



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 01:03 PM JST

PDB ID : 7FGY  
Title : Toxoplasma gondii dihydrofolate reductase thymidylate synthase (TgDHFR-TS) complexed with P40, 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 : 2.67 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 : 2.36  
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) : 2.36

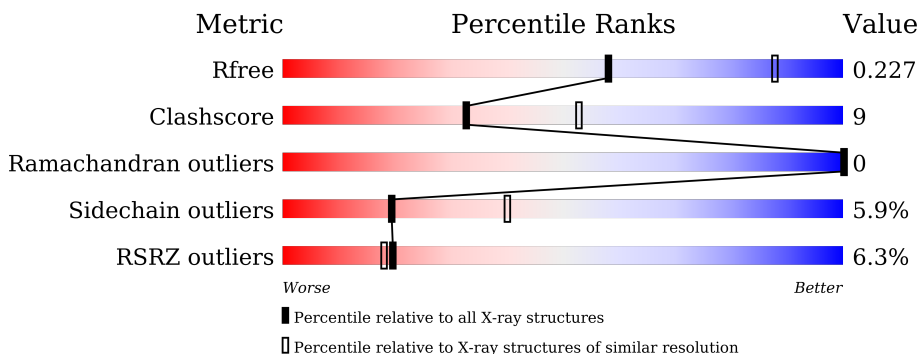
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 5% 67% 24% • 8%
1	B	610	 6% 67% 23% • 8%
1	C	610	 6% 71% 20% • 9%
1	D	610	 6% 69% 21% • 8%

## 2 Entry composition [i](#)

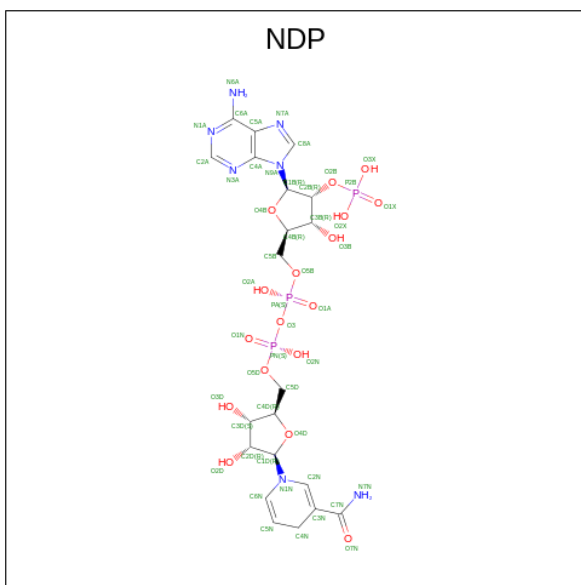
There are 5 unique types of molecules in this entry. The entry contains 18628 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	Total	C	N	O	S	0	0	0
			4465	2840	787	813	25			
1	B	562	Total	C	N	O	S	0	0	0
			4480	2850	790	815	25			
1	C	557	Total	C	N	O	S	0	0	0
			4453	2833	785	810	25			
1	D	562	Total	C	N	O	S	0	0	0
			4483	2851	790	817	25			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



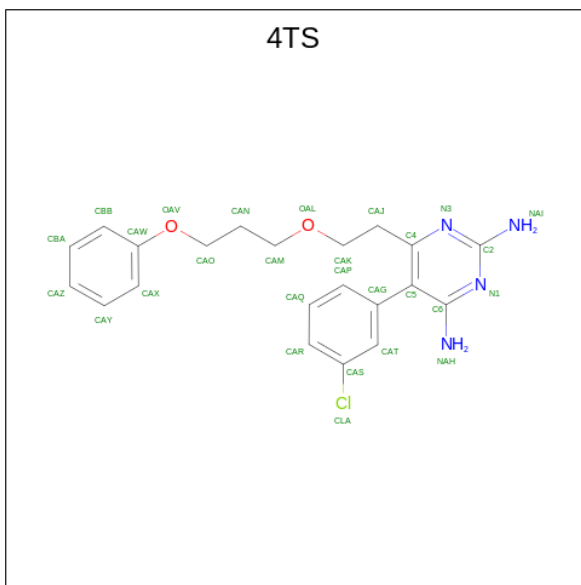
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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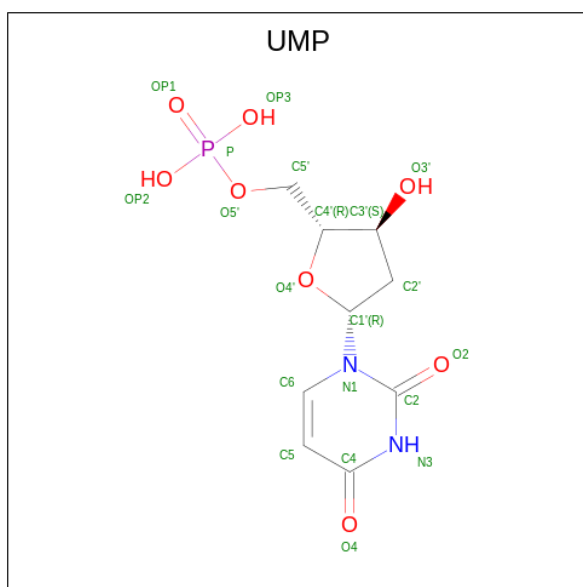
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 5-(3-chlorophenyl)-6-[2-(3-phenoxypropoxy)ethyl]pyrimidine-2,4-diamine (three-letter code: 4TS) (formula:  $C_{21}H_{23}ClN_4O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	B	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	C	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	D	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		

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

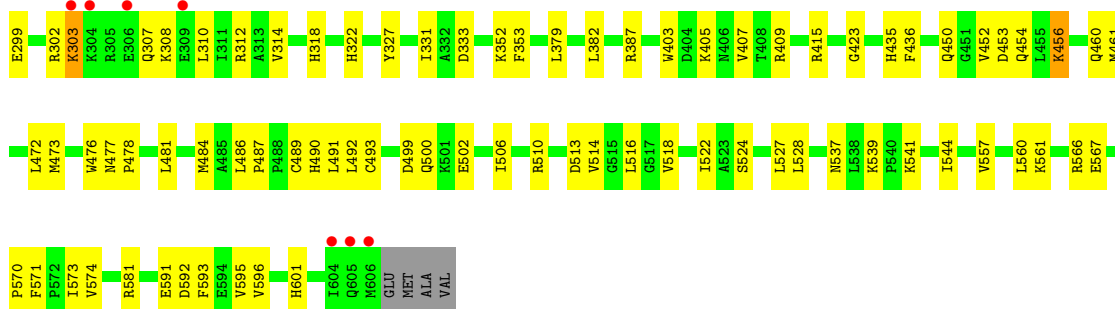


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	20	9	2	8	1	0	0
4	B	1	20	9	2	8	1	0	0
4	C	1	20	9	2	8	1	0	0
4	D	1	20	9	2	8	1	0	0

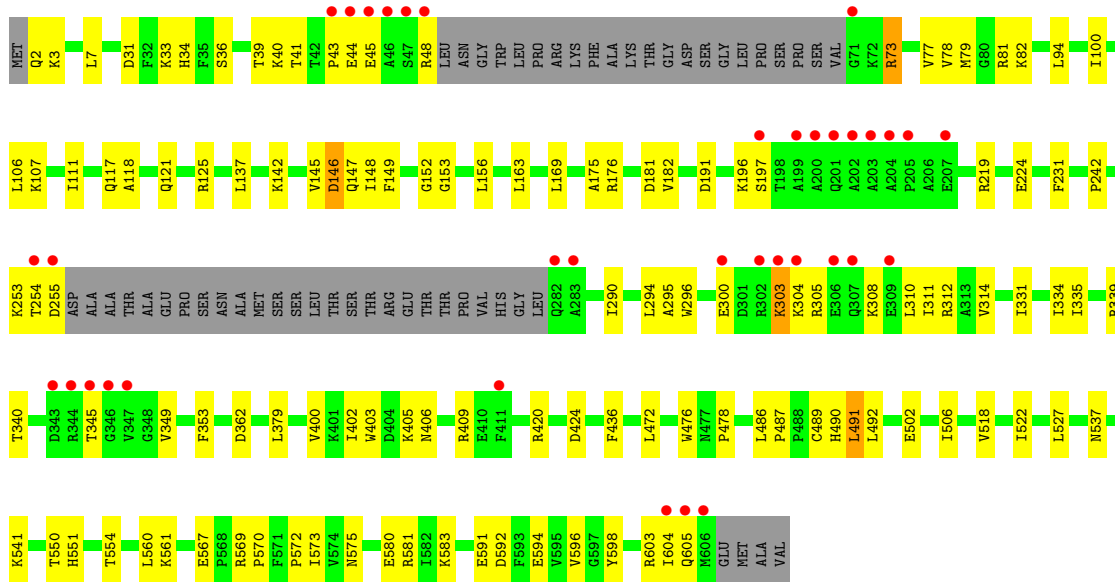
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	102	102	102	0	0
5	B	91	91	91	0	0
5	C	84	84	84	0	0
5	D	86	86	86	0	0

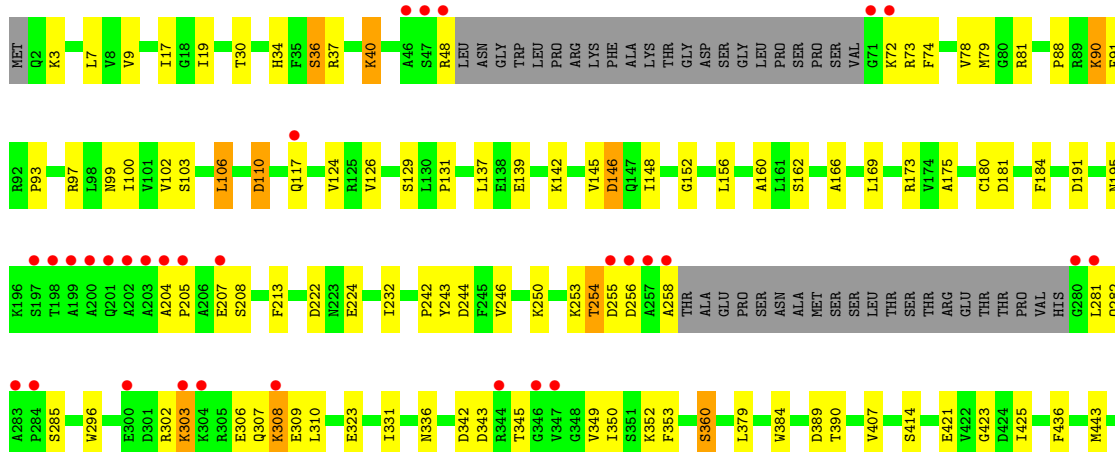


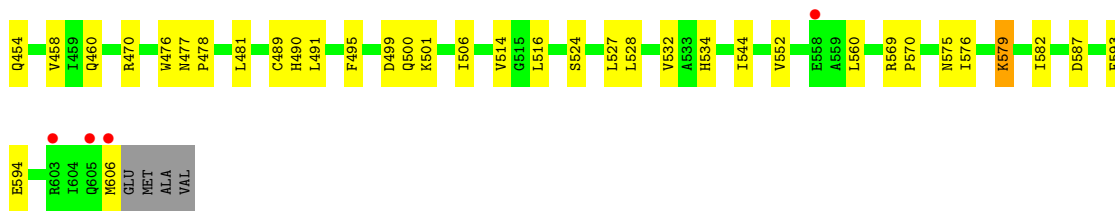


● Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



● 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, $\alpha$ , $\beta$ , $\gamma$	70.12Å 100.71Å 106.04Å 85.54° 83.52° 84.67°	Depositor
Resolution (Å)	41.04 – 2.67 49.62 – 2.67	Depositor EDS
% Data completeness (in resolution range)	85.1 (41.04-2.67) 85.2 (49.62-2.67)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.166 , 0.227 0.169 , 0.227	Depositor DCC
$R_{free}$ test set	3491 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtrriage
Anisotropy	0.084	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: UMP, NDP, 4TS

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	0.50	0/4572	0.67	1/6192 (0.0%)
1	B	0.50	0/4587	0.66	0/6212
1	C	0.49	0/4560	0.65	0/6175
1	D	0.48	0/4590	0.66	0/6216
All	All	0.49	0/18309	0.66	1/24795 (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	A	492	LEU	CA-CB-CG	5.42	127.77	115.30

