WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 06:57 PM EDT

PDB ID	:	4IQG
Title	:	Crystal structure of BPRO0239 oxidoreductase from Polaromonas sp. JS666 in NADP bound form
Authors	:	Niedzialkowska, E.; Majorek, K.A.; Porebski, P.J.; Al Obaidi, N.; Hammonds, J.; Hillerich, B.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; Minor, W.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2013-01-11
Resolution	:	1.85 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

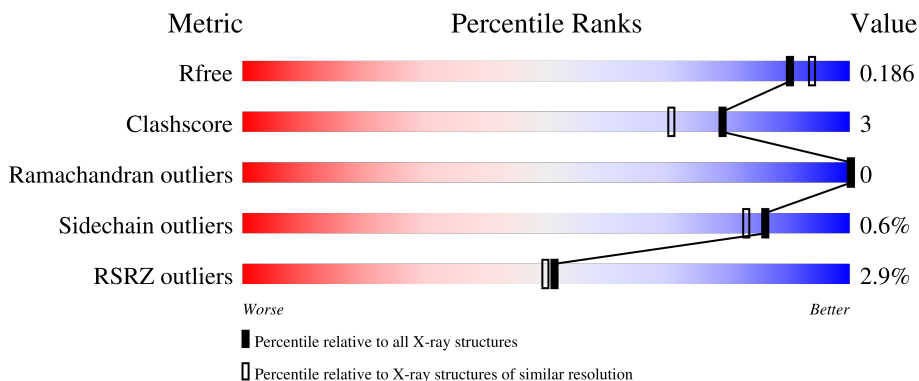|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 1.85 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		0.186
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		2.9%

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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	271	3% / 81% 6% 13%
1	B	271	.% / 86% 6% 9%
1	C	271	6% / 85% 7% 9%
1	D	271	.% / 83% 8% 8%

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
4	GOL	A	303	-	-	X	-
5	PEG	D	302	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7931 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 Short-chain dehydrogenase/reductase SDR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	247	Total	C	N	O	S	Se	0	4	0
			1792	1115	324	348	1	4			
1	A	235	Total	C	N	O	S	Se	0	4	0
			1707	1066	307	329	1	4			
1	B	247	Total	C	N	O	S	Se	0	4	0
			1805	1121	330	349	1	4			
1	D	248	Total	C	N	O	S	Se	0	5	0
			1827	1133	335	354	1	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MSE	-	expression tag	UNP Q12GY8
C	-21	HIS	-	expression tag	UNP Q12GY8
C	-20	HIS	-	expression tag	UNP Q12GY8
C	-19	HIS	-	expression tag	UNP Q12GY8
C	-18	HIS	-	expression tag	UNP Q12GY8
C	-17	HIS	-	expression tag	UNP Q12GY8
C	-16	HIS	-	expression tag	UNP Q12GY8
C	-15	SER	-	expression tag	UNP Q12GY8
C	-14	SER	-	expression tag	UNP Q12GY8
C	-13	GLY	-	expression tag	UNP Q12GY8
C	-12	VAL	-	expression tag	UNP Q12GY8
C	-11	ASP	-	expression tag	UNP Q12GY8
C	-10	LEU	-	expression tag	UNP Q12GY8
C	-9	GLY	-	expression tag	UNP Q12GY8
C	-8	THR	-	expression tag	UNP Q12GY8
C	-7	GLU	-	expression tag	UNP Q12GY8
C	-6	ASN	-	expression tag	UNP Q12GY8
C	-5	LEU	-	expression tag	UNP Q12GY8
C	-4	TYR	-	expression tag	UNP Q12GY8
C	-3	PHE	-	expression tag	UNP Q12GY8
C	-2	GLN	-	expression tag	UNP Q12GY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q12GY8
C	0	MSE	-	expression tag	UNP Q12GY8
C	1	LEU	-	expression tag	UNP Q12GY8
A	-22	MSE	-	expression tag	UNP Q12GY8
A	-21	HIS	-	expression tag	UNP Q12GY8
A	-20	HIS	-	expression tag	UNP Q12GY8
A	-19	HIS	-	expression tag	UNP Q12GY8
A	-18	HIS	-	expression tag	UNP Q12GY8
A	-17	HIS	-	expression tag	UNP Q12GY8
A	-16	HIS	-	expression tag	UNP Q12GY8
A	-15	SER	-	expression tag	UNP Q12GY8
A	-14	SER	-	expression tag	UNP Q12GY8
A	-13	GLY	-	expression tag	UNP Q12GY8
A	-12	VAL	-	expression tag	UNP Q12GY8
A	-11	ASP	-	expression tag	UNP Q12GY8
A	-10	LEU	-	expression tag	UNP Q12GY8
A	-9	GLY	-	expression tag	UNP Q12GY8
A	-8	THR	-	expression tag	UNP Q12GY8
A	-7	GLU	-	expression tag	UNP Q12GY8
A	-6	ASN	-	expression tag	UNP Q12GY8
A	-5	LEU	-	expression tag	UNP Q12GY8
A	-4	TYR	-	expression tag	UNP Q12GY8
A	-3	PHE	-	expression tag	UNP Q12GY8
A	-2	GLN	-	expression tag	UNP Q12GY8
A	-1	SER	-	expression tag	UNP Q12GY8
A	0	MSE	-	expression tag	UNP Q12GY8
A	1	LEU	-	expression tag	UNP Q12GY8
B	-22	MSE	-	expression tag	UNP Q12GY8
B	-21	HIS	-	expression tag	UNP Q12GY8
B	-20	HIS	-	expression tag	UNP Q12GY8
B	-19	HIS	-	expression tag	UNP Q12GY8
B	-18	HIS	-	expression tag	UNP Q12GY8
B	-17	HIS	-	expression tag	UNP Q12GY8
B	-16	HIS	-	expression tag	UNP Q12GY8
B	-15	SER	-	expression tag	UNP Q12GY8
B	-14	SER	-	expression tag	UNP Q12GY8
B	-13	GLY	-	expression tag	UNP Q12GY8
B	-12	VAL	-	expression tag	UNP Q12GY8
B	-11	ASP	-	expression tag	UNP Q12GY8
B	-10	LEU	-	expression tag	UNP Q12GY8
B	-9	GLY	-	expression tag	UNP Q12GY8
B	-8	THR	-	expression tag	UNP Q12GY8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLU	-	expression tag	UNP Q12GY8
B	-6	ASN	-	expression tag	UNP Q12GY8
B	-5	LEU	-	expression tag	UNP Q12GY8
B	-4	TYR	-	expression tag	UNP Q12GY8
B	-3	PHE	-	expression tag	UNP Q12GY8
B	-2	GLN	-	expression tag	UNP Q12GY8
B	-1	SER	-	expression tag	UNP Q12GY8
B	0	MSE	-	expression tag	UNP Q12GY8
B	1	LEU	-	expression tag	UNP Q12GY8
D	-22	MSE	-	expression tag	UNP Q12GY8
D	-21	HIS	-	expression tag	UNP Q12GY8
D	-20	HIS	-	expression tag	UNP Q12GY8
D	-19	HIS	-	expression tag	UNP Q12GY8
D	-18	HIS	-	expression tag	UNP Q12GY8
D	-17	HIS	-	expression tag	UNP Q12GY8
D	-16	HIS	-	expression tag	UNP Q12GY8
D	-15	SER	-	expression tag	UNP Q12GY8
D	-14	SER	-	expression tag	UNP Q12GY8
D	-13	GLY	-	expression tag	UNP Q12GY8
D	-12	VAL	-	expression tag	UNP Q12GY8
D	-11	ASP	-	expression tag	UNP Q12GY8
D	-10	LEU	-	expression tag	UNP Q12GY8
D	-9	GLY	-	expression tag	UNP Q12GY8
D	-8	THR	-	expression tag	UNP Q12GY8
D	-7	GLU	-	expression tag	UNP Q12GY8
D	-6	ASN	-	expression tag	UNP Q12GY8
D	-5	LEU	-	expression tag	UNP Q12GY8
D	-4	TYR	-	expression tag	UNP Q12GY8
D	-3	PHE	-	expression tag	UNP Q12GY8
D	-2	GLN	-	expression tag	UNP Q12GY8
D	-1	SER	-	expression tag	UNP Q12GY8
D	0	MSE	-	expression tag	UNP Q12GY8
D	1	LEU	-	expression tag	UNP Q12GY8

