



# Full wwPDB X-ray Structure Validation Report

Aug 17, 2023 – 02:08 PM JST

PDB ID : 8JFB  
Title : V1/S quadruple mutant Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with compound 4 (B21588), NADPH and dUMP  
Authors : Vanichtanankul, J.; Saeyang, T.; Vitsupakorn, D.; Saepua, S.; Thongpanchang, C.; Yuthavong, Y.; Kamchonwongpaisan, S.; Hoarau, M.  
Deposited on : 2023-05-17  
Resolution : 2.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

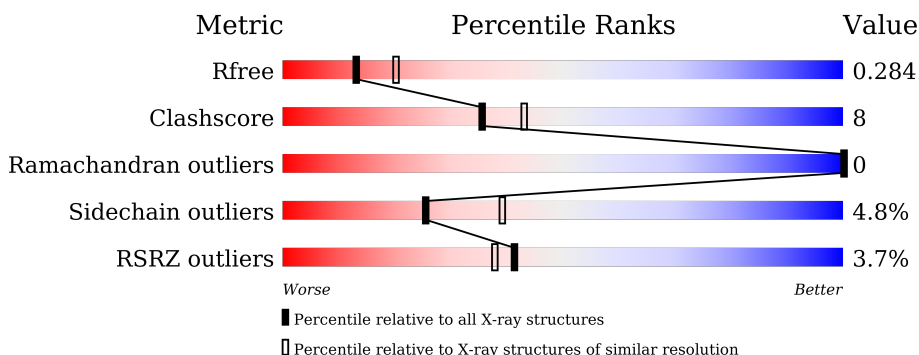
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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  $\geq 3$ , 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	
1	B	608	

## 2 Entry composition [i](#)

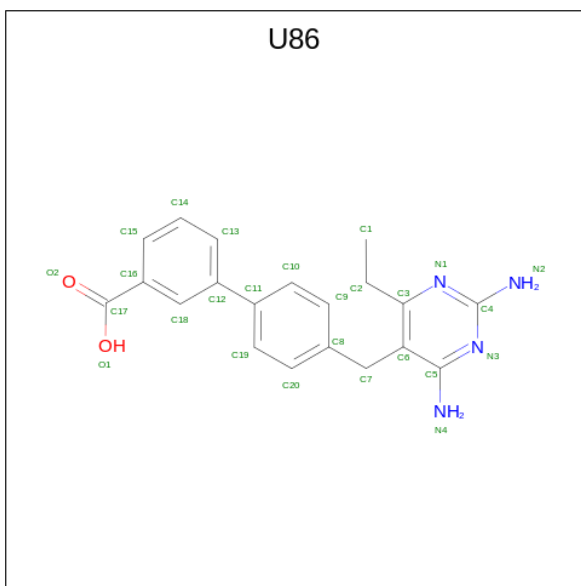
There are 5 unique types of molecules in this entry. The entry contains 9249 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bifunctional dihydrofolate reductase-thymidylate synthase.

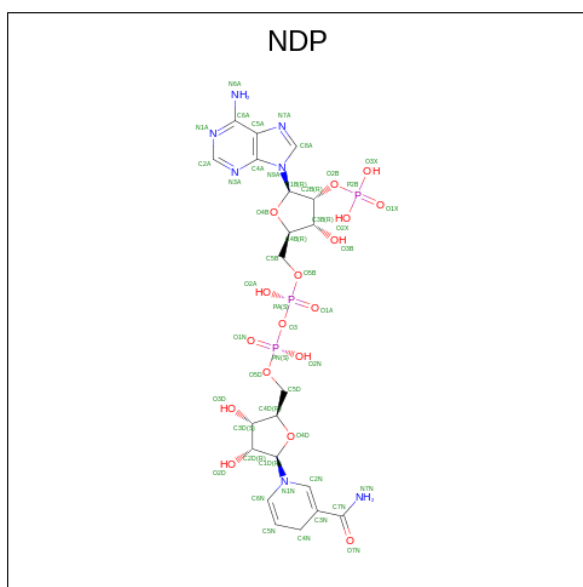
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	530	Total 4416	C 2858	N 728	O 805	S 25	0	0	0
1	B	525	Total 4360	C 2825	N 722	O 789	S 24	0	0	0

- Molecule 2 is 3-[4-[[2,4-bis(azanyl)-6-ethyl-pyrimidin-5-yl]methyl]phenyl]benzoic acid (three-letter code: U86) (formula: C<sub>20</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



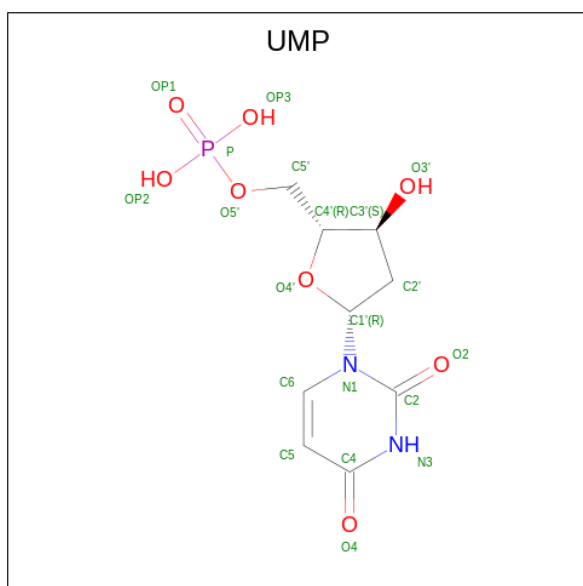
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 26	C 20	N 4	O 2	0	0
2	B	1	Total 26	C 20	N 4	O 2	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

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



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

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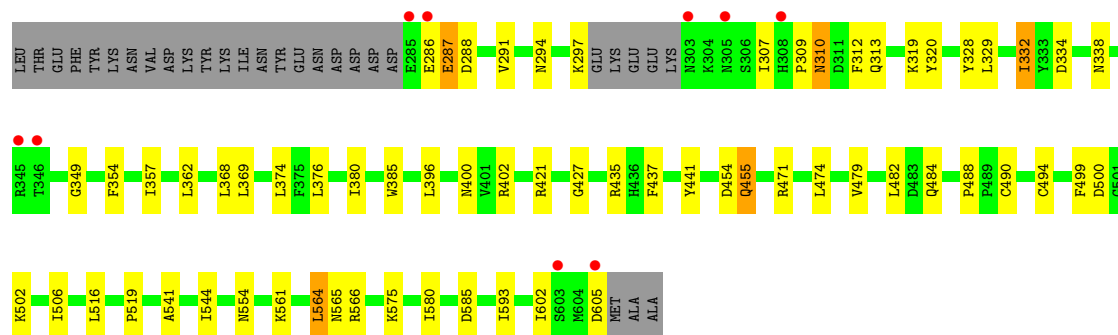
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	20	9	2	8	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	153	Total	O	0	0
			153	153		
5	B	132	Total	O	0	0
			132	132		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.78Å 156.23Å 167.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.32 – 2.65 16.32 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.7 (16.32-2.65) 93.7 (16.32-2.65)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.66Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 5.0	Depositor
R, $R_{free}$	0.211 , 0.280 0.213 , 0.284	Depositor DCC
$R_{free}$ test set	2143 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtrriage
Anisotropy	0.542	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: U86, NDP, 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	0.47	0/4519	0.63	0/6102
1	B	0.45	0/4461	0.60	0/6025
All	All	0.46	0/8980	0.62	0/12127

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	4416	0	4367	68	0
1	B	4360	0	4320	83	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
3	A	48	0	26	5	0
3	B	48	0	26	3	0
4	A	20	0	11	0	0
4	B	20	0	11	1	0
5	A	153	0	0	2	0
5	B	132	0	0	1	0
All	All	9249	0	8761	144	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 8.

