WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2023 – 08:57 PM EDT

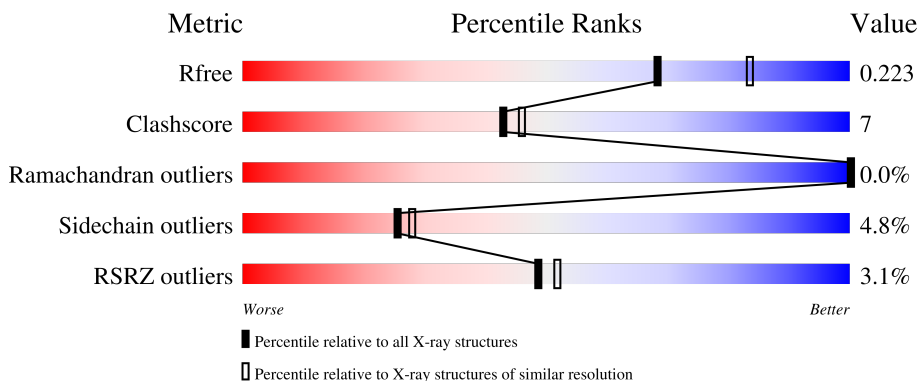|		
PDB ID	:	3SZG
Title	:	Crystal structure of C176A glutamine-dependent NAD+ synthetase from M. tuberculosis bound to AMP/PPi and NaAD+
Authors	:	Chuenchor, W.; Doukov, T.; Gerratana, B.
Deposited on	:	2011-07-19
Resolution	:	2.25 Å(reported)

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 2.25 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		0.223
Clashscore		7
Ramachandran outliers		0.0%
Sidechain outliers		4.8%
RSRZ outliers		3.1%

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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	680	4% ... 81% 13% · ·
1	B	680	2% ... 80% 13% · 5%
1	C	680	3% ... 82% 13% · ·
1	D	680	3% ... 82% 12% · ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 21381 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 Glutamine-dependent NAD(+) synthetase.

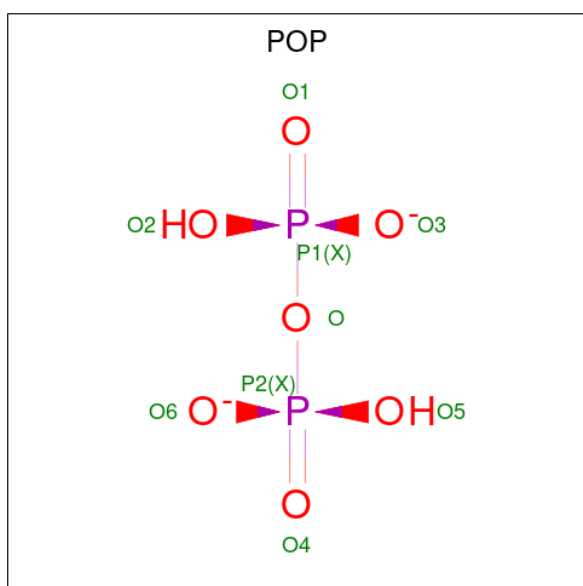| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5040	3191	902	932	15			
1	B	649	Total	C	N	O	S	0	0	0
			5039	3188	902	934	15			
1	C	660	Total	C	N	O	S	0	0	0
			5119	3243	913	948	15			
1	D	658	Total	C	N	O	S	0	0	0
			5116	3242	912	947	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0A5L6
A	176	ALA	CYS	engineered mutation	UNP P0A5L6
B	0	SER	-	expression tag	UNP P0A5L6
B	176	ALA	CYS	engineered mutation	UNP P0A5L6
C	0	SER	-	expression tag	UNP P0A5L6
C	176	ALA	CYS	engineered mutation	UNP P0A5L6
D	0	SER	-	expression tag	UNP P0A5L6
D	176	ALA	CYS	engineered mutation	UNP P0A5L6

- Molecule 2 is NICOTINIC ACID ADENINE DINUCLEOTIDE (three-letter code: DND) (formula: $C_{21}H_{27}N_6O_{15}P_2$).

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DND

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

AMP

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

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 9	O 7	P 2	0	0
4	B	1	Total 9	O 7	P 2	0	0
4	C	1	Total 9	O 7	P 2	0	0
4	D	1	Total 9	O 7	P 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO

O1

OH

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0

- Molecule 6 is water.

