



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:11 PM UTC

PDB ID : 6CM2 / pdb_00006cm2
Title : SAMHD1 HD domain bound to decitabine triphosphate
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Deposited on : 2018-03-02
Resolution : 2.14 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)

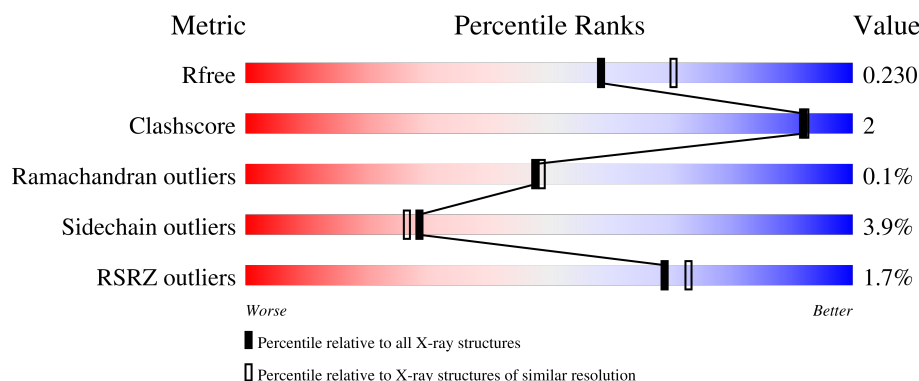
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	2% 87% 6% 7%
1	B	514	2% 86% 8% 6%
1	C	514	2% 86% 8% 6%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	514	2% 84% 9% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16496 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.

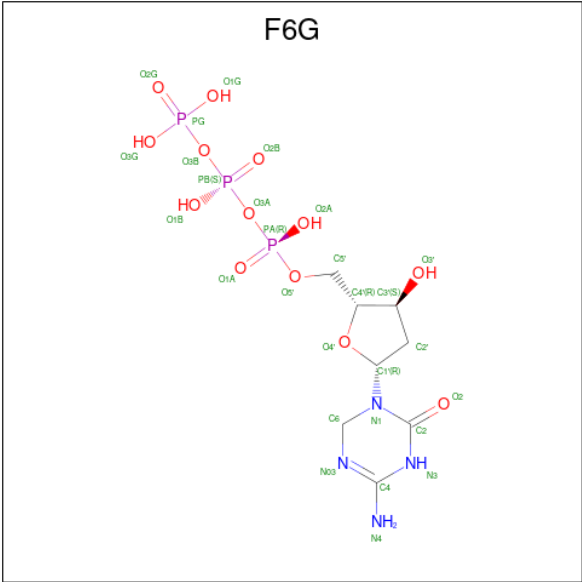
- Molecule 1 is a protein called Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	481	Total	C	N	O	S	0	3	0
			3956	2529	689	717	21			
1	C	481	Total	C	N	O	S	0	1	0
			3941	2521	687	713	20			
1	B	481	Total	C	N	O	S	0	2	0
			3944	2523	687	713	21			
1	A	480	Total	C	N	O	S	0	1	0
			3931	2516	685	709	21			

There are 8 discrepancies between the modelled and reference sequences:

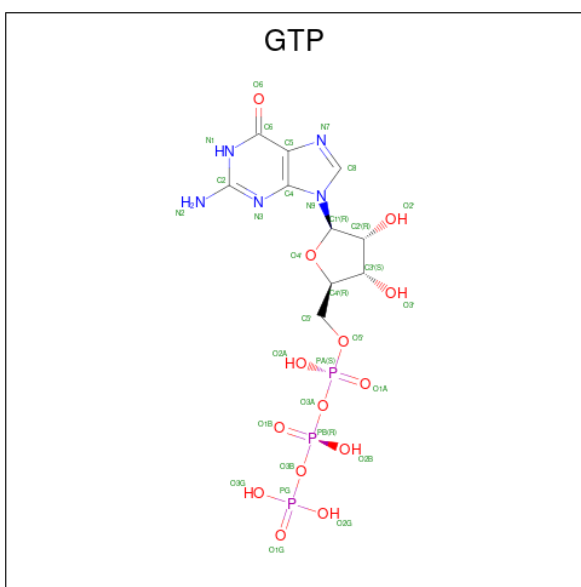
Chain	Residue	Modelled	Actual	Comment	Reference
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation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

- Molecule 2 is 6-amino-3-{2-deoxy-5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-erythro-pentofuranosyl}-3,4-dihydro-1,3,5-triazin-2(1H)-one (CCD ID: F6G) (formula: C₈H₁₇N₄O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			28	8	4	13	3		
2	D	1	Total	C	N	O	P	0	0
			28	8	4	13	3		
2	C	1	Total	C	N	O	P	0	0
			28	8	4	13	3		
2	C	1	Total	C	N	O	P	0	0
			28	8	4	13	3		
2	B	1	Total	C	N	O	P	0	0
			28	8	4	13	3		
2	B	1	Total	C	N	O	P	0	0
			28	8	4	13	3		
2	A	1	Total	C	N	O	P	0	0
			28	8	4	13	3		
2	A	1	Total	C	N	O	P	0	0
			28	8	4	13	3		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	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	B	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		

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	98	Total	O	0	0
			98	98		
5	C	88	Total	O	0	0
			88	88		

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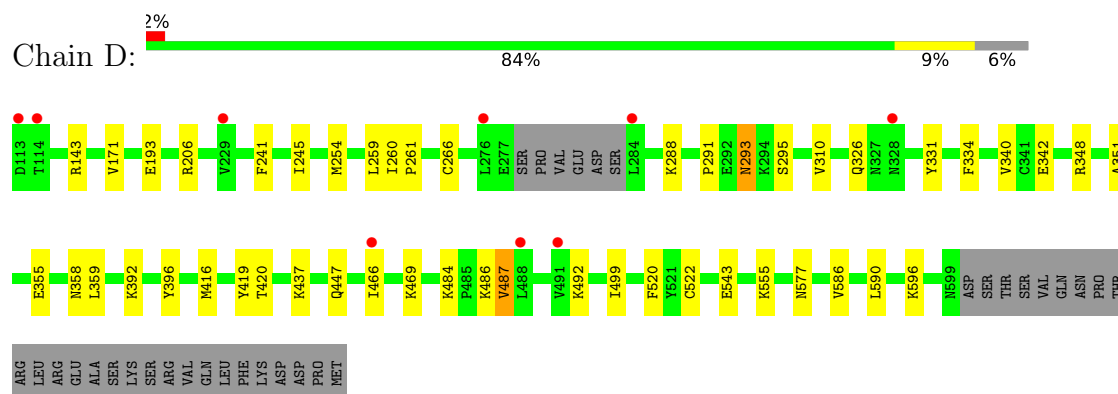
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	78	Total 78	O 78	0	0
5	A	104	Total 104	O 104	0	0

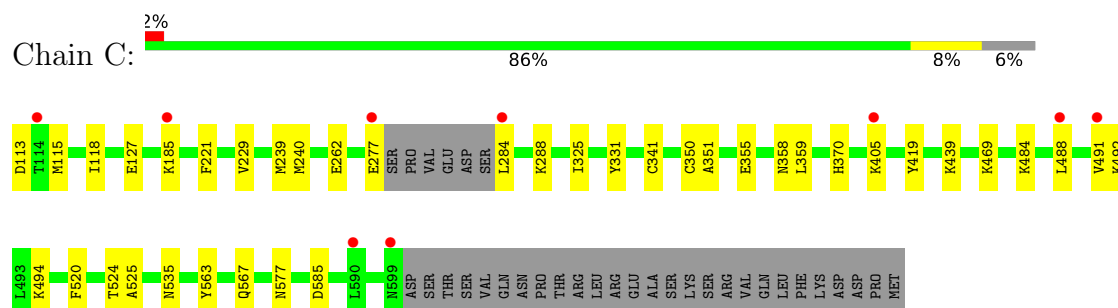
3 Residue-property plots

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.

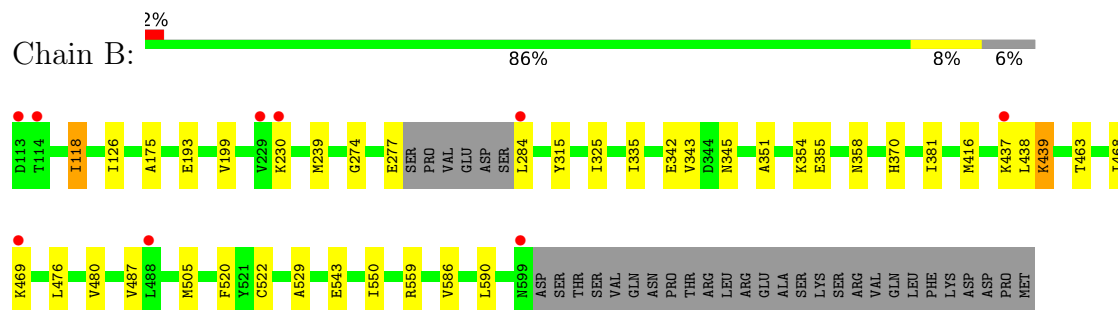
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



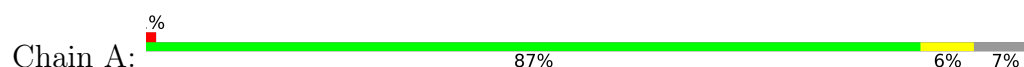
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

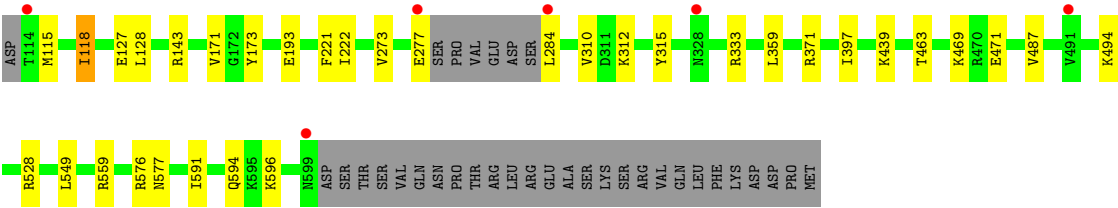


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- 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	87.49Å 146.54Å 98.55Å 90.00° 114.61° 90.00°	Depositor
Resolution (Å)	50.00 – 2.14 50.00 – 2.14	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.14) 99.0 (50.00-2.14)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.174 , 0.225 0.177 , 0.230	Depositor DCC
R_{free} test set	6373 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16496	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: GTP, F6G, 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	1.07	4/4023 (0.1%)	1.11	2/5430 (0.0%)
1	B	1.02	2/4039 (0.0%)	1.09	4/5452 (0.1%)
1	C	1.02	1/4033 (0.0%)	1.04	4/5444 (0.1%)
1	D	1.03	2/4048 (0.0%)	1.07	1/5464 (0.0%)
All	All	1.04	9/16143 (0.1%)	1.08	11/21790 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	TYR	C-O	-5.84	1.17	1.24
1	A	222	ILE	CA-C	5.71	1.57	1.52
1	D	419	TYR	C-O	-5.71	1.17	1.24
1	C	325	ILE	C-O	-5.68	1.18	1.24
1	A	221	PHE	CA-C	5.37	1.59	1.52
1	D	266	CYS	C-O	-5.13	1.18	1.24
1	B	335	ILE	C-O	-5.11	1.18	1.24
1	B	354	LYS	C-O	-5.06	1.17	1.24
1	A	577	ASN	CA-C	5.01	1.59	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	ILE	N-CA-C	-6.10	99.34	108.12
1	A	576	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	C	525	ALA	CA-C-N	5.75	125.42	119.56
1	C	525	ALA	C-N-CA	5.75	125.42	119.56
1	A	333	ARG	N-CA-C	-5.40	105.47	111.36
1	D	487	VAL	CB-CA-C	-5.32	104.41	111.80
1	B	274	GLY	CA-C-N	5.32	126.49	119.84
1	B	274	GLY	C-N-CA	5.32	126.49	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	325	ILE	N-CA-C	-5.18	100.41	108.86
1	C	221	PHE	N-CA-C	5.16	116.71	111.14
1	B	345	ASN	N-CA-C	5.05	119.29	113.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3931	0	3921	7	0
1	B	3944	0	3931	14	0
1	C	3941	0	3926	9	0
1	D	3956	0	3935	22	0
2	A	56	0	0	2	0
2	B	56	0	0	0	0
2	C	56	0	0	1	0
2	D	56	0	0	1	0
3	A	32	0	12	0	0
3	B	64	0	24	0	0
3	D	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	104	0	0	0	0
5	B	78	0	0	0	0
5	C	88	0	0	0	0
5	D	98	0	0	0	0
All	All	16496	0	15761	51	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 2.

