



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:18 pm BST

PDB ID : 6A2P  
Title : Crystal structure of quadruple mutant (N51I+C59R+S108N+I164L) Plasmodium falciparum DHFR-TS complexed with BT3, NADPH, and dUMP  
Authors : Chitnumsub, P.; Jaruwat, A.; Tarnchampoo, B.; Yuthavong, Y.  
Deposited on : 2018-06-12  
Resolution : 2.60 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](mailto: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 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 : 2.11  
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) : 2.11

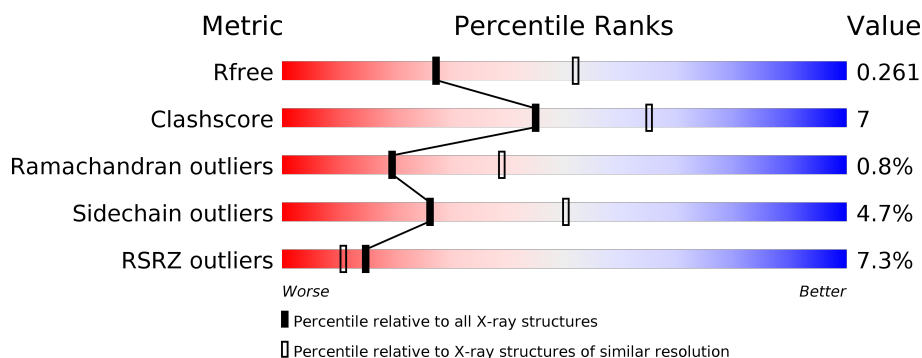
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>10%</div> </div> </div>
1	B	608	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>9%</div> </div> </div>

## 2 Entry composition [i](#)

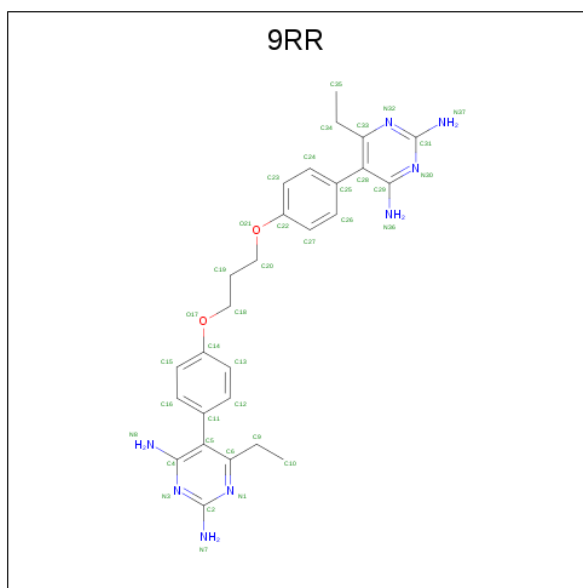
There are 5 unique types of molecules in this entry. The entry contains 9490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

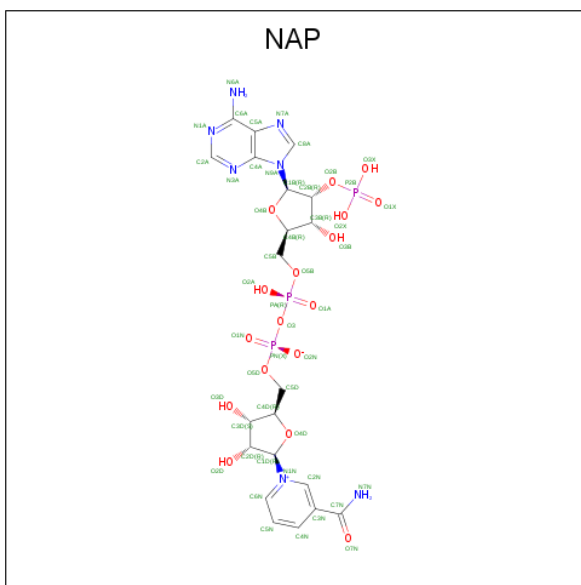
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4550	2937	753	833	27			
1	B	551	Total	C	N	O	S	0	0	0
			4580	2955	759	839	27			

- Molecule 2 is 5,5'-[propane-1,3-diylbis(oxy-4,1-phenylene)]bis(6-ethylpyrimidine-2,4-diamine) (three-letter code: 9RR) (formula: C<sub>27</sub>H<sub>32</sub>N<sub>8</sub>O<sub>2</sub>).



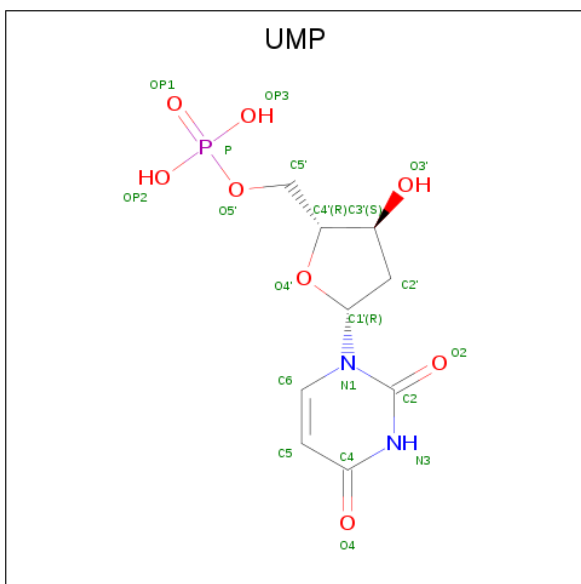
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	27	8	2		
2	B	1	Total	C	N	O	0	0
			37	27	8	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	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:  $\text{C}_9\text{H}_{13}\text{N}_2\text{O}_8\text{P}$ ).



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

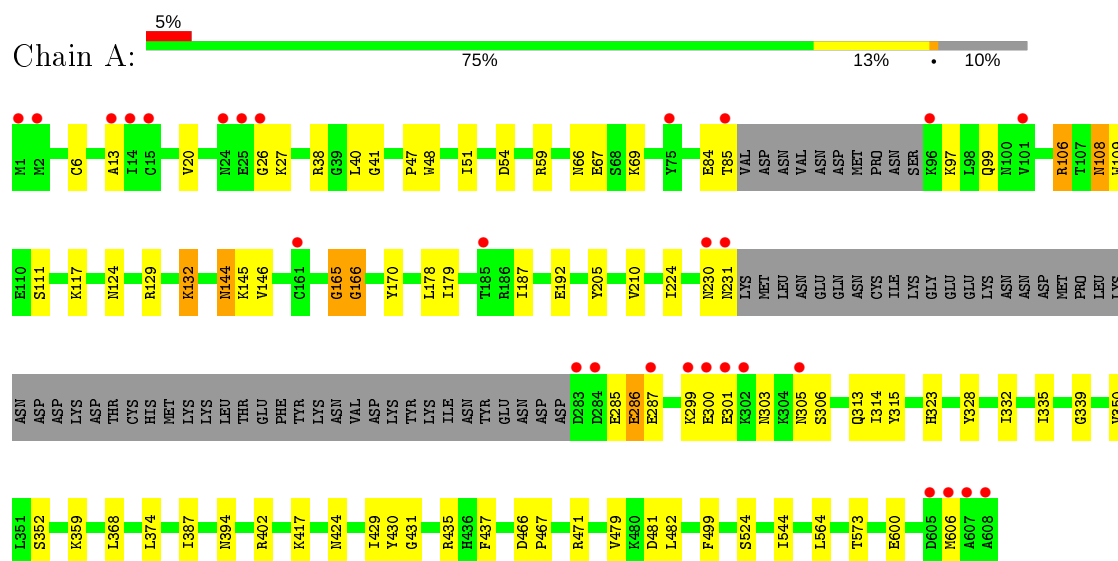
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	100	Total 100	O 100	0	0
5	B	98	Total 98	O 98	0	0

