Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 07:23 PM JST

PDB ID	:	6A2N
Title	:	Crystal structure of quadruple mutant (N51I+C59R+S108N+I164L) Plasmodium falciparum DHFR-TS complexed with BT2, NADPH, and dUMP
Authors	:	Chitnumsub, P.; Jaruwat, A.; Tarnchampoo, B.; Yuthavong, Y.
Deposited on	:	2018-06-12
Resolution	:	2.45 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

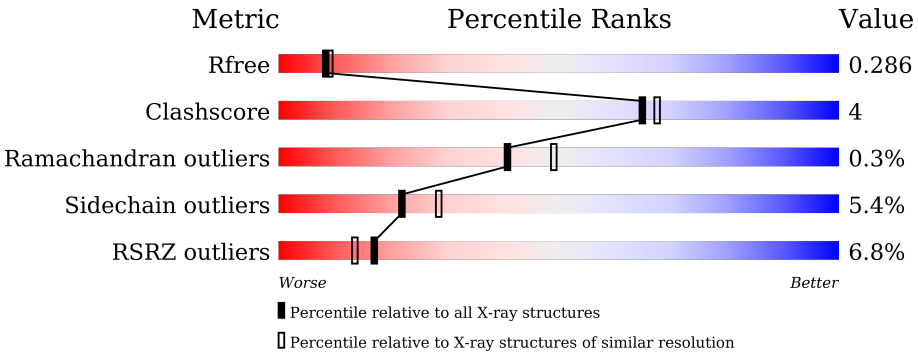
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	5% 77% 12% • 10%
1	B	608	7% 77% 12% • 10%

2 Entry composition (i)

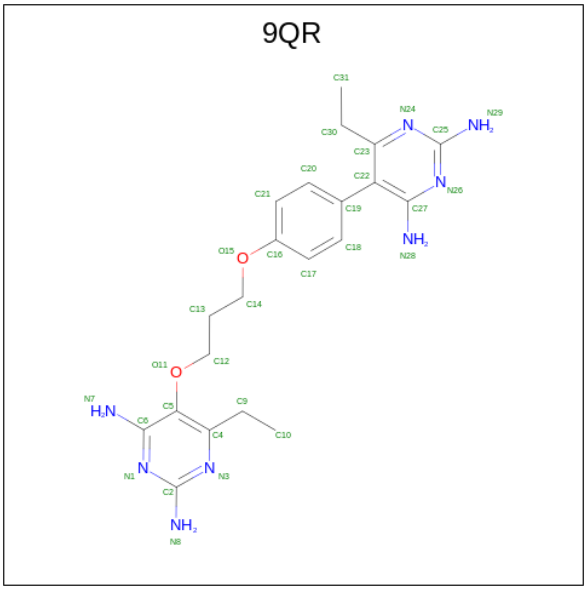
There are 5 unique types of molecules in this entry. The entry contains 9956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

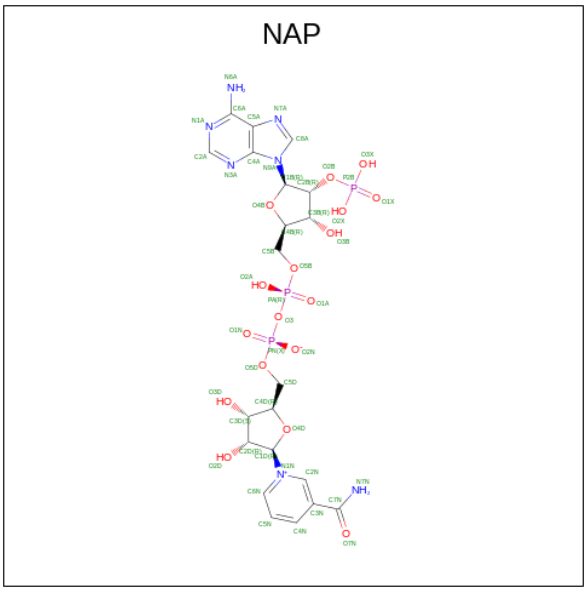
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4550	2937	753	833	27			
1	B	547	Total	C	N	O	S	0	0	0
			4550	2937	753	833	27			

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



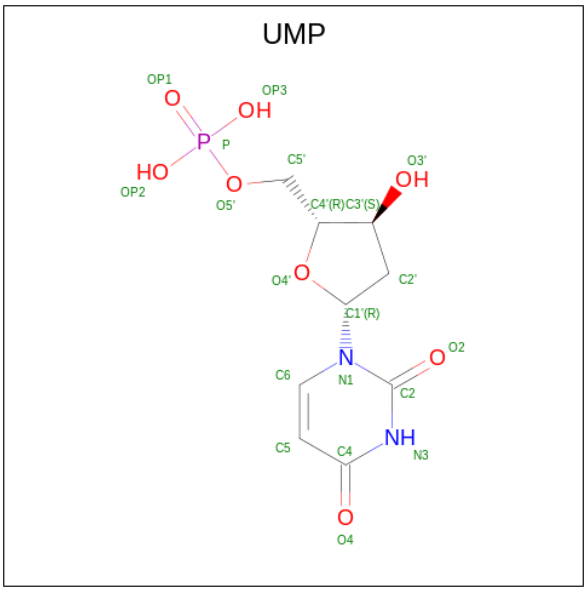
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	21	8	2		
2	B	1	Total	C	N	O	0	0
			31	21	8	2		

- 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	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		

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



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

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

- Molecule 5 is water.

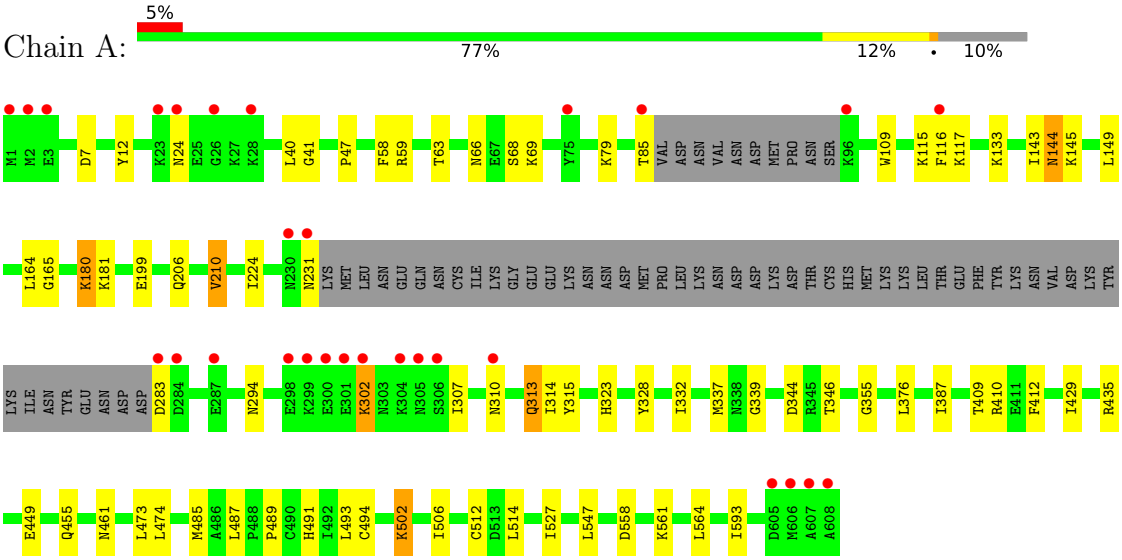
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total	O	0	0
			354	354		
5	B	304	Total	O	0	0
			304	304		

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.

