wwPDB X-ray Structure Validation Summary Report (i)

Jun 14, 2020 – 12:12 pm BST

PDB ID	:	2J4E
Title	:	THE ITP COMPLEX OF HUMAN INOSINE TRIPHOSPHATASE
Authors	:	Stenmark, P.; Kursula, P.; Arrowsmith, C.; Berglund, H.; Busam, R.; Collins, R.; Edwards, A.; Ehn, M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Holmbergschiavone, L.; Hogbom, M.; Kotenyova, T.; Landry, R.; Loppnau, P.; Magnusdottir, A.; Nilsson-Ehle, P.; Nyman, T.; Ogg, D.; Persson, C.; Sagemark, J.; Sundstrom, M.; Uppenberg, J.; Thorsell, A.G.; Schuler, H.; Van Den Berg, S.; Wallden, K.; Weigelt, J.; Nordlund, P.
Deposited on	:	2006-08-29
Resolution	:	2.80 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
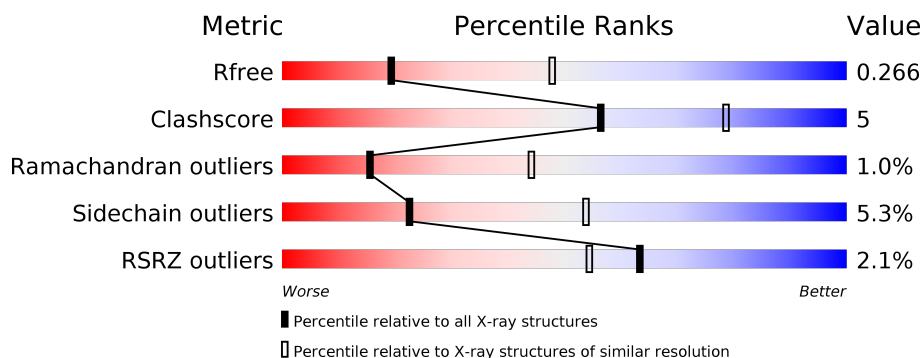
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 <=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	196	4% / 84% / 10% / 6%
1	B	196	2% / 85% / 14% / ·
1	C	196	% / 81% / 16% / ··
1	D	196	3% / 84% / 14% / ··
1	E	196	2% / 83% / 13% / ··

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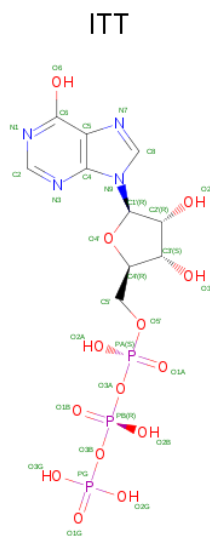| Mol	Chain	Length	Quality of chain
1	F	196	% 80% 18%
1	G	196	2% 82% 11% 5%
1	H	196	4% 83% 10% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12296 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 INOSINE TRIPHOSPHATE PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1442	928	242	264	8			
1	B	194	Total	C	N	O	S	0	0	0
			1509	967	253	280	9			
1	C	194	Total	C	N	O	S	0	0	0
			1509	967	253	280	9			
1	D	195	Total	C	N	O	S	0	0	0
			1515	970	254	282	9			
1	E	190	Total	C	N	O	S	0	0	0
			1486	953	249	275	9			
1	F	194	Total	C	N	O	S	0	0	0
			1509	967	253	280	9			
1	G	186	Total	C	N	O	S	0	0	0
			1456	936	244	267	9			
1	H	184	Total	C	N	O	S	0	0	0
			1446	930	243	265	8			

- Molecule 2 is INOSINE 5'-TRIPHOSPHATE (three-letter code: ITT) (formula: $C_{10}H_{15}N_4O_{14}P_3$).

