wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 11:20 am GMT

PDB ID	:	6YQ0
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	:	1.08 Å(reported)

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   ⓘ

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

The reported resolution of this entry is 1.08 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		0.172
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		3.0%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
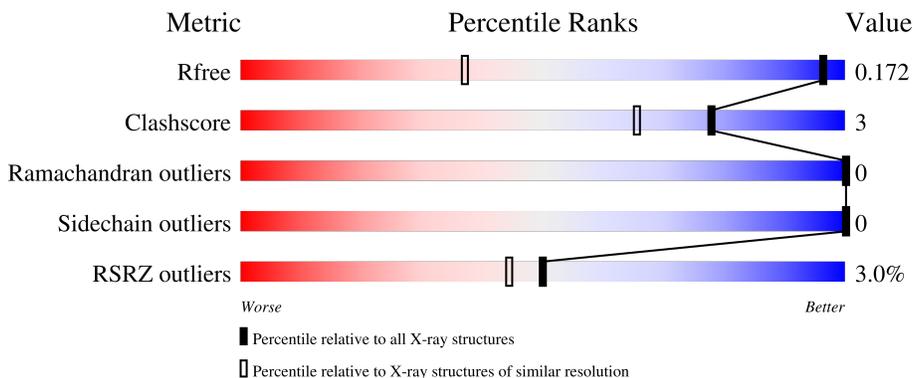
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1386 (1.12-1.04)
Clashscore	141614	1021 (1.10-1.06)
Ramachandran outliers	138981	1381 (1.12-1.04)
Sidechain outliers	138945	1379 (1.12-1.04)
RSRZ outliers	127900	1359 (1.12-1.04)

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	2% 94% 6%
1	BBB	255	4% 92% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	AAA	301	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 4583 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
1	AAA	254	Total 1918	C 1196	N 344	O 372	S 6	0	7	0
1	BBB	254	Total 1911	C 1191	N 341	O 373	S 6	0	6	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
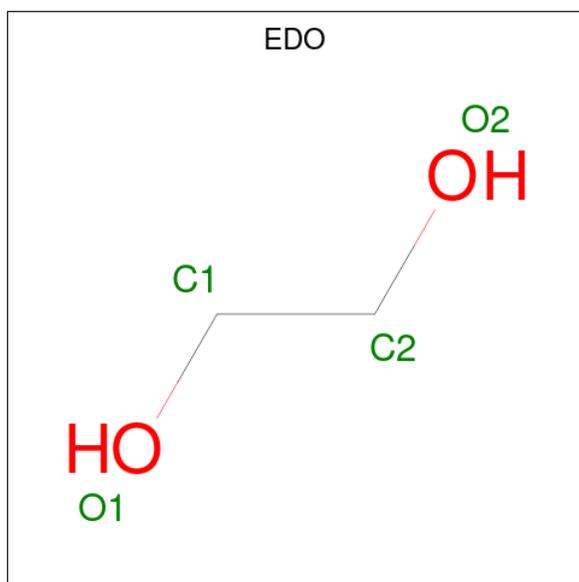
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total 4	C 2	O 2	0	0
2	AAA	1	Total 4	C 2	O 2	0	0
2	AAA	1	Total 4	C 2	O 2	0	0
2	AAA	1	Total 4	C 2	O 2	0	0

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

- Molecule 3 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).

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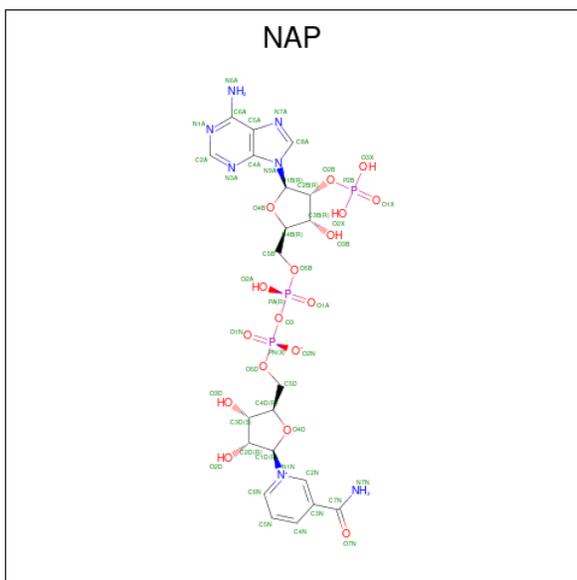
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total 48	C 21	N 7	O 17	P 3	0	0