All (51) 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:487:VAL:HG13	1:D:590:LEU:HD12	1.75	0.68
1:B:118:ILE:HG22	1:B:126:ILE:HB	1.78	0.66
2:A:703:F6G:O1G	2:A:703:F6G:O2A	2.18	0.62
1:D:396:TYR:CD1	1:D:437:LYS:HD2	2.34	0.62
1:A:312:LYS:NZ	2:A:703:F6G:O2B	2.32	0.62
1:D:522[A]:CYS:SG	1:B:586:VAL:HG11	2.43	0.59
1:D:331:TYR:C	1:D:331:TYR:CD1	2.81	0.57
1:D:355:GLU:OE1	1:D:358:ASN:ND2	2.38	0.57
1:C:351:ALA:O	1:C:520:PHE:HA	2.07	0.54
1:D:396:TYR:CE1	1:D:437:LYS:HD2	2.42	0.54
1:C:331:TYR:C	1:C:331:TYR:CD1	2.87	0.52
1:D:416:MET:HA	1:D:416:MET:HE2	1.91	0.51
1:B:370:HIS:HB3	1:B:505:MET:HE1	1.93	0.51
1:C:240:MET:HE2	1:C:419:TYR:HD2	1.77	0.50
1:D:291:PRO:HG2	1:D:293:ASN:HD21	1.78	0.49
1:D:334:PHE:HE2	1:D:359:LEU:HD11	1.76	0.49
1:D:351:ALA:O	1:D:520:PHE:HA	2.12	0.49
1:A:487:VAL:HG23	1:A:591:ILE:HD11	1.96	0.48
1:D:499:ILE:HD11	1:D:555:LYS:HE2	1.95	0.48
1:A:171:VAL:HG13	1:A:310:VAL:HG23	1.97	0.47
1:D:171:VAL:HG13	1:D:310:VAL:HG23	1.97	0.47
1:C:115:MET:HE3	1:C:127:GLU:HB3	1.97	0.47
1:D:334:PHE:CE2	1:D:359:LEU:HD11	2.50	0.46
1:B:438:LEU:O	1:B:439:LYS:C	2.58	0.46
1:D:586:VAL:HG11	1:B:522[A]:CYS:SG	2.55	0.46
1:D:241:PHE:CE1	1:D:245:ILE:HD11	2.51	0.46
1:B:175:ALA:HB1	1:B:199:VAL:HG12	1.98	0.45
2:D:701:F6G:O1G	2:D:701:F6G:O2A	2.33	0.45
1:D:143:ARG:HD2	1:D:420:THR:HA	1.98	0.45
1:C:341:CYS:HB2	1:C:350:CYS:SG	2.57	0.45
1:B:476:LEU:O	1:B:480:VAL:HG23	2.17	0.45
1:A:371:ARG:NH1	1:A:549:LEU:HD21	2.31	0.45
1:D:254:MET:HE3	1:D:259:LEU:HD23	1.99	0.45
1:D:260:ILE:O	1:D:261:PRO:C	2.59	0.44
1:D:487:VAL:CG1	1:D:590:LEU:HD12	2.44	0.44
1:C:370:HIS:NE2	2:C:701:F6G:O2A	2.48	0.44
1:B:239:MET:HE2	1:B:416:MET:HE3	2.00	0.44
1:A:118:ILE:HD11	1:A:128:LEU:HD12	2.01	0.43
1:B:468:ILE:HD12	1:B:550:ILE:HD11	1.99	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:A:115:MET:HE3	1:A:127:GLU:HB3	2.00	0.43
1:D:340:VAL:HA	1:D:348:ARG:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:VAL:HG13	1:D:590:LEU:CD1	2.46	0.42
1:C:355:GLU:OE1	1:C:358:ASN:ND2	2.51	0.42
1:B:355:GLU:OE1	1:B:358:ASN:ND2	2.52	0.42
1:D:241:PHE:O	1:D:245:ILE:HG12	2.19	0.42
1:B:487:VAL:HG22	1:B:590:LEU:CD1	2.50	0.42
1:C:563:TYR:O	1:C:567:GLN:HG2	2.20	0.42
1:C:585:ASP:O	1:A:528:ARG:NH2	2.53	0.42
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.95	0.41
1:B:343:VAL:HG22	1:B:529:ALA:CB	2.51	0.41

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	477/514 (93%)	468 (98%)	9 (2%)	0	100	100
1	B	479/514 (93%)	464 (97%)	15 (3%)	0	100	100
1	C	478/514 (93%)	461 (96%)	16 (3%)	1 (0%)	43	42
1	D	480/514 (93%)	466 (97%)	14 (3%)	0	100	100
All	All	1914/2056 (93%)	1859 (97%)	54 (3%)	1 (0%)	48	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	488	LEU

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/459 (93%)	410 (96%)	17 (4%)	28	25
1	B	429/459 (94%)	416 (97%)	13 (3%)	36	37
1	C	428/459 (93%)	408 (95%)	20 (5%)	23	19
1	D	430/459 (94%)	413 (96%)	17 (4%)	28	25
All	All	1714/1836 (93%)	1647 (96%)	67 (4%)	28	26

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	193	GLU
1	D	206	ARG
1	D	288	LYS
1	D	293	ASN
1	D	295	SER
1	D	326	GLN
1	D	342	GLU
1	D	392	LYS
1	D	447	GLN
1	D	466	ILE
1	D	469	LYS
1	D	484	LYS
1	D	486	LYS
1	D	492	LYS
1	D	543	GLU
1	D	577	ASN
1	D	596	LYS
1	C	113	ASP
1	C	118	ILE
1	C	185	LYS
1	C	229	VAL
1	C	239	MET
1	C	262	GLU
1	C	277	GLU
1	C	284	LEU
1	C	288	LYS
1	C	359	LEU
1	C	405	LYS

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Mol	Chain	Res	Type
1	C	439	LYS
1	C	469	LYS
1	C	484	LYS
1	C	491	VAL
1	C	492	LYS
1	C	494	LYS
1	C	524	THR
1	C	535	ASN
1	C	577	ASN
1	B	118	ILE
1	B	193	GLU
1	B	230	LYS
1	B	277	GLU
1	B	284	LEU
1	B	315	TYR
1	B	342	GLU
1	B	437	LYS
1	B	439	LYS
1	B	463	THR
1	B	469	LYS
1	B	543	GLU
1	B	559	ARG
1	A	118	ILE
1	A	143	ARG
1	A	193	GLU
1	A	273	VAL
1	A	277	GLU
1	A	284	LEU
1	A	315	TYR
1	A	359	LEU
1	A	397	ILE
1	A	439	LYS
1	A	463	THR
1	A	469	LYS
1	A	471	GLU
1	A	494	LYS
1	A	559	ARG
1	A	594	GLN
1	A	596	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	149	GLN
1	D	180	HIS
1	D	200	GLN
1	D	207	ASN
1	D	215	HIS
1	D	293	ASN
1	D	321	HIS
1	C	149	GLN
1	C	200	GLN
1	C	215	HIS
1	C	243	HIS
1	C	322	HIS
1	C	358	ASN
1	C	364	HIS
1	C	517	HIS
1	B	140	GLN
1	B	149	GLN
1	B	215	HIS
1	B	235	GLN
1	B	243	HIS
1	B	248	ASN
1	B	293	ASN
1	B	326	GLN
1	B	364	HIS
1	B	367	ASN
1	B	594	GLN
1	A	149	GLN
1	A	200	GLN
1	A	215	HIS
1	A	243	HIS
1	A	326	GLN
1	A	328	ASN
1	A	425	ASN
1	A	535	ASN
1	A	539	GLN

5.3.3 RNA ⓘ

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 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	F6G	A	703	-	25,29,29	4.19	11 (44%)	37,45,45	2.20	10 (27%)
3	GTP	B	705	4	33,34,34	1.53	5 (15%)	50,54,54	1.72	11 (22%)
2	F6G	C	701	-	25,29,29	4.29	12 (48%)	37,45,45	1.78	9 (24%)
2	F6G	C	703	4	25,29,29	3.60	10 (40%)	37,45,45	2.39	11 (29%)
3	GTP	B	703	4	33,34,34	1.35	6 (18%)	50,54,54	1.68	10 (20%)
3	GTP	D	702	4	33,34,34	1.19	3 (9%)	50,54,54	1.74	12 (24%)
2	F6G	B	704	-	25,29,29	4.16	10 (40%)	37,45,45	1.92	9 (24%)
3	GTP	A	704	4	33,34,34	1.47	6 (18%)	50,54,54	1.65	14 (28%)
2	F6G	A	701	4	25,29,29	3.56	10 (40%)	37,45,45	2.43	9 (24%)
2	F6G	D	703	4	25,29,29	3.45	9 (36%)	37,45,45	2.39	11 (29%)
2	F6G	B	701	4	25,29,29	3.76	10 (40%)	37,45,45	2.34	12 (32%)
2	F6G	D	701	-	25,29,29	4.38	10 (40%)	37,45,45	1.71	8 (21%)

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	F6G	A	703	-	-	3/22/47/47	0/1/2/2
3	GTP	B	705	4	-	8/22/38/38	0/3/3/3
2	F6G	C	701	-	-	8/22/47/47	0/1/2/2
2	F6G	C	703	4	-	6/22/47/47	0/1/2/2
3	GTP	B	703	4	-	5/22/38/38	0/3/3/3
3	GTP	D	702	4	-	4/22/38/38	0/3/3/3
2	F6G	B	704	-	-	3/22/47/47	0/1/2/2
3	GTP	A	704	4	-	2/22/38/38	0/3/3/3
2	F6G	A	701	4	-	7/22/47/47	0/1/2/2
2	F6G	D	703	4	-	3/22/47/47	0/1/2/2
2	F6G	B	701	4	-	9/22/47/47	0/1/2/2
2	F6G	D	701	-	-	1/22/47/47	0/1/2/2

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	F6G	PB-O3B	10.65	1.71	1.59
2	D	701	F6G	C6-N03	-10.54	1.35	1.46
2	A	703	F6G	PB-O3B	10.54	1.70	1.59
2	C	701	F6G	PB-O3B	10.28	1.70	1.59
2	B	701	F6G	C6-N03	-10.16	1.36	1.46
2	C	701	F6G	C6-N03	-9.78	1.36	1.46
2	A	703	F6G	C2'-C3'	-9.48	1.28	1.52
2	D	703	F6G	C6-N03	-9.40	1.37	1.46
2	A	703	F6G	C6-N03	-9.22	1.37	1.46
2	B	704	F6G	C6-N03	-9.13	1.37	1.46
2	C	703	F6G	C6-N03	-8.96	1.37	1.46
2	C	701	F6G	C2'-C3'	-8.91	1.30	1.52
2	A	701	F6G	C2'-C3'	-8.87	1.30	1.52
2	D	701	F6G	C2'-C3'	-8.83	1.30	1.52
2	B	704	F6G	C2'-C3'	-8.79	1.30	1.52
2	A	701	F6G	C6-N03	-8.57	1.37	1.46
2	B	704	F6G	PB-O3B	8.26	1.68	1.59
2	C	703	F6G	C2'-C3'	-8.19	1.32	1.52
2	D	701	F6G	O4'-C4'	-8.17	1.26	1.45
2	D	703	F6G	C2'-C3'	-7.83	1.33	1.52
2	B	701	F6G	C2'-C3'	-7.69	1.33	1.52
2	B	704	F6G	PA-O3A	7.39	1.67	1.59
2	A	703	F6G	O4'-C4'	-7.21	1.29	1.45
2	C	701	F6G	O4'-C4'	-7.17	1.29	1.45
2	B	704	F6G	O4'-C4'	-7.12	1.29	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	703	F6G	O4'-C4'	-7.08	1.29	1.45
2	B	701	F6G	O4'-C4'	-6.91	1.29	1.45
2	C	703	F6G	O4'-C4'	-6.63	1.30	1.45
2	C	703	F6G	C4-N4	6.56	1.49	1.34
2	A	701	F6G	C4-N4	6.38	1.49	1.34
2	A	701	F6G	O4'-C4'	-6.33	1.30	1.45
2	B	701	F6G	C4-N4	5.82	1.47	1.34
2	B	701	F6G	O4'-C1'	5.80	1.55	1.42
2	D	703	F6G	C4-N4	5.67	1.47	1.34
2	B	704	F6G	O4'-C1'	5.39	1.54	1.42
2	D	701	F6G	O4'-C1'	5.03	1.53	1.42
2	C	701	F6G	C4-N4	5.00	1.45	1.34
2	C	701	F6G	O4'-C1'	4.93	1.53	1.42
2	C	703	F6G	O4'-C1'	4.79	1.53	1.42
2	D	701	F6G	C3'-C4'	4.79	1.65	1.53
2	C	701	F6G	C3'-C4'	4.73	1.65	1.53
2	A	703	F6G	C4-N4	4.68	1.45	1.34
2	A	703	F6G	O4'-C1'	4.66	1.52	1.42
2	D	701	F6G	PA-O3A	4.64	1.64	1.59
2	B	704	F6G	C3'-C4'	4.50	1.64	1.53
2	A	701	F6G	O4'-C1'	4.47	1.52	1.42
2	B	701	F6G	C3'-C4'	4.43	1.64	1.53
2	C	703	F6G	C3'-C4'	4.38	1.64	1.53
2	B	704	F6G	C4-N4	4.33	1.44	1.34
2	C	701	F6G	PA-O3A	4.13	1.64	1.59
2	D	703	F6G	O4'-C1'	4.11	1.51	1.42
2	A	703	F6G	C3'-C4'	4.00	1.63	1.53
2	A	701	F6G	C3'-C4'	3.83	1.63	1.53
2	B	701	F6G	PA-O3A	3.72	1.63	1.59
3	B	703	GTP	C5-N7	-3.59	1.31	1.39
3	B	705	GTP	PA-O3A	3.49	1.63	1.59
2	D	701	F6G	C4-N4	3.48	1.42	1.34
2	D	703	F6G	C3'-C4'	3.46	1.62	1.53
2	B	701	F6G	PB-O3B	3.40	1.63	1.59
3	B	705	GTP	C5-C4	3.39	1.48	1.38
3	B	705	GTP	C5-N7	-3.39	1.32	1.39
2	A	701	F6G	C2-N3	-3.37	1.32	1.38
3	A	704	GTP	C5-C4	3.34	1.47	1.38
2	C	703	F6G	PB-O3A	3.29	1.63	1.59
2	C	703	F6G	PB-O3B	3.29	1.63	1.59
2	D	703	F6G	PB-O3A	3.13	1.62	1.59
3	B	705	GTP	C6-N1	-3.10	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	GTP	PB-O3A	3.10	1.62	1.59
2	B	704	F6G	PA-O5'	3.07	1.71	1.59
3	B	705	GTP	C4-N9	-3.06	1.30	1.38
2	A	701	F6G	PB-O3A	-3.03	1.56	1.59
3	A	704	GTP	PB-O3B	2.99	1.62	1.59
3	A	704	GTP	C4-N9	-2.98	1.30	1.38
3	D	702	GTP	C5-C4	2.98	1.46	1.38
2	A	703	F6G	O3'-C3'	2.90	1.49	1.43
2	C	701	F6G	O3'-C3'	2.84	1.49	1.43
2	D	701	F6G	O3'-C3'	2.80	1.49	1.43
2	B	704	F6G	PB-O3A	2.80	1.62	1.59
2	A	703	F6G	PA-O3A	2.79	1.62	1.59
2	C	701	F6G	PA-O5'	2.75	1.70	1.59
2	B	701	F6G	O3'-C3'	2.72	1.49	1.43
3	A	704	GTP	C5-N7	-2.69	1.33	1.39
2	A	703	F6G	PA-O5'	2.63	1.69	1.59
2	D	701	F6G	PA-O5'	2.58	1.69	1.59
3	D	702	GTP	C4-N9	-2.54	1.31	1.38
3	B	703	GTP	C6-N1	-2.53	1.34	1.38
3	D	702	GTP	PB-O3B	2.44	1.62	1.59
3	B	703	GTP	C5-C4	2.43	1.45	1.38
3	B	703	GTP	C4-N9	-2.41	1.31	1.38
2	A	701	F6G	PB-O3B	2.40	1.62	1.59
2	C	703	F6G	C2-N1	2.34	1.38	1.35
2	C	701	F6G	PB-O3A	2.31	1.62	1.59
2	D	703	F6G	C2-N3	-2.29	1.34	1.38
2	C	701	F6G	C2'-C1'	2.19	1.58	1.52
3	B	703	GTP	PB-O3A	2.19	1.61	1.59
3	B	703	GTP	PB-O3B	2.16	1.61	1.59
2	D	703	F6G	O3'-C3'	2.16	1.47	1.43
3	A	704	GTP	C6-N1	-2.15	1.34	1.38
2	C	703	F6G	C2-N3	-2.10	1.34	1.38
2	A	703	F6G	C2'-C1'	2.09	1.58	1.52
2	B	701	F6G	C2-N3	-2.06	1.34	1.38
2	A	701	F6G	C2-N1	2.01	1.38	1.35