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	4465	0	4419	95	0
1	B	4480	0	4433	95	0
1	C	4453	0	4413	71	0
1	D	4483	0	4441	80	0
2	A	48	0	26	3	0
2	B	48	0	26	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	26	3	0
2	D	48	0	26	4	0
3	A	28	0	0	1	0
3	B	28	0	0	0	0
3	C	28	0	0	1	0
3	D	28	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	102	0	0	3	0
5	B	91	0	0	7	0
5	C	84	0	0	3	0
5	D	86	0	0	2	0
All	All	18628	0	17854	314	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (314) 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:D:302:ARG:NH1	1:D:306:GLU:OE2	2.16	0.77
1:A:339:ARG:NH1	1:B:500:GLN:OE1	2.19	0.76
1:A:48:ARG:HH21	1:B:295:ALA:HB1	1.51	0.76
1:B:106:LEU:HD23	1:B:111:ILE:HD11	1.68	0.74
1:A:562:GLU:HG2	1:A:604:ILE:HG23	1.72	0.72
1:A:2:GLN:NE2	5:A:801:HOH:O	2.23	0.71
1:C:137:LEU:HD13	1:C:148:ILE:HG12	1.72	0.71
1:C:118:ALA:HB3	1:C:121:GLN:HG2	1.72	0.70
1:C:175:ALA:HB3	1:C:242:PRO:HG2	1.74	0.70
1:B:314:VAL:HG11	1:B:567:GLU:HG3	1.74	0.70
1:C:73:ARG:HD3	1:C:146:ASP:OD2	1.92	0.70
1:B:181:ASP:OD1	1:B:182:VAL:HG23	1.92	0.70
1:A:164:GLY:O	1:A:250:LYS:NZ	2.25	0.69
1:B:302:ARG:NH1	5:B:801:HOH:O	2.26	0.69
1:B:415:ARG:NH1	1:B:484:MET:O	2.26	0.68
1:D:204:ALA:HA	1:D:207:GLU:HG2	1.76	0.68
1:C:224:GLU:HG2	1:C:253:LYS:HE3	1.76	0.67
1:C:191:ASP:HB3	1:C:196:LYS:HD2	1.77	0.66
1:B:453:ASP:OD2	1:B:456:LYS:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LYS:NZ	5:D:802:HOH:O	2.29	0.66
1:B:81:ARG:NE	2:B:701:NDP:O3X	2.29	0.65
1:B:102:VAL:O	2:B:701:NDP:H1B	1.97	0.65
1:D:204:ALA:O	1:D:208:SER:N	2.29	0.64
1:A:436:PHE:CE1	1:B:478:PRO:HD2	2.33	0.64
1:C:331:ILE:HD13	1:C:560:LEU:HD22	1.80	0.64
1:A:478:PRO:HD2	1:B:436:PHE:CE1	2.33	0.63
1:A:73:ARG:NH1	1:A:143:ASP:O	2.31	0.63
1:C:2:GLN:N	5:C:803:HOH:O	2.31	0.63
1:B:472:LEU:HD23	1:B:492:LEU:HD11	1.82	0.62
1:A:478:PRO:HA	1:A:481:LEU:HG	1.82	0.61
1:B:478:PRO:HA	1:B:481:LEU:HG	1.81	0.61
1:D:379:LEU:HD13	1:D:527:LEU:HD21	1.83	0.61
1:A:175:ALA:HB3	1:A:242:PRO:HG2	1.83	0.60
1:D:36:SER:O	1:D:40:LYS:HB2	2.01	0.60
1:D:576:ILE:HB	1:D:579:LYS:HZ3	1.65	0.60
1:C:81:ARG:NE	2:C:701:NDP:O3X	2.33	0.60
1:C:314:VAL:HG11	1:C:567:GLU:HG3	1.83	0.60
1:C:506:ILE:HG13	1:D:353:PHE:CE2	2.36	0.60
1:C:502:GLU:HB3	1:C:541:LYS:HB2	1.84	0.60
1:B:403:TRP:CZ3	1:B:486:LEU:HD12	2.37	0.60
1:C:339:ARG:NH1	1:D:499:ASP:OD1	2.35	0.59
1:D:195:ASN:OD1	1:D:569:ARG:NH1	2.35	0.59
1:A:82:LYS:HG3	2:A:701:NDP:H51A	1.83	0.59
1:D:73:ARG:NE	1:D:146:ASP:OD2	2.35	0.59
1:D:137:LEU:HD13	1:D:148:ILE:HG12	1.84	0.59
1:C:575:ASN:HB2	1:C:594:GLU:HG2	1.85	0.58
1:A:204:ALA:HA	1:A:207:GLU:HG2	1.84	0.58
1:D:303:LYS:O	1:D:307:GLN:HG2	2.03	0.58
1:B:73:ARG:NH1	1:B:143:ASP:O	2.37	0.57
1:A:368:LEU:HD12	1:A:519:PRO:HB3	1.85	0.57
1:C:583:LYS:NZ	5:C:804:HOH:O	2.36	0.57
1:D:213:PHE:O	1:D:250:LYS:NZ	2.36	0.57
1:D:97:ARG:O	1:D:99:ASN:ND2	2.37	0.57
1:A:106:LEU:HD13	1:A:111:ILE:HD11	1.86	0.56
1:B:290:ILE:HG22	1:B:294:LEU:HG	1.86	0.56
1:A:476:TRP:HB2	1:A:491:LEU:HB2	1.87	0.56
1:B:581:ARG:NH2	1:B:592:ASP:OD2	2.36	0.56
1:C:349:VAL:HG12	1:C:551:HIS:HB2	1.87	0.56
1:A:513:ASP:OD2	1:A:516:LEU:HB2	2.05	0.56
1:A:324:GLU:HG3	1:A:368:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:ILE:HG22	1:A:606:MET:H	1.70	0.56
1:B:188:PRO:HB3	1:B:253:LYS:NZ	2.21	0.56
1:A:19:ILE:HB	1:A:180:CYS:HA	1.88	0.56
1:A:137:LEU:HD13	1:A:148:ILE:HG12	1.88	0.56
1:D:81:ARG:HE	2:D:701:NDP:P2B	2.29	0.55
1:B:167:SER:OG	1:B:168:HIS:ND1	2.38	0.55
1:C:572:PRO:HG3	1:C:598:TYR:CD1	2.41	0.55
1:A:17:ILE:O	2:A:701:NDP:H2N	2.06	0.55
1:C:176:ARG:HD2	1:C:596:VAL:CG1	2.36	0.55
1:C:82:LYS:HD2	2:C:701:NDP:H51A	1.88	0.55
1:D:175:ALA:HB3	1:D:242:PRO:HG2	1.88	0.55
1:B:499:ASP:N	1:B:499:ASP:OD1	2.40	0.54
1:C:106:LEU:HD23	1:C:111:ILE:HD11	1.89	0.54
1:A:353:PHE:CE2	1:B:506:ILE:HG13	2.42	0.54
1:A:34:HIS:HB2	1:B:296:TRP:CZ2	2.43	0.54
1:A:107:LYS:HB2	1:A:110:ASP:OD2	2.09	0.53
1:C:295:ALA:HB1	1:D:48:ARG:HH21	1.74	0.53
1:A:555:ASN:OD1	1:A:555:ASN:N	2.37	0.53
1:C:490:HIS:CD2	1:C:490:HIS:H	2.26	0.53
1:B:454:GLN:HB2	1:B:473:MET:HG3	1.91	0.53
1:C:436:PHE:CE1	1:D:478:PRO:HD2	2.42	0.53
1:A:302:ARG:HH11	1:A:303:LYS:HZ2	1.55	0.53
1:C:242:PRO:HB3	1:C:573:ILE:HG13	1.91	0.53
1:D:17:ILE:O	2:D:701:NDP:H2N	2.09	0.53
1:D:500:GLN:NE2	5:D:805:HOH:O	2.41	0.53
1:B:81:ARG:HE	2:B:701:NDP:P2B	2.31	0.52
1:C:603:ARG:HG2	1:C:604:ILE:H	1.75	0.52
1:C:78:VAL:HG12	1:C:156:LEU:HD21	1.92	0.52
1:C:476:TRP:HB2	1:C:491:LEU:HB2	1.91	0.52
1:D:102:VAL:O	2:D:701:NDP:H1B	2.09	0.52
1:A:334:ILE:HG12	1:A:352:LYS:HG3	1.91	0.52
1:C:296:TRP:HB3	1:D:37:ARG:HG3	1.91	0.52
1:B:82:LYS:HG3	2:B:701:NDP:H51A	1.91	0.52
1:A:84:TRP:CH2	1:A:92:ARG:HG2	2.44	0.52
1:D:3:LYS:NZ	1:D:145:VAL:O	2.29	0.52
1:D:575:ASN:HB2	1:D:594:GLU:HG3	1.92	0.52
1:B:228:ARG:HG3	1:B:251:ARG:HG3	1.92	0.52
1:D:582:ILE:HG23	1:D:587:ASP:HB2	1.91	0.51
1:A:192:ILE:HD13	1:A:229:PRO:HG3	1.92	0.51
1:B:242:PRO:HB3	1:B:573:ILE:HG13	1.91	0.51
1:B:2:GLN:NE2	5:B:809:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:HIS:CD2	1:B:282:GLN:HB3	2.46	0.51
1:D:224:GLU:HG2	1:D:253:LYS:HD3	1.92	0.51
1:D:232:ILE:HG12	1:D:246:VAL:HG12	1.91	0.51
1:A:576:ILE:HB	1:A:579:LYS:HD3	1.92	0.51
1:A:37:ARG:NH1	1:B:299:GLU:OE1	2.34	0.51
1:D:454:GLN:O	1:D:458:VAL:HG23	2.11	0.51
1:C:39:THR:HA	1:C:149:PHE:CE2	2.46	0.51
1:A:231:PHE:CD2	1:B:290:ILE:HG23	2.47	0.50
1:B:78:VAL:HG12	1:B:156:LEU:HD21	1.94	0.50
1:B:436:PHE:CE2	1:B:477:ASN:HB2	2.47	0.50
1:D:129:SER:HB2	1:D:131:PRO:HD2	1.93	0.50
1:D:331:ILE:HD13	1:D:560:LEU:HD22	1.94	0.50
1:C:478:PRO:HD2	1:D:436:PHE:CE1	2.47	0.50
1:B:379:LEU:HD11	1:B:593:PHE:CE1	2.47	0.50
1:C:406:ASN:OD1	1:C:486:LEU:HD11	2.12	0.50
1:D:7:LEU:HD11	1:D:160:ALA:HB1	1.94	0.50
1:B:175:ALA:HB3	1:B:242:PRO:HG2	1.93	0.49
1:A:173:ARG:HB2	1:A:244:ASP:OD1	2.12	0.49
1:B:85:GLU:HA	1:B:92:ARG:NH1	2.27	0.49
1:C:400:VAL:HG12	1:C:402:ILE:HG12	1.94	0.49
1:B:216:GLU:HG2	1:B:217:LEU:HG	1.95	0.49
1:A:77:VAL:HG21	1:A:94:LEU:HD12	1.93	0.49
1:A:89:ARG:NH1	1:A:89:ARG:HB2	2.27	0.49
1:B:81:ARG:HB2	1:B:103:SER:HB2	1.94	0.49
1:A:296:TRP:CZ2	1:B:34:HIS:HB2	2.47	0.49
1:A:506:ILE:HG13	1:B:353:PHE:CE2	2.48	0.49
1:B:303:LYS:O	1:B:307:GLN:HG2	2.13	0.49
1:A:129:SER:HB2	1:A:131:PRO:HD2	1.95	0.49
1:A:299:GLU:OE2	1:B:37:ARG:NH1	2.46	0.49
1:B:2:GLN:N	5:B:810:HOH:O	2.45	0.49
1:D:7:LEU:HB2	1:D:169:LEU:HD22	1.95	0.49
1:B:513:ASP:OD2	1:B:516:LEU:HB2	2.13	0.49
2:D:701:NDP:H8A	2:D:701:NDP:H52A	1.95	0.49
1:A:566:ARG:HD3	1:A:601:HIS:CD2	2.48	0.48
1:C:353:PHE:CE2	1:D:506:ILE:HG13	2.48	0.48
1:D:255:ASP:HB2	1:D:258:ALA:HA	1.95	0.48
1:A:374:PHE:CE1	1:A:376:LYS:HB3	2.49	0.48
1:B:387:ARG:NH2	5:B:813:HOH:O	2.47	0.48
1:A:506:ILE:HG12	1:A:544:ILE:HB	1.95	0.48
1:B:7:LEU:HB2	1:B:169:LEU:HD22	1.96	0.48
1:A:498:ASN:OD1	1:A:502:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:MET:HG2	5:B:877:HOH:O	2.13	0.48
1:A:210:PHE:CD1	1:A:219:ARG:HG3	2.49	0.48
1:B:518:VAL:O	1:B:522:ILE:HG13	2.14	0.48
1:C:518:VAL:O	1:C:522:ILE:HG13	2.14	0.48
1:B:95:VAL:HG13	1:B:96:ASP:OD2	2.14	0.48
1:B:333:ASP:OD2	1:B:352:LYS:HE2	2.14	0.48
1:B:476:TRP:HB2	1:B:491:LEU:HB2	1.95	0.48
1:C:305:ARG:HG2	1:C:310:LEU:HD11	1.96	0.48
1:D:173:ARG:HB2	1:D:244:ASP:OD1	2.14	0.48
1:A:229:PRO:HG2	1:A:567:GLU:OE2	2.14	0.47
1:A:436:PHE:CD1	1:B:478:PRO:HD2	2.49	0.47
1:D:93:PRO:HB3	1:D:124:VAL:HG21	1.96	0.47
1:D:204:ALA:HB3	1:D:205:PRO:HD3	1.96	0.47
1:D:478:PRO:HA	1:D:481:LEU:HG	1.97	0.47
1:A:384:TRP:CH2	1:A:425:ILE:HD13	2.49	0.47
1:A:499:ASP:OD1	1:A:499:ASP:N	2.47	0.47
1:D:506:ILE:HG12	1:D:544:ILE:HB	1.96	0.47
1:C:569:ARG:HB3	1:C:570:PRO:HD2	1.95	0.47
1:D:323:GLU:OE2	1:D:360:SER:OG	2.31	0.47
1:D:436:PHE:CE2	1:D:477:ASN:HB2	2.50	0.47
1:A:490:HIS:CD2	1:A:490:HIS:H	2.32	0.47
1:D:78:VAL:HG12	1:D:156:LEU:HD21	1.96	0.47
1:C:219:ARG:NH2	5:C:812:HOH:O	2.47	0.47
1:C:77:VAL:HG21	1:C:94:LEU:HD12	1.96	0.47
1:A:454:GLN:O	1:A:458:VAL:HG23	2.14	0.47
1:C:403:TRP:CZ3	1:C:486:LEU:HD12	2.49	0.47
1:D:9:VAL:HG21	1:D:184:PHE:CD1	2.50	0.47
1:B:331:ILE:HG12	1:B:514:VAL:CG1	2.45	0.47
1:B:331:ILE:HG12	1:B:514:VAL:HG11	1.96	0.47
1:D:74:PHE:O	1:D:145:VAL:HA	2.15	0.47
1:C:334:ILE:HD11	1:C:550:THR:HG22	1.98	0.46
1:D:110:ASP:N	1:D:110:ASP:OD1	2.48	0.46
1:B:85:GLU:HA	1:B:92:ARG:HH12	1.79	0.46
1:B:224:GLU:HG2	1:B:253:LYS:HD2	1.97	0.46
1:C:472:LEU:HD23	1:C:492:LEU:HD11	1.98	0.46
1:B:502:GLU:HB3	1:B:541:LYS:HB2	1.97	0.46
1:A:99:ASN:HB2	1:A:124:VAL:HG22	1.97	0.46
1:C:254:THR:HG22	1:C:254:THR:O	2.15	0.46
1:D:19:ILE:HB	1:D:180:CYS:HA	1.96	0.46
1:A:476:TRP:CZ2	1:A:481:LEU:HD11	2.51	0.46
1:B:487:PRO:O	1:B:510:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:HB2	1:B:110:ASP:OD2	2.16	0.46
1:B:379:LEU:HD13	1:B:527:LEU:HD21	1.97	0.46
1:B:74:PHE:O	1:B:145:VAL:HA	2.16	0.46
1:D:458:VAL:HG11	1:D:495:PHE:CD1	2.51	0.46
1:A:300:GLU:O	1:A:304:LYS:HG2	2.17	0.45
1:B:436:PHE:HB3	1:B:452:VAL:HB	1.98	0.45
1:D:7:LEU:HD13	1:D:166:ALA:HB2	1.99	0.45
1:D:19:ILE:HA	1:D:181:ASP:CG	2.36	0.45
1:D:528:LEU:O	1:D:532:VAL:HG23	2.16	0.45
1:A:2:GLN:N	5:A:816:HOH:O	2.49	0.45
1:D:106:LEU:O	1:D:126:VAL:HG11	2.16	0.45
1:B:188:PRO:HB3	1:B:253:LYS:HZ1	1.81	0.45
1:D:79:MET:HA	1:D:152:GLY:O	2.15	0.45
1:A:181:ASP:OD1	1:A:182:VAL:HG23	2.16	0.45
1:C:420:ARG:HD2	1:C:424:ASP:HB3	1.98	0.45
1:B:331:ILE:HD13	1:B:560:LEU:HD22	1.98	0.45
1:C:537:ASN:O	1:C:537:ASN:ND2	2.49	0.45
1:C:296:TRP:CE2	1:D:34:HIS:HB2	2.52	0.45
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.67	0.45
1:D:254:THR:HB	1:D:256:ASP:OD2	2.17	0.45
1:A:6:CYS:SG	1:A:168:HIS:HB2	2.57	0.44
1:A:117:GLN:OE1	1:A:117:GLN:HA	2.18	0.44
1:B:460:GLN:NE2	5:B:811:HOH:O	2.50	0.44
1:D:514:VAL:HB	1:D:552:VAL:HG12	2.00	0.44
1:A:88:PRO:HD3	3:A:702:4TS:CAZ	2.47	0.44
1:A:176:ARG:HD2	1:A:596:VAL:CG1	2.47	0.44
1:C:41:THR:HG23	1:C:45:GLU:HB2	1.98	0.44
1:B:574:VAL:HG22	1:B:595:VAL:HG22	1.99	0.44
1:C:7:LEU:HB2	1:C:169:LEU:HD22	2.00	0.44
1:D:81:ARG:HB2	1:D:103:SER:HB2	2.00	0.44
1:B:153:GLY:HA3	2:B:701:NDP:O5D	2.18	0.44
1:D:421:GLU:HB3	1:D:443:MET:HE2	2.00	0.44
1:A:48:ARG:NH2	1:B:295:ALA:HB1	2.28	0.44
1:A:445:THR:HB	1:A:447:TYR:CZ	2.52	0.44
1:B:237:SER:HA	1:B:241:VAL:O	2.18	0.44
1:C:3:LYS:HD3	1:C:145:VAL:HG12	1.99	0.44
1:A:78:VAL:HG12	1:A:156:LEU:HD21	1.99	0.43
1:A:84:TRP:CZ2	1:A:92:ARG:HG2	2.54	0.43
1:A:441:LYS:HE2	1:A:441:LYS:HB3	1.64	0.43
1:B:176:ARG:HD2	1:B:596:VAL:CG1	2.48	0.43
1:C:36:SER:O	1:C:40:LYS:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:ARG:NH2	1:C:592:ASP:OD2	2.35	0.43
1:D:88:PRO:HB2	1:D:90:LYS:HG2	1.99	0.43
1:D:255:ASP:C	1:D:258:ALA:H	2.22	0.43
1:C:308:LYS:HB3	1:C:308:LYS:HE2	1.83	0.43
1:D:569:ARG:HB3	1:D:570:PRO:HD2	2.00	0.43
1:C:43:PRO:HG3	1:C:147:GLN:HE21	1.83	0.43
1:B:490:HIS:H	1:B:490:HIS:CD2	2.35	0.43
1:D:99:ASN:N	1:D:99:ASN:HD22	2.17	0.43
1:A:79:MET:O	1:A:101:VAL:HA	2.18	0.43
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.99	0.43
1:B:557:VAL:O	1:B:561:LYS:HG3	2.18	0.43
1:C:405:LYS:HE2	1:C:405:LYS:HB3	1.84	0.43
1:B:435:HIS:HB3	1:B:450:GLN:O	2.18	0.43
1:D:384:TRP:CD1	1:D:389:ASP:HB3	2.53	0.43
1:A:461:MET:SD	1:A:465:ASN:HB3	2.58	0.43
1:A:302:ARG:HH11	1:A:303:LYS:NZ	2.17	0.42
1:A:539:LYS:HB2	1:A:539:LYS:HE3	1.86	0.42
1:B:79:MET:HA	1:B:152:GLY:O	2.19	0.42
1:A:478:PRO:HD2	1:B:436:PHE:CZ	2.54	0.42
1:C:34:HIS:HB2	1:D:296:TRP:CZ2	2.53	0.42
1:A:39:THR:HA	1:A:149:PHE:CE2	2.55	0.42
1:B:566:ARG:HD3	1:B:601:HIS:ND1	2.33	0.42
1:A:384:TRP:HH2	1:A:425:ILE:HD13	1.85	0.42
1:B:88:PRO:HB2	1:B:90:LYS:HD2	2.01	0.42
1:B:407:VAL:HB	1:B:423:GLY:H	1.84	0.42
1:B:539:LYS:HE3	1:B:539:LYS:HB2	1.73	0.42
1:C:379:LEU:HD13	1:C:527:LEU:HD21	2.00	0.42
1:D:88:PRO:HD2	1:D:91:PHE:HD2	1.84	0.42
1:A:567:GLU:O	1:A:601:HIS:HE1	2.02	0.42
1:A:186:ALA:O	1:A:209:VAL:HG22	2.19	0.42
1:B:99:ASN:HB2	1:B:124:VAL:HG22	2.02	0.42
1:C:100:ILE:HD13	1:C:125:ARG:HB2	2.01	0.42
1:C:349:VAL:CG1	1:C:551:HIS:HB2	2.48	0.42
1:B:177:GLU:HB2	5:B:834:HOH:O	2.19	0.42
1:C:79:MET:HA	1:C:152:GLY:O	2.20	0.42
1:D:476:TRP:HB2	1:D:491:LEU:HB2	2.00	0.42
1:C:153:GLY:HA3	2:C:701:NDP:O5D	2.20	0.42
1:D:379:LEU:HD11	1:D:593:PHE:CE2	2.55	0.42
1:A:102:VAL:O	2:A:701:NDP:H1B	2.20	0.42
1:A:72:LYS:HD3	5:A:811:HOH:O	2.20	0.41
1:A:282:GLN:OE1	1:B:318:HIS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:TYR:CZ	1:B:331:ILE:HD11	2.55	0.41
1:C:296:TRP:CB	1:D:37:ARG:HG3	2.50	0.41
1:D:343:ASP:OD2	1:D:345:THR:OG1	2.38	0.41
1:A:74:PHE:O	1:A:145:VAL:HA	2.19	0.41
1:A:487:PRO:HA	1:A:488:PRO:HD3	1.95	0.41
1:A:516:LEU:HD11	1:A:556:HIS:CE1	2.55	0.41
1:A:118:ALA:HB3	1:A:121:GLN:HG2	2.02	0.41
1:A:408:THR:O	1:A:411:PHE:N	2.53	0.41
1:C:181:ASP:OD1	1:C:182:VAL:HG23	2.20	0.41
1:B:382:LEU:HD11	1:B:528:LEU:HD13	2.01	0.41
1:C:311:ILE:HG13	1:C:335:ILE:HG21	2.01	0.41
1:A:37:ARG:HA	1:A:37:ARG:HD3	1.91	0.41
1:A:74:PHE:CZ	1:A:144:SER:HB2	2.56	0.41
1:B:77:VAL:HG21	1:B:94:LEU:HD12	2.03	0.41
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.78	0.41
1:C:31:ASP:OD2	3:C:702:4TS:N3	2.53	0.41
1:C:487:PRO:HG3	1:D:470:ARG:NH1	2.35	0.41
1:D:390:THR:HB	1:D:425:ILE:HG12	2.03	0.41
1:A:566:ARG:HD3	1:A:601:HIS:CG	2.56	0.41
1:C:580:GLU:H	1:C:580:GLU:CD	2.23	0.41
1:B:39:THR:HA	1:B:149:PHE:CE2	2.55	0.41
1:B:322:HIS:HE1	1:B:571:PHE:CE1	2.39	0.41
1:D:407:VAL:HG21	1:D:423:GLY:HA2	2.02	0.41
1:D:490:HIS:CD2	1:D:490:HIS:H	2.38	0.41
1:A:163:LEU:O	1:A:215:PRO:HB3	2.20	0.41
1:A:469:ARG:O	1:B:510:ARG:HD2	2.21	0.41
1:A:493:CYS:HA	1:A:506:ILE:O	2.20	0.41
1:B:173:ARG:CZ	1:B:570:PRO:HD3	2.50	0.41
1:B:234:LYS:HA	1:B:322:HIS:HA	2.02	0.41
1:C:163:LEU:HA	1:C:163:LEU:HD12	1.68	0.41
1:C:303:LYS:H	1:C:303:LYS:HG3	1.69	0.41
1:D:7:LEU:HD11	1:D:160:ALA:CB	2.51	0.41
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.20	0.41
1:C:290:ILE:HG22	1:C:294:LEU:HG	2.03	0.41
1:D:30:THR:HB	1:D:243:TYR:OH	2.20	0.41
1:A:231:PHE:HD2	1:B:290:ILE:HG23	1.86	0.40
1:A:518:VAL:O	1:A:522:ILE:HG13	2.20	0.40
1:D:19:ILE:HA	1:D:181:ASP:OD1	2.21	0.40
1:A:74:PHE:CE1	1:A:144:SER:HB2	2.57	0.40
1:B:211:VAL:HG12	1:B:225:ALA:HB3	2.04	0.40
1:C:340:THR:HA	1:C:349:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ASP:OD1	1:C:362:ASP:N	2.43	0.40
1:D:534:HIS:CE1	1:D:579:LYS:HB3	2.56	0.40
2:B:701:NDP:H52A	2:B:701:NDP:H8A	2.04	0.40
1:A:18:GLY:O	1:A:180:CYS:HB3	2.21	0.40
1:A:455:LEU:O	1:A:459:ILE:HD12	2.21	0.40
1:A:563:GLN:O	1:A:566:ARG:HG3	2.21	0.40
1:C:303:LYS:HD2	1:C:304:LYS:HG3	2.04	0.40
1:D:308:LYS:NZ	1:D:336:ASN:HA	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/610 (91%)	534 (97%)	19 (3%)	0	100	100
1	B	556/610 (91%)	529 (95%)	27 (5%)	0	100	100
1	C	551/610 (90%)	527 (96%)	24 (4%)	0	100	100
1	D	556/610 (91%)	535 (96%)	21 (4%)	0	100	100
All	All	2216/2440 (91%)	2125 (96%)	91 (4%)	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	482/525 (92%)	454 (94%)	28 (6%)	20	41
1	B	482/525 (92%)	454 (94%)	28 (6%)	20	41
1	C	482/525 (92%)	460 (95%)	22 (5%)	27	51
1	D	484/525 (92%)	449 (93%)	35 (7%)	14	31
All	All	1930/2100 (92%)	1817 (94%)	113 (6%)	19	40