All (144) 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:A:119:LEU:H	1:A:124:ASN:HD21	1.22	0.85
1:B:119:LEU:H	1:B:124:ASN:HD21	1.27	0.83
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.73	0.70
1:B:8:VAL:HA	1:B:76:LYS:HD3	1.73	0.69
1:A:12:TYR:HD2	1:A:181:LYS:HB2	1.62	0.65
1:A:7:ASP:O	1:A:76:LYS:NZ	2.25	0.64
1:B:309:PRO:HA	1:B:312:PHE:HD2	1.63	0.63
1:A:106:ARG:NH1	5:A:802:HOH:O	2.31	0.62
1:A:324:PRO:HB2	1:A:571:PHE:HE2	1.64	0.61
1:A:201:ASN:HB3	1:A:204:GLU:HB2	1.83	0.61
1:B:329:LEU:HD22	1:B:564:LEU:HD12	1.82	0.60
1:B:19:LYS:HG2	1:B:36:THR:HG22	1.82	0.60
1:B:119:LEU:H	1:B:124:ASN:ND2	1.99	0.59
1:B:210:VAL:HG12	1:B:224:ILE:HG22	1.87	0.57
1:B:112:ILE:HB	1:B:117:LYS:HD3	1.85	0.57
1:B:294:ASN:HD22	1:B:297:LYS:HG3	1.70	0.57
1:A:153:LEU:HD22	1:A:158:TYR:CZ	2.39	0.57
1:B:312:PHE:HA	1:B:565:ASN:HD21	1.70	0.56
1:A:327:GLN:HB3	1:A:358:MET:HG2	1.86	0.56
1:A:166:GLY:HA3	3:A:702:NDP:O5D	2.05	0.56
1:B:101:VAL:HG22	1:B:123:ILE:HB	1.88	0.56
1:B:209:SER:HB2	1:B:225:ILE:HD12	1.88	0.56
1:A:501:GLY:HA2	1:A:538:LEU:HD22	1.88	0.55
1:A:160:LYS:NZ	1:B:288:ASP:OD2	2.30	0.55
1:B:106:ARG:NH1	3:B:701:NDP:O3X	2.39	0.55
1:B:376:LEU:HD12	1:B:593:ILE:HG13	1.89	0.55
1:A:314:ILE:O	1:A:318:LEU:HD13	2.07	0.54
1:B:400:ASN:ND2	1:B:402:ARG:HH21	2.05	0.54
1:B:500:ASP:HB3	1:B:502:LYS:HE3	1.90	0.54
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.43	0.54
1:B:4:GLN:HB2	1:B:7:ASP:OD2	2.08	0.54
1:A:69:LYS:O	1:A:73:LEU:HG	2.08	0.53
1:A:455:GLN:HB3	1:A:474:LEU:HD12	1.89	0.53
1:A:124:ASN:HB2	1:A:140:VAL:HG22	1.90	0.53
1:B:104:MET:HG2	1:B:164:LEU:HD12	1.90	0.52
1:B:334:ASP:OD1	1:B:338:ASN:ND2	2.34	0.52
1:A:12:TYR:CD2	1:A:181:LYS:HB2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASN:HA	1:B:56:LYS:NZ	2.25	0.52
1:B:70:TYR:CE2	1:B:74:LYS:HB2	2.45	0.52
1:A:127:LEU:O	3:A:702:NDP:H1B	2.11	0.51
1:B:368:LEU:HD11	1:B:374:LEU:HB2	1.93	0.51
1:B:490:CYS:SG	4:B:703:UMP:H5'	2.50	0.51
1:A:485:MET:SD	1:A:489:PRO:HD3	2.50	0.51
1:A:376:LEU:HD23	1:A:593:ILE:HG13	1.92	0.50
1:A:357:ILE:HA	1:A:545:HIS:O	2.11	0.50
1:B:328:TYR:CZ	1:B:332:ILE:HD11	2.46	0.50
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.92	0.50
1:B:70:TYR:CZ	1:B:74:LYS:HB2	2.45	0.50
1:A:315:TYR:HB2	1:A:564:LEU:O	2.12	0.49
1:A:170:TYR:HE2	3:A:702:NDP:H41N	1.78	0.49
1:A:42:ASN:HB2	1:A:193:CYS:HA	1.94	0.48
1:A:112:ILE:HB	1:A:117:LYS:HD3	1.95	0.48
1:A:8:VAL:HG13	1:A:76:LYS:HG2	1.95	0.48
1:A:488:PRO:HG2	1:B:471:ARG:HD3	1.95	0.48
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.94	0.48
1:B:580:ILE:HG23	1:B:585:ASP:HB2	1.95	0.48
1:B:132:LYS:HG2	1:B:134:GLU:O	2.14	0.48
1:B:385:TRP:CE3	1:B:396:LEU:HD11	2.49	0.48
1:A:575:LYS:NZ	1:A:594:GLN:OE1	2.27	0.47
1:B:184:PHE:HB3	1:B:224:ILE:HG13	1.96	0.47
1:B:206:GLN:HE21	1:B:229:THR:HG21	1.79	0.47
1:B:132:LYS:HB3	1:B:132:LYS:HE2	1.63	0.47
1:A:51:ILE:HD13	1:A:187:ILE:HD12	1.96	0.47
1:B:109:TRP:CH2	1:B:117:LYS:HB3	2.49	0.47
1:B:421:ARG:HH11	1:B:421:ARG:HG2	1.80	0.47
1:A:348:VAL:HG11	1:A:555:ASN:OD1	2.14	0.47
1:A:350:VAL:HG12	1:A:553:TYR:HA	1.96	0.47
1:A:383:LEU:HD11	1:A:528:PHE:CD1	2.49	0.46
1:A:479:VAL:HB	1:B:437:PHE:CE1	2.50	0.46
1:B:455:GLN:HB3	1:B:474:LEU:CD1	2.46	0.46
1:A:479:VAL:HB	1:B:437:PHE:CD1	2.50	0.46
1:A:305:ASN:OD1	1:A:341:LYS:HE3	2.15	0.46
1:B:126:ILE:HB	1:B:142:ILE:HD13	1.98	0.46
1:B:312:PHE:CE1	1:B:561:LYS:HG2	2.51	0.46
1:B:310:ASN:N	1:B:310:ASN:OD1	2.47	0.46
