



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2022 – 08:21 AM JST

PDB ID : 7FGX
Title : Toxoplasma gondii dihydrofolate reductase thymidylate synthase (TgDHFR-TS) complexed with P39, NADPH and dUMP
Authors : Vanichtanankul, J.; Yoomuang, A.; Taweechai, S.; Saeyang, T.; Yuvaniyama, J.; Tarnchompoo, B.; Yuthavong, Y.; Kamchonwongpaisan, S.
Deposited on : 2021-07-28
Resolution : 2.05 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 ⓘ](#)) 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

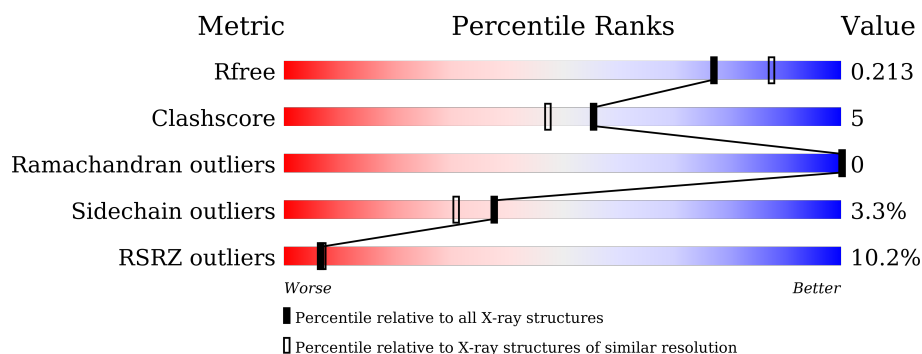
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	610	<div> <div>9%</div> <div>81% 10% 8%</div> </div>
1	B	610	<div> <div>10%</div> <div>79% 12% 8%</div> </div>
1	C	610	<div> <div>9%</div> <div>78% 12% 9%</div> </div>
1	D	610	<div> <div>10%</div> <div>80% 12% 8%</div> </div>

2 Entry composition ⓘ

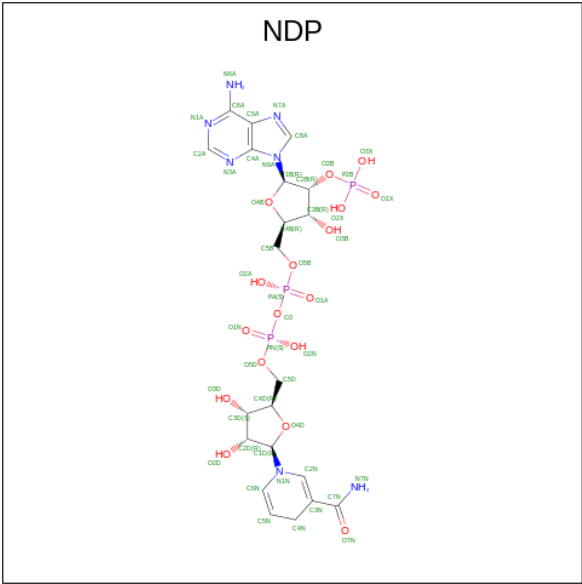
There are 5 unique types of molecules in this entry. The entry contains 19328 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	560	Total	C	N	O	S	0	0	0
			4473	2845	788	814	26			
1	B	560	Total	C	N	O	S	0	0	0
			4470	2845	788	811	26			
1	C	558	Total	C	N	O	S	0	0	0
			4461	2838	786	811	26			
1	D	563	Total	C	N	O	S	0	0	0
			4491	2856	791	818	26			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



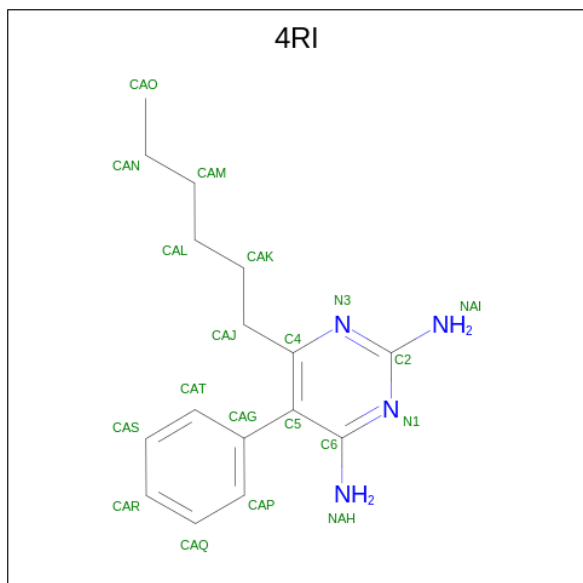
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

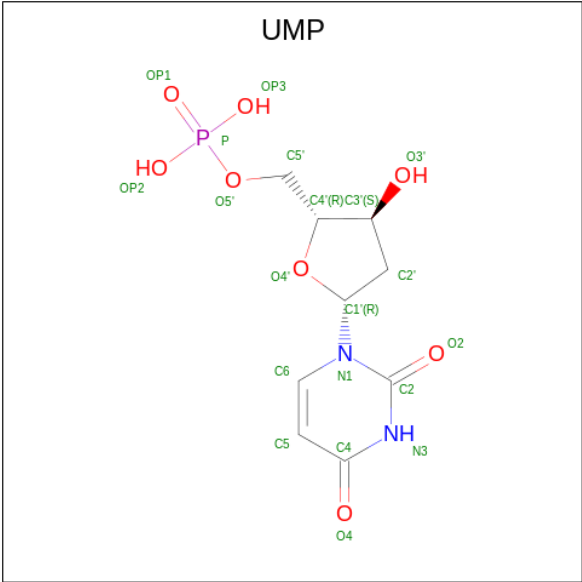
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 6-hexyl-5-phenyl-pyrimidine-2,4-diamine (three-letter code: 4RI) (formula: $C_{16}H_{22}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			20	16	4		
3	B	1	Total	C	N	0	0
			20	16	4		
3	C	1	Total	C	N	0	0
			20	16	4		
3	D	1	Total	C	N	0	0
			20	16	4		

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



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

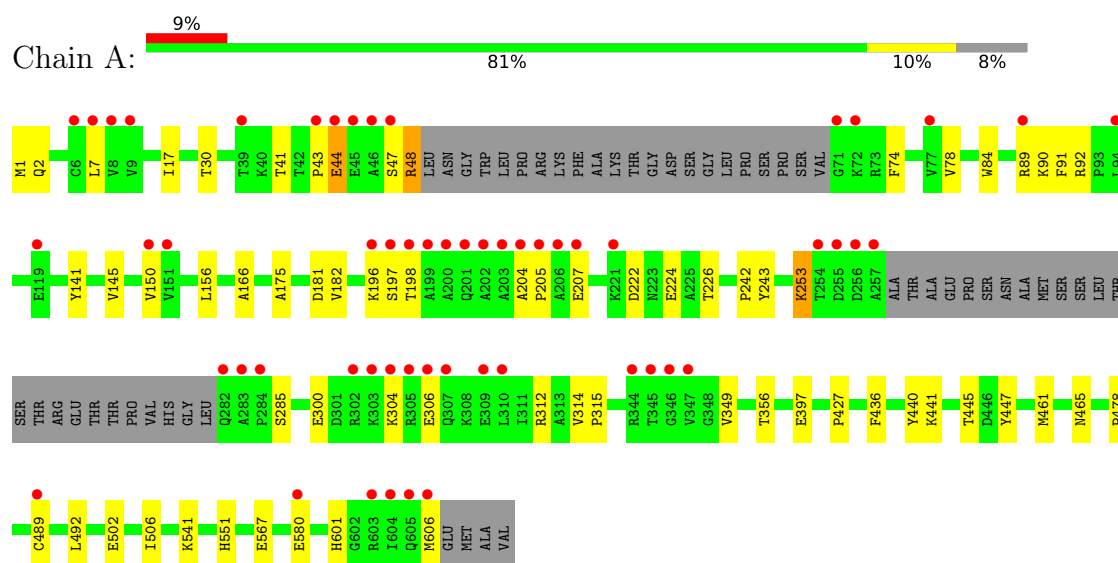
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	284	Total	O	0	0
			284	284		
5	B	253	Total	O	0	0
			253	253		
5	C	303	Total	O	0	0
			303	303		
5	D	241	Total	O	0	0
			241	241		

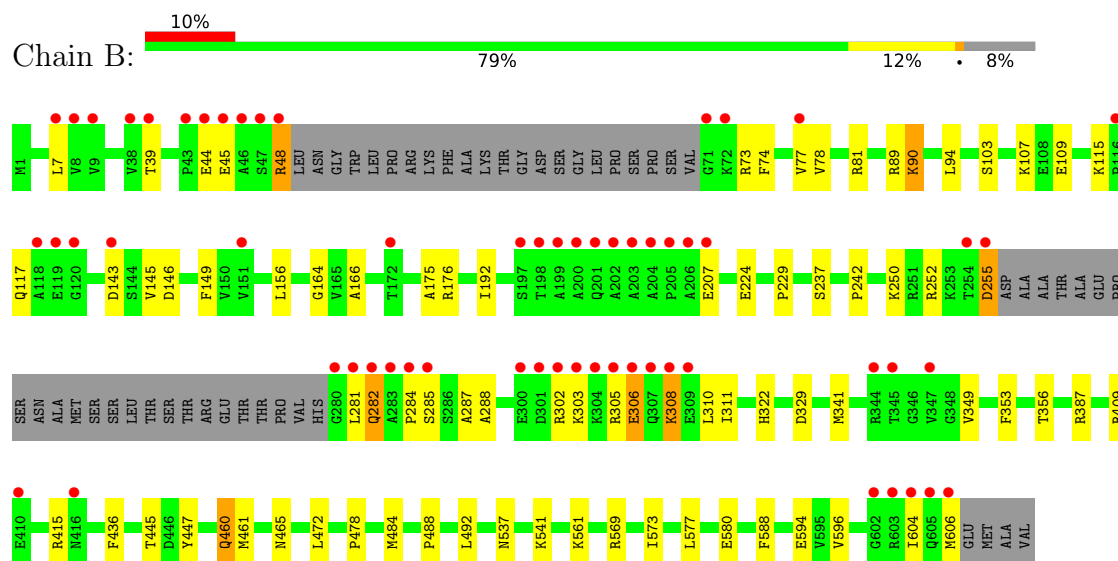
3 Residue-property plots [i](#)

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.

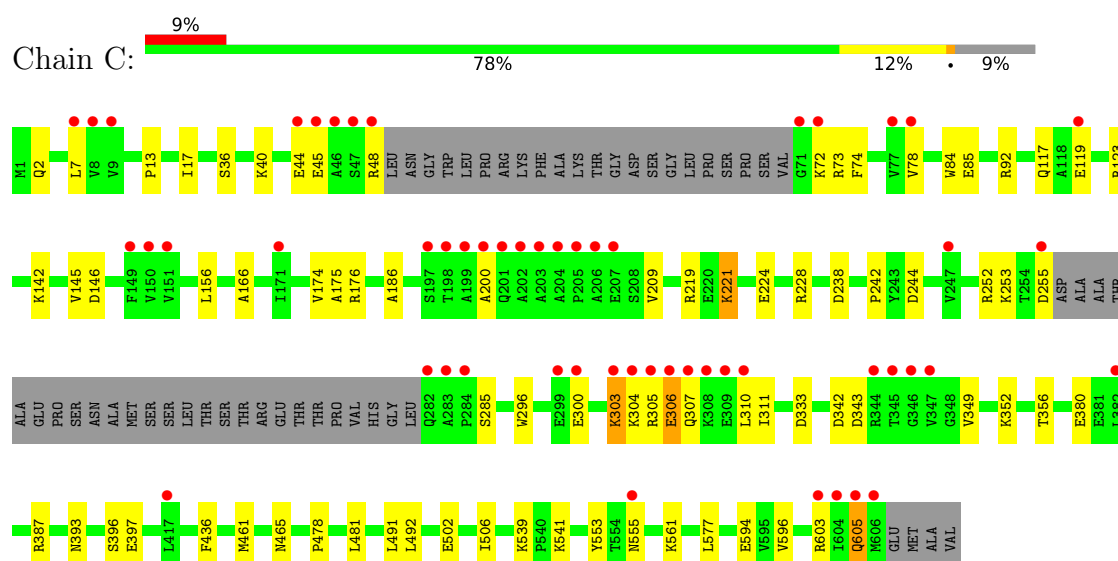
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



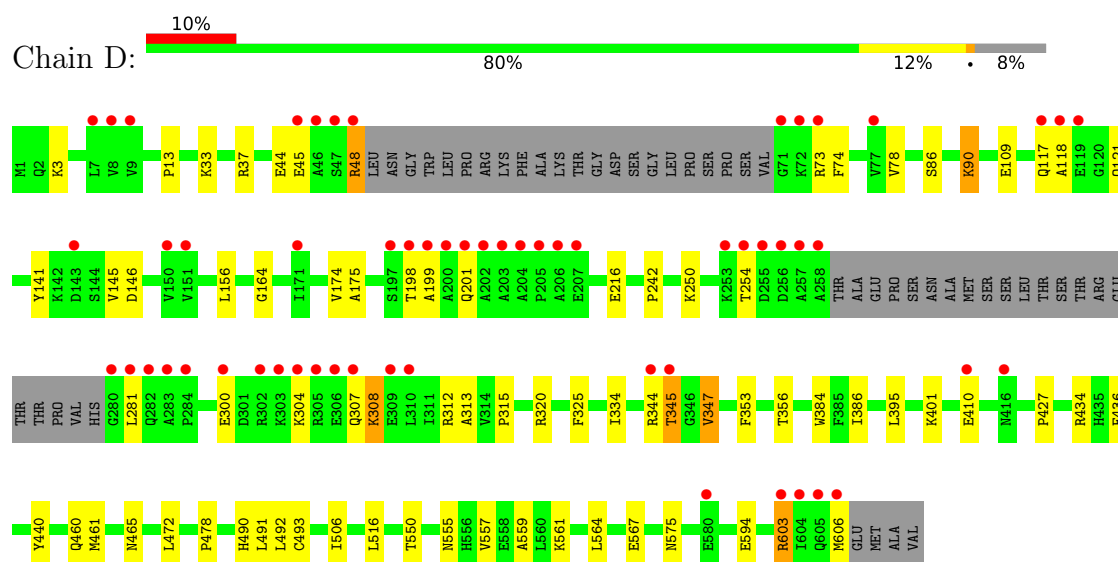
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



- 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 1	Depositor
Cell constants a, b, c, α , β , γ	68.40Å 102.54Å 106.20Å 88.95° 87.74° 84.69°	Depositor
Resolution (Å)	30.05 – 2.05 30.05 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.8 (30.05-2.05) 94.8 (30.05-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.180 , 0.214 0.180 , 0.213	Depositor DCC
R_{free} test set	8538 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19328	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 4RI, 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	0.42	0/4580	0.61	0/6202
1	B	0.43	0/4577	0.63	0/6197
1	C	0.44	0/4568	0.61	1/6185 (0.0%)
1	D	0.40	0/4598	0.61	0/6226
All	All	0.42	0/18323	0.61	1/24810 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	244	ASP	CB-CG-OD1	5.68	123.42	118.30

