



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:35 PM UTC

PDB ID : 8JFB / pdb_00008jfb
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

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](#) ①) 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

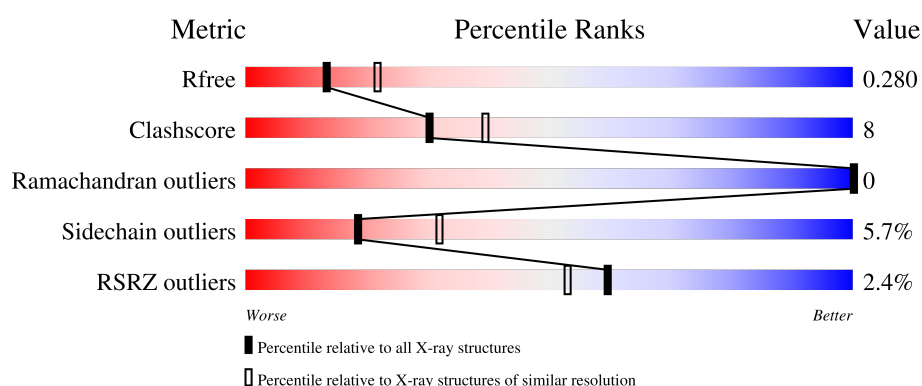
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	% 66% 20% • 13%
1	B	608	3% 64% 22% • 14%

2 Entry composition [i](#)

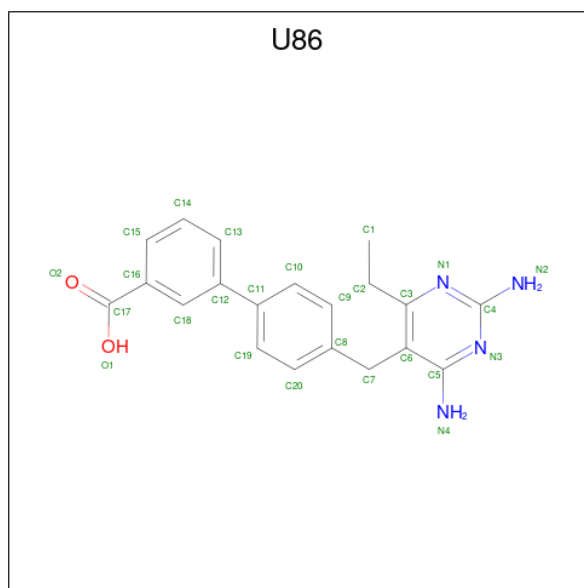
There are 5 unique types of molecules in this entry. The entry contains 9249 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

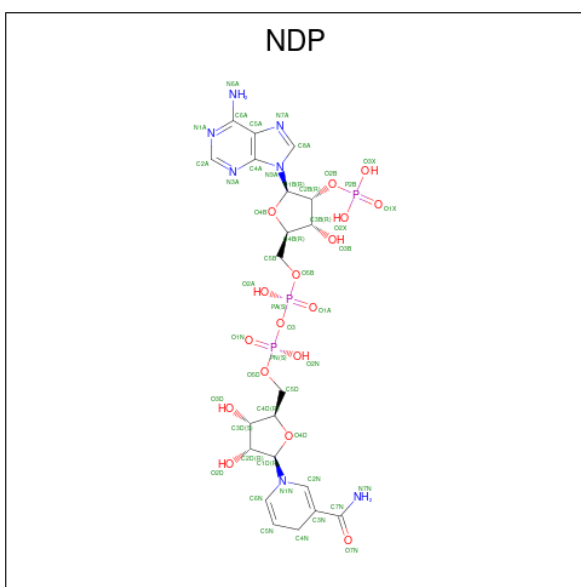
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	0	0
			4416	2858	728	805	25			
1	B	525	Total	C	N	O	S	0	0	0
			4360	2825	722	789	24			

- Molecule 2 is 3-[4-[[2,4-bis(azanyl)-6-ethyl-pyrimidin-5-yl]methyl]phenyl]benzoic acid (CCD ID: U86) (formula: C₂₀H₂₀N₄O₂) (labeled as "Ligand of Interest" by depositor).



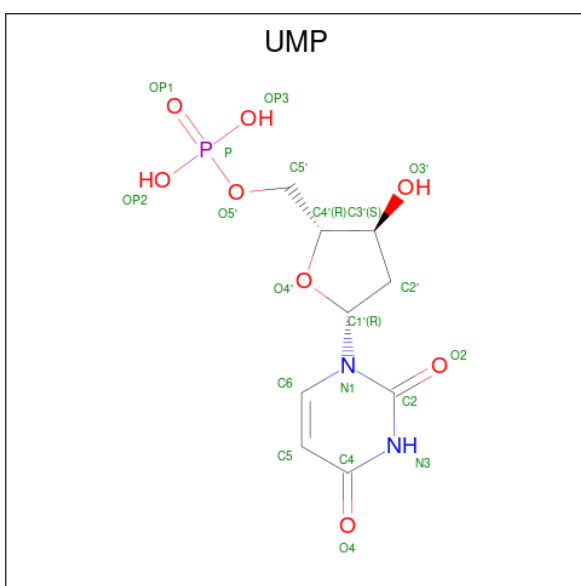
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	20	4	2		
2	B	1	Total	C	N	O	0	0
			26	20	4	2		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