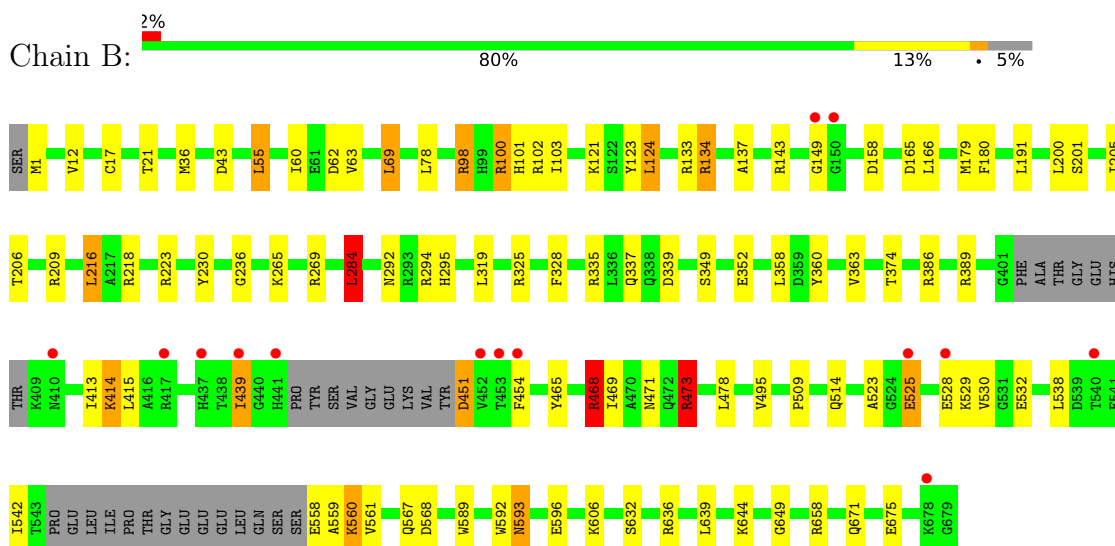| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	162	Total 162	O 162	0	0
6	B	190	Total 190	O 190	0	0
6	C	216	Total 216	O 216	0	0
6	D	177	Total 177	O 177	0	0

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.
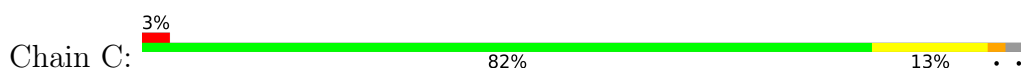
- Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain A:

- Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain B:

- Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain C:

S0 M1 S5 Q8 V12 R13 V14 C17 T21 M36 D43 L55 I60 V63 L69 L70 V73 L78 D79 L80 P96 L97 R98 H99 R100 H101 R102 K121 S122 Y123 R128 R133 R134 A137 R143 G149 D158 L166

M179 F180 L191 L200 S201 I205 T206 R209 L216 R223 V229 G236 R269 L284 N292 R293 R294 E298 A314 L319 L320 R321 R325 F328 Q334 R335 L336 Q337 Q338 D339 S349 E352 Q353 R354 L358 D359 Y360 V363

R386 R389 F402 ALA THR GLY GLU HIS THR K409 N410 I413 R417 A418 H437 T438 I439 G440 H441 P442 Y443 S444 K448 V449 Y450 V457 Y465 R468 I469 A470 N471 Q472 R473 L478 V495 G496 D497 P509 Q514 R518 S522 A523 G524 E525

F526 G527 E528 K529 V530 G531 E532 L538 I542 THR PRO GLU LEU ILE PRO THR GLY GLU GLU GLU LEU GLN SER S557 E558 A559 Q567 W592 N593 E596 K606 S632 R636 S637 A638 L639 K644 G649 Q671 E675 K678 G679

• Molecule 1: Glutamine-dependent NAD(+) synthetase

Chain D:

3%

82%

12%

SER M1 V12 C17 T21 C40 D43 L55 D62 V63 L64 L69 L78 R98 H99 R100 H101 R102 K121 S122 Y123 R128 R134 A137 D140 R143 R147 I148 G149 G150 D158 D165 L166 M179 F180 L200 S201 I205

T206 R209 R213 L216 R223 G236 A243 K265 R269 L284 N292 R293 R294 E298 R305 A314 L319 L320 R321 R325 F328 P333 Q334 R335 L336 Q337 Q338 D339 S349 E352 Q353 R354 Y360 V363 S368 T374

R386 R389 F402 ALA THR GLY GLU HIS THR K409 N410 I413 K414 L415 A416 R417 M435 I439 P442 V445 G446 E447 K448 V449 Y450 Y465 R468 I469 A470 N471 Q472 R473 L478 V495 G496 D497 P509 Q514 R518 A523 G524 E525 F526 G527 E528

