



wwPDB X-ray Structure Validation Summary Report ⓘ

May 4, 2024 – 12:34 pm BST

PDB ID : 6I6P
Title : SEPIAPTERIN REDUCTASE IN COMPLEX WITH COMPOUND 3
Authors : Alen, J.; Schade, M.; Wagener, M.; Blaesse, M.
Deposited on : 2018-11-15
Resolution : 1.62 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 ⓘ 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

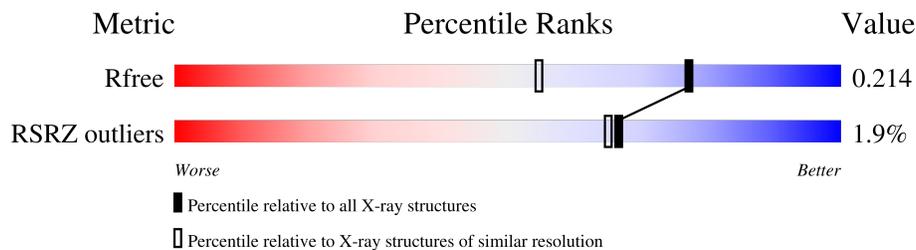
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4693 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4709 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 Sepiapterin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2127	1337	379	398	13	26	10	0
1	B	258	2003	1261	354	376	12	33	8	0

There are 30 discrepancies between the modelled and reference sequences:

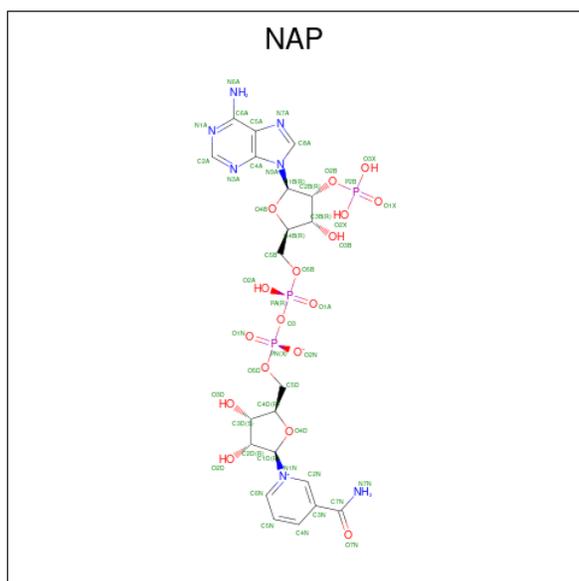
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP P35270
A	-13	GLY	-	expression tag	UNP P35270
A	-12	HIS	-	expression tag	UNP P35270
A	-11	HIS	-	expression tag	UNP P35270
A	-10	HIS	-	expression tag	UNP P35270
A	-9	HIS	-	expression tag	UNP P35270
A	-8	HIS	-	expression tag	UNP P35270
A	-7	HIS	-	expression tag	UNP P35270
A	-6	GLU	-	expression tag	UNP P35270
A	-5	ASN	-	expression tag	UNP P35270
A	-4	LEU	-	expression tag	UNP P35270
A	-3	TYR	-	expression tag	UNP P35270
A	-2	PHE	-	expression tag	UNP P35270
A	-1	GLN	-	expression tag	UNP P35270
A	0	GLY	-	expression tag	UNP P35270
B	-14	MET	-	initiating methionine	UNP P35270
B	-13	GLY	-	expression tag	UNP P35270
B	-12	HIS	-	expression tag	UNP P35270
B	-11	HIS	-	expression tag	UNP P35270
B	-10	HIS	-	expression tag	UNP P35270
B	-9	HIS	-	expression tag	UNP P35270
B	-8	HIS	-	expression tag	UNP P35270
B	-7	HIS	-	expression tag	UNP P35270
B	-6	GLU	-	expression tag	UNP P35270
B	-5	ASN	-	expression tag	UNP P35270