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	4473	0	4431	42	0
1	B	4470	0	4431	58	0
1	C	4461	0	4425	47	0
1	D	4491	0	4453	48	0
2	A	48	0	26	3	0
2	B	48	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	26	1	0
2	D	48	0	26	0	0
3	A	20	0	0	1	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
4	A	20	0	11	0	0
4	B	20	0	11	0	0
4	C	20	0	11	0	0
4	D	20	0	11	0	0
5	A	284	0	0	6	0
5	B	253	0	0	15	1
5	C	303	0	0	11	1
5	D	241	0	0	7	0
All	All	19328	0	17888	183	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 (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASP:OD1	5:B:801:HOH:O	1.92	0.85
1:B:588:PHE:O	5:B:802:HOH:O	1.94	0.83
1:A:224:GLU:HG2	1:A:253:LYS:HD3	1.60	0.83
1:B:308:LYS:O	5:B:803:HOH:O	1.95	0.82
1:C:73:ARG:NH1	1:C:146:ASP:OD1	2.12	0.82
1:C:342:ASP:O	5:C:801:HOH:O	1.98	0.81
1:D:603:ARG:HH11	1:D:603:ARG:HA	1.47	0.79
1:B:465:ASN:ND2	5:B:807:HOH:O	2.15	0.79
1:B:73:ARG:NH2	5:B:804:HOH:O	2.01	0.78
1:B:302:ARG:HG2	1:B:305:ARG:HH21	1.49	0.78
1:D:216:GLU:OE1	5:D:801:HOH:O	2.03	0.77
1:B:329:ASP:OD2	5:B:805:HOH:O	2.03	0.75
1:C:85:GLU:OE1	5:C:803:HOH:O	2.05	0.74
1:A:312:ARG:HG2	1:A:315:PRO:HB3	1.70	0.74
1:D:86:SER:O	5:D:802:HOH:O	2.04	0.74
1:B:460:GLN:NE2	5:B:808:HOH:O	2.23	0.71
2:A:701:NDP:O1X	5:A:802:HOH:O	2.07	0.71
1:C:380:GLU:OE2	5:C:804:HOH:O	2.08	0.70
1:C:343:ASP:HB2	1:C:349:VAL:HG23	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:LYS:HE3	1:D:90:LYS:H	1.56	0.69
1:D:401:LYS:O	5:D:803:HOH:O	2.09	0.69
1:A:465:ASN:ND2	5:A:808:HOH:O	2.26	0.67
1:B:284:PRO:O	5:B:806:HOH:O	2.11	0.67
1:C:200:ALA:HB2	1:C:605:GLN:HE22	1.59	0.67
1:B:175:ALA:HB3	1:B:242:PRO:HG2	1.75	0.66
1:C:387:ARG:HD2	5:C:806:HOH:O	1.96	0.65
1:A:78:VAL:HG12	1:A:156:LEU:HD21	1.77	0.65
1:C:84:TRP:O	1:C:92:ARG:HD2	1.95	0.65
1:C:303:LYS:HE2	1:C:304:LYS:HG3	1.79	0.65
1:A:43:PRO:O	5:A:803:HOH:O	2.14	0.64
1:C:387:ARG:NH1	5:C:806:HOH:O	2.20	0.63
1:B:48:ARG:HH11	1:B:48:ARG:HB2	1.63	0.63
1:D:73:ARG:NH2	1:D:146:ASP:OD1	2.33	0.62
1:D:313:ALA:HB2	1:D:564:LEU:HG	1.80	0.62
1:B:461:MET:HG2	5:B:1016:HOH:O	2.02	0.60
1:D:472:LEU:HD23	1:D:492:LEU:HD21	1.85	0.59
1:D:78:VAL:HG12	1:D:156:LEU:HD21	1.84	0.59
1:B:604:ILE:HG22	1:B:606:MET:H	1.67	0.59
1:B:73:ARG:NH1	1:B:143:ASP:O	2.36	0.59
1:D:344:ARG:HD3	5:D:820:HOH:O	2.02	0.59
1:B:288:ALA:N	5:B:806:HOH:O	2.07	0.58
1:D:461:MET:SD	1:D:465:ASN:HB3	2.44	0.57
1:C:175:ALA:HB3	1:C:242:PRO:HG2	1.87	0.56
1:A:44:GLU:O	5:A:805:HOH:O	2.18	0.56
1:A:436:PHE:CE1	1:B:478:PRO:HD2	2.40	0.56
1:D:164:GLY:O	1:D:250:LYS:NZ	2.38	0.55
1:B:164:GLY:O	1:B:250:LYS:NZ	2.38	0.55
1:C:356:THR:HG21	1:D:356:THR:HG21	1.88	0.55
1:A:567:GLU:O	1:A:601:HIS:HE1	1.89	0.54
1:D:300:GLU:OE2	1:D:304:LYS:HE2	2.07	0.54
1:C:478:PRO:HA	1:C:481:LEU:HG	1.89	0.54
1:D:312:ARG:HG2	1:D:315:PRO:HB3	1.90	0.54
1:B:460:GLN:HE21	1:B:460:GLN:HA	1.73	0.54
1:A:175:ALA:HB3	1:A:242:PRO:HG2	1.91	0.53
1:C:176:ARG:HD2	1:C:596:VAL:CG1	2.38	0.53
1:A:478:PRO:HD2	1:B:436:PHE:CE1	2.43	0.53
1:D:175:ALA:HB3	1:D:242:PRO:HG2	1.90	0.52
1:B:282:GLN:HG2	1:B:287:ALA:HB2	1.92	0.52
1:D:45:GLU:O	1:D:48:ARG:NE	2.42	0.52
1:C:491:LEU:HD11	1:D:492:LEU:HD11	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:HG21	1:B:356:THR:HG21	1.92	0.52
2:A:701:NDP:H42N	3:A:702:4RI:CAP	2.39	0.52
1:A:1:MET:N	5:A:804:HOH:O	2.17	0.51
1:C:123:ARG:NH1	5:C:814:HOH:O	2.36	0.51
1:B:45:GLU:O	1:B:48:ARG:NH1	2.44	0.51
1:B:224:GLU:HG3	5:B:829:HOH:O	2.10	0.51
1:B:77:VAL:HG21	1:B:94:LEU:HD12	1.92	0.51
1:D:118:ALA:HB3	1:D:121:GLN:HG3	1.93	0.51
1:C:305:ARG:HG2	1:C:310:LEU:HD11	1.93	0.51
1:D:386:ILE:O	1:D:434:ARG:NH1	2.40	0.51
1:B:308:LYS:HD3	5:B:905:HOH:O	2.11	0.50
1:B:78:VAL:HG12	1:B:156:LEU:HD21	1.93	0.50
1:D:334:ILE:HD11	1:D:550:THR:HG22	1.93	0.50
1:A:198:THR:H	1:D:199:ALA:HB2	1.77	0.50
1:D:490:HIS:CD2	1:D:490:HIS:H	2.29	0.50
1:B:73:ARG:NE	1:B:146:ASP:OD1	2.42	0.49
1:C:7:LEU:HD13	1:C:166:ALA:HB2	1.95	0.49
1:C:502:GLU:HB3	1:C:541:LYS:HB2	1.93	0.49
1:B:472:LEU:HD23	1:B:492:LEU:HD11	1.95	0.49
1:D:3:LYS:NZ	1:D:145:VAL:O	2.39	0.49
1:A:84:TRP:CZ2	1:A:92:ARG:HG2	2.48	0.48
1:B:90:LYS:H	1:B:90:LYS:HD2	1.77	0.48
1:B:302:ARG:HG2	1:B:305:ARG:NH2	2.23	0.48
1:C:311:ILE:HD11	1:C:561:LYS:HE2	1.94	0.48
1:D:320:ARG:HB3	1:D:325:PHE:CD2	2.48	0.48
1:A:222:ASP:OD2	5:A:806:HOH:O	2.20	0.48
1:C:117:GLN:HE22	1:C:123:ARG:HA	1.79	0.48
1:A:226:THR:HB	1:A:253:LYS:HD2	1.96	0.48
1:B:7:LEU:HD13	1:B:166:ALA:HB2	1.96	0.48
1:C:461:MET:SD	1:C:465:ASN:HB3	2.53	0.48
1:C:78:VAL:HG12	1:C:156:LEU:HD21	1.95	0.47
1:A:74:PHE:O	1:A:145:VAL:HA	2.15	0.47
1:D:74:PHE:O	1:D:145:VAL:HA	2.15	0.47
1:C:36:SER:O	1:C:40:LYS:HB2	2.16	0.46
1:C:478:PRO:HD2	1:D:436:PHE:CE1	2.51	0.46
1:C:17:ILE:O	2:C:701:NDP:H2N	2.16	0.46
1:A:89:ARG:HB2	1:A:89:ARG:NH1	2.31	0.46
1:A:349:VAL:HG12	1:A:551:HIS:HB2	1.97	0.46
1:A:181:ASP:OD1	1:A:182:VAL:HG23	2.16	0.46
1:B:81:ARG:HB2	1:B:103:SER:HB2	1.98	0.45
1:B:580:GLU:H	1:B:580:GLU:CD	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ARG:NE	5:C:805:HOH:O	2.16	0.45
1:C:221:LYS:NZ	5:C:817:HOH:O	2.41	0.45
1:C:117:GLN:NE2	5:C:802:HOH:O	2.04	0.45
1:D:384:TRP:CD2	1:D:395:LEU:HD11	2.51	0.45
1:A:204:ALA:HB3	1:A:205:PRO:HD3	1.99	0.45
1:C:224:GLU:OE2	1:C:253:LYS:NZ	2.39	0.45
1:B:577:LEU:HD21	1:B:594:GLU:HG2	1.99	0.44
1:C:506:ILE:HG13	1:D:353:PHE:CE2	2.52	0.44
1:D:491:LEU:HD12	1:D:492:LEU:HB2	1.99	0.44
1:A:478:PRO:HD2	1:B:436:PHE:CZ	2.52	0.44
1:C:343:ASP:HA	5:C:801:HOH:O	2.16	0.44
1:D:37:ARG:NH1	5:D:822:HOH:O	2.51	0.44
1:B:192:ILE:HD13	1:B:229:PRO:HG3	1.99	0.44
1:A:461:MET:SD	1:A:465:ASN:HB3	2.58	0.44
1:C:306:GLU:H	1:C:306:GLU:HG2	1.63	0.44
1:D:141:TYR:HB3	1:D:145:VAL:HG23	2.00	0.44
1:D:216:GLU:CD	5:D:801:HOH:O	2.52	0.44
1:A:30:THR:HB	1:A:243:TYR:OH	2.18	0.44
1:C:252:ARG:O	1:C:255:ASP:HB3	2.18	0.44
1:C:539:LYS:HE3	1:C:539:LYS:HB2	1.76	0.44
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.74	0.44
1:B:176:ARG:HD2	1:B:596:VAL:CG1	2.48	0.44
1:A:7:LEU:HD13	1:A:166:ALA:HB2	1.99	0.44
1:B:90:LYS:H	1:B:90:LYS:CD	2.31	0.44
1:D:575:ASN:HB2	1:D:594:GLU:HG2	1.98	0.44
1:B:109:GLU:H	1:B:109:GLU:CD	2.21	0.43
1:B:461:MET:HE3	5:B:1016:HOH:O	2.18	0.43
1:A:7:LEU:HD12	1:A:150:VAL:HB	2.00	0.43
1:A:48:ARG:HD3	1:B:302:ARG:HH12	1.84	0.43
1:D:13:PRO:HD3	1:D:174:VAL:O	2.19	0.43
1:D:559:ALA:HA	1:D:606:MET:HB2	2.01	0.43
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.73	0.42
1:B:415:ARG:NH1	1:B:484:MET:O	2.52	0.42
1:C:186:ALA:O	1:C:209:VAL:HG22	2.18	0.42
1:B:252:ARG:O	1:B:255:ASP:HB2	2.19	0.42
1:C:577:LEU:HD21	1:C:594:GLU:HG2	2.01	0.42
1:C:349:VAL:HG22	1:C:553:TYR:CD1	2.54	0.42
1:C:491:LEU:HD12	1:C:492:LEU:HB2	2.02	0.42
1:A:502:GLU:HB3	1:A:541:LYS:HB2	2.01	0.42
1:A:580:GLU:H	1:A:580:GLU:CD	2.22	0.42
1:D:109:GLU:H	1:D:109:GLU:CD	2.21	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:PHE:O	1:C:145:VAL:HA	2.19	0.42
1:D:427:PRO:HB3	1:D:440:TYR:HB2	2.00	0.42
1:B:89:ARG:HD2	1:B:115:LYS:HD3	2.01	0.42
1:B:322:HIS:NE2	1:B:569:ARG:O	2.43	0.42
1:B:387:ARG:NH2	5:B:821:HOH:O	2.50	0.42
1:D:557:VAL:O	1:D:561:LYS:HG3	2.19	0.42
1:B:305:ARG:HG3	1:B:310:LEU:HD11	2.01	0.42
1:B:306:GLU:H	1:B:306:GLU:HG3	1.66	0.42
1:A:89:ARG:NH2	1:A:92:ARG:HH22	2.17	0.42
1:A:90:LYS:HE3	1:A:91:PHE:CZ	2.54	0.42
1:A:506:ILE:HG13	1:B:353:PHE:CE2	2.55	0.41
1:B:74:PHE:O	1:B:145:VAL:HA	2.20	0.41
1:C:13:PRO:HD3	1:C:174:VAL:O	2.20	0.41
1:D:345:THR:HB	1:D:347:VAL:HG12	2.02	0.41
1:A:300:GLU:O	1:A:304:LYS:HG2	2.19	0.41
1:C:393:ASN:O	1:C:397:GLU:HG3	2.20	0.41
1:C:296:TRP:CE3	1:D:33:LYS:HE3	2.56	0.41
1:D:308:LYS:HB3	1:D:308:LYS:HE2	1.84	0.41
1:C:436:PHE:CE1	1:D:478:PRO:HD2	2.56	0.41
1:B:284:PRO:C	5:B:806:HOH:O	2.56	0.41
1:C:45:GLU:O	1:C:48:ARG:HG3	2.21	0.41
1:C:333:ASP:OD2	1:C:352:LYS:HE2	2.21	0.41
1:D:117:GLN:OE1	1:D:117:GLN:N	2.32	0.41
1:A:314:VAL:HG11	1:A:567:GLU:HG3	2.03	0.41
1:B:39:THR:HA	1:B:149:PHE:CE2	2.56	0.41
1:B:237:SER:HB2	1:B:573:ILE:HD11	2.02	0.41
1:A:141:TYR:HB3	1:A:145:VAL:HG23	2.03	0.41
1:B:311:ILE:CD1	1:B:561:LYS:HE3	2.51	0.41
1:B:445:THR:HB	1:B:447:TYR:CZ	2.56	0.41
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.69	0.40
1:A:17:ILE:O	2:A:701:NDP:H2N	2.21	0.40
1:A:47:SER:O	1:A:48:ARG:HB2	2.21	0.40
1:A:197:SER:HB2	1:D:199:ALA:HB3	2.03	0.40
1:A:606:MET:SD	1:A:606:MET:N	2.94	0.40
1:B:484:MET:SD	1:B:488:PRO:HD3	2.61	0.40
1:D:567:GLU:OE1	5:D:804:HOH:O	2.22	0.40
1:B:311:ILE:HD11	1:B:561:LYS:HE3	2.03	0.40
1:C:238:ASP:OD1	5:C:807:HOH:O	2.22	0.40
1:D:493:CYS:HA	1:D:506:ILE:O	2.21	0.40
1:A:427:PRO:HB3	1:A:440:TYR:HB2	2.03	0.40
1:A:445:THR:HB	1:A:447:TYR:CZ	2.57	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)
5:B:1012:HOH:O	5:C:1071:HOH:O[1_644]	1.99	0.21