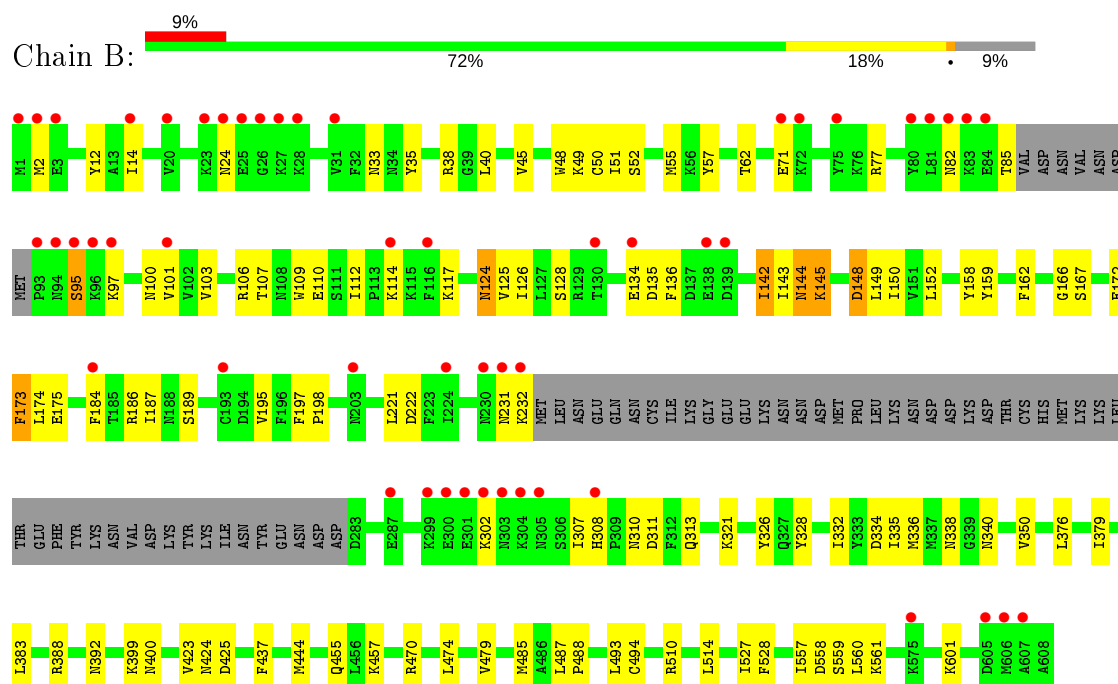
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.24Å 158.90Å 167.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.28 – 2.60 25.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.8 (25.28-2.60) 93.0 (25.27-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.206 , 0.267 0.204 , 0.261	Depositor DCC
$R_{free}$ test set	2304 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9490	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.81	1/4655 (0.0%)	0.93	1/6281 (0.0%)
1	B	0.80	0/4686	0.92	1/6322 (0.0%)
All	All	0.81	1/9341 (0.0%)	0.93	2/12603 (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	5
1	B	0	4
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	GLY	N-CA	-5.39	1.38	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	471	ARG	NE-CZ-NH1	-5.11	117.74	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain
1	A	165	GLY	Peptide
1	A	350	VAL	Peptide
1	A	352	SER	Peptide
1	A	402	ARG	Sidechain
1	B	350	VAL	Peptide
1	B	388	ARG	Sidechain
1	B	510	ARG	Sidechain
1	B	77	ARG	Sidechain

## 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	48	0
1	B	4580	0	4543	70	0
2	A	37	0	0	2	0
2	B	37	0	0	3	0
3	A	48	0	25	12	0
4	A	20	0	11	0	0
4	B	20	0	11	0	0
5	A	100	0	0	5	0
5	B	98	0	0	1	0
All	All	9490	0	9101	120	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 7.

