



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:17 PM UTC

PDB ID : 4TNX / pdb_00004tnx
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dGTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.31 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

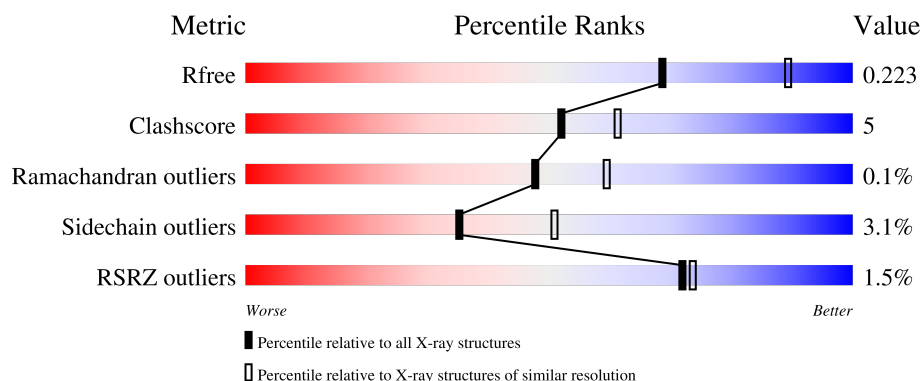
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	514	0% 81% 12% 6%
1	B	514	0% 84% 9% 7%
1	C	514	2% 85% 8% 6%
1	D	514	2% 84% 9% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16322 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.

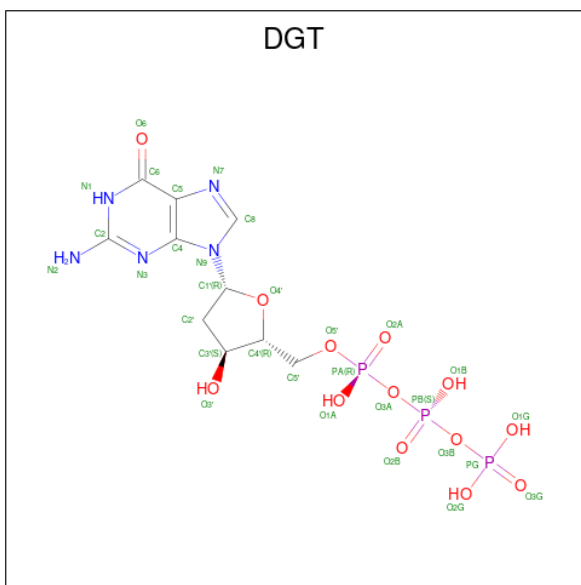
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	3	0
			3956	2529	689	717	21			
1	B	479	Total	C	N	O	S	0	3	0
			3940	2521	686	712	21			
1	C	481	Total	C	N	O	S	0	2	0
			3947	2524	688	714	21			
1	D	483	Total	C	N	O	S	0	2	0
			3961	2531	690	719	21			

There are 8 discrepancies between the modelled and reference sequences:

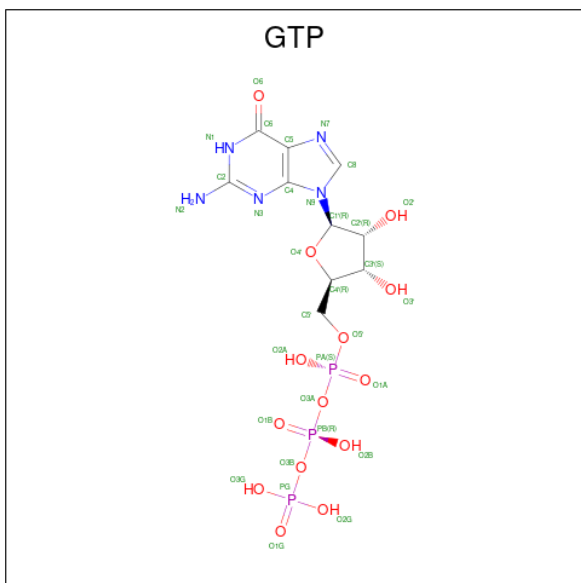
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation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

- Molecule 2 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
2	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).

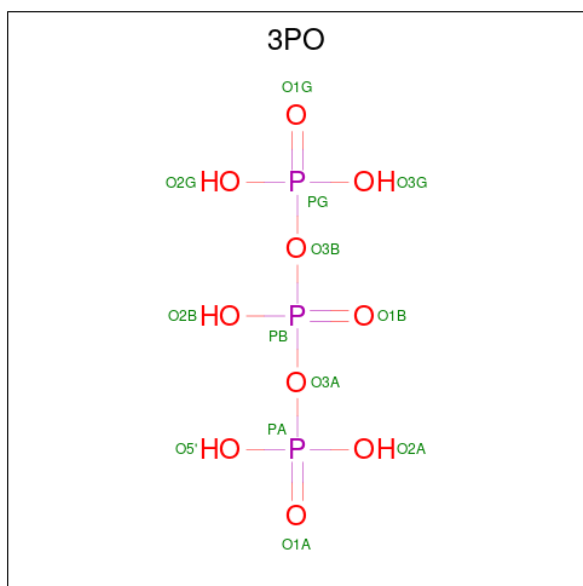


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TRIPHOSPHATE (CCD ID: 3PO) (formula: $\text{H}_5\text{O}_{10}\text{P}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			13	10	3		

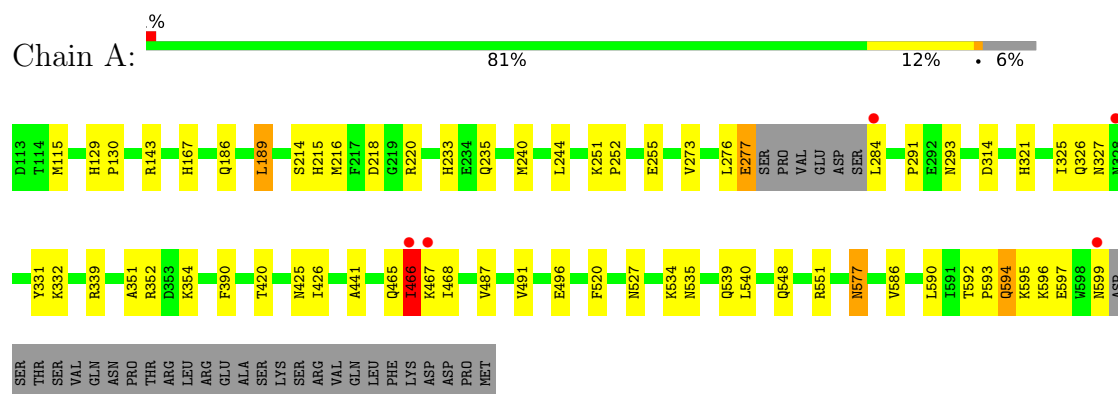
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total 80	O 80	0	0
6	B	49	Total 49	O 49	0	0
6	C	47	Total 47	O 47	0	0
6	D	73	Total 73	O 73	0	0

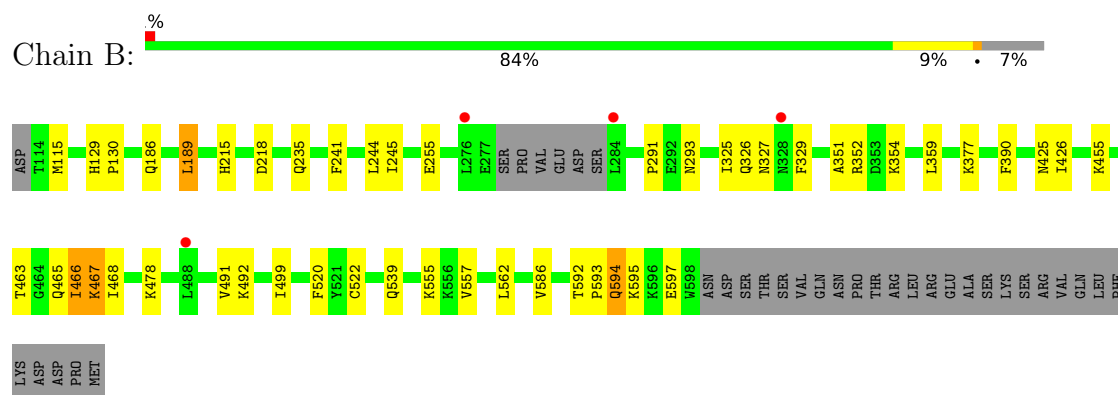
3 Residue-property plots

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.

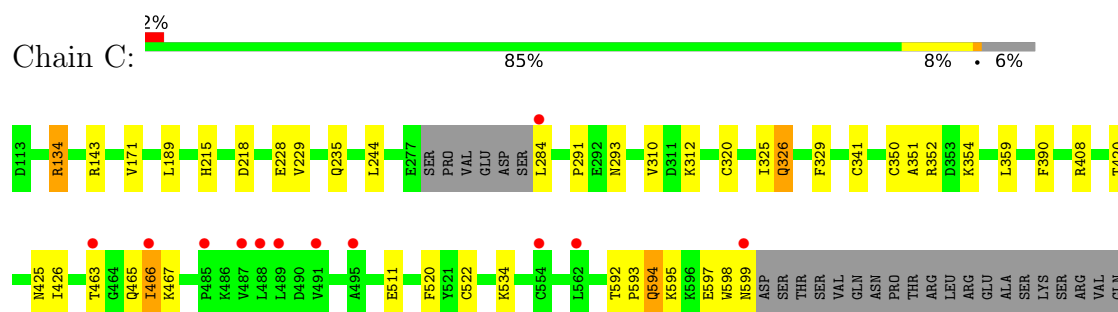
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



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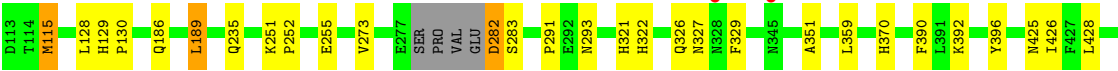
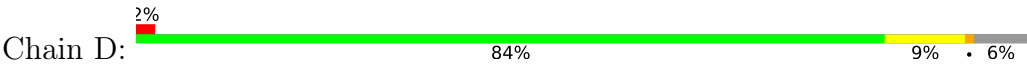


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



LEU
PHE
LYS
ASP
ASP
PRO
PRO
MET

● Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



PHE
LYS
ASP
ASP
PRO
PRO
MET

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.89Å 140.73Å 97.60Å 90.00° 114.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.31 50.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.31) 99.5 (50.00-2.31)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.188 , 0.226 0.192 , 0.223	Depositor DCC
R_{free} test set	4335 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16322	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PO, GTP, DGT, 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	1.01	2/4048 (0.0%)	0.96	2/5464 (0.0%)
1	B	0.89	1/4032 (0.0%)	0.94	1/5442 (0.0%)
1	C	0.86	0/4039	0.92	1/5452 (0.0%)
1	D	0.99	0/4053	0.99	1/5471 (0.0%)
All	All	0.94	3/16172 (0.0%)	0.96	5/21829 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	ALA	C-O	-5.95	1.17	1.24
1	A	214	SER	CA-C	5.68	1.58	1.52
1	B	478	LYS	N-CA	5.28	1.52	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	MET	CG-SD-CE	-6.41	86.80	100.90
1	B	329	PHE	N-CA-C	6.35	119.08	108.73
1	D	329	PHE	N-CA-C	5.85	118.77	109.24
1	A	551	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	C	329	PHE	N-CA-C	5.03	117.44	109.24

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	3956	0	3935	57	0
1	B	3940	0	3925	35	0
1	C	3947	0	3930	35	0
1	D	3961	0	3939	49	0
2	A	31	0	12	4	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
2	D	31	0	12	2	0
3	A	64	0	24	0	0
3	B	32	0	12	0	0
3	C	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	13	0	0	1	0
6	A	80	0	0	4	0
6	B	49	0	0	0	0
6	C	47	0	0	2	0
6	D	73	0	0	6	0
All	All	16322	0	15825	162	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 5.