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	F6G	C2'-C1'-N1	8.66	125.88	115.59
2	D	703	F6G	C2'-C1'-N1	7.65	124.68	115.59
2	C	703	F6G	N1-C6-N03	7.35	124.93	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	F6G	C2'-C1'-N1	6.98	123.88	115.59
2	C	703	F6G	C2'-C1'-N1	6.86	123.75	115.59
2	D	703	F6G	N1-C6-N03	6.56	123.80	114.46
2	A	703	F6G	N1-C6-N03	6.26	123.37	114.46
2	B	701	F6G	N1-C6-N03	6.22	123.31	114.46
2	A	701	F6G	N1-C6-N03	6.07	123.10	114.46
2	B	704	F6G	N1-C6-N03	5.51	122.30	114.46
2	B	701	F6G	N3-C2-N1	5.50	122.18	116.65
2	C	701	F6G	N1-C6-N03	5.42	122.18	114.46
3	B	705	GTP	C5-C4-N3	-5.13	120.23	128.39
3	D	702	GTP	C5-C4-N3	-5.11	120.25	128.39
2	A	701	F6G	O4'-C1'-N1	-5.04	102.14	108.39
3	A	704	GTP	O3G-PG-O2G	4.91	126.22	107.80
2	B	704	F6G	O4'-C1'-N1	4.78	114.31	108.39
2	D	703	F6G	N3-C2-N1	4.65	121.32	116.65
2	D	701	F6G	N1-C6-N03	4.58	120.97	114.46
3	B	705	GTP	O3A-PB-O1B	-4.40	97.47	110.70
3	B	703	GTP	C5-C4-N3	-4.33	121.49	128.39
2	A	703	F6G	O4'-C1'-N1	4.32	113.74	108.39
3	D	702	GTP	N9-C4-N3	4.31	134.57	125.95
2	C	703	F6G	O1B-PB-O3A	4.27	118.81	107.27
2	D	701	F6G	N3-C2-N1	4.15	120.82	116.65
2	C	703	F6G	O4'-C1'-N1	-4.08	103.32	108.39
2	A	703	F6G	N3-C2-N1	4.04	120.71	116.65
2	A	703	F6G	O3G-PG-O3B	4.03	118.17	104.64
2	D	703	F6G	O4'-C1'-N1	-3.93	103.51	108.39
2	A	701	F6G	N3-C2-N1	3.92	120.59	116.65
3	B	703	GTP	C2-N3-C4	3.80	118.85	112.30
3	B	703	GTP	N9-C4-N3	3.77	133.49	125.95
3	B	705	GTP	N9-C4-N3	3.66	133.27	125.95
3	D	702	GTP	C2-N3-C4	3.62	118.53	112.30
2	D	701	F6G	O3A-PB-O2B	-3.61	99.84	110.70
2	A	703	F6G	O3B-PB-O2B	3.57	121.44	110.70
2	C	701	F6G	O1B-PB-O3A	-3.56	97.66	107.27
2	A	703	F6G	C6-N1-C2	-3.55	115.65	121.70
2	A	703	F6G	O3A-PB-O2B	-3.42	100.41	110.70
2	D	703	F6G	O3A-PB-O2B	-3.38	100.55	110.70
2	B	701	F6G	C6-N1-C2	-3.31	116.06	121.70
2	D	701	F6G	O3G-PG-O3B	3.24	115.51	104.64
2	C	703	F6G	C6-N1-C2	-3.23	116.18	121.70
3	B	703	GTP	C6-C5-N7	3.20	136.10	130.29
3	B	705	GTP	C2-N3-C4	3.18	117.78	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	F6G	N3-C2-N1	3.12	119.79	116.65
2	B	704	F6G	N3-C2-N1	3.11	119.77	116.65
2	D	703	F6G	C6-N1-C2	-3.07	116.46	121.70
3	A	704	GTP	C5-C4-N3	-3.07	123.50	128.39
2	C	703	F6G	O2A-PA-O3A	3.06	115.55	107.27
2	B	701	F6G	O3B-PB-O2B	-2.96	101.78	110.70
2	C	701	F6G	C6-N1-C2	-2.94	116.69	121.70
2	A	701	F6G	C6-N1-C2	-2.94	116.69	121.70
3	A	704	GTP	O2A-PA-O3A	2.91	115.13	107.27
2	B	704	F6G	O2-C2-N3	-2.90	116.14	121.49
2	C	703	F6G	O3A-PB-O2B	-2.90	101.97	110.70
3	B	703	GTP	O3A-PB-O1B	-2.90	101.99	110.70
3	A	704	GTP	C3'-C2'-C1'	2.88	106.92	101.46
2	D	703	F6G	O4'-C1'-C2'	-2.88	100.86	106.25
2	B	704	F6G	C6-N1-C2	-2.85	116.84	121.70
2	B	701	F6G	O1B-PB-O3B	2.85	114.97	107.27
2	D	701	F6G	O2-C2-N3	-2.81	116.31	121.49
3	D	702	GTP	O6-C6-C5	-2.80	119.14	126.53
2	B	701	F6G	O2-C2-N3	-2.80	116.32	121.49
2	C	701	F6G	O3G-PG-O3B	2.74	113.81	104.64
2	A	701	F6G	O2A-PA-O3A	-2.71	99.95	107.27
3	D	702	GTP	O2B-PB-O3A	-2.67	100.07	107.27
2	A	701	F6G	O2A-PA-O1A	2.65	124.76	112.44
2	D	701	F6G	C6-N1-C2	-2.64	117.20	121.70
3	A	704	GTP	O2G-PG-O3B	-2.62	95.85	104.64
3	D	702	GTP	C2-N1-C6	-2.62	120.36	125.11
2	C	701	F6G	O2-C2-N3	-2.58	116.72	121.49
2	B	704	F6G	O1B-PB-O3A	2.54	114.14	107.27
3	B	705	GTP	O5'-PA-O1A	-2.53	98.92	108.94
3	A	704	GTP	O2B-PB-O3A	-2.51	100.49	107.27
2	A	703	F6G	O1B-PB-O3B	2.50	114.04	107.27
3	A	704	GTP	N9-C4-N3	2.50	130.95	125.95
2	C	701	F6G	O1G-PG-O3B	2.49	113.00	104.64
3	B	703	GTP	C3'-C2'-C1'	2.48	106.16	101.46
2	D	703	F6G	C3'-C2'-C1'	2.48	108.67	102.60
2	A	701	F6G	O2-C2-N3	-2.48	116.92	121.49
3	B	705	GTP	O2A-PA-O3A	2.46	113.92	107.27
3	A	704	GTP	O6-C6-N1	2.46	124.74	120.11
2	D	701	F6G	O2A-PA-O3A	2.45	113.89	107.27
3	B	705	GTP	O2B-PB-O3A	2.43	113.85	107.27
2	B	701	F6G	O2A-PA-O3A	2.43	113.84	107.27
2	C	703	F6G	N3-C2-N1	2.40	119.06	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	GTP	O3G-PG-O2G	2.39	116.76	107.80
2	B	701	F6G	O3'-C3'-C2'	2.39	119.17	110.88
3	B	703	GTP	O2B-PB-O3B	2.38	113.72	107.27
3	D	702	GTP	C6-C5-N7	2.37	134.61	130.29
3	B	705	GTP	C3'-C2'-C1'	2.36	105.93	101.46
2	A	701	F6G	O4'-C1'-C2'	-2.36	101.84	106.25
3	A	704	GTP	C2-N3-C4	2.34	116.32	112.30
3	B	703	GTP	O2B-PB-O3A	2.33	113.56	107.27
2	B	704	F6G	O1G-PG-O3B	2.33	112.43	104.64
3	A	704	GTP	O2B-PB-O1B	2.30	123.14	112.44
3	D	702	GTP	O2A-PA-O3A	2.28	113.43	107.27
3	D	702	GTP	N2-C2-N3	-2.27	115.23	119.67
3	D	702	GTP	O3'-C3'-C2'	2.27	119.10	111.82
2	C	701	F6G	N3-C4-N03	-2.27	119.15	123.32
2	B	704	F6G	O3A-PB-O2B	-2.27	103.88	110.70
2	D	703	F6G	O1G-PG-O3B	2.26	112.23	104.64
3	A	704	GTP	O6-C6-C5	-2.25	120.60	126.53
3	B	705	GTP	C6-C5-N7	2.23	134.36	130.29
2	C	701	F6G	O2A-PA-O3A	-2.22	101.28	107.27
2	A	703	F6G	O4'-C1'-C2'	-2.18	102.18	106.25
3	A	704	GTP	N2-C2-N3	-2.17	115.43	119.67
2	C	703	F6G	O1G-PG-O3B	2.16	111.89	104.64
3	B	703	GTP	O6-C6-C5	-2.16	120.83	126.53
2	C	703	F6G	N4-C4-N3	2.14	121.27	116.76
3	B	705	GTP	C4-C5-N7	-2.13	107.29	110.67
2	B	701	F6G	O3A-PB-O2B	2.11	117.06	110.70
2	D	703	F6G	O2-C2-N3	-2.11	117.60	121.49
3	A	704	GTP	O2'-C2'-C1'	-2.10	102.87	110.10
3	D	702	GTP	O2A-PA-O5'	-2.09	98.11	107.57
2	B	704	F6G	N3-C4-N03	-2.08	119.49	123.32
3	B	703	GTP	C8-N7-C5	2.08	107.96	104.26
3	B	705	GTP	O3G-PG-O3B	2.07	111.58	104.64
2	B	701	F6G	O1G-PG-O3G	2.06	115.53	107.80
2	C	703	F6G	C3'-C2'-C1'	2.06	107.64	102.60
2	D	703	F6G	O1B-PB-O3A	2.04	112.79	107.27
3	A	704	GTP	C4'-O4'-C1'	-2.04	104.97	109.47
2	D	701	F6G	O3A-PA-O1A	-2.03	104.59	110.70
2	A	703	F6G	O2A-PA-O3A	2.02	112.74	107.27
2	B	701	F6G	C2'-C3'-C4'	2.00	106.86	102.80