1:A:340:ASN:HB3	1:B:499:PHE:CE1	2.51	0.46
1:B:171:GLN:HG2	1:B:198:PRO:HG3	1.98	0.45
1:A:437:PHE:CD1	1:B:479:VAL:HB	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:VAL:HB	1:B:164:LEU:HD11	1.99	0.45
1:B:455:GLN:HB3	1:B:474:LEU:HD12	1.99	0.44
1:B:605:ASP:OD1	1:B:605:ASP:N	2.50	0.44
1:B:309:PRO:HA	1:B:312:PHE:CD2	2.49	0.44
1:A:329:LEU:HD22	1:A:564:LEU:HD12	2.00	0.44
1:B:494:CYS:HA	1:B:506:ILE:O	2.18	0.44
1:B:173:PHE:HB3	1:B:179:ILE:HD11	1.99	0.44
1:A:506:ILE:HG13	1:B:354:PHE:CE2	2.52	0.44
1:B:575:LYS:HA	1:B:575:LYS:HD2	1.78	0.44
1:B:201:ASN:O	1:B:204:GLU:N	2.51	0.44
1:A:459:ILE:HG13	1:A:460:ILE:N	2.33	0.43
1:B:566:ARG:CZ	1:B:602:ILE:HD11	2.48	0.43
1:A:332:ILE:CD1	1:A:514:LEU:HB3	2.48	0.43
1:A:82:ASN:HB2	5:A:874:HOH:O	2.18	0.43
1:A:208:ILE:HD13	1:A:227:LYS:HD2	2.00	0.43
1:A:126:ILE:HD12	1:A:140:VAL:HG11	1.99	0.43
1:A:510:ARG:HG3	1:A:511:SER:N	2.33	0.43
1:B:179:ILE:HB	1:B:205:TYR:OH	2.19	0.43
1:A:502:LYS:HB3	1:A:541:ALA:HB2	2.01	0.43
1:B:208:ILE:HG12	1:B:227:LYS:HB2	2.01	0.43
1:B:484:GLN:HG3	5:B:838:HOH:O	2.18	0.43
1:A:79:LYS:HE3	1:A:79:LYS:HB3	1.84	0.42
1:A:170:TYR:CE2	3:A:702:NDP:H41N	2.54	0.42
1:A:319:LYS:HG3	1:A:320:TYR:CD2	2.54	0.42
1:A:172:GLU:O	1:A:176:LYS:HG3	2.19	0.42
1:B:208:ILE:HG21	1:B:227:LYS:HD2	2.01	0.42
1:B:287:GLU:O	1:B:291:VAL:HG23	2.20	0.42
1:A:173:PHE:HB3	1:A:179:ILE:HD11	2.00	0.42
1:A:292:TYR:O	1:A:295:PHE:HB3	2.19	0.42
1:A:376:LEU:HG	1:A:379:ILE:HD11	2.01	0.42
1:B:113:PRO:HB3	1:B:115:LYS:HZ3	1.85	0.42
1:B:16:ALA:HA	1:B:185:THR:HB	2.02	0.42
1:A:371:THR:HB	1:A:563:GLN:HG3	2.02	0.41
1:A:19:LYS:HG2	1:A:36:THR:HG22	2.03	0.41
1:B:156:LEU:HD23	1:B:156:LEU:HA	1.87	0.41
1:B:362:LEU:N	1:B:541:ALA:O	2.43	0.41
1:B:376:LEU:O	1:B:380:ILE:HG13	2.20	0.41
3:B:701:NDP:H71N	3:B:701:NDP:H2N	1.67	0.41
1:A:16:ALA:HA	1:A:185:THR:HB	2.02	0.41
1:A:383:LEU:HD21	1:A:528:PHE:HB2	2.02	0.41
1:A:103:VAL:HA	1:A:125:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TRP:CE3	1:A:126:ILE:HD11	2.56	0.41
1:A:373:LYS:HE2	1:A:598:HIS:CE1	2.56	0.41
1:B:369:LEU:HD12	1:B:519:PRO:HB3	2.01	0.41
1:A:98:LEU:HD12	1:A:98:LEU:HA	1.88	0.41
1:A:164:LEU:O	3:A:702:NDP:H5N	2.21	0.41
1:B:83:LYS:HE3	1:B:83:LYS:HB2	1.84	0.41
1:B:349:GLY:O	1:B:554:ASN:ND2	2.53	0.41
1:B:385:TRP:CD2	1:B:396:LEU:HD11	2.55	0.41
1:A:448:TYR:O	1:A:451:LYS:HB2	2.21	0.41
1:B:115:LYS:H	1:B:115:LYS:HG2	1.64	0.41
1:B:435:ARG:NE	1:B:454:ASP:OD1	2.49	0.41
1:B:5:VAL:HG11	1:B:150:ILE:HG12	2.03	0.41
1:B:109:TRP:O	1:B:117:LYS:NZ	2.49	0.41
1:B:113:PRO:O	1:B:117:LYS:HG3	2.21	0.41
1:B:427:GLY:HA2	1:B:441:TYR:CE2	2.56	0.41
1:B:593:ILE:HD12	1:B:593:ILE:HG23	1.76	0.41
1:B:319:LYS:HE3	1:B:320:TYR:CE1	2.56	0.41
1:A:133:LYS:HB3	1:A:133:LYS:HE3	1.55	0.40
1:B:127:LEU:HA	1:B:143:ILE:HG13	2.03	0.40
1:B:150:ILE:H	1:B:150:ILE:HD12	1.86	0.40
1:B:482:LEU:HD22	1:B:488:PRO:HB3	2.03	0.40
1:A:325:GLU:HG3	1:A:369:LEU:HD22	2.04	0.40
1:A:369:LEU:HB2	1:A:374:LEU:HD11	2.03	0.40
1:A:121:ASN:O	1:A:122:ARG:HG3	2.21	0.40
1:B:195:VAL:HG21	3:B:701:NDP:H4D	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	520/608 (86%)	492 (95%)	28 (5%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	513/608 (84%)	483 (94%)	30 (6%)	0	100	100
All	All	1033/1216 (85%)	975 (94%)	58 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	496/570 (87%)	473 (95%)	23 (5%)	27	41
1	B	488/570 (86%)	464 (95%)	24 (5%)	25	38
All	All	984/1140 (86%)	937 (95%)	47 (5%)	25	39

