



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:13 AM UTC

PDB ID : 6DWD / pdb_00006dwd
Title : SAMHD1 Bound to Clofarabine-TP in the Catalytic Pocket and Allosteric Pocket
Authors : Knecht, K.M.; Buzovetsky, O.; Schneider, C.; Thomas, D.; Srikanth, V.; Kaderali, L.; Tofoleanu, F.; Reiss, K.; Ferreira, N.; Geisslinger, G.; Batista, V.S.; Ji, X.; Cinatl, J.; Keppler, O.T.; Xiong, Y.
Deposited on : 2018-06-26
Resolution : 1.70 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

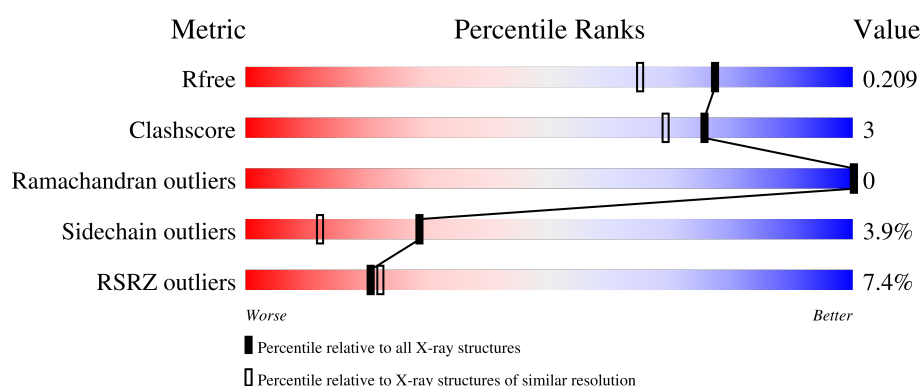
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	550	7% 75% 8% 15%
1	B	550	8% 78% 8% 13%
1	C	550	6% 79% 8% 13%
1	D	550	4% 79% 8% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GLY	A	716	-	X	-	-
7	SIN	D	714	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17162 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	1	0
			3939	2520	686	712	21			
1	C	481	Total	C	N	O	S	0	2	0
			3941	2522	686	712	21			
1	B	481	Total	C	N	O	S	0	0	0
			3933	2517	685	711	20			
1	A	466	Total	C	N	O	S	0	0	0
			3810	2436	665	689	20			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	77	MET	-	initiating methionine	UNP Q9Y3Z3
D	78	GLY	-	expression tag	UNP Q9Y3Z3
D	79	SER	-	expression tag	UNP Q9Y3Z3
D	80	SER	-	expression tag	UNP Q9Y3Z3
D	81	HIS	-	expression tag	UNP Q9Y3Z3
D	82	HIS	-	expression tag	UNP Q9Y3Z3
D	83	HIS	-	expression tag	UNP Q9Y3Z3
D	84	HIS	-	expression tag	UNP Q9Y3Z3
D	85	HIS	-	expression tag	UNP Q9Y3Z3
D	86	HIS	-	expression tag	UNP Q9Y3Z3
D	87	SER	-	expression tag	UNP Q9Y3Z3
D	88	SER	-	expression tag	UNP Q9Y3Z3
D	89	GLY	-	expression tag	UNP Q9Y3Z3
D	90	LEU	-	expression tag	UNP Q9Y3Z3
D	91	VAL	-	expression tag	UNP Q9Y3Z3
D	92	PRO	-	expression tag	UNP Q9Y3Z3
D	93	ARG	-	expression tag	UNP Q9Y3Z3
D	94	GLY	-	expression tag	UNP Q9Y3Z3
D	95	SER	-	expression tag	UNP Q9Y3Z3
D	96	HIS	-	expression tag	UNP Q9Y3Z3
D	97	MET	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	98	ALA	-	expression tag	UNP Q9Y3Z3
D	99	SER	-	expression tag	UNP Q9Y3Z3
D	100	MET	-	expression tag	UNP Q9Y3Z3
D	101	THR	-	expression tag	UNP Q9Y3Z3
D	102	GLY	-	expression tag	UNP Q9Y3Z3
D	103	GLY	-	expression tag	UNP Q9Y3Z3
D	104	GLN	-	expression tag	UNP Q9Y3Z3
D	105	GLN	-	expression tag	UNP Q9Y3Z3
D	106	MET	-	expression tag	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	ARG	-	expression tag	UNP Q9Y3Z3
D	109	ASP	-	expression tag	UNP Q9Y3Z3
D	110	PRO	-	expression tag	UNP Q9Y3Z3
D	111	ASN	-	expression tag	UNP Q9Y3Z3
D	112	SER	-	expression tag	UNP Q9Y3Z3
D	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
D	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
C	77	MET	-	initiating methionine	UNP Q9Y3Z3
C	78	GLY	-	expression tag	UNP Q9Y3Z3
C	79	SER	-	expression tag	UNP Q9Y3Z3
C	80	SER	-	expression tag	UNP Q9Y3Z3
C	81	HIS	-	expression tag	UNP Q9Y3Z3
C	82	HIS	-	expression tag	UNP Q9Y3Z3
C	83	HIS	-	expression tag	UNP Q9Y3Z3
C	84	HIS	-	expression tag	UNP Q9Y3Z3
C	85	HIS	-	expression tag	UNP Q9Y3Z3
C	86	HIS	-	expression tag	UNP Q9Y3Z3
C	87	SER	-	expression tag	UNP Q9Y3Z3
C	88	SER	-	expression tag	UNP Q9Y3Z3
C	89	GLY	-	expression tag	UNP Q9Y3Z3
C	90	LEU	-	expression tag	UNP Q9Y3Z3
C	91	VAL	-	expression tag	UNP Q9Y3Z3
C	92	PRO	-	expression tag	UNP Q9Y3Z3
C	93	ARG	-	expression tag	UNP Q9Y3Z3
C	94	GLY	-	expression tag	UNP Q9Y3Z3
C	95	SER	-	expression tag	UNP Q9Y3Z3
C	96	HIS	-	expression tag	UNP Q9Y3Z3
C	97	MET	-	expression tag	UNP Q9Y3Z3
C	98	ALA	-	expression tag	UNP Q9Y3Z3
C	99	SER	-	expression tag	UNP Q9Y3Z3
C	100	MET	-	expression tag	UNP Q9Y3Z3
C	101	THR	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	102	GLY	-	expression tag	UNP Q9Y3Z3
C	103	GLY	-	expression tag	UNP Q9Y3Z3
C	104	GLN	-	expression tag	UNP Q9Y3Z3
C	105	GLN	-	expression tag	UNP Q9Y3Z3
C	106	MET	-	expression tag	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	ARG	-	expression tag	UNP Q9Y3Z3
C	109	ASP	-	expression tag	UNP Q9Y3Z3
C	110	PRO	-	expression tag	UNP Q9Y3Z3
C	111	ASN	-	expression tag	UNP Q9Y3Z3
C	112	SER	-	expression tag	UNP Q9Y3Z3
C	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
C	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
B	77	MET	-	initiating methionine	UNP Q9Y3Z3
B	78	GLY	-	expression tag	UNP Q9Y3Z3
B	79	SER	-	expression tag	UNP Q9Y3Z3
B	80	SER	-	expression tag	UNP Q9Y3Z3
B	81	HIS	-	expression tag	UNP Q9Y3Z3
B	82	HIS	-	expression tag	UNP Q9Y3Z3
B	83	HIS	-	expression tag	UNP Q9Y3Z3
B	84	HIS	-	expression tag	UNP Q9Y3Z3
B	85	HIS	-	expression tag	UNP Q9Y3Z3
B	86	HIS	-	expression tag	UNP Q9Y3Z3
B	87	SER	-	expression tag	UNP Q9Y3Z3
B	88	SER	-	expression tag	UNP Q9Y3Z3
B	89	GLY	-	expression tag	UNP Q9Y3Z3
B	90	LEU	-	expression tag	UNP Q9Y3Z3
B	91	VAL	-	expression tag	UNP Q9Y3Z3
B	92	PRO	-	expression tag	UNP Q9Y3Z3
B	93	ARG	-	expression tag	UNP Q9Y3Z3
B	94	GLY	-	expression tag	UNP Q9Y3Z3
B	95	SER	-	expression tag	UNP Q9Y3Z3
B	96	HIS	-	expression tag	UNP Q9Y3Z3
B	97	MET	-	expression tag	UNP Q9Y3Z3
B	98	ALA	-	expression tag	UNP Q9Y3Z3
B	99	SER	-	expression tag	UNP Q9Y3Z3
B	100	MET	-	expression tag	UNP Q9Y3Z3
B	101	THR	-	expression tag	UNP Q9Y3Z3
B	102	GLY	-	expression tag	UNP Q9Y3Z3
B	103	GLY	-	expression tag	UNP Q9Y3Z3
B	104	GLN	-	expression tag	UNP Q9Y3Z3
B	105	GLN	-	expression tag	UNP Q9Y3Z3

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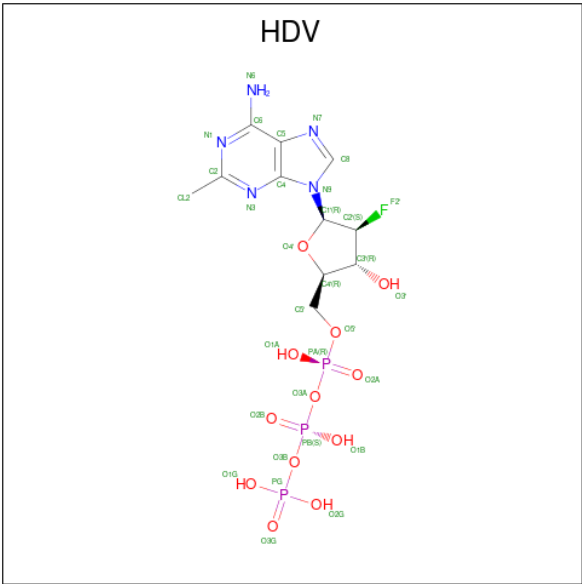
Chain	Residue	Modelled	Actual	Comment	Reference
B	106	MET	-	expression tag	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	ARG	-	expression tag	UNP Q9Y3Z3
B	109	ASP	-	expression tag	UNP Q9Y3Z3
B	110	PRO	-	expression tag	UNP Q9Y3Z3
B	111	ASN	-	expression tag	UNP Q9Y3Z3
B	112	SER	-	expression tag	UNP Q9Y3Z3
B	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
B	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3
A	77	MET	-	initiating methionine	UNP Q9Y3Z3
A	78	GLY	-	expression tag	UNP Q9Y3Z3
A	79	SER	-	expression tag	UNP Q9Y3Z3
A	80	SER	-	expression tag	UNP Q9Y3Z3
A	81	HIS	-	expression tag	UNP Q9Y3Z3
A	82	HIS	-	expression tag	UNP Q9Y3Z3
A	83	HIS	-	expression tag	UNP Q9Y3Z3
A	84	HIS	-	expression tag	UNP Q9Y3Z3
A	85	HIS	-	expression tag	UNP Q9Y3Z3
A	86	HIS	-	expression tag	UNP Q9Y3Z3
A	87	SER	-	expression tag	UNP Q9Y3Z3
A	88	SER	-	expression tag	UNP Q9Y3Z3
A	89	GLY	-	expression tag	UNP Q9Y3Z3
A	90	LEU	-	expression tag	UNP Q9Y3Z3
A	91	VAL	-	expression tag	UNP Q9Y3Z3
A	92	PRO	-	expression tag	UNP Q9Y3Z3
A	93	ARG	-	expression tag	UNP Q9Y3Z3
A	94	GLY	-	expression tag	UNP Q9Y3Z3
A	95	SER	-	expression tag	UNP Q9Y3Z3
A	96	HIS	-	expression tag	UNP Q9Y3Z3
A	97	MET	-	expression tag	UNP Q9Y3Z3
A	98	ALA	-	expression tag	UNP Q9Y3Z3
A	99	SER	-	expression tag	UNP Q9Y3Z3
A	100	MET	-	expression tag	UNP Q9Y3Z3
A	101	THR	-	expression tag	UNP Q9Y3Z3
A	102	GLY	-	expression tag	UNP Q9Y3Z3
A	103	GLY	-	expression tag	UNP Q9Y3Z3
A	104	GLN	-	expression tag	UNP Q9Y3Z3
A	105	GLN	-	expression tag	UNP Q9Y3Z3
A	106	MET	-	expression tag	UNP Q9Y3Z3
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	ARG	-	expression tag	UNP Q9Y3Z3
A	109	ASP	-	expression tag	UNP Q9Y3Z3

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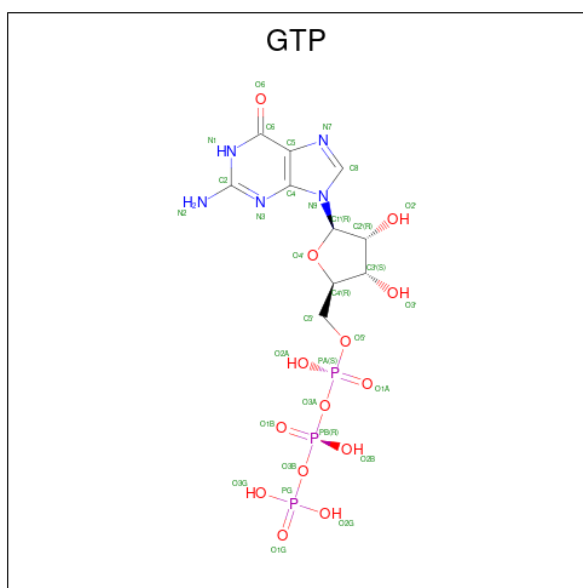
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	PRO	-	expression tag	UNP Q9Y3Z3
A	111	ASN	-	expression tag	UNP Q9Y3Z3
A	112	SER	-	expression tag	UNP Q9Y3Z3
A	206	ARG	HIS	engineered mutation	UNP Q9Y3Z3
A	207	ASN	ASP	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is 9-{2-deoxy-2-fluoro-5-O-[(R)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]oxy}phosphoryl]-beta-D-arabinofuranosyl}-2-me thyl-9H-purin-6-amine (CCD ID: HDV) (formula: C₁₁H₁₇FN₅O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		
2	D	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		
2	C	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		
2	C	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		
2	B	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		
2	B	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		
2	A	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		
2	A	1	Total	C	F	N	O	P	0	0
			32	11	1	5	12	3		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	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	D	2	Total	Mg	0	0
			2	2		
4	C	4	Total	Mg	0	0
			4	4		
4	B	1	Total	Mg	0	0
			1	1		
4	A	3	Total	Mg	0	0
			3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

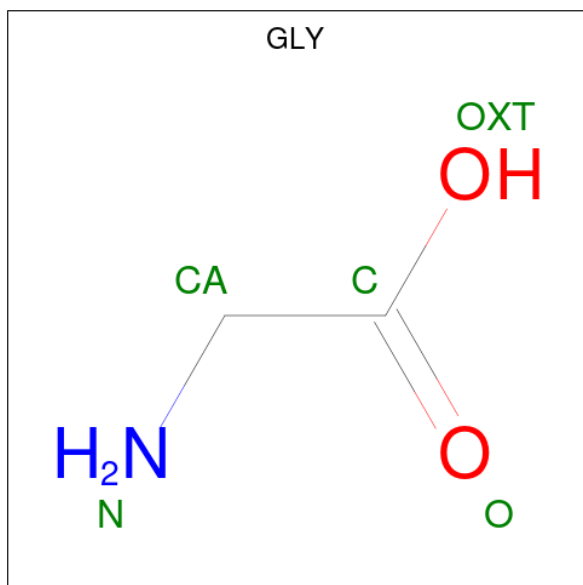
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	6	Total	Na	0	0
			6	6		

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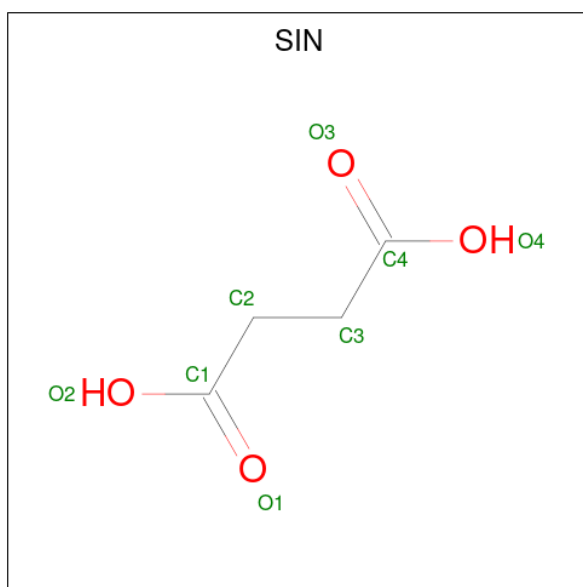
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	4	Total	Na	0	0
			4	4		
5	B	4	Total	Na	0	0
			4	4		
5	A	9	Total	Na	0	0
			9	9		

- Molecule 6 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



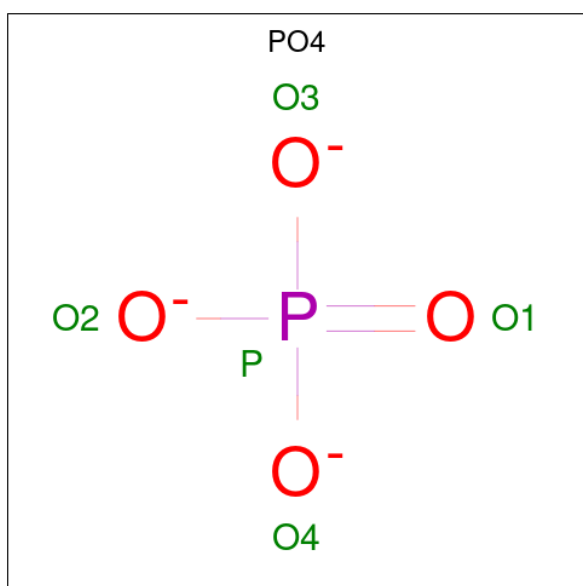
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			5	2	1	2		
6	C	1	Total	C	N	O	0	0
			5	2	1	2		
6	C	1	Total	C	N	O	0	0
			5	2	1	2		
6	B	1	Total	C	N	O	0	0
			5	2	1	2		
6	A	1	Total	C	N	O	0	0
			5	2	1	2		
6	A	1	Total	C	N	O	0	0
			5	2	1	2		
6	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 7 is SUCCINIC ACID (CCD ID: SIN) (formula: $C_4H_6O_4$).



