



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 PM UTC

PDB ID : 8JFD / pdb_00008jfd
Title : V1/S quadruple mutant Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with compound 8 (B21594), 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 : 2.30 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

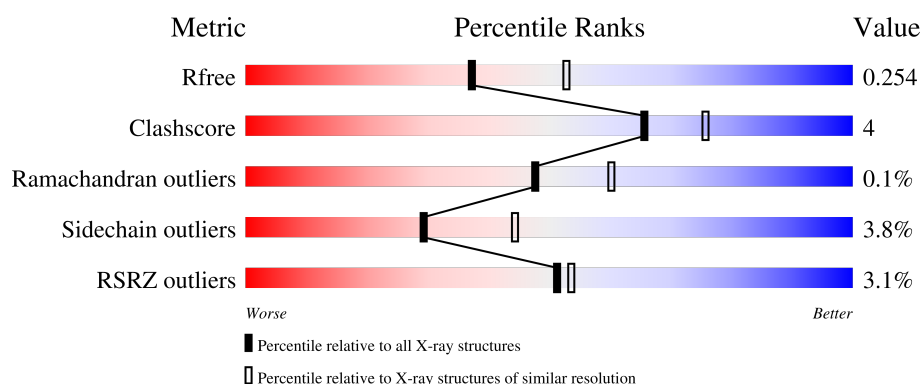
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	608	2% 77% 9% 13%
1	B	608	3% 74% 12% 13%

2 Entry composition [i](#)

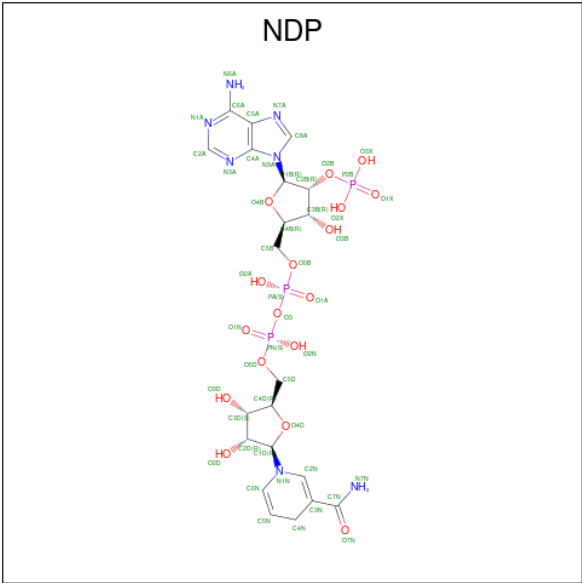
There are 6 unique types of molecules in this entry. The entry contains 9583 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

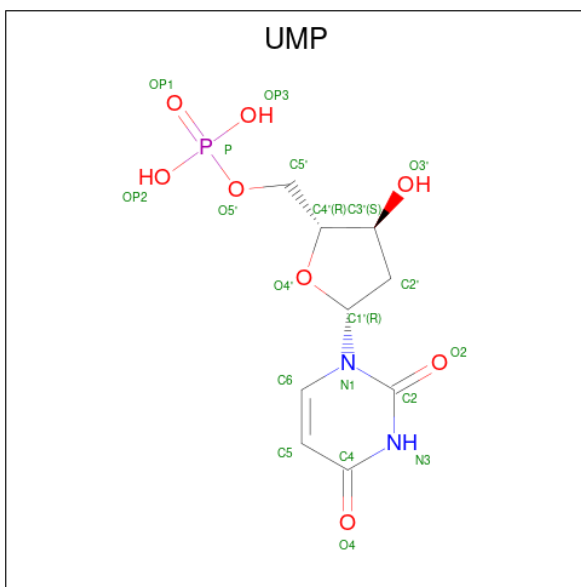
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	526	Total	C	N	O	S	0	0	0
			4372	2835	721	792	24			
1	B	528	Total	C	N	O	S	0	0	0
			4391	2845	724	798	24			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



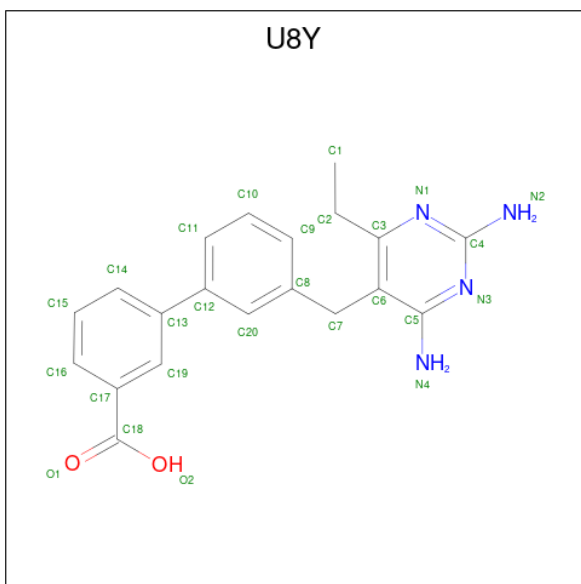
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



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

- Molecule 4 is 3-[3-[[2,4-bis(azanyl)-6-ethyl-pyrimidin-5-yl]methyl]phenyl]benzoic acid (CCD ID: U8Y) (formula: C₂₀H₂₀N₄O₂) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	332	Total	O	0	0
			332	332		
6	B	288	Total	O	0	0
			288	288		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.35Å 156.50Å 165.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.79 – 2.30 16.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (16.79-2.30) 98.2 (16.79-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.30Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.202 , 0.256 (Not available) , 0.254	Depositor DCC
R_{free} test set	3328 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9583	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, GOL, U8Y, NDP

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	0.34	0/4475	0.52	0/6045
1	B	0.32	0/4494	0.49	0/6072
All	All	0.33	0/8969	0.50	0/12117