All (162) 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:596:LYS:HB3	6:D:907:HOH:O	1.63	0.98
1:A:597:GLU:OE1	1:A:597:GLU:N	1.97	0.96
1:A:216:MET:HA	6:A:869:HOH:O	1.67	0.94
1:D:577:ASN:ND2	1:D:595:LYS:NZ	2.19	0.89
1:C:465:GLN:HG2	1:C:466:ILE:HD13	1.56	0.87
1:C:390:PHE:CE2	1:C:426:ILE:HD11	2.10	0.87
1:A:327:ASN:O	1:C:326:GLN:HG2	1.75	0.86
1:D:577:ASN:HD22	1:D:595:LYS:NZ	1.75	0.85
1:C:465:GLN:CG	1:C:466:ILE:HD13	2.08	0.84
1:D:390:PHE:CE2	1:D:426:ILE:HD11	2.11	0.84
1:D:115:MET:HE2	1:D:129:HIS:HA	1.60	0.84
1:A:467:LYS:HB2	1:A:548:GLN:CD	2.04	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:PHE:CE2	1:A:426:ILE:HD11	2.17	0.80
2:A:701:DGT:H5'A	6:D:971:HOH:O	1.81	0.80
2:A:701:DGT:C5'	6:D:971:HOH:O	2.31	0.77
1:D:577:ASN:ND2	1:D:595:LYS:HZ3	1.80	0.77
1:D:466:ILE:HD13	1:D:466:ILE:N	2.01	0.76
1:C:466:ILE:HD13	1:C:466:ILE:N	2.01	0.74
1:A:467:LYS:HG3	1:A:468:ILE:N	2.00	0.74
1:D:577:ASN:HD22	1:D:595:LYS:HZ3	1.32	0.74
1:B:466:ILE:N	1:B:466:ILE:HD13	2.00	0.74
1:D:577:ASN:ND2	1:D:595:LYS:HZ1	1.86	0.72
1:A:467:LYS:HG3	1:A:468:ILE:H	1.53	0.71
1:A:593:PRO:HA	1:A:599:ASN:HD21	1.52	0.71
1:A:467:LYS:HB2	1:A:548:GLN:OE1	1.91	0.71
1:B:325:ILE:HG22	2:D:800:DGT:N2	2.06	0.71
1:B:377:LYS:NZ	2:D:800:DGT:O2G	2.24	0.70
1:A:277:GLU:CG	1:A:277:GLU:O	2.39	0.70
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.26	0.69
1:C:465:GLN:CG	1:C:466:ILE:CD1	2.70	0.69
1:C:408:ARG:NH2	6:C:801:HOH:O	2.25	0.69
1:D:465:GLN:HG3	1:D:466:ILE:CD1	2.26	0.66
1:C:465:GLN:HG2	1:C:466:ILE:CD1	2.26	0.66
1:A:425:ASN:ND2	1:D:425:ASN:HD22	1.94	0.65
1:A:167:HIS:HD2	1:A:314:ASP:OD2	1.79	0.65
1:C:390:PHE:CE2	1:C:426:ILE:CD1	2.80	0.65
1:A:390:PHE:CE2	1:A:426:ILE:CD1	2.80	0.64
1:D:390:PHE:CE2	1:D:426:ILE:CD1	2.80	0.64
1:A:425:ASN:HD21	1:D:425:ASN:ND2	1.94	0.64
1:A:465:GLN:C	1:A:466:ILE:HG23	2.23	0.64
1:C:465:GLN:HG3	1:C:466:ILE:CD1	2.28	0.64
1:A:592:THR:OG1	1:A:593:PRO:HD3	1.98	0.63
1:A:597:GLU:H	1:A:597:GLU:CD	2.02	0.62
1:A:425:ASN:HD21	1:D:425:ASN:HD22	1.48	0.60
1:B:597:GLU:OE1	1:B:597:GLU:N	2.27	0.60
1:D:465:GLN:HG3	1:D:466:ILE:HD13	1.84	0.59
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.41	0.59
2:A:701:DGT:H5'	6:D:971:HOH:O	2.00	0.59
1:D:115:MET:HE2	1:D:129:HIS:CA	2.31	0.59
1:B:390:PHE:CE2	1:B:426:ILE:CD1	2.85	0.59
1:B:522[A]:CYS:SG	1:D:586:VAL:HG11	2.43	0.59
1:A:466:ILE:O	1:A:467:LYS:HG2	2.03	0.58
1:D:115:MET:HG3	1:D:128:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.04	0.58
1:A:339:ARG:NH1	1:A:527:ASN:OD1	2.24	0.58
1:B:465:GLN:CG	1:B:466:ILE:HD13	2.34	0.58
1:C:325:ILE:HG22	2:C:703:DGT:N2	2.19	0.57
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.05	0.57
1:A:321:HIS:CE1	1:D:321:HIS:CE1	2.93	0.56
1:A:465:GLN:O	1:A:466:ILE:HG23	2.05	0.56
1:C:465:GLN:HG3	1:C:466:ILE:HD13	1.82	0.56
1:D:466:ILE:N	1:D:466:ILE:CD1	2.69	0.56
1:A:277:GLU:O	1:A:277:GLU:HG3	2.05	0.56
1:A:535:ASN:OD1	1:A:535:ASN:N	2.35	0.55
1:D:465:GLN:CG	1:D:466:ILE:HD13	2.35	0.55
1:B:425:ASN:ND2	1:C:425:ASN:ND2	2.54	0.55
1:B:354:LYS:NZ	2:B:703:DGT:O1A	2.33	0.54
1:A:390:PHE:CZ	1:A:426:ILE:CD1	2.91	0.54
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.07	0.54
1:D:291:PRO:HG2	1:D:293:ASN:OD1	2.07	0.54
1:B:291:PRO:HG2	1:B:293:ASN:OD1	2.07	0.54
1:B:465:GLN:HG2	1:B:466:ILE:HD13	1.88	0.53
1:A:143:ARG:HD3	6:A:819:HOH:O	2.08	0.53
1:D:465:GLN:CG	1:D:466:ILE:CD1	2.87	0.53
1:C:594:GLN:HG2	1:C:595:LYS:N	2.23	0.52
1:D:322:HIS:HE1	6:D:944:HOH:O	1.92	0.52
1:B:327:ASN:O	1:D:326:GLN:HG2	2.10	0.52
1:D:186:GLN:HB2	1:D:189:LEU:HD22	1.91	0.52
1:C:291:PRO:HG2	1:C:293:ASN:OD1	2.10	0.52
1:A:467:LYS:CG	1:A:468:ILE:H	2.21	0.51
1:A:594:GLN:HG2	1:A:595:LYS:N	2.25	0.51
1:D:322:HIS:CE1	6:D:944:HOH:O	2.63	0.50
1:C:592:THR:N	1:C:593:PRO:CD	2.75	0.50
1:A:115:MET:C	1:A:115:MET:SD	2.94	0.50
1:C:134:ARG:NE	1:C:134:ARG:HA	2.27	0.49
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.93	0.49
1:A:351:ALA:O	1:A:520:PHE:HA	2.13	0.49
1:B:465:GLN:HG2	1:B:466:ILE:CD1	2.43	0.49
1:A:327:ASN:O	1:C:326:GLN:CG	2.54	0.49
1:A:325:ILE:HG22	2:A:701:DGT:N2	2.28	0.49
1:D:577:ASN:HD21	1:D:595:LYS:NZ	2.09	0.49
1:B:592:THR:N	1:B:593:PRO:CD	2.76	0.48
1:A:220:ARG:HG3	6:A:869:HOH:O	2.14	0.48
1:B:326:GLN:HG3	1:D:326:GLN:CG	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:GLN:CG	1:B:466:ILE:CD1	2.91	0.48
1:B:351:ALA:O	1:B:520:PHE:HA	2.13	0.48
1:A:216:MET:CA	6:A:869:HOH:O	2.43	0.47
1:D:351:ALA:O	1:D:520:PHE:HA	2.14	0.47
1:A:487:VAL:HG13	1:A:590:LEU:HD12	1.95	0.47
1:D:598:TRP:O	1:D:599:ASN:CB	2.62	0.47
1:B:352:ARG:HG3	1:B:354:LYS:HG2	1.97	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.15	0.46
1:C:598:TRP:O	1:C:599:ASN:CB	2.62	0.46
1:D:282:ASP:OD2	1:D:282:ASP:N	2.48	0.46
1:A:466:ILE:O	1:A:466:ILE:HD12	2.14	0.46
1:A:425:ASN:HB2	1:D:428:LEU:HD13	1.97	0.46
1:C:228:GLU:OE2	1:C:229:VAL:HG23	2.15	0.46
1:D:592:THR:N	1:D:593:PRO:CD	2.78	0.46
1:B:186:GLN:HB2	1:B:189:LEU:HD22	1.97	0.46
1:A:215:HIS:HA	1:A:218:ASP:OD2	2.15	0.46
1:A:390:PHE:CZ	1:A:426:ILE:HD11	2.51	0.45
1:B:390:PHE:CZ	1:B:426:ILE:CD1	3.00	0.45
1:C:352:ARG:HG3	1:C:354:LYS:HG2	1.97	0.45
1:B:244:LEU:C	1:B:244:LEU:HD23	2.42	0.45
1:B:326:GLN:HG3	1:D:326:GLN:HG2	1.97	0.45
1:A:331:TYR:CE1	1:A:332:LYS:HG3	2.52	0.45
1:A:276:LEU:O	1:A:277:GLU:C	2.59	0.45
1:A:277:GLU:O	1:A:277:GLU:HG2	2.15	0.45
1:C:215:HIS:HA	1:C:218:ASP:OD2	2.17	0.45
1:A:291:PRO:HG2	1:A:293:ASN:OD1	2.17	0.44
1:B:594:GLN:HG2	1:B:595:LYS:N	2.33	0.44
1:D:392:LYS:HB3	1:D:441:ALA:HB2	2.00	0.44
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.52	0.44
1:A:143:ARG:HD2	1:A:420:THR:HA	2.00	0.44
1:A:251:LYS:HB2	1:A:252:PRO:HD3	2.00	0.44
1:A:577:ASN:ND2	1:A:595:LYS:NZ	2.66	0.44
1:B:467:LYS:HG3	1:B:468:ILE:N	2.32	0.43
1:B:499:ILE:HD11	1:B:555:LYS:HE2	1.99	0.43
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.53	0.43
1:A:352:ARG:HG3	1:A:354:LYS:HG2	2.00	0.43
1:C:390:PHE:CZ	1:C:426:ILE:CD1	3.01	0.43
1:D:390:PHE:CZ	1:D:426:ILE:CD1	3.01	0.43
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.53	0.43
1:B:465:GLN:HG3	1:B:466:ILE:CD1	2.48	0.43
1:D:251:LYS:HB2	1:D:252:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:CYS:HB3	1:C:325:ILE:O	2.19	0.43
1:B:326:GLN:HB3	1:D:327:ASN:O	2.19	0.43
1:B:562:LEU:HD12	1:B:562:LEU:HA	1.87	0.42
1:C:171:VAL:HG13	1:C:310:VAL:HG23	2.01	0.42
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.53	0.42
1:D:488:LEU:HA	1:D:488:LEU:HD13	1.78	0.42
1:D:390:PHE:CZ	1:D:426:ILE:HG13	2.54	0.42
1:A:592:THR:N	1:A:593:PRO:CD	2.83	0.42
1:B:241:PHE:O	1:B:245:ILE:HG12	2.20	0.42
1:C:341:CYS:HB2	1:C:350:CYS:SG	2.59	0.42
1:D:435:ASP:HA	1:D:436:PRO:HD3	1.90	0.42
1:C:597:GLU:OE1	1:C:597:GLU:N	2.37	0.42
1:A:244:LEU:C	1:A:244:LEU:HD23	2.45	0.41
1:C:598:TRP:O	1:C:599:ASN:HB2	2.20	0.41
1:A:326:GLN:HG3	1:C:326:GLN:CG	2.51	0.41
1:A:425:ASN:ND2	1:D:425:ASN:ND2	2.59	0.41
1:B:215:HIS:HA	1:B:218:ASP:OD2	2.20	0.41
1:C:143:ARG:HD2	1:C:420:THR:HA	2.02	0.41
1:A:167:HIS:CD2	1:A:314:ASP:OD2	2.67	0.41
1:B:455:LYS:HG2	1:B:557:VAL:HG12	2.02	0.41
1:D:370:HIS:HB3	1:D:505:MET:HE1	2.03	0.41
1:D:491:VAL:C	1:D:492:LYS:HD2	2.46	0.41
1:C:244:LEU:C	1:C:244:LEU:HD23	2.46	0.41
1:A:233:HIS:NE2	5:A:705:3PO:O2G	2.54	0.40
1:C:312:LYS:HG3	6:C:836:HOH:O	2.20	0.40
1:B:586:VAL:HG11	1:D:522[A]:CYS:SG	2.61	0.40
1:A:390:PHE:CZ	1:A:426:ILE:HG13	2.57	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	480/514 (93%)	474 (99%)	5 (1%)	1 (0%)	43	53
1	B	478/514 (93%)	470 (98%)	8 (2%)	0	100	100
1	C	479/514 (93%)	474 (99%)	5 (1%)	0	100	100
1	D	481/514 (94%)	474 (98%)	7 (2%)	0	100	100
All	All	1918/2056 (93%)	1892 (99%)	25 (1%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/459 (94%)	415 (96%)	15 (4%)	32	46
1	B	428/459 (93%)	416 (97%)	12 (3%)	38	55
1	C	429/459 (94%)	417 (97%)	12 (3%)	38	55
1	D	431/459 (94%)	417 (97%)	14 (3%)	34	50
All	All	1718/1836 (94%)	1665 (97%)	53 (3%)	35	51

