wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 11:35 am GMT

PDB ID	:	6YQ3
Title	:	Promiscuous Reductase LugOII Catalyzes Keto-reduction at C1 during Lugdunomycin Biosynthesis
Authors	:	Xiao, X.; Elsayed, S.S.; Wu, C.; van der Heul, H.; Prota, A.; Huang, J.; Guo, R.; Abrahams, J.P.; van Wezel, G.P.
Deposited on	:	2020-04-16
Resolution	:	1.57 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:

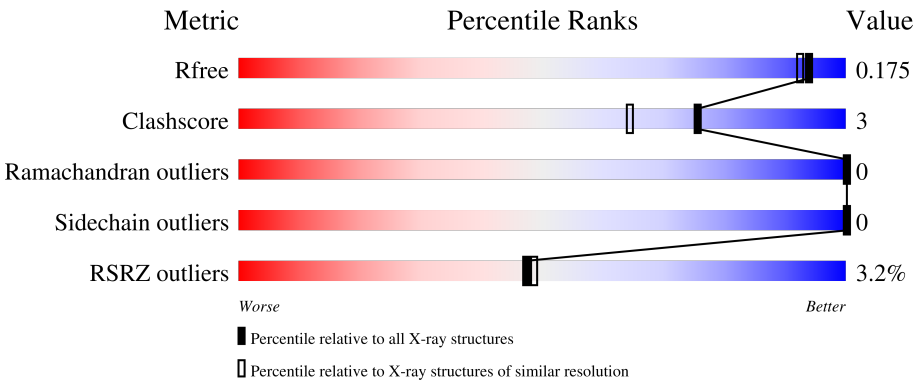
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	AAA	255	4% 91% 7%
1	BBB	255	3% 95%

2 Entry composition (i)

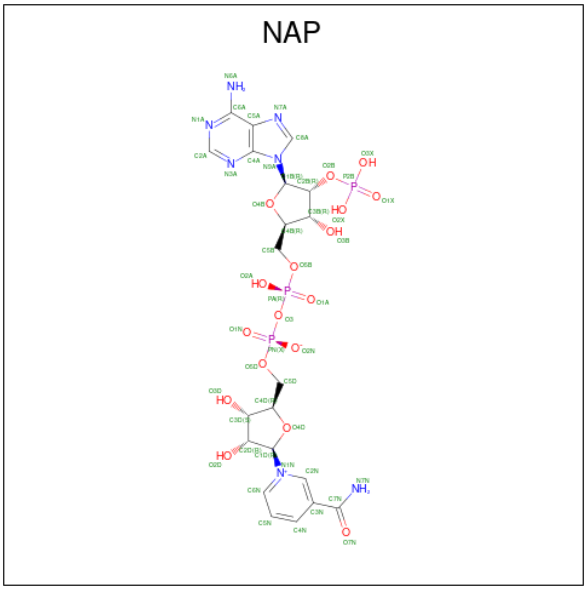
There are 5 unique types of molecules in this entry. The entry contains 4421 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Monooxygenase.

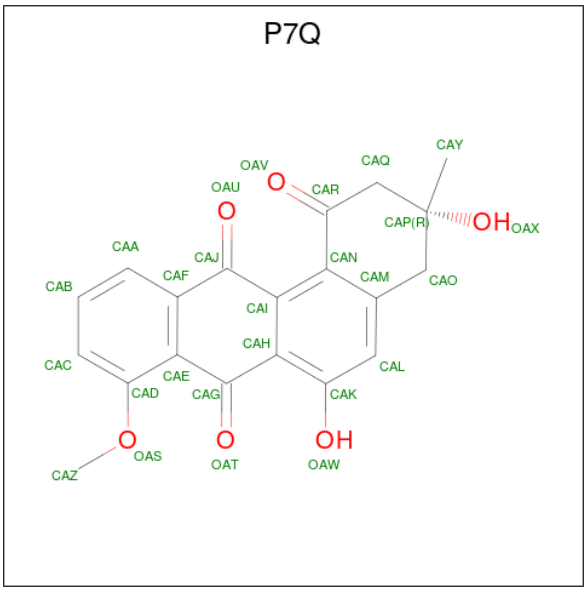
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	252	1889	1176	341	366	6	0	4	0
1	BBB	254	1892	1178	340	368	6	0	3	0

- 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).