All (120) 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:392:ASN:HA	1:B:444:MET:CE	1.74	1.15
1:B:392:ASN:HA	1:B:444:MET:HE2	1.32	1.06
1:B:425:ASP:HA	1:B:444:MET:HE3	1.49	0.91
1:A:166:GLY:H	3:A:702:NAP:H5N	1.35	0.89
1:B:392:ASN:CA	1:B:444:MET:HE2	2.03	0.89
3:A:702:NAP:O3B	3:A:702:NAP:O1X	1.96	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:LEU:HD22	1:B:379:ILE:HD11	1.64	0.79
1:B:392:ASN:HA	1:B:444:MET:HE1	1.67	0.73
1:A:166:GLY:H	3:A:702:NAP:C5N	2.01	0.73
1:A:166:GLY:N	3:A:702:NAP:H5N	2.07	0.66
1:A:54:ASP:OD2	2:A:701:9RR:N32	2.28	0.66
1:B:493:LEU:HD12	1:B:493:LEU:C	2.16	0.65
1:A:108:ASN:OD1	3:A:702:NAP:C6N	2.45	0.64
1:A:132:LYS:HE3	1:A:132:LYS:HA	1.82	0.62
1:B:106:ARG:NH1	1:B:110:GLU:OE1	2.33	0.61
1:A:129:ARG:HG3	3:A:702:NAP:C2A	2.31	0.61
1:B:392:ASN:CB	1:B:444:MET:HE2	2.31	0.60
1:B:186:ARG:NH2	1:B:222:ASP:OD2	2.17	0.60
1:B:455:GLN:HB3	1:B:474:LEU:HD12	1.82	0.60
1:B:172:GLU:O	1:B:173:PHE:C	2.39	0.60
1:A:303:ASN:HA	5:A:821:HOH:O	2.02	0.59
1:A:99:GLN:NE2	5:A:801:HOH:O	2.15	0.58
1:B:197:PHE:CD1	1:B:198:PRO:HD2	2.39	0.58
1:B:166:GLY:O	1:B:167:SER:C	2.42	0.58
1:A:335:ILE:O	1:A:339:GLY:N	2.37	0.58
1:B:112:ILE:HB	1:B:117:LYS:HE2	1.84	0.58
1:B:392:ASN:CA	1:B:444:MET:CE	2.63	0.58
1:A:315:TYR:HB2	1:A:564:LEU:O	2.03	0.57
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.41	0.55
1:A:179:ILE:O	1:A:205:TYR:OH	2.17	0.55
1:B:485:MET:HE2	1:B:488:PRO:HA	1.89	0.54
2:B:701:9RR:C10	2:B:701:9RR:C12	2.85	0.54
1:B:124:ASN:HD22	1:B:124:ASN:N	2.06	0.54
1:B:487:LEU:H	1:B:487:LEU:HD23	1.71	0.54
1:B:62:THR:O	1:B:100:ASN:ND2	2.37	0.54
1:A:210:VAL:HG12	1:A:323:HIS:HB2	1.90	0.54
2:B:701:9RR:C9	2:B:701:9RR:C12	2.85	0.54
1:B:493:LEU:HD12	1:B:493:LEU:O	2.07	0.54
1:A:40:LEU:O	3:A:702:NAP:H2N	2.08	0.53
1:A:430:TYR:O	1:A:431:GLY:C	2.47	0.53
1:B:336:MET:HE1	1:B:557:ILE:HG23	1.91	0.53
1:A:437:PHE:CD1	1:B:479:VAL:HB	2.45	0.52
1:B:172:GLU:O	1:B:174:LEU:N	2.42	0.52
1:B:335:ILE:HD12	1:B:514:LEU:HD13	1.91	0.52
1:B:35:TYR:CE1	1:B:38:ARG:HD3	2.45	0.51
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.92	0.51
1:B:142:ILE:HG13	1:B:143:ILE:N	2.25	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:LEU:O	1:B:152:LEU:N	2.44	0.51
1:B:57:TYR:HE2	5:B:803:HOH:O	1.93	0.51
1:A:285:GLU:C	1:A:287:GLU:H	2.14	0.51
1:B:143:ILE:HD12	1:B:145:LYS:O	2.11	0.51
1:B:142:ILE:HG13	1:B:143:ILE:O	2.12	0.50
1:B:332:ILE:HD13	1:B:560:LEU:HD22	1.92	0.50
1:A:328:TYR:CZ	1:A:332:ILE:HD11	2.47	0.50
1:B:144:ASN:ND2	1:B:148:ASP:OD2	2.45	0.50
1:B:307:ILE:HG21	1:B:336:MET:HB3	1.94	0.50
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.93	0.49
1:A:600:GLU:HB3	5:A:816:HOH:O	2.11	0.49
1:B:40:LEU:HB2	1:B:195:VAL:O	2.12	0.49
1:A:387:ILE:O	1:A:435:ARG:NH1	2.44	0.49
1:A:230:ASN:OD1	1:A:230:ASN:N	2.45	0.48
1:B:172:GLU:O	1:B:175:GLU:N	2.46	0.48
1:B:487:LEU:N	1:B:487:LEU:HD23	2.28	0.48
1:A:108:ASN:OD1	3:A:702:NAP:H6N	2.13	0.48
1:B:308:HIS:O	1:B:311:ASP:HB2	2.14	0.48
1:B:336:MET:CE	1:B:557:ILE:HG23	2.43	0.48
1:B:100:ASN:OD1	1:B:159:TYR:HB3	2.14	0.48
1:A:20:VAL:CG2	1:A:38:ARG:NH2	2.77	0.48
1:B:437:PHE:CD1	1:B:437:PHE:C	2.87	0.47
1:B:12:TYR:O	1:B:162:PHE:HA	2.15	0.47
1:A:145:LYS:O	1:A:146:VAL:C	2.53	0.46
1:A:479:VAL:HB	1:B:437:PHE:CD1	2.50	0.46
1:B:51:ILE:CD1	1:B:187:ILE:HD12	2.45	0.46
1:B:48:TRP:O	1:B:49:LYS:C	2.54	0.46
1:A:6:CYS:CB	1:A:178:LEU:O	2.64	0.46
1:A:51:ILE:CD1	1:A:187:ILE:HD12	2.46	0.46
1:A:314:ILE:O	1:A:315:TYR:C	2.53	0.46
1:B:33:ASN:OD1	1:B:35:TYR:HB3	2.15	0.45
1:A:144:ASN:C	1:A:144:ASN:HD22	2.19	0.45
1:A:165:GLY:HA3	1:A:170:TYR:CZ	2.52	0.45
1:A:6:CYS:HB3	1:A:178:LEU:O	2.16	0.45
1:B:221:LEU:HD23	1:B:221:LEU:N	2.32	0.45
1:B:376:LEU:CD2	1:B:379:ILE:HD11	2.40	0.45
2:A:701:9RR:C24	3:A:702:NAP:C7N	2.95	0.45
1:B:197:PHE:CD1	1:B:198:PRO:CD	2.99	0.45
1:B:109:TRP:CZ2	1:B:117:LYS:HD3	2.52	0.44
1:B:109:TRP:CH2	1:B:117:LYS:HD3	2.52	0.44
1:A:210:VAL:HG22	1:A:224:ILE:HG22	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ILE:O	1:A:430:TYR:C	2.55	0.44
1:A:466:ASP:N	1:A:467:PRO:CD	2.81	0.44
1:A:306:SER:N	5:A:810:HOH:O	2.51	0.44
1:B:85:THR:HG22	1:B:85:THR:O	2.18	0.44
1:A:106:ARG:HE	3:A:702:NAP:P2B	2.41	0.43
1:A:359:LYS:HG2	1:A:544:ILE:HG12	2.00	0.43
1:B:231:ASN:O	1:B:232:LYS:HB2	2.18	0.43
1:B:383:LEU:HD12	1:B:383:LEU:HA	1.86	0.43
3:A:702:NAP:P2B	3:A:702:NAP:HO3A	2.39	0.43
1:B:101:VAL:HG23	1:B:158:TYR:HB2	2.01	0.43
1:B:35:TYR:CZ	1:B:38:ARG:HD3	2.54	0.43
1:A:368:LEU:HD11	1:A:374:LEU:HB2	2.01	0.42
1:A:66:ASN:ND2	1:A:69:LYS:HE3	2.34	0.42
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.54	0.42
1:A:166:GLY:HA3	3:A:702:NAP:PA	2.60	0.42
1:B:321:LYS:HD2	1:B:326:TYR:CE1	2.54	0.42
1:A:394:ASN:ND2	1:A:424:ASN:OD1	2.52	0.42
1:B:527:ILE:O	1:B:528:PHE:C	2.56	0.42
1:B:399:LYS:O	1:B:400:ASN:HB2	2.20	0.42
1:B:328:TYR:CZ	1:B:332:ILE:HD11	2.55	0.42
1:A:481:ASP:O	1:A:482:LEU:C	2.58	0.41
1:A:306:SER:HB3	5:A:810:HOH:O	2.20	0.41
1:B:125:VAL:CG1	1:B:126:ILE:N	2.84	0.41
1:B:423:VAL:O	1:B:424:ASN:HB2	2.20	0.41
1:B:558:ASP:O	1:B:561:LYS:HB2	2.21	0.41
1:B:114:LYS:HA	1:B:117:LYS:HB2	2.02	0.41
1:B:14:ILE:O	2:B:701:9RR:N36	2.54	0.41
1:A:48:TRP:CD1	1:A:51:ILE:HG13	2.56	0.41
1:B:125:VAL:HG12	1:B:126:ILE:N	2.36	0.41
1:B:103:VAL:O	1:B:103:VAL:HG12	2.21	0.40
1:B:334:ASP:OD1	1:B:338:ASN:ND2	2.54	0.40
1:A:13:ALA:HB2	1:A:179:ILE:HD12	2.02	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	541/608 (89%)	503 (93%)	34 (6%)	4 (1%)	22	43
1	B	545/608 (90%)	493 (90%)	47 (9%)	5 (1%)	17	35
All	All	1086/1216 (89%)	996 (92%)	81 (8%)	9 (1%)	19	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	ASN
1	B	173	PHE
1	A	300	GLU
1	A	305	ASN
1	B	95	SER
1	A	26	GLY
1	A	286	GLU
1	B	82	ASN
1	B	150	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	510/570 (90%)	489 (96%)	21 (4%)	30	56
1	B	514/570 (90%)	487 (95%)	27 (5%)	22	45
All	All	1024/1140 (90%)	976 (95%)	48 (5%)	26	50