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	554/610 (91%)	540 (98%)	14 (2%)	0	100	100
1	B	554/610 (91%)	536 (97%)	18 (3%)	0	100	100
1	C	552/610 (90%)	536 (97%)	16 (3%)	0	100	100
1	D	557/610 (91%)	543 (98%)	14 (2%)	0	100	100
All	All	2217/2440 (91%)	2155 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/525 (92%)	470 (97%)	13 (3%)	44	38
1	B	482/525 (92%)	463 (96%)	19 (4%)	32	25
1	C	483/525 (92%)	467 (97%)	16 (3%)	38	31
1	D	485/525 (92%)	469 (97%)	16 (3%)	38	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1933/2100 (92%)	1869 (97%)	64 (3%)	38 31

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	41	THR
1	A	44	GLU
1	A	48	ARG
1	A	196	LYS
1	A	207	GLU
1	A	253	LYS
1	A	285	SER
1	A	306	GLU
1	A	397	GLU
1	A	441	LYS
1	A	489	CYS
1	A	492	LEU
1	B	44	GLU
1	B	48	ARG
1	B	90	LYS
1	B	107	LYS
1	B	117	GLN
1	B	207	GLU
1	B	255	ASP
1	B	281	LEU
1	B	282	GLN
1	B	285	SER
1	B	303	LYS
1	B	306	GLU
1	B	308	LYS
1	B	341	MET
1	B	349	VAL
1	B	409	ARG
1	B	460	GLN
1	B	537	ASN
1	B	541	LYS
1	C	2	GLN
1	C	44	GLU
1	C	72	LYS
1	C	119	GLU
1	C	142	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	221	LYS
1	C	228	ARG
1	C	285	SER
1	C	300	GLU
1	C	303	LYS
1	C	306	GLU
1	C	307	GLN
1	C	396	SER
1	C	555	ASN
1	C	603	ARG
1	C	605	GLN
1	D	44	GLU
1	D	48	ARG
1	D	90	LYS
1	D	198	THR
1	D	201	GLN
1	D	254	THR
1	D	281	LEU
1	D	307	GLN
1	D	308	LYS
1	D	345	THR
1	D	347	VAL
1	D	410	GLU
1	D	460	GLN
1	D	516	LEU
1	D	555	ASN
1	D	603	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	ASN
1	A	601	HIS
1	B	307	GLN
1	B	460	GLN
1	B	605	GLN
1	C	2	GLN
1	C	117	GLN
1	C	282	GLN
1	C	307	GLN
1	C	460	GLN
1	D	282	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	307	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	4RI	A	702	-	21,21,21	3.17	10 (47%)	27,27,27	1.52	4 (14%)
4	UMP	D	703	-	21,21,21	0.85	0	31,31,31	1.59	6 (19%)
4	UMP	A	703	-	21,21,21	0.78	1 (4%)	31,31,31	1.48	4 (12%)
2	NDP	C	701	-	45,52,52	2.04	7 (15%)	53,80,80	1.42	11 (20%)
4	UMP	B	703	-	21,21,21	0.87	1 (4%)	31,31,31	1.58	6 (19%)
3	4RI	B	702	-	21,21,21	3.12	9 (42%)	27,27,27	1.23	3 (11%)
3	4RI	C	702	-	21,21,21	3.02	9 (42%)	27,27,27	1.39	4 (14%)
2	NDP	B	701	-	45,52,52	2.28	8 (17%)	53,80,80	1.48	8 (15%)
2	NDP	D	701	-	45,52,52	2.24	10 (22%)	53,80,80	1.45	9 (16%)
2	NDP	A	701	-	45,52,52	2.20	7 (15%)	53,80,80	1.46	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UMP	C	703	-	21,21,21	0.82	1 (4%)	31,31,31	1.62	4 (12%)
3	4RI	D	702	-	21,21,21	3.11	10 (47%)	27,27,27	1.58	5 (18%)

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	4RI	A	702	-	-	1/10/10/10	0/2/2/2
4	UMP	D	703	-	-	3/10/22/22	0/2/2/2
4	UMP	A	703	-	-	1/10/22/22	0/2/2/2
2	NDP	C	701	-	-	2/30/77/77	0/5/5/5
4	UMP	B	703	-	-	5/10/22/22	0/2/2/2
3	4RI	B	702	-	-	1/10/10/10	0/2/2/2
3	4RI	C	702	-	-	1/10/10/10	0/2/2/2
2	NDP	B	701	-	-	3/30/77/77	0/5/5/5
2	NDP	D	701	-	-	4/30/77/77	0/5/5/5
2	NDP	A	701	-	-	4/30/77/77	0/5/5/5
4	UMP	C	703	-	-	2/10/22/22	0/2/2/2
3	4RI	D	702	-	-	0/10/10/10	0/2/2/2

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NDP	P2B-O2B	11.77	1.81	1.59
2	D	701	NDP	P2B-O2B	11.38	1.80	1.59
2	B	701	NDP	P2B-O2B	11.37	1.80	1.59
2	C	701	NDP	P2B-O2B	10.28	1.78	1.59
3	A	702	4RI	CAQ-CAP	6.81	1.53	1.38
3	B	702	4RI	CAQ-CAP	6.68	1.53	1.38
3	D	702	4RI	CAQ-CAP	6.60	1.52	1.38
3	C	702	4RI	CAQ-CAP	6.48	1.52	1.38
3	A	702	4RI	CAT-CAG	6.21	1.52	1.39
3	B	702	4RI	CAT-CAG	6.21	1.52	1.39
3	D	702	4RI	CAT-CAG	6.01	1.52	1.39
3	C	702	4RI	CAT-CAG	5.82	1.51	1.39
3	A	702	4RI	CAS-CAR	5.68	1.53	1.38
3	D	702	4RI	CAS-CAR	5.65	1.53	1.38
3	B	702	4RI	CAS-CAR	5.62	1.52	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	4RI	C2-NAI	5.56	1.45	1.33
3	D	702	4RI	C2-NAI	5.51	1.44	1.33
3	C	702	4RI	CAS-CAR	5.38	1.52	1.38
3	A	702	4RI	C2-NAI	5.34	1.44	1.33
3	C	702	4RI	C2-NAI	5.32	1.44	1.33
3	A	702	4RI	C6-NAH	4.85	1.46	1.34
3	D	702	4RI	C6-NAH	4.66	1.45	1.34
3	B	702	4RI	C6-NAH	4.46	1.45	1.34
3	C	702	4RI	C6-NAH	4.28	1.44	1.34
2	D	701	NDP	O4B-C1B	3.96	1.46	1.41
2	B	701	NDP	C7N-N7N	3.66	1.43	1.33
2	B	701	NDP	C3B-C2B	3.60	1.61	1.52
2	A	701	NDP	PN-O5D	3.49	1.73	1.59
2	D	701	NDP	O2B-C2B	-3.44	1.31	1.44
2	D	701	NDP	PN-O5D	3.39	1.73	1.59
2	C	701	NDP	O4B-C1B	3.22	1.45	1.41
2	A	701	NDP	C7N-N7N	3.15	1.41	1.33
3	B	702	4RI	CAS-CAT	-3.14	1.32	1.38
3	A	702	4RI	CAS-CAT	-3.09	1.32	1.38
2	B	701	NDP	O2B-C2B	-3.05	1.33	1.44
2	B	701	NDP	PN-O5D	3.05	1.71	1.59
2	B	701	NDP	C6N-N1N	3.04	1.44	1.37
3	D	702	4RI	CAS-CAT	-2.99	1.32	1.38
3	C	702	4RI	CAS-CAT	-2.98	1.32	1.38
2	C	701	NDP	C7N-N7N	2.93	1.41	1.33
3	C	702	4RI	CAP-CAG	-2.90	1.33	1.39
2	A	701	NDP	C6N-N1N	2.90	1.44	1.37
2	C	701	NDP	C6N-N1N	2.88	1.44	1.37
2	A	701	NDP	C7N-C3N	-2.82	1.42	1.48
3	A	702	4RI	CAP-CAG	-2.82	1.33	1.39
3	B	702	4RI	CAP-CAG	-2.80	1.33	1.39
2	A	701	NDP	O2B-C2B	-2.79	1.33	1.44
2	B	701	NDP	O4B-C1B	2.74	1.44	1.41
3	D	702	4RI	CAP-CAG	-2.70	1.33	1.39
2	C	701	NDP	O2B-C2B	-2.69	1.34	1.44
3	D	702	4RI	C6-N1	-2.68	1.31	1.35
2	C	701	NDP	C3B-C2B	2.65	1.58	1.52
3	A	702	4RI	C6-N1	-2.56	1.31	1.35
2	B	701	NDP	C2A-N1A	2.48	1.38	1.33
2	C	701	NDP	PN-O5D	2.44	1.69	1.59
3	C	702	4RI	CAR-CAQ	-2.39	1.31	1.38
3	B	702	4RI	C5-C6	-2.33	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	NDP	C7N-N7N	2.29	1.39	1.33
3	D	702	4RI	C5-C6	-2.28	1.38	1.43
2	D	701	NDP	C4A-N3A	2.27	1.38	1.35
3	D	702	4RI	CAR-CAQ	-2.23	1.32	1.38
2	D	701	NDP	C2A-N1A	2.22	1.38	1.33
3	A	702	4RI	CAR-CAQ	-2.17	1.32	1.38
2	D	701	NDP	C6N-N1N	2.17	1.42	1.37
2	D	701	NDP	C3B-C2B	2.16	1.57	1.52
3	A	702	4RI	C5-C6	-2.16	1.39	1.43
3	C	702	4RI	C5-C6	-2.11	1.39	1.43
2	D	701	NDP	C7N-C3N	-2.10	1.44	1.48
4	A	703	UMP	C6-C5	2.06	1.39	1.35
3	B	702	4RI	CAR-CAQ	-2.05	1.32	1.38
4	C	703	UMP	C6-C5	2.03	1.39	1.35
2	A	701	NDP	C3B-C2B	2.02	1.57	1.52
4	B	703	UMP	C6-C5	2.01	1.39	1.35

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	703	UMP	C4-N3-C2	-5.09	119.86	126.58
4	B	703	UMP	C4-N3-C2	-4.57	120.55	126.58
4	A	703	UMP	C4-N3-C2	-4.56	120.56	126.58
4	D	703	UMP	C4-N3-C2	-4.51	120.64	126.58
3	A	702	4RI	C5-C6-N1	-4.31	120.10	122.52
3	D	702	4RI	C5-C6-N1	-4.08	120.22	122.52
3	D	702	4RI	C6-C5-C4	4.07	119.27	115.91
4	C	703	UMP	N3-C2-N1	4.02	120.22	114.89
3	A	702	4RI	C6-C5-C4	3.88	119.11	115.91
2	B	701	NDP	PN-O3-PA	-3.87	119.53	132.83
3	C	702	4RI	C6-C5-C4	3.83	119.06	115.91
4	D	703	UMP	N3-C2-N1	3.70	119.80	114.89
4	B	703	UMP	C5-C4-N3	3.54	120.14	114.84
4	A	703	UMP	N3-C2-N1	3.49	119.53	114.89
2	A	701	NDP	O2B-P2B-O1X	-3.45	96.08	109.39
2	D	701	NDP	PN-O3-PA	-3.42	121.10	132.83
4	A	703	UMP	C5-C4-N3	3.37	119.89	114.84
4	B	703	UMP	N3-C2-N1	3.37	119.36	114.89
2	A	701	NDP	PN-O3-PA	-3.34	121.35	132.83
2	C	701	NDP	PN-O3-PA	-3.21	121.80	132.83
2	A	701	NDP	C3B-C2B-C1B	-3.06	97.14	102.89
4	C	703	UMP	O4-C4-C5	-3.02	119.85	125.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	703	UMP	C5-C4-N3	3.02	119.36	114.84
2	C	701	NDP	O2B-P2B-O1X	-2.98	97.88	109.39
4	D	703	UMP	O4-C4-C5	-2.96	119.96	125.16
4	D	703	UMP	C1'-N1-C2	2.96	123.47	117.64
3	C	702	4RI	C5-C4-N3	-2.89	120.05	123.61
4	B	703	UMP	O4-C4-C5	-2.87	120.11	125.16
2	C	701	NDP	C3B-C2B-C1B	-2.80	97.63	102.89
2	B	701	NDP	C3B-C2B-C1B	-2.80	97.63	102.89
3	B	702	4RI	C5-C6-N1	-2.77	120.97	122.52
4	D	703	UMP	C5-C4-N3	2.76	118.97	114.84
3	B	702	4RI	C6-C5-C4	2.74	118.17	115.91
2	B	701	NDP	PN-O5D-C5D	-2.65	106.16	121.68
2	B	701	NDP	O3X-P2B-O2X	2.63	117.68	107.64
3	D	702	4RI	CAG-C5-C4	-2.60	121.36	123.46
3	A	702	4RI	CAG-C5-C4	-2.59	121.36	123.46
2	A	701	NDP	O3X-P2B-O2X	2.57	117.47	107.64
2	D	701	NDP	O3X-P2B-O2X	2.57	117.45	107.64
2	D	701	NDP	O2B-P2B-O1X	-2.51	99.70	109.39
2	D	701	NDP	O3X-P2B-O2B	-2.51	94.75	105.99
3	D	702	4RI	C5-C4-N3	-2.51	120.52	123.61
2	B	701	NDP	O2B-P2B-O1X	-2.47	99.84	109.39
2	D	701	NDP	C3B-C2B-C1B	-2.47	98.25	102.89
2	C	701	NDP	O3X-P2B-O2X	2.46	117.03	107.64
4	B	703	UMP	C1'-N1-C2	2.42	122.41	117.64
4	D	703	UMP	C1'-N1-C6	-2.38	116.85	121.55
2	B	701	NDP	O3X-P2B-O2B	-2.37	95.36	105.99
3	C	702	4RI	C2-N1-C6	-2.37	114.38	116.99
3	D	702	4RI	CAJ-C4-C5	-2.37	120.17	124.22
2	A	701	NDP	PA-O5B-C5B	-2.35	107.93	121.68
3	A	702	4RI	C5-C4-N3	-2.33	120.74	123.61
2	C	701	NDP	O2B-C2B-C1B	-2.33	101.73	110.10
2	D	701	NDP	PA-O5B-C5B	-2.29	108.26	121.68
2	B	701	NDP	PA-O5B-C5B	-2.24	108.55	121.68
2	A	701	NDP	PN-O5D-C5D	-2.23	108.63	121.68
2	D	701	NDP	PN-O5D-C5D	-2.20	108.78	121.68
3	B	702	4RI	C5-C4-N3	-2.19	120.91	123.61
2	C	701	NDP	C2A-N1A-C6A	-2.16	115.07	118.75
4	A	703	UMP	O4-C4-C5	-2.13	121.41	125.16
2	D	701	NDP	O5B-C5B-C4B	-2.13	101.65	108.99
2	D	701	NDP	O2A-PA-O1A	2.11	122.69	112.24
2	B	701	NDP	C2A-N1A-C6A	-2.11	115.15	118.75
2	C	701	NDP	O7N-C7N-N7N	-2.09	117.98	122.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	NDP	C3N-C2N-N1N	-2.07	120.15	123.10
2	C	701	NDP	PA-O5B-C5B	-2.03	109.75	121.68
2	A	701	NDP	O2B-C2B-C1B	-2.03	102.79	110.10
4	B	703	UMP	C1'-N1-C6	-2.03	117.54	121.55
3	C	702	4RI	CAG-C5-C4	-2.03	121.81	123.46
2	C	701	NDP	O5D-PN-O1N	-2.03	101.15	109.07
2	C	701	NDP	O2A-PA-O1A	2.01	122.15	112.24

There are no chirality outliers.

