



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:57 AM UTC

PDB ID : 6A2K / pdb_00006a2k
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

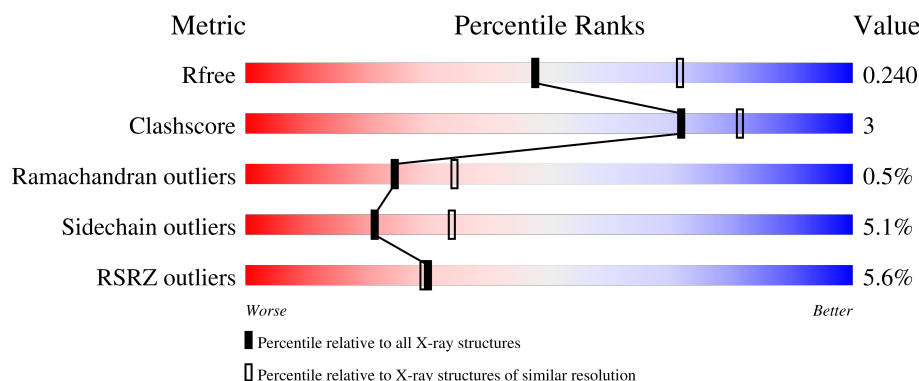
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 $\leq 5\%$. 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	2% 79% 9% • 11%
1	B	608	8% 72% 14% • 13%

2 Entry composition [i](#)

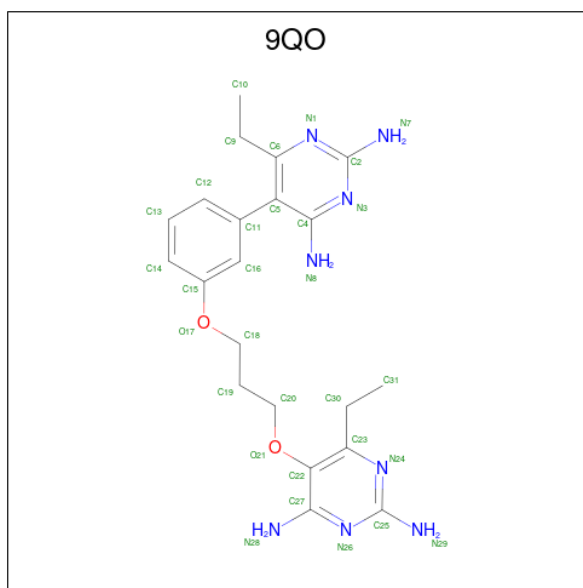
There are 5 unique types of molecules in this entry. The entry contains 9429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	543	Total	C	N	O	S	0	0	0
			4507	2910	745	824	28			
1	B	527	Total	C	N	O	S	0	0	0
			4373	2831	723	793	26			

- Molecule 2 is 5-(3-{3-[(2,4-diamino-6-ethylpyrimidin-5-yl)oxy]propoxy}phenyl)-6-ethylpyrimidine-2,4-diamine (CCD ID: 9QO) (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 (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

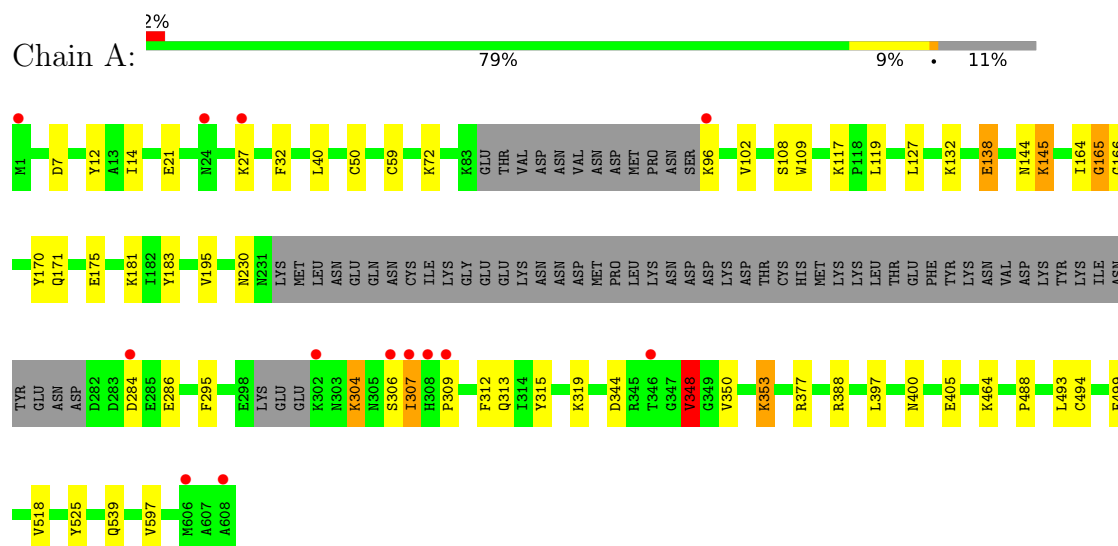
- Molecule 5 is water.