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	59	ARG
1	A	67	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	84	GLU
1	A	85	THR
1	A	97	LYS
1	A	108	ASN
1	A	111	SER
1	A	124	ASN
1	A	132	LYS
1	A	144	ASN
1	A	192	GLU
1	A	231	ASN
1	A	286	GLU
1	A	299	LYS
1	A	301	GLU
1	A	313	GLN
1	A	417	LYS
1	A	524	SER
1	A	573	THR
1	A	606	MET
1	B	2	MET
1	B	45	VAL
1	B	50	CYS
1	B	52	SER
1	B	55	MET
1	B	71	GLU
1	B	95	SER
1	B	97	LYS
1	B	107	THR
1	B	124	ASN
1	B	128	SER
1	B	134	GLU
1	B	135	ASP
1	B	136	PHE
1	B	142	ILE
1	B	144	ASN
1	B	145	LYS
1	B	148	ASP
1	B	184	PHE
1	B	189	SER
1	B	302	LYS
1	B	310	ASN
1	B	313	GLN
1	B	457	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	494	CYS
1	B	559	SER
1	B	601	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	144	ASN
1	A	171	GLN
1	A	394	ASN
1	A	424	ASN
1	B	121	ASN
1	B	144	ASN
1	B	394	ASN
1	B	424	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	702	-	18,21,21	1.23	2 (11%)	21,31,31	1.60	5 (23%)
2	9RR	A	701	-	40,40,40	1.55	9 (22%)	55,55,55	2.99	23 (41%)
2	9RR	B	701	-	40,40,40	0.95	3 (7%)	55,55,55	2.51	18 (32%)
3	NAP	A	702	-	45,52,52	2.54	18 (40%)	56,80,80	2.26	18 (32%)
4	UMP	A	703	-	18,21,21	1.16	2 (11%)	21,31,31	1.51	4 (19%)

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	702	-	-	1/7/22/22	0/2/2/2
2	9RR	A	701	-	-	3/20/20/20	0/4/4/4
2	9RR	B	701	-	-	8/20/20/20	0/4/4/4
3	NAP	A	702	-	-	9/31/67/67	0/5/5/5
4	UMP	A	703	-	-	3/7/22/22	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAP	C3N-C7N	7.07	1.61	1.50
3	A	702	NAP	O4D-C1D	6.44	1.50	1.41
3	A	702	NAP	C7N-N7N	4.91	1.42	1.33
3	A	702	NAP	O4B-C1B	4.84	1.47	1.41
3	A	702	NAP	C2N-C3N	3.88	1.45	1.39
2	A	701	9RR	C33-N32	3.70	1.40	1.34
3	A	702	NAP	C4A-N3A	3.67	1.40	1.35
2	A	701	9RR	C5-C4	3.40	1.50	1.43
3	A	702	NAP	P2B-O1X	3.38	1.61	1.50
3	A	702	NAP	O7N-C7N	3.34	1.30	1.24
3	A	702	NAP	C5A-C4A	3.27	1.49	1.40
3	A	702	NAP	C2N-N1N	3.27	1.38	1.35
3	A	702	NAP	PA-O1A	3.10	1.61	1.50
2	A	701	9RR	C5-C6	2.93	1.47	1.40
2	B	701	9RR	C28-C33	2.84	1.47	1.40
2	A	701	9RR	C2-N3	2.75	1.40	1.35
4	B	702	UMP	C2-N3	-2.70	1.32	1.38
2	A	701	9RR	C4-N3	2.63	1.38	1.35
3	A	702	NAP	C8A-N7A	2.56	1.39	1.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	UMP	C4-N3	2.44	1.37	1.33
3	A	702	NAP	O4D-C4D	2.41	1.50	1.45
3	A	702	NAP	C6N-C5N	2.36	1.43	1.38
2	B	701	9RR	C5-C11	-2.27	1.45	1.50
3	A	702	NAP	O3B-C3B	2.26	1.48	1.43
3	A	702	NAP	PN-O1N	2.24	1.58	1.50
3	A	702	NAP	PA-O5B	2.23	1.68	1.59
4	B	702	UMP	P-O5'	-2.20	1.53	1.60
2	A	701	9RR	C27-C26	2.15	1.42	1.38
3	A	702	NAP	C2A-N1A	2.14	1.37	1.33
2	A	701	9RR	C29-N36	2.12	1.39	1.34
2	B	701	9RR	C5-C6	2.11	1.45	1.40
2	A	701	9RR	C12-C13	-2.06	1.35	1.38
2	A	701	9RR	C29-N30	2.01	1.37	1.35
4	A	703	UMP	O4'-C4'	-2.01	1.40	1.45

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	9RR	C9-C6-C5	-9.71	115.82	122.57
2	A	701	9RR	C34-C33-C28	-7.75	117.19	122.57
2	A	701	9RR	C5-C4-N3	-7.62	118.23	122.52
2	B	701	9RR	C31-N32-C33	7.08	122.14	116.24
2	B	701	9RR	C2-N1-C6	6.71	121.84	116.24
2	B	701	9RR	C5-C4-N3	-6.39	118.93	122.52
3	A	702	NAP	C3N-C2N-N1N	6.18	126.47	120.43
2	A	701	9RR	C28-C29-N30	-6.14	119.07	122.52
2	A	701	9RR	C35-C34-C33	-5.91	100.31	114.88
2	B	701	9RR	C28-C33-N32	-4.91	117.56	123.61
2	A	701	9RR	N36-C29-N30	4.81	123.84	117.03
3	A	702	NAP	C6N-N1N-C2N	-4.79	117.61	121.97
2	B	701	9RR	C5-C6-N1	-4.57	117.97	123.61
3	A	702	NAP	C1B-N9A-C4A	-4.38	118.95	126.64
2	A	701	9RR	C31-N30-C29	4.34	121.78	116.99
2	B	701	9RR	C28-C29-N30	-4.31	120.10	122.52
2	B	701	9RR	C24-C25-C28	-4.21	113.81	120.79
3	A	702	NAP	O3X-P2B-O2X	4.08	123.25	107.64
3	A	702	NAP	N3A-C2A-N1A	-4.06	122.33	128.68
3	A	702	NAP	C6N-C5N-C4N	3.99	125.24	119.44
2	A	701	9RR	C31-N32-C33	3.98	119.56	116.24
3	A	702	NAP	PN-O3-PA	-3.97	119.21	132.83
3	A	702	NAP	C3D-C2D-C1D	3.74	106.60	100.98