All (27) torsion outliers are listed below:

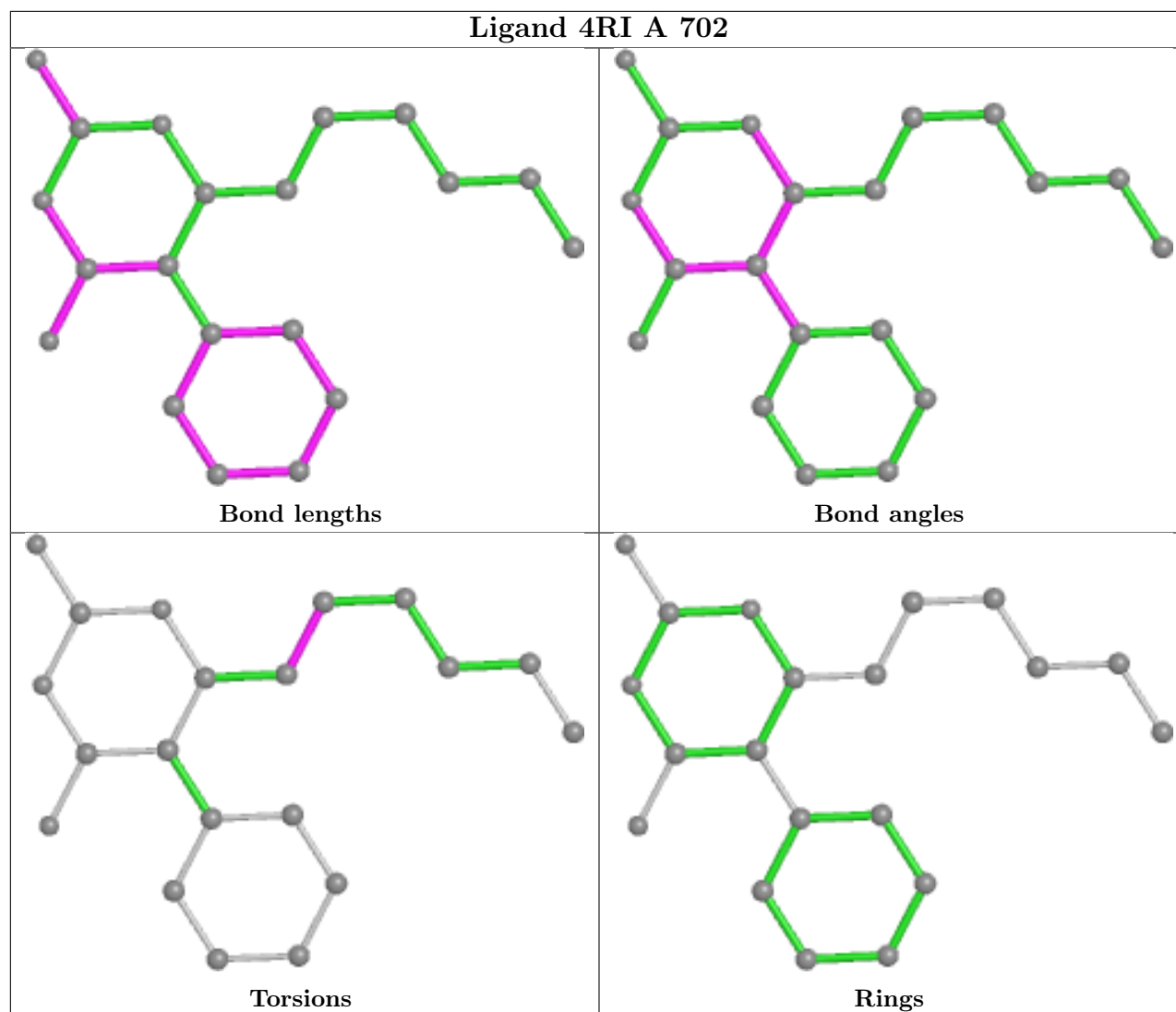
Mol	Chain	Res	Type	Atoms
2	B	701	NDP	PA-O3-PN-O5D
2	D	701	NDP	PA-O3-PN-O5D
4	B	703	UMP	C5'-O5'-P-OP1
4	B	703	UMP	C5'-O5'-P-OP3
4	B	703	UMP	C3'-C4'-C5'-O5'
4	B	703	UMP	O4'-C4'-C5'-O5'
2	A	701	NDP	PA-O3-PN-O5D
4	C	703	UMP	O4'-C4'-C5'-O5'
4	D	703	UMP	O4'-C4'-C5'-O5'
4	B	703	UMP	C5'-O5'-P-OP2
2	B	701	NDP	O4D-C1D-N1N-C2N
3	C	702	4RI	C4-CAJ-CAK-CAL
4	D	703	UMP	C5'-O5'-P-OP1
2	C	701	NDP	O4D-C1D-N1N-C2N
2	C	701	NDP	C2D-C1D-N1N-C2N
2	A	701	NDP	O4D-C1D-N1N-C2N
2	D	701	NDP	O4D-C1D-N1N-C2N
2	A	701	NDP	C2D-C1D-N1N-C2N
2	A	701	NDP	C4D-C5D-O5D-PN
3	B	702	4RI	C4-CAJ-CAK-CAL
2	D	701	NDP	C2D-C1D-N1N-C2N
4	C	703	UMP	C3'-C4'-C5'-O5'
4	D	703	UMP	C3'-C4'-C5'-O5'
4	A	703	UMP	O4'-C4'-C5'-O5'
2	B	701	NDP	C2N-C3N-C7N-N7N
2	D	701	NDP	C2N-C3N-C7N-N7N
3	A	702	4RI	C4-CAJ-CAK-CAL

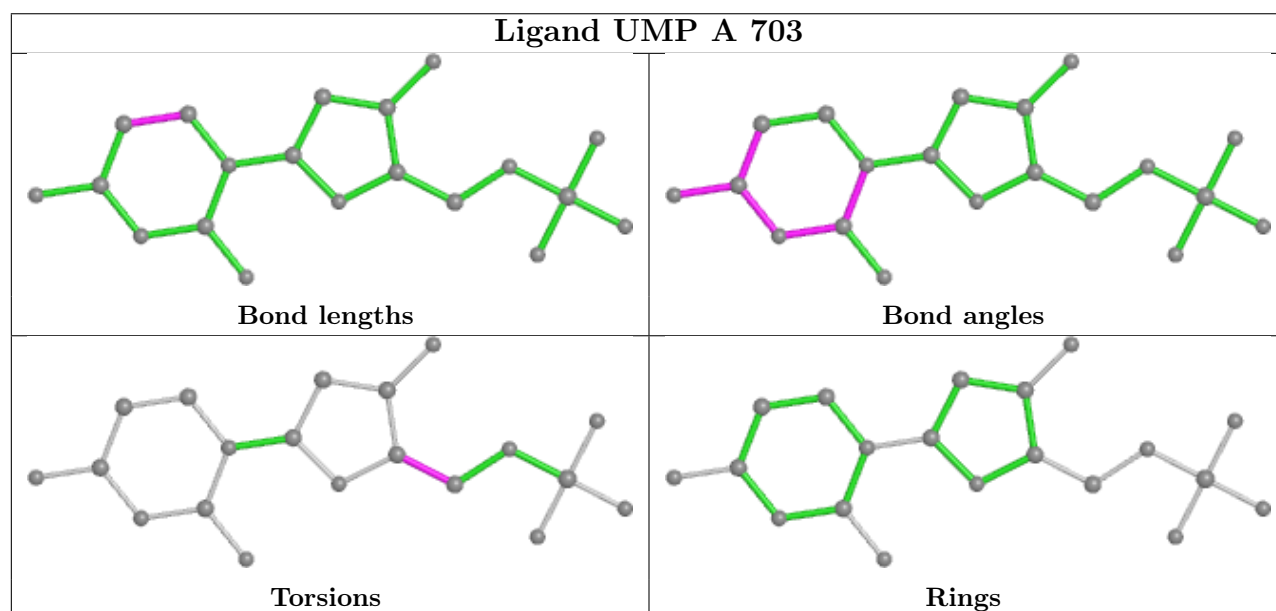
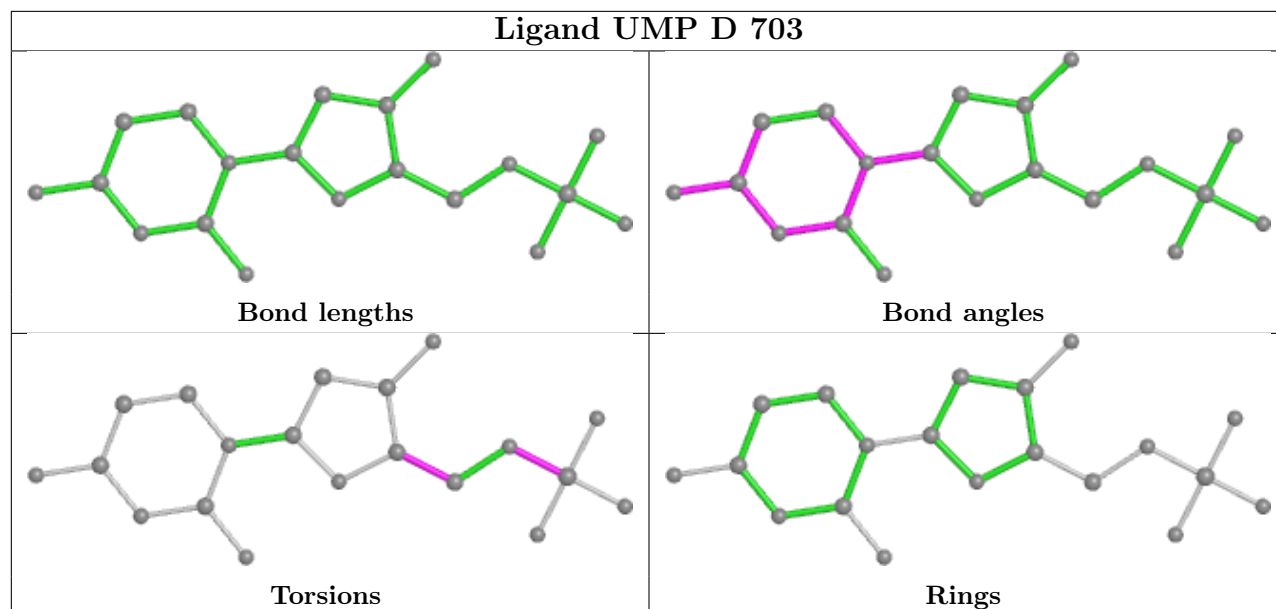
There are no ring outliers.

