



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2022 – 06:37 PM EDT

PDB ID : 4TO5
Title : Structure basis of cellular dNTP regulation, SAMHD1-GTP-dTTP-dCTP complex
Authors : Ji, X.; Tang, C.; Zhao, Q.; Wang, W.; Xiong, Y.
Deposited on : 2014-06-05
Resolution : 2.80 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 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 : 2.27
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) : 2.27

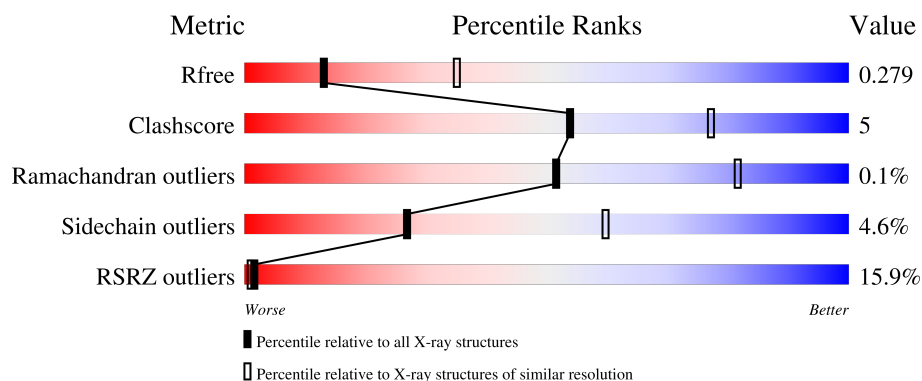
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	<div> <div>16%</div> <div>81% 10% • 7%</div> </div>
1	B	514	<div> <div>18%</div> <div>81% 11% • 7%</div> </div>
1	C	514	<div> <div>11%</div> <div>81% 12% • 7%</div> </div>
1	D	514	<div> <div>15%</div> <div>83% 9% • 7%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16073 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.

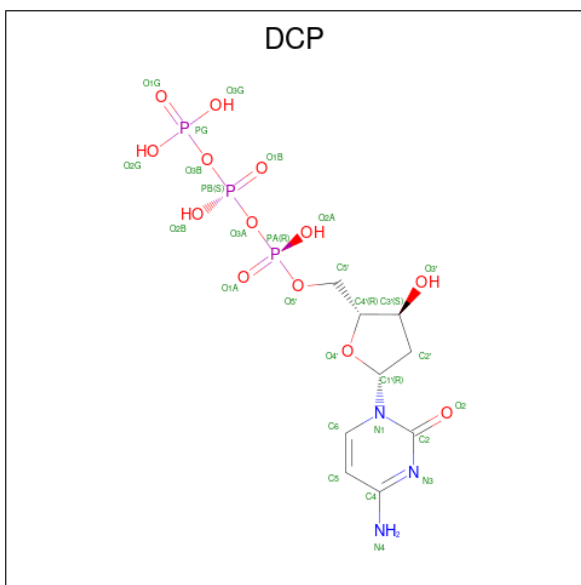
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3932	2517	684	711	20			
1	C	479	Total	C	N	O	S	0	1	0
			3922	2511	684	706	21			
1	D	480	Total	C	N	O	S	0	2	0
			3933	2518	684	710	21			
1	B	480	Total	C	N	O	S	0	0	0
			3922	2512	683	707	20			

There are 8 discrepancies between the modelled and reference sequences:

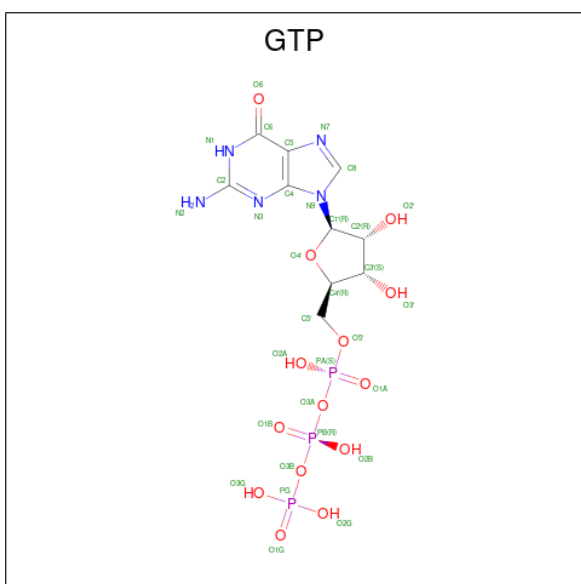
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation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

- Molecule 2 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



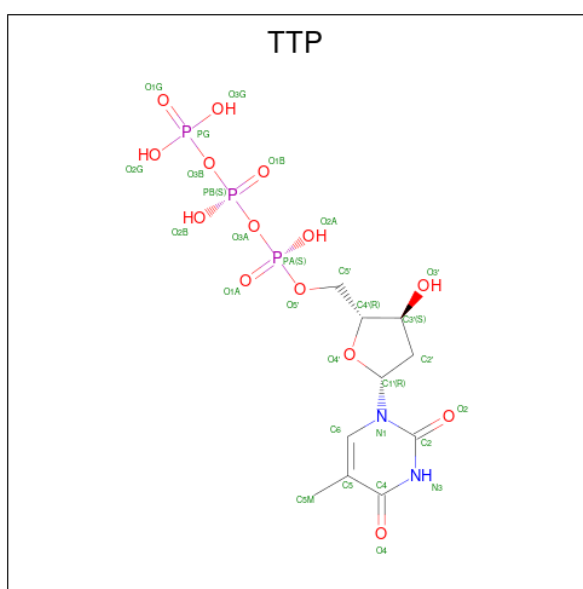
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	C	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	D	1	Total 28	C 9	N 3	O 13	P 3	0	0
2	B	1	Total 28	C 9	N 3	O 13	P 3	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: 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 32	C 10	N 5	O 14	P 3	0	0
3	D	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	B	1	Total 32	C 10	N 5	O 14	P 3	0	0
3	B	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 4 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_2\text{O}_{14}\text{P}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total 29	C 10	N 2	O 14	P 3	0	0
4	C	1	Total 29	C 10	N 2	O 14	P 3	0	0
4	D	1	Total 29	C 10	N 2	O 14	P 3	0	0
4	B	1	Total 29	C 10	N 2	O 14	P 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Mg 1	0	0
5	D	1	Total 1	Mg 1	0	0

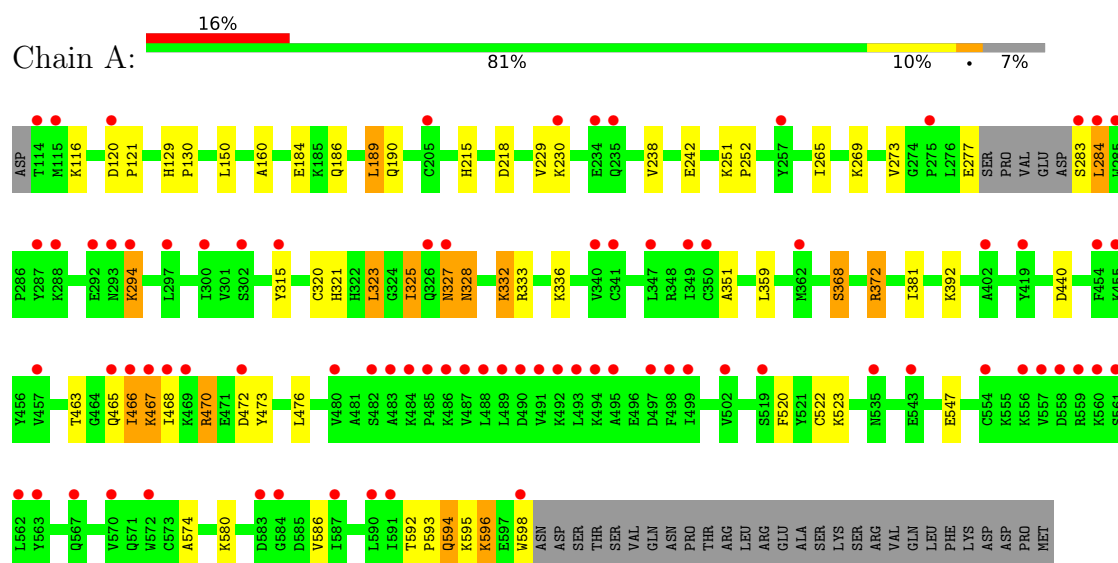
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	O 1	0	0
6	C	1	Total 1	O 1	0	0
6	D	1	Total 1	O 1	0	0
6	B	1	Total 1	O 1	0	0

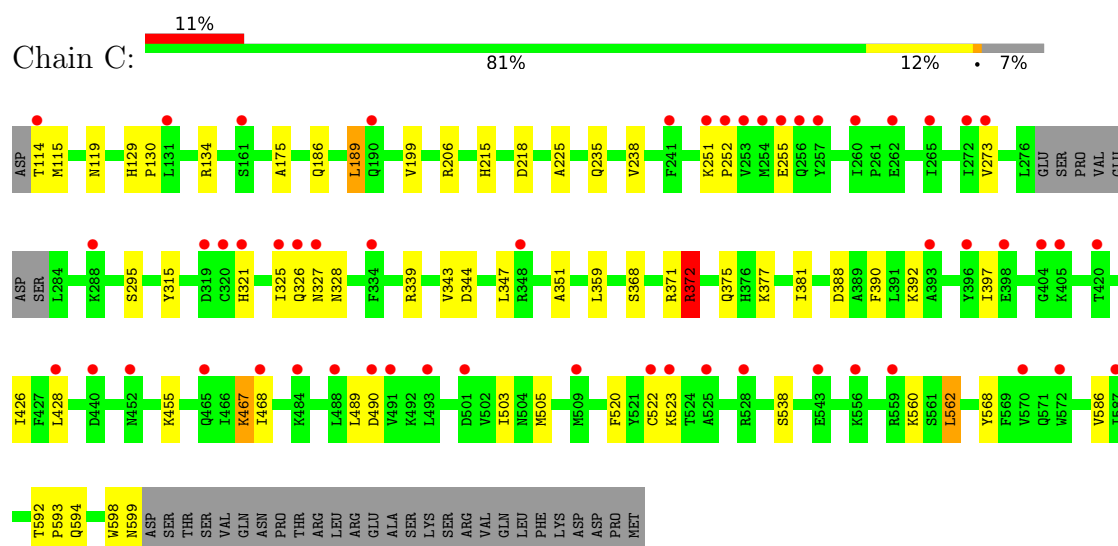
3 Residue-property plots

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.

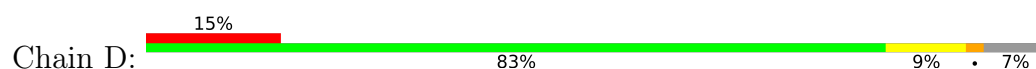
• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

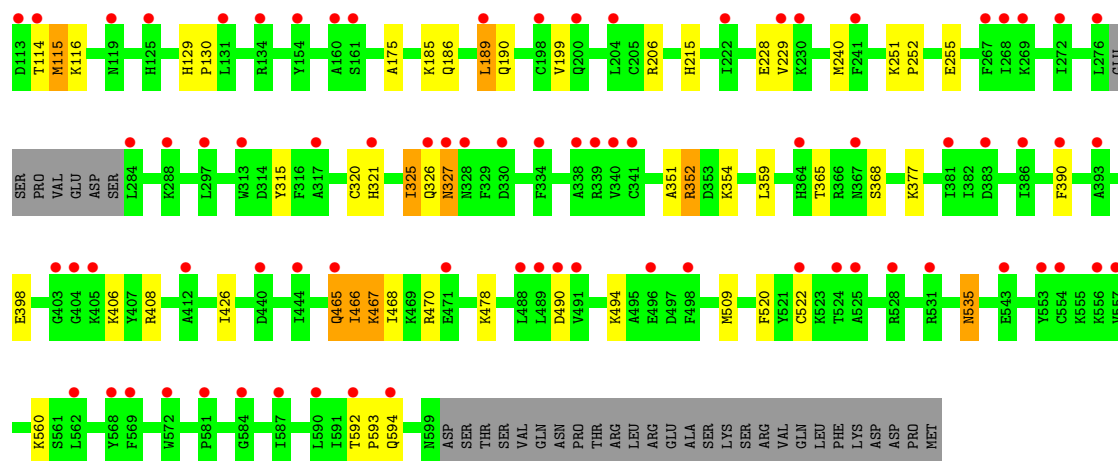


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

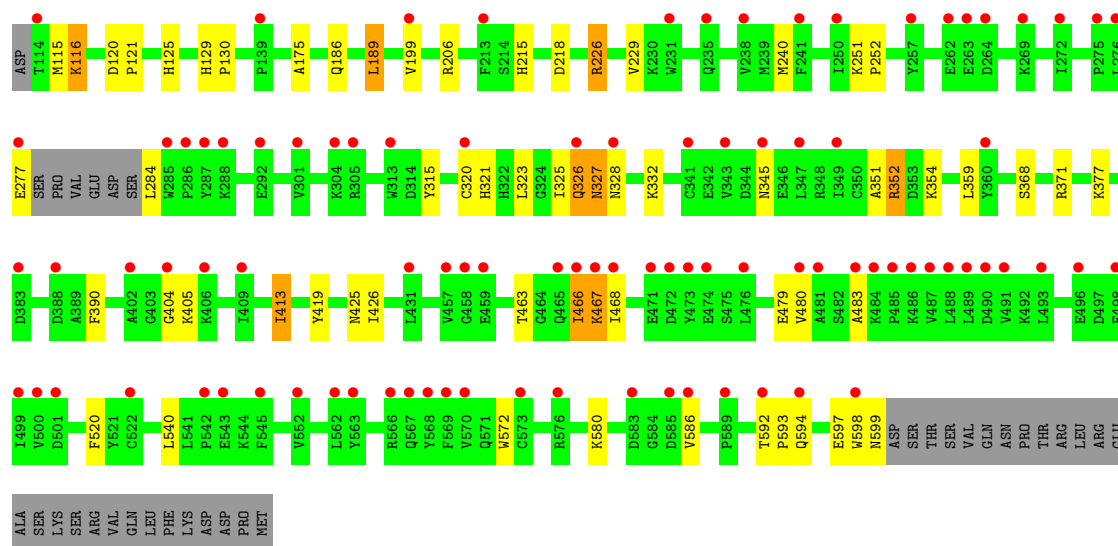
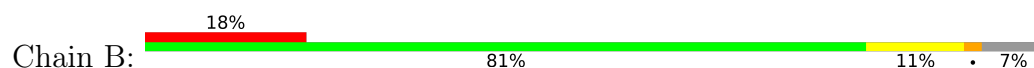


• Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





• 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	86.46Å 145.12Å 98.23Å 90.00° 114.13° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.39 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.80) 96.6 (48.39-2.73)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.271 , 0.285 0.266 , 0.279	Depositor DCC
R_{free} test set	2852 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16073	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: TTP, GTP, DCP, 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	0.56	0/4024	0.70	2/5431 (0.0%)
1	B	0.60	0/4014	0.75	7/5418 (0.1%)
1	C	0.56	0/4014	0.71	3/5418 (0.1%)
1	D	0.58	0/4025	0.72	3/5433 (0.1%)
All	All	0.57	0/16077	0.72	15/21700 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	LYS	CD-CE-NZ	7.83	129.70	111.70
1	B	371	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	B	352	ARG	CG-CD-NE	-7.02	97.05	111.80
1	D	352	ARG	CG-CD-NE	-6.81	97.51	111.80
1	D	470	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	115	MET	CG-SD-CE	6.46	110.53	100.20
1	A	372	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	B	226	ARG	CG-CD-NE	6.12	124.66	111.80
1	B	483	ALA	N-CA-C	5.70	126.38	111.00
1	B	226	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	D	470	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	372	ARG	CG-CD-NE	5.32	122.97	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	371	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	B	371	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	B	405	LYS	N-CA-CB	-5.01	101.59	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	404	GLY	Peptide

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	3932	0	3920	63	0
1	B	3922	0	3913	46	0
1	C	3922	0	3915	38	1
1	D	3933	0	3916	30	1
2	A	28	0	12	7	0
2	B	28	0	12	5	0
2	C	28	0	12	0	0
2	D	28	0	12	1	0
3	A	32	0	12	1	0
3	B	64	0	24	0	0
3	D	32	0	12	2	0
4	A	29	0	13	2	0
4	B	29	0	13	2	0
4	C	29	0	13	1	0
4	D	29	0	13	1	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	1	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	16073	0	15812	169	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (169) 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:390:PHE:CZ	1:D:426:ILE:HD11	1.78	1.18
1:A:283:SER:HB2	1:A:284:LEU:CA	1.84	1.07
1:A:283:SER:CB	1:A:284:LEU:HA	1.89	1.03
1:A:466:ILE:H	1:A:466:ILE:HD12	0.90	1.03
1:D:390:PHE:CE2	1:D:426:ILE:HD11	1.94	1.02
1:A:466:ILE:H	1:A:466:ILE:CD1	1.70	1.02
1:A:283:SER:HB2	1:A:284:LEU:HA	1.04	1.00
1:A:466:ILE:HD12	1:A:466:ILE:N	1.74	1.00
1:A:463:THR:O	1:A:466:ILE:HD13	1.63	0.98
1:A:470:ARG:HB2	1:A:470:ARG:NH1	1.87	0.90
1:D:390:PHE:CZ	1:D:426:ILE:CD1	2.55	0.89
1:A:328:ASN:HD21	1:C:326:GLN:HE21	1.20	0.89
1:A:215:HIS:HE1	2:A:701:DCP:O4'	1.56	0.88
1:C:490:ASP:OD2	1:C:560:LYS:HE2	1.74	0.86
1:A:473:TYR:HA	1:A:476:LEU:CD1	2.06	0.85
1:B:463:THR:O	1:B:466:ILE:HG12	1.76	0.84
1:A:463:THR:O	1:A:466:ILE:CD1	2.26	0.84
1:A:215:HIS:CE1	2:A:701:DCP:O4'	2.33	0.81
1:B:466:ILE:N	1:B:466:ILE:HD13	1.95	0.81
1:D:115:MET:C	1:D:115:MET:SD	2.59	0.80
1:A:473:TYR:HA	1:A:476:LEU:HD13	1.64	0.80
1:D:377:LYS:NZ	4:B:702:TTP:O2B	2.16	0.78
1:B:215:HIS:CD2	2:B:703:DCP:C6	2.67	0.77
1:A:470:ARG:HB2	1:A:470:ARG:CZ	2.14	0.76
1:A:522:CYS:SG	1:C:586:VAL:HG11	2.28	0.73
1:D:466:ILE:HD13	1:D:466:ILE:N	2.05	0.72
1:A:470:ARG:HA	1:A:473:TYR:CE2	2.24	0.72
1:A:328:ASN:HD22	1:A:328:ASN:C	1.94	0.71
1:C:327:ASN:O	1:C:328:ASN:HB2	1.92	0.70
1:B:390:PHE:CE2	1:B:426:ILE:HD11	2.26	0.70
1:A:472:ASP:O	1:A:476:LEU:HD12	1.92	0.69
1:A:215:HIS:CE1	2:A:701:DCP:C6	2.76	0.69
4:A:703:TTP:O4	1:C:372:ARG:HG2	1.94	0.67
1:B:326:GLN:O	1:B:326:GLN:HG3	1.94	0.67
1:A:470:ARG:CZ	1:A:470:ARG:CB	2.73	0.66
1:A:320:CYS:SG	1:A:327:ASN:O	2.53	0.65
1:A:190:GLN:O	1:A:294:LYS:NZ	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:GLU:OE2	1:D:406:LYS:HD3	1.98	0.64
1:D:326:GLN:O	1:D:327:ASN:CB	2.47	0.63
1:A:265:ILE:O	1:A:269:LYS:HG3	1.98	0.63
1:D:490:ASP:OD2	1:D:560:LYS:HD3	2.00	0.62
1:A:238:VAL:O	1:A:242:GLU:HG3	2.00	0.62
1:A:328:ASN:C	1:A:328:ASN:ND2	2.52	0.62
1:B:466:ILE:HD13	1:B:466:ILE:H	1.65	0.61
1:B:215:HIS:CE1	2:B:703:DCP:O2A	2.52	0.61
1:B:466:ILE:N	1:B:466:ILE:CD1	2.62	0.61
1:A:586:VAL:HG11	1:C:522[A]:CYS:SG	2.40	0.60
1:D:535:ASN:OD1	1:D:535:ASN:N	2.31	0.60
1:A:596:LYS:N	1:A:596:LYS:CD	2.63	0.60
1:C:235:GLN:O	1:C:238:VAL:HG22	2.01	0.60
1:A:215:HIS:ND1	2:A:701:DCP:C6	2.65	0.59
1:B:327:ASN:HD22	1:B:328:ASN:N	1.99	0.59
1:A:392:LYS:NZ	1:A:440:ASP:OD1	2.35	0.59
1:C:321:HIS:CE1	1:B:321:HIS:CE1	2.91	0.59
4:A:703:TTP:O1B	1:C:377:LYS:NZ	2.34	0.58
1:A:472:ASP:O	1:A:476:LEU:CD1	2.51	0.57
1:C:372:ARG:HG2	1:C:372:ARG:HH21	1.68	0.57
1:A:473:TYR:CA	1:A:476:LEU:CD1	2.81	0.57
1:B:413:ILE:CD1	1:B:419:TYR:CE1	2.88	0.56
1:D:215:HIS:CD2	2:D:702:DCP:C6	2.89	0.56
1:C:375:GLN:HG3	1:C:505:MET:CE	2.36	0.55
1:A:470:ARG:HA	1:A:473:TYR:CD2	2.42	0.55
1:A:116:LYS:NZ	3:D:703:GTP:O2A	2.39	0.55
1:C:388:ASP:OD2	1:C:392:LYS:HE3	2.06	0.55
1:C:455:LYS:HG3	1:C:562:LEU:HD11	1.89	0.55
1:D:390:PHE:CE1	1:D:426:ILE:CD1	2.89	0.55
1:D:465:GLN:HA	1:D:465:GLN:OE1	2.07	0.55
1:C:119:ASN:ND2	1:B:323:LEU:O	2.40	0.55
1:D:522[A]:CYS:SG	1:B:586:VAL:HG11	2.47	0.54
1:A:596:LYS:N	1:A:596:LYS:HD3	2.22	0.54
1:C:467:LYS:HG3	1:C:468:ILE:N	2.24	0.53
6:A:801:HOH:O	1:B:116:LYS:HE2	2.08	0.53
1:A:547:GLU:OE1	1:C:538:SER:OG	2.24	0.52
1:B:467:LYS:HG3	1:B:468:ILE:N	2.24	0.52
4:D:704:TTP:O1B	1:B:377:LYS:NZ	2.42	0.51
1:B:327:ASN:HD22	1:B:328:ASN:H	1.58	0.51
1:C:428:LEU:HD13	1:B:425:ASN:HB2	1.93	0.51
1:A:238:VAL:HG13	1:A:269:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLN:O	1:B:326:GLN:CG	2.59	0.50
1:A:592:THR:OG1	1:A:593:PRO:HD3	2.12	0.50
1:A:467:LYS:HG3	1:A:468:ILE:N	2.27	0.50
1:D:467:LYS:HG3	1:D:468:ILE:N	2.26	0.49
1:A:476:LEU:HD12	1:A:476:LEU:H	1.76	0.49
1:D:390:PHE:CE1	1:D:426:ILE:HD12	2.47	0.49
1:A:129:HIS:CG	1:A:130:PRO:HD2	2.47	0.49
1:C:592:THR:OG1	1:C:593:PRO:HD3	2.12	0.49
1:D:592:THR:OG1	1:D:593:PRO:HD3	2.13	0.49
1:B:351:ALA:O	1:B:520:PHE:HA	2.13	0.49
1:A:368:SER:O	1:A:372:ARG:HG3	2.12	0.48
3:A:702:GTP:O2A	1:D:116:LYS:HE3	2.13	0.48
1:B:592:THR:OG1	1:B:593:PRO:HD3	2.13	0.48
1:C:489:LEU:CD1	1:C:568:TYR:HE2	2.27	0.48
1:A:215:HIS:NE2	2:A:701:DCP:O1A	2.46	0.48
1:C:129:HIS:CG	1:C:130:PRO:HD2	2.49	0.47
1:D:351:ALA:O	1:D:520:PHE:HA	2.15	0.47
1:D:115:MET:SD	1:D:115:MET:O	2.72	0.47
1:B:129:HIS:CG	1:B:130:PRO:HD2	2.50	0.47
1:B:463:THR:O	1:B:466:ILE:CG1	2.54	0.47
1:D:186:GLN:HB2	1:D:189:LEU:HD22	1.97	0.47
1:D:129:HIS:CG	1:D:130:PRO:HD2	2.50	0.47
2:A:701:DCP:O2G	2:A:701:DCP:O2B	2.32	0.46
1:B:226:ARG:NH2	1:B:229:VAL:HG21	2.30	0.46
1:D:466:ILE:N	1:D:466:ILE:CD1	2.74	0.46
1:A:320:CYS:HB3	1:A:325:ILE:O	2.16	0.46
1:B:390:PHE:CE2	1:B:426:ILE:CD1	2.98	0.46
1:A:215:HIS:ND1	2:A:701:DCP:N1	2.64	0.46
1:B:390:PHE:CZ	1:B:426:ILE:CD1	2.99	0.46
1:B:390:PHE:CZ	1:B:426:ILE:HD11	2.51	0.46
1:C:397:ILE:HG21	1:C:426:ILE:HD11	1.96	0.45
1:A:351:ALA:O	1:A:520:PHE:HA	2.16	0.45
1:A:277:GLU:O	1:A:277:GLU:HG3	2.16	0.45
1:C:598:TRP:O	1:C:599:ASN:CB	2.64	0.45
1:A:150:LEU:CD1	1:A:323:LEU:HD21	2.47	0.45
1:A:574:ALA:HB1	1:A:595:LYS:HD2	1.99	0.45
1:C:351:ALA:O	1:C:520:PHE:HA	2.16	0.45
1:B:186:GLN:HB2	1:B:189:LEU:HD22	1.98	0.45
1:A:251:LYS:HB2	1:A:252:PRO:HD3	1.99	0.45
1:B:320:CYS:SG	1:B:327:ASN:O	2.72	0.45
1:A:160:ALA:HB2	1:A:323:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:THR:N	1:D:593:PRO:CD	2.80	0.45
1:A:592:THR:N	1:A:593:PRO:CD	2.80	0.44
1:B:592:THR:N	1:B:593:PRO:CD	2.81	0.44
1:A:215:HIS:HA	1:A:218:ASP:OD2	2.17	0.44
1:C:186:GLN:HB2	1:C:189:LEU:HD22	1.98	0.44
1:C:598:TRP:O	1:C:599:ASN:HB2	2.17	0.44
1:B:120:ASP:OD2	1:B:121:PRO:HD2	2.17	0.44
1:D:251:LYS:HB2	1:D:252:PRO:HD3	2.00	0.44
1:D:320:CYS:HB3	1:D:325:ILE:O	2.18	0.44
1:C:390:PHE:CZ	1:C:426:ILE:CG2	3.01	0.44
1:C:592:THR:N	1:C:593:PRO:CD	2.81	0.44
1:B:251:LYS:HB2	1:B:252:PRO:HD3	2.00	0.44
1:B:320:CYS:HB3	1:B:325:ILE:O	2.18	0.44
1:D:352:ARG:HG3	1:D:354:LYS:HG2	2.00	0.44
1:C:215:HIS:HA	1:C:218:ASP:OD2	2.18	0.43
1:C:372:ARG:HH21	1:C:372:ARG:CG	2.31	0.43
1:C:327:ASN:O	1:C:328:ASN:CB	2.59	0.43
1:A:186:GLN:HB2	1:A:189:LEU:HD22	1.99	0.43
1:B:215:HIS:CD2	2:B:703:DCP:N1	2.86	0.43
1:A:332:LYS:NZ	1:A:336:LYS:HE2	2.34	0.43
1:C:343:VAL:O	1:C:344:ASP:HB2	2.18	0.43
1:B:352:ARG:HG3	1:B:354:LYS:HG2	2.00	0.43
1:A:120:ASP:OD2	1:A:121:PRO:HD2	2.19	0.43
1:C:375:GLN:HG3	1:C:505:MET:HE2	1.99	0.43
1:B:215:HIS:HE2	2:B:703:DCP:PA	2.41	0.43
1:A:372:ARG:HD2	4:C:701:TTP:O4	2.18	0.43
1:B:175:ALA:HB1	1:B:199:VAL:HG12	2.01	0.43
1:B:215:HIS:HA	1:B:218:ASP:OD2	2.19	0.42
1:C:295:SER:OG	1:C:347:LEU:O	2.37	0.42
1:B:598:TRP:O	1:B:599:ASN:CB	2.67	0.42
1:B:215:HIS:NE2	2:B:703:DCP:O2A	2.52	0.42
1:B:480:VAL:HG22	1:B:572:TRP:CD2	2.55	0.42
1:B:479:GLU:HB3	1:B:572:TRP:HE1	1.85	0.42
1:C:375:GLN:HG3	1:C:505:MET:HE1	2.02	0.42
1:A:381:ILE:HD12	1:A:381:ILE:HA	1.93	0.41
1:B:598:TRP:O	1:B:599:ASN:HB2	2.20	0.41
1:A:283:SER:HB2	1:A:284:LEU:C	2.35	0.41
1:D:175:ALA:HB1	1:D:199:VAL:HG12	2.03	0.41
1:A:321:HIS:CE1	1:D:321:HIS:NE2	2.89	0.41
1:A:333:ARG:HB2	1:B:125:HIS:CE1	2.56	0.41
1:C:175:ALA:HB1	1:C:199:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:LYS:HB2	1:C:252:PRO:HD3	2.02	0.41
1:A:580:LYS:HD2	1:A:598:TRP:HB3	2.03	0.41
1:D:327:ASN:O	1:D:365:THR:HG21	2.21	0.41
3:D:703:GTP:H5''	4:B:702:TTP:O1B	2.20	0.41
1:A:594:GLN:O	1:A:596:LYS:HE2	2.21	0.41
1:C:381:ILE:HD12	1:C:381:ILE:HA	1.94	0.41
1:C:503:ILE:HG21	1:C:505:MET:HE2	2.02	0.41
1:B:597:GLU:OE1	1:B:597:GLU:N	2.37	0.40
1:B:580:LYS:HD2	1:B:598:TRP:HB3	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ALA:O	1:D:494:LYS:NZ[1_656]	1.87	0.33