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	9RR	C31-N30-C29	3.59	120.95	116.99
2	B	701	9RR	C26-C25-C28	3.58	126.74	120.79
3	A	702	NAP	O4B-C4B-C3B	3.51	112.06	105.11
2	B	701	9RR	C2-N3-C4	3.46	120.81	116.99
2	A	701	9RR	C25-C28-C33	-3.45	120.67	123.46
2	A	701	9RR	C28-C33-N32	-3.39	119.43	123.61
3	A	702	NAP	O5D-PN-O1N	-3.36	95.92	109.07
2	B	701	9RR	N8-C4-N3	3.35	121.77	117.03
4	A	703	UMP	OP2-P-O5'	-3.34	97.85	106.73
2	B	701	9RR	C11-C5-C6	-3.29	120.79	123.46
4	A	703	UMP	OP3-P-OP1	3.23	123.34	110.68
4	B	702	UMP	P-O5'-C5'	3.18	127.06	118.30
2	A	701	9RR	C11-C5-C6	-3.08	120.96	123.46
2	A	701	9RR	C34-C33-N32	3.06	123.36	116.66
3	A	702	NAP	O3B-C3B-C2B	3.04	119.79	111.17
2	A	701	9RR	N8-C4-N3	3.01	121.29	117.03
3	A	702	NAP	C2N-C3N-C4N	-2.94	114.92	118.26
3	A	702	NAP	C2A-N1A-C6A	2.94	123.78	118.75
2	A	701	9RR	C27-C22-C23	-2.91	115.69	120.18
4	B	702	UMP	C2'-C1'-N1	2.90	120.96	114.27
2	A	701	9RR	C28-C29-N36	-2.88	116.82	120.86
4	B	702	UMP	OP3-P-OP2	2.88	118.64	107.64
2	A	701	9RR	O17-C18-C19	-2.80	97.93	108.33
3	A	702	NAP	O3X-P2B-O2B	-2.60	94.34	105.99
2	A	701	9RR	C2-N1-C6	2.55	118.37	116.24
2	B	701	9RR	C18-C19-C20	-2.55	105.22	113.70
2	A	701	9RR	C2-N3-C4	2.49	119.74	116.99
3	A	702	NAP	O2A-PA-O1A	2.43	124.26	112.24
2	B	701	9RR	C9-C6-C5	-2.43	120.89	122.57
2	A	701	9RR	C9-C6-N1	2.39	121.90	116.66
4	A	703	UMP	OP3-P-OP2	2.30	116.42	107.64
2	A	701	9RR	C29-C28-C33	2.27	117.78	115.91
3	A	702	NAP	O2N-PN-O1N	2.23	123.25	112.24
3	A	702	NAP	O2B-C2B-C1B	-2.22	102.10	110.10
2	B	701	9RR	C20-O21-C22	2.18	123.64	117.93
4	B	702	UMP	OP2-P-O5'	-2.14	101.05	106.73
3	A	702	NAP	O3X-P2B-O1X	2.14	119.04	110.68
2	A	701	9RR	N37-C31-N32	2.13	120.57	117.25
4	A	703	UMP	O5'-C5'-C4'	-2.12	101.68	108.99
4	B	702	UMP	C4'-O4'-C1'	2.11	114.55	109.45
2	B	701	9RR	C4-C5-C6	2.08	117.63	115.91
2	B	701	9RR	N36-C29-N30	2.07	119.95	117.03

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	9RR	N32-C31-N30	-2.06	122.19	125.42
2	A	701	9RR	C24-C23-C22	2.05	122.23	119.73
2	B	701	9RR	C9-C6-N1	2.04	121.12	116.66

There are no chirality outliers.

All (24) torsion outliers are listed below:

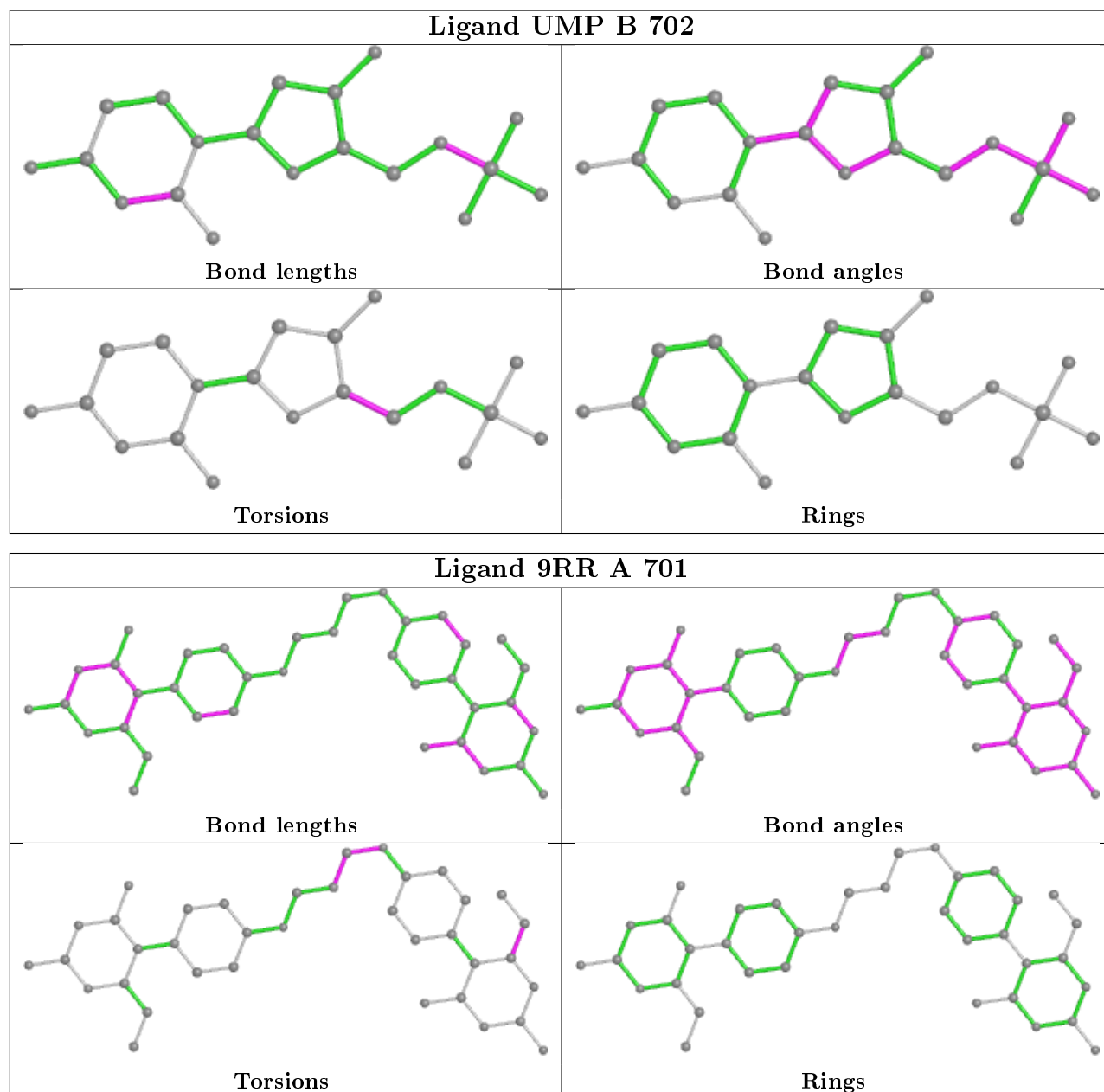
Mol	Chain	Res	Type	Atoms
3	A	702	NAP	C5D-O5D-PN-O3
3	A	702	NAP	C5D-O5D-PN-O1N
4	A	703	UMP	O4'-C1'-N1-C6
3	A	702	NAP	C3B-C2B-O2B-P2B
2	A	701	9RR	C18-C19-C20-O21
2	B	701	9RR	C23-C22-O21-C20
2	B	701	9RR	C27-C22-O21-C20
3	A	702	NAP	C1B-C2B-O2B-P2B
2	B	701	9RR	O17-C18-C19-C20
2	A	701	9RR	C19-C20-O21-C22
2	B	701	9RR	C16-C11-C5-C4
2	B	701	9RR	C16-C11-C5-C6
2	B	701	9RR	C19-C20-O21-C22
2	B	701	9RR	C12-C11-C5-C6
3	A	702	NAP	C5D-O5D-PN-O2N
2	B	701	9RR	C12-C11-C5-C4
3	A	702	NAP	C3D-C4D-C5D-O5D
3	A	702	NAP	O4D-C4D-C5D-O5D
3	A	702	NAP	PA-O3-PN-O2N
4	B	702	UMP	O4'-C4'-C5'-O5'
4	A	703	UMP	C5'-O5'-P-OP3
4	A	703	UMP	O4'-C4'-C5'-O5'
3	A	702	NAP	PN-O3-PA-O2A
2	A	701	9RR	N32-C33-C34-C35

There are no ring outliers.