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LEU
1	A	235	GLN
1	A	255	GLU
1	A	273	VAL
1	A	277	GLU
1	A	284	LEU
1	A	466	ILE
1	A	491	VAL
1	A	496	GLU
1	A	534	LYS

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Mol	Chain	Res	Type
1	A	539	GLN
1	A	540	LEU
1	A	577	ASN
1	A	594	GLN
1	A	596	LYS
1	B	115	MET
1	B	189	LEU
1	B	235	GLN
1	B	255	GLU
1	B	359	LEU
1	B	463	THR
1	B	466	ILE
1	B	467	LYS
1	B	491	VAL
1	B	492	LYS
1	B	539	GLN
1	B	594	GLN
1	C	134	ARG
1	C	189	LEU
1	C	235	GLN
1	C	284	LEU
1	C	326	GLN
1	C	359	LEU
1	C	463	THR
1	C	466	ILE
1	C	467	LYS
1	C	511	GLU
1	C	534	LYS
1	C	594	GLN
1	D	115	MET
1	D	189	LEU
1	D	235	GLN
1	D	255	GLU
1	D	273	VAL
1	D	282	ASP
1	D	283	SER
1	D	359	LEU
1	D	463	THR
1	D	466	ILE
1	D	467	LYS
1	D	488	LEU
1	D	491	VAL

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Mol	Chain	Res	Type
1	D	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	A	149	GLN
1	A	167	HIS
1	A	190	GLN
1	A	200	GLN
1	A	243	HIS
1	A	248	ASN
1	A	322	HIS
1	A	364	HIS
1	A	577	ASN
1	B	149	GLN
1	B	200	GLN
1	B	233	HIS
1	B	326	GLN
1	B	425	ASN
1	B	447	GLN
1	B	539	GLN
1	C	140	GLN
1	C	149	GLN
1	C	200	GLN
1	C	233	HIS
1	C	243	HIS
1	C	248	ASN
1	C	322	HIS
1	C	370	HIS
1	C	375	GLN
1	C	380	ASN
1	C	425	ASN
1	D	190	GLN
1	D	200	GLN
1	D	243	HIS
1	D	322	HIS
1	D	370	HIS
1	D	375	GLN
1	D	380	ASN
1	D	425	ASN
1	D	571	GLN

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Mol	Chain	Res	Type
1	D	577	ASN
1	D	594	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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
3	GTP	A	704	4	33,34,34	1.46	4 (12%)	50,54,54	1.78	12 (24%)
3	GTP	C	704	4	33,34,34	1.22	4 (12%)	50,54,54	1.86	13 (26%)
5	3PO	A	705	-	10,12,12	2.01	2 (20%)	17,20,20	1.24	3 (17%)
3	GTP	B	701	4	33,34,34	1.66	6 (18%)	50,54,54	1.87	12 (24%)
2	DGT	A	701	4	32,33,33	1.31	4 (12%)	48,52,52	1.82	11 (22%)
3	GTP	A	702	4	33,34,34	1.45	5 (15%)	50,54,54	1.59	8 (16%)
2	DGT	D	800	4	32,33,33	1.40	5 (15%)	48,52,52	1.73	12 (25%)
2	DGT	C	703	4	32,33,33	1.45	6 (18%)	48,52,52	1.94	11 (22%)
2	DGT	B	703	4	32,33,33	1.82	8 (25%)	48,52,52	1.69	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	704	4	-	8/22/38/38	0/3/3/3
3	GTP	C	704	4	-	6/22/38/38	0/3/3/3
5	3PO	A	705	-	-	2/12/12/12	-
3	GTP	B	701	4	-	3/22/38/38	0/3/3/3
2	DGT	A	701	4	-	3/22/34/34	0/3/3/3
3	GTP	A	702	4	-	2/22/38/38	0/3/3/3
2	DGT	D	800	4	-	2/22/34/34	0/3/3/3
2	DGT	C	703	4	-	3/22/34/34	0/3/3/3
2	DGT	B	703	4	-	5/22/34/34	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GTP	PB-O3B	5.24	1.65	1.59
3	B	701	GTP	PB-O3A	5.21	1.65	1.59
2	C	703	DGT	PB-O3B	4.56	1.64	1.59
5	A	705	3PO	PB-O3B	4.42	1.64	1.59
5	A	705	3PO	PB-O3A	4.14	1.64	1.59
2	B	703	DGT	PA-O3A	3.96	1.63	1.59
3	B	701	GTP	PA-O3A	3.96	1.63	1.59
3	A	702	GTP	C5-C4	3.89	1.49	1.38
2	B	703	DGT	PB-O3A	3.82	1.63	1.59
3	A	704	GTP	C5-C4	3.54	1.48	1.38
2	A	701	DGT	C5-C4	3.53	1.48	1.38
3	B	701	GTP	C5-C4	3.48	1.48	1.38
2	D	800	DGT	PA-O3A	3.47	1.63	1.59
2	D	800	DGT	C6-N1	-3.44	1.32	1.38
2	B	703	DGT	C5-N7	-3.41	1.32	1.39
3	A	704	GTP	C5-N7	-3.21	1.32	1.39
2	B	703	DGT	C6-N1	-3.11	1.33	1.38
3	C	704	GTP	C5-C4	3.07	1.47	1.38
3	A	704	GTP	PB-O3B	-3.05	1.56	1.59
2	C	703	DGT	C5-C4	3.02	1.47	1.38
2	B	703	DGT	PB-O3B	3.01	1.62	1.59
3	C	704	GTP	PB-O3B	3.00	1.62	1.59
2	D	800	DGT	C5-C4	2.99	1.47	1.38
2	B	703	DGT	C4-N9	-2.98	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	GTP	C5-N7	-2.93	1.33	1.39
3	A	704	GTP	PB-O3A	2.90	1.62	1.59
2	B	703	DGT	C5-C4	2.81	1.46	1.38
2	B	703	DGT	C2-N1	-2.57	1.31	1.37
2	C	703	DGT	PB-O3A	2.54	1.62	1.59
2	A	701	DGT	C4-N9	-2.49	1.31	1.38
3	C	704	GTP	C5-N7	-2.44	1.34	1.39
2	A	701	DGT	O4'-C4'	-2.41	1.39	1.45
2	C	703	DGT	C4-N9	-2.39	1.32	1.38
3	C	704	GTP	PB-O3A	2.37	1.62	1.59
2	D	800	DGT	C5-N7	-2.35	1.34	1.39
2	D	800	DGT	C4-N9	-2.34	1.32	1.38
2	A	701	DGT	PB-O3B	2.28	1.62	1.59
2	C	703	DGT	C5-N7	-2.25	1.34	1.39
3	B	701	GTP	C4-N9	-2.23	1.32	1.38
2	C	703	DGT	PA-O3A	2.18	1.61	1.59
3	A	702	GTP	PG-O2G	-2.08	1.47	1.54
3	A	702	GTP	C4-N9	-2.06	1.32	1.38
3	B	701	GTP	C6-N1	-2.02	1.35	1.38
3	A	702	GTP	C5-N7	-2.02	1.35	1.39