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	F6G	PB-O3B-PG-O1G
2	B	701	F6G	C2'-C1'-N1-C6
2	B	701	F6G	O4'-C1'-N1-C6
2	A	701	F6G	C2'-C1'-N1-C6
2	A	701	F6G	O4'-C1'-N1-C6
3	B	705	GTP	PB-O3B-PG-O3G
2	C	701	F6G	O4'-C4'-C5'-O5'
3	B	705	GTP	PB-O3B-PG-O1G
3	B	705	GTP	PG-O3B-PB-O1B
2	B	704	F6G	O4'-C4'-C5'-O5'
2	C	703	F6G	PB-O3B-PG-O3G
2	B	701	F6G	PB-O3B-PG-O1G
2	B	704	F6G	C3'-C4'-C5'-O5'
2	D	703	F6G	PG-O3B-PB-O2B
2	C	701	F6G	PB-O3A-PA-O1A
2	B	701	F6G	PB-O3A-PA-O2A
2	B	701	F6G	PG-O3B-PB-O1B
2	A	701	F6G	PG-O3B-PB-O1B
3	D	702	GTP	PG-O3B-PB-O1B
3	B	703	GTP	C5'-O5'-PA-O2A
3	B	705	GTP	C5'-O5'-PA-O3A
3	B	703	GTP	C4'-C5'-O5'-PA
3	B	705	GTP	C4'-C5'-O5'-PA
2	A	701	F6G	C2'-C1'-N1-C2
2	C	703	F6G	PB-O3A-PA-O2A
2	C	703	F6G	PG-O3B-PB-O2B
3	B	703	GTP	PG-O3B-PB-O2B
3	B	705	GTP	PG-O3B-PB-O2B
3	B	705	GTP	PB-O3A-PA-O2A
2	C	701	F6G	C3'-C4'-C5'-O5'
2	A	703	F6G	O4'-C4'-C5'-O5'
3	D	702	GTP	C4'-C5'-O5'-PA
2	C	703	F6G	C2'-C1'-N1-C2
2	B	701	F6G	C2'-C1'-N1-C2
2	C	701	F6G	C2'-C1'-N1-C6
3	A	704	GTP	C4'-C5'-O5'-PA
2	B	701	F6G	O4'-C1'-N1-C2
2	C	701	F6G	PB-O3B-PG-O2G
2	D	703	F6G	PB-O3B-PG-O3G
2	C	701	F6G	PB-O3B-PG-O3G
2	B	701	F6G	PB-O3B-PG-O3G
2	A	701	F6G	O4'-C1'-N1-C2
2	D	703	F6G	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	D	701	F6G	PB-O3A-PA-O2A
2	B	701	F6G	PG-O3B-PB-O2B
2	A	701	F6G	PG-O3B-PB-O2B
2	A	703	F6G	PA-O3A-PB-O1B
3	B	703	GTP	PG-O3B-PB-O1B
3	B	703	GTP	PB-O3A-PA-O2A
3	B	705	GTP	PB-O3A-PA-O1A
2	C	703	F6G	O4'-C1'-N1-C2
2	C	701	F6G	PB-O3A-PA-O2A
2	C	703	F6G	PG-O3B-PB-O1B
2	B	704	F6G	PB-O3A-PA-O2A
2	A	701	F6G	PB-O3A-PA-O2A
2	A	703	F6G	PA-O3A-PB-O2B
3	D	702	GTP	PG-O3B-PB-O2B
3	D	702	GTP	PB-O3A-PA-O2A
3	A	704	GTP	PB-O3A-PA-O2A

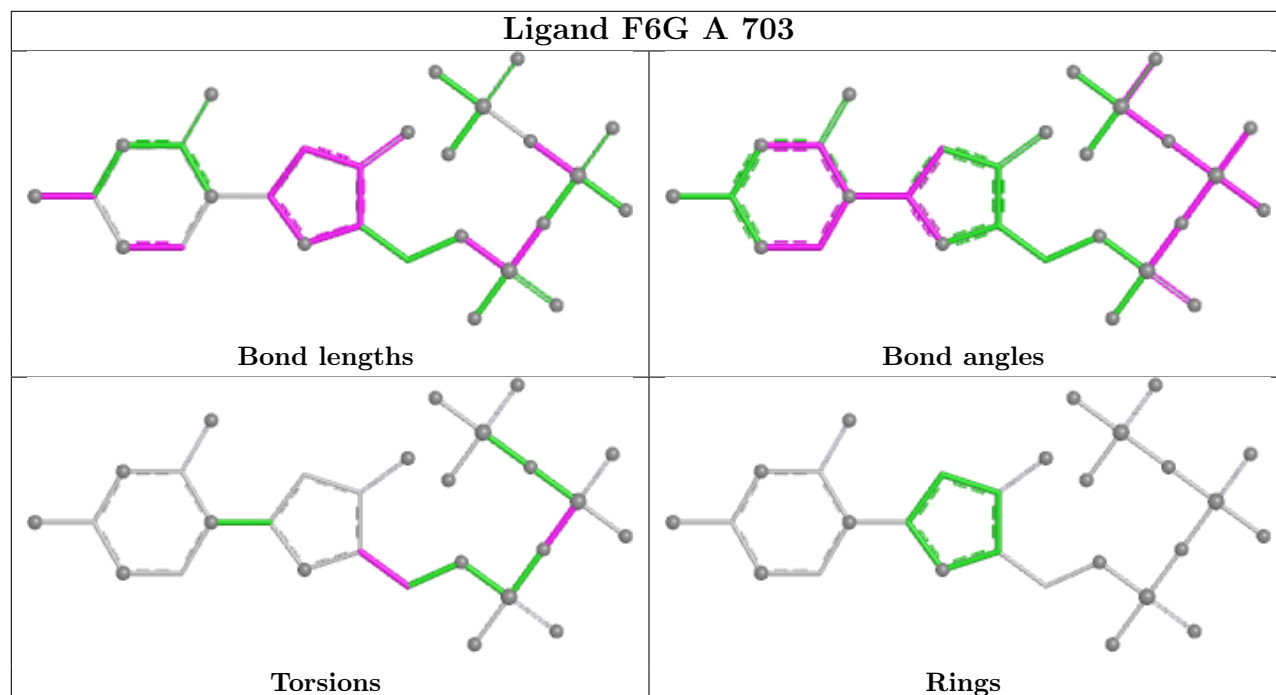
There are no ring outliers.

3 monomers are involved in 4 short contacts:

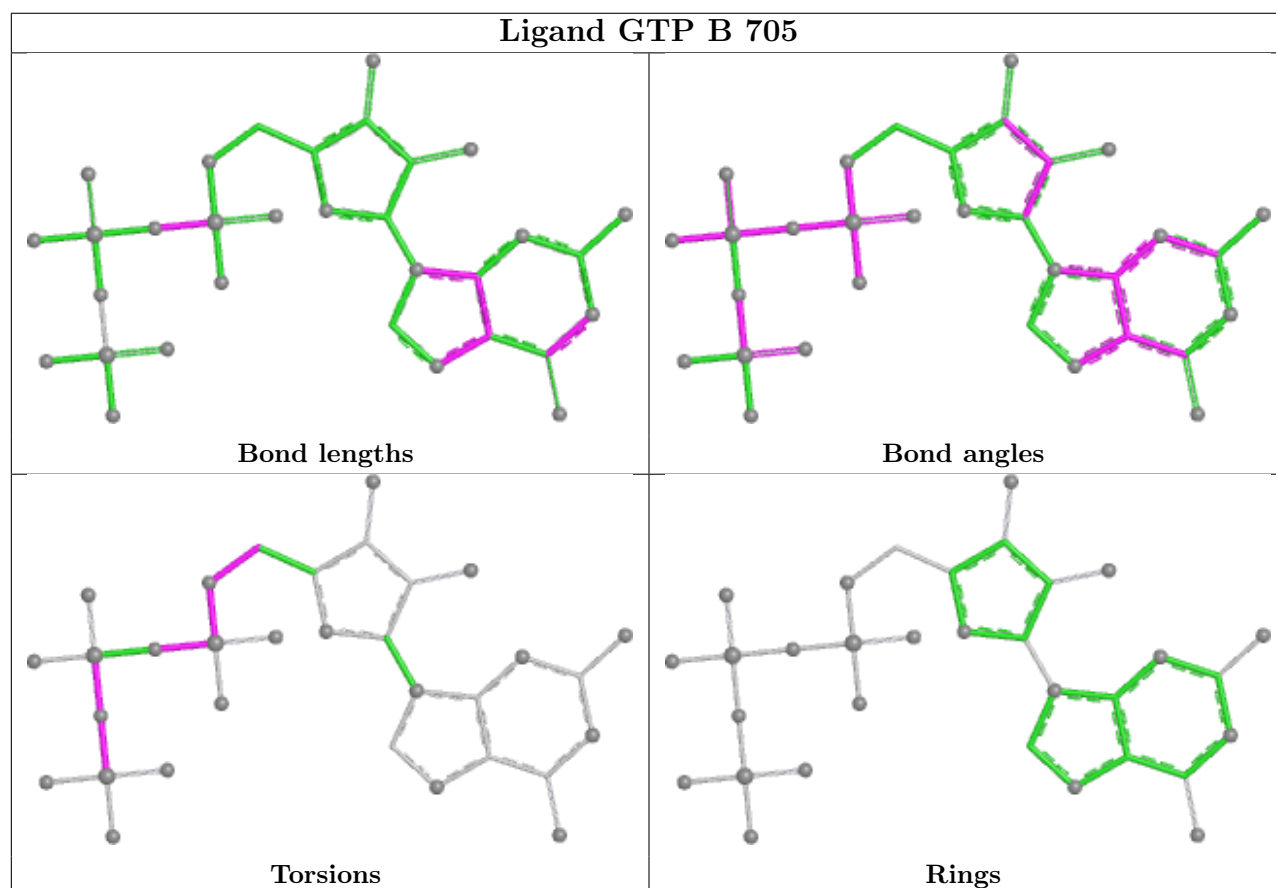
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	703	F6G	2	0
2	C	701	F6G	1	0
2	D	701	F6G	1	0

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.