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	73	ARG
1	A	90	LYS
1	A	100	ILE
1	A	142	LYS
1	A	144	SER
1	A	191	ASP
1	A	196	LYS
1	A	198	THR
1	A	208	SER
1	A	216	GLU
1	A	222	ASP
1	A	255	ASP
1	A	282	GLN
1	A	285	SER
1	A	301	ASP
1	A	303	LYS
1	A	305	ARG
1	A	307	GLN
1	A	341	MET
1	A	344	ARG
1	A	349	VAL
1	A	489	CYS
1	A	554	THR
1	A	555	ASN
1	A	577	LEU
1	A	586	ASP
1	A	603	ARG
1	B	33	LYS
1	B	44	GLU
1	B	48	ARG
1	B	90	LYS
1	B	107	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	117	GLN
1	B	142	LYS
1	B	144	SER
1	B	156	LEU
1	B	167	SER
1	B	201	GLN
1	B	207	GLU
1	B	219	ARG
1	B	221	LYS
1	B	234	LYS
1	B	254	THR
1	B	282	GLN
1	B	303	LYS
1	B	308	LYS
1	B	312	ARG
1	B	405	LYS
1	B	409	ARG
1	B	456	LYS
1	B	489	CYS
1	B	493	CYS
1	B	524	SER
1	B	537	ASN
1	B	591	GLU
1	C	33	LYS
1	C	44	GLU
1	C	48	ARG
1	C	73	ARG
1	C	107	LYS
1	C	117	GLN
1	C	142	LYS
1	C	146	ASP
1	C	197	SER
1	C	231	PHE
1	C	255	ASP
1	C	300	GLU
1	C	303	LYS
1	C	312	ARG
1	C	345	THR
1	C	409	ARG
1	C	489	CYS
1	C	491	LEU
1	C	554	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	561	LYS
1	C	591	GLU
1	C	605	GLN
1	D	36	SER
1	D	40	LYS
1	D	72	LYS
1	D	90	LYS
1	D	100	ILE
1	D	106	LEU
1	D	110	ASP
1	D	117	GLN
1	D	139	GLU
1	D	142	LYS
1	D	146	ASP
1	D	162	SER
1	D	191	ASP
1	D	222	ASP
1	D	254	THR
1	D	281	LEU
1	D	282	GLN
1	D	285	SER
1	D	303	LYS
1	D	308	LYS
1	D	309	GLU
1	D	310	LEU
1	D	342	ASP
1	D	349	VAL
1	D	350	ILE
1	D	352	LYS
1	D	360	SER
1	D	414	SER
1	D	460	GLN
1	D	489	CYS
1	D	501	LYS
1	D	516	LEU
1	D	524	SER
1	D	579	LYS
1	D	606	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	393	ASN
1	A	465	ASN
1	A	601	HIS
1	B	2	GLN
1	B	460	GLN
1	B	465	ASN
1	C	117	GLN
1	C	147	GLN
1	C	307	GLN
1	C	537	ASN
1	C	605	GLN
1	D	2	GLN
1	D	27	HIS
1	D	477	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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
4	UMP	B	703	-	21,21,21	0.92	1 (4%)	31,31,31	1.43	6 (19%)
3	4TS	C	702	-	30,30,30	3.73	16 (53%)	38,39,39	1.78	7 (18%)
4	UMP	C	703	-	21,21,21	0.82	1 (4%)	31,31,31	1.61	6 (19%)
4	UMP	D	703	-	21,21,21	0.85	1 (4%)	31,31,31	1.57	6 (19%)
4	UMP	A	703	-	21,21,21	0.79	0	31,31,31	1.59	4 (12%)
2	NDP	C	701	-	45,52,52	1.92	5 (11%)	53,80,80	1.54	12 (22%)
2	NDP	A	701	-	45,52,52	2.12	4 (8%)	53,80,80	1.58	10 (18%)
2	NDP	D	701	-	45,52,52	1.98	6 (13%)	53,80,80	1.57	9 (16%)
2	NDP	B	701	-	45,52,52	2.05	7 (15%)	53,80,80	1.50	11 (20%)
3	4TS	A	702	-	30,30,30	3.72	17 (56%)	38,39,39	1.61	7 (18%)
3	4TS	B	702	-	30,30,30	3.81	16 (53%)	38,39,39	1.83	7 (18%)
3	4TS	D	702	-	30,30,30	3.76	16 (53%)	38,39,39	1.74	7 (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
4	UMP	B	703	-	-	5/10/22/22	0/2/2/2
3	4TS	C	702	-	-	1/14/14/14	0/3/3/3
4	UMP	C	703	-	-	2/10/22/22	0/2/2/2
4	UMP	D	703	-	-	4/10/22/22	0/2/2/2
4	UMP	A	703	-	-	5/10/22/22	0/2/2/2
2	NDP	C	701	-	-	12/30/77/77	0/5/5/5
2	NDP	A	701	-	-	8/30/77/77	0/5/5/5
2	NDP	D	701	-	-	8/30/77/77	0/5/5/5
2	NDP	B	701	-	-	6/30/77/77	0/5/5/5
3	4TS	A	702	-	-	0/14/14/14	0/3/3/3
3	4TS	B	702	-	-	0/14/14/14	0/3/3/3
3	4TS	D	702	-	-	2/14/14/14	0/3/3/3

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NDP	P2B-O2B	11.44	1.80	1.59
2	B	701	NDP	P2B-O2B	10.29	1.78	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	NDP	P2B-O2B	9.98	1.78	1.59
2	D	701	NDP	P2B-O2B	9.90	1.78	1.59
3	C	702	4TS	CAR-CAS	8.35	1.53	1.38
3	B	702	4TS	CAR-CAS	8.08	1.53	1.38
3	D	702	4TS	CAR-CAS	8.00	1.53	1.38
3	C	702	4TS	CAX-CAW	7.33	1.53	1.38
3	A	702	4TS	CAX-CAW	7.25	1.53	1.38
3	D	702	4TS	CAT-CAG	7.20	1.52	1.39
3	B	702	4TS	CAX-CAW	7.20	1.53	1.38
3	B	702	4TS	CAT-CAG	7.18	1.52	1.39
3	D	702	4TS	CAX-CAW	7.02	1.52	1.38
3	A	702	4TS	CAR-CAS	6.95	1.51	1.38
3	C	702	4TS	CBA-CBB	6.76	1.53	1.38
3	D	702	4TS	CAQ-CAP	6.75	1.53	1.38
3	B	702	4TS	CAQ-CAP	6.71	1.53	1.38
3	A	702	4TS	CBA-CBB	6.60	1.52	1.38
3	A	702	4TS	CAT-CAG	6.57	1.51	1.39
3	C	702	4TS	CAT-CAG	6.55	1.51	1.39
3	C	702	4TS	CAQ-CAP	6.50	1.52	1.38
3	D	702	4TS	CBA-CBB	6.45	1.52	1.38
3	B	702	4TS	CBA-CBB	6.44	1.52	1.38
3	A	702	4TS	CAQ-CAP	6.28	1.52	1.38
3	B	702	4TS	CAZ-CAY	5.83	1.53	1.38
3	B	702	4TS	C2-NAI	5.81	1.45	1.33
3	C	702	4TS	CAZ-CAY	5.63	1.52	1.38
3	D	702	4TS	CAZ-CAY	5.61	1.52	1.38
3	A	702	4TS	C2-NAI	5.54	1.45	1.33
3	A	702	4TS	CAZ-CAY	5.49	1.52	1.38
3	D	702	4TS	C2-NAI	5.43	1.44	1.33
3	C	702	4TS	C2-NAI	4.97	1.43	1.33
3	D	702	4TS	C6-NAH	4.65	1.45	1.34
3	A	702	4TS	CAT-CAS	-4.62	1.30	1.38
3	B	702	4TS	C6-NAH	4.49	1.45	1.34
3	A	702	4TS	C6-NAH	4.46	1.45	1.34
3	C	702	4TS	C6-NAH	4.25	1.44	1.34
2	B	701	NDP	PN-O5D	4.11	1.75	1.59
2	A	701	NDP	PN-O5D	4.06	1.75	1.59
3	B	702	4TS	CAT-CAS	-4.02	1.31	1.38
3	C	702	4TS	CAT-CAS	-4.00	1.31	1.38
2	D	701	NDP	PN-O5D	3.97	1.75	1.59
2	C	701	NDP	PN-O5D	3.84	1.74	1.59
3	A	702	4TS	CAQ-CAR	-3.78	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	4TS	CAQ-CAR	-3.70	1.31	1.38
3	A	702	4TS	CAP-CAG	-3.61	1.31	1.39
3	D	702	4TS	CAY-CAX	-3.48	1.31	1.38
3	D	702	4TS	CAT-CAS	-3.45	1.32	1.38
3	A	702	4TS	CBB-CAW	-3.43	1.31	1.38
3	B	702	4TS	CAY-CAX	-3.38	1.31	1.38
3	B	702	4TS	CAQ-CAR	-3.37	1.31	1.38
3	D	702	4TS	CBB-CAW	-3.37	1.31	1.38
3	A	702	4TS	CAY-CAX	-3.29	1.32	1.38
3	B	702	4TS	CBB-CAW	-3.29	1.32	1.38
3	C	702	4TS	CBB-CAW	-3.25	1.32	1.38
3	C	702	4TS	CAQ-CAR	-3.20	1.32	1.38
3	C	702	4TS	CAY-CAX	-3.20	1.32	1.38
2	A	701	NDP	C7N-C3N	-3.19	1.41	1.48
3	B	702	4TS	CAP-CAG	-2.99	1.32	1.39
2	C	701	NDP	O2B-C2B	-2.99	1.33	1.44
2	B	701	NDP	C7N-N7N	2.97	1.41	1.33
3	D	702	4TS	CAP-CAG	-2.88	1.33	1.39
2	B	701	NDP	O2B-C2B	-2.86	1.33	1.44
2	D	701	NDP	C2A-N1A	2.86	1.39	1.33
2	B	701	NDP	C7N-C3N	-2.85	1.42	1.48
2	D	701	NDP	O2B-C2B	-2.76	1.34	1.44
3	C	702	4TS	C5-C6	-2.65	1.38	1.43
3	A	702	4TS	C6-N1	-2.64	1.31	1.35
2	A	701	NDP	O2B-C2B	-2.61	1.34	1.44
3	C	702	4TS	C2-N3	-2.59	1.30	1.35
3	A	702	4TS	C5-CAG	2.45	1.54	1.50
3	C	702	4TS	CAP-CAG	-2.41	1.34	1.39
3	D	702	4TS	C5-CAG	2.31	1.54	1.50
3	B	702	4TS	C5-C6	-2.30	1.38	1.43
4	D	703	UMP	C5-C4	-2.28	1.38	1.43
2	B	701	NDP	O4B-C1B	2.26	1.44	1.41
3	A	702	4TS	CBA-CAZ	-2.23	1.32	1.38
3	B	702	4TS	CBA-CAZ	-2.22	1.32	1.38
3	A	702	4TS	C5-C6	-2.20	1.39	1.43
2	D	701	NDP	C2A-N3A	2.18	1.35	1.32
3	C	702	4TS	CBA-CAZ	-2.17	1.32	1.38
4	B	703	UMP	C5-C4	-2.17	1.38	1.43
2	C	701	NDP	C7N-C3N	-2.13	1.44	1.48
3	D	702	4TS	CBA-CAZ	-2.13	1.32	1.38
3	B	702	4TS	C6-N1	-2.11	1.32	1.35
2	D	701	NDP	C4A-N3A	2.10	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	4TS	C5-C6	-2.10	1.39	1.43
2	C	701	NDP	C7N-N7N	2.03	1.38	1.33
2	B	701	NDP	C3B-C2B	2.02	1.57	1.52
4	C	703	UMP	C5-C4	-2.01	1.39	1.43