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	GTP	C5-C4-N3	-6.19	118.54	128.39
3	C	704	GTP	C5-C4-N3	-5.66	119.37	128.39
2	C	703	DGT	C2-N3-C4	5.63	122.00	112.30
3	A	704	GTP	C5-C4-N3	-5.36	119.86	128.39
3	C	704	GTP	C2-N3-C4	5.14	121.16	112.30
3	B	701	GTP	C2-N3-C4	5.03	120.97	112.30
2	A	701	DGT	C2-N3-C4	4.88	120.70	112.30
2	A	701	DGT	C5-C4-N3	-4.88	120.63	128.39
3	A	702	GTP	C5-C4-N3	-4.86	120.65	128.39
2	C	703	DGT	C5-C4-N3	-4.81	120.74	128.39
3	A	704	GTP	C2-N3-C4	4.62	120.26	112.30
2	D	800	DGT	C5-C4-N3	-4.46	121.29	128.39
3	A	702	GTP	N9-C4-N3	4.39	134.74	125.95
3	A	702	GTP	C2-N3-C4	4.36	119.81	112.30
2	A	701	DGT	C6-C5-N7	4.19	137.92	130.29
2	B	703	DGT	C5-C4-N3	-4.13	121.81	128.39
3	A	704	GTP	N9-C4-N3	4.11	134.16	125.95
3	C	704	GTP	N9-C4-N3	4.07	134.09	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	DGT	C2-N3-C4	4.02	119.23	112.30
2	B	703	DGT	C6-C5-N7	3.95	137.47	130.29
2	C	703	DGT	C6-C5-N7	3.92	137.43	130.29
3	B	701	GTP	N9-C4-N3	3.83	133.62	125.95
3	A	704	GTP	O3A-PB-O1B	-3.78	99.33	110.70
2	C	703	DGT	O6-C6-C5	-3.61	117.01	126.53
2	A	701	DGT	N2-C2-N3	-3.60	112.65	119.67
2	B	703	DGT	O1B-PB-O2B	3.60	129.17	112.44
2	D	800	DGT	C6-C5-N7	3.58	136.81	130.29
2	C	703	DGT	N2-C2-N1	3.56	124.28	116.76
2	B	703	DGT	C2-N3-C4	3.55	118.42	112.30
2	D	800	DGT	N9-C4-N3	3.51	132.97	125.95
2	C	703	DGT	N9-C4-N3	3.47	132.90	125.95
3	B	701	GTP	C6-C5-N7	3.44	136.54	130.29
2	A	701	DGT	N2-C2-N1	3.41	123.95	116.76
3	A	702	GTP	O2A-PA-O3A	3.39	116.44	107.27
2	A	701	DGT	N9-C4-N3	3.31	132.56	125.95
3	C	704	GTP	C3'-C2'-C1'	3.26	107.63	101.46
2	C	703	DGT	N2-C2-N3	-3.13	113.56	119.67
3	A	702	GTP	C6-C5-N7	3.12	135.97	130.29
3	C	704	GTP	O2A-PA-O3A	3.05	115.51	107.27
3	C	704	GTP	C6-C5-N7	3.04	135.83	130.29
3	B	701	GTP	N2-C2-N3	-3.00	113.81	119.67
2	B	703	DGT	N9-C4-N3	2.87	131.69	125.95
2	D	800	DGT	O2G-PG-O1G	2.86	118.53	107.80
2	C	703	DGT	C6-C5-C4	-2.76	114.67	118.83
2	C	703	DGT	O2G-PG-O3B	-2.76	95.39	104.64
2	B	703	DGT	O2G-PG-O3B	-2.72	95.50	104.64
3	B	701	GTP	C3'-C2'-C1'	2.71	106.58	101.46
2	D	800	DGT	C2'-C3'-C4'	2.68	108.25	102.80
3	B	701	GTP	C4-C5-N7	-2.67	106.44	110.67
3	A	704	GTP	C6-C5-N7	2.65	135.11	130.29
3	B	701	GTP	N2-C2-N1	2.64	122.33	116.76
3	A	704	GTP	C3'-C2'-C1'	2.63	106.44	101.46
3	A	702	GTP	O2G-PG-O1G	2.59	120.92	110.83
2	B	703	DGT	C6-C5-C4	-2.57	114.96	118.83
2	A	701	DGT	C4-C5-N7	-2.57	106.59	110.67
2	D	800	DGT	O1B-PB-O2B	2.55	124.31	112.44
3	C	704	GTP	O3A-PB-O1B	-2.49	103.23	110.70
2	B	703	DGT	C2'-C3'-C4'	2.47	107.81	102.80
3	A	704	GTP	O3G-PG-O2G	2.46	117.04	107.80
3	C	704	GTP	C4-C5-N7	-2.44	106.80	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	GTP	O2B-PB-O3B	2.42	113.81	107.27
2	D	800	DGT	O3B-PG-O3G	-2.41	98.36	111.04
2	D	800	DGT	O1A-PA-O2A	2.41	123.65	112.44
2	A	701	DGT	O2G-PG-O1G	2.40	116.80	107.80
3	A	704	GTP	O2B-PB-O3A	2.39	113.74	107.27
2	D	800	DGT	C6-C5-C4	-2.38	115.25	118.83
3	B	701	GTP	O3B-PB-O1B	-2.37	103.57	110.70
3	A	704	GTP	N2-C2-N1	2.37	121.76	116.76
2	B	703	DGT	O1G-PG-O3G	2.34	119.95	110.83
5	A	705	3PO	O3G-PG-O2G	2.29	116.38	107.80
3	C	704	GTP	O2B-PB-O3B	2.26	113.39	107.27
3	B	701	GTP	O3B-PG-O1G	-2.24	99.23	111.04
2	A	701	DGT	C6-C5-C4	-2.23	115.47	118.83
2	A	701	DGT	O6-C6-C5	-2.22	120.67	126.53
2	C	703	DGT	O6-C6-N1	2.21	124.28	120.11
3	A	704	GTP	O6-C6-C5	-2.16	120.82	126.53
2	A	701	DGT	O3B-PG-O3G	-2.14	99.80	111.04
2	C	703	DGT	C5-C6-N1	2.13	118.68	113.25
3	A	704	GTP	N2-C2-N3	-2.13	115.52	119.67
3	C	704	GTP	O2A-PA-O1A	2.12	122.33	112.44
3	A	704	GTP	O2'-C2'-C1'	-2.11	102.84	110.10
3	C	704	GTP	N2-C2-N1	2.11	121.21	116.76
3	C	704	GTP	O6-C6-C5	-2.10	120.98	126.53
3	B	701	GTP	O3G-PG-O3B	2.08	111.62	104.64
3	C	704	GTP	O2G-PG-O1G	2.08	118.92	110.83
5	A	705	3PO	O2B-PB-O3A	2.07	112.87	107.27
2	D	800	DGT	O6-C6-C5	-2.07	121.07	126.53
3	A	702	GTP	C6-C5-C4	-2.07	115.72	118.83
5	A	705	3PO	O5'-PA-O2A	2.05	115.50	107.80
3	A	702	GTP	C3'-C2'-C1'	2.04	105.31	101.46
2	D	800	DGT	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DGT	PB-O3B-PG-O1G
2	C	703	DGT	PB-O3B-PG-O1G
2	D	800	DGT	PB-O3B-PG-O1G
3	A	704	GTP	PB-O3B-PG-O2G
3	A	704	GTP	PB-O3B-PG-O3G
3	A	704	GTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	A	705	3PO	PB-O3B-PG-O2G
3	C	704	GTP	PB-O3B-PG-O2G
3	C	704	GTP	PB-O3B-PG-O3G
2	B	703	DGT	PB-O3A-PA-O2A
3	C	704	GTP	PG-O3B-PB-O2B
3	A	704	GTP	C4'-C5'-O5'-PA
3	A	702	GTP	PG-O3B-PB-O2B
3	A	704	GTP	PG-O3B-PB-O1B
3	B	701	GTP	PG-O3B-PB-O2B
3	C	704	GTP	PG-O3B-PB-O1B
2	D	800	DGT	PB-O3B-PG-O3G
3	A	702	GTP	C4'-C5'-O5'-PA
3	C	704	GTP	C4'-C5'-O5'-PA
2	B	703	DGT	PG-O3B-PB-O2B
3	A	704	GTP	PG-O3B-PB-O2B
3	A	704	GTP	PB-O3B-PG-O1G
2	A	701	DGT	PB-O3B-PG-O2G
2	B	703	DGT	PB-O3B-PG-O2G
2	C	703	DGT	PB-O3B-PG-O2G
3	B	701	GTP	PB-O3B-PG-O2G
5	A	705	3PO	PB-O3B-PG-O3G
2	B	703	DGT	PA-O3A-PB-O1B
2	C	703	DGT	PB-O3A-PA-O1A
2	A	701	DGT	PB-O3A-PA-O1A
2	B	703	DGT	PB-O3A-PA-O1A
3	A	704	GTP	PB-O3A-PA-O2A
3	B	701	GTP	PB-O3A-PA-O2A
3	C	704	GTP	PB-O3A-PA-O2A

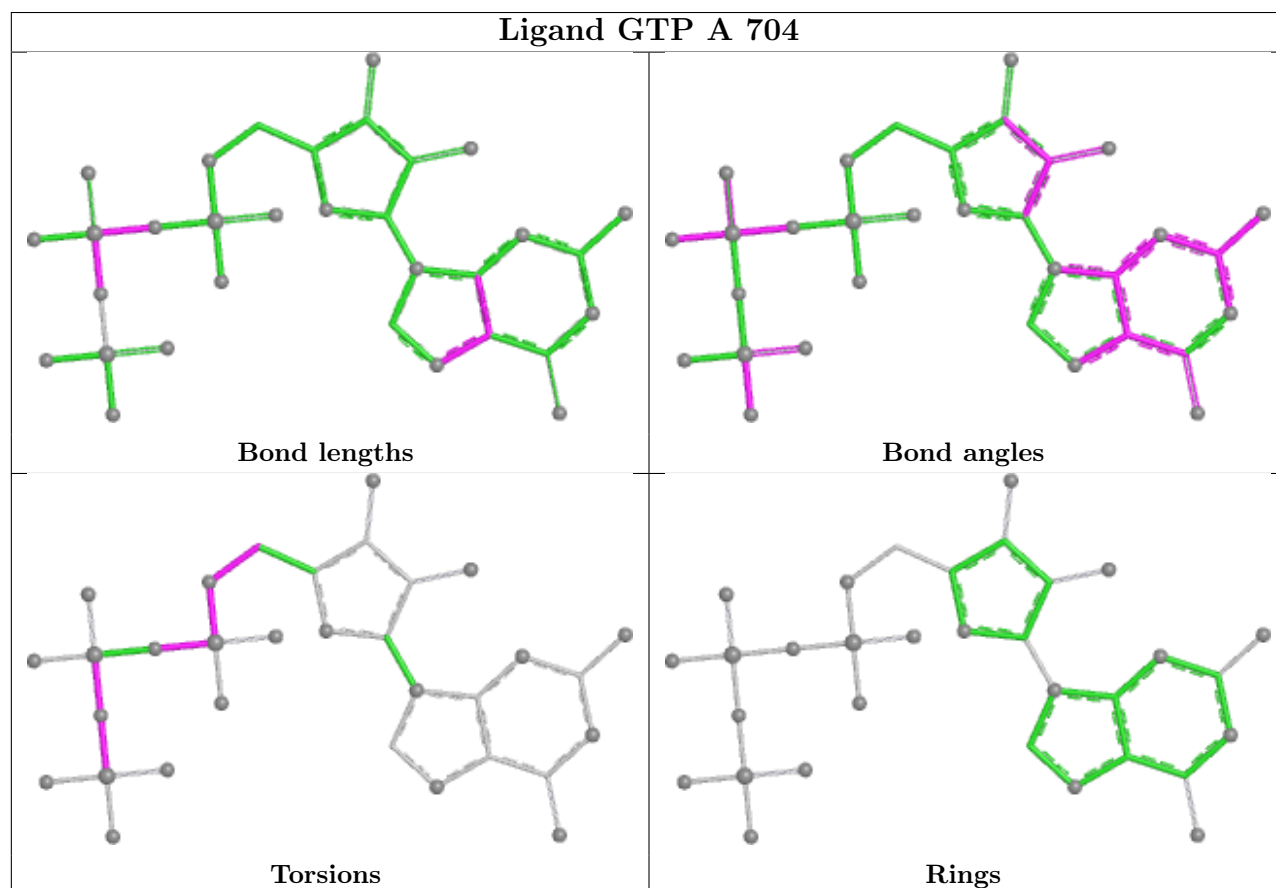
There are no ring outliers.