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

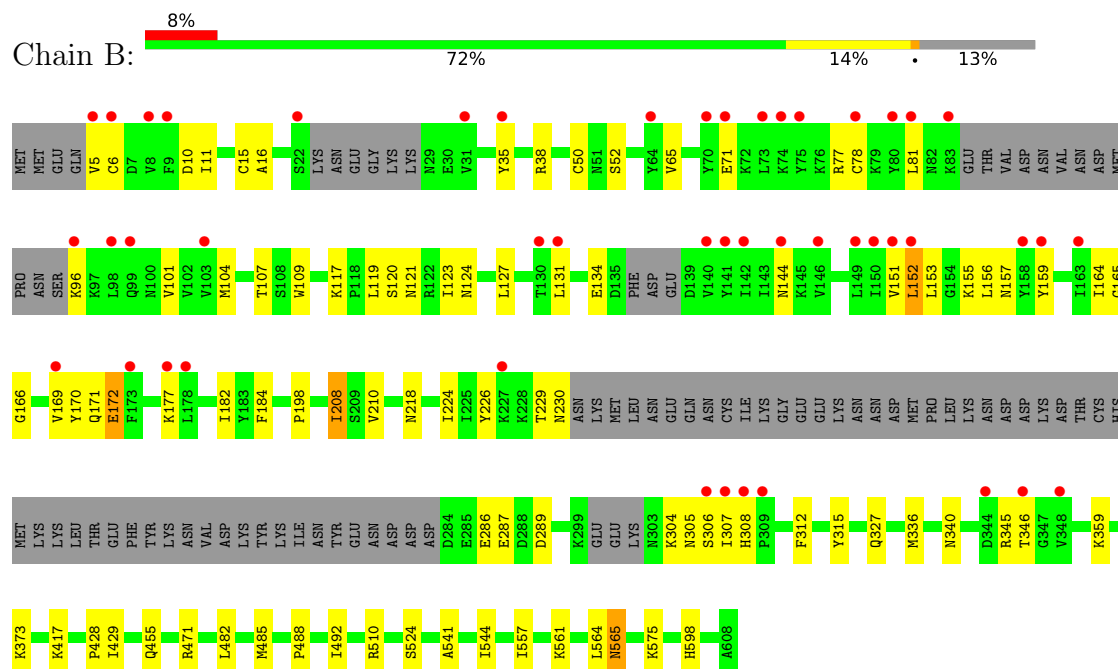
3 Residue-property plots [i](#)

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



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4 Data and refinement statistics

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) 97.9 (27.83-2.38)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2925 reflections (5.00%)	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)	0.32 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.85	0/4611	1.05	15/6223 (0.2%)
1	B	0.86	1/4474 (0.0%)	1.03	4/6040 (0.1%)
All	All	0.86	1/9085 (0.0%)	1.04	19/12263 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	ALA	CA-C	9.05	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ILE	CB-CA-C	-8.74	101.35	110.88
1	A	307	ILE	N-CA-C	-8.38	100.92	110.05
1	B	308	HIS	N-CA-C	6.60	119.84	110.40
1	B	305	ASN	N-CA-C	6.13	119.92	110.42
1	A	539	GLN	CA-C-N	-5.66	114.13	119.85
1	A	539	GLN	C-N-CA	-5.66	114.13	119.85
1	A	377	ARG	CA-C-N	5.66	126.38	119.99
1	A	377	ARG	C-N-CA	5.66	126.38	119.99
1	A	165	GLY	N-CA-C	5.64	119.35	111.00
1	A	350	VAL	N-CA-C	5.59	117.71	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	GLN	CB-CA-C	-5.37	101.88	110.79
1	A	304	LYS	N-CA-C	-5.36	99.39	110.80
1	A	518	VAL	CA-C-N	-5.32	113.14	119.05
1	A	518	VAL	C-N-CA	-5.32	113.14	119.05
1	A	348	VAL	N-CA-C	-5.19	102.04	108.89
1	A	138	GLU	N-CA-C	5.18	118.13	110.46
1	A	164	ILE	CA-C-N	-5.11	113.08	122.27
1	A	164	ILE	C-N-CA	-5.11	113.08	122.27
1	A	295	PHE	N-CA-C	5.07	118.57	112.38

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

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	29	0
1	B	4373	0	4338	34	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	5	0
5	B	159	0	0	1	0
All	All	9429	0	8872	59	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 (59) 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
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:104:MET:HE2	1:B:164:ILE:HD11	1.96	0.47
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:493:LEU:C	1:A:493:LEU:HD12	2.40	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:153:LEU:C	1:B:155:LYS:H	2.26	0.43
1:B:492:ILE:HD11	1:B:510:ARG:HD3	2.01	0.43
1:A:464:LYS:NZ	5:A:810:HOH:O	2.51	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:152:LEU:O	1:B:156:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLY:HA2	1:B:170:TYR:CZ	2.55	0.42
1:B:428:PRO:O	1:B:485:MET:HE2	2.20	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: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:336:MET:HE2	1:B:557:ILE:HG23	2.02	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

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	535/608 (88%)	499 (93%)	33 (6%)	3 (1%)	21	30
1	B	515/608 (85%)	476 (92%)	37 (7%)	2 (0%)	30	40
All	All	1050/1216 (86%)	975 (93%)	70 (7%)	5 (0%)	24	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	GLU

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

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	506/570 (89%)	490 (97%)	16 (3%)	34	53
1	B	491/570 (86%)	456 (93%)	35 (7%)	13	21
All	All	997/1140 (88%)	946 (95%)	51 (5%)	21	34

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	27	LYS
1	A	50	CYS
1	A	72	LYS
1	A	96	LYS
1	A	132	LYS
1	A	138	GLU
1	A	145	LYS
1	A	195	VAL
1	A	284	ASP
1	A	286	GLU
1	A	307	ILE
1	A	313	GLN
1	A	348	VAL
1	A	353	LYS
1	A	400	ASN
1	B	5	VAL
1	B	6	CYS
1	B	11	ILE

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Mol	Chain	Res	Type
1	B	50	CYS
1	B	52	SER
1	B	71	GLU
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	144	ASN
1	B	151	VAL
1	B	152	LEU
1	B	157	ASN
1	B	172	GLU
1	B	208	ILE
1	B	218	ASN
1	B	229	THR
1	B	230	ASN
1	B	287	GLU
1	B	304	LYS
1	B	307	ILE
1	B	327	GLN
1	B	345	ARG
1	B	346	THR
1	B	417	LYS
1	B	524	SER
1	B	564	LEU
1	B	565	ASN
1	B	575	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	316	ASN
1	A	407	ASN
1	A	530	HIS
1	B	82	ASN
1	B	157	ASN

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Mol	Chain	Res	Type
1	B	206	GLN
1	B	294	ASN
1	B	313	GLN
1	B	407	ASN
1	B	563	GLN
1	B	565	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.44	2 (9%)	30,31,31	1.97	8 (26%)
3	NAP	B	702	-	50,52,52	1.24	5 (10%)	71,80,80	1.57	9 (12%)
2	9QO	B	701	-	33,33,33	0.86	0	42,45,45	2.81	17 (40%)
4	UMP	B	703	-	21,21,21	1.54	2 (9%)	30,31,31	2.25	13 (43%)
2	9QO	A	701	-	33,33,33	0.87	0	42,45,45	2.61	16 (38%)
3	NAP	A	702	-	50,52,52	1.35	7 (14%)	71,80,80	1.74	16 (22%)