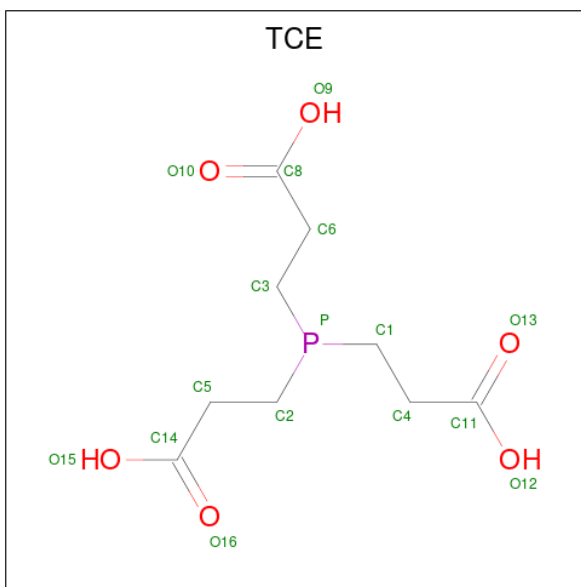
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			8	4	4		
7	B	1	Total	C	O	0	0
			8	4	4		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is 3,3',3''-phosphanetriyltripropanoic acid (CCD ID: TCE) (formula: $C_9H_{15}O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O	P	0	0
			16	9	6	1		

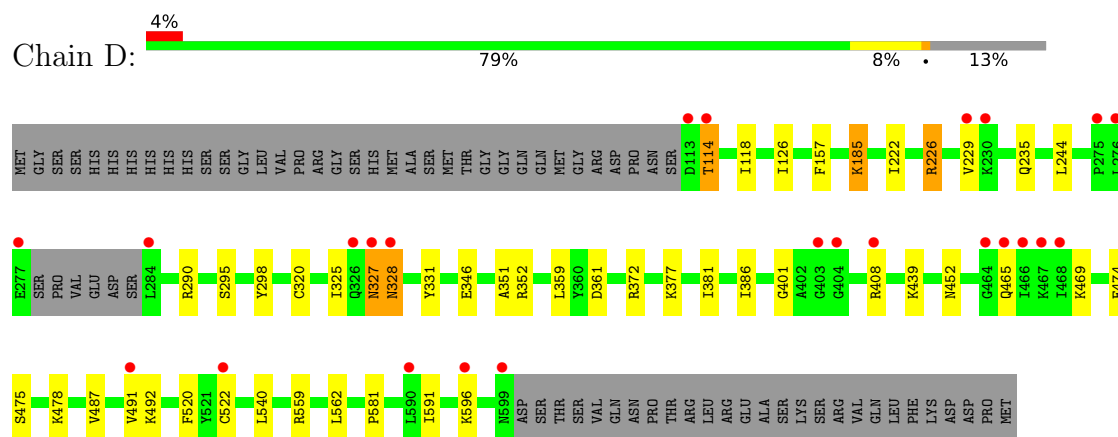
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	287	Total	O	0	0
			287	287		
10	C	252	Total	O	0	0
			252	252		
10	B	227	Total	O	0	0
			227	227		
10	A	284	Total	O	0	0
			284	284		

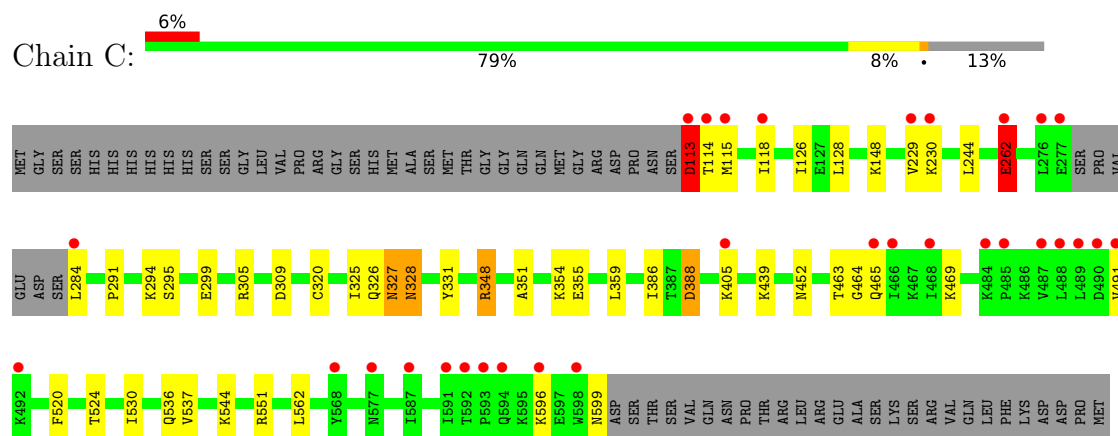
3 Residue-property plots [i](#)

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.

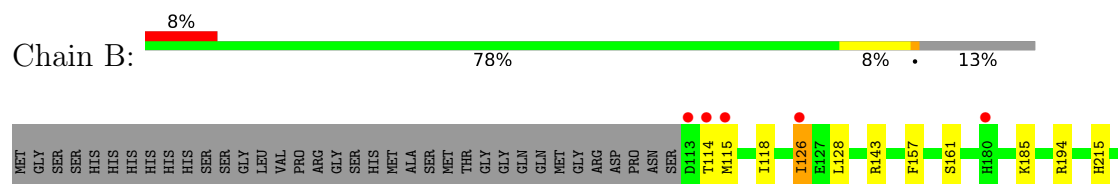
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

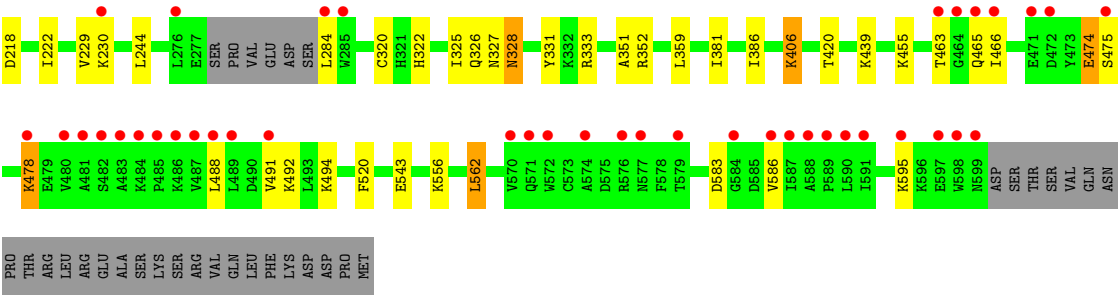


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1

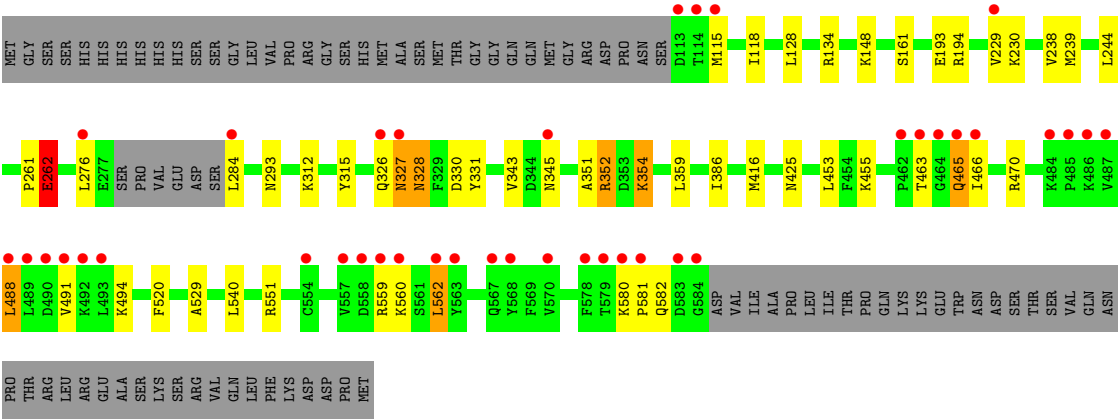
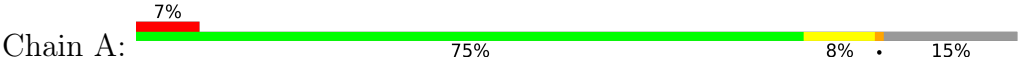


- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1





● 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	80.48Å 142.23Å 98.79Å 90.00° 114.10° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.0 (50.00-1.70) 94.1 (50.00-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.176 , 0.202 0.185 , 0.209	Depositor DCC
R_{free} test set	10589 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17162	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: HDV, SIN, GTP, TCE, PO4, MG, NA

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	1.25	8/3898 (0.2%)	1.18	15/5258 (0.3%)
1	B	1.18	7/4025 (0.2%)	1.11	6/5433 (0.1%)
1	C	1.22	10/4039 (0.2%)	1.16	12/5452 (0.2%)
1	D	1.20	8/4031 (0.2%)	1.12	8/5441 (0.1%)
All	All	1.21	33/15993 (0.2%)	1.14	41/21584 (0.2%)

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	C	0	1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	ASN	CA-C	12.72	1.70	1.52
1	C	388	ASP	CB-CG	-8.99	1.29	1.52
1	B	328	ASN	CA-C	8.93	1.64	1.52
1	A	161	SER	CB-OG	8.46	1.59	1.42
1	D	328	ASN	CA-C	8.34	1.63	1.52
1	A	327	ASN	C-O	-7.57	1.14	1.24
1	C	328[A]	ASN	CA-C	7.37	1.62	1.52
1	C	328[B]	ASN	CA-C	7.37	1.62	1.52
1	C	530	ILE	C-O	-7.19	1.14	1.23
1	D	157	PHE	C-O	-6.66	1.18	1.24
1	A	262	GLU	CA-C	6.51	1.61	1.52
1	B	327	ASN	C-O	-6.40	1.16	1.24
1	C	309	ASP	C-O	6.17	1.31	1.23
1	D	226	ARG	CG-CD	-6.13	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	401	GLY	C-O	-6.08	1.18	1.24
1	C	113	ASP	CB-CG	5.90	1.66	1.52
1	D	222	ILE	CA-C	5.80	1.57	1.52
1	A	330	ASP	C-O	5.78	1.30	1.23
1	C	524	THR	C-O	-5.71	1.16	1.24
1	C	327	ASN	C-O	-5.67	1.17	1.24
1	A	262	GLU	C-O	5.64	1.30	1.24
1	B	194	ARG	CA-C	5.63	1.59	1.52
1	D	581	PRO	CA-C	-5.55	1.46	1.52
1	B	161	SER	CB-OG	5.45	1.53	1.42
1	A	194	ARG	CA-C	5.30	1.59	1.52
1	D	327	ASN	CG-ND2	5.30	1.44	1.33
1	B	157	PHE	C-O	-5.23	1.19	1.24
1	A	345	ASN	CA-CB	5.15	1.61	1.53
1	B	222	ILE	CA-C	5.12	1.56	1.52
1	B	333	ARG	C-O	5.09	1.29	1.24
1	C	291	PRO	C-O	5.08	1.30	1.23
1	D	361	ASP	C-O	5.08	1.30	1.24
1	C	126	ILE	N-CA	-5.06	1.40	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ASN	CA-C-N	10.50	138.52	120.68
1	A	327	ASN	C-N-CA	10.50	138.52	120.68
1	A	328	ASN	N-CA-CB	-10.16	94.66	110.30
1	A	328	ASN	CB-CA-C	-8.17	93.70	110.38
1	C	115	MET	N-CA-C	8.12	122.48	110.30
1	D	226	ARG	CA-CB-CG	-7.50	99.10	114.10
1	B	115	MET	N-CA-C	7.48	121.51	110.30
1	A	352	ARG	CG-CD-NE	-6.98	96.65	112.00
1	B	352	ARG	CG-CD-NE	-6.90	96.81	112.00
1	A	328	ASN	CA-C-O	6.89	127.92	119.79
1	B	115	MET	CB-CA-C	-6.74	100.70	110.06
1	D	114	THR	N-CA-CB	6.58	120.56	110.49
1	D	328	ASN	CA-C-O	6.57	126.63	119.15
1	D	290	ARG	O-C-N	6.37	125.79	121.71
1	D	352	ARG	CG-CD-NE	-6.37	97.98	112.00
1	C	115	MET	CB-CA-C	-6.30	101.31	110.06
1	C	537	VAL	N-CA-C	6.19	117.55	111.67
1	A	262	GLU	CB-CG-CD	6.10	122.96	112.60
1	A	354	LYS	CB-CG-CD	5.72	124.46	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	LEU	CA-C-O	-5.70	114.92	121.47
1	C	348	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	C	328[A]	ASN	CA-C-O	5.58	125.51	119.15
1	C	328[B]	ASN	CA-C-O	5.58	125.51	119.15
1	C	294	LYS	CD-CE-NZ	-5.49	94.34	111.90
1	C	295	SER	N-CA-C	5.40	117.87	111.33
1	A	386	ILE	N-CA-C	-5.39	105.27	110.72
1	B	386	ILE	N-CA-C	-5.38	105.29	110.72
1	D	386	ILE	N-CA-C	-5.31	105.36	110.72
1	A	328	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	345	ASN	CA-CB-CG	5.21	117.81	112.60
1	C	348	ARG	CG-CD-NE	5.20	123.45	112.00
1	A	238	VAL	CA-C-O	-5.20	115.66	121.17
1	C	262	GLU	CB-CG-CD	5.17	121.39	112.60
1	D	185	LYS	CD-CE-NZ	5.15	128.39	111.90
1	C	386	ILE	N-CA-C	-5.14	105.53	110.72
1	B	406	LYS	CB-CG-CD	5.13	123.11	111.30
1	B	328	ASN	CA-C-O	5.11	124.97	119.15
1	A	465	GLN	CA-CB-CG	5.09	124.29	114.10
1	A	551	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	D	295	SER	N-CA-C	5.04	117.43	111.33
1	C	294	LYS	CA-CB-CG	-5.04	104.03	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	464	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	3810	0	3793	33	0
1	B	3933	0	3921	22	0
1	C	3941	0	3932	28	0
1	D	3939	0	3925	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	64	0	0	0	0
2	B	64	0	0	2	0
2	C	64	0	0	1	0
2	D	64	0	0	1	0
3	B	32	0	12	0	0
3	C	32	0	12	0	0
3	D	64	0	24	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	2	0	0	0	0
5	A	9	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	6	0	0	0	0
6	A	15	0	6	0	0
6	B	5	0	2	1	0
6	C	10	0	4	0	0
6	D	5	0	2	0	0
7	B	8	0	4	0	0
7	D	8	0	4	2	0
8	C	5	0	0	0	0
9	A	16	0	12	2	0
10	A	284	0	0	6	0
10	B	227	0	0	6	0
10	C	252	0	0	7	0
10	D	287	0	0	10	0
All	All	17162	0	15653	95	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 3.

