Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2023 – 07:22 PM JST

PDB ID	:	6A2K
Title	:	Crystal structure of wild type Plasmodium falciparum DHFR-TS complexed with BT1, NADPH, and dUMP
Authors	:	Chitnumsub, P.; Jaruwat, A.; Tarnchampoo, B.; Yuthavong, Y.
Deposited on	:	2018-06-12
Resolution	:	2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

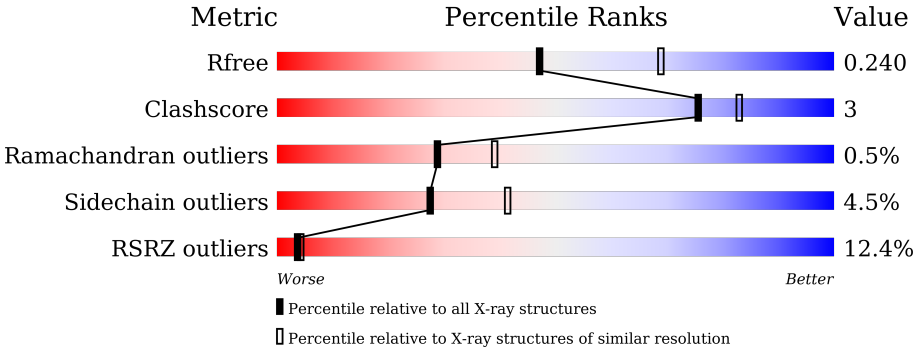
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	608	8%, 81%, 8%, 11%
1	B	608	14%, 74%, 12%, •, 13%

2 Entry composition (i)

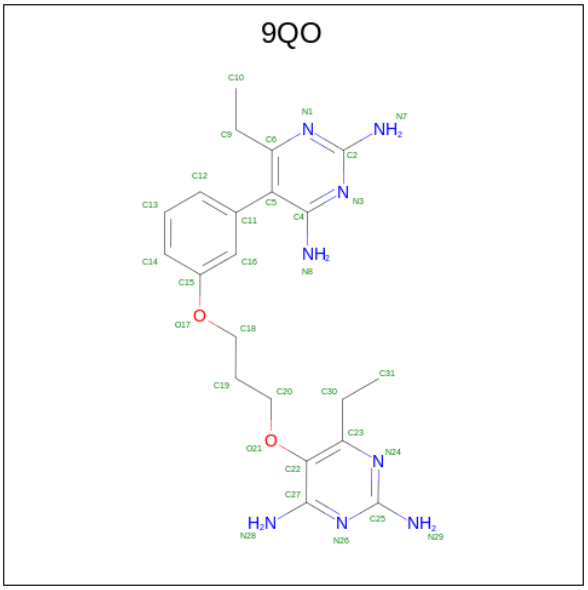
There are 5 unique types of molecules in this entry. The entry contains 9429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

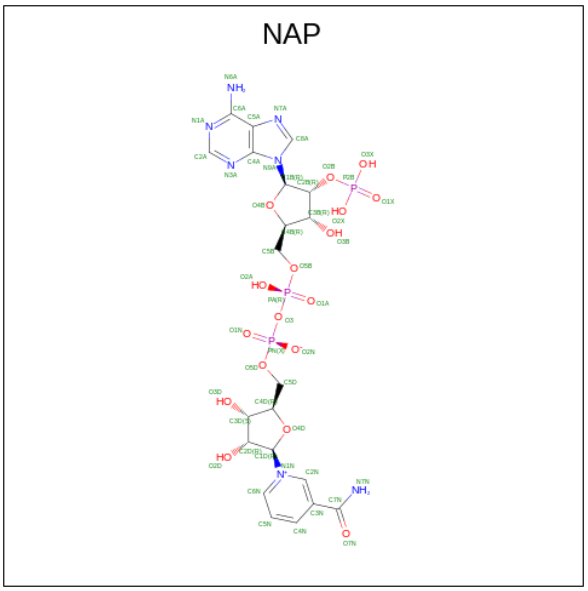
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4507	2910	745	824	28	0	0	0
1	B	527	4373	2831	723	793	26	0	0	0

- Molecule 2 is 5-(3-{3-[(2,4-diamino-6-ethylpyrimidin-5-yl)oxy]propoxy}phenyl)-6-ethylpyrimidine-2,4-diamine (three-letter code: 9QO) (formula: $C_{21}H_{28}N_8O_2$).



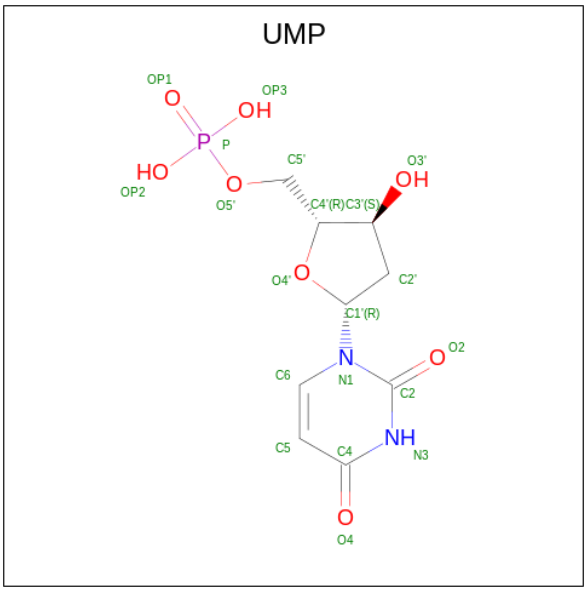
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	31	21	8	2	0	0
2	B	1	31	21	8	2	0	0

- 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
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	20	9	2	8	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	20	9	2	8	1	0	0

- Molecule 5 is water.

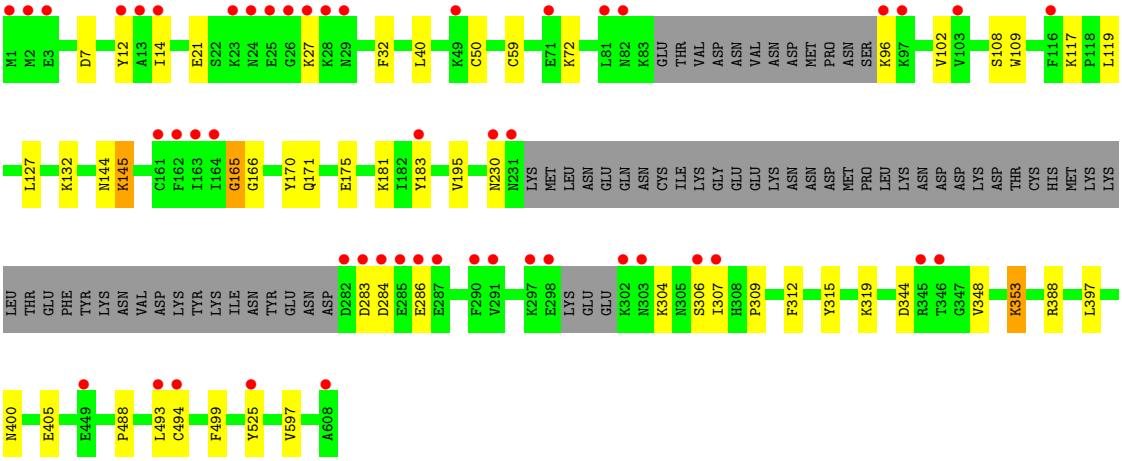
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	192	192	192	0	0
			Total	O		
5	B	159	159	159	0	0

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.