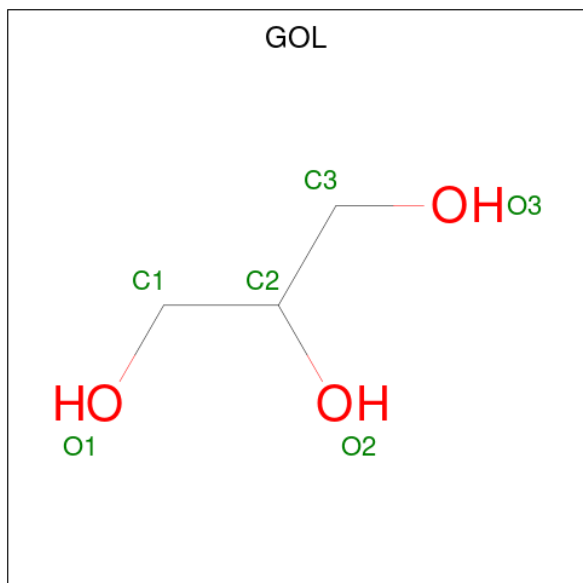- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

FMT

C

OH O2

O

O1

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

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

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
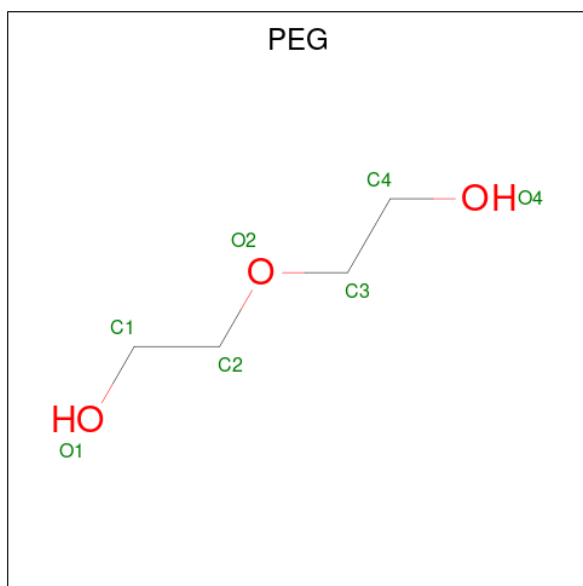
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 7	C 4	O 3	0	0

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	129	Total 129	O 129	0	0
6	A	124	Total 124	O 124	0	0
6	B	154	Total 154	O 154	0	0
6	D	161	Total 161	O 161	0	1

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.
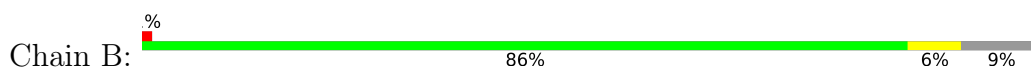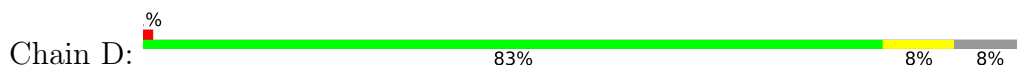
- Molecule 1: Short-chain dehydrogenase/reductase SDR
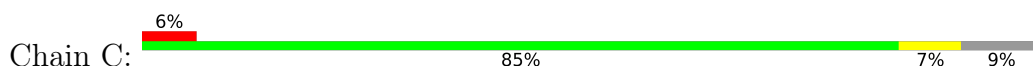
- Molecule 1: Short-chain dehydrogenase/reductase SDR

- Molecule 1: Short-chain dehydrogenase/reductase SDR

- Molecule 1: Short-chain dehydrogenase/reductase SDR

K173 R181 G188 Y236 R248
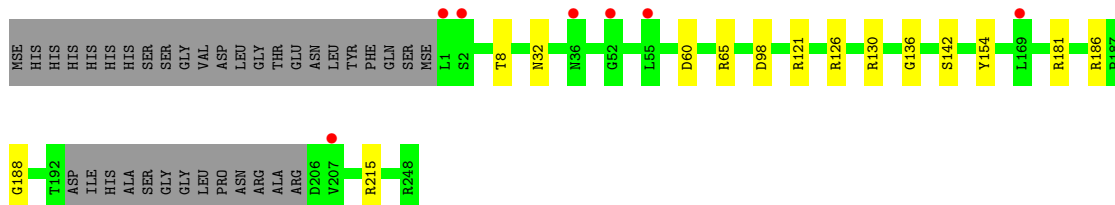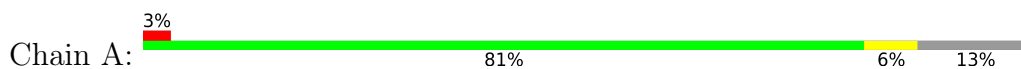
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.14Å　97.71Å　70.67Å 90.00°　97.32°　90.00°	Depositor
Resolution (Å)	40.11　–　1.85 40.08　–　1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.11-1.85) 99.6 (40.08-1.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.148　,　0.173 0.160　,　0.186	Depositor DCC
R_{free} test set	3944 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7931	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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 $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, NAP, GOL, PEG

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	0.80	0/1730	0.91	6/2338 (0.3%)
1	B	0.89	0/1828	0.96	7/2470 (0.3%)
1	C	0.87	0/1815	0.93	5/2455 (0.2%)
1	D	0.94	1/1856 (0.1%)	1.02	8/2507 (0.3%)
All	All	0.88	1/7229 (0.0%)	0.96	26/9770 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	TYR	CE1-CZ	-5.22	1.31	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	65	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	D	65	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	60	ASP	CB-CG-OD1	7.04	124.63	118.30
1	B	65	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	C	126	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	126	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	D	126	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	D	147	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	126	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	181	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	65	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	126	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	65	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	181	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	248	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	B	126	ARG	NE-CZ-NH2	-5.57	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	D	24	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	248	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	60	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	24	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	C	60	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	215	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	147	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	126	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	147	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	A	1707	0	1738	10	0
1	B	1805	0	1826	7	0
1	C	1792	0	1810	10	0
1	D	1827	0	1865	17	0
2	A	6	0	3	0	0
2	B	6	0	3	0	0
2	C	9	0	3	0	0
2	D	6	0	4	0	0
3	A	48	0	25	1	0
3	B	48	0	25	2	0
3	C	48	0	25	2	0
3	D	48	0	25	3	0
4	A	6	0	8	5	0
5	D	7	0	10	6	0
6	A	124	0	0	3	0
6	B	154	0	0	1	0
6	C	129	0	0	0	0
6	D	161	0	0	0	0
All	All	7931	0	7370	41	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.