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

- Molecule 4 is (3 {R})-8-methoxy-3-methyl-3-oxidanyl-2,4-dihydrobenzo[a]anthracene-1,7, 12-trione (three-letter code: P7K) (formula: $C_{20}H_{16}O_5$) (labeled as "Ligand of Interest" by depositor).
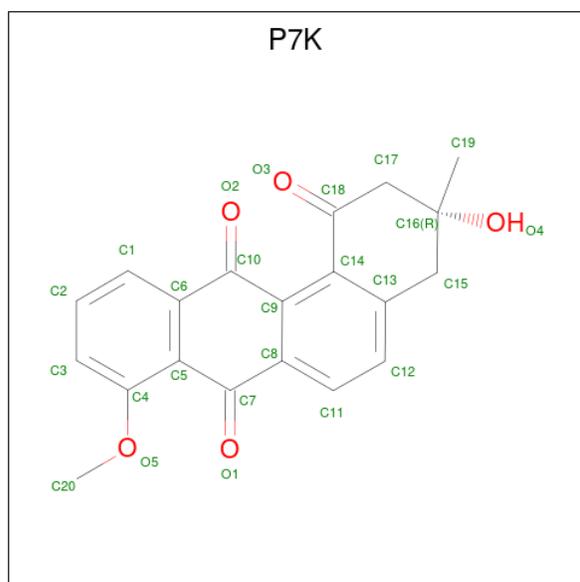
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			25	20	5		
4	BBB	1	Total	C	O	0	0
			25	20	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	287	Total	O	0	0
			287	287		
5	BBB	265	Total	O	0	0
			265	265		

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: Monooxygenase

Chain AAA:
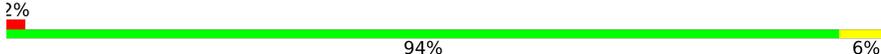
• Molecule 1: Monooxygenase

Chain BBB:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.10Å 60.38Å 88.22Å 90.00° 102.42° 90.00°	Depositor
Resolution (Å)	49.49 – 1.08 49.45 – 1.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.49-1.08) 99.8 (49.45-1.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.08Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.155 , 0.170 0.157 , 0.172	Depositor DCC
R_{free} test set	9703 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	8.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4583	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAP, P7K

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	1.07	5/1964 (0.3%)	1.07	4/2662 (0.2%)
1	BBB	1.11	8/1954 (0.4%)	1.07	7/2648 (0.3%)
All	All	1.09	13/3918 (0.3%)	1.07	11/5310 (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	BBB	0	2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	158	GLU	CD-OE1	10.91	1.37	1.25
1	AAA	109	GLU	CD-OE1	-8.43	1.16	1.25
1	BBB	179	HIS	CE1-NE2	-7.99	1.14	1.32
1	BBB	79	GLU	CD-OE2	-7.47	1.17	1.25
1	BBB	158	GLU	CD-OE2	6.26	1.32	1.25

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	183	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	AAA	140	ASP	CB-CG-OD1	8.47	125.92	118.30
1	BBB	183	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	BBB	3	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	AAA	53	ARG	NE-CZ-NH1	7.31	123.95	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	BBB	153[A]	ARG	Sidechain
1	BBB	153[B]	ARG	Sidechain

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	1918	0	1940	11	0
1	BBB	1911	0	1928	9	0
2	AAA	44	0	62	7	0
2	BBB	12	0	17	2	0
3	AAA	48	0	25	1	0
3	BBB	48	0	25	0	0
4	AAA	25	0	0	1	0
4	BBB	25	0	0	2	0
5	AAA	287	0	0	4	2
5	BBB	265	0	0	1	2
All	All	4583	0	3997	23	2

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 23 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:154[B]:CYS:SG	1:BBB:253:LEU:CD2	2.52	0.98
1:BBB:153[B]:ARG:NH1	2:BBB:305:EDO:O2	1.99	0.95
1:AAA:153[A]:ARG:NH2	5:AAA:401:HOH:O	1.97	0.95
1:BBB:154[B]:CYS:SG	1:BBB:253:LEU:HD22	2.20	0.81
1:AAA:73[B]:GLU:HG2	5:AAA:402:HOH:O	1.83	0.79