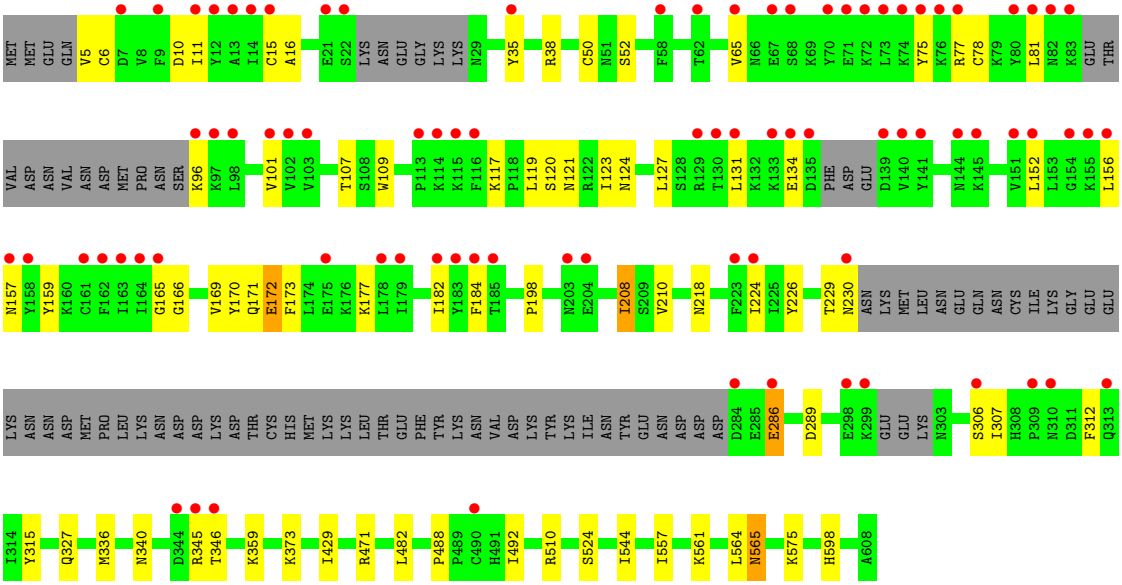
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain A:



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.29Å 154.25Å 163.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.83 – 2.38 27.83 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.7 (27.83-2.38) 97.8 (27.83-2.38)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.248 0.188 , 0.240	Depositor DCC
R_{free} test set	2911 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9429	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: 9QO, UMP, NAP

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	0.70	0/4611	0.80	1/6223 (0.0%)
1	B	0.68	0/4474	0.78	1/6040 (0.0%)
All	All	0.69	0/9085	0.79	2/12263 (0.0%)

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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	ILE	CB-CA-C	-5.12	101.35	111.60
1	A	165	GLY	CA-C-N	-5.07	106.06	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	SER	Peptide

5.2 Too-close contacts (i)

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4507	0	4462	28	0
1	B	4373	0	4338	31	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
3	A	48	0	25	7	0
3	B	48	0	25	3	0
4	A	20	0	11	0	0
4	B	20	0	11	0	0
5	A	192	0	0	4	0
5	B	159	0	0	1	0
All	All	9429	0	8872	55	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 (55) 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:B:312:PHE:HA	1:B:565:ASN:HD21	1.41	0.86
1:A:165:GLY:HA3	3:A:702:NAP:H5N	1.65	0.79
1:A:166:GLY:HA3	3:A:702:NAP:O1A	1.88	0.73
1:B:312:PHE:HA	1:B:565:ASN:ND2	2.05	0.72
1:B:373:LYS:HG3	1:B:598:HIS:CE1	2.32	0.64
1:B:119:LEU:H	1:B:124:ASN:HD21	1.47	0.62
1:B:10:ASP:HB2	1:B:77:ARG:HH21	1.65	0.61
1:A:166:GLY:HA3	3:A:702:NAP:PA	2.42	0.60
1:A:488:PRO:HG2	1:B:471:ARG:HD3	1.87	0.56
1:A:165:GLY:HA3	3:A:702:NAP:C5N	2.37	0.55
1:A:108:SER:OG	3:A:702:NAP:H6N	2.07	0.54
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.89	0.53
1:B:306:SER:HA	5:B:944:HOH:O	2.08	0.53
1:A:59:CYS:SG	5:A:983:HOH:O	2.34	0.53
1:B:312:PHE:CA	1:B:565:ASN:HD21	2.16	0.52
1:A:353:LYS:HG3	5:A:875:HOH:O	2.10	0.50
1:B:359:LYS:HG2	1:B:544:ILE:HG12	1.92	0.50
1:A:127:LEU:O	3:A:702:NAP:H1B	2.12	0.50
1:A:397:LEU:HD21	1:A:405:GLU:HB2	1.94	0.49
1:B:16:ALA:H	3:B:702:NAP:H72N	1.60	0.49
1:A:109:TRP:CH2	1:A:117:LYS:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:VAL:HG21	1:A:119:LEU:HD12	1.95	0.48
1:A:312:PHE:HB3	1:A:315:TYR:HB3	1.94	0.48
1:B:482:LEU:HD22	1:B:488:PRO:HB3	1.96	0.48
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.79	0.48
1:B:171:GLN:HA	1:B:198:PRO:HG3	1.97	0.47
1:A:319:LYS:HE2	1:B:286:GLU:HG3	1.97	0.46
1:A:40:LEU:HD22	3:A:702:NAP:C7N	2.46	0.46
1:B:166:GLY:HA3	3:B:702:NAP:O1A	2.15	0.46
1:A:304:LYS:HB2	5:A:813:HOH:O	2.15	0.46
1:B:101:VAL:HG22	1:B:123:ILE:HB	1.97	0.46
1:B:312:PHE:CE1	1:B:561:LYS:HG2	2.52	0.45
1:A:181:LYS:NZ	1:B:289:ASP:OD2	2.47	0.44
1:B:172:GLU:H	1:B:172:GLU:HG3	1.63	0.44
1:B:492:ILE:HD11	1:B:510:ARG:HD3	2.01	0.43
1:A:171:GLN:HG3	1:A:175:GLU:OE2	2.19	0.43
1:A:32:PHE:CD1	1:A:597:VAL:HG13	2.54	0.42
1:B:336:MET:HE2	1:B:557:ILE:HG23	2.00	0.42
1:B:152:LEU:O	1:B:156:LEU:HG	2.19	0.42
1:B:165:GLY:HA2	1:B:170:TYR:CZ	2.55	0.42
1:A:388:ARG:HG2	5:A:934:HOH:O	2.19	0.42
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.55	0.42
1:B:65:VAL:HG13	1:B:159:TYR:CD1	2.55	0.42
1:A:165:GLY:HA2	1:A:170:TYR:CZ	2.55	0.42
1:A:493:LEU:C	1:A:493:LEU:HD12	2.40	0.42
1:B:15:CYS:SG	1:B:184:PHE:CD2	3.13	0.42
1:A:344:ASP:N	1:A:348:VAL:O	2.53	0.41
1:B:35:TYR:CE1	1:B:38:ARG:HD2	2.55	0.41
1:B:109:TRP:CH2	1:B:117:LYS:HB3	2.56	0.41
1:B:210:VAL:HG12	1:B:224:ILE:HG22	2.03	0.41
1:B:169:VAL:HG23	3:B:702:NAP:O1A	2.20	0.41
1:A:494:CYS:SG	1:A:525:TYR:CE1	3.14	0.40
1:A:14:ILE:HA	1:A:183:TYR:O	2.21	0.40
1:B:312:PHE:HB3	1:B:315:TYR:HB3	2.03	0.40
1:A:144:ASN:OD1	1:A:145:LYS:HG3	2.21	0.40

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	A	535/608 (88%)	499 (93%)	33 (6%)	3 (1%)	25	34
1	B	515/608 (85%)	476 (92%)	37 (7%)	2 (0%)	34	46
All	All	1050/1216 (86%)	975 (93%)	70 (7%)	5 (0%)	29	39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLU
1	B	177	LYS
1	A	230	ASN
1	A	309	PRO
1	B	429	ILE

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	A	506/570 (89%)	492 (97%)	14 (3%)	43	61
1	B	491/570 (86%)	460 (94%)	31 (6%)	18	26
All	All	997/1140 (88%)	952 (96%)	45 (4%)	27	41

