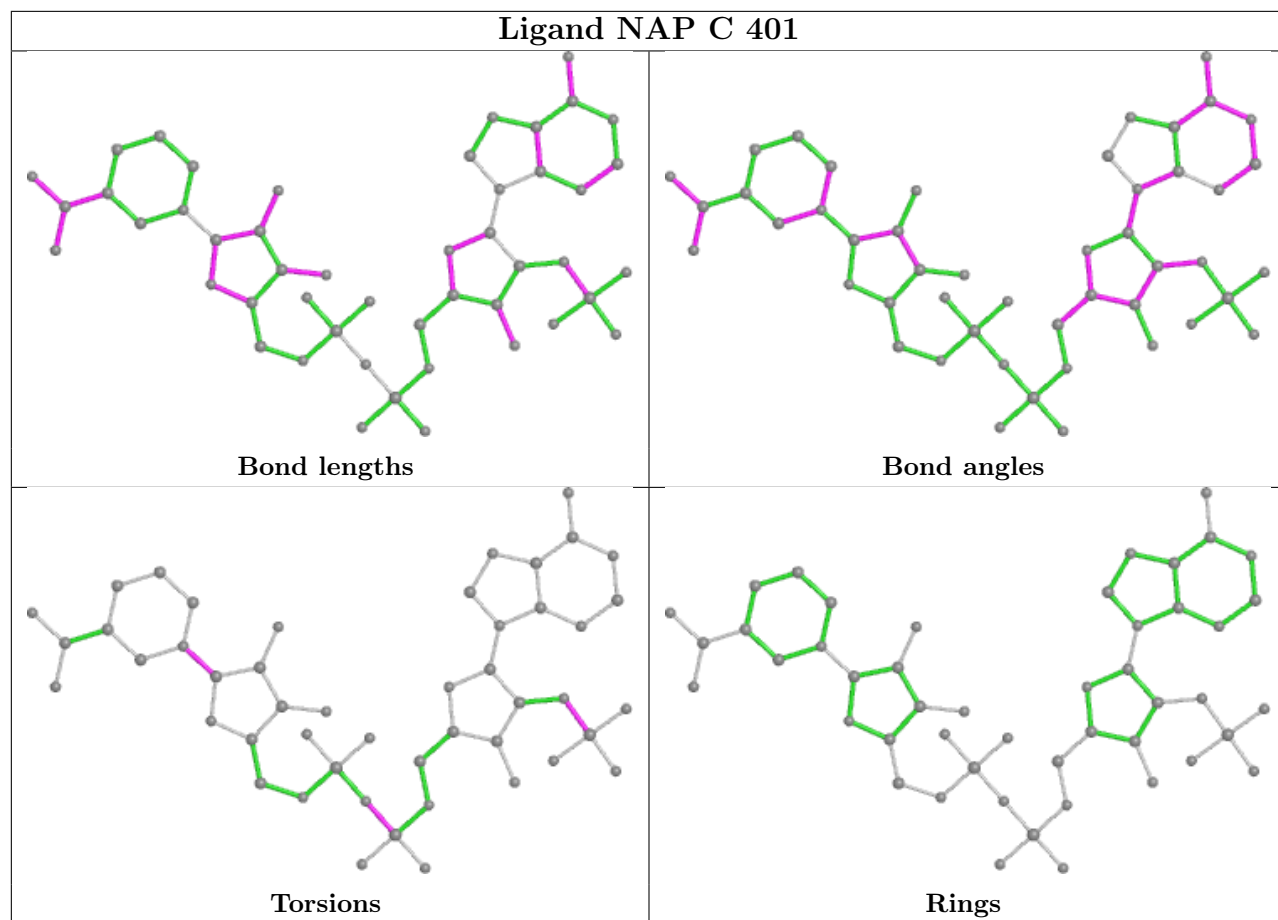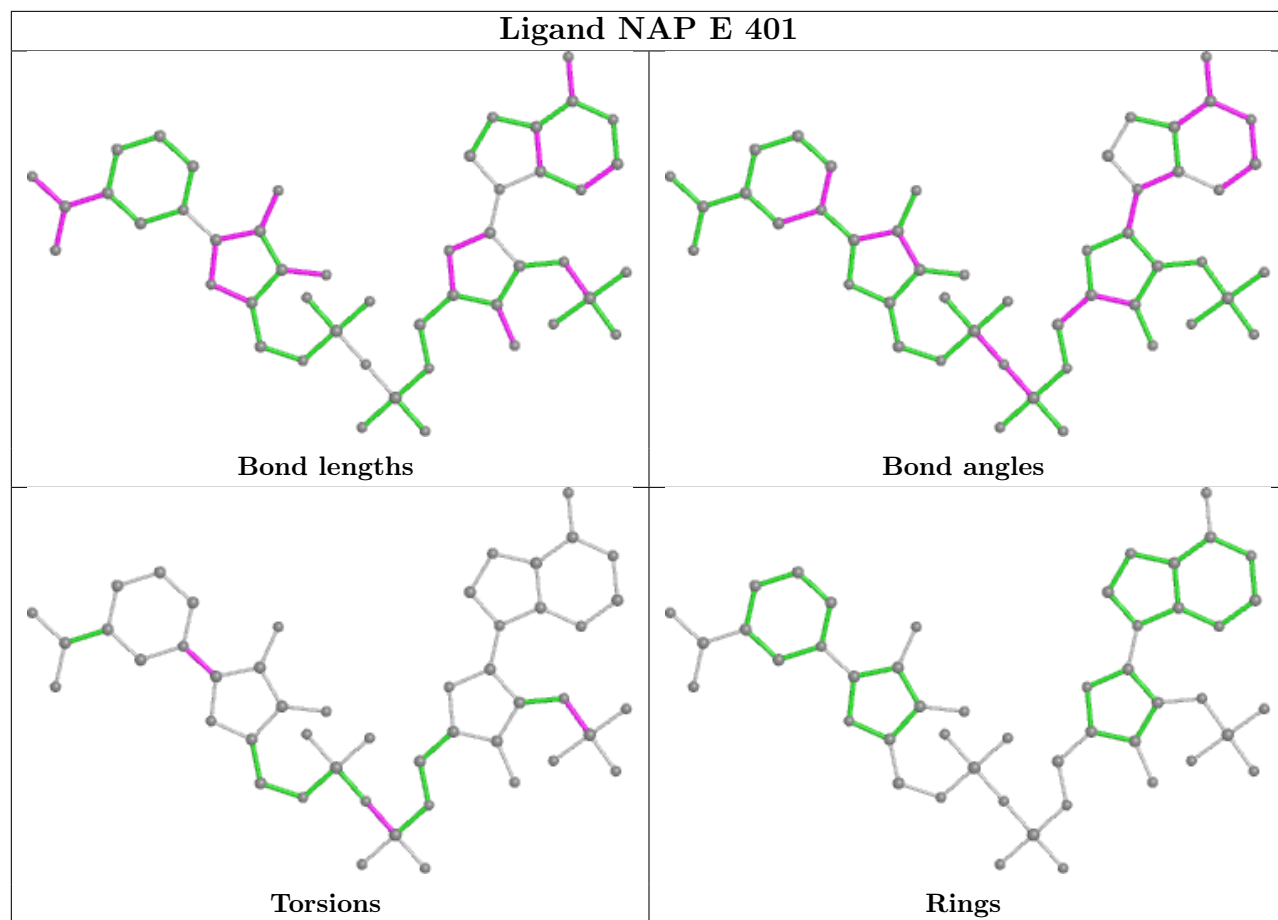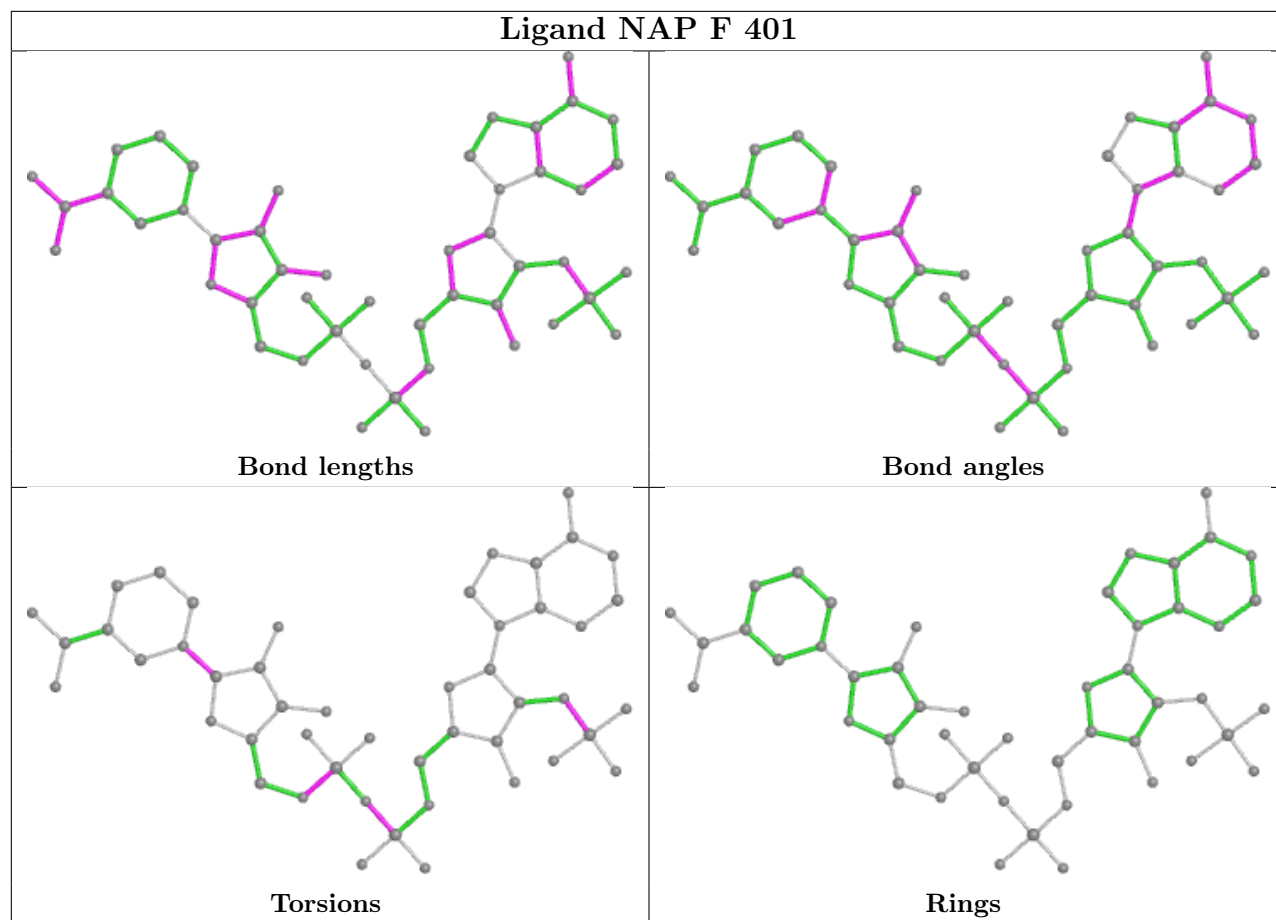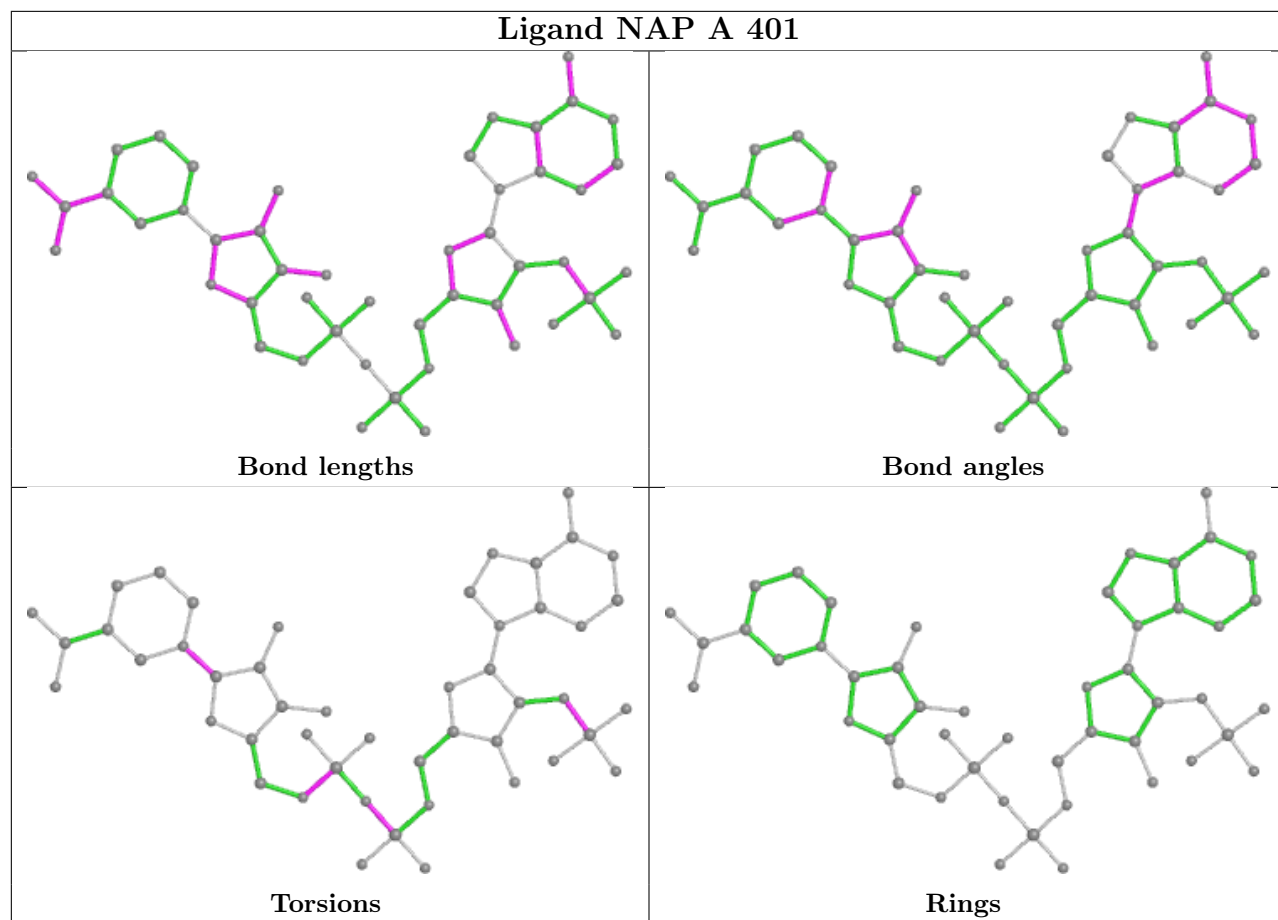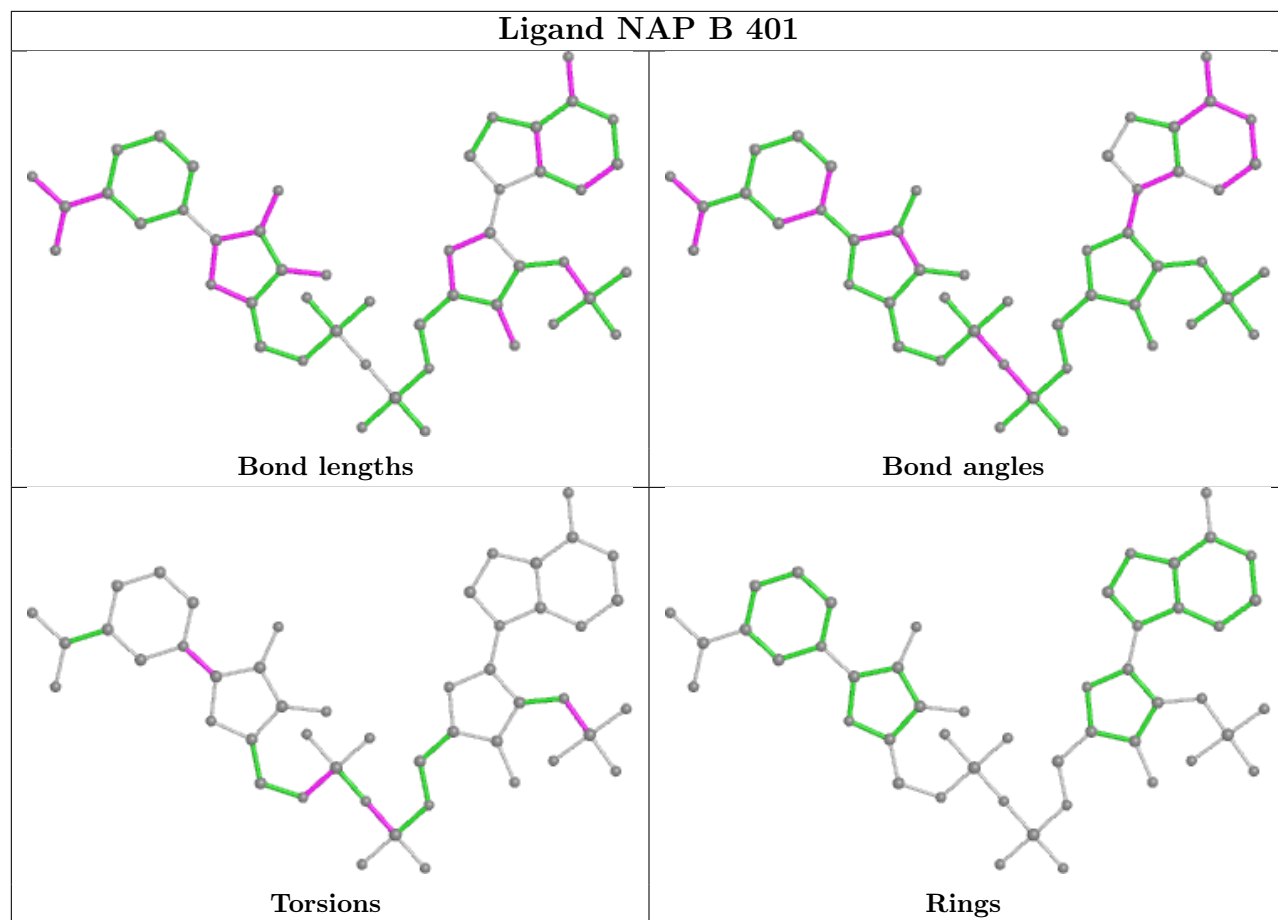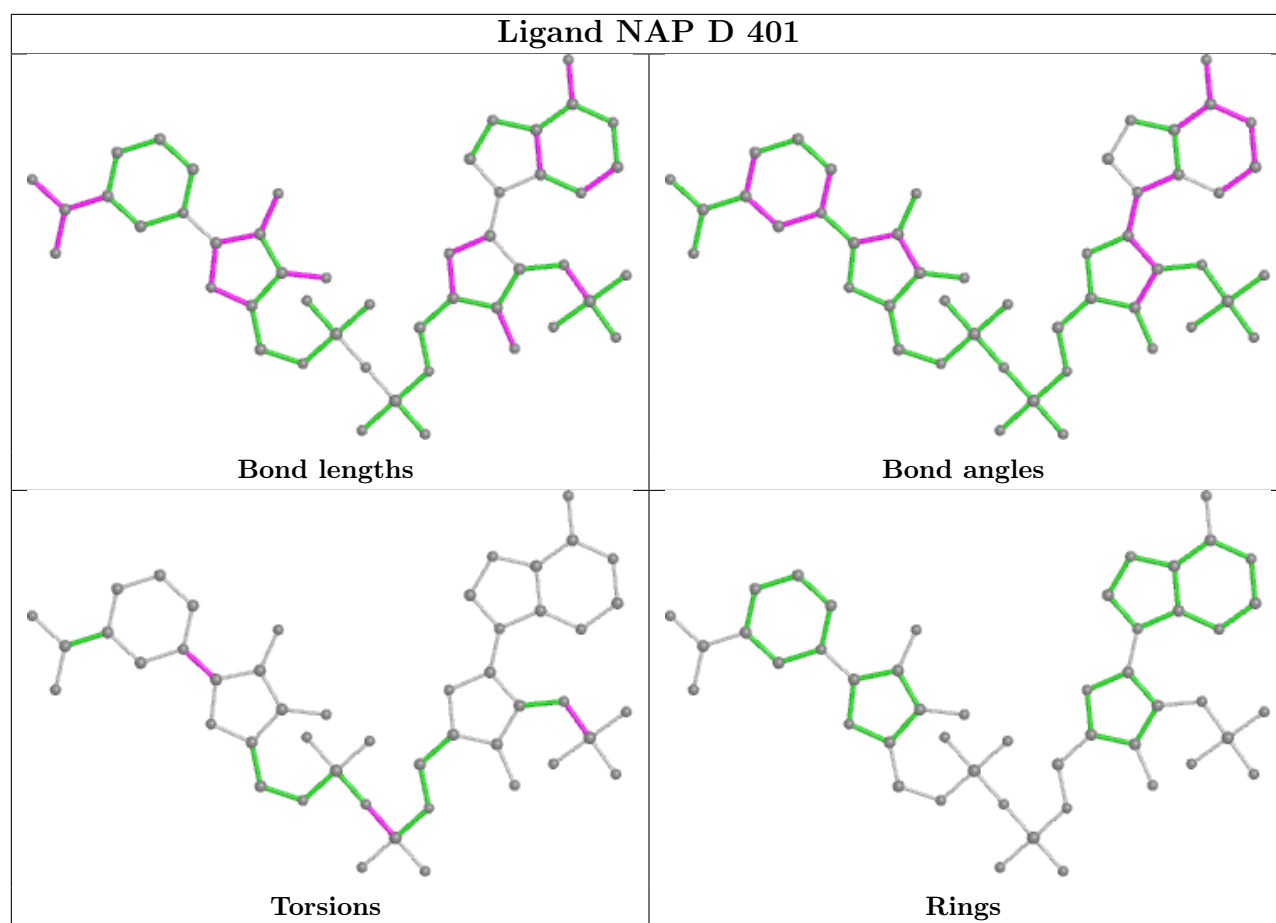
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	298/306 (97%)	-0.31	0 100	100	20, 29, 42, 67	0
