



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2022 – 08:14 AM JST

PDB ID : 7FGW  
Title : Toxoplasma gondii dihydrofolate reductase thymidylate synthase (TgDHFR-TS) complexed with pyrimethamine, NADPH and dUMP  
Authors : Vanichtanankul, J.; Yoomuang, A.; Taweechai, S.; Saeyang, T.; Yuvaniyama, Y.; Tarnchompoo, B.; Yuthavong, Y.; Kamchonwongpaisan, S.  
Deposited on : 2021-07-28  
Resolution : 2.15 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

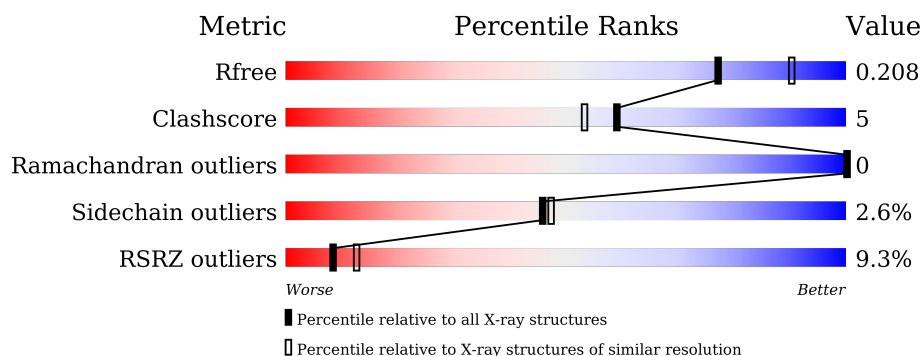
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	610	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	610	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	610	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	610	<div> <div>10%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>

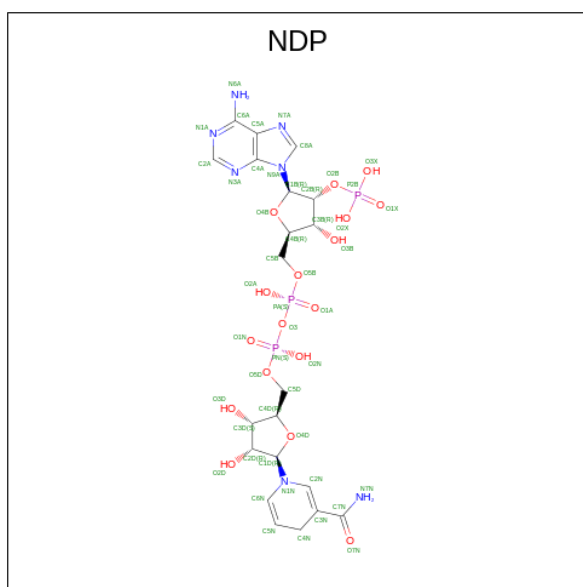


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total 4460	C 2837	N 785	O 812	S 26	0	0	0
1	B	560	Total 4473	C 2845	N 788	O 815	S 25	0	0	0
1	C	556	Total 4441	C 2827	N 783	O 806	S 25	0	0	0
1	D	559	Total 4465	C 2841	N 786	O 812	S 26	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



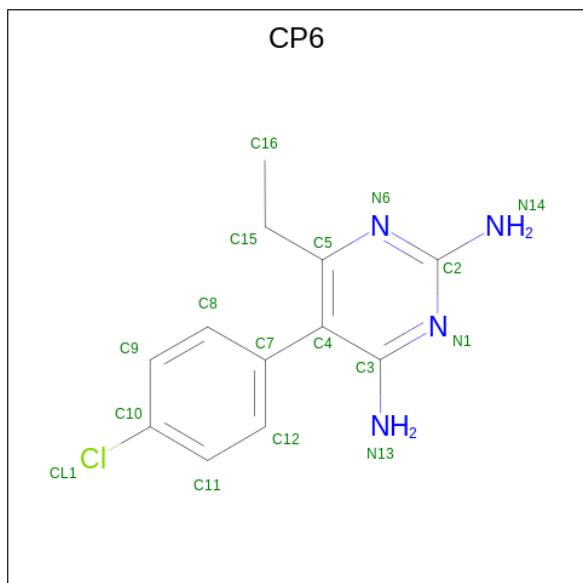
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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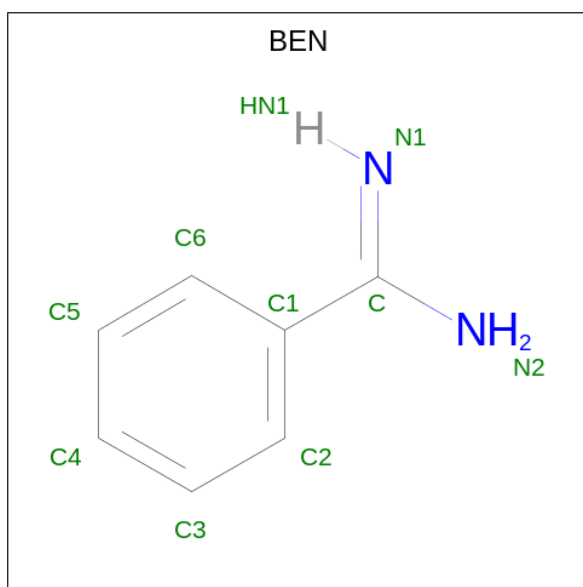
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-(4-CHLORO-PHENYL)-6-ETHYL-PYRIMIDINE-2,4-DIAMINE (three-letter code: CP6) (formula:  $C_{12}H_{13}ClN_4$ ) (labeled as "Ligand of Interest" by depositor).



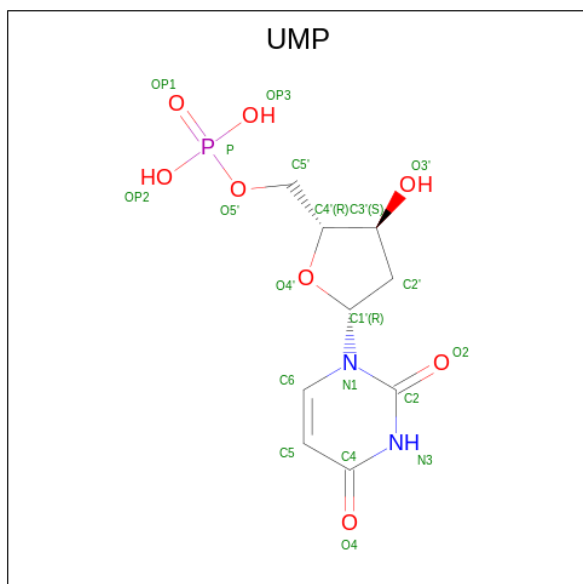
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			17	12	1	4		
3	B	1	Total	C	Cl	N	0	0
			17	12	1	4		
3	C	1	Total	C	Cl	N	0	0
			17	12	1	4		
3	D	1	Total	C	Cl	N	0	0
			17	12	1	4		

- Molecule 4 is BENZAMIDINE (three-letter code: BEN) (formula:  $C_7H_8N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			9	7	2		
4	C	1	Total	C	N	0	0
			9	7	2		

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



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

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

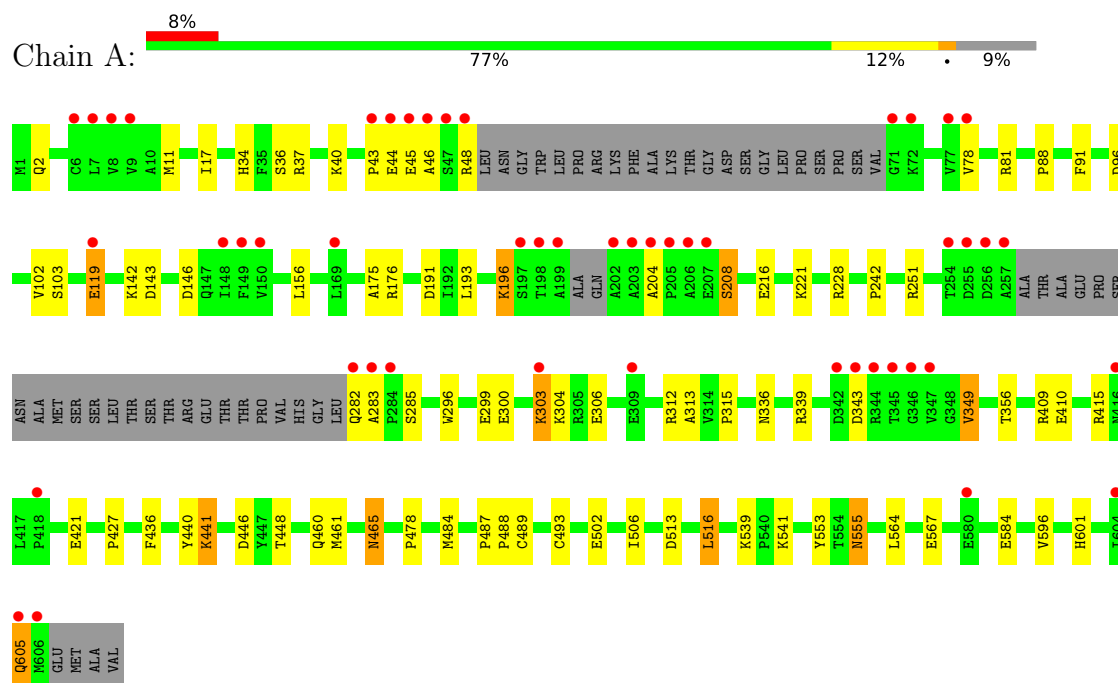
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	394	Total	O	0	0
			394	394		
6	B	397	Total	O	0	0
			397	397		
6	C	414	Total	O	0	0
			414	414		
6	D	326	Total	O	0	0
			326	326		

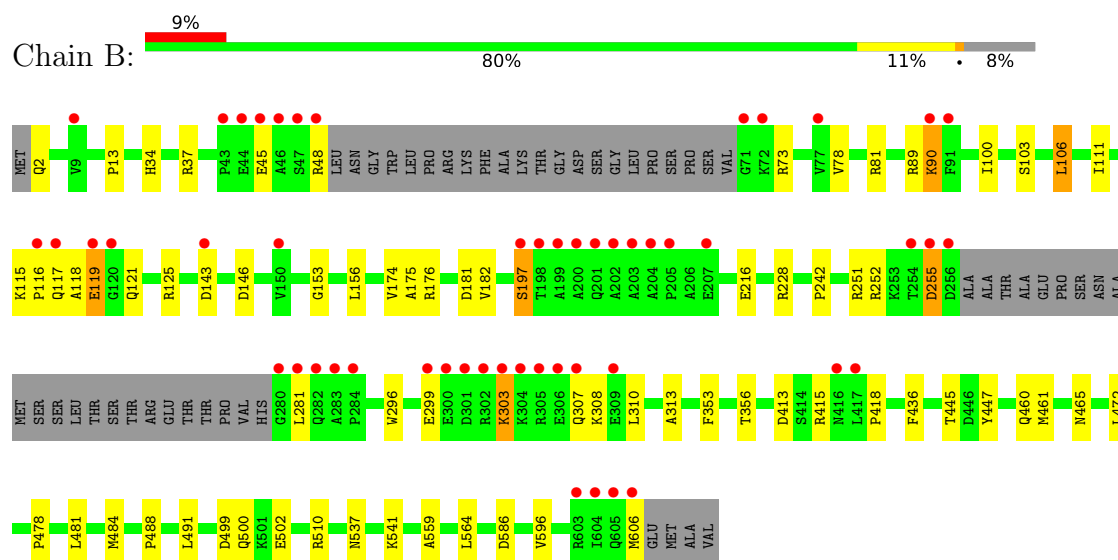
### 3 Residue-property plots

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.


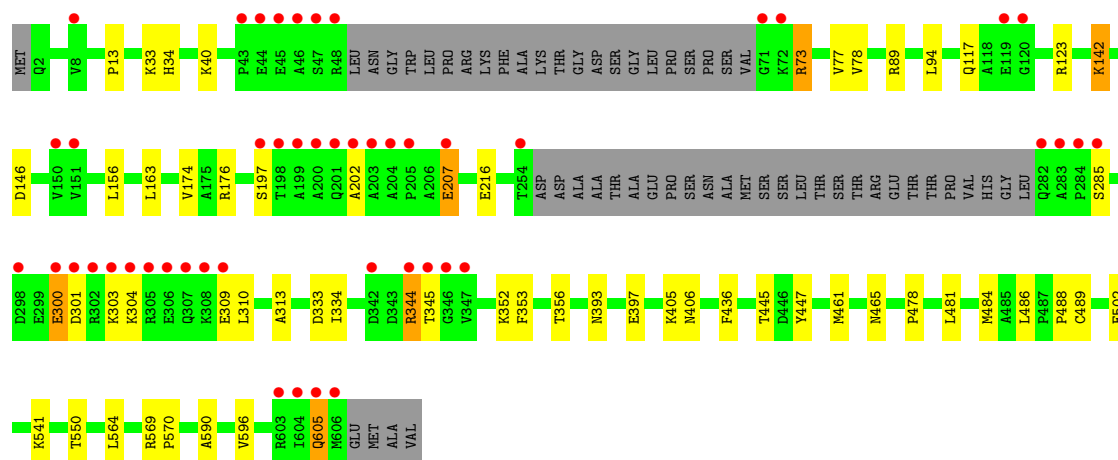
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase




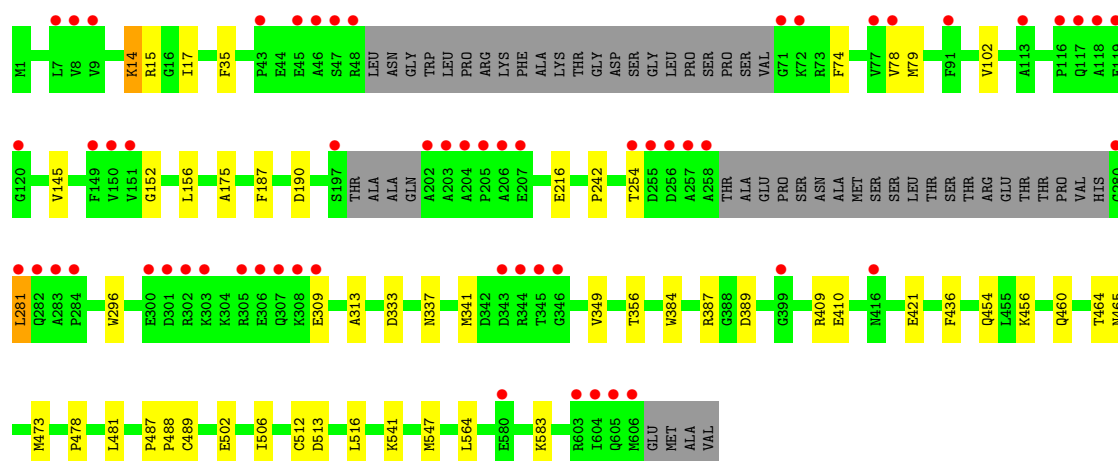
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



## ● Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain C:  8% 81% 9% 9%

## ● Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain D:  10% 83% 8% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.28Å 101.12Å 107.21Å 85.45° 83.70° 84.25°	Depositor
Resolution (Å)	29.29 – 2.15 29.29 – 2.15	Depositor EDS
% Data completeness (in resolution range)	87.2 (29.29-2.15) 87.2 (29.29-2.15)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.160 , 0.209 0.160 , 0.208	Depositor DCC
$R_{free}$ test set	6943 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: BEN, NDP, UMP, CP6

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	0.45	0/4566	0.63	0/6181
1	B	0.46	0/4580	0.63	0/6202
1	C	0.45	0/4548	0.62	0/6159
1	D	0.43	0/4571	0.61	0/6187
All	All	0.45	0/18265	0.62	0/24729

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	4460	0	4420	60	0
1	B	4473	0	4431	48	0
1	C	4441	0	4403	39	0
1	D	4465	0	4427	34	0
2	A	48	0	26	2	0
2	B	48	0	26	2	0
2	C	48	0	26	0	0
2	D	48	0	26	2	0
3	A	17	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	13	0	0
3	C	17	0	13	1	0
3	D	17	0	13	2	0
4	A	9	0	7	1	0
4	C	9	0	7	2	0
5	A	20	0	11	0	0
5	B	20	0	11	0	0
5	C	20	0	11	0	0
5	D	20	0	11	0	0
6	A	394	0	0	12	0
6	B	397	0	0	7	1
6	C	414	0	0	5	1
6	D	326	0	0	6	0
All	All	19728	0	17895	170	1

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 5.