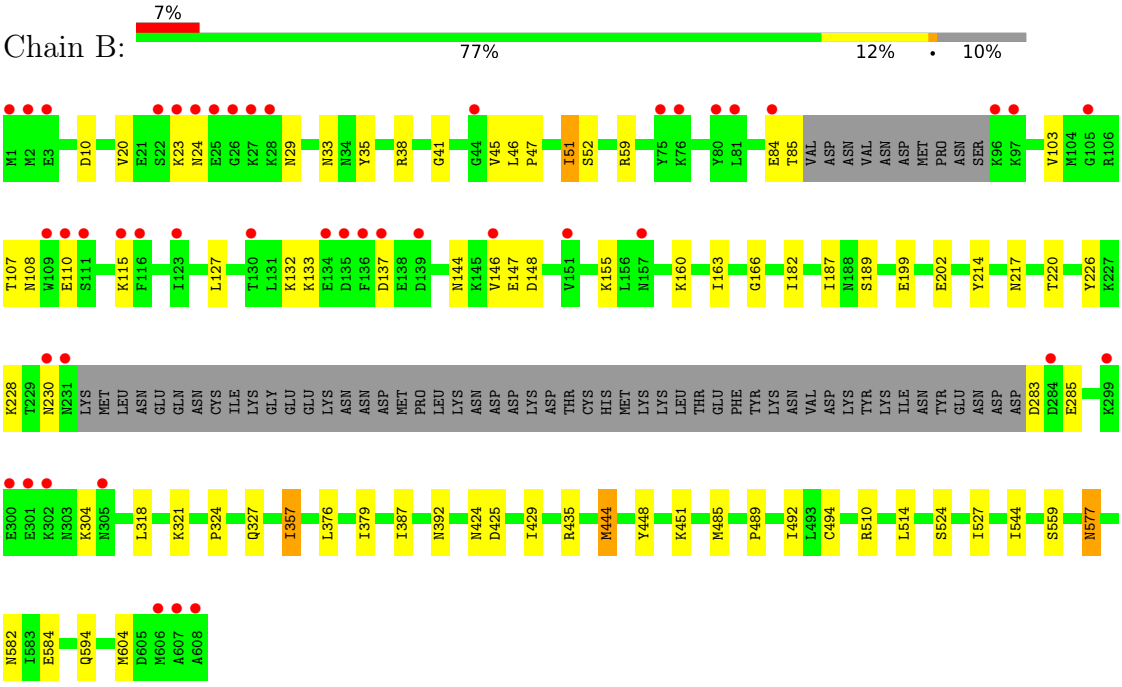
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

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	59.71Å 157.11Å 166.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.45 29.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	83.1 (30.00-2.45) 83.2 (29.85-2.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.58 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.203 , 0.291 0.201 , 0.286	Depositor DCC
R_{free} test set	2456 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9956	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 9QR, UMP

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	0.63	0/4655	0.77	0/6281
1	B	0.63	0/4655	0.75	0/6281
All	All	0.63	0/9310	0.76	0/12562

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4550	0	4511	38	0
1	B	4550	0	4511	36	0
2	A	31	0	0	1	0
2	B	31	0	0	1	0
3	A	48	0	25	3	0
3	B	48	0	25	4	0
4	A	20	0	11	0	0
4	B	20	0	11	0	0
5	A	354	0	0	5	0
5	B	304	0	0	1	0
All	All	9956	0	9094	76	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 4.

All (76) 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:425:ASP:HA	1:B:444:MET:HE3	1.36	1.07
1:B:392:ASN:HA	1:B:444:MET:HE2	1.40	1.02
1:A:561:LYS:HD3	5:A:1075:HOH:O	1.67	0.92
1:B:392:ASN:HA	1:B:444:MET:CE	2.04	0.88
1:B:425:ASP:HA	1:B:444:MET:CE	2.07	0.83
2:B:701:9QR:C12	3:B:702:NAP:H4N	2.14	0.77
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.58	0.69
1:B:424:ASN:O	1:B:444:MET:HE1	1.95	0.66
1:A:376:LEU:HD13	1:A:527:ILE:HD11	1.79	0.63
1:B:582:ASN:HB3	1:B:584:GLU:OE2	2.00	0.61
2:A:701:9QR:C20	2:A:701:9QR:C30	2.78	0.59
1:B:425:ASP:CA	1:B:444:MET:HE3	2.24	0.57
1:A:307:ILE:HG21	1:A:337:MET:SD	2.45	0.57
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.40	0.56
1:B:392:ASN:CA	1:B:444:MET:HE2	2.26	0.56
1:B:35:TYR:CE1	1:B:38:ARG:HD2	2.41	0.56
1:A:494:CYS:HA	1:A:506:ILE:O	2.05	0.55
1:A:12:TYR:CD1	1:A:181:LYS:HB2	2.39	0.55
1:A:461:ASN:HB3	5:A:805:HOH:O	2.09	0.52
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.91	0.52
1:B:376:LEU:HD13	1:B:527:ILE:HD11	1.92	0.52
1:A:165:GLY:HA3	3:A:702:NAP:H5N	1.92	0.51
1:A:315:TYR:HB2	1:A:564:LEU:O	2.10	0.51
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.94	0.50
1:A:409:THR:HG23	1:A:412:PHE:H	1.76	0.50
1:A:376:LEU:HD12	1:A:593:ILE:HD11	1.94	0.50
1:A:455:GLN:HB3	1:A:474:LEU:HD12	1.93	0.50
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.47	0.49
1:B:85:THR:HG21	1:B:155:LYS:HA	1.95	0.49
1:B:20:VAL:HG21	1:B:38:ARG:NH2	2.27	0.49
1:B:379:ILE:HD13	1:B:524:SER:HB2	1.94	0.49
1:A:302:LYS:HE2	1:A:339:GLY:O	2.12	0.48
1:A:210:VAL:CG1	1:A:323:HIS:HB2	2.43	0.48
1:A:144:ASN:ND2	1:A:145:LYS:HG3	2.29	0.48
1:A:485:MET:SD	1:A:489:PRO:HD3	2.54	0.48
1:B:41:GLY:HA3	3:B:702:NAP:H1D	1.96	0.48
1:B:577:ASN:C	1:B:577:ASN:HD22	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ILE:O	1:B:435:ARG:NH1	2.47	0.48
1:A:387:ILE:O	1:A:435:ARG:NH1	2.47	0.47
1:A:12:TYR:CZ	1:A:180:LYS:HE3	2.50	0.47
1:B:127:LEU:HD22	3:B:702:NAP:N1A	2.30	0.46
1:A:502:LYS:HG2	5:A:918:HOH:O	2.15	0.46
1:B:214:TYR:O	1:B:220:THR:HA	2.15	0.46
1:B:485:MET:SD	1:B:489:PRO:HD3	2.56	0.46
1:A:58:PHE:HE1	1:A:164:LEU:HD22	1.81	0.46
1:A:40:LEU:O	3:A:702:NAP:H2N	2.15	0.45
1:B:318:LEU:HB2	1:B:321:LYS:HD2	1.99	0.45
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.99	0.45
1:A:376:LEU:HD12	1:A:593:ILE:CD1	2.46	0.45
1:B:304:LYS:HA	1:B:304:LYS:HD2	1.82	0.45
1:A:558:ASP:HA	1:A:561:LYS:HE2	1.98	0.45
1:A:59:ARG:O	1:A:63:THR:HG23	2.17	0.44
1:A:310:ASN:HB2	5:A:1120:HOH:O	2.17	0.44
1:A:344:ASP:OD2	1:A:346:THR:HG22	2.17	0.44
1:A:66:ASN:HD22	1:A:69:LYS:HE3	1.82	0.44
1:B:35:TYR:CZ	1:B:38:ARG:HD2	2.52	0.44
1:A:313:GLN:HE21	1:A:314:ILE:HG13	1.82	0.44
1:A:512:CYS:SG	1:A:547:LEU:HD22	2.57	0.44
1:A:115:LYS:HE3	1:A:116:PHE:HE1	1.83	0.44
1:B:448:TYR:O	1:B:451:LYS:HB2	2.17	0.43
1:B:103:VAL:HB	1:B:163:ILE:HD13	2.00	0.43
1:B:23:LYS:HA	1:B:24:ASN:HA	1.79	0.43
1:B:324:PRO:O	1:B:327:GLN:HB2	2.19	0.42
1:B:357:ILE:HD11	1:B:544:ILE:HG23	2.01	0.42
1:B:492:ILE:HD11	1:B:510:ARG:HD3	2.01	0.42
1:B:33:ASN:OD1	1:B:35:TYR:HB3	2.19	0.42
1:B:132:LYS:HG2	5:B:1054:HOH:O	2.18	0.42
1:A:143:ILE:HD13	1:A:149:LEU:HB2	2.02	0.41
1:B:182:ILE:HB	1:B:226:TYR:HB2	2.02	0.41
1:B:10:ASP:HB3	1:B:160:LYS:HG2	2.02	0.41
1:A:328:TYR:CZ	1:A:332:ILE:HD11	2.54	0.41
1:A:355:GLY:HA2	1:A:547:LEU:O	2.20	0.41
1:B:166:GLY:HA3	3:B:702:NAP:O5D	2.20	0.41
1:A:493:LEU:HD22	1:B:492:ILE:HG21	2.02	0.41
3:A:702:NAP:H4D	5:A:971:HOH:O	2.21	0.41
1:A:210:VAL:HG22	1:A:224:ILE:HG22	2.03	0.41