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	4372	0	4322	33	0
1	B	4391	0	4342	36	0
2	A	48	0	26	0	0
2	B	48	0	26	1	0
3	A	20	0	11	0	0
3	B	20	0	11	0	0
4	A	26	0	0	0	0
4	B	26	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	332	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	288	0	0	2	0
All	All	9583	0	8754	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (67) 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:319:LYS:HG2	1:B:286:GLU:HG2	1.58	0.85
1:A:70:TYR:OH	1:A:157:ASN:ND2	2.20	0.71
1:A:491:HIS:HD2	6:A:1003:HOH:O	1.78	0.67
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.78	0.66
1:B:133:LYS:H	1:B:133:LYS:HE2	1.61	0.65
1:A:332:ILE:HD13	1:A:560:LEU:HD22	1.80	0.62
1:A:376:LEU:HD22	1:A:379:ILE:HD11	1.83	0.60
1:A:51:ILE:HD13	1:A:187:ILE:HD12	1.83	0.60
1:B:12:TYR:HE1	1:B:181:LYS:HD3	1.69	0.57
1:B:4:GLN:N	6:B:808:HOH:O	2.38	0.57
1:B:145:LYS:HD3	1:B:146:VAL:H	1.69	0.56
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.87	0.56
1:A:177:LYS:HB3	1:A:228:LYS:HZ1	1.70	0.56
1:A:376:LEU:HD12	1:A:593:ILE:HG13	1.89	0.55
1:B:312:PHE:HA	1:B:565:ASN:HD21	1.72	0.53
1:B:336:MET:HE1	1:B:560:LEU:HB2	1.91	0.53
1:A:329:LEU:HD22	1:A:564:LEU:HD12	1.91	0.53
1:B:195:VAL:HG21	2:B:701:NDP:H4D	1.90	0.53
1:A:12:TYR:HD2	1:A:181:LYS:HB2	1.75	0.52
1:B:573:THR:HG22	1:B:594:GLN:HB2	1.91	0.52
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.91	0.52
1:B:201:ASN:HD22	1:B:204:GLU:HG3	1.75	0.52
1:A:66:ASN:HB3	1:A:69:LYS:HD2	1.93	0.51
1:B:309:PRO:HA	1:B:312:PHE:HD2	1.77	0.50
1:A:171:GLN:HE21	1:A:175:GLU:HG3	1.77	0.50
1:A:145:LYS:HE2	1:A:148:ASP:OD2	2.13	0.49
1:B:42:ASN:HB2	1:B:193:CYS:HA	1.96	0.48
1:B:572:PRO:HB3	1:B:596:TYR:HA	1.96	0.47
1:A:425:ASP:OD1	1:A:441:TYR:OH	2.30	0.47
1:A:480:LYS:HD3	6:A:1046:HOH:O	2.14	0.47
1:B:128:SER:OG	1:B:131:LEU:HB2	2.15	0.46
1:A:171:GLN:NE2	1:A:175:GLU:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ASN:O	1:B:307:ILE:HG12	2.15	0.46
1:A:72:LYS:HD3	1:A:72:LYS:HA	1.61	0.46
1:A:516:LEU:HD23	1:A:516:LEU:HA	1.83	0.46
1:A:375:PHE:CD1	1:A:375:PHE:N	2.85	0.45
1:B:325:GLU:HG3	1:B:369:LEU:HD22	1.99	0.44
1:A:10:ASP:OD2	1:A:77:ARG:NH2	2.50	0.44
1:A:387:ILE:O	1:A:435:ARG:NH1	2.45	0.44
1:A:479:VAL:HB	1:B:437:PHE:CD1	2.52	0.44
1:A:500:ASP:HB3	1:A:502:LYS:HE2	1.98	0.44
1:B:214:TYR:O	1:B:220:THR:HA	2.18	0.44
1:B:201:ASN:HD21	1:B:203:ASN:HB2	1.83	0.43
1:B:346:THR:HB	1:B:348:VAL:HG23	2.00	0.43
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.90	0.43
1:A:310:ASN:HA	1:A:313:GLN:HG3	2.00	0.43
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.19	0.43
1:A:159:TYR:CD2	1:A:160:LYS:HG3	2.54	0.42
1:A:305:ASN:OD1	1:A:341:LYS:NZ	2.52	0.42
1:A:294:ASN:HD22	1:A:297:LYS:HG3	1.84	0.42
1:B:601:LYS:HE3	1:B:601:LYS:HB2	1.73	0.42
1:A:398:ASN:ND2	6:A:807:HOH:O	2.35	0.42
1:B:12:TYR:HD1	1:B:181:LYS:HB2	1.84	0.42
1:A:21:GLU:H	1:A:21:GLU:HG2	1.72	0.41
1:A:327:GLN:HB3	1:A:358:MET:HG2	2.02	0.41
1:B:376:LEU:HD12	1:B:593:ILE:HG13	2.02	0.41
1:B:569:TYR:CG	1:B:597:VAL:HG12	2.55	0.41
1:A:477:TRP:O	6:A:801:HOH:O	2.22	0.41
1:B:177:LYS:HG2	1:B:228:LYS:HZ1	1.85	0.41
1:B:119:LEU:HB3	1:B:122:ARG:CZ	2.51	0.41
1:B:312:PHE:HB3	1:B:315:TYR:HB3	2.02	0.41
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.92	0.41
1:B:314:ILE:H	1:B:314:ILE:HD12	1.86	0.40
1:B:492:ILE:HD11	1:B:510:ARG:HD3	2.03	0.40
1:B:210:VAL:HG12	1:B:224:ILE:HG22	2.02	0.40
1:B:579:ASP:OD2	6:B:801:HOH:O	2.22	0.40
1:B:76:LYS:HE2	1:B:76:LYS:HB3	1.94	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	516/608 (85%)	499 (97%)	17 (3%)	0	100	100
1	B	518/608 (85%)	500 (96%)	17 (3%)	1 (0%)	43	55
All	All	1034/1216 (85%)	999 (97%)	34 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	429	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	488/570 (86%)	478 (98%)	10 (2%)	48	67
1	B	492/570 (86%)	465 (94%)	27 (6%)	19	28
All	All	980/1140 (86%)	943 (96%)	37 (4%)	29	44

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLU
1	A	171	GLN
1	A	202	GLU
1	A	286	GLU
1	A	307	ILE

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Mol	Chain	Res	Type
1	A	375	PHE
1	A	487	LEU
1	A	514	LEU
1	A	516	LEU
1	A	537	ASN
1	B	20	VAL
1	B	21	GLU
1	B	29	ASN
1	B	45	VAL
1	B	110	GLU
1	B	127	LEU
1	B	132	LYS
1	B	133	LYS
1	B	134	GLU
1	B	135	ASP
1	B	137	ASP
1	B	139	ASP
1	B	144	ASN
1	B	145	LYS
1	B	155	LYS
1	B	202	GLU
1	B	215	THR
1	B	229	THR
1	B	283	ASP
1	B	341	LYS
1	B	346	THR
1	B	457	LYS
1	B	514	LEU
1	B	516	LEU
1	B	564	LEU
1	B	573	THR
1	B	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	42	ASN
1	A	157	ASN
1	A	171	GLN
1	A	294	ASN
1	A	316	ASN

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Mol	Chain	Res	Type
1	A	407	ASN
1	A	415	ASN
1	A	491	HIS
1	A	563	GLN
1	B	201	ASN
1	B	203	ASN
1	B	316	ASN
1	B	338	ASN
1	B	340	ASN
1	B	491	HIS
1	B	537	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 ⓘ