All (41) 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:150:SER:HA	5:D:302:PEG:H21	1.54	0.87
1:D:150:SER:CA	5:D:302:PEG:H21	2.14	0.78
1:D:150:SER:H	5:D:302:PEG:H21	1.48	0.78
1:D:150:SER:N	5:D:302:PEG:H21	2.01	0.75
1:A:181:ARG:HH21	4:A:303:GOL:H11	1.54	0.72
1:C:188:GLY:O	3:C:304:NAP:H4N	1.97	0.64
1:D:150:SER:HA	5:D:302:PEG:C2	2.26	0.64
4:A:303:GOL:H12	6:A:511:HOH:O	1.98	0.64
1:A:181:ARG:HH21	4:A:303:GOL:C1	2.12	0.62
1:D:188:GLY:O	3:D:301:NAP:H4N	1.99	0.62
1:A:136:GLY:O	4:A:303:GOL:H32	2.03	0.59
1:B:188:GLY:O	3:B:301:NAP:H4N	2.09	0.53
1:D:169[B]:LEU:HD11	1:D:173:LYS:HE3	1.90	0.52
1:D:169[B]:LEU:CD1	1:D:173:LYS:HE3	2.40	0.52
1:A:188:GLY:O	3:A:304:NAP:H4N	2.09	0.52
1:C:121:ARG:HG3	1:A:98:ASP:HA	1.95	0.49
1:D:45:ARG:NH1	1:D:49:GLU:OE2	2.45	0.49
1:C:9:GLY:HA2	3:C:304:NAP:H1B	1.94	0.48
1:B:82:SER:C	1:B:127:MSE:HE2	2.34	0.47
1:B:53:GLN:NE2	6:B:540:HOH:O	2.48	0.47
1:A:181:ARG:NH2	4:A:303:GOL:H11	2.27	0.46
1:D:142:SER:O	3:D:301:NAP:H6N	2.16	0.46
6:A:442:HOH:O	1:B:220:ARG:HG3	2.16	0.45
1:C:98:ASP:HA	1:A:121:ARG:HG3	2.00	0.44
1:C:169[A]:LEU:HD11	1:C:173:LYS:HE3	2.00	0.44
1:A:8:THR:HA	1:A:32:ASN:HB3	1.99	0.44
1:C:169[A]:LEU:HD12	1:C:169[A]:LEU:HA	1.75	0.42
1:B:121:ARG:HG3	1:D:98:ASP:HA	2.02	0.42
1:A:130:ARG:NH1	6:A:454:HOH:O	2.53	0.42
1:D:8:THR:HA	1:D:32:ASN:HB3	2.01	0.42
1:C:32:ASN:HA	1:C:57:VAL:O	2.20	0.42
1:C:213:MSE:HE2	1:C:213:MSE:HB3	1.88	0.41
1:B:9:GLY:HA2	3:B:301:NAP:H1B	2.03	0.41
1:D:145:ALA:HA	5:D:302:PEG:H12	2.03	0.41
1:B:98:ASP:HA	1:D:121:ARG:HG3	2.03	0.41
1:C:81:LEU:HG	1:C:127:MSE:HE3	2.02	0.40
1:A:142:SER:HB3	1:A:186:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LEU:O	1:C:175:VAL:HG22	2.21	0.40
1:D:11:SER:OG	3:D:301:NAP:O3X	2.37	0.40
1:D:82:SER:C	1:D:127:MSE:HE2	2.41	0.40

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	235/271 (87%)	228 (97%)	7 (3%)	0	100	100
1	B	249/271 (92%)	241 (97%)	8 (3%)	0	100	100
1	C	249/271 (92%)	241 (97%)	8 (3%)	0	100	100
1	D	251/271 (93%)	243 (97%)	8 (3%)	0	100	100
All	All	984/1084 (91%)	953 (97%)	31 (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	A	168/194 (87%)	167 (99%)	1 (1%)	86	83
1	B	177/194 (91%)	176 (99%)	1 (1%)	86	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	176/194 (91%)	175 (99%)	1 (1%)	86	83
1	D	183/194 (94%)	182 (100%)	1 (0%)	88	86
All	All	704/776 (91%)	700 (99%)	4 (1%)	86	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	154	TYR
1	A	154	TYR
1	B	154	TYR
1	D	154	TYR

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 ⓘ

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
2	FMT	D	304	-	0,2,2	-	-	0,1,1	-	-
3	NAP	B	301	-	45,52,52	1.56	8 (17%)	56,80,80	1.48	11 (19%)
2	FMT	C	302	-	0,2,2	-	-	0,1,1	-	-
3	NAP	D	301	-	45,52,52	1.33	4 (8%)	56,80,80	1.61	10 (17%)
4	GOL	A	303	-	5,5,5	0.40	0	5,5,5	0.61	0
2	FMT	B	303	-	0,2,2	-	-	0,1,1	-	-
3	NAP	C	304	-	45,52,52	1.40	6 (13%)	56,80,80	1.21	5 (8%)
5	PEG	D	302	-	6,6,6	1.00	1 (16%)	5,5,5	2.15	1 (20%)
2	FMT	A	302	-	0,2,2	-	-	0,1,1	-	-
3	NAP	A	304	-	45,52,52	1.32	5 (11%)	56,80,80	1.72	14 (25%)
2	FMT	D	303	-	0,2,2	-	-	0,1,1	-	-
2	FMT	A	301	-	0,2,2	-	-	0,1,1	-	-
2	FMT	C	303	-	0,2,2	-	-	0,1,1	-	-
2	FMT	C	301	-	0,2,2	-	-	0,1,1	-	-
2	FMT	B	302	-	0,2,2	-	-	0,1,1	-	-