1	B	298/306 (97%)	-0.23	2 (0%) 87	89	22, 32, 47, 65	0
1	C	298/306 (97%)	-0.33	0 100	100	20, 30, 43, 79	0
1	D	298/306 (97%)	-0.28	1 (0%) 94	94	22, 32, 47, 71	0
1	E	298/306 (97%)	-0.10	2 (0%) 87	89	23, 36, 58, 67	0
1	F	298/306 (97%)	0.01	3 (1%) 82	85	23, 39, 64, 81	0
All	All	1788/1836 (97%)	-0.21	8 (0%) 92	93	20, 32, 54, 81	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	222	CYS	3.4
1	E	118	ALA	3.2
1	F	34	LEU	2.9
1	F	222	CYS	2.5
1	B	222	CYS	2.5

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
3	ACT	A	402	4/4	0.77	0.19	38,39,40,44	0
3	ACT	C	403	4/4	0.84	0.20	41,41,43,46	0
3	ACT	B	403	4/4	0.85	0.18	38,40,41,45	0
3	ACT	B	402	4/4	0.86	0.17	41,46,47,48	0
3	ACT	C	402	4/4	0.88	0.12	34,43,46,46	0
4	PEG	A	403	7/7	0.91	0.25	29,37,41,43	0
4	PEG	B	404	7/7	0.91	0.16	22,34,46,47	0
4	PEG	F	402	7/7	0.91	0.13	39,41,48,51	0
2	NAP	F	401	48/48	0.92	0.11	29,47,61,63	0
3	ACT	A	405	4/4	0.93	0.13	34,38,38,42	0
4	PEG	A	404	7/7	0.93	0.22	33,36,41,44	0
2	NAP	E	401	48/48	0.94	0.10	27,42,54,62	0