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	477/514 (93%)	469 (98%)	8 (2%)	0	100	100
1	B	476/514 (93%)	468 (98%)	8 (2%)	0	100	100
1	C	476/514 (93%)	468 (98%)	8 (2%)	0	100	100
1	D	478/514 (93%)	470 (98%)	7 (2%)	1 (0%)	47	78
All	All	1907/2056 (93%)	1875 (98%)	31 (2%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	ASN

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	427/459 (93%)	406 (95%)	21 (5%)	25	57
1	B	425/459 (93%)	406 (96%)	19 (4%)	27	60
1	C	426/459 (93%)	410 (96%)	16 (4%)	33	67
1	D	426/459 (93%)	404 (95%)	22 (5%)	23	55
All	All	1704/1836 (93%)	1626 (95%)	78 (5%)	27	60

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	189	LEU
1	A	229	VAL
1	A	230	LYS
1	A	273	VAL
1	A	284	LEU
1	A	315	TYR
1	A	323	LEU
1	A	325	ILE
1	A	327	ASN
1	A	328	ASN
1	A	332	LYS
1	A	359	LEU
1	A	368	SER
1	A	465	GLN
1	A	466	ILE
1	A	467	LYS
1	A	470	ARG
1	A	523	LYS
1	A	594	GLN
1	A	596	LYS
1	C	114	THR
1	C	134	ARG
1	C	189	LEU

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Mol	Chain	Res	Type
1	C	206	ARG
1	C	255	GLU
1	C	273	VAL
1	C	315	TYR
1	C	325	ILE
1	C	339	ARG
1	C	359	LEU
1	C	368	SER
1	C	372	ARG
1	C	467	LYS
1	C	523	LYS
1	C	562	LEU
1	C	594	GLN
1	D	114	THR
1	D	115	MET
1	D	185	LYS
1	D	189	LEU
1	D	190	GLN
1	D	206	ARG
1	D	228	GLU
1	D	229	VAL
1	D	240	MET
1	D	255	GLU
1	D	315	TYR
1	D	325	ILE
1	D	359	LEU
1	D	368	SER
1	D	408	ARG
1	D	465	GLN
1	D	466	ILE
1	D	467	LYS
1	D	478	LYS
1	D	509	MET
1	D	535	ASN
1	D	594	GLN
1	B	115	MET
1	B	116	LYS
1	B	189	LEU
1	B	206	ARG
1	B	240	MET
1	B	277	GLU
1	B	284	LEU

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Mol	Chain	Res	Type
1	B	315	TYR
1	B	326	GLN
1	B	327	ASN
1	B	332	LYS
1	B	345	ASN
1	B	359	LEU
1	B	368	SER
1	B	413	ILE
1	B	466	ILE
1	B	467	LYS
1	B	540	LEU
1	B	594	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	327	ASN
1	A	328	ASN
1	A	425	ASN
1	C	425	ASN
1	D	190	GLN
1	D	322	HIS
1	D	425	ASN
1	B	233	HIS
1	B	327	ASN
1	B	425	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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
2	DCP	D	702	-	23,29,29	0.67	0	30,45,45	1.38	4 (13%)
2	DCP	B	703	-	23,29,29	0.67	0	30,45,45	1.34	3 (10%)
3	GTP	B	704	5	26,34,34	1.17	2 (7%)	33,54,54	2.04	10 (30%)
3	GTP	B	701	5	26,34,34	1.33	2 (7%)	33,54,54	1.88	9 (27%)
3	GTP	A	702	5	26,34,34	1.23	3 (11%)	33,54,54	2.12	10 (30%)
2	DCP	C	702	-	23,29,29	0.65	0	30,45,45	1.39	3 (10%)
2	DCP	A	701	-	23,29,29	0.69	0	30,45,45	1.55	4 (13%)
3	GTP	D	703	5	26,34,34	1.12	2 (7%)	33,54,54	1.90	9 (27%)
4	TTP	C	701	5	23,30,30	1.00	1 (4%)	29,47,47	2.14	6 (20%)
4	TTP	D	704	5	23,30,30	1.01	1 (4%)	29,47,47	2.14	6 (20%)
4	TTP	B	702	5	23,30,30	0.93	1 (4%)	29,47,47	1.95	4 (13%)
4	TTP	A	703	5	23,30,30	0.94	1 (4%)	29,47,47	2.10	4 (13%)

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
2	DCP	D	702	-	-	6/19/34/34	0/2/2/2
2	DCP	B	703	-	-	8/19/34/34	0/2/2/2
3	GTP	B	704	5	-	5/18/38/38	0/3/3/3
3	GTP	B	701	5	-	4/18/38/38	0/3/3/3
3	GTP	A	702	5	-	6/18/38/38	0/3/3/3
2	DCP	C	702	-	-	3/19/34/34	0/2/2/2
2	DCP	A	701	-	-	9/19/34/34	0/2/2/2
3	GTP	D	703	5	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TTP	C	701	5	-	6/19/34/34	0/2/2/2
4	TTP	D	704	5	-	5/19/34/34	0/2/2/2
4	TTP	B	702	5	-	7/19/34/34	0/2/2/2
4	TTP	A	703	5	-	3/19/34/34	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	704	GTP	C5-C6	4.14	1.48	1.41
3	A	702	GTP	C5-C6	4.08	1.48	1.41
3	B	701	GTP	O4'-C1'	3.76	1.46	1.41
4	C	701	TTP	C5-C4	3.18	1.48	1.41
4	D	704	TTP	C5-C4	3.06	1.48	1.41
4	B	702	TTP	C5-C4	2.80	1.47	1.41
3	B	701	GTP	C8-N7	2.45	1.39	1.34
3	B	704	GTP	C5-C4	2.40	1.47	1.40
4	A	703	TTP	C5-C4	2.39	1.46	1.41
3	A	702	GTP	C5-C4	2.35	1.47	1.40
3	D	703	GTP	C5-C4	2.24	1.46	1.40
3	A	702	GTP	O4'-C1'	2.04	1.43	1.41
3	D	703	GTP	C5-C6	2.04	1.44	1.41

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	704	TTP	C2-N3-C4	9.08	122.81	115.14
4	A	703	TTP	C2-N3-C4	8.84	122.61	115.14
4	B	702	TTP	C2-N3-C4	8.13	122.01	115.14
4	C	701	TTP	C2-N3-C4	7.85	121.77	115.14
3	A	702	GTP	C2-N3-C4	5.33	121.44	115.36
3	B	704	GTP	C2-N3-C4	4.88	120.92	115.36
3	B	704	GTP	PA-O3A-PB	-4.85	116.18	132.83
2	A	701	DCP	C4-N3-C2	4.50	120.90	116.34
3	B	701	GTP	C2-N3-C4	4.35	120.33	115.36
4	C	701	TTP	O2G-PG-O1G	4.14	126.87	110.68
3	B	701	GTP	C4-C5-C6	-4.04	116.94	120.80
3	D	703	GTP	C5-C6-N1	-4.01	117.95	123.43
3	A	702	GTP	C4-C5-C6	-3.97	117.00	120.80
3	D	703	GTP	PA-O3A-PB	-3.96	119.23	132.83
2	A	701	DCP	PB-O3B-PG	-3.89	119.47	132.83
3	A	702	GTP	C5-C6-N1	-3.84	118.19	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	GTP	C2-N1-C6	3.79	121.95	115.93
3	B	704	GTP	C5-C6-N1	-3.76	118.29	123.43
2	B	703	DCP	C4-N3-C2	3.69	120.08	116.34
4	A	703	TTP	PB-O3B-PG	-3.68	120.21	132.83
3	B	704	GTP	C4-C5-C6	-3.66	117.30	120.80
3	D	703	GTP	C2-N3-C4	3.63	119.50	115.36
3	D	703	GTP	PB-O3B-PG	-3.63	120.39	132.83
2	C	702	DCP	C4-N3-C2	3.57	119.95	116.34
4	A	703	TTP	PB-O3A-PA	-3.53	120.70	132.83
2	D	702	DCP	PB-O3B-PG	-3.53	120.71	132.83
3	D	703	GTP	C3'-C2'-C1'	3.53	106.29	100.98
3	B	704	GTP	C2-N1-C6	3.51	121.51	115.93
3	A	702	GTP	N3-C2-N1	-3.48	122.58	127.22
4	B	702	TTP	PB-O3A-PA	-3.48	120.89	132.83
3	B	704	GTP	C3'-C2'-C1'	3.46	106.18	100.98
3	D	703	GTP	C2-N1-C6	3.44	121.39	115.93
3	A	702	GTP	PA-O3A-PB	-3.43	121.06	132.83
2	D	702	DCP	C4-N3-C2	3.42	119.81	116.34
2	C	702	DCP	PB-O3B-PG	-3.42	121.11	132.83
2	B	703	DCP	PB-O3B-PG	-3.37	121.26	132.83
3	B	701	GTP	C5-C6-N1	-3.35	118.85	123.43
4	C	701	TTP	PB-O3B-PG	-3.31	121.45	132.83
3	A	702	GTP	C3'-C2'-C1'	3.30	105.95	100.98
4	C	701	TTP	C5-C6-N1	-3.29	118.65	122.19
3	B	701	GTP	C2-N1-C6	3.24	121.08	115.93
2	A	701	DCP	PB-O3A-PA	-3.24	121.72	132.83
4	D	704	TTP	PB-O3B-PG	-3.23	121.76	132.83
3	B	701	GTP	PA-O3A-PB	-3.19	121.89	132.83
3	B	704	GTP	N3-C2-N1	-3.13	123.05	127.22
2	D	702	DCP	PB-O3A-PA	-3.09	122.22	132.83
2	C	702	DCP	PB-O3A-PA	-3.09	122.23	132.83
4	C	701	TTP	PB-O3A-PA	-3.08	122.24	132.83
4	B	702	TTP	O3G-PG-O2G	3.08	119.41	107.64
3	D	703	GTP	C4-C5-C6	-3.04	117.89	120.80
3	D	703	GTP	N3-C2-N1	-2.97	123.26	127.22
3	A	702	GTP	PB-O3B-PG	-2.96	122.67	132.83
4	B	702	TTP	PB-O3B-PG	-2.91	122.83	132.83
3	B	701	GTP	PB-O3B-PG	-2.86	123.01	132.83
3	B	701	GTP	N3-C2-N1	-2.82	123.45	127.22
4	D	704	TTP	PB-O3A-PA	-2.77	123.32	132.83
3	B	701	GTP	C3'-C2'-C1'	2.77	105.14	100.98
2	B	703	DCP	PB-O3A-PA	-2.69	123.60	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	TTP	O2A-PA-O1A	2.50	124.62	112.24
4	D	704	TTP	C5-C6-N1	-2.49	119.51	122.19
3	A	702	GTP	O3G-PG-O2G	2.43	116.91	107.64
3	B	704	GTP	N2-C2-N1	2.41	121.01	117.25
4	D	704	TTP	O2A-PA-O1A	2.38	124.01	112.24
3	B	704	GTP	PB-O3B-PG	-2.36	124.72	132.83
3	B	704	GTP	C4-C5-N7	-2.31	106.99	109.40
2	D	702	DCP	C2'-C1'-N1	-2.27	109.02	114.27
3	A	702	GTP	C4-C5-N7	-2.26	107.05	109.40
3	D	703	GTP	O3G-PG-O2G	2.20	116.03	107.64
4	A	703	TTP	C2'-C3'-C4'	2.17	107.28	102.76
4	D	704	TTP	O2G-PG-O1G	2.13	119.03	110.68
2	A	701	DCP	N4-C4-N3	2.08	119.77	116.49
3	B	701	GTP	O4'-C4'-C3'	-2.05	101.06	105.11

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	DCP	C5'-O5'-PA-O2A
2	D	702	DCP	C5'-O5'-PA-O2A
2	D	702	DCP	PB-O3A-PA-O5'
2	B	703	DCP	C5'-O5'-PA-O1A
3	A	702	GTP	PB-O3B-PG-O3G
4	A	703	TTP	O4'-C1'-N1-C6
4	C	701	TTP	PB-O3B-PG-O3G
4	C	701	TTP	O4'-C1'-N1-C6
4	D	704	TTP	PB-O3B-PG-O2G
4	D	704	TTP	O4'-C1'-N1-C6
4	B	702	TTP	O4'-C1'-N1-C6
2	A	701	DCP	C3'-C4'-C5'-O5'
2	A	701	DCP	O4'-C4'-C5'-O5'
3	B	704	GTP	PB-O3B-PG-O1G
2	B	703	DCP	C3'-C4'-C5'-O5'
2	A	701	DCP	C4'-C5'-O5'-PA
2	C	702	DCP	C4'-C5'-O5'-PA
2	D	702	DCP	C4'-C5'-O5'-PA
2	B	703	DCP	C4'-C5'-O5'-PA
2	A	701	DCP	PB-O3A-PA-O5'
2	C	702	DCP	PB-O3A-PA-O5'
2	B	703	DCP	PB-O3A-PA-O5'
3	B	704	GTP	PB-O3B-PG-O3G