All (170) 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:299:GLU:OE1	1:B:37:ARG:NH1	2.16	0.76
1:A:421:GLU:OE2	6:A:802:HOH:O	2.04	0.76
1:A:96:ASP:OD2	6:A:801:HOH:O	2.03	0.75
1:D:465:ASN:OD1	6:D:801:HOH:O	2.08	0.71
1:B:106:LEU:HD23	1:B:111:ILE:HD11	1.74	0.70
1:B:73:ARG:NH1	1:B:143:ASP:O	2.25	0.70
1:D:513:ASP:OD2	1:D:516:LEU:HB2	1.92	0.70
1:A:539:LYS:NZ	6:A:806:HOH:O	2.19	0.68
1:A:175:ALA:HB3	1:A:242:PRO:HG2	1.74	0.68
1:B:465:ASN:ND2	6:B:805:HOH:O	2.25	0.67
1:C:216:GLU:OE1	1:C:216:GLU:N	2.24	0.67
1:D:175:ALA:HB3	1:D:242:PRO:HG2	1.75	0.66
1:D:421:GLU:OE2	6:D:802:HOH:O	2.14	0.66
1:D:456:LYS:NZ	6:D:805:HOH:O	2.28	0.66
1:B:460:GLN:NE2	6:B:807:HOH:O	2.28	0.65
1:A:584:GLU:OE2	6:A:803:HOH:O	2.15	0.64
1:A:436:PHE:CE1	1:B:478:PRO:HD2	2.34	0.63
1:C:73:ARG:NH1	1:C:146:ASP:OD1	2.30	0.62
1:A:567:GLU:O	1:A:601:HIS:HE1	1.82	0.62
1:C:590:ALA:O	6:C:801:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:GLU:OE1	6:C:802:HOH:O	2.16	0.61
1:C:436:PHE:CE1	1:D:478:PRO:HD2	2.36	0.60
1:B:78:VAL:HG12	1:B:156:LEU:HD21	1.84	0.60
1:A:441:LYS:NZ	6:A:816:HOH:O	2.35	0.59
1:C:13:PRO:HD3	1:C:174:VAL:O	2.02	0.59
1:A:300:GLU:O	1:A:304:LYS:HG2	2.02	0.58
1:B:252:ARG:O	1:B:255:ASP:HB2	2.04	0.58
1:A:119:GLU:O	6:A:804:HOH:O	2.17	0.58
1:A:191:ASP:HB3	1:A:196:LYS:NZ	2.19	0.58
1:A:343:ASP:HB3	1:A:349:VAL:HG21	1.85	0.58
1:A:605:GLN:HA	1:A:605:GLN:HE21	1.69	0.57
1:B:2:GLN:N	6:B:812:HOH:O	2.38	0.57
1:C:356:THR:HG21	1:D:356:THR:HG21	1.87	0.57
1:B:460:GLN:NE2	6:B:811:HOH:O	2.37	0.56
1:C:478:PRO:HD2	1:D:436:PHE:CE1	2.42	0.55
1:C:461:MET:SD	1:C:465:ASN:HB3	2.46	0.55
1:A:282:GLN:NE2	6:A:818:HOH:O	2.39	0.55
1:A:228:ARG:NH2	1:A:251:ARG:HH12	2.05	0.55
1:B:81:ARG:HB2	1:B:103:SER:HB2	1.89	0.55
1:B:461:MET:SD	1:B:465:ASN:HB3	2.48	0.54
1:A:11:MET:SD	1:A:193:LEU:HD11	2.48	0.54
1:B:303:LYS:O	1:B:307:GLN:HG2	2.07	0.53
1:D:281:LEU:H	1:D:281:LEU:HD23	1.73	0.53
1:A:478:PRO:HD2	1:B:436:PHE:CE1	2.44	0.53
1:A:48:ARG:NH2	6:A:807:HOH:O	2.26	0.53
1:B:484:MET:SD	1:B:488:PRO:HD3	2.48	0.53
1:B:175:ALA:HB3	1:B:242:PRO:HG2	1.89	0.53
1:A:356:THR:HG21	1:B:356:THR:HG21	1.91	0.53
1:B:478:PRO:HA	1:B:481:LEU:HG	1.90	0.53
1:B:13:PRO:HD3	1:B:174:VAL:O	2.09	0.52
1:C:334:ILE:HD11	1:C:550:THR:HG22	1.90	0.52
1:C:197:SER:O	1:C:202:ALA:HB2	2.09	0.52
1:A:228:ARG:HH21	1:A:251:ARG:HH12	1.56	0.52
1:D:333:ASP:OD1	1:D:337:ASN:ND2	2.39	0.52
1:B:45:GLU:O	1:B:48:ARG:NH1	2.39	0.52
1:A:313:ALA:HB2	1:A:564:LEU:HG	1.91	0.51
1:A:502:GLU:HB3	1:A:541:LYS:HB2	1.91	0.51
1:C:77:VAL:HG21	1:C:94:LEU:HD12	1.92	0.51
1:C:393:ASN:O	1:C:397:GLU:HG3	2.10	0.50
1:D:387:ARG:NH1	6:D:817:HOH:O	2.43	0.50
1:C:333:ASP:OD2	1:C:352:LYS:HE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASP:OD1	6:A:805:HOH:O	2.19	0.50
1:A:216:GLU:OE1	1:A:216:GLU:N	2.33	0.50
1:A:78:VAL:HG12	1:A:156:LEU:HD21	1.93	0.50
1:D:216:GLU:OE1	1:D:216:GLU:N	2.28	0.49
1:D:478:PRO:HA	1:D:481:LEU:HG	1.94	0.49
1:B:586:ASP:OD2	6:B:801:HOH:O	2.20	0.49
1:B:559:ALA:HA	1:B:606:MET:HG3	1.94	0.48
1:A:191:ASP:HB3	1:A:196:LYS:HZ1	1.79	0.48
1:A:312:ARG:HG2	1:A:315:PRO:HB3	1.96	0.48
2:B:701:NDP:H8A	2:B:701:NDP:H52A	1.96	0.47
1:A:513:ASP:OD2	1:A:516:LEU:HB2	2.15	0.47
1:C:156:LEU:HA	1:C:156:LEU:HD12	1.67	0.47
1:C:304:LYS:NZ	6:C:821:HOH:O	2.46	0.47
1:D:583:LYS:NZ	6:D:819:HOH:O	2.47	0.47
1:A:296:TRP:CZ2	1:B:34:HIS:HB2	2.50	0.47
3:A:702:CP6:C10	4:A:703:BEN:H5	2.45	0.46
1:B:502:GLU:HB3	1:B:541:LYS:HB2	1.97	0.46
1:B:197:SER:OG	6:B:802:HOH:O	2.21	0.46
1:B:118:ALA:HB3	1:B:121:GLN:HG3	1.97	0.46
1:C:40:LYS:NZ	6:C:815:HOH:O	2.47	0.46
1:C:484:MET:SD	1:C:488:PRO:HD3	2.56	0.46
1:A:43:PRO:HA	1:A:46:ALA:HB3	1.97	0.46
1:A:102:VAL:O	2:A:701:NDP:H1B	2.16	0.45
1:C:94:LEU:HD21	4:C:703:BEN:H4	1.98	0.45
1:D:78:VAL:HG12	1:D:156:LEU:HD21	1.98	0.45
1:A:336:ASN:ND2	6:A:810:HOH:O	2.31	0.45
1:B:313:ALA:HB2	1:B:564:LEU:HG	1.99	0.45
1:B:181:ASP:OD1	1:B:182:VAL:HG23	2.16	0.45
1:B:413:ASP:OD1	1:B:418:PRO:HA	2.16	0.45
1:C:123:ARG:HD3	6:C:1143:HOH:O	2.16	0.45
1:C:300:GLU:HG3	1:C:301:ASP:N	2.32	0.45
1:D:74:PHE:O	1:D:145:VAL:HA	2.17	0.45
1:A:555:ASN:OD1	1:A:555:ASN:N	2.43	0.45
1:C:605:GLN:H	1:C:605:GLN:HG2	1.66	0.45
1:D:512:CYS:SG	1:D:547:MET:HG2	2.57	0.45
1:C:478:PRO:HA	1:C:481:LEU:HG	1.99	0.45
1:A:17:ILE:O	2:A:701:NDP:H2N	2.17	0.44
1:C:313:ALA:HB2	1:C:564:LEU:HG	1.99	0.44
1:A:282:GLN:HE21	1:A:283:ALA:H	1.64	0.44
1:A:460:GLN:HB3	6:A:1097:HOH:O	2.16	0.44
1:C:300:GLU:HA	1:C:303:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:CYS:HA	1:A:506:ILE:O	2.18	0.44
1:A:446:ASP:OD1	1:A:448:THR:OG1	2.23	0.44
1:B:303:LYS:NZ	6:B:827:HOH:O	2.50	0.44
1:B:491:LEU:HD21	1:B:510:ARG:HB3	1.99	0.44
1:B:73:ARG:HB3	1:B:146:ASP:OD1	2.18	0.44
1:C:34:HIS:HB2	1:D:296:TRP:CZ2	2.53	0.44
1:A:142:LYS:HE3	1:A:142:LYS:HB2	1.75	0.43
1:A:204:ALA:O	1:A:208:SER:N	2.42	0.43
1:B:115:LYS:HB2	1:B:116:PRO:HD2	1.99	0.43
1:C:502:GLU:HB3	1:C:541:LYS:HB2	1.99	0.43
1:C:569:ARG:HB3	1:C:570:PRO:HD2	2.01	0.43
1:B:445:THR:HB	1:B:447:TYR:CZ	2.53	0.43
1:C:78:VAL:HG12	1:C:156:LEU:HD21	2.00	0.43
1:A:303:LYS:O	1:A:306:GLU:HG2	2.19	0.43
1:C:142:LYS:HB3	1:C:142:LYS:HE2	1.86	0.43
1:D:79:MET:HA	1:D:152:GLY:O	2.19	0.43
1:D:313:ALA:HB2	1:D:564:LEU:HG	2.00	0.43
1:A:176:ARG:HD2	1:A:596:VAL:CG1	2.48	0.42
1:C:310:LEU:HD23	1:C:310:LEU:HA	1.81	0.42
1:A:221:LYS:HB3	1:A:221:LYS:HE3	1.83	0.42
1:A:415:ARG:HD2	6:A:995:HOH:O	2.18	0.42
1:C:406:ASN:ND2	1:C:486:LEU:HD21	2.34	0.42
1:A:37:ARG:NH1	1:B:299:GLU:OE1	2.50	0.42
1:A:282:GLN:NE2	1:A:283:ALA:H	2.16	0.42
1:C:344:ARG:HG2	1:C:345:THR:N	2.35	0.42
1:D:17:ILE:O	2:D:701:NDP:H2N	2.20	0.42
1:A:45:GLU:O	1:A:48:ARG:HG3	2.20	0.42
1:B:90:LYS:H	1:B:90:LYS:HG3	1.39	0.42
1:B:415:ARG:NH1	1:B:484:MET:O	2.50	0.42
1:D:454:GLN:HB2	1:D:473:MET:HG3	2.01	0.42
1:C:176:ARG:HD2	1:C:596:VAL:CG1	2.50	0.41
1:D:502:GLU:HB3	1:D:541:LYS:HB2	2.01	0.41
1:A:81:ARG:HB2	1:A:103:SER:HB2	2.02	0.41
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.73	0.41
1:A:427:PRO:HB3	1:A:440:TYR:HB2	2.02	0.41
1:B:153:GLY:HA3	2:B:701:NDP:O5D	2.19	0.41
1:D:35:PHE:CZ	3:D:702:CP6:H12	2.55	0.41
1:D:384:TRP:CD1	1:D:389:ASP:HB3	2.54	0.41
1:A:339:ARG:NH1	1:B:500:GLN:OE1	2.49	0.41
1:B:119:GLU:H	1:B:119:GLU:CD	2.22	0.41
1:A:487:PRO:HA	1:A:488:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HD12	1:B:125:ARG:HB2	2.02	0.41
1:B:176:ARG:HD2	1:B:596:VAL:CG1	2.50	0.41
1:D:102:VAL:O	2:D:701:NDP:H1B	2.21	0.41
1:A:461:MET:SD	1:A:465:ASN:HB3	2.60	0.41
1:C:353:PHE:CE2	1:D:506:ILE:HG13	2.56	0.41
1:C:445:THR:HB	1:C:447:TYR:CZ	2.55	0.41
3:C:702:CP6:C8	3:C:702:CP6:H152	2.51	0.41
1:D:460:GLN:O	1:D:464:THR:HG23	2.20	0.41
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.90	0.41
1:B:216:GLU:H	1:B:216:GLU:CD	2.24	0.41
1:D:387:ARG:NH2	6:D:823:HOH:O	2.48	0.41
1:D:487:PRO:HA	1:D:488:PRO:HD3	1.97	0.41
1:A:88:PRO:HG2	1:A:91:PHE:HD2	1.85	0.41
1:C:94:LEU:CD2	4:C:703:BEN:H4	2.51	0.40
1:A:34:HIS:HB2	1:B:296:TRP:CZ2	2.57	0.40
1:A:36:SER:O	1:A:40:LYS:HB2	2.21	0.40
1:B:499:ASP:OD1	1:B:499:ASP:N	2.46	0.40
1:C:33:LYS:HE3	1:D:296:TRP:CE3	2.57	0.40
1:C:163:LEU:HD12	1:C:163:LEU:HA	1.89	0.40
1:A:484:MET:SD	1:A:488:PRO:HD3	2.61	0.40
1:A:506:ILE:HG13	1:B:353:PHE:CE2	2.57	0.40
1:D:187:PHE:CE1	1:D:190:ASP:HB3	2.56	0.40
1:A:349:VAL:HG13	1:A:553:TYR:CD1	2.57	0.40
1:D:14:LYS:O	1:D:15:ARG:HB2	2.21	0.40
1:D:35:PHE:CE1	3:D:702:CP6:H12	2.56	0.40
3:A:702:CP6:C8	3:A:702:CP6:H152	2.51	0.40
1:B:228:ARG:HG3	1:B:251:ARG:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1122:HOH:O	6:C:1177:HOH:O[1_646]	2.19	0.01