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



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

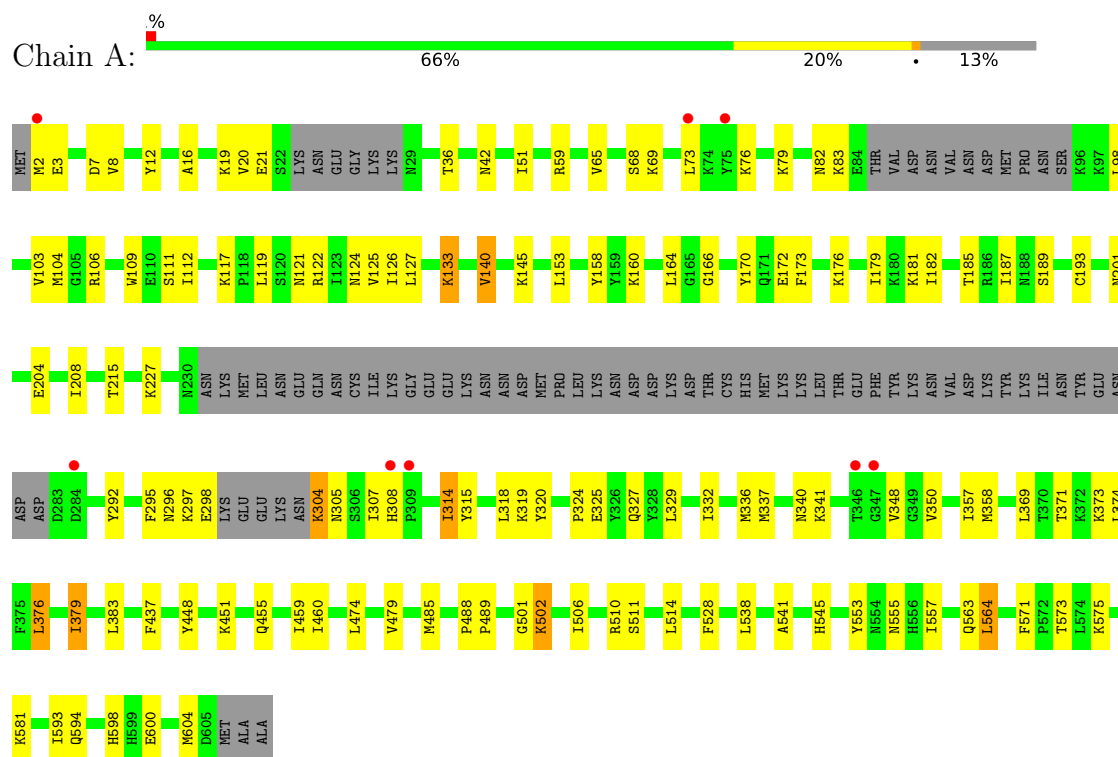
- Molecule 5 is water.

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

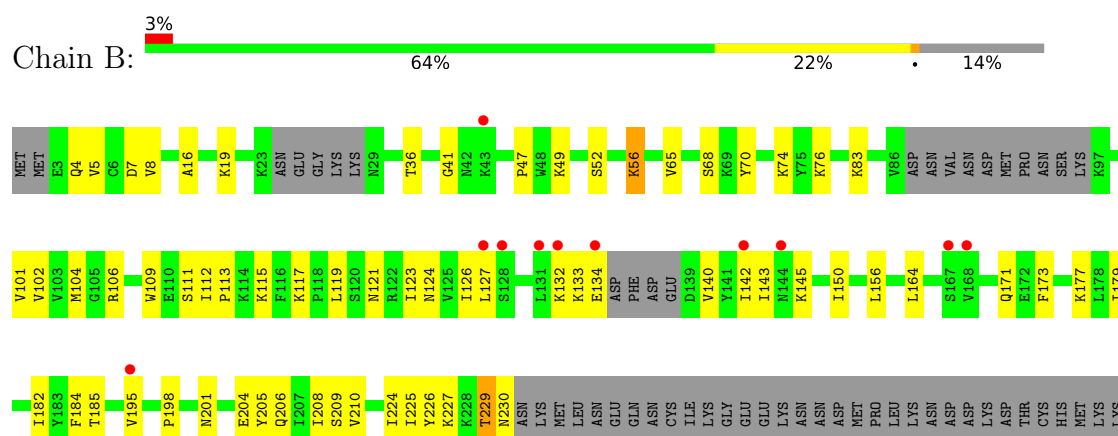
3 Residue-property plots [i](#)

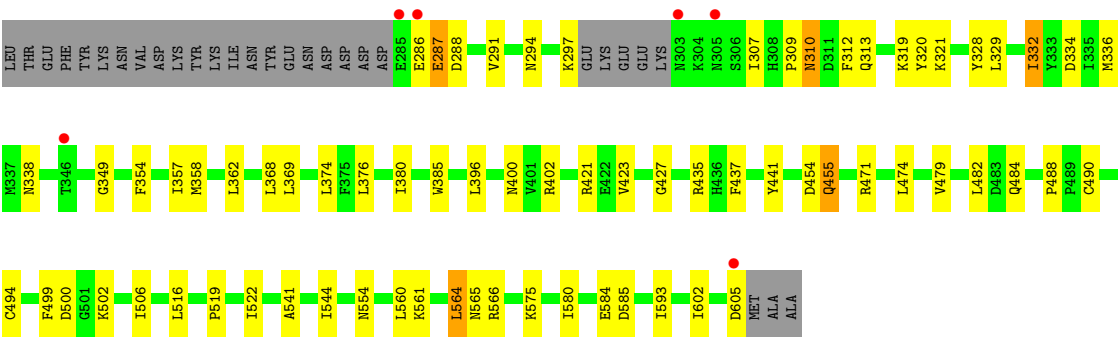
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



- 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, α , β , γ	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) 93.2 (16.32-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.66Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 5.0	Depositor
R, R_{free}	0.211 , 0.280 0.211 , 0.280	Depositor DCC
R_{free} test set	2156 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9249	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, U86, 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	0.39	0/4519	0.56	0/6102
1	B	0.37	0/4461	0.54	0/6025
All	All	0.38	0/8980	0.55	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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4416	0	4367	71	0
1	B	4360	0	4320	86	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	149	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 (149) 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:304:LYS:HD2	1:A:337:MET:HE3	1.82	0.61
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: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:336:MET:HE2	1:A:557:ILE:HG23	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:TYR:CD2	1:A:181:LYS:HB2	2.43	0.52
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:160:LYS:NZ	1:B:288:ASP:OD2	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:109:TRP:O	1:B:117:LYS:NZ	2.49	0.43
1:A:126:ILE:HD12	1:A:140:VAL:HG11	1.99	0.43
1:A:459:ILE:HG13	1:A:460:ILE:N	2.33	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:B:115:LYS:HZ3	1:B:115:LYS:HG2	1.65	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:B:358:MET:HE1	1:B:522:ILE:HD11	2.02	0.42
1:A:376:LEU:HG	1:A:379:ILE:HD11	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG2	1:B:115:LYS:H	1.64	0.41
1:B:435:ARG:NE	1:B:454:ASP:OD1	2.49	0.41
1:A:296:ASN:HA	1:B:56:LYS:HZ1	1.85	0.41
1:B:5:VAL:HG11	1:B:150:ILE:HG12	2.03	0.41
1:B:113:PRO:O	1:B:117:LYS:HG3	2.21	0.41
1:B:336:MET:HE1	1:B:560:LEU:HB2	2.03	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 ⓘ

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	520/608 (86%)	492 (95%)	28 (5%)	0	100	100
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 ⓘ