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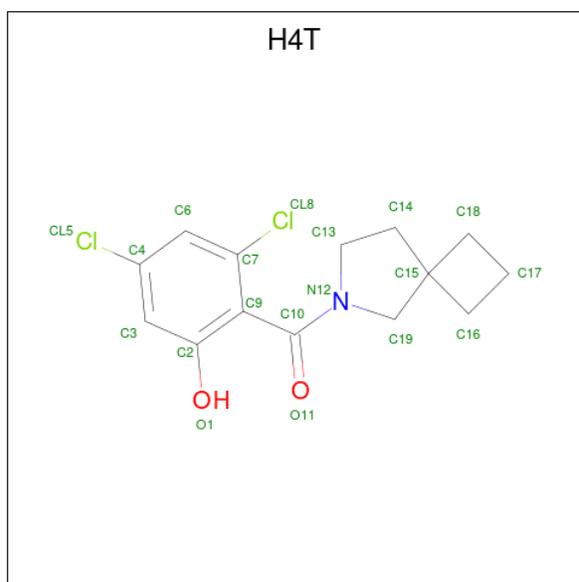
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	LEU	-	expression tag	UNP P35270
B	-3	TYR	-	expression tag	UNP P35270
B	-2	PHE	-	expression tag	UNP P35270
B	-1	GLN	-	expression tag	UNP P35270
B	0	GLY	-	expression tag	UNP P35270

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



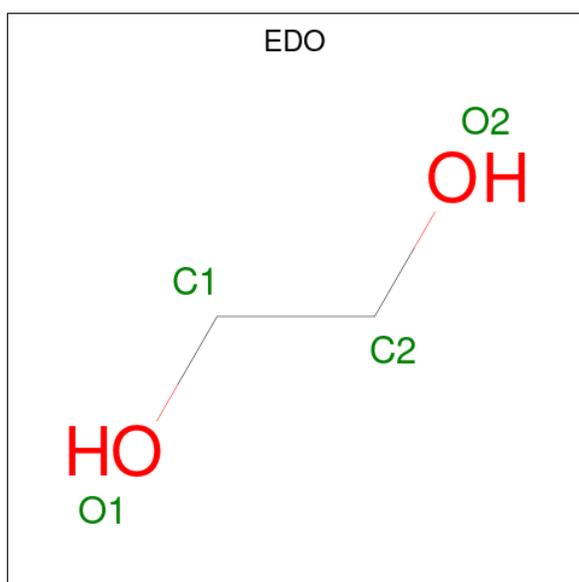
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 6-azaspiro[3.4]octan-6-yl-[2,4-bis(chloranyl)-6-oxidanyl-phenyl]methanone (three-letter code: H4T) (formula: C₁₄H₁₅Cl₂NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	Cl	N			O	
3	A	1	Total	19	14	2	1	2	0	0
3	B	1	Total	19	14	2	1	2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	227	Total	O	0	0
			227	227		
5	B	206	Total	O	0	0
			206	206		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.53Å 77.71Å 59.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.30 – 1.62 46.10 – 1.62	Depositor EDS
% Data completeness (in resolution range)	97.9 (64.30-1.62) 97.9 (46.10-1.62)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.62Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.154 , 0.208 0.167 , 0.214	Depositor DCC
R_{free} test set	3577 reflections (5.34%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4709	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

7 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
4	EDO	B	303	-	3,3,3	0.38	0	2,2,2	0.32	0
3	H4T	A	302	-	21,21,21	1.15	3 (14%)	24,32,32	1.56	5 (20%)
2	NAP	B	301	-	45,52,52	0.85	2 (4%)	56,80,80	1.27	3 (5%)
4	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.31	0
2	NAP	A	301	-	45,52,52	0.84	2 (4%)	56,80,80	1.15	5 (8%)
3	H4T	B	302	-	21,21,21	1.15	2 (9%)	24,32,32	1.59	6 (25%)
4	EDO	B	304	-	3,3,3	0.50	0	2,2,2	0.30	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
4	EDO	B	303	-	-	1/1/1/1	-
3	H4T	A	302	-	-	0/8/27/27	0/3/3/3
2	NAP	B	301	-	-	6/31/67/67	0/5/5/5
4	EDO	A	303	-	-	0/1/1/1	-
2	NAP	A	301	-	-	7/31/67/67	0/5/5/5
3	H4T	B	302	-	-	0/8/27/27	0/3/3/3
4	EDO	B	304	-	-	0/1/1/1	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	H4T	C9-C10	-3.42	1.46	1.51
3	A	302	H4T	C9-C10	-3.10	1.47	1.51
2	A	301	NAP	C5A-C4A	2.52	1.47	1.40
3	A	302	H4T	C16-C15	-2.49	1.52	1.55
2	B	301	NAP	C5A-C4A	2.34	1.47	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C3N-C7N-N7N	4.13	122.71	117.75
2	A	301	NAP	C3N-C7N-N7N	3.63	122.11	117.75
3	A	302	H4T	C13-C14-C15	-3.51	98.84	104.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	H4T	C17-C18-C15	-3.46	86.41	89.16
2	B	301	NAP	C4A-C5A-N7A	-3.45	105.80	109.40

