



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:30 PM EDT

PDB ID : 4TO1 / pdb_00004to1
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dATP/dCTP-dCTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.55 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

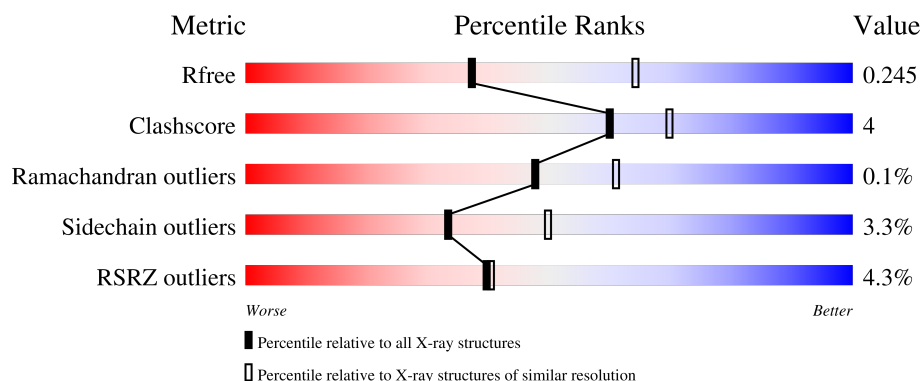
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	514	3% 84% 9% 7%
1	B	514	8% 86% 7% 7%
1	C	514	% 84% 9% 6%
1	D	514	4% 84% 10% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16149 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

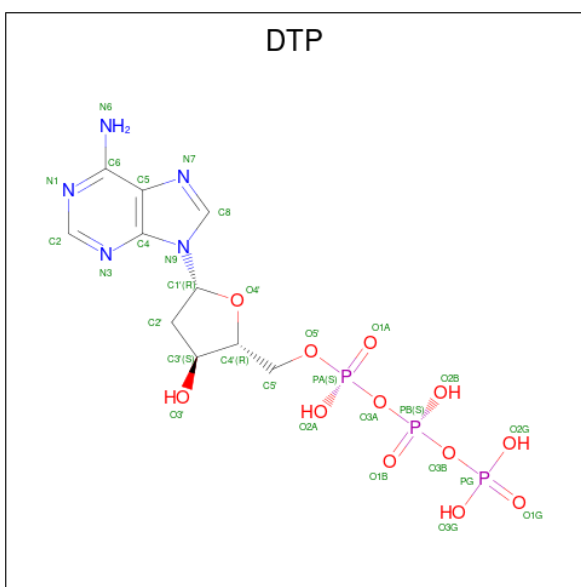
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	1	0
			3922	2511	684	706	21			
1	B	480	Total	C	N	O	S	0	0	0
			3924	2512	684	708	20			
1	C	481	Total	C	N	O	S	0	2	0
			3944	2522	687	715	20			
1	D	484	Total	C	N	O	S	0	1	0
			3961	2535	689	716	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



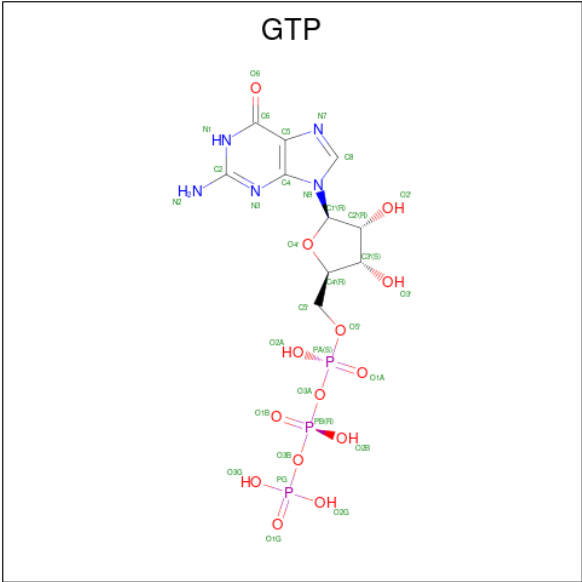


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
3	B	1	Total 30	C 10	N 5	O 12	P 3	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

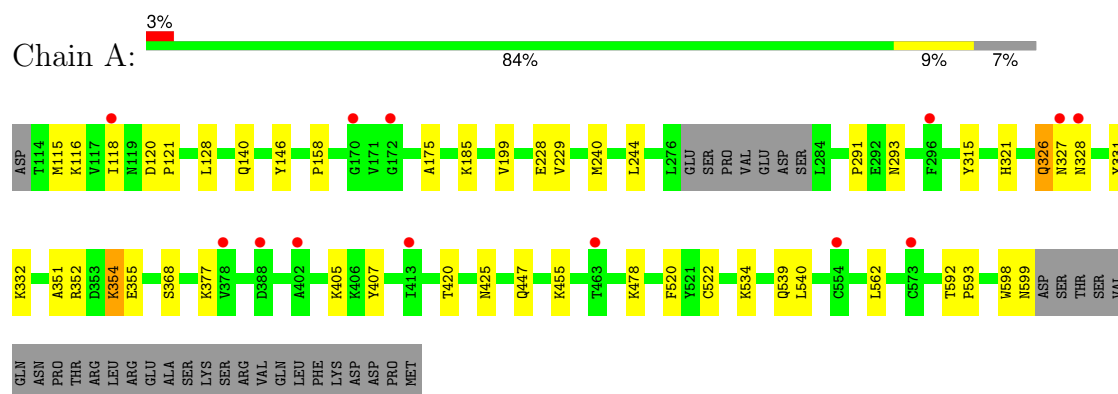
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	6	Total	O	0	0
			6	6		
6	C	22	Total	O	0	0
			22	22		
6	D	3	Total	O	0	0
			3	3		

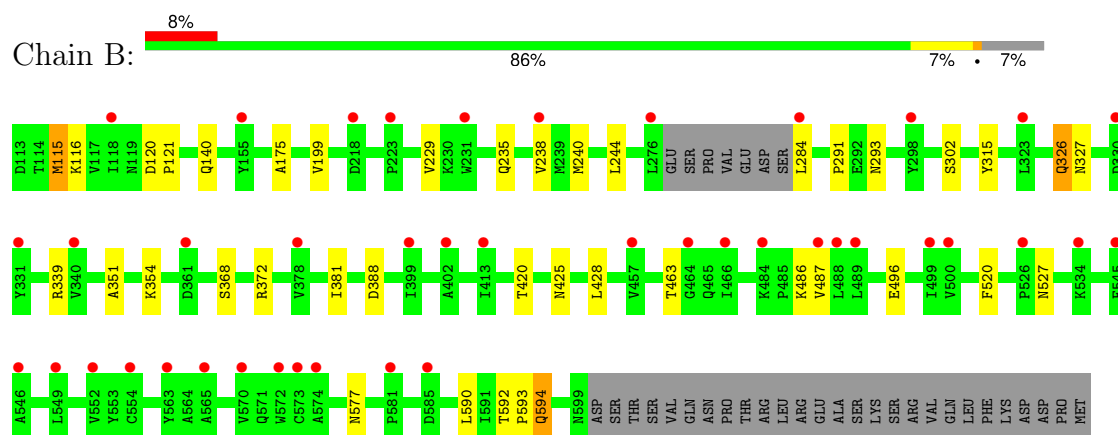
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

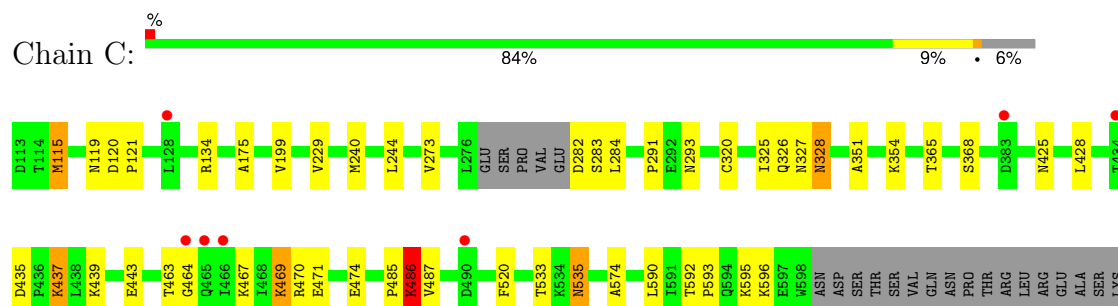
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



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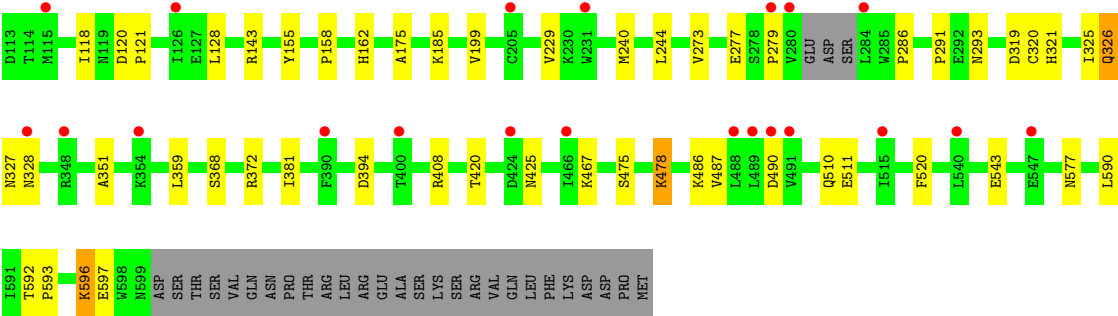
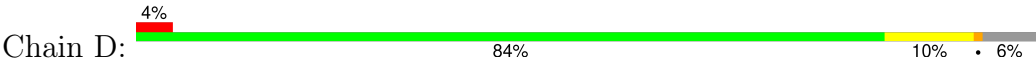


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



SER
ARG
VAL
GLN
LEU
PHE
LYS
ASP
PRO
MET

● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.20Å 141.59Å 98.19Å 90.00° 115.79° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 50.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.55) 96.0 (50.00-2.55)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.221 , 0.235 0.233 , 0.245	Depositor DCC
R_{free} test set	3206 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.877	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16149	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DCP, DTP, GTP, MG

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	0.72	1/4014 (0.0%)	0.88	1/5418 (0.0%)
1	B	0.71	0/4016	0.87	1/5421 (0.0%)
1	C	0.84	1/4036 (0.0%)	0.90	1/5448 (0.0%)
1	D	0.74	0/4054	0.85	0/5473
All	All	0.75	2/16120 (0.0%)	0.88	3/21760 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	GLN	CA-C	6.29	1.60	1.52
1	C	464	GLY	C-O	5.46	1.31	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	THR	N-CA-C	-7.32	104.47	113.41
1	C	463	THR	N-CA-C	6.24	118.88	108.96
1	A	326	GLN	CB-CA-C	5.40	118.66	109.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3922	0	3915	41	0
1	B	3924	0	3915	35	0
1	C	3944	0	3927	49	0
1	D	3961	0	3950	31	0
2	A	28	0	12	1	0
2	B	28	0	12	1	0
2	C	56	0	24	1	0
2	D	56	0	24	1	0
3	A	30	0	12	0	0
3	B	30	0	12	1	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	C	64	0	24	0	0
5	D	64	0	24	0	0
6	A	7	0	0	4	0
6	B	6	0	0	1	0
6	C	22	0	0	1	0
6	D	3	0	0	1	0
All	All	16149	0	15851	138	0