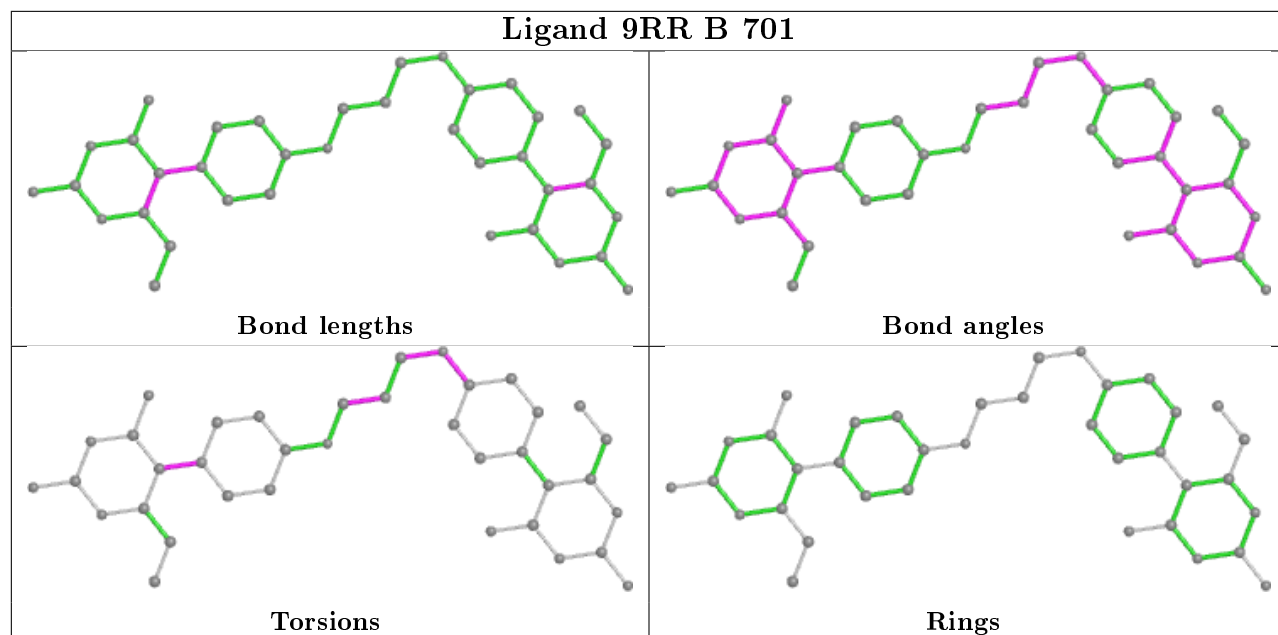
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	9RR	2	0
2	B	701	9RR	3	0
3	A	702	NAP	12	0

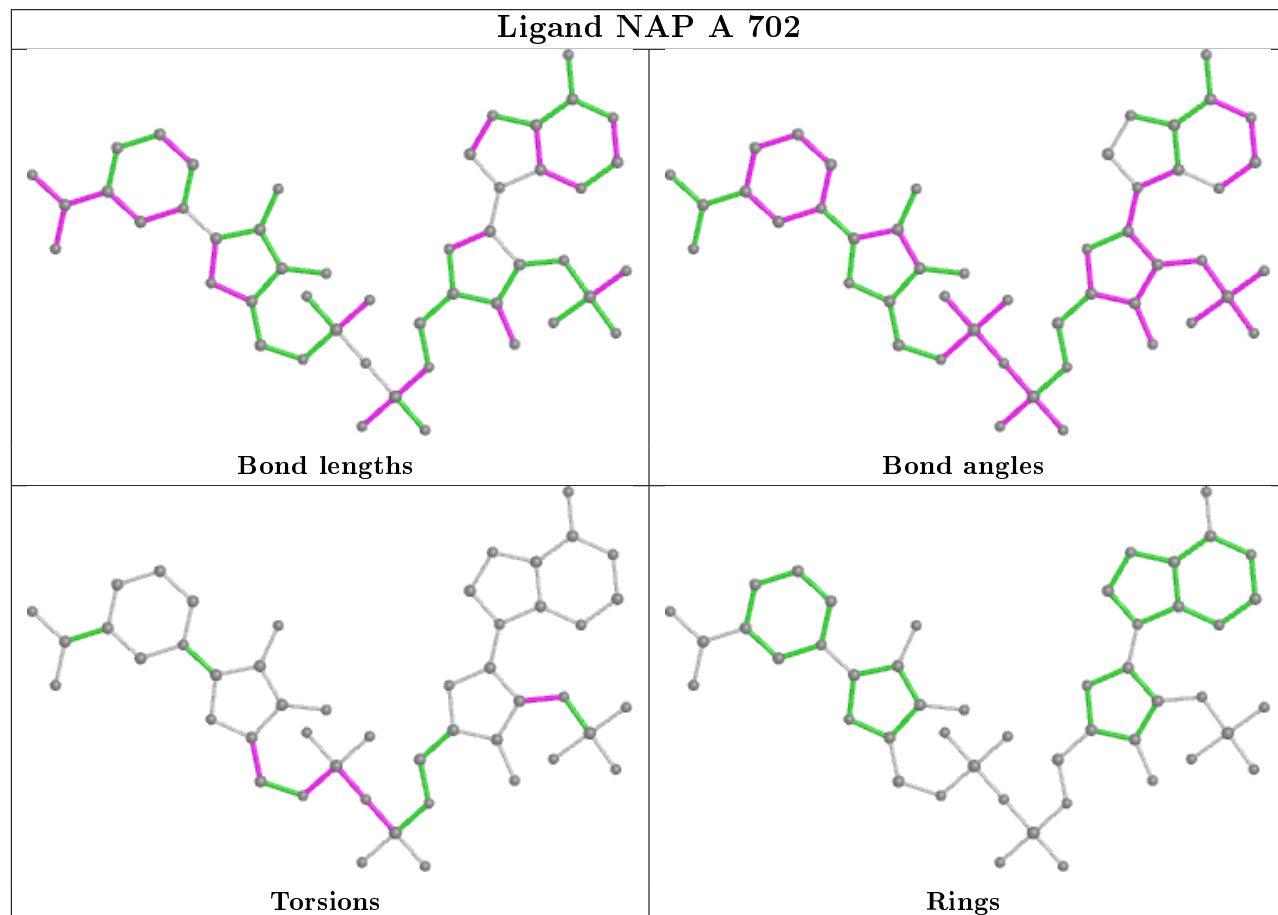
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