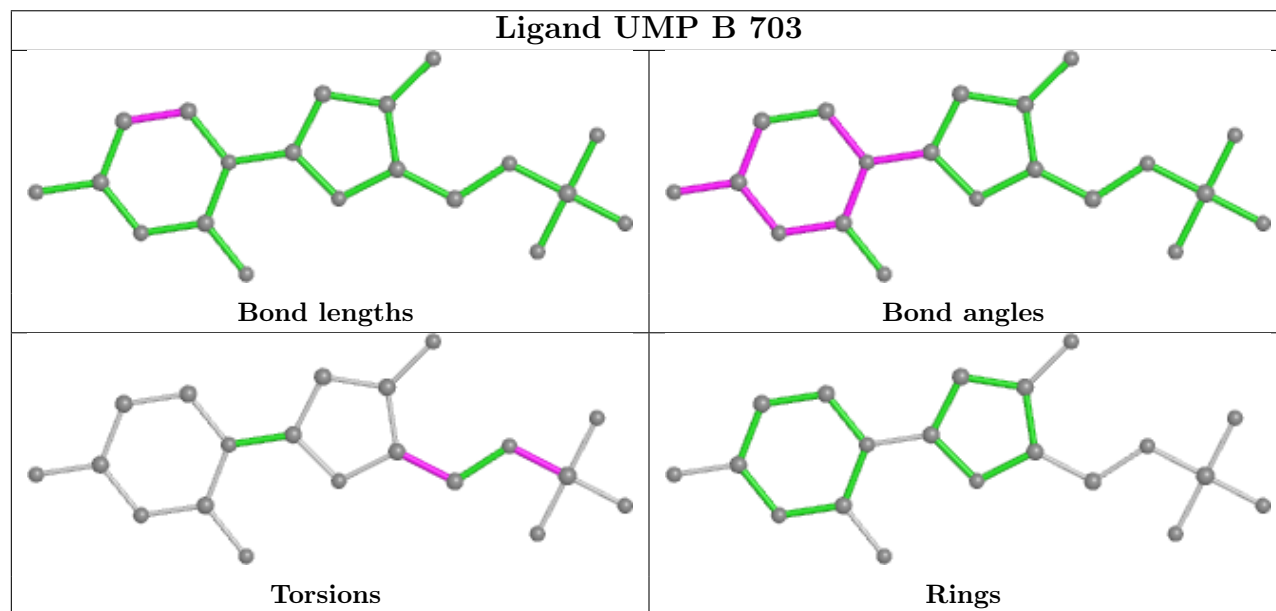
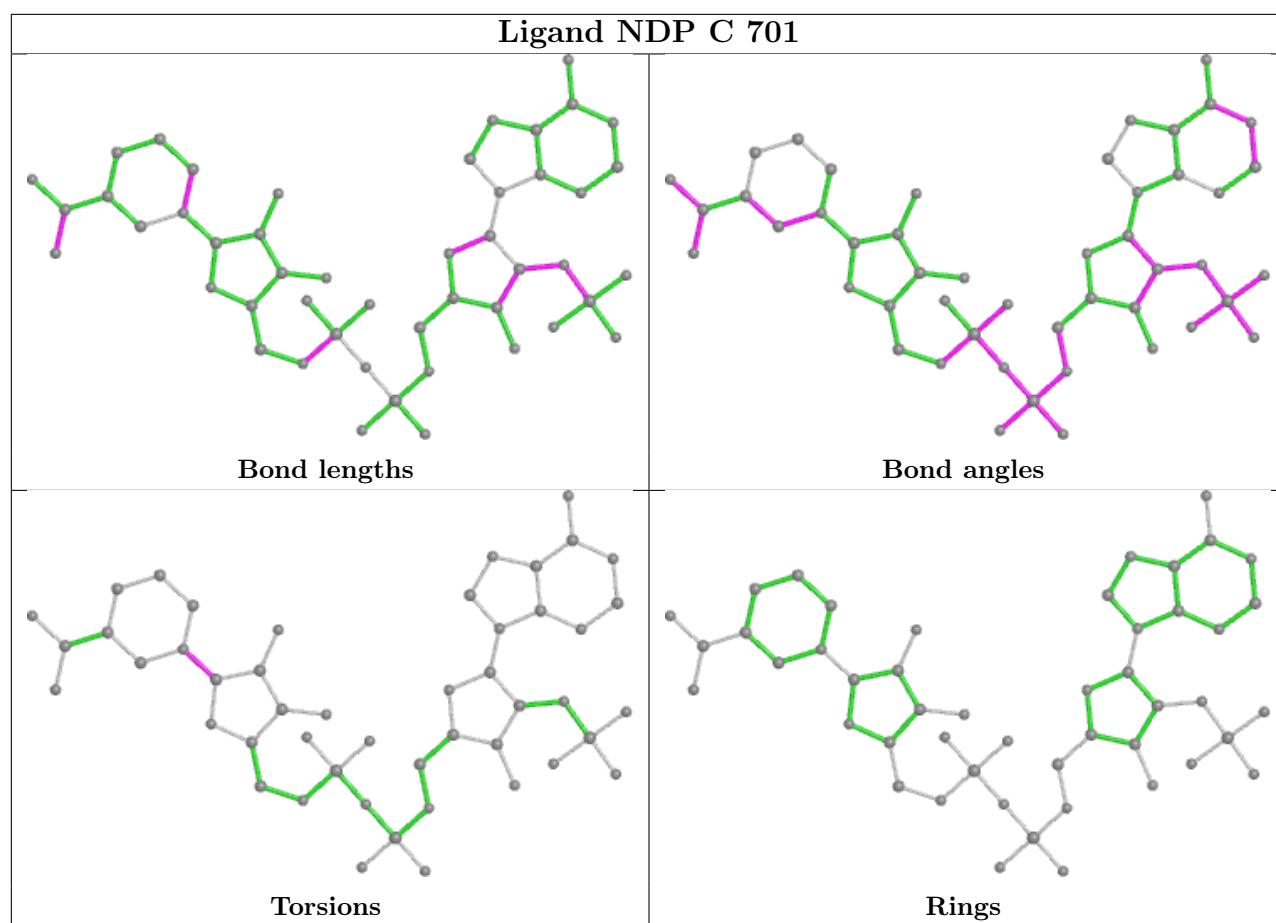
3 monomers are involved in 4 short contacts:

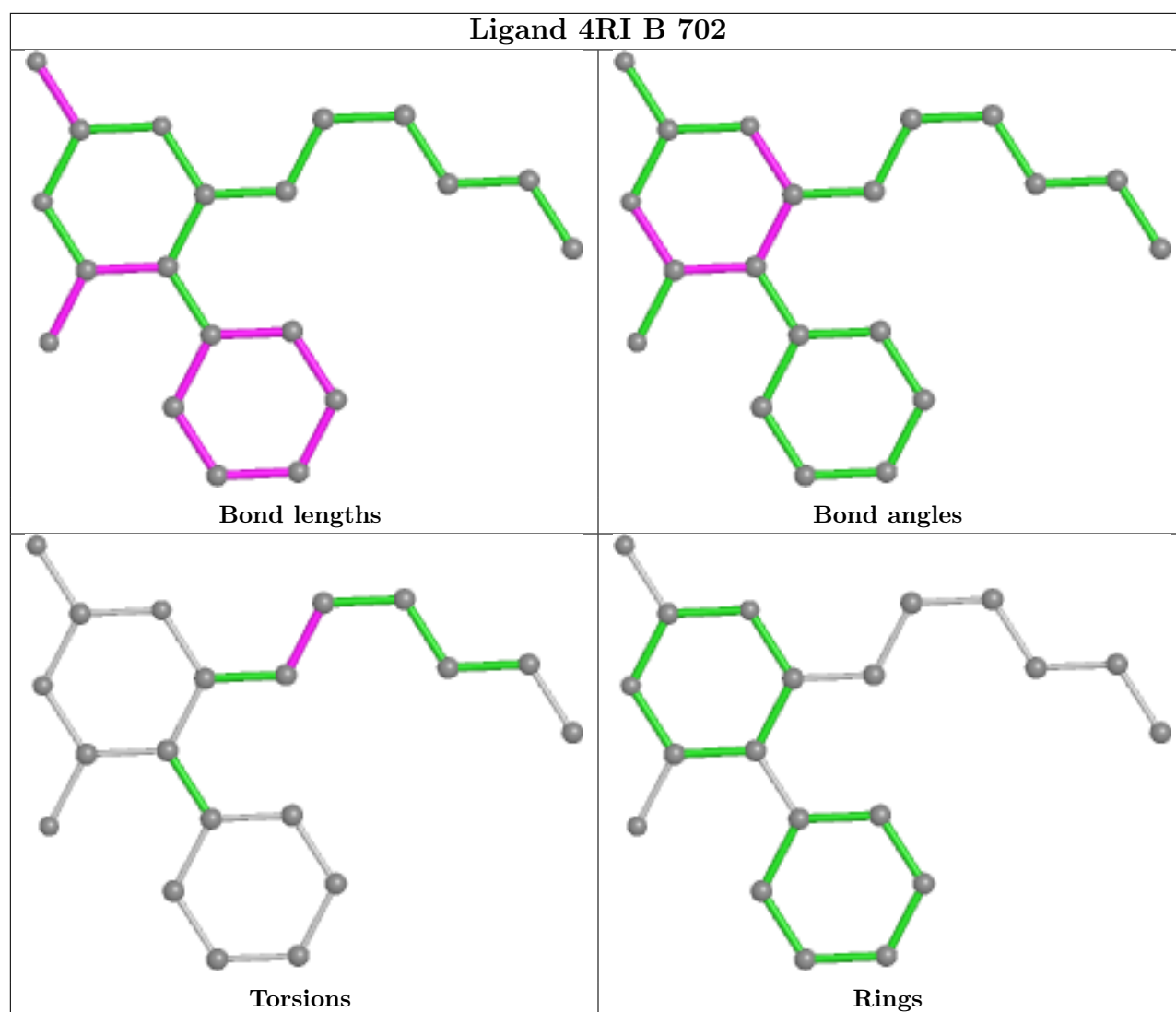
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	4RI	1	0
2	C	701	NDP	1	0
2	A	701	NDP	3	0

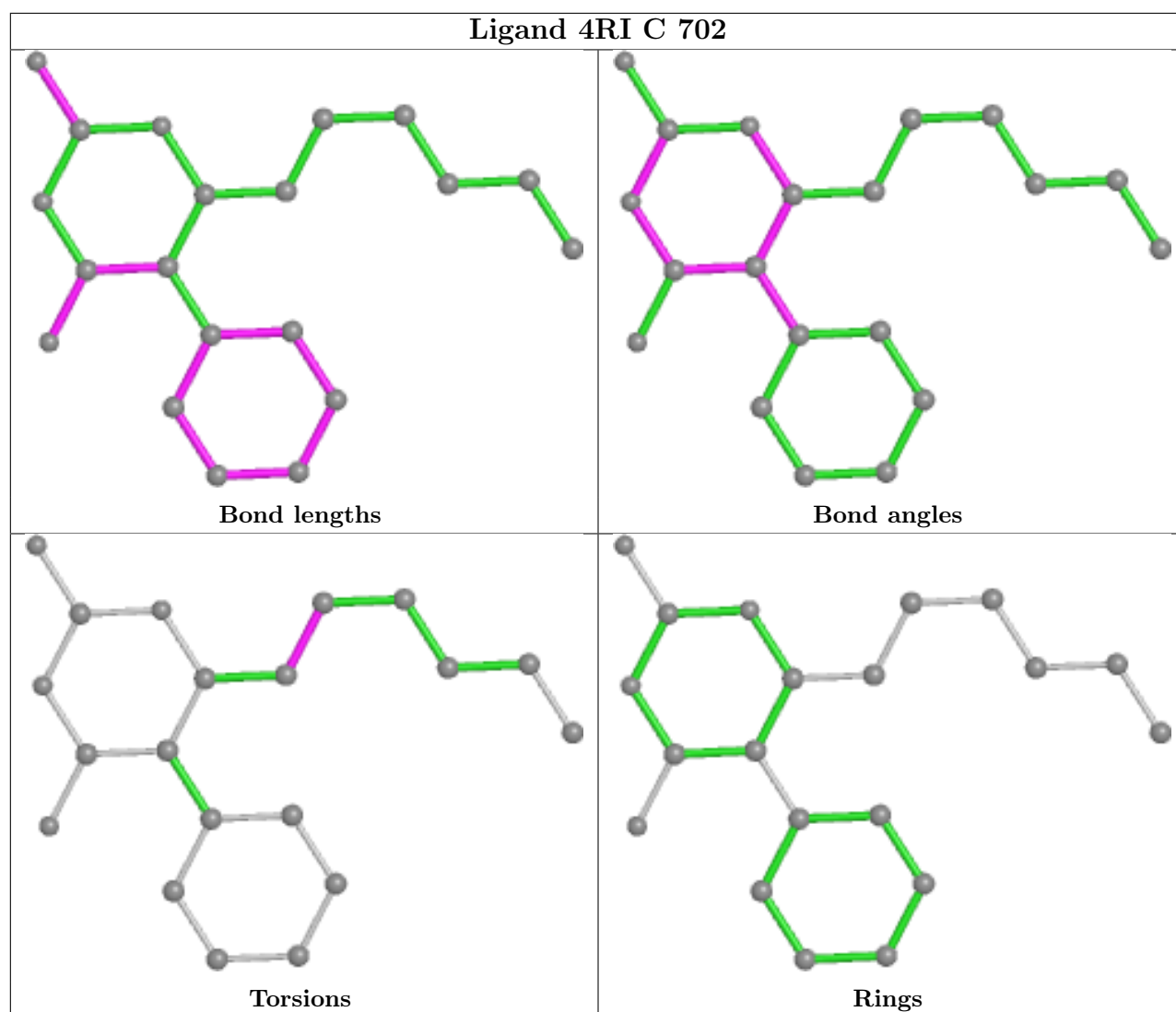
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