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%)	466 (94%)	30 (6%)	17	30
1	B	488/570 (86%)	462 (95%)	26 (5%)	20	35
All	All	984/1140 (86%)	928 (94%)	56 (6%)	18	32

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	3	GLU
1	A	20	VAL
1	A	21	GLU
1	A	59	ARG
1	A	65	VAL
1	A	68	SER
1	A	83	LYS
1	A	104	MET
1	A	111	SER
1	A	133	LYS
1	A	140	VAL
1	A	145	LYS
1	A	182	ILE
1	A	189	SER

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Mol	Chain	Res	Type
1	A	215	THR
1	A	297	LYS
1	A	298	GLU
1	A	304	LYS
1	A	307	ILE
1	A	308	HIS
1	A	314	ILE
1	A	376	LEU
1	A	379	ILE
1	A	502	LYS
1	A	564	LEU
1	A	573	THR
1	A	581	LYS
1	A	600	GLU
1	A	604	MET
1	B	49	LYS
1	B	52	SER
1	B	56	LYS
1	B	65	VAL
1	B	68	SER
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	321	LYS
1	B	332	ILE
1	B	357	ILE
1	B	423	VAL
1	B	455	GLN
1	B	516	LEU
1	B	564	LEU
1	B	584	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	42	ASN
1	A	124	ASN
1	A	144	ASN
1	A	171	GLN
1	A	313	GLN
1	A	424	ASN
1	A	436	HIS
1	A	450	ASN
1	A	461	ASN
1	A	554	ASN
1	B	66	ASN
1	B	124	ASN
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	491	HIS
1	B	554	ASN
1	B	582	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
2	U86	A	701	-	28,28,28	0.48	0	37,39,39	0.86	3 (8%)
3	NDP	A	702	-	51,52,52	2.55	11 (21%)	71,80,80	1.44	12 (16%)
4	UMP	B	703	-	21,21,21	1.01	2 (9%)	30,31,31	1.78	6 (20%)
4	UMP	A	703	-	21,21,21	0.83	0	30,31,31	1.76	7 (23%)
2	U86	B	702	-	28,28,28	0.52	0	37,39,39	0.77	2 (5%)
3	NDP	B	701	-	51,52,52	2.62	11 (21%)	71,80,80	1.48	14 (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
2	U86	A	701	-	-	0/14/14/14	0/3/3/3
3	NDP	A	702	-	-	3/34/77/77	0/5/5/5
4	UMP	B	703	-	-	4/10/22/22	0/2/2/2
4	UMP	A	703	-	-	6/10/22/22	0/2/2/2
2	U86	B	702	-	-	0/14/14/14	0/3/3/3
3	NDP	B	701	-	-	4/34/77/77	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NDP	P2B-O2B	13.05	1.82	1.59
3	B	701	NDP	P2B-O2B	13.02	1.82	1.59
3	B	701	NDP	PA-O3	7.78	1.67	1.59
3	A	702	NDP	PA-O3	7.44	1.67	1.59
3	B	701	NDP	PN-O5D	4.72	1.77	1.59
3	A	702	NDP	PN-O5D	4.32	1.76	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	NDP	C2B-C1B	3.51	1.61	1.53
3	A	702	NDP	C4A-N3A	3.03	1.40	1.34
3	B	701	NDP	O2B-C2B	-3.00	1.33	1.44
3	B	701	NDP	C5A-C4A	2.98	1.44	1.39
3	A	702	NDP	C2A-N1A	2.93	1.39	1.33
3	A	702	NDP	O2B-C2B	-2.85	1.34	1.44
3	B	701	NDP	C2A-N1A	2.83	1.39	1.33
3	A	702	NDP	C5A-C4A	2.76	1.44	1.39
3	A	702	NDP	C8A-N9A	2.61	1.42	1.37
3	B	701	NDP	C4A-N3A	2.58	1.39	1.34
3	A	702	NDP	C7N-N7N	2.38	1.40	1.33
3	B	701	NDP	C8A-N9A	2.34	1.41	1.37
3	B	701	NDP	PN-O3	2.23	1.61	1.59
3	A	702	NDP	C2B-C1B	2.21	1.58	1.53
4	B	703	UMP	C2-N1	2.11	1.41	1.38
4	B	703	UMP	C5-C4	-2.10	1.39	1.43
3	B	701	NDP	C7N-N7N	2.07	1.39	1.33
3	A	702	NDP	C6A-N6A	2.06	1.39	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	UMP	C4-N3-C2	-4.66	120.83	126.61
4	B	703	UMP	C4-N3-C2	-4.63	120.86	126.61
3	B	701	NDP	P2B-O2B-C2B	-4.13	112.40	123.43
4	B	703	UMP	C5-C4-N3	4.08	120.52	114.80
4	A	703	UMP	C5-C4-N3	3.82	120.15	114.80
3	A	702	NDP	P2B-O2B-C2B	-3.66	113.65	123.43
3	B	701	NDP	O2B-P2B-O1X	-3.64	96.35	109.33
4	B	703	UMP	O4-C4-C5	-3.58	118.99	125.16
3	A	702	NDP	O2B-P2B-O1X	-3.50	96.87	109.33
4	A	703	UMP	N3-C2-N1	3.13	118.97	114.89
4	B	703	UMP	C1'-N1-C2	3.08	123.69	117.66
4	A	703	UMP	C1'-N1-C2	3.05	123.62	117.66
3	A	702	NDP	O2N-PN-O3	2.98	115.33	107.27
4	B	703	UMP	C1'-N1-C6	-2.96	115.71	121.53
4	A	703	UMP	C1'-N1-C6	-2.82	115.99	121.53
4	A	703	UMP	O2-C2-N3	-2.79	116.35	121.49
3	B	701	NDP	O2N-PN-O3	2.70	114.57	107.27
3	B	701	NDP	PA-O5B-C5B	-2.67	106.05	121.35
3	B	701	NDP	PN-O5D-C5D	-2.65	106.14	121.35
3	B	701	NDP	C3N-C2N-N1N	-2.64	119.33	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NDP	C3N-C2N-N1N	-2.59	119.41	123.20
2	B	702	U86	C6-C3-N1	-2.53	121.54	123.48
3	B	701	NDP	O3X-P2B-O2X	2.50	117.19	107.80
3	B	701	NDP	O2A-PA-O1A	2.49	124.02	112.44
3	A	702	NDP	O3X-P2B-O2X	2.46	117.03	107.80
3	A	702	NDP	PN-O5D-C5D	-2.44	107.36	121.35
3	B	701	NDP	O3-PA-O1A	-2.42	103.42	110.70
3	B	701	NDP	O5D-PN-O1N	-2.42	99.34	108.94
2	A	701	U86	C6-C7-C8	-2.42	108.75	114.22
2	A	701	U86	C6-C3-N1	-2.38	121.65	123.48
4	B	703	UMP	N3-C2-N1	2.35	117.95	114.89
4	A	703	UMP	O4-C4-C5	-2.30	121.20	125.16
3	A	702	NDP	O5B-C5B-C4B	-2.27	101.25	108.99
2	B	702	U86	C5-C6-C3	2.27	117.20	115.90
3	A	702	NDP	PA-O5B-C5B	-2.27	108.34	121.35
3	B	701	NDP	C2A-N1A-C6A	-2.25	115.03	118.73
3	A	702	NDP	C2B-C3B-C4B	-2.16	97.35	101.99
3	B	701	NDP	N3A-C4A-N9A	2.16	130.84	127.17
2	A	701	U86	C5-C6-C3	2.15	117.13	115.90
3	B	701	NDP	O2N-PN-O1N	2.15	122.46	112.44
3	A	702	NDP	O2A-PA-O1A	2.11	122.27	112.44
3	A	702	NDP	O7N-C7N-N7N	-2.11	118.17	122.89
3	B	701	NDP	O3X-P2B-O2B	-2.08	97.74	105.85
3	A	702	NDP	O2N-PN-O1N	2.06	122.03	112.44