All (95) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328[B]:ASN:HD22	1:A:328:ASN:ND2	1.36	1.20
1:C:452:ASN:HB3	10:C:1023:HOH:O	1.49	1.12
2:D:703:HDV:CL2	10:D:830:HOH:O	2.02	1.07
2:B:701:HDV:CL2	10:B:842:HOH:O	2.03	1.03
1:C:465:GLN:HE22	1:C:544:LYS:HE2	1.20	1.01
1:C:328[B]:ASN:HD22	1:A:328:ASN:HD21	1.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:1040:HOH:O	1:B:328:ASN:HB2	1.71	0.90
1:C:328[B]:ASN:ND2	1:A:328:ASN:ND2	2.21	0.88
1:C:328[B]:ASN:ND2	1:A:328:ASN:HD21	1.74	0.85
1:C:465:GLN:NE2	1:C:544:LYS:HE2	1.92	0.82
2:C:704:HDV:CL2	10:C:814:HOH:O	2.29	0.80
1:C:113:ASP:HB2	10:C:912:HOH:O	1.88	0.73
1:D:522[A]:CYS:SG	1:B:586:VAL:HG21	2.30	0.72
6:B:709:GLY:HA3	10:B:862:HOH:O	1.93	0.67
1:B:218:ASP:OD2	10:B:801:HOH:O	2.13	0.66
1:C:262:GLU:H	1:C:262:GLU:CD	2.04	0.66
1:A:354:LYS:NZ	10:A:803:HOH:O	2.31	0.64
1:D:298:TYR:O	10:D:801:HOH:O	2.15	0.64
1:A:262:GLU:H	1:A:262:GLU:CD	2.07	0.63
9:A:718:TCE:H6A	10:A:1011:HOH:O	1.99	0.63
1:C:326:GLN:HG2	1:A:326:GLN:HG2	1.82	0.62
1:D:185:LYS:HE2	10:D:1046:HOH:O	1.99	0.62
1:D:408:ARG:HD2	10:D:1012:HOH:O	1.98	0.61
1:C:452:ASN:CB	10:C:1023:HOH:O	2.25	0.61
1:B:463:THR:O	1:B:466:ILE:HD12	2.00	0.61
1:D:452:ASN:ND2	7:D:714:SIN:H31	2.16	0.60
1:D:452:ASN:HD21	7:D:714:SIN:H31	1.66	0.60
1:A:463:THR:O	1:A:466:ILE:HD12	2.03	0.58
1:C:326:GLN:CG	1:A:326:GLN:CG	2.84	0.55
1:C:328[B]:ASN:HD22	1:A:328:ASN:HD22	1.42	0.54
1:A:239:MET:HE2	1:A:416:MET:HE3	1.88	0.53
1:C:326:GLN:HG2	1:A:326:GLN:CG	2.38	0.53
1:B:583:ASP:OD2	10:B:802:HOH:O	2.17	0.52
1:C:326:GLN:CG	1:A:326:GLN:HG2	2.40	0.52
1:D:235:GLN:HG2	10:D:1076:HOH:O	2.10	0.52
1:D:346:GLU:HA	10:D:803:HOH:O	2.09	0.52
1:A:455:LYS:HB2	1:A:562:LEU:HD11	1.91	0.51
1:D:328:ASN:HB2	1:B:328:ASN:HB3	1.93	0.50
1:A:293:ASN:ND2	9:A:718:TCE:O16	2.41	0.50
1:D:474:GLU:O	1:D:478:LYS:CE	2.60	0.49
1:B:215:HIS:NE2	2:B:702:HDV:O2A	2.45	0.48
1:B:455:LYS:HB2	1:B:562:LEU:HD11	1.94	0.48
1:C:113:ASP:CB	10:C:912:HOH:O	2.56	0.48
1:B:331:TYR:CD1	1:B:331:TYR:C	2.92	0.48
1:C:354:LYS:HG3	1:C:355:GLU:OE2	2.14	0.47
1:D:331:TYR:C	1:D:331:TYR:CD1	2.93	0.47
1:C:331:TYR:C	1:C:331:TYR:CD1	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ARG:HD2	10:D:886:HOH:O	2.13	0.47
1:B:474:GLU:O	1:B:478:LYS:CE	2.63	0.46
1:A:331:TYR:C	1:A:331:TYR:CD1	2.93	0.46
1:C:351:ALA:O	1:C:520:PHE:HA	2.15	0.46
1:A:134:ARG:HD2	10:A:1069:HOH:O	2.15	0.46
1:A:351:ALA:O	1:A:520:PHE:HA	2.15	0.46
1:B:351:ALA:O	1:B:520:PHE:HA	2.15	0.46
1:A:261:PRO:HD2	10:A:912:HOH:O	2.15	0.46
1:C:327:ASN:O	1:A:326:GLN:HG2	2.16	0.46
1:D:118:ILE:HG23	1:D:126:ILE:HG12	1.99	0.45
1:B:143:ARG:HD2	1:B:420:THR:HA	1.97	0.45
1:C:148:LYS:NZ	10:C:816:HOH:O	2.50	0.45
1:B:475:SER:HA	1:B:478:LYS:HE2	1.99	0.45
1:A:470:ARG:HH11	1:A:470:ARG:HG3	1.81	0.45
1:D:351:ALA:O	1:D:520:PHE:HA	2.16	0.45
1:A:244:LEU:C	1:A:244:LEU:HD23	2.42	0.45
1:C:299:GLU:OE2	1:C:348:ARG:HD2	2.17	0.45
1:B:322:HIS:HE1	10:B:956:HOH:O	1.99	0.45
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.90	0.44
1:C:244:LEU:C	1:C:244:LEU:HD23	2.43	0.44
1:D:244:LEU:C	1:D:244:LEU:HD23	2.42	0.44
1:C:118:ILE:HD12	1:C:128:LEU:HD11	1.99	0.44
1:B:118:ILE:HD12	1:B:128:LEU:HD11	2.00	0.44
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.89	0.44
1:D:475:SER:HA	1:D:478:LYS:HE2	2.00	0.44
1:B:244:LEU:C	1:B:244:LEU:HD23	2.43	0.43
1:A:262:GLU:CG	10:A:979:HOH:O	2.67	0.43
1:A:352:ARG:CZ	1:A:354:LYS:HD2	2.48	0.43
1:D:487:VAL:HG23	1:D:591:ILE:HD11	2.01	0.43
1:C:320:CYS:HB3	1:C:325:ILE:O	2.19	0.43
1:C:551:ARG:NH1	10:C:823:HOH:O	2.53	0.42
1:A:262:GLU:CD	1:A:262:GLU:N	2.77	0.42
1:B:126:ILE:HD13	1:B:126:ILE:HG21	1.85	0.42
1:B:320:CYS:HB3	1:B:325:ILE:O	2.20	0.42
1:D:327:ASN:O	1:B:326:GLN:HG2	2.20	0.41
1:D:320:CYS:HB3	1:D:325:ILE:O	2.20	0.41
1:D:372:ARG:NH2	10:D:822:HOH:O	2.53	0.41
1:C:326:GLN:HG2	1:A:327:ASN:O	2.19	0.41
1:A:118:ILE:HD12	1:A:128:LEU:HD11	2.02	0.41
1:A:312:LYS:HA	1:A:315:TYR:CE2	2.56	0.41
1:A:148:LYS:NZ	10:A:806:HOH:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LYS:HE2	10:B:999:HOH:O	2.21	0.41
1:D:185:LYS:CE	10:D:1046:HOH:O	2.62	0.41
1:C:536:GLN:HE21	1:A:582:GLN:HG2	1.86	0.41
1:A:488:LEU:O	1:A:488:LEU:HD23	2.21	0.40
1:A:580:LYS:HD2	1:A:581:PRO:HD2	2.02	0.40
1:D:328:ASN:ND2	1:B:326:GLN:O	2.52	0.40
1:A:343:VAL:HG22	1:A:529:ALA:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/550 (84%)	452 (98%)	10 (2%)	0	100	100
1	B	477/550 (87%)	469 (98%)	8 (2%)	0	100	100
1	C	479/550 (87%)	473 (99%)	6 (1%)	0	100	100
1	D	478/550 (87%)	470 (98%)	8 (2%)	0	100	100
All	All	1896/2200 (86%)	1864 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/488 (85%)	396 (96%)	17 (4%)	27	11
1	B	427/488 (88%)	408 (96%)	19 (4%)	25	10
1	C	429/488 (88%)	412 (96%)	17 (4%)	28	12
1	D	428/488 (88%)	415 (97%)	13 (3%)	36	19
All	All	1697/1952 (87%)	1631 (96%)	66 (4%)	28	12

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	114	THR
1	D	229	VAL
1	D	359	LEU
1	D	377	LYS
1	D	439	LYS
1	D	465	GLN
1	D	469	LYS
1	D	491	VAL
1	D	492	LYS
1	D	540	LEU
1	D	559	ARG
1	D	562	LEU
1	D	596	LYS
1	C	113	ASP
1	C	114	THR
1	C	229	VAL
1	C	230	LYS
1	C	262	GLU
1	C	284	LEU
1	C	305	ARG
1	C	359	LEU
1	C	388	ASP
1	C	405	LYS
1	C	439	LYS
1	C	463	THR
1	C	469	LYS
1	C	491	VAL
1	C	562	LEU
1	C	596	LYS
1	C	599	ASN
1	B	114	THR
1	B	126	ILE
1	B	229	VAL

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Mol	Chain	Res	Type
1	B	230	LYS
1	B	284	LEU
1	B	359	LEU
1	B	406	LYS
1	B	439	LYS
1	B	465	GLN
1	B	474	GLU
1	B	478	LYS
1	B	488	LEU
1	B	491	VAL
1	B	492	LYS
1	B	494	LYS
1	B	543	GLU
1	B	556	LYS
1	B	562	LEU
1	B	595	LYS
1	A	115	MET
1	A	193	GLU
1	A	229	VAL
1	A	230	LYS
1	A	262	GLU
1	A	276	LEU
1	A	284	LEU
1	A	359	LEU
1	A	425	ASN
1	A	465	GLN
1	A	488	LEU
1	A	491	VAL
1	A	494	LYS
1	A	540	LEU
1	A	559	ARG
1	A	560	LYS
1	A	562	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	190	GLN
1	D	248	ASN
1	D	535	ASN
1	D	571	GLN
1	D	594	GLN

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Mol	Chain	Res	Type
1	C	149	GLN
1	C	163	ASN
1	C	200	GLN
1	C	248	ASN
1	C	465	GLN
1	C	510	GLN
1	C	535	ASN
1	C	571	GLN
1	C	594	GLN
1	C	599	ASN
1	B	149	GLN
1	B	163	ASN
1	B	321	HIS
1	B	364	HIS
1	B	367	ASN
1	B	465	GLN
1	B	510	GLN
1	B	535	ASN
1	B	571	GLN
1	B	594	GLN
1	A	149	GLN
1	A	163	ASN
1	A	248	ASN
1	A	256	GLN
1	A	321	HIS
1	A	328	ASN
1	A	345	ASN
1	A	364	HIS
1	A	367	ASN
1	A	510	GLN
1	A	567	GLN
1	A	571	GLN
1	A	577	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 33 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	GTP	B	703	4	33,34,34	1.39	5 (15%)	50,54,54	1.62	9 (18%)
2	HDV	A	702	4	33,34,34	1.98	15 (45%)	50,54,54	2.31	14 (28%)
3	GTP	D	704	4	33,34,34	1.87	3 (9%)	50,54,54	1.14	4 (8%)
6	GLY	A	716	-	4,4,4	1.27	1 (25%)	3,4,4	2.25	1 (33%)
9	TCE	A	718	-	12,15,15	1.39	1 (8%)	12,18,18	3.38	5 (41%)
6	GLY	A	717	-	4,4,4	0.95	0	3,4,4	1.43	1 (33%)
2	HDV	D	701	4	33,34,34	2.40	10 (30%)	50,54,54	2.72	21 (42%)
2	HDV	B	702	4	33,34,34	1.90	9 (27%)	50,54,54	2.60	17 (34%)
2	HDV	B	701	4	33,34,34	2.20	15 (45%)	50,54,54	2.54	16 (32%)
6	GLY	C	712	-	4,4,4	1.20	0	3,4,4	1.72	1 (33%)
6	GLY	D	713	-	4,4,4	1.16	1 (25%)	3,4,4	1.45	0
3	GTP	D	702	4	33,34,34	1.77	5 (15%)	50,54,54	1.38	8 (16%)
2	HDV	C	701	4	33,34,34	2.24	9 (27%)	50,54,54	2.57	17 (34%)
2	HDV	D	703	4	33,34,34	2.42	11 (33%)	50,54,54	2.33	16 (32%)
7	SIN	D	714	5	7,7,7	1.22	0	8,8,8	2.47	3 (37%)
6	GLY	C	713	-	4,4,4	1.01	0	3,4,4	1.25	0
6	GLY	A	715	-	4,4,4	1.04	0	3,4,4	0.62	0
2	HDV	C	704	4	33,34,34	1.97	11 (33%)	50,54,54	2.16	15 (30%)
8	PO4	C	714	-	4,4,4	0.94	0	6,6,6	1.16	0
3	GTP	C	702	4	33,34,34	1.56	4 (12%)	50,54,54	1.52	8 (16%)
2	HDV	A	704	4	33,34,34	2.23	11 (33%)	50,54,54	3.03	25 (50%)
7	SIN	B	710	-	7,7,7	1.40	1 (14%)	8,8,8	1.34	1 (12%)
6	GLY	B	709	-	4,4,4	0.69	0	3,4,4	1.93	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	B	703	4	-	5/22/38/38	0/3/3/3
2	HDV	A	702	4	-	3/22/38/38	0/3/3/3
3	GTP	D	704	4	-	4/22/38/38	0/3/3/3
6	GLY	A	716	-	-	2/2/2/2	-
9	TCE	A	718	-	-	9/15/15/15	-
6	GLY	A	717	-	-	2/2/2/2	-
2	HDV	D	701	4	-	3/22/38/38	0/3/3/3
2	HDV	B	702	4	-	3/22/38/38	0/3/3/3
2	HDV	B	701	4	-	5/22/38/38	0/3/3/3
6	GLY	C	712	-	-	2/2/2/2	-
6	GLY	D	713	-	-	2/2/2/2	-
3	GTP	D	702	4	-	3/22/38/38	0/3/3/3
2	HDV	C	701	4	-	4/22/38/38	0/3/3/3
2	HDV	D	703	4	-	3/22/38/38	0/3/3/3
7	SIN	D	714	5	-	5/5/5/5	-
6	GLY	C	713	-	-	0/2/2/2	-
6	GLY	A	715	-	-	0/2/2/2	-
2	HDV	C	704	4	-	3/22/38/38	0/3/3/3
3	GTP	C	702	4	-	6/22/38/38	0/3/3/3
2	HDV	A	704	4	-	4/22/38/38	0/3/3/3
7	SIN	B	710	-	-	3/5/5/5	-
6	GLY	B	709	-	-	0/2/2/2	-

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	HDV	PB-O3A	7.97	1.68	1.59
3	D	704	GTP	PB-O3A	7.41	1.67	1.59
3	D	702	GTP	PB-O3A	7.33	1.67	1.59
2	D	703	HDV	C6-N1	-6.32	1.26	1.35
2	C	701	HDV	C2'-C3'	-6.01	1.44	1.52
2	C	701	HDV	C2'-C1'	-5.51	1.46	1.53
2	A	704	HDV	C6-N6	5.33	1.47	1.34
2	D	703	HDV	O4'-C1'	5.28	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	704	GTP	PB-O3B	-5.28	1.53	1.59
2	A	704	HDV	PB-O3A	5.23	1.65	1.59
2	A	702	HDV	C6-N1	-4.98	1.28	1.35
2	D	703	HDV	PA-O3A	4.77	1.64	1.59
2	B	702	HDV	C2'-C3'	-4.62	1.46	1.52
2	C	704	HDV	C6-N1	-4.60	1.28	1.35
2	C	701	HDV	C6-N6	4.57	1.45	1.34
2	B	701	HDV	PA-O3A	4.31	1.64	1.59
2	D	701	HDV	C2'-C1'	-4.29	1.47	1.53
2	B	701	HDV	C6-N1	-4.28	1.29	1.35
2	B	702	HDV	C6-N6	4.21	1.45	1.34
3	B	703	GTP	PB-O3B	-4.17	1.55	1.59
3	C	702	GTP	PB-O3A	4.11	1.63	1.59
2	B	702	HDV	C2'-C1'	-4.00	1.48	1.53
3	C	702	GTP	PB-O3B	-3.97	1.55	1.59
2	D	701	HDV	C6-N6	3.95	1.44	1.34
2	D	701	HDV	C2'-C3'	-3.90	1.47	1.52
2	D	703	HDV	C5-N7	3.84	1.46	1.39
2	C	701	HDV	C5-N7	3.83	1.46	1.39
2	A	704	HDV	C2'-C3'	-3.74	1.47	1.52
2	A	704	HDV	C2'-C1'	-3.70	1.48	1.53
2	A	704	HDV	C4-N9	-3.62	1.30	1.37
2	C	704	HDV	O4'-C1'	3.58	1.50	1.42
3	B	703	GTP	C6-N1	-3.50	1.32	1.38
2	C	704	HDV	PB-O3A	3.48	1.63	1.59
2	B	701	HDV	PG-O1G	-3.46	1.41	1.54
2	B	701	HDV	O4'-C1'	3.39	1.49	1.42
3	C	702	GTP	C6-N1	-3.39	1.32	1.38
2	D	701	HDV	C5-C4	3.26	1.44	1.39
2	B	701	HDV	C2'-C1'	-3.24	1.49	1.53
2	D	703	HDV	C6-N6	3.22	1.42	1.34
2	B	701	HDV	PB-O3A	3.15	1.62	1.59
2	A	704	HDV	C5-C4	3.09	1.44	1.39
2	B	701	HDV	C6-N6	3.08	1.42	1.34
2	A	702	HDV	PA-O3A	3.05	1.62	1.59
2	C	701	HDV	PG-O1G	-3.04	1.43	1.54
2	D	703	HDV	PB-O3A	3.03	1.62	1.59
2	A	702	HDV	C6-N6	2.99	1.41	1.34
2	C	701	HDV	PA-O3A	2.91	1.62	1.59
2	B	701	HDV	C4-N3	-2.90	1.30	1.34
2	C	704	HDV	PG-O1G	-2.89	1.44	1.54
2	A	702	HDV	PG-O2G	-2.88	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	HDV	C8-N9	-2.85	1.32	1.37
2	A	704	HDV	PA-O1A	-2.85	1.42	1.55
2	B	702	HDV	PG-O2G	-2.83	1.44	1.54
2	A	702	HDV	C2'-C1'	-2.83	1.49	1.53
2	D	701	HDV	O4'-C1'	2.82	1.48	1.42
2	C	704	HDV	PG-O3G	-2.81	1.41	1.50
2	B	702	HDV	C5-N7	2.80	1.44	1.39
2	C	704	HDV	C5-C4	2.73	1.44	1.39
2	D	701	HDV	PA-O1A	-2.73	1.42	1.55
2	D	703	HDV	PB-O1B	-2.69	1.42	1.55
2	C	701	HDV	C5-C4	2.62	1.43	1.39
2	B	702	HDV	PB-O3A	-2.61	1.56	1.59
2	C	701	HDV	CL2-C2	2.59	1.56	1.49
2	B	701	HDV	PG-O2G	-2.58	1.45	1.54
2	C	704	HDV	C6-N6	2.58	1.40	1.34
2	A	704	HDV	F2'-C2'	2.58	1.45	1.40
2	B	701	HDV	C4-N9	-2.58	1.32	1.37
2	D	701	HDV	C2-N1	2.57	1.38	1.34
2	D	701	HDV	PB-O3B	2.55	1.62	1.59
2	B	701	HDV	C2'-C3'	-2.55	1.49	1.52
2	A	702	HDV	C5-N7	2.53	1.43	1.39
2	D	703	HDV	PG-O2G	-2.52	1.45	1.54
2	D	701	HDV	C8-N7	2.52	1.36	1.31
6	A	716	GLY	OXT-C	-2.47	1.22	1.30
2	A	704	HDV	CL2-C2	2.45	1.56	1.49
2	D	703	HDV	C3'-C4'	-2.44	1.46	1.53
2	B	702	HDV	O4'-C1'	2.41	1.47	1.42
2	A	702	HDV	C8-N7	2.37	1.36	1.31
2	C	701	HDV	O4'-C1'	2.34	1.47	1.42
2	A	702	HDV	O4'-C1'	2.32	1.47	1.42
2	B	701	HDV	PA-O1A	-2.32	1.44	1.55
2	A	704	HDV	C2-N3	2.32	1.38	1.34
2	A	702	HDV	PB-O3B	-2.30	1.57	1.59
2	A	704	HDV	PG-O1G	-2.28	1.46	1.54
2	A	702	HDV	C4-N3	-2.27	1.31	1.34
3	D	704	GTP	C4-N3	2.27	1.39	1.34
2	D	703	HDV	C8-N9	-2.26	1.33	1.37
3	D	702	GTP	PG-O2G	-2.25	1.46	1.54
2	B	702	HDV	PG-O1G	-2.24	1.46	1.54
6	D	713	GLY	OXT-C	-2.21	1.23	1.30
3	D	702	GTP	PA-O5'	2.21	1.68	1.59
3	B	703	GTP	PB-O3A	2.21	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	HDV	C8-N9	-2.21	1.33	1.37
3	D	702	GTP	PA-O3A	-2.16	1.57	1.59
2	A	702	HDV	PA-O2A	-2.16	1.43	1.50
2	A	702	HDV	PB-O1B	-2.13	1.45	1.55
2	C	704	HDV	O4'-C4'	2.12	1.49	1.45
3	B	703	GTP	O4'-C4'	-2.11	1.40	1.45
2	A	702	HDV	F2'-C2'	2.10	1.44	1.40
9	A	718	TCE	P-C3	2.10	1.87	1.84
3	C	702	GTP	PA-O2A	-2.09	1.45	1.55
2	B	701	HDV	PB-O1B	-2.08	1.45	1.55
2	A	702	HDV	C5-C4	2.07	1.42	1.39
2	D	703	HDV	O4'-C4'	2.07	1.49	1.45
2	C	704	HDV	C8-N7	2.06	1.35	1.31
3	B	703	GTP	C2-N1	-2.05	1.32	1.37
3	D	702	GTP	PB-O2B	-2.05	1.45	1.55
7	B	710	SIN	O4-C4	-2.03	1.24	1.30
2	C	704	HDV	PB-O2B	-2.03	1.43	1.50
2	B	701	HDV	C5-C4	2.03	1.42	1.39
2	A	702	HDV	PA-O1A	-2.02	1.46	1.55
2	C	704	HDV	O3'-C3'	2.01	1.47	1.43