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AAA:645:HOH:O	5:BBB:616:HOH:O[2_555]	1.92	0.28
5:AAA:645:HOH:O	5:BBB:572:HOH:O[2_555]	2.07	0.13

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	AAA	259/255 (102%)	252 (97%)	7 (3%)	0	100	100
1	BBB	258/255 (101%)	251 (97%)	7 (3%)	0	100	100
All	All	517/510 (101%)	503 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains   ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	198/192 (103%)	198 (100%)	0	100	100
1	BBB	197/192 (103%)	197 (100%)	0	100	100
All	All	395/384 (103%)	395 (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 ⓘ

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 ⓘ

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	EDO	AAA	301	-	3,3,3	0.73	0	2,2,2	1.43	0
2	EDO	BBB	305	-	3,3,3	0.82	0	2,2,2	0.22	0
2	EDO	AAA	304	-	3,3,3	3.33	1 (33%)	2,2,2	1.05	0
2	EDO	AAA	302	-	3,3,3	0.56	0	2,2,2	0.45	0
2	EDO	AAA	309	-	3,3,3	1.01	0	2,2,2	0.98	0
2	EDO	AAA	313	-	3,3,3	1.29	1 (33%)	2,2,2	0.36	0
3	NAP	AAA	306	-	45,52,52	1.32	6 (13%)	56,80,80	1.15	4 (7%)
3	NAP	BBB	303	-	45,52,52	1.22	6 (13%)	56,80,80	1.17	4 (7%)
4	P7K	AAA	307	-	28,28,28	1.16	2 (7%)	41,44,44	1.43	7 (17%)
4	P7K	BBB	304	-	28,28,28	1.34	5 (17%)	41,44,44	1.35	6 (14%)
2	EDO	AAA	305	-	3,3,3	0.76	0	2,2,2	0.79	0
2	EDO	AAA	303	-	3,3,3	0.84	0	2,2,2	0.25	0
2	EDO	AAA	311	-	3,3,3	1.51	1 (33%)	2,2,2	0.87	0
2	EDO	BBB	302	-	3,3,3	0.76	0	2,2,2	0.26	0
2	EDO	AAA	310	-	3,3,3	0.64	0	2,2,2	0.63	0
2	EDO	AAA	308	-	3,3,3	0.88	0	2,2,2	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	EDO	AAA	312	-	3,3,3	0.50	0	2,2,2	0.12	0
2	EDO	BBB	301	-	3,3,3	2.60	1 (33%)	2,2,2	1.56	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
2	EDO	AAA	301	-	-	0/1/1/1	-
2	EDO	BBB	305	-	-	0/1/1/1	-
2	EDO	AAA	304	-	-	0/1/1/1	-
2	EDO	AAA	302	-	-	0/1/1/1	-
2	EDO	AAA	309	-	-	0/1/1/1	-
2	EDO	AAA	313	-	-	0/1/1/1	-
3	NAP	AAA	306	-	-	2/31/67/67	0/5/5/5
3	NAP	BBB	303	-	-	1/31/67/67	0/5/5/5
4	P7K	AAA	307	-	-	0/2/32/32	0/4/4/4
4	P7K	BBB	304	-	-	0/2/32/32	0/4/4/4
2	EDO	AAA	305	-	-	0/1/1/1	-
2	EDO	AAA	303	-	-	0/1/1/1	-
2	EDO	AAA	311	-	-	0/1/1/1	-
2	EDO	BBB	302	-	-	0/1/1/1	-
2	EDO	AAA	310	-	-	0/1/1/1	-
2	EDO	AAA	308	-	-	0/1/1/1	-
2	EDO	AAA	312	-	-	0/1/1/1	-
2	EDO	BBB	301	-	-	0/1/1/1	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	304	EDO	O2-C2	-5.75	1.12	1.42
2	BBB	301	EDO	O2-C2	-4.49	1.18	1.42
3	BBB	303	NAP	C3N-C7N	-3.81	1.44	1.50
3	AAA	306	NAP	C8A-N7A	-3.42	1.28	1.34
4	AAA	307	P7K	O3-C18	3.33	1.27	1.22