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	541/608 (89%)	511 (94%)	29 (5%)	1 (0%)	47 57
1	B	541/608 (89%)	503 (93%)	36 (7%)	2 (0%)	34 41
All	All	1082/1216 (89%)	1014 (94%)	65 (6%)	3 (0%)	41 49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	ILE
1	B	429	ILE
1	A	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	510/570 (90%)	487 (96%)	23 (4%)	27 36
1	B	510/570 (90%)	478 (94%)	32 (6%)	18 22
All	All	1020/1140 (90%)	965 (95%)	55 (5%)	22 28

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	24	ASN
1	A	68	SER

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Mol	Chain	Res	Type
1	A	79	LYS
1	A	85	THR
1	A	133	LYS
1	A	144	ASN
1	A	180	LYS
1	A	199	GLU
1	A	206	GLN
1	A	210	VAL
1	A	231	ASN
1	A	283	ASP
1	A	294	ASN
1	A	302	LYS
1	A	313	GLN
1	A	410	ARG
1	A	449	GLU
1	A	473	LEU
1	A	487	LEU
1	A	491	HIS
1	A	502	LYS
1	A	514	LEU
1	B	29	ASN
1	B	45	VAL
1	B	46	LEU
1	B	52	SER
1	B	59	ARG
1	B	84	GLU
1	B	107	THR
1	B	108	ASN
1	B	110	GLU
1	B	115	LYS
1	B	133	LYS
1	B	137	ASP
1	B	144	ASN
1	B	146	VAL
1	B	147	GLU
1	B	148	ASP
1	B	189	SER
1	B	199	GLU
1	B	202	GLU
1	B	217	ASN
1	B	228	LYS
1	B	230	ASN

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Mol	Chain	Res	Type
1	B	283	ASP
1	B	285	GLU
1	B	357	ILE
1	B	444	MET
1	B	494	CYS
1	B	514	LEU
1	B	559	SER
1	B	577	ASN
1	B	594	GLN
1	B	604	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	206	GLN
1	A	313	GLN
1	A	394	ASN
1	A	424	ASN
1	B	82	ASN
1	B	394	ASN
1	B	424	ASN
1	B	534	GLN
1	B	577	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	A	703	-	21,21,21	1.28	2 (9%)	31,31,31	1.98	8 (25%)
2	9QR	A	701	-	32,33,33	0.91	0	42,45,45	2.45	15 (35%)
3	NAP	B	702	-	45,52,52	0.92	3 (6%)	56,80,80	1.21	6 (10%)
4	UMP	B	703	-	21,21,21	1.32	3 (14%)	31,31,31	1.88	7 (22%)
2	9QR	B	701	-	32,33,33	0.80	0	42,45,45	2.38	12 (28%)
3	NAP	A	702	-	45,52,52	1.04	4 (8%)	56,80,80	1.50	14 (25%)

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	A	703	-	-	1/10/22/22	0/2/2/2
2	9QR	A	701	-	-	9/16/16/16	0/3/3/3
3	NAP	B	702	-	-	13/31/67/67	0/5/5/5
4	UMP	B	703	-	-	1/10/22/22	0/2/2/2
2	9QR	B	701	-	-	3/16/16/16	0/3/3/3
3	NAP	A	702	-	-	2/31/67/67	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	UMP	C2-N1	3.41	1.43	1.38
4	A	703	UMP	C2-N1	2.98	1.43	1.38
4	A	703	UMP	C6-C5	2.90	1.41	1.35
3	B	702	NAP	C5A-C4A	2.74	1.48	1.40
3	A	702	NAP	O4D-C1D	2.72	1.44	1.41
3	A	702	NAP	C5A-C4A	2.70	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAP	C2N-C3N	2.41	1.42	1.39
4	B	703	UMP	C2-N3	-2.26	1.33	1.38
3	B	702	NAP	P2B-O2B	2.14	1.63	1.59
4	B	703	UMP	C6-C5	2.03	1.39	1.35
3	B	702	NAP	O4B-C1B	2.03	1.43	1.41
3	A	702	NAP	O4B-C1B	2.02	1.43	1.41