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	HDV	C4-N9-C8	9.95	116.19	105.74
2	B	702	HDV	C4-N9-C8	8.65	114.82	105.74
2	C	701	HDV	C4-N9-C8	8.17	114.32	105.74
2	D	701	HDV	N6-C6-N1	8.03	127.86	117.03
2	A	702	HDV	C5-C4-N3	-7.28	119.51	127.18
2	C	701	HDV	N6-C6-N1	7.09	126.59	117.03
2	B	701	HDV	C5-C4-N3	-7.04	119.76	127.18
2	A	704	HDV	N6-C6-N1	7.04	126.52	117.03
2	D	701	HDV	CL2-C2-N1	6.82	127.34	117.13
2	C	704	HDV	C5-C4-N3	-6.68	120.14	127.18
9	A	718	TCE	C1-P-C3	6.44	121.47	100.95
2	D	703	HDV	C4-N9-C8	6.39	112.45	105.74
2	B	701	HDV	N3-C4-N9	6.35	135.04	126.99
2	B	701	HDV	C4-N9-C8	6.32	112.37	105.74
9	A	718	TCE	C1-P-C2	6.23	120.81	100.95
2	B	702	HDV	N3-C4-N9	6.15	134.80	126.99
2	A	702	HDV	N3-C4-N9	5.96	134.55	126.99
2	A	704	HDV	N3-C4-N9	5.88	134.46	126.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	HDV	C5-C4-N3	-5.81	121.06	127.18
2	D	701	HDV	C4-N9-C8	5.57	111.59	105.74
2	C	704	HDV	N3-C4-N9	5.48	133.94	126.99
2	C	701	HDV	N3-C4-N9	5.43	133.88	126.99
2	A	704	HDV	N9-C8-N7	-5.36	106.33	113.94
2	B	702	HDV	C5-C4-N3	-5.27	121.63	127.18
9	A	718	TCE	C3-P-C2	5.26	117.72	100.95
2	B	701	HDV	C2'-C1'-N9	5.11	123.07	113.92
2	A	704	HDV	CL2-C2-N1	5.09	124.75	117.13
7	D	714	SIN	C2-C3-C4	5.05	127.06	113.67
2	D	703	HDV	N3-C4-N9	4.96	133.28	126.99
2	D	701	HDV	C5-C4-N3	-4.92	121.99	127.18
2	B	702	HDV	N9-C8-N7	-4.83	107.08	113.94
2	D	701	HDV	C2-N1-C6	4.64	125.24	118.10
2	B	702	HDV	N1-C2-N3	-4.60	117.66	125.77
2	D	703	HDV	C2'-C1'-N9	4.48	121.94	113.92
2	C	704	HDV	C2'-C1'-N9	4.47	121.92	113.92
2	D	701	HDV	O3A-PA-O2A	-4.42	97.40	110.70
2	C	704	HDV	C4-N9-C8	4.42	110.38	105.74
2	A	702	HDV	C2'-C3'-C4'	4.38	108.20	102.43
2	C	701	HDV	C2-N1-C6	4.35	124.79	118.10
2	C	704	HDV	C3'-C2'-C1'	4.35	108.15	103.10
2	D	701	HDV	N3-C4-N9	4.33	132.49	126.99
2	B	701	HDV	N6-C6-N1	4.28	122.80	117.03
2	A	704	HDV	C2-N1-C6	4.23	124.61	118.10
2	D	701	HDV	N1-C2-N3	-4.20	118.36	125.77
2	A	704	HDV	O1A-PA-O5'	4.16	126.42	107.57
2	C	701	HDV	CL2-C2-N1	4.14	123.32	117.13
2	B	701	HDV	N9-C8-N7	-4.08	108.15	113.94
2	D	703	HDV	C3'-C2'-C1'	4.07	107.83	103.10
2	C	701	HDV	C5-C4-N3	-4.07	122.89	127.18
2	C	701	HDV	C3'-C2'-C1'	4.04	107.79	103.10
2	C	701	HDV	N1-C2-N3	-4.02	118.68	125.77
2	A	702	HDV	O3A-PB-O2B	-4.02	98.62	110.70
2	B	702	HDV	CL2-C2-N1	4.01	123.14	117.13
2	A	704	HDV	C5-C4-N3	-4.01	122.96	127.18
2	A	702	HDV	O4'-C1'-N9	-4.00	100.41	108.09
2	A	704	HDV	O3A-PA-O2A	-3.98	98.74	110.70
2	D	703	HDV	O3A-PB-O2B	-3.98	98.74	110.70
3	C	702	GTP	C5-C4-N3	-3.94	122.11	128.39
2	A	702	HDV	C2'-C1'-N9	3.93	120.97	113.92
2	A	702	HDV	C4-N9-C8	3.91	109.84	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	GTP	C5-C4-N3	-3.90	122.18	128.39
2	B	701	HDV	C4-C5-N7	-3.85	106.19	110.58
3	B	703	GTP	O3G-PG-O3B	3.76	117.25	104.64
2	A	702	HDV	N6-C6-N1	3.75	122.09	117.03
2	B	701	HDV	O1A-PA-O3A	3.74	117.39	107.27
2	D	703	HDV	C4-C5-N7	-3.66	106.40	110.58
2	B	702	HDV	N6-C6-N1	3.66	121.97	117.03
7	D	714	SIN	O2-C1-O1	-3.64	113.96	123.33
2	B	701	HDV	O1G-PG-O2G	3.60	121.32	107.80
2	D	701	HDV	N9-C8-N7	-3.57	108.88	113.94
2	B	701	HDV	C3'-C2'-C1'	3.54	107.20	103.10
2	A	704	HDV	C5-C4-N9	-3.50	102.00	105.81
3	B	703	GTP	N9-C4-N3	3.48	132.90	125.95
2	D	703	HDV	O4'-C1'-C2'	-3.47	102.18	105.84
2	A	704	HDV	N1-C2-N3	-3.41	119.76	125.77
3	C	702	GTP	N9-C4-N3	3.40	132.76	125.95
2	A	704	HDV	F2'-C2'-C1'	3.39	115.68	108.88
6	A	716	GLY	OXT-C-O	-3.35	114.73	123.33
2	A	704	HDV	C5-C6-N6	-3.34	115.00	123.29
2	D	701	HDV	C5-C6-N6	-3.34	115.01	123.29
2	A	704	HDV	O1B-PB-O3B	3.34	116.30	107.27
2	B	702	HDV	C2-N1-C6	3.34	123.23	118.10
2	D	701	HDV	O1A-PA-O5'	3.31	122.55	107.57
2	B	702	HDV	O3A-PB-O2B	3.29	120.61	110.70
2	B	701	HDV	C2'-C3'-C4'	3.26	106.72	102.43
2	D	701	HDV	C4-C5-N7	-3.25	106.86	110.58
2	A	704	HDV	O3A-PB-O2B	-3.25	100.93	110.70
2	A	702	HDV	C6-C5-C4	3.23	121.59	117.18
2	C	701	HDV	C5-C6-N6	-3.22	115.31	123.29
2	C	701	HDV	F2'-C2'-C1'	3.17	115.24	108.88
2	C	701	HDV	N9-C8-N7	-3.16	109.45	113.94
3	C	702	GTP	C2-N3-C4	3.15	117.72	112.30
2	D	703	HDV	N6-C6-N1	3.14	121.27	117.03
3	D	704	GTP	C5-C4-N3	-3.11	123.44	128.39
2	C	704	HDV	C2'-C3'-C4'	3.11	106.53	102.43
2	D	703	HDV	C2'-C3'-C4'	3.09	106.51	102.43
2	C	704	HDV	C4-C5-N7	-3.05	107.09	110.58
2	D	703	HDV	O3B-PB-O2B	3.05	119.87	110.70
2	A	704	HDV	C4-N9-C1'	-3.02	119.58	126.63
3	D	702	GTP	O3G-PG-O2G	3.01	119.07	107.80
3	D	702	GTP	N2-C2-N3	-2.99	113.83	119.67
9	A	718	TCE	O9-C8-C6	2.97	123.38	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	704	HDV	C5-N7-C8	2.96	108.10	103.45
2	B	702	HDV	C4-N9-C1'	-2.96	119.72	126.63
2	B	702	HDV	C6-C5-N7	2.95	137.79	132.09
2	D	701	HDV	O1B-PB-O3B	2.94	115.22	107.27
2	A	704	HDV	C4-C5-N7	-2.93	107.23	110.58
2	B	701	HDV	C5-N7-C8	2.90	108.01	103.45
2	C	701	HDV	C4-N9-C1'	-2.89	119.87	126.63
3	C	702	GTP	O3G-PG-O3B	2.88	114.28	104.64
2	D	701	HDV	O1B-PB-O3A	2.86	115.00	107.27
3	C	702	GTP	O6-C6-C5	-2.84	119.03	126.53
2	D	703	HDV	N9-C8-N7	-2.83	109.92	113.94
2	A	702	HDV	O4'-C1'-C2'	-2.79	102.89	105.84
3	C	702	GTP	C2'-C1'-N9	2.78	120.98	113.25
2	A	702	HDV	CL2-C2-N1	-2.77	112.98	117.13
3	D	702	GTP	C5-C4-N3	-2.77	123.99	128.39
2	B	702	HDV	O2G-PG-O3B	2.76	113.88	104.64
2	C	704	HDV	O4'-C1'-C2'	-2.75	102.94	105.84
2	B	702	HDV	C4-C5-N7	-2.72	107.47	110.58
2	C	704	HDV	O1A-PA-O3A	2.70	114.58	107.27
6	B	709	GLY	OXT-C-CA	2.68	124.05	113.38
2	B	701	HDV	O3A-PB-O2B	-2.68	102.64	110.70
2	C	704	HDV	N6-C6-N1	2.67	120.64	117.03
3	D	702	GTP	N9-C4-N3	2.64	131.24	125.95
2	D	701	HDV	C2'-C3'-C4'	2.62	105.89	102.43
2	A	704	HDV	O1A-PA-O3A	2.62	114.36	107.27
2	C	701	HDV	C4-C5-N7	-2.58	107.63	110.58
3	B	703	GTP	C6-C5-N7	2.58	134.99	130.29
2	B	702	HDV	C5-C6-N6	-2.55	116.98	123.29
2	D	701	HDV	F2'-C2'-C3'	-2.54	104.12	109.14
3	B	703	GTP	C8-N9-C4	2.54	110.78	106.03
2	A	704	HDV	O1B-PB-O3A	2.53	114.10	107.27
2	B	701	HDV	C4-N9-C1'	-2.53	120.73	126.63
2	C	701	HDV	C5-C4-N9	-2.47	103.12	105.81
7	B	710	SIN	O4-C4-O3	-2.47	116.99	123.33
2	A	704	HDV	C3'-C2'-C1'	2.43	105.92	103.10
2	B	701	HDV	O1B-PB-O3A	2.43	113.83	107.27
2	C	704	HDV	N9-C8-N7	-2.42	110.50	113.94
3	B	703	GTP	N9-C8-N7	-2.41	108.93	113.40
3	B	703	GTP	O3A-PA-O1A	-2.41	103.45	110.70
2	B	702	HDV	O1A-PA-O3A	-2.41	100.76	107.27
2	C	704	HDV	O4'-C1'-N9	-2.41	103.47	108.09
2	C	701	HDV	O1A-PA-O3A	-2.39	100.82	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	714	SIN	O2-C1-C2	2.36	121.47	114.00
3	D	704	GTP	O3G-PG-O2G	2.36	116.67	107.80
2	D	703	HDV	C4-N9-C1'	-2.36	121.11	126.63
9	A	718	TCE	O15-C14-C5	2.36	121.45	114.00
2	A	702	HDV	C4-N9-C1'	-2.35	121.13	126.63
2	D	703	HDV	O4'-C1'-N9	-2.35	103.58	108.09
2	D	701	HDV	C5-N7-C8	2.33	107.11	103.45
2	A	704	HDV	O1A-PA-O2A	-2.32	101.64	112.44
2	C	701	HDV	C6-C5-N7	2.32	136.57	132.09
3	B	703	GTP	C2-N3-C4	2.32	116.29	112.30
2	B	702	HDV	C5-N7-C8	2.26	107.01	103.45
3	B	703	GTP	O4'-C4'-C3'	-2.23	100.72	105.15
2	C	704	HDV	O1B-PB-O2B	2.23	122.81	112.44
2	C	704	HDV	O3A-PA-O2A	-2.22	104.02	110.70
2	A	704	HDV	PA-O5'-C5'	-2.22	108.61	121.35
2	A	702	HDV	O1B-PB-O3A	2.21	113.25	107.27
3	D	702	GTP	O2B-PB-O3B	2.21	113.24	107.27
2	A	702	HDV	N1-C2-N3	2.20	129.65	125.77
6	C	712	GLY	OXT-C-CA	2.20	122.13	113.38
2	C	704	HDV	O3'-C3'-C4'	-2.19	104.79	111.08
3	D	704	GTP	C6-C5-N7	2.18	134.27	130.29
3	D	704	GTP	C3'-C2'-C1'	2.18	105.59	101.46
3	D	702	GTP	O6-C6-N1	2.16	124.17	120.11
2	A	704	HDV	C6-C5-N7	2.14	136.21	132.09
3	C	702	GTP	O2G-PG-O1G	2.12	119.10	110.83
2	D	701	HDV	C3'-C2'-C1'	2.12	105.56	103.10
3	D	702	GTP	C3'-C2'-C1'	2.11	105.45	101.46
2	D	703	HDV	O1G-PG-O3G	2.11	119.04	110.83
2	B	701	HDV	C6-C5-C4	2.10	120.04	117.18
2	D	703	HDV	C6-C5-C4	2.08	120.02	117.18
2	D	701	HDV	C4-N9-C1'	-2.08	121.77	126.63
2	B	702	HDV	C5-C4-N9	-2.06	103.57	105.81
2	C	701	HDV	O4'-C1'-C2'	-2.06	103.67	105.84
2	A	704	HDV	O4'-C1'-C2'	-2.04	103.68	105.84
3	C	702	GTP	O6-C6-N1	2.04	123.95	120.11
2	D	701	HDV	C6-C5-N7	2.04	136.02	132.09
2	D	701	HDV	O3A-PB-O2B	-2.04	104.57	110.70
6	A	717	GLY	OXT-C-CA	2.02	121.40	113.38
3	D	702	GTP	N9-C8-N7	-2.01	109.68	113.40

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	HDV	PB-O3B-PG-O1G
3	D	704	GTP	PB-O3B-PG-O3G
6	D	713	GLY	O-C-CA-N
6	D	713	GLY	OXT-C-CA-N
6	C	712	GLY	O-C-CA-N
6	A	716	GLY	O-C-CA-N
6	A	716	GLY	OXT-C-CA-N
6	A	717	GLY	O-C-CA-N
9	A	718	TCE	P-C2-C5-C14
9	A	718	TCE	C5-C2-P-C1
9	A	718	TCE	C6-C3-P-C2
9	A	718	TCE	C4-C1-P-C3
7	B	710	SIN	C1-C2-C3-C4
2	D	701	HDV	C3'-C4'-C5'-O5'
2	D	701	HDV	O4'-C4'-C5'-O5'
2	C	701	HDV	C3'-C4'-C5'-O5'
2	C	701	HDV	O4'-C4'-C5'-O5'
2	B	702	HDV	C3'-C4'-C5'-O5'
2	B	702	HDV	O4'-C4'-C5'-O5'
2	A	704	HDV	C3'-C4'-C5'-O5'
2	A	704	HDV	O4'-C4'-C5'-O5'
6	C	712	GLY	OXT-C-CA-N
6	A	717	GLY	OXT-C-CA-N
7	D	714	SIN	C1-C2-C3-C4
9	A	718	TCE	C3-C6-C8-O9
3	C	702	GTP	PB-O3B-PG-O1G
2	B	702	HDV	C4'-C5'-O5'-PA
9	A	718	TCE	C3-C6-C8-O10
9	A	718	TCE	O13-C11-C4-C1
2	B	701	HDV	PB-O3A-PA-O1A
2	B	701	HDV	PG-O3B-PB-O2B
2	A	702	HDV	PG-O3B-PB-O2B
3	C	702	GTP	PG-O3B-PB-O2B
3	B	703	GTP	PG-O3B-PB-O2B
9	A	718	TCE	P-C3-C6-C8
2	A	704	HDV	C5'-O5'-PA-O1A
2	D	701	HDV	C4'-C5'-O5'-PA
2	C	701	HDV	C4'-C5'-O5'-PA
2	A	704	HDV	C4'-C5'-O5'-PA
3	C	702	GTP	C4'-C5'-O5'-PA
9	A	718	TCE	O12-C11-C4-C1
3	B	703	GTP	PB-O3B-PG-O1G
3	B	703	GTP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	B	703	GTP	C4'-C5'-O5'-PA
3	D	704	GTP	C4'-C5'-O5'-PA
7	B	710	SIN	O2-C1-C2-C3
7	B	710	SIN	O1-C1-C2-C3
2	D	703	HDV	PG-O3B-PB-O2B
2	C	704	HDV	PA-O3A-PB-O2B
2	C	701	HDV	PB-O3A-PA-O5'
3	D	702	GTP	C4'-C5'-O5'-PA
7	D	714	SIN	O2-C1-C2-C3
7	D	714	SIN	C2-C3-C4-O4
7	D	714	SIN	C2-C3-C4-O3
7	D	714	SIN	O1-C1-C2-C3
2	C	704	HDV	PA-O3A-PB-O1B
2	C	704	HDV	PG-O3B-PB-O1B
2	B	701	HDV	PB-O3A-PA-O2A
2	B	701	HDV	PG-O3B-PB-O1B
3	D	702	GTP	PB-O3A-PA-O2A
3	C	702	GTP	PG-O3B-PB-O1B
3	C	702	GTP	PB-O3A-PA-O2A
3	B	703	GTP	PG-O3B-PB-O1B
2	D	703	HDV	PB-O3A-PA-O1A
2	D	703	HDV	PG-O3B-PB-O1B
2	A	702	HDV	PB-O3A-PA-O1A
2	A	702	HDV	PG-O3B-PB-O1B
3	D	702	GTP	PG-O3B-PB-O2B
3	D	704	GTP	PG-O3B-PB-O2B
3	D	704	GTP	PB-O3A-PA-O2A
3	C	702	GTP	PB-O3A-PA-O1A