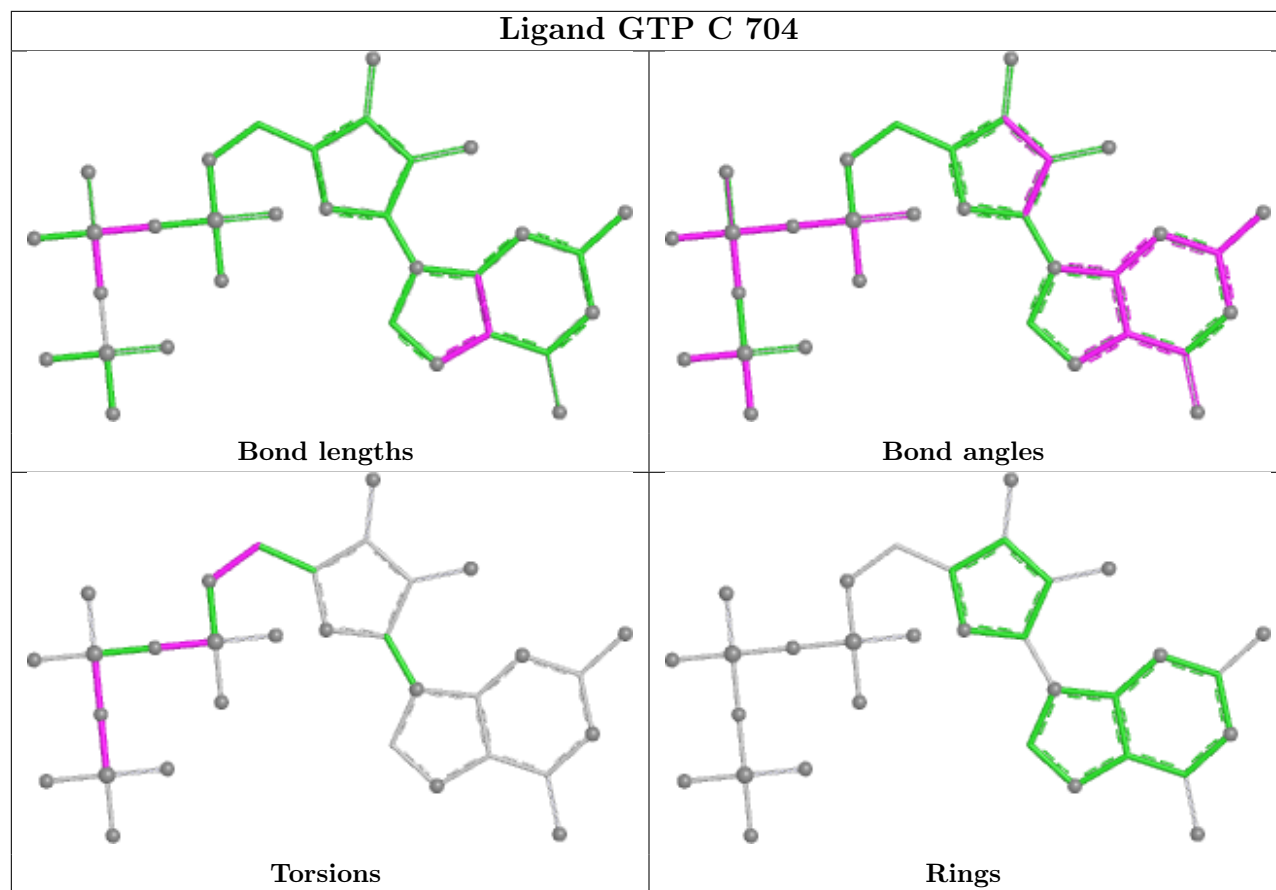
5 monomers are involved in 9 short contacts:

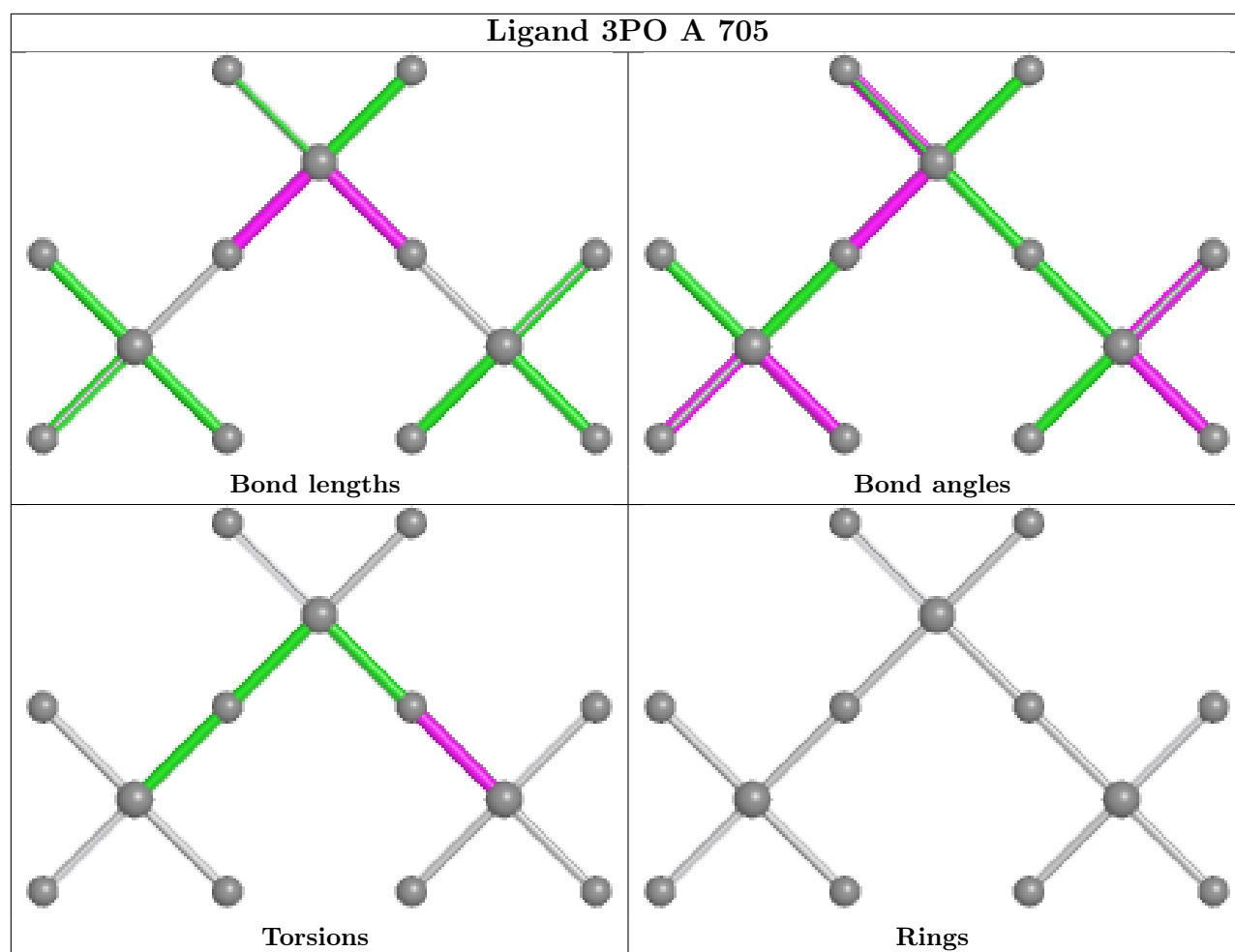
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	3PO	1	0
2	A	701	DGT	4	0
2	D	800	DGT	2	0
2	C	703	DGT	1	0
2	B	703	DGT	1	0

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

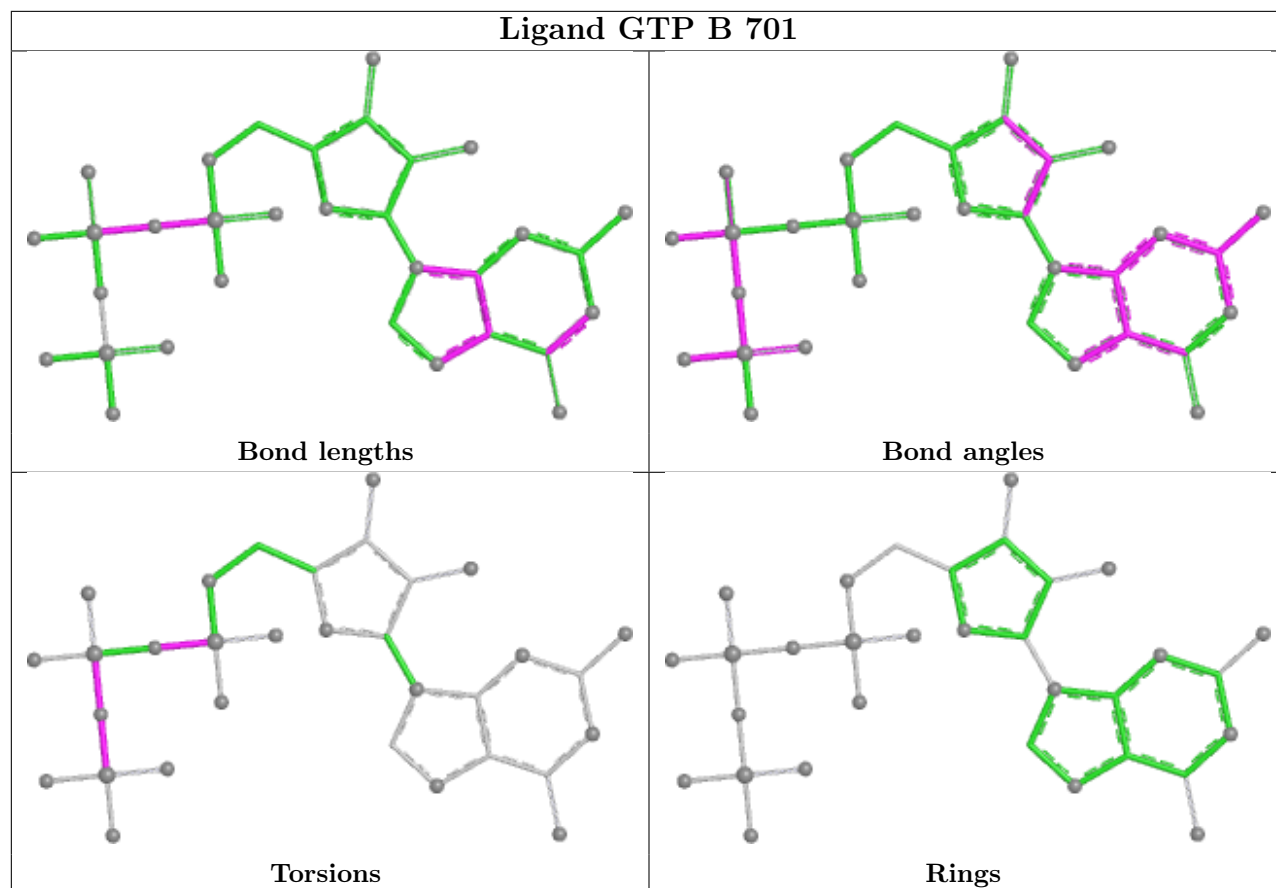
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