3	ACT	E	402	4/4	0.94	0.12	48,49,53,54	0
2	NAP	D	401	48/48	0.95	0.12	26,37,45,47	0
2	NAP	B	401	48/48	0.96	0.09	23,37,44,45	0
2	NAP	C	401	48/48	0.96	0.10	25,32,39,43	0
2	NAP	A	401	48/48	0.97	0.09	23,31,37,39	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 F 401:

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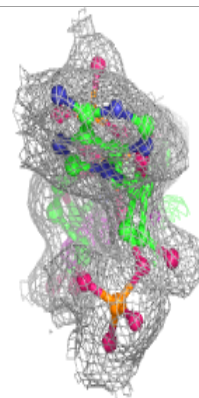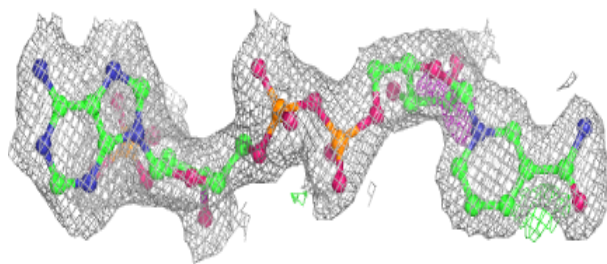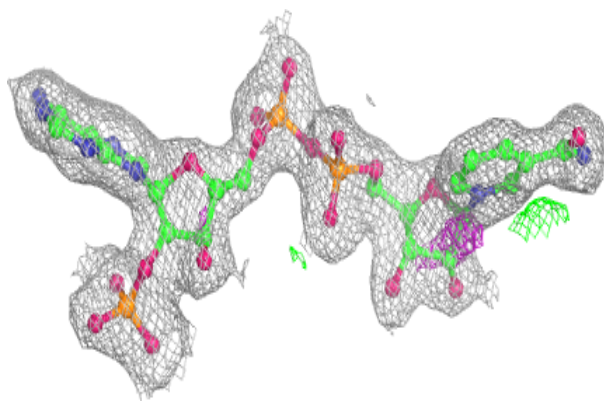and green (positive)
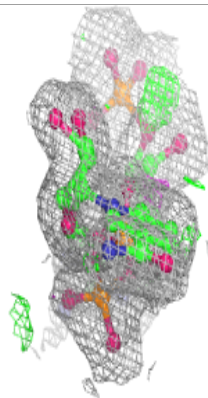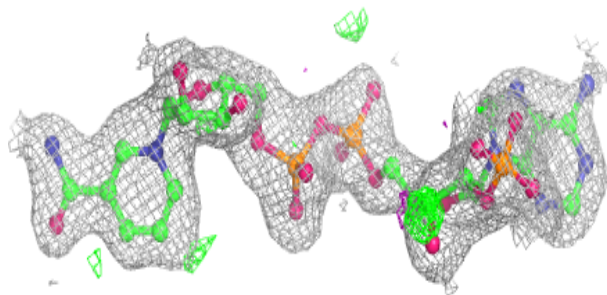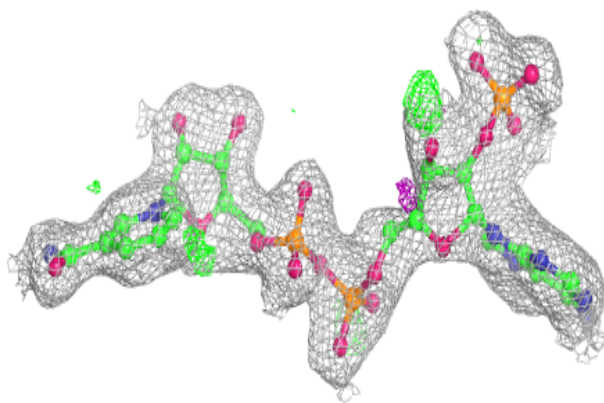
Electron density around NAP E 401:

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