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

All (138) 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:C:574:ALA:O	1:C:595:LYS:NZ	1.67	1.26
1:B:115:MET:HE2	1:B:115:MET:C	1.60	1.24
1:B:115:MET:HE2	1:B:116:LYS:N	1.55	1.21
2:B:701:DCP:N3	6:B:801:HOH:O	1.91	1.01
1:B:115:MET:HE1	1:B:116:LYS:C	1.86	0.99
1:C:328:ASN:ND2	1:C:365:THR:OG1	1.96	0.99
1:C:439:LYS:O	1:C:443:GLU:HG3	1.63	0.96
1:B:115:MET:CE	1:B:116:LYS:C	2.41	0.93
1:C:435:ASP:OD1	1:C:437:LYS:HG2	1.69	0.93
1:C:533:THR:OG1	1:C:535[A]:ASN:ND2	2.03	0.92
1:B:115:MET:HE1	1:B:116:LYS:O	1.70	0.91
1:B:115:MET:C	1:B:115:MET:CE	2.44	0.89
1:B:115:MET:HE2	1:B:116:LYS:CA	2.03	0.88
1:B:115:MET:CE	1:B:116:LYS:N	2.35	0.88
1:C:435:ASP:CG	1:C:437:LYS:HG3	1.98	0.88
1:C:535[A]:ASN:HD22	1:C:535[A]:ASN:H	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ASP:CG	1:C:437:LYS:CG	2.52	0.83
1:B:115:MET:CE	1:B:116:LYS:O	2.28	0.82
1:C:467:LYS:CE	1:C:469:LYS:HE3	2.12	0.80
1:C:485:PRO:O	1:C:486:LYS:HB2	1.81	0.79
1:A:326:GLN:NE2	1:C:326:GLN:HE21	1.81	0.77
1:C:435:ASP:OD2	1:C:437:LYS:HD2	1.85	0.76
1:A:326:GLN:NE2	1:C:326:GLN:NE2	2.33	0.75
1:C:435:ASP:OD1	1:C:437:LYS:CG	2.33	0.75
1:C:535[A]:ASN:HD22	1:C:535[A]:ASN:N	1.86	0.73
1:A:326:GLN:HE22	1:C:326:GLN:NE2	1.86	0.72
1:A:326:GLN:HE22	1:C:326:GLN:HE21	1.37	0.72
1:C:467:LYS:HE2	1:C:469:LYS:HE3	1.70	0.72
1:A:327:ASN:O	1:C:326:GLN:HB2	1.92	0.70
1:A:140:GLN:HG3	1:A:240:MET:CE	2.21	0.70
1:B:594:GLN:N	1:B:594:GLN:OE1	2.25	0.70
1:B:372:ARG:HH22	1:D:328:ASN:HD21	1.39	0.69
1:D:596:LYS:HE2	1:D:597:GLU:OE1	1.93	0.68
1:B:140:GLN:HG3	1:B:240:MET:CE	2.25	0.67
1:B:425:ASN:ND2	1:C:425:ASN:OD1	2.30	0.64
1:C:470:ARG:HB2	1:C:470:ARG:CZ	2.27	0.64
1:B:327:ASN:O	1:D:326:GLN:HB2	1.96	0.64
1:C:574:ALA:C	1:C:595:LYS:NZ	2.56	0.62
1:B:326:GLN:HB2	1:D:327:ASN:O	2.01	0.61
1:A:331:TYR:OH	6:A:801:HOH:O	2.13	0.61
1:B:339:ARG:HH11	1:B:527:ASN:HD21	1.47	0.60
1:A:425:ASN:OD1	1:D:425:ASN:ND2	2.34	0.60
1:C:435:ASP:OD2	1:C:437:LYS:CD	2.49	0.59
1:C:435:ASP:OD2	1:C:437:LYS:CG	2.51	0.58
1:A:405:LYS:HD3	1:A:407:TYR:OH	2.04	0.58
1:A:331:TYR:C	1:A:331:TYR:CD1	2.83	0.57
1:C:574:ALA:C	1:C:595:LYS:HZ2	2.13	0.56
1:A:140:GLN:CG	1:A:240:MET:CE	2.84	0.56
1:B:487:VAL:HG23	1:B:590:LEU:HD12	1.89	0.55
1:D:487:VAL:HG23	1:D:590:LEU:HD12	1.89	0.54
1:A:326:GLN:HE21	1:A:327:ASN:H	1.55	0.54
1:B:115:MET:CE	1:B:116:LYS:CA	2.75	0.54
1:C:487:VAL:HG23	1:C:590:LEU:HD12	1.89	0.54
1:A:326:GLN:HE21	1:A:327:ASN:N	2.05	0.53
1:B:339:ARG:HH11	1:B:527:ASN:ND2	2.06	0.53
1:C:485:PRO:O	1:C:486:LYS:CB	2.51	0.53
1:D:162:HIS:HE1	1:D:319:ASP:OD1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLN:CG	1:B:240:MET:CE	2.87	0.52
1:A:228:GLU:OE1	1:A:228:GLU:N	2.41	0.51
1:A:355:GLU:OE1	6:A:806:HOH:O	2.19	0.51
1:C:469:LYS:HB3	1:C:471:GLU:OE1	2.11	0.51
1:A:140:GLN:CG	1:A:240:MET:HE3	2.41	0.51
1:A:377:LYS:HE2	6:D:801:HOH:O	2.10	0.51
1:B:235:GLN:O	1:B:238:VAL:HG22	2.11	0.50
1:A:116:LYS:NZ	6:A:805:HOH:O	2.44	0.50
1:A:146:TYR:HH	1:D:155:TYR:HH	1.59	0.49
1:C:435:ASP:OD2	1:C:437:LYS:HG3	2.10	0.49
1:C:467:LYS:HE3	1:C:469:LYS:HE3	1.93	0.49
1:A:352:ARG:CZ	1:A:354:LYS:HD3	2.43	0.49
1:D:511:GLU:H	1:D:511:GLU:CD	2.22	0.48
1:C:244:LEU:C	1:C:244:LEU:HD23	2.39	0.48
1:A:146:TYR:OH	1:D:155:TYR:OH	2.30	0.48
1:B:140:GLN:CG	1:B:240:MET:HE3	2.44	0.48
1:C:535[A]:ASN:ND2	1:C:535[A]:ASN:N	2.56	0.48
1:A:240:MET:HE1	1:A:420:THR:OG1	2.14	0.48
1:D:394:ASP:O	1:D:408:ARG:HD2	2.14	0.48
1:B:240:MET:HE1	1:B:420:THR:OG1	2.14	0.48
1:C:467:LYS:CE	1:C:469:LYS:CE	2.90	0.47
1:B:120:ASP:OD1	1:B:121:PRO:HD2	2.15	0.47
1:D:244:LEU:C	1:D:244:LEU:HD23	2.39	0.47
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.47
1:C:592:THR:N	1:C:593:PRO:CD	2.78	0.47
1:D:351:ALA:O	1:D:520:PHE:HA	2.15	0.47
1:A:321:HIS:CE1	1:D:321:HIS:CE1	3.03	0.46
1:A:405:LYS:HD3	1:A:407:TYR:CZ	2.50	0.46
1:A:244:LEU:C	1:A:244:LEU:HD23	2.40	0.46
1:A:522:CYS:HB3	6:A:804:HOH:O	2.16	0.46
1:C:467:LYS:HE3	1:C:469:LYS:CE	2.46	0.46
1:B:244:LEU:C	1:B:244:LEU:HD23	2.41	0.46
1:B:351:ALA:O	1:B:520:PHE:HA	2.16	0.45
1:D:475:SER:HA	1:D:478:LYS:HE2	1.98	0.45
1:B:326:GLN:O	1:D:328:ASN:ND2	2.49	0.45
1:A:592:THR:N	1:A:593:PRO:CD	2.79	0.45
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.90	0.45
1:B:592:THR:N	1:B:593:PRO:CD	2.79	0.45
1:D:279:PRO:HG3	1:D:286:PRO:HB3	1.99	0.45
1:A:293:ASN:OD1	1:A:293:ASN:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ILE:HD12	1:D:128:LEU:HD11	1.98	0.44
1:A:118:ILE:HD12	1:A:128:LEU:HD11	2.00	0.44
1:D:118:ILE:HD13	1:D:118:ILE:HG21	1.79	0.44
1:C:115:MET:HE3	1:C:115:MET:HB2	1.93	0.44
1:A:328:ASN:ND2	1:C:326:GLN:O	2.51	0.44
1:B:327:ASN:O	1:D:326:GLN:CB	2.63	0.44
1:B:428:LEU:HD13	1:C:425:ASN:HB2	2.00	0.44
1:D:120:ASP:OD2	1:D:121:PRO:HD2	2.17	0.44
1:A:598:TRP:O	1:A:599:ASN:HB2	2.18	0.43
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.17	0.43
1:A:118:ILE:HG21	1:A:118:ILE:HD13	1.80	0.43
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.19	0.43
1:B:175:ALA:HB1	1:B:199:VAL:HG12	2.00	0.43
1:C:437:LYS:HB3	1:C:437:LYS:HE2	1.82	0.43
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.19	0.43
1:A:351:ALA:O	1:A:520:PHE:HA	2.19	0.43
2:A:701:DCP:O2G	2:A:701:DCP:O2B	2.36	0.43
1:C:119:ASN:HB2	2:D:702:DCP:H1'	2.00	0.43
1:C:120:ASP:OD2	1:C:121:PRO:HD2	2.17	0.43
1:C:535[A]:ASN:ND2	1:C:535[A]:ASN:H	2.01	0.43
1:A:158:PRO:HG3	1:D:118:ILE:HG21	2.00	0.42
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.18	0.42
1:A:120:ASP:OD2	1:A:121:PRO:HD2	2.18	0.42
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.92	0.42
1:A:326:GLN:CG	1:C:327:ASN:O	2.68	0.42
1:A:455:LYS:CB	1:A:562:LEU:HD21	2.50	0.42
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.02	0.42
1:C:320:CYS:HB3	1:C:325:ILE:O	2.19	0.42
1:B:425:ASN:HB2	1:C:428:LEU:HD13	2.01	0.42
1:A:118:ILE:HG21	1:D:158:PRO:HG3	2.02	0.42
1:D:467:LYS:HD3	1:D:467:LYS:HA	1.91	0.41
2:C:705:DCP:H5'1	6:C:816:HOH:O	2.20	0.41
1:D:143:ARG:HD2	1:D:420:THR:HA	2.03	0.41
3:B:702:DTP:N6	1:D:372:ARG:HG2	2.36	0.41
1:D:320:CYS:HB3	1:D:325:ILE:O	2.21	0.41
1:A:331:TYR:CD1	1:A:332:LYS:N	2.89	0.40
1:C:467:LYS:HG2	1:C:469:LYS:CD	2.52	0.40
1:B:115:MET:HE2	1:B:115:MET:O	2.07	0.40
1:A:175:ALA:HB1	1:A:199:VAL:HG12	2.03	0.40
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/514 (93%)	469 (98%)	7 (2%)	0	100	100
1	B	476/514 (93%)	465 (98%)	11 (2%)	0	100	100
1	C	479/514 (93%)	467 (98%)	11 (2%)	1 (0%)	43	56
1	D	481/514 (94%)	470 (98%)	11 (2%)	0	100	100
All	All	1912/2056 (93%)	1871 (98%)	40 (2%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	LYS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/459 (93%)	415 (97%)	11 (3%)	40	59
1	B	426/459 (93%)	413 (97%)	13 (3%)	35	53
1	C	429/459 (94%)	410 (96%)	19 (4%)	25	38
1	D	431/459 (94%)	416 (96%)	15 (4%)	32	48
All	All	1712/1836 (93%)	1654 (97%)	58 (3%)	33	48

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	185	LYS
1	A	229	VAL
1	A	315	TYR
1	A	354	LYS
1	A	368	SER
1	A	447	GLN
1	A	478	LYS
1	A	534	LYS
1	A	539	GLN
1	A	540	LEU
1	B	115	MET
1	B	229	VAL
1	B	284	LEU
1	B	302	SER
1	B	315	TYR
1	B	326	GLN
1	B	354	LYS
1	B	368	SER
1	B	388	ASP
1	B	486	LYS
1	B	496	GLU
1	B	577	ASN
1	B	594	GLN
1	C	115	MET
1	C	134	ARG
1	C	229	VAL
1	C	240	MET
1	C	273	VAL
1	C	282	ASP
1	C	283	SER
1	C	284	LEU
1	C	328	ASN
1	C	354	LYS
1	C	368[A]	SER
1	C	368[B]	SER
1	C	437	LYS
1	C	469	LYS
1	C	474	GLU
1	C	486	LYS
1	C	535[A]	ASN
1	C	535[B]	ASN
1	C	596	LYS

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Mol	Chain	Res	Type
1	D	185	LYS
1	D	229	VAL
1	D	240	MET
1	D	273	VAL
1	D	277	GLU
1	D	326	GLN
1	D	359	LEU
1	D	368	SER
1	D	478	LYS
1	D	486	LYS
1	D	490	ASP
1	D	510	GLN
1	D	543	GLU
1	D	577	ASN
1	D	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	210	HIS
1	A	233	HIS
1	A	243	HIS
1	A	326	GLN
1	A	328	ASN
1	A	364	HIS
1	A	367	ASN
1	A	370	HIS
1	A	375	GLN
1	A	380	ASN
1	A	567	GLN
1	A	571	GLN
1	A	594	GLN
1	B	200	GLN
1	B	322	HIS
1	B	364	HIS
1	B	367	ASN
1	B	370	HIS
1	B	375	GLN
1	B	380	ASN
1	B	425	ASN
1	B	527	ASN