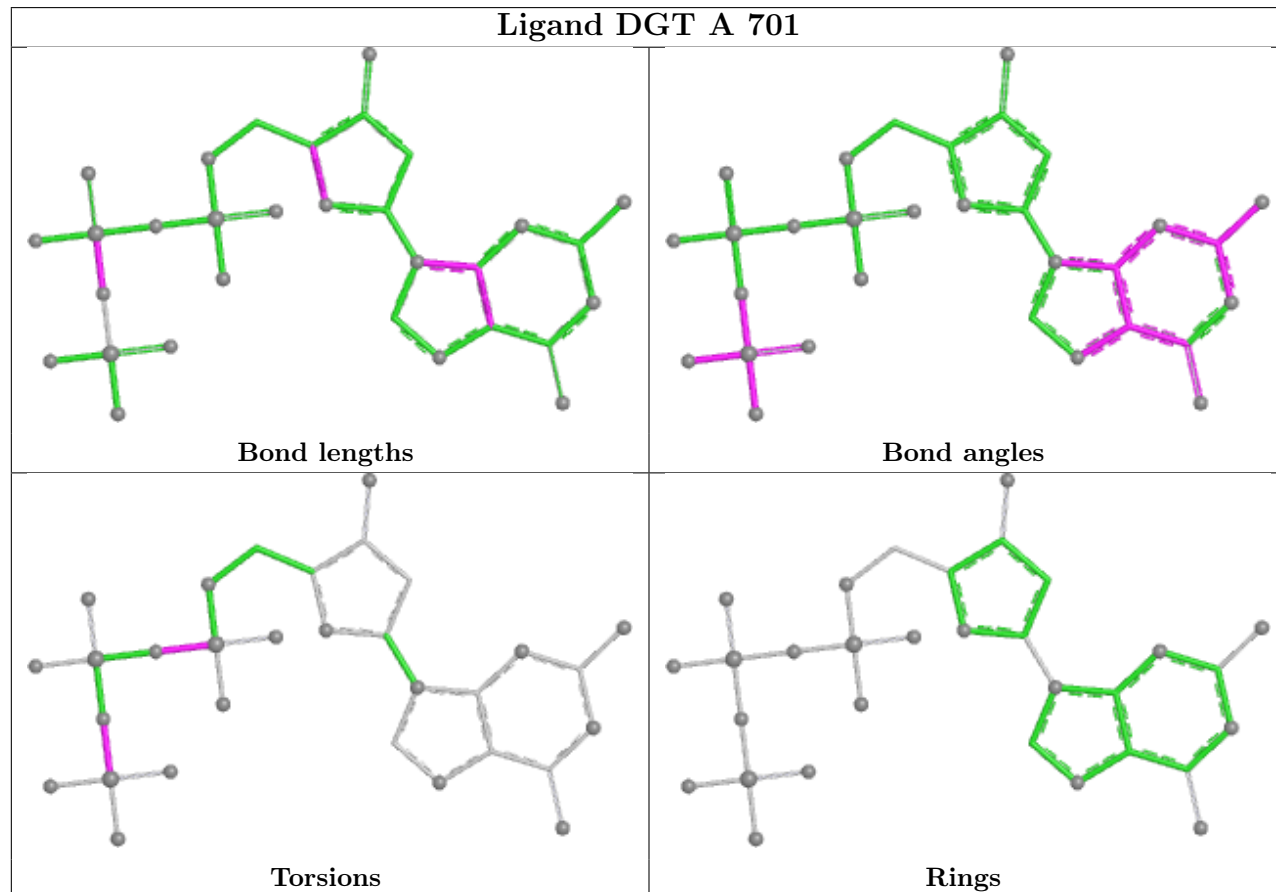


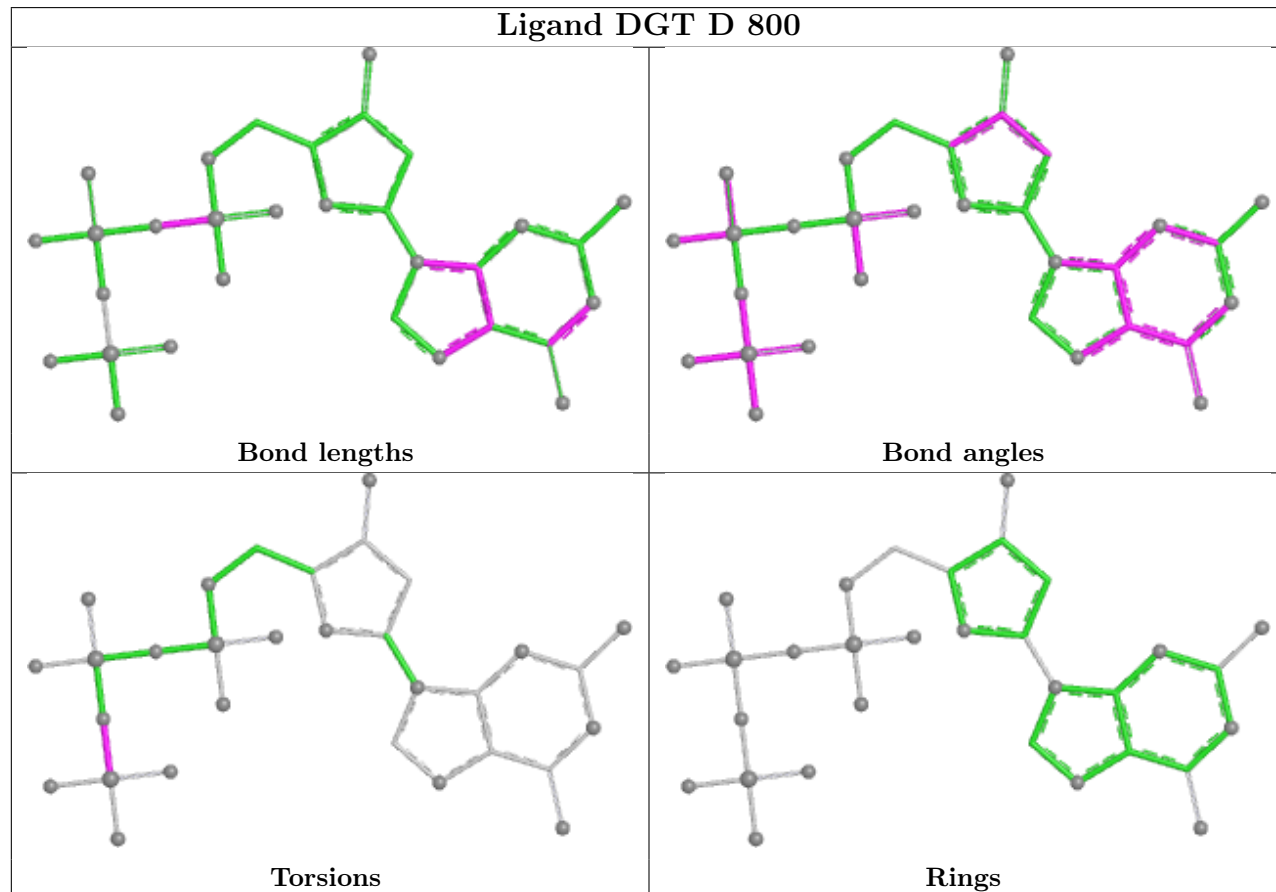
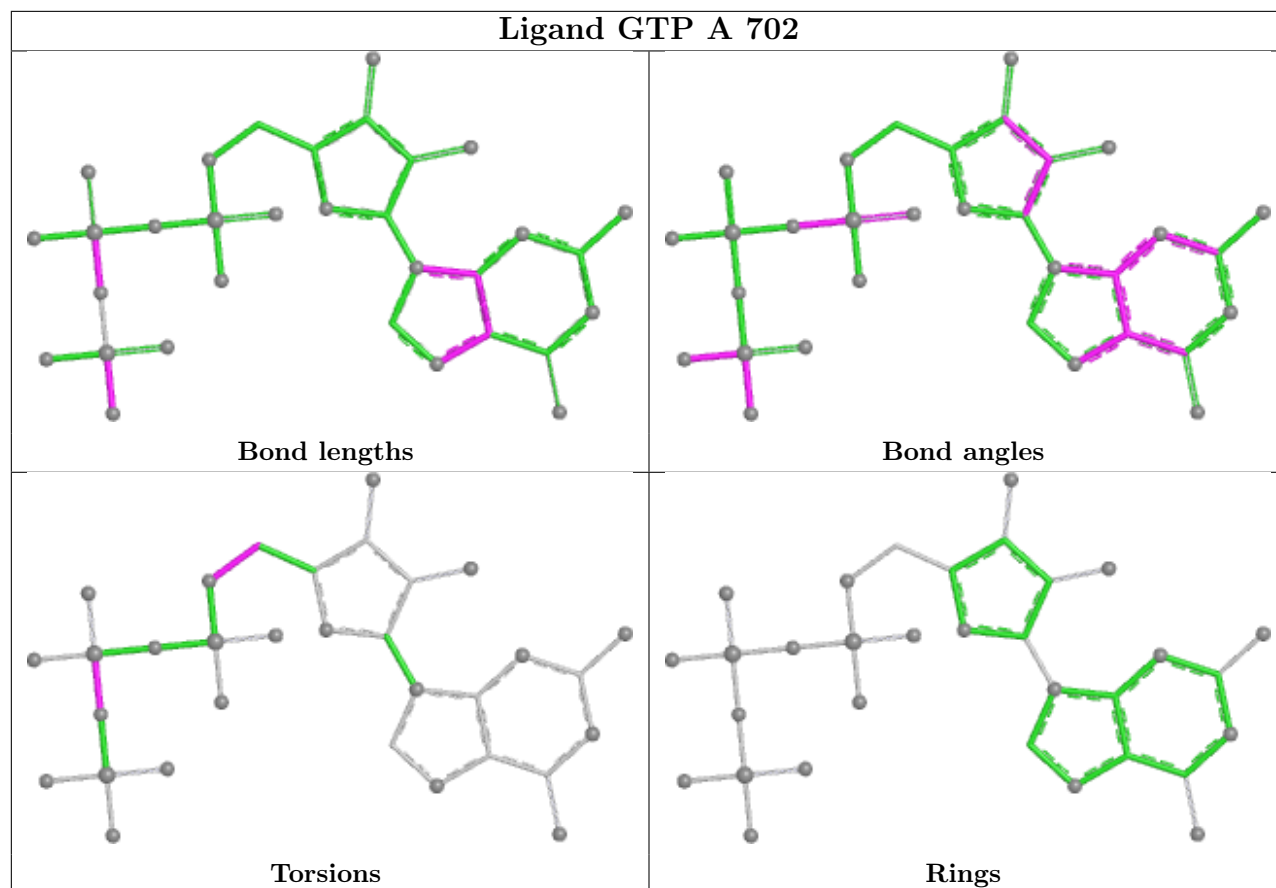