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	4TS	C2-N3-C4	6.18	121.39	116.24
3	C	702	4TS	C2-N3-C4	6.10	121.33	116.24
3	D	702	4TS	C2-N3-C4	5.79	121.07	116.24
4	A	703	UMP	C4-N3-C2	-5.17	119.75	126.58
3	A	702	4TS	C2-N3-C4	5.11	120.50	116.24
2	A	701	NDP	PN-O3-PA	-5.10	115.33	132.83
3	B	702	4TS	C5-C6-N1	-5.06	119.68	122.52
2	D	701	NDP	PN-O3-PA	-4.93	115.92	132.83
4	C	703	UMP	C4-N3-C2	-4.69	120.39	126.58
3	C	702	4TS	C5-C6-N1	-4.64	119.91	122.52
2	C	701	NDP	PN-O3-PA	-4.63	116.93	132.83
2	B	701	NDP	PN-O3-PA	-4.55	117.20	132.83
4	D	703	UMP	C4-N3-C2	-4.54	120.59	126.58
3	A	702	4TS	C5-C6-N1	-4.54	119.97	122.52
3	D	702	4TS	C5-C6-N1	-3.97	120.29	122.52
4	C	703	UMP	N3-C2-N1	3.92	120.09	114.89
4	B	703	UMP	C4-N3-C2	-3.80	121.57	126.58
3	B	702	4TS	C2-N1-C6	3.77	121.15	116.99
4	D	703	UMP	C5-C4-N3	3.62	120.25	114.84
4	A	703	UMP	N3-C2-N1	3.61	119.69	114.89
3	A	702	4TS	C2-N1-C6	3.44	120.78	116.99
3	C	702	4TS	C2-N1-C6	3.37	120.71	116.99
3	B	702	4TS	C5-C4-N3	-3.35	119.48	123.61
4	A	703	UMP	C5-C4-N3	3.30	119.78	114.84
3	D	702	4TS	C5-C4-N3	-3.29	119.55	123.61
4	C	703	UMP	O4-C4-C5	-3.27	119.40	125.16
3	A	702	4TS	C5-C4-N3	-3.26	119.59	123.61
3	D	702	4TS	C2-N1-C6	3.12	120.43	116.99
2	A	701	NDP	O2B-P2B-O1X	-3.12	97.36	109.39
2	D	701	NDP	O2B-P2B-O1X	-3.09	97.46	109.39
3	B	702	4TS	N3-C2-N1	-3.09	120.58	125.42
3	C	702	4TS	NAI-C2-N1	3.07	122.03	117.25
3	C	702	4TS	N3-C2-N1	-2.99	120.74	125.42
4	D	703	UMP	O4-C4-C5	-2.93	120.01	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	UMP	C5-C4-N3	2.92	119.21	114.84
2	D	701	NDP	C3B-C2B-C1B	-2.91	97.42	102.89
4	A	703	UMP	O4-C4-C5	-2.86	120.13	125.16
4	B	703	UMP	O4-C4-C5	-2.85	120.15	125.16
4	D	703	UMP	C1'-N1-C6	-2.84	115.95	121.55
3	C	702	4TS	C5-C4-N3	-2.83	120.12	123.61
4	D	703	UMP	N3-C2-N1	2.81	118.62	114.89
4	C	703	UMP	C5-C4-N3	2.80	119.02	114.84
2	C	701	NDP	PA-O5B-C5B	-2.77	105.46	121.68
3	D	702	4TS	CAT-CAG-C5	2.75	125.04	120.57
2	A	701	NDP	O3X-P2B-O2X	2.73	118.05	107.64
4	D	703	UMP	C1'-N1-C2	2.71	122.98	117.64
2	D	701	NDP	O3X-P2B-O2X	2.69	117.92	107.64
2	C	701	NDP	O3X-P2B-O2X	2.68	117.89	107.64
2	B	701	NDP	O3X-P2B-O2X	2.68	117.86	107.64
3	D	702	4TS	N3-C2-N1	-2.57	121.38	125.42
4	B	703	UMP	C1'-N1-C2	2.57	122.71	117.64
4	B	703	UMP	N3-C2-N1	2.57	118.30	114.89
2	B	701	NDP	PA-O5B-C5B	-2.53	106.87	121.68
2	B	701	NDP	O2B-P2B-O1X	-2.53	99.64	109.39
2	C	701	NDP	C3B-C2B-C1B	-2.51	98.16	102.89
2	C	701	NDP	O3X-P2B-O2B	-2.51	94.75	105.99
3	A	702	4TS	N3-C2-N1	-2.48	121.53	125.42
2	A	701	NDP	PA-O5B-C5B	-2.45	107.33	121.68
2	D	701	NDP	PN-O5D-C5D	-2.43	107.44	121.68
2	D	701	NDP	C2B-C3B-C4B	-2.42	96.73	101.99
3	D	702	4TS	CAP-CAG-C5	-2.42	116.78	120.79
4	B	703	UMP	C1'-N1-C6	-2.40	116.81	121.55
2	A	701	NDP	PN-O5D-C5D	-2.38	107.73	121.68
2	D	701	NDP	PA-O5B-C5B	-2.38	107.74	121.68
2	C	701	NDP	PN-O5D-C5D	-2.37	107.78	121.68
3	B	702	4TS	NAI-C2-N1	2.33	120.87	117.25
2	B	701	NDP	PN-O5D-C5D	-2.32	108.05	121.68
2	D	701	NDP	O3X-P2B-O2B	-2.32	95.59	105.99
2	B	701	NDP	C2B-C3B-C4B	-2.31	96.97	101.99
2	B	701	NDP	C1D-N1N-C2N	-2.31	117.26	121.11
2	C	701	NDP	O2B-P2B-O1X	-2.27	100.64	109.39
2	A	701	NDP	C3B-C2B-C1B	-2.26	98.65	102.89
2	B	701	NDP	C3B-C2B-C1B	-2.24	98.68	102.89
2	B	701	NDP	O3X-P2B-O2B	-2.24	95.95	105.99
2	B	701	NDP	C2A-N1A-C6A	-2.21	114.97	118.75
3	B	702	4TS	C6-C5-C4	2.20	117.72	115.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NDP	C2A-N1A-C6A	-2.19	115.02	118.75
2	C	701	NDP	O2A-PA-O1A	2.18	123.00	112.24
2	D	701	NDP	C2A-N1A-C6A	-2.16	115.07	118.75
3	C	702	4TS	CAT-CAS-CLA	-2.15	116.47	119.15
2	C	701	NDP	O2N-PN-O1N	2.12	122.73	112.24
4	C	703	UMP	O2-C2-N1	-2.11	119.98	122.79
2	B	701	NDP	O2A-PA-O1A	2.11	122.66	112.24
2	A	701	NDP	C3N-C2N-N1N	-2.10	120.10	123.10
2	C	701	NDP	C4A-C5A-N7A	2.10	111.59	109.40
2	A	701	NDP	O5D-PN-O1N	-2.10	100.87	109.07
2	C	701	NDP	O2B-C2B-C1B	-2.10	102.55	110.10
4	C	703	UMP	C1'-N1-C2	2.08	121.75	117.64
3	A	702	4TS	C6-C5-C4	2.08	117.62	115.91
2	C	701	NDP	C5D-C4D-C3D	-2.07	107.41	115.18
3	A	702	4TS	CAO-OAV-CAW	-2.05	112.57	117.93
2	A	701	NDP	O2N-PN-O1N	2.03	122.27	112.24

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NDP	PA-O3-PN-O5D
2	C	701	NDP	C5D-O5D-PN-O2N
4	A	703	UMP	O4'-C4'-C5'-O5'
4	B	703	UMP	C5'-O5'-P-OP2
4	B	703	UMP	C5'-O5'-P-OP3
4	B	703	UMP	C3'-C4'-C5'-O5'
4	B	703	UMP	O4'-C4'-C5'-O5'
4	D	703	UMP	C3'-C4'-C5'-O5'
4	D	703	UMP	O4'-C4'-C5'-O5'
4	A	703	UMP	C3'-C4'-C5'-O5'
2	A	701	NDP	C3B-C4B-C5B-O5B
4	B	703	UMP	C5'-O5'-P-OP1
4	D	703	UMP	C5'-O5'-P-OP1
2	B	701	NDP	PA-O3-PN-O5D
2	C	701	NDP	PA-O3-PN-O5D
2	D	701	NDP	PA-O3-PN-O5D
4	A	703	UMP	C5'-O5'-P-OP2
4	A	703	UMP	C5'-O5'-P-OP3
2	A	701	NDP	C5B-O5B-PA-O3
2	C	701	NDP	C5B-O5B-PA-O3
2	D	701	NDP	C2B-O2B-P2B-O2X

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Mol	Chain	Res	Type	Atoms
2	A	701	NDP	O4B-C4B-C5B-O5B
2	C	701	NDP	C5D-O5D-PN-O1N
3	D	702	4TS	CBB-CAW-OAV-CAO
3	D	702	4TS	CAX-CAW-OAV-CAO
4	C	703	UMP	O4'-C4'-C5'-O5'
4	A	703	UMP	C5'-O5'-P-OP1
2	A	701	NDP	C4D-C5D-O5D-PN
2	D	701	NDP	C4D-C5D-O5D-PN
2	C	701	NDP	C3B-C4B-C5B-O5B
2	A	701	NDP	O4D-C1D-N1N-C2N
2	B	701	NDP	O4D-C1D-N1N-C2N
2	C	701	NDP	O4D-C1D-N1N-C2N
2	D	701	NDP	O4D-C1D-N1N-C2N
2	B	701	NDP	C4D-C5D-O5D-PN
2	C	701	NDP	C4D-C5D-O5D-PN
2	B	701	NDP	C2D-C1D-N1N-C2N
2	C	701	NDP	C2D-C1D-N1N-C2N
2	A	701	NDP	C2D-C1D-N1N-C2N
2	D	701	NDP	C2D-C1D-N1N-C2N
2	C	701	NDP	O4B-C4B-C5B-O5B
2	B	701	NDP	O4B-C4B-C5B-O5B
4	D	703	UMP	C5'-O5'-P-OP3
3	C	702	4TS	CAN-CAO-OAV-CAW
2	B	701	NDP	C3B-C4B-C5B-O5B
4	C	703	UMP	C3'-C4'-C5'-O5'
2	C	701	NDP	C5D-O5D-PN-O3
2	D	701	NDP	C2B-O2B-P2B-O3X
2	A	701	NDP	C5B-O5B-PA-O1A
2	C	701	NDP	C5B-O5B-PA-O1A
2	C	701	NDP	C2N-C3N-C7N-N7N
2	D	701	NDP	C5B-O5B-PA-O1A
2	D	701	NDP	C2N-C3N-C7N-N7N

There are no ring outliers.

6 monomers are involved in 18 short contacts:

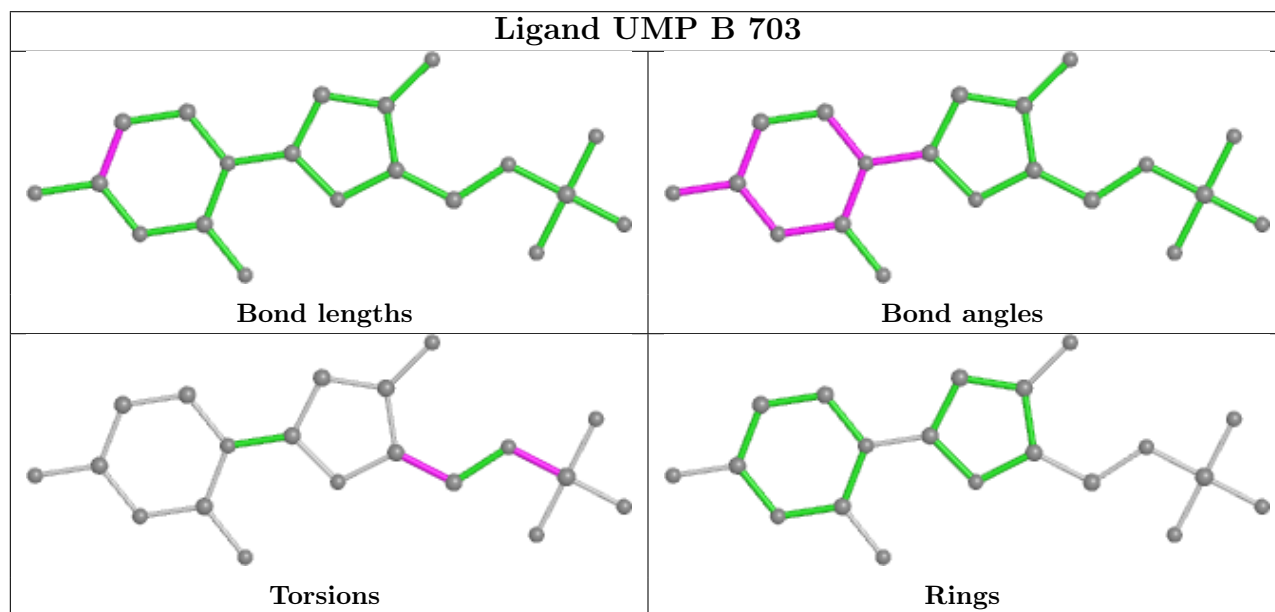
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	4TS	1	0
2	C	701	NDP	3	0
2	A	701	NDP	3	0
2	D	701	NDP	4	0
2	B	701	NDP	6	0