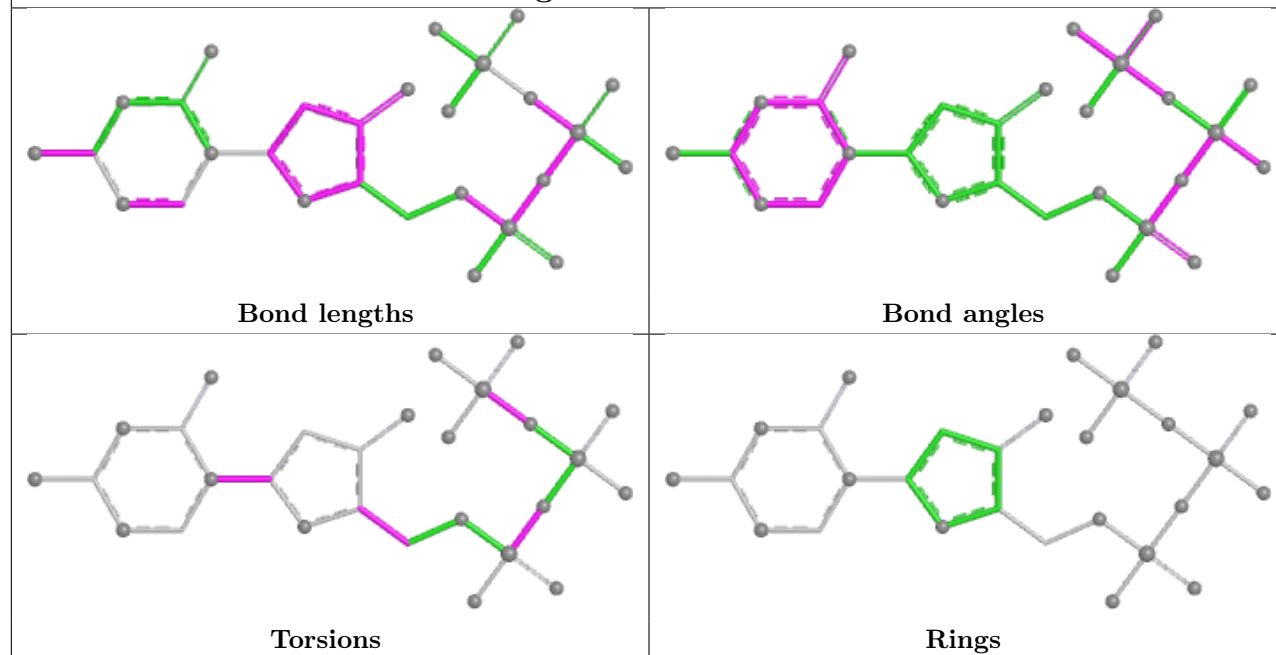
Ligand F6G A 703



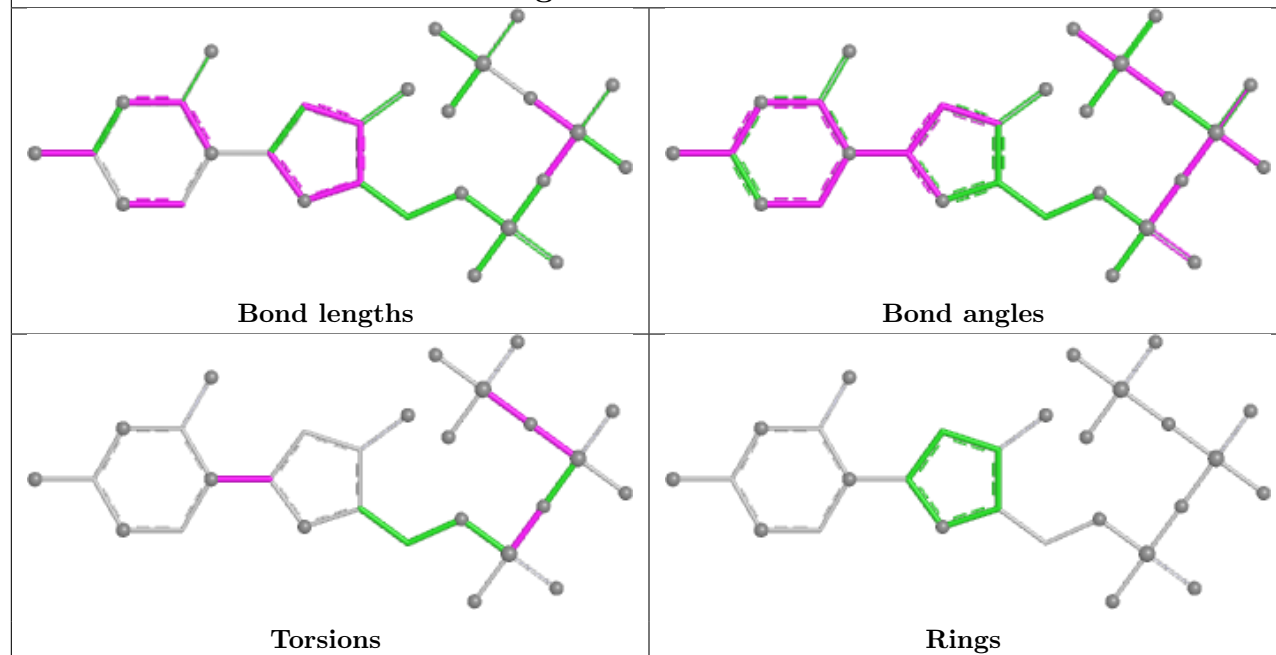
Ligand GTP B 705



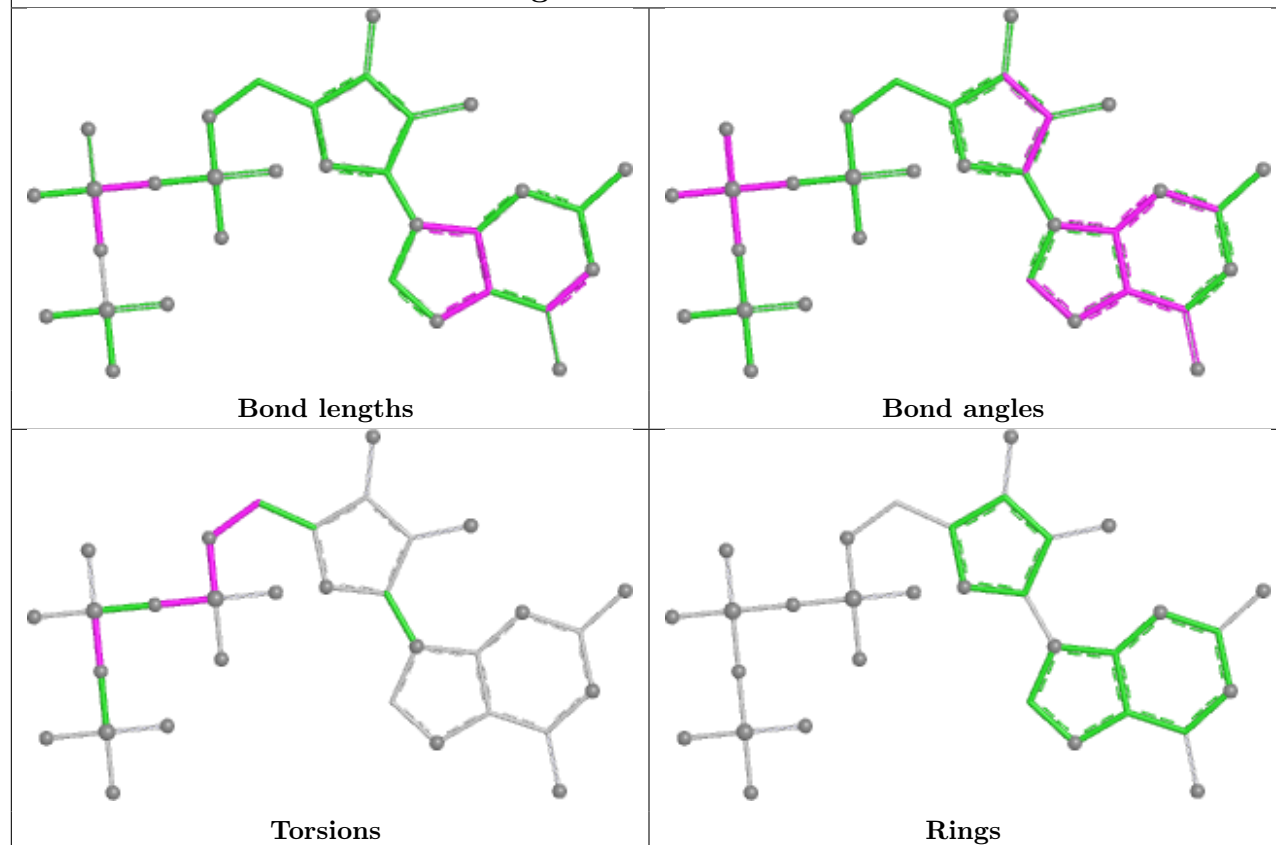
Ligand F6G C 701



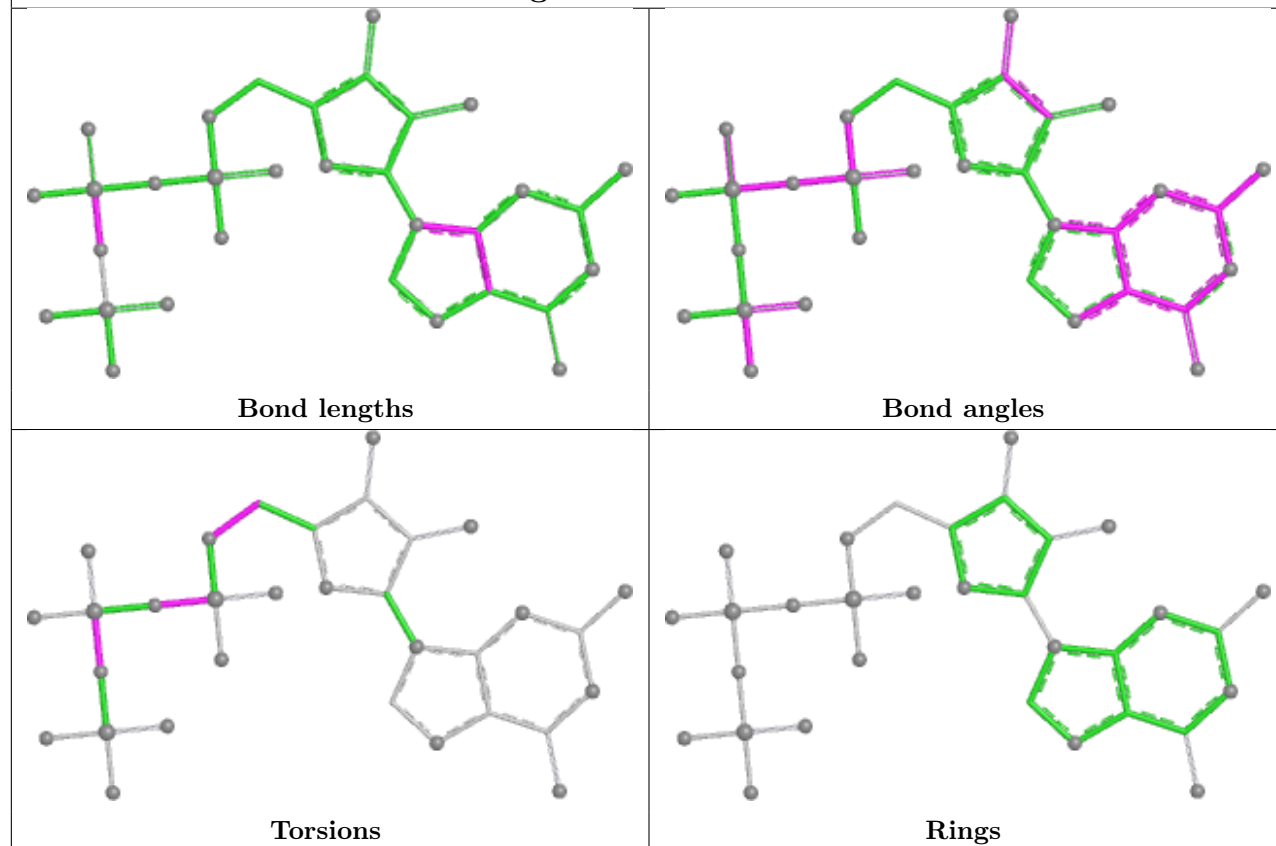
Ligand F6G C 703



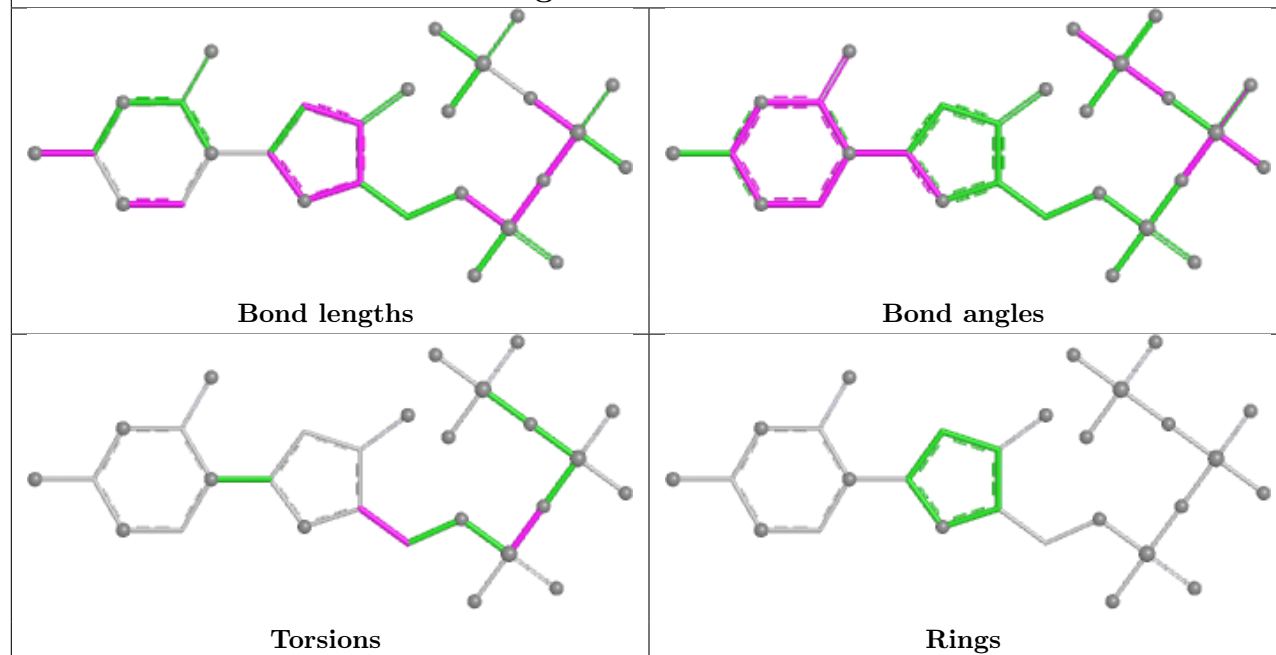
Ligand GTP B 703



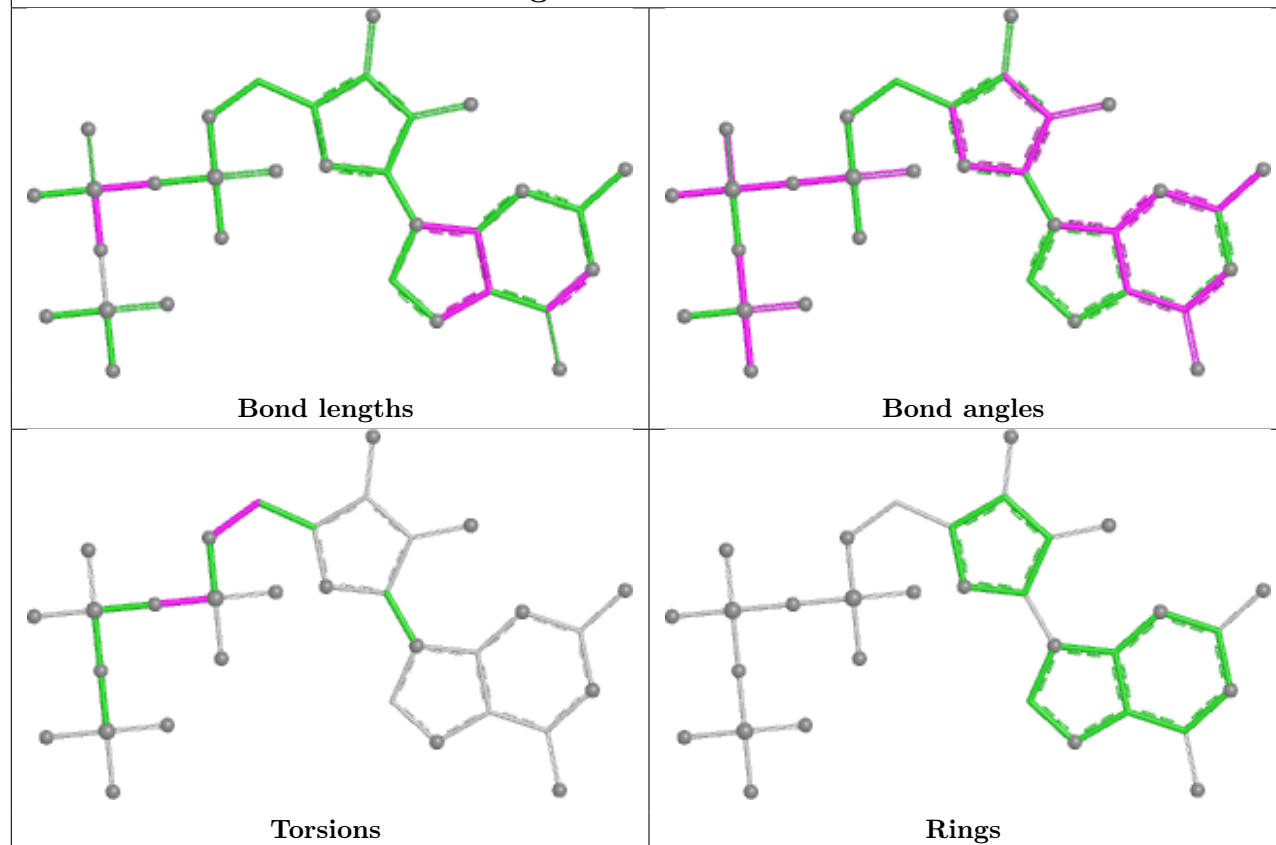
Ligand GTP D 702



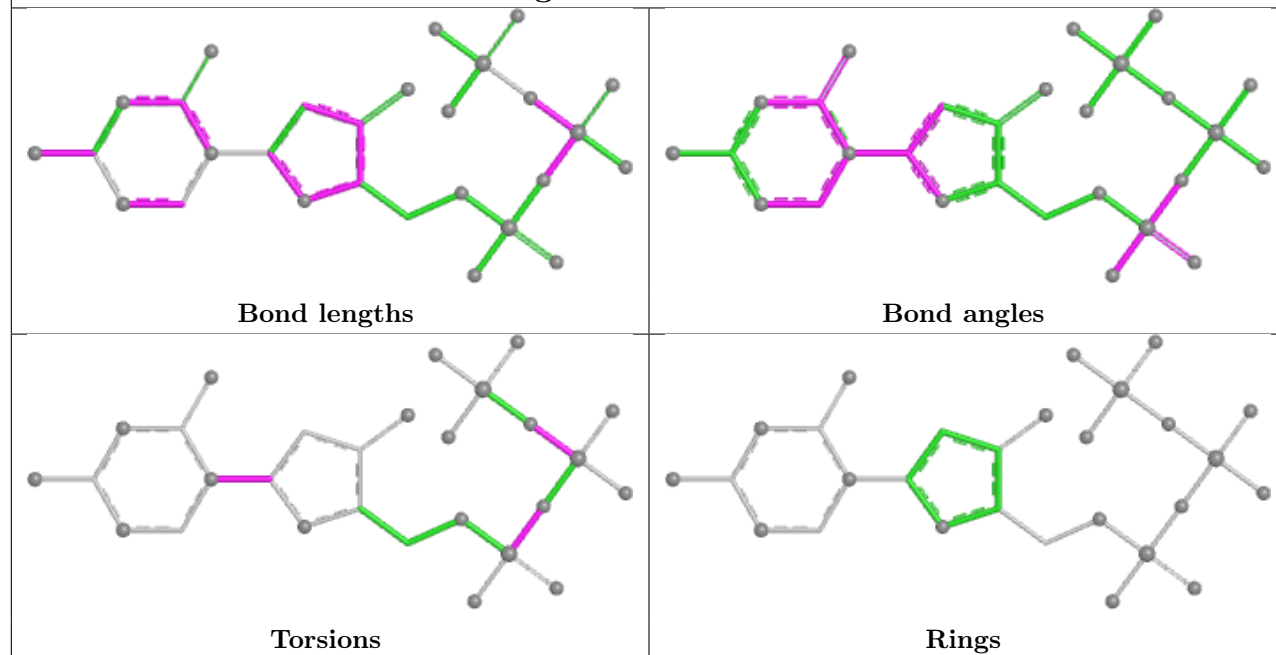
Ligand F6G B 704



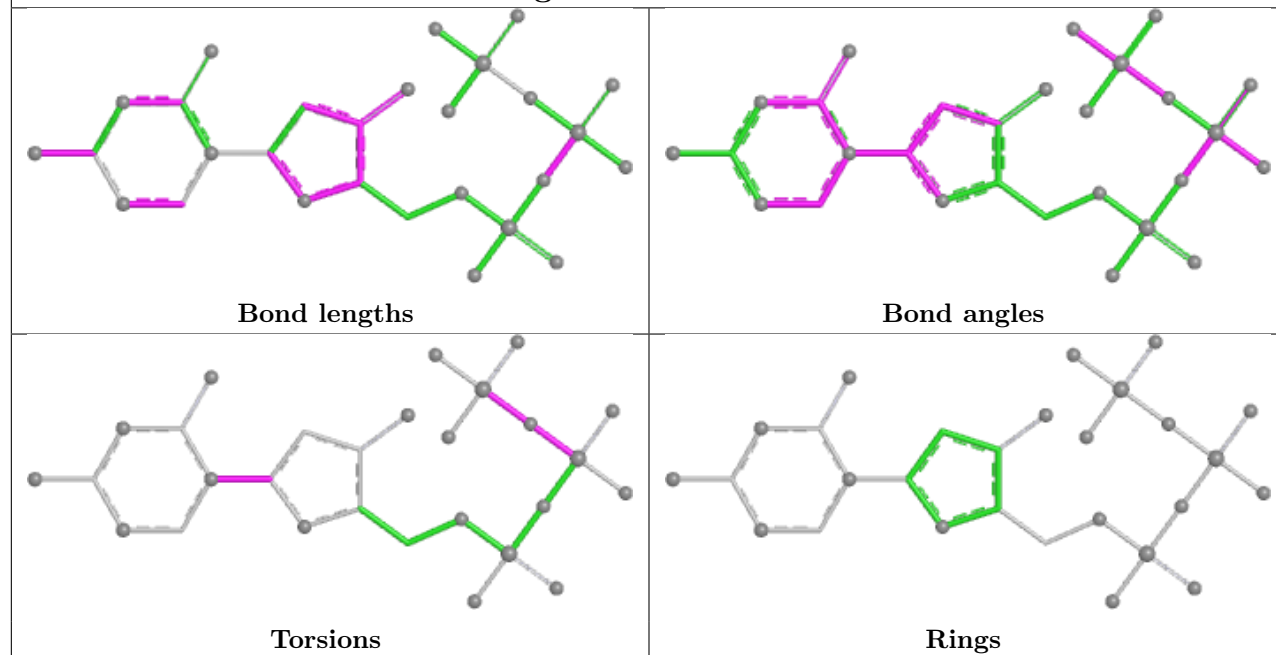
Ligand GTP A 704

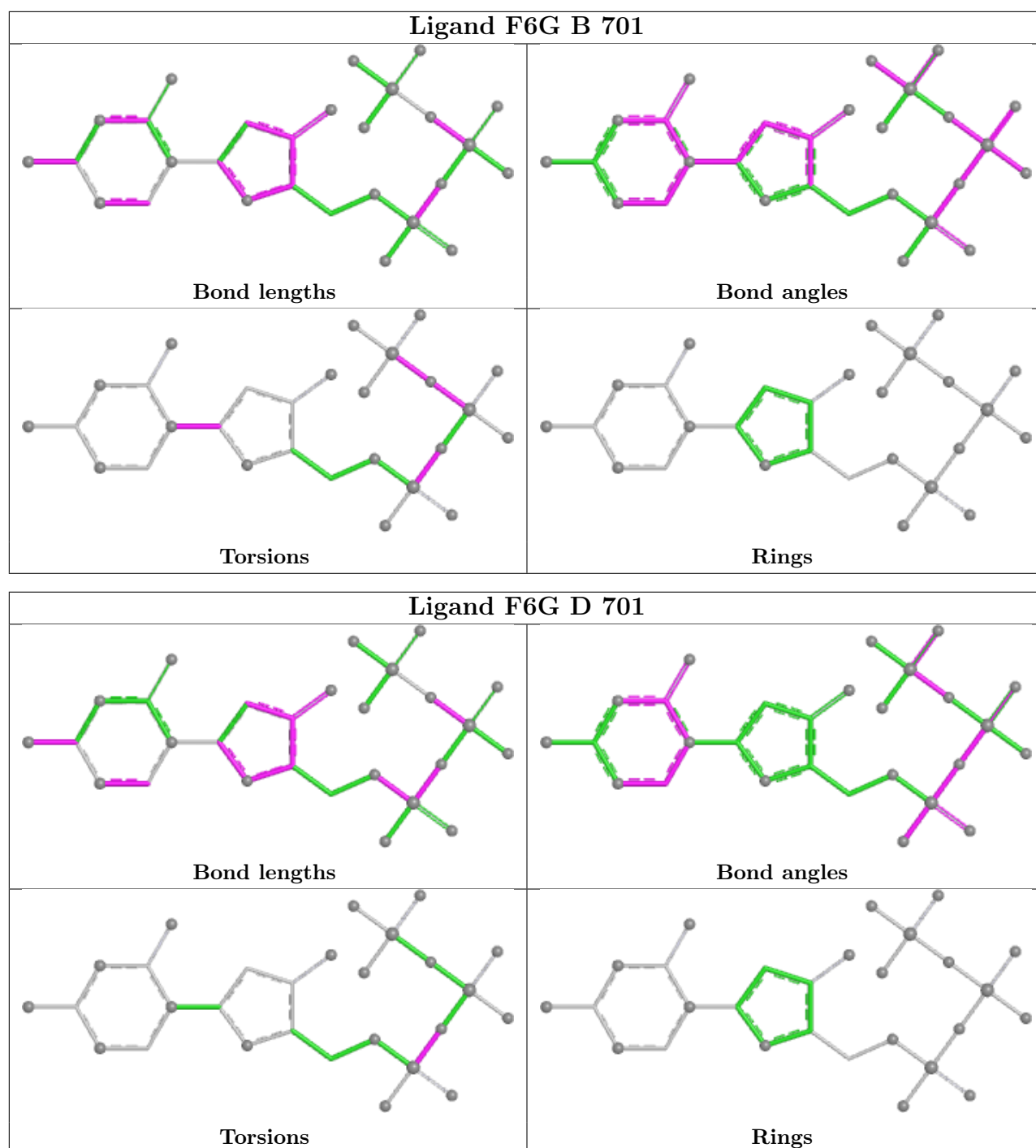


Ligand F6G A 701



Ligand F6G D 703





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%)	-0.24	6 (1%) 75 79	17, 35, 63, 91	1 (0%)
1	B	481/514 (93%)	0.01	9 (1%) 66 70	15, 42, 72, 96	2 (0%)
1	C	481/514 (93%)	-0.04	9 (1%) 66 70	19, 40, 72, 101	1 (0%)
1	D	481/514 (93%)	-0.09	9 (1%) 66 70	16, 38, 70, 96	3 (0%)
All	All	1923/2056 (93%)	-0.09	33 (1%) 69 73	15, 38, 70, 101	7 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	284	LEU	7.0
1	A	284	LEU	6.1
1	B	284	LEU	5.5
1	D	488	LEU	4.9