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Mol	Chain	Res	Type
1	B	539	GLN
1	B	571	GLN
1	B	599	ASN
1	C	149	GLN
1	C	210	HIS
1	C	235	GLN
1	C	243	HIS
1	C	248	ASN
1	C	322	HIS
1	C	326	GLN
1	C	367	ASN
1	C	370	HIS
1	C	375	GLN
1	C	380	ASN
1	C	510	GLN
1	C	539	GLN
1	C	571	GLN
1	C	594	GLN
1	D	162	HIS
1	D	200	GLN
1	D	210	HIS
1	D	233	HIS
1	D	235	GLN
1	D	243	HIS
1	D	248	ASN
1	D	322	HIS
1	D	328	ASN
1	D	367	ASN
1	D	370	HIS
1	D	375	GLN
1	D	380	ASN
1	D	425	ASN
1	D	594	GLN
1	D	599	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	D	701	4	33,34,34	1.36	5 (15%)	50,54,54	1.84	13 (26%)
2	DCP	D	702	4	28,29,29	1.19	2 (7%)	41,45,45	1.13	3 (7%)
2	DCP	B	701	-	28,29,29	0.95	1 (3%)	41,45,45	1.08	2 (4%)
2	DCP	C	705	-	28,29,29	1.18	2 (7%)	41,45,45	0.95	2 (4%)
5	GTP	C	704	4	33,34,34	1.28	5 (15%)	50,54,54	1.62	8 (16%)
2	DCP	A	701	-	28,29,29	1.17	2 (7%)	41,45,45	0.90	1 (2%)
5	GTP	D	704	4	33,34,34	1.37	6 (18%)	50,54,54	1.55	7 (14%)
2	DCP	D	703	-	28,29,29	1.19	4 (14%)	41,45,45	0.90	0
2	DCP	C	701	4	28,29,29	1.29	4 (14%)	41,45,45	1.10	2 (4%)
3	DTP	A	702	4	31,32,32	1.76	6 (19%)	46,50,50	1.65	9 (19%)
3	DTP	B	702	4	31,32,32	1.81	7 (22%)	46,50,50	1.61	7 (15%)
5	GTP	C	706	4	33,34,34	1.76	5 (15%)	50,54,54	1.60	8 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	701	4	-	4/22/38/38	0/3/3/3
2	DCP	D	702	4	-	6/22/34/34	0/2/2/2
2	DCP	B	701	-	-	7/22/34/34	0/2/2/2
2	DCP	C	705	-	-	3/22/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	704	4	-	2/22/38/38	0/3/3/3
2	DCP	A	701	-	-	8/22/34/34	0/2/2/2
5	GTP	D	704	4	-	3/22/38/38	0/3/3/3
2	DCP	D	703	-	-	4/22/34/34	0/2/2/2
2	DCP	C	701	4	-	2/22/34/34	0/2/2/2
3	DTP	A	702	4	-	6/22/34/34	0/3/3/3
3	DTP	B	702	4	-	5/22/34/34	0/3/3/3
5	GTP	C	706	4	-	3/22/38/38	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	706	GTP	PA-O3A	5.49	1.65	1.59
3	A	702	DTP	C5-C4	5.47	1.48	1.39
3	B	702	DTP	C5-C4	5.26	1.48	1.39
5	C	706	GTP	PB-O3A	4.53	1.64	1.59
3	A	702	DTP	C5-N7	-3.84	1.32	1.39
2	C	705	DCP	PB-O3B	3.81	1.63	1.59
3	B	702	DTP	PA-O3A	3.79	1.63	1.59
2	D	702	DCP	PA-O3A	3.69	1.63	1.59
5	D	701	GTP	C5-N7	-3.49	1.32	1.39
3	A	702	DTP	C8-N7	3.45	1.38	1.31
5	C	704	GTP	C6-N1	-3.37	1.32	1.38
5	D	704	GTP	PA-O3A	3.34	1.63	1.59
3	B	702	DTP	C5-N7	-3.33	1.33	1.39
5	D	704	GTP	C5-C4	3.33	1.47	1.38
5	C	706	GTP	C5-N7	-3.14	1.32	1.39
2	A	701	DCP	PA-O3A	3.10	1.62	1.59
5	C	706	GTP	C5-C4	3.05	1.47	1.38
5	D	701	GTP	C5-C4	3.05	1.47	1.38
2	C	701	DCP	PB-O3B	3.04	1.62	1.59
5	D	701	GTP	C4-N9	-3.03	1.30	1.38
5	D	704	GTP	PB-O3A	3.03	1.62	1.59
5	C	704	GTP	C5-C4	2.91	1.46	1.38
2	A	701	DCP	PB-O3B	2.82	1.62	1.59
5	C	704	GTP	C5-N7	-2.79	1.33	1.39
2	B	701	DCP	PA-O3A	2.77	1.62	1.59
2	D	703	DCP	PB-O3B	2.75	1.62	1.59
3	B	702	DTP	C4-N9	-2.75	1.32	1.37
3	A	702	DTP	C2-N1	2.66	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	DCP	PA-O3A	2.65	1.62	1.59
5	C	704	GTP	PA-O3A	2.64	1.62	1.59
3	B	702	DTP	PB-O3B	2.61	1.62	1.59
5	D	704	GTP	C6-N1	-2.60	1.34	1.38
5	C	706	GTP	C6-N1	-2.57	1.34	1.38
2	C	701	DCP	PA-O3A	2.53	1.62	1.59
3	A	702	DTP	C4-N9	-2.51	1.32	1.37
5	D	701	GTP	PB-O3A	2.48	1.62	1.59
5	D	701	GTP	PA-O3A	2.47	1.62	1.59
2	D	703	DCP	C5-C4	-2.40	1.37	1.42
2	C	705	DCP	C5-C4	-2.37	1.37	1.42
5	D	704	GTP	C5-N7	-2.36	1.34	1.39
2	D	703	DCP	PB-O3A	2.34	1.62	1.59
3	B	702	DTP	C8-N7	2.28	1.36	1.31
2	C	701	DCP	O4'-C4'	-2.27	1.39	1.45
3	B	702	DTP	C5-C6	2.15	1.47	1.41
5	D	704	GTP	C4-N9	-2.15	1.32	1.38
2	C	701	DCP	C5-C4	-2.12	1.38	1.42
2	D	702	DCP	C6-C5	2.08	1.39	1.35
3	A	702	DTP	O4'-C4'	-2.02	1.40	1.45
5	C	704	GTP	C4-N9	-2.02	1.32	1.38

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	704	GTP	C5-C4-N3	-5.52	119.61	128.39
5	D	704	GTP	C5-C4-N3	-5.34	119.89	128.39
5	D	701	GTP	C5-C4-N3	-5.28	119.99	128.39
5	C	706	GTP	C5-C4-N3	-5.06	120.34	128.39
3	A	702	DTP	N6-C6-N1	4.49	128.37	118.38
5	D	704	GTP	C2-N3-C4	4.44	119.95	112.30
3	B	702	DTP	C5-C4-N3	-4.28	120.82	126.72
5	D	701	GTP	N9-C4-N3	4.21	134.37	125.95
5	C	704	GTP	C2-N3-C4	4.20	119.54	112.30
5	C	704	GTP	N9-C4-N3	4.03	134.01	125.95
3	B	702	DTP	N3-C4-N9	4.03	134.02	127.17
5	D	701	GTP	C2-N3-C4	4.01	119.20	112.30
5	D	701	GTP	O6-C6-C5	-3.99	116.01	126.53
5	D	704	GTP	N9-C4-N3	3.86	133.67	125.95
3	B	702	DTP	N3-C2-N1	-3.73	122.94	128.58
3	A	702	DTP	C5-C4-N3	-3.71	121.60	126.72
5	C	706	GTP	N9-C4-N3	3.71	133.37	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	706	GTP	C2-N3-C4	3.69	118.66	112.30
3	B	702	DTP	C2-N3-C4	3.43	120.20	111.83
3	A	702	DTP	N3-C4-N9	3.40	132.95	127.17
3	A	702	DTP	C5-C6-N6	-3.37	114.94	123.29
5	C	704	GTP	C6-C5-N7	3.31	136.32	130.29
5	D	704	GTP	C6-C5-N7	3.28	136.26	130.29
5	D	701	GTP	N2-C2-N3	-3.27	113.28	119.67
2	B	701	DCP	O4'-C1'-N1	3.18	113.50	107.86
3	A	702	DTP	O4'-C1'-N9	-3.06	102.46	107.96
3	B	702	DTP	N6-C6-N1	2.96	124.97	118.38
5	D	701	GTP	O6-C6-N1	2.89	125.55	120.11
5	C	706	GTP	C6-C5-N7	2.83	135.44	130.29
5	D	701	GTP	N2-C2-N1	2.82	122.72	116.76
2	D	702	DCP	O4'-C1'-N1	2.74	112.72	107.86
5	D	704	GTP	C3'-C2'-C1'	2.72	106.61	101.46
2	B	701	DCP	O3G-PG-O2G	2.69	117.90	107.80
5	D	701	GTP	O2B-PB-O1B	2.64	124.70	112.44
5	C	706	GTP	C4-C5-N7	-2.61	106.54	110.67
3	A	702	DTP	O3G-PG-O1G	2.60	120.96	110.83
5	C	706	GTP	C3'-C2'-C1'	2.60	106.38	101.46
2	D	702	DCP	O2A-PA-O1A	2.57	124.41	112.44
2	C	701	DCP	O3G-PG-O2G	2.54	117.31	107.80
3	B	702	DTP	C5-C6-N6	-2.46	117.20	123.29
2	C	705	DCP	N4-C4-N3	2.43	122.25	117.91
3	A	702	DTP	C4-N9-C8	2.42	108.27	105.74
2	C	705	DCP	C5-C4-N4	-2.41	116.42	120.63
3	B	702	DTP	C4-N9-C8	2.36	108.22	105.74
5	D	701	GTP	O3A-PB-O1B	-2.35	103.64	110.70
5	D	701	GTP	C6-C5-N7	2.33	134.54	130.29
2	C	701	DCP	C2'-C3'-C4'	2.32	107.51	102.80
5	C	704	GTP	C4-C5-N7	-2.31	107.02	110.67
2	D	702	DCP	O2-C2-N3	-2.30	118.70	122.33
5	D	704	GTP	C4-C5-N7	-2.29	107.04	110.67
5	D	704	GTP	O2A-PA-O1A	2.28	123.05	112.44
5	D	701	GTP	C2-N1-C6	-2.26	121.01	125.11
5	C	706	GTP	O2A-PA-O1A	2.23	122.80	112.44
3	A	702	DTP	C2-N3-C4	2.21	117.23	111.83
5	C	704	GTP	C5-C6-N1	2.20	118.85	113.25
5	D	701	GTP	O3G-PG-O2G	2.16	115.89	107.80
5	C	706	GTP	C8-N7-C5	2.13	108.06	104.26
5	C	704	GTP	O6-C6-C5	-2.05	121.13	126.53
5	C	704	GTP	O2B-PB-O1B	2.05	121.97	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	DTP	O2B-PB-O3A	2.04	112.79	107.27
5	D	701	GTP	C5'-C6'-N1	2.04	118.44	113.25
2	A	701	DCP	O4'-C1'-N1	2.04	111.48	107.86

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DCP	C5'-O5'-PA-O2A
2	B	701	DCP	C5'-O5'-PA-O1A
2	D	702	DCP	PB-O3B-PG-O2G
2	D	702	DCP	PB-O3B-PG-O3G
2	D	703	DCP	C5'-O5'-PA-O2A
3	A	702	DTP	PB-O3B-PG-O3G
3	B	702	DTP	PB-O3B-PG-O2G
3	B	702	DTP	PB-O3B-PG-O3G
2	A	701	DCP	C3'-C4'-C5'-O5'
2	A	701	DCP	O4'-C4'-C5'-O5'
2	B	701	DCP	C3'-C4'-C5'-O5'
2	B	701	DCP	O4'-C4'-C5'-O5'
3	A	702	DTP	PB-O3B-PG-O1G
2	A	701	DCP	C4'-C5'-O5'-PA
2	C	705	DCP	C4'-C5'-O5'-PA
2	D	703	DCP	C4'-C5'-O5'-PA
2	B	701	DCP	C4'-C5'-O5'-PA
2	A	701	DCP	PB-O3A-PA-O5'
2	B	701	DCP	PB-O3A-PA-O5'
2	C	705	DCP	PB-O3A-PA-O5'
2	D	703	DCP	PB-O3A-PA-O5'
5	D	701	GTP	PB-O3B-PG-O1G
3	A	702	DTP	PG-O3B-PB-O1B
2	A	701	DCP	C5'-O5'-PA-O3A
2	B	701	DCP	C5'-O5'-PA-O2A
2	B	701	DCP	C5'-O5'-PA-O3A
2	D	702	DCP	PG-O3B-PB-O1B
3	A	702	DTP	PB-O3A-PA-O2A
3	B	702	DTP	PB-O3A-PA-O2A
5	C	706	GTP	PG-O3B-PB-O2B
5	D	701	GTP	PG-O3B-PB-O2B
2	C	705	DCP	C3'-C4'-C5'-O5'
5	D	704	GTP	PG-O3B-PB-O1B
5	C	704	GTP	C4'-C5'-O5'-PA