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AAA	307	P7K	C19-C16-C15	-4.65	106.67	110.86
3	BBB	303	NAP	C3N-C7N-N7N	4.37	123.00	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	BBB	304	P7K	O3-C18-C17	-4.28	115.26	121.16
3	BBB	303	NAP	C5A-C6A-N6A	3.40	125.52	120.35
3	AAA	306	NAP	C5A-C6A-N6A	3.12	125.09	120.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	306	NAP	O4B-C4B-C5B-O5B
3	AAA	306	NAP	PN-O3-PA-O2A
3	BBB	303	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	301	EDO	4	0
2	BBB	305	EDO	2	0
3	AAA	306	NAP	1	0
4	AAA	307	P7K	1	0
4	BBB	304	P7K	2	0
2	AAA	310	EDO	3	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 AAA 306

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP BBB 303

Bond lengths

Bond angles

Torsions

Rings

Ligand P7K AAA 307

Bond lengths

Bond angles

Torsions

Rings

Ligand P7K BBB 304

Bond lengths

Bond angles

Torsions

Rings
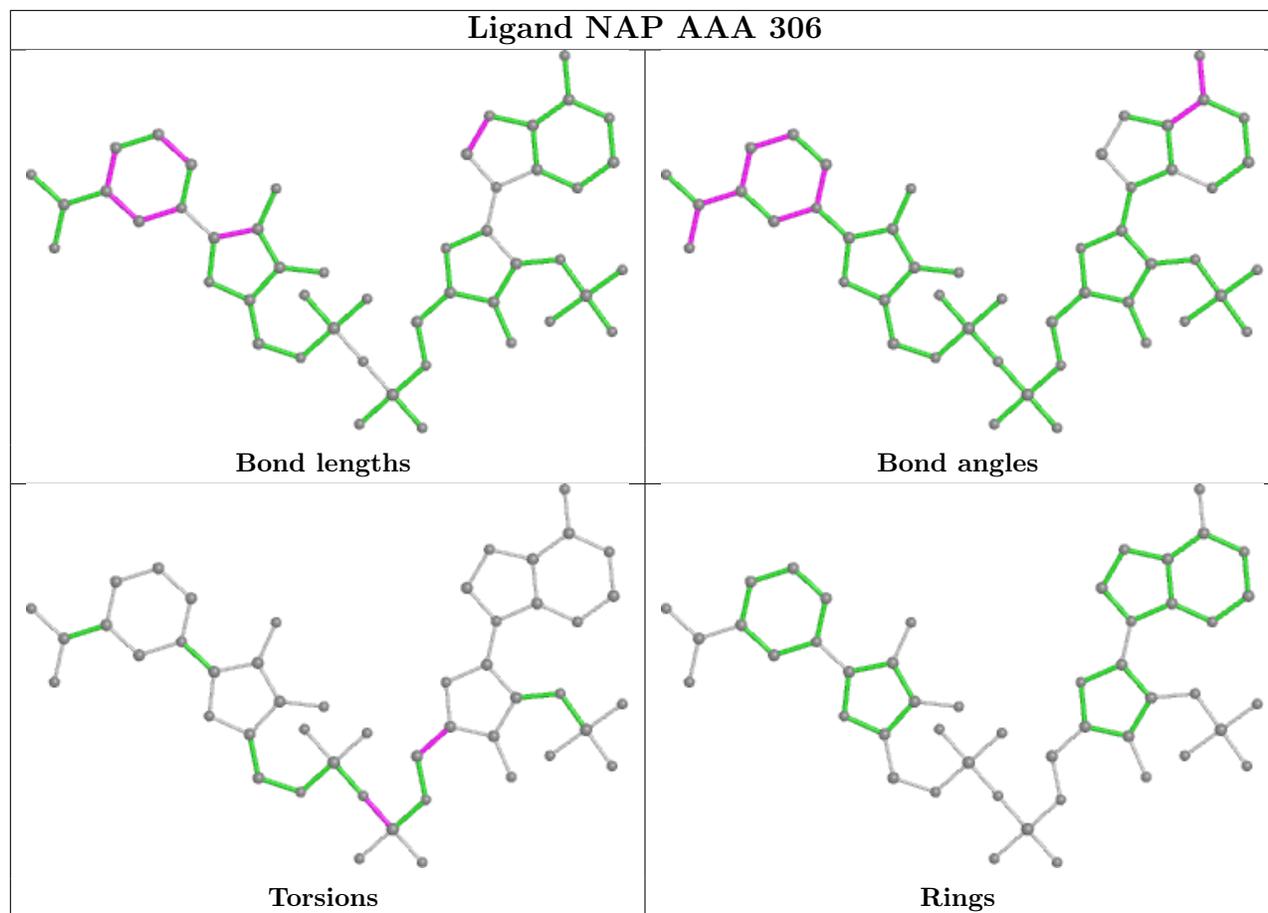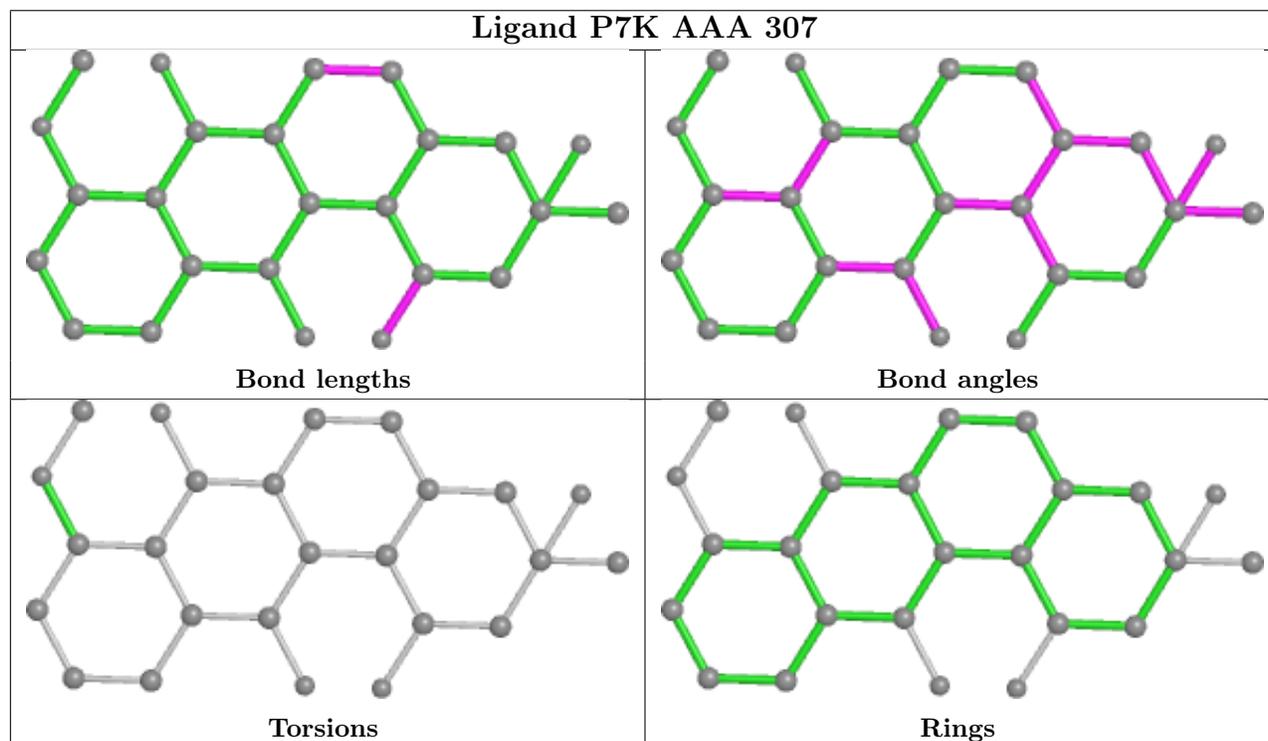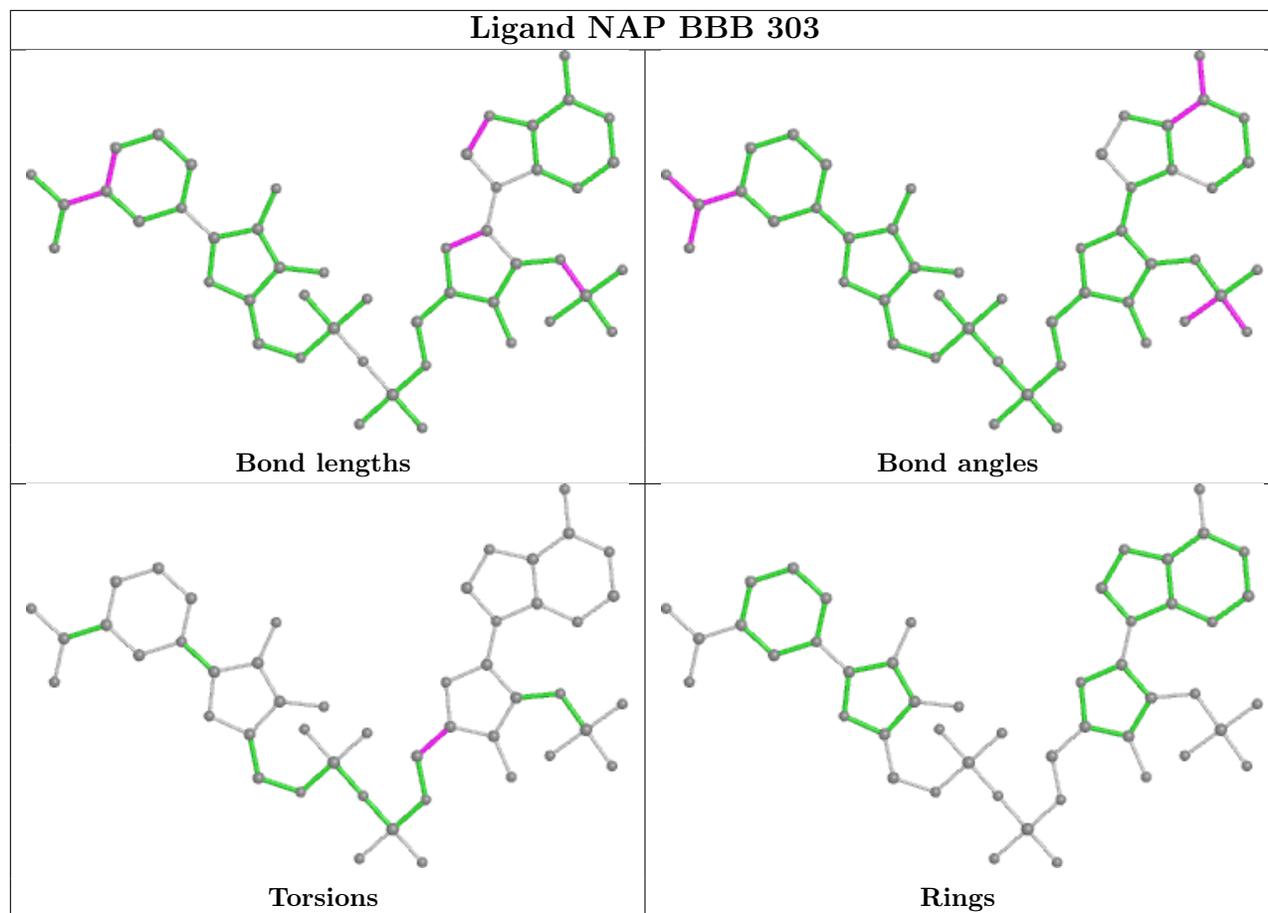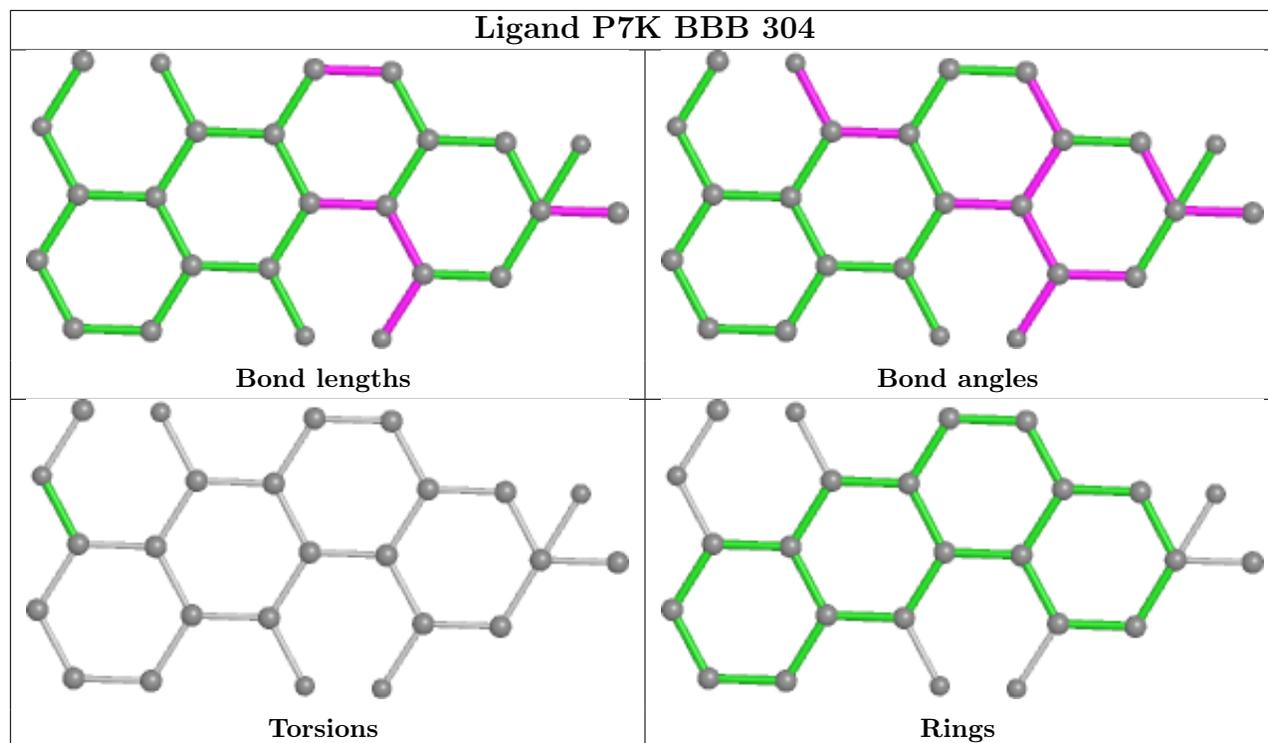
5.7 Other polymers (i)