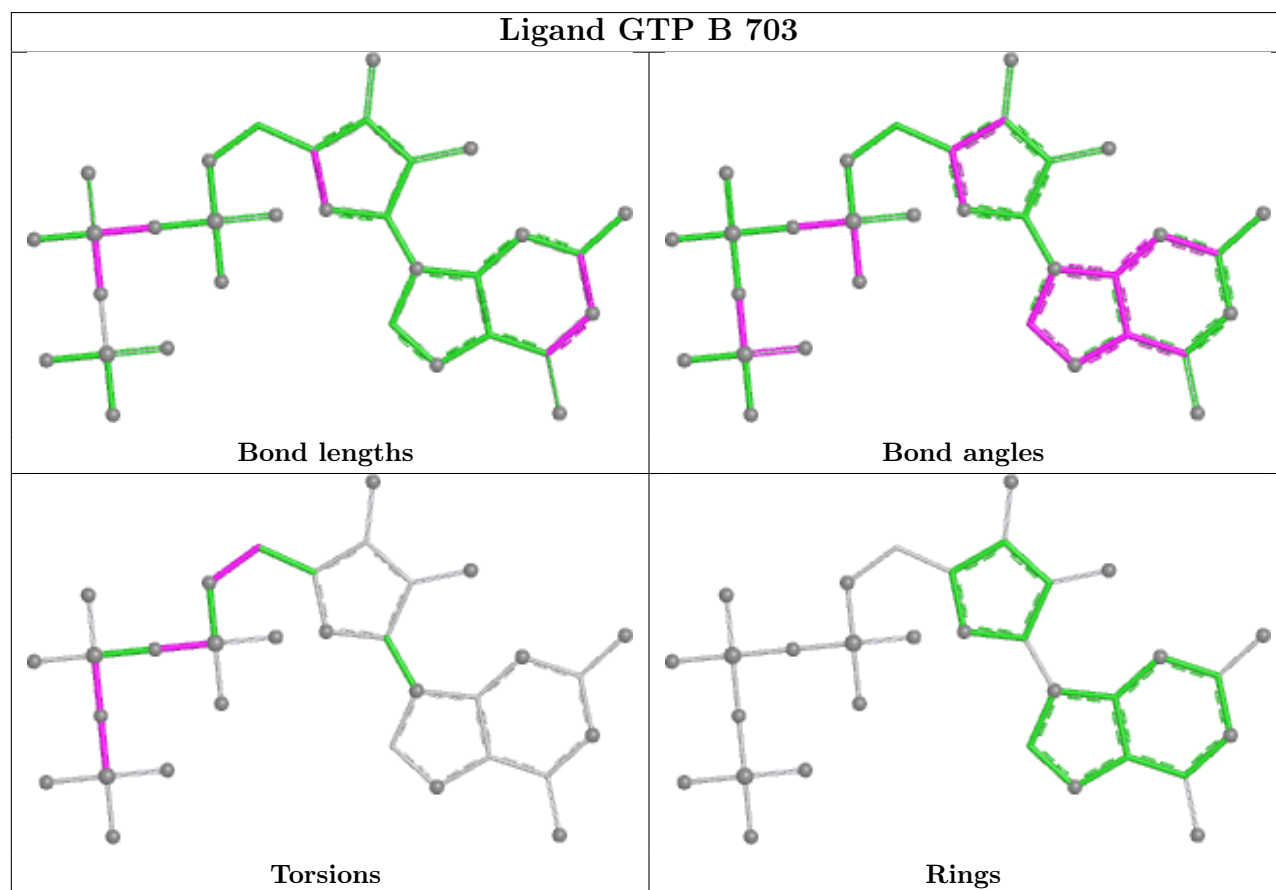
There are no ring outliers.

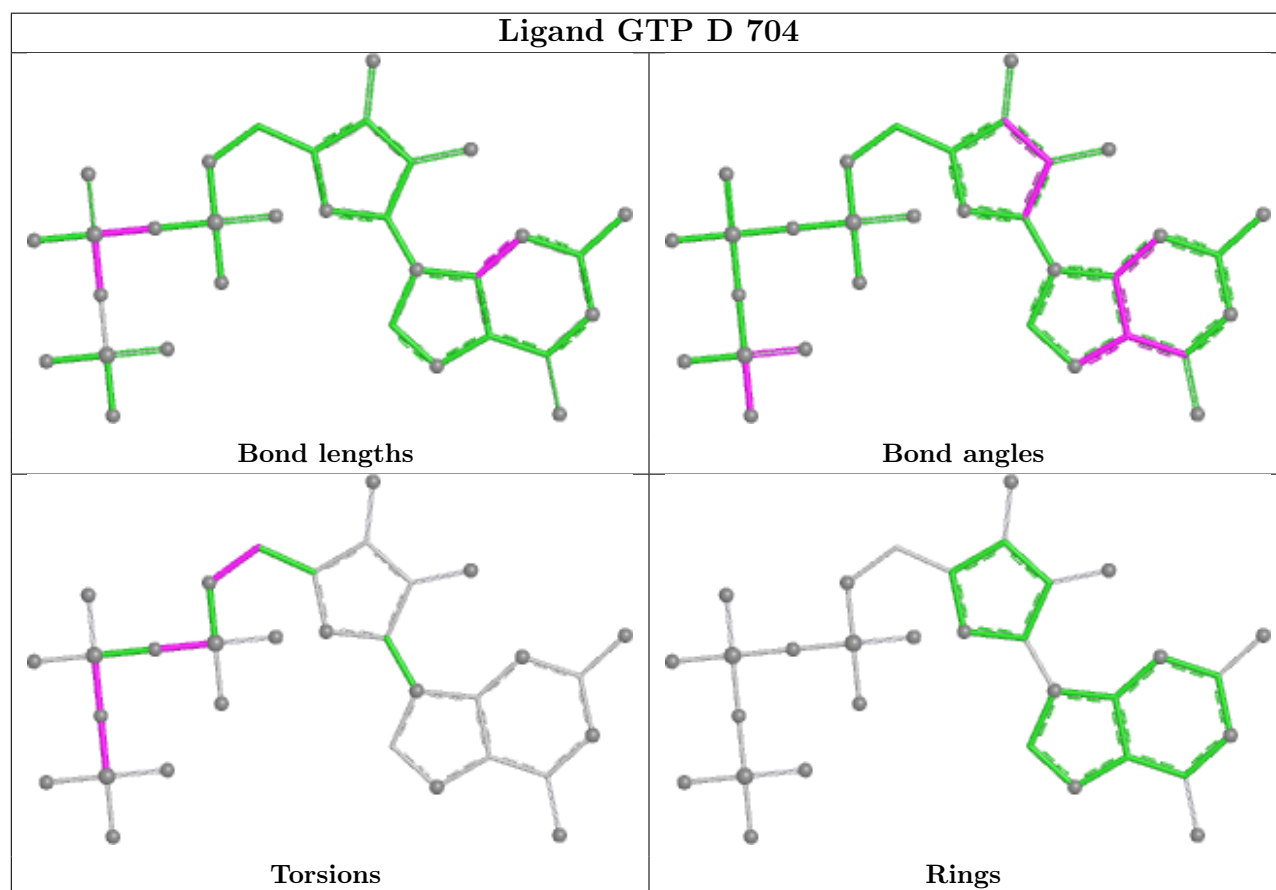
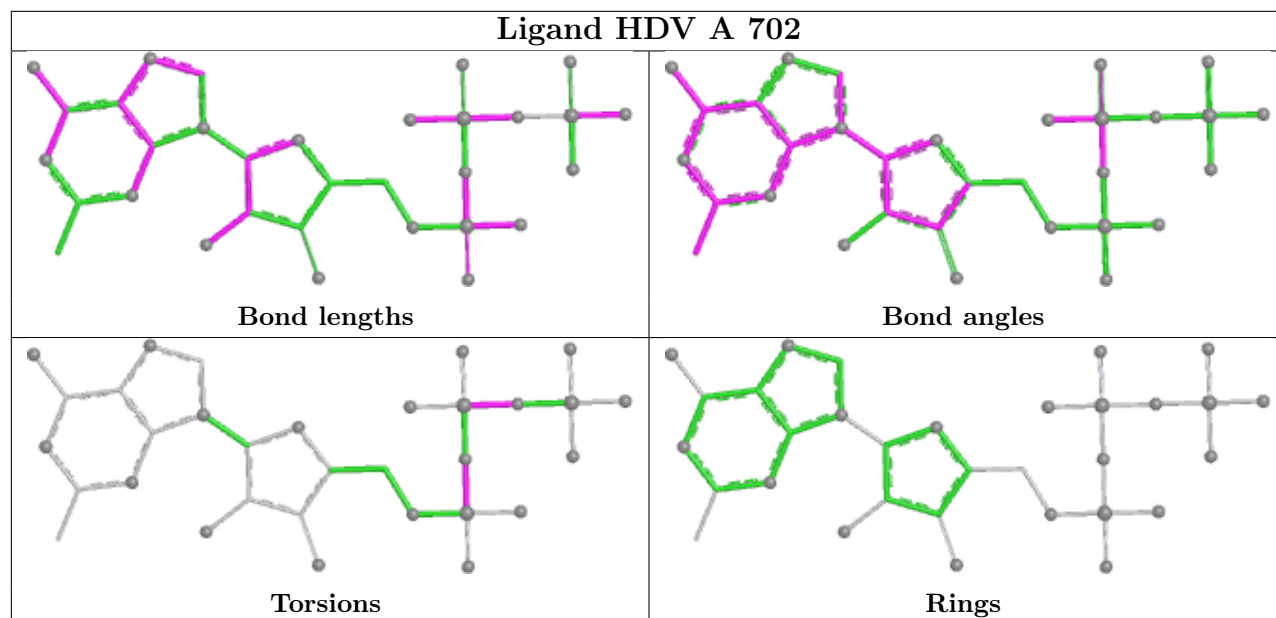
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	718	TCE	2	0
2	B	702	HDV	1	0
2	B	701	HDV	1	0
2	D	703	HDV	1	0
7	D	714	SIN	2	0
2	C	704	HDV	1	0
6	B	709	GLY	1	0

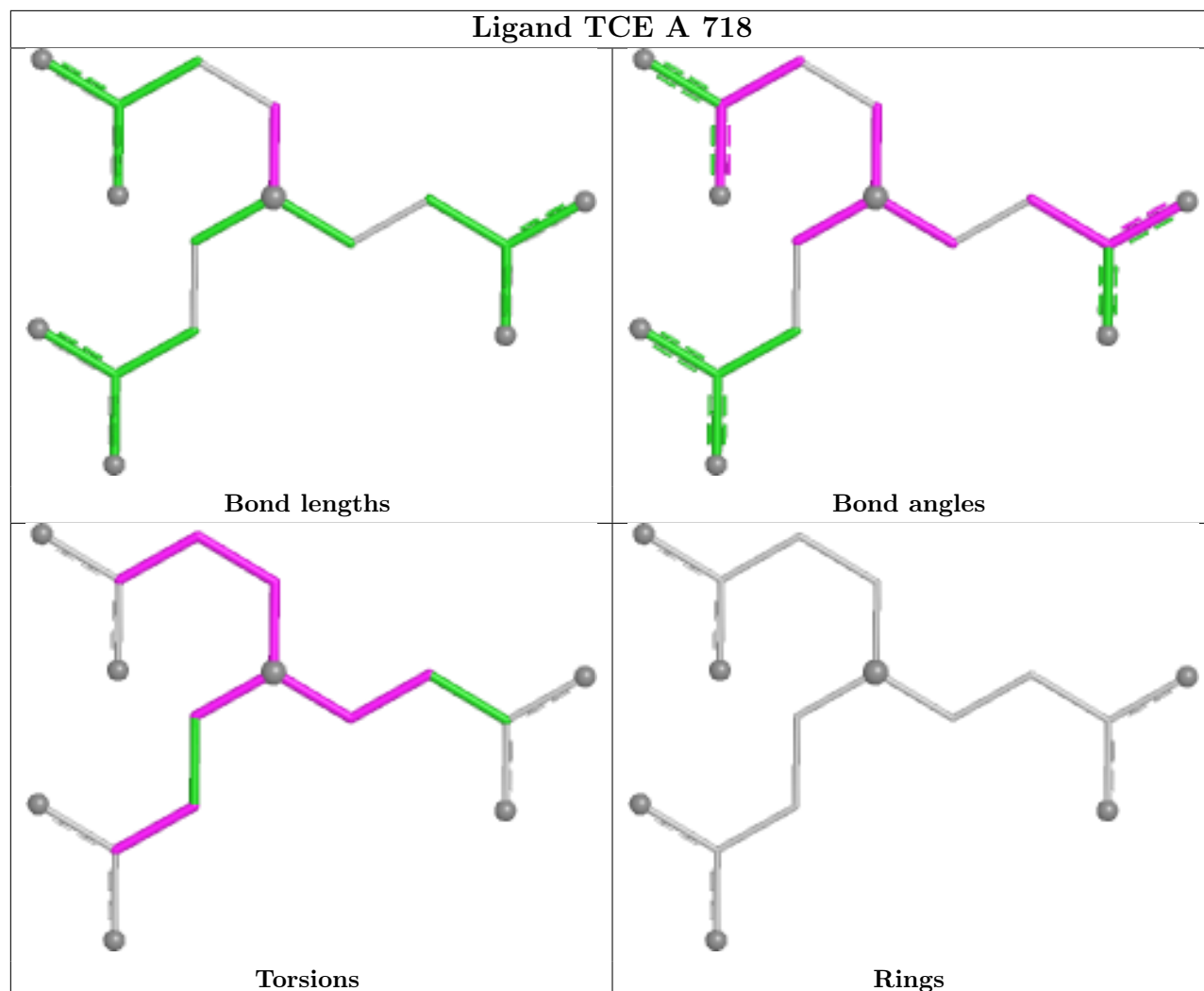
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