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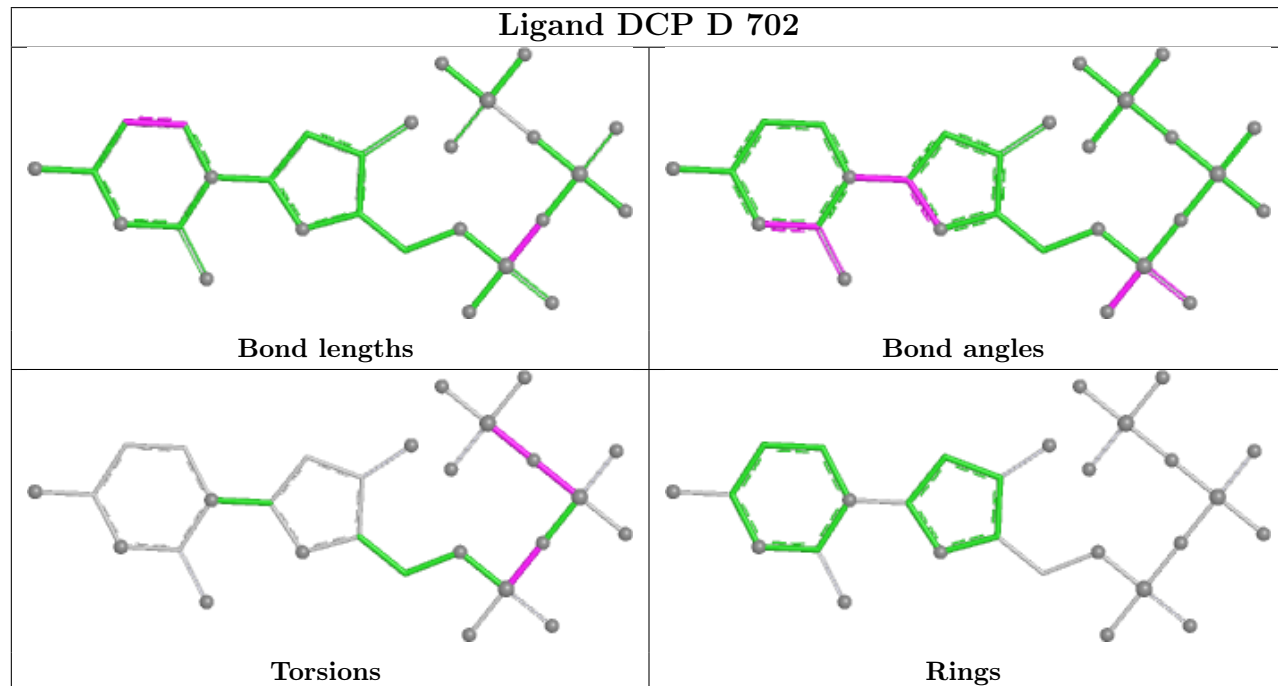
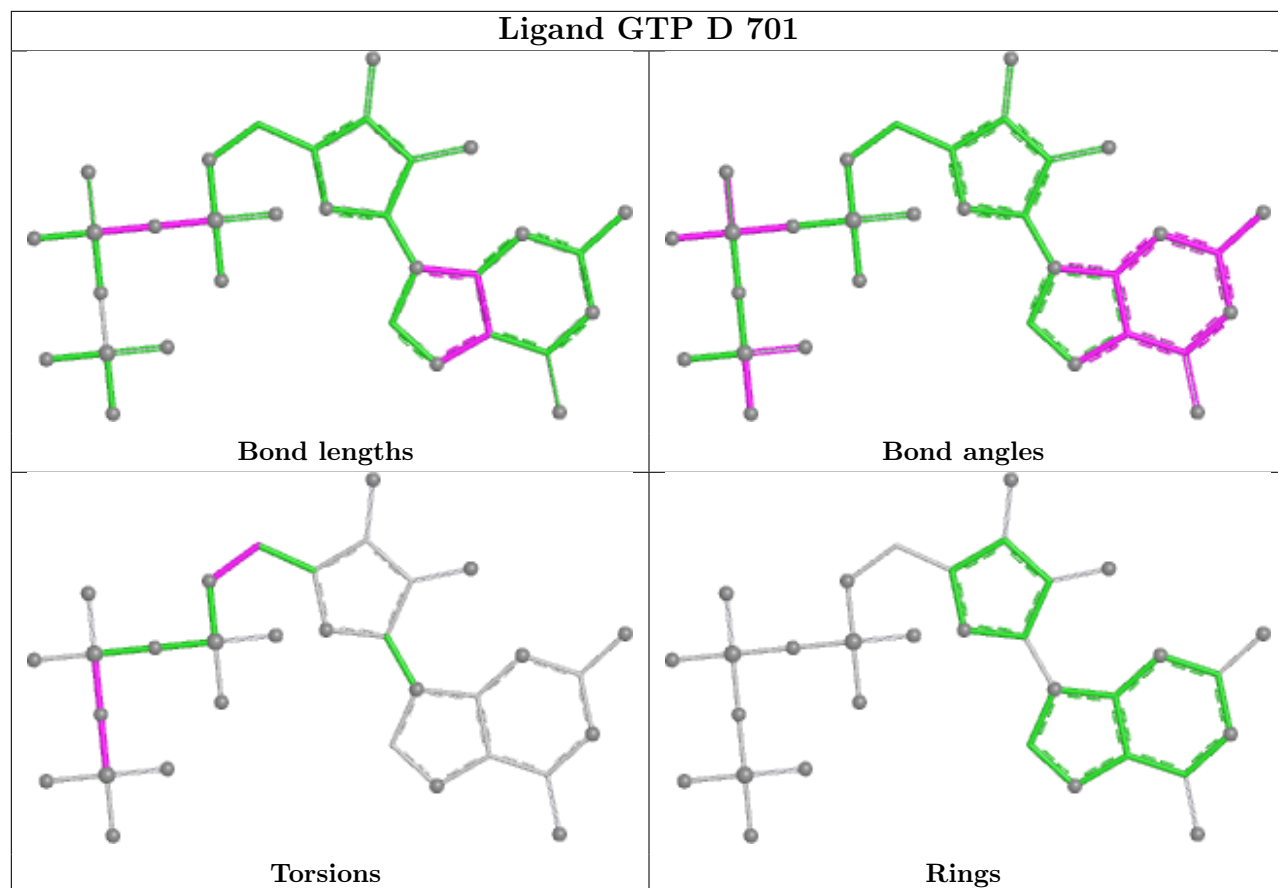
Mol	Chain	Res	Type	Atoms
5	C	706	GTP	C4'-C5'-O5'-PA
5	D	701	GTP	C4'-C5'-O5'-PA
5	D	704	GTP	C4'-C5'-O5'-PA
2	A	701	DCP	PG-O3B-PB-O1B
2	C	701	DCP	PA-O3A-PB-O2B
3	A	702	DTP	PB-O3A-PA-O1A
5	C	704	GTP	PG-O3B-PB-O1B
5	D	701	GTP	PG-O3B-PB-O1B
5	D	704	GTP	PB-O3A-PA-O2A
2	D	702	DCP	PB-O3B-PG-O1G
2	A	701	DCP	PG-O3B-PB-O2B
2	C	701	DCP	PG-O3B-PB-O2B
2	D	702	DCP	PB-O3A-PA-O2A
2	D	702	DCP	PG-O3B-PB-O2B
2	D	703	DCP	PG-O3B-PB-O2B
3	A	702	DTP	PG-O3B-PB-O2B
3	B	702	DTP	PG-O3B-PB-O1B
3	B	702	DTP	PG-O3B-PB-O2B
5	C	706	GTP	PB-O3A-PA-O2A

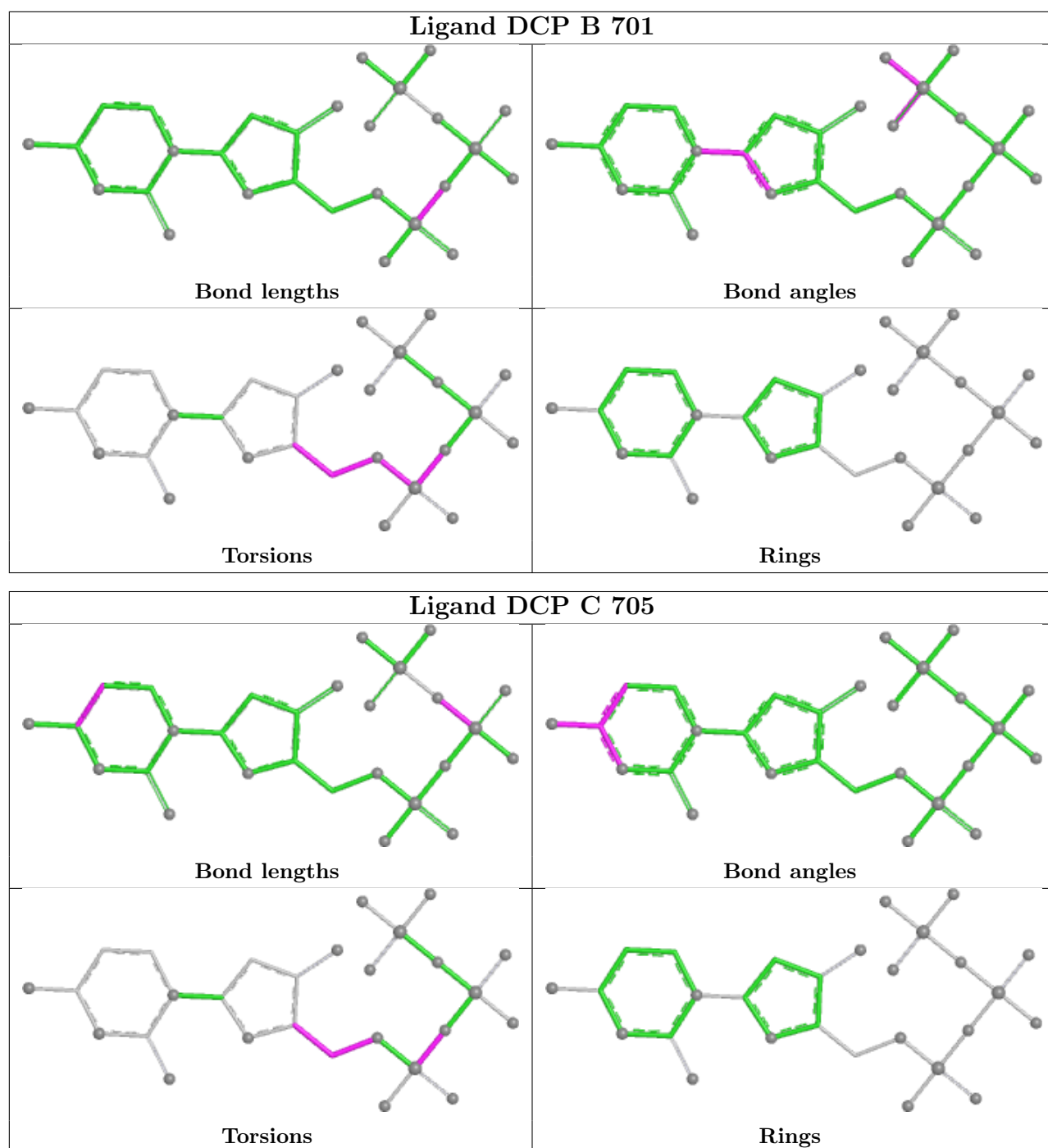
There are no ring outliers.

5 monomers are involved in 5 short contacts:

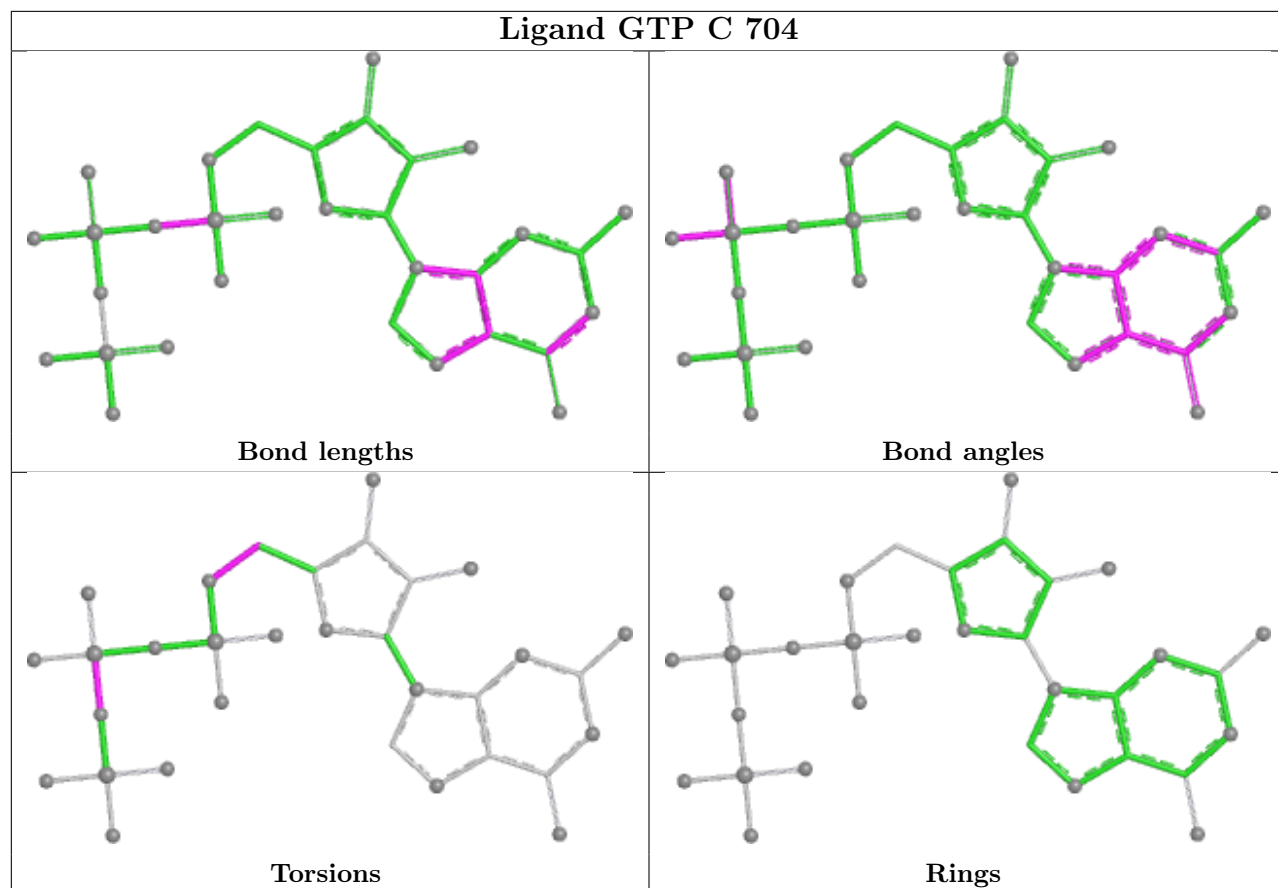
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	702	DCP	1	0
2	B	701	DCP	1	0
2	C	705	DCP	1	0
2	A	701	DCP	1	0
3	B	702	DTP	1	0