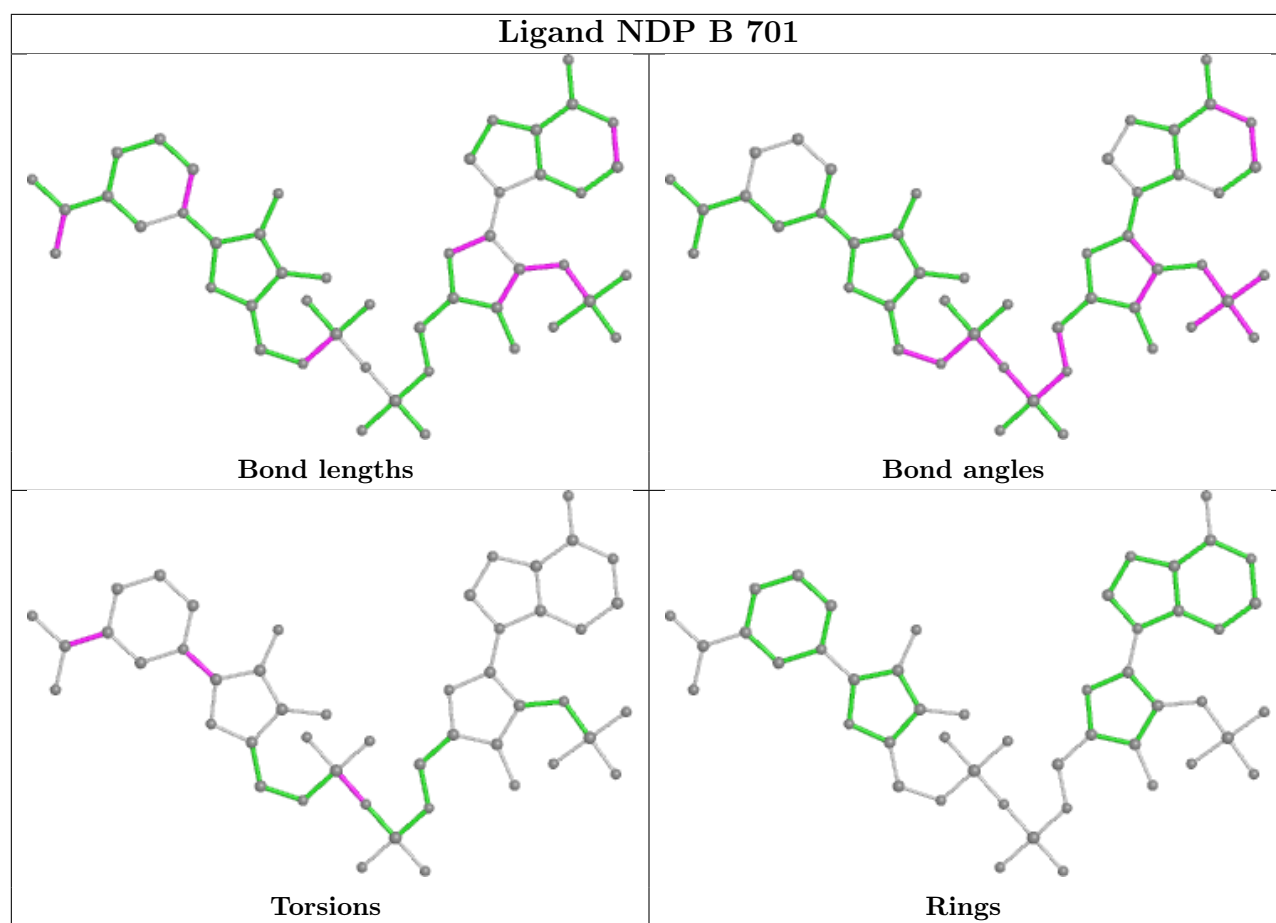


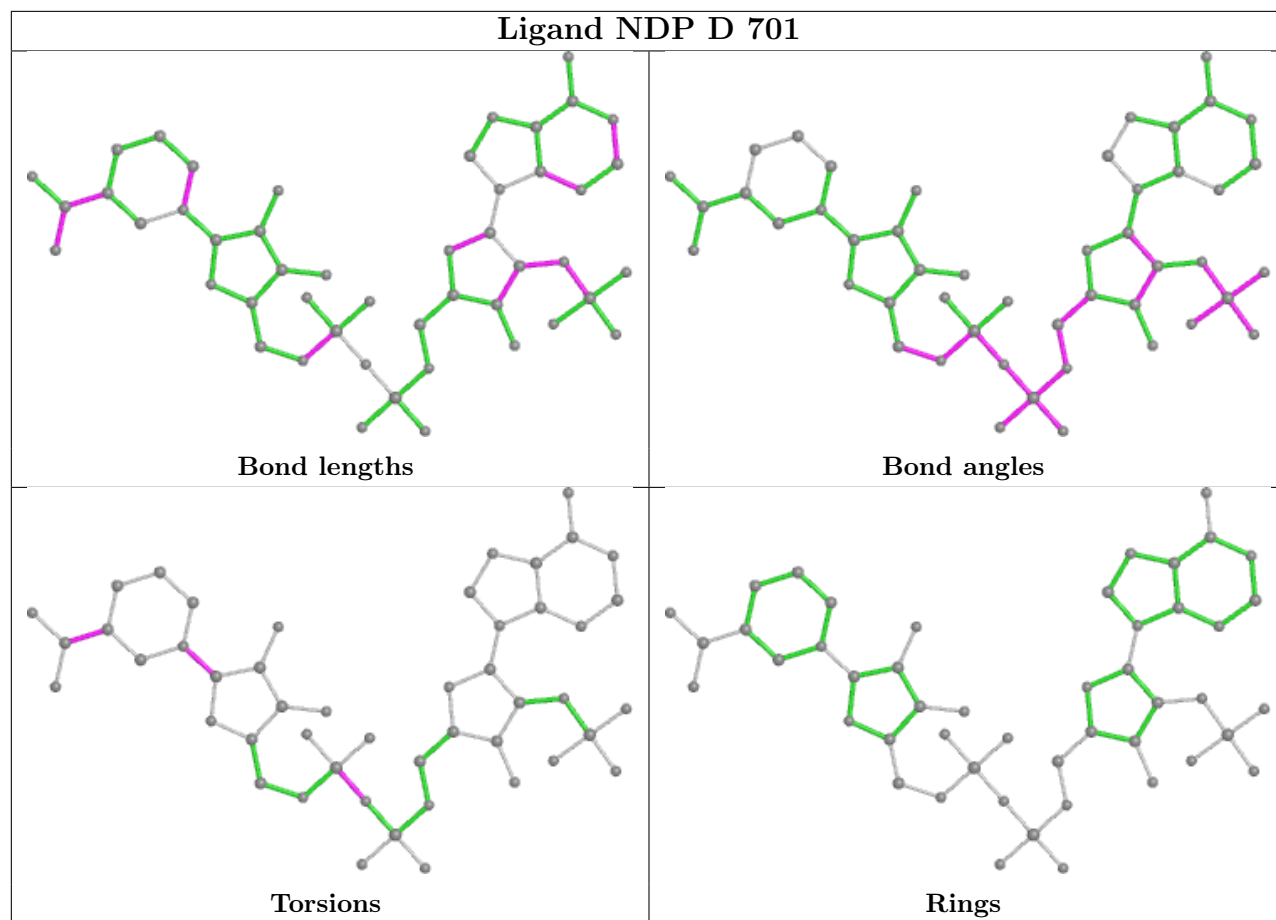


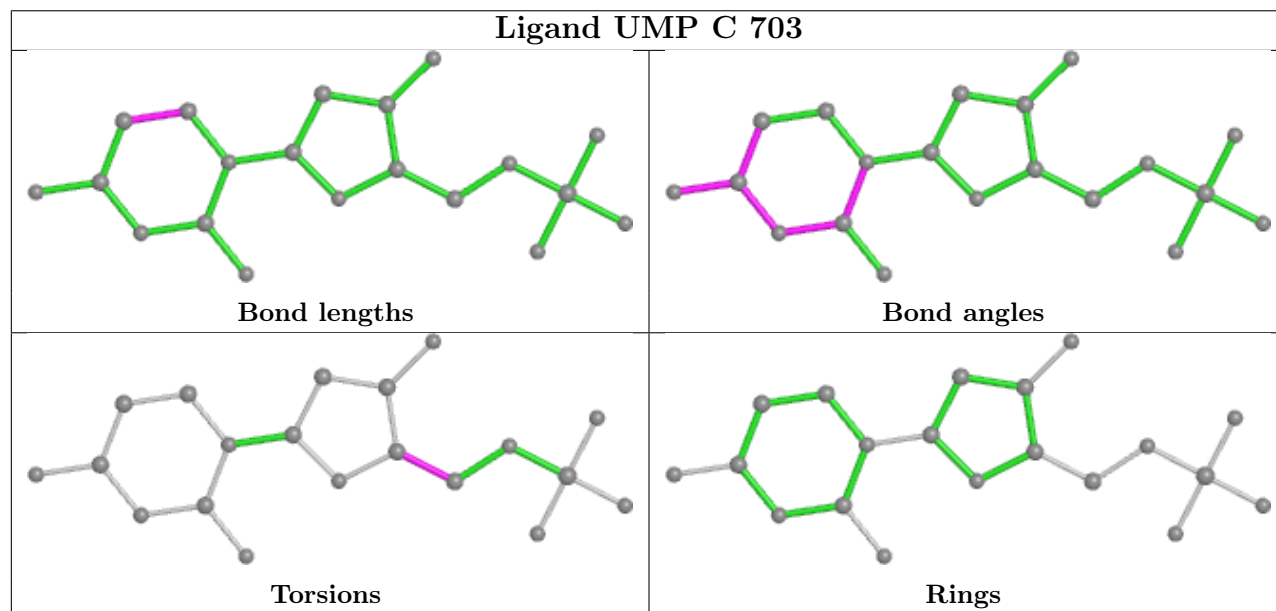
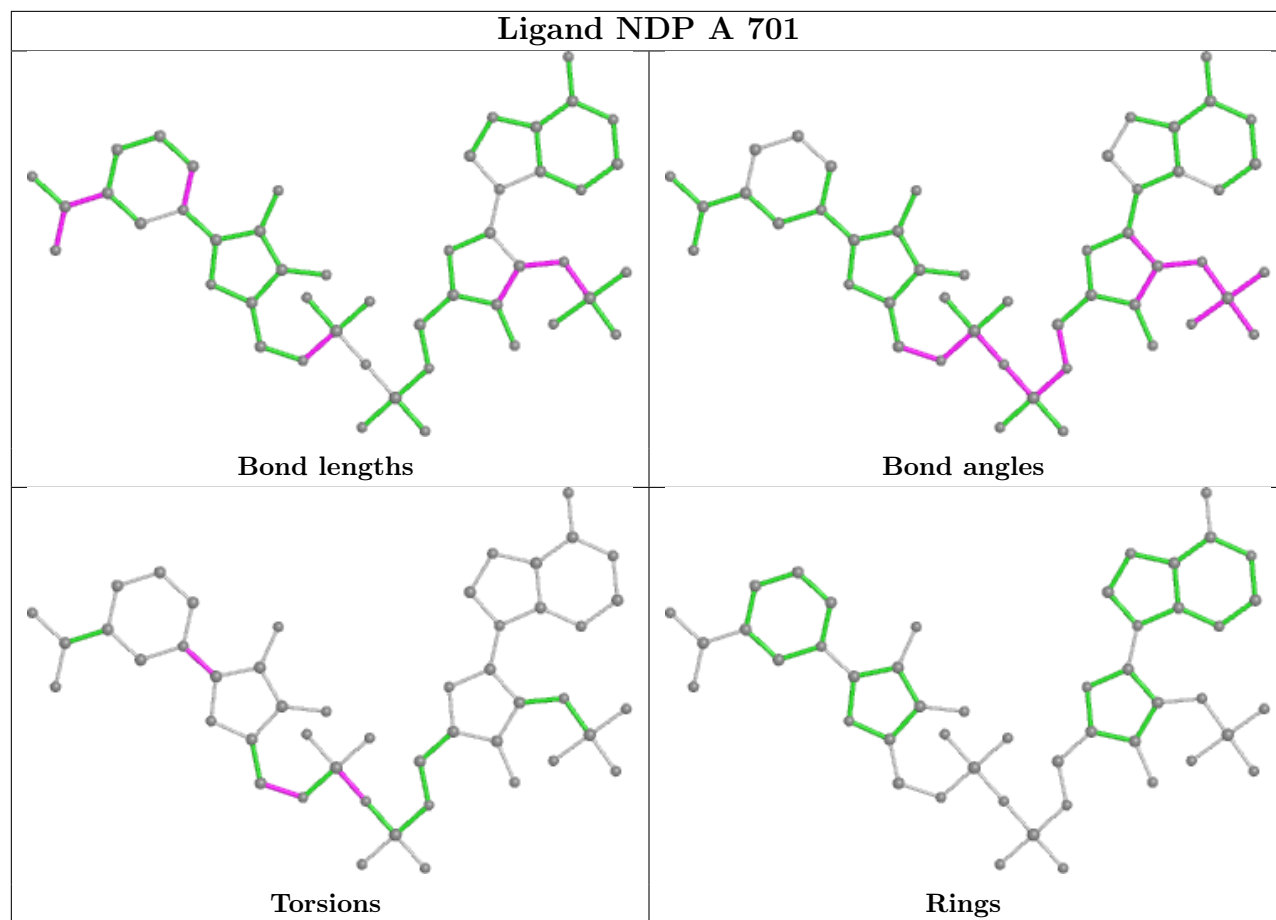