8 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	UMP	B	702	-	21,21,21	0.92	1 (4%)	30,31,31	1.64	5 (16%)
2	NDP	B	701	-	51,52,52	2.67	11 (21%)	71,80,80	1.50	17 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	704	-	5,5,5	0.90	0	5,5,5	1.03	0
4	U8Y	A	703	-	28,28,28	0.52	0	37,39,39	0.99	2 (5%)
3	UMP	A	702	-	21,21,21	0.89	0	30,31,31	1.77	8 (26%)
5	GOL	A	704	-	5,5,5	1.01	0	5,5,5	1.03	0
4	U8Y	B	703	-	28,28,28	0.49	0	37,39,39	0.81	2 (5%)
2	NDP	A	701	-	51,52,52	2.24	9 (17%)	71,80,80	1.44	12 (16%)

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	UMP	B	702	-	-	5/10/22/22	0/2/2/2
2	NDP	B	701	-	-	12/34/77/77	0/5/5/5
5	GOL	B	704	-	-	0/4/4/4	-
4	U8Y	A	703	-	-	3/14/14/14	0/3/3/3
3	UMP	A	702	-	-	0/10/22/22	0/2/2/2
5	GOL	A	704	-	-	0/4/4/4	-
4	U8Y	B	703	-	-	3/14/14/14	0/3/3/3
2	NDP	A	701	-	-	7/34/77/77	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	NDP	P2B-O2B	14.89	1.85	1.59
2	A	701	NDP	P2B-O2B	10.21	1.77	1.59
2	A	701	NDP	PA-O3	6.79	1.66	1.59
2	B	701	NDP	PA-O3	6.02	1.66	1.59
2	A	701	NDP	PN-O5D	4.85	1.78	1.59
2	B	701	NDP	PN-O5D	4.27	1.76	1.59
2	A	701	NDP	O2B-C2B	-3.52	1.32	1.44
2	A	701	NDP	PN-O3	3.07	1.62	1.59
2	B	701	NDP	C5A-C4A	3.00	1.44	1.39
2	A	701	NDP	C5A-C4A	2.95	1.44	1.39
2	B	701	NDP	C2A-N1A	2.80	1.38	1.33
2	B	701	NDP	O2B-C2B	-2.74	1.34	1.44
2	B	701	NDP	C2B-C1B	2.66	1.59	1.53
2	A	701	NDP	C2A-N1A	2.48	1.38	1.33
2	B	701	NDP	C4A-N3A	2.46	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	NDP	C7N-N7N	2.24	1.39	1.33
2	A	701	NDP	C8A-N9A	2.18	1.41	1.37
2	A	701	NDP	C7N-N7N	2.17	1.39	1.33
2	B	701	NDP	C8A-N7A	2.09	1.35	1.31
2	B	701	NDP	C8A-N9A	2.08	1.41	1.37
3	B	702	UMP	C5-C4	-2.07	1.39	1.43

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	UMP	C4-N3-C2	-4.72	120.76	126.61
2	B	701	NDP	O2N-PN-O3	4.34	119.01	107.27
3	B	702	UMP	C4-N3-C2	-4.03	121.60	126.61
3	A	702	UMP	C5-C4-N3	3.86	120.21	114.80
3	B	702	UMP	C5-C4-N3	3.70	119.98	114.80
2	A	701	NDP	P2B-O2B-C2B	-3.66	113.66	123.43
2	A	701	NDP	O2B-P2B-O1X	-3.60	96.50	109.33
2	B	701	NDP	O2B-P2B-O1X	-3.57	96.61	109.33
4	A	703	U8Y	C5-C6-C3	3.42	117.85	115.90
3	B	702	UMP	C1'-N1-C6	-3.42	114.81	121.53
2	A	701	NDP	O2N-PN-O3	3.41	116.50	107.27
3	B	702	UMP	O4-C4-C5	-3.40	119.29	125.16
3	A	702	UMP	C1'-N1-C6	-3.22	115.20	121.53
3	B	702	UMP	C1'-N1-C2	3.13	123.79	117.66
3	A	702	UMP	C1'-N1-C2	3.10	123.72	117.66
2	B	701	NDP	P2B-O2B-C2B	-3.09	115.18	123.43
3	A	702	UMP	O4-C4-C5	-2.90	120.16	125.16
3	A	702	UMP	N3-C2-N1	2.89	118.65	114.89
4	A	703	U8Y	C6-C3-N1	-2.88	121.26	123.48
2	B	701	NDP	PA-O5B-C5B	-2.83	105.12	121.35
2	A	701	NDP	O3X-P2B-O2X	2.71	117.95	107.80
4	B	703	U8Y	C5-C6-C3	2.65	117.41	115.90
2	B	701	NDP	O3X-P2B-O2X	2.63	117.67	107.80
2	B	701	NDP	PN-O5D-C5D	-2.59	106.49	121.35
2	B	701	NDP	O2A-PA-O3	-2.58	100.29	107.27
4	B	703	U8Y	C6-C3-N1	-2.54	121.53	123.48
2	B	701	NDP	O3-PA-O1A	-2.45	103.33	110.70
2	B	701	NDP	C3N-C2N-N1N	-2.42	119.66	123.20
2	A	701	NDP	O3X-P2B-O2B	-2.34	96.74	105.85
2	A	701	NDP	PA-O5B-C5B	-2.30	108.17	121.35
3	A	702	UMP	O2-C2-N3	-2.25	117.33	121.49
2	B	701	NDP	O2N-PN-O1N	2.24	122.88	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NDP	C5A-C4A-N3A	-2.20	123.69	126.72
2	A	701	NDP	N3A-C4A-N9A	2.17	130.86	127.17
2	B	701	NDP	N3A-C4A-N9A	2.17	130.86	127.17
2	B	701	NDP	O4B-C4B-C3B	2.15	109.43	105.15
2	B	701	NDP	C2A-N1A-C6A	-2.14	115.22	118.73
3	A	702	UMP	OP3-P-O5'	2.14	112.24	106.67
2	A	701	NDP	C2A-N1A-C6A	-2.13	115.23	118.73
2	B	701	NDP	O2A-PA-O1A	2.12	122.33	112.44
2	B	701	NDP	O5D-PN-O1N	-2.12	100.52	108.94
2	A	701	NDP	O7N-C7N-N7N	-2.06	118.27	122.89
2	A	701	NDP	O3-PA-O1A	-2.06	104.51	110.70
2	A	701	NDP	O3-PN-O1N	-2.02	104.64	110.70
2	B	701	NDP	O7N-C7N-C3N	2.01	124.67	120.90
2	B	701	NDP	C5A-C4A-N3A	-2.00	123.96	126.72