## 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	550/610 (90%)	535 (97%)	15 (3%)	0	100	100
1	B	554/610 (91%)	536 (97%)	18 (3%)	0	100	100
1	C	550/610 (90%)	535 (97%)	15 (3%)	0	100	100
1	D	551/610 (90%)	536 (97%)	15 (3%)	0	100	100
All	All	2205/2440 (90%)	2142 (97%)	63 (3%)	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	483/525 (92%)	466 (96%)	17 (4%)	36	34
1	B	484/525 (92%)	471 (97%)	13 (3%)	44	46
1	C	480/525 (91%)	468 (98%)	12 (2%)	47	49
1	D	483/525 (92%)	474 (98%)	9 (2%)	57	61
All	All	1930/2100 (92%)	1879 (97%)	51 (3%)	46	47

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

Mol	Chain	Res	Type
1	A	2	GLN
1	A	44	GLU
1	A	119	GLU
1	A	146	ASP
1	A	196	LYS
1	A	208	SER
1	A	285	SER
1	A	303	LYS

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Mol	Chain	Res	Type
1	A	349	VAL
1	A	409	ARG
1	A	410	GLU
1	A	441	LYS
1	A	465	ASN
1	A	489	CYS
1	A	516	LEU
1	A	555	ASN
1	A	605	GLN
1	B	89	ARG
1	B	90	LYS
1	B	106	LEU
1	B	117	GLN
1	B	119	GLU
1	B	197	SER
1	B	255	ASP
1	B	281	LEU
1	B	303	LYS
1	B	308	LYS
1	B	310	LEU
1	B	472	LEU
1	B	537	ASN
1	C	73	ARG
1	C	89	ARG
1	C	117	GLN
1	C	142	LYS
1	C	207	GLU
1	C	285	SER
1	C	300	GLU
1	C	309	GLU
1	C	344	ARG
1	C	405	LYS
1	C	489	CYS
1	C	605	GLN
1	D	14	LYS
1	D	254	THR
1	D	281	LEU
1	D	309	GLU
1	D	341	MET
1	D	349	VAL
1	D	409	ARG
1	D	410	GLU

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Mol	Chain	Res	Type
1	D	489	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	GLN
1	A	465	ASN
1	A	601	HIS
1	A	605	GLN
1	B	2	GLN
1	B	460	GLN
1	B	465	ASN
1	C	2	GLN
1	C	416	ASN
1	C	605	GLN
1	D	282	GLN
1	D	307	GLN
1	D	460	GLN
1	D	556	HIS

### 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](#)

14 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
5	UMP	B	703	-	21,21,21	0.89	1 (4%)	31,31,31	1.48	5 (16%)
3	CP6	B	702	-	17,18,18	1.99	4 (23%)	21,25,25	2.23	6 (28%)
4	BEN	A	703	-	9,9,9	1.26	1 (11%)	7,11,11	1.27	1 (14%)
4	BEN	C	703	-	9,9,9	1.40	1 (11%)	7,11,11	1.06	0
5	UMP	A	704	-	21,21,21	0.83	1 (4%)	31,31,31	1.44	4 (12%)
5	UMP	C	704	-	21,21,21	0.82	0	31,31,31	1.42	4 (12%)
2	NDP	A	701	-	45,52,52	2.30	8 (17%)	53,80,80	1.43	7 (13%)
2	NDP	B	701	-	45,52,52	2.16	8 (17%)	53,80,80	1.42	10 (18%)
2	NDP	C	701	-	45,52,52	2.29	7 (15%)	53,80,80	1.41	9 (16%)
3	CP6	D	702	-	17,18,18	2.15	4 (23%)	21,25,25	2.57	6 (28%)
3	CP6	A	702	-	17,18,18	2.09	4 (23%)	21,25,25	2.20	6 (28%)
3	CP6	C	702	-	17,18,18	2.09	4 (23%)	21,25,25	2.25	6 (28%)
5	UMP	D	703	-	21,21,21	0.85	0	31,31,31	1.46	6 (19%)
2	NDP	D	701	-	45,52,52	2.33	8 (17%)	53,80,80	1.47	9 (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
5	UMP	B	703	-	-	5/10/22/22	0/2/2/2
3	CP6	B	702	-	-	1/2/6/6	0/2/2/2
4	BEN	A	703	-	-	3/4/4/4	0/1/1/1
4	BEN	C	703	-	-	4/4/4/4	0/1/1/1
5	UMP	A	704	-	-	1/10/22/22	0/2/2/2
5	UMP	C	704	-	-	2/10/22/22	0/2/2/2
2	NDP	A	701	-	-	2/30/77/77	0/5/5/5
2	NDP	B	701	-	-	5/30/77/77	0/5/5/5
2	NDP	C	701	-	-	2/30/77/77	0/5/5/5
3	CP6	D	702	-	-	1/2/6/6	0/2/2/2
3	CP6	A	702	-	-	1/2/6/6	0/2/2/2
3	CP6	C	702	-	-	0/2/6/6	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	UMP	D	703	-	-	2/10/22/22	0/2/2/2
2	NDP	D	701	-	-	3/30/77/77	0/5/5/5

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NDP	P2B-O2B	12.82	1.83	1.59
2	C	701	NDP	P2B-O2B	12.53	1.83	1.59
2	D	701	NDP	P2B-O2B	12.28	1.82	1.59
2	B	701	NDP	P2B-O2B	11.12	1.80	1.59
3	D	702	CP6	C2-N14	5.81	1.45	1.33
3	A	702	CP6	C2-N14	5.57	1.45	1.33
3	C	702	CP6	C5-C4	-5.09	1.35	1.43
3	C	702	CP6	C2-N14	4.66	1.43	1.33
3	B	702	CP6	C2-N14	4.59	1.43	1.33
3	D	702	CP6	C5-C4	-4.26	1.36	1.43
3	A	702	CP6	C5-C4	-4.20	1.36	1.43
3	B	702	CP6	C5-C4	-4.02	1.37	1.43
4	C	703	BEN	C1-C	-3.77	1.40	1.47
2	D	701	NDP	O4B-C1B	3.62	1.46	1.41
4	A	703	BEN	C1-C	-3.44	1.41	1.47
2	D	701	NDP	PN-O5D	3.39	1.73	1.59
2	B	701	NDP	C7N-N7N	3.39	1.42	1.33
2	C	701	NDP	C3D-C4D	3.15	1.61	1.53
3	B	702	CP6	C3-N13	3.14	1.45	1.34
3	D	702	CP6	C3-N13	3.11	1.45	1.34
2	B	701	NDP	PN-O5D	3.07	1.71	1.59
2	C	701	NDP	C7N-N7N	3.03	1.41	1.33
2	D	701	NDP	O2B-C2B	-3.02	1.33	1.44
3	C	702	CP6	C3-N13	3.02	1.45	1.34
3	A	702	CP6	C3-N13	2.94	1.44	1.34
2	B	701	NDP	O2B-C2B	-2.84	1.33	1.44
2	A	701	NDP	O2B-C2B	-2.79	1.33	1.44
2	D	701	NDP	C3B-C2B	2.79	1.59	1.52
3	D	702	CP6	C10-CL1	2.76	1.80	1.74
2	D	701	NDP	C7N-N7N	2.74	1.40	1.33
3	B	702	CP6	C10-CL1	2.60	1.80	1.74
3	A	702	CP6	C10-CL1	2.58	1.80	1.74
2	C	701	NDP	PN-O5D	2.56	1.69	1.59
2	B	701	NDP	O4B-C1B	2.54	1.44	1.41
2	A	701	NDP	PN-O5D	2.53	1.69	1.59
2	B	701	NDP	C2A-N1A	2.48	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	NDP	O4B-C1B	2.46	1.44	1.41
2	A	701	NDP	C7N-N7N	2.42	1.39	1.33
2	A	701	NDP	O3B-C3B	-2.38	1.37	1.43
2	B	701	NDP	C3B-C2B	2.37	1.58	1.52
2	A	701	NDP	C3B-C2B	2.35	1.58	1.52
2	A	701	NDP	C2A-N1A	2.33	1.38	1.33
2	D	701	NDP	C2A-N1A	2.23	1.38	1.33
2	C	701	NDP	O2B-C2B	-2.20	1.36	1.44
3	C	702	CP6	C10-CL1	2.16	1.79	1.74
5	B	703	UMP	C6-C5	2.14	1.40	1.35
5	A	704	UMP	C6-C5	2.13	1.40	1.35
2	C	701	NDP	C3B-C2B	2.09	1.57	1.52
2	D	701	NDP	C2A-N3A	2.05	1.35	1.32
2	B	701	NDP	O2D-C2D	-2.01	1.38	1.43
2	A	701	NDP	O4B-C1B	2.00	1.43	1.41

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	CP6	C2-N6-C5	6.44	121.61	116.24
3	D	702	CP6	C5-C4-C3	-6.40	117.61	123.34
3	A	702	CP6	C5-C4-C3	-6.07	117.91	123.34
3	C	702	CP6	C2-N6-C5	5.28	120.64	116.24
3	B	702	CP6	C2-N6-C5	5.09	120.48	116.24
3	C	702	CP6	C5-C4-C3	-5.00	118.87	123.34
3	B	702	CP6	C5-C4-C3	-4.98	118.89	123.34
3	A	702	CP6	C2-N6-C5	4.79	120.23	116.24
3	C	702	CP6	C16-C15-C5	-4.55	103.76	114.88
3	D	702	CP6	N6-C2-N1	-4.22	118.80	125.42
3	B	702	CP6	C4-C5-N6	-4.14	119.43	122.44
5	B	703	UMP	C4-N3-C2	-4.11	121.15	126.58
5	D	703	UMP	C4-N3-C2	-4.11	121.15	126.58
5	C	704	UMP	C4-N3-C2	-4.10	121.17	126.58
5	A	704	UMP	C4-N3-C2	-4.04	121.25	126.58
2	D	701	NDP	PN-O3-PA	-3.91	119.40	132.83
3	B	702	CP6	C16-C15-C5	-3.78	105.63	114.88
2	A	701	NDP	PN-O3-PA	-3.67	120.25	132.83
2	B	701	NDP	PN-O3-PA	-3.53	120.72	132.83
3	A	702	CP6	N6-C2-N1	-3.49	119.95	125.42
3	D	702	CP6	C16-C15-C5	-3.44	106.47	114.88
5	C	704	UMP	C5-C4-N3	3.42	119.96	114.84
5	A	704	UMP	N3-C2-N1	3.28	119.25	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	NDP	C3B-C2B-C1B	-3.25	96.78	102.89
5	B	703	UMP	N3-C2-N1	3.19	119.12	114.89
2	D	701	NDP	C3B-C2B-C1B	-3.17	96.92	102.89
2	A	701	NDP	C3B-C2B-C1B	-3.17	96.93	102.89
3	A	702	CP6	C16-C15-C5	-3.13	107.21	114.88
5	B	703	UMP	C5-C4-N3	3.09	119.46	114.84
2	B	701	NDP	C3B-C2B-C1B	-3.08	97.10	102.89
3	C	702	CP6	C4-C5-N6	-3.07	120.21	122.44
2	C	701	NDP	PN-O3-PA	-3.07	122.29	132.83
5	C	704	UMP	O4-C4-C5	-3.06	119.78	125.16
2	D	701	NDP	O2B-P2B-O1X	-3.04	97.67	109.39
5	D	703	UMP	N3-C2-N1	3.02	118.90	114.89
5	D	703	UMP	C5-C4-N3	2.96	119.27	114.84
3	D	702	CP6	C4-C5-N6	-2.92	120.32	122.44
5	A	704	UMP	C5-C4-N3	2.88	119.14	114.84
3	C	702	CP6	N14-C2-N1	2.86	121.70	117.25
5	D	703	UMP	O4-C4-C5	-2.83	120.18	125.16
5	B	703	UMP	O4-C4-C5	-2.81	120.23	125.16
3	C	702	CP6	N6-C2-N1	-2.80	121.03	125.42
2	A	701	NDP	O2B-P2B-O1X	-2.75	98.78	109.39
2	A	701	NDP	O3X-P2B-O2X	2.72	118.03	107.64
2	C	701	NDP	O3X-P2B-O2X	2.72	118.03	107.64
2	B	701	NDP	C2A-N1A-C6A	-2.71	114.12	118.75
5	C	704	UMP	N3-C2-N1	2.70	118.48	114.89
3	B	702	CP6	N6-C2-N1	-2.70	121.19	125.42
2	D	701	NDP	O3X-P2B-O2X	2.69	117.91	107.64
5	D	703	UMP	C1'-N1-C2	2.65	122.86	117.64
3	D	702	CP6	N14-C2-N1	2.63	121.35	117.25
2	B	701	NDP	O3X-P2B-O2X	2.60	117.58	107.64
2	C	701	NDP	O2B-P2B-O1X	-2.54	99.58	109.39
2	B	701	NDP	O2B-P2B-O1X	-2.50	99.74	109.39
2	A	701	NDP	O2B-C2B-C1B	-2.48	101.17	110.10
2	D	701	NDP	O3X-P2B-O2B	-2.48	94.88	105.99
4	A	703	BEN	C1-C-N2	2.43	121.72	118.05
3	A	702	CP6	C4-C5-N6	-2.40	120.70	122.44
2	C	701	NDP	PA-O5B-C5B	-2.38	107.69	121.68
2	A	701	NDP	O3X-P2B-O2B	-2.31	95.64	105.99
5	A	704	UMP	O4-C4-C5	-2.30	121.12	125.16
5	D	703	UMP	C1'-N1-C6	-2.29	117.02	121.55
2	B	701	NDP	O7N-C7N-N7N	-2.28	117.56	122.88
2	B	701	NDP	PA-O5B-C5B	-2.28	108.33	121.68
2	C	701	NDP	O3X-P2B-O2B	-2.26	95.86	105.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	NDP	O3X-P2B-O2B	-2.26	95.87	105.99
2	C	701	NDP	C2A-N1A-C6A	-2.23	114.94	118.75
2	D	701	NDP	PN-O5D-C5D	-2.19	108.84	121.68
5	B	703	UMP	O4'-C1'-N1	2.16	111.72	107.86
2	D	701	NDP	PA-O5B-C5B	-2.16	109.02	121.68
2	C	701	NDP	O7N-C7N-N7N	-2.14	117.89	122.88
2	B	701	NDP	PN-O5D-C5D	-2.12	109.24	121.68
3	A	702	CP6	N14-C2-N1	2.10	120.52	117.25
2	A	701	NDP	O2X-P2B-O1X	2.07	118.79	110.68
2	B	701	NDP	O2B-C2B-C1B	-2.07	102.66	110.10
3	B	702	CP6	N14-C2-N6	2.06	120.45	117.25
2	C	701	NDP	PN-O5D-C5D	-2.05	109.65	121.68
2	D	701	NDP	C2A-N1A-C6A	-2.04	115.27	118.75
2	D	701	NDP	O7N-C7N-N7N	-2.03	118.12	122.88