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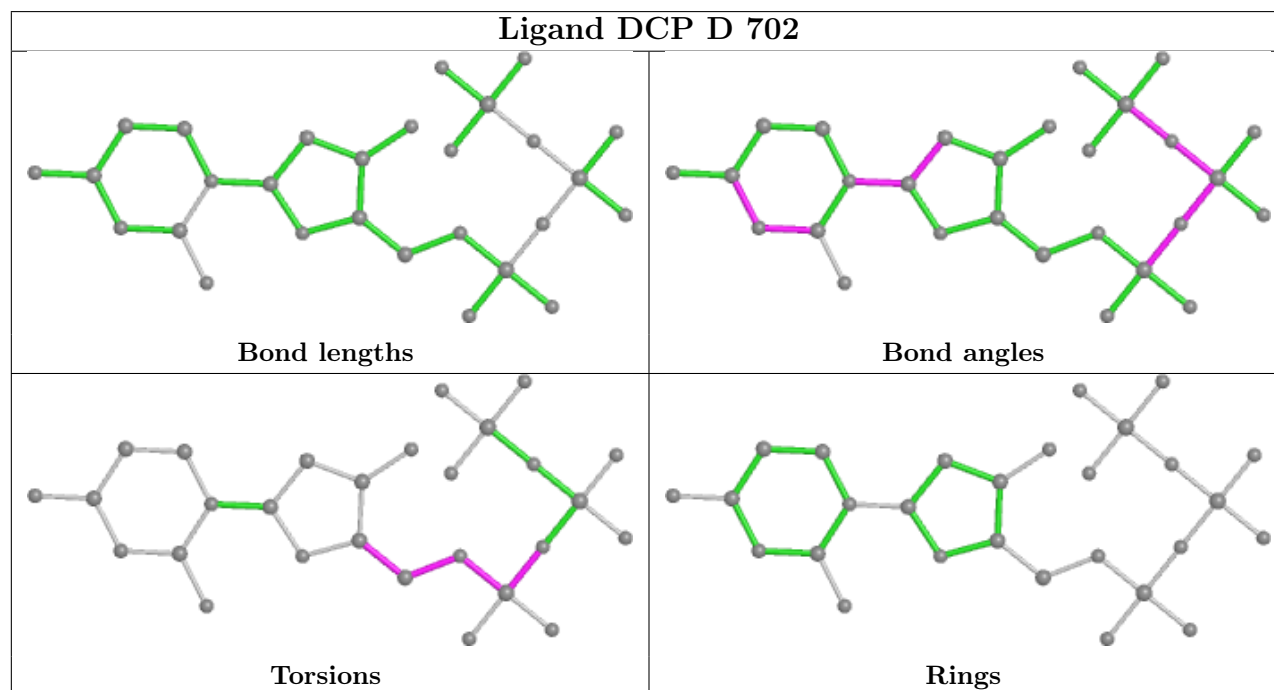
Mol	Chain	Res	Type	Atoms
4	D	704	TTP	PB-O3B-PG-O3G
4	B	702	TTP	PB-O3B-PG-O2G
2	A	701	DCP	C5'-O5'-PA-O3A
2	D	702	DCP	C5'-O5'-PA-O3A
2	B	703	DCP	C5'-O5'-PA-O3A
4	B	702	TTP	C5'-O5'-PA-O3A
3	A	702	GTP	PG-O3B-PB-O1B
3	B	704	GTP	PG-O3B-PB-O1B
4	A	703	TTP	PG-O3B-PB-O1B
4	C	701	TTP	PG-O3B-PB-O1B
4	D	704	TTP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

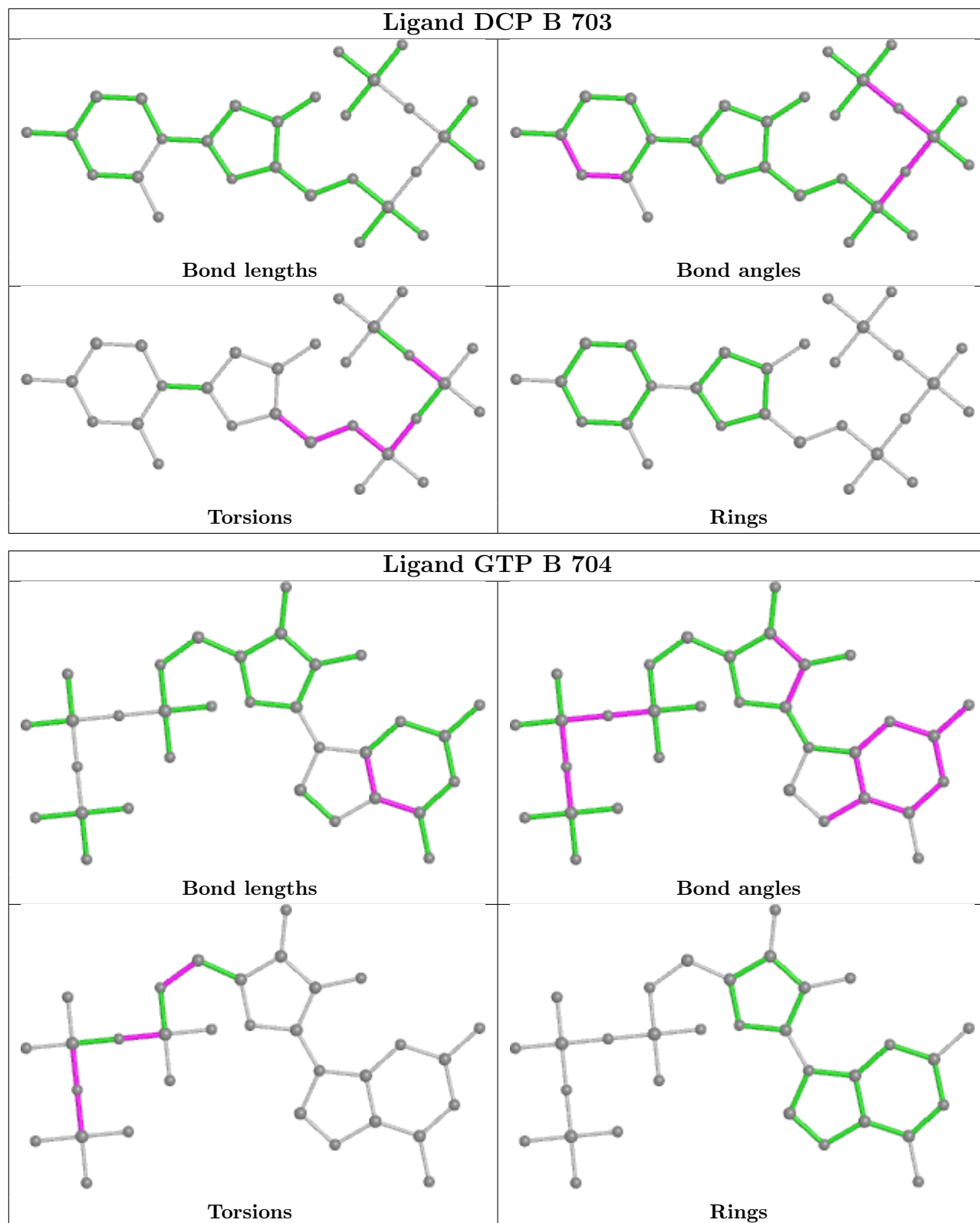
There are no ring outliers.

9 monomers are involved in 21 short contacts:

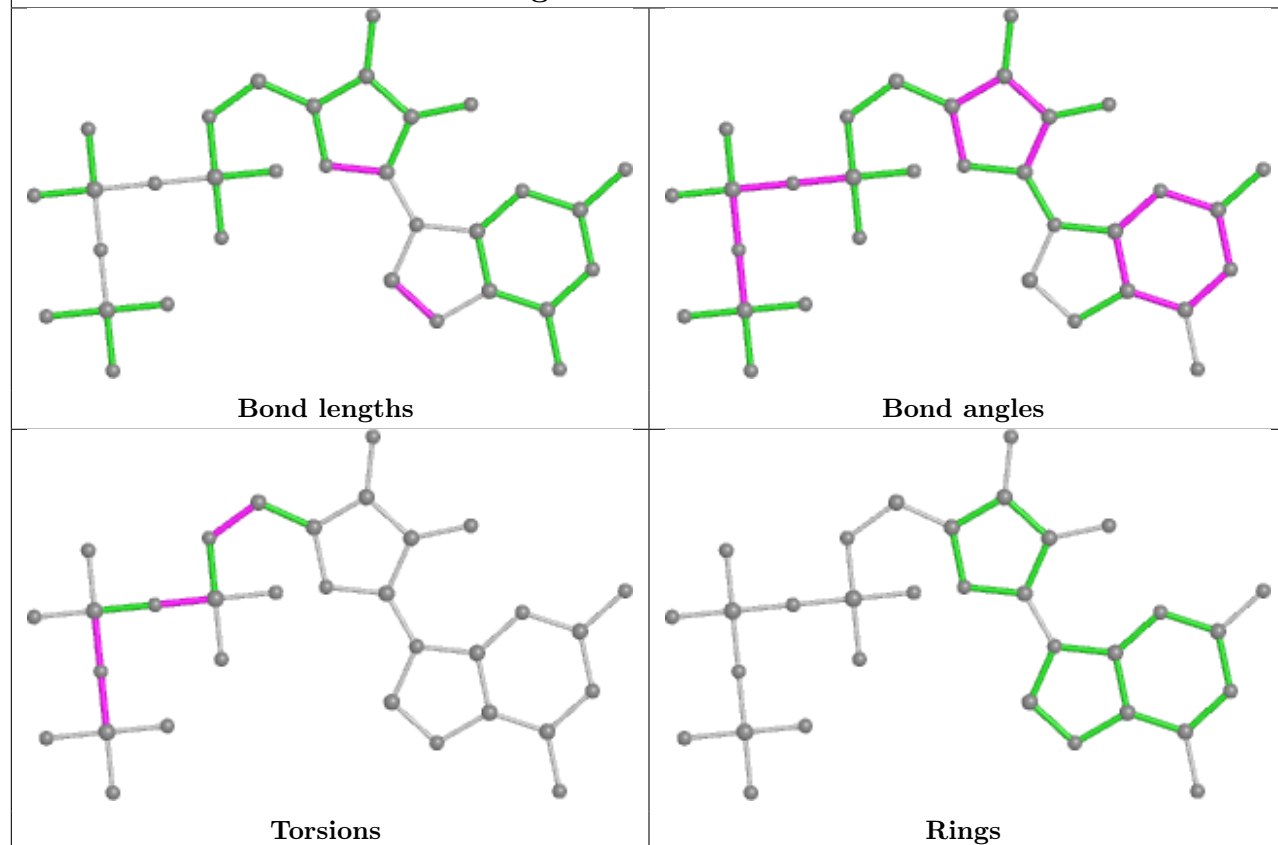
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	702	DCP	1	0
2	B	703	DCP	5	0
3	A	702	GTP	1	0
2	A	701	DCP	7	0
3	D	703	GTP	2	0
4	C	701	TTP	1	0
4	D	704	TTP	1	0
4	B	702	TTP	2	0
4	A	703	TTP	2	0