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP

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Mol	Chain	Res	Type
1	A	27	LYS
1	A	50	CYS
1	A	72	LYS
1	A	96	LYS
1	A	132	LYS
1	A	145	LYS
1	A	195	VAL
1	A	283	ASP
1	A	284	ASP
1	A	286	GLU
1	A	307	ILE
1	A	353	LYS
1	A	400	ASN
1	B	5	VAL
1	B	6	CYS
1	B	11	ILE
1	B	50	CYS
1	B	52	SER
1	B	75	TYR
1	B	78	CYS
1	B	81	LEU
1	B	96	LYS
1	B	107	THR
1	B	120	SER
1	B	121	ASN
1	B	127	LEU
1	B	131	LEU
1	B	134	GLU
1	B	157	ASN
1	B	172	GLU
1	B	173	PHE
1	B	208	ILE
1	B	218	ASN
1	B	229	THR
1	B	230	ASN
1	B	286	GLU
1	B	307	ILE
1	B	327	GLN
1	B	345	ARG
1	B	346	THR
1	B	524	SER
1	B	564	LEU

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Mol	Chain	Res	Type
1	B	565	ASN
1	B	575	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	338	ASN
1	A	530	HIS
1	B	42	ASN
1	B	157	ASN
1	B	294	ASN
1	B	310	ASN
1	B	565	ASN

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	$\#\|Z\| > 2$
4	UMP	B	703	-	21,21,21	1.51	2 (9%)	31,31,31	2.23	13 (41%)
2	9QO	A	701	-	32,33,33	0.86	0	42,45,45	2.53	17 (40%)
2	9QO	B	701	-	32,33,33	0.85	0	42,45,45	2.64	17 (40%)
3	NAP	A	702	-	45,52,52	1.00	2 (4%)	56,80,80	1.24	7 (12%)
3	NAP	B	702	-	45,52,52	0.94	1 (2%)	56,80,80	1.15	4 (7%)
4	UMP	A	703	-	21,21,21	1.41	2 (9%)	31,31,31	1.94	9 (29%)

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	UMP	B	703	-	-	8/10/22/22	0/2/2/2
2	9QO	A	701	-	-	3/16/16/16	0/3/3/3
2	9QO	B	701	-	-	8/16/16/16	0/3/3/3
3	NAP	A	702	-	-	4/31/67/67	0/5/5/5
3	NAP	B	702	-	-	5/31/67/67	0/5/5/5
4	UMP	A	703	-	-	4/10/22/22	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	UMP	C2-N1	4.66	1.45	1.38
4	A	703	UMP	C2-N1	4.32	1.45	1.38
3	B	702	NAP	C5A-C4A	2.85	1.48	1.40
4	A	703	UMP	O2-C2	2.80	1.28	1.23
4	B	703	UMP	O2-C2	2.63	1.27	1.23
3	A	702	NAP	O4D-C1D	2.50	1.44	1.41
3	A	702	NAP	C5A-C4A	2.10	1.46	1.40

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	9QO	C2-N1-C6	8.21	123.09	116.24
2	A	701	9QO	C25-N24-C23	6.80	121.91	116.24
2	B	701	9QO	C25-N24-C23	6.74	121.86	116.24
2	A	701	9QO	C2-N1-C6	5.87	121.14	116.24
2	A	701	9QO	C5-C4-N3	-5.30	119.54	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	703	UMP	C1'-N1-C2	5.06	127.62	117.64
2	A	701	9QO	C20-O21-C22	4.49	127.81	114.23
4	A	703	UMP	O4-C4-C5	-4.29	117.61	125.16
2	B	701	9QO	N3-C2-N1	-4.29	118.69	125.42
4	B	703	UMP	O4-C4-C5	-4.28	117.64	125.16
2	B	701	9QO	C9-C6-C5	4.19	125.49	122.57
4	A	703	UMP	C5-C4-N3	4.10	120.98	114.84
2	B	701	9QO	C2-N3-C4	4.07	121.48	116.99
4	B	703	UMP	C1'-N1-C6	-3.87	113.91	121.55
2	A	701	9QO	N26-C25-N24	-3.74	119.55	125.42
4	A	703	UMP	C1'-N1-C2	3.73	124.99	117.64
2	A	701	9QO	C25-N26-C27	3.71	121.09	116.99
2	B	701	9QO	C25-N26-C27	3.70	121.08	116.99
2	B	701	9QO	N26-C25-N24	-3.67	119.67	125.42
2	A	701	9QO	C2-N3-C4	3.58	120.94	116.99
4	B	703	UMP	C5-C4-N3	3.56	120.16	114.84
2	B	701	9QO	C18-O17-C15	3.45	126.94	117.93
2	B	701	9QO	C20-O21-C22	3.44	124.63	114.23
2	A	701	9QO	C18-O17-C15	3.43	126.88	117.93
4	A	703	UMP	C1'-N1-C6	-3.39	114.85	121.55
3	A	702	NAP	N3A-C2A-N1A	-3.38	123.40	128.68
4	A	703	UMP	C4-N3-C2	-3.28	122.25	126.58
4	A	703	UMP	OP3-P-OP2	3.27	120.15	107.64
3	B	702	NAP	PN-O3-PA	-3.24	121.70	132.83
2	A	701	9QO	C5-C6-N1	-3.24	119.62	123.61
3	B	702	NAP	C4A-C5A-N7A	-3.19	106.07	109.40
2	A	701	9QO	N3-C2-N1	-3.13	120.51	125.42
4	B	703	UMP	O5'-P-OP1	-3.07	97.86	106.47
3	B	702	NAP	N3A-C2A-N1A	-3.02	123.95	128.68
3	A	702	NAP	C4A-C5A-N7A	-3.01	106.26	109.40
2	B	701	9QO	C5-C6-N1	-2.99	119.92	123.61
2	A	701	9QO	O21-C22-C23	2.87	123.38	119.17
4	B	703	UMP	C4-N3-C2	-2.87	122.80	126.58
2	A	701	9QO	N7-C2-N3	2.82	121.64	117.25
2	A	701	9QO	C4-C5-C6	2.82	118.24	115.91
2	A	701	9QO	N29-C25-N26	2.82	121.64	117.25
4	B	703	UMP	O5'-C5'-C4'	2.73	118.37	108.99
4	B	703	UMP	O4'-C1'-N1	2.72	112.73	107.86
3	A	702	NAP	C3N-C2N-N1N	2.65	123.01	120.43
4	B	703	UMP	P-O5'-C5'	2.57	125.37	118.30
2	B	701	9QO	C22-C23-N24	-2.55	119.30	122.46
2	A	701	9QO	C11-C5-C6	-2.53	121.41	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	NAP	O2B-C2B-C1B	-2.52	101.04	110.10
3	A	702	NAP	O3X-P2B-O1X	2.51	120.51	110.68
2	B	701	9QO	N29-C25-N26	2.51	121.15	117.25
2	B	701	9QO	O21-C22-C23	2.50	122.84	119.17
2	A	701	9QO	C22-C23-N24	-2.50	119.36	122.46
4	B	703	UMP	C2'-C1'-N1	2.50	119.53	113.77
2	B	701	9QO	N7-C2-N1	2.48	121.11	117.25
4	A	703	UMP	O4'-C1'-N1	2.46	112.26	107.86
4	B	703	UMP	O2-C2-N3	-2.40	117.04	121.50
2	B	701	9QO	C11-C16-C15	2.38	123.04	119.94
4	A	703	UMP	OP3-P-O5'	-2.36	100.45	106.73
2	B	701	9QO	C5-C4-N8	2.36	124.17	120.86
2	A	701	9QO	C10-C9-C6	-2.32	109.16	114.88
4	A	703	UMP	P-O5'-C5'	2.31	124.66	118.30
3	A	702	NAP	O2A-PA-O1A	2.22	123.21	112.24
4	B	703	UMP	N3-C2-N1	2.17	117.77	114.89
3	B	702	NAP	O2A-PA-O1A	2.16	122.91	112.24
3	A	702	NAP	C2N-N1N-C1D	-2.05	114.58	119.14
2	B	701	9QO	N8-C4-N3	-2.05	114.14	117.03
4	B	703	UMP	C6-N1-C2	-2.02	118.41	120.99