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

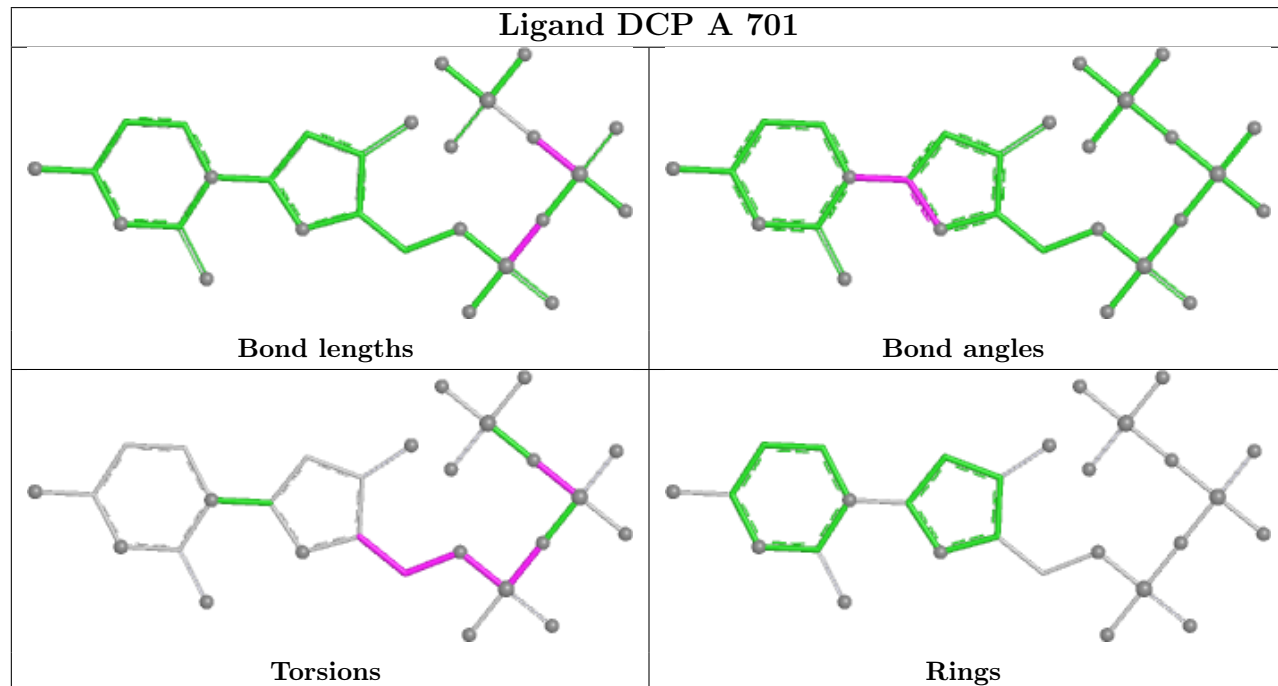


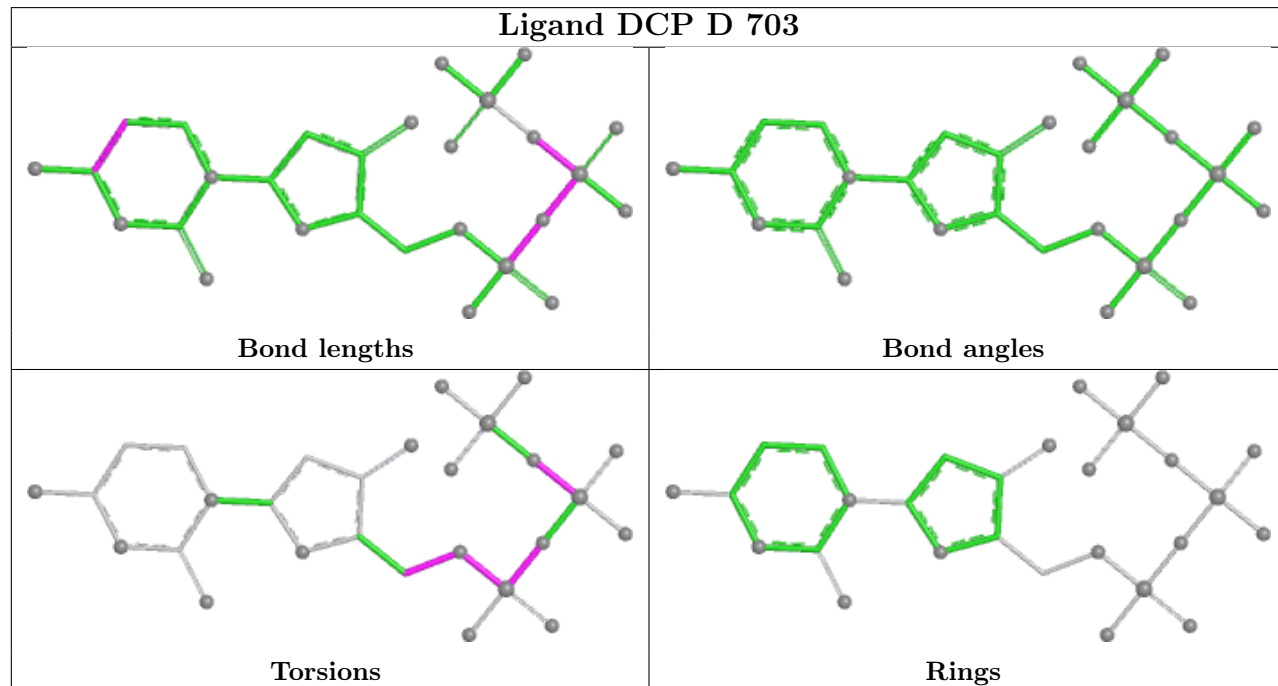
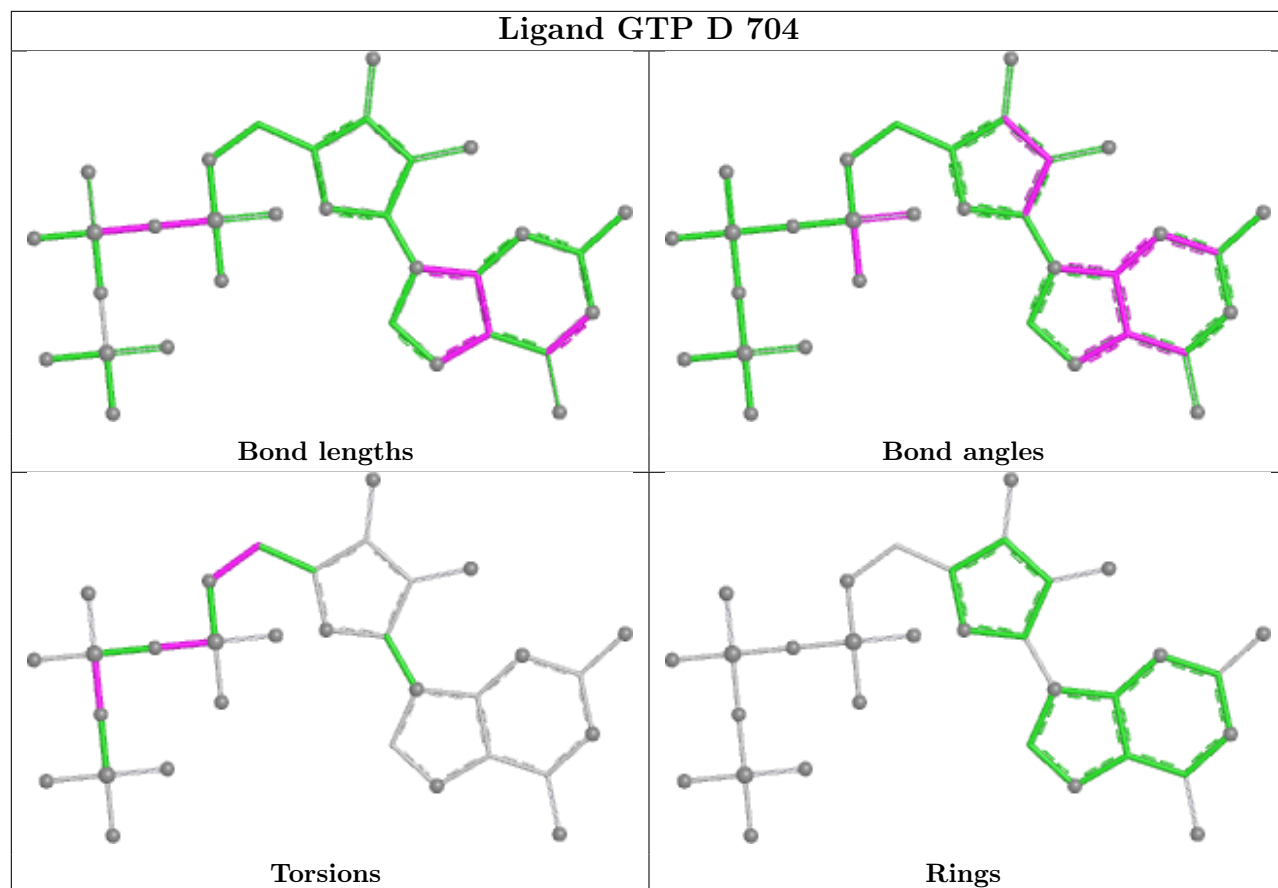