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	-	-	4/10/22/22	0/2/2/2
3	NAP	B	702	-	-	5/35/67/67	0/5/5/5
2	9QO	B	701	-	-	9/16/16/16	0/3/3/3
4	UMP	B	703	-	-	8/10/22/22	0/2/2/2
2	9QO	A	701	-	-	3/16/16/16	0/3/3/3
3	NAP	A	702	-	-	4/35/67/67	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAP	C5A-C4A	5.26	1.48	1.39
4	B	703	UMP	C2-N1	4.77	1.45	1.38
4	A	703	UMP	C2-N1	4.42	1.45	1.38
3	A	702	NAP	C5A-C4A	4.15	1.46	1.39
3	A	702	NAP	PA-O3	3.34	1.63	1.59
3	B	702	NAP	C5A-C6A	3.12	1.49	1.41
4	A	703	UMP	O2-C2	2.88	1.28	1.23
3	A	702	NAP	O4D-C1D	2.81	1.44	1.40
3	A	702	NAP	PN-O3	2.78	1.62	1.59
4	B	703	UMP	O2-C2	2.70	1.27	1.23
3	A	702	NAP	C5A-C6A	2.67	1.48	1.41
3	A	702	NAP	C4A-N9A	-2.53	1.32	1.37
3	A	702	NAP	C5A-N7A	-2.40	1.34	1.39
3	B	702	NAP	C5A-N7A	-2.35	1.34	1.39
3	B	702	NAP	C8A-N7A	2.19	1.35	1.31
3	B	702	NAP	O4D-C1D	2.05	1.43	1.40

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	9QO	C2-N1-C6	9.36	123.09	116.26
2	A	701	9QO	C25-N24-C23	7.75	121.91	116.26
2	B	701	9QO	C25-N24-C23	7.68	121.86	116.26
2	A	701	9QO	C2-N1-C6	6.68	121.14	116.26
3	B	702	NAP	C5A-C4A-N3A	-6.04	118.40	126.72
3	A	702	NAP	C5A-C4A-N3A	-5.57	119.04	126.72
2	A	701	9QO	C5-C4-N3	-5.19	119.54	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	UMP	C1'-N1-C2	5.09	127.62	117.66
3	A	702	NAP	N3A-C4A-N9A	4.70	135.16	127.17
2	B	701	9QO	C9-C6-C5	4.53	125.49	122.47
3	B	702	NAP	N3A-C4A-N9A	4.53	134.88	127.17
2	A	701	9QO	C20-O21-C22	4.53	127.81	114.22
2	B	701	9QO	N3-C2-N1	-4.43	118.69	125.48
4	A	703	UMP	C5-C4-N3	4.41	120.98	114.80
4	A	703	UMP	O4-C4-C5	-4.38	117.61	125.16
4	B	703	UMP	O4-C4-C5	-4.36	117.64	125.16
3	B	702	NAP	C4A-C5A-N7A	-3.94	106.07	110.58
4	B	703	UMP	C1'-N1-C6	-3.87	113.91	121.53
2	A	701	9QO	N26-C25-N24	-3.87	119.55	125.48
3	A	702	NAP	C4A-N9A-C8A	3.83	109.76	105.74
4	B	703	UMP	C5-C4-N3	3.83	120.16	114.80
2	B	701	9QO	N26-C25-N24	-3.79	119.67	125.48
3	A	702	NAP	C4A-C5A-N7A	-3.78	106.26	110.58
3	B	702	NAP	C2A-N3A-C4A	3.77	121.05	111.83
4	A	703	UMP	C1'-N1-C2	3.75	124.99	117.66
3	A	702	NAP	C2A-N3A-C4A	3.68	120.83	111.83
4	A	703	UMP	C4-N3-C2	-3.51	122.25	126.61
2	B	701	9QO	C2-N3-C4	3.50	121.48	117.28
2	B	701	9QO	C20-O21-C22	3.47	124.63	114.22
2	B	701	9QO	C18-O17-C15	3.47	126.94	117.93
2	A	701	9QO	C18-O17-C15	3.44	126.88	117.93
3	A	702	NAP	N3A-C2A-N1A	-3.42	123.40	128.58
4	A	703	UMP	C1'-N1-C6	-3.40	114.85	121.53
2	A	701	9QO	C5-C6-N1	-3.36	119.62	123.47
4	A	703	UMP	OP3-P-OP2	3.29	120.15	107.80
2	A	701	9QO	N3-C2-N1	-3.24	120.51	125.48
3	A	702	NAP	C5A-N7A-C8A	3.23	108.52	103.45
4	B	703	UMP	O5'-P-OP1	-3.17	97.86	106.44
2	A	701	9QO	C25-N26-C27	3.17	121.09	117.28
2	B	701	9QO	C25-N26-C27	3.16	121.08	117.28
2	A	701	9QO	C4-C5-C6	3.15	118.24	115.97
2	B	701	9QO	C5-C6-N1	-3.10	119.92	123.47
4	B	703	UMP	C4-N3-C2	-3.07	122.80	126.61
3	B	702	NAP	N3A-C2A-N1A	-3.06	123.95	128.58
2	A	701	9QO	C2-N3-C4	3.05	120.94	117.28
3	A	702	NAP	N9A-C8A-N7A	-3.00	109.68	113.94
2	A	701	9QO	O21-C22-C23	2.95	123.38	119.18
2	A	701	9QO	N7-C2-N3	2.95	121.64	117.22
2	A	701	9QO	N29-C25-N26	2.94	121.64	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAP	C5A-N7A-C8A	2.77	107.80	103.45
4	B	703	UMP	O5'-C5'-C4'	2.75	118.37	108.99
4	B	703	UMP	O4'-C1'-N1	2.74	112.73	107.86
3	A	702	NAP	O3-PN-O1N	-2.69	102.60	110.70
2	B	701	9QO	C11-C16-C15	2.65	123.04	119.85
2	B	701	9QO	C5-C4-N8	2.64	124.17	120.82
2	B	701	9QO	N29-C25-N26	2.62	121.15	117.22
2	B	701	9QO	N7-C2-N1	2.59	121.11	117.22
2	B	701	9QO	O21-C22-C23	2.57	122.84	119.18
3	A	702	NAP	O2B-C2B-C1B	-2.56	101.04	110.05
3	A	702	NAP	C6A-C5A-N7A	2.55	137.01	132.09
2	B	701	9QO	C22-C23-N24	-2.55	119.30	122.46
3	B	702	NAP	O4B-C1B-N9A	2.54	112.97	108.09
2	A	701	9QO	C22-C23-N24	-2.50	119.36	122.46
3	A	702	NAP	O3X-P2B-O1X	2.48	120.51	110.83
4	A	703	UMP	O4'-C1'-N1	2.48	112.26	107.86
3	B	702	NAP	C6A-C5A-N7A	2.43	136.78	132.09
4	B	703	UMP	O2-C2-N3	-2.41	117.04	121.49
4	A	703	UMP	OP3-P-O5'	-2.38	100.45	106.67
3	A	702	NAP	C6N-N1N-C1D	2.37	124.38	119.73
3	A	702	NAP	O2A-PA-O1A	2.31	123.21	112.44
4	B	703	UMP	C2'-C1'-N1	2.29	119.53	113.81
3	B	702	NAP	O2A-PA-O1A	2.25	122.91	112.44
4	B	703	UMP	N3-C2-N1	2.21	117.77	114.89
2	B	701	9QO	N8-C4-N3	-2.14	114.14	117.03
4	B	703	UMP	C6-N1-C2	-2.13	118.41	121.00
3	A	702	NAP	C2N-N1N-C1D	-2.06	114.58	119.13
4	B	703	UMP	O4-C4-N3	2.02	122.20	119.27
3	A	702	NAP	O2N-PN-O1N	2.02	121.84	112.44
2	A	701	9QO	C10-C9-C6	-2.01	109.16	114.59