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	9QO	C12-C11-C5-C4
2	B	701	9QO	C16-C11-C5-C4
3	A	702	NAP	PA-O3-PN-O5D
3	A	702	NAP	O4D-C1D-N1N-C2N
3	A	702	NAP	O4D-C1D-N1N-C6N
3	B	702	NAP	O4D-C1D-N1N-C2N
3	B	702	NAP	O4D-C1D-N1N-C6N
3	B	702	NAP	C2D-C1D-N1N-C2N
4	B	703	UMP	C5'-O5'-P-OP2
4	B	703	UMP	C5'-O5'-P-OP3
2	B	701	9QO	C16-C11-C5-C6
4	B	703	UMP	C3'-C4'-C5'-O5'
4	B	703	UMP	O4'-C4'-C5'-O5'
2	B	701	9QO	C14-C15-O17-C18
2	B	701	9QO	C16-C15-O17-C18
2	B	701	9QO	C12-C11-C5-C6
2	B	701	9QO	O17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
2	A	701	9QO	O17-C18-C19-C20
2	A	701	9QO	C18-C19-C20-O21
2	A	701	9QO	C19-C18-O17-C15
4	A	703	UMP	C3'-C4'-C5'-O5'
4	A	703	UMP	O4'-C4'-C5'-O5'
4	B	703	UMP	C5'-O5'-P-OP1
4	A	703	UMP	C2'-C1'-N1-C2
4	A	703	UMP	C2'-C1'-N1-C6
4	B	703	UMP	C4'-C5'-O5'-P
4	B	703	UMP	C2'-C1'-N1-C2
3	B	702	NAP	C3B-C4B-C5B-O5B
4	B	703	UMP	C2'-C1'-N1-C6
2	B	701	9QO	N24-C23-C30-C31
3	A	702	NAP	C2D-C1D-N1N-C2N
3	B	702	NAP	C2D-C1D-N1N-C6N

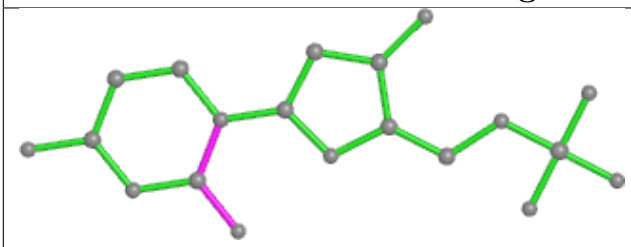
There are no ring outliers.

2 monomers are involved in 10 short contacts:

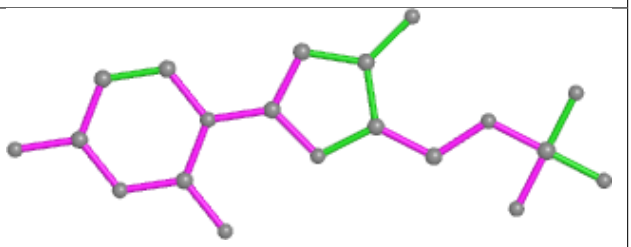
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NAP	7	0
3	B	702	NAP	3	0

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.