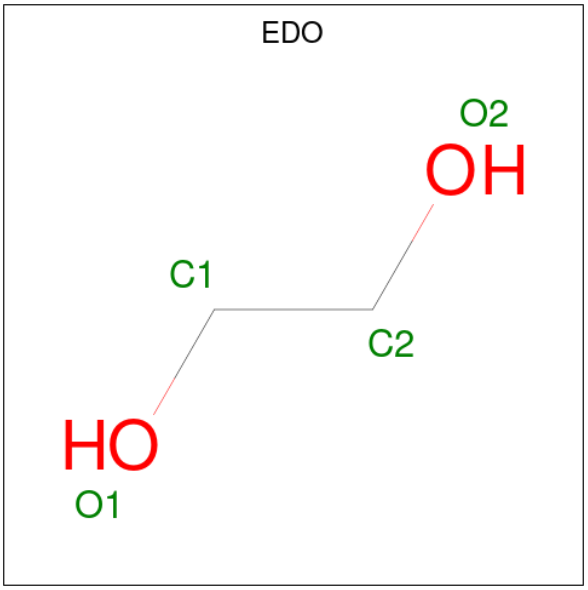
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	AAA	1	48	21	7	17	3	0	0
2	BBB	1	48	21	7	17	3	0	0

- Molecule 3 is (3 {R})-8-methoxy-3-methyl-3,6-bis(oxidanyl)-2,4-dihydrobenzo[a]anthracene-1,7,12-trione (three-letter code: P7Q) (formula: $C_{20}H_{16}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	AAA	1	26	20	6	0	0
			Total	C	O		
3	BBB	1	26	20	6	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

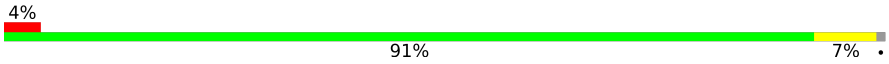
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	AAA	224	224	224	0	0
			Total	O		
5	BBB	260	260	260	0	0

3 Residue-property plots (i)

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

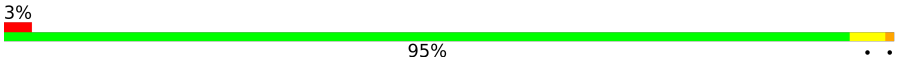
- Molecule 1: Monooxygenase

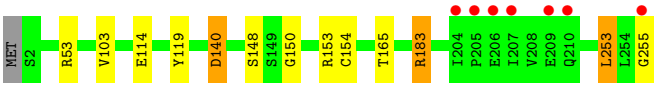
Chain AAA:



- Molecule 1: Monooxygenase

Chain BBB:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	87.97Å 60.21Å 88.31Å 90.00° 102.46° 90.00°	Depositor
Resolution (Å)	24.70 – 1.57 24.68 – 1.57	Depositor EDS
% Data completeness (in resolution range)	96.1 (24.70-1.57) 96.1 (24.68-1.57)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.142 , 0.166 0.155 , 0.175	Depositor DCC
R_{free} test set	3027 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4421	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, P7Q, EDO

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	AAA	0.92	1/1925 (0.1%)	1.08	8/2609 (0.3%)
1	BBB	0.92	3/1926 (0.2%)	1.02	7/2613 (0.3%)
All	All	0.92	4/3851 (0.1%)	1.05	15/5222 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	158	GLU	CD-OE1	8.49	1.34	1.25
1	BBB	114	GLU	CD-OE2	6.44	1.32	1.25
1	BBB	114	GLU	CD-OE1	5.96	1.32	1.25
1	BBB	253	LEU	C-O	5.43	1.33	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	183[A]	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	AAA	183[B]	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	AAA	183[A]	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	AAA	183[B]	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	BBB	140	ASP	CB-CG-OD1	6.83	124.45	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1889	0	1903	11	0
1	BBB	1892	0	1903	9	0
2	AAA	48	0	25	2	0
2	BBB	48	0	25	2	0
3	AAA	26	0	0	1	0
3	BBB	26	0	0	8	0
4	AAA	8	0	12	1	0
5	AAA	224	0	0	1	0
5	BBB	260	0	0	0	0
All	All	4421	0	3868	24	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 3.

The worst 5 of 24 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:BBB:103:VAL:HA	3:BBB:302:P7Q:CAQ	2.06	0.84
1:AAA:154[B]:CYS:SG	1:AAA:253:LEU:CD2	2.72	0.78
1:AAA:154[B]:CYS:SG	1:AAA:253:LEU:HD23	2.35	0.66
1:AAA:154[B]:CYS:SG	1:AAA:253:LEU:HD22	2.44	0.57
1:BBB:150:GLY:HA3	3:BBB:302:P7Q:CAZ	2.35	0.56