There are no chirality outliers.

All (33) 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
2	B	701	9QO	C22-C23-C30-C31
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

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Mol	Chain	Res	Type	Atoms
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
2	B	701	9QO	C14-C15-O17-C18
2	B	701	9QO	C16-C15-O17-C18
4	B	703	UMP	O4'-C4'-C5'-O5'
2	B	701	9QO	C12-C11-C5-C6
2	B	701	9QO	O17-C18-C19-C20
4	B	703	UMP	C3'-C4'-C5'-O5'
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	B	703	UMP	C5'-O5'-P-OP1
4	A	703	UMP	C3'-C4'-C5'-O5'
4	A	703	UMP	C2'-C1'-N1-C2
4	A	703	UMP	O4'-C4'-C5'-O5'
4	A	703	UMP	C2'-C1'-N1-C6
4	B	703	UMP	C2'-C1'-N1-C2
3	A	702	NAP	C2D-C1D-N1N-C2N
3	B	702	NAP	C2D-C1D-N1N-C6N
4	B	703	UMP	C4'-C5'-O5'-P
3	B	702	NAP	C3B-C4B-C5B-O5B
4	B	703	UMP	C2'-C1'-N1-C6
2	B	701	9QO	N24-C23-C30-C31

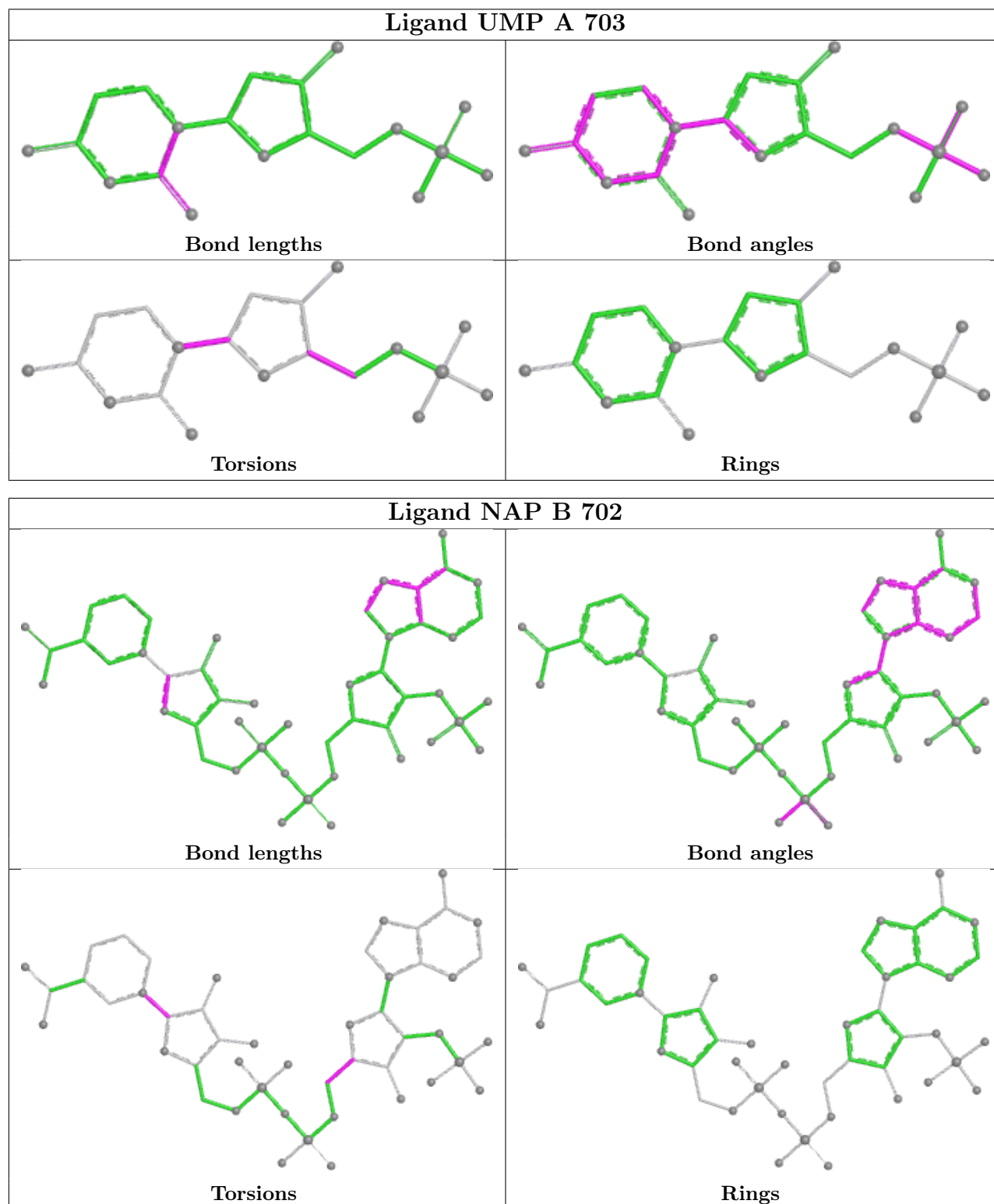
There are no ring outliers.