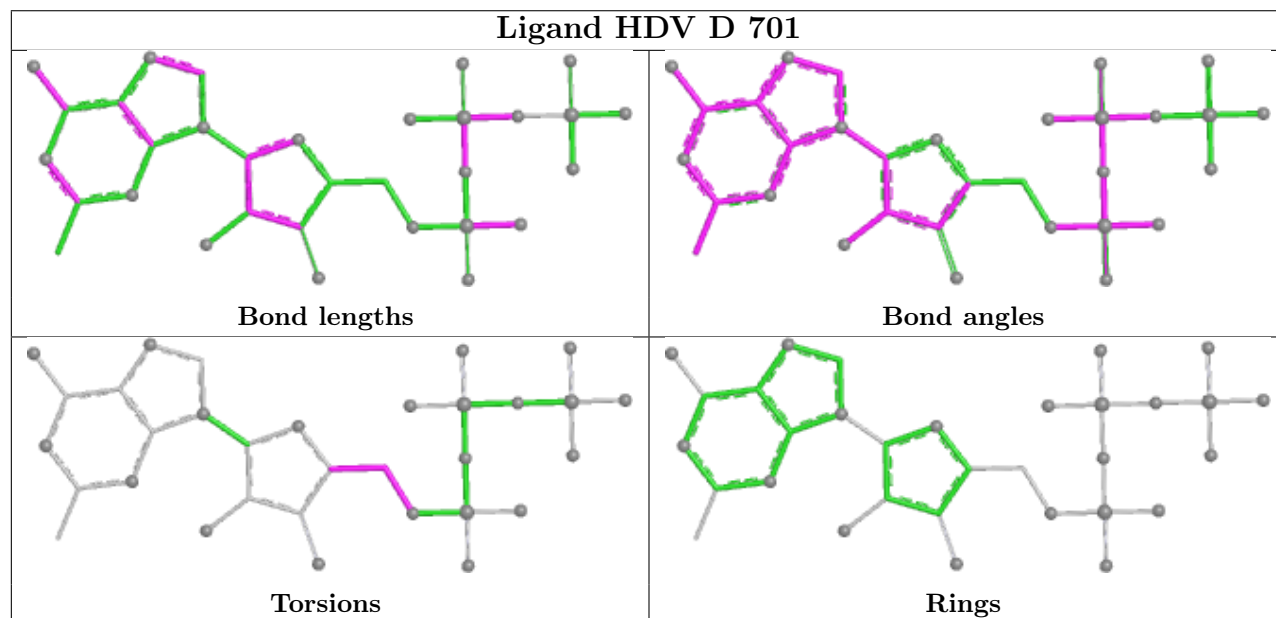


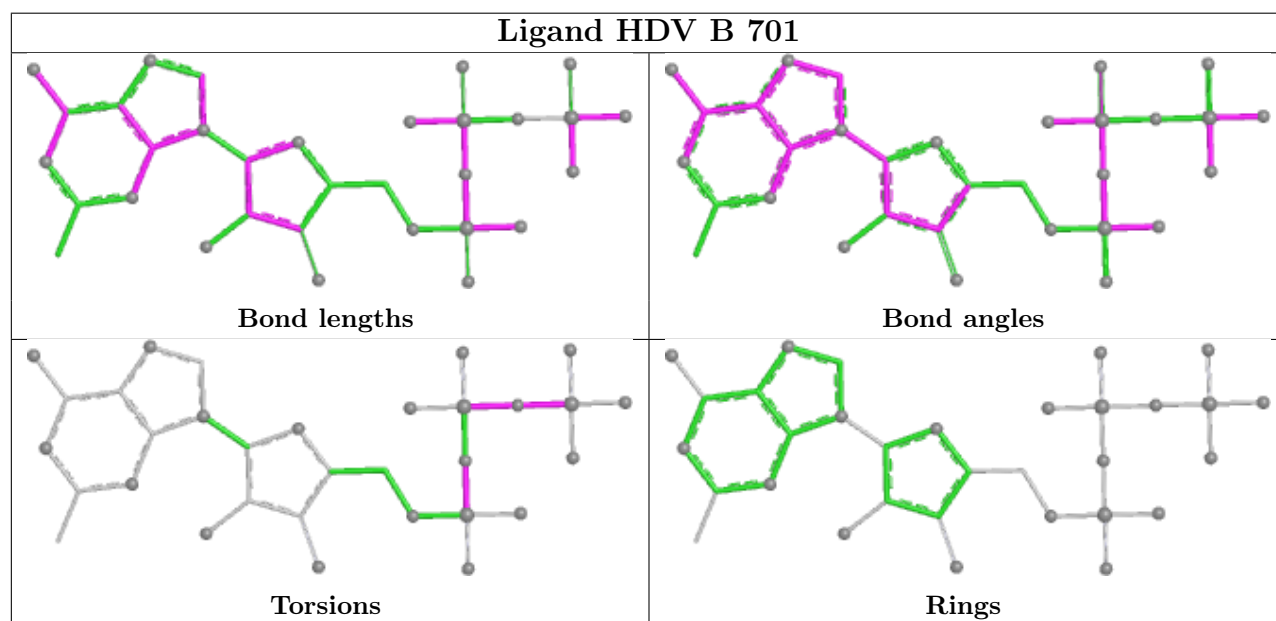
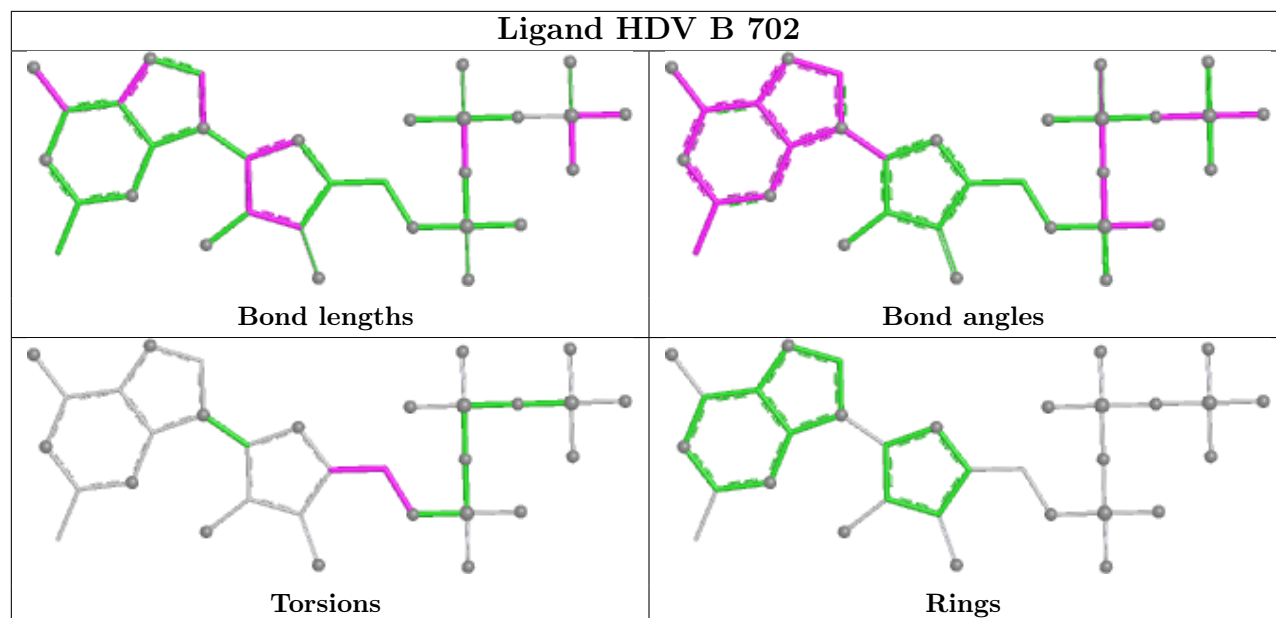


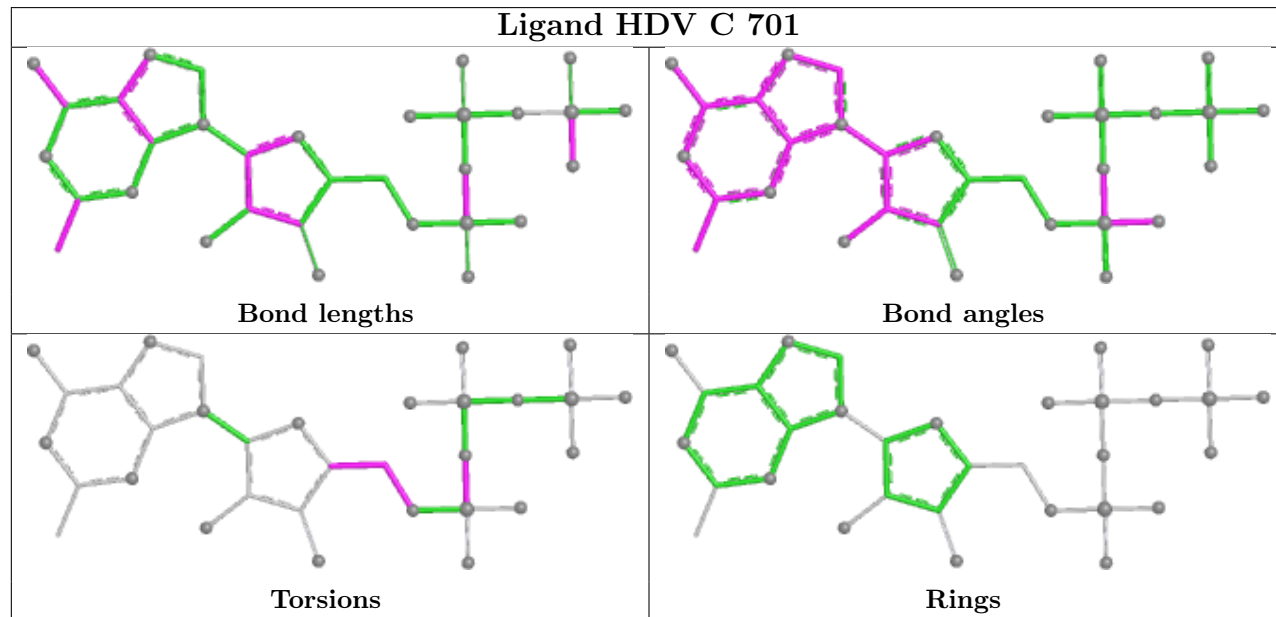
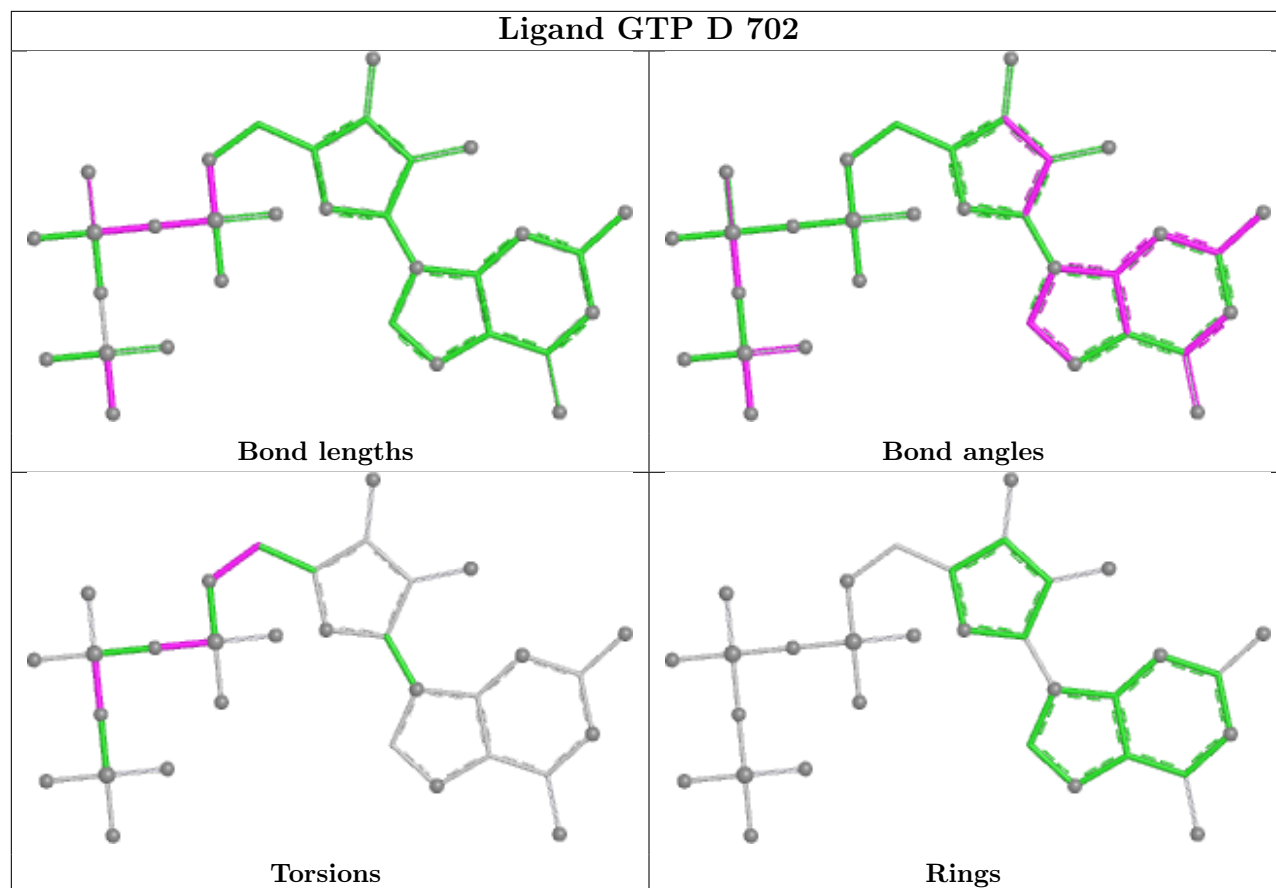
Ligand TCE A 718

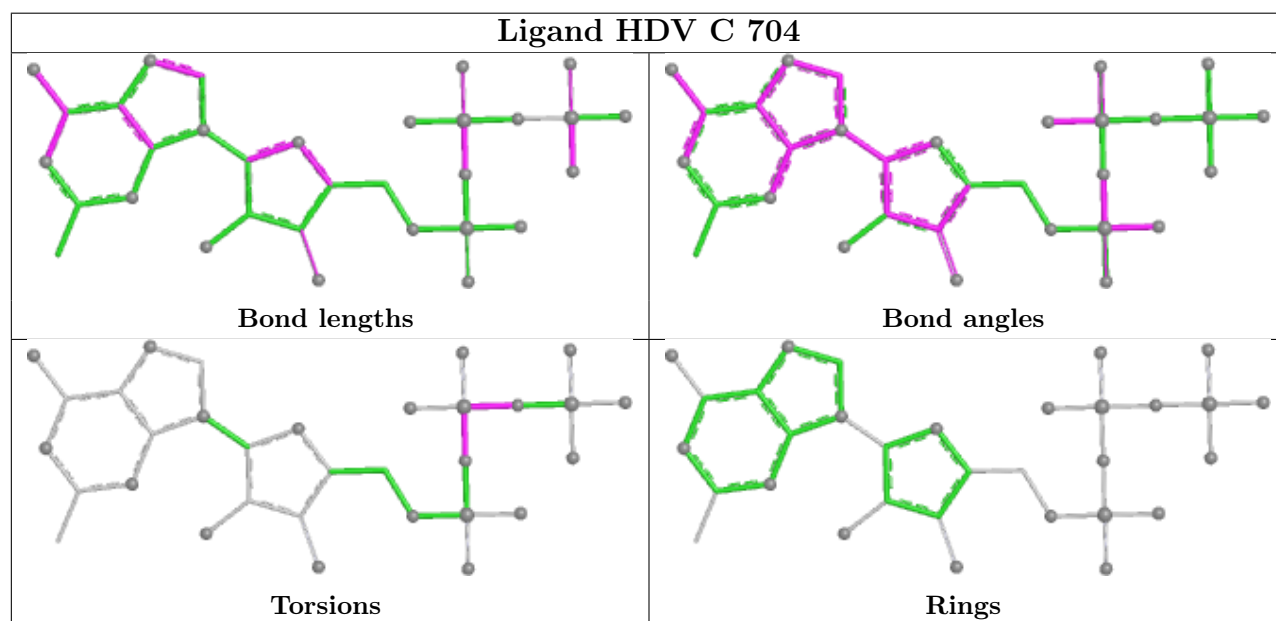
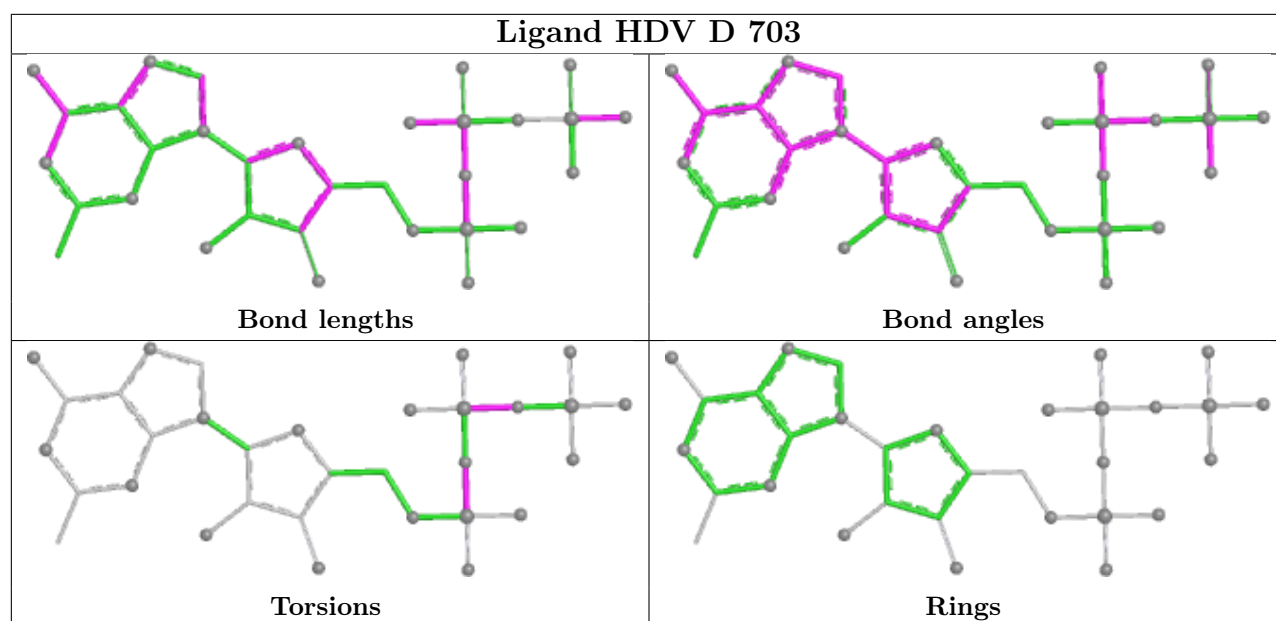