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	252/255 (99%)	247 (98%)	5 (2%)	0	100	100
1	BBB	255/255 (100%)	247 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	507/510 (99%)	494 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	AAA	194/192 (101%)	194 (100%)	0	100	100
1	BBB	194/192 (101%)	194 (100%)	0	100	100
All	All	388/384 (101%)	388 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	P7Q	AAA	302	-	29,29,29	2.44	9 (31%)	43,46,46	2.76	19 (44%)
2	NAP	BBB	301	-	45,52,52	1.58	7 (15%)	56,80,80	1.11	4 (7%)
2	NAP	AAA	301	-	45,52,52	1.35	5 (11%)	56,80,80	1.10	5 (8%)
4	EDO	AAA	303	-	3,3,3	0.54	0	2,2,2	2.22	1 (50%)
3	P7Q	BBB	302	-	29,29,29	3.73	14 (48%)	43,46,46	2.85	20 (46%)
4	EDO	AAA	304	-	3,3,3	0.51	0	2,2,2	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	P7Q	AAA	302	-	-	0/2/32/32	0/4/4/4
2	NAP	BBB	301	-	-	1/31/67/67	0/5/5/5
2	NAP	AAA	301	-	-	2/31/67/67	0/5/5/5
4	EDO	AAA	303	-	-	0/1/1/1	-
3	P7Q	BBB	302	-	-	0/2/32/32	0/4/4/4
4	EDO	AAA	304	-	-	1/1/1/1	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	302	P7Q	CAQ-CAP	11.98	1.66	1.53
3	BBB	302	P7Q	OAX-CAP	8.65	1.56	1.44
3	AAA	302	P7Q	CAQ-CAR	-7.01	1.40	1.50
3	BBB	302	P7Q	CAY-CAP	5.87	1.59	1.52
2	BBB	301	NAP	C4N-C3N	5.55	1.48	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	302	P7Q	OAV-CAR-CAQ	-7.89	110.28	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BBB	302	P7Q	CAZ-OAS-CAD	-7.11	106.80	117.53
3	AAA	302	P7Q	CAI-CAN-CAR	5.70	128.09	121.12
3	AAA	302	P7Q	CAL-CAK-CAH	5.48	127.30	120.93
3	BBB	302	P7Q	CAL-CAK-CAH	5.42	127.23	120.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	304	EDO	O1-C1-C2-O2
2	AAA	301	NAP	PN-O3-PA-O2A
2	BBB	301	NAP	O4B-C4B-C5B-O5B
2	AAA	301	NAP	O4B-C4B-C5B-O5B

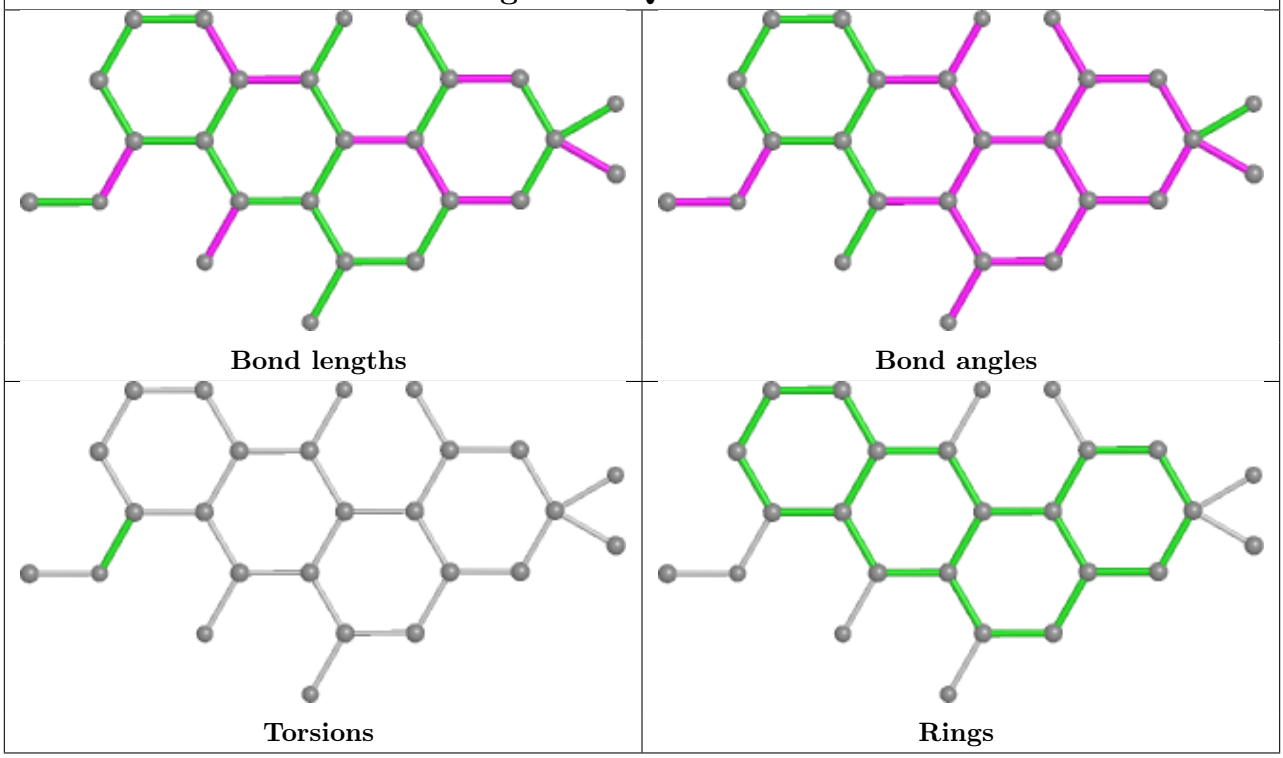
There are no ring outliers.