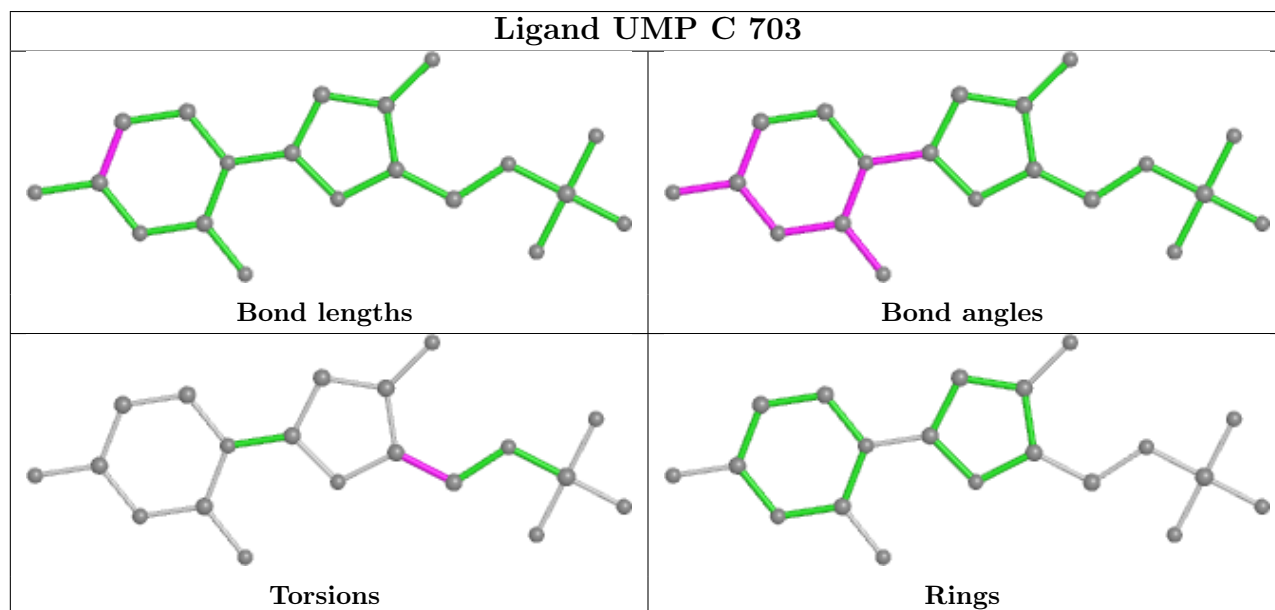
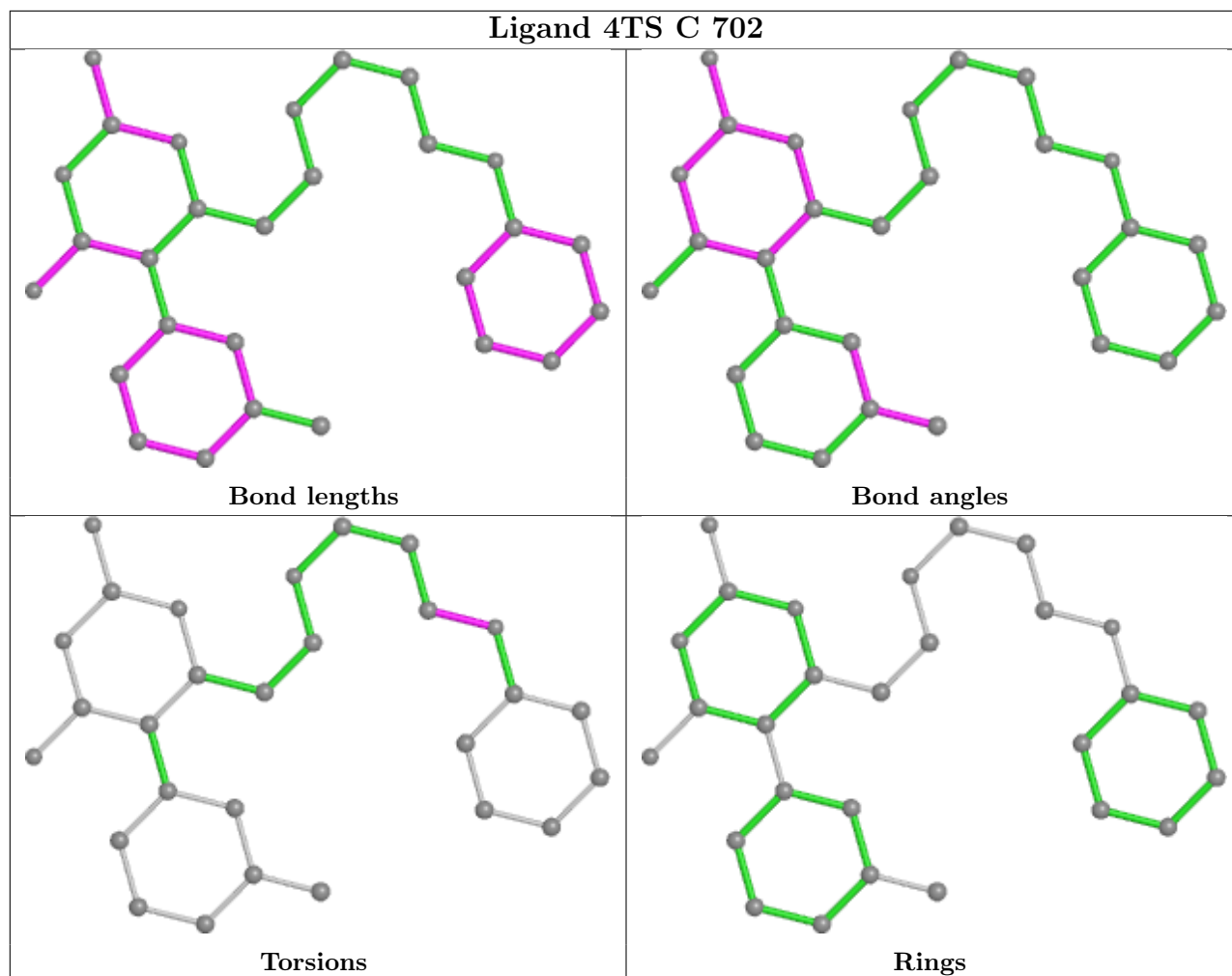
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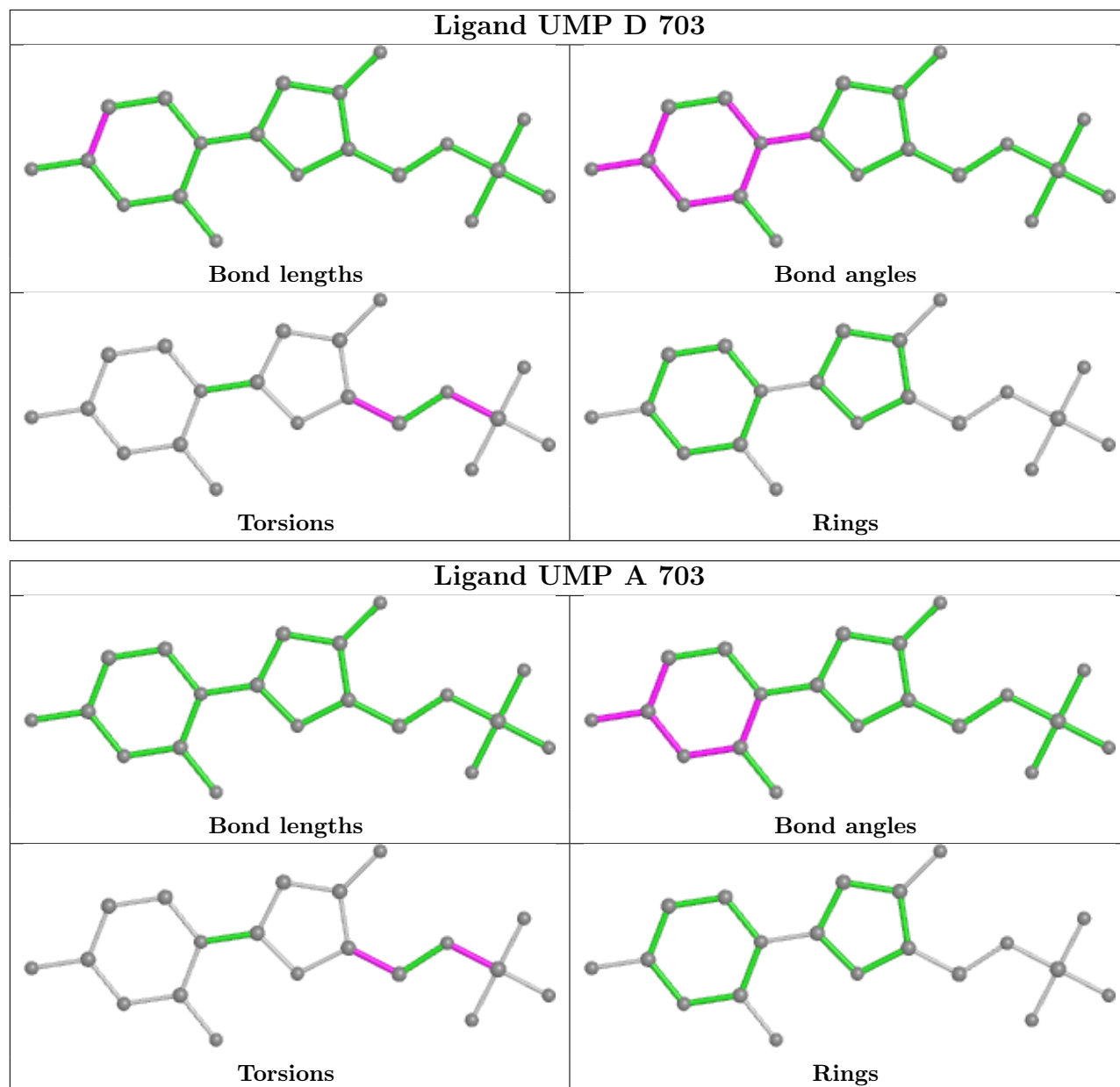
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	4TS	1	0

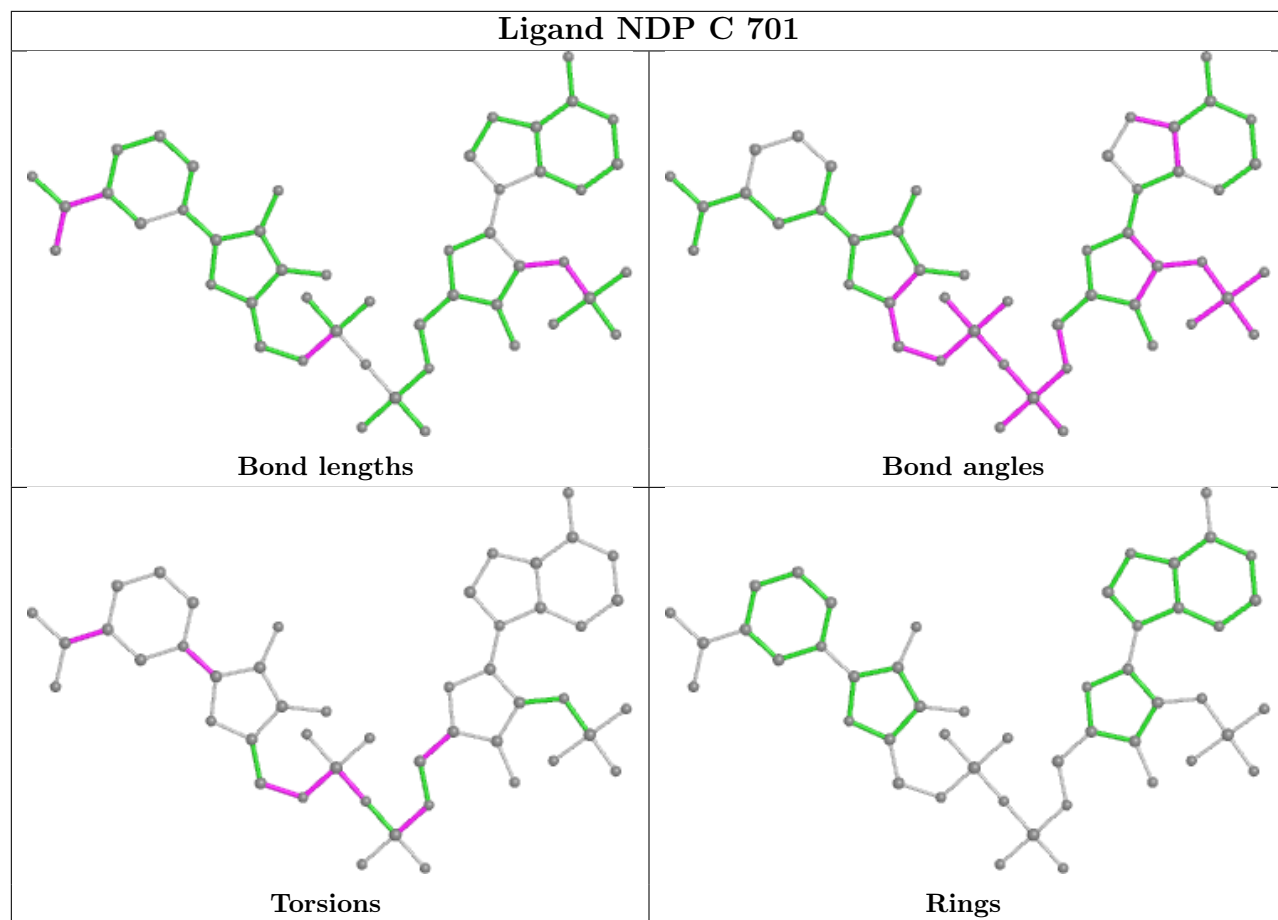
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