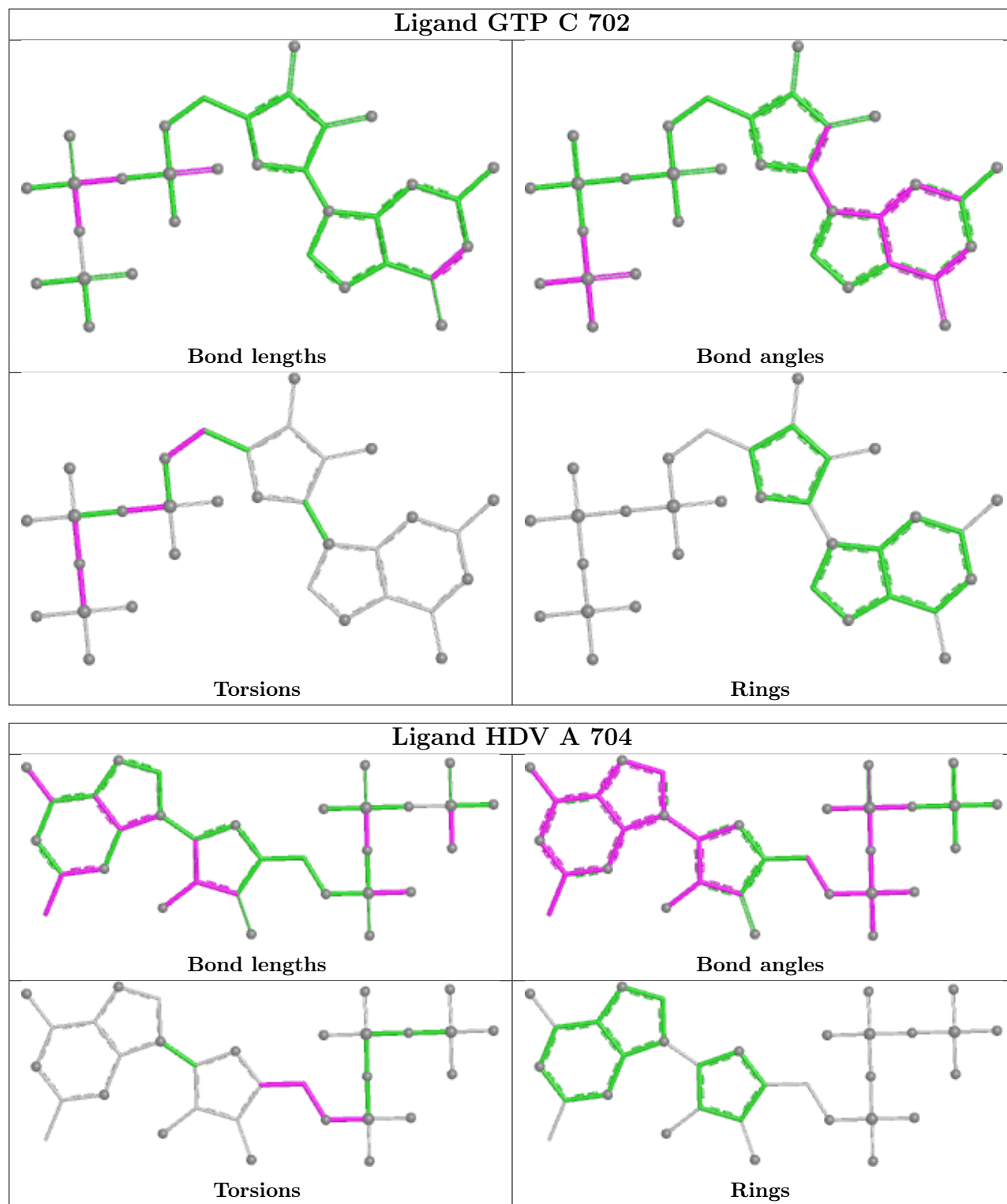
Ligand HDV D 701











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	466/550 (84%)	0.31	40 (8%) 16 17	10, 23, 62, 133	0
1	B	481/550 (87%)	0.51	46 (9%) 13 14	12, 27, 61, 98	0
1	C	481/550 (87%)	0.31	31 (6%) 25 27	12, 25, 62, 91	2 (0%)
1	D	481/550 (87%)	0.15	24 (4%) 34 38	9, 22, 52, 110	1 (0%)
All	All	1909/2200 (86%)	0.32	141 (7%) 20 22	9, 24, 61, 133	3 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	LEU	6.2
1	D	284	LEU	5.7
1	C	114	THR	5.7
1	A	466	ILE	5.3
1	D	466	ILE	5.3
1	C	284	LEU	5.2
1	A	489	LEU	5.2
1	A	115	MET	5.1
1	A	284	LEU	5.1
1	A	487	VAL	5.1
1	C	488	LEU	5.0
1	C	487	VAL	4.9
1	B	284	LEU	4.8
1	C	276	LEU	4.8
1	A	491	VAL	4.7
1	D	464	GLY	4.3
1	B	114	THR	4.2
1	A	562	LEU	4.2
1	B	587	ILE	4.2
1	A	584	GLY	4.1
1	B	485	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	586	VAL	4.0
1	B	589	PRO	3.9
1	D	113	ASP	3.9
1	B	466	ILE	3.9
1	D	114	THR	3.9
1	A	563	TYR	3.9
1	A	113	ASP	3.8
1	A	464	GLY	3.8
1	A	114	THR	3.8
1	B	591	ILE	3.7
1	C	466	ILE	3.7
1	C	485	PRO	3.7
1	B	590	LEU	3.7
1	B	574	ALA	3.7
1	B	572	TRP	3.7
1	A	276	LEU	3.6
1	B	489	LEU	3.5
1	C	113	ASP	3.5
1	C	492	LYS	3.4
1	A	557	VAL	3.4
1	C	568	TYR	3.4
1	D	465	GLN	3.3
1	A	490	ASP	3.3
1	C	491	VAL	3.2
1	C	489	LEU	3.2
1	D	468	ILE	3.1
1	B	276	LEU	3.1
1	B	570	VAL	3.1
1	B	464	GLY	3.1
1	A	463	THR	3.1
1	A	581	PRO	3.1
1	B	115	MET	3.1
1	A	560	LYS	3.1
1	B	480	VAL	3.0
1	A	568	TYR	3.0
1	D	276	LEU	3.0
1	B	488	LEU	3.0
1	B	597	GLU	3.0
1	B	483	ALA	3.0
1	B	230	LYS	2.9
1	A	583	ASP	2.9
1	A	486	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	599	ASN	2.9
1	D	327	ASN	2.9
1	B	481	ALA	2.8
1	B	584	GLY	2.8
1	C	465	GLN	2.8
1	B	595	LYS	2.8
1	B	113	ASP	2.8
1	D	599	ASN	2.7
1	B	472	ASP	2.7
1	A	579	THR	2.7
1	C	591	ILE	2.7
1	D	596	LYS	2.6
1	B	486	LYS	2.6
1	A	493	LEU	2.6
1	B	465	GLN	2.6
1	B	491	VAL	2.6
1	A	485	PRO	2.6
1	D	408	ARG	2.6
1	B	571	GLN	2.5
1	B	577	ASN	2.5
1	C	468	ILE	2.5
1	A	462	PRO	2.5
1	C	592	THR	2.5
1	B	285	TRP	2.5
1	C	594	GLN	2.5
1	A	492	LYS	2.5
1	C	484	LYS	2.4
1	D	229	VAL	2.4
1	A	326	GLN	2.4
1	D	467	LYS	2.4
1	D	522[A]	CYS	2.4
1	B	588	ALA	2.4
1	C	229	VAL	2.4
1	C	598	TRP	2.4
1	B	487	VAL	2.4
1	A	570	VAL	2.4
1	C	277	GLU	2.3
1	C	490	ASP	2.3
1	C	596	LYS	2.3
1	A	578	PHE	2.3
1	B	126	ILE	2.3
1	B	475	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	598	TRP	2.3
1	A	559	ARG	2.3
1	A	484	LYS	2.3
1	A	558	ASP	2.2
1	A	580	LYS	2.2
1	C	587	ILE	2.2
1	C	593	PRO	2.2
1	D	277	GLU	2.2
1	D	328	ASN	2.2
1	C	577	ASN	2.2
1	B	579	THR	2.2
1	D	590	LEU	2.1
1	C	405	LYS	2.1
1	A	345	ASN	2.1
1	C	115	MET	2.1
1	B	482	SER	2.1
1	A	465	GLN	2.1
1	A	567	GLN	2.1
1	B	576	ARG	2.1
1	D	491	VAL	2.1
1	D	403	GLY	2.1
1	C	230	LYS	2.1
1	C	262	GLU	2.1
1	B	463	THR	2.1
1	B	484	LYS	2.1
1	A	229	VAL	2.1
1	D	275	PRO	2.1
1	D	230	LYS	2.1
1	C	118	ILE	2.1
1	A	327	ASN	2.0
1	B	471	GLU	2.0
1	D	326	GLN	2.0
1	D	404	GLY	2.0
1	A	554	CYS	2.0
1	B	180	HIS	2.0
1	B	478	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
6	GLY	C	713	5/5	0.72	0.16	50,53,61,66	0
9	TCE	A	718	16/16	0.74	0.17	50,64,95,97	0
6	GLY	D	713	5/5	0.79	0.14	47,48,52,52	0
6	GLY	C	712	5/5	0.79	0.14	40,42,48,58	0
6	GLY	A	716	5/5	0.81	0.16	47,51,62,64	0
6	GLY	A	715	5/5	0.81	0.17	37,40,52,62	0
8	PO4	C	714	5/5	0.82	0.12	61,64,68,73	0
7	SIN	B	710	8/8	0.82	0.13	43,48,54,56	0
5	NA	A	710	1/1	0.85	0.11	49,49,49,49	0
5	NA	D	712	1/1	0.85	0.14	49,49,49,49	0
5	NA	C	710	1/1	0.85	0.17	48,48,48,48	0
7	SIN	D	714	8/8	0.86	0.12	44,48,55,59	0
4	MG	D	706	1/1	0.86	0.15	45,45,45,45	0
6	GLY	B	709	5/5	0.86	0.13	29,31,38,39	0
6	GLY	A	717	5/5	0.86	0.11	33,33,41,45	0
5	NA	A	714	1/1	0.87	0.14	55,55,55,55	0
5	NA	B	706	1/1	0.88	0.15	46,46,46,46	0
5	NA	A	709	1/1	0.88	0.14	49,49,49,49	0
4	MG	C	707	1/1	0.88	0.15	49,49,49,49	0
5	NA	A	713	1/1	0.88	0.15	47,47,47,47	0
5	NA	B	708	1/1	0.89	0.12	53,53,53,53	0
5	NA	A	708	1/1	0.89	0.20	40,40,40,40	0
5	NA	D	707	1/1	0.89	0.28	52,52,52,52	0
5	NA	D	708	1/1	0.89	0.13	48,48,48,48	0
5	NA	A	711	1/1	0.89	0.13	54,54,54,54	0
5	NA	D	709	1/1	0.89	0.18	48,48,48,48	0
5	NA	A	707	1/1	0.90	0.09	39,39,39,39	0
5	NA	B	707	1/1	0.90	0.13	42,42,42,42	0
5	NA	D	710	1/1	0.92	0.13	50,50,50,50	0
5	NA	B	705	1/1	0.93	0.17	44,44,44,44	0
5	NA	D	711	1/1	0.93	0.14	47,47,47,47	0
5	NA	A	712	1/1	0.93	0.09	48,48,48,48	0

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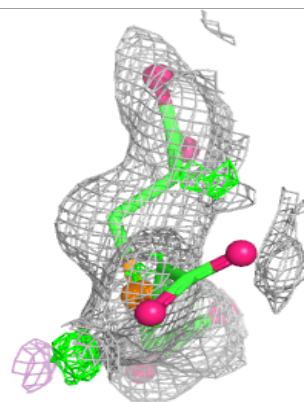
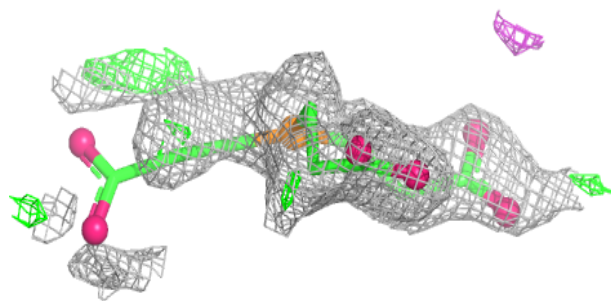
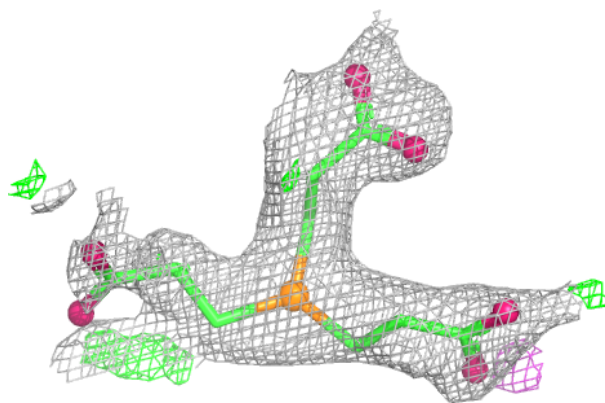
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	A	706	1/1	0.93	0.16	34,34,34,34	0
5	NA	C	709	1/1	0.94	0.11	34,34,34,34	0
5	NA	C	708	1/1	0.94	0.18	38,38,38,38	0
5	NA	C	711	1/1	0.94	0.08	47,47,47,47	0
2	HDV	B	702	32/32	0.97	0.05	15,25,32,36	0
4	MG	A	701	1/1	0.98	0.03	15,15,15,15	0
4	MG	A	705	1/1	0.98	0.07	18,18,18,18	0
2	HDV	A	704	32/32	0.98	0.05	11,20,27,30	0
3	GTP	C	702	32/32	0.98	0.04	13,16,23,25	0
2	HDV	C	701	32/32	0.98	0.05	14,22,29,32	0
2	HDV	D	701	32/32	0.98	0.05	11,18,26,29	0
2	HDV	B	701	32/32	0.99	0.04	10,14,18,26	0
3	GTP	B	703	32/32	0.99	0.03	12,13,23,24	0
4	MG	D	705	1/1	0.99	0.04	17,17,17,17	0
2	HDV	D	703	32/32	0.99	0.04	11,15,20,26	0
4	MG	C	703	1/1	0.99	0.02	16,16,16,16	0
2	HDV	A	702	32/32	0.99	0.04	13,16,19,25	0
4	MG	B	704	1/1	0.99	0.09	24,24,24,24	0
2	HDV	C	704	32/32	0.99	0.03	9,12,16,21	0
4	MG	A	703	1/1	0.99	0.02	18,18,18,18	0
3	GTP	D	702	32/32	0.99	0.04	10,12,19,22	0
3	GTP	D	704	32/32	0.99	0.03	9,11,14,16	0
4	MG	C	706	1/1	1.00	0.05	22,22,22,22	0
4	MG	C	705	1/1	1.00	0.01	12,12,12,12	0

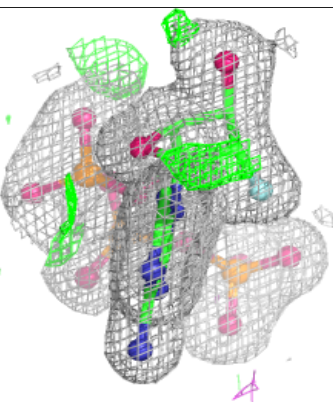
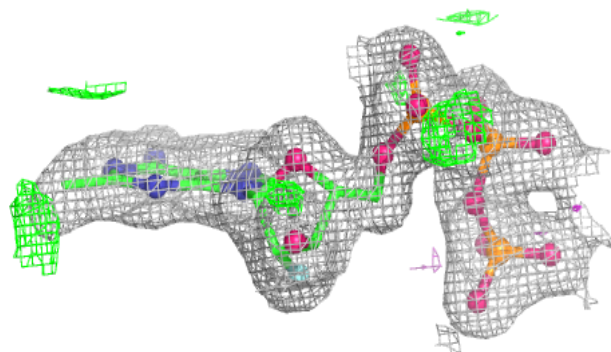
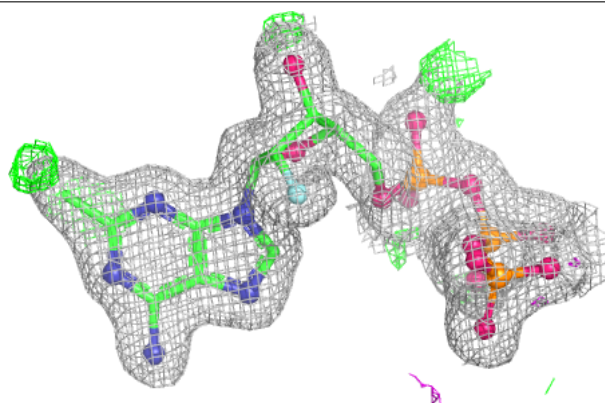
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TCE A 718:

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

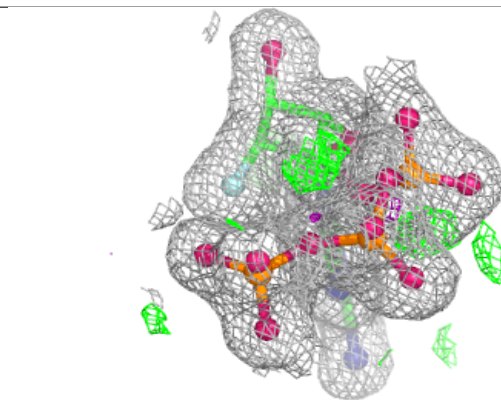
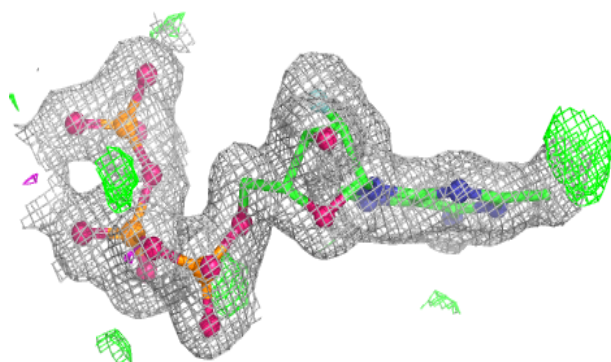
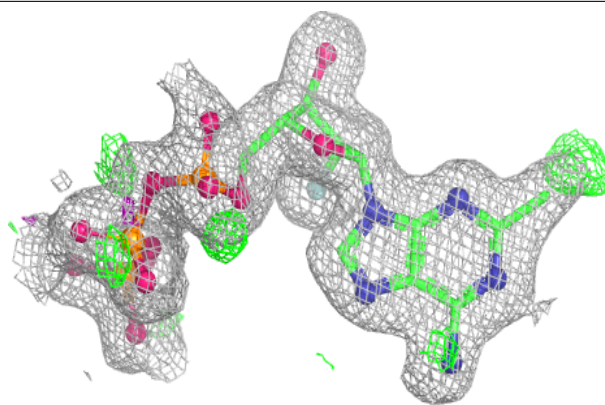
**Electron density around HDV B 702:**

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

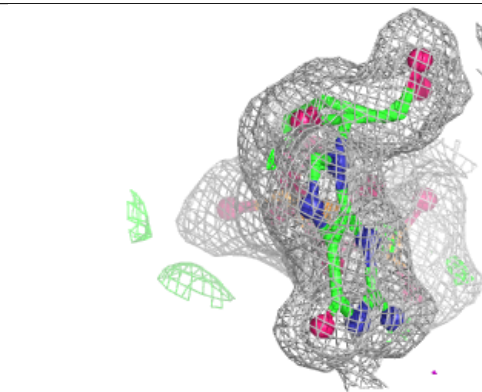
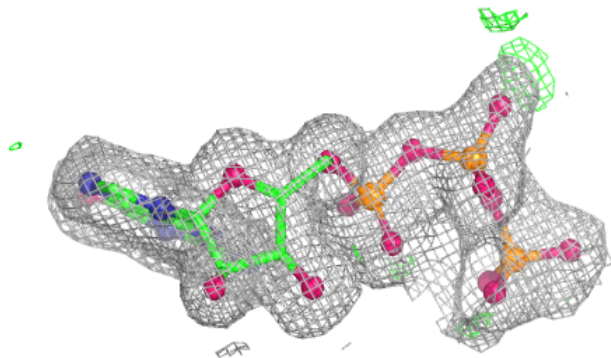
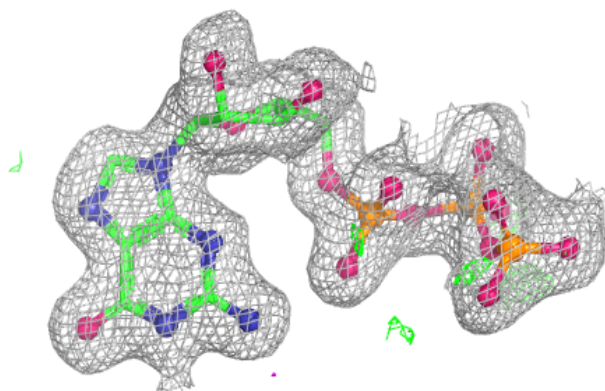