5 monomers are involved in 12 short contacts:

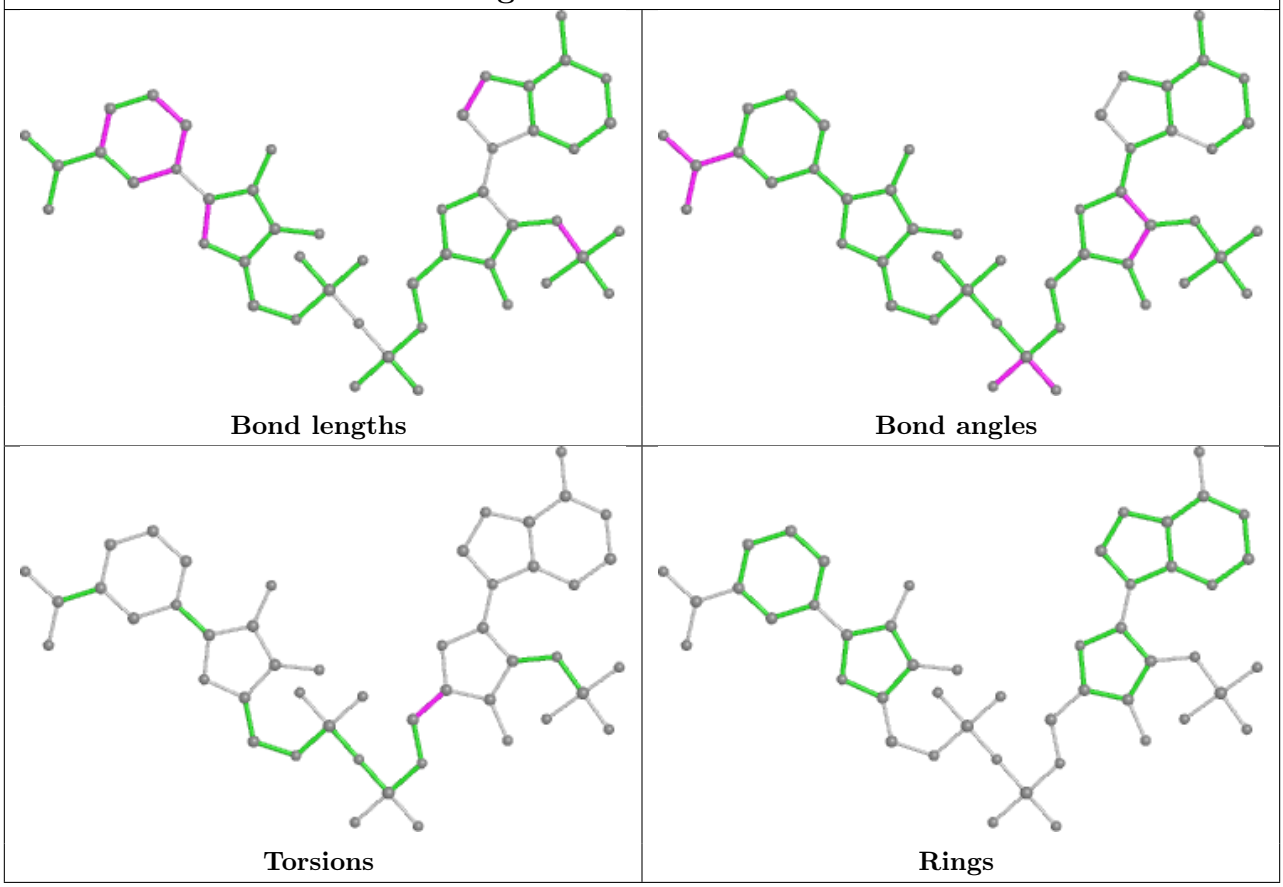
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	302	P7Q	1	0
2	BBB	301	NAP	2	0
2	AAA	301	NAP	2	0
4	AAA	303	EDO	1	0
3	BBB	302	P7Q	8	0

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.