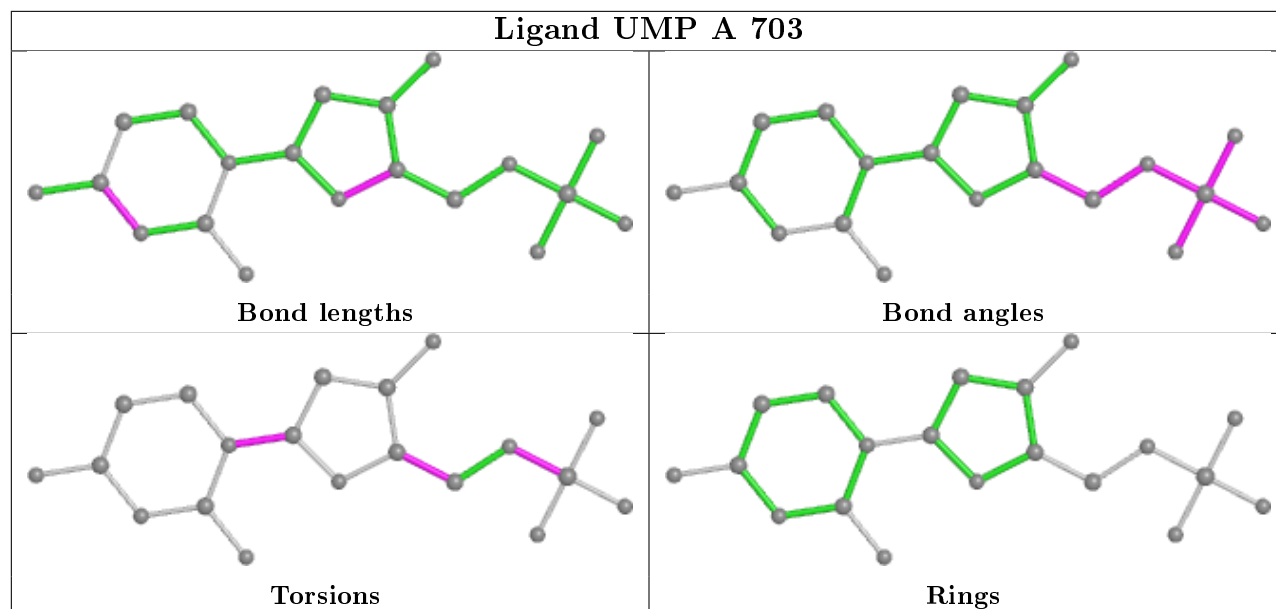


## Ligand 9RR B 701



## Ligand NAP A 702





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	547/608 (89%)	-0.27	28 (5%)	28 22	30, 52, 115, 120	0
1	B	551/608 (90%)	0.03	52 (9%)	8 5	31, 59, 119, 120	0
All	All	1098/1216 (90%)	-0.12	80 (7%)	15 11	30, 54, 118, 120	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	608	ALA	6.5
1	B	2	MET	6.1
1	B	301	GLU	6.0
1	B	93	PRO	5.9
1	B	1	MET	5.8
1	A	1	MET	5.7
1	A	2	MET	5.6
1	A	305	ASN	5.5
1	B	24	ASN	5.4
1	B	26	GLY	5.4
1	B	230	ASN	5.3
1	B	95	SER	5.3
1	B	232	LYS	5.0
1	A	24	ASN	5.0
1	B	231	ASN	4.9
1	B	134	GLU	4.9
1	A	607	ALA	4.5
1	A	231	ASN	4.2
1	B	116	PHE	4.2
1	B	305	ASN	4.2
1	B	607	ALA	4.0
1	A	25	GLU	4.0
1	A	26	GLY	3.9
1	B	302	LYS	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	96	LYS	3.9
1	A	283	ASP	3.9
1	A	75	TYR	3.8
1	A	301	GLU	3.8
1	A	606	MET	3.7
1	B	23	LYS	3.7
1	B	139	ASP	3.7
1	B	94	ASN	3.5
1	B	28	LYS	3.4
1	B	606	MET	3.3
1	B	27	LYS	3.3
1	B	304	LYS	3.3
1	B	83	LYS	3.2
1	B	299	LYS	3.2
1	B	84	GLU	3.1
1	A	230	ASN	2.8
1	B	303	ASN	2.7
1	B	300	GLU	2.7
1	B	3	GLU	2.7
1	B	130	THR	2.7
1	A	161	CYS	2.7
1	B	605	ASP	2.6
1	B	101	VAL	2.6
1	B	287	GLU	2.6
1	B	308	HIS	2.5
1	A	605	ASP	2.5
1	A	284	ASP	2.5
1	A	14	ILE	2.4
1	B	82	ASN	2.4
1	B	81	LEU	2.4
1	B	75	TYR	2.4
1	B	138	GLU	2.4
1	A	299	LYS	2.4
1	B	72	LYS	2.4
1	B	31	VAL	2.4
1	A	302	LYS	2.4
1	B	14	ILE	2.4
1	B	114	LYS	2.3
1	B	203	ASN	2.3
1	A	96	LYS	2.3
1	B	97	LYS	2.3
1	B	575	LYS	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	184	PHE	2.2
1	B	80	TYR	2.2
1	B	193	CYS	2.2
1	A	185	THR	2.1
1	A	300	GLU	2.1
1	A	15	CYS	2.1
1	B	20	VAL	2.1
1	A	101	VAL	2.1
1	A	85	THR	2.1
1	B	71	GLU	2.1
1	A	13	ALA	2.0
1	B	25	GLU	2.0
1	B	224	ILE	2.0
1	A	287	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

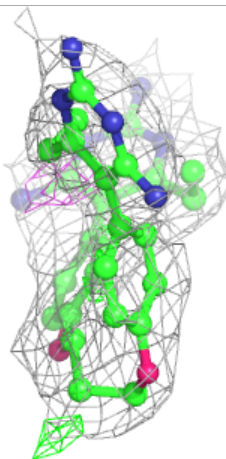
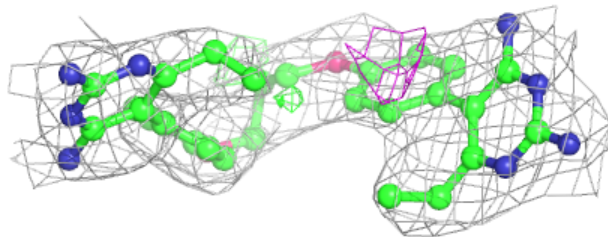
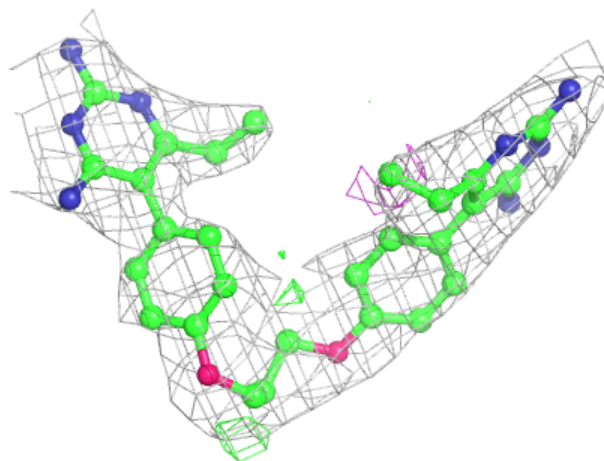
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	9RR	B	701	37/37	0.88	0.18	61,82,100,104	0
2	9RR	A	701	37/37	0.90	0.17	29,48,64,74	0
3	NAP	A	702	48/48	0.92	0.27	44,68,92,107	0
4	UMP	B	702	20/20	0.98	0.10	42,53,69,78	0
4	UMP	A	703	20/20	0.98	0.09	40,47,70,72	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.