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NDP	C5B-O5B-PA-O1A
2	A	701	NDP	C5B-O5B-PA-O3
2	A	701	NDP	PA-O3-PN-O5D
2	B	701	NDP	C5B-O5B-PA-O2A
2	B	701	NDP	C5D-O5D-PN-O3
2	B	701	NDP	C5D-O5D-PN-O1N
3	B	702	UMP	C5'-O5'-P-OP2
3	B	702	UMP	C5'-O5'-P-OP3
2	B	701	NDP	C3D-C4D-C5D-O5D
2	B	701	NDP	O4B-C4B-C5B-O5B
3	B	702	UMP	C3'-C4'-C5'-O5'
3	B	702	UMP	O4'-C4'-C5'-O5'
2	B	701	NDP	C3B-C4B-C5B-O5B
4	B	703	U8Y	C20-C12-C13-C19
4	A	703	U8Y	C20-C12-C13-C19
2	B	701	NDP	O4D-C4D-C5D-O5D
3	B	702	UMP	C5'-O5'-P-OP1
2	A	701	NDP	C3B-C4B-C5B-O5B
2	A	701	NDP	O4B-C4B-C5B-O5B
4	A	703	U8Y	C20-C12-C13-C14
2	B	701	NDP	C2D-C1D-N1N-C2N
4	A	703	U8Y	C11-C12-C13-C19
4	B	703	U8Y	C20-C12-C13-C14

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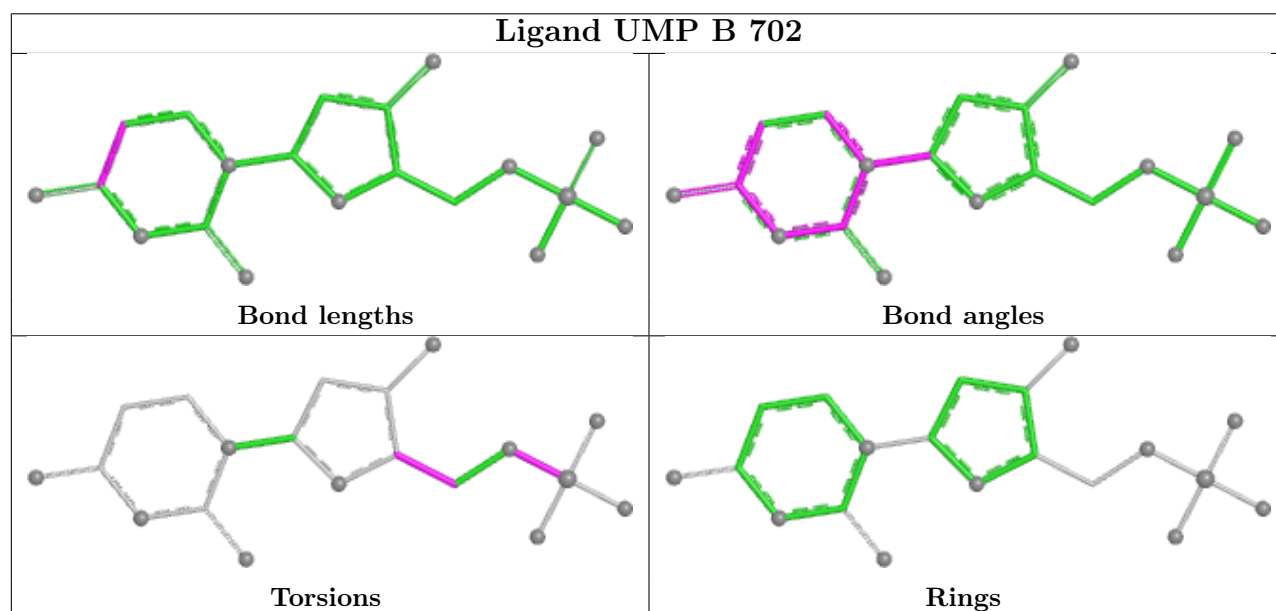
Mol	Chain	Res	Type	Atoms
2	A	701	NDP	O4D-C1D-N1N-C2N
2	B	701	NDP	O4D-C1D-N1N-C2N
4	B	703	U8Y	C11-C12-C13-C19
2	B	701	NDP	C2B-O2B-P2B-O1X
2	A	701	NDP	C2D-C1D-N1N-C2N
2	B	701	NDP	C2D-C1D-N1N-C6N
2	B	701	NDP	C2B-O2B-P2B-O3X

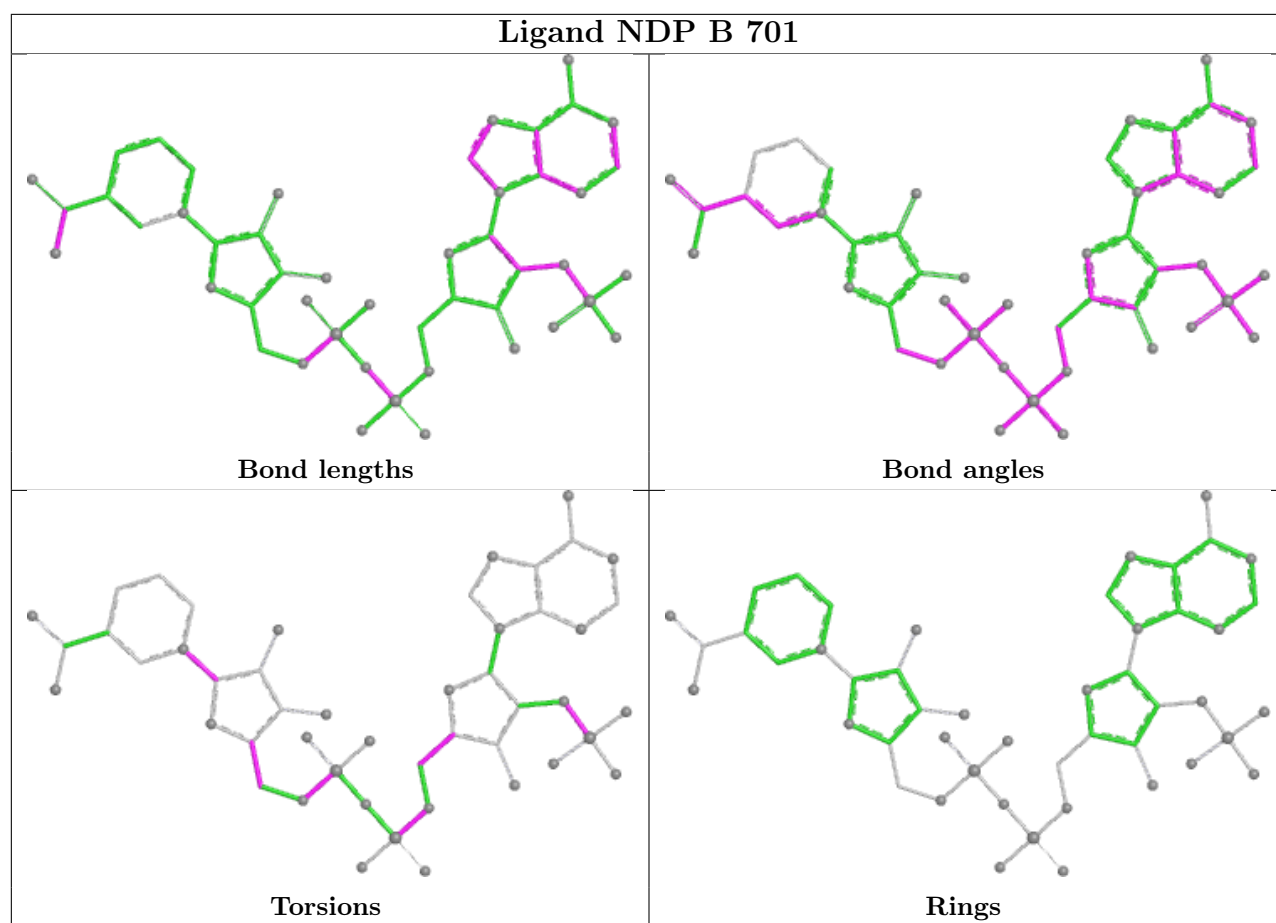
There are no ring outliers.