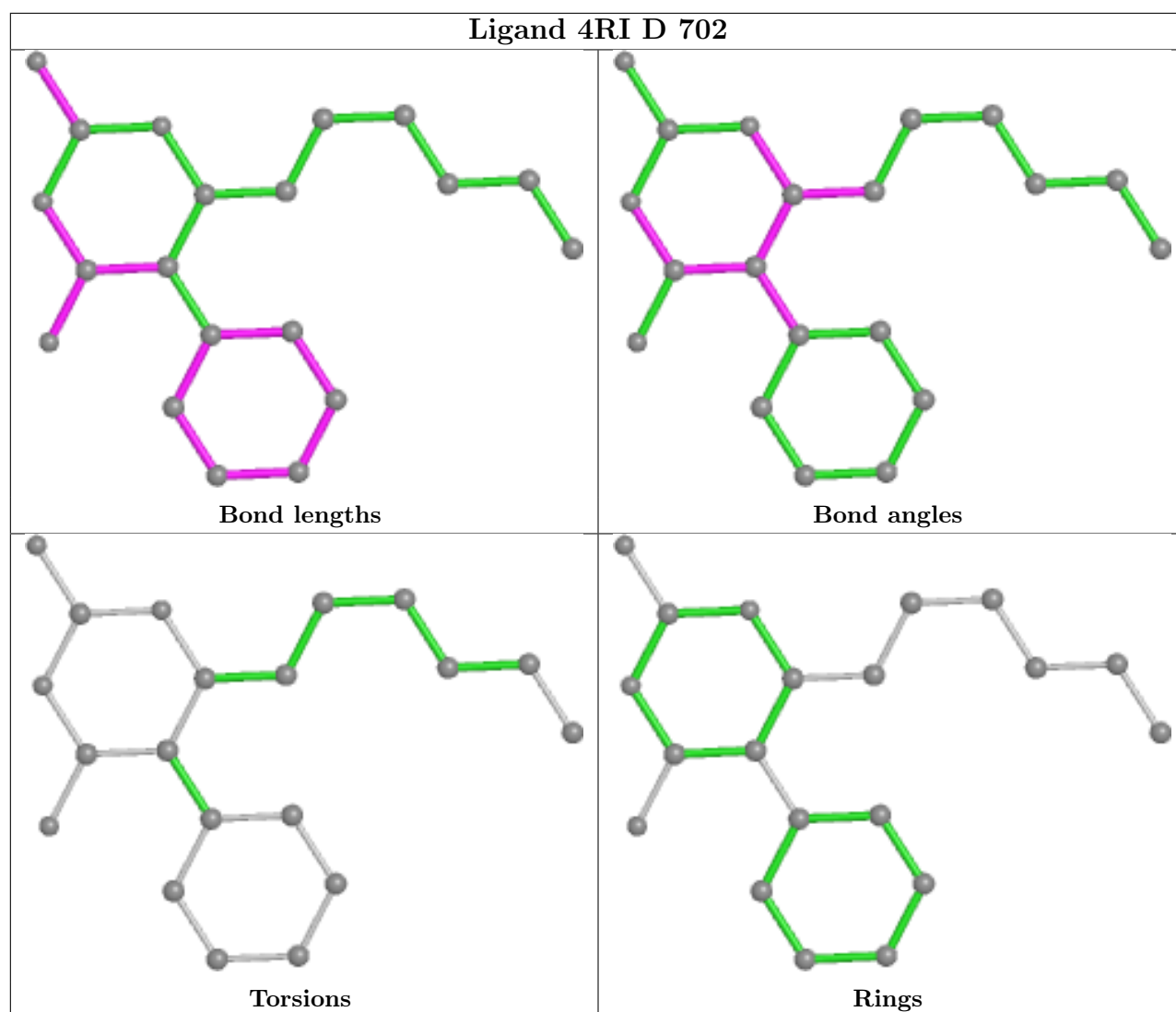












5.7 Other polymers [i](#)

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	560/610 (91%)	0.48	56 (10%) 7 7	24, 38, 76, 114	0
1	B	560/610 (91%)	0.45	60 (10%) 6 6	27, 39, 77, 98	0
1	C	558/610 (91%)	0.34	54 (9%) 7 8	24, 37, 72, 107	0
1	D	563/610 (92%)	0.57	58 (10%) 6 6	28, 40, 82, 118	0
All	All	2241/2440 (91%)	0.46	228 (10%) 6 7	24, 39, 77, 118	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	ALA	16.8
1	A	257	ALA	13.2
1	D	200	ALA	12.1
1	D	205	PRO	12.1
1	D	257	ALA	12.0
1	C	203	ALA	11.1
1	D	203	ALA	10.9
1	D	258	ALA	10.8
1	D	280	GLY	10.8
1	D	256	ASP	10.7
1	D	202	ALA	10.7
1	D	281	LEU	10.4
1	B	281	LEU	10.2
1	B	205	PRO	9.8
1	B	307	GLN	9.7
1	A	205	PRO	9.6
1	A	199	ALA	9.5
1	C	204	ALA	9.4
1	D	199	ALA	9.3
1	A	206	ALA	9.1
1	C	283	ALA	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	200	ALA	9.0
1	C	200	ALA	8.9
1	B	280	GLY	8.8
1	D	284	PRO	8.6
1	C	606	MET	8.5
1	C	201	GLN	8.4
1	B	283	ALA	8.4
1	B	606	MET	8.4
1	D	201	GLN	8.3
1	A	201	GLN	8.0
1	B	203	ALA	7.7
1	D	255	ASP	7.7
1	A	606	MET	7.7
1	A	200	ALA	7.6
1	D	206	ALA	7.5
1	B	204	ALA	7.5
1	A	284	PRO	7.4
1	D	606	MET	7.4
1	C	199	ALA	7.4
1	D	204	ALA	7.3
1	B	282	GLN	7.1
1	B	201	GLN	7.0
1	A	203	ALA	7.0
1	D	71	GLY	6.8
1	A	204	ALA	6.7
1	B	306	GLU	6.7
1	B	605	GLN	6.6
1	B	284	PRO	6.5
1	A	256	ASP	6.4
1	C	71	GLY	6.4
1	B	202	ALA	6.3
1	C	202	ALA	6.3
1	A	198	THR	6.2
1	C	197	SER	6.2
1	D	604	ILE	6.0
1	B	206	ALA	6.0
1	C	284	PRO	5.9
1	C	207	GLU	5.8
1	B	71	GLY	5.7
1	B	303	LYS	5.7
1	A	605	GLN	5.7
1	B	304	LYS	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	283	ALA	5.5
1	D	283	ALA	5.5
1	D	198	THR	5.5
1	C	605	GLN	5.4
1	B	604	ILE	5.3
1	C	282	GLN	5.2
1	C	205	PRO	5.2
1	D	254	THR	5.1
1	D	605	GLN	4.9
1	A	282	GLN	4.9
1	A	45	GLU	4.8
1	A	71	GLY	4.8
1	A	254	THR	4.8
1	C	46	ALA	4.8
1	B	603	ARG	4.7
1	A	197	SER	4.7
1	C	603	ARG	4.6
1	C	307	GLN	4.6
1	A	119	GLU	4.5
1	B	199	ALA	4.5
1	A	307	GLN	4.5
1	B	119	GLU	4.5
1	B	198	THR	4.4
1	D	303	LYS	4.3
1	D	48	ARG	4.3
1	A	44	GLU	4.3
1	B	44	GLU	4.3
1	A	306	GLU	4.3
1	D	197	SER	4.2
1	B	207	GLU	4.1
1	B	197	SER	4.1
1	A	347	VAL	4.1
1	A	346	GLY	4.1
1	C	303	LYS	4.1
1	A	207	GLU	4.1
1	B	308	LYS	4.1
1	B	345	THR	4.0
1	A	303	LYS	4.0
1	A	345	THR	4.0
1	A	255	ASP	3.9
1	C	47	SER	3.9
1	B	305	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	304	LYS	3.8
1	D	119	GLU	3.7
1	D	603	ARG	3.7
1	C	198	THR	3.6
1	D	72	LYS	3.6
1	C	48	ARG	3.6
1	B	72	LYS	3.5
1	C	308	LYS	3.5
1	D	45	GLU	3.5
1	C	206	ALA	3.5
1	D	345	THR	3.5
1	A	304	LYS	3.5
1	A	603	ARG	3.5
1	D	344	ARG	3.4
1	D	8	VAL	3.4
1	B	301	ASP	3.4
1	D	151	VAL	3.3
1	D	305	ARG	3.3
1	C	604	ILE	3.3
1	C	44	GLU	3.3
1	D	47	SER	3.3
1	B	151	VAL	3.3
1	B	9	VAL	3.2
1	D	46	ALA	3.2
1	B	46	ALA	3.2
1	D	282	GLN	3.2
1	A	309	GLU	3.2
1	D	300	GLU	3.2
1	A	7	LEU	3.1
1	B	255	ASP	3.0
1	B	302	ARG	3.0
1	B	254	THR	3.0
1	B	344	ARG	3.0
1	B	45	GLU	3.0
1	B	47	SER	3.0
1	A	6	CYS	2.9
1	C	119	GLU	2.9
1	C	309	GLU	2.9
1	B	118	ALA	2.9
1	B	48	ARG	2.9
1	D	150	VAL	2.8
1	A	43	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	8	VAL	2.8
1	C	344	ARG	2.8
1	A	47	SER	2.8
1	A	151	VAL	2.7
1	B	7	LEU	2.7
1	C	300	GLU	2.7
1	C	45	GLU	2.7
1	C	306	GLU	2.7
1	D	77	VAL	2.7
1	D	304	LYS	2.7
1	D	307	GLN	2.7
1	A	8	VAL	2.7
1	A	305	ARG	2.7
1	D	73	ARG	2.7
1	B	43	PRO	2.7
1	B	300	GLU	2.6
1	A	72	LYS	2.6
1	C	345	THR	2.6
1	C	305	ARG	2.6
1	C	382	LEU	2.6
1	B	116	PRO	2.6
1	D	416	ASN	2.6
1	C	346	GLY	2.6
1	C	7	LEU	2.6
1	A	77	VAL	2.5
1	B	309	GLU	2.5
1	D	9	VAL	2.5
1	C	310	LEU	2.5
1	C	9	VAL	2.5
1	D	117	GLN	2.5
1	C	171	ILE	2.5
1	B	39	THR	2.4
1	C	8	VAL	2.4
1	D	309	GLU	2.4
1	C	149	PHE	2.4
1	D	310	LEU	2.4
1	C	347	VAL	2.4
1	A	580	GLU	2.4
1	D	253	LYS	2.4
1	A	89	ARG	2.4
1	D	207	GLU	2.4
1	A	344	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	78	VAL	2.3
1	D	410	GLU	2.3
1	B	416	ASN	2.3
1	A	302	ARG	2.3
1	C	299	GLU	2.3
1	B	38	VAL	2.3
1	B	347	VAL	2.3
1	B	285	SER	2.3
1	C	150	VAL	2.3
1	B	602	GLY	2.3
1	A	150	VAL	2.3
1	D	171	ILE	2.3
1	A	46	ALA	2.2
1	C	255	ASP	2.2
1	A	9	VAL	2.2
1	D	143	ASP	2.2
1	A	221	LYS	2.2
1	B	410	GLU	2.2
1	C	151	VAL	2.1
1	A	39	THR	2.1
1	B	77	VAL	2.1
1	C	77	VAL	2.1
1	D	306	GLU	2.1
1	C	417	LEU	2.1
1	A	196	LYS	2.1
1	C	72	LYS	2.1
1	A	604	ILE	2.1
1	A	310	LEU	2.1
1	C	247	VAL	2.1
1	C	555	ASN	2.1
1	D	580	GLU	2.0
1	D	7	LEU	2.0
1	D	118	ALA	2.0
1	B	120	GLY	2.0
1	D	302	ARG	2.0
1	A	489	CYS	2.0
1	A	94	LEU	2.0
1	B	172	THR	2.0
1	B	143	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](#)

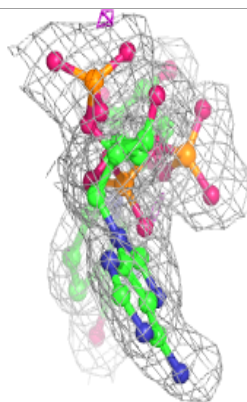
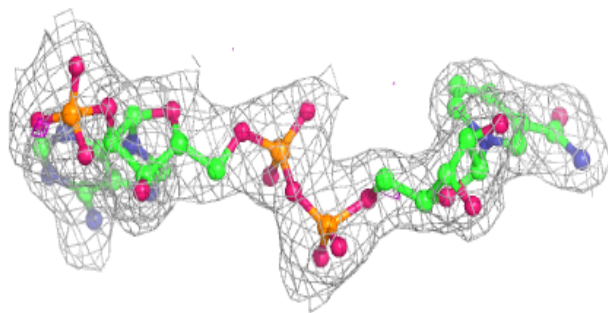
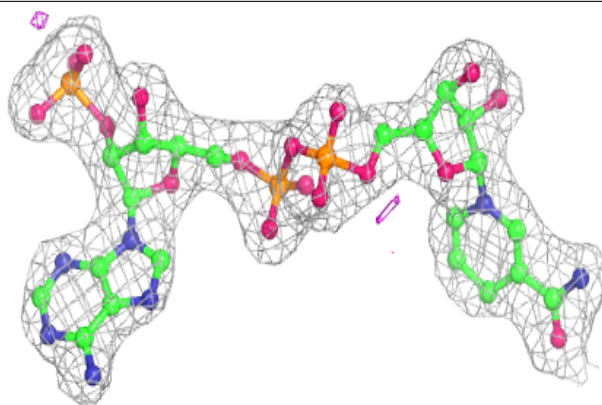
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NDP	D	701	48/48	0.95	0.10	29,38,48,49	0
4	UMP	A	703	20/20	0.95	0.10	38,44,49,52	0
4	UMP	C	703	20/20	0.95	0.13	42,47,52,52	0
3	4RI	B	702	20/20	0.96	0.21	29,34,39,40	0
2	NDP	B	701	48/48	0.96	0.08	30,37,48,50	0
2	NDP	A	701	48/48	0.96	0.09	24,34,42,45	0
3	4RI	C	702	20/20	0.97	0.18	22,27,32,33	0
3	4RI	A	702	20/20	0.97	0.16	24,27,33,34	0
4	UMP	B	703	20/20	0.97	0.09	40,47,52,54	0
2	NDP	C	701	48/48	0.97	0.09	24,31,43,47	0
3	4RI	D	702	20/20	0.98	0.16	28,34,40,45	0
4	UMP	D	703	20/20	0.98	0.06	39,44,47,49	0

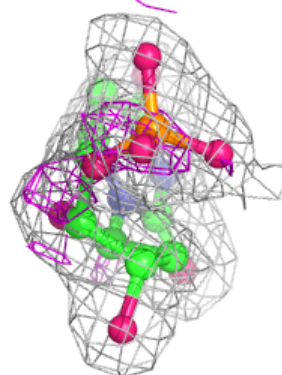
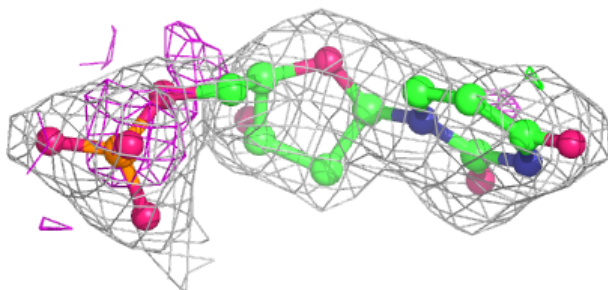
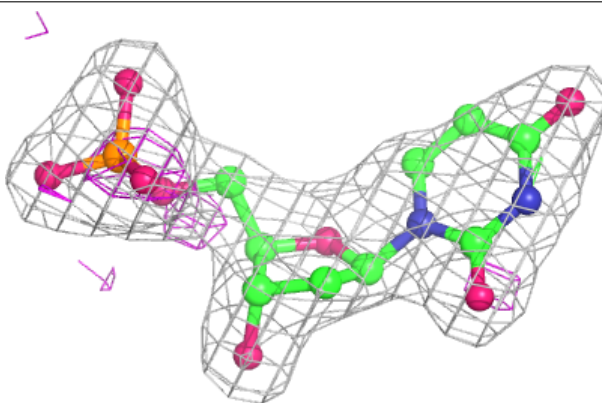
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP 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)

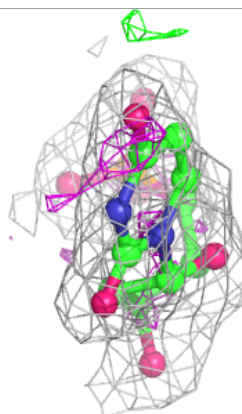
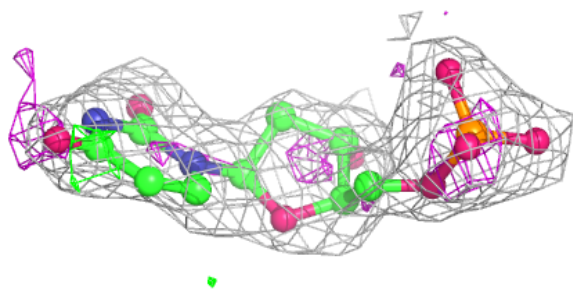
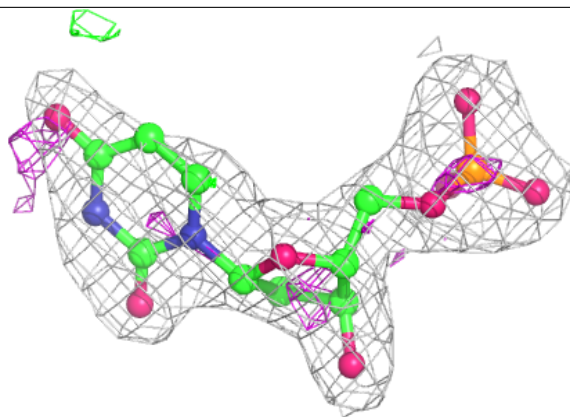
**Electron density around UMP A 703:**

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

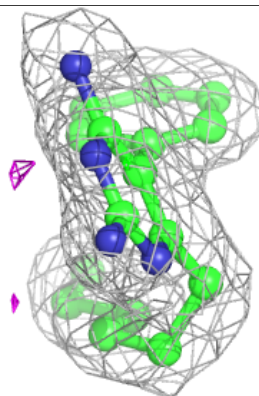
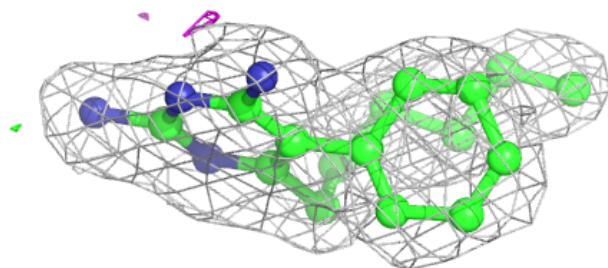
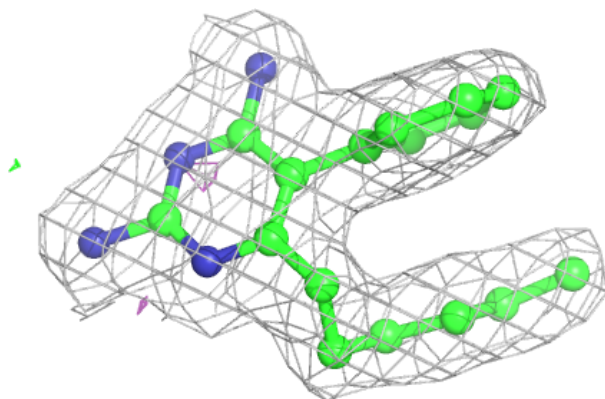