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	703	BEN	N2-C-C1-C2
4	C	703	BEN	N2-C-C1-C6
5	B	703	UMP	C5'-O5'-P-OP3
5	B	703	UMP	C3'-C4'-C5'-O5'
5	B	703	UMP	C5'-O5'-P-OP1
5	B	703	UMP	O4'-C4'-C5'-O5'
3	A	702	CP6	C16-C15-C5-C4
3	B	702	CP6	C16-C15-C5-C4
3	D	702	CP6	C16-C15-C5-C4
2	B	701	NDP	PA-O3-PN-O5D
2	D	701	NDP	PA-O3-PN-O5D
4	A	703	BEN	N1-C-C1-C2
4	C	703	BEN	N1-C-C1-C2
4	C	703	BEN	N1-C-C1-C6
5	C	704	UMP	C5'-O5'-P-OP1
2	B	701	NDP	O4D-C1D-N1N-C2N
5	D	703	UMP	O4'-C4'-C5'-O5'
2	A	701	NDP	O4D-C1D-N1N-C2N
2	C	701	NDP	O4D-C1D-N1N-C2N
2	D	701	NDP	O4D-C1D-N1N-C2N
2	C	701	NDP	C2D-C1D-N1N-C2N
4	A	703	BEN	N2-C-C1-C2
4	A	703	BEN	N2-C-C1-C6

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Mol	Chain	Res	Type	Atoms
2	D	701	NDP	C2D-C1D-N1N-C2N
2	A	701	NDP	C2D-C1D-N1N-C2N
2	B	701	NDP	C2D-C1D-N1N-C2N
5	B	703	UMP	C5'-O5'-P-OP2
2	B	701	NDP	C2N-C3N-C7N-N7N
5	A	704	UMP	O4'-C4'-C5'-O5'
5	C	704	UMP	O4'-C4'-C5'-O5'
5	D	703	UMP	C3'-C4'-C5'-O5'
2	B	701	NDP	C4D-C5D-O5D-PN

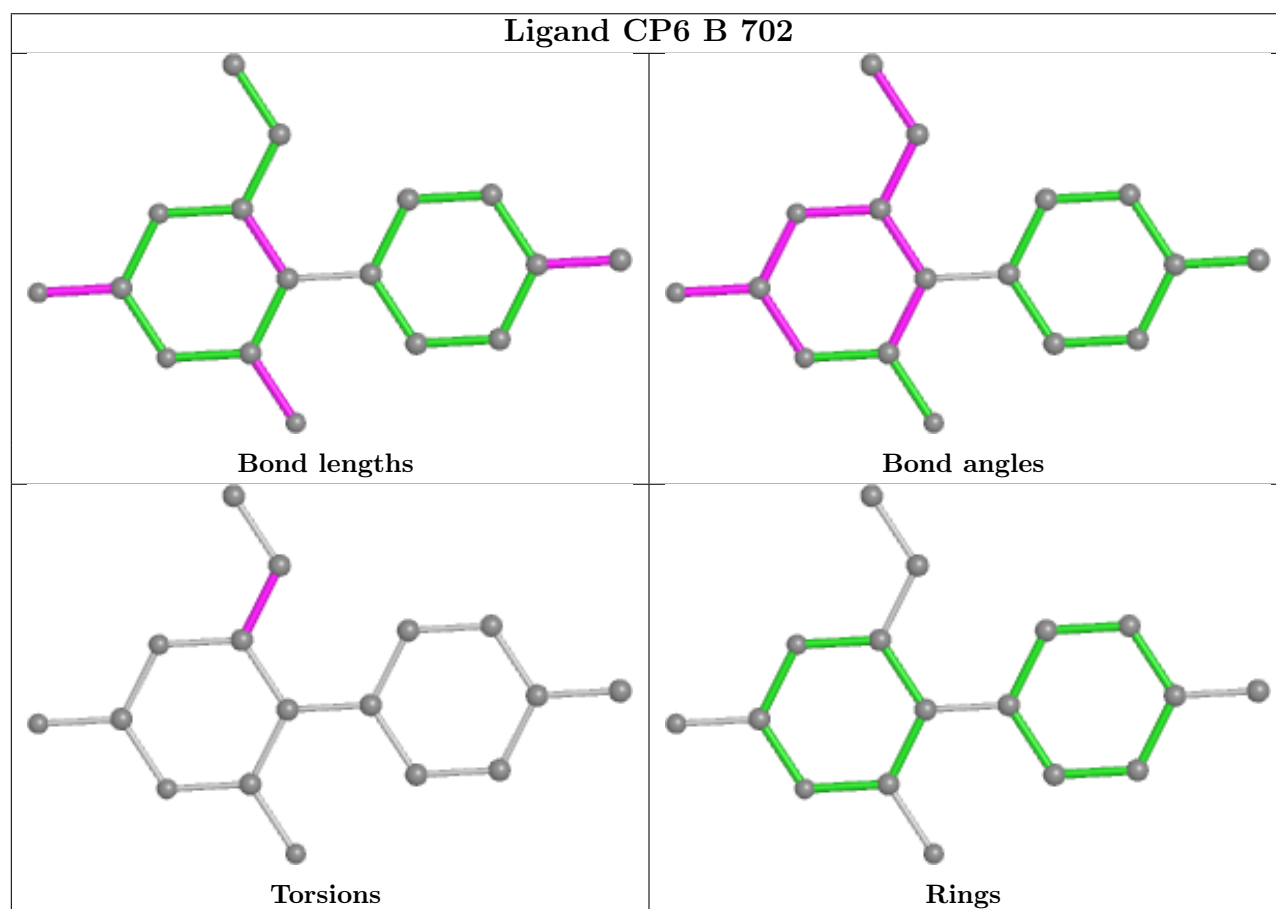
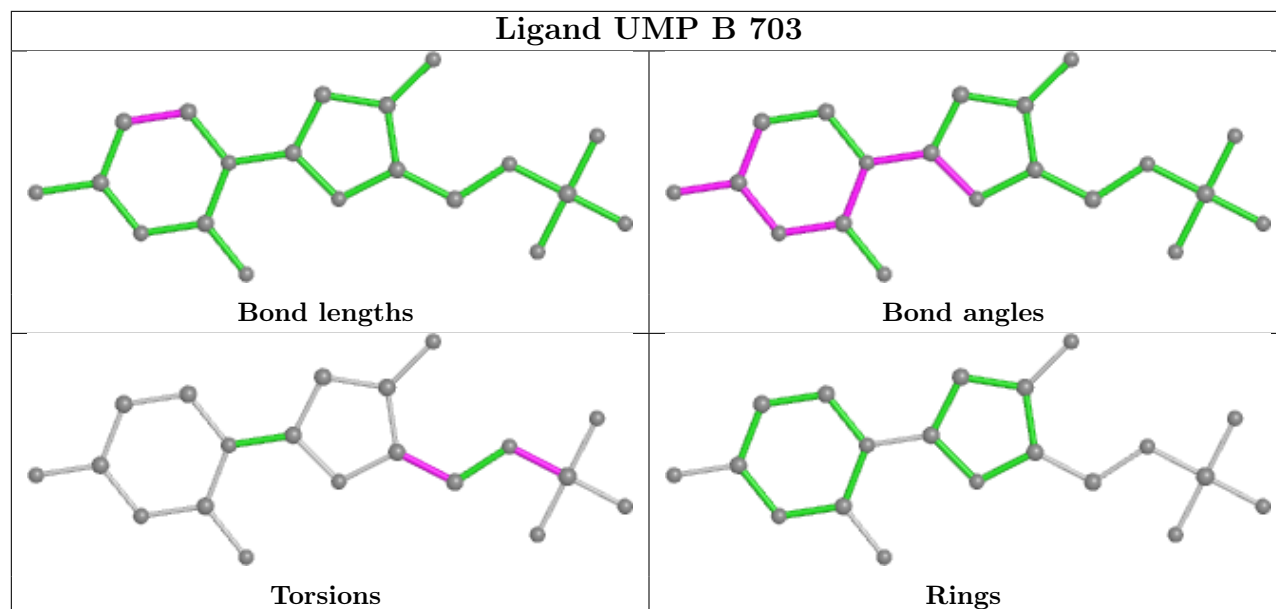
There are no ring outliers.

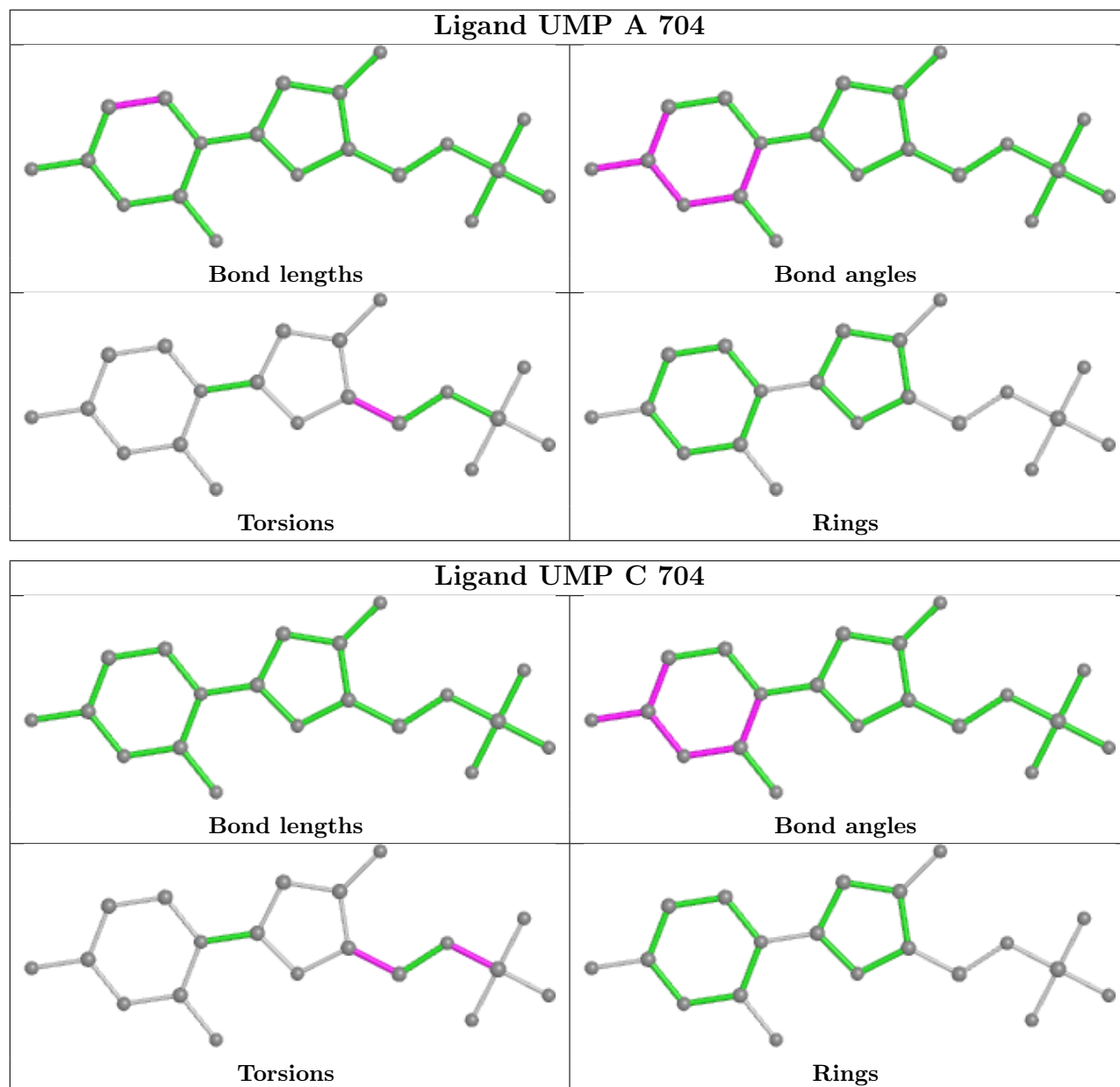
8 monomers are involved in 13 short contacts:

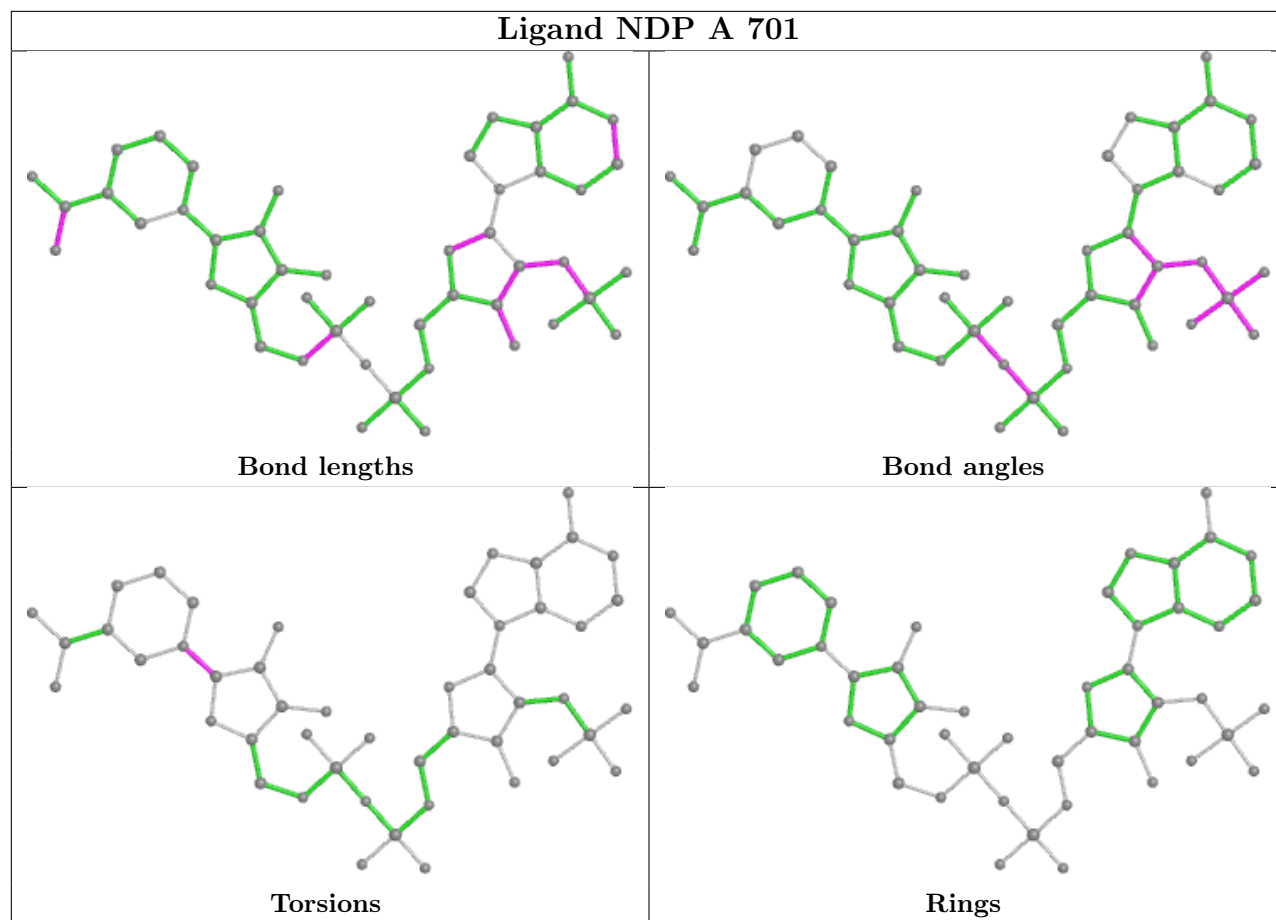
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	BEN	1	0
4	C	703	BEN	2	0
2	A	701	NDP	2	0
2	B	701	NDP	2	0
3	D	702	CP6	2	0
3	A	702	CP6	2	0
3	C	702	CP6	1	0
2	D	701	NDP	2	0

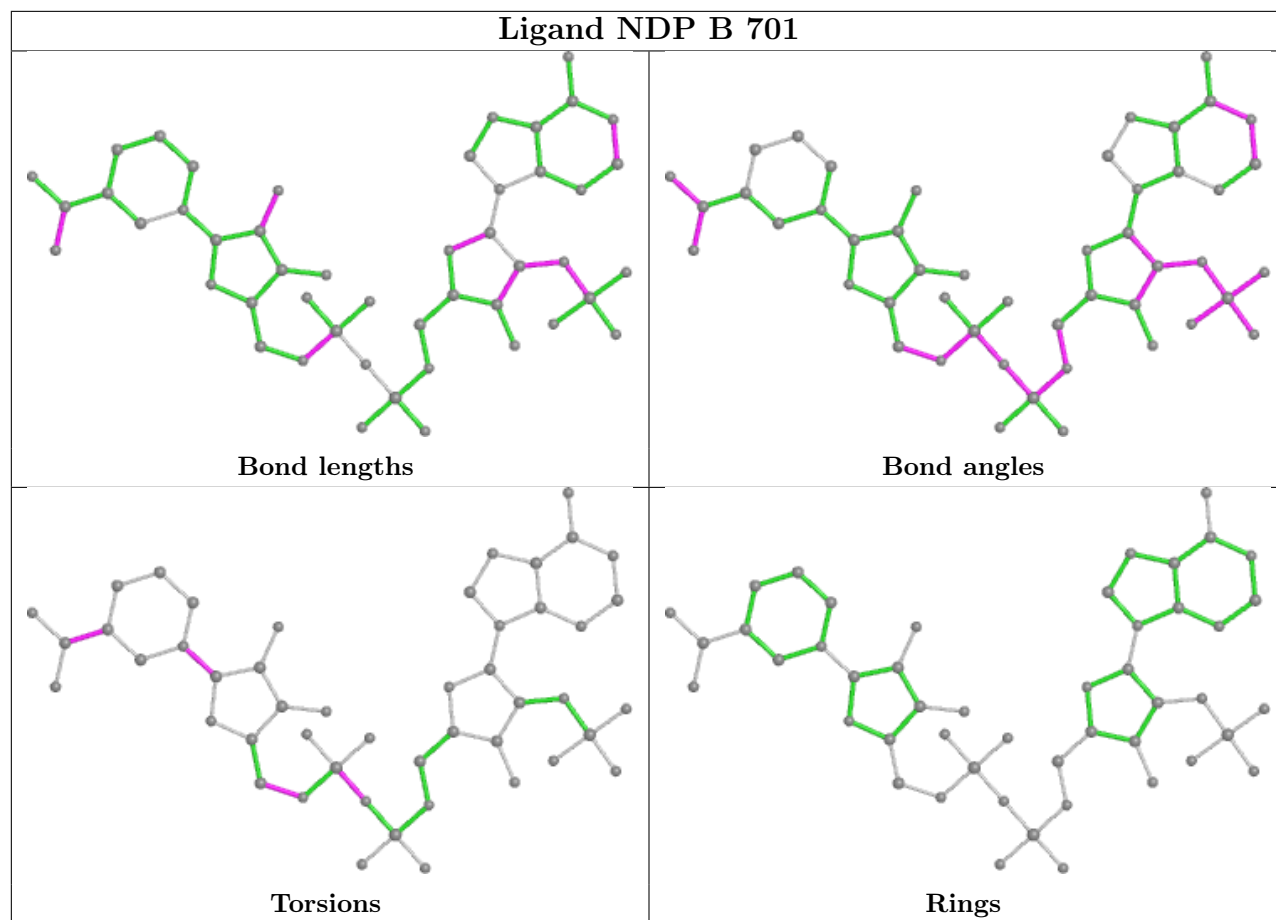
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