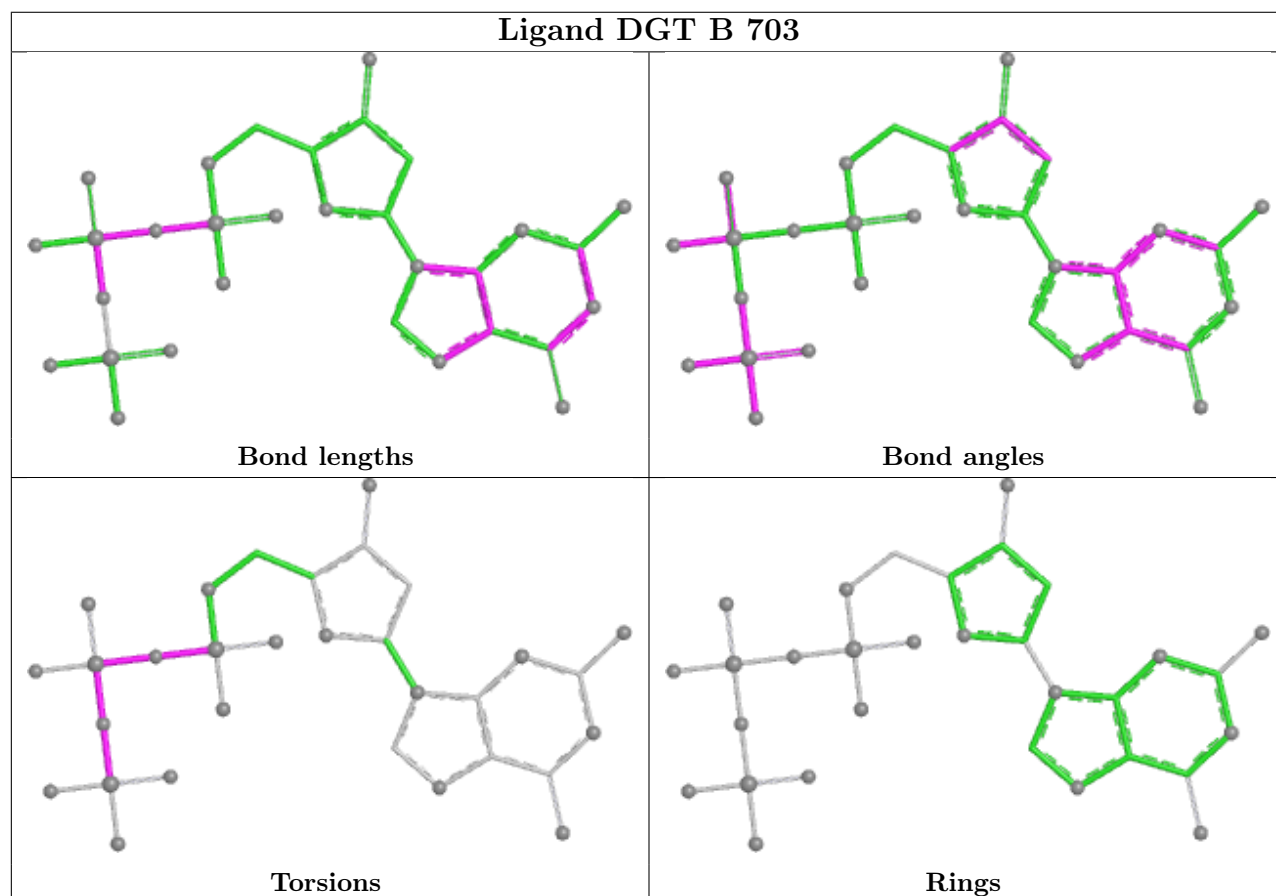
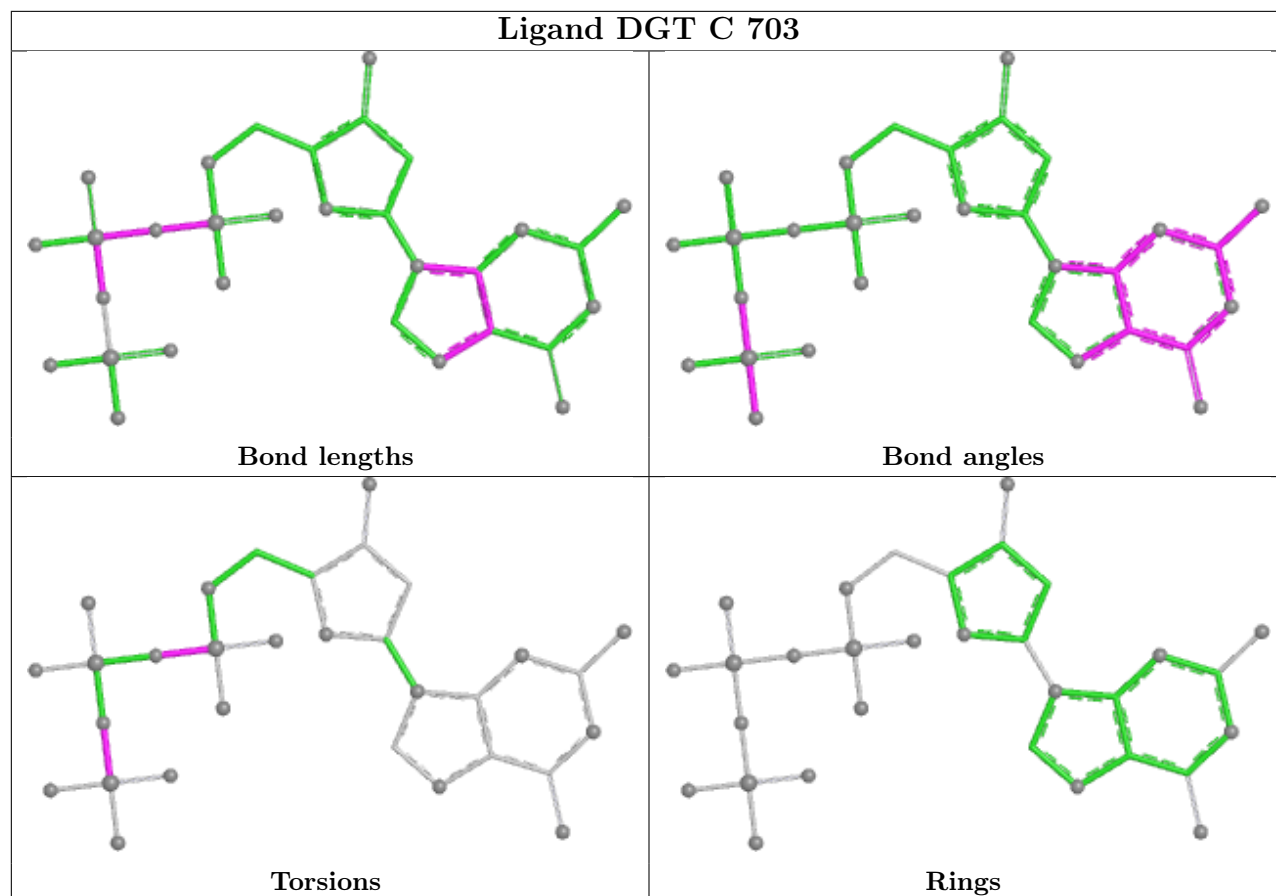
Ligand GTP B 701



Ligand DGT 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	481/514 (93%)	-0.12	5 (1%) 79 81	18, 44, 71, 98	3 (0%)
1	B	479/514 (93%)	0.06	4 (0%) 82 84	22, 54, 86, 113	3 (0%)
1	C	481/514 (93%)	0.20	12 (2%) 58 61	22, 55, 101, 129	2 (0%)
1	D	483/514 (93%)	-0.02	8 (1%) 69 71	18, 45, 86, 112	2 (0%)
All	All	1924/2056 (93%)	0.03	29 (1%) 72 73	18, 50, 88, 129	10 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	284	LEU	4.4
1	B	284	LEU	3.9
1	D	475	SER	3.0
1	A	466	ILE	3.0
1	C	466	ILE	3.0
1	C	491	VAL	2.9
1	A	284	LEU	2.7
1	D	466	ILE	2.5
1	A	599	ASN	2.5
1	D	472	ASP	2.5
1	C	489	LEU	2.4
1	D	465	GLN	2.4
1	A	328	ASN	2.4
1	A	467	LYS	2.4
1	C	495	ALA	2.3
1	D	463	THR	2.3
1	B	328	ASN	2.3
1	C	463	THR	2.3
1	B	488	LEU	2.2
1	C	554	CYS	2.2
1	D	464	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	488	LEU	2.1
1	C	485	PRO	2.1
1	B	276	LEU	2.1
1	C	487	VAL	2.1
1	C	562	LEU	2.0
1	C	599	ASN	2.0
1	D	328	ASN	2.0
1	D	345	ASN	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.

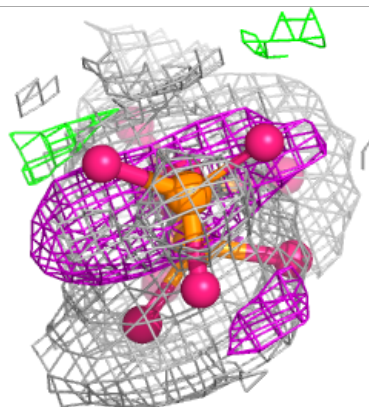
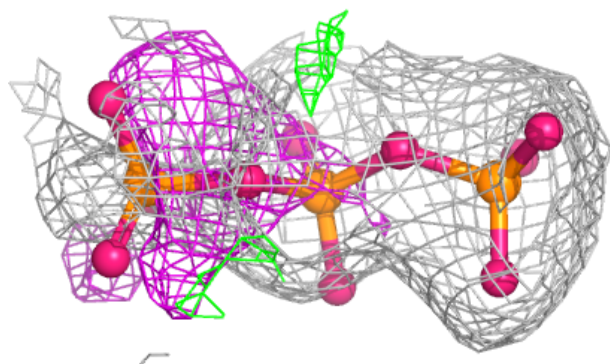
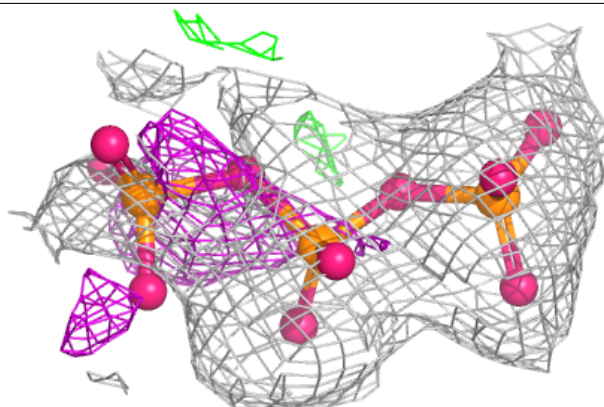
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	3PO	A	705	13/13	0.84	0.13	62,89,154,155	0
2	DGT	C	703	31/31	0.97	0.05	37,40,48,49	0
2	DGT	A	701	31/31	0.98	0.05	31,34,38,39	0
2	DGT	D	800	31/31	0.98	0.05	34,36,38,38	0
3	GTP	A	702	32/32	0.98	0.04	30,31,34,35	0
3	GTP	A	704	32/32	0.98	0.05	29,30,32,32	0
3	GTP	B	701	32/32	0.98	0.05	37,40,44,45	0
3	GTP	C	704	32/32	0.98	0.05	36,43,49,50	0
2	DGT	B	703	31/31	0.98	0.05	29,30,34,36	0
4	MG	B	702	1/1	0.99	0.03	49,49,49,49	0
4	MG	C	702	1/1	0.99	0.03	49,49,49,49	0
4	MG	A	703	1/1	0.99	0.03	34,34,34,34	0
4	MG	C	701	1/1	1.00	0.04	43,43,43,43	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.

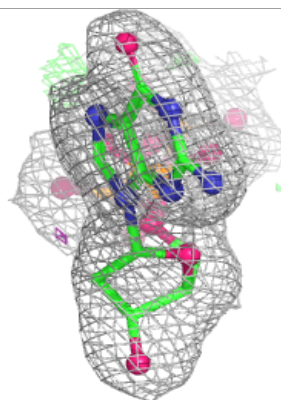
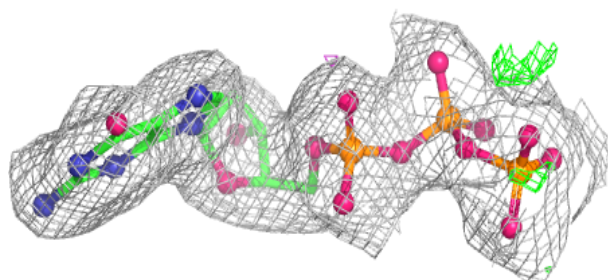
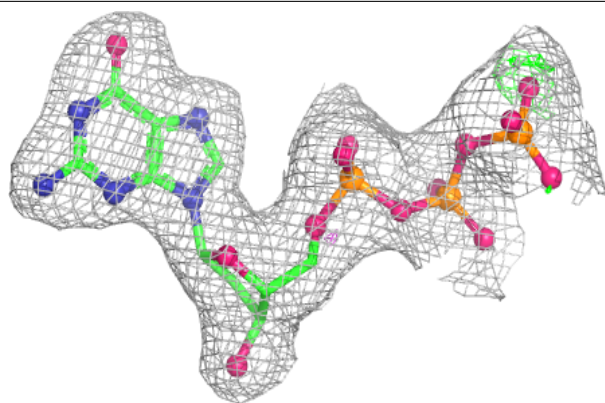
Electron density around 3PO A 705:

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

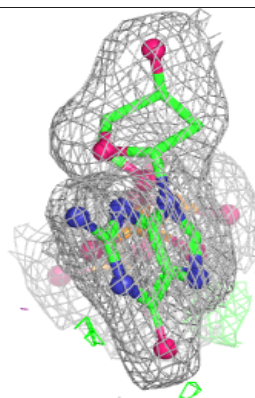
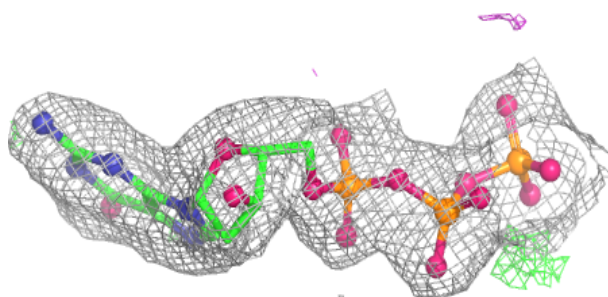
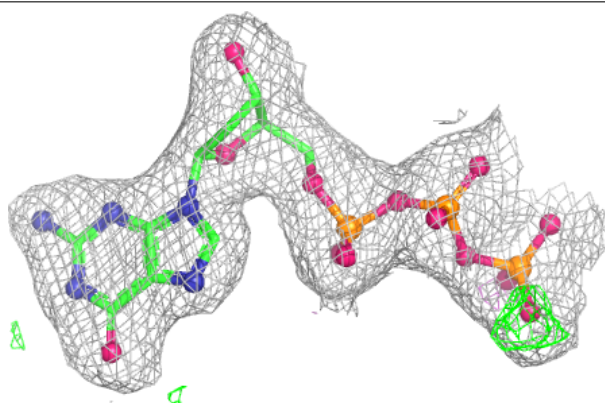