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	9QR	C2-N3-C4	7.14	122.20	116.24
2	A	701	9QR	C2-N3-C4	6.95	122.03	116.24
2	B	701	9QR	C25-N24-C23	6.76	121.87	116.24
2	A	701	9QR	C25-N24-C23	5.88	121.14	116.24
4	B	703	UMP	C5-C4-N3	4.64	121.77	114.84
4	B	703	UMP	C4-N3-C2	-4.50	120.64	126.58
4	A	703	UMP	N3-C2-N1	4.43	120.77	114.89
2	A	701	9QR	C22-C27-N26	-4.36	120.07	122.52
4	A	703	UMP	C4-N3-C2	-4.29	120.92	126.58
2	A	701	9QR	C25-N26-C27	4.29	121.72	116.99
3	B	702	NAP	N3A-C2A-N1A	-4.12	122.23	128.68
4	A	703	UMP	C5-C4-N3	4.04	120.89	114.84
2	B	701	9QR	C22-C23-N24	-3.89	118.81	123.61
4	B	703	UMP	O4-C4-C5	-3.85	118.39	125.16
2	B	701	9QR	C5-C4-N3	-3.78	117.78	122.46
2	B	701	9QR	C22-C27-N26	-3.76	120.41	122.52
2	A	701	9QR	C5-C4-N3	-3.73	117.84	122.46
4	B	703	UMP	N3-C2-N1	3.63	119.71	114.89
2	B	701	9QR	C25-N26-C27	3.63	121.00	116.99
2	A	701	9QR	C22-C23-N24	-3.52	119.27	123.61
2	A	701	9QR	N3-C2-N1	-3.50	119.93	125.42
2	B	701	9QR	C12-O11-C5	3.50	124.79	114.23
2	B	701	9QR	N24-C25-N26	-3.49	119.94	125.42
4	A	703	UMP	O4-C4-C5	-3.47	119.06	125.16
3	A	702	NAP	N3A-C2A-N1A	-3.41	123.35	128.68
2	A	701	9QR	N24-C25-N26	-3.40	120.09	125.42
3	A	702	NAP	C4A-C5A-N7A	-3.38	105.88	109.40
2	B	701	9QR	N3-C2-N1	-3.32	120.22	125.42
4	A	703	UMP	C2'-C1'-N1	3.28	121.32	113.77
4	A	703	UMP	P-O5'-C5'	3.27	127.30	118.30
2	A	701	9QR	C20-C19-C22	-3.26	115.38	120.79
2	A	701	9QR	C18-C19-C22	3.07	125.89	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	NAP	C3D-C2D-C1D	2.97	105.45	100.98
2	A	701	9QR	N7-C6-N1	2.96	121.22	117.03
2	A	701	9QR	C2-N1-C6	2.91	120.21	116.99
3	A	702	NAP	C3D-C2D-C1D	2.81	105.21	100.98
4	B	703	UMP	C1'-N1-C2	2.79	123.13	117.64
2	A	701	9QR	N29-C25-N24	2.71	121.46	117.25
3	B	702	NAP	C4A-C5A-N7A	-2.67	106.62	109.40
3	A	702	NAP	C6N-N1N-C2N	-2.60	119.61	121.97
2	B	701	9QR	C2-N1-C6	2.59	119.85	116.99
3	A	702	NAP	C3N-C2N-N1N	2.51	122.88	120.43
3	A	702	NAP	O2B-C2B-C1B	-2.51	101.08	110.10
2	B	701	9QR	C27-C22-C23	2.48	117.95	115.91
2	B	701	9QR	N29-C25-N24	2.47	121.09	117.25
4	B	703	UMP	P-O5'-C5'	2.42	124.95	118.30
2	A	701	9QR	C19-C22-C23	-2.41	121.50	123.46
3	A	702	NAP	O2A-PA-O1A	2.38	124.00	112.24
3	A	702	NAP	PN-O3-PA	-2.31	124.91	132.83
3	B	702	NAP	PN-O3-PA	-2.29	124.97	132.83
3	A	702	NAP	C5A-C6A-N6A	2.25	123.78	120.35
4	A	703	UMP	OP3-P-OP2	2.24	116.20	107.64
3	A	702	NAP	C5D-C4D-C3D	-2.24	106.80	115.18
3	B	702	NAP	C2A-N1A-C6A	2.24	122.58	118.75
4	A	703	UMP	O5'-P-OP1	-2.20	100.30	106.47
3	A	702	NAP	O4D-C4D-C5D	2.20	116.61	109.37
2	A	701	9QR	C27-C22-C23	2.15	117.68	115.91
3	A	702	NAP	C2A-N1A-C6A	2.14	122.42	118.75
3	A	702	NAP	C2D-C3D-C4D	2.13	106.77	102.64
4	B	703	UMP	C1'-N1-C6	-2.09	117.42	121.55
3	A	702	NAP	C3N-C7N-N7N	2.06	120.23	117.75
3	B	702	NAP	O2B-C2B-C1B	2.02	117.37	110.10

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	9QR	C18-C19-C22-C27
3	B	702	NAP	C1B-C2B-O2B-P2B
3	B	702	NAP	C2B-O2B-P2B-O3X
3	B	702	NAP	C5D-O5D-PN-O1N
3	B	702	NAP	O4D-C1D-N1N-C2N
3	B	702	NAP	C2D-C1D-N1N-C2N
3	B	702	NAP	C2N-C3N-C7N-O7N

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Mol	Chain	Res	Type	Atoms
3	B	702	NAP	C2N-C3N-C7N-N7N
3	B	702	NAP	C4N-C3N-C7N-O7N
3	B	702	NAP	C4N-C3N-C7N-N7N
2	A	701	9QR	C12-C13-C14-O15
2	A	701	9QR	C18-C19-C22-C23
2	A	701	9QR	C20-C19-C22-C27
2	A	701	9QR	C17-C16-O15-C14
2	A	701	9QR	C21-C16-O15-C14
2	A	701	9QR	C20-C19-C22-C23
2	B	701	9QR	C17-C16-O15-C14
2	B	701	9QR	C21-C16-O15-C14
3	A	702	NAP	O4D-C4D-C5D-O5D
3	A	702	NAP	C3D-C4D-C5D-O5D
2	B	701	9QR	C13-C12-O11-C5
3	B	702	NAP	C2B-O2B-P2B-O1X
3	B	702	NAP	C4D-C5D-O5D-PN
3	B	702	NAP	C5D-O5D-PN-O3
4	A	703	UMP	O4'-C4'-C5'-O5'
3	B	702	NAP	C2D-C1D-N1N-C6N
4	B	703	UMP	O4'-C4'-C5'-O5'
2	A	701	9QR	C13-C14-O15-C16
2	A	701	9QR	C22-C23-C30-C31

There are no ring outliers.

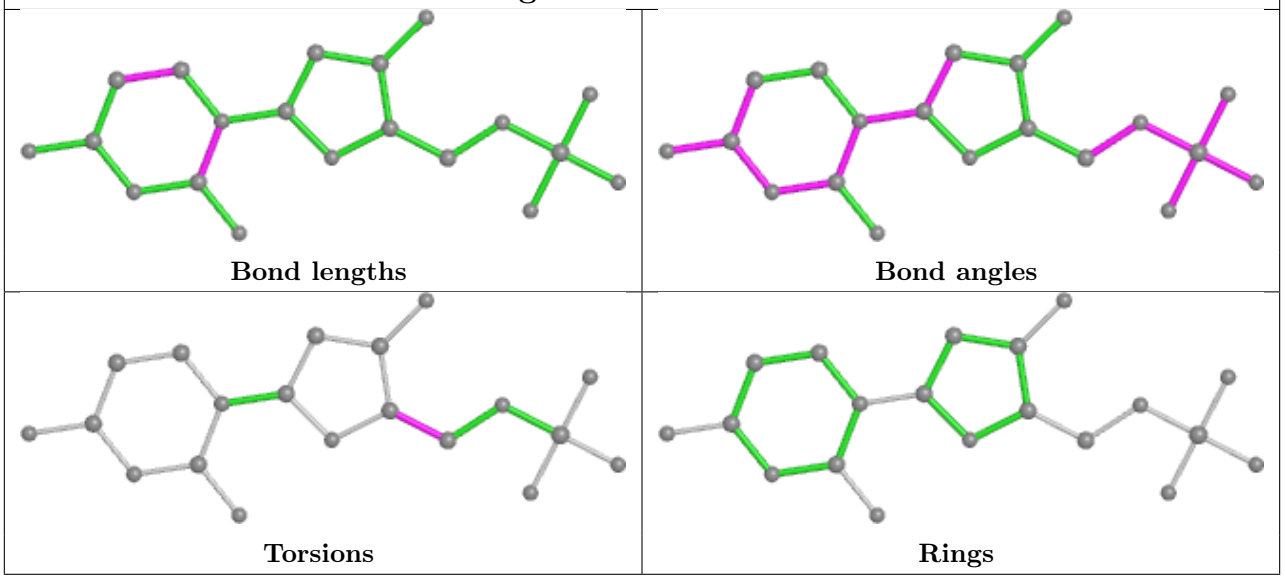
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	9QR	1	0
3	B	702	NAP	4	0
2	B	701	9QR	1	0
3	A	702	NAP	3	0