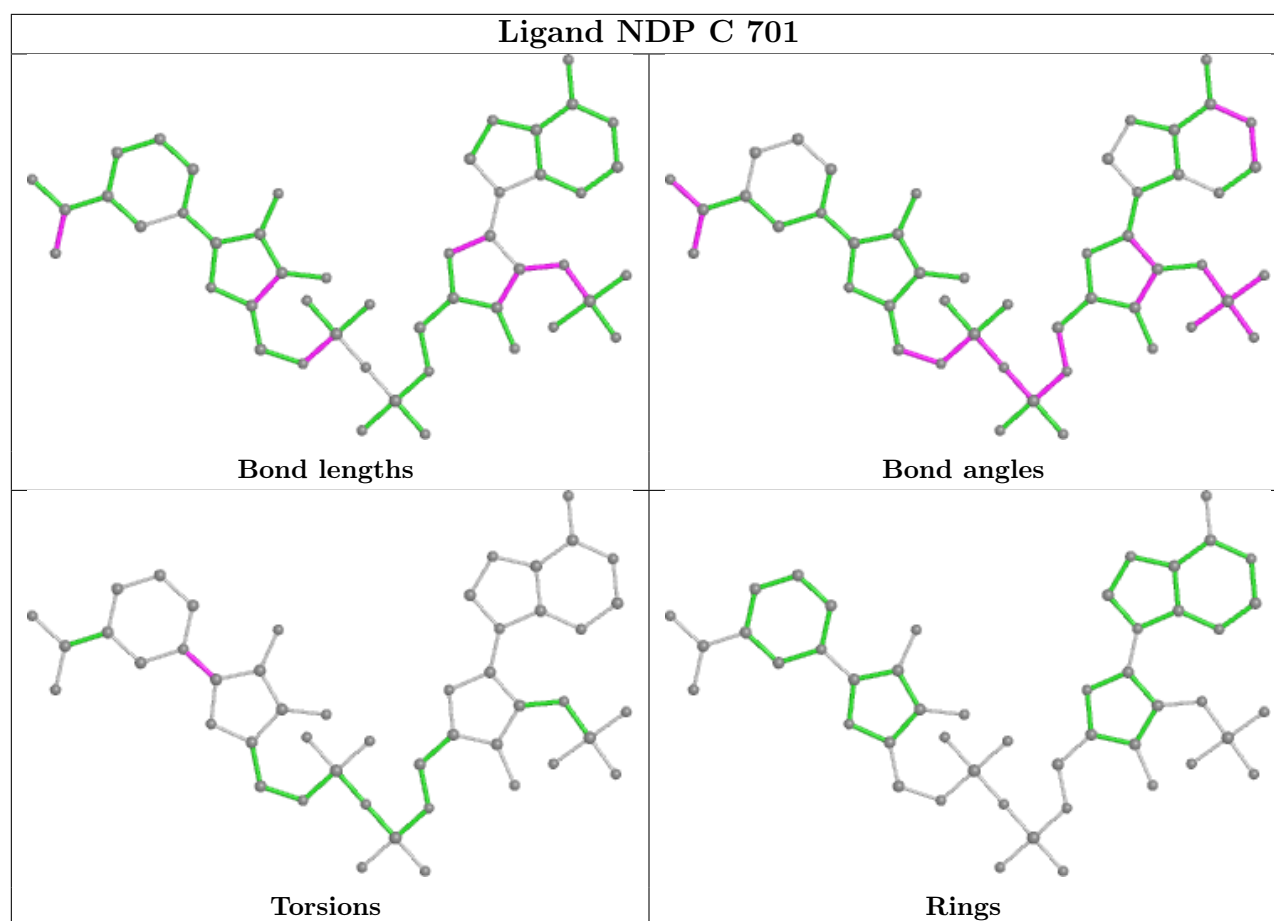


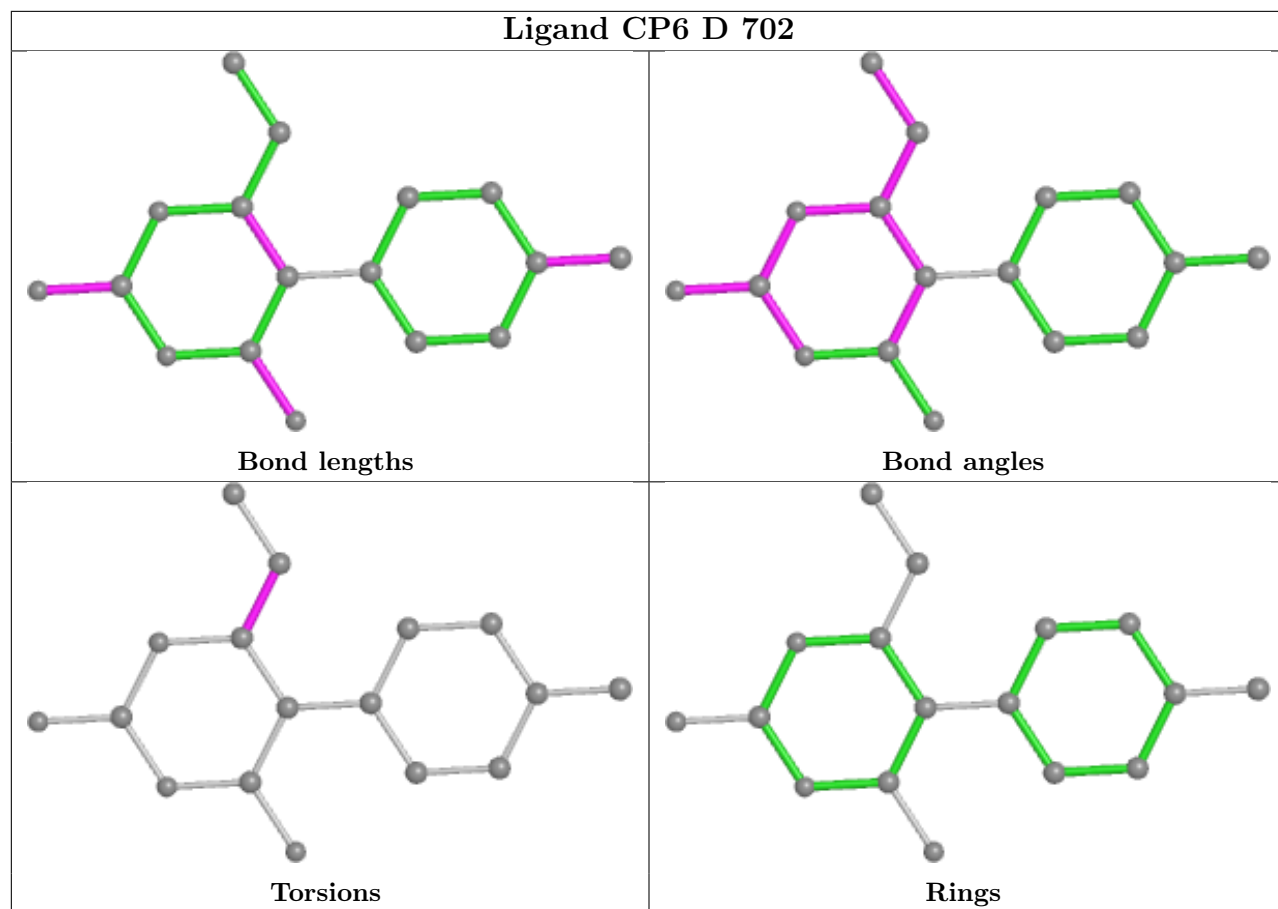


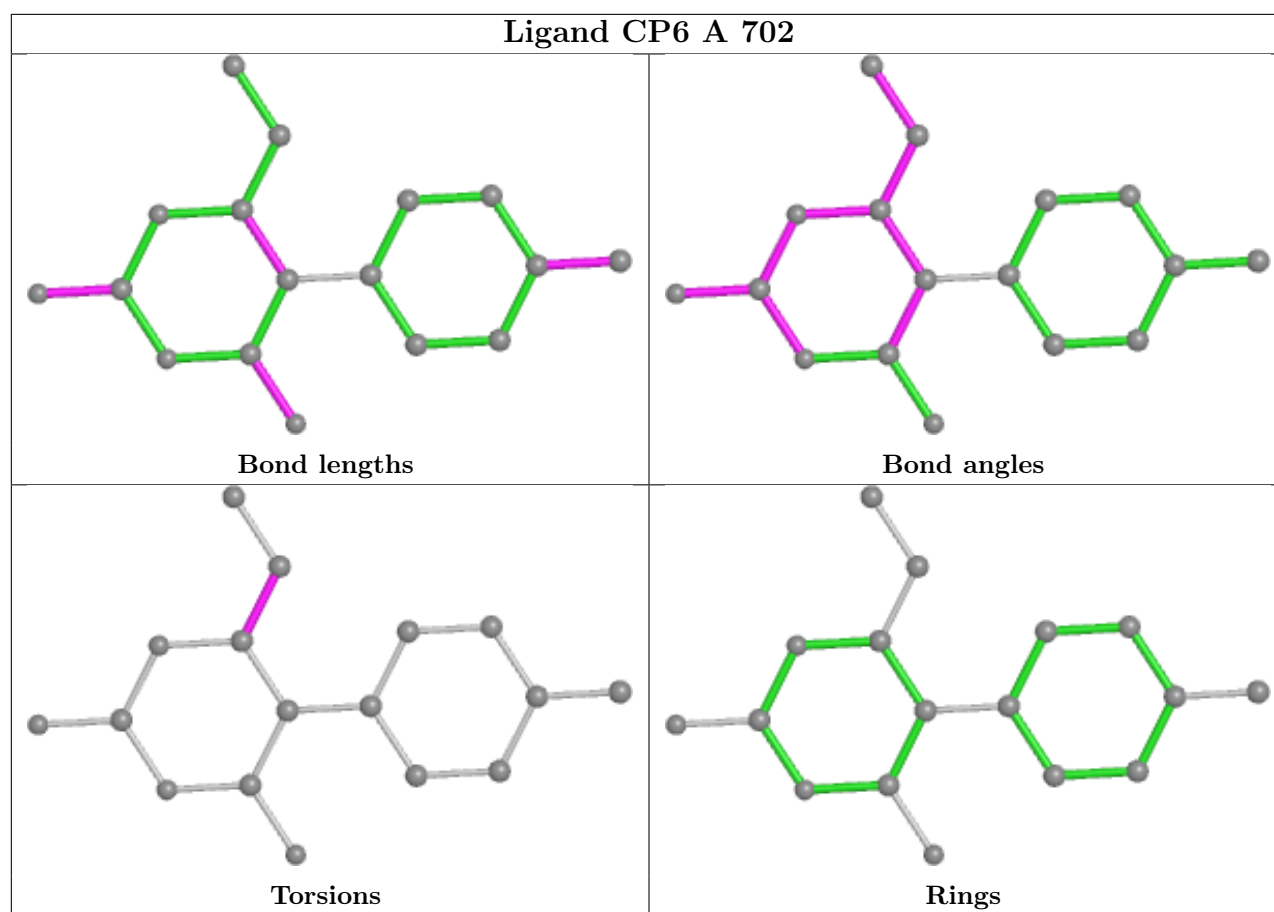




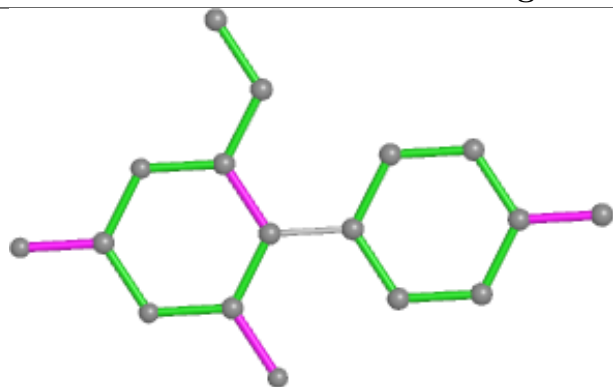




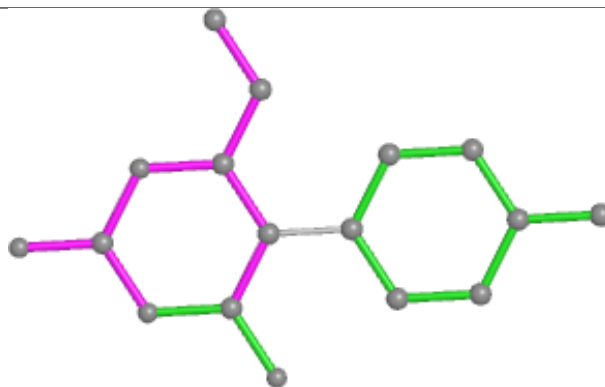




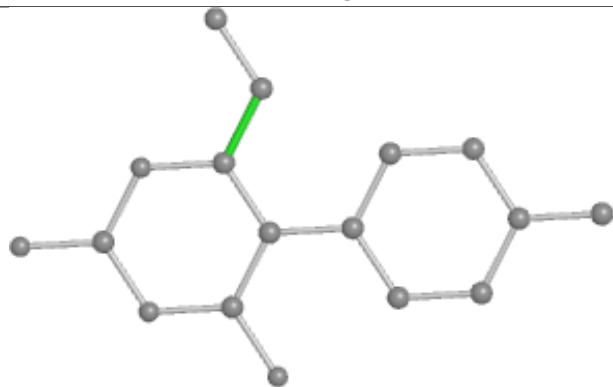
## Ligand CP6 C 702



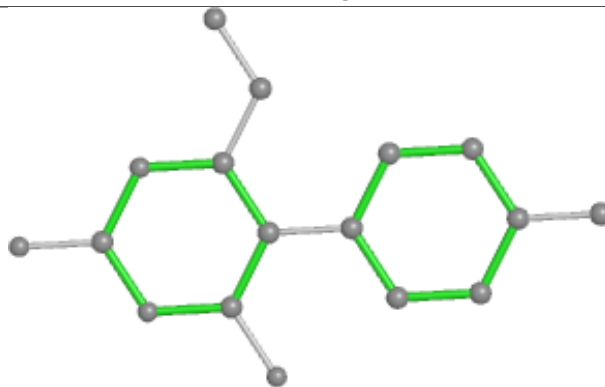
Bond lengths



Bond angles

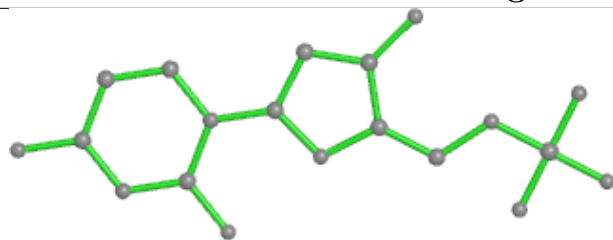


Torsions

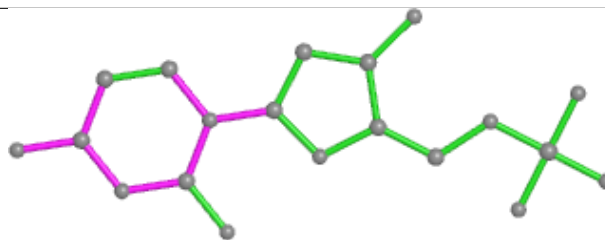


Rings

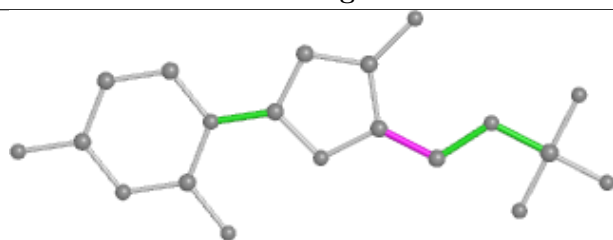
## Ligand UMP D 703



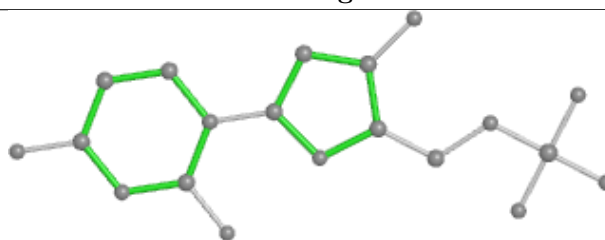
Bond lengths



Bond angles

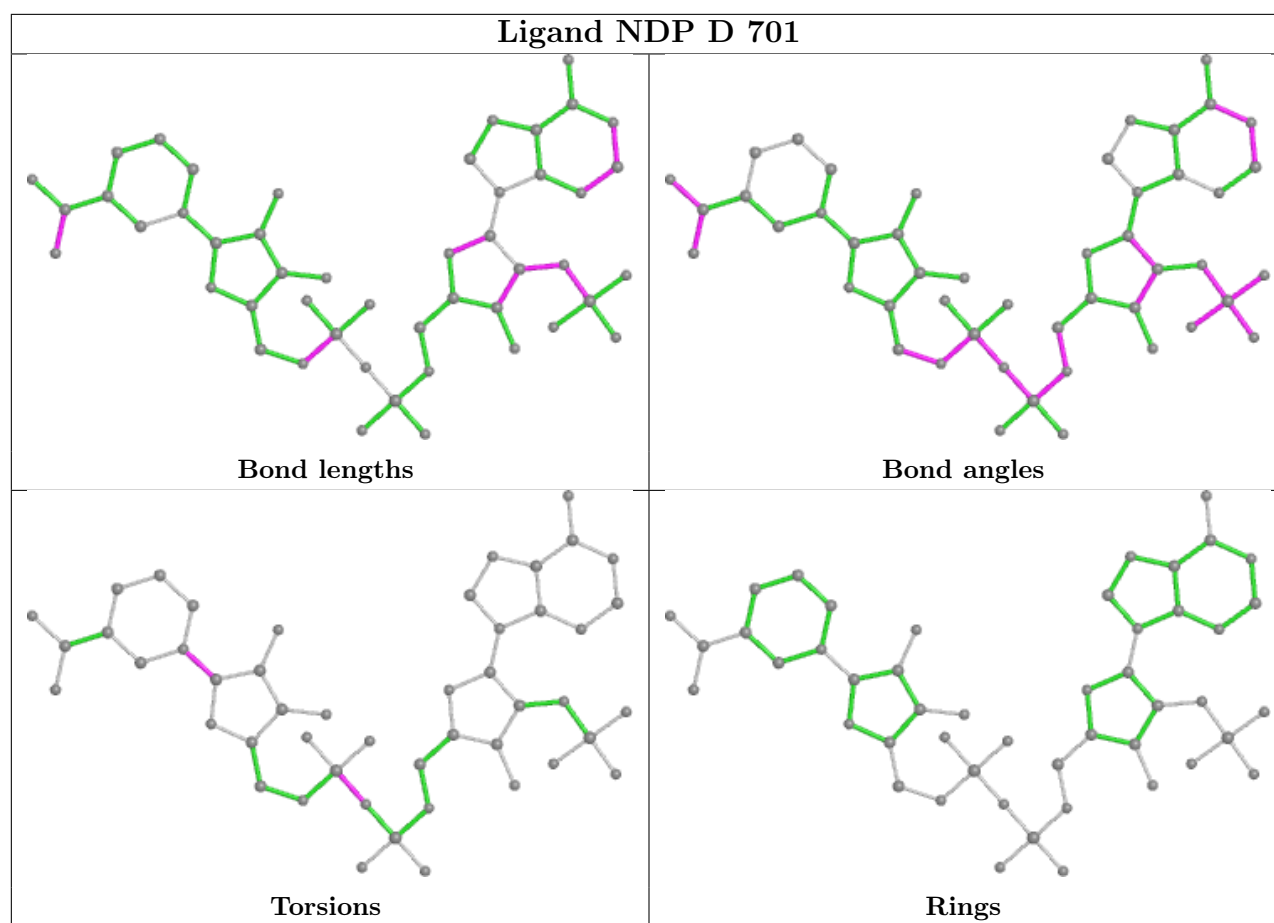


Torsions



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, 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	558/610 (91%)	0.40	49 (8%) 10 14	11, 27, 62, 90	0
1	B	560/610 (91%)	0.36	52 (9%) 8 13	13, 26, 67, 93	0
1	C	556/610 (91%)	0.26	48 (8%) 10 15	14, 25, 70, 93	0
1	D	559/610 (91%)	0.53	59 (10%) 6 9	16, 29, 72, 109	0
All	All	2233/2440 (91%)	0.39	208 (9%) 8 13	11, 27, 68, 109	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	202	ALA	14.5
1	D	258	ALA	14.4
1	D	257	ALA	12.4
1	D	281	LEU	12.1
1	A	202	ALA	12.1
1	B	281	LEU	11.8
1	D	203	ALA	11.7
1	B	200	ALA	11.2
1	A	199	ALA	11.0
1	D	47	SER	10.5
1	B	280	GLY	10.3
1	C	47	SER	9.7
1	A	71	GLY	9.6
1	B	199	ALA	9.3
1	C	203	ALA	9.1
1	A	205	PRO	9.0
1	D	46	ALA	8.8
1	A	203	ALA	8.8
1	B	203	ALA	8.7
1	C	200	ALA	8.4
1	D	71	GLY	8.4