2 monomers are involved in 10 short contacts:

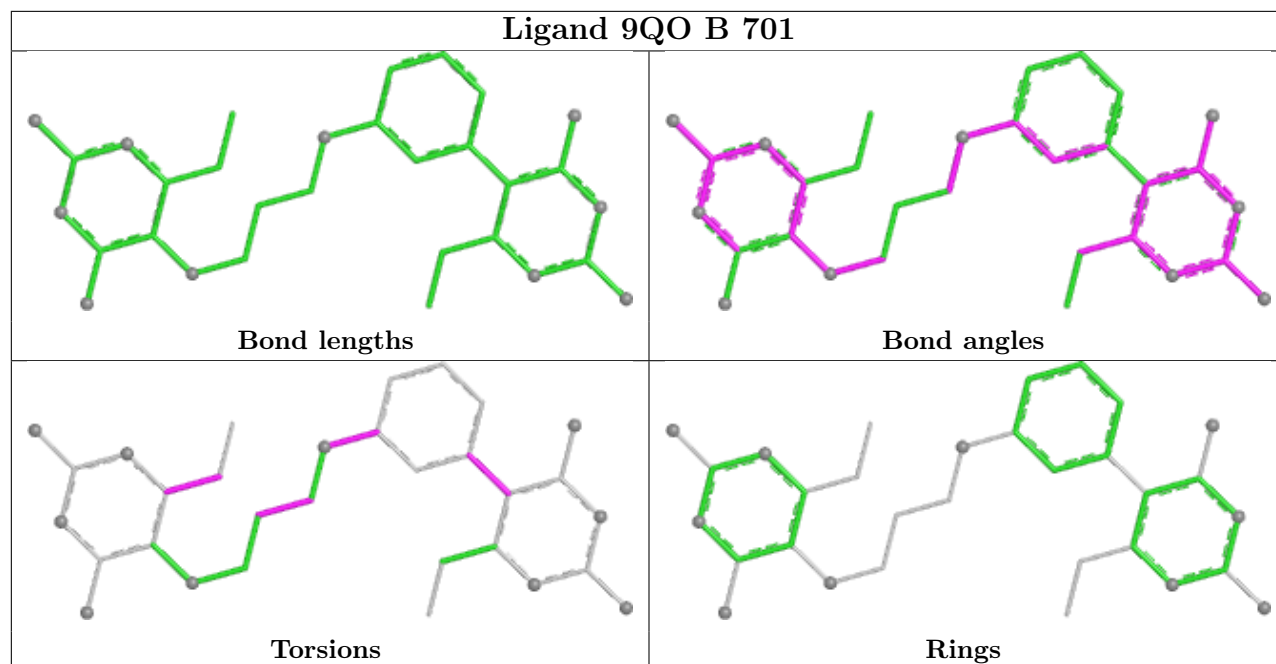
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	NAP	3	0
3	A	702	NAP	7	0

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 than 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

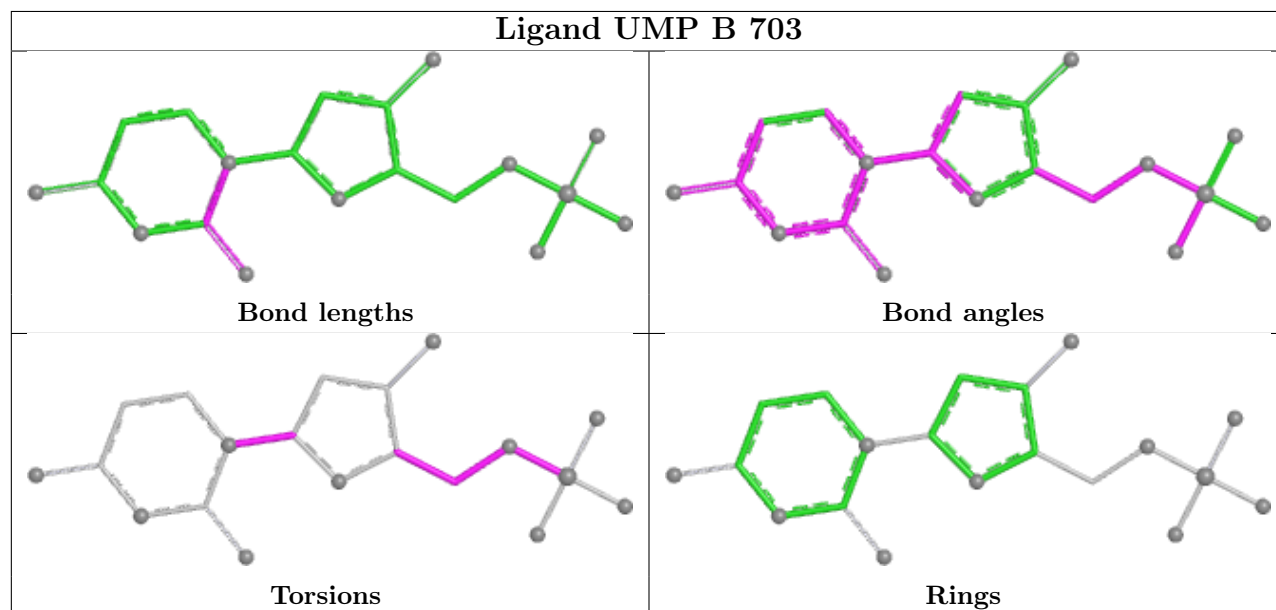
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