1 monomer is involved in 1 short contact:

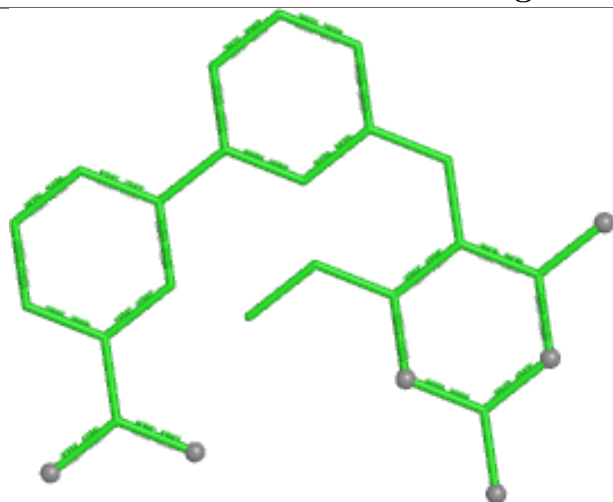
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	NDP	1	0

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.

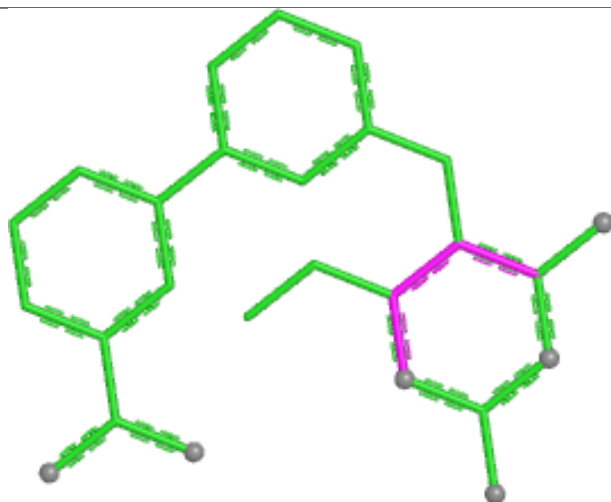




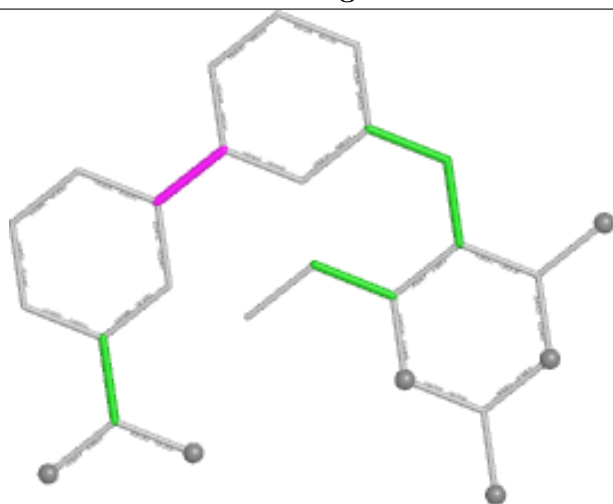
Ligand U8Y A 703



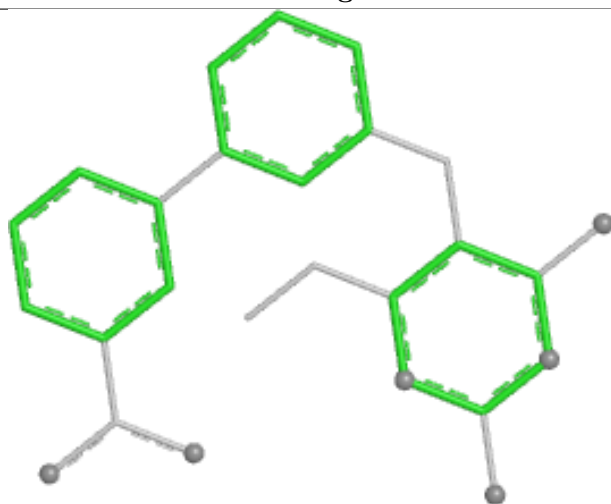
Bond lengths



Bond angles

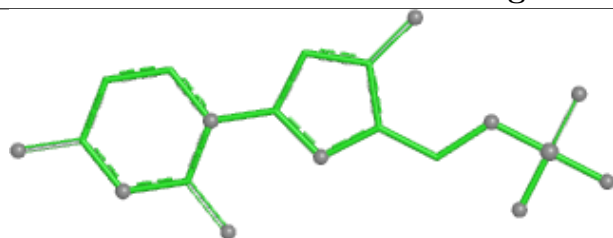


Torsions

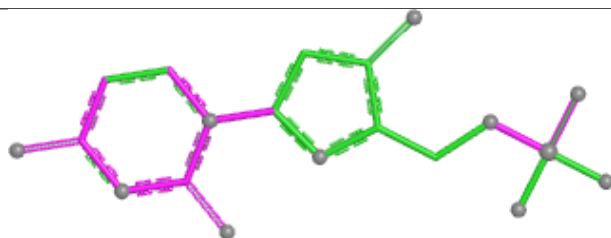


Rings

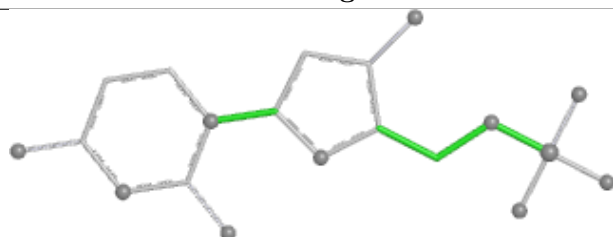
Ligand UMP A 702



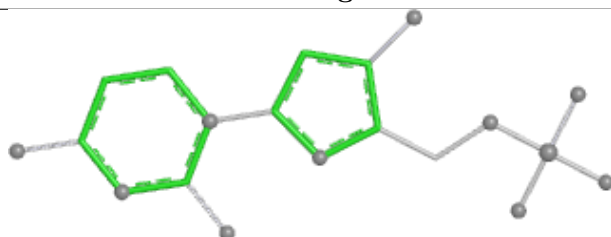
Bond lengths



Bond angles

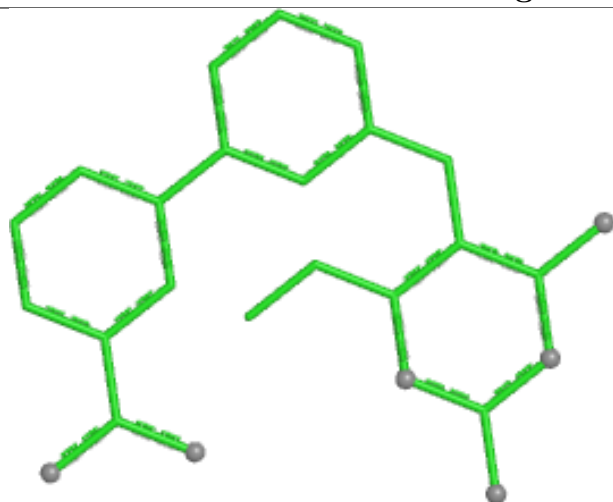


Torsions

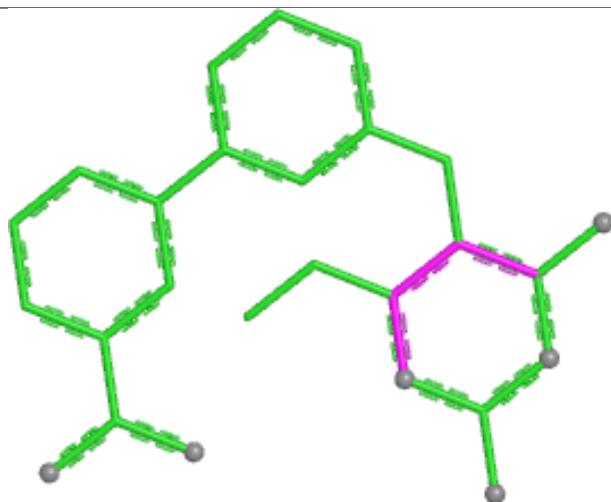


Rings

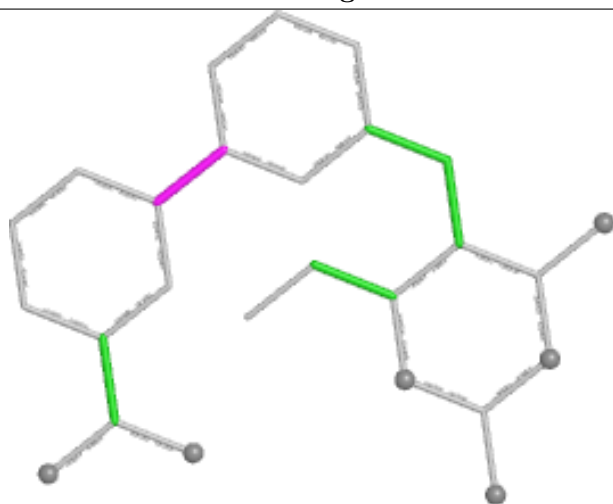
Ligand U8Y B 703



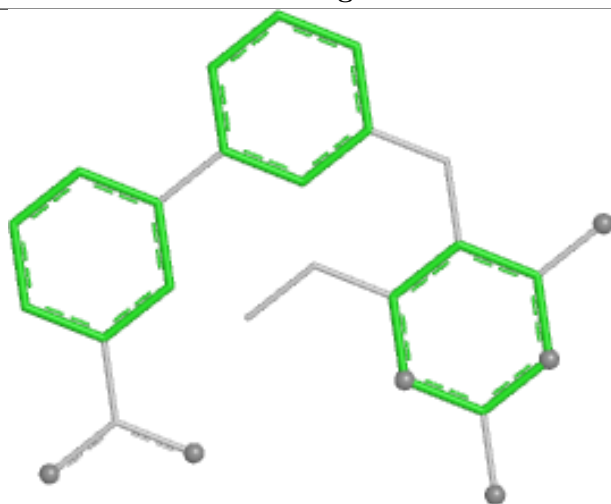
Bond lengths



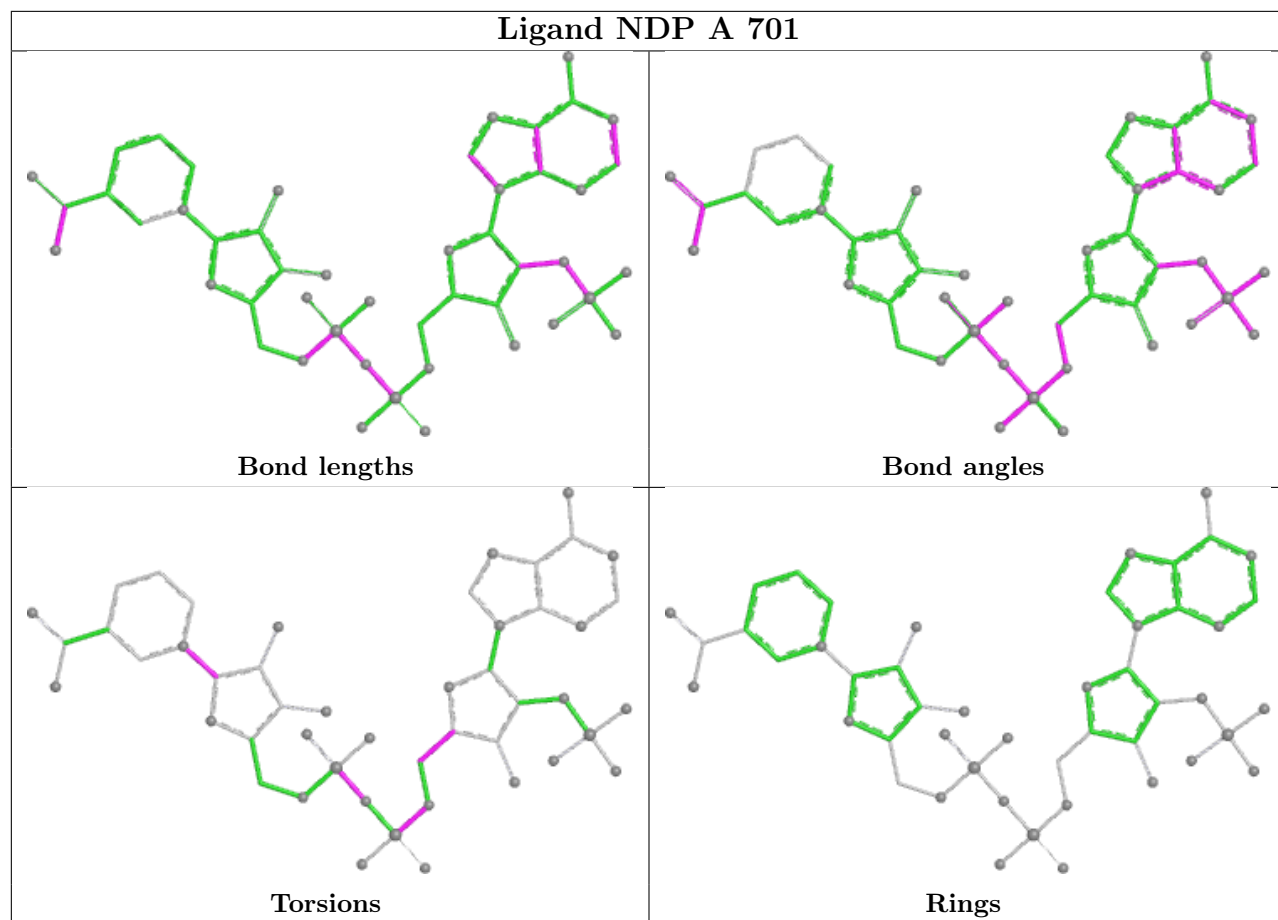