1	C	284	LEU	4.0
1	B	488	LEU	3.5
1	C	488	LEU	3.5
1	D	114	THR	3.2
1	D	328	ASN	3.0
1	B	114	THR	2.8
1	C	599	ASN	2.7
1	C	590	LEU	2.6
1	C	185	LYS	2.5
1	C	114	THR	2.4
1	D	229	VAL	2.4
1	A	599	ASN	2.4
1	B	113	ASP	2.4
1	A	328	ASN	2.3
1	C	405	LYS	2.3
1	D	466	ILE	2.3
1	C	491	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	599	ASN	2.3
1	D	113	ASP	2.3
1	C	277	GLU	2.3
1	B	469	LYS	2.2
1	B	230	LYS	2.2
1	B	437	LYS	2.2
1	B	229	VAL	2.2
1	A	491	VAL	2.1
1	A	277	GLU	2.1
1	A	114	THR	2.1
1	D	491	VAL	2.1
1	D	276	LEU	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
2	F6G	C	701	28/28	0.90	0.08	24,36,72,77	0
2	F6G	D	701	28/28	0.92	0.08	25,32,78,85	0
2	F6G	B	704	28/28	0.92	0.08	26,38,82,89	0
2	F6G	A	703	28/28	0.93	0.08	18,28,70,73	0
2	F6G	A	701	28/28	0.98	0.05	20,30,39,46	0
3	GTP	B	705	32/32	0.98	0.04	22,26,35,40	0
2	F6G	C	703	28/28	0.99	0.04	20,24,32,34	0
2	F6G	B	701	28/28	0.99	0.04	22,24,33,37	0
3	GTP	D	702	32/32	0.99	0.03	20,24,30,31	0
3	GTP	B	703	32/32	0.99	0.04	23,28,34,37	0
2	F6G	D	703	28/28	0.99	0.04	23,28,36,45	0