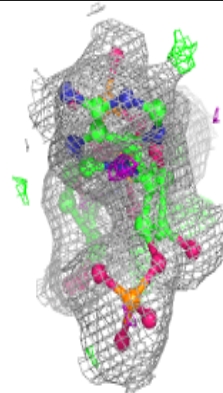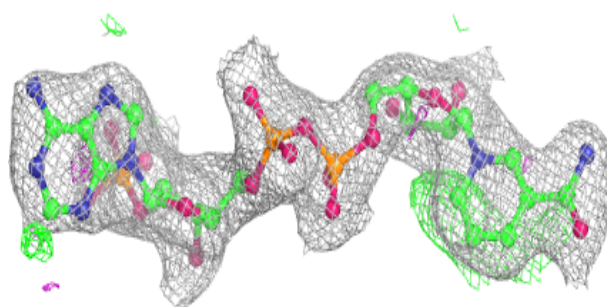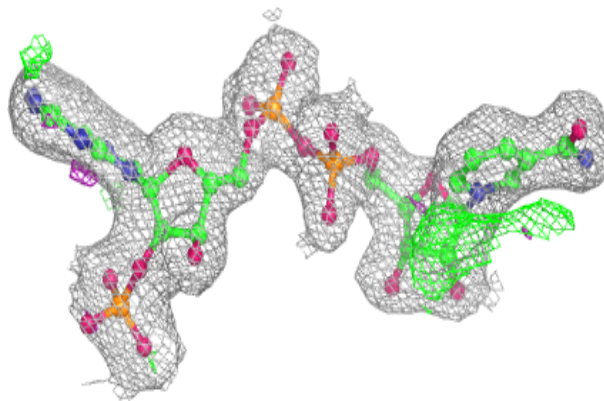
**Electron density around NAP D 401:**

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

Electron density around NAP 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 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)