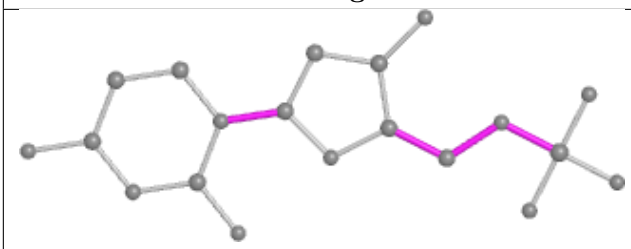
Ligand UMP B 703



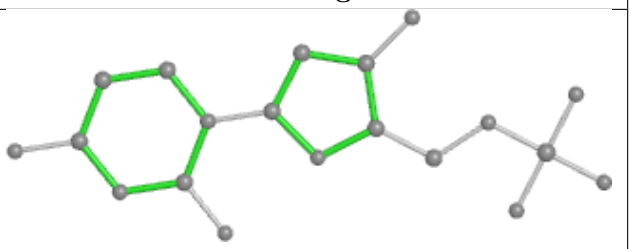
Bond lengths



Bond angles

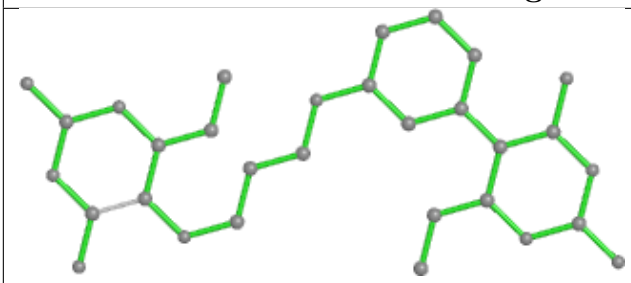


Torsions

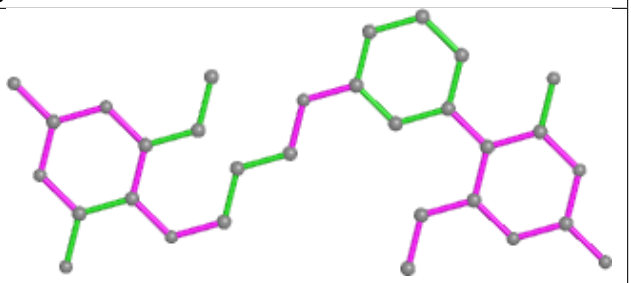


Rings

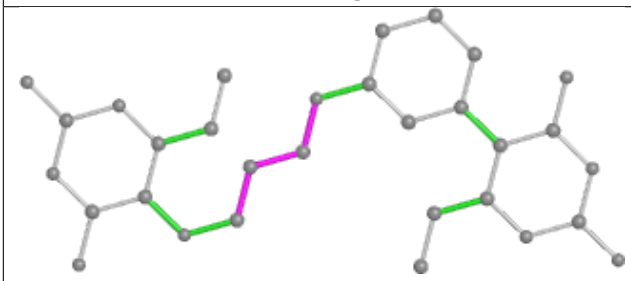
Ligand 9QO A 701



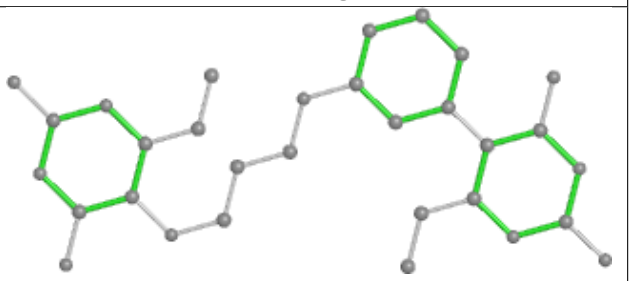
Bond lengths



Bond angles

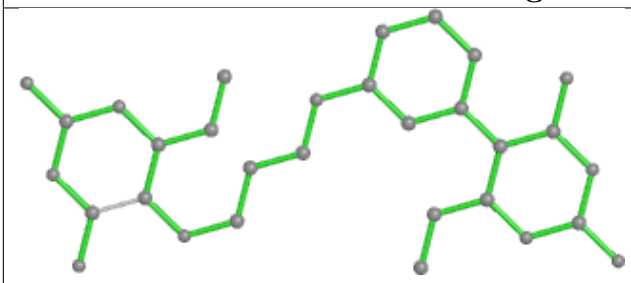


Torsions

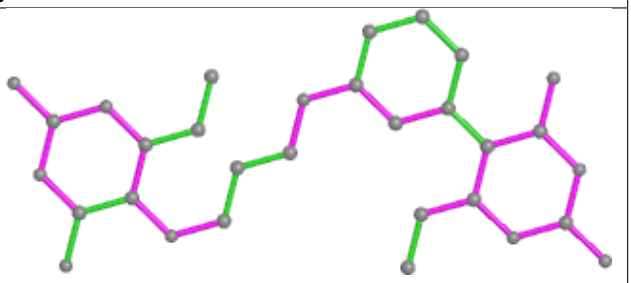


Rings

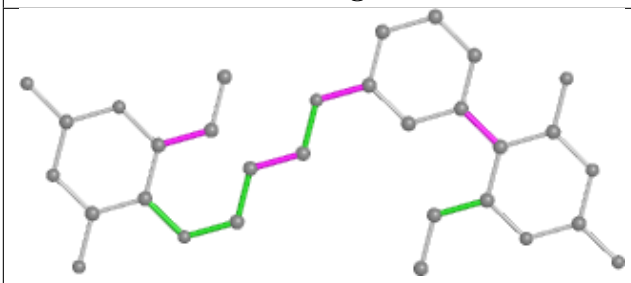
Ligand 9QO B 701



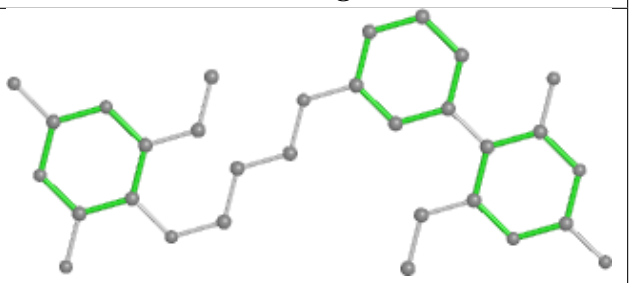
Bond lengths



Bond angles

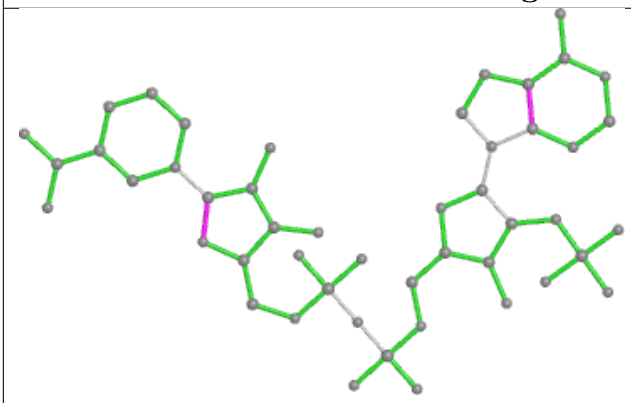


Torsions

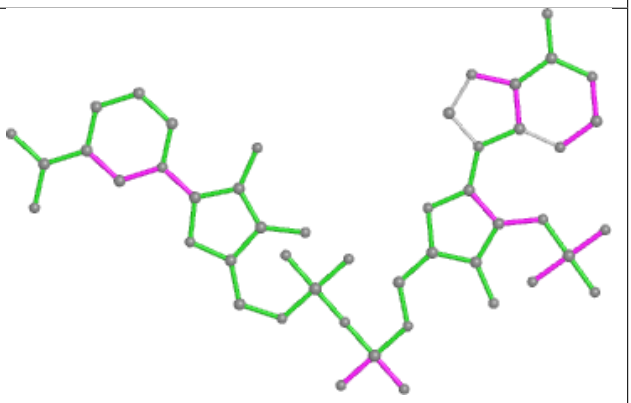


Rings

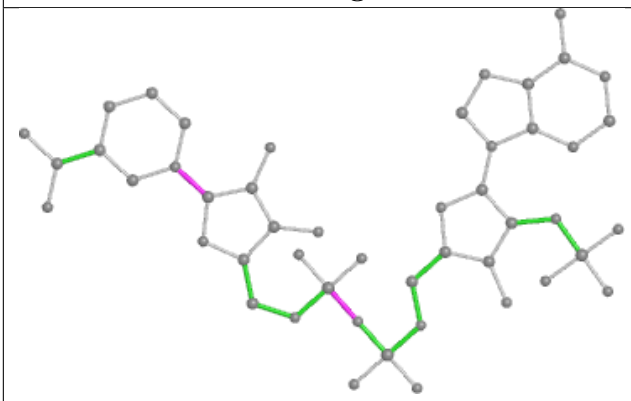
Ligand NAP A 702



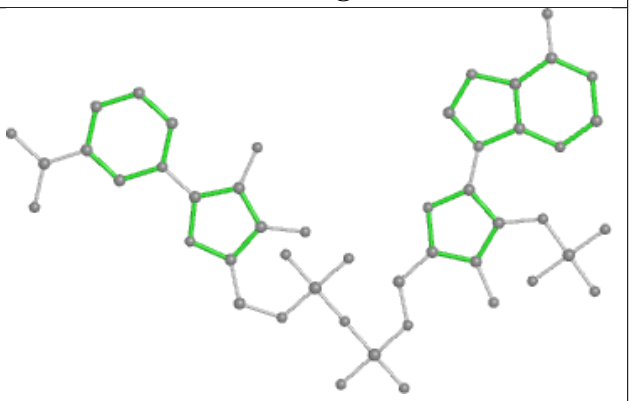
Bond lengths



Bond angles

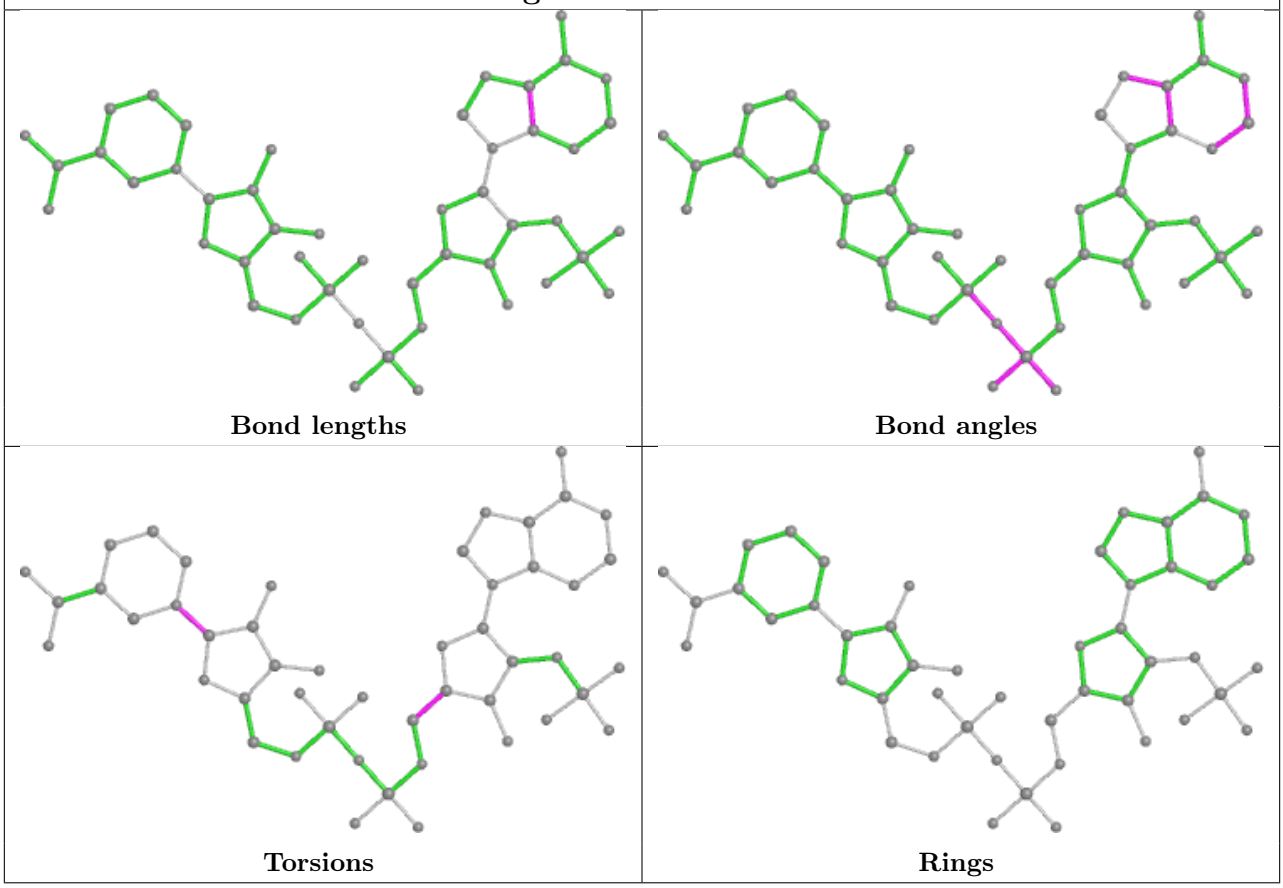


Torsions

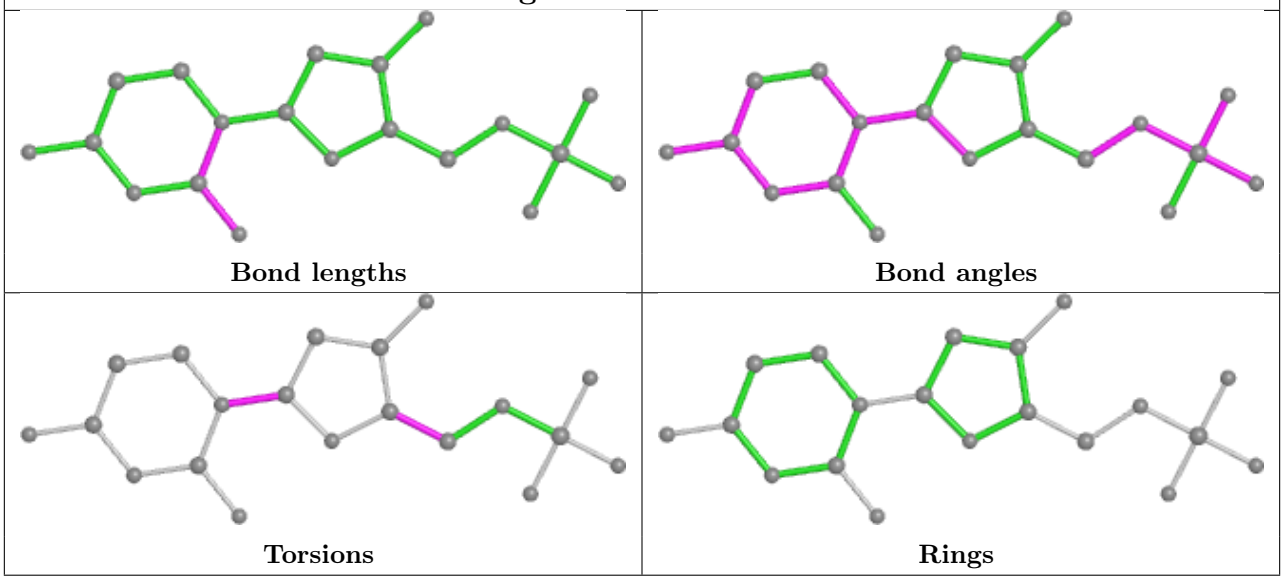


Rings

Ligand NAP B 702



Ligand UMP A 703



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	A	543/608 (89%)	0.15	49 (9%) 9 10	28, 39, 100, 120	0
1	B	527/608 (86%)	0.50	84 (15%) 1 2	28, 44, 119, 120	0
All	All	1070/1216 (87%)	0.32	133 (12%) 4 4	28, 41, 118, 120	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	12.7
1	A	2	MET	11.2
1	B	75	TYR	9.4
1	B	80	TYR	9.3
1	B	70	TYR	9.1
1	A	282	ASP	8.5
1	A	345	ARG	7.5
1	B	81	LEU	7.5
1	B	151	VAL	6.8
1	A	283	ASP	6.6
1	A	284	ASP	6.6
1	B	130	THR	6.1
1	A	25	GLU	6.0
1	B	12	TYR	5.8
1	B	82	ASN	5.5
1	B	14	ILE	5.3
1	B	97	LYS	5.2
1	A	231	ASN	5.2
1	A	26	GLY	5.1
1	B	71	GLU	5.0
1	B	346	THR	4.7
1	B	133	LYS	4.7
1	B	13	ALA	4.5
1	B	96	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	23	LYS	4.4
1	B	155	LYS	4.4
1	B	77	ARG	4.4
1	B	162	PHE	4.4