There are no chirality outliers.

All (17) 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
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
4	A	703	UMP	C2'-C1'-N1-C2
3	B	701	NDP	O4D-C1D-N1N-C2N
3	B	701	NDP	C4D-C5D-O5D-PN
3	A	702	NDP	C4D-C5D-O5D-PN

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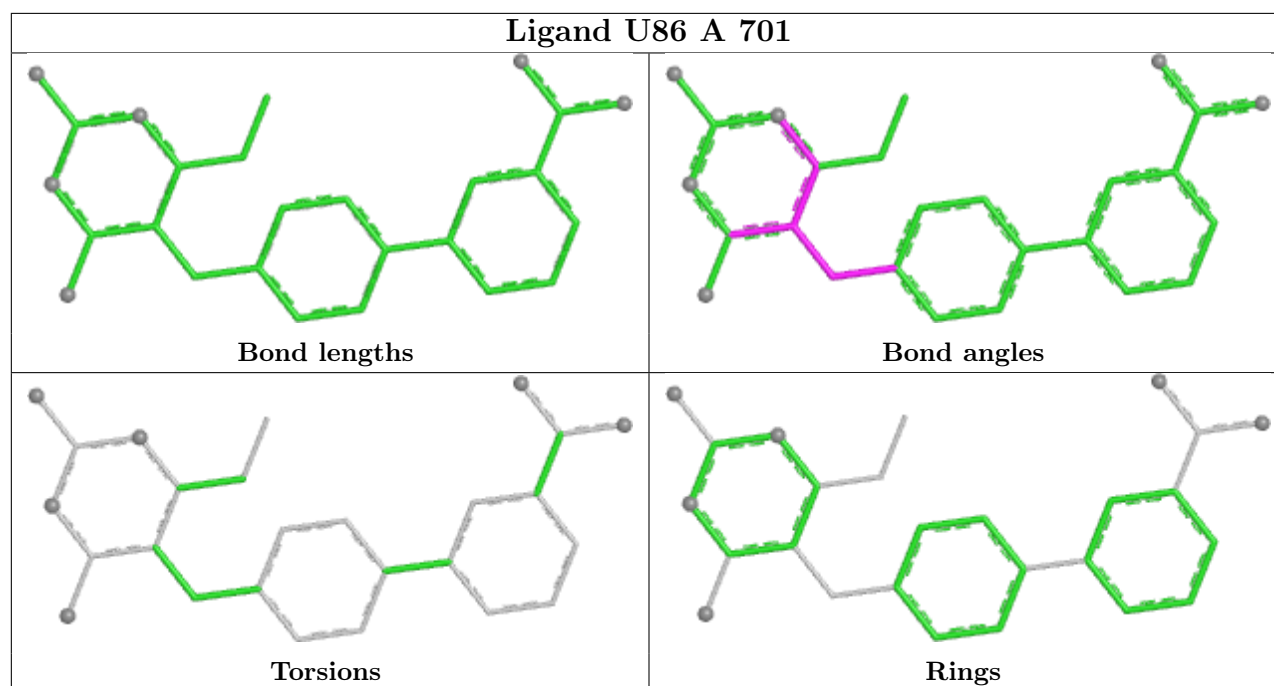
Mol	Chain	Res	Type	Atoms
4	A	703	UMP	C2'-C1'-N1-C6
4	B	703	UMP	C5'-O5'-P-OP3
3	B	701	NDP	C2D-C1D-N1N-C2N
3	A	702	NDP	C2B-O2B-P2B-O3X