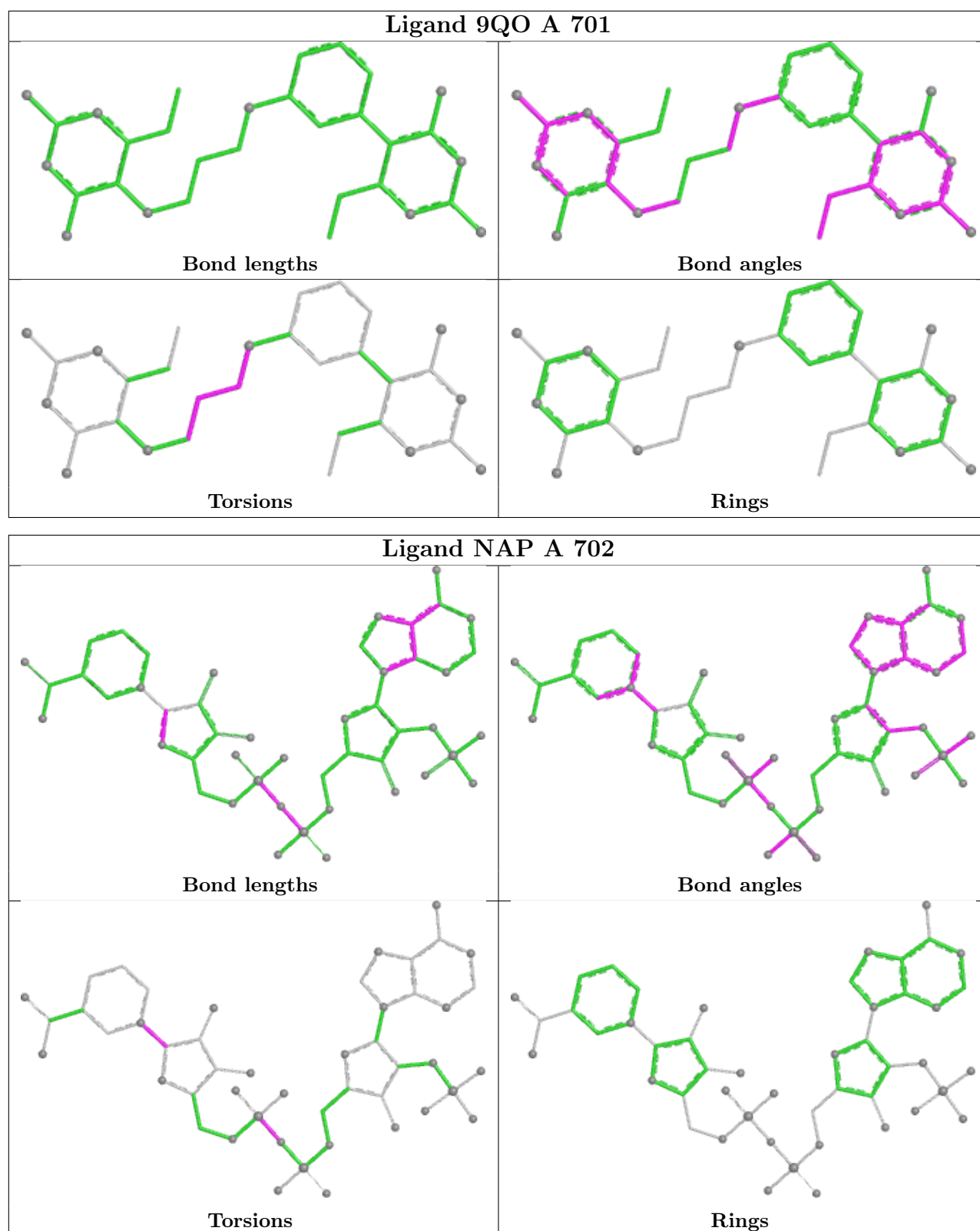


Ligand 9QO B 701



Ligand UMP B 703





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	543/608 (89%)	-0.18	13 (2%) 59 59	28, 39, 100, 120	0
1	B	527/608 (86%)	0.25	47 (8%) 15 14	28, 44, 119, 120	0
All	All	1070/1216 (87%)	0.03	60 (5%) 30 29	28, 41, 118, 120	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	VAL	6.0
1	B	151	VAL	4.9
1	B	178	LEU	4.7
1	B	70	TYR	4.3
1	B	141	TYR	4.3
1	B	309	PRO	4.2
1	B	5	VAL	4.0
1	B	75	TYR	4.0
1	B	81	LEU	3.8
1	A	307	ILE	3.7
1	A	309	PRO	3.7
1	B	8	VAL	3.6
1	B	131	LEU	3.3
1	B	80	TYR	3.3
1	B	149	LEU	3.3
1	A	306	SER	3.0
1	A	608	ALA	3.0
1	B	158	TYR	2.9
1	B	173	PHE	2.9
1	B	307	ILE	2.9
1	B	306	SER	2.8
1	B	344	ASP	2.7
1	A	346	THR	2.7
1	B	83	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	9	PHE	2.6
1	A	96	LYS	2.6
1	B	346	THR	2.6
1	B	98	LEU	2.6
1	B	169	VAL	2.6
1	B	22	SER	2.6
1	B	150	ILE	2.6
1	B	348	VAL	2.6
1	A	27	LYS	2.6
1	B	71	GLU	2.5
1	B	142	ILE	2.5
1	B	73	LEU	2.5
1	B	74	LYS	2.5
1	B	103	VAL	2.5
1	A	606	MET	2.5
1	B	152	LEU	2.4
1	B	144	ASN	2.4
1	A	1	MET	2.4
1	B	163	ILE	2.4
1	A	308	HIS	2.3
1	B	130	THR	2.2
1	B	31	VAL	2.2
1	A	284	ASP	2.2
1	B	96	LYS	2.2
1	B	78	CYS	2.2
1	B	64	TYR	2.1
1	B	177	LYS	2.1
1	B	227	LYS	2.1
1	B	6	CYS	2.1
1	A	302	LYS	2.1
1	B	35	TYR	2.1
1	A	24	ASN	2.1
1	B	99	GLN	2.1
1	B	308	HIS	2.0
1	B	159	TYR	2.0
1	B	146	VAL	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