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	20	VAL
1	A	21	GLU
1	A	50	CYS
1	A	59	ARG
1	A	68	SER
1	A	104	MET
1	A	111	SER
1	A	133	LYS
1	A	145	LYS
1	A	189	SER
1	A	285	GLU
1	A	297	LYS
1	A	298	GLU
1	A	304	LYS
1	A	307	ILE
1	A	314	ILE
1	A	376	LEU

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Mol	Chain	Res	Type
1	A	410	ARG
1	A	451	LYS
1	A	502	LYS
1	A	573	THR
1	A	581	LYS
1	B	49	LYS
1	B	52	SER
1	B	59	ARG
1	B	65	VAL
1	B	68	SER
1	B	74	LYS
1	B	111	SER
1	B	121	ASN
1	B	133	LYS
1	B	140	VAL
1	B	145	LYS
1	B	177	LYS
1	B	229	THR
1	B	230	ASN
1	B	286	GLU
1	B	287	GLU
1	B	307	ILE
1	B	310	ASN
1	B	313	GLN
1	B	332	ILE
1	B	357	ILE
1	B	455	GLN
1	B	516	LEU
1	B	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	124	ASN
1	A	144	ASN
1	A	171	GLN
1	A	313	GLN
1	A	424	ASN
1	A	450	ASN
1	A	461	ASN
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	206	GLN
1	B	230	ASN
1	B	294	ASN
1	B	313	GLN
1	B	316	ASN
1	B	394	ASN
1	B	400	ASN
1	B	415	ASN
1	B	424	ASN
1	B	554	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$
3	NDP	A	702	-	45,52,52	2.25	6 (13%)	53,80,80	1.58	10 (18%)
3	NDP	B	701	-	45,52,52	2.29	6 (13%)	53,80,80	1.55	10 (18%)
4	UMP	B	703	-	21,21,21	1.00	2 (9%)	31,31,31	1.69	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	U86	A	701	-	27,28,28	0.48	0	34,39,39	0.79	2 (5%)
2	U86	B	702	-	27,28,28	0.51	0	34,39,39	0.67	1 (2%)
4	UMP	A	703	-	21,21,21	0.82	0	31,31,31	1.68	7 (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
3	NDP	A	702	-	-	4/30/77/77	0/5/5/5
3	NDP	B	701	-	-	4/30/77/77	0/5/5/5
4	UMP	B	703	-	-	4/10/22/22	0/2/2/2
2	U86	A	701	-	-	0/14/14/14	0/3/3/3
2	U86	B	702	-	-	0/14/14/14	0/3/3/3
4	UMP	A	703	-	-	6/10/22/22	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NDP	P2B-O2B	12.22	1.82	1.59
3	B	701	NDP	P2B-O2B	12.20	1.82	1.59
3	B	701	NDP	PN-O5D	4.59	1.77	1.59
3	A	702	NDP	PN-O5D	4.20	1.76	1.59
3	A	702	NDP	C4A-N3A	3.22	1.40	1.35
3	B	701	NDP	O2B-C2B	-2.82	1.33	1.44
3	A	702	NDP	C2A-N1A	2.81	1.39	1.33
3	B	701	NDP	C2A-N1A	2.72	1.39	1.33
3	A	702	NDP	O2B-C2B	-2.68	1.34	1.44
3	B	701	NDP	C4A-N3A	2.60	1.39	1.35
3	A	702	NDP	C7N-N7N	2.59	1.40	1.33
3	B	701	NDP	C7N-N7N	2.26	1.39	1.33
4	B	703	UMP	C2-N1	2.07	1.41	1.38
4	B	703	UMP	C5-C4	-2.03	1.39	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NDP	PN-O3-PA	-5.20	114.97	132.83
3	B	701	NDP	PN-O3-PA	-5.11	115.31	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	UMP	C4-N3-C2	-4.36	120.83	126.58
4	B	703	UMP	C4-N3-C2	-4.33	120.86	126.58
4	B	703	UMP	C5-C4-N3	3.80	120.52	114.84
4	A	703	UMP	C5-C4-N3	3.55	120.15	114.84
4	B	703	UMP	O4-C4-C5	-3.51	118.99	125.16
3	B	701	NDP	O2B-P2B-O1X	-3.38	96.35	109.39
3	A	702	NDP	O2B-P2B-O1X	-3.25	96.87	109.39
4	A	703	UMP	N3-C2-N1	3.07	118.97	114.89
4	B	703	UMP	C1'-N1-C2	3.07	123.69	117.64
4	A	703	UMP	C1'-N1-C2	3.03	123.62	117.64
4	B	703	UMP	C1'-N1-C6	-2.96	115.71	121.55
4	A	703	UMP	C1'-N1-C6	-2.82	115.99	121.55
4	A	703	UMP	O2-C2-N3	-2.77	116.35	121.50
3	B	701	NDP	PA-O5B-C5B	-2.66	106.05	121.68
3	B	701	NDP	PN-O5D-C5D	-2.65	106.14	121.68
3	B	701	NDP	C3N-C2N-N1N	-2.64	119.33	123.10
3	A	702	NDP	C3N-C2N-N1N	-2.58	119.41	123.10
3	B	701	NDP	O3X-P2B-O2X	2.50	117.19	107.64
3	B	701	NDP	O5D-PN-O1N	-2.49	99.35	109.07
3	A	702	NDP	O3X-P2B-O2X	2.46	117.03	107.64
3	A	702	NDP	PN-O5D-C5D	-2.44	107.36	121.68
3	B	701	NDP	O2A-PA-O1A	2.38	124.03	112.24
2	A	701	U86	C6-C7-C8	-2.31	108.75	114.06
2	B	702	U86	C6-C3-N1	-2.31	121.54	123.49
4	B	703	UMP	N3-C2-N1	2.30	117.95	114.89
3	A	702	NDP	PA-O5B-C5B	-2.27	108.34	121.68
4	A	703	UMP	O4-C4-C5	-2.25	121.20	125.16
3	A	702	NDP	O5B-C5B-C4B	-2.25	101.26	108.99
2	A	701	U86	C6-C3-N1	-2.18	121.65	123.49
3	B	701	NDP	C2A-N1A-C6A	-2.17	115.03	118.75
3	A	702	NDP	C2B-C3B-C4B	-2.14	97.35	101.99
3	B	701	NDP	O2N-PN-O1N	2.07	122.45	112.24
3	A	702	NDP	O2A-PA-O1A	2.03	122.27	112.24
3	A	702	NDP	O7N-C7N-N7N	-2.01	118.17	122.88

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	NDP	PA-O3-PN-O5D
4	A	703	UMP	C5'-O5'-P-OP1
4	A	703	UMP	C5'-O5'-P-OP2