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

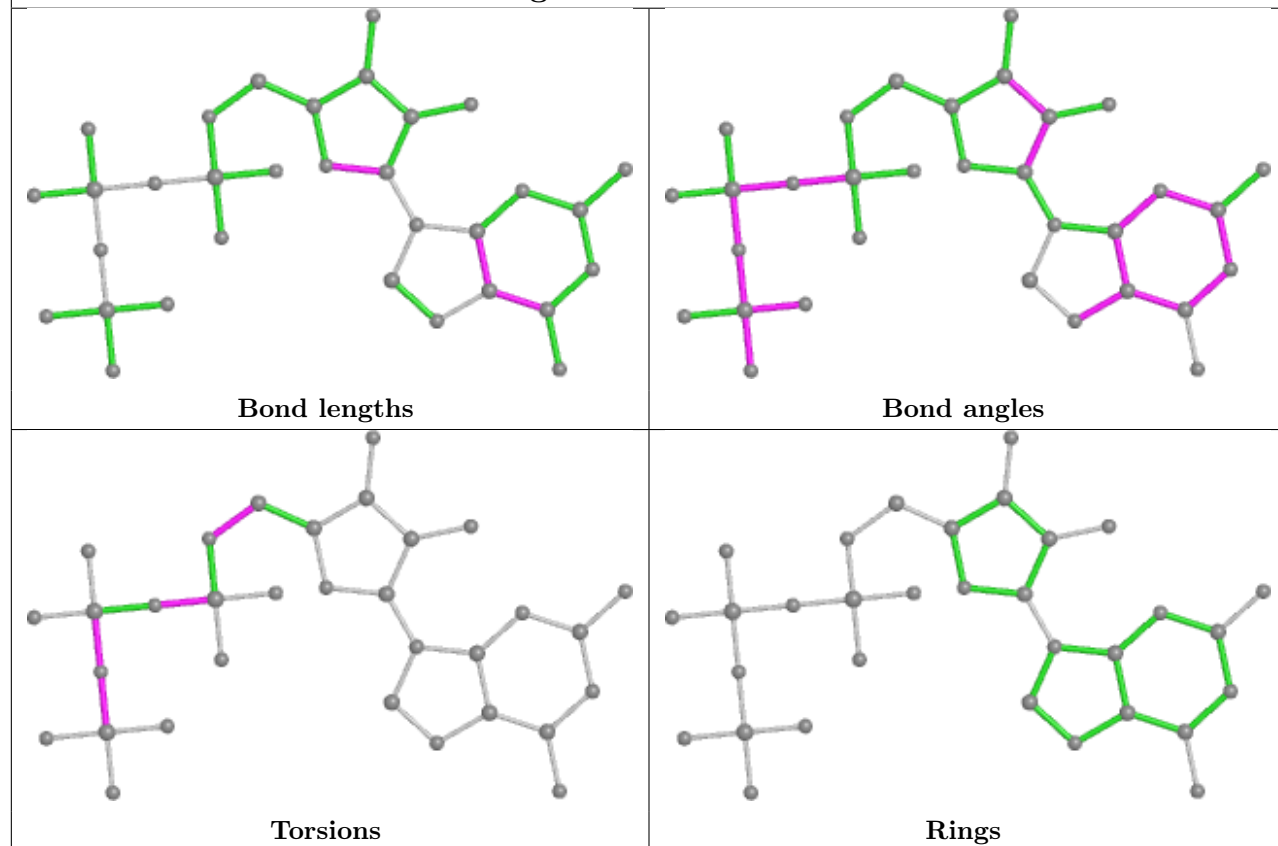


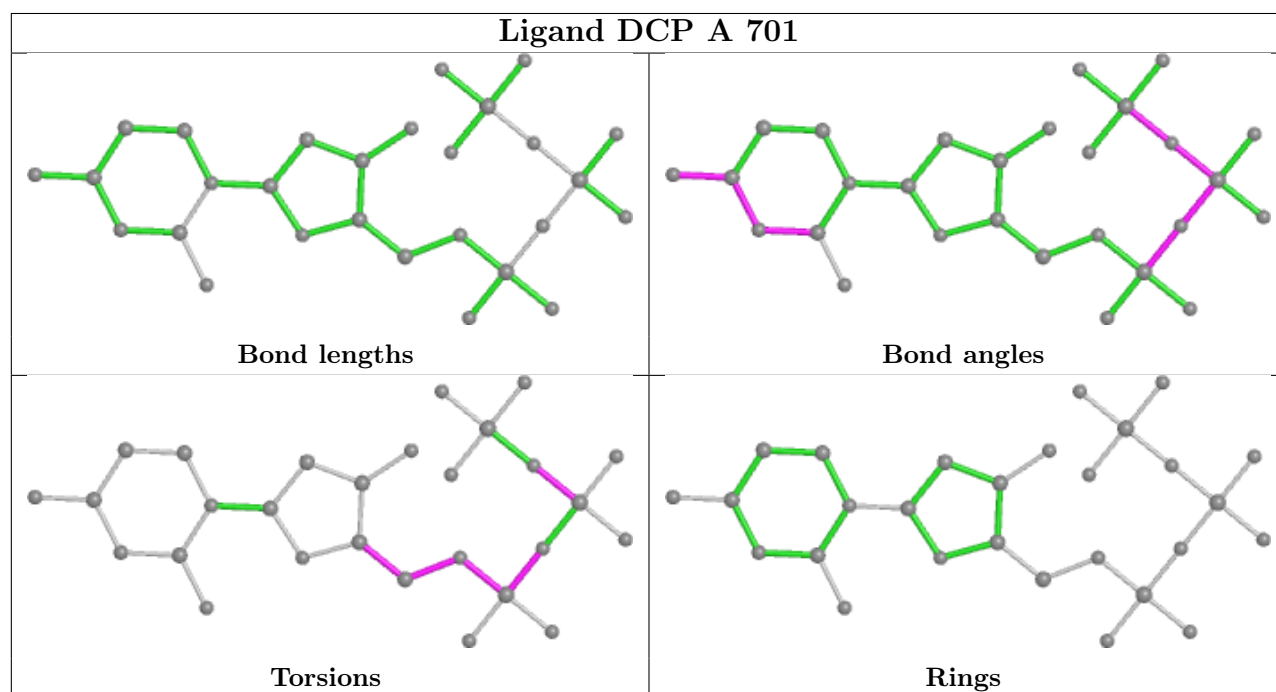
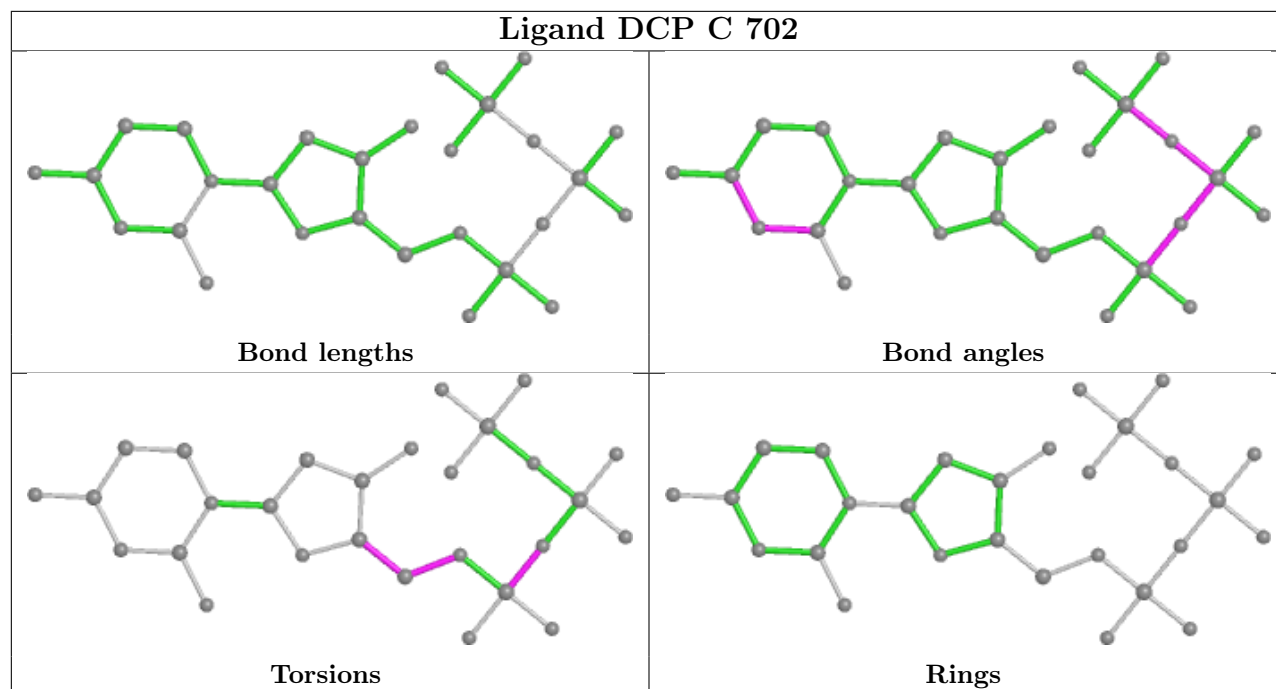


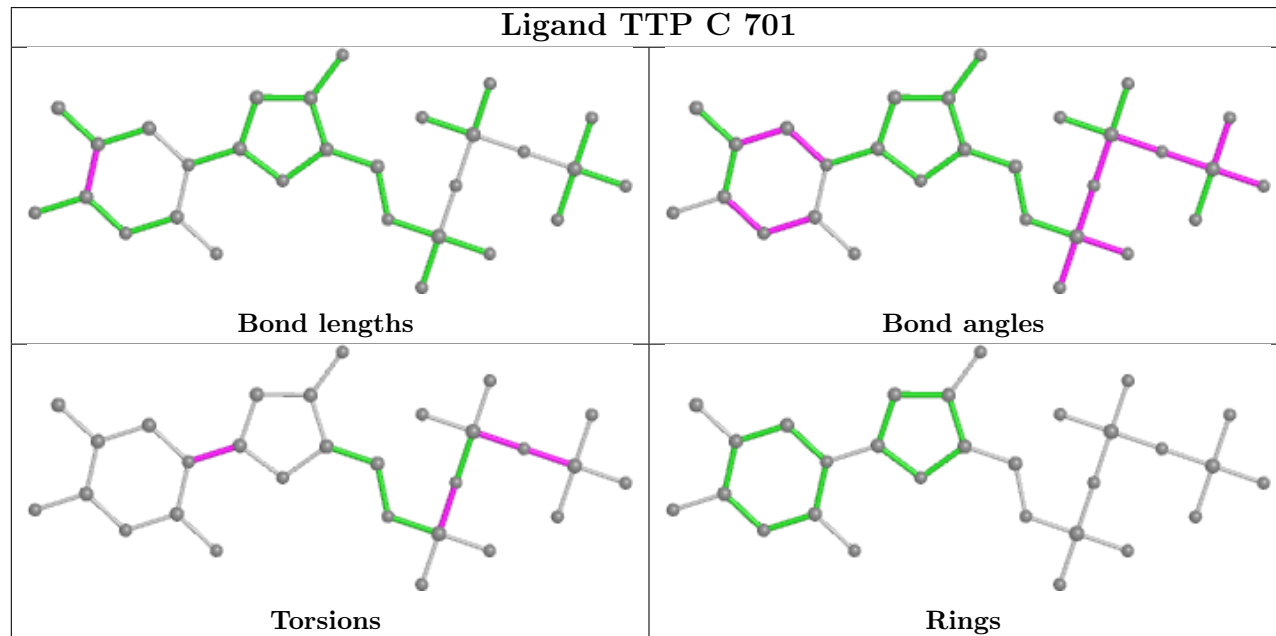
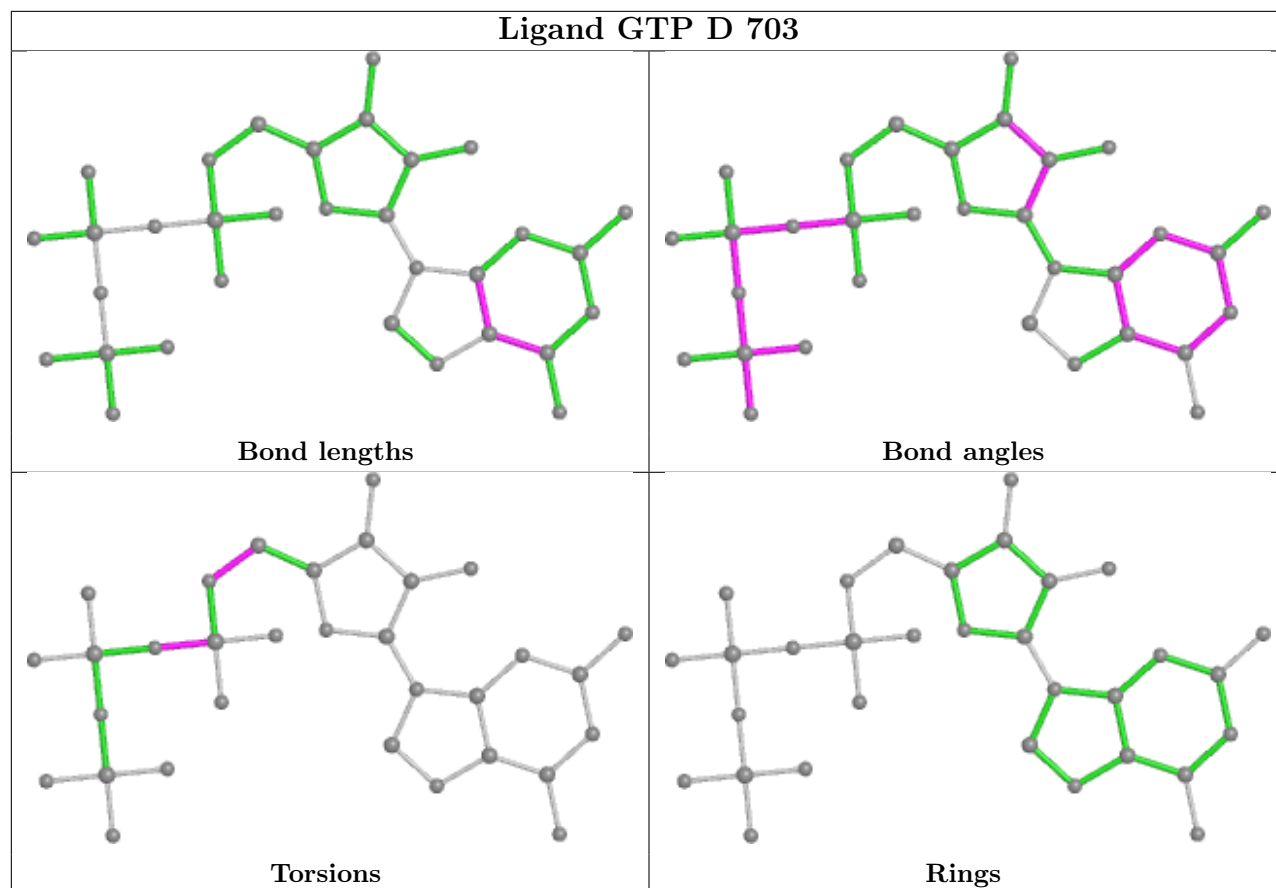
Ligand GTP B 701