1	B	182	ILE	4.3
1	B	140	VAL	4.3
1	A	303	ASN	4.2
1	A	302	LYS	4.2
1	A	286	GLU	4.2
1	A	3	GLU	4.1
1	B	141	TYR	4.0
1	A	287	GLU	4.0
1	A	14	ILE	4.0
1	B	183	TYR	4.0
1	B	175	GLU	3.8
1	A	96	LYS	3.8
1	B	163	ILE	3.8
1	A	24	ASN	3.7
1	B	144	ASN	3.7
1	B	15	CYS	3.7
1	A	163	ILE	3.7
1	B	178	LEU	3.7
1	B	11	ILE	3.7
1	B	74	LYS	3.6
1	A	82	ASN	3.6
1	B	345	ARG	3.5
1	B	131	LEU	3.5
1	B	184	PHE	3.5
1	B	299	LYS	3.5
1	A	230	ASN	3.4
1	B	309	PRO	3.4
1	A	162	PHE	3.4
1	A	346	THR	3.4
1	B	230	ASN	3.4
1	B	139	ASP	3.3
1	A	28	LYS	3.3
1	B	145	LYS	3.3
1	B	83	LYS	3.3
1	B	156	LEU	3.2
1	A	27	LYS	3.2
1	B	152	LEU	3.2
1	A	81	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	76	LYS	3.2
1	A	298	GLU	3.1
1	B	158	TYR	3.1
1	A	290	PHE	3.1
1	B	103	VAL	3.1
1	B	154	GLY	3.1
1	B	7	ASP	3.0
1	B	35	TYR	3.0
1	B	102	VAL	3.0
1	B	9	PHE	3.0
1	A	29	ASN	2.9
1	A	164	ILE	2.9
1	B	164	ILE	2.9
1	A	103	VAL	2.9
1	B	73	LEU	2.8
1	B	114	LYS	2.8
1	B	313	GLN	2.8
1	B	161	CYS	2.8
1	B	113	PRO	2.7
1	B	286	GLU	2.8
1	A	97	LYS	2.7
1	A	13	ALA	2.7
1	B	101	VAL	2.7
1	B	185	THR	2.7
1	B	179	ILE	2.6
1	B	165	GLY	2.6
1	B	204	GLU	2.6
1	B	67	GLU	2.6
1	B	135	ASP	2.6
1	B	134	GLU	2.6
1	A	12	TYR	2.5
1	A	285	GLU	2.5
1	A	297	LYS	2.5
1	B	72	LYS	2.5
1	B	224	ILE	2.4
1	B	98	LEU	2.4
1	A	608	ALA	2.4
1	B	58	PHE	2.4
1	A	71	GLU	2.4
1	B	157	ASN	2.4
1	A	116	PHE	2.3
1	B	116	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	VAL	2.3
1	B	203	ASN	2.3
1	A	306	SER	2.3
1	B	22	SER	2.3
1	B	306	SER	2.3
1	A	307	ILE	2.3
1	A	183	TYR	2.2
1	B	310	ASN	2.2
1	A	449	GLU	2.2
1	B	68	SER	2.2
1	B	490	CYS	2.2
1	B	62	THR	2.2
1	A	49	LYS	2.2
1	B	344	ASP	2.2
1	B	284	ASP	2.2
1	A	494	CYS	2.1
1	B	21	GLU	2.1
1	B	115	LYS	2.1
1	A	493	LEU	2.1
1	B	129	ARG	2.1
1	B	298	GLU	2.1
1	B	223	PHE	2.1
1	A	161	CYS	2.1
1	A	525	TYR	2.1
1	B	65	VAL	2.0