Electron density around UMP C 703:

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

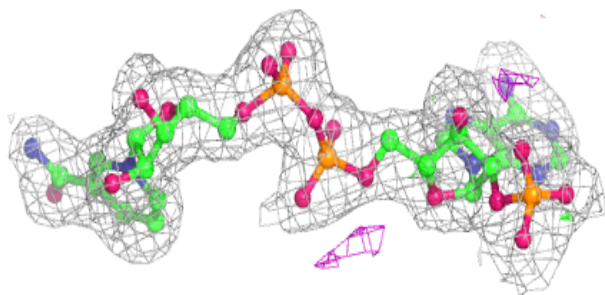
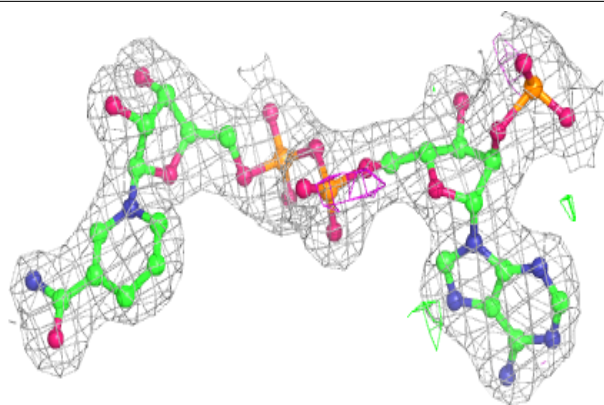
**Electron density around 4RI B 702:**

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

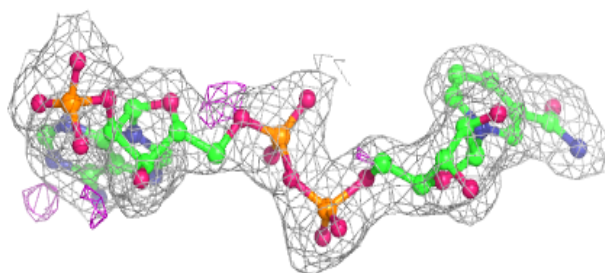
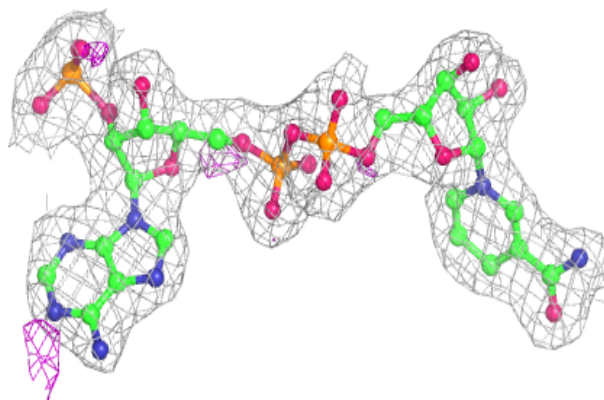


Electron density around NDP B 701:

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

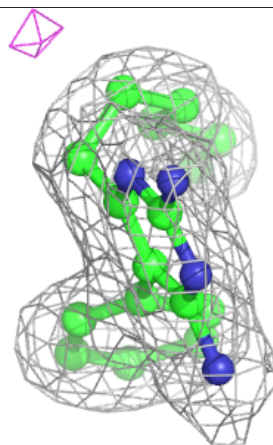
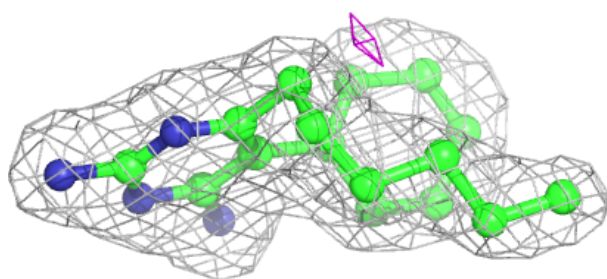
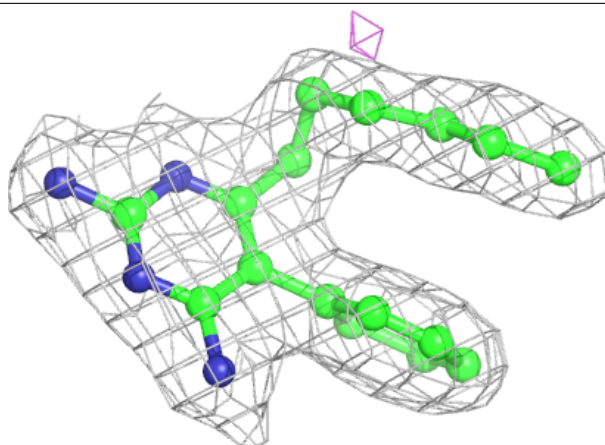
**Electron density around NDP A 701:**

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

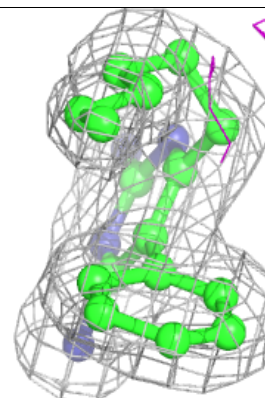
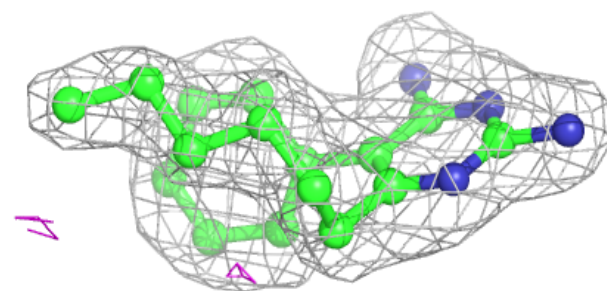
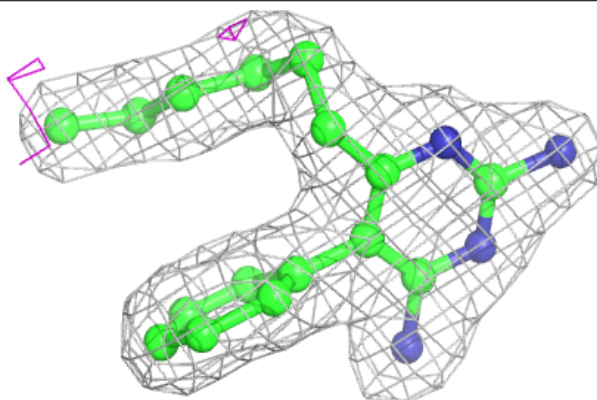


Electron density around 4RI C 702:

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

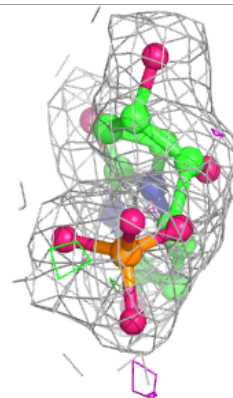
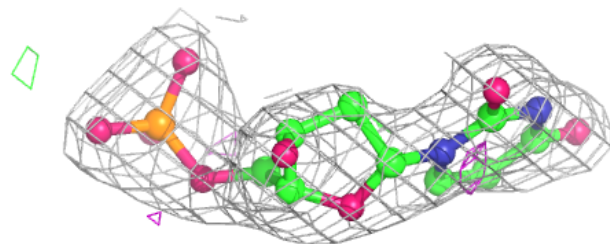
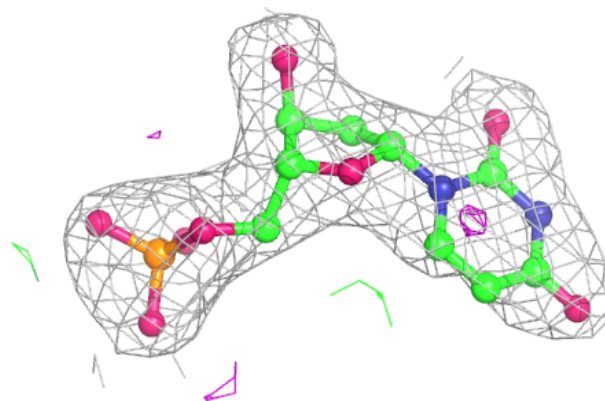
**Electron density around 4RI A 702:**

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

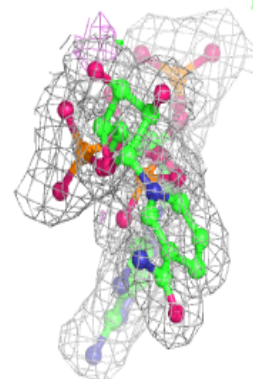
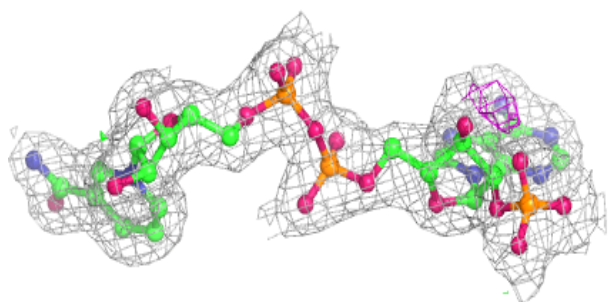
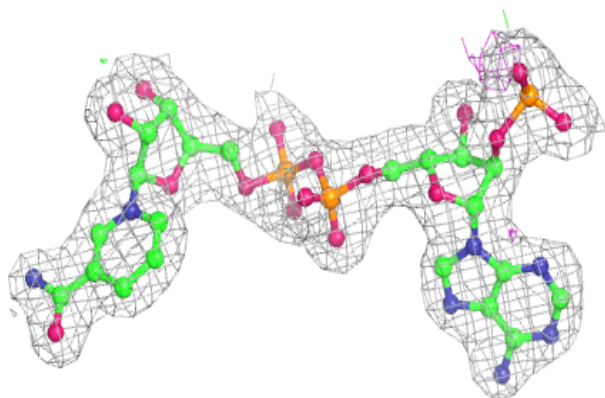


Electron density around UMP B 703:

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

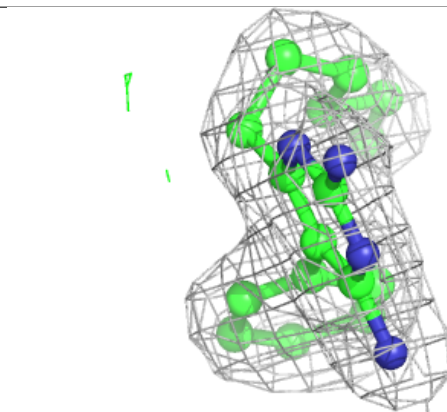
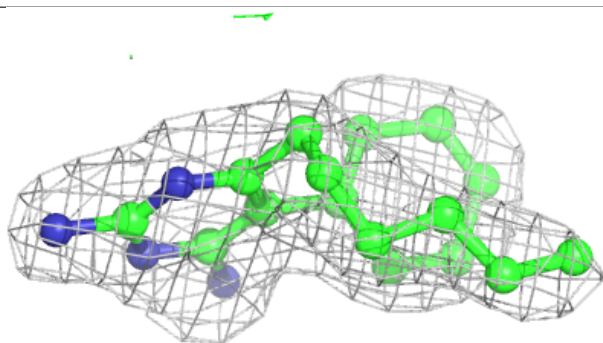
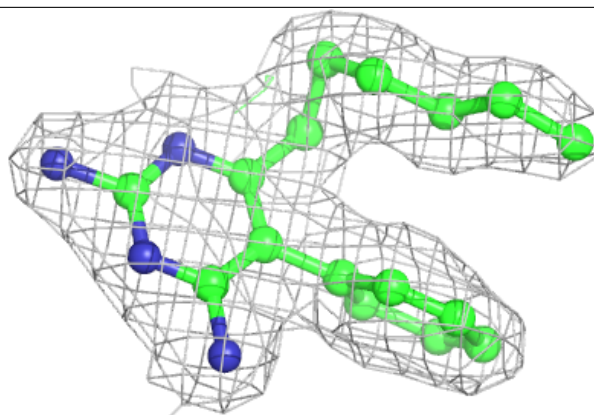
**Electron density around NDP C 701:**

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

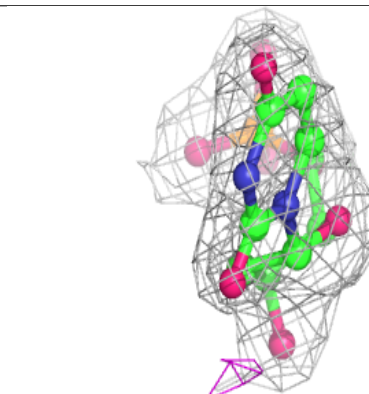
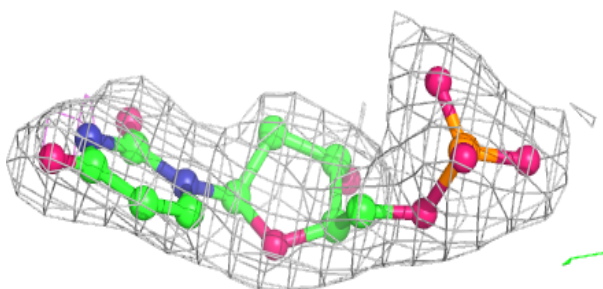
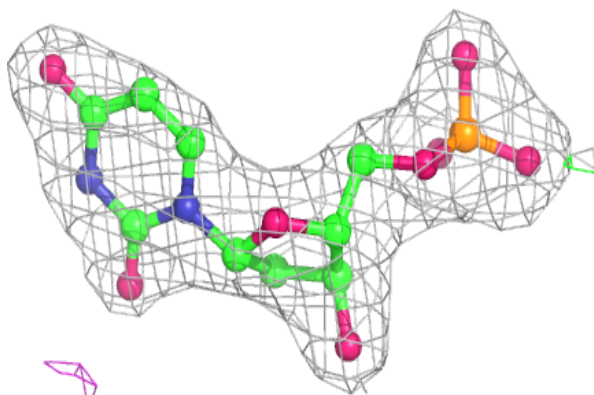


Electron density around 4RI D 702:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.