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	NAP	B	301	-	-	8/31/67/67	0/5/5/5
4	GOL	A	303	-	-	0/4/4/4	-
5	PEG	D	302	-	-	3/4/4/4	-
3	NAP	A	304	-	-	6/31/67/67	0/5/5/5
3	NAP	D	301	-	-	8/31/67/67	0/5/5/5
3	NAP	C	304	-	-	8/31/67/67	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NAP	C2N-N1N	4.08	1.39	1.35
3	C	304	NAP	O4B-C1B	3.62	1.46	1.41
3	A	304	NAP	O4B-C1B	3.50	1.46	1.41
3	A	304	NAP	P2B-O2B	3.46	1.65	1.59
3	D	301	NAP	C5A-C4A	3.37	1.49	1.40
3	B	301	NAP	C4N-C3N	3.11	1.44	1.39
3	B	301	NAP	P2B-O3X	-3.10	1.42	1.54
3	A	304	NAP	C6N-C5N	3.09	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	NAP	C8A-N7A	2.98	1.40	1.34
3	C	304	NAP	C5A-C4A	2.85	1.48	1.40
3	C	304	NAP	C6N-C5N	2.80	1.44	1.38
3	B	301	NAP	P2B-O2B	2.79	1.64	1.59
3	C	304	NAP	P2B-O2B	2.76	1.64	1.59
3	C	304	NAP	C2N-C3N	2.75	1.43	1.39
3	C	304	NAP	C2A-N3A	2.70	1.36	1.32
3	D	301	NAP	P2B-O2B	2.69	1.64	1.59
3	B	301	NAP	O4B-C1B	2.59	1.44	1.41
3	A	304	NAP	C5A-C4A	2.58	1.47	1.40
3	B	301	NAP	C5A-C4A	2.56	1.47	1.40
3	B	301	NAP	C7N-N7N	-2.56	1.28	1.33
3	D	301	NAP	C2A-N1A	2.50	1.38	1.33
3	B	301	NAP	C2A-N1A	2.43	1.38	1.33
5	D	302	PEG	O1-C1	2.14	1.53	1.42
3	A	304	NAP	C2A-N1A	2.03	1.37	1.33

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	NAP	O7N-C7N-C3N	-5.36	113.22	119.63
3	D	301	NAP	N3A-C2A-N1A	-5.27	120.45	128.68
3	A	304	NAP	N3A-C2A-N1A	-4.44	121.74	128.68
5	D	302	PEG	O2-C2-C1	4.31	129.01	110.07
3	A	304	NAP	C2N-C3N-C4N	4.14	122.95	118.26
3	A	304	NAP	C3N-C2N-N1N	-3.78	116.73	120.43
3	D	301	NAP	C3N-C7N-N7N	-3.72	113.28	117.75
3	C	304	NAP	N3A-C2A-N1A	-3.59	123.07	128.68
3	B	301	NAP	N3A-C2A-N1A	-3.57	123.09	128.68
3	D	301	NAP	C1B-N9A-C4A	-3.50	120.49	126.64
3	D	301	NAP	O4D-C1D-C2D	-3.37	102.00	106.93
3	C	304	NAP	O4D-C1D-C2D	-3.22	102.22	106.93
3	D	301	NAP	O2X-P2B-O1X	3.12	122.91	110.68
3	D	301	NAP	O2N-PN-O1N	3.05	127.30	112.24
3	D	301	NAP	O5B-PA-O1A	3.04	120.96	109.07
3	D	301	NAP	O7N-C7N-N7N	2.94	126.75	122.58
3	A	304	NAP	C6N-C5N-C4N	-2.93	115.18	119.44
3	B	301	NAP	O3X-P2B-O2X	2.73	118.09	107.64
3	B	301	NAP	C3N-C2N-N1N	-2.69	117.80	120.43
3	B	301	NAP	O2X-P2B-O1X	2.59	120.83	110.68
3	A	304	NAP	C3N-C7N-N7N	2.52	120.78	117.75
3	B	301	NAP	C1B-N9A-C4A	-2.51	122.23	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	304	NAP	N6A-C6A-N1A	2.46	123.69	118.57
3	A	304	NAP	C1B-N9A-C4A	-2.41	122.40	126.64
3	B	301	NAP	C2N-C3N-C4N	2.37	120.95	118.26
3	A	304	NAP	O7N-C7N-N7N	2.32	125.88	122.58
3	B	301	NAP	O2N-PN-O1N	2.29	123.56	112.24
3	A	304	NAP	C3B-C2B-C1B	-2.25	98.67	102.89
3	C	304	NAP	O3X-P2B-O2X	2.24	116.21	107.64
3	B	301	NAP	C3N-C7N-N7N	-2.20	115.11	117.75
3	B	301	NAP	O2A-PA-O1A	2.13	122.78	112.24
3	A	304	NAP	C5A-C6A-N6A	-2.09	117.17	120.35
3	D	301	NAP	C5A-C6A-N6A	-2.08	117.19	120.35
3	C	304	NAP	O2A-PA-O1A	2.06	122.42	112.24
3	B	301	NAP	N6A-C6A-N1A	2.06	122.85	118.57
3	A	304	NAP	C5N-C6N-N1N	2.06	123.35	120.40
3	A	304	NAP	C2A-N1A-C6A	2.04	122.25	118.75
3	C	304	NAP	C3N-C7N-N7N	-2.04	115.30	117.75
3	D	301	NAP	C6N-N1N-C2N	-2.03	120.12	121.97
3	A	304	NAP	O2N-PN-O1N	2.02	122.24	112.24
3	B	301	NAP	O3X-P2B-O1X	-2.02	102.77	110.68

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	304	NAP	C5D-O5D-PN-O1N
3	A	304	NAP	C5D-O5D-PN-O1N
3	B	301	NAP	C5D-O5D-PN-O1N
3	D	301	NAP	C2B-O2B-P2B-O3X
3	D	301	NAP	C5D-O5D-PN-O1N
3	B	301	NAP	C3B-C4B-C5B-O5B
3	D	301	NAP	PN-O3-PA-O1A
3	B	301	NAP	O4B-C4B-C5B-O5B
5	D	302	PEG	C4-C3-O2-C2
3	C	304	NAP	C5D-O5D-PN-O3
3	A	304	NAP	C5D-O5D-PN-O3
3	B	301	NAP	C5D-O5D-PN-O3
3	D	301	NAP	C5D-O5D-PN-O3
5	D	302	PEG	O1-C1-C2-O2
3	B	301	NAP	PN-O3-PA-O2A
5	D	302	PEG	C1-C2-O2-C3
3	C	304	NAP	C5D-O5D-PN-O2N
3	B	301	NAP	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
3	D	301	NAP	C5D-O5D-PN-O2N
3	A	304	NAP	PN-O3-PA-O2A
3	C	304	NAP	O4B-C4B-C5B-O5B
3	B	301	NAP	C1B-C2B-O2B-P2B
3	C	304	NAP	C1B-C2B-O2B-P2B
3	A	304	NAP	C1B-C2B-O2B-P2B
3	C	304	NAP	PN-O3-PA-O1A
3	C	304	NAP	C3B-C2B-O2B-P2B
3	A	304	NAP	C3B-C2B-O2B-P2B
3	B	301	NAP	C3B-C2B-O2B-P2B
3	D	301	NAP	C1B-C2B-O2B-P2B
3	A	304	NAP	O4B-C4B-C5B-O5B
3	C	304	NAP	PN-O3-PA-O2A
3	D	301	NAP	O4B-C4B-C5B-O5B
3	D	301	NAP	C3B-C2B-O2B-P2B