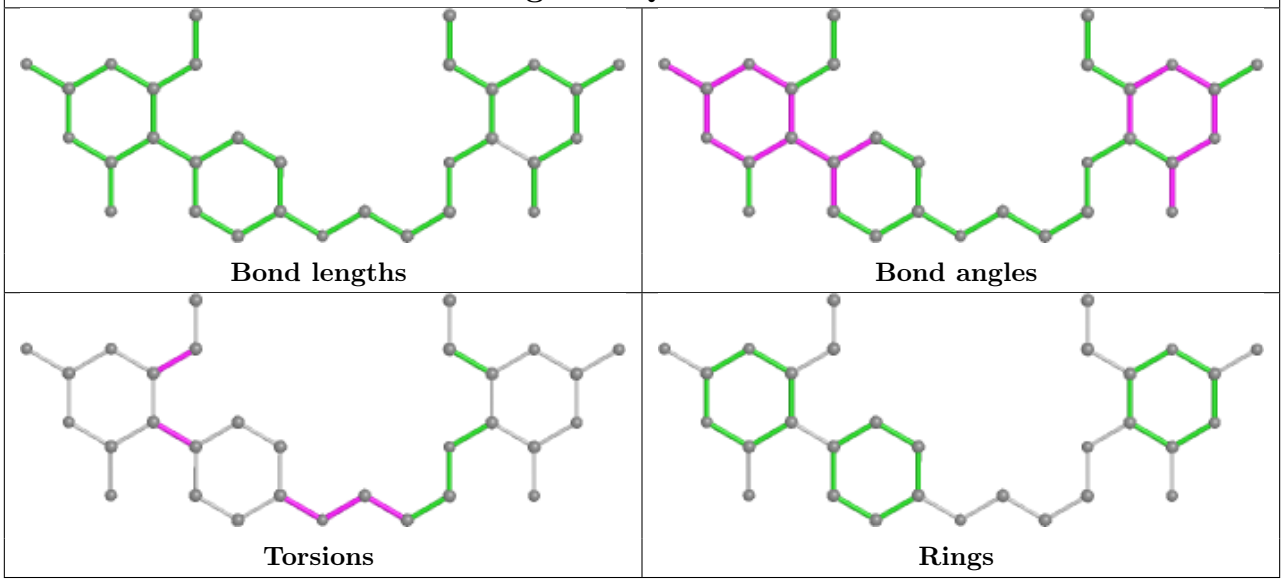
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