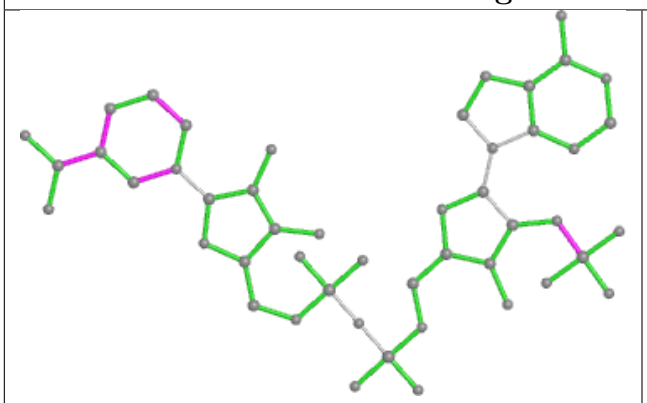
Ligand P7Q AAA 302



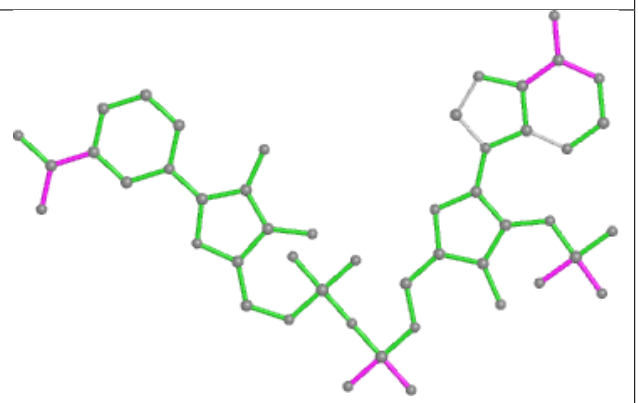
Ligand NAP BBB 301



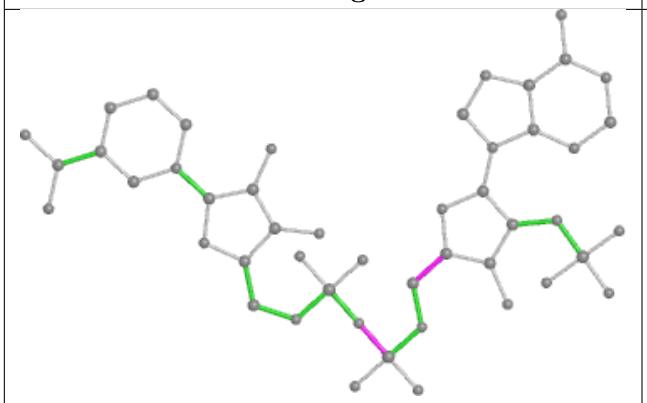
Ligand NAP AAA 301



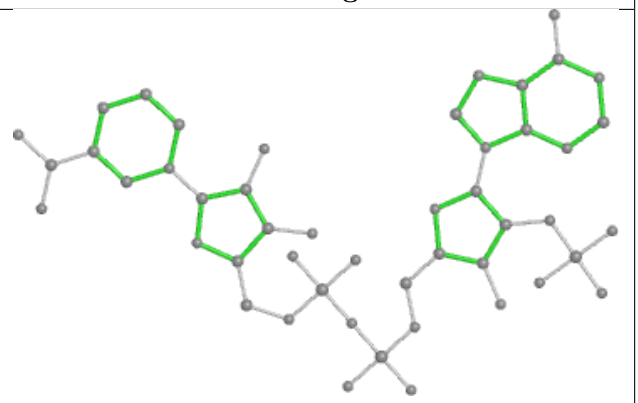
Bond lengths



Bond angles

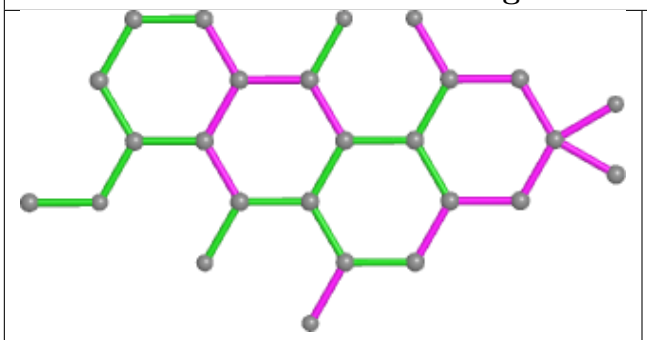


Torsions

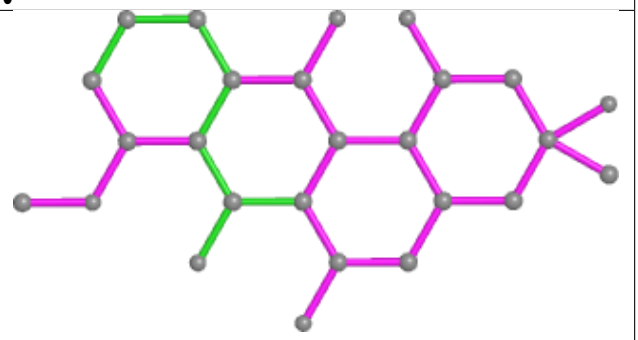


Rings

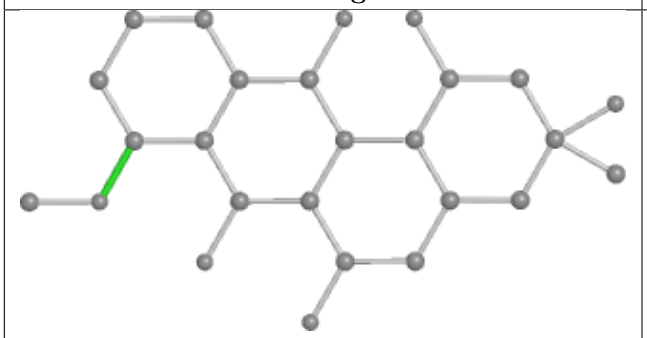
Ligand P7Q BBB 302



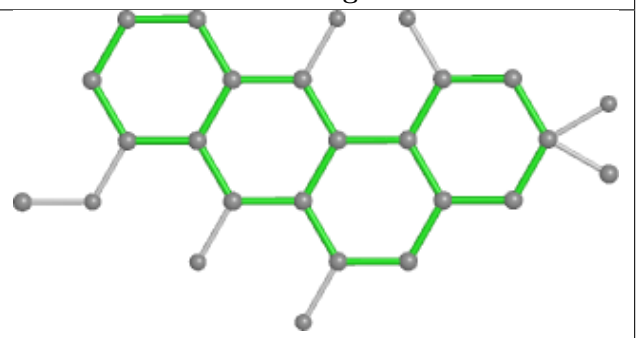
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	252/255 (98%)	-0.09	9 (3%)	42	44	10, 15, 31, 53	0
1	BBB	254/255 (99%)	-0.24	7 (2%)	53	54	10, 14, 29, 45	0