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C2B-O2B-P2B-O3X
2	A	301	NAP	O4D-C1D-N1N-C2N
2	B	301	NAP	C2B-O2B-P2B-O3X
2	B	301	NAP	C5D-O5D-PN-O2N
2	B	301	NAP	O4D-C1D-N1N-C2N

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

5.1 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	270/276 (97%)	-0.15	9 (3%) 46 42	14, 23, 44, 68	12 (4%)
1	B	258/276 (93%)	-0.21	1 (0%) 92 92	14, 25, 43, 53	13 (5%)
All	All	528/552 (95%)	-0.18	10 (1%) 66 65	14, 24, 43, 68	25 (4%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	PRO	5.6
1	A	58	ARG	5.3
1	A	59	SER	4.0
1	A	60	GLY	3.2
1	A	55	GLY	2.9

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

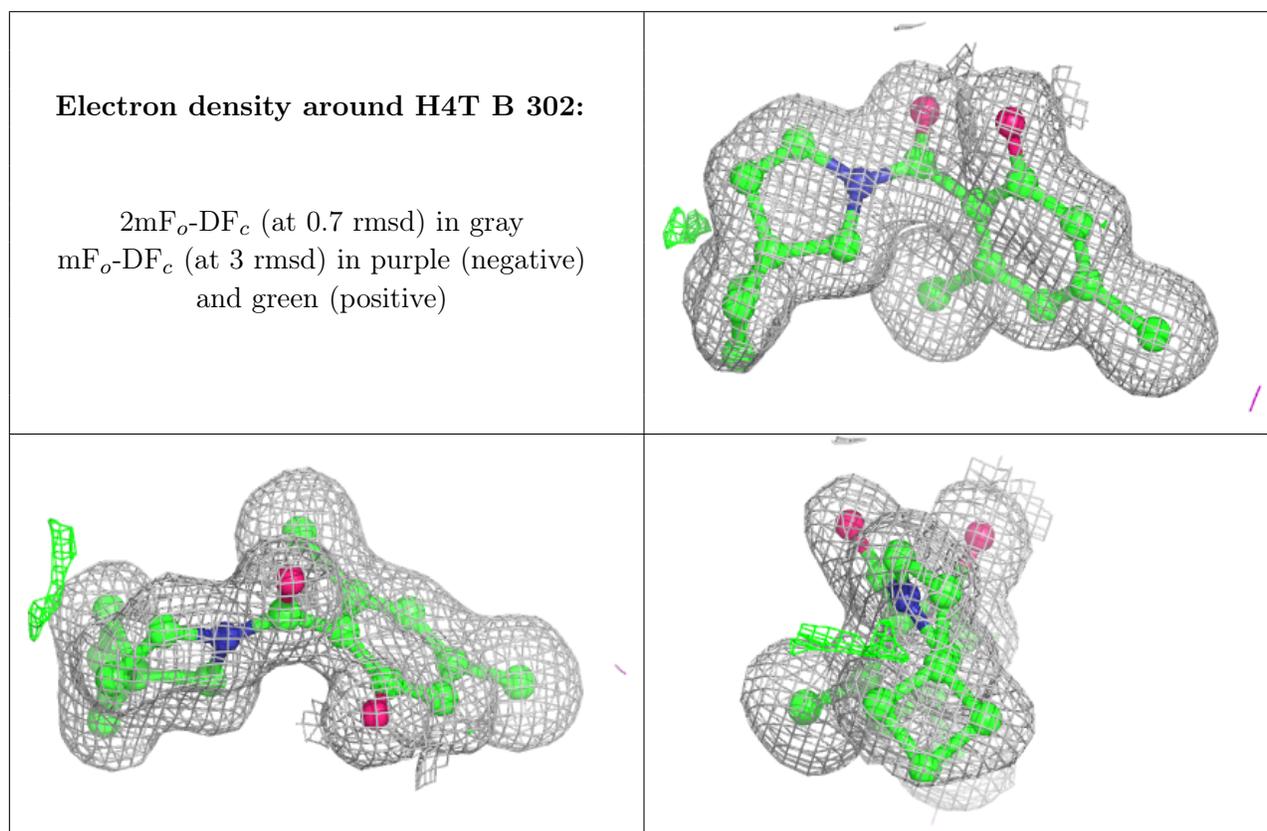
There are no monosaccharides in this entry.