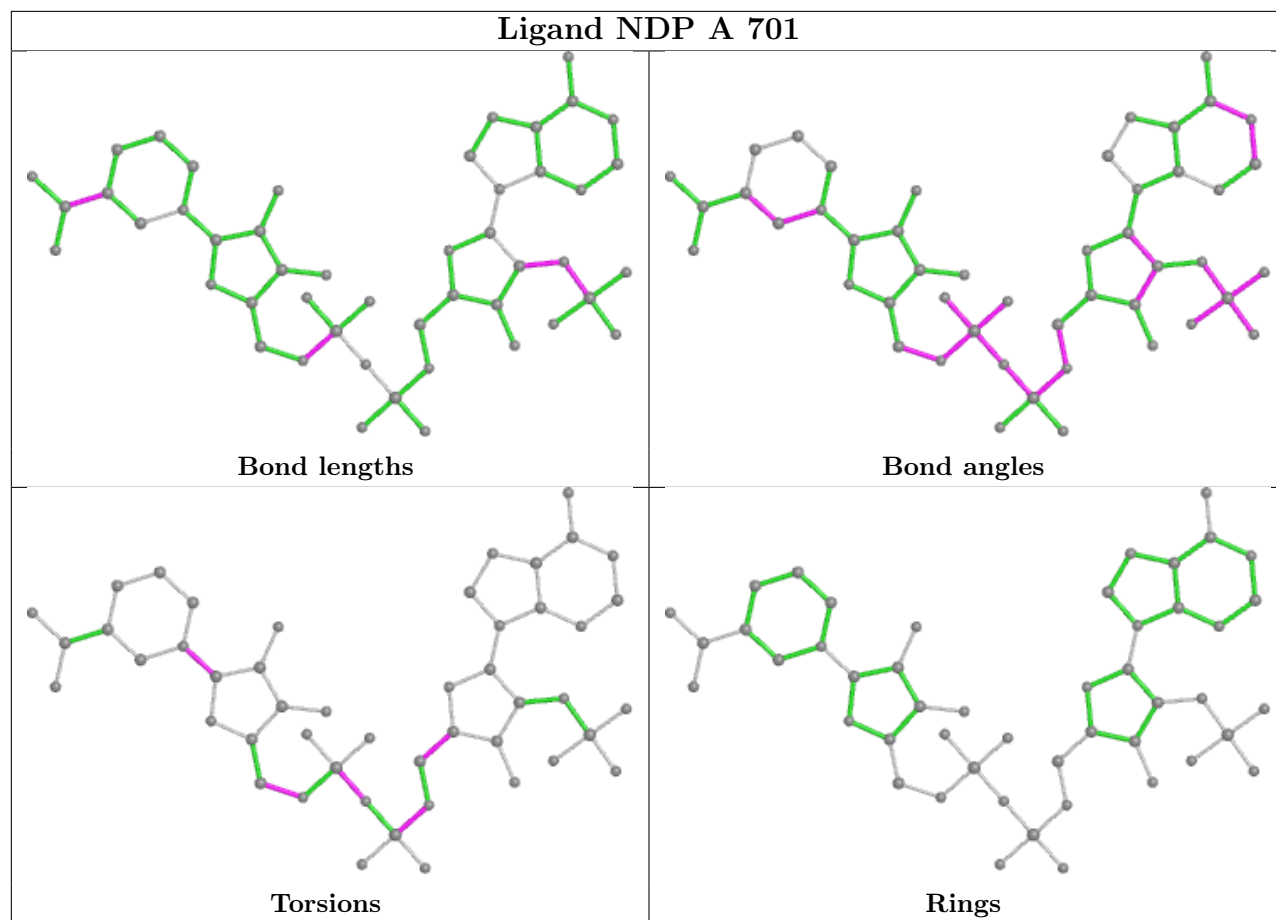


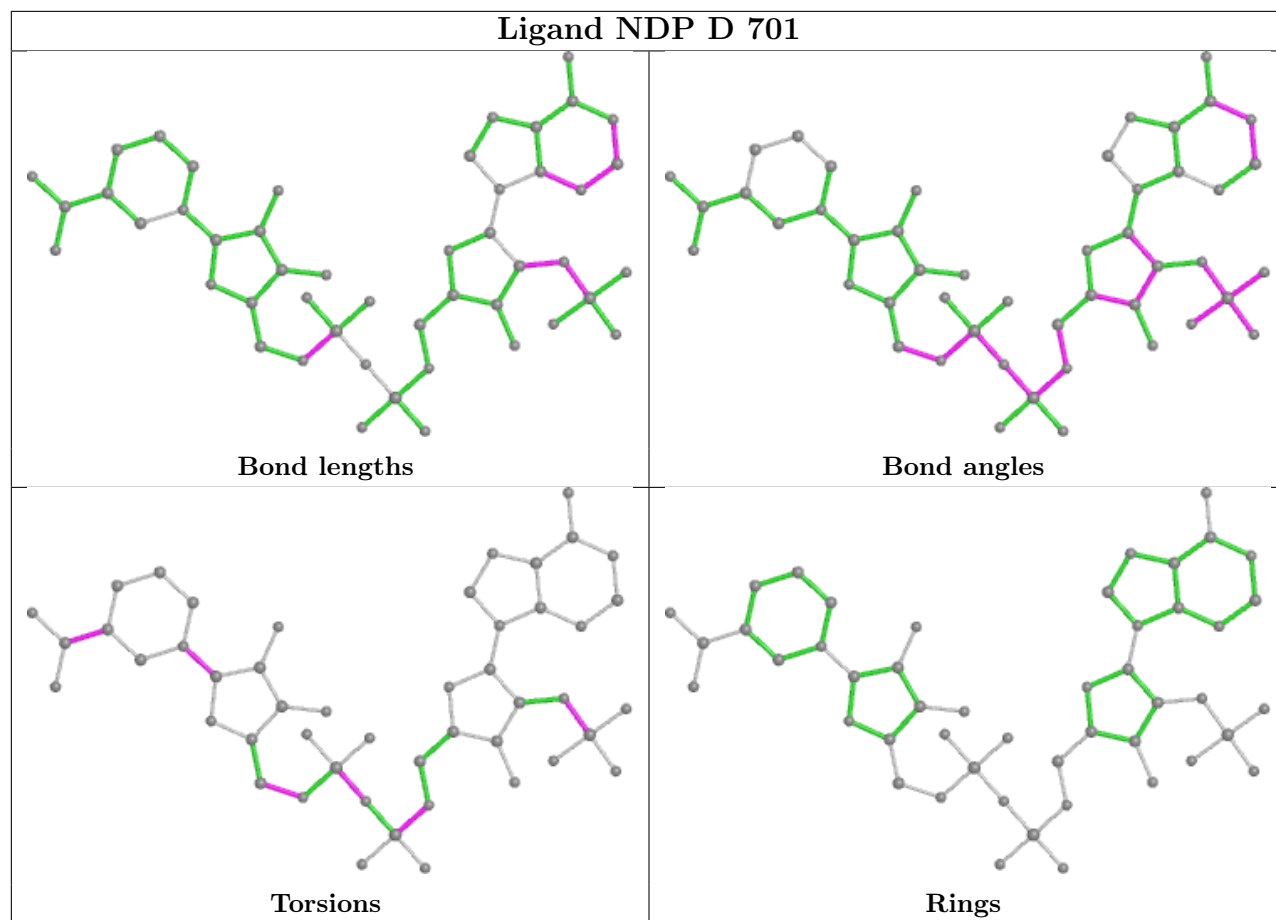


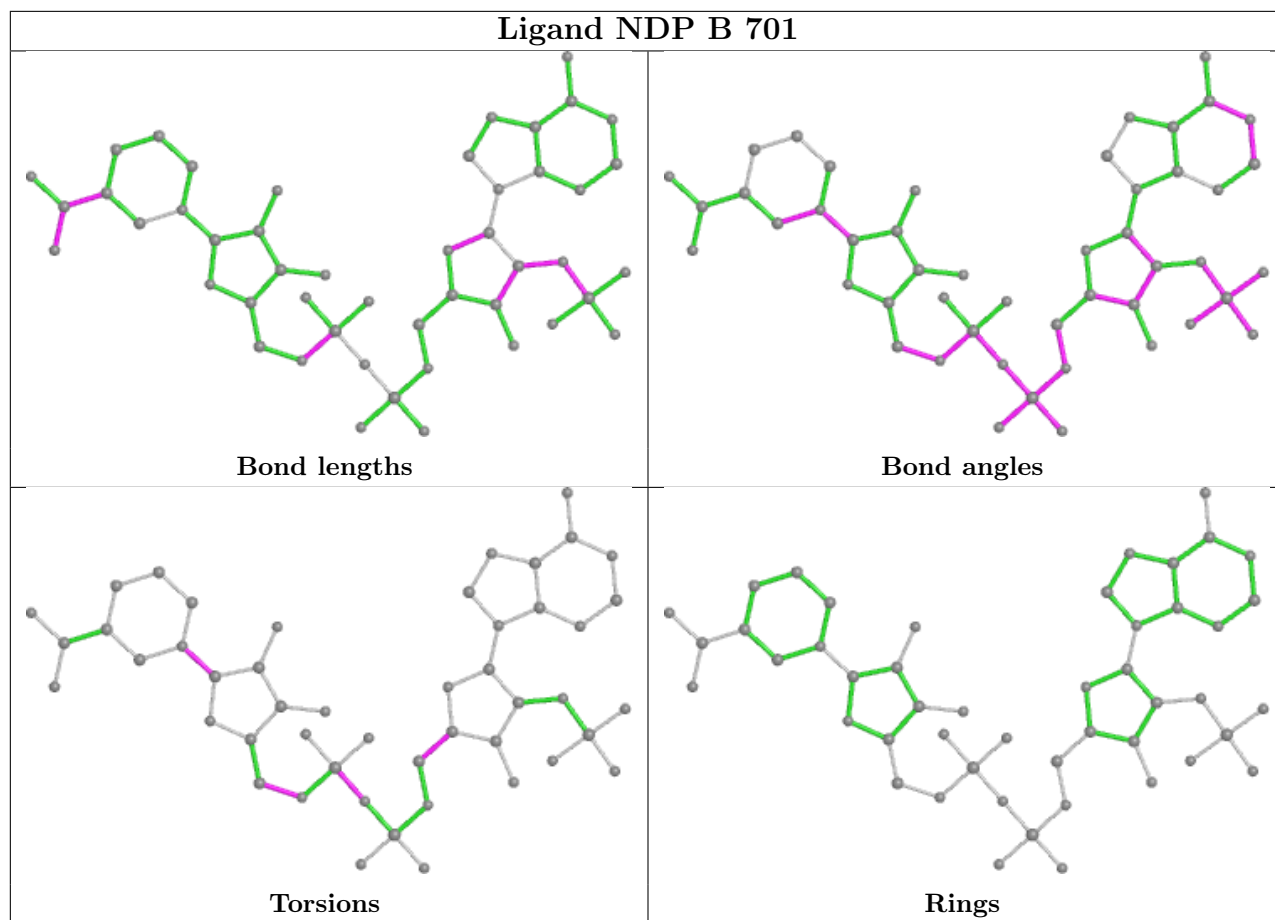


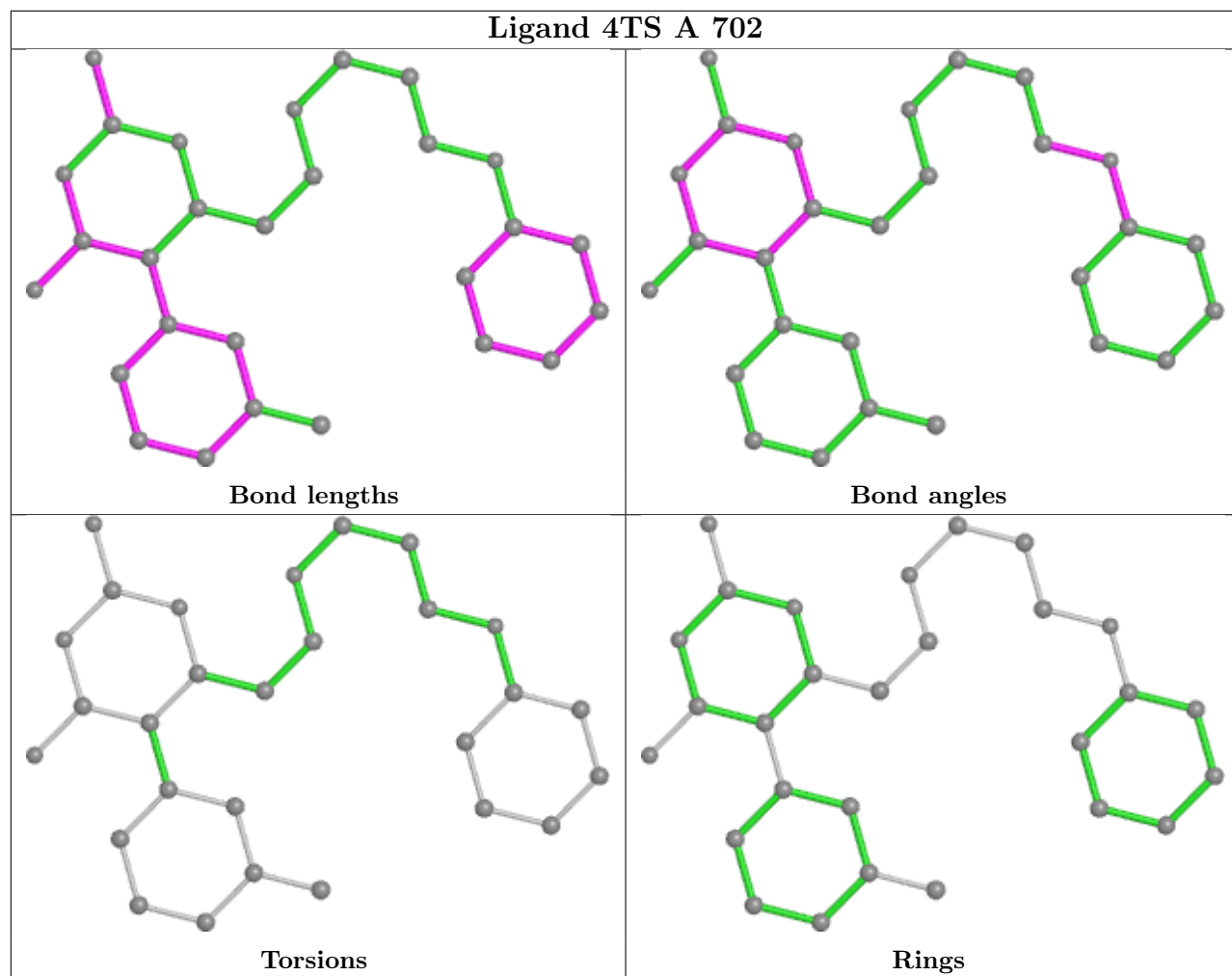


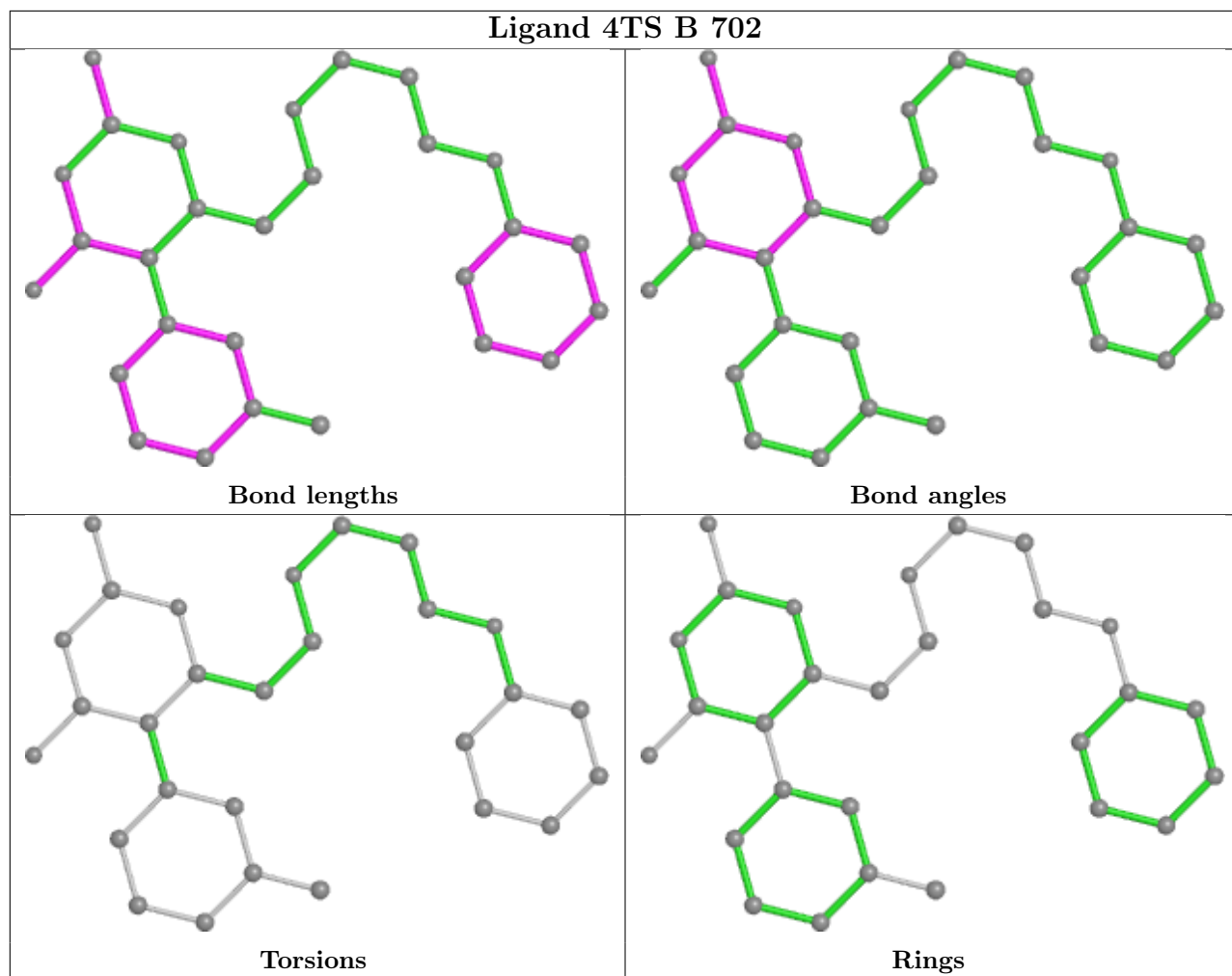


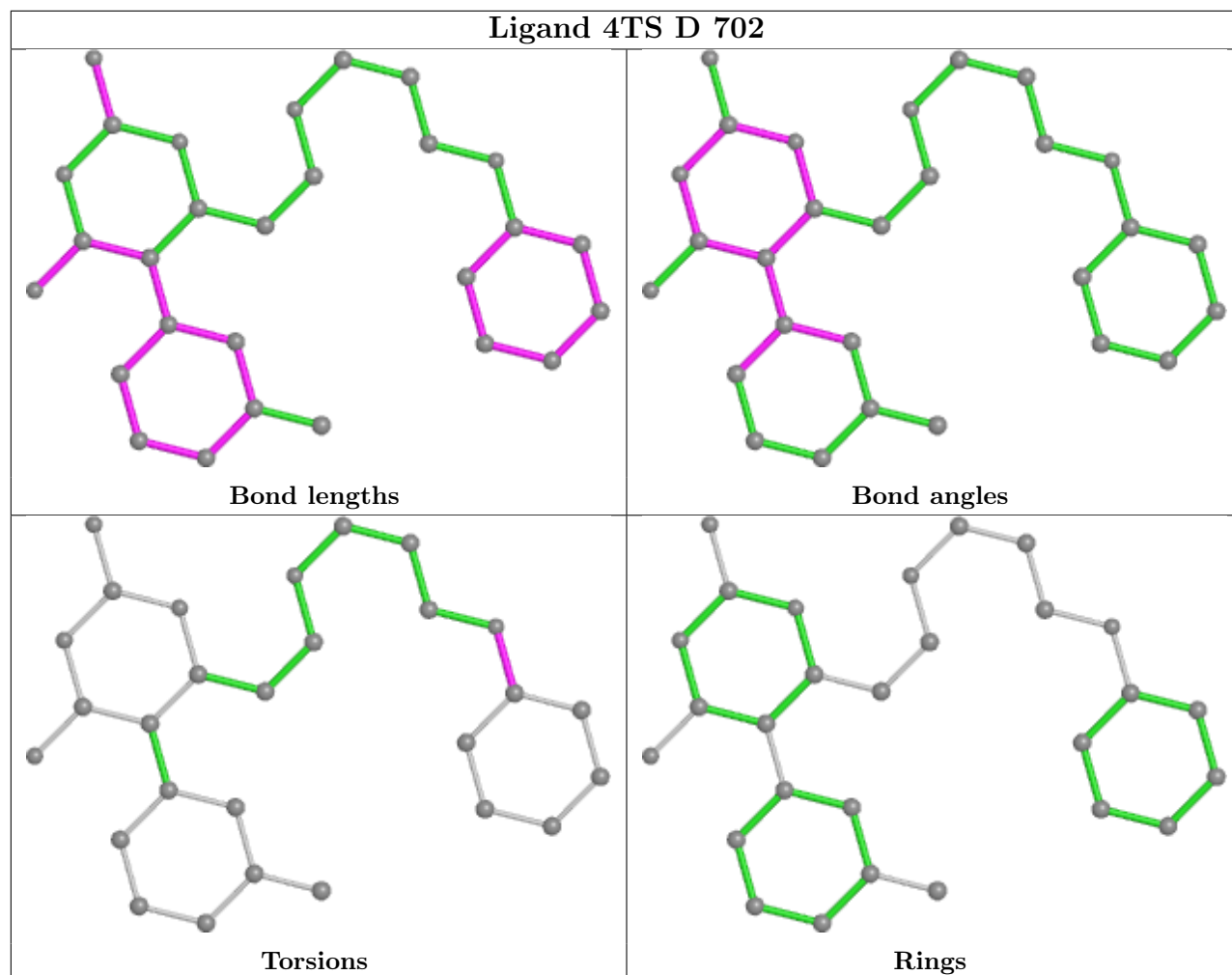












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 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	559/610 (91%)	0.07	33 (5%) 22 20	22, 35, 80, 114	0
1	B	562/610 (92%)	0.10	37 (6%) 18 16	20, 36, 90, 123	0
1	C	557/610 (91%)	0.17	36 (6%) 18 16	24, 35, 87, 123	0
1	D	562/610 (92%)	0.24	35 (6%) 20 18	23, 37, 89, 132	0
All	All	2240/2440 (91%)	0.14	141 (6%) 20 18	20, 36, 86, 132	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	202	ALA	13.1
1	D	257	ALA	13.1
1	B	257	ALA	12.5
1	D	258	ALA	12.5
1	C	203	ALA	12.2
1	A	201	GLN	12.0
1	B	202	ALA	11.9
1	A	199	ALA	11.3
1	D	200	ALA	10.8
1	B	203	ALA	10.0
1	D	606	MET	9.7
1	B	258	ALA	9.6
1	C	201	GLN	9.4
1	A	257	ALA	9.2
1	D	256	ASP	9.2
1	A	202	ALA	8.5
1	A	200	ALA	8.5
1	B	281	LEU	8.4
1	D	199	ALA	8.3
1	B	256	ASP	8.3
1	D	202	ALA	8.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	198	THR	7.9
1	A	256	ASP	7.4
1	B	47	SER	7.4
1	A	345	THR	7.3
1	D	201	GLN	7.2
1	C	200	ALA	7.2
1	C	46	ALA	7.1
1	A	284	PRO	7.0
1	C	606	MET	6.9
1	D	48	ARG	6.7
1	D	284	PRO	6.5
1	B	280	GLY	6.4
1	C	45	GLU	6.2
1	C	204	ALA	6.2
1	D	203	ALA	6.2
1	A	606	MET	5.8
1	D	197	SER	5.6
1	A	198	THR	5.6
1	D	204	ALA	5.4
1	A	71	GLY	5.4
1	A	205	PRO	5.4
1	B	71	GLY	5.3
1	A	203	ALA	5.2
1	C	48	ARG	5.0
1	B	46	ALA	5.0
1	A	197	SER	4.9
1	A	283	ALA	4.9
1	B	282	GLN	4.9
1	B	204	ALA	4.8
1	D	47	SER	4.8
1	A	255	ASP	4.8
1	B	255	ASP	4.8
1	C	199	ALA	4.8
1	D	71	GLY	4.7
1	A	347	VAL	4.6
1	C	255	ASP	4.6
1	B	200	ALA	4.6
1	B	119	GLU	4.5
1	B	201	GLN	4.5
1	A	346	GLY	4.5
1	D	344	ARG	4.4
1	A	254	THR	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	91	PHE	4.4
1	C	283	ALA	4.4
1	C	346	GLY	4.3
1	A	47	SER	4.2
1	A	204	ALA	4.2
1	B	48	ARG	4.1
1	D	205	PRO	4.0
1	A	46	ALA	4.0
1	C	347	VAL	4.0
1	C	43	PRO	3.9
1	D	283	ALA	3.9
1	C	303	LYS	3.8
1	D	255	ASP	3.8
1	C	344	ARG	3.7
1	A	45	GLU	3.7
1	B	303	LYS	3.7
1	C	282	GLN	3.7
1	B	45	GLU	3.6
1	B	254	THR	3.6
1	B	605	GLN	3.6
1	D	304	LYS	3.6
1	C	604	ILE	3.5
1	C	345	THR	3.5
1	B	604	ILE	3.4
1	B	199	ALA	3.4
1	D	72	LYS	3.4
1	B	88	PRO	3.4
1	C	309	GLU	3.3
1	D	46	ALA	3.3