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	526/608 (86%)	-0.09	12 (2%) 61 63	15, 28, 56, 75	0
1	B	528/608 (86%)	0.17	21 (3%) 42 44	16, 32, 65, 95	0
All	All	1054/1216 (86%)	0.04	33 (3%) 51 53	15, 29, 62, 95	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	PHE	4.8
1	B	303	ASN	4.7
1	A	303	ASN	4.1
1	B	131	LEU	4.1
1	B	135	ASP	3.2
1	A	346	THR	3.1
1	A	309	PRO	3.1
1	B	106	ARG	3.0
1	A	348	VAL	2.9
1	B	132	LYS	2.9
1	A	307	ILE	2.8
1	A	347	GLY	2.8
1	A	605	ASP	2.7
1	B	107	THR	2.7
1	A	85	THR	2.7
1	B	285	GLU	2.6
1	B	137	ASP	2.6
1	A	343	SER	2.6
1	B	128	SER	2.6
1	B	346	THR	2.5
1	B	142	ILE	2.5
1	B	109	TRP	2.4
1	B	110	GLU	2.4
1	A	449	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	307	ILE	2.3
1	B	75	TYR	2.3
1	B	348	VAL	2.3
1	B	345	ARG	2.2
1	B	143	ILE	2.2
1	B	144	ASN	2.2
1	A	286	GLU	2.1
1	A	82	ASN	2.1
1	B	127	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