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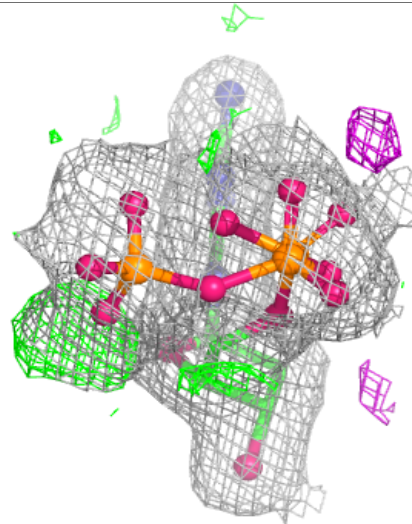
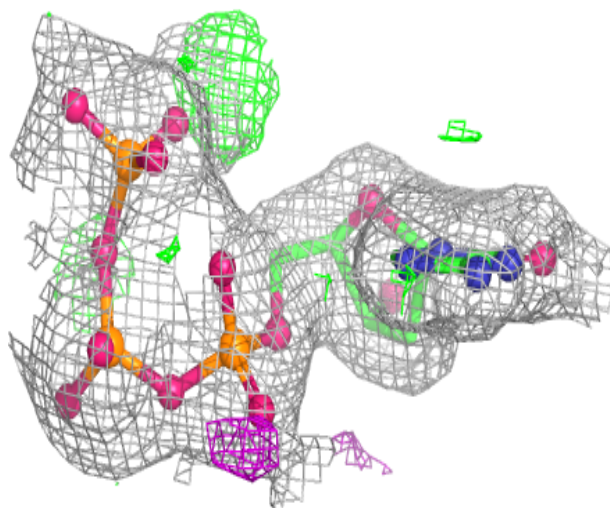
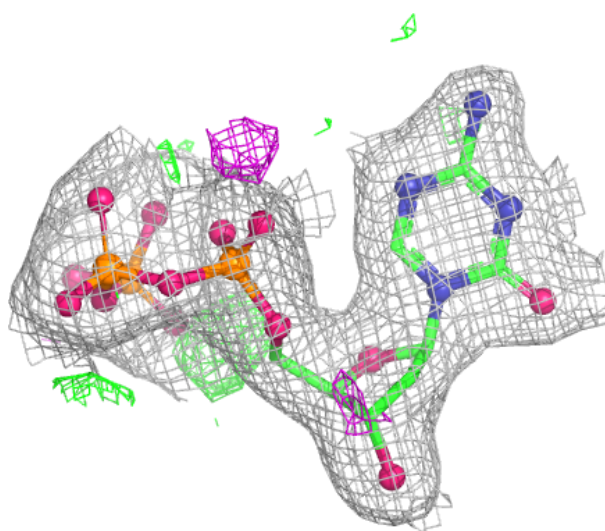
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GTP	A	704	32/32	0.99	0.03	17,22,29,35	0
4	MG	C	702	1/1	0.99	0.02	25,25,25,25	0
4	MG	C	704	1/1	0.99	0.02	22,22,22,22	0
4	MG	B	702	1/1	0.99	0.02	23,23,23,23	0
4	MG	A	702	1/1	1.00	0.01	31,31,31,31	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.

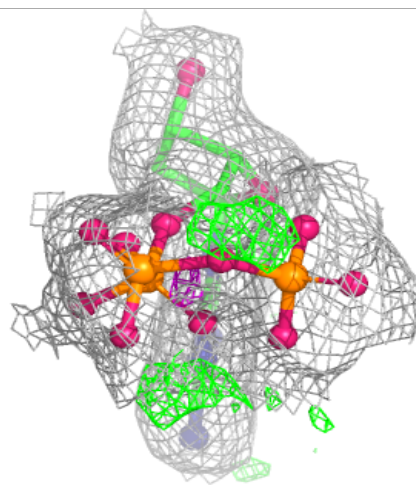
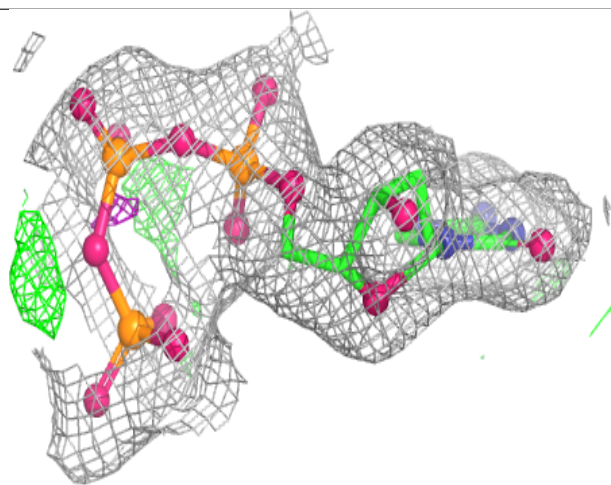
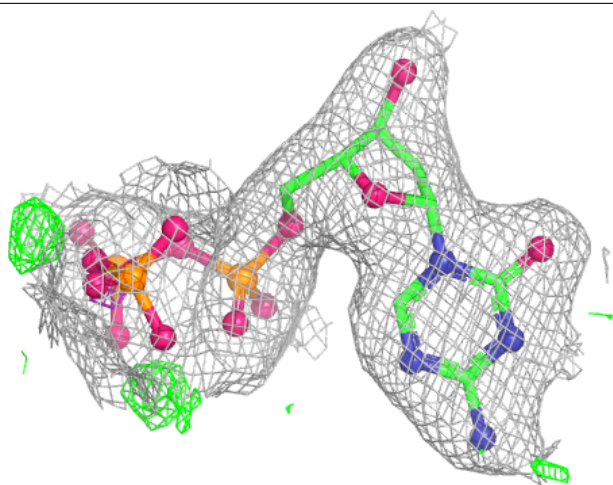
Electron density around F6G C 701:

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



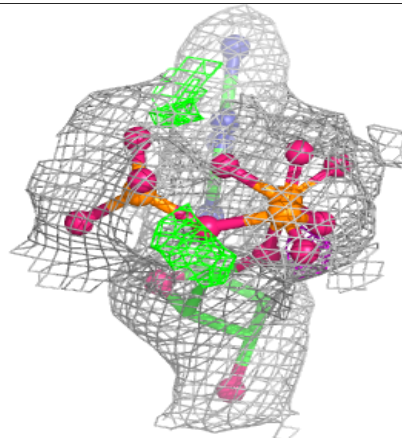
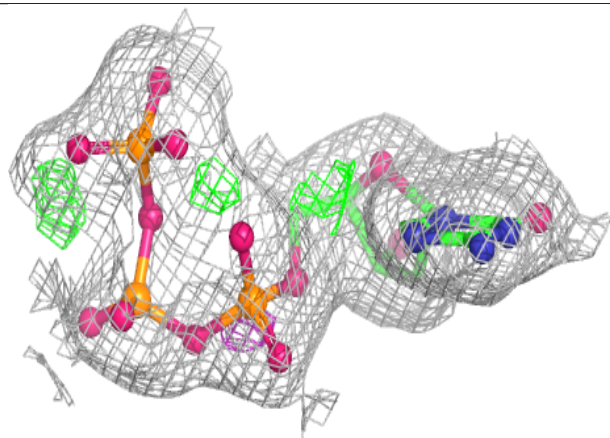
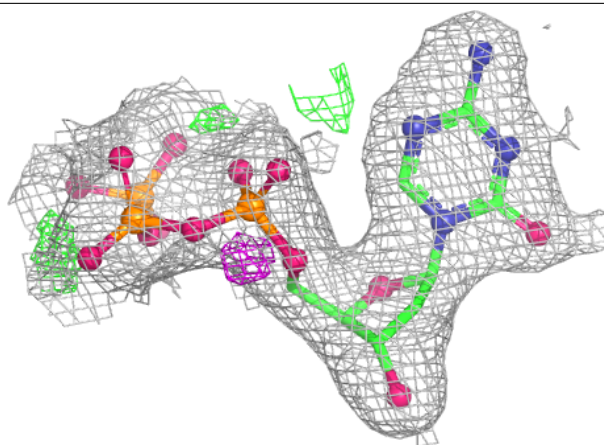
Electron density around F6G D 701:

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



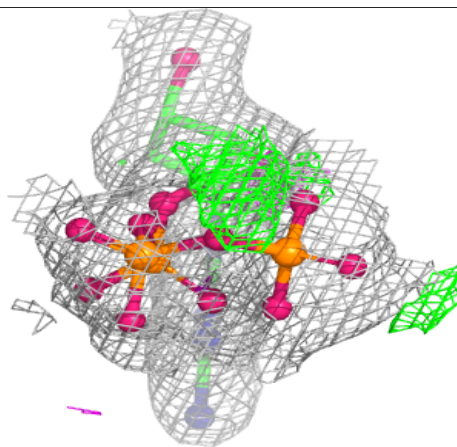
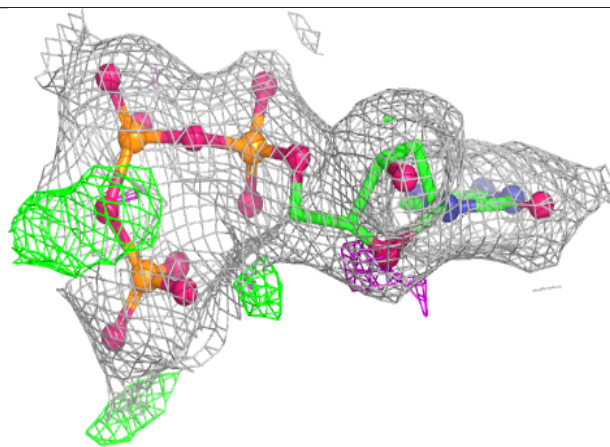
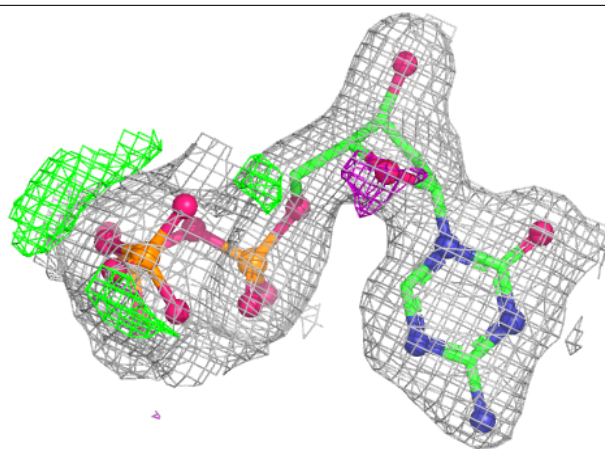
Electron density around F6G B 704:

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



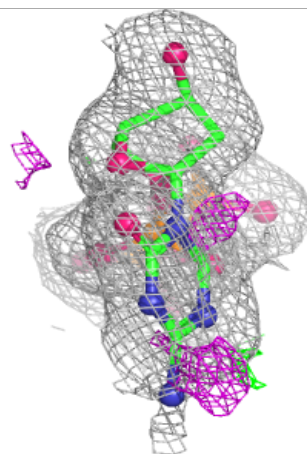
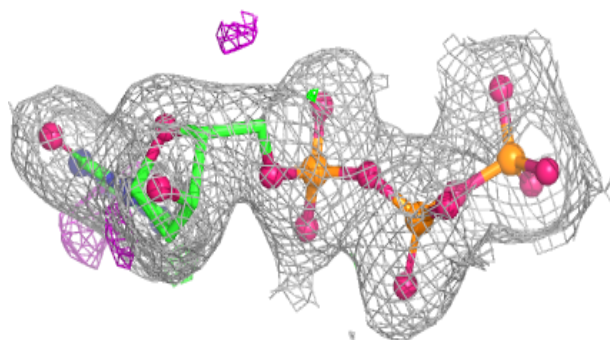
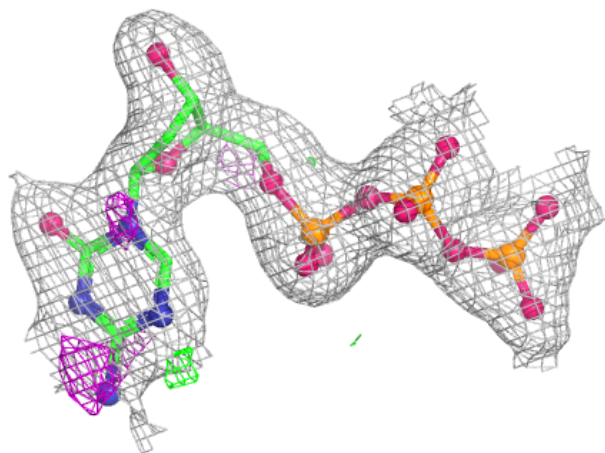
Electron density around F6G A 703:

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



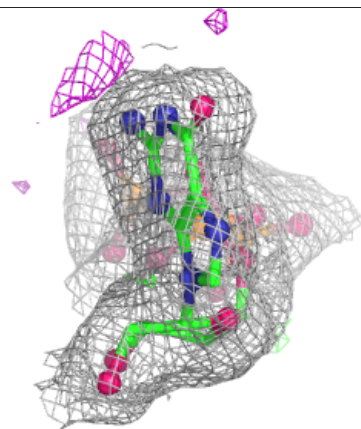
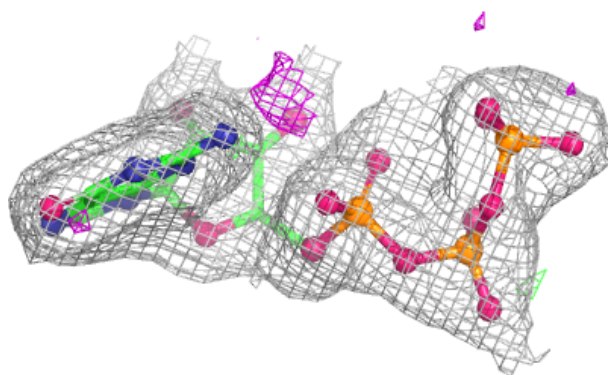
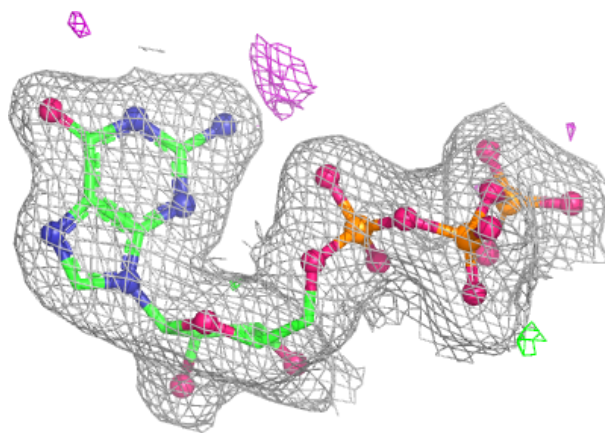
Electron density around F6G A 701:

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



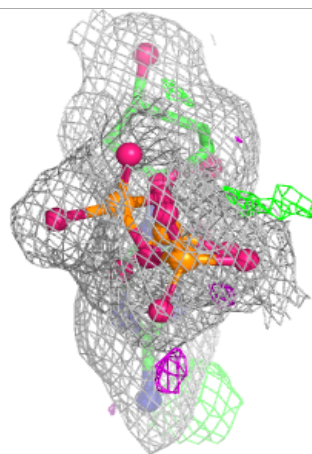
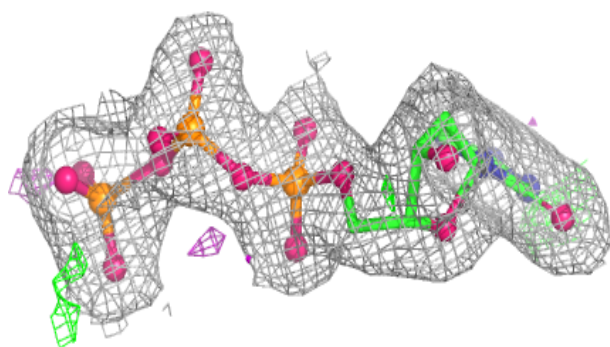
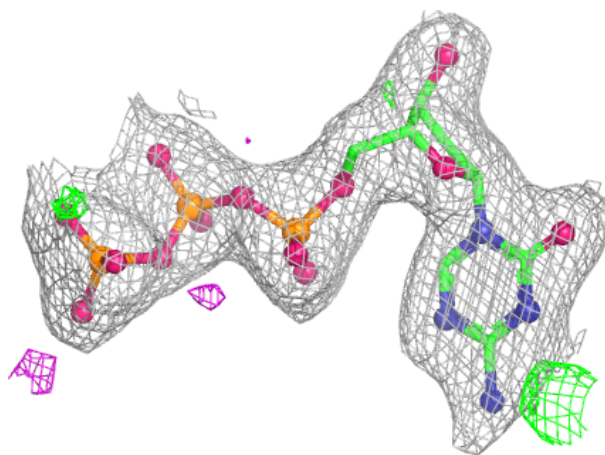
Electron density around GTP B 705:

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



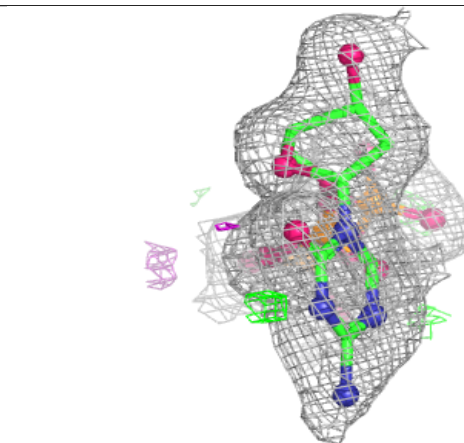
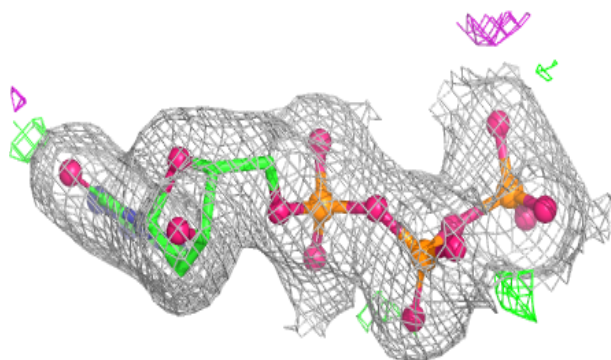
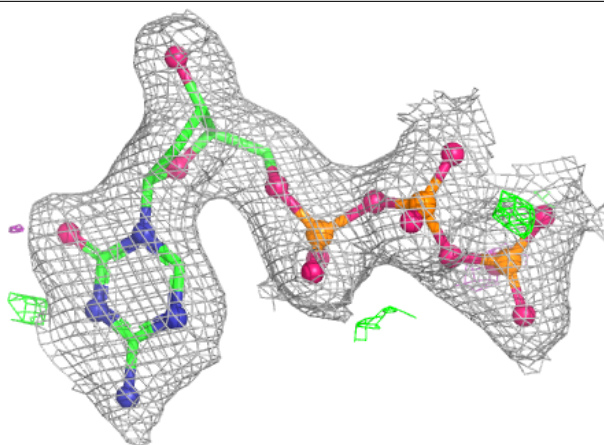
Electron density around F6G C 703:

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

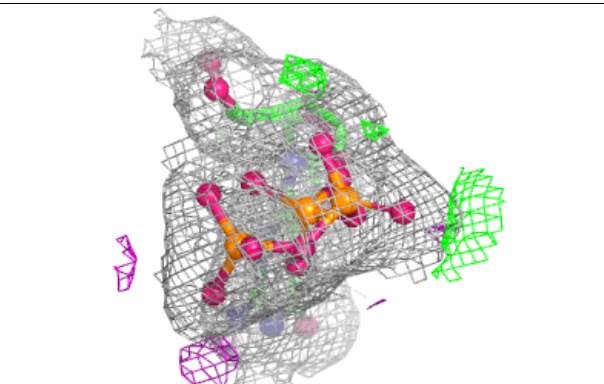
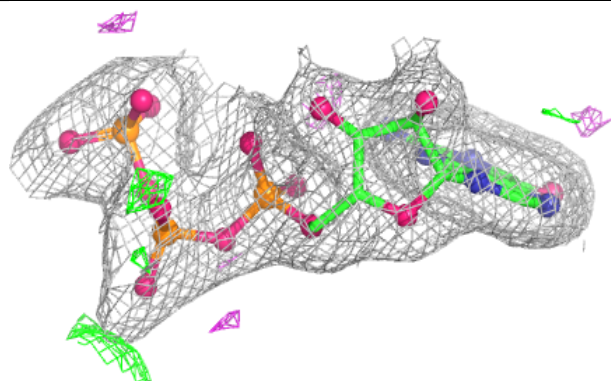
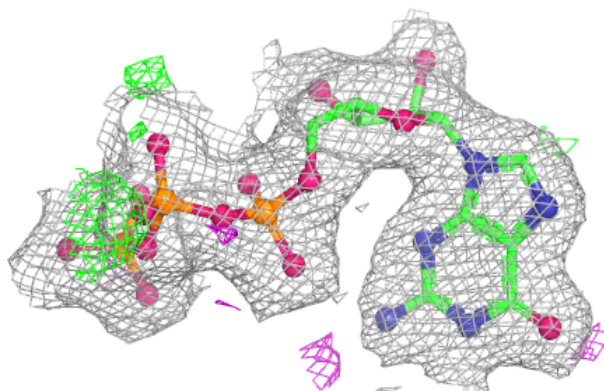


Electron density around F6G B 701:

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

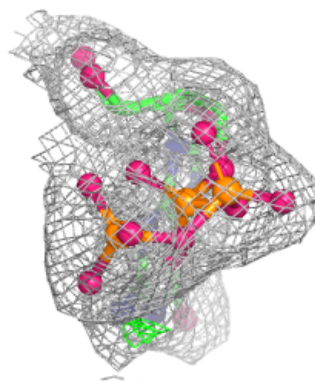
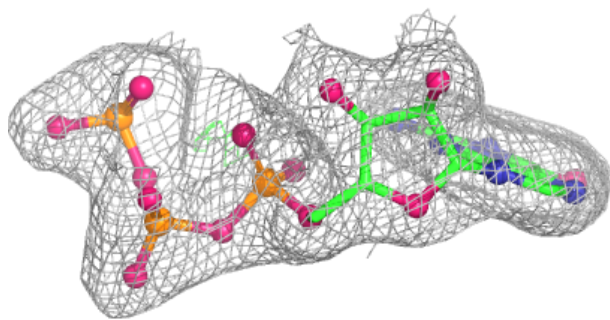
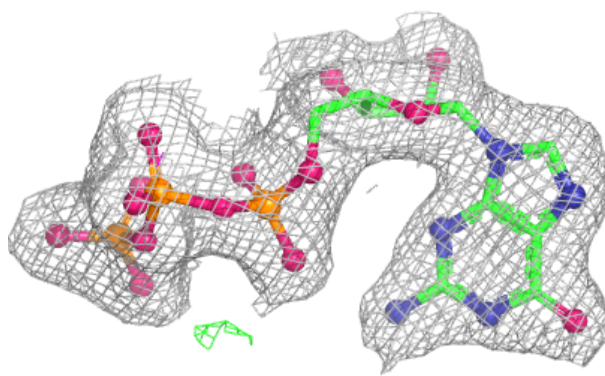
**Electron density around GTP D 702:**

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

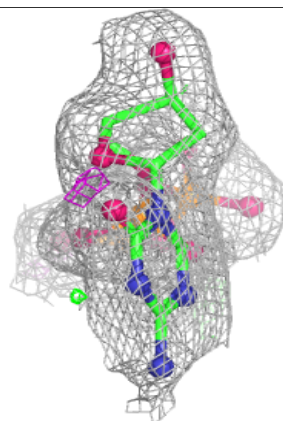
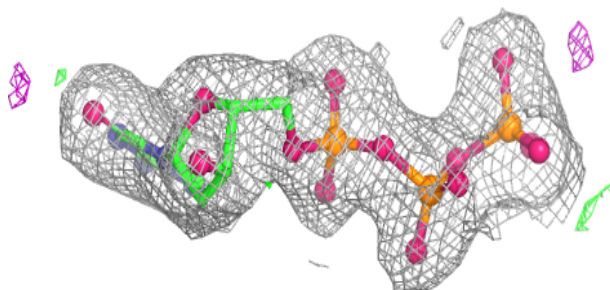
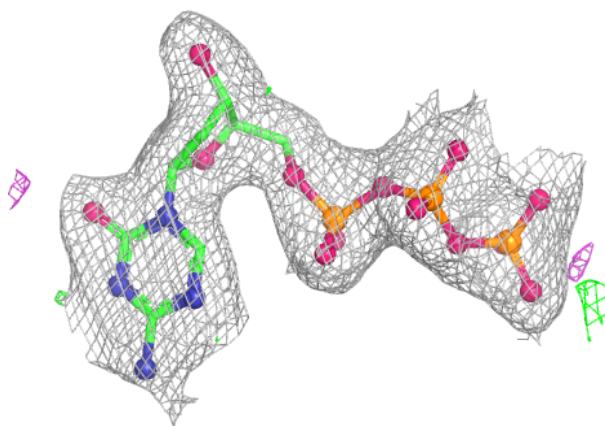


Electron density around GTP B 703:

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

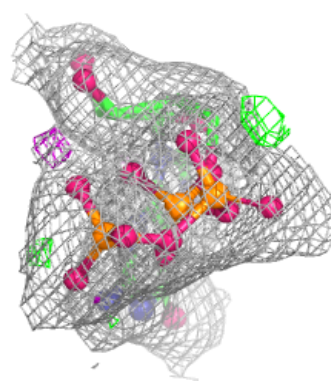
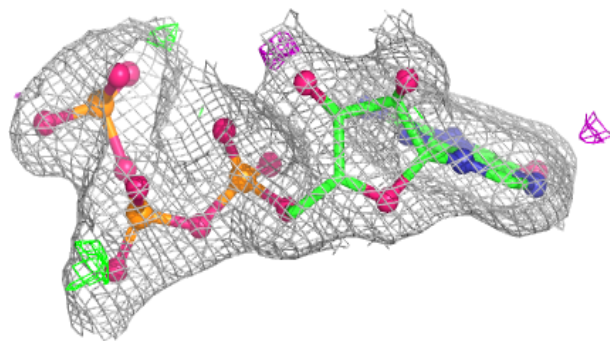
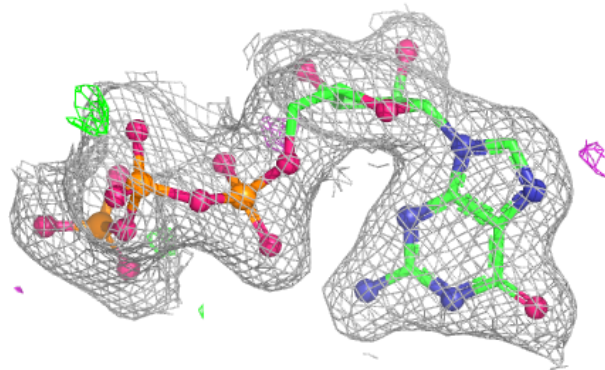
**Electron density around F6G D 703:**

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



Electron density around GTP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.