Electron density around DGT C 703:

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

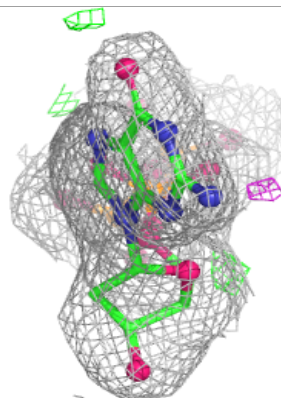
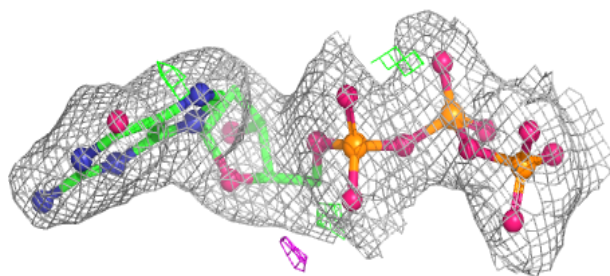
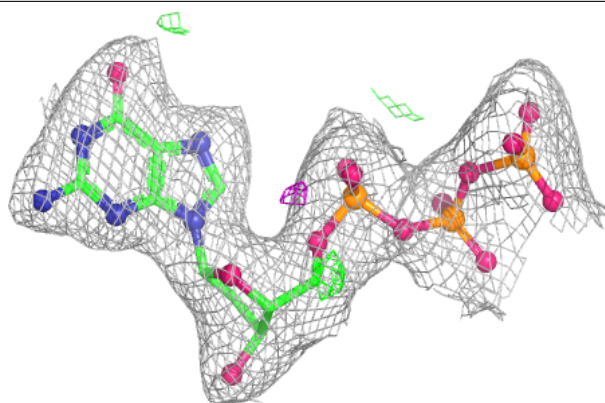
**Electron density around DGT A 701:**

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

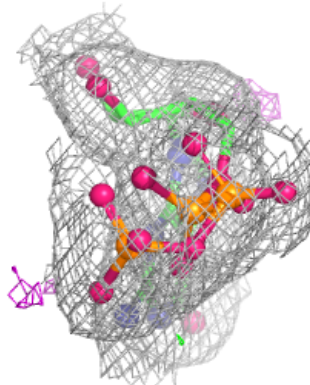
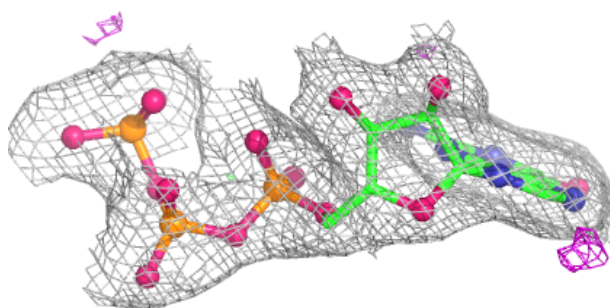
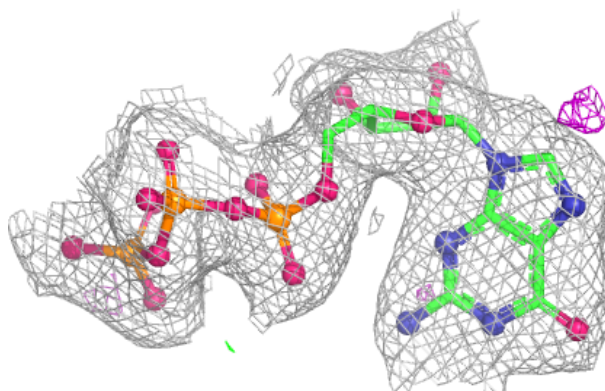


Electron density around DGT D 800:

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

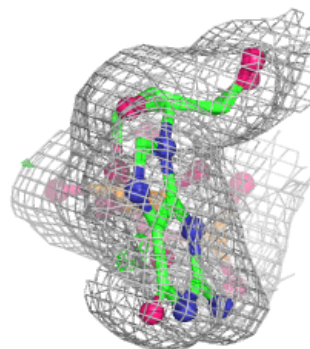
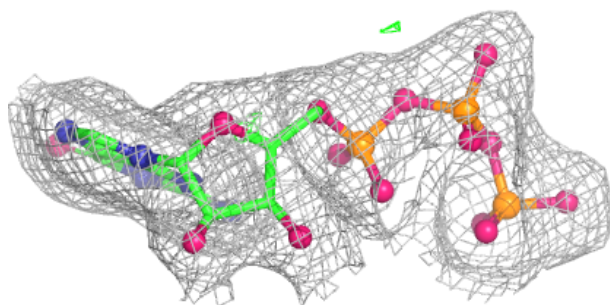
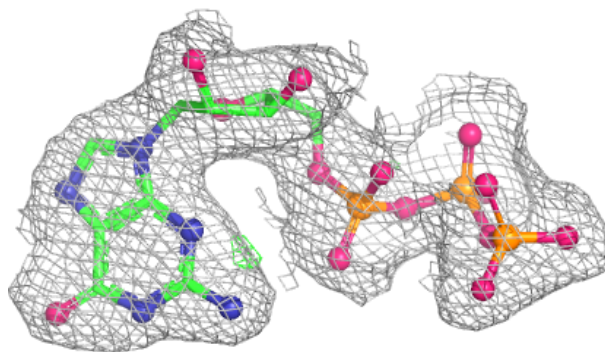
**Electron density around GTP A 702:**

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

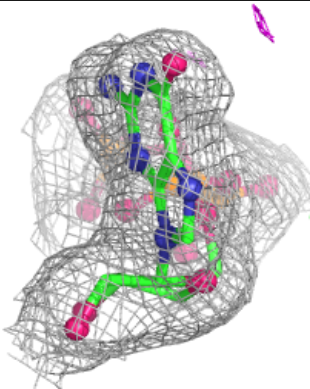
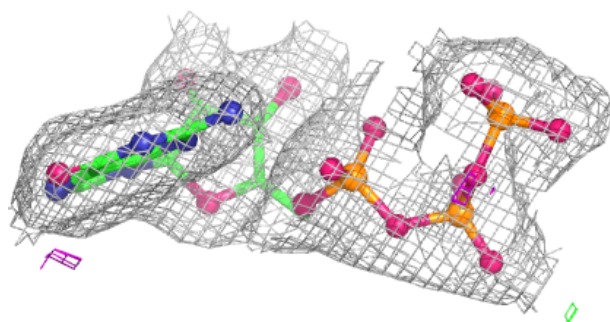
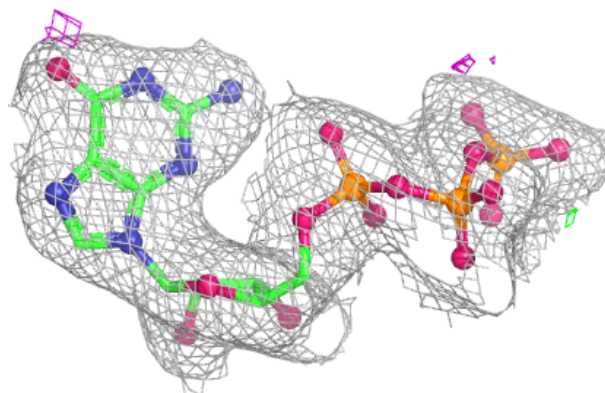


Electron density around GTP A 704:

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

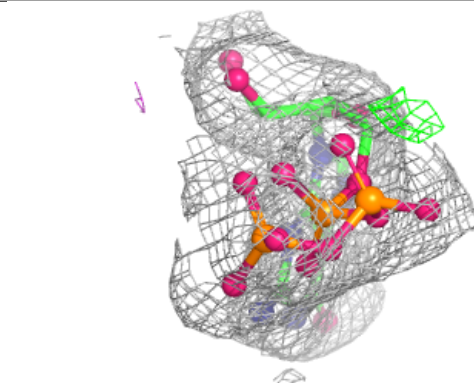
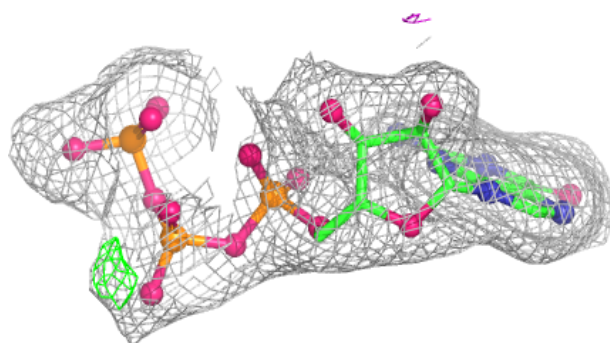
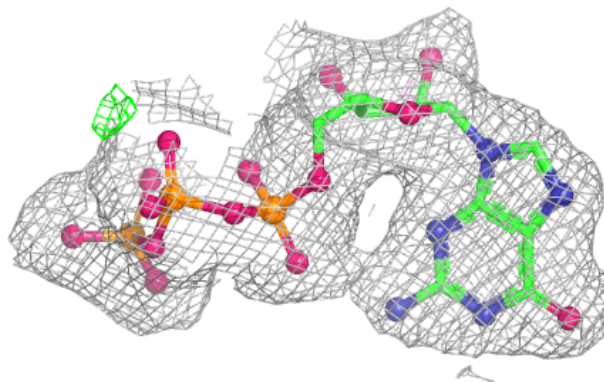
**Electron density around GTP B 701:**

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

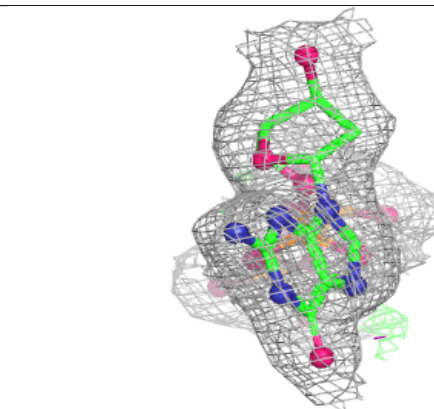
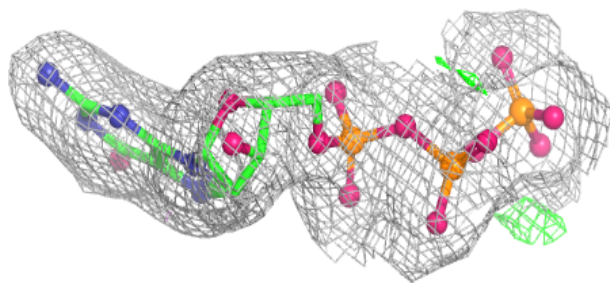
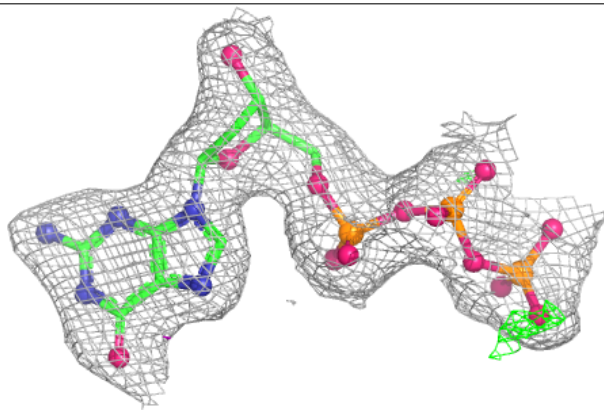


Electron density around GTP C 704:

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

**Electron density around DGT 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.