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 ⓘ

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	AAA	254/255 (99%)	0.14	5 (1%)	65	58	5, 8, 18, 38	0
1	BBB	254/255 (99%)	0.18	10 (3%)	39	33	5, 9, 21, 34	0
All	All	508/510 (99%)	0.16	15 (2%)	50	44	5, 9, 20, 38	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	255	GLY	6.0
1	BBB	103	VAL	4.5
1	BBB	104	ASP	4.4
1	BBB	102	GLY	3.9
1	AAA	255	GLY	3.4

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
4	P7K	BBB	304	25/25	0.79	0.22	16,21,30,33	0
2	EDO	BBB	305	4/4	0.82	0.23	14,14,14,15	0
2	EDO	AAA	301	4/4	0.83	0.18	18,26,29,30	0
2	EDO	AAA	305	4/4	0.87	0.19	19,25,25,31	0
2	EDO	AAA	302	4/4	0.89	0.09	15,16,16,22	0
2	EDO	AAA	310	4/4	0.92	0.15	18,22,24,25	0
2	EDO	AAA	312	4/4	0.93	0.15	19,19,20,20	0
4	P7K	AAA	307	25/25	0.94	0.11	10,13,18,22	0
2	EDO	AAA	308	4/4	0.94	0.15	14,14,15,15	0
2	EDO	AAA	303	4/4	0.95	0.11	12,13,13,15	0
2	EDO	AAA	311	4/4	0.95	0.13	14,19,20,20	0
2	EDO	BBB	302	4/4	0.96	0.11	10,10,11,12	0