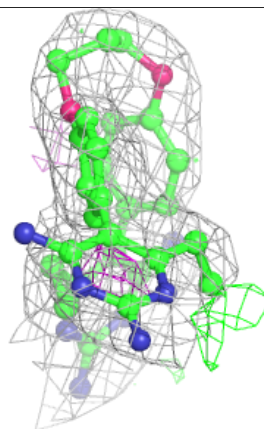
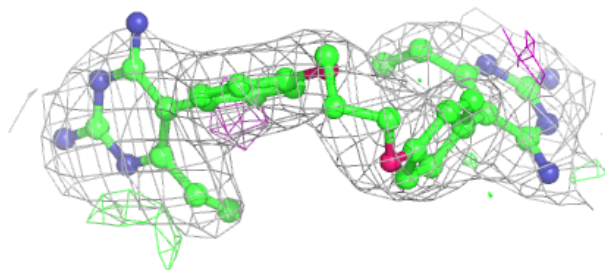
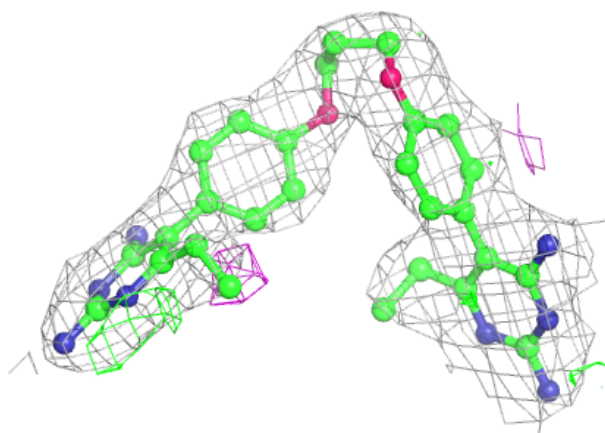
**Electron density around 9RR B 701:**

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

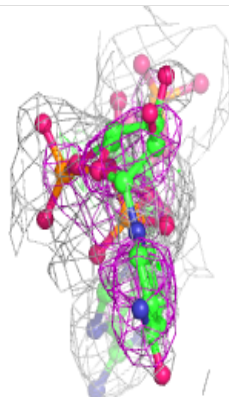
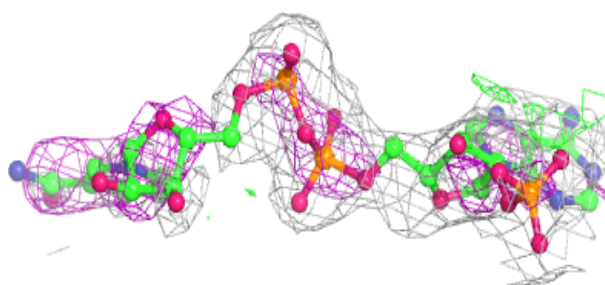
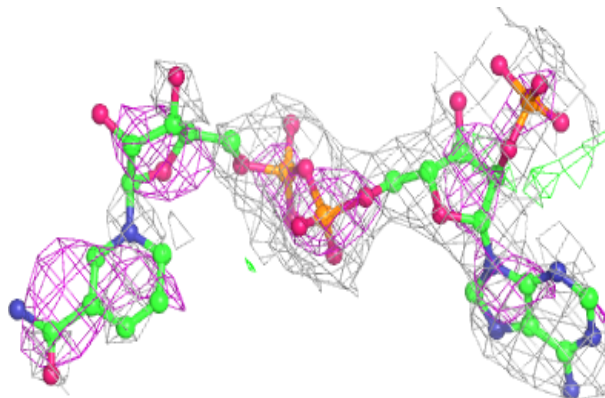


**Electron density around 9RR A 701:**

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

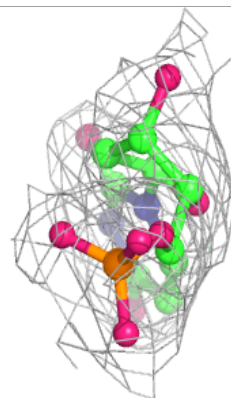
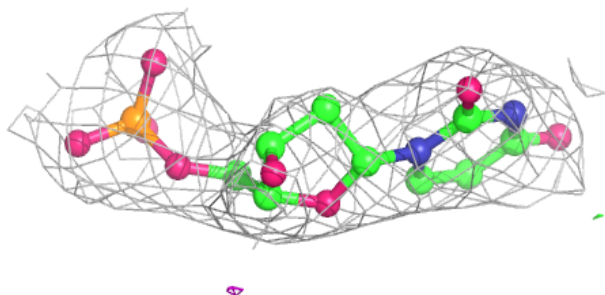
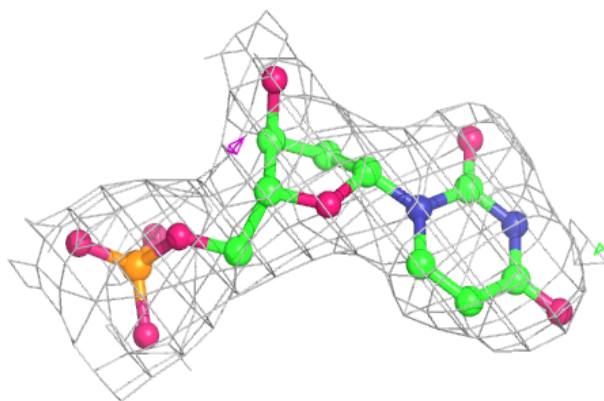
**Electron density around NAP A 702:**

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

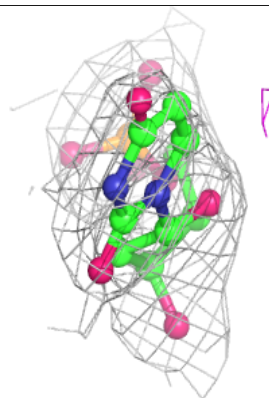
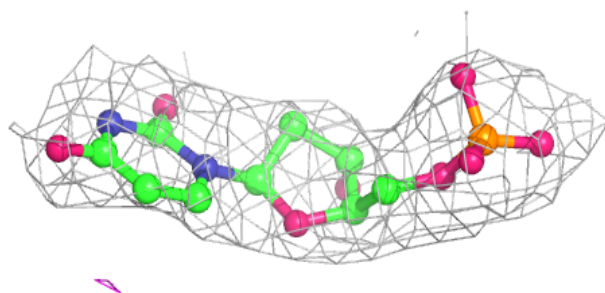
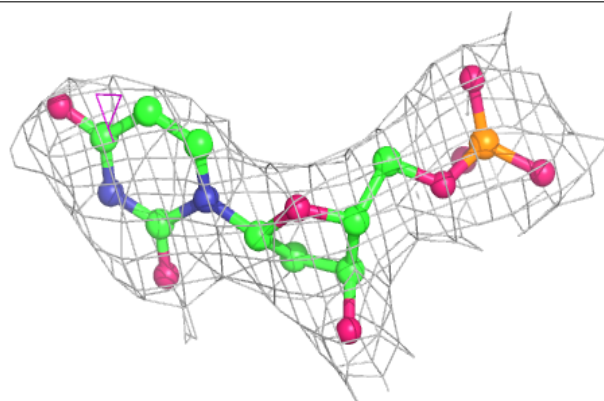


**Electron density around UMP B 702:**

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

**Electron density around UMP 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

There are no such residues in this entry.