5.4 Ligands [i](#)

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

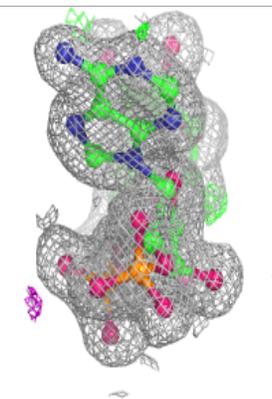
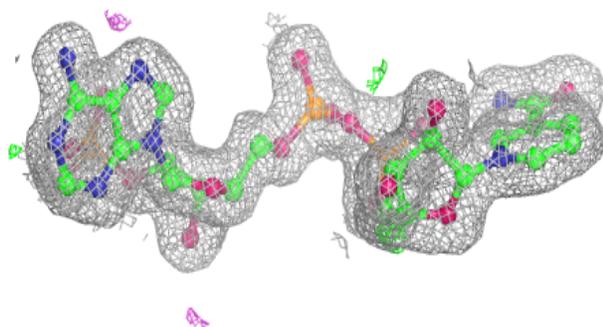
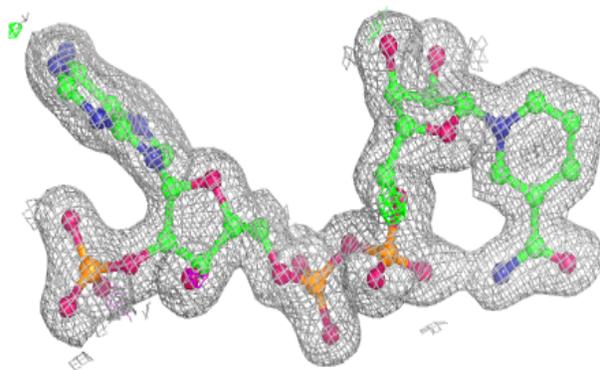
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	303	4/4	0.82	0.15	33,35,44,48	0
4	EDO	B	304	4/4	0.92	0.12	26,36,41,52	0
4	EDO	A	303	4/4	0.96	0.12	23,32,36,47	0
3	H4T	B	302	19/19	0.97	0.08	17,21,32,34	0
2	NAP	B	301	48/48	0.97	0.07	15,20,24,27	0
2	NAP	A	301	48/48	0.98	0.07	12,15,17,18	0
3	H4T	A	302	19/19	0.98	0.07	14,19,30,32	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.

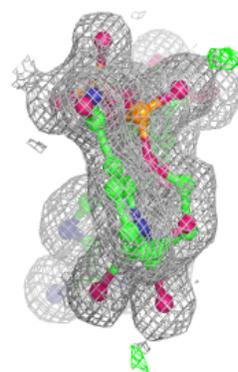
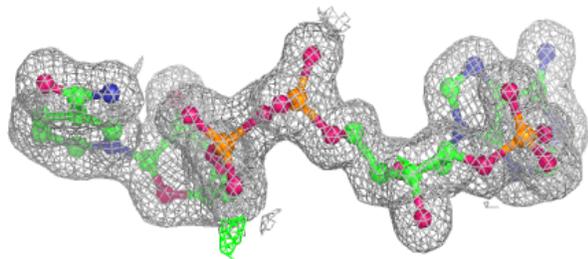
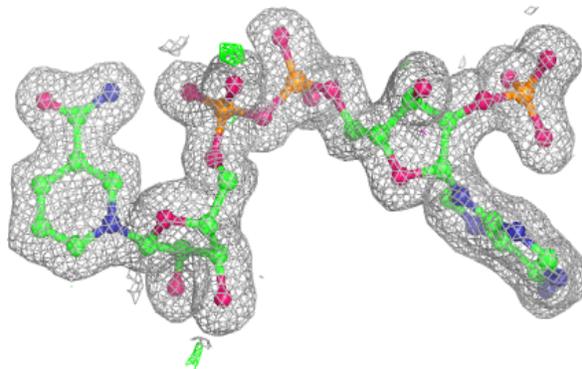