All	All	506/510 (99%)	-0.17	16 (3%)	47	49	10, 15, 30, 53	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	207	ILE	4.5
1	AAA	206	GLU	3.7
1	BBB	205	PRO	3.6
1	AAA	204	ILE	3.5
1	BBB	207	ILE	3.4

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

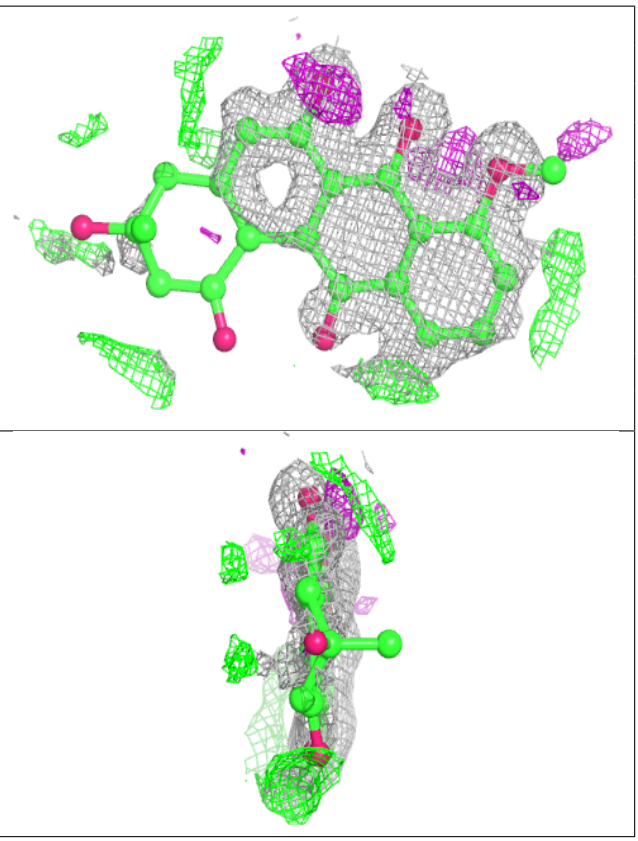
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	P7Q	AAA	302	26/26	0.80	0.25	32,45,82,89	0
3	P7Q	BBB	302	26/26	0.86	0.18	20,26,52,66	0
4	EDO	AAA	303	4/4	0.92	0.12	22,24,25,27	0
4	EDO	AAA	304	4/4	0.95	0.11	22,28,30,32	0
2	NAP	AAA	301	48/48	0.98	0.05	12,14,17,21	0
2	NAP	BBB	301	48/48	0.98	0.06	11,13,16,16	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.