1	B	198	THR	3.3
1	B	304	LYS	3.3
1	C	47	SER	3.2
1	B	197	SER	3.2
1	C	205	PRO	3.0
1	A	303	LYS	3.0
1	A	114	GLU	3.0
1	B	606	MET	3.0
1	D	117	GLN	3.0
1	C	197	SER	3.0
1	C	306	GLU	2.9
1	C	302	ARG	2.9
1	A	344	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	605	GLN	2.9
1	C	411	PHE	2.8
1	A	72	LYS	2.8
1	C	300	GLU	2.8
1	B	44	GLU	2.7
1	C	207	GLU	2.7
1	A	48	ARG	2.7
1	B	207	GLU	2.6
1	D	303	LYS	2.6
1	A	605	GLN	2.6
1	C	304	LYS	2.6
1	C	254	THR	2.6
1	D	605	GLN	2.6
1	C	307	GLN	2.5
1	A	417	LEU	2.5
1	D	347	VAL	2.5
1	B	72	LYS	2.5
1	A	282	GLN	2.4
1	B	43	PRO	2.4
1	D	346	GLY	2.3
1	D	603	ARG	2.3
1	B	309	GLU	2.3
1	A	206	ALA	2.3
1	B	306	GLU	2.3
1	D	558	GLU	2.3
1	D	281	LEU	2.3
1	C	44	GLU	2.3
1	B	283	ALA	2.2
1	B	90	LYS	2.2
1	C	71	GLY	2.2
1	D	300	GLU	2.2
1	A	343	ASP	2.1
1	D	207	GLU	2.1
1	D	280	GLY	2.1
1	C	343	ASP	2.0
1	D	308	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

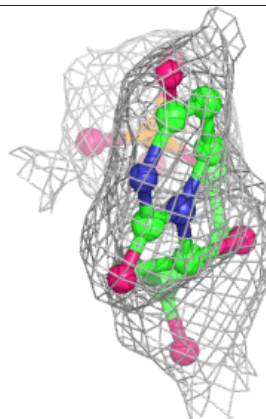
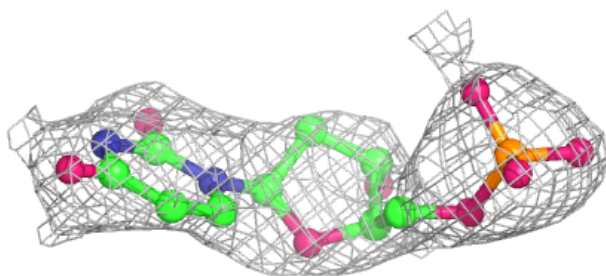
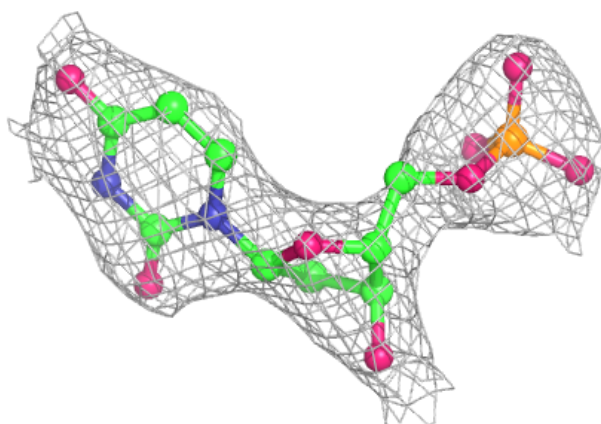
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	UMP	C	703	20/20	0.96	0.15	43,53,60,61	0
3	4TS	A	702	28/28	0.97	0.15	24,28,46,50	0
3	4TS	B	702	28/28	0.97	0.18	29,36,47,49	0
3	4TS	C	702	28/28	0.97	0.18	26,31,44,48	0
3	4TS	D	702	28/28	0.97	0.16	27,35,47,51	0
4	UMP	A	703	20/20	0.97	0.14	35,41,51,53	0
4	UMP	B	703	20/20	0.97	0.12	39,46,53,55	0
2	NDP	B	701	48/48	0.97	0.14	29,36,47,55	0
4	UMP	D	703	20/20	0.97	0.16	40,47,51,53	0
2	NDP	D	701	48/48	0.98	0.14	25,38,46,50	0
2	NDP	A	701	48/48	0.98	0.12	21,33,41,44	0
2	NDP	C	701	48/48	0.98	0.14	23,31,37,42	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.

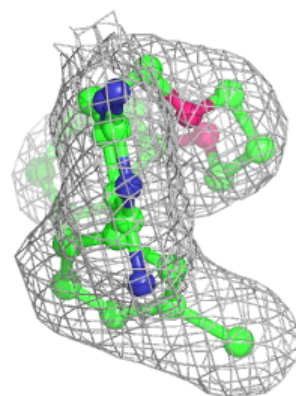
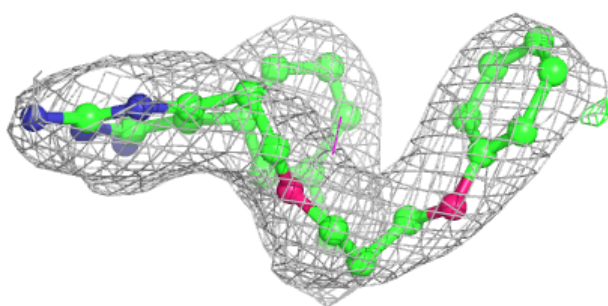
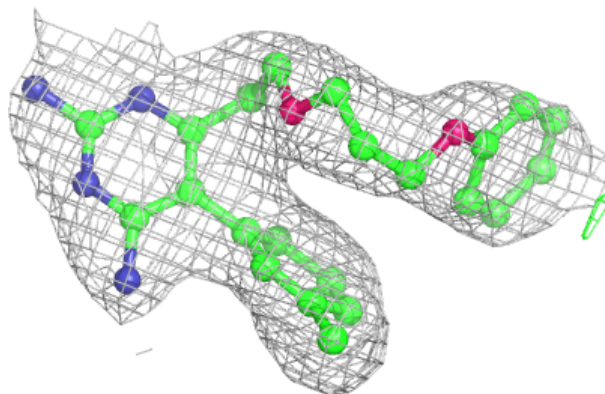
**Electron density around UMP C 703:**

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

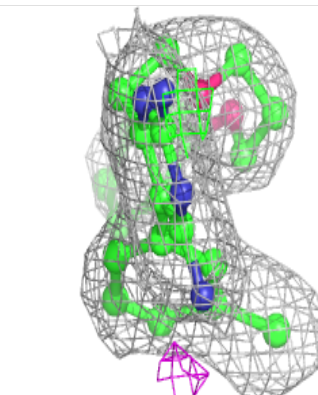
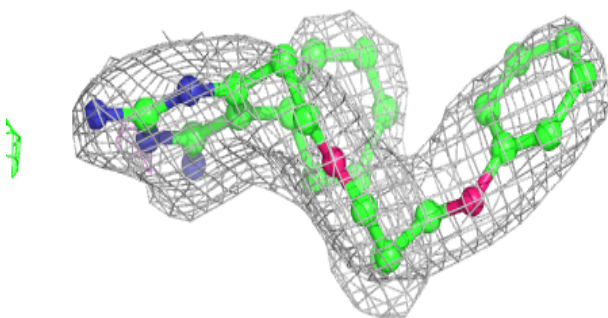
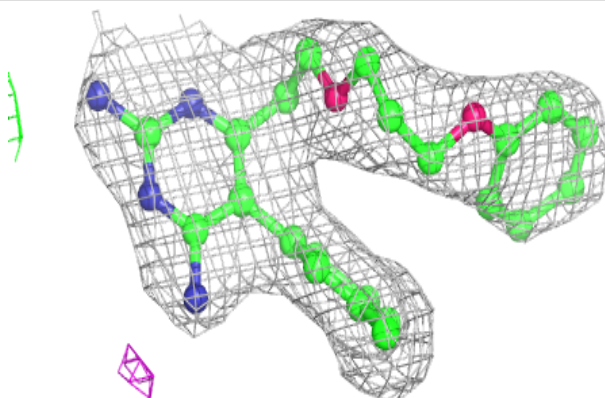


**Electron density around 4TS A 702:**

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

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

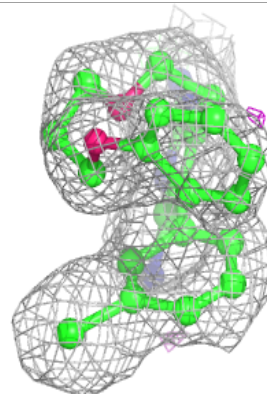
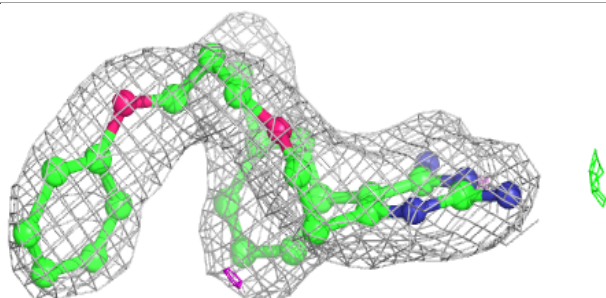
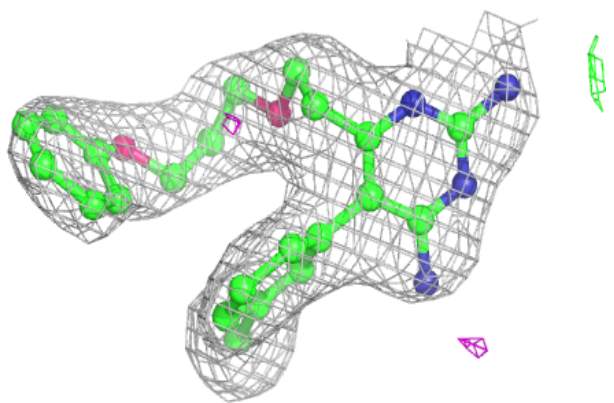
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