E532 L538 D539 I542 THR PRO GLU LEU ILE PRO THR GLY GLU GLU GLU LEU GLN SER SER E558 A559 Q567 W589 W592 N593 E596 R597 K606 S607 E608 S632 R636 K644 G649 S664 Q671 E675 G679

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	177.94Å 177.94Å 214.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.12 – 2.25 39.12 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.12-2.25) 99.4 (39.12-2.25)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.192 , 0.229 0.184 , 0.223	Depositor DCC
R_{free} test set	8068 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	1.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 63.0	EDS
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21381	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, AMP, DND, POP

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	0.82	2/5156 (0.0%)	0.95	15/7003 (0.2%)
1	B	0.85	2/5154 (0.0%)	0.91	14/6999 (0.2%)
1	C	0.85	2/5239 (0.0%)	0.91	14/7118 (0.2%)
1	D	0.90	6/5236 (0.1%)	0.92	14/7112 (0.2%)
All	All	0.85	12/20785 (0.1%)	0.92	57/28232 (0.2%)

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	B	0	1
1	D	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	CYS	CB-SG	20.02	2.16	1.82
1	D	17	CYS	CB-SG	12.07	2.02	1.82
1	C	284	LEU	CG-CD2	-7.48	1.24	1.51
1	A	284	LEU	CG-CD2	-6.98	1.26	1.51
1	B	284	LEU	CG-CD2	-6.83	1.26	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	ARG	NE-CZ-NH1	-18.65	110.98	120.30
1	A	134	ARG	NE-CZ-NH2	-18.09	111.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	ARG	NE-CZ-NH2	17.31	128.96	120.30
1	D	134	ARG	NE-CZ-NH2	-16.60	112.00	120.30
1	C	134	ARG	NE-CZ-NH1	-16.36	112.12	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	559	ALA	Peptide
1	D	559	ALA	Peptide

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	5040	0	4938	69	0
1	B	5039	0	4949	79	0
1	C	5119	0	5014	75	0
1	D	5116	0	5021	70	0
2	A	44	0	25	0	0
2	B	44	0	25	1	0
2	C	44	0	25	1	0
2	D	44	0	25	0	0
3	A	23	0	12	2	0
3	B	23	0	12	0	0
3	C	23	0	12	0	0
3	D	23	0	12	0	0
4	A	9	0	0	0	0
4	B	9	0	0	1	0
4	C	9	0	0	0	0
4	D	9	0	0	1	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	162	0	0	5	0
6	B	190	0	0	6	0
6	C	216	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	177	0	0	4	0
All	All	21381	0	20094	276	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 7.

The worst 5 of 276 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:D:17:CYS:CB	1:D:17:CYS:SG	2.02	1.47
1:D:40:CYS:CB	1:D:40:CYS:SG	2.16	1.33
1:B:69:LEU:C	1:B:69:LEU:HD12	1.76	1.06
1:D:143:ARG:HG2	1:D:143:ARG:HH11	1.27	0.98
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.32	0.93

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	642/680 (94%)	615 (96%)	26 (4%)	1 (0%)	47	55
1	B	641/680 (94%)	616 (96%)	25 (4%)	0	100	100
1	C	654/680 (96%)	624 (95%)	30 (5%)	0	100	100
1	D	652/680 (96%)	626 (96%)	26 (4%)	0	100	100
All	All	2589/2720 (95%)	2481 (96%)	107 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU

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	519/548 (95%)	497 (96%)	22 (4%)	30	34
1	B	521/548 (95%)	498 (96%)	23 (4%)	28	32
1	C	528/548 (96%)	502 (95%)	26 (5%)	25	27
1	D	529/548 (96%)	500 (94%)	29 (6%)	21	21
All	All	2097/2192 (96%)	1997 (95%)	100 (5%)	25	28

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	410	ASN
1	D	1	MET
1	D	664	SER
1	C	439	ILE
1	C	525	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	295	HIS
1	C	515	HIS
1	C	626	GLN
1	D	295	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 ⓘ