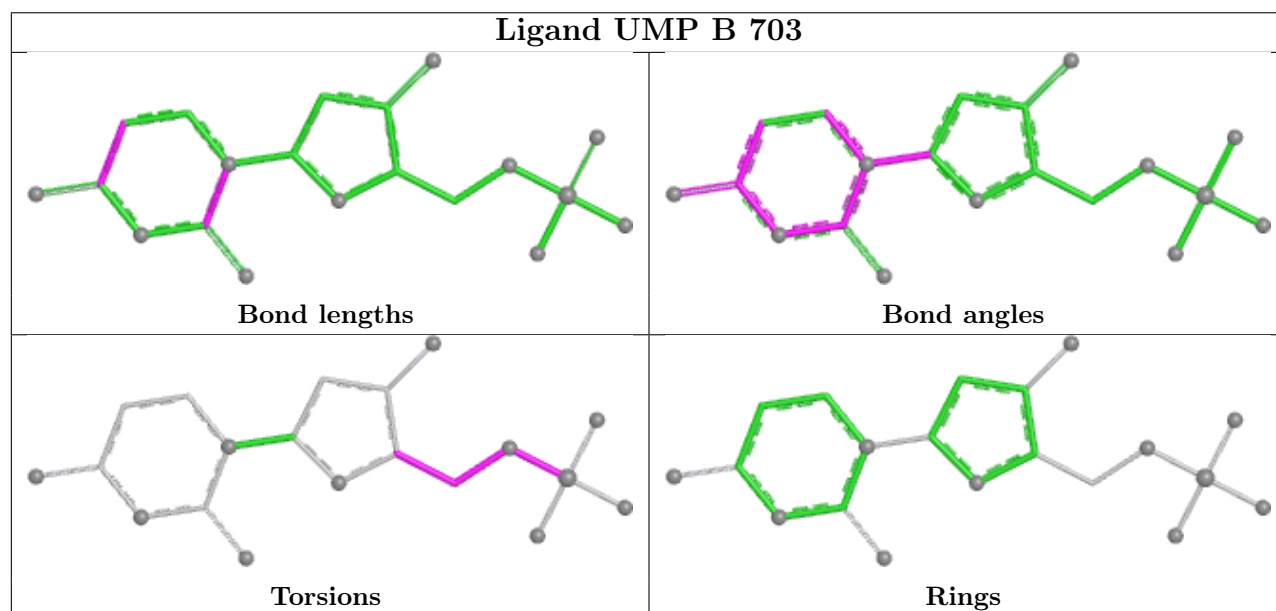
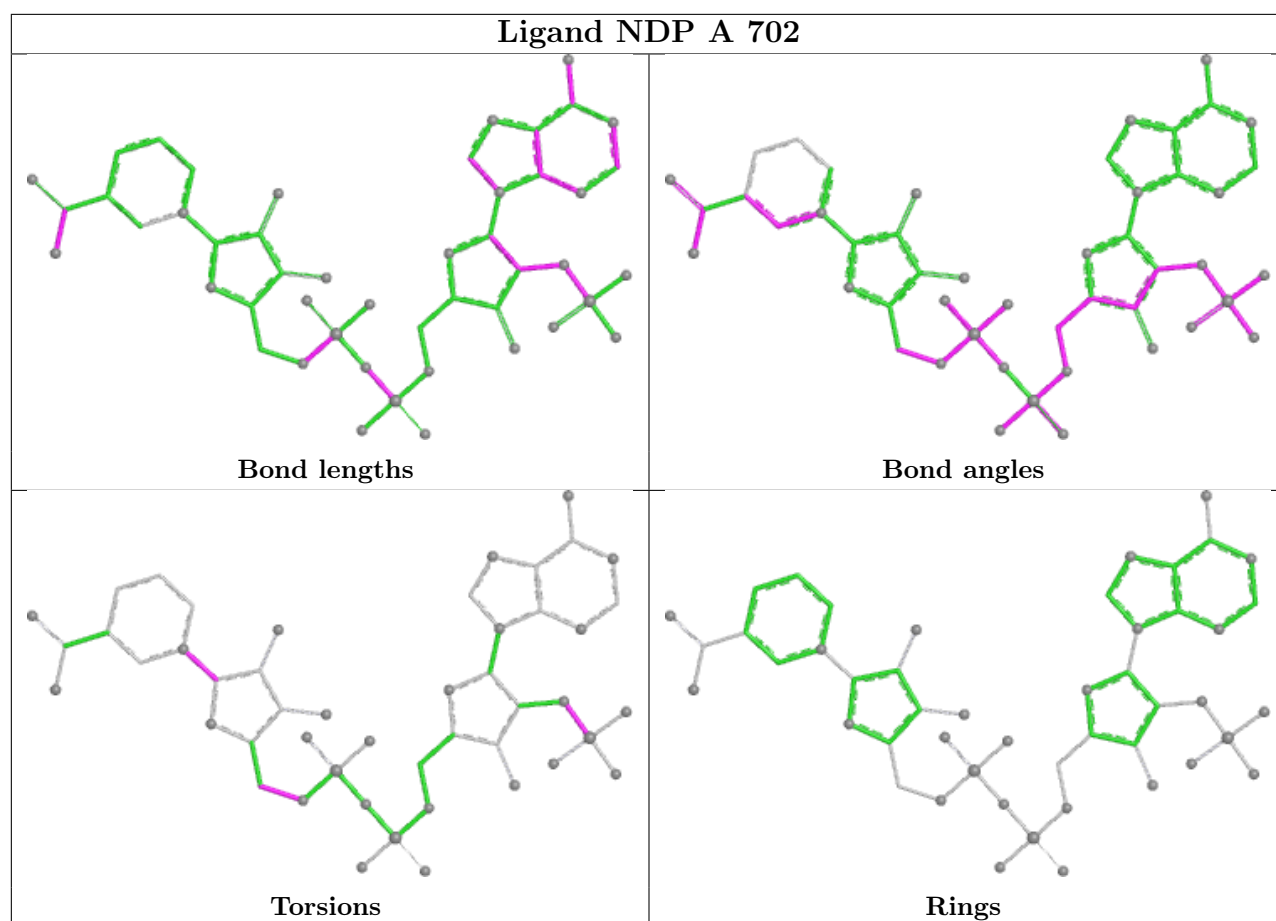
There are no ring outliers.