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	NAP	2	0
3	D	301	NAP	3	0
4	A	303	GOL	5	0
3	C	304	NAP	2	0
5	D	302	PEG	6	0
3	A	304	NAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Full wwPDB X-ray Structure Validation Report

Ligand NAP B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 304

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 304

Bond lengths

Bond angles

Torsions

Rings
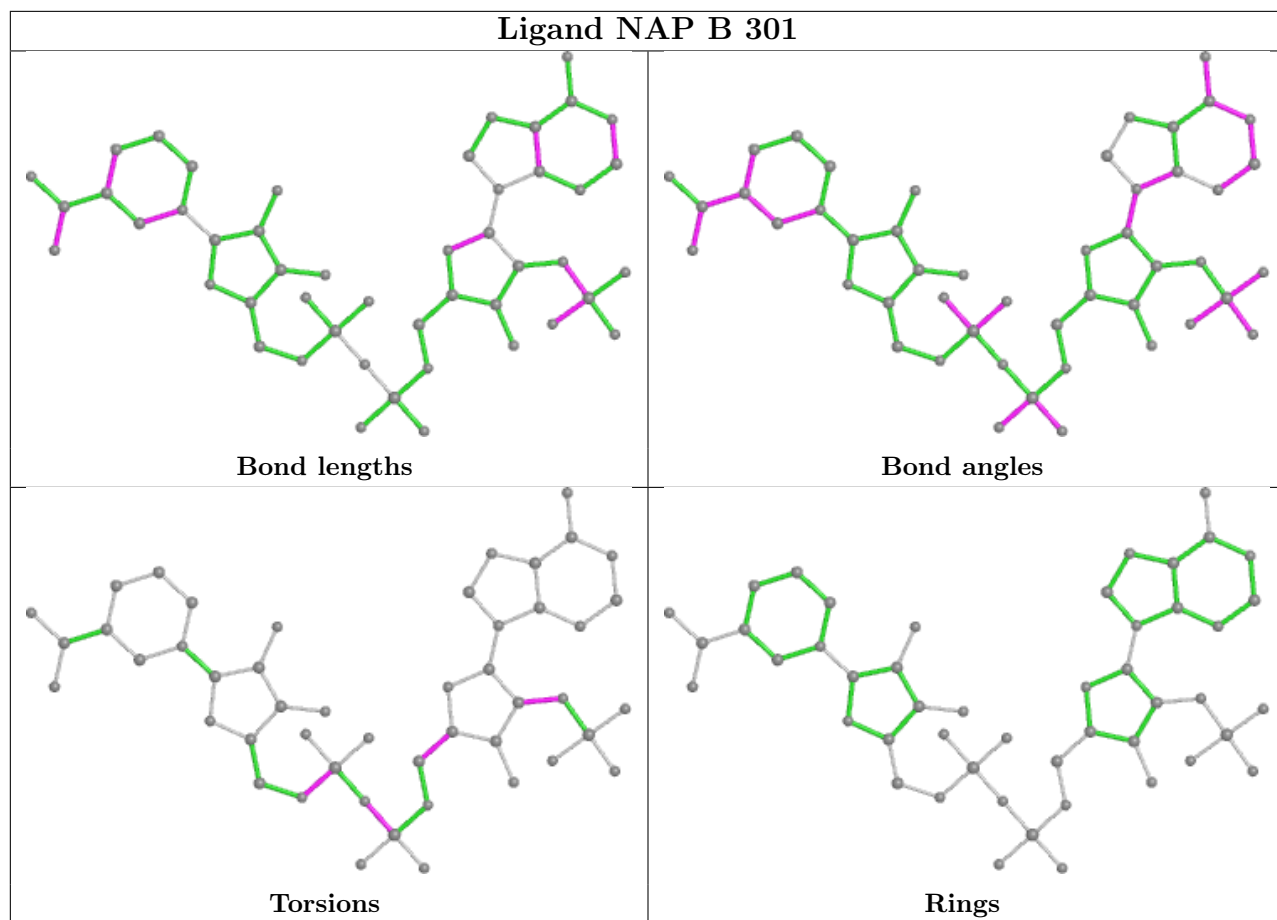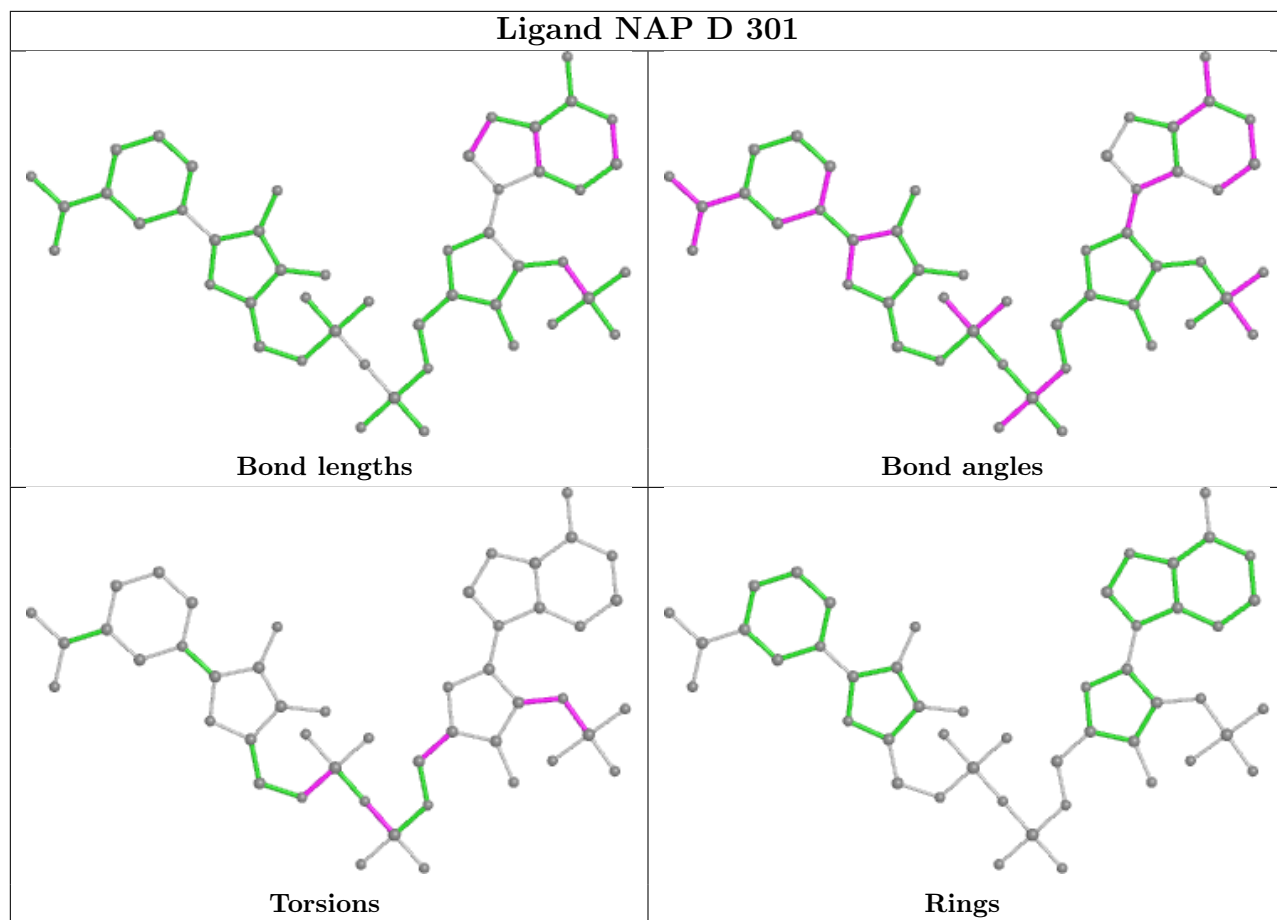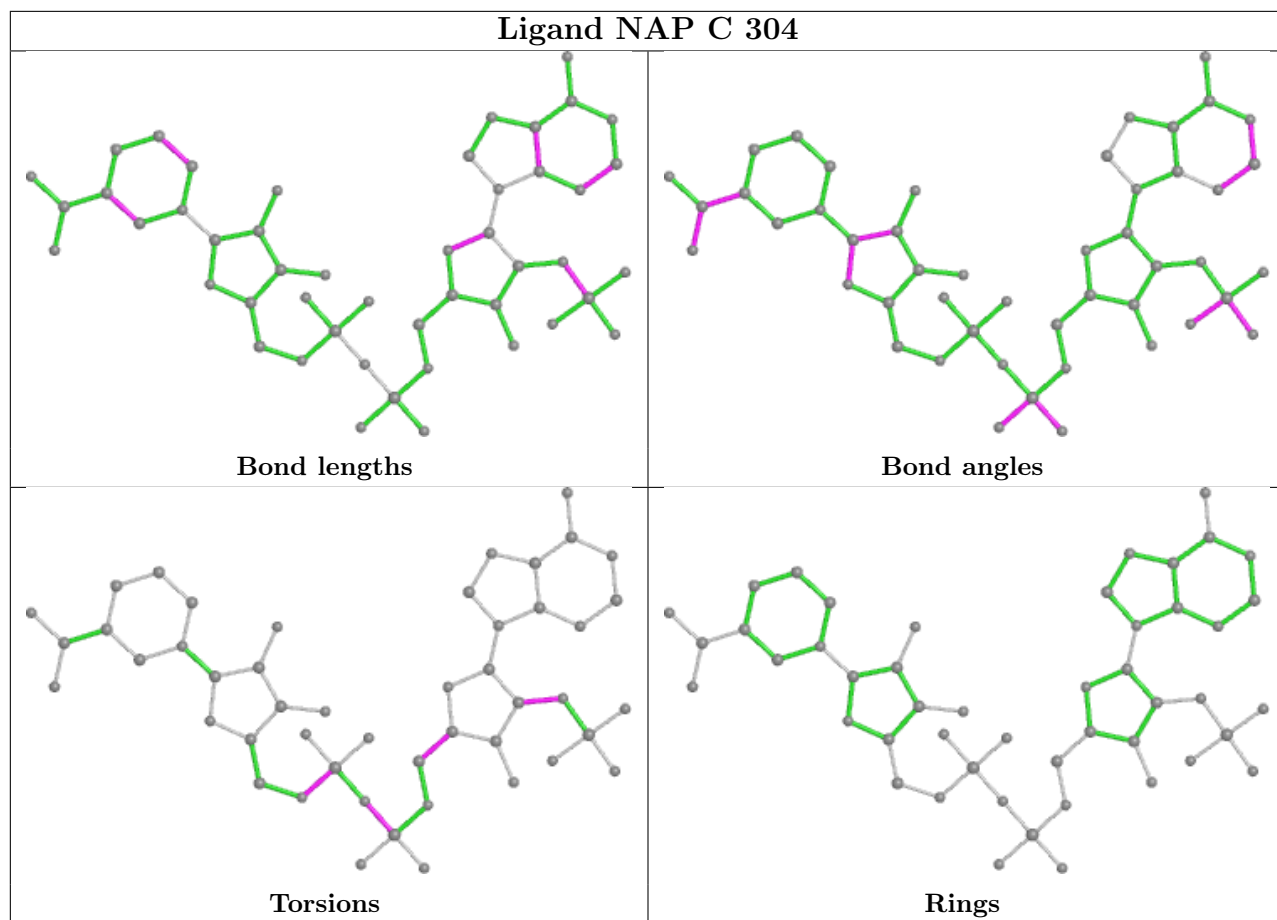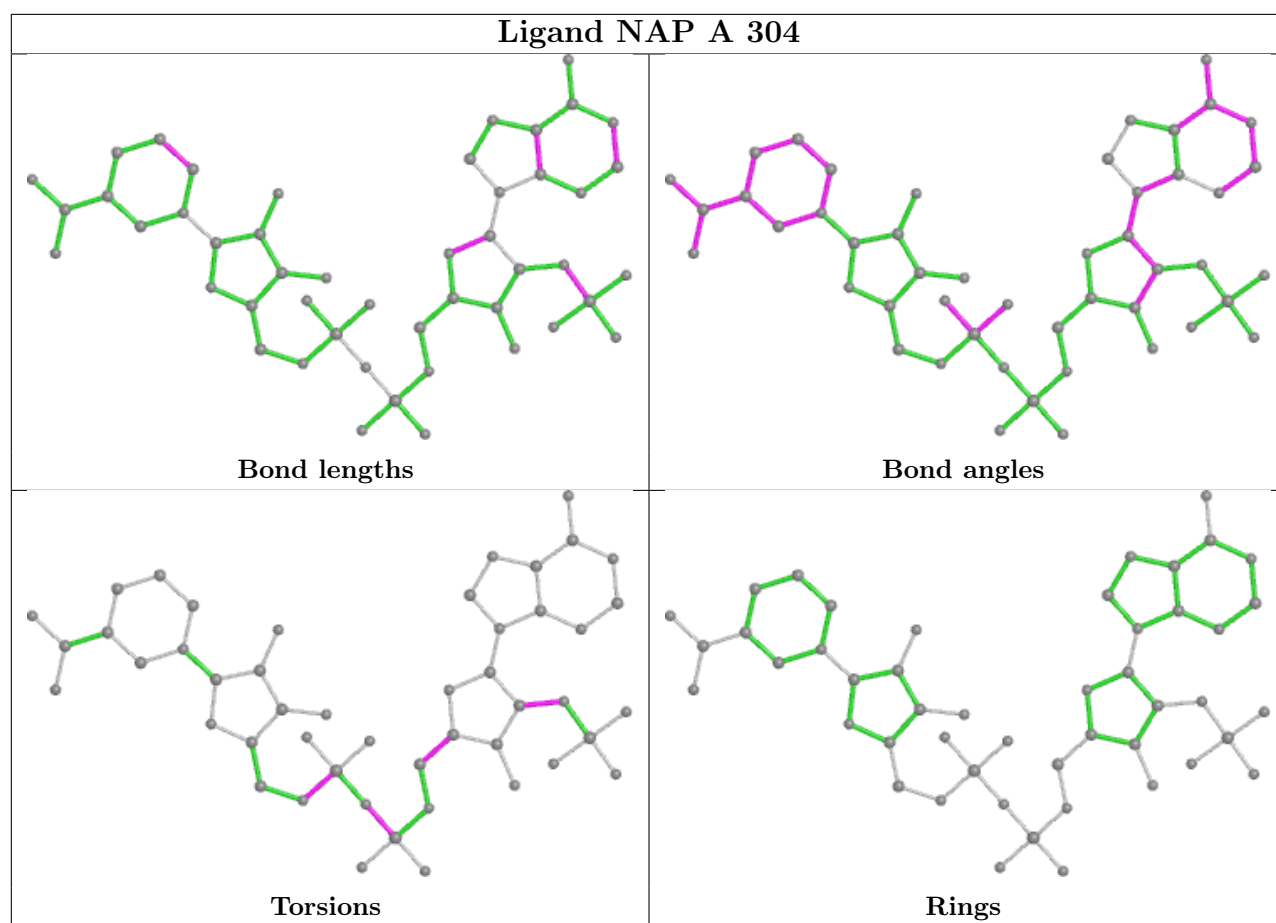
5.7   Other polymers ⓘ