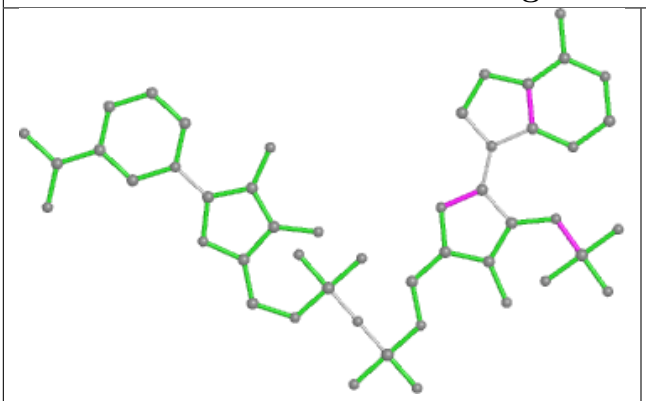
Ligand UMP A 703



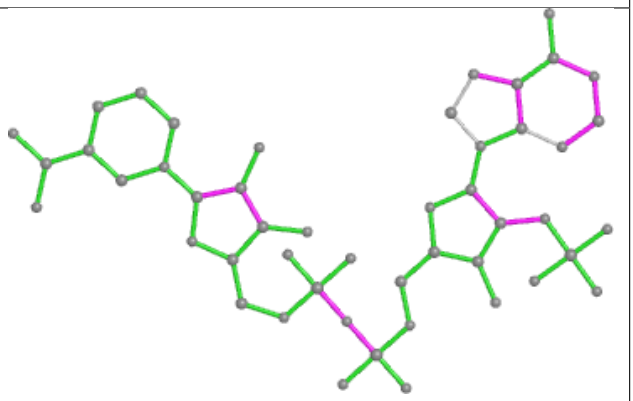
Ligand 9QR A 701



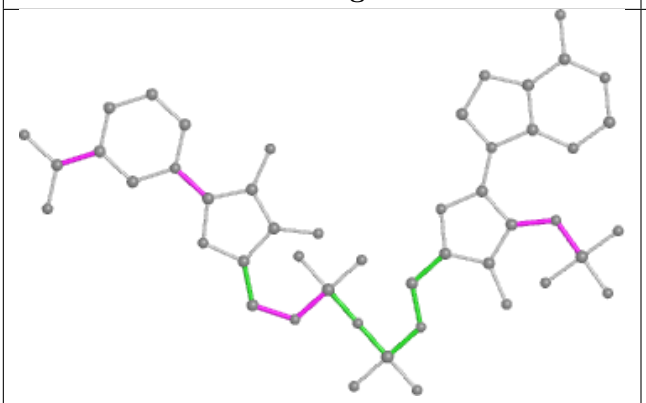
Ligand NAP B 702



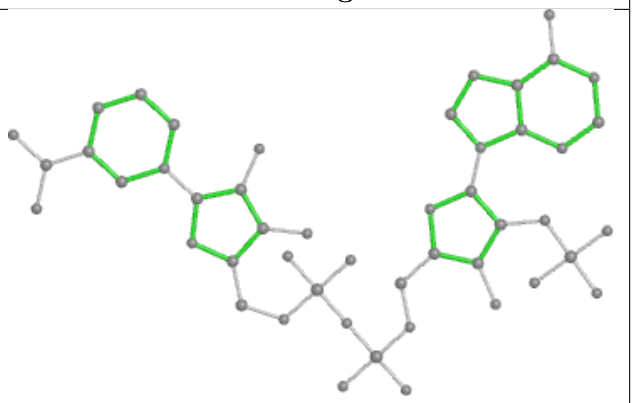
Bond lengths



Bond angles

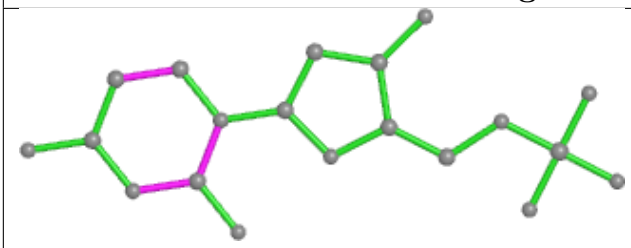


Torsions

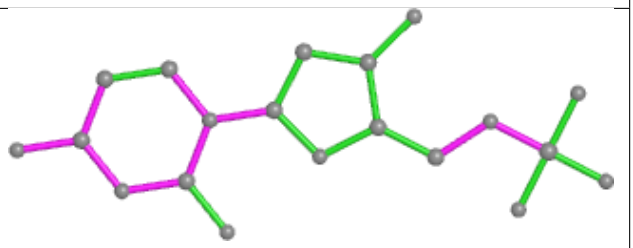


Rings

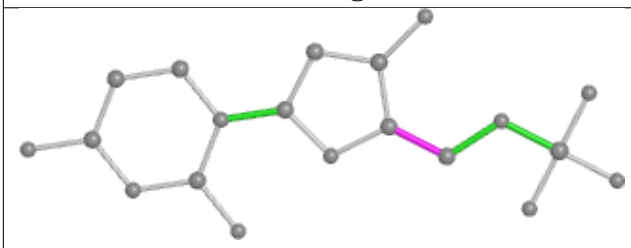
Ligand UMP B 703



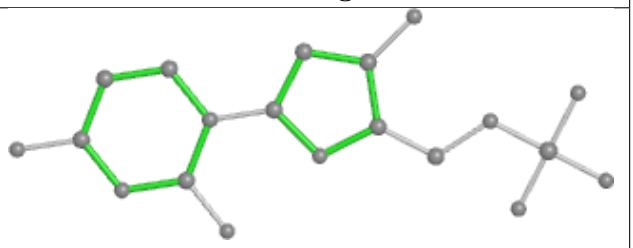
Bond lengths



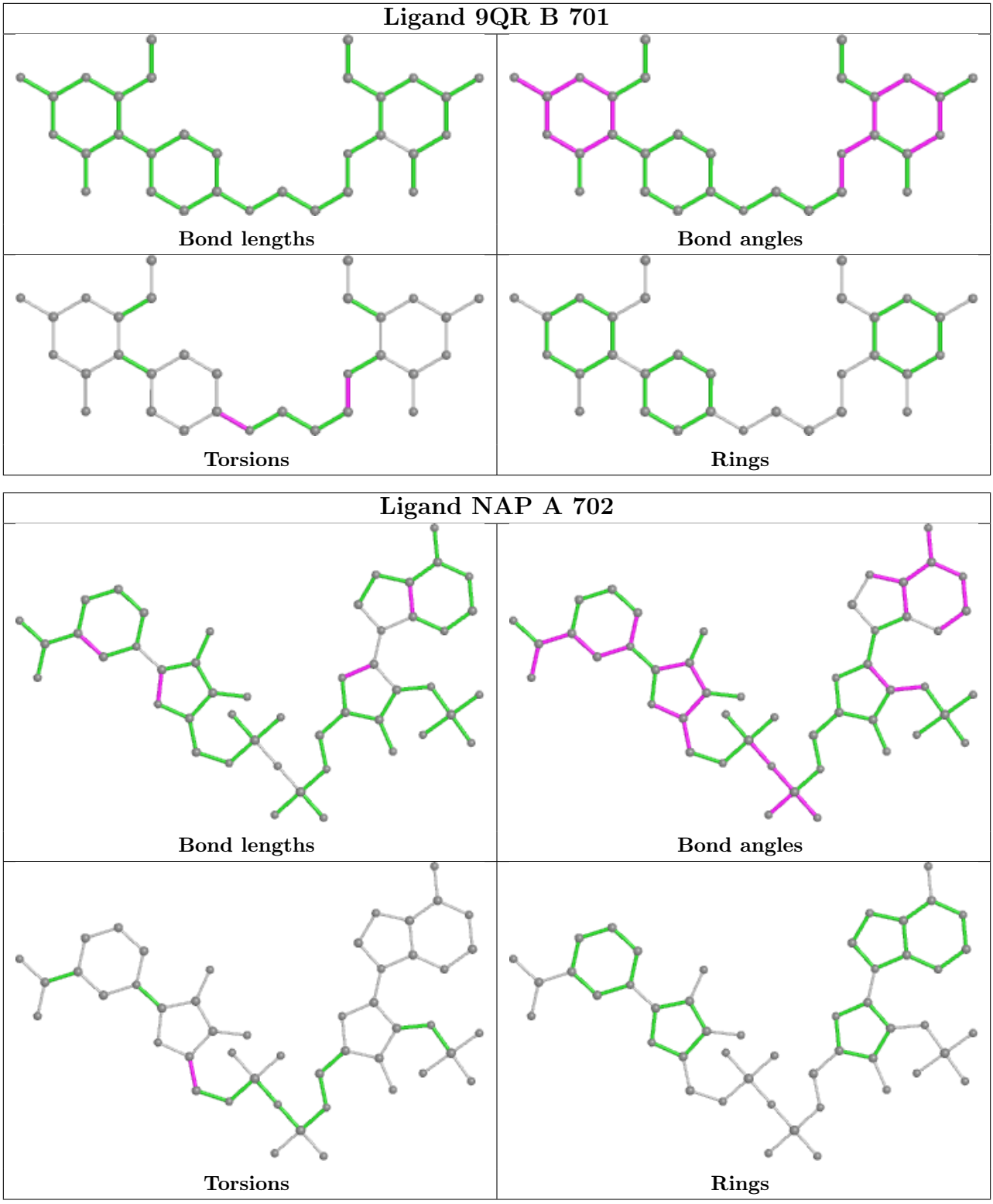
Bond angles



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, 95^{th} 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	547/608 (89%)	-0.15	29 (5%)	26	23	8, 21, 92, 120	0
1	B	547/608 (89%)	0.17	45 (8%)	11	8	8, 27, 113, 120	0
All	All	1094/1216 (89%)	0.01	74 (6%)	17	13	8, 23, 108, 120	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	ALA	13.4
1	A	607	ALA	8.8
1	B	607	ALA	8.4
1	B	2	MET	8.4
1	A	1	MET	8.2
1	A	2	MET	8.0
1	A	305	ASN	8.0
1	B	24	ASN	7.7
1	B	75	TYR	7.5
1	B	608	ALA	7.4
1	A	306	SER	6.9
1	B	1	MET	6.8
1	A	24	ASN	6.6
1	B	302	LYS	6.3
1	B	606	MET	6.2
1	B	301	GLU	5.8
1	B	27	LYS	5.8
1	A	606	MET	5.6
1	B	231	ASN	5.5
1	A	23	LYS	5.2
1	A	231	ASN	5.1
1	B	28	LYS	5.0
1	B	96	LYS	4.8
1	B	84	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	300	GLU	4.5
1	B	26	GLY	4.5
1	B	305	ASN	4.4
1	A	75	TYR	4.3
1	A	301	GLU	4.0
1	A	26	GLY	3.8
1	A	3	GLU	3.6
1	B	135	ASP	3.6
1	B	23	LYS	3.6
1	B	230	ASN	3.5
1	B	25	GLU	3.5
1	B	134	GLU	3.5
1	B	3	GLU	3.5
1	A	85	THR	3.5
1	B	151	VAL	3.5
1	B	130	THR	3.4
1	B	300	GLU	3.3
1	A	96	LYS	3.3
1	B	116	PHE	3.2
1	B	97	LYS	3.2
1	A	299	LYS	3.1
1	B	80	TYR	3.0
1	B	137	ASP	3.0
1	B	81	LEU	2.9
1	A	283	ASP	2.9
1	A	304	LYS	2.8
1	B	299	LYS	2.8
1	A	302	LYS	2.7
1	B	105	GLY	2.6
1	B	110	GLU	2.6
1	B	284	ASP	2.6
1	B	109	TRP	2.6
1	B	111	SER	2.6
1	B	136	PHE	2.5
1	A	284	ASP	2.5
1	B	157	ASN	2.5
1	B	44	GLY	2.4
1	A	28	LYS	2.4
1	A	230	ASN	2.3
1	B	146	VAL	2.2
1	A	310	ASN	2.2
1	B	22	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	298	GLU	2.2
1	A	116	PHE	2.1
1	B	123	ILE	2.1
1	B	76	LYS	2.1
1	B	115	LYS	2.1
1	B	139	ASP	2.0
1	A	287	GLU	2.0
1	A	605	ASP	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)