Electron density around HDV A 704:

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

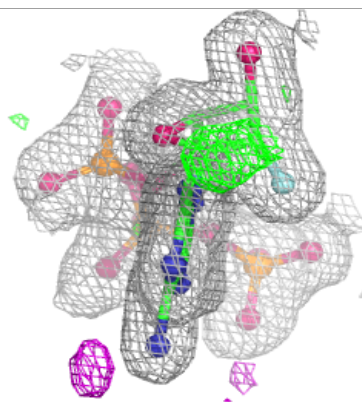
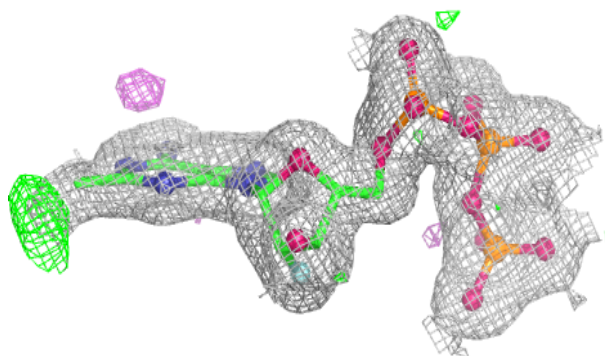
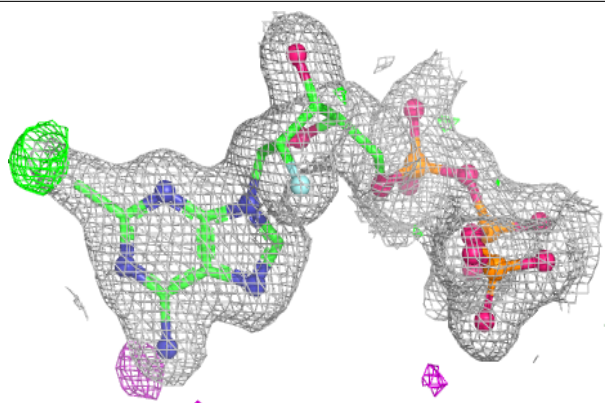
**Electron density around GTP C 702:**

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

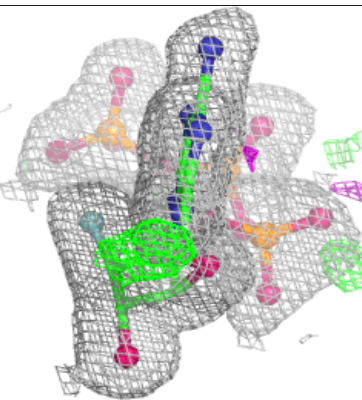
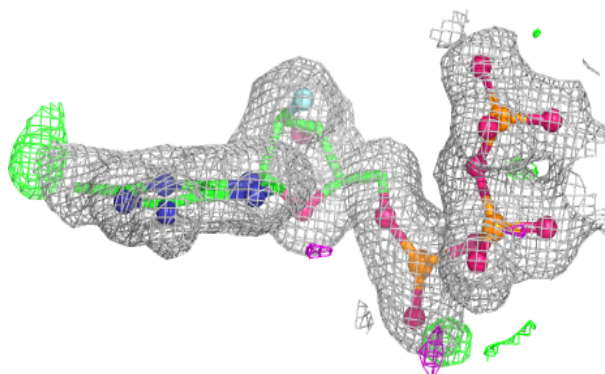
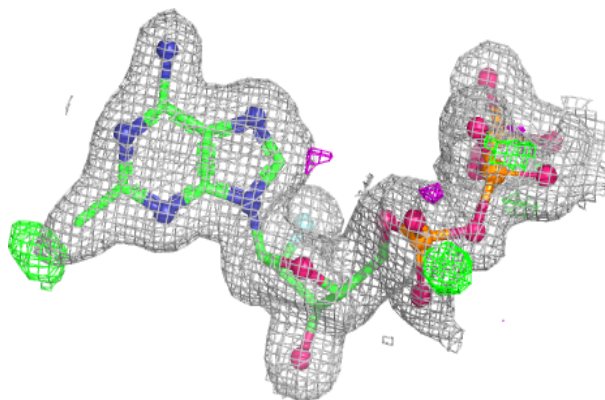


Electron density around HDV C 701:

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

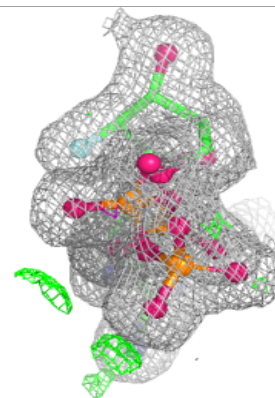
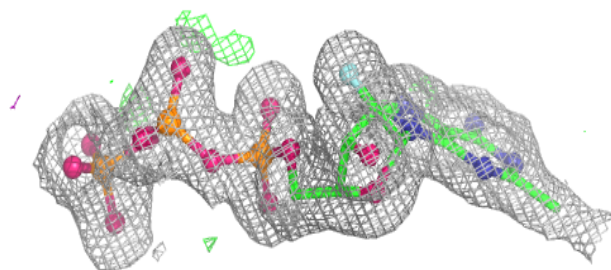
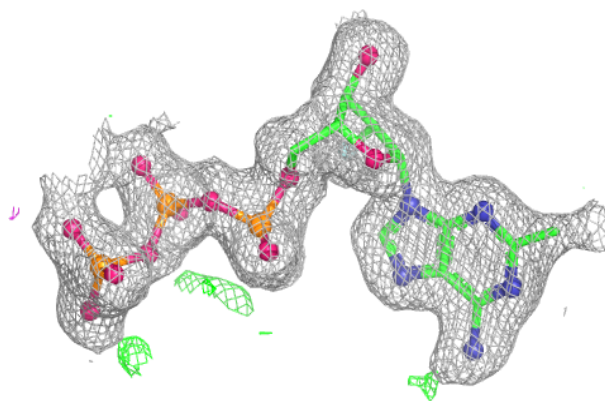
**Electron density around HDV D 701:**

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

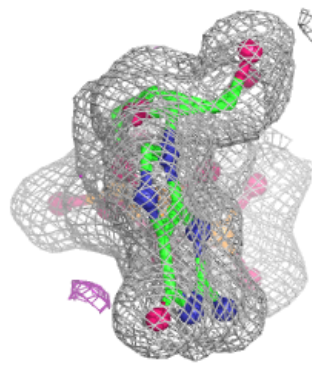
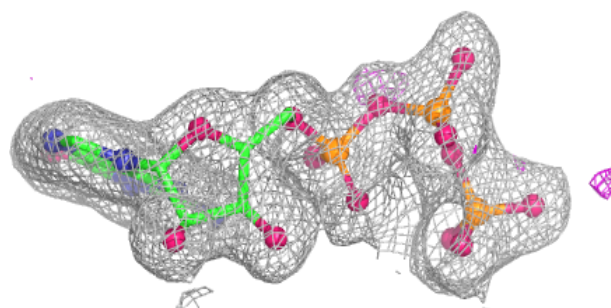
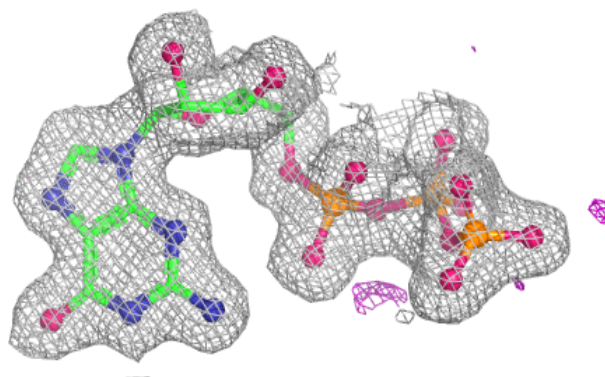


Electron density around HDV B 701:

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

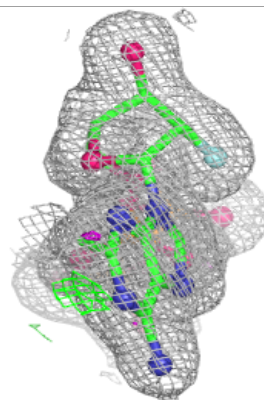
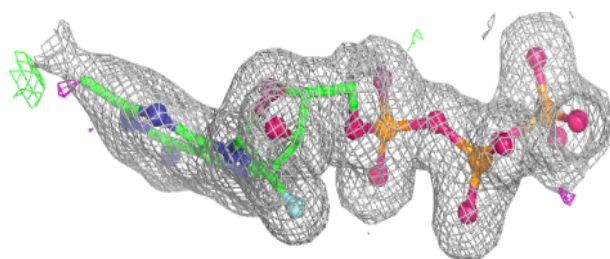
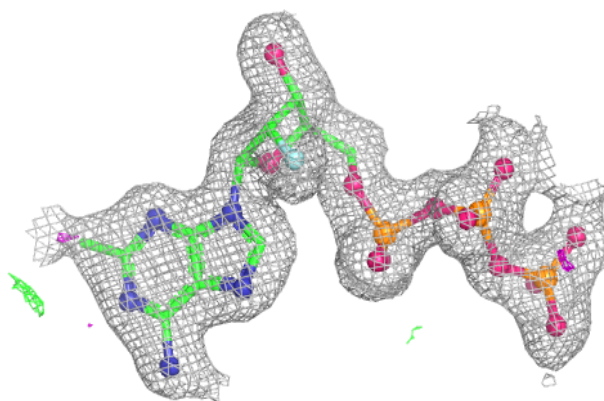
**Electron density around GTP B 703:**

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

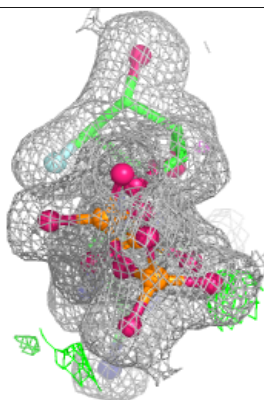
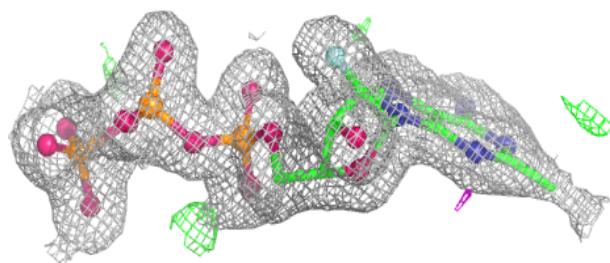
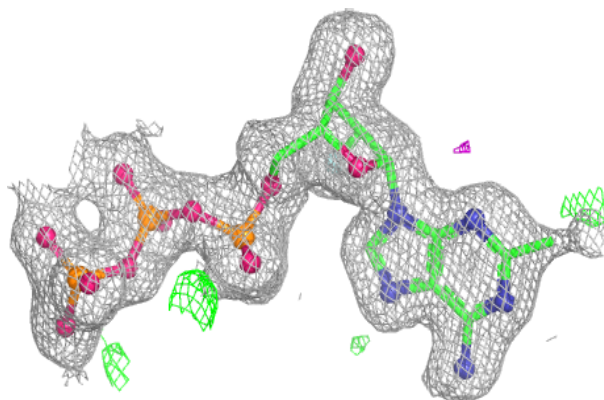


Electron density around HDV D 703:

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

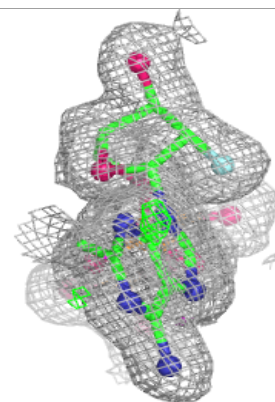
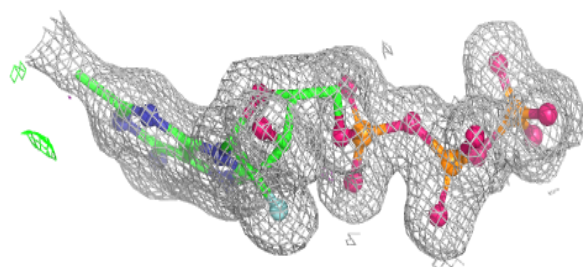
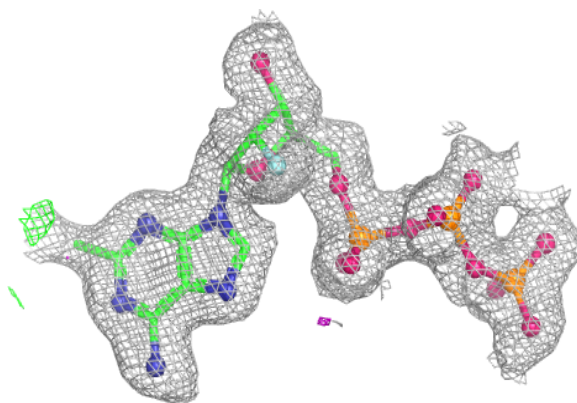
**Electron density around HDV A 702:**

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

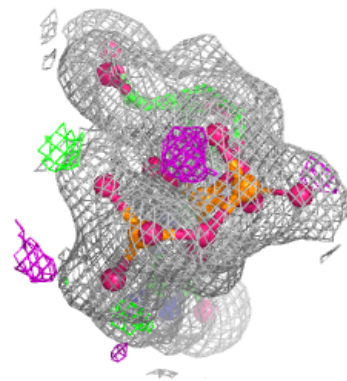
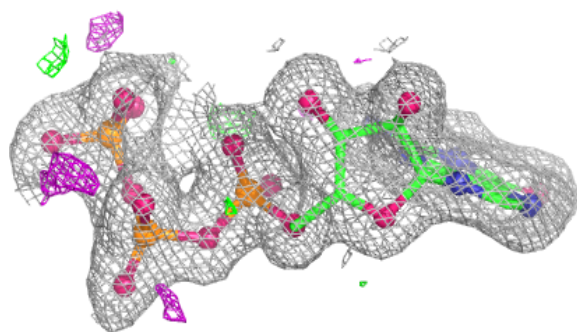
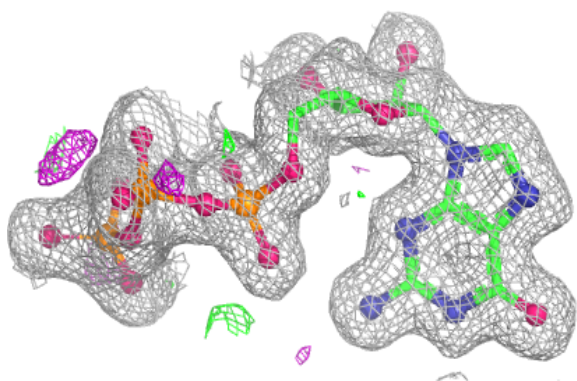


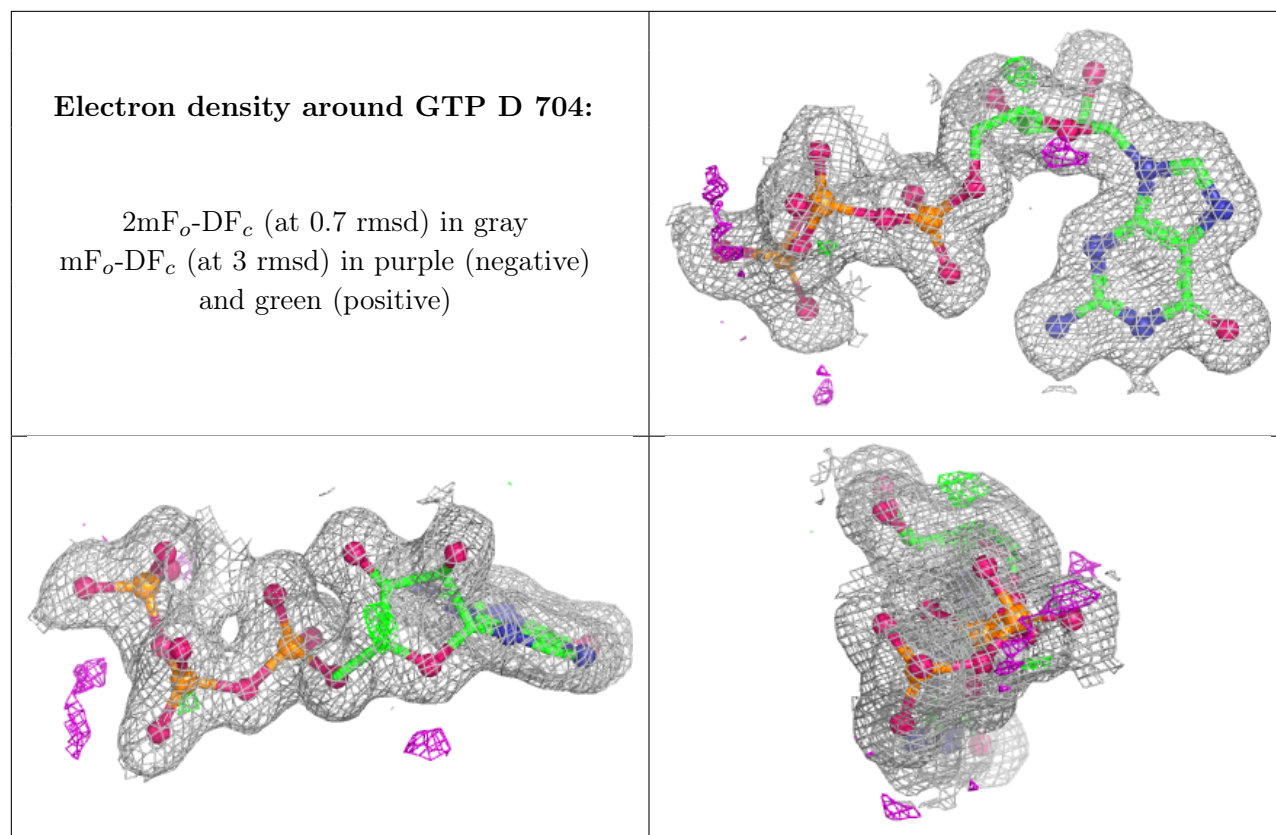
Electron density around HDV C 704:

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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)





6.5 Other polymers [i](#)

There are no such residues in this entry.