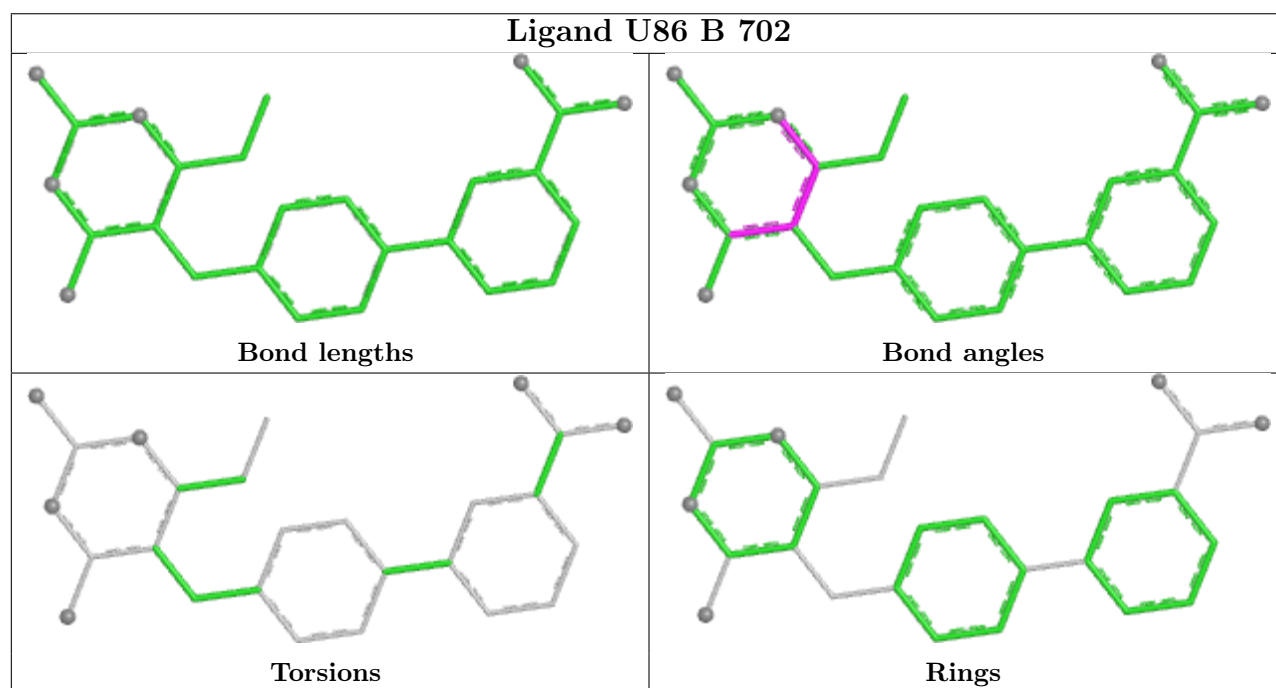
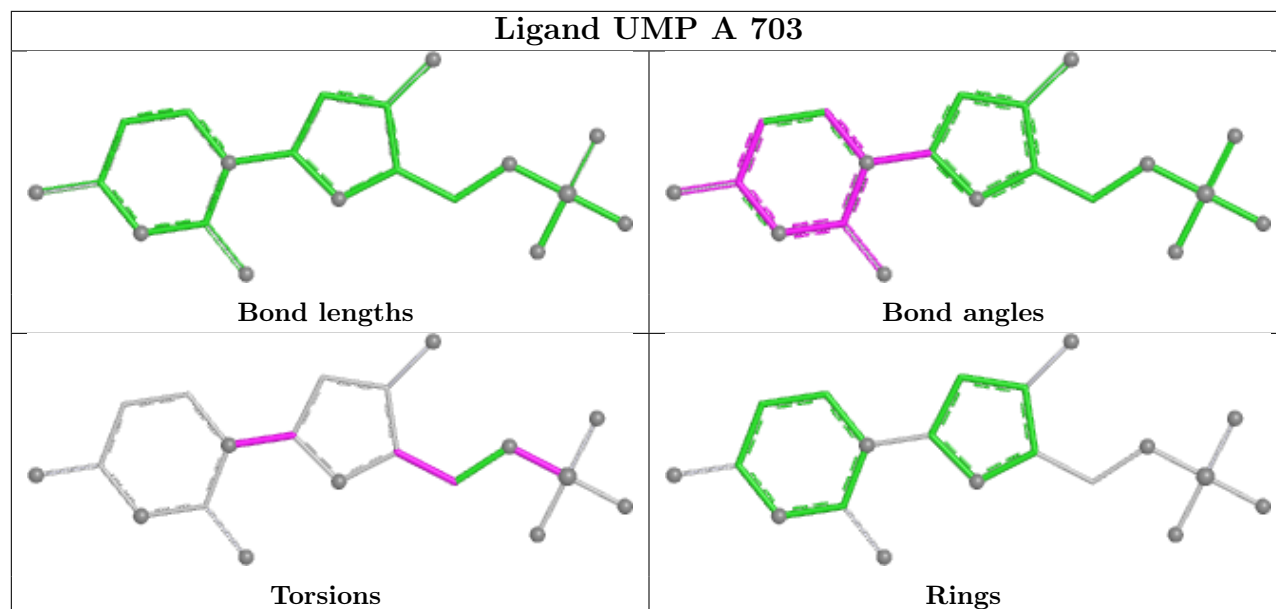
3 monomers are involved in 9 short contacts:

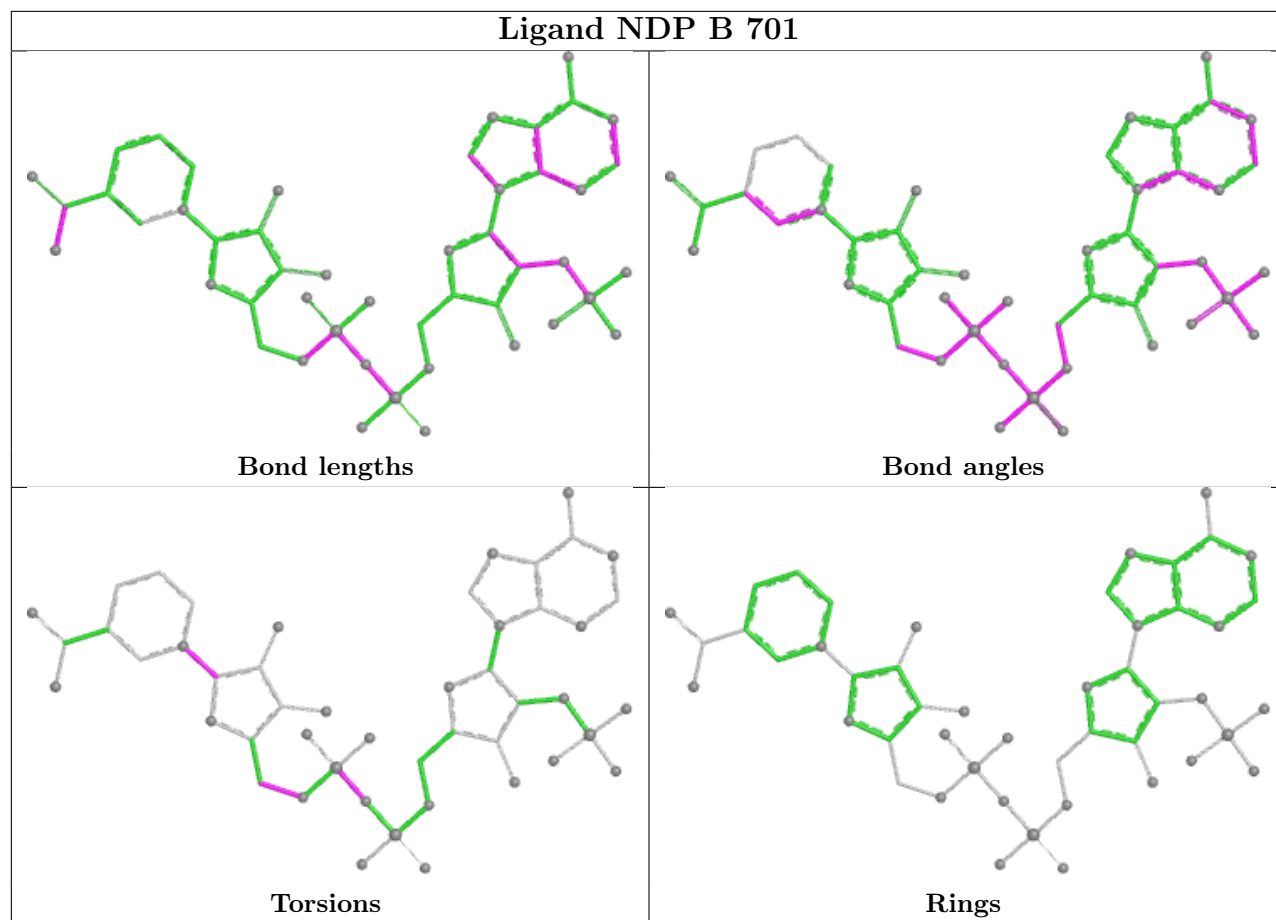
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NDP	5	0
4	B	703	UMP	1	0
3	B	701	NDP	3	0