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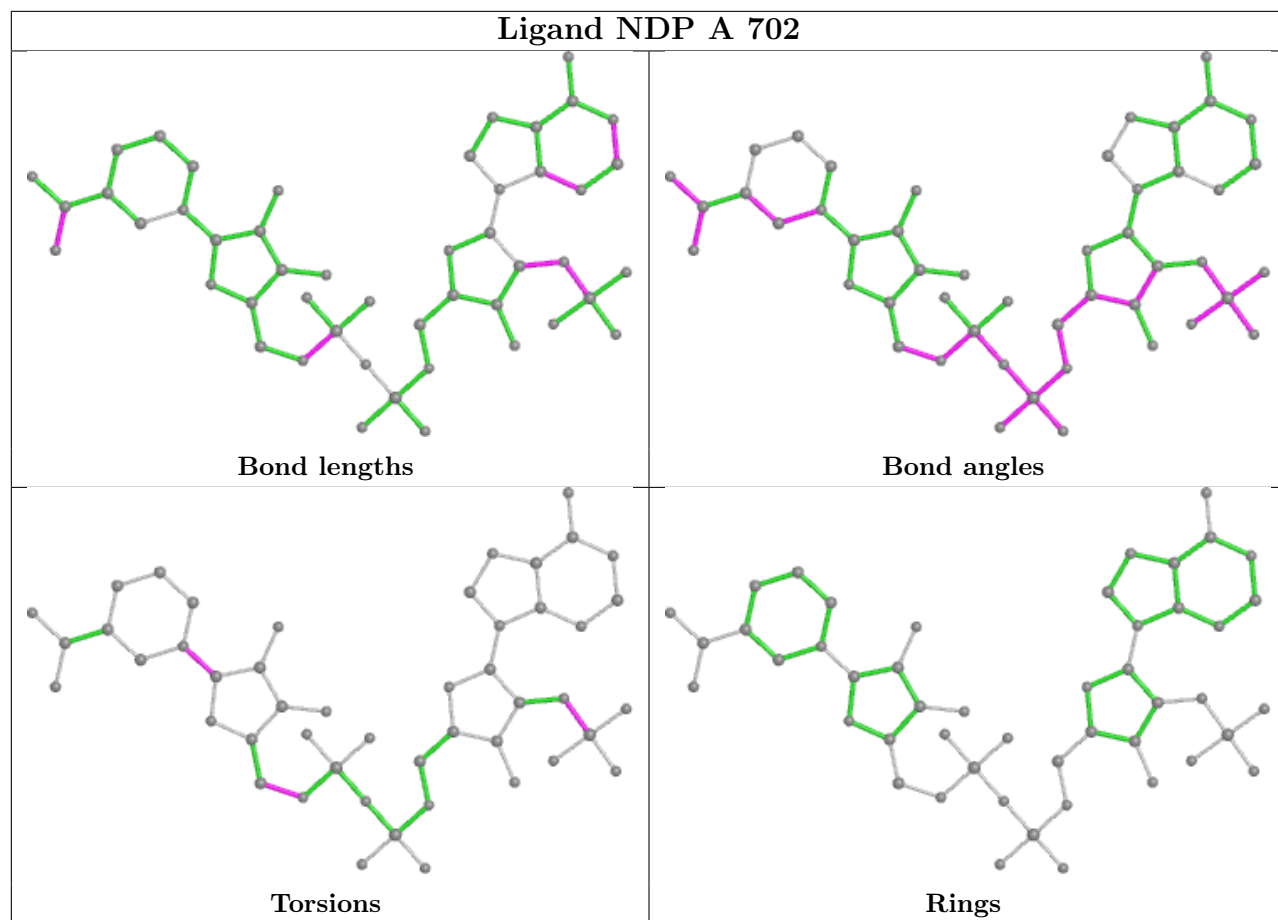
Mol	Chain	Res	Type	Atoms
4	A	703	UMP	C5'-O5'-P-OP3
4	B	703	UMP	C3'-C4'-C5'-O5'
4	B	703	UMP	O4'-C4'-C5'-O5'
4	A	703	UMP	O4'-C4'-C5'-O5'
4	B	703	UMP	C4'-C5'-O5'-P
3	A	702	NDP	O4D-C1D-N1N-C2N
3	B	701	NDP	C4D-C5D-O5D-PN
3	B	701	NDP	O4D-C1D-N1N-C2N
4	A	703	UMP	C2'-C1'-N1-C2
3	B	701	NDP	C2D-C1D-N1N-C2N
3	A	702	NDP	C4D-C5D-O5D-PN
4	A	703	UMP	C2'-C1'-N1-C6
4	B	703	UMP	C5'-O5'-P-OP3
3	A	702	NDP	C2B-O2B-P2B-O3X
3	A	702	NDP	C2D-C1D-N1N-C2N

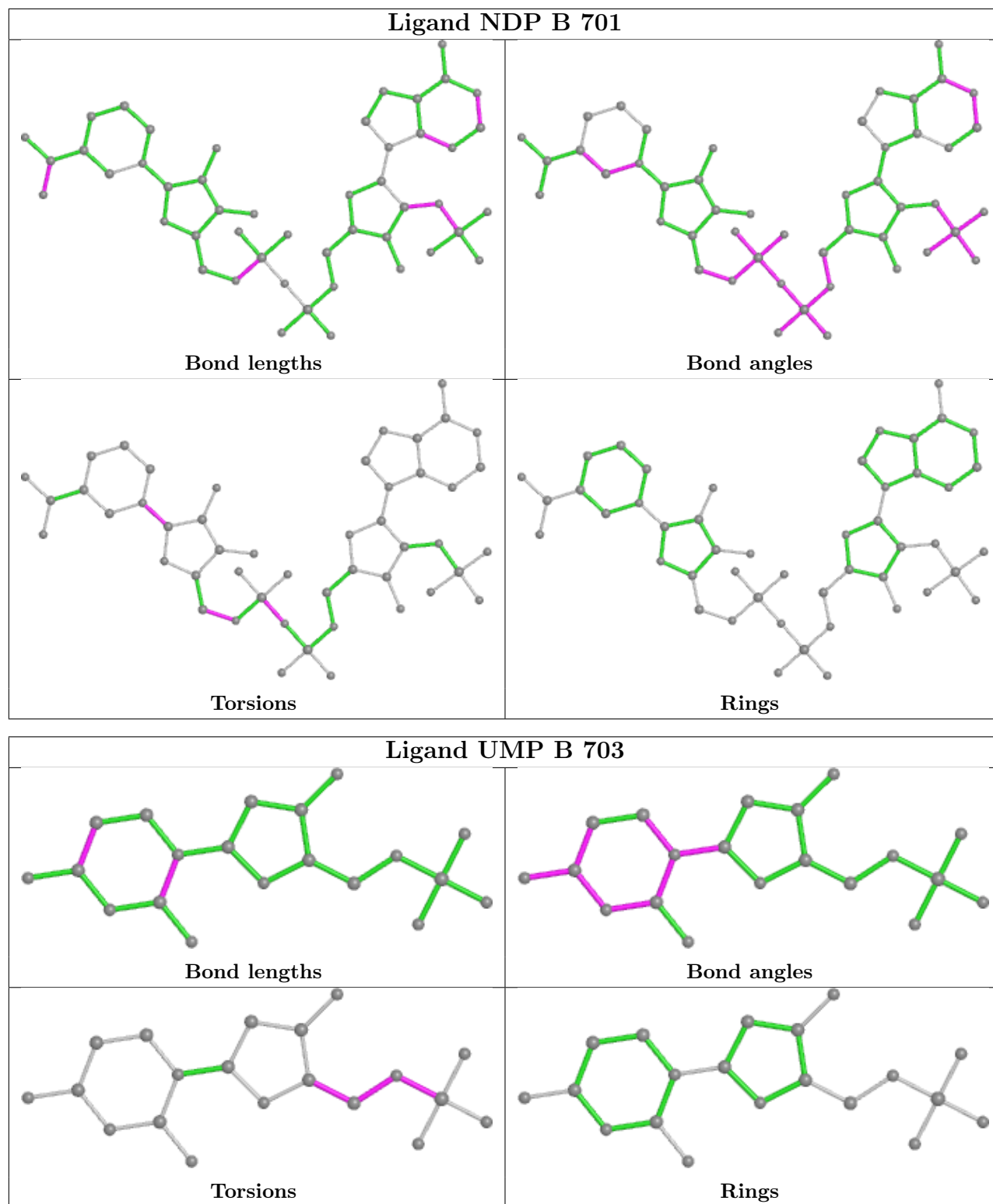
There are no ring outliers.