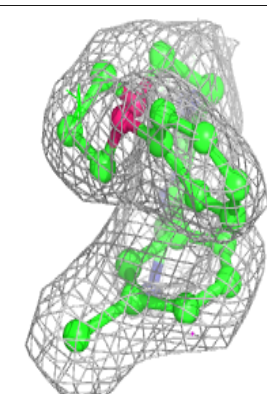
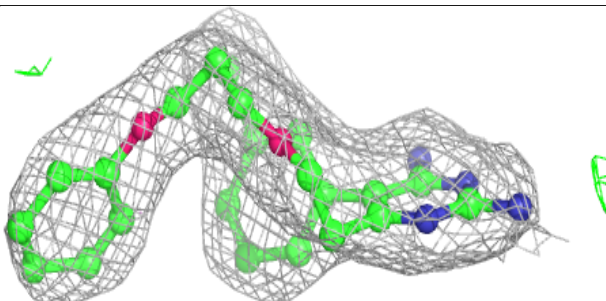
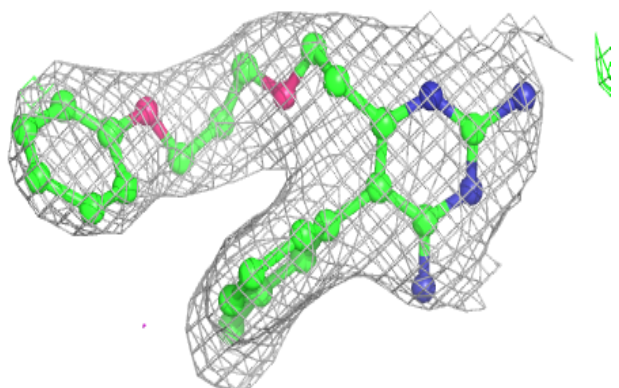


**Electron density around 4TS C 702:**

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

**Electron density around 4TS D 702:**

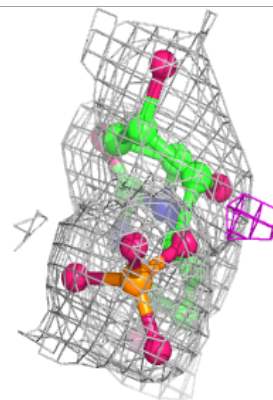
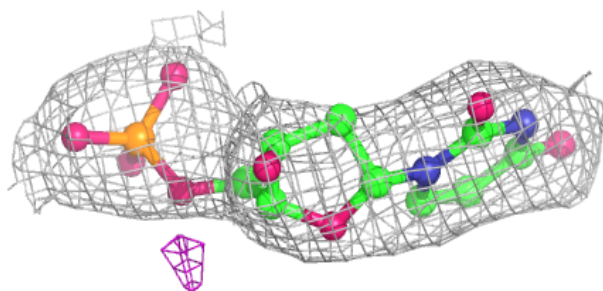
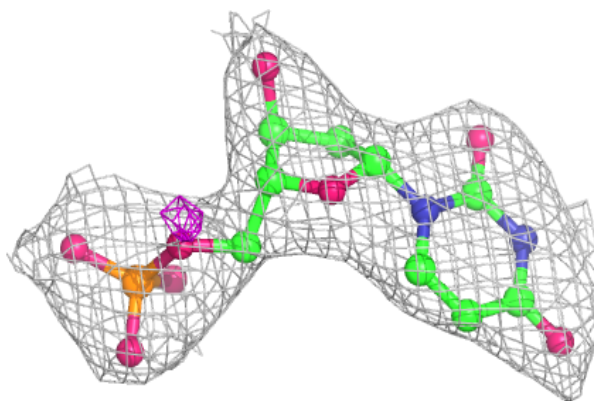
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



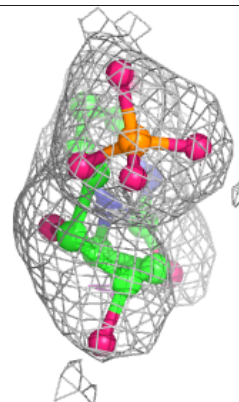
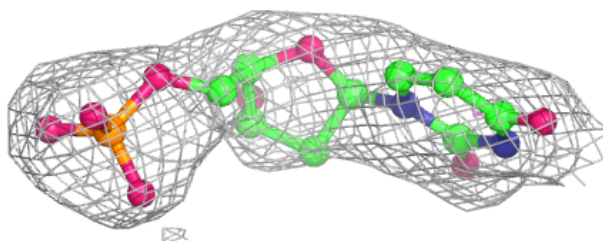
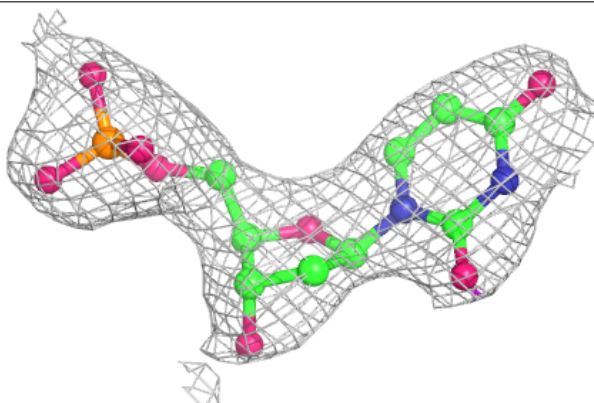


**Electron density around UMP A 703:**

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

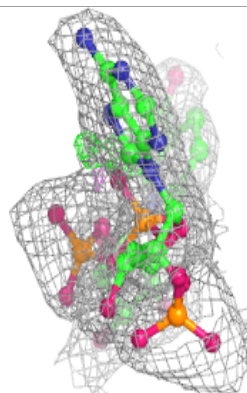
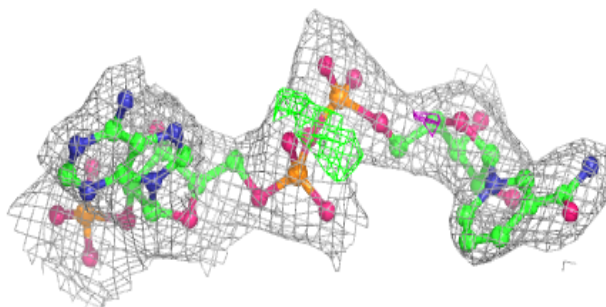
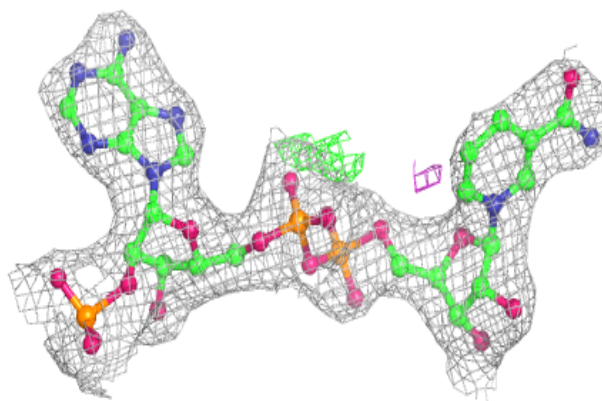
**Electron density around UMP B 703:**

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

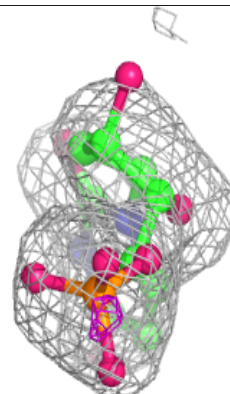
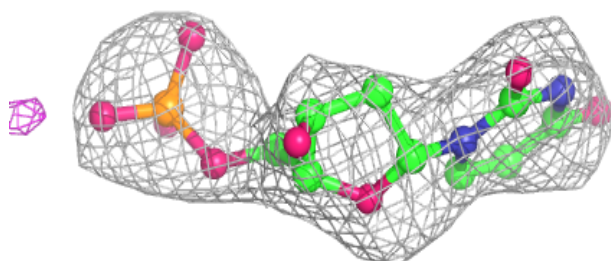
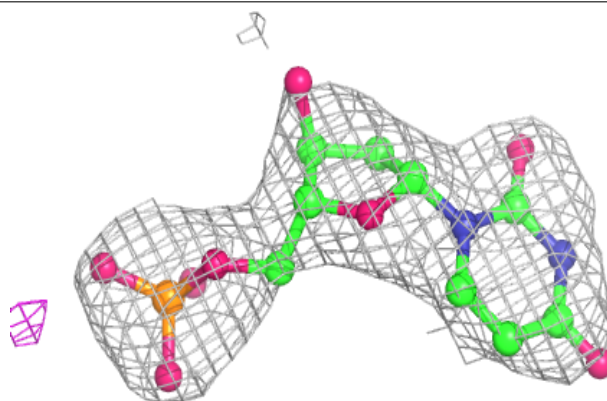


**Electron density around NDP B 701:**

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

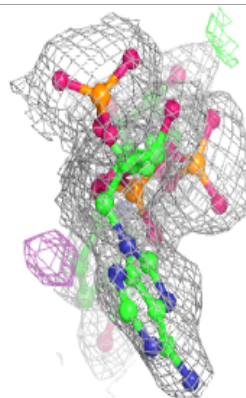
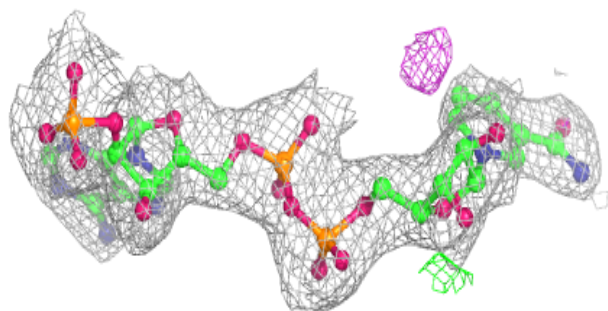
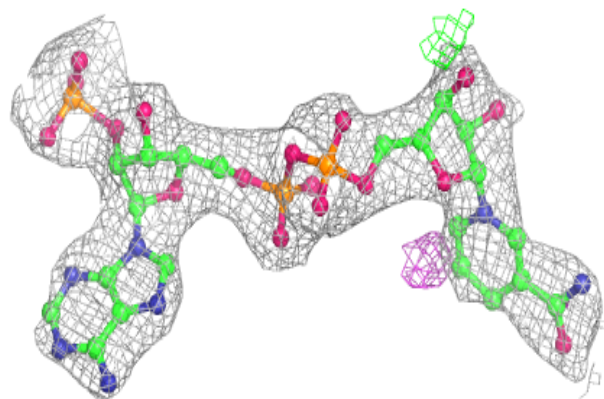
**Electron density around UMP D 703:**

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

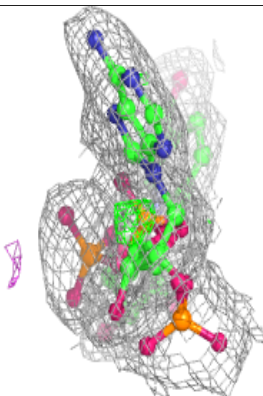
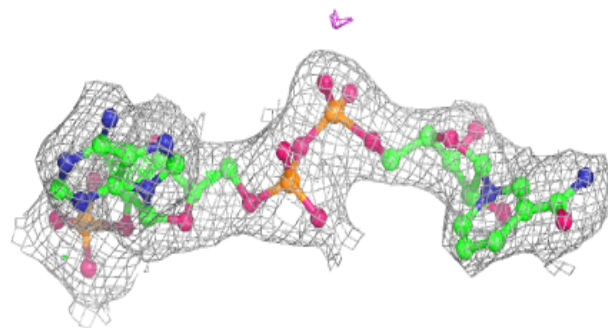
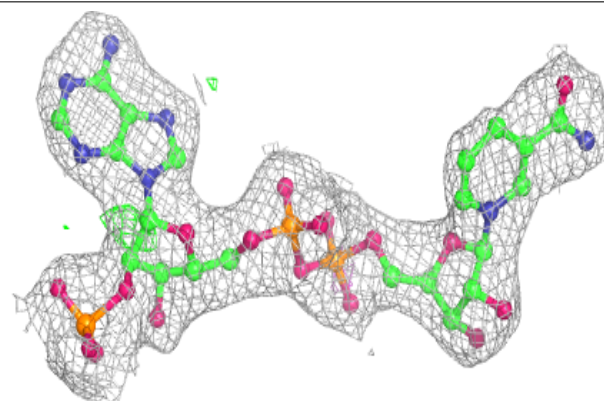


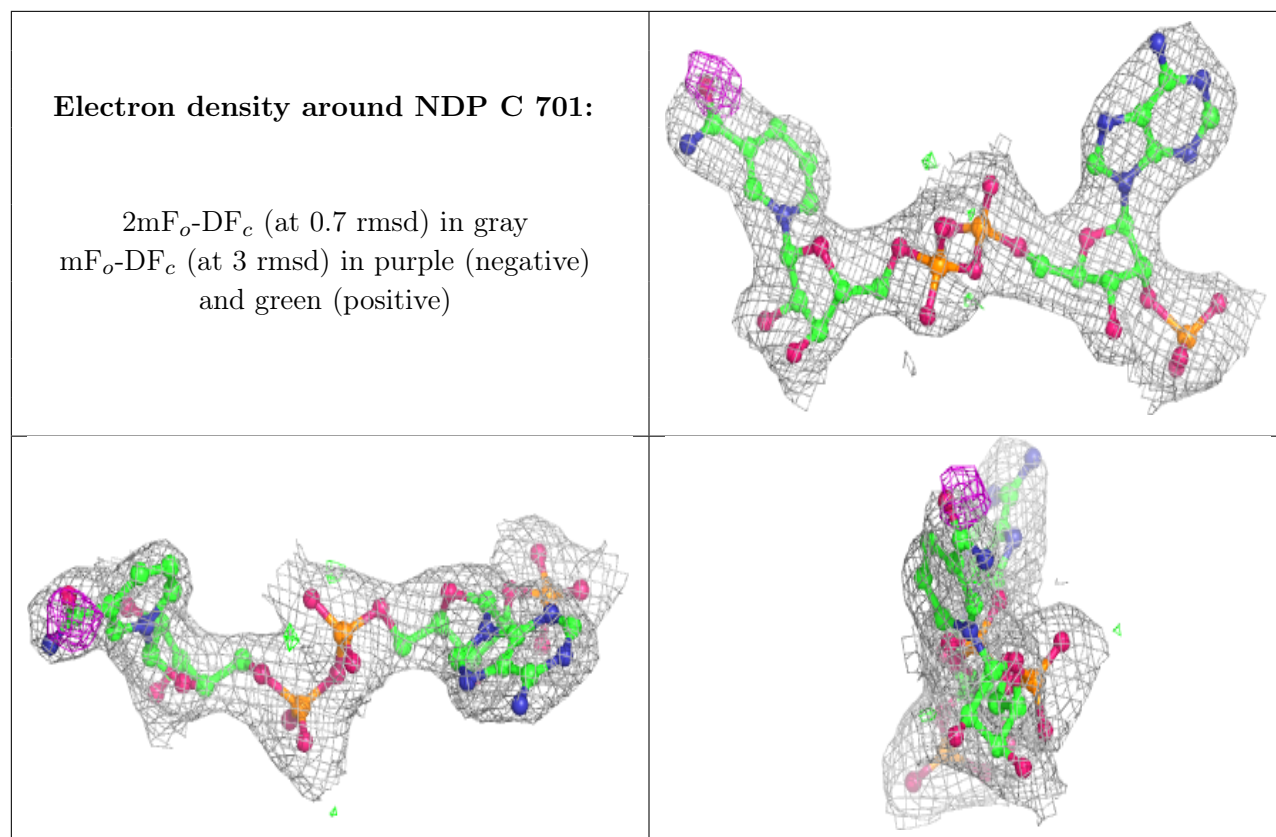
**Electron density around NDP D 701:**

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

**Electron density around NDP A 701:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.