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

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	530/608 (87%)	-0.03	8 (1%) 72 67	17, 32, 64, 92	0
1	B	525/608 (86%)	0.13	17 (3%) 50 42	17, 35, 71, 104	0
All	All	1055/1216 (86%)	0.05	25 (2%) 59 53	17, 33, 68, 104	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	GLY	3.3
1	B	605	ASP	3.2
1	A	309	PRO	3.0
1	B	286	GLU	2.9
1	A	284	ASP	2.7
1	A	75	TYR	2.7
1	B	303	ASN	2.5
1	B	134	GLU	2.5
1	B	285	GLU	2.5
1	A	308	HIS	2.4
1	B	168	VAL	2.4
1	B	346	THR	2.3
1	B	128	SER	2.3
1	B	132	LYS	2.2
1	B	195	VAL	2.2
1	B	131	LEU	2.2
1	B	167	SER	2.2
1	B	142	ILE	2.2
1	B	144	ASN	2.1
1	B	127	LEU	2.1
1	B	305	ASN	2.1
1	B	43	LYS	2.1
1	A	73	LEU	2.1
1	A	346	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2	MET	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

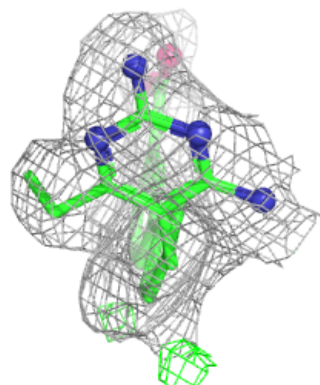
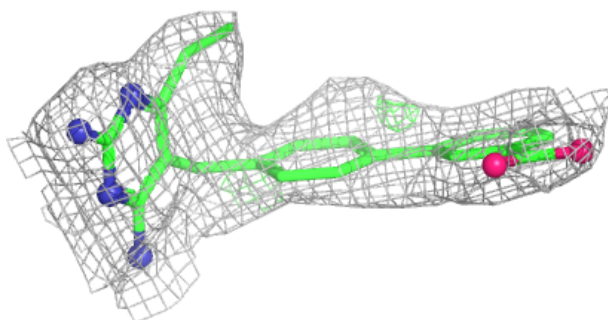
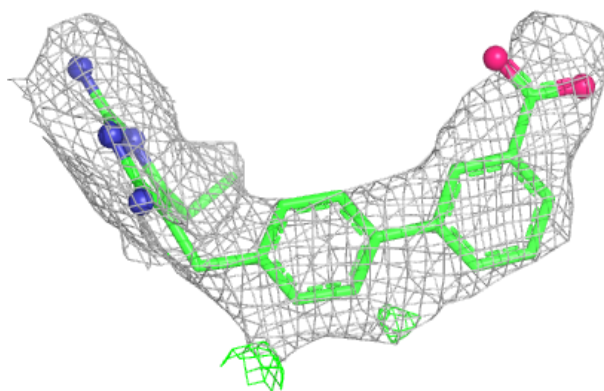
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	U86	B	702	26/26	0.77	0.15	40,54,69,73	0
3	NDP	B	701	48/48	0.81	0.14	50,69,77,78	0
3	NDP	A	702	48/48	0.89	0.11	29,46,54,56	0
4	UMP	A	703	20/20	0.90	0.12	38,45,48,52	0
4	UMP	B	703	20/20	0.90	0.12	35,41,48,51	0
2	U86	A	701	26/26	0.93	0.09	26,31,39,47	0

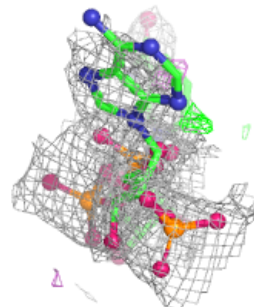
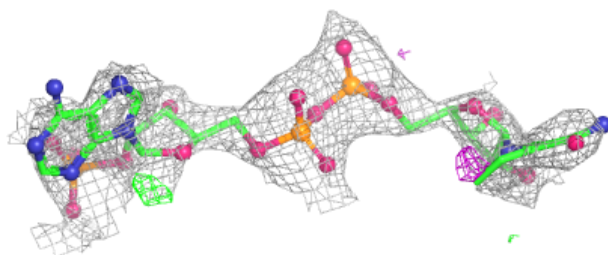
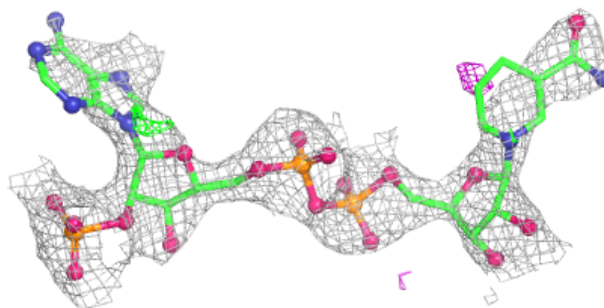
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U86 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)