15 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	AMP	A	681	-	22,25,25	0.68	0	25,38,38	1.39	2 (8%)
2	DND	D	680	-	42,48,48	0.99	2 (4%)	50,73,73	1.19	4 (8%)
2	DND	C	680	-	42,48,48	0.93	1 (2%)	50,73,73	1.20	3 (6%)
4	POP	B	682	-	6,8,8	0.93	0	13,13,13	1.18	1 (7%)
4	POP	D	682	-	6,8,8	0.71	0	13,13,13	1.21	1 (7%)
4	POP	C	682	-	6,8,8	0.62	0	13,13,13	1.29	1 (7%)
5	GOL	C	683	-	5,5,5	0.55	0	5,5,5	1.04	0
3	AMP	C	681	-	22,25,25	0.78	0	25,38,38	1.50	4 (16%)
3	AMP	D	681	-	22,25,25	0.83	0	25,38,38	1.55	3 (12%)
5	GOL	B	683	-	5,5,5	0.53	0	5,5,5	0.71	0
5	GOL	D	683	-	5,5,5	0.63	0	5,5,5	0.57	0
2	DND	B	680	-	42,48,48	0.86	1 (2%)	50,73,73	1.36	8 (16%)
3	AMP	B	681	-	22,25,25	0.92	0	25,38,38	1.53	3 (12%)
2	DND	A	680	-	42,48,48	0.91	0	50,73,73	1.28	4 (8%)
4	POP	A	682	-	6,8,8	0.81	0	13,13,13	0.95	0

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	AMP	A	681	-	-	2/6/26/26	0/3/3/3
2	DND	D	680	-	-	8/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DND	C	680	-	-	7/26/62/62	0/5/5/5
4	POP	B	682	-	-	3/6/6/6	-
4	POP	D	682	-	-	0/6/6/6	-
4	POP	C	682	-	-	0/6/6/6	-
5	GOL	C	683	-	-	2/4/4/4	-
3	AMP	C	681	-	-	1/6/26/26	0/3/3/3
3	AMP	D	681	-	-	2/6/26/26	0/3/3/3
5	GOL	B	683	-	-	4/4/4/4	-
5	GOL	D	683	-	-	2/4/4/4	-
2	DND	B	680	-	-	6/26/62/62	0/5/5/5
3	AMP	B	681	-	-	5/6/26/26	0/3/3/3
2	DND	A	680	-	-	8/26/62/62	0/5/5/5
4	POP	A	682	-	-	0/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	680	DND	O4B-C1B	3.29	1.45	1.41
2	D	680	DND	O4B-C1B	3.16	1.45	1.41
2	B	680	DND	O4D-C1D	2.50	1.44	1.41
2	D	680	DND	C2A-N3A	2.40	1.36	1.32

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	681	AMP	N3-C2-N1	-5.65	119.85	128.68
2	B	680	DND	N3A-C2A-N1A	-5.59	119.94	128.68
2	D	680	DND	N3A-C2A-N1A	-5.06	120.77	128.68
3	B	681	AMP	N3-C2-N1	-4.87	121.07	128.68
3	C	681	AMP	N3-C2-N1	-4.45	121.73	128.68

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	680	DND	PN-O3P-PA-O5B
2	A	680	DND	C2N-C3N-C7N-O7N
2	A	680	DND	C2N-C3N-C7N-O8N
2	B	680	DND	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	C	680	DND	PN-O3P-PA-O5B

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	681	AMP	2	0
2	C	680	DND	1	0
4	B	682	POP	1	0
4	D	682	POP	1	0
2	B	680	DND	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 AMP A 681

Bond lengths   Bond angles

Torsions   Rings

Ligand DND D 680

Bond lengths

Bond angles

Torsions

Rings

Ligand DND C 680

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP C 681

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP D 681

Bond lengths

Bond angles

Torsions

Rings

Ligand DND B 680

Bond lengths

Bond angles

Torsions

Rings

Ligand AMP B 681

Bond lengths

Bond angles

Torsions

Rings

Ligand DND A 680

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	650/680 (95%)	-0.07	24 (3%)	41	44	26, 42, 71, 108	0
1	B	649/680 (95%)	-0.12	14 (2%)	62	65	23, 38, 68, 108	0
1	C	660/680 (97%)	-0.07	20 (3%)	50	53	22, 38, 68, 108	0
1	D	658/680 (96%)	-0.05	22 (3%)	46	48	23, 40, 71, 109	0
All	All	2617/2720 (96%)	-0.08	80 (3%)	49	52	22, 40, 70, 109	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	448	LYS	5.0
1	D	410	ASN	4.6
1	C	449	VAL	4.6
1	C	524	GLY	4.4
1	A	452	VAL	4.4