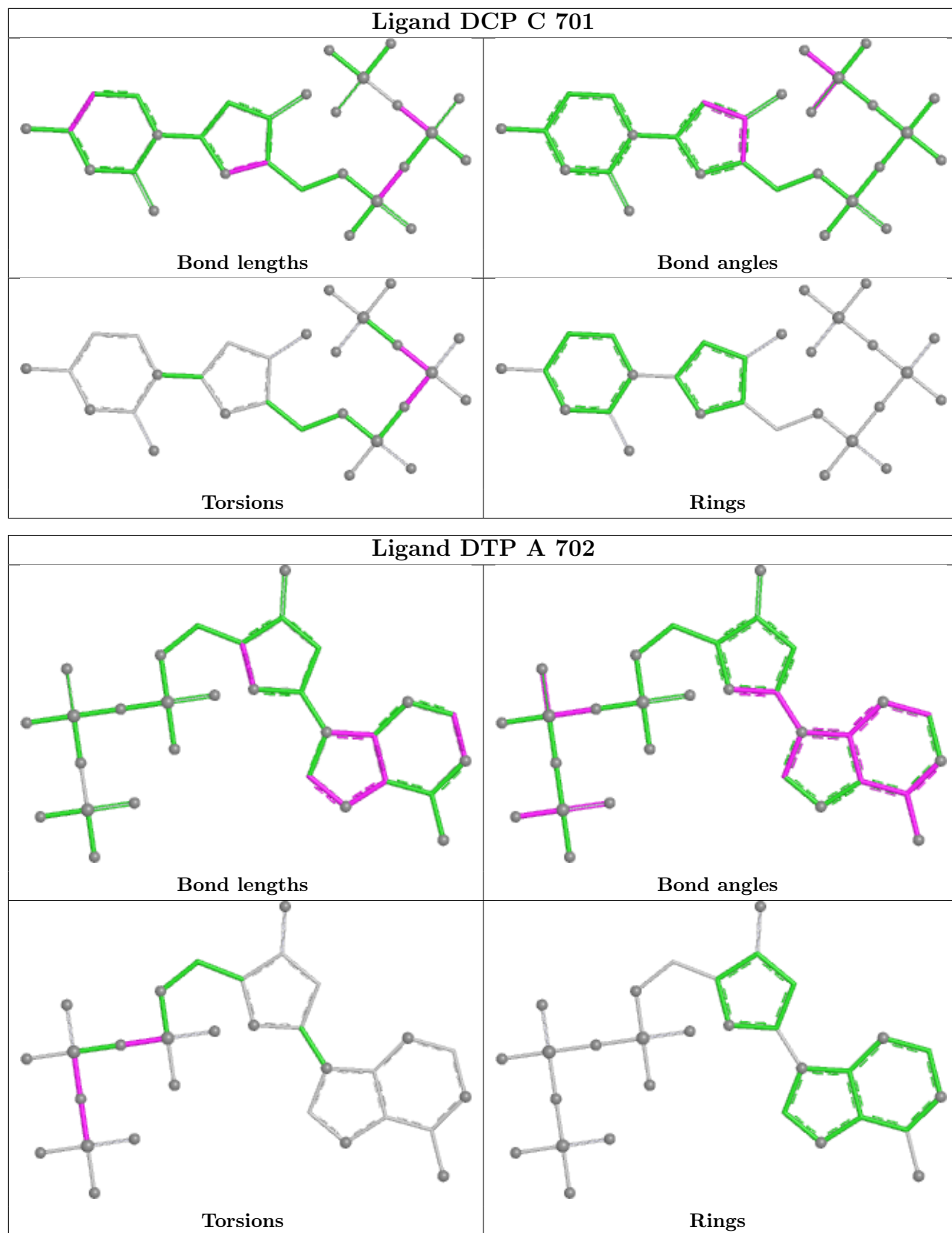
Ligand GTP C 704

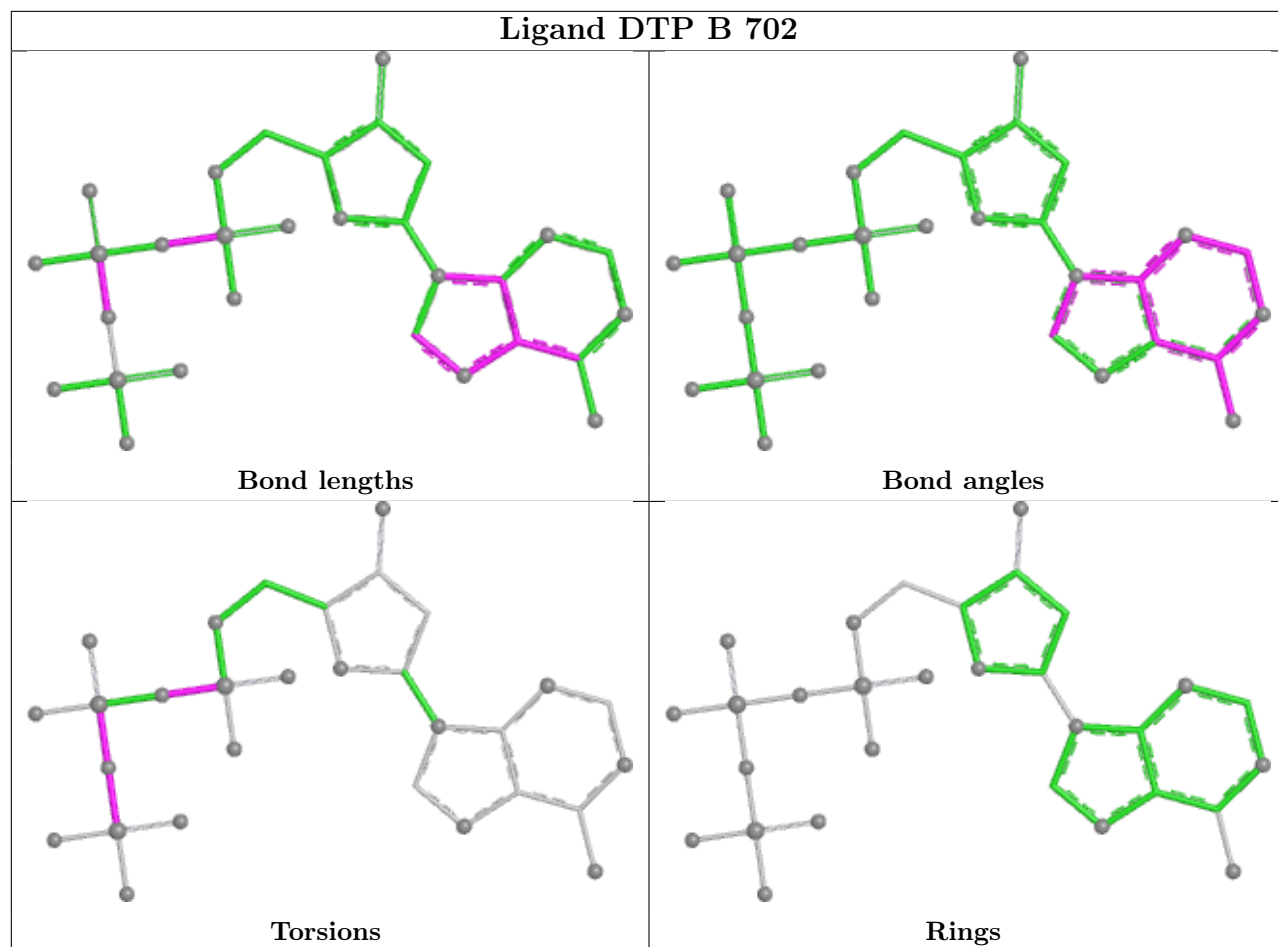


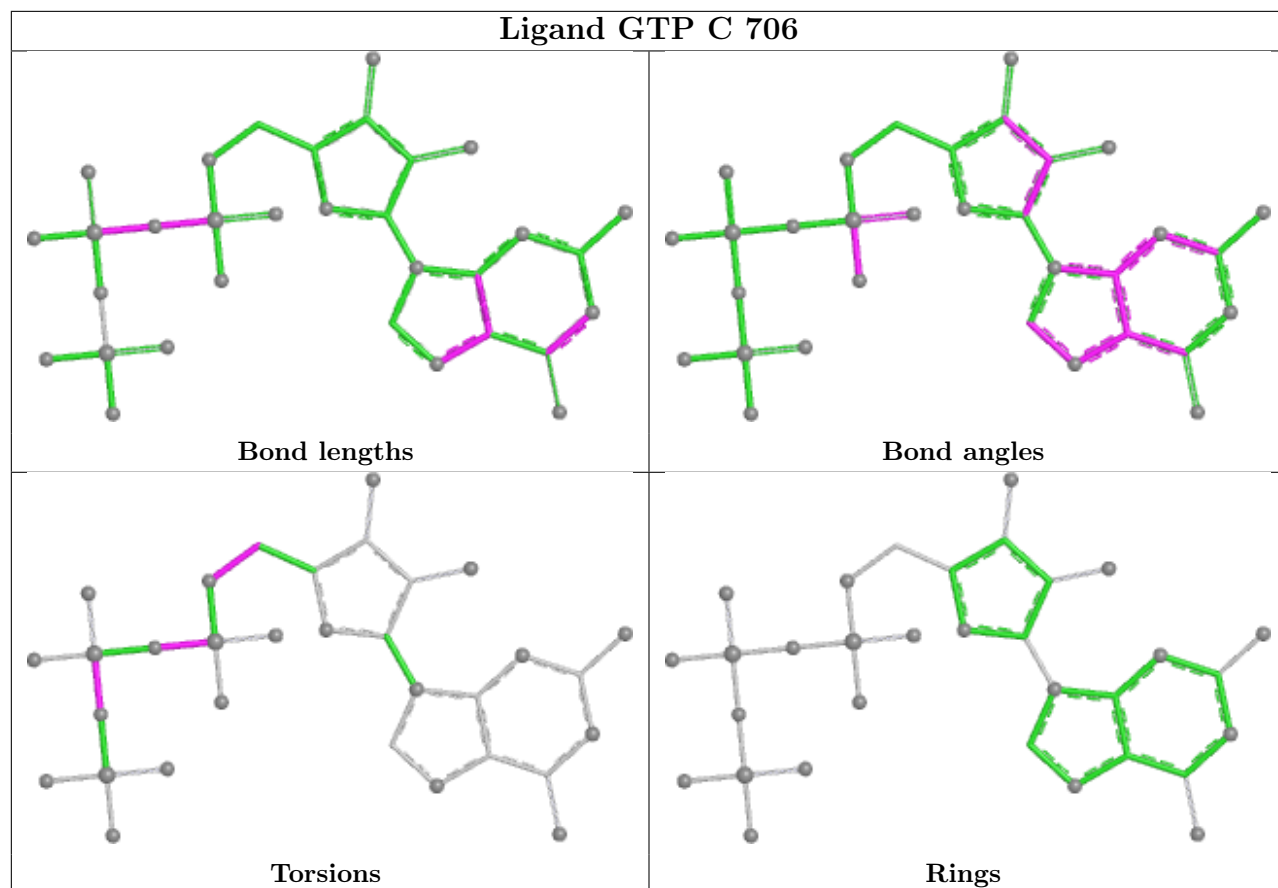
Ligand DCP A 701











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	479/514 (93%)	0.45	13 (2%) 56 57	25, 74, 123, 162	1 (0%)
1	B	480/514 (93%)	0.88	42 (8%) 15 15	38, 99, 174, 214	0
1	C	481/514 (93%)	0.32	7 (1%) 72 73	19, 62, 104, 153	2 (0%)
1	D	484/514 (94%)	0.50	21 (4%) 40 40	35, 76, 126, 181	1 (0%)
All	All	1924/2056 (93%)	0.54	83 (4%) 40 40	19, 76, 143, 214	4 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	ILE	4.4
1	B	284	LEU	3.5
1	B	378	VAL	3.3
1	B	223	PRO	3.3
1	D	284	LEU	3.3
1	B	276	LEU	3.2
1	A	554	CYS	3.2
1	B	585	ASP	3.1
1	B	457	VAL	3.1
1	D	490	ASP	3.1
1	D	488	LEU	3.0
1	B	464	GLY	2.9
1	D	115[A]	MET	2.9
1	B	554	CYS	2.8
1	D	126	ILE	2.8
1	D	280	VAL	2.8
1	B	572	TRP	2.7
1	A	172	GLY	2.7
1	A	413	ILE	2.7
1	D	354	LYS	2.7
1	B	340	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	490	ASP	2.6
1	B	413	ILE	2.6
1	A	327	ASN	2.6
1	D	424	ASP	2.6
1	B	488	LEU	2.6
1	A	328	ASN	2.6
1	B	573	CYS	2.5
1	A	388	ASP	2.5
1	B	231	TRP	2.5
1	B	526	PRO	2.4
1	A	296	PHE	2.4
1	B	570	VAL	2.4
1	C	464	GLY	2.4
1	C	466	ILE	2.4
1	D	491	VAL	2.4
1	B	402	ALA	2.4
1	C	383	ASP	2.3
1	B	552	VAL	2.3
1	B	546	ALA	2.3
1	D	390	PHE	2.3
1	B	238	VAL	2.3
1	B	298	TYR	2.3
1	B	487	VAL	2.3
1	D	540	LEU	2.3
1	B	218	ASP	2.3
1	D	547	GLU	2.3
1	B	581	PRO	2.3
1	A	463	THR	2.2
1	D	400	THR	2.2
1	B	489	LEU	2.2
1	D	489	LEU	2.2
1	B	500	VAL	2.2
1	B	155	TYR	2.2
1	C	465	GLN	2.2
1	B	499	ILE	2.2
1	A	378	VAL	2.2
1	D	328	ASN	2.2
1	B	484	LYS	2.2
1	B	399	ILE	2.2
1	B	545	PHE	2.2
1	C	434	THR	2.2
1	D	515	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	231	TRP	2.2
1	A	170	GLY	2.1
1	D	205	CYS	2.1
1	B	565	ALA	2.1
1	B	323	LEU	2.1
1	B	549	LEU	2.1
1	C	128	LEU	2.1
1	D	466	ILE	2.1
1	D	348	ARG	2.1
1	B	361	ASP	2.1
1	D	279	PRO	2.1
1	B	331	TYR	2.1
1	A	573	CYS	2.1
1	A	402	ALA	2.0
1	B	574	ALA	2.0
1	A	118	ILE	2.0
1	B	118	ILE	2.0
1	B	534	LYS	2.0
1	B	330	ASP	2.0
1	B	563	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

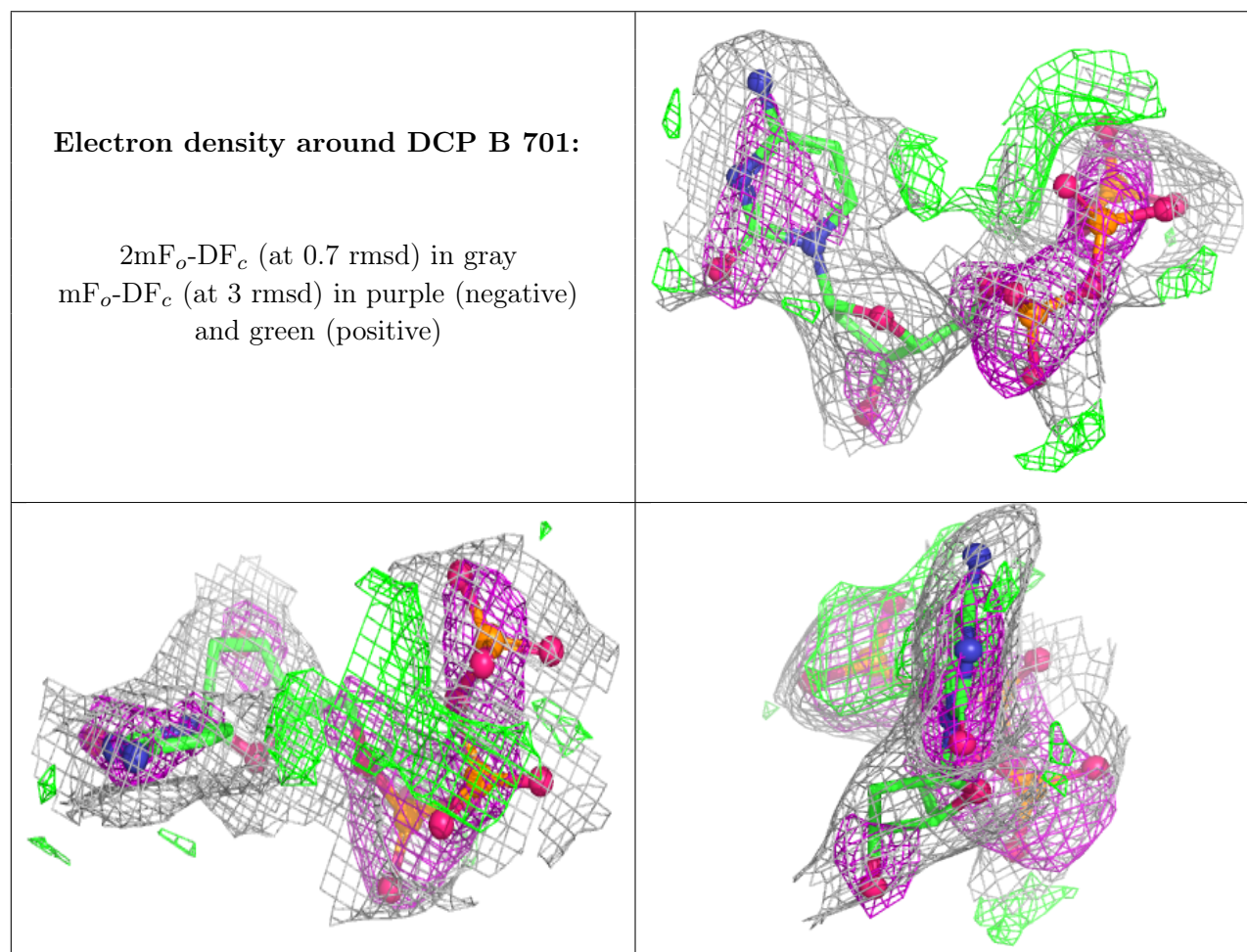
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DCP	B	701	28/28	0.76	0.14	28,40,55,57	0
5	GTP	C	704	32/32	0.80	0.12	20,23,28,31	0
2	DCP	D	703	28/28	0.85	0.11	32,39,58,64	0