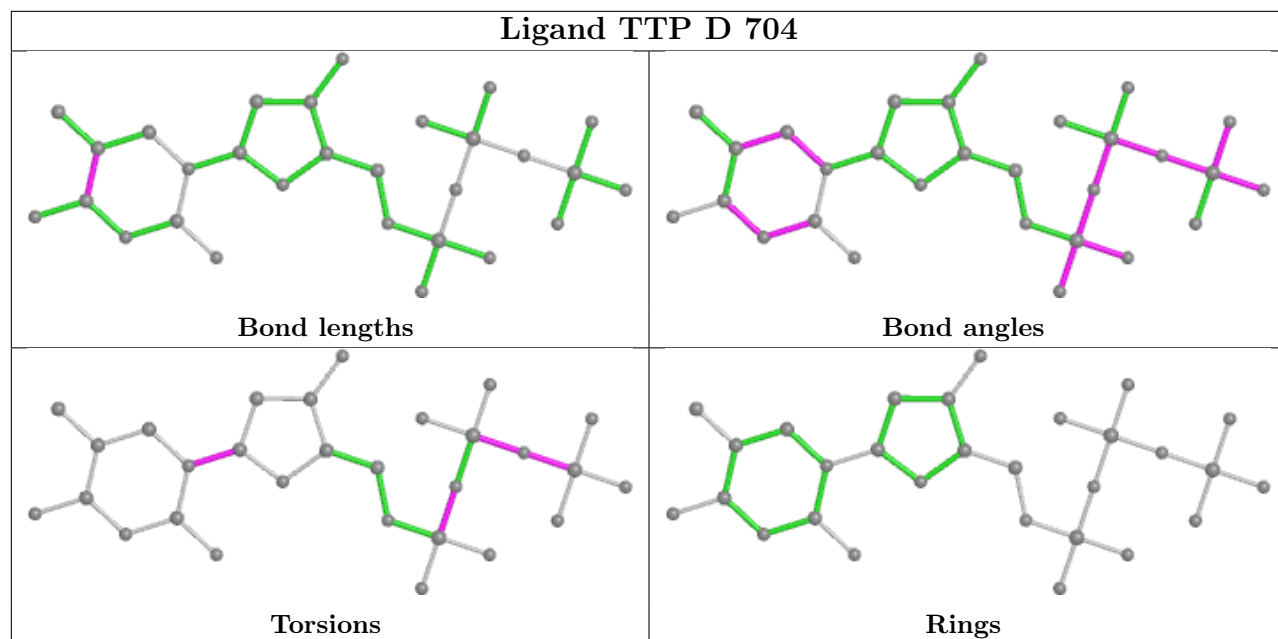
Ligand GTP A 702



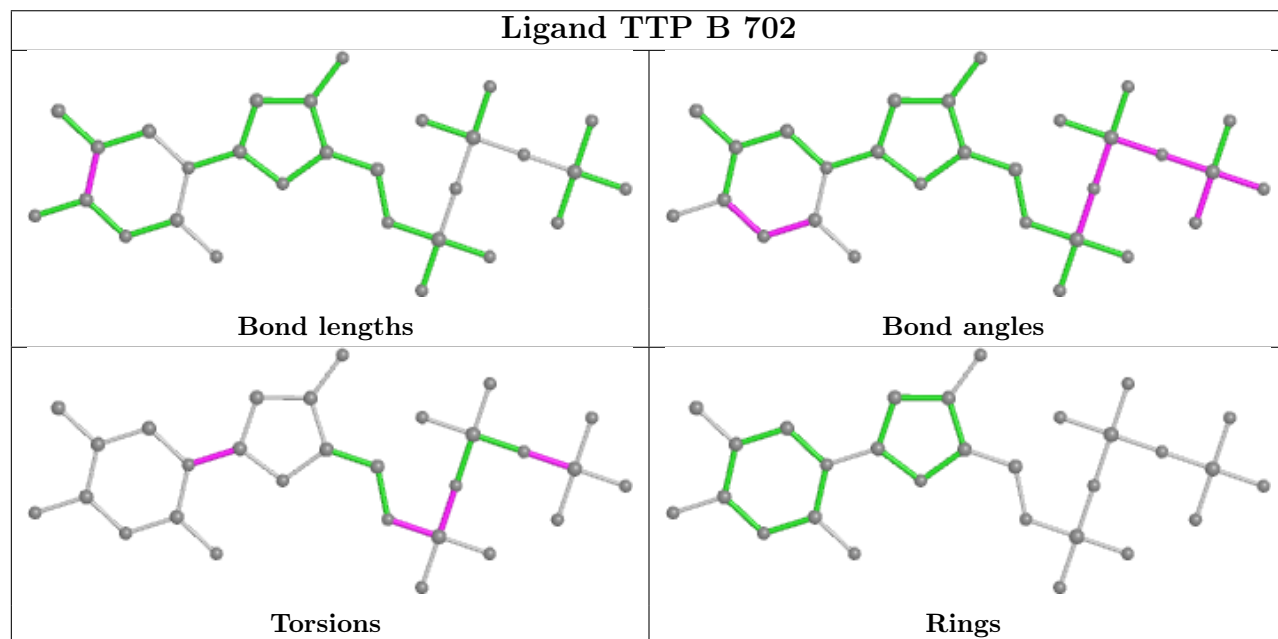


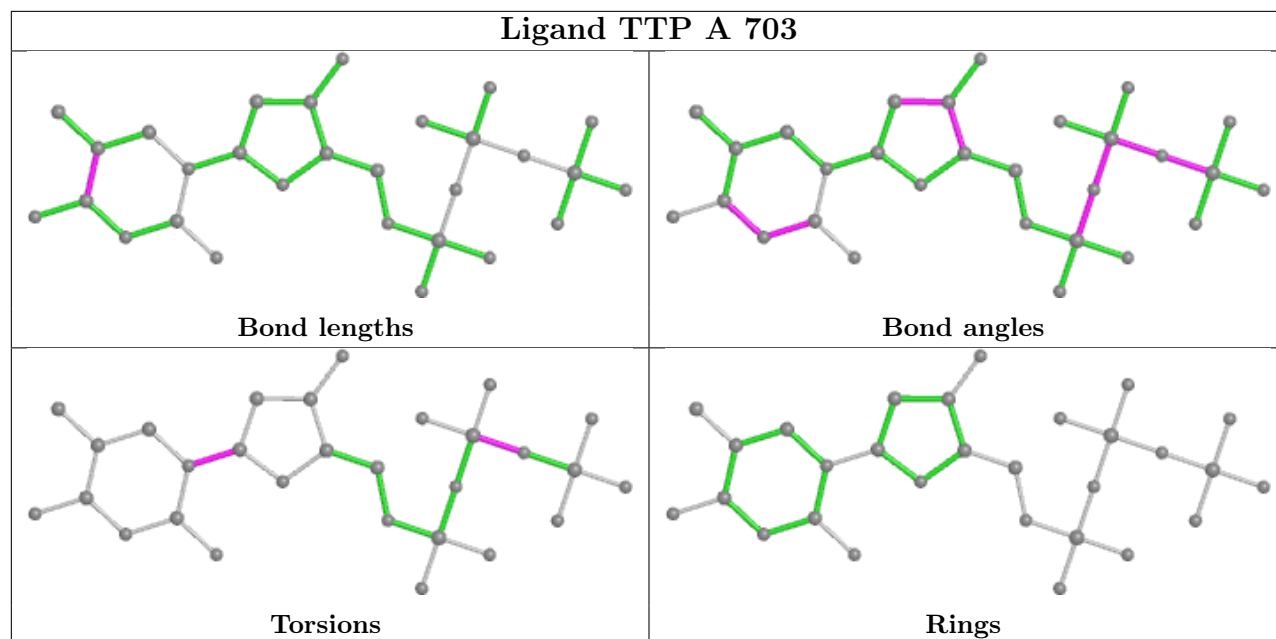


Ligand TTP D 704



Ligand TTP B 702





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	480/514 (93%)	1.13	80 (16%) 1 1	74, 96, 122, 142	0
1	B	480/514 (93%)	1.20	93 (19%) 1 0	74, 96, 126, 152	0
1	C	479/514 (93%)	0.96	54 (11%) 5 3	68, 92, 110, 121	0
1	D	480/514 (93%)	1.08	78 (16%) 1 1	86, 108, 134, 148	0
All	All	1919/2056 (93%)	1.09	305 (15%) 1 1	68, 98, 127, 152	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	489	LEU	8.0
1	D	522[A]	CYS	7.3
1	A	490	ASP	6.5
1	A	488	LEU	6.2
1	B	486	LYS	6.1
1	A	288	LYS	6.1
1	B	286	PRO	6.1
1	D	590	LEU	5.9
1	A	487	VAL	5.8
1	B	404	GLY	5.7
1	C	251	LYS	5.6
1	A	563	TYR	5.5
1	A	491	VAL	5.4
1	B	570	VAL	5.4
1	D	276	LEU	5.0
1	B	465	GLN	5.0
1	A	115	MET	4.9
1	D	490	ASP	4.8
1	A	486	LYS	4.8
1	D	326	GLN	4.7
1	B	498	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	490	ASP	4.6
1	A	347	LEU	4.6
1	B	488	LEU	4.4
1	B	500	VAL	4.3
1	B	487	VAL	4.3
1	C	522[A]	CYS	4.3
1	A	205	CYS	4.2
1	A	557	VAL	4.2
1	D	269	LYS	4.1
1	D	230	LYS	4.1
1	A	554	CYS	4.1
1	C	257	TYR	4.0
1	B	586	VAL	4.0
1	B	360	TYR	4.0
1	A	327	ASN	3.9
1	B	499	ILE	3.9
1	B	272	ILE	3.9
1	C	131	LEU	3.9
1	B	313	TRP	3.9
1	C	543	GLU	3.8
1	B	598	TRP	3.8
1	A	284	LEU	3.8
1	D	491	VAL	3.8
1	D	543	GLU	3.7
1	B	406	LYS	3.7
1	B	583	ASP	3.7
1	A	485	PRO	3.7
1	B	483	ALA	3.7
1	B	276	LEU	3.7
1	D	113	ASP	3.7
1	D	241	PHE	3.6
1	A	350	CYS	3.6
1	B	493	LEU	3.6
1	A	492	LYS	3.6
1	C	523	LYS	3.6
1	B	285	TRP	3.6
1	A	467	LYS	3.6
1	A	591	ILE	3.6
1	B	213	PHE	3.6
1	B	328	ASN	3.6
1	D	341	CYS	3.5
1	B	472	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	562	LEU	3.5
1	C	468	ILE	3.5
1	B	471	GLU	3.5
1	B	563	TYR	3.5
1	B	585	ASP	3.5
1	B	480	VAL	3.4
1	A	493	LEU	3.4
1	D	268	ILE	3.4
1	B	568	TYR	3.4
1	C	493	LEU	3.4
1	A	465	GLN	3.4
1	D	272	ILE	3.4
1	D	405	LYS	3.4
1	D	568	TYR	3.4
1	D	498	PHE	3.3
1	B	476	LEU	3.3
1	B	484	LYS	3.3
1	A	419	TYR	3.3
1	A	584	GLY	3.3
1	D	587	ILE	3.3
1	B	468	ILE	3.3
1	A	495	ALA	3.3
1	C	398	GLU	3.3
1	A	326	GLN	3.3
1	B	562	LEU	3.3
1	B	485	PRO	3.3
1	A	285	TRP	3.3
1	D	390	PHE	3.2
1	C	326	GLN	3.2
1	D	488	LEU	3.2
1	D	327	ASN	3.2
1	D	489	LEU	3.2
1	D	321	HIS	3.2
1	A	468	ILE	3.1
1	B	592	THR	3.1
1	D	465	GLN	3.1
1	A	230	LYS	3.1
1	D	592	THR	3.1
1	B	241	PHE	3.1
1	D	496	GLU	3.1
1	B	114	THR	3.1
1	C	241	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	262	GLU	3.0
1	D	581	PRO	3.0
1	B	287	TYR	3.0
1	D	556	LYS	3.0
1	B	250	ILE	3.0
1	D	328	ASN	2.9
1	B	489	LEU	2.9
1	B	459	GLU	2.9
1	A	498	PHE	2.9
1	D	572	TRP	2.9
1	A	483	ALA	2.9
1	D	297	LEU	2.9
1	D	313	TRP	2.9
1	C	393	ALA	2.9
1	B	304	LYS	2.8
1	B	238	VAL	2.8
1	D	204	LEU	2.8
1	D	557	VAL	2.8
1	A	567	GLN	2.8
1	B	569	PHE	2.8
1	C	327	ASN	2.8
1	B	347	LEU	2.8
1	B	573	CYS	2.8
1	C	253	VAL	2.8
1	B	474	GLU	2.8
1	A	562	LEU	2.8
1	B	275	PRO	2.8
1	A	535	ASN	2.8
1	B	231	TRP	2.8
1	A	257	TYR	2.8
1	C	572	TRP	2.7
1	A	556	LYS	2.7
1	D	134	ARG	2.7
1	D	444	ILE	2.7
1	C	528	ARG	2.7
1	B	589	PRO	2.7
1	C	484	LYS	2.7
1	B	594	GLN	2.7
1	B	235	GLN	2.7
1	D	317	ALA	2.7
1	A	454	PHE	2.7
1	D	154	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	566	ARG	2.7
1	B	349	ILE	2.7
1	A	297	LEU	2.7
1	B	457	VAL	2.7
1	B	501	ASP	2.7
1	C	570	VAL	2.6
1	A	543	GLU	2.6
1	A	587	ILE	2.6
1	D	386	ILE	2.6
1	B	576	ARG	2.6
1	A	292	GLU	2.6
1	D	569	PHE	2.6
1	B	320	CYS	2.6
1	C	273	VAL	2.6
1	C	525	ALA	2.6
1	D	383	ASP	2.6
1	B	301	VAL	2.6
1	B	388	ASP	2.6
1	D	554	CYS	2.6
1	D	339	ARG	2.6
1	B	567	GLN	2.5
1	D	364	HIS	2.5
1	A	469	LYS	2.5
1	A	287	TYR	2.5
1	A	482	SER	2.5
1	C	265	ILE	2.5
1	A	457	VAL	2.5
1	B	491	VAL	2.5
1	C	465	GLN	2.5
1	D	471	GLU	2.5
1	C	420	THR	2.5
1	B	466	ILE	2.5
1	B	552	VAL	2.5
1	A	519	SER	2.5
1	D	222	ILE	2.5
1	B	409	ILE	2.5
1	B	343	VAL	2.5
1	D	288	LYS	2.5
1	B	305	ARG	2.5
1	D	584	GLY	2.5
1	B	467	LYS	2.5
1	C	288	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	559	ARG	2.5
1	C	256	GLN	2.5
1	D	131	LEU	2.5
1	A	455	LYS	2.4
1	C	252	PRO	2.4
1	A	583	ASP	2.4
1	D	267	PHE	2.4
1	C	556	LYS	2.4
1	B	402	ALA	2.4
1	D	229	VAL	2.4
1	C	319	ASP	2.4
1	C	452	ASN	2.4
1	C	255	GLU	2.4
1	A	561	SER	2.4
1	D	161	SER	2.4
1	A	294	LYS	2.4
1	C	405	LYS	2.4
1	B	496	GLU	2.3
1	C	321	HIS	2.3
1	C	254	MET	2.3
1	D	125	HIS	2.3
1	A	275	PRO	2.3
1	A	349	ILE	2.3
1	D	524	THR	2.3
1	B	262	GLU	2.3
1	B	345	ASN	2.3
1	B	522	CYS	2.3
1	B	542	PRO	2.3
1	A	484	LYS	2.3
1	C	587	ILE	2.3
1	D	381	ILE	2.3
1	D	528	ARG	2.3
1	D	531	ARG	2.3
1	A	558	ASP	2.3
1	B	277	GLU	2.3
1	A	494	LYS	2.3
1	D	160	ALA	2.3
1	A	300	ILE	2.3
1	A	114	THR	2.3
1	A	499	ILE	2.3
1	B	288	LYS	2.3
1	A	293	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	292	GLU	2.3
1	C	440	ASP	2.3
1	B	481	ALA	2.3
1	C	334	PHE	2.3
1	D	200	GLN	2.3
1	D	334	PHE	2.2
1	B	543	GLU	2.2
1	C	404	GLY	2.2
1	B	139	PRO	2.2
1	B	473	TYR	2.2
1	A	340	VAL	2.2
1	D	340	VAL	2.2
1	D	440	ASP	2.2
1	B	341	CYS	2.2
1	B	545	PHE	2.2
1	A	572	TRP	2.2
1	D	367	ASN	2.2
1	D	525	ALA	2.2
1	B	431	LEU	2.2
1	A	362	MET	2.2
1	A	598	TRP	2.2
1	A	570	VAL	2.2
1	A	559	ARG	2.2
1	B	383	ASP	2.2
1	C	491	VAL	2.2
1	A	234	GLU	2.2
1	C	348	ARG	2.2
1	B	458	GLY	2.2
1	A	590	LEU	2.2
1	D	189	LEU	2.2
1	D	198	CYS	2.2
1	A	466	ILE	2.1
1	A	283	SER	2.1
1	A	341	CYS	2.1
1	A	502	VAL	2.1
1	C	428	LEU	2.1
1	D	403	GLY	2.1
1	B	264	ASP	2.1
1	D	393	ALA	2.1
1	C	488	LEU	2.1
1	A	472	ASP	2.1
1	C	190	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	594	GLN	2.1
1	A	560	LYS	2.1
1	D	119	ASN	2.1
1	B	263	GLU	2.1
1	B	490	ASP	2.1
1	B	269	LYS	2.1
1	D	284	LEU	2.1
1	B	326	GLN	2.1
1	C	325	ILE	2.1
1	A	480	VAL	2.1
1	A	302	SER	2.1
1	A	402	ALA	2.1
1	C	114	THR	2.1
1	C	260	ILE	2.1
1	C	272	ILE	2.1
1	D	338	ALA	2.1
1	C	320	CYS	2.0
1	D	404	GLY	2.0
1	C	161	SER	2.0
1	A	315	TYR	2.0
1	D	553	TYR	2.0
1	B	257	TYR	2.0
1	A	120	ASP	2.0
1	D	330	ASP	2.0
1	B	199	VAL	2.0
1	A	497	ASP	2.0
1	C	501	ASP	2.0
1	D	412	ALA	2.0
1	C	396	TYR	2.0
1	D	114	THR	2.0
1	C	509	MET	2.0
1	A	235	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