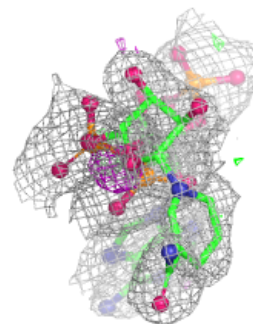
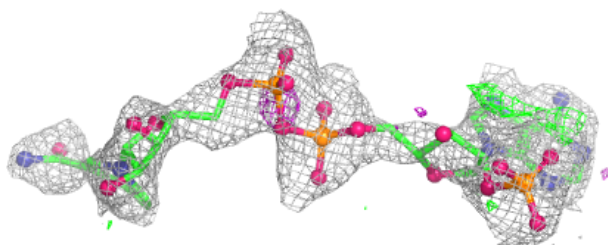
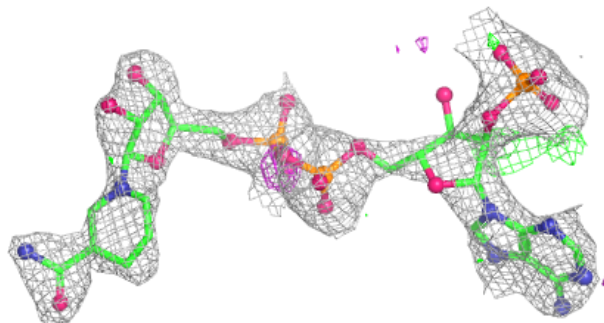
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NDP	B	701	48/48	0.83	0.13	36,62,72,75	0
4	U8Y	B	703	26/26	0.87	0.10	33,41,55,60	0
5	GOL	A	704	6/6	0.88	0.11	22,26,27,32	0
5	GOL	B	704	6/6	0.90	0.10	23,27,29,32	0
4	U8Y	A	703	26/26	0.92	0.08	17,22,32,35	0
3	UMP	B	702	20/20	0.92	0.10	27,36,42,43	0
3	UMP	A	702	20/20	0.94	0.09	28,33,38,40	0
2	NDP	A	701	48/48	0.95	0.07	20,32,37,38	0

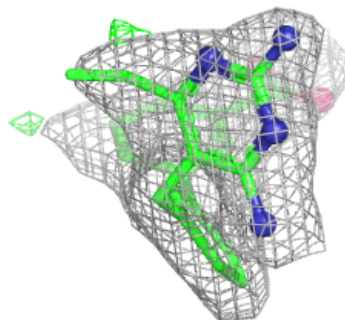
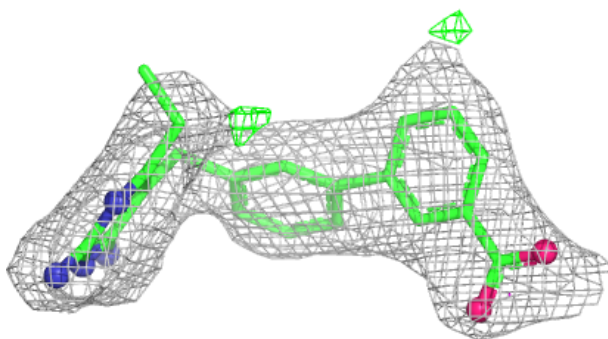
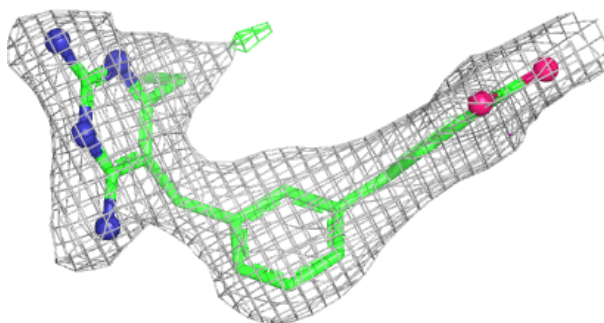
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