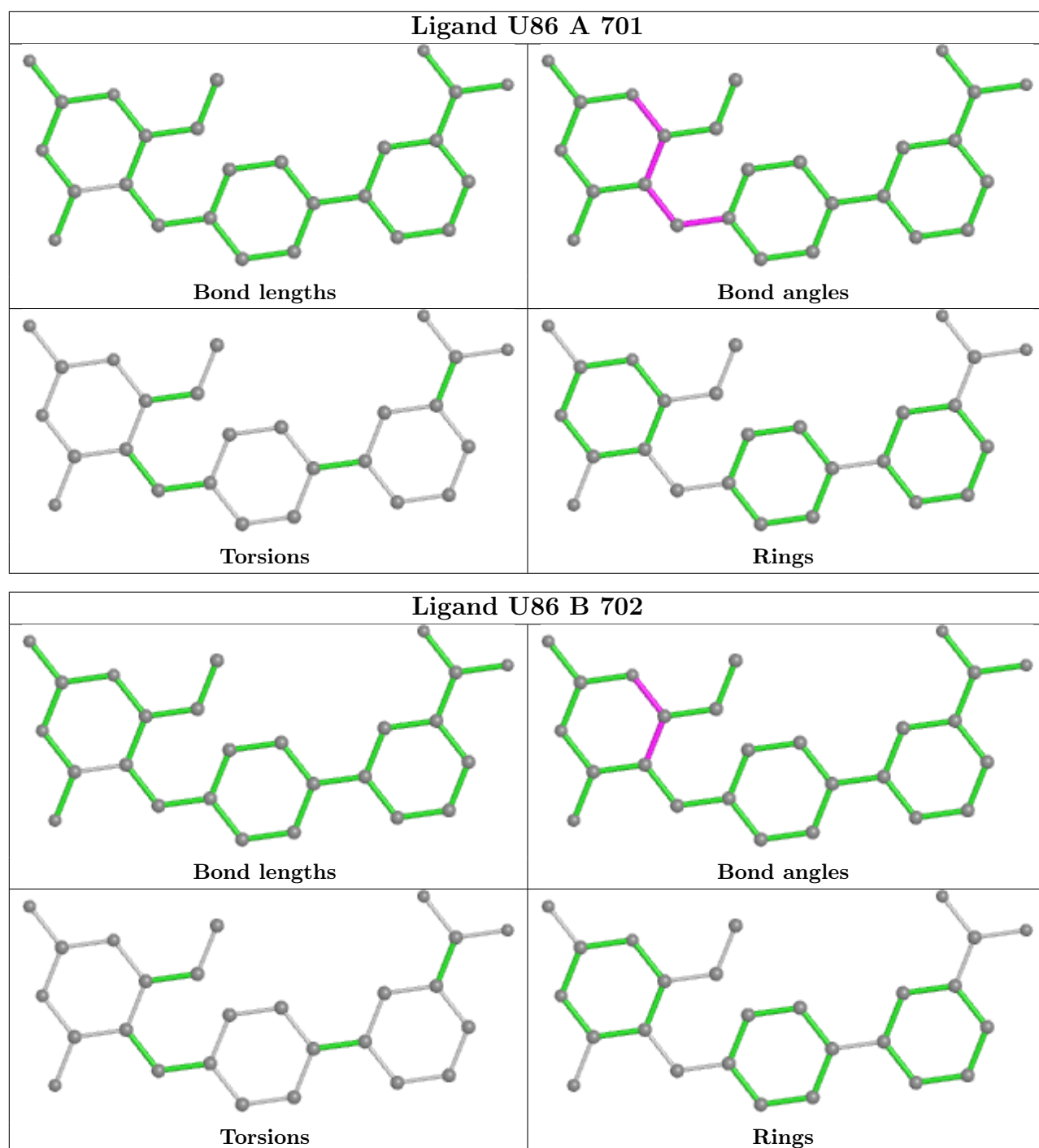
3 monomers are involved in 9 short contacts:

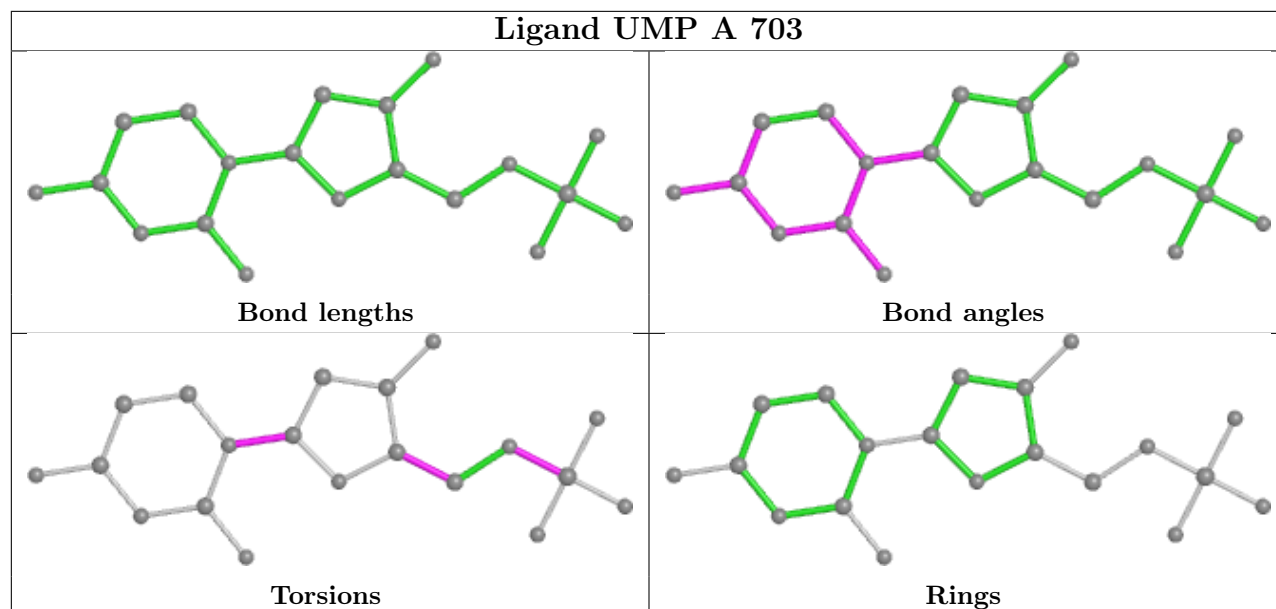
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NDP	5	0
3	B	701	NDP	3	0
4	B	703	UMP	1	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	530/608 (87%)	-0.23	18 (3%) 45 41	17, 32, 64, 92	0
1	B	525/608 (86%)	-0.08	21 (4%) 38 34	17, 35, 71, 104	0
All	All	1055/1216 (86%)	-0.16	39 (3%) 41 38	17, 33, 68, 104	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	GLU	6.1
1	A	2	MET	4.7
1	B	22	SER	4.0
1	A	284	ASP	3.8
1	B	230	ASN	3.8
1	B	286	GLU	3.6
1	B	346	THR	3.4
1	A	75	TYR	3.4
1	B	605	ASP	3.3
1	A	298	GLU	3.2
1	A	230	ASN	3.1
1	A	29	ASN	3.1
1	B	3	GLU	2.9
1	A	309	PRO	2.9
1	B	97	LYS	2.8
1	B	345	ARG	2.8
1	A	22	SER	2.6
1	B	29	ASN	2.6
1	A	21	GLU	2.5
1	A	306	SER	2.4
1	A	96	LYS	2.3
1	B	82	ASN	2.3
1	A	347	GLY	2.3
1	B	303	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	132	LYS	2.2
1	B	603	SER	2.2
1	A	283	ASP	2.2
1	B	202	GLU	2.2
1	A	49	LYS	2.2
1	A	30	GLU	2.1
1	A	308	HIS	2.1
1	A	4	GLN	2.1
1	B	35	TYR	2.1
1	A	296	ASN	2.1
1	B	85	THR	2.1
1	B	308	HIS	2.0
1	B	305	ASN	2.0
1	B	285	GLU	2.0
1	B	49	LYS	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.