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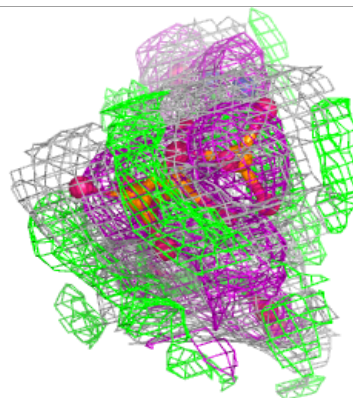
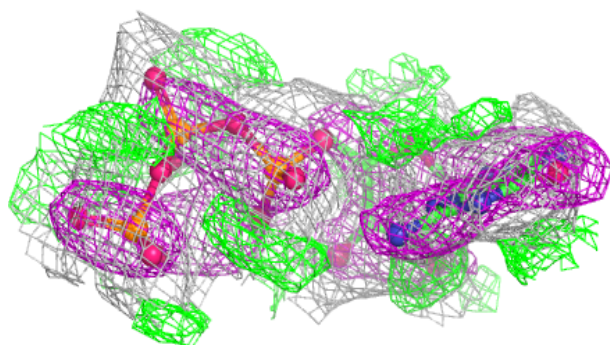
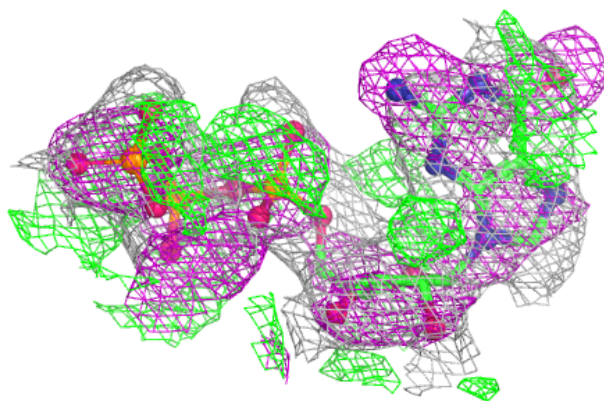
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DCP	A	701	28/28	0.87	0.09	38,46,67,75	0
2	DCP	D	702	28/28	0.88	0.12	16,20,34,35	0
5	GTP	D	704	32/32	0.88	0.10	16,20,26,26	0
2	DCP	C	705	28/28	0.90	0.09	27,35,65,72	0
3	DTP	B	702	30/30	0.93	0.10	16,20,33,36	0
5	GTP	D	701	32/32	0.93	0.09	22,26,29,30	0
4	MG	A	704	1/1	0.93	0.07	48,48,48,48	0
2	DCP	C	701	28/28	0.95	0.09	19,25,37,51	0
5	GTP	C	706	32/32	0.95	0.07	16,22,25,26	0
4	MG	C	702	1/1	0.96	0.14	32,32,32,32	0
4	MG	C	703	1/1	0.96	0.21	15,15,15,15	0
3	DTP	A	702	30/30	0.96	0.07	15,21,37,42	0
4	MG	A	703	1/1	0.97	0.07	28,28,28,28	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.

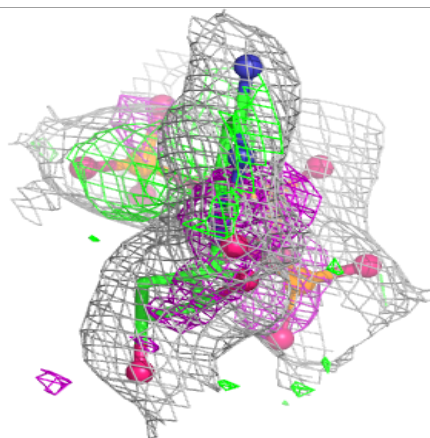
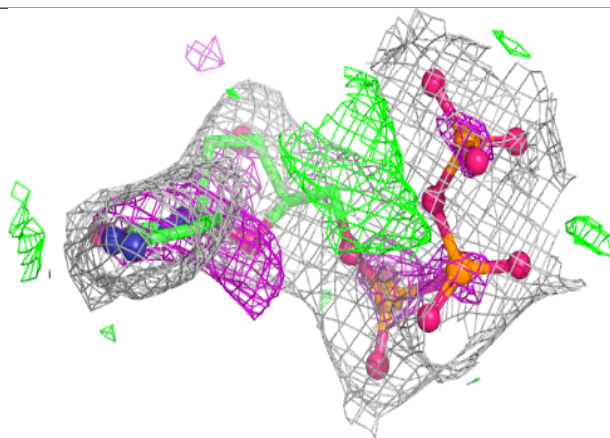
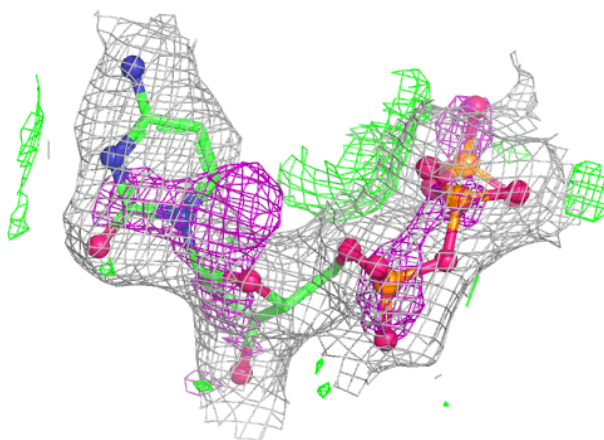


Electron density around GTP C 704:

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

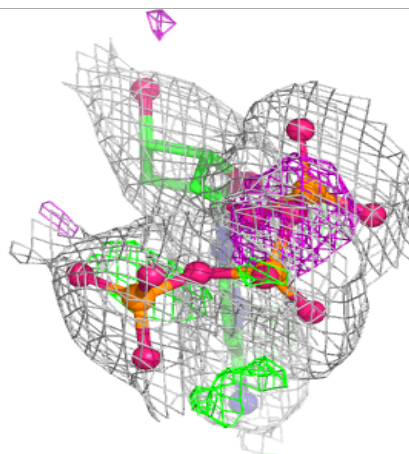
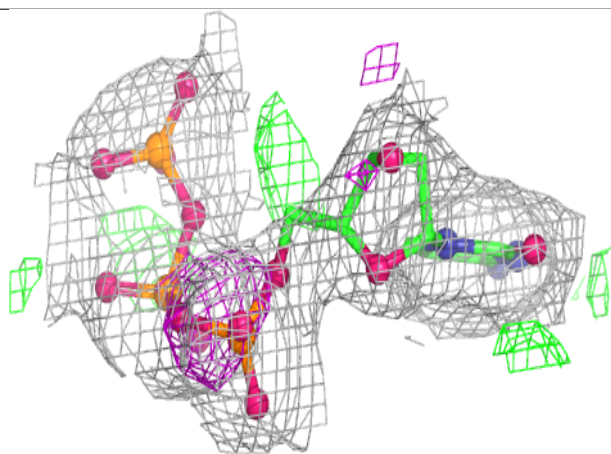
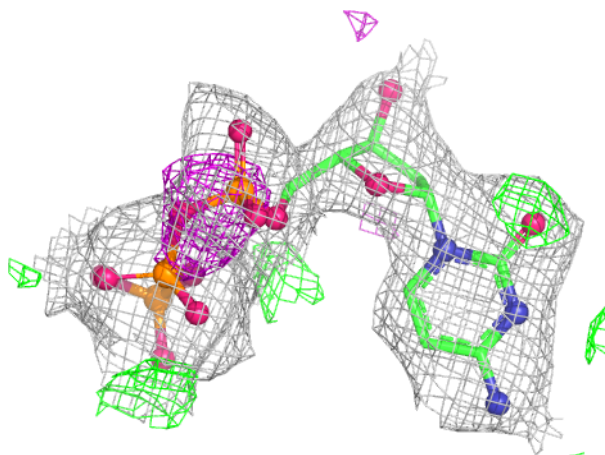
**Electron density around DCP D 703:**

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



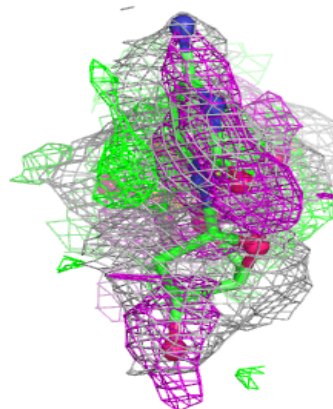
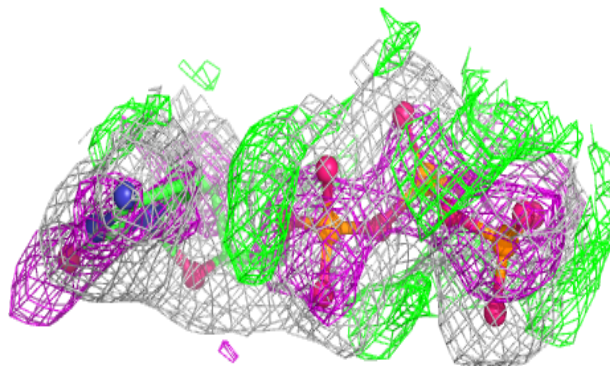
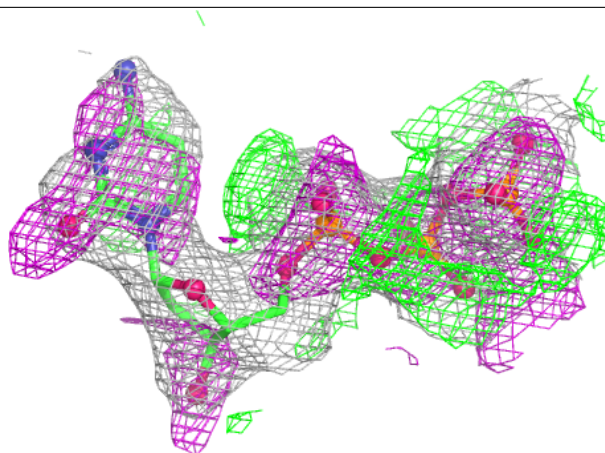
Electron density around DCP A 701:

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

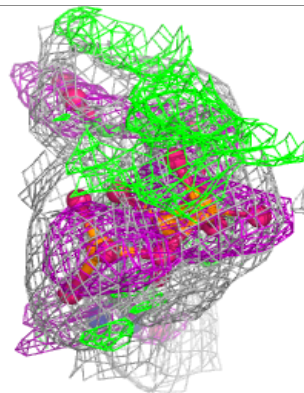
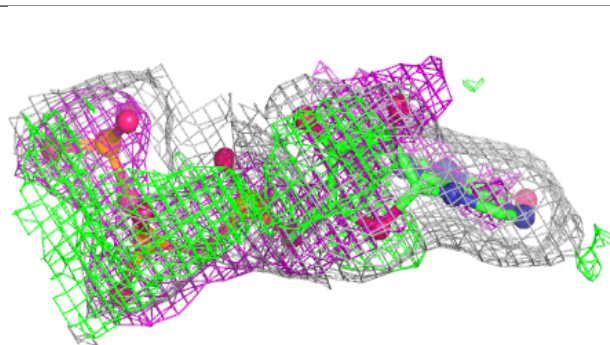
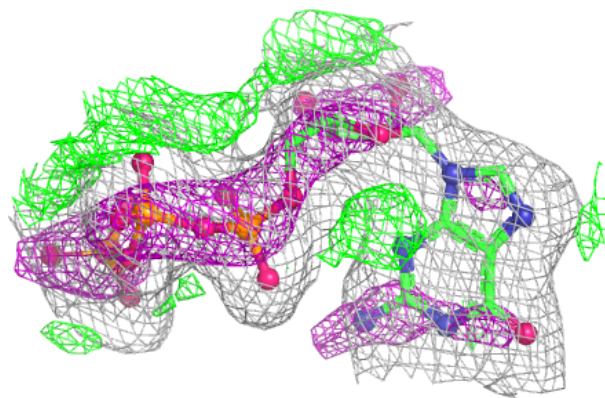