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	231/271 (85%)	-0.00	7 (3%)	50	48	19, 30, 53, 64	0
1	B	243/271 (89%)	-0.28	3 (1%)	79	79	17, 25, 43, 60	0
1	C	243/271 (89%)	0.08	16 (6%)	18	17	17, 28, 59, 69	0
1	D	244/271 (90%)	-0.28	2 (0%)	86	86	15, 24, 43, 65	0
All	All	961/1084 (88%)	-0.12	28 (2%)	51	50	15, 26, 50, 69	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	LEU	6.9
1	C	198	GLY	6.4
1	C	204	ALA	5.8
1	C	199	GLY	5.3
1	C	202	ASN	5.3
1	C	201	PRO	5.0
1	A	1	LEU	4.4
1	C	203	ARG	4.1
1	C	197	SER	4.1
1	C	194	ILE	4.0
1	C	196	ALA	3.9
1	D	1	LEU	3.9
1	C	195	HIS	3.5
1	A	207	VAL	3.3
1	C	207	VAL	2.8
1	A	55	LEU	2.8
1	C	169[A]	LEU	2.7
1	B	2	SER	2.6
1	A	169[A]	LEU	2.3
1	C	208	ALA	2.3
1	A	52	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	2	SER	2.2
1	B	198	GLY	2.2
1	C	90	VAL	2.2
1	C	193	ASP	2.2
1	D	169[A]	LEU	2.1
1	A	36	ASN	2.0
1	B	200	LEU	2.0