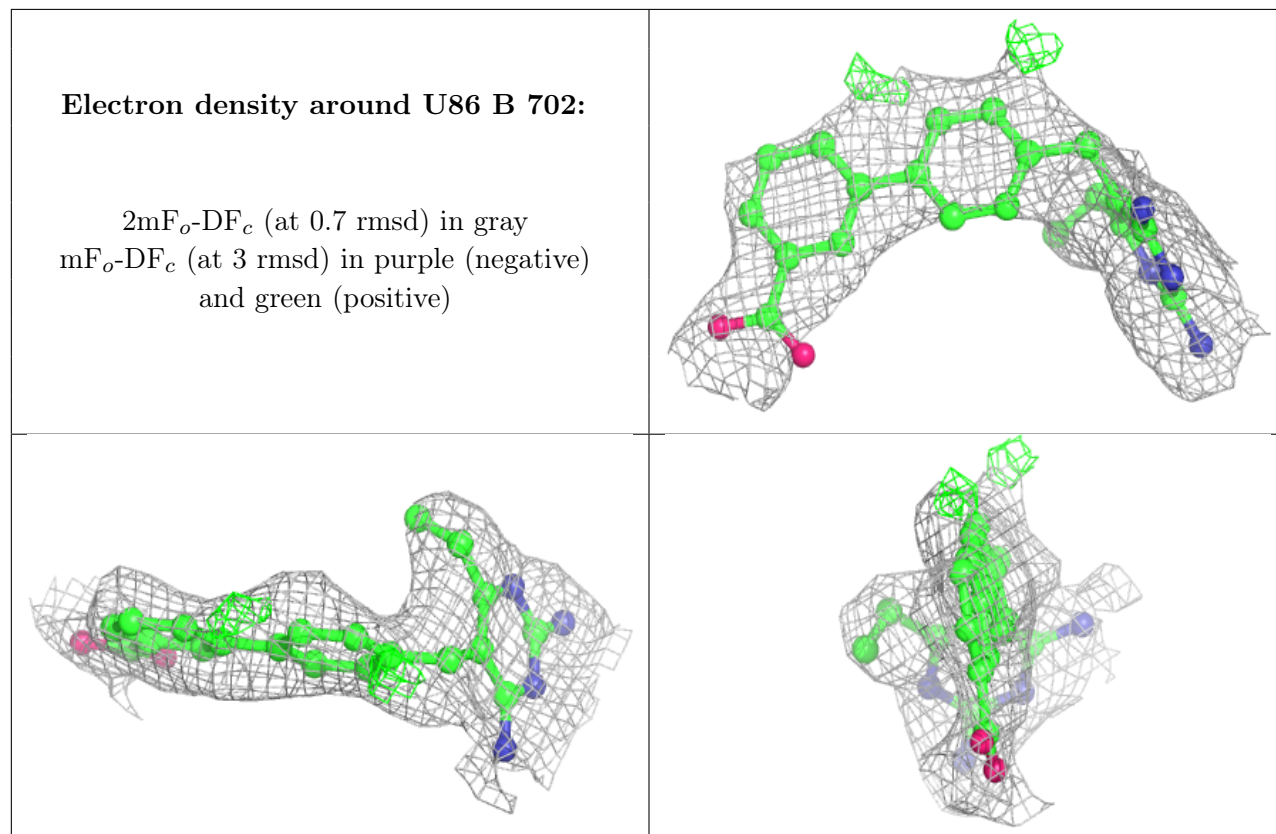
## 6.4 Ligands [i](#)

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<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(Å <sup>2</sup> )	Q<0.9
2	U86	B	702	26/26	0.85	0.21	40,54,69,73	0
3	NDP	B	701	48/48	0.90	0.23	50,69,77,78	0
3	NDP	A	702	48/48	0.93	0.17	29,46,54,56	0
4	UMP	B	703	20/20	0.93	0.24	35,41,48,51	0
4	UMP	A	703	20/20	0.94	0.25	38,45,48,52	0
2	U86	A	701	26/26	0.96	0.14	26,31,39,47	0

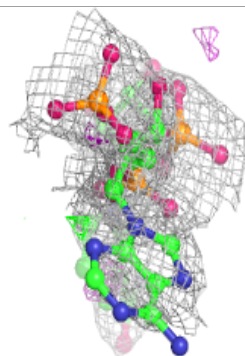
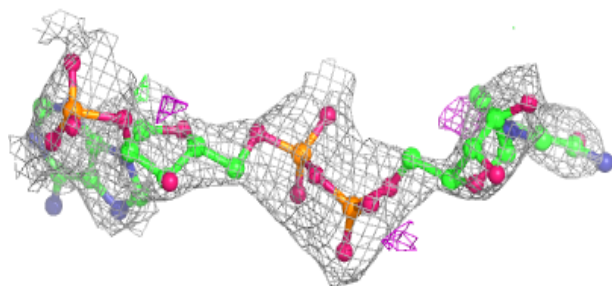
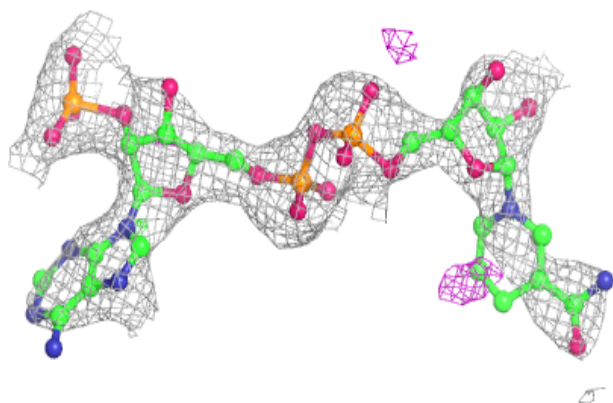
The following is a graphical depiction of the model fit to experimental electron density of all

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.

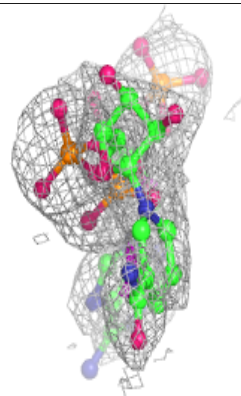
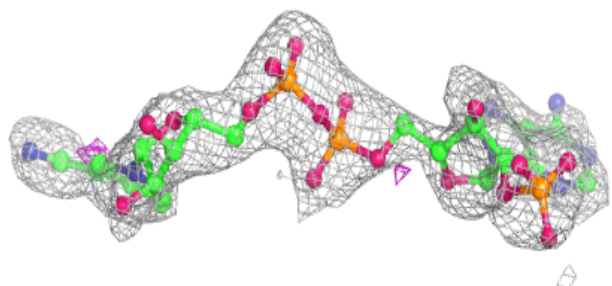
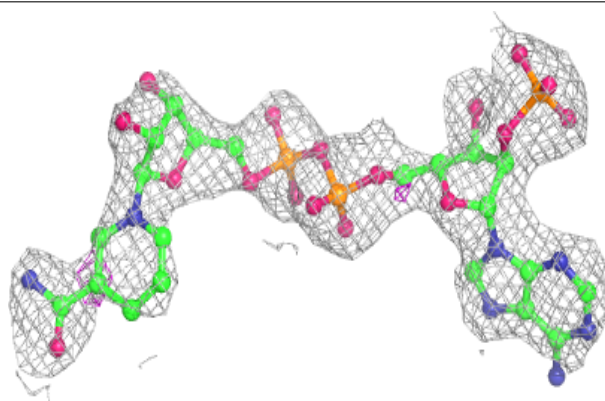