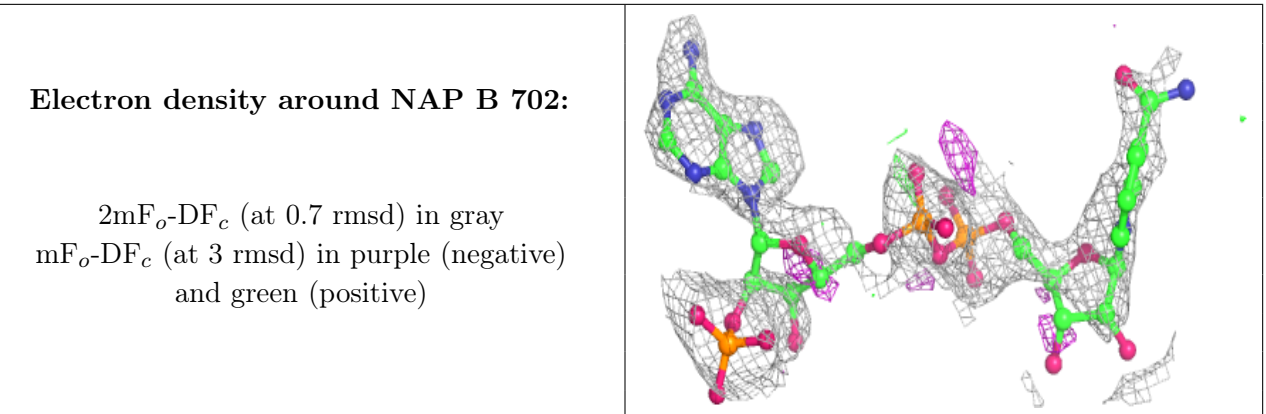
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

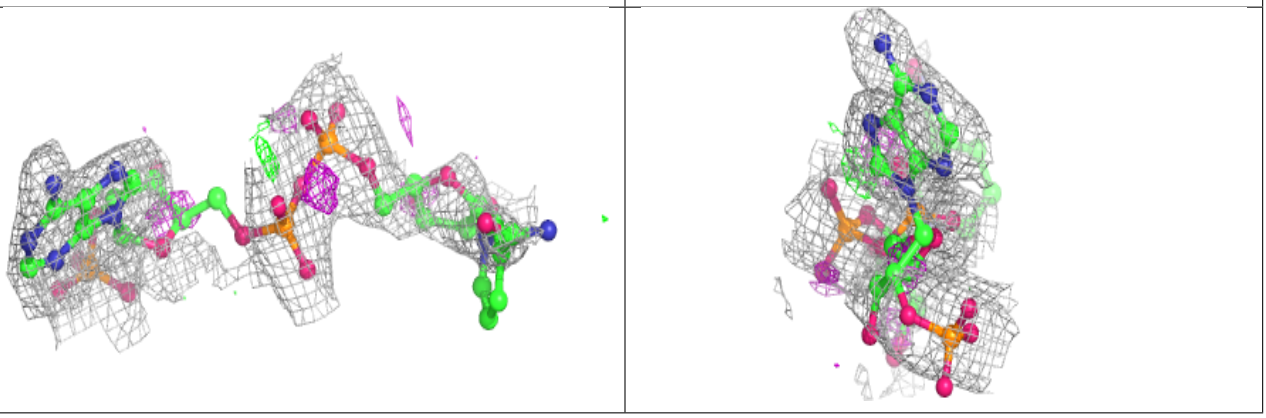
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	B	702	48/48	0.76	0.30	85,105,118,120	0
2	9QR	B	701	31/31	0.80	0.28	42,72,101,103	0
2	9QR	A	701	31/31	0.84	0.23	21,46,61,63	0
3	NAP	A	702	48/48	0.92	0.14	38,50,55,61	0
4	UMP	A	703	20/20	0.98	0.10	11,13,14,15	0
4	UMP	B	703	20/20	0.98	0.11	15,19,23,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAP B 702:

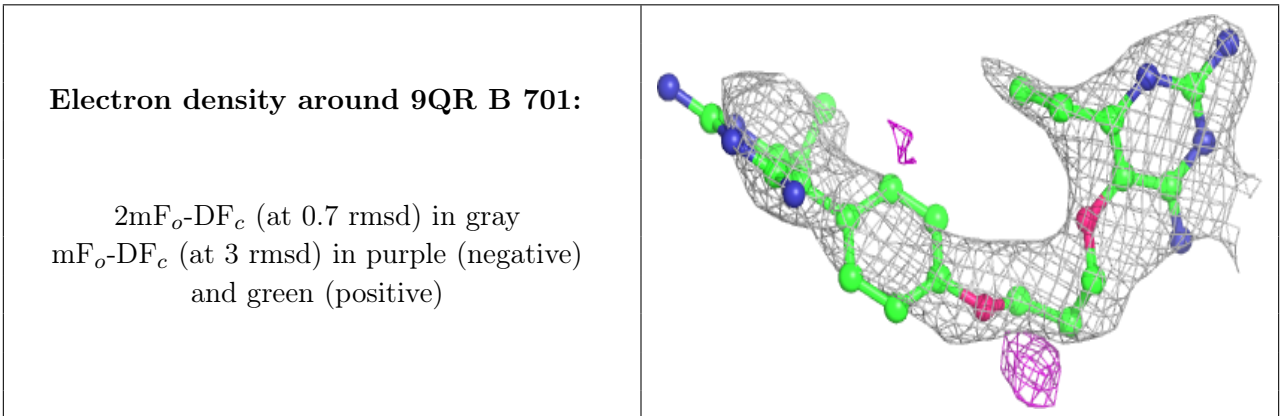
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

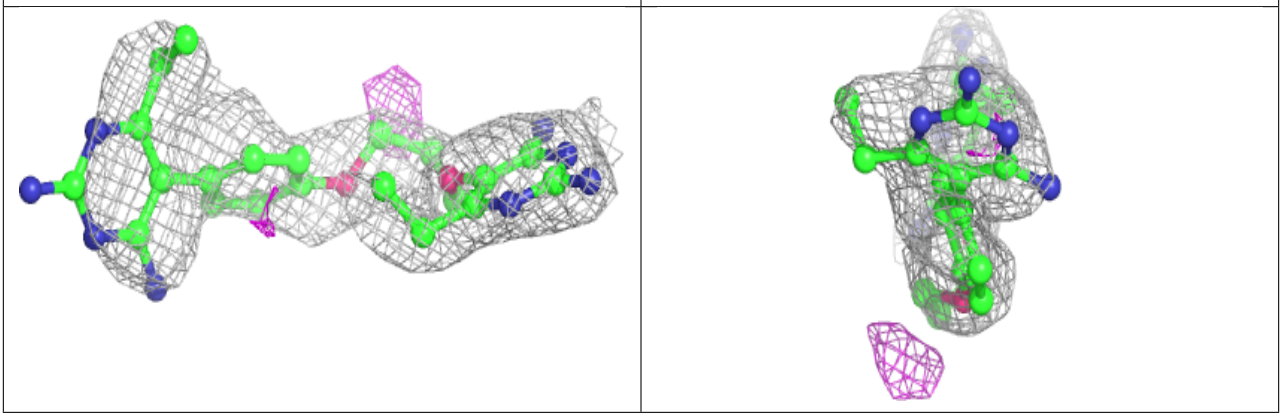




Electron density around 9QR B 701:

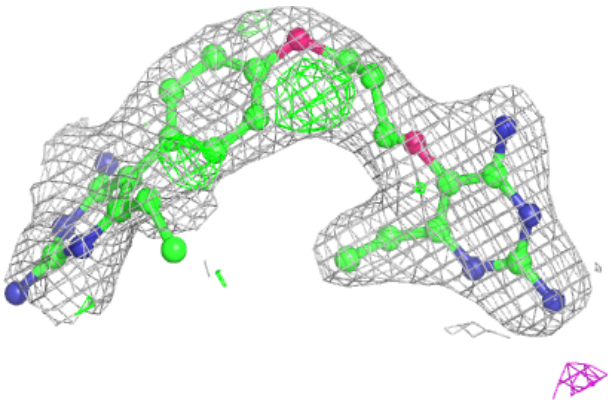
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

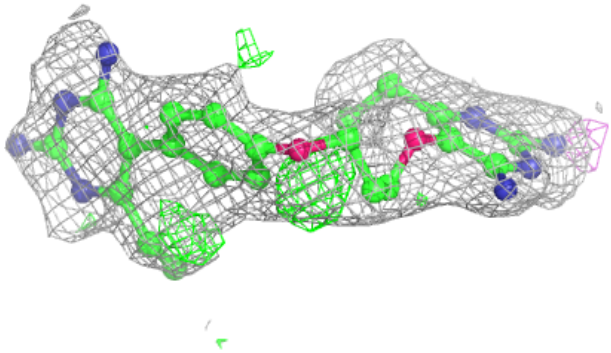


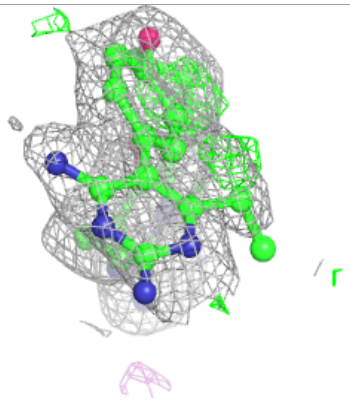


Electron density around 9QR A 701:

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

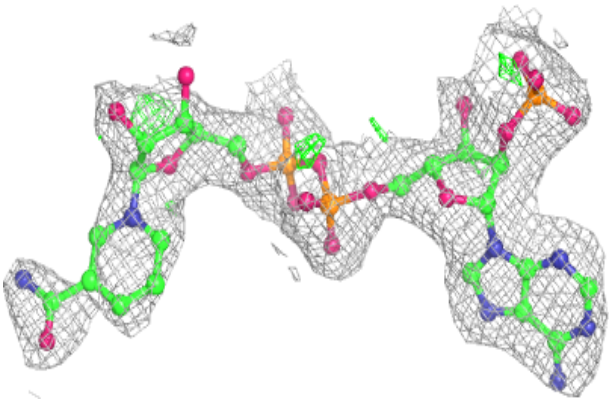


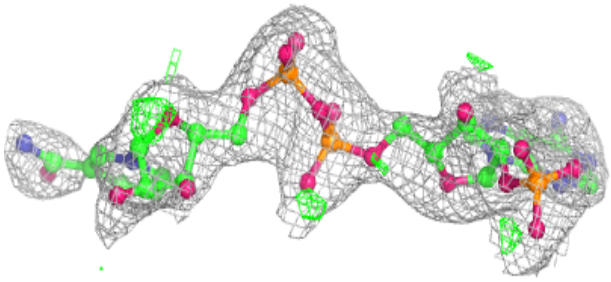


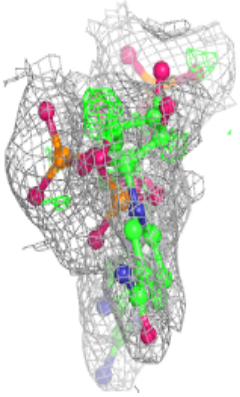


Electron density around NAP A 702:

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

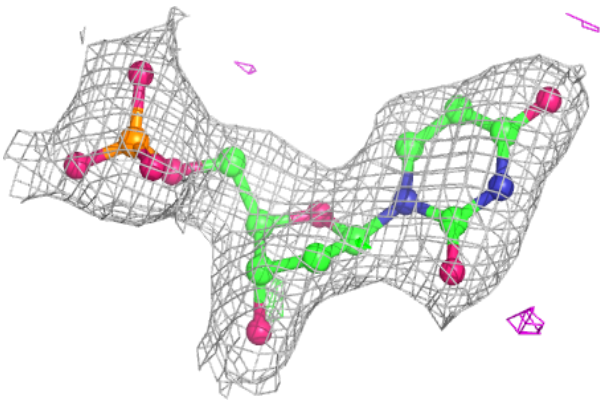


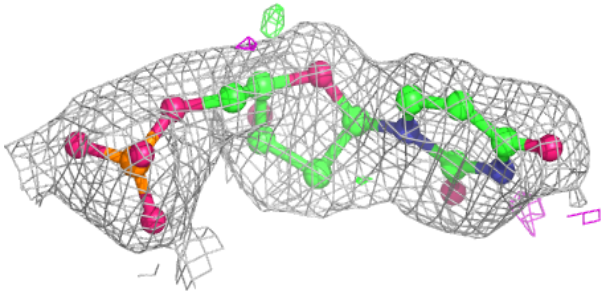


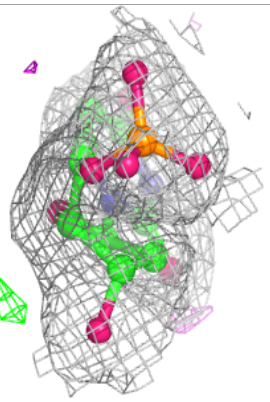


Electron density around UMP A 703:

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

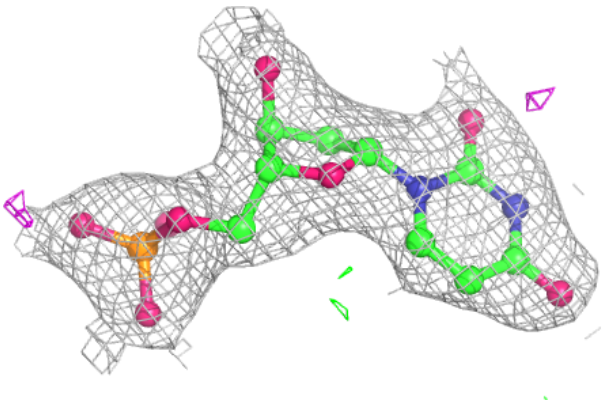


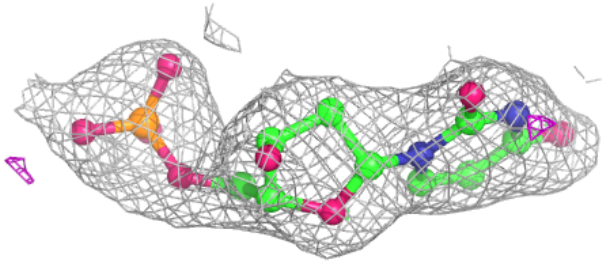


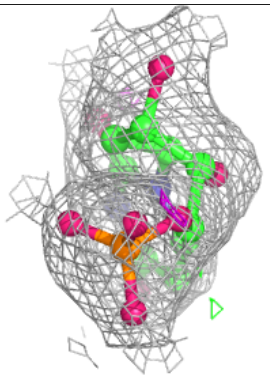


Electron density around UMP B 703:

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







6.5 Other polymers (i)

There are no such residues in this entry.