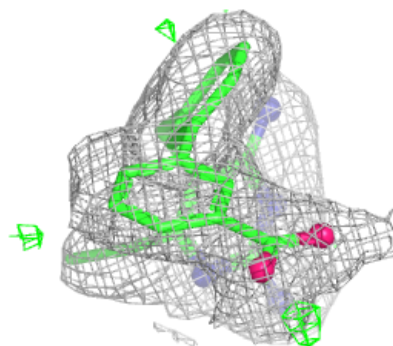
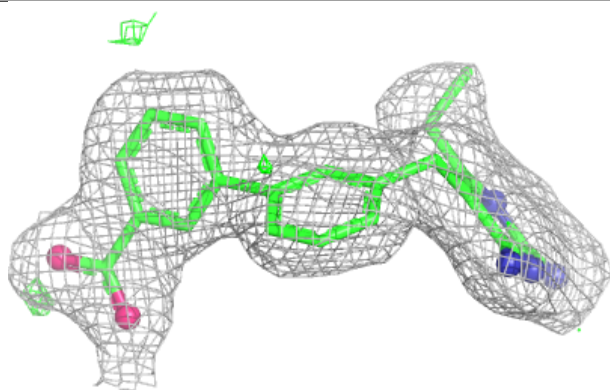
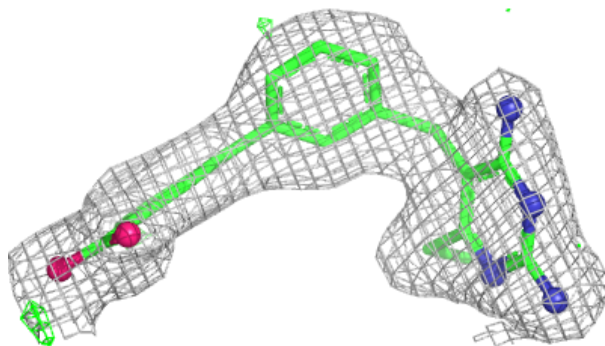
**Electron density around U8Y B 703:**

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



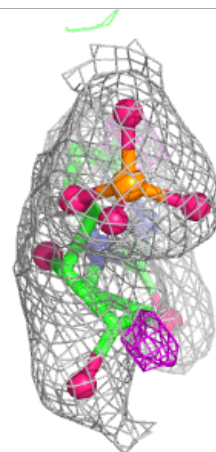
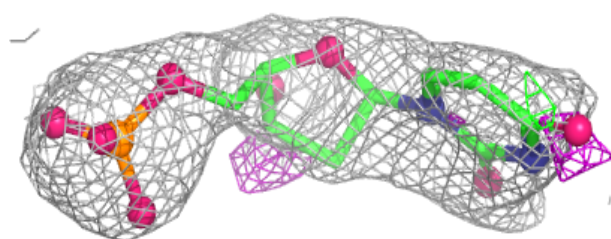
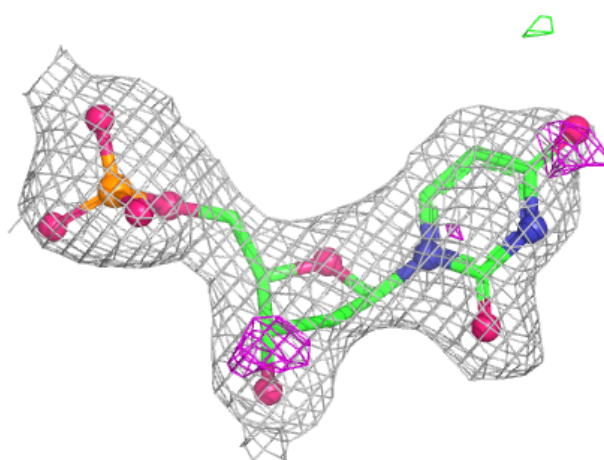
Electron density around U8Y A 703:

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



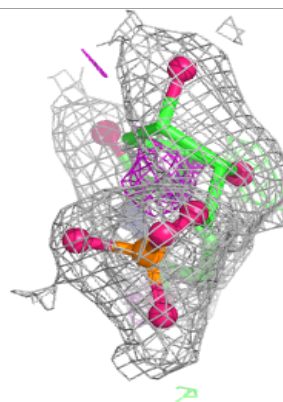
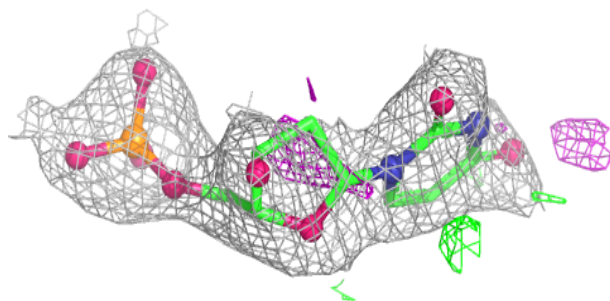
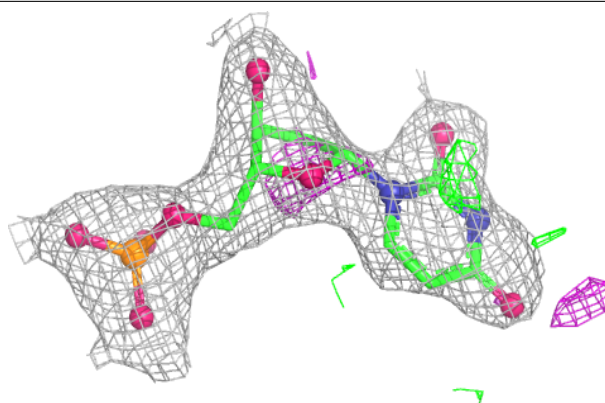
Electron density around UMP B 702:

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

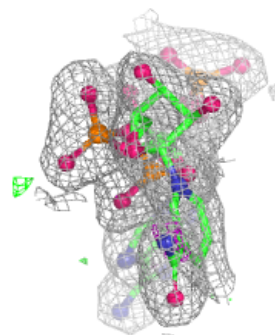
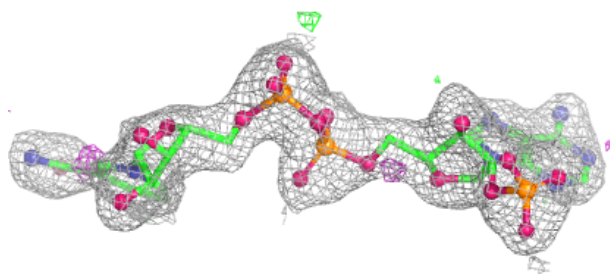
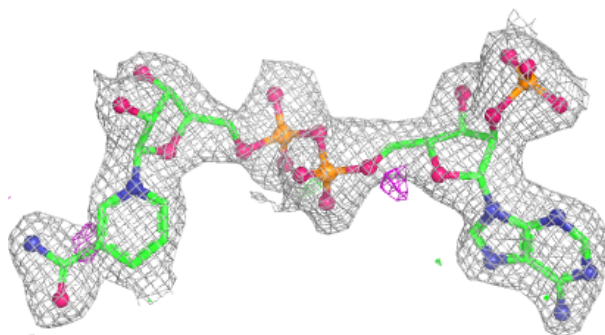


Electron density around UMP A 702:

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

**Electron density around NDP 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.