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Mol	Chain	Res	Type	RSRZ
1	B	47	SER	8.3
1	A	282	GLN	8.1
1	C	204	ALA	8.1
1	D	204	ALA	8.1
1	D	205	PRO	8.0
1	A	198	THR	7.8
1	A	47	SER	7.8
1	D	280	GLY	7.7
1	C	202	ALA	7.6
1	A	606	MET	7.6
1	D	43	PRO	7.4
1	C	46	ALA	7.4
1	A	204	ALA	7.3
1	C	201	GLN	7.3
1	B	256	ASP	7.2
1	A	46	ALA	7.1
1	A	255	ASP	7.0
1	D	48	ARG	7.0
1	D	256	ASP	7.0
1	B	282	GLN	6.9
1	B	606	MET	6.9
1	A	48	ARG	6.7
1	B	202	ALA	6.6
1	D	255	ASP	6.6
1	A	345	THR	6.4
1	D	72	LYS	6.4
1	B	201	GLN	6.3
1	D	284	PRO	6.3
1	A	206	ALA	6.3
1	D	254	THR	6.2
1	D	283	ALA	6.2
1	D	197	SER	6.1
1	C	606	MET	6.0
1	C	283	ALA	6.0
1	C	71	GLY	6.0
1	C	282	GLN	6.0
1	A	256	ASP	5.9
1	B	48	ARG	5.9
1	D	344	ARG	5.8
1	A	284	PRO	5.8
1	B	283	ALA	5.7
1	B	303	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	347	VAL	5.6
1	C	199	ALA	5.6
1	A	283	ALA	5.5
1	A	43	PRO	5.4
1	A	257	ALA	5.4
1	D	206	ALA	5.3
1	C	45	GLU	5.2
1	A	254	THR	5.1
1	D	606	MET	5.0
1	D	282	GLN	4.9
1	D	605	GLN	4.9
1	B	605	GLN	4.9
1	B	46	ALA	4.9
1	B	71	GLY	4.9
1	C	48	ARG	4.9
1	A	605	GLN	4.9
1	A	119	GLU	4.8
1	A	346	GLY	4.8
1	A	197	SER	4.8
1	B	204	ALA	4.7
1	C	44	GLU	4.7
1	D	117	GLN	4.6
1	B	284	PRO	4.5
1	D	45	GLU	4.5
1	C	344	ARG	4.4
1	A	45	GLU	4.4
1	C	43	PRO	4.4
1	B	91	PHE	4.4
1	D	345	THR	4.3
1	C	205	PRO	4.3
1	C	284	PRO	4.3
1	B	44	GLU	4.3
1	C	605	GLN	4.3
1	B	255	ASP	4.2
1	D	307	GLN	4.1
1	A	72	LYS	4.1
1	B	45	GLU	4.1
1	C	304	LYS	4.1
1	C	347	VAL	4.1
1	C	603	ARG	4.1
1	B	307	GLN	4.1
1	C	345	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	304	LYS	4.0
1	B	205	PRO	3.8
1	D	301	ASP	3.7
1	C	300	GLU	3.7
1	B	603	ARG	3.7
1	B	306	GLU	3.7
1	C	604	ILE	3.6
1	D	119	GLU	3.6
1	C	197	SER	3.6
1	B	119	GLU	3.5
1	B	604	ILE	3.5
1	B	198	THR	3.5
1	D	303	LYS	3.5
1	B	301	ASP	3.5
1	D	603	ARG	3.5
1	B	254	THR	3.4
1	C	120	GLY	3.4
1	A	207	GLU	3.4
1	D	8	VAL	3.4
1	C	119	GLU	3.3
1	C	309	GLU	3.3
1	C	307	GLN	3.3
1	C	72	LYS	3.3
1	A	344	ARG	3.3
1	D	151	VAL	3.2
1	A	416	ASN	3.2
1	D	150	VAL	3.2
1	A	343	ASP	3.2
1	C	303	LYS	3.2
1	B	309	GLU	3.1
1	D	580	GLU	3.1
1	D	77	VAL	3.1
1	D	207	GLU	3.1
1	D	91	PHE	3.1
1	B	207	GLU	3.1
1	B	43	PRO	3.1
1	D	399	GLY	3.0
1	D	306	GLU	3.0
1	C	254	THR	3.0
1	B	72	LYS	3.0
1	D	116	PRO	3.0
1	C	302	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	7	LEU	3.0
1	D	343	ASP	3.0
1	D	305	ARG	3.0
1	A	44	GLU	2.9
1	B	300	GLU	2.9
1	C	306	GLU	2.9
1	B	302	ARG	2.9
1	B	197	SER	2.9
1	C	346	GLY	2.8
1	A	150	VAL	2.8
1	B	90	LYS	2.8
1	D	9	VAL	2.8
1	C	207	GLU	2.7
1	D	300	GLU	2.7
1	D	346	GLY	2.7
1	A	418	PRO	2.7
1	B	299	GLU	2.7
1	A	303	LYS	2.7
1	C	342	ASP	2.7
1	A	309	GLU	2.7
1	D	416	ASN	2.7
1	A	580	GLU	2.6
1	D	78	VAL	2.6
1	D	309	GLU	2.6
1	C	198	THR	2.6
1	C	301	ASP	2.6
1	B	120	GLY	2.6
1	C	308	LYS	2.6
1	A	148	ILE	2.5
1	A	604	ILE	2.5
1	D	308	LYS	2.5
1	C	305	ARG	2.5
1	D	120	GLY	2.5
1	D	118	ALA	2.4
1	A	149	PHE	2.4
1	D	149	PHE	2.4
1	A	9	VAL	2.4
1	D	113	ALA	2.4
1	D	302	ARG	2.4
1	C	285	SER	2.4
1	A	7	LEU	2.3
1	B	416	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	150	VAL	2.3
1	C	298	ASP	2.3
1	A	77	VAL	2.3
1	B	143	ASP	2.3
1	B	116	PRO	2.3
1	B	417	LEU	2.3
1	C	151	VAL	2.3
1	B	9	VAL	2.3
1	C	150	VAL	2.3
1	A	169	LEU	2.3
1	A	6	CYS	2.2
1	C	8	VAL	2.2
1	B	117	GLN	2.2
1	D	604	ILE	2.2
1	A	8	VAL	2.2
1	A	78	VAL	2.1
1	B	77	VAL	2.1
1	B	305	ARG	2.1
1	A	342	ASP	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.

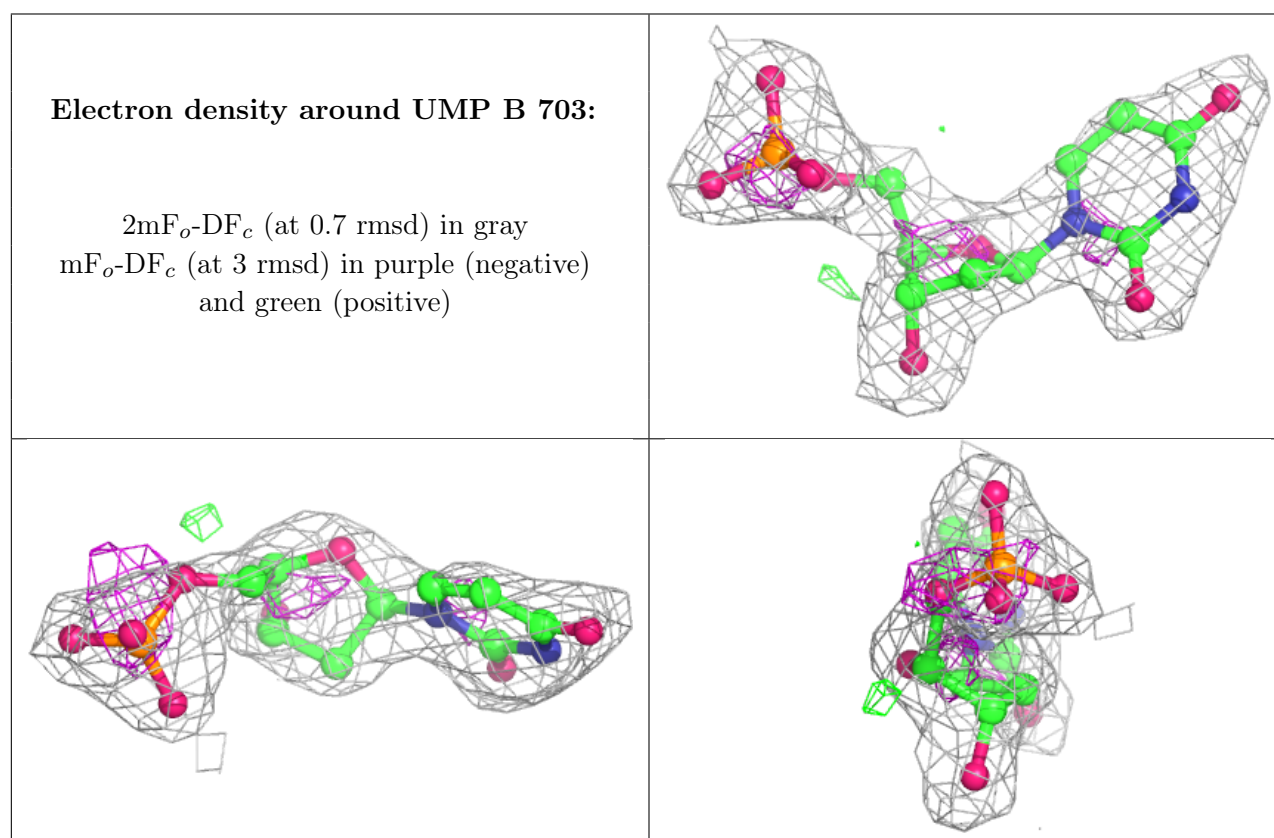
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	BEN	C	703	9/9	0.78	0.27	35,46,51,51	0
4	BEN	A	703	9/9	0.81	0.29	36,45,49,50	0
5	UMP	B	703	20/20	0.92	0.15	34,43,51,54	0
5	UMP	C	704	20/20	0.94	0.14	36,43,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	UMP	D	703	20/20	0.95	0.17	34,45,50,52	0
5	UMP	A	704	20/20	0.96	0.11	29,36,41,45	0
2	NDP	D	701	48/48	0.97	0.10	14,24,33,36	0
3	CP6	D	702	17/17	0.97	0.18	17,20,24,33	0
2	NDP	A	701	48/48	0.97	0.10	10,19,28,36	0
2	NDP	B	701	48/48	0.97	0.09	16,26,37,42	0
3	CP6	C	702	17/17	0.98	0.15	13,18,23,27	0
2	NDP	C	701	48/48	0.98	0.08	14,23,32,40	0
3	CP6	A	702	17/17	0.98	0.16	12,15,22,24	0
3	CP6	B	702	17/17	0.98	0.14	13,19,26,31	0

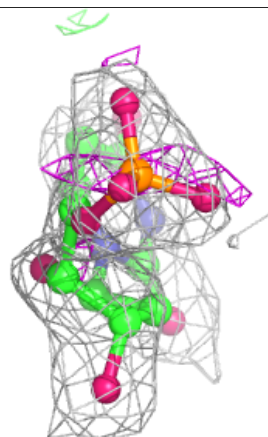
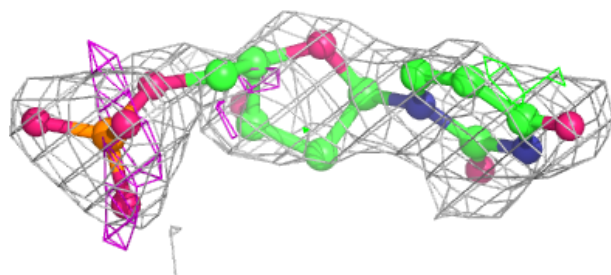
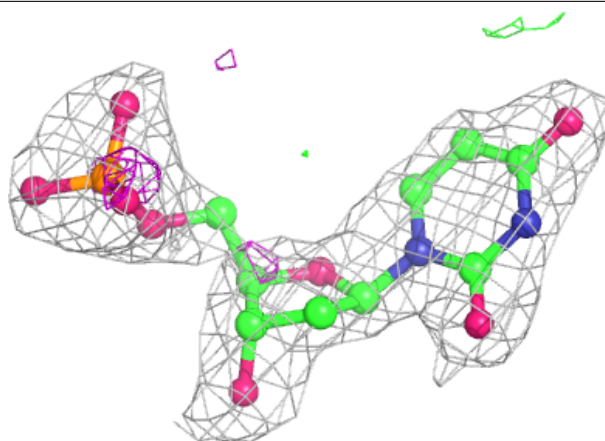
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





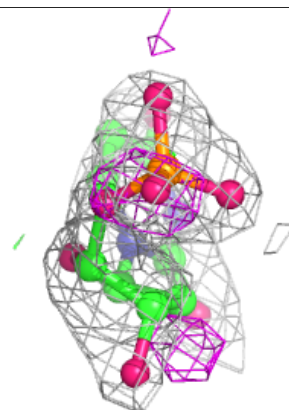
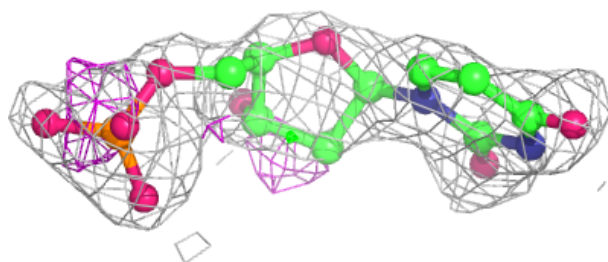
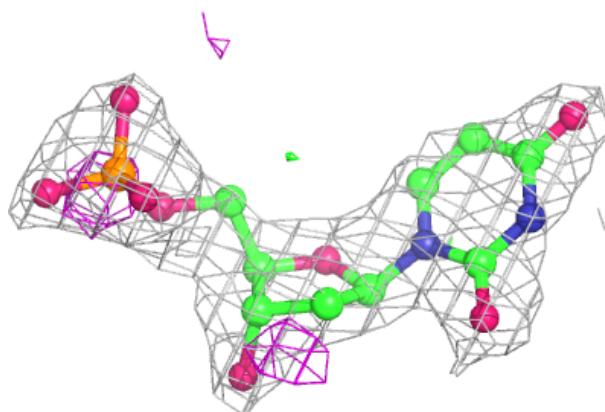
**Electron density around UMP C 704:**

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

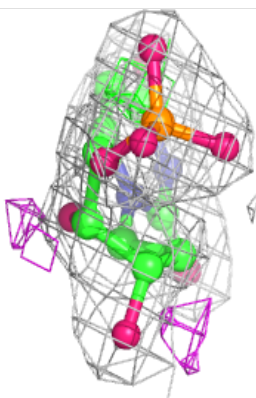
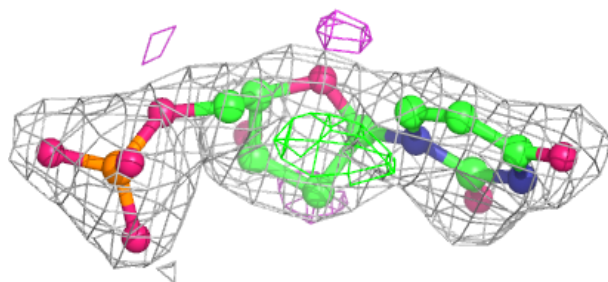
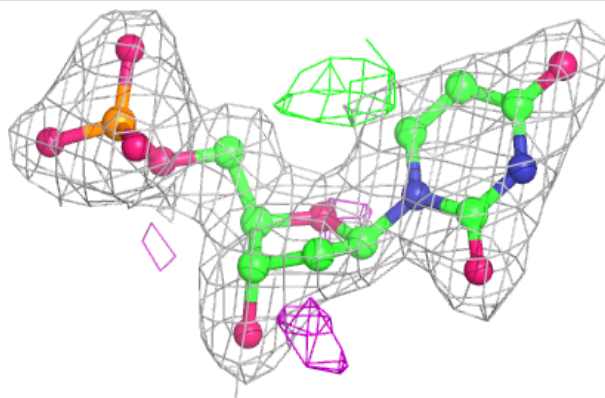