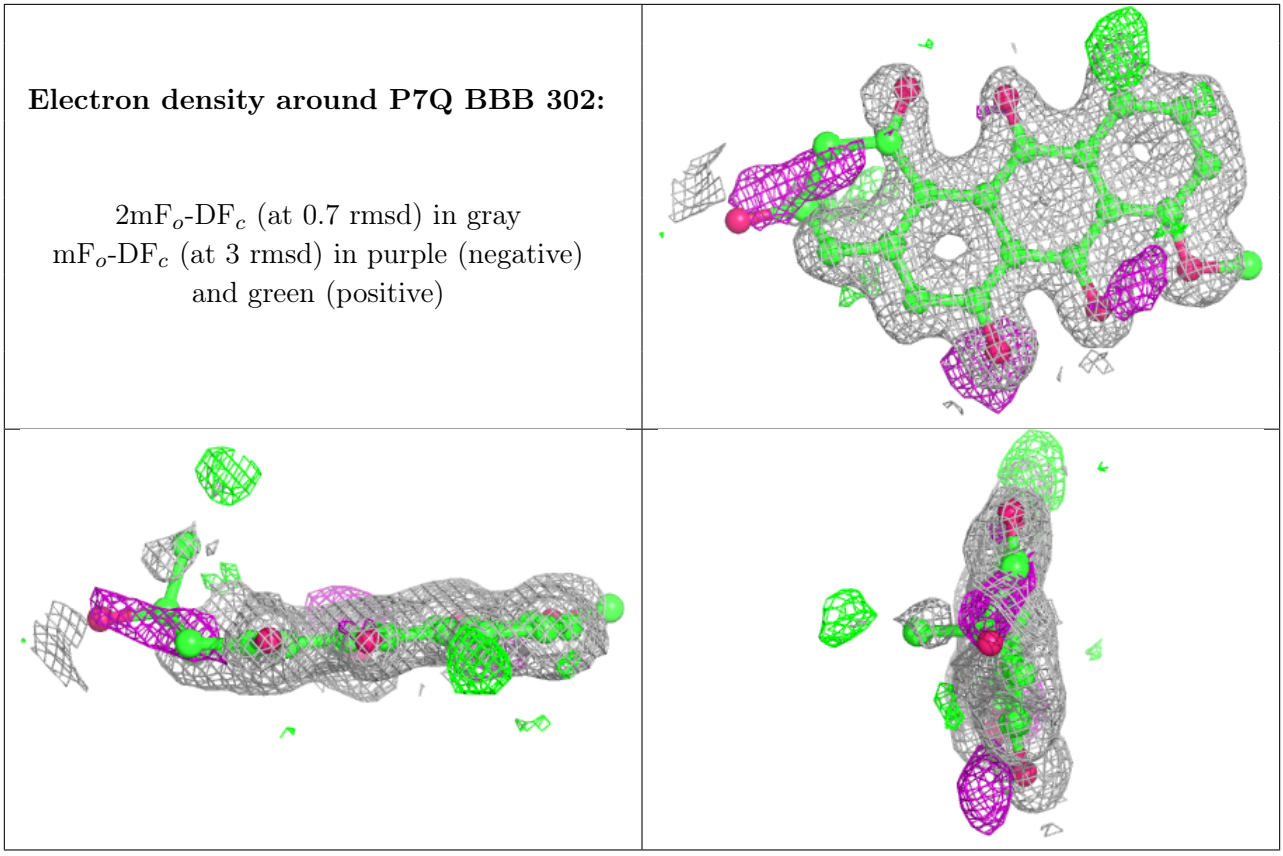
Electron density around P7Q AAA 302:

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



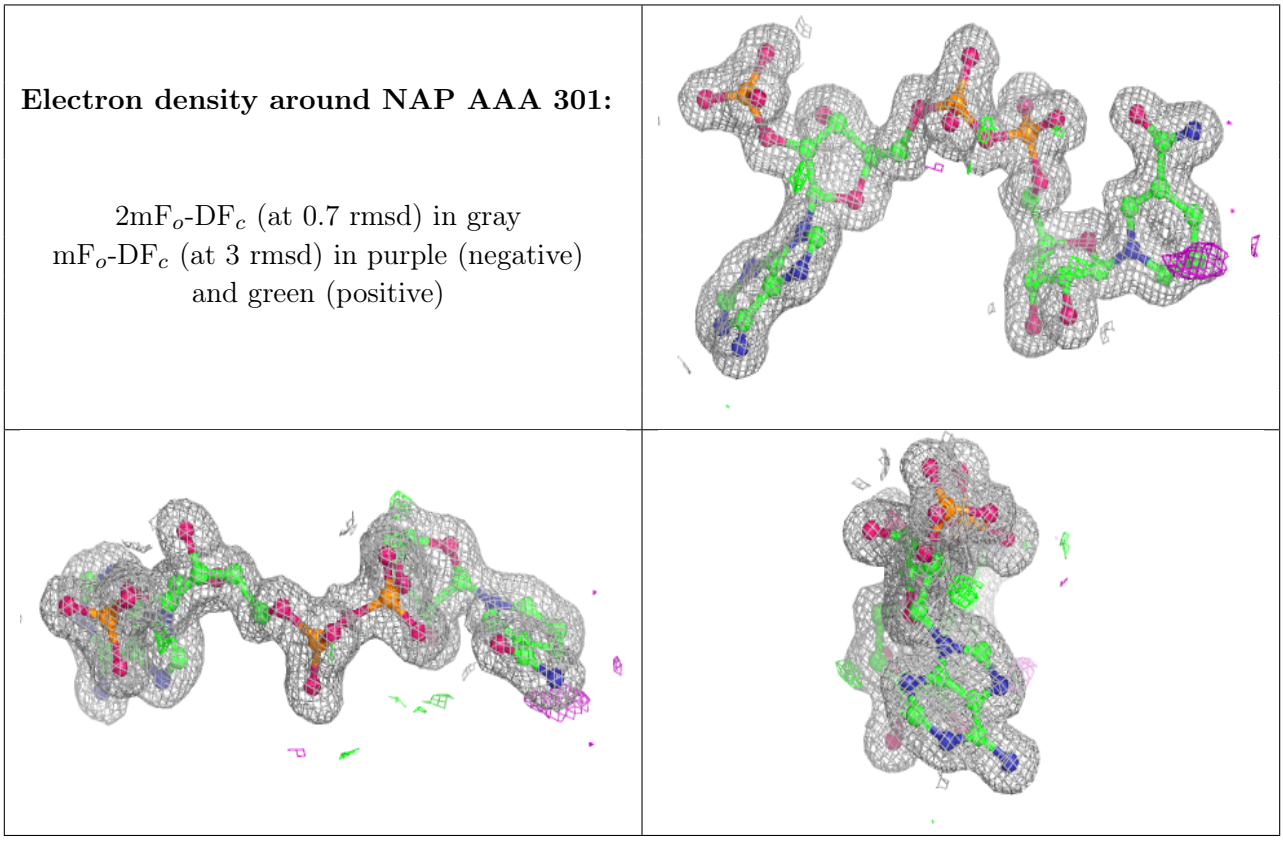
Electron density around P7Q BBB 302:

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



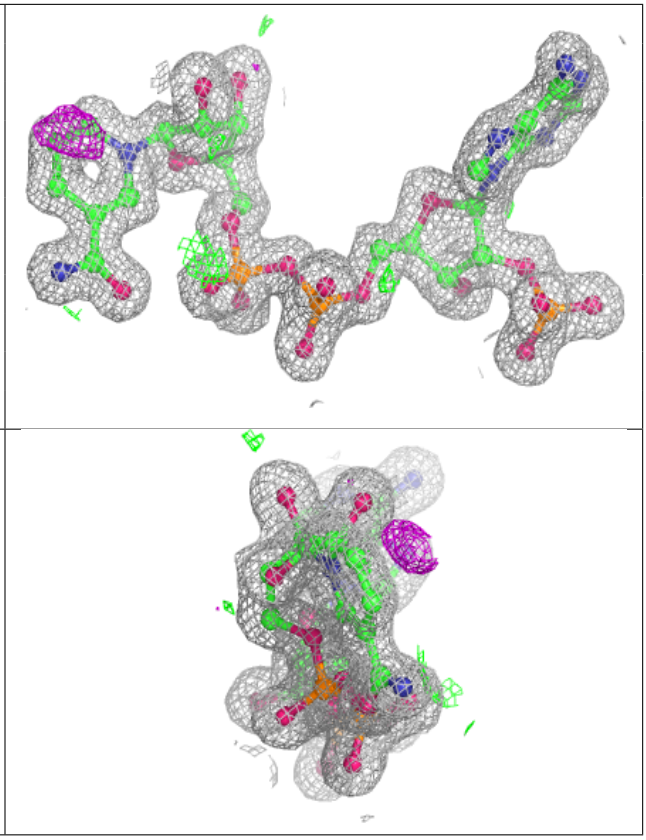
Electron density around NAP AAA 301:

$2mF_o$-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 BBB 301:

$2mF_o$-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.