ITT

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	4	14	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	4	14	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	4	14	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	4	14	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	4	14	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	4	14	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	4	14	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

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W O R L D W I D E
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).
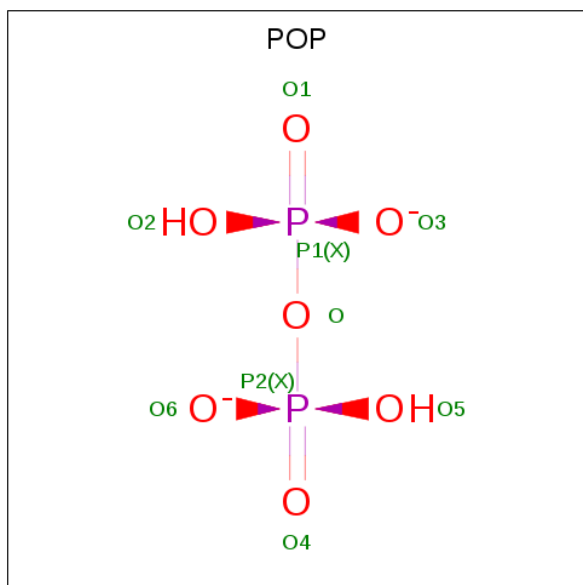
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 9	O 7	P 2	0	0

- Molecule 5 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).

IMP
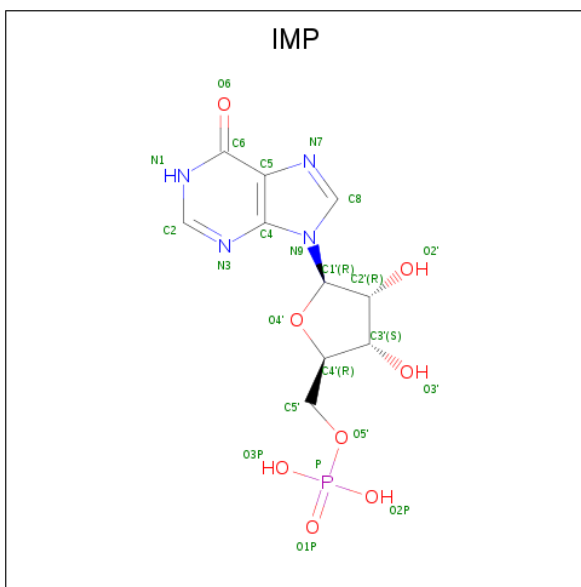
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	D	1	23	10	4	8	1	0	0

- Molecule 6 is water.