Electron density around NAP A 401:

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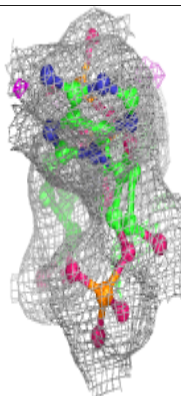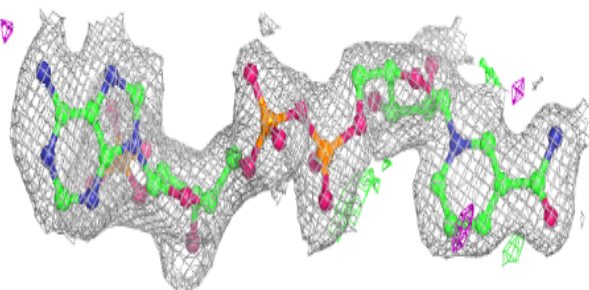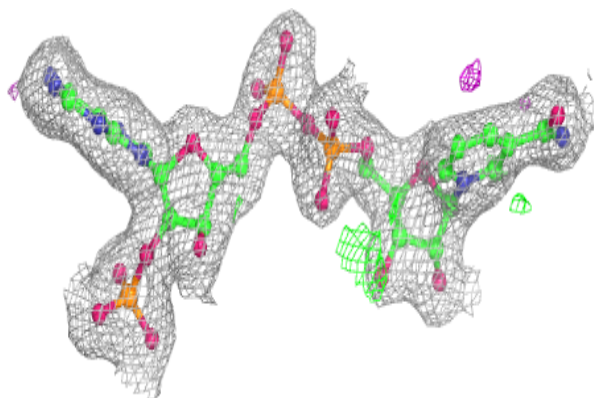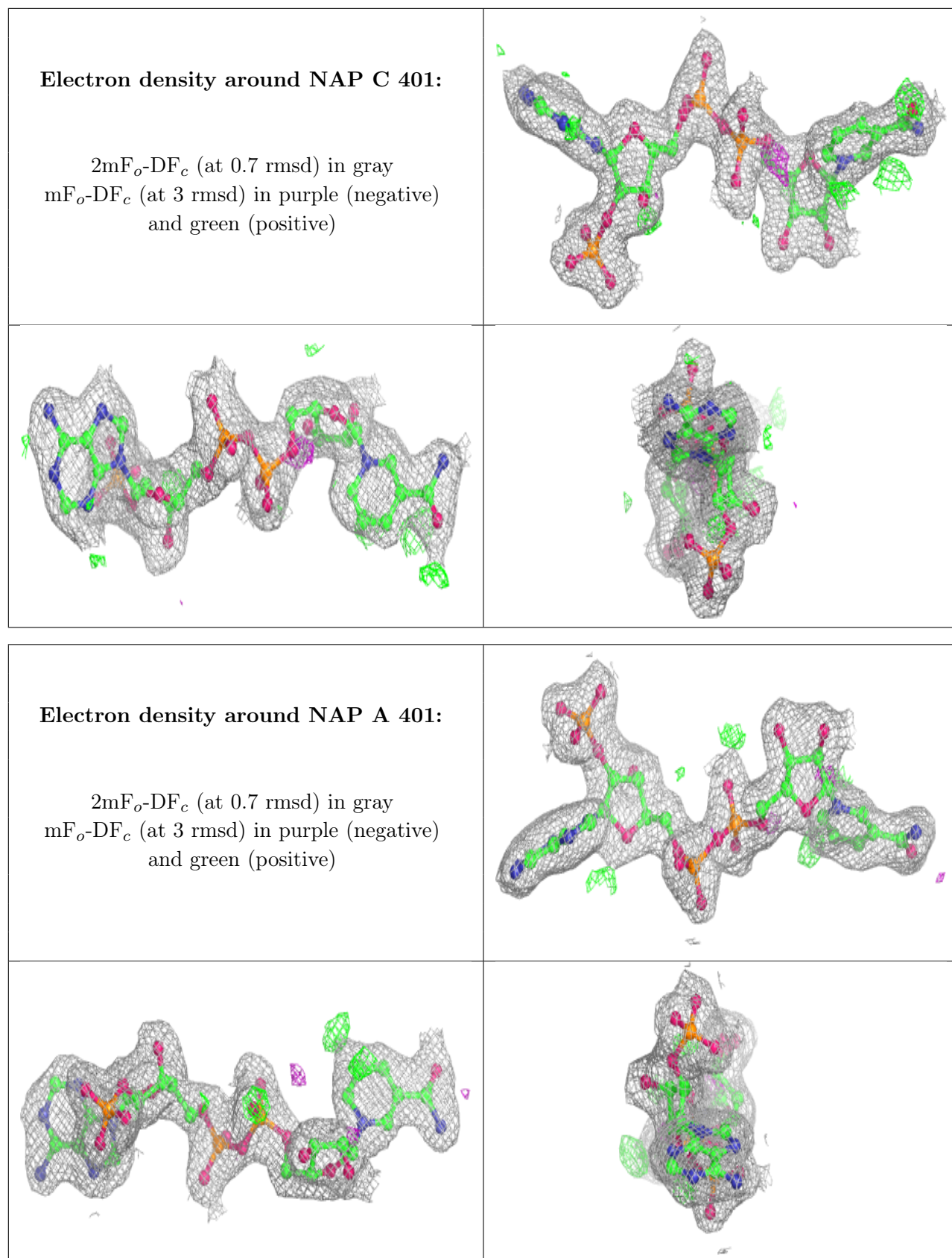
6.5 Other polymers (i)

There are no such residues in this entry.