**Electron density around UMP D 703:**

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

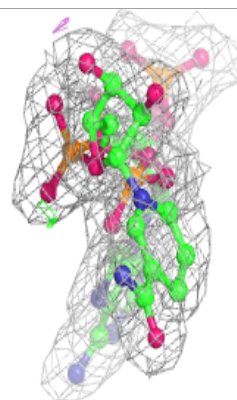
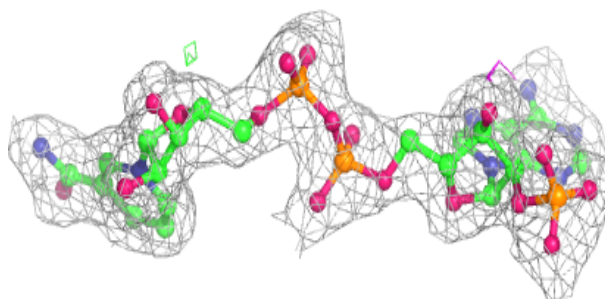
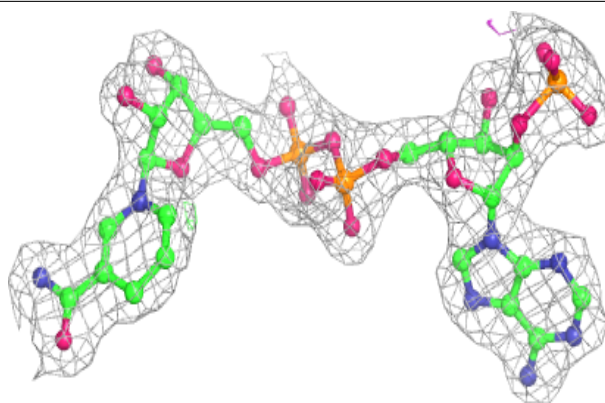
**Electron density around UMP A 704:**

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

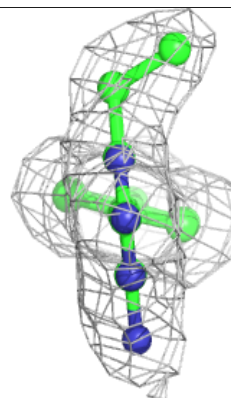
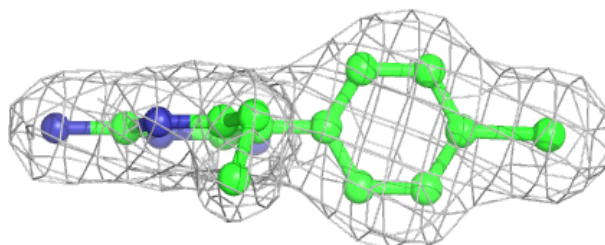
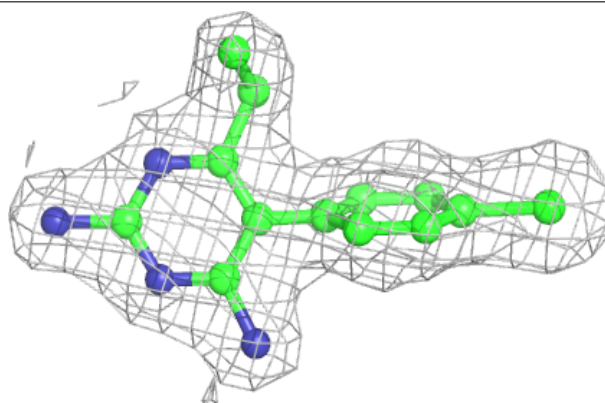


**Electron density around NDP D 701:**

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

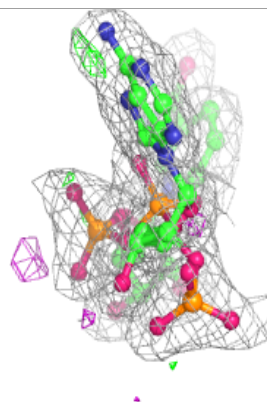
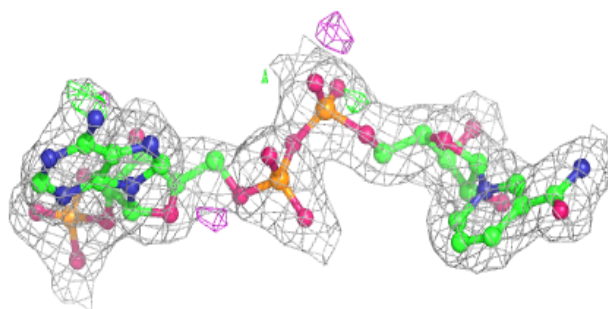
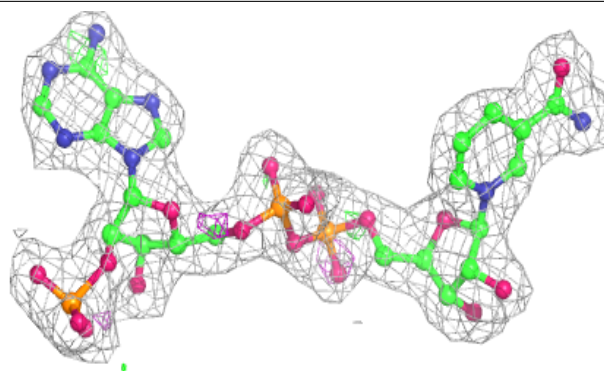
**Electron density around CP6 D 702:**

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

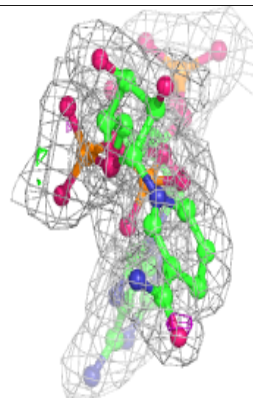
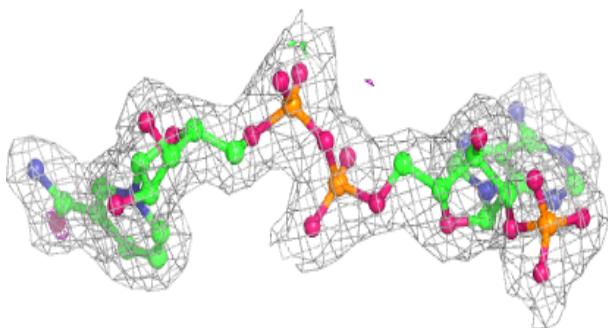
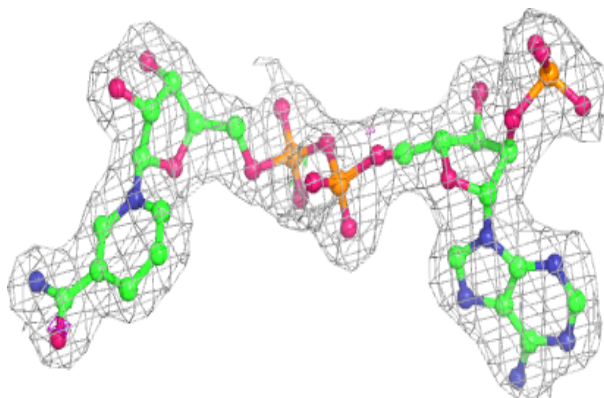


**Electron density around NDP A 701:**

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

**Electron density around NDP B 701:**

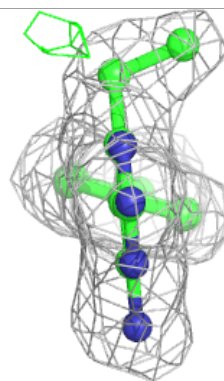
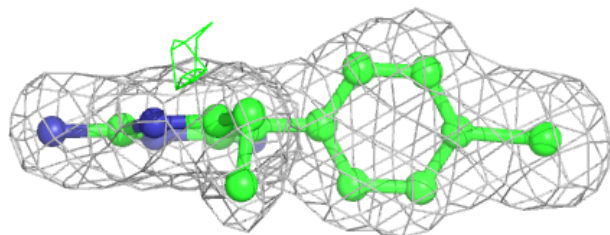
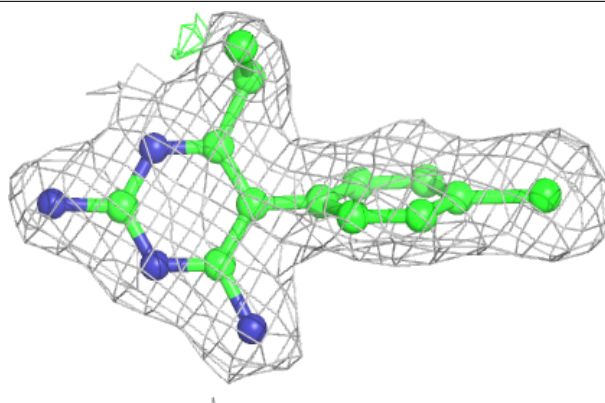
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



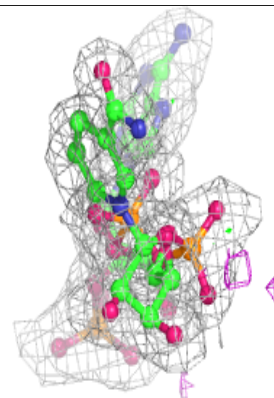
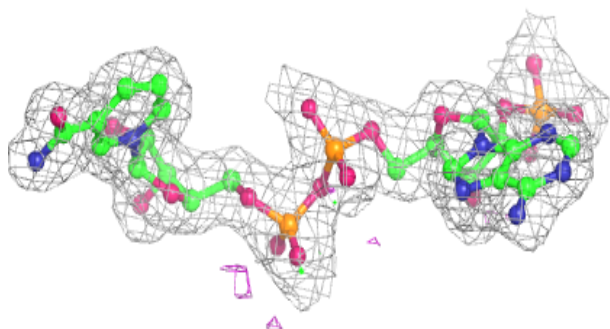
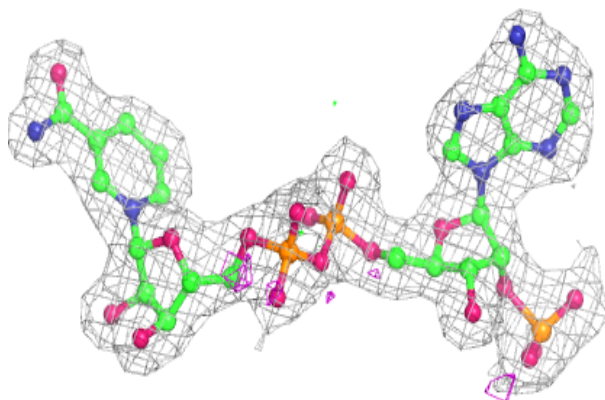


**Electron density around CP6 C 702:**

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

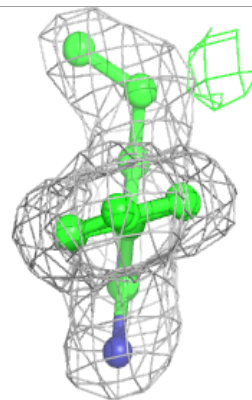
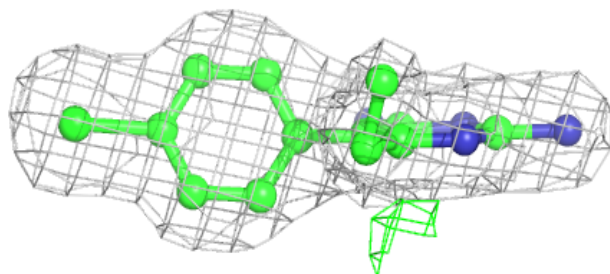
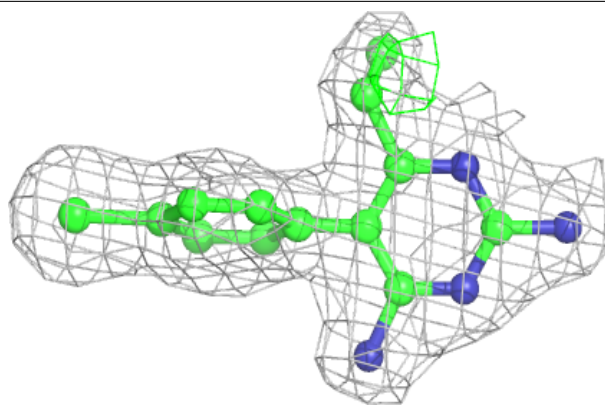
**Electron density around NDP C 701:**

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

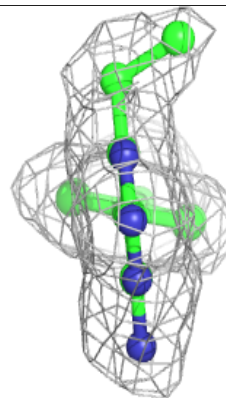
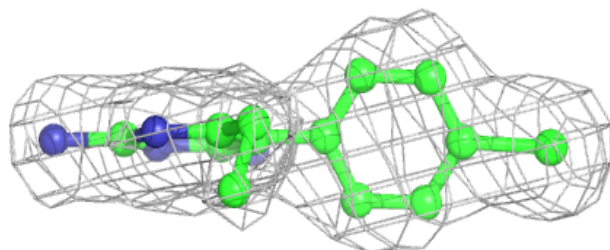
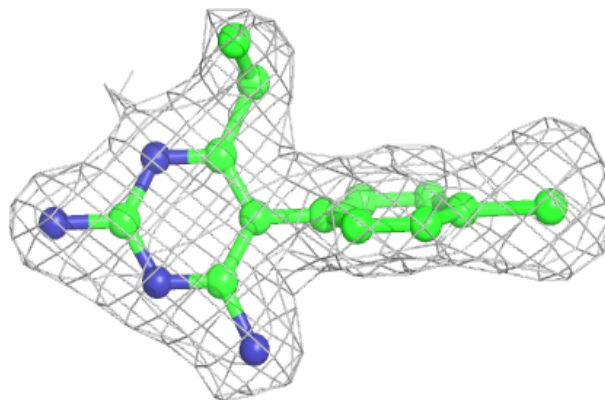


**Electron density around CP6 A 702:**

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

**Electron density around CP6 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.