2	EDO	AAA	304	4/4	0.96	0.15	7,11,12,14	0
2	EDO	AAA	313	4/4	0.97	0.12	13,19,21,21	0
2	EDO	BBB	301	4/4	0.97	0.12	8,11,12,15	0
2	EDO	AAA	309	4/4	0.97	0.14	9,9,13,14	0
3	NAP	BBB	303	48/48	0.98	0.06	6,8,10,14	0
3	NAP	AAA	306	48/48	0.99	0.06	5,6,8,10	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 P7K BBB 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
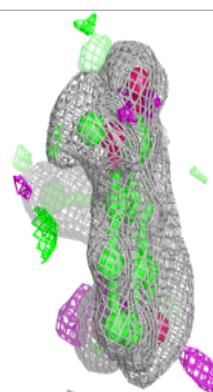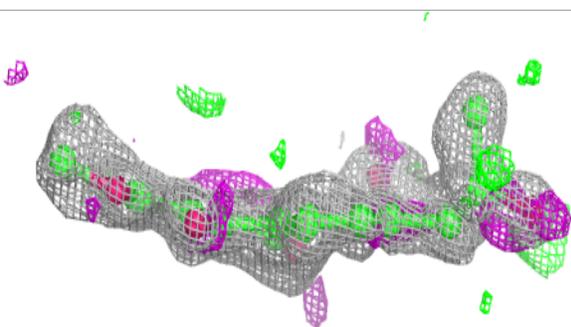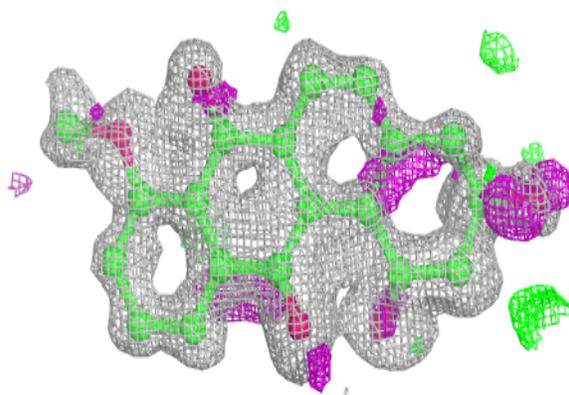
**Electron density around P7K AAA 307:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
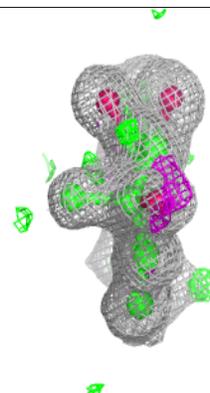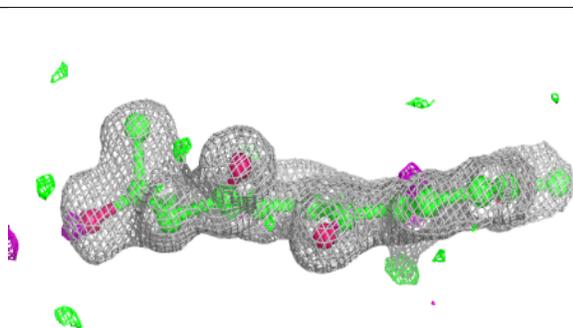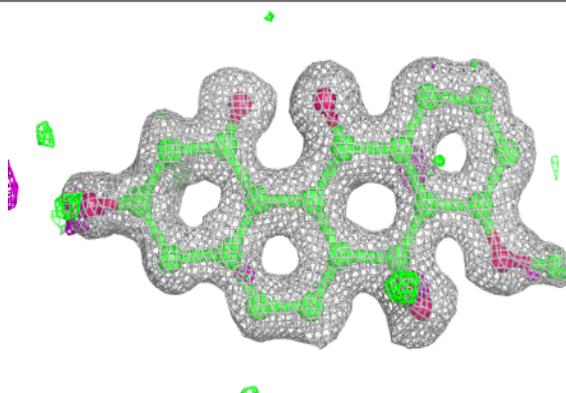
Electron density around NAP BBB 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
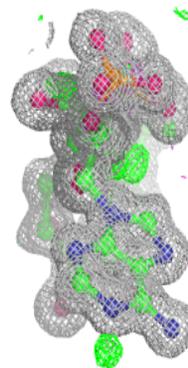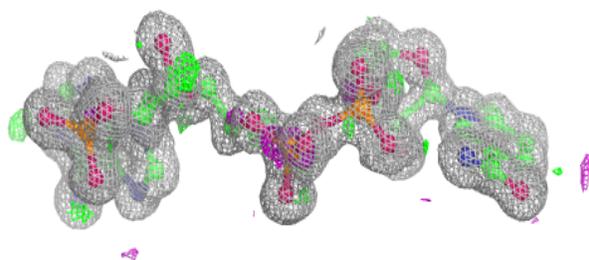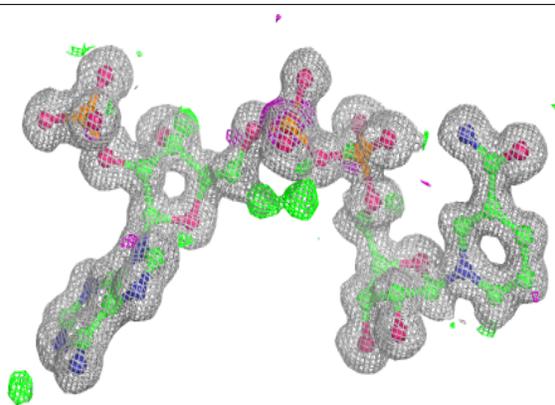
Electron density around NAP AAA 306:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.