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)

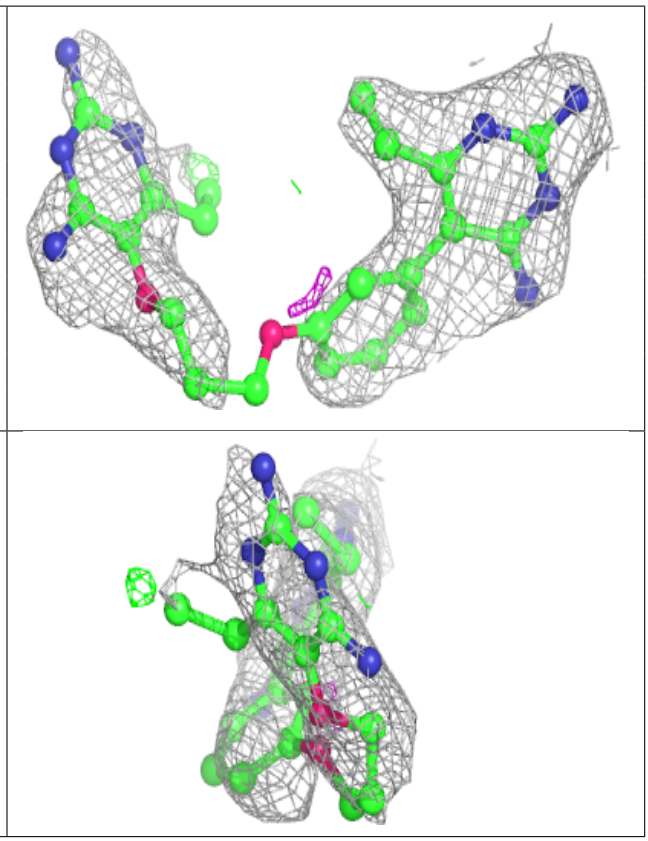
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	9QO	B	701	31/31	0.74	0.31	50,96,116,119	0
2	9QO	A	701	31/31	0.85	0.22	29,51,93,94	0
3	NAP	B	702	48/48	0.88	0.15	76,98,120,120	0
4	UMP	B	703	20/20	0.90	0.21	55,80,105,108	0
4	UMP	A	703	20/20	0.94	0.18	51,78,120,120	0
3	NAP	A	702	48/48	0.97	0.08	34,40,46,49	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.

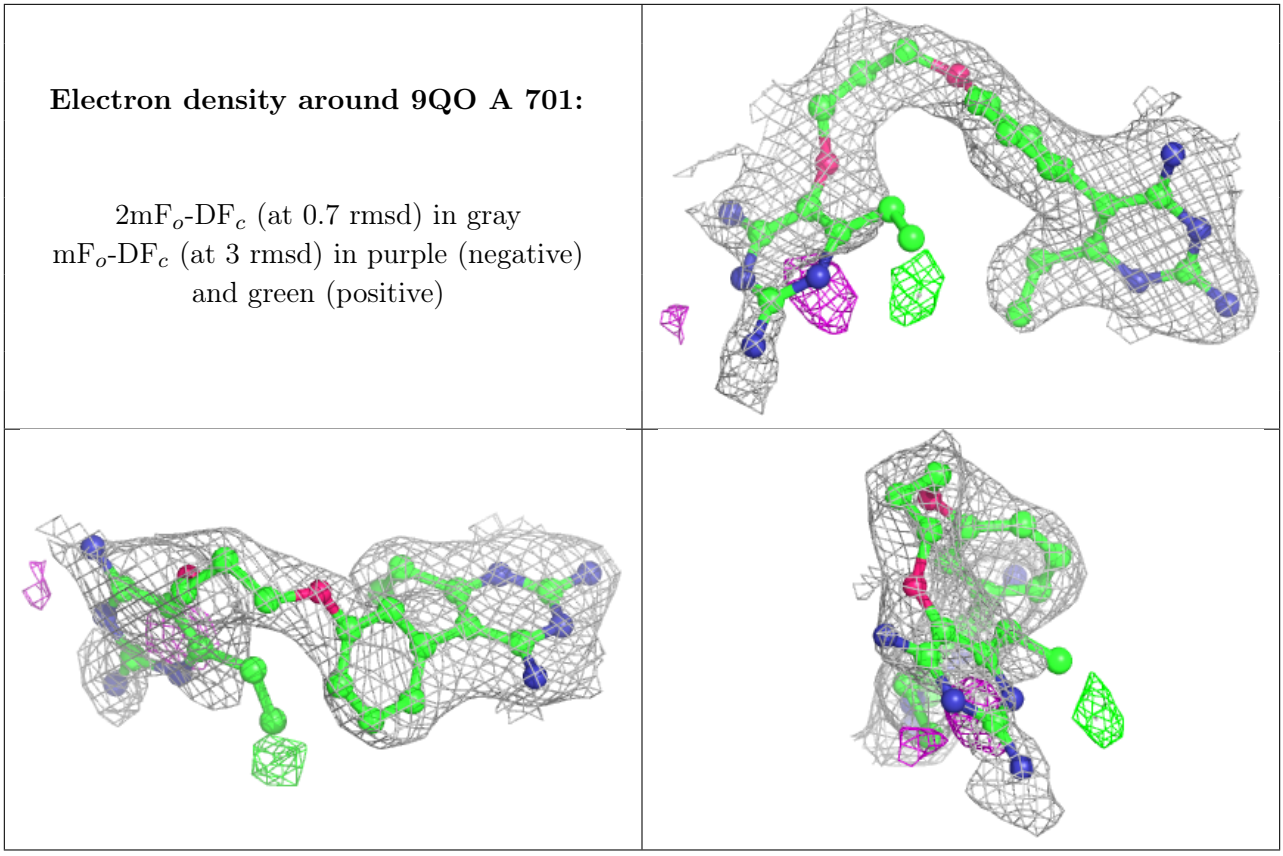
Electron density around 9QO B 701:

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



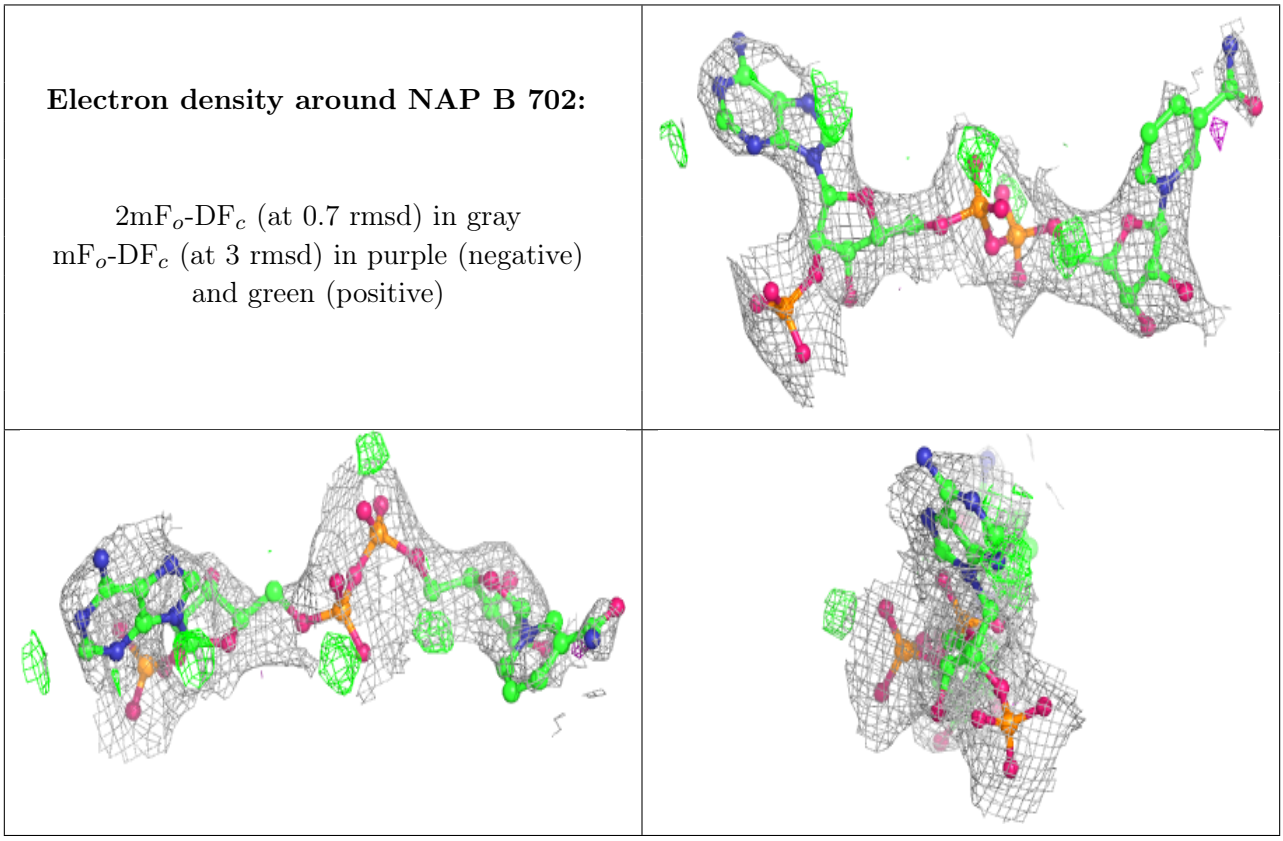
Electron density around 9QO A 701:

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



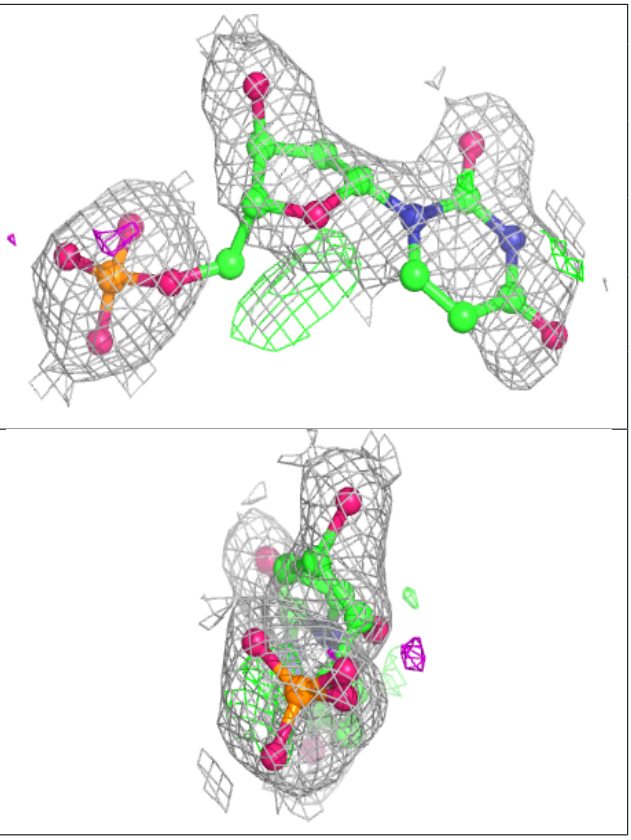
Electron density around NAP B 702:

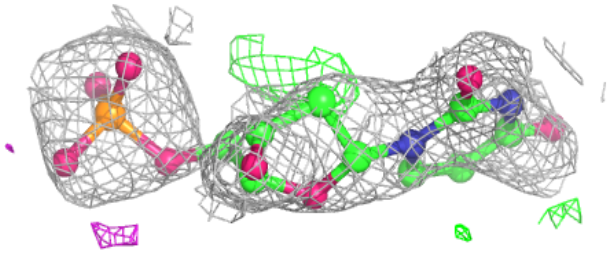
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UMP B 703:

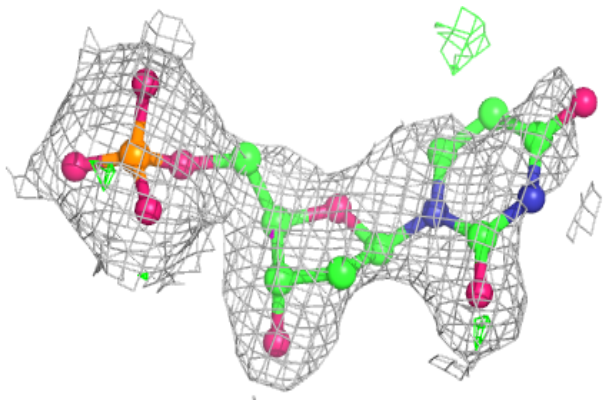
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

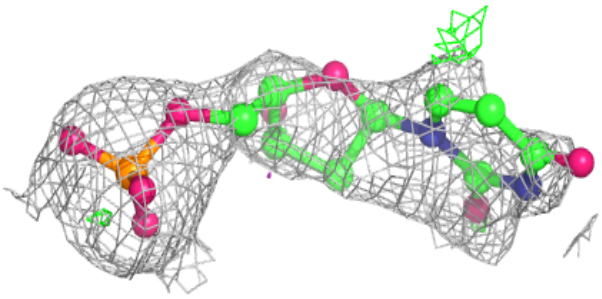


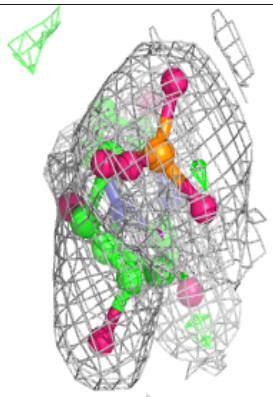


Electron density around UMP A 703:

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

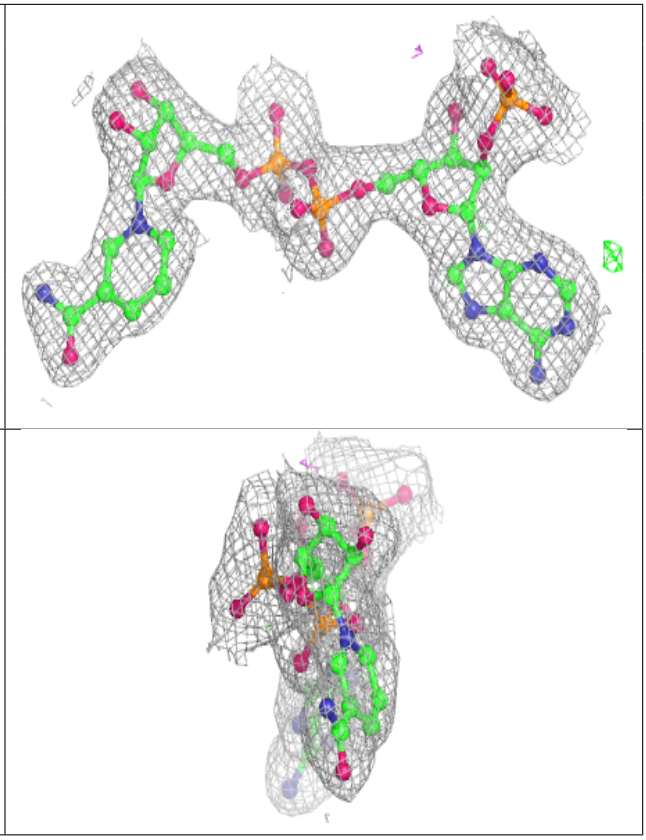






Electron density around NAP A 702:

$2mF_o$-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.