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

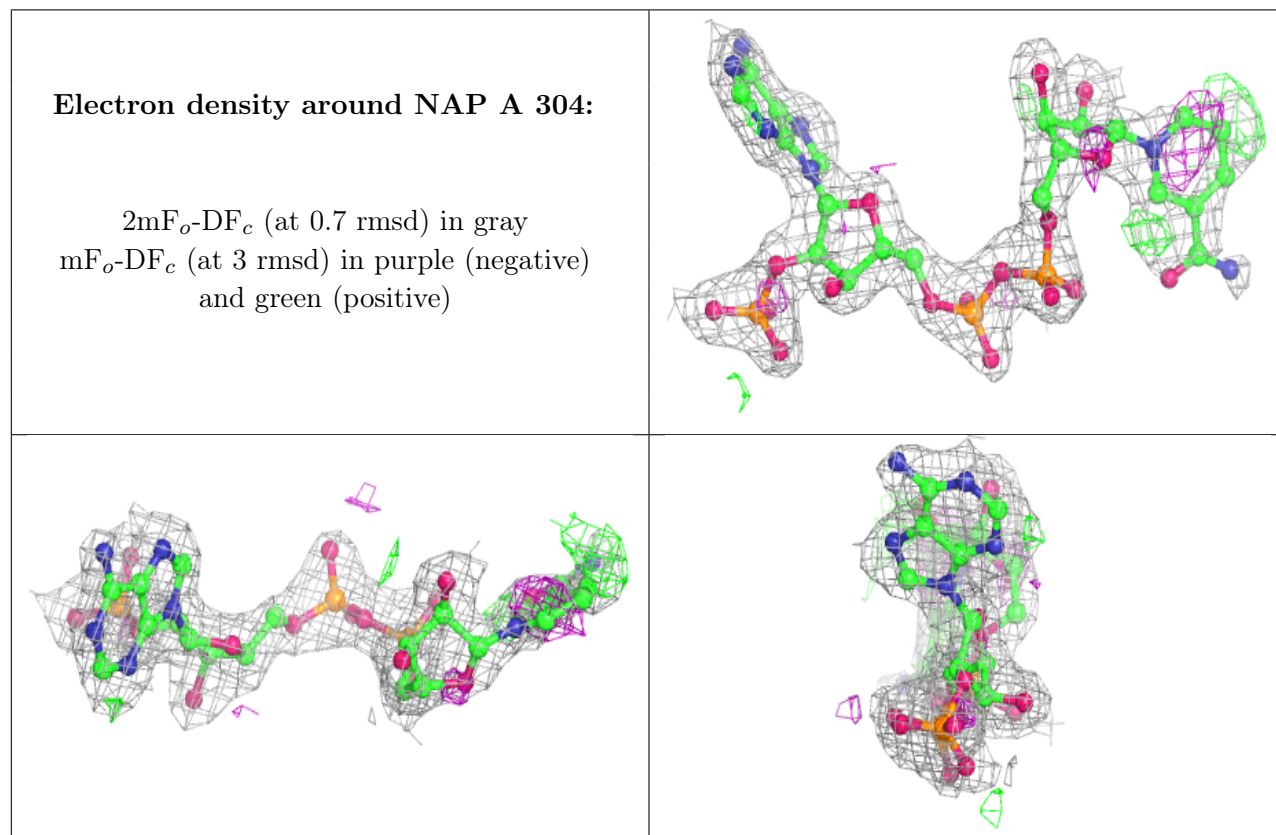There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	D	302	7/7	0.74	0.20	34,40,56,58	0
2	FMT	B	302	3/3	0.79	0.19	41,41,47,53	0
2	FMT	D	303	3/3	0.85	0.28	39,39,39,49	0
4	GOL	A	303	6/6	0.87	0.23	27,27,31,36	6
3	NAP	A	304	48/48	0.87	0.16	29,38,48,61	48
2	FMT	C	302	3/3	0.88	0.23	37,37,43,43	0
2	FMT	C	303	3/3	0.89	0.16	58,58,58,64	0
2	FMT	D	304	3/3	0.90	0.23	31,31,37,42	0
2	FMT	A	302	3/3	0.90	0.25	32,32,38,40	0
3	NAP	C	304	48/48	0.91	0.16	25,35,42,43	48
2	FMT	C	301	3/3	0.94	0.13	45,45,50,54	0
2	FMT	B	303	3/3	0.94	0.12	51,51,53,57	0
2	FMT	A	301	3/3	0.95	0.18	32,32,40,47	0
3	NAP	B	301	48/48	0.96	0.09	17,21,26,28	48
3	NAP	D	301	48/48	0.97	0.07	19,25,29,30	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.
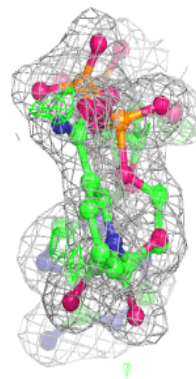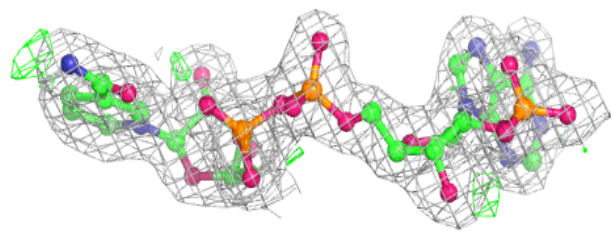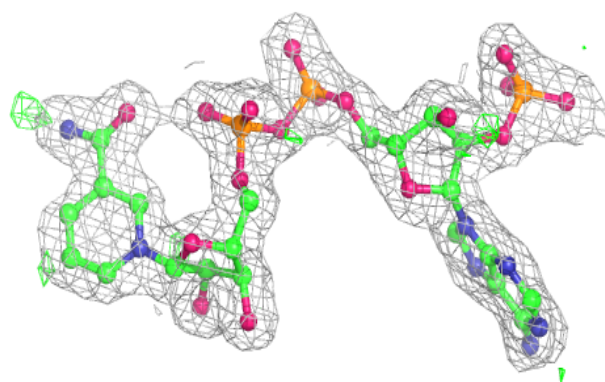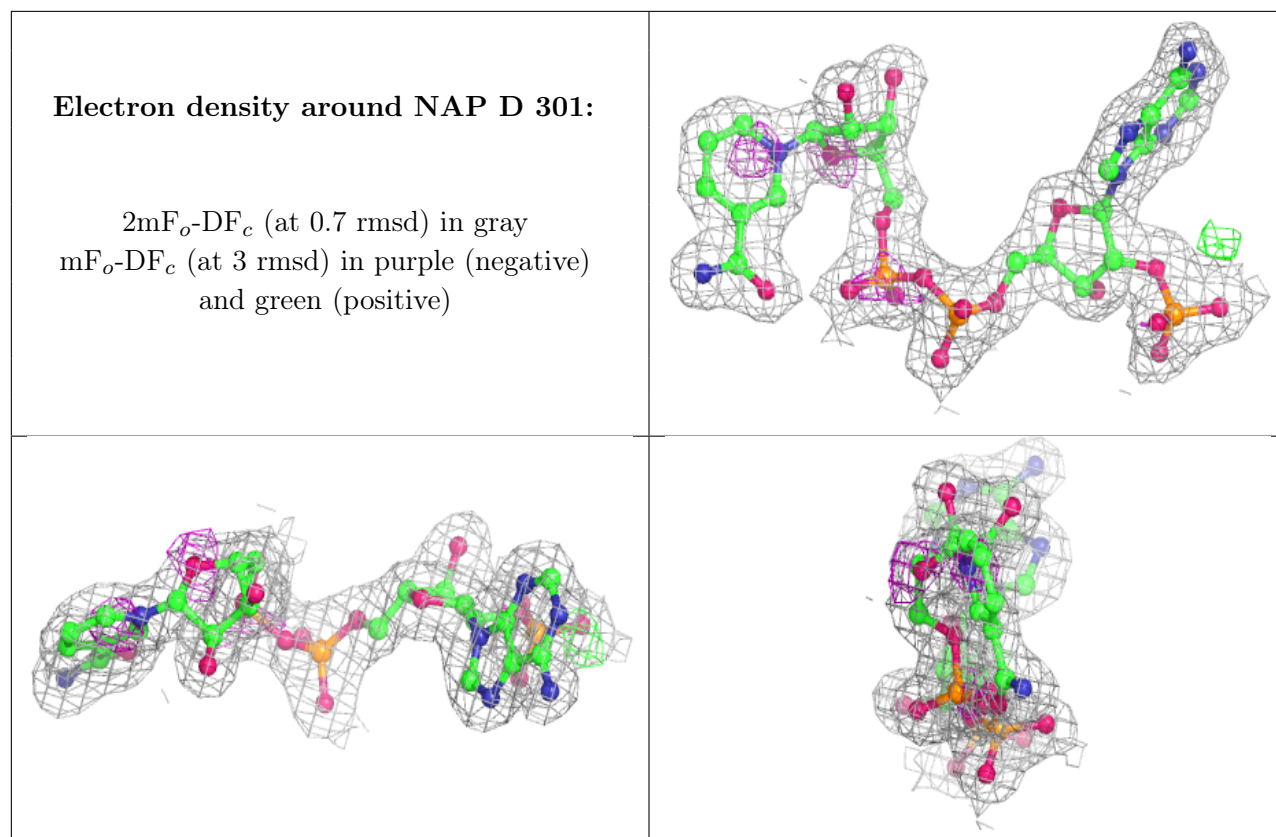
Electron density around NAP A 304:

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

Electron density around NAP C 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
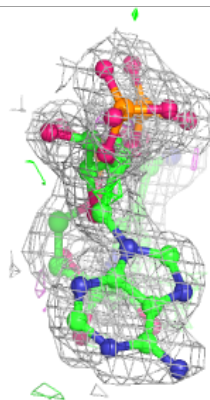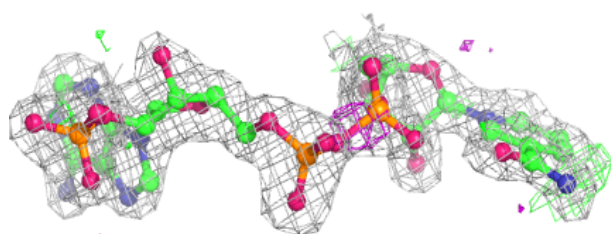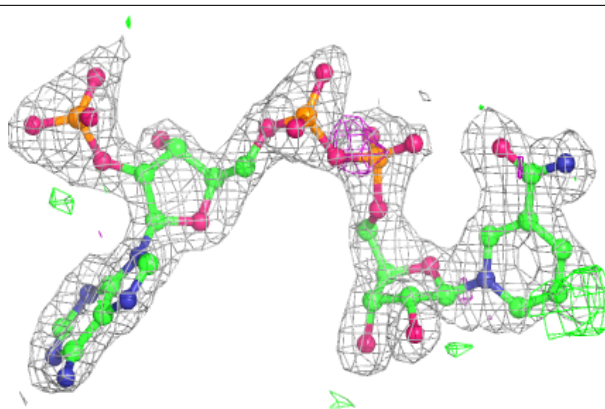
Electron density around NAP B 301:

$2mF_o$-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 D 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 ⓘ

There are no such residues in this entry.