Electron density around DCP D 702:

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

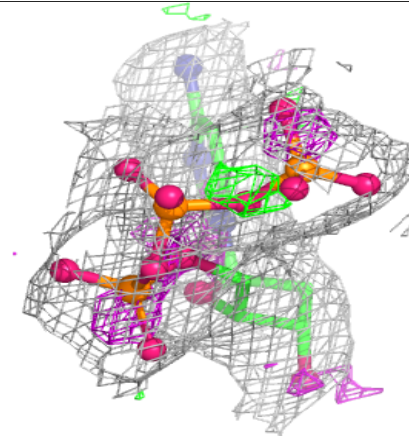
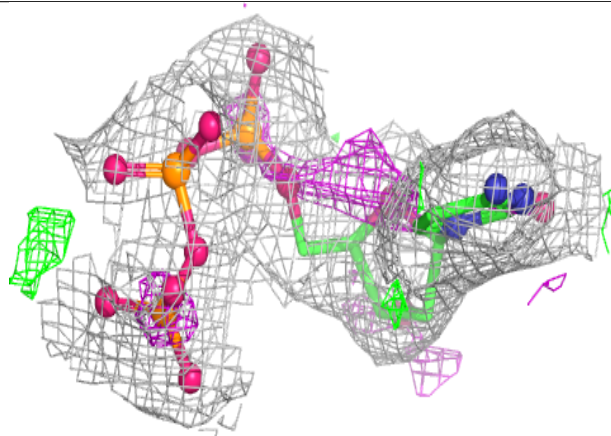
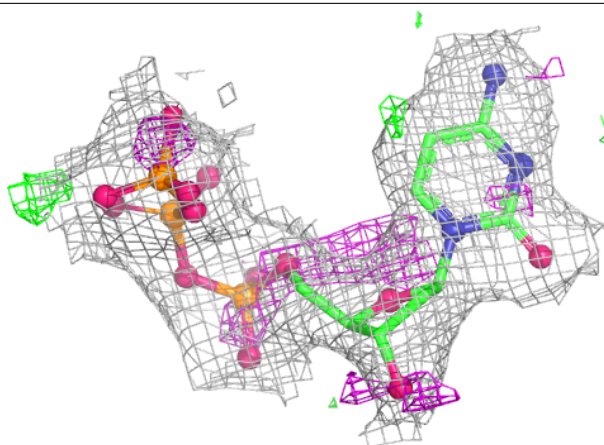
**Electron density around GTP D 704:**

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

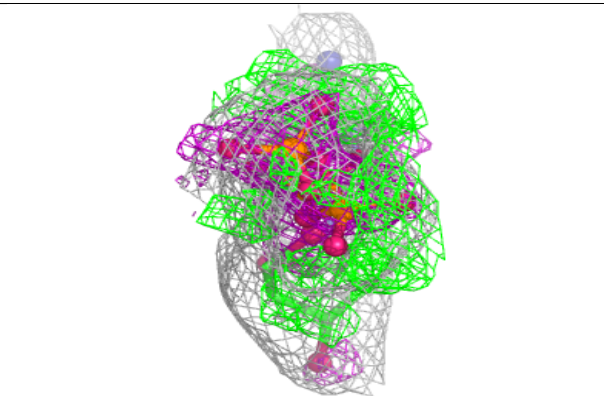
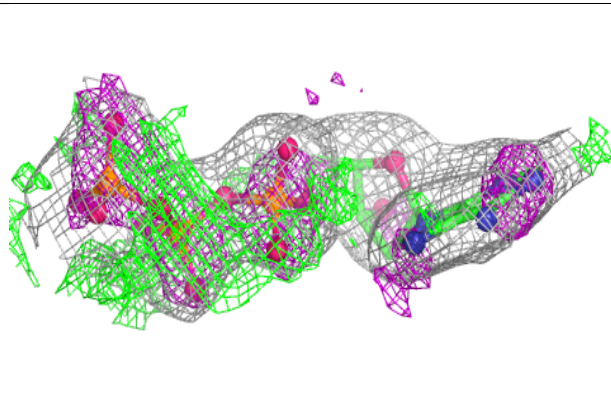
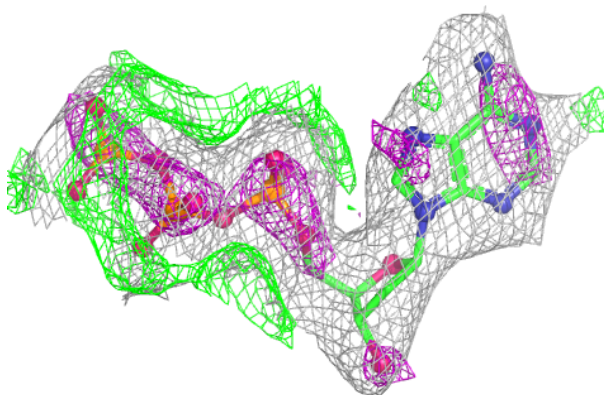


Electron density around DCP C 705:

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

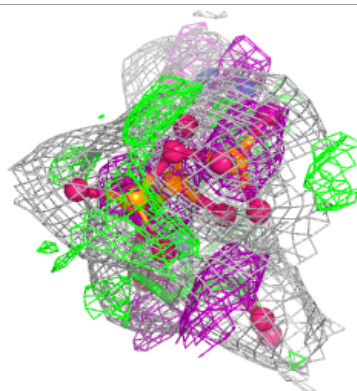
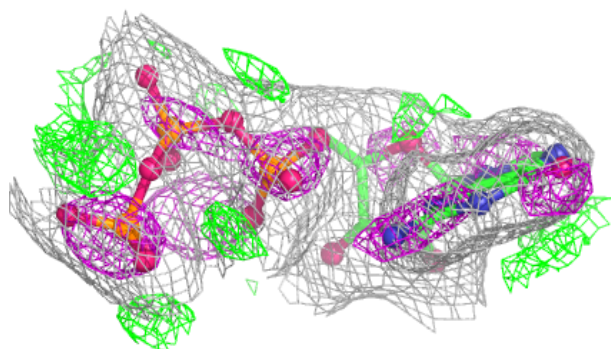
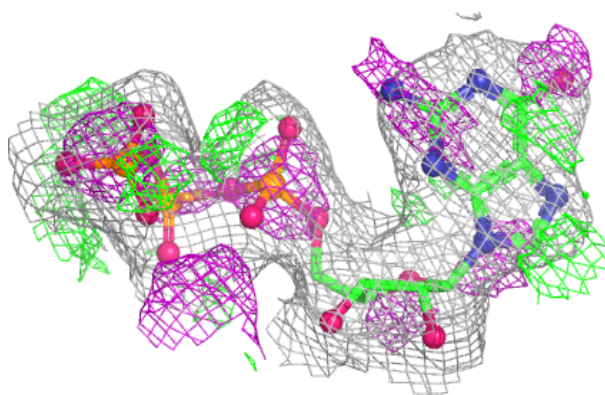
**Electron density around DTP B 702:**

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

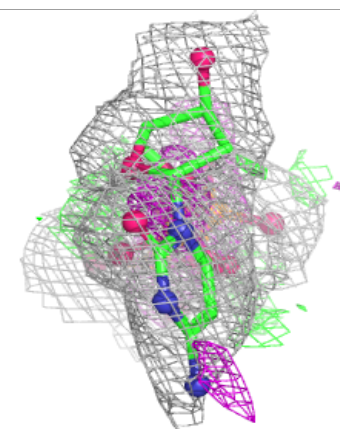
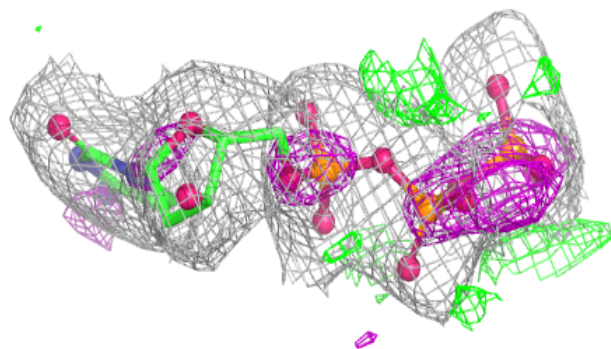
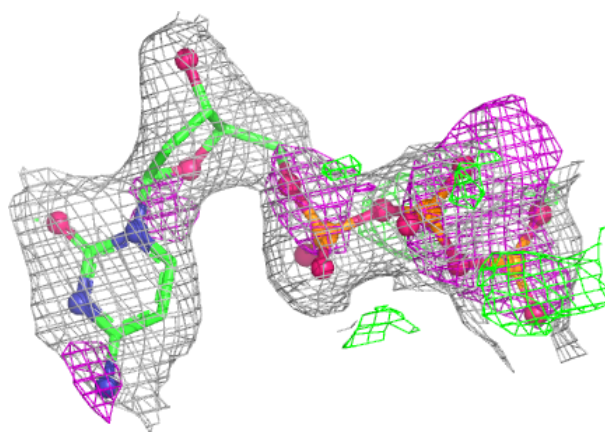


Electron density around GTP D 701:

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

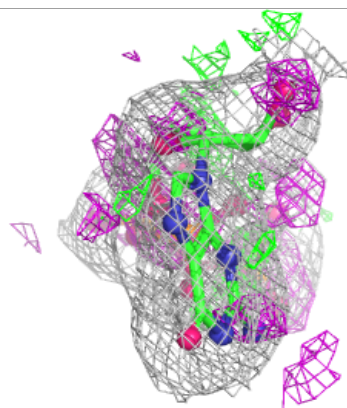
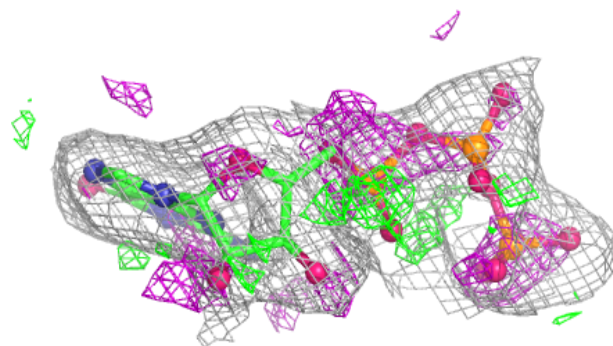
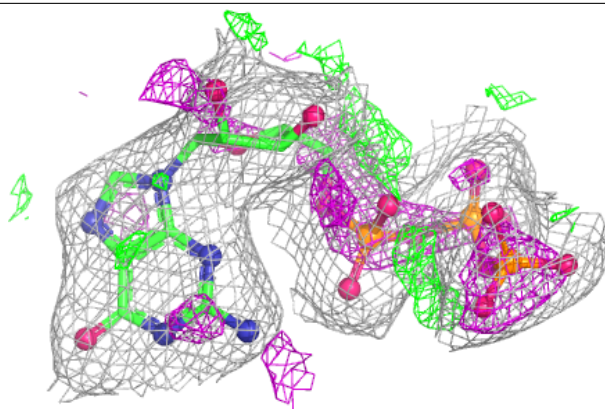
**Electron density around DCP C 701:**

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

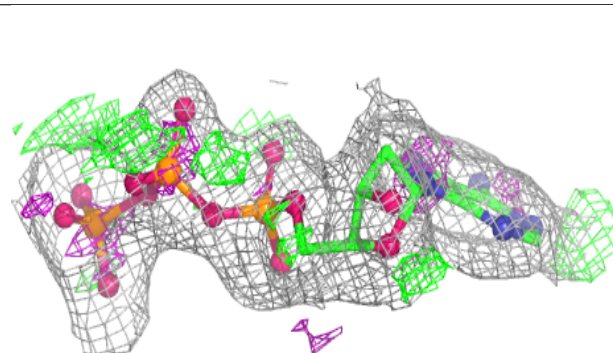
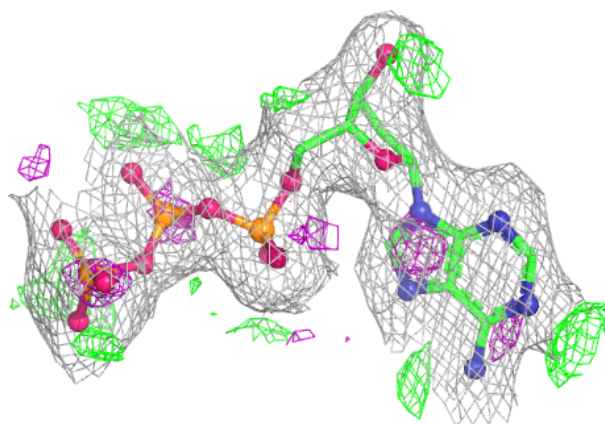


Electron density around GTP C 706:

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

**Electron density around DTP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.