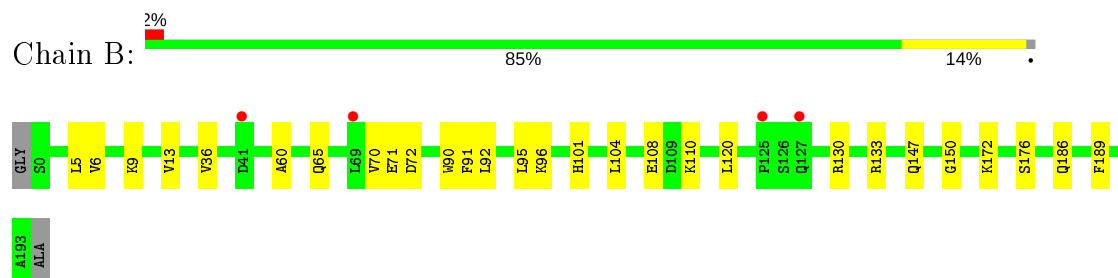| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	19	Total	O	0	0
			19	19		
6	C	26	Total	O	0	0
			26	26		
6	D	30	Total	O	0	0
			30	30		
6	E	29	Total	O	0	0
			29	29		
6	F	23	Total	O	0	0
			23	23		
6	G	27	Total	O	0	0
			27	27		
6	H	8	Total	O	0	0
			8	8		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
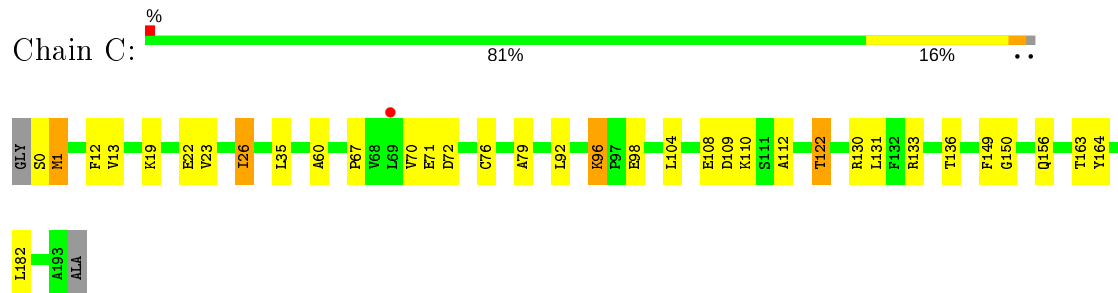
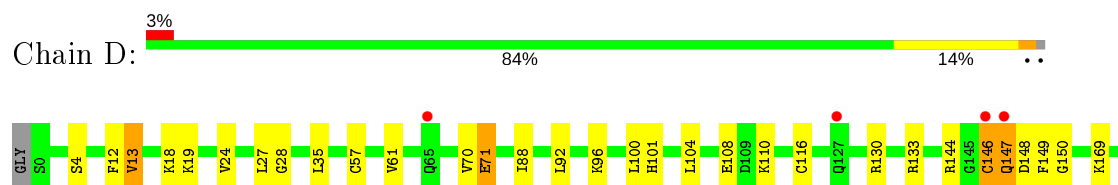- Molecule 1: INOSINE TRIPHOSPHATE PYROPHOSPHATASE
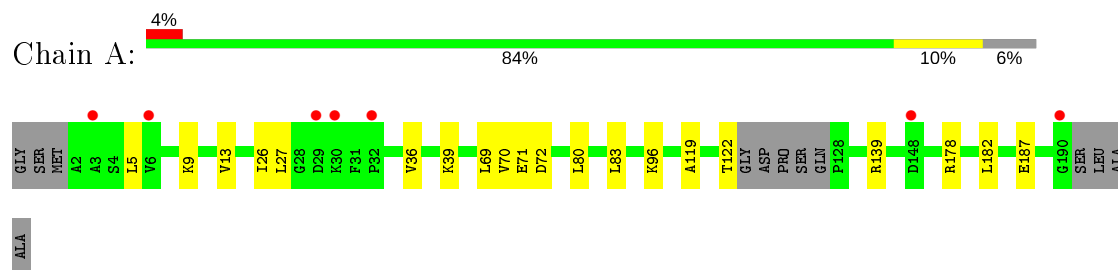
- Molecule 1: INOSINE TRIPHOSPHATE PYROPHOSPHATASE

- Molecule 1: INOSINE TRIPHOSPHATE PYROPHOSPHATASE
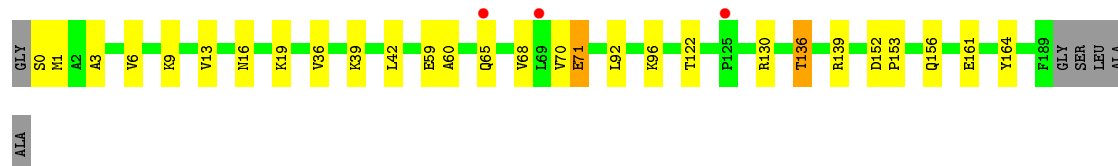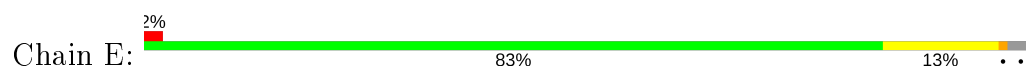

- Molecule 1: INOSINE TRIPHOSPHATE PYROPHOSPHATASE

A194

• Molecule 1: INOSINE TRIPHOSPHATE PYROPHOSPHATASE

Chain E:

2%

83%   13%

GLY S0 M1 A2 A3 V6 K9 V13 N16 K19 V36 K39 L42 E59 A60 Q65 V68 L69 V70 E71 L92 K96 T122 P125 R130 T136 R139 D152 P153 Q156 E161 Y164 F189 GLY SER LEU ALA
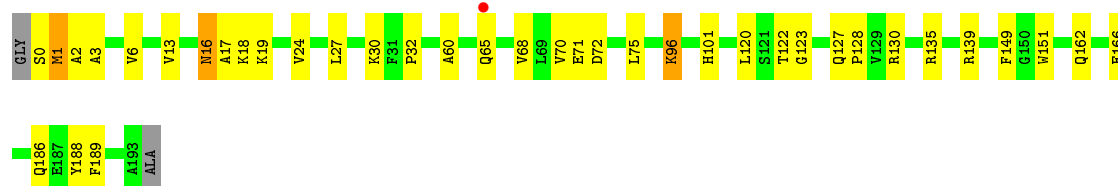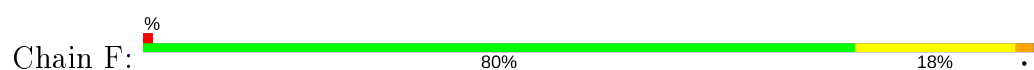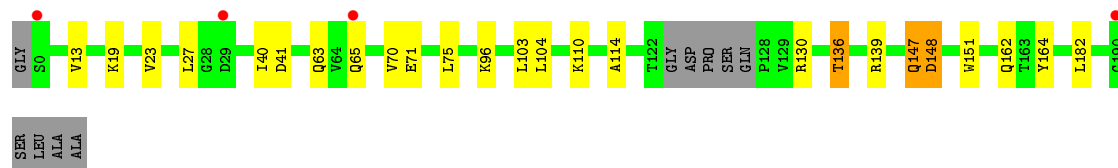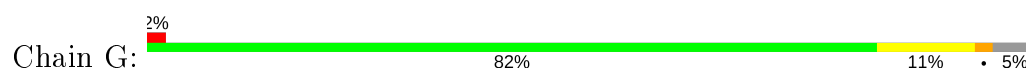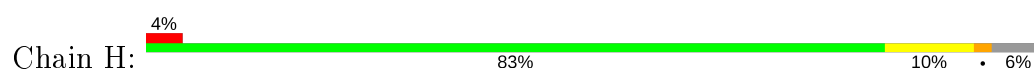
ALA

• Molecule 1: INOSINE TRIPHOSPHATE PYROPHOSPHATASE

Chain F:

%

80%   18%

GLY S0 M1 A2 A3 V6 V13 N16 A17 K18 K19 V24 L27 K30 F31 P32 A60 Q65 V68 L69 V70 E71 D72 L75 K96 H101 L120 S121 T122 G123 Q127 P128 V129 R130 R135 R139 F149 G150 W151 Q162 E166

Q186 E187 Y188 F189 A193 ALA

• Molecule 1: INOSINE TRIPHOSPHATE PYROPHOSPHATASE

Chain G:

2%

82%   11%   5%

GLY S0 V13 K19 V23 L27 G28 D29 I40 D41 Q63 V64 Q65 V70 E71 L75 K96 L103 L104 K110 A114 T122 GLY ASP PRO SER GLN P128 V129 R130 T136 R139 Q147 D148 W151 Q162 T163 Y164 L182 G190

SER LEU ALA ALA

• Molecule 1: INOSINE TRIPHOSPHATE PYROPHOSPHATASE

Chain H:

4%

83%   10%   6%

GLY SER MET ALA A3 S4 L5 V6 F12 V13 K19 L20 E21 L27 G28 D29 L35 K39 V64 Q65 L69 V70 E71 L92 E98 T122 GLY ASP PRO SER Q127 P128 V129 R130 R135 D148 F149 G150 K169 G190 SER LEU ALA ALA

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.00Å 75.29Å 110.79Å 85.12° 77.72° 69.19°	Depositor
Resolution (Å)	19.81 – 2.80 19.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.81-2.80) 97.8 (19.81-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.265 0.205 , 0.266	Depositor DCC
R_{free} test set	2461 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	38.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.2	EDS
L-test for twinning [2]	$< |L| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12296	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: IMP, ITT, MG, POP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.37	0/1475	0.55	0/1993
1	B	0.41	0/1544	0.56	0/2089
1	C	0.39	0/1544	0.55	0/2089
1	D	0.42	0/1550	0.61	0/2096
1	E	0.40	0/1521	0.54	0/2058
1	F	0.40	0/1544	0.57	0/2089
1	G	0.40	0/1489	0.58	0/2011
1	H	0.37	0/1479	0.54	0/1999
All	All	0.39	0/12146	0.56	0/16424