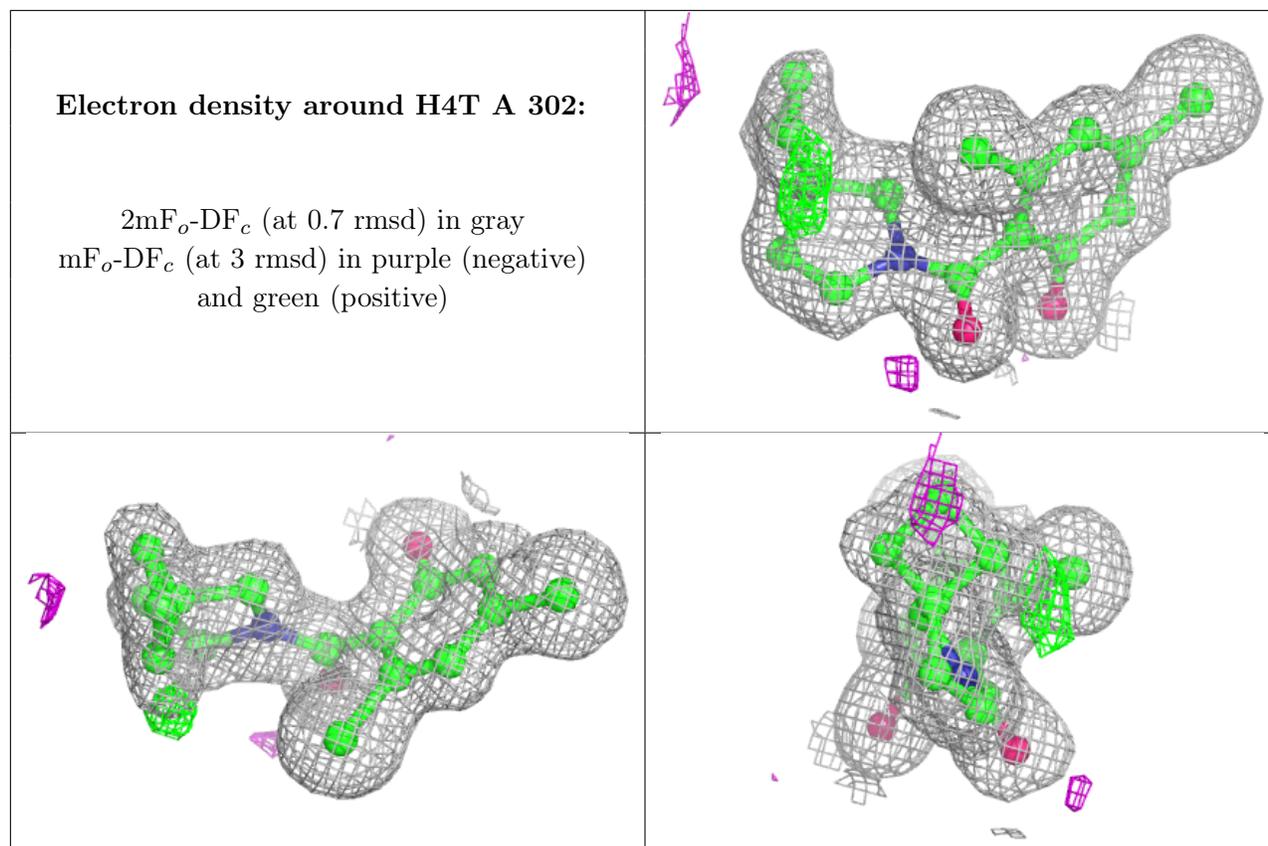
Electron density around NAP B 301:

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

**Electron density around NAP A 301:**

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





5.5 Other polymers [i](#)

There are no such residues in this entry.