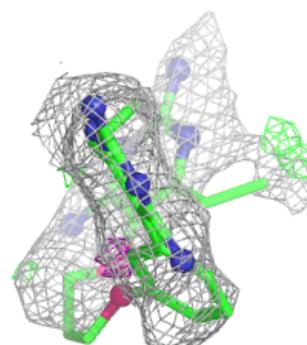
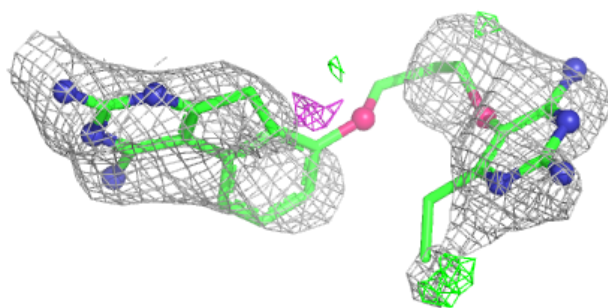
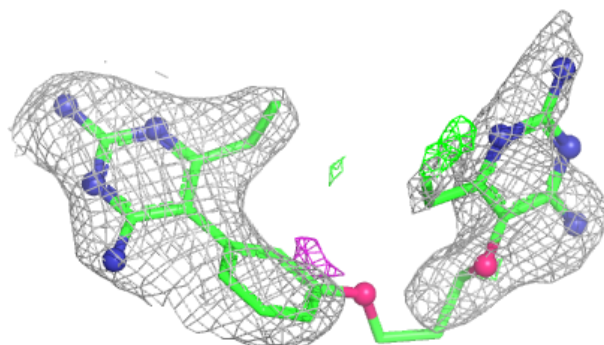
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	9QO	B	701	31/31	0.82	0.16	50,96,116,119	0
3	NAP	B	702	48/48	0.83	0.12	76,98,120,120	0
4	UMP	B	703	20/20	0.87	0.13	55,80,105,108	0
2	9QO	A	701	31/31	0.89	0.13	29,51,93,94	0
4	UMP	A	703	20/20	0.91	0.13	51,78,120,120	0
3	NAP	A	702	48/48	0.97	0.06	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.

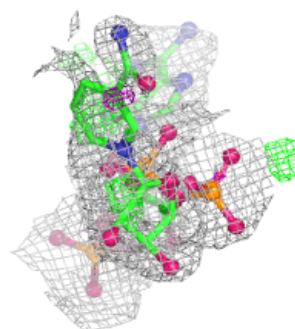
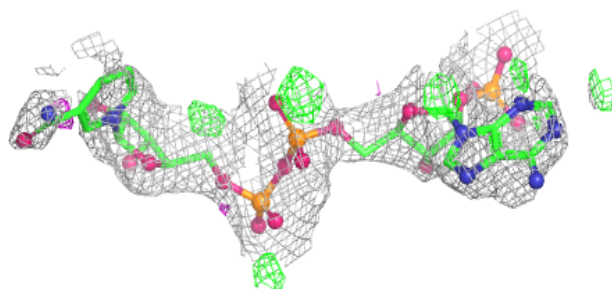
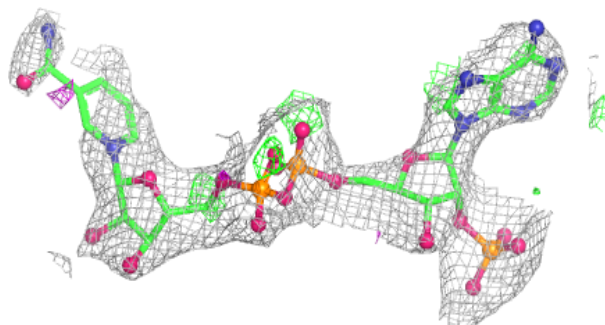
Electron density around 9QO B 701:

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

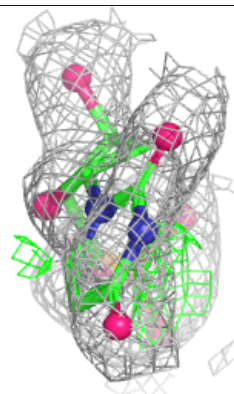
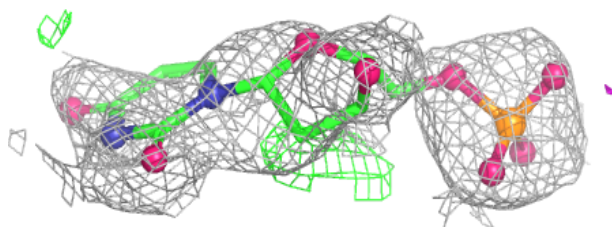
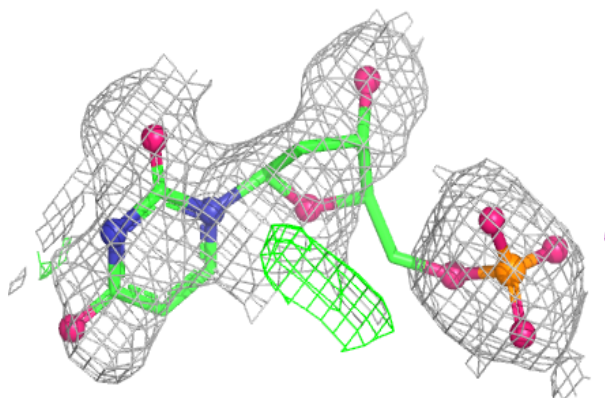


Electron density around NAP B 702:

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

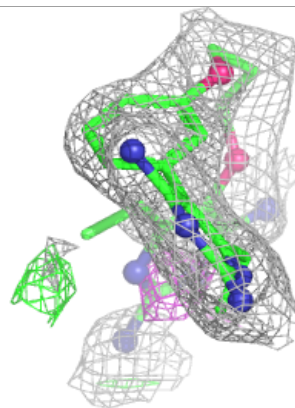
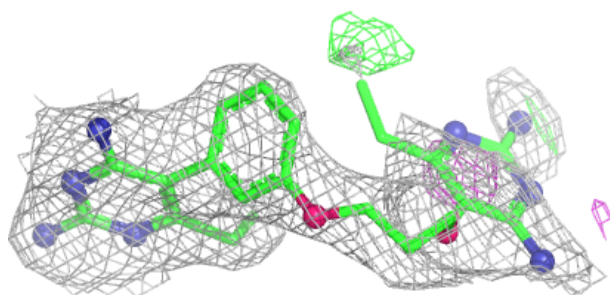
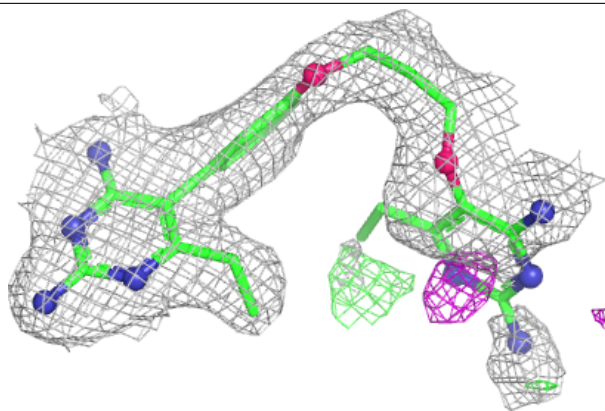
**Electron density around UMP B 703:**

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

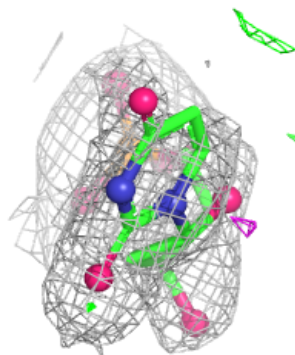
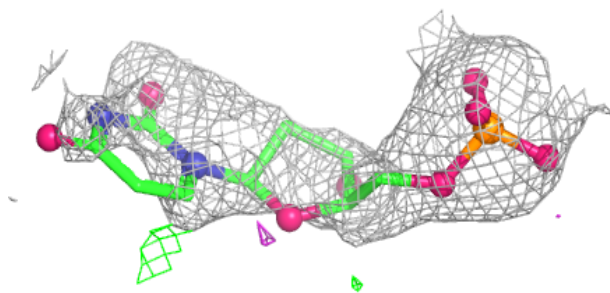
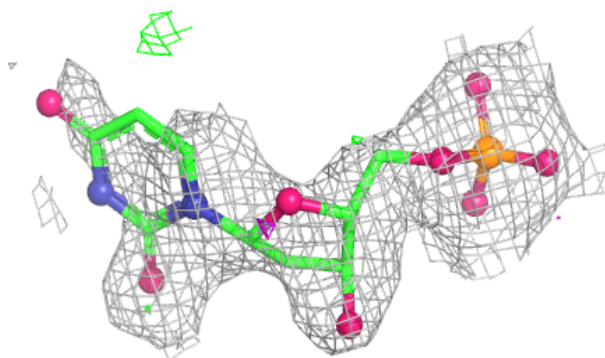


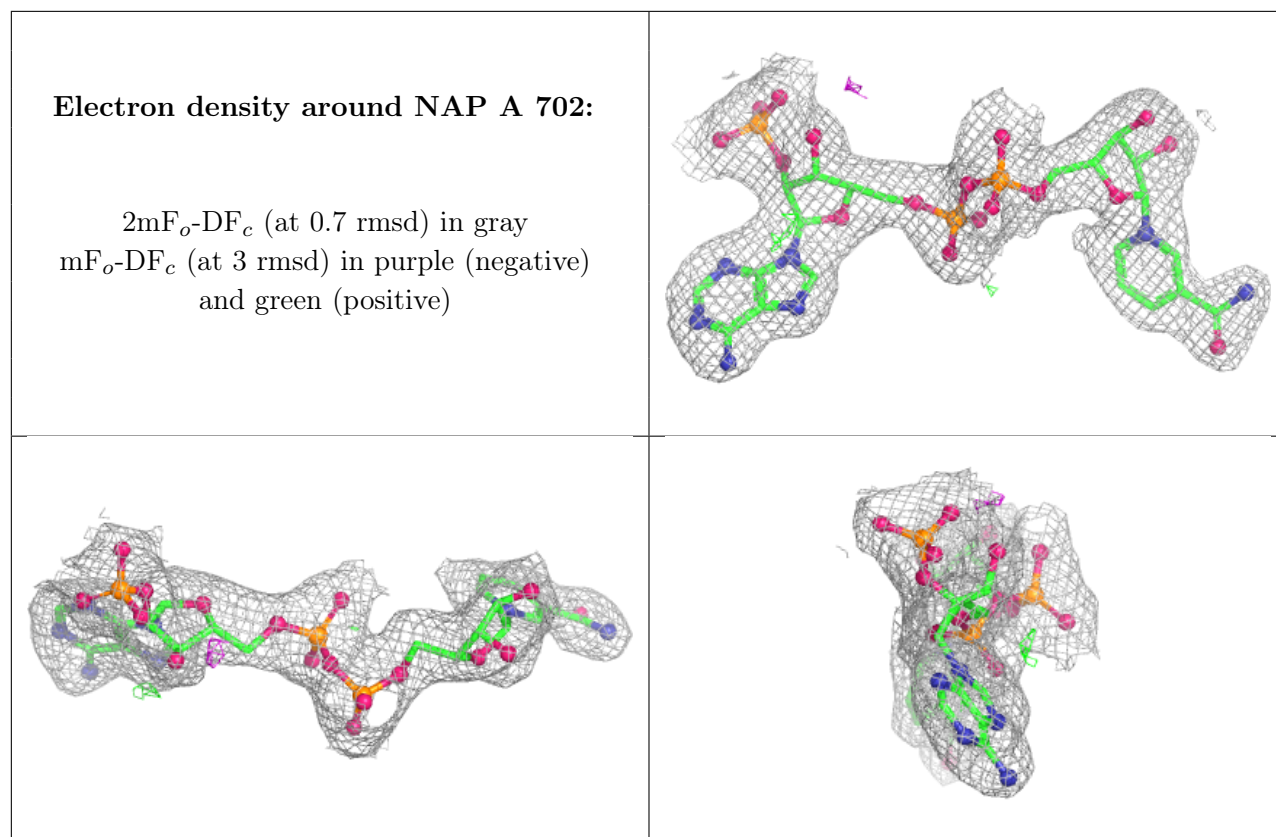
Electron density around 9QO A 701:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.