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(Å²)	Q<0.9
3	AMP	C	681	23/23	0.69	0.30	58,93,202,206	0
3	AMP	B	681	23/23	0.72	0.25	51,80,139,151	0
3	AMP	A	681	23/23	0.80	0.22	55,89,150,153	0
3	AMP	D	681	23/23	0.80	0.23	44,80,192,196	0
4	POP	B	682	9/9	0.87	0.20	40,77,168,292	0
4	POP	A	682	9/9	0.88	0.19	53,83,179,264	0
5	GOL	D	683	6/6	0.89	0.21	34,49,54,56	0
5	GOL	C	683	6/6	0.90	0.17	33,47,62,62	0
4	POP	C	682	9/9	0.91	0.16	49,103,170,272	0
5	GOL	B	683	6/6	0.92	0.14	30,45,52,57	0
4	POP	D	682	9/9	0.93	0.13	68,95,173,228	0
2	DND	D	680	44/44	0.95	0.13	34,52,87,121	0
2	DND	A	680	44/44	0.96	0.13	27,49,112,127	0
2	DND	B	680	44/44	0.96	0.12	32,45,103,132	0
2	DND	C	680	44/44	0.96	0.11	25,46,76,87	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.
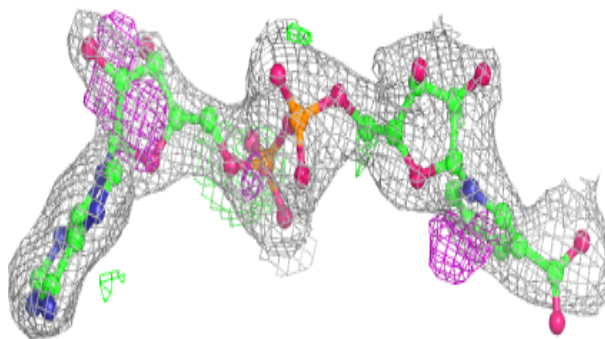
Electron density around AMP C 681:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
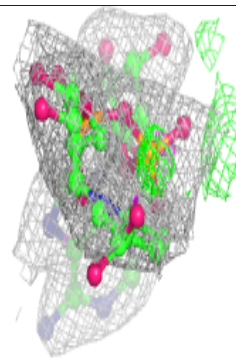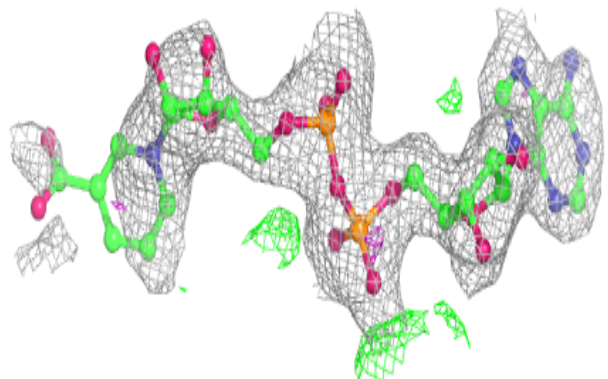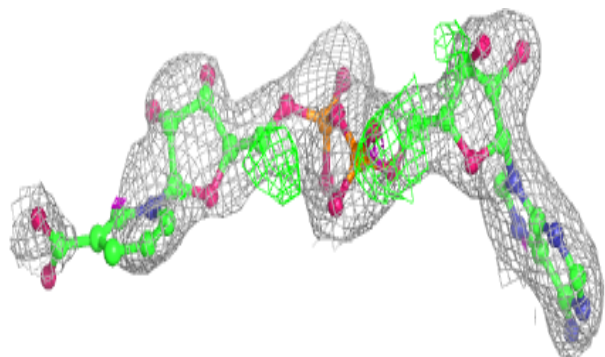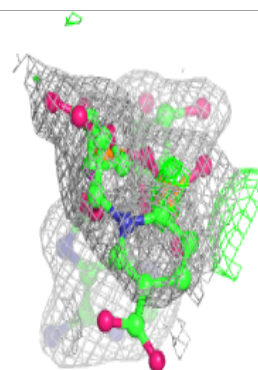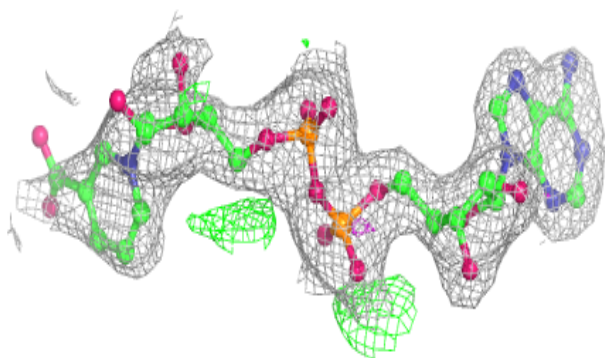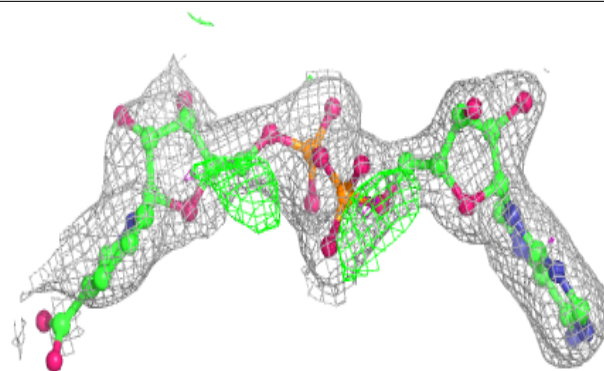mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
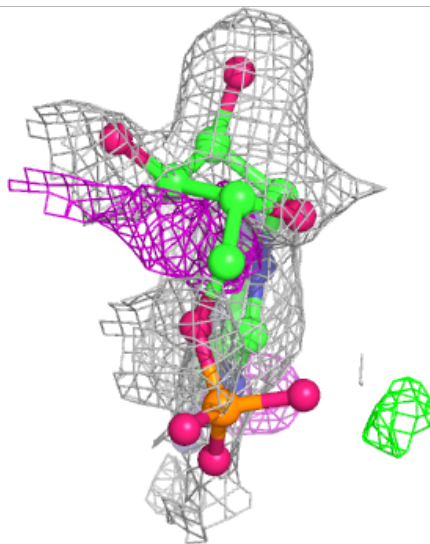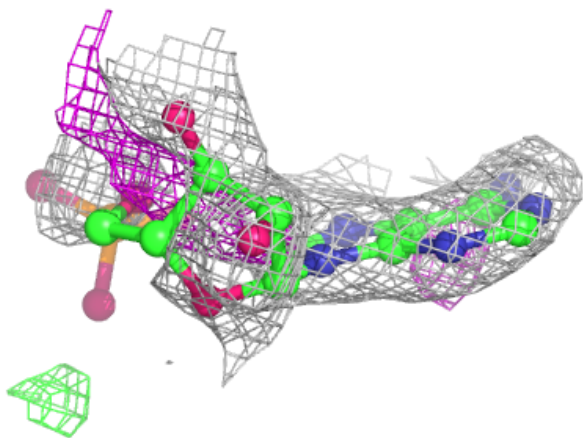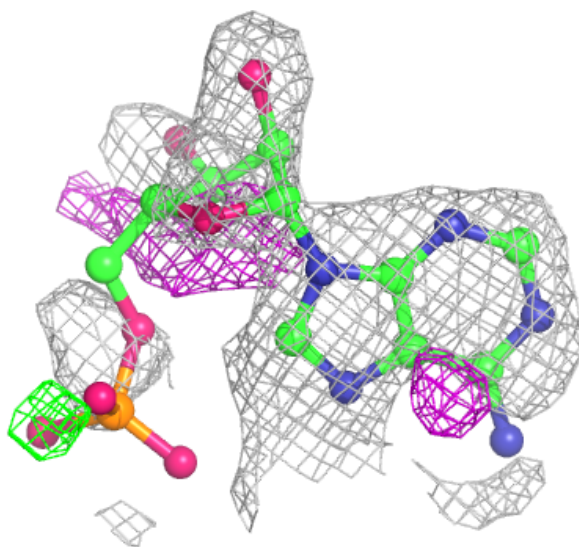
Electron density around AMP B 681:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