**Electron density around NDP B 701:**

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

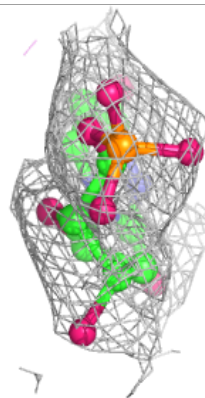
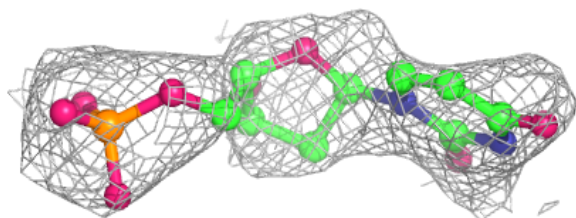
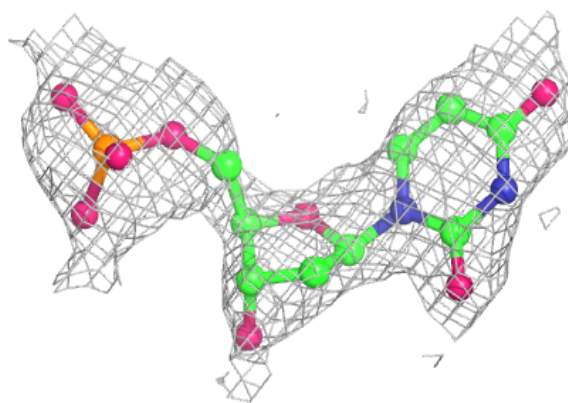
**Electron density around NDP A 702:**

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

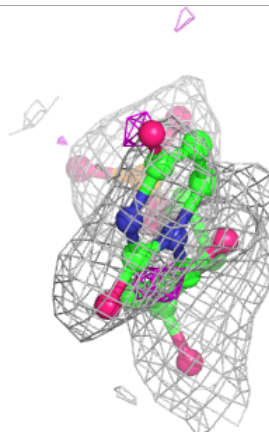
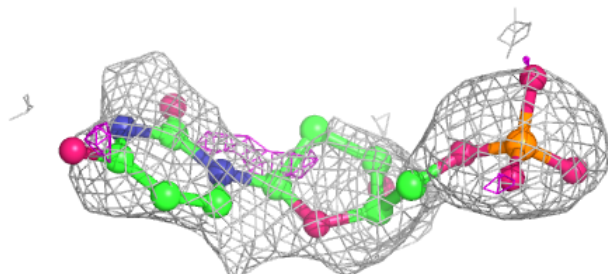
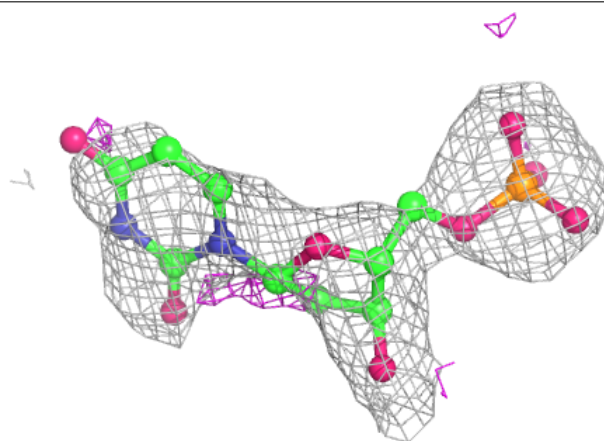


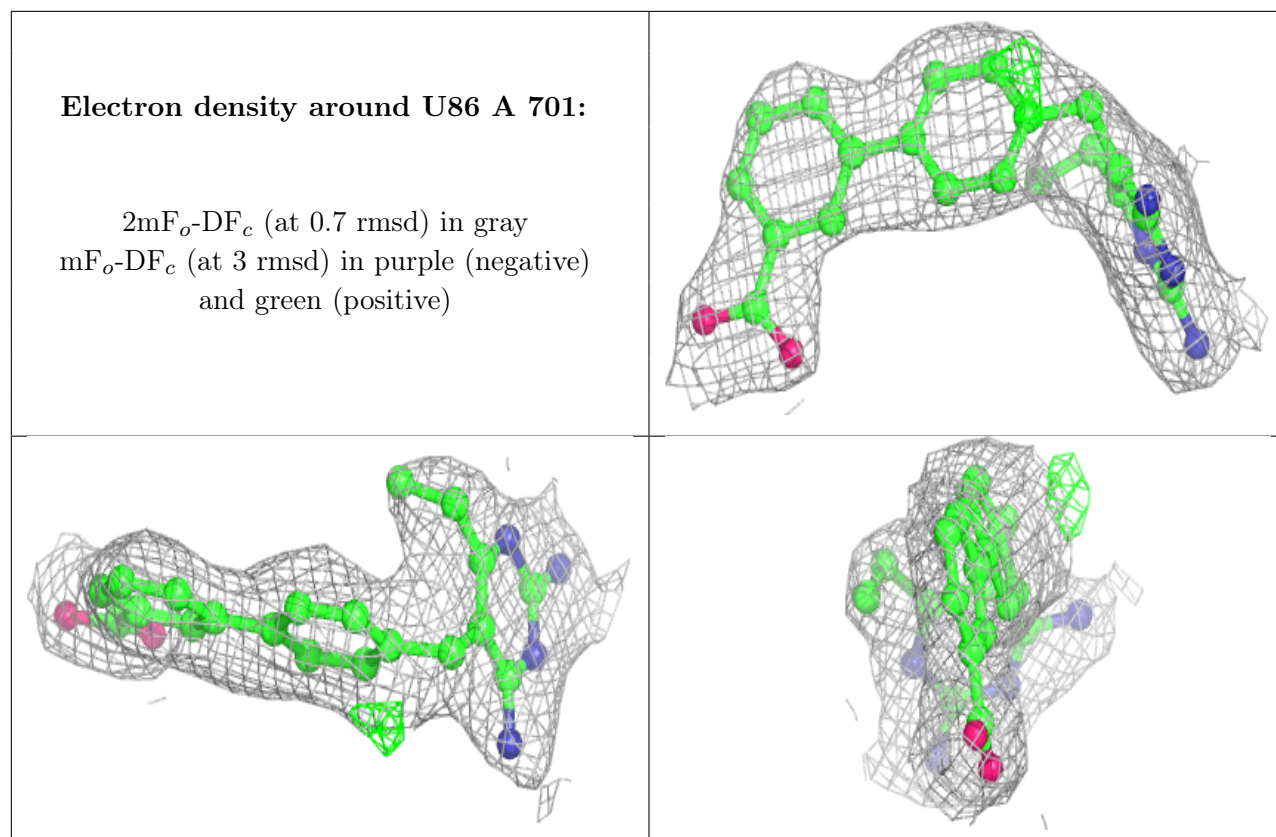
**Electron density around UMP B 703:**

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

**Electron density around UMP A 703:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.