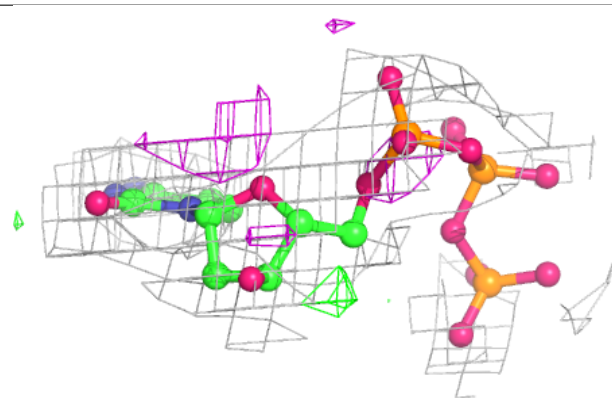
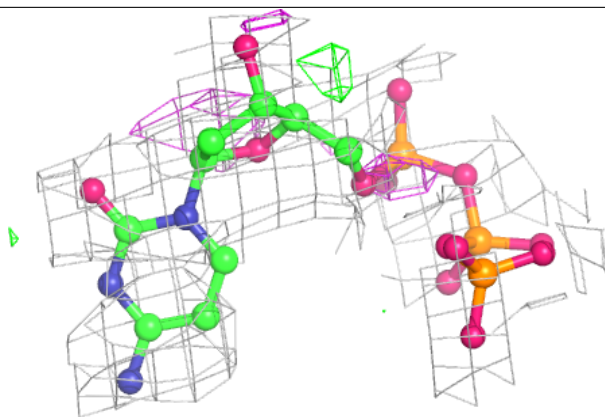
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	705	1/1	0.31	0.18	93,93,93,93	0
5	MG	A	704	1/1	0.55	0.10	148,148,148,148	0
2	DCP	A	701	28/28	0.71	0.27	84,95,129,131	0
2	DCP	B	703	28/28	0.71	0.25	90,106,123,126	0
2	DCP	D	702	28/28	0.74	0.30	93,106,131,133	0
2	DCP	C	702	28/28	0.75	0.27	112,120,135,137	0
5	MG	D	701	1/1	0.76	0.16	85,85,85,85	0
5	MG	C	703	1/1	0.81	0.10	101,101,101,101	0
3	GTP	D	703	32/32	0.85	0.22	59,78,98,106	0
3	GTP	B	701	32/32	0.87	0.25	48,78,103,108	0
3	GTP	A	702	32/32	0.89	0.19	70,84,97,103	0
3	GTP	B	704	32/32	0.91	0.18	80,87,111,114	0
4	TTP	C	701	29/29	0.91	0.18	66,81,100,103	0
4	TTP	D	704	29/29	0.91	0.20	79,89,100,102	0
4	TTP	B	702	29/29	0.91	0.23	56,83,101,106	0
4	TTP	A	703	29/29	0.92	0.25	70,85,98,106	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.

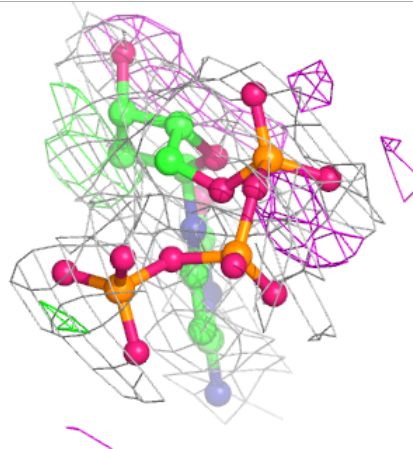
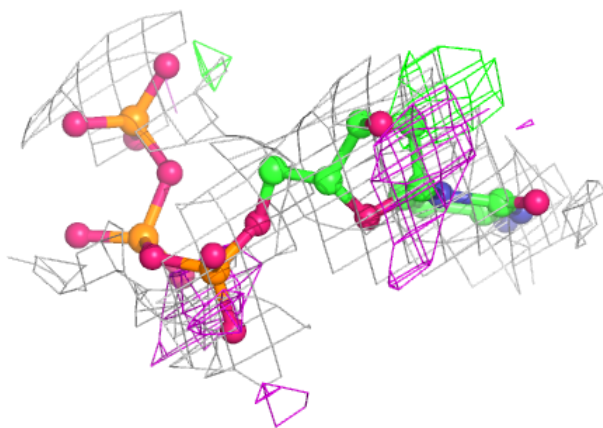
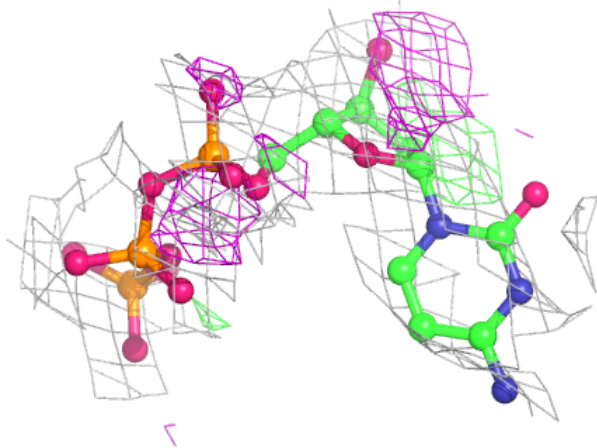
Electron density around DCP A 701:

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



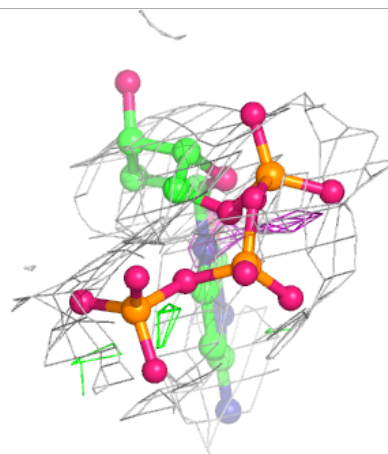
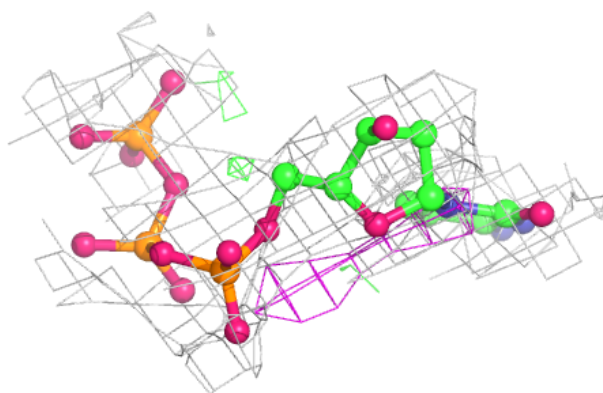
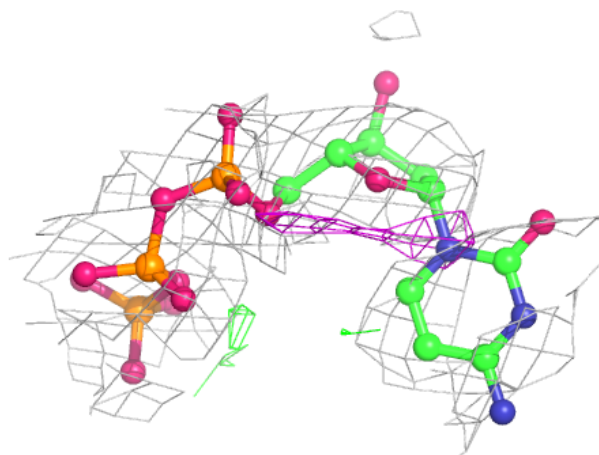
Electron density around DCP B 703:

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



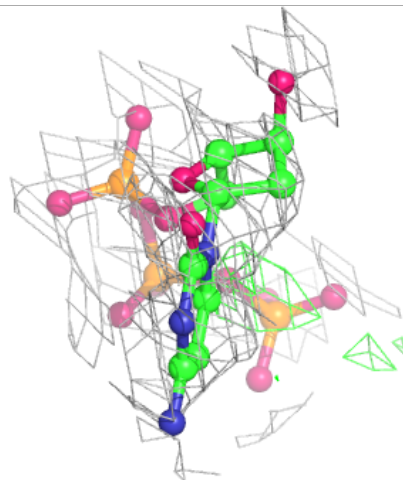
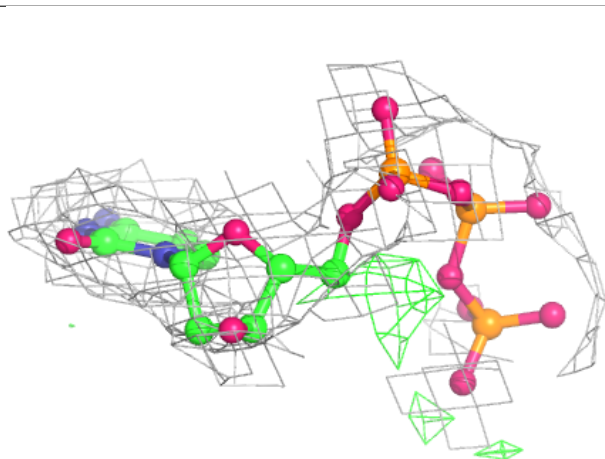
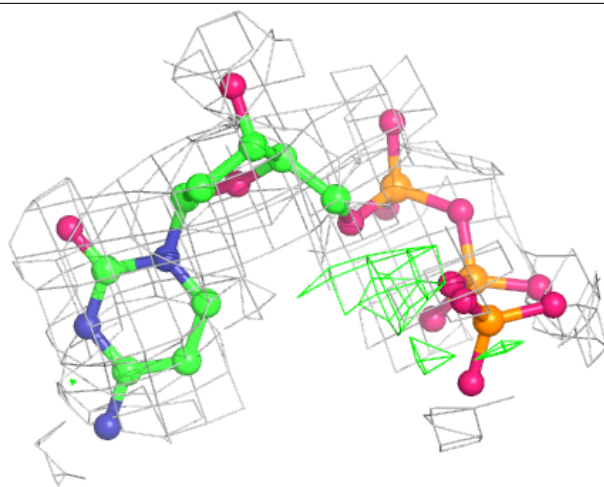
Electron density around DCP D 702:

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



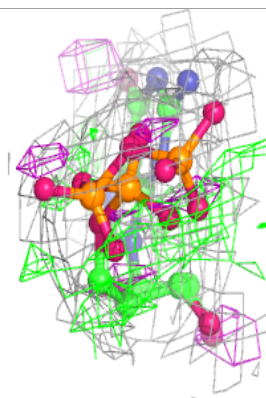
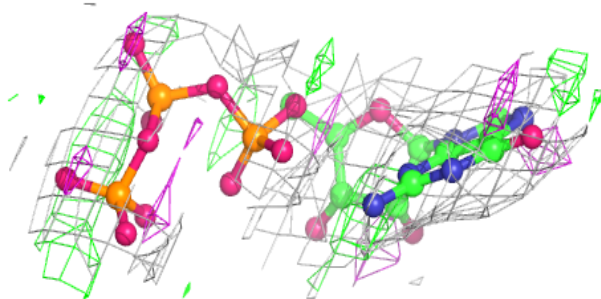
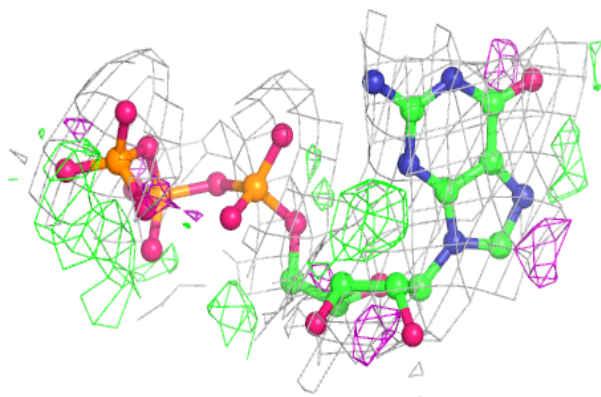
Electron density around DCP C 702:

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

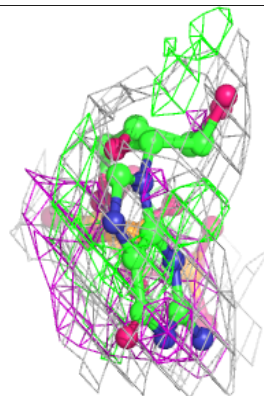
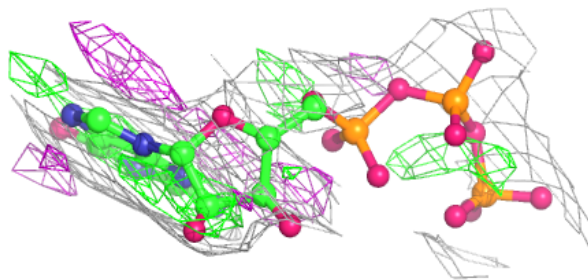
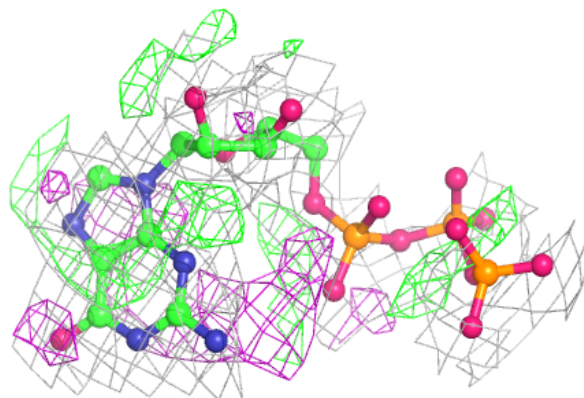


Electron density around GTP D 703:

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

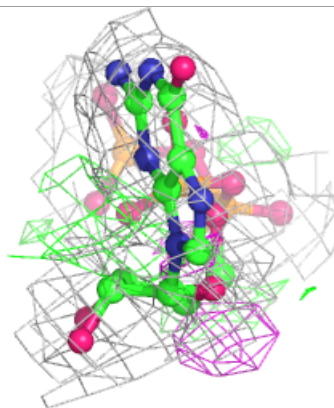
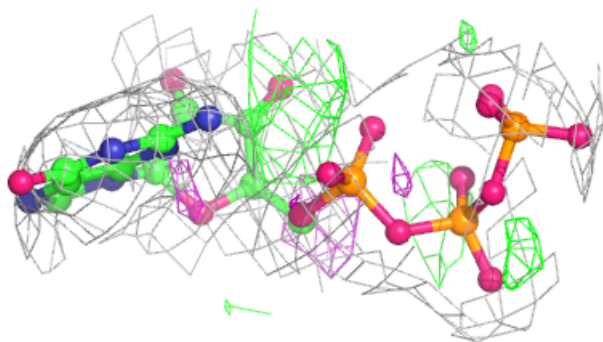
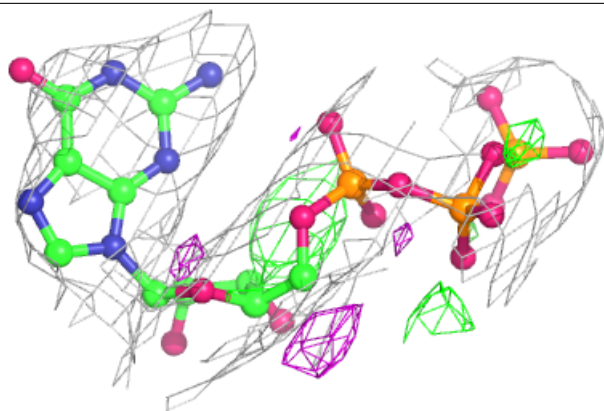
**Electron density around GTP B 701:**

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

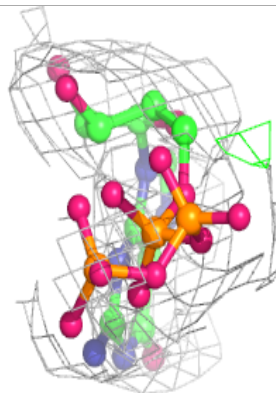
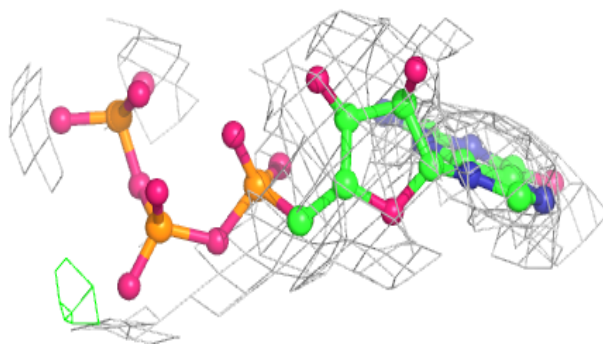
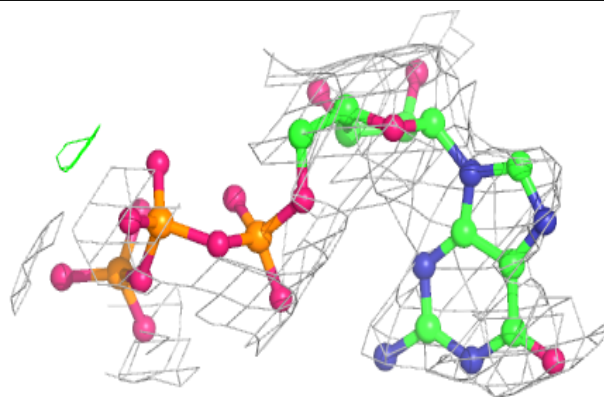


Electron density around GTP A 702:

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

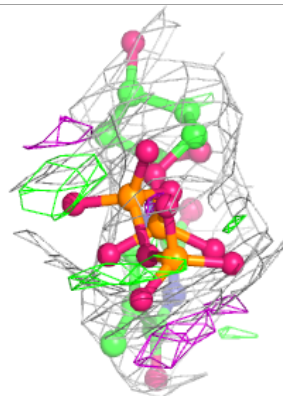
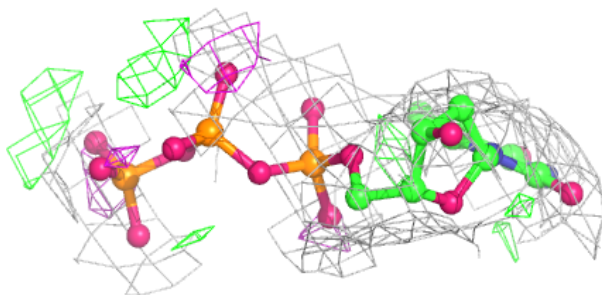
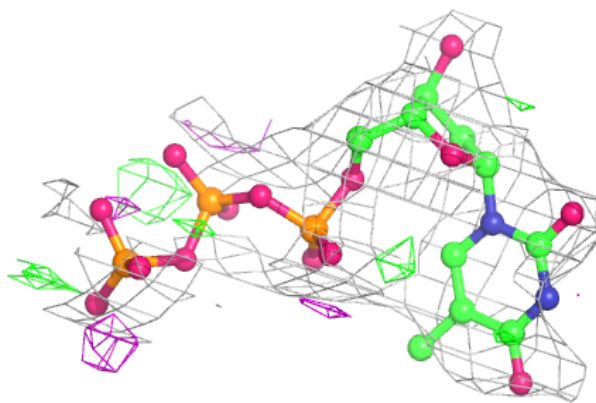
**Electron density around GTP B 704:**

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

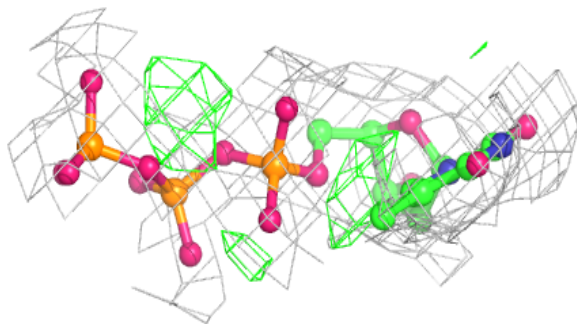
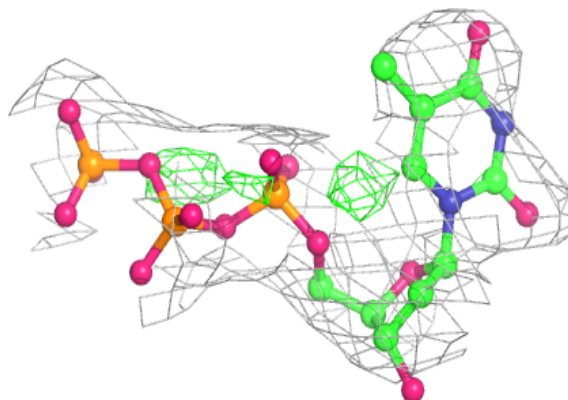


Electron density around TTP C 701:

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

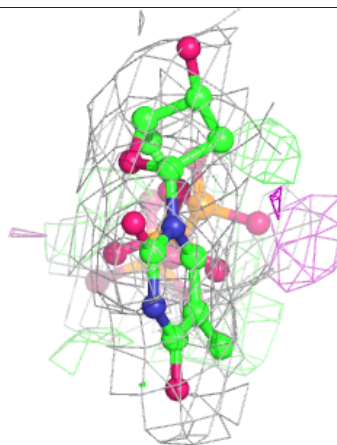
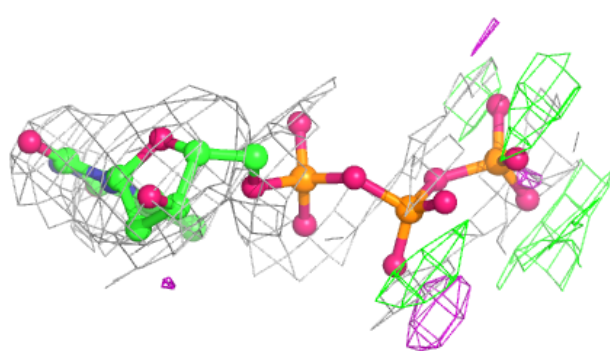
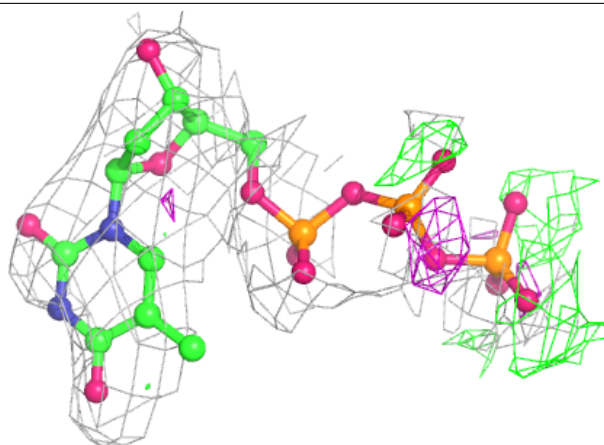
**Electron density around TTP D 704:**

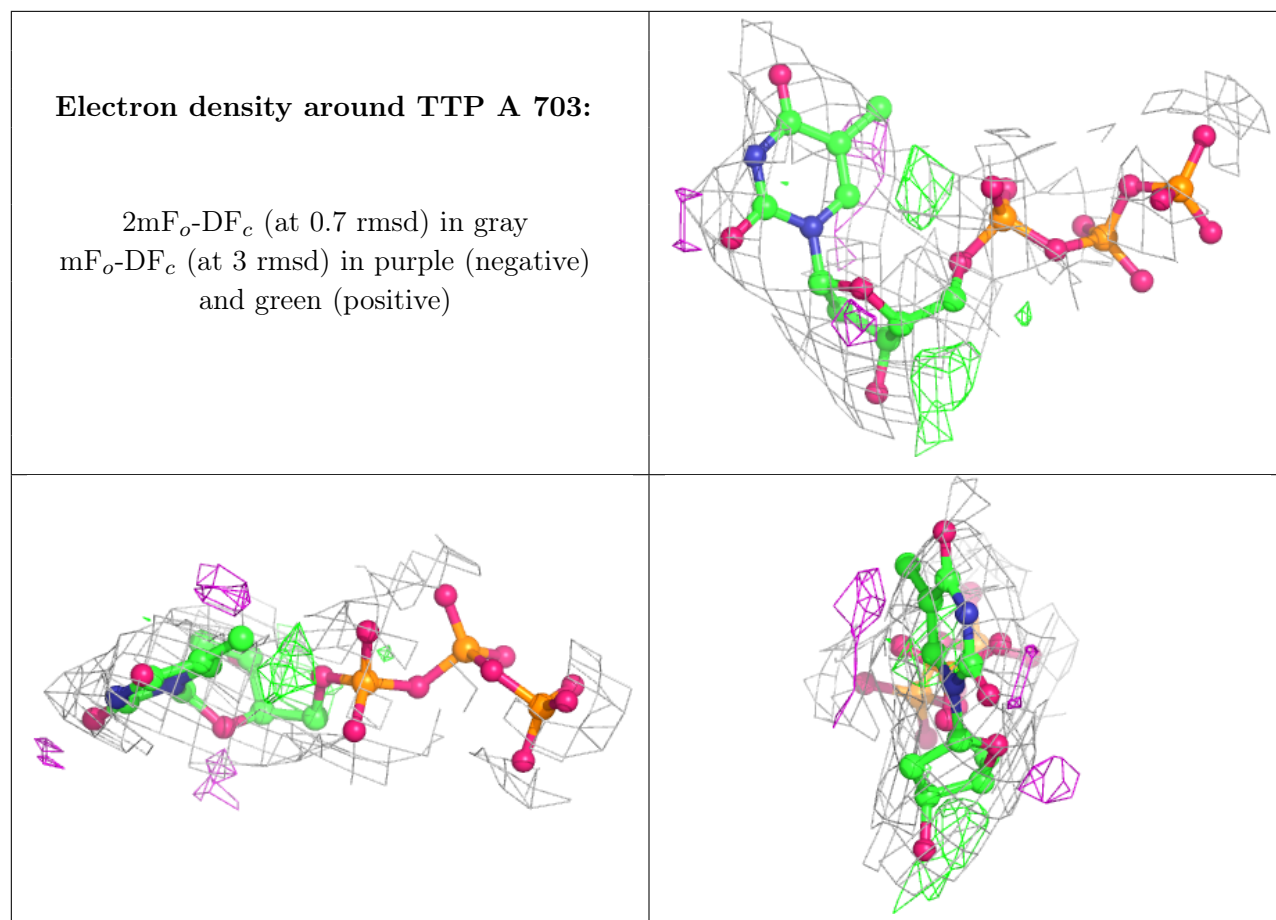
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TTP B 702:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.