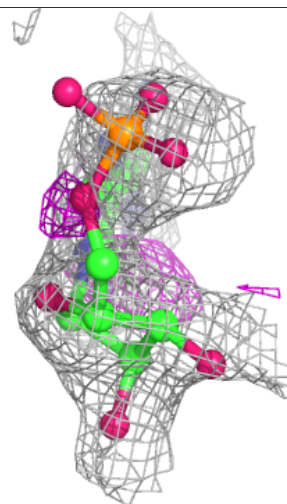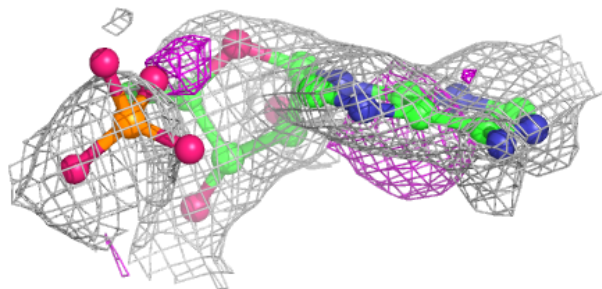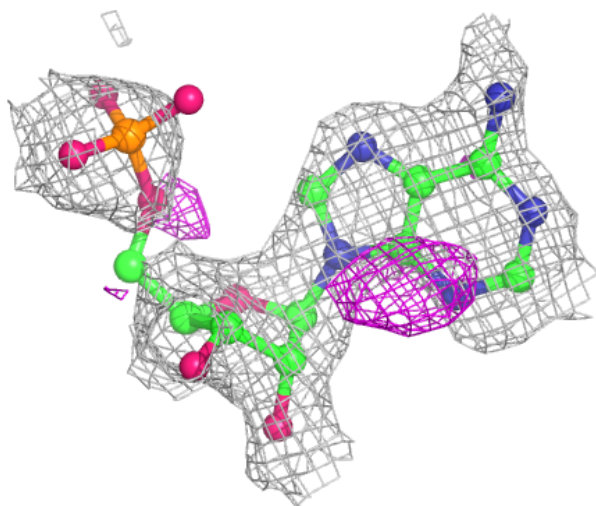
Electron density around AMP A 681:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
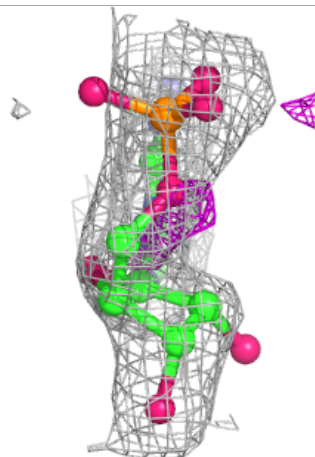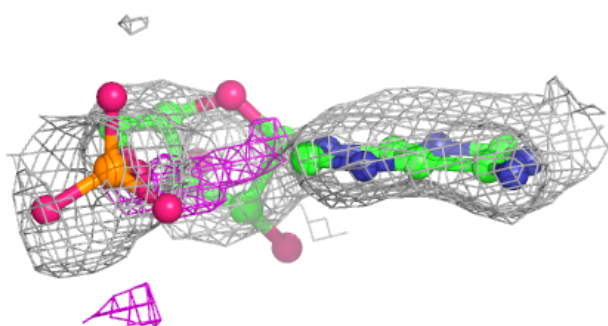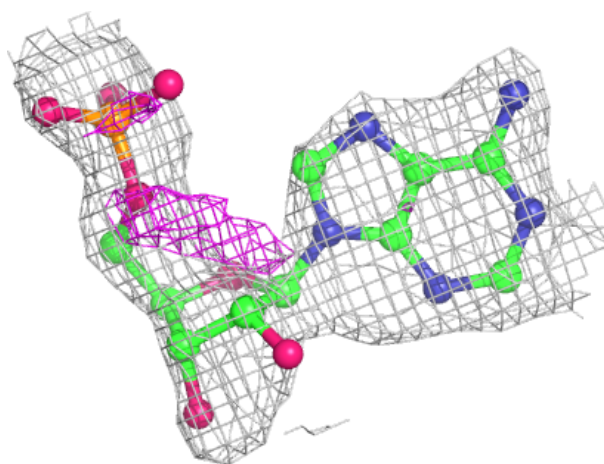
Electron density around AMP D 681:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
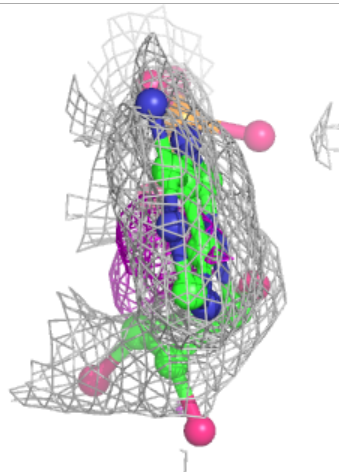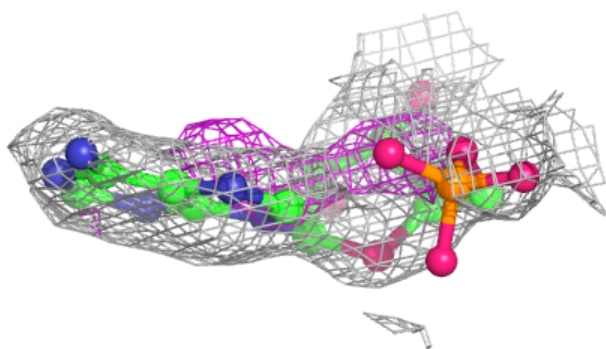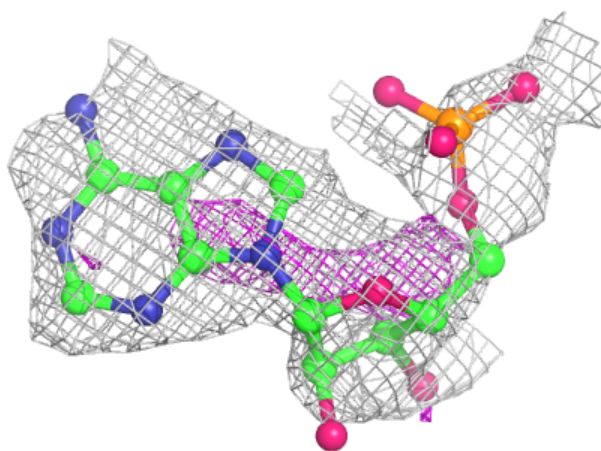
Electron density around DND D 680:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
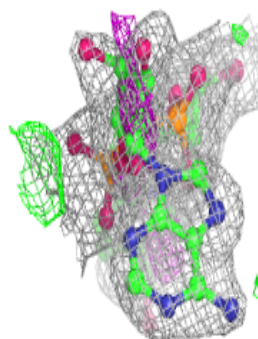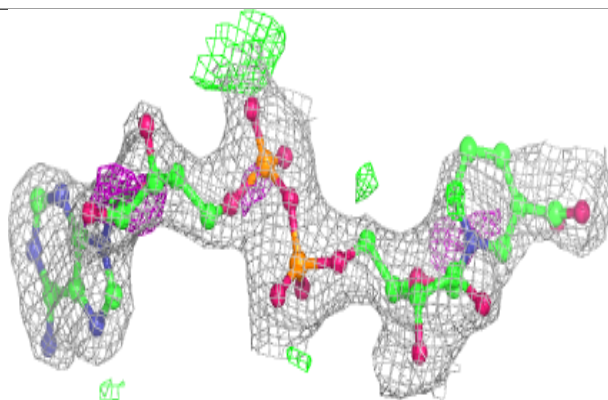
Electron density around DND A 680:

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

Electron density around DND B 680:

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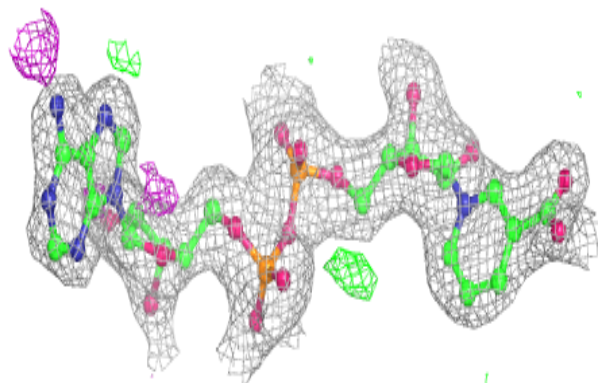mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

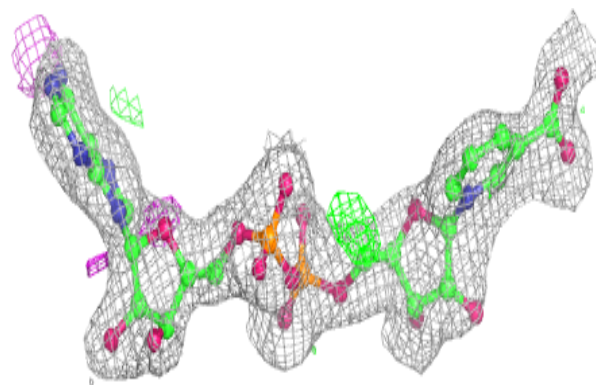**Electron density around DND C 680:**

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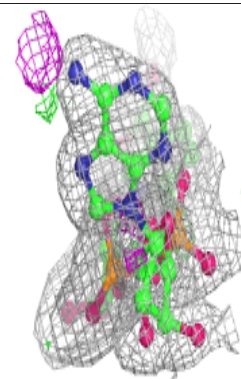
6.5 Other polymers (i)

There are no such residues in this entry.