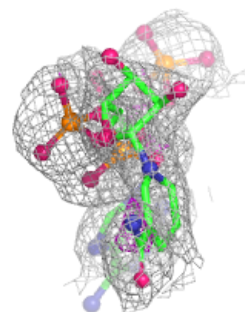
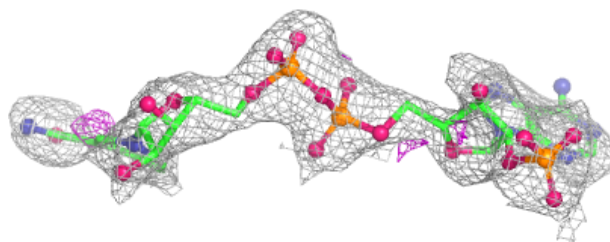
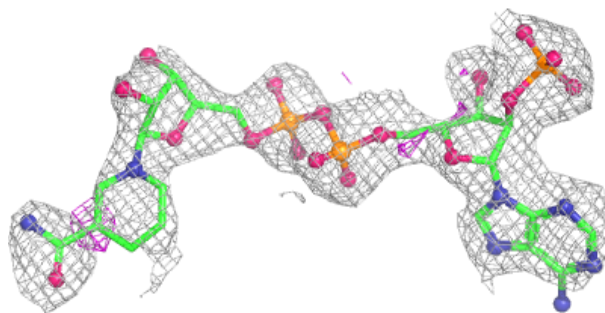
**Electron density around NDP B 701:**

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

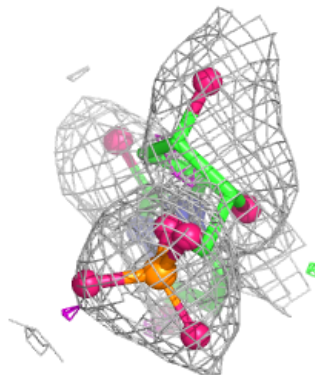
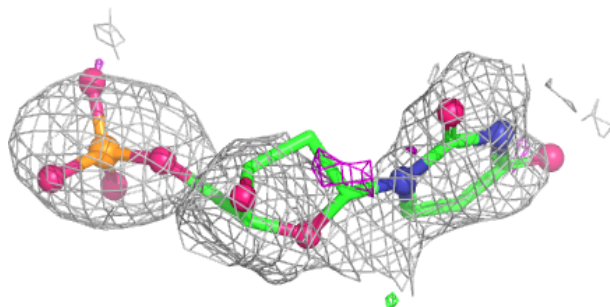
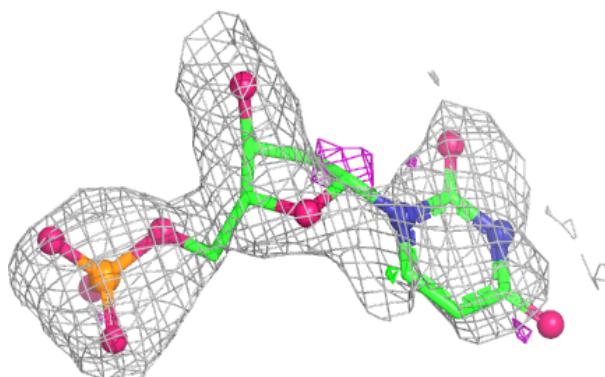


Electron density around NDP A 702:

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

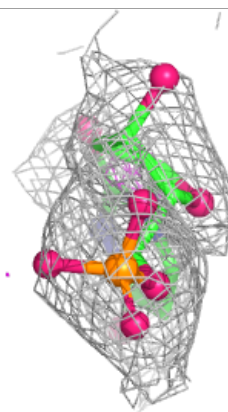
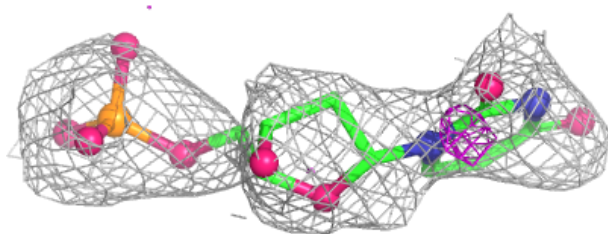
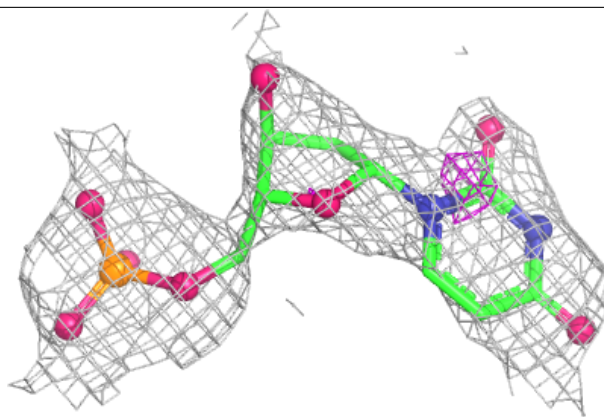
**Electron density around UMP A 703:**

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

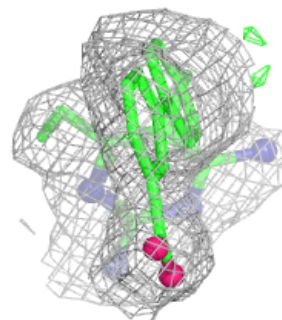
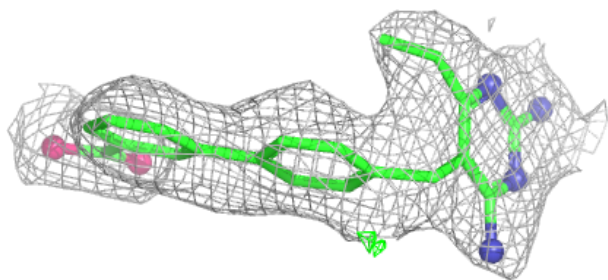
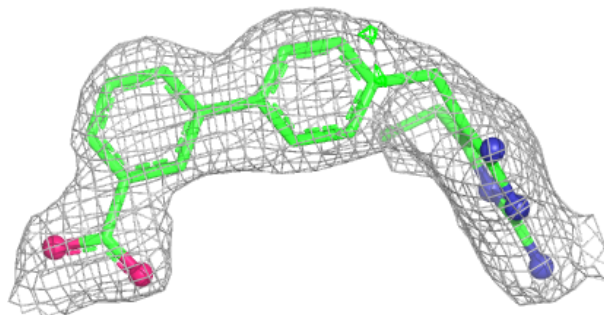


Electron density around UMP B 703:

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

**Electron density around U86 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.