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	144	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1442	0	1439	12	0
1	B	1509	0	1504	15	0
1	C	1509	0	1504	24	0
1	D	1515	0	1509	19	0
1	E	1486	0	1480	15	0
1	F	1509	0	1504	19	0
1	G	1456	0	1456	14	0
1	H	1446	0	1441	10	0
2	A	31	0	10	1	0
2	B	31	0	10	0	0
2	C	31	0	10	0	0
2	E	31	0	10	0	0
2	F	31	0	10	0	0
2	G	31	0	10	0	0
2	H	31	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	D	9	0	0	0	0
5	D	23	0	11	0	0
6	A	5	0	0	0	0
6	B	19	0	0	0	0
6	C	26	0	0	0	0
6	D	30	0	0	1	0
6	E	29	0	0	0	0
6	F	23	0	0	2	0
6	G	27	0	0	0	0
6	H	8	0	0	0	0
All	All	12296	0	11918	121	0

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

The worst 5 of 121 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:146:CYS:HA	1:D:147:GLN:HB2	1.35	1.06
1:G:147:GLN:HA	1:G:148:ASP:HB2	1.54	0.90
1:D:146:CYS:HA	1:D:147:GLN:CB	2.01	0.88
1:G:114:ALA:HB3	1:G:136:THR:HG22	1.55	0.88
1:G:147:GLN:HA	1:G:148:ASP:CB	2.02	0.87

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	180/196 (92%)	170 (94%)	9 (5%)	1 (1%)	25	56
1	B	192/196 (98%)	184 (96%)	7 (4%)	1 (0%)	29	61
1	C	192/196 (98%)	184 (96%)	6 (3%)	2 (1%)	15	44
1	D	193/196 (98%)	182 (94%)	8 (4%)	3 (2%)	9	31
1	E	188/196 (96%)	180 (96%)	7 (4%)	1 (0%)	29	61
1	F	192/196 (98%)	185 (96%)	4 (2%)	3 (2%)	9	31
1	G	182/196 (93%)	176 (97%)	4 (2%)	2 (1%)	14	41
1	H	180/196 (92%)	167 (93%)	11 (6%)	2 (1%)	14	41
All	All	1499/1568 (96%)	1428 (95%)	56 (4%)	15 (1%)	15	44

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	147	GLN
1	C	1	MET
1	F	65	GLN

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Mol	Chain	Res	Type
1	D	146	CYS
1	H	4	SER

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	153/161 (95%)	146 (95%)	7 (5%)	27	60
1	B	161/161 (100%)	154 (96%)	7 (4%)	29	62
1	C	161/161 (100%)	153 (95%)	8 (5%)	24	56
1	D	161/161 (100%)	153 (95%)	8 (5%)	24	56
1	E	159/161 (99%)	151 (95%)	8 (5%)	24	56
1	F	161/161 (100%)	149 (92%)	12 (8%)	13	37
1	G	155/161 (96%)	146 (94%)	9 (6%)	20	50
1	H	154/161 (96%)	146 (95%)	8 (5%)	23	55
All	All	1265/1288 (98%)	1198 (95%)	67 (5%)	22	54

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	0	SER
1	E	139	ARG
1	H	71	GLU
1	E	39	LYS
1	E	92	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	101	HIS
1	E	102	GLN
1	H	65	GLN

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Mol	Chain	Res	Type
1	E	78	ASN
1	F	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	ITT	H	1001	3	25,33,33	1.62	5 (20%)	29,52,52	1.82	8 (27%)
2	ITT	B	1001	3	25,33,33	1.63	5 (20%)	29,52,52	1.56	3 (10%)
2	ITT	F	1001	3	25,33,33	1.62	5 (20%)	29,52,52	1.70	6 (20%)
2	ITT	A	1001	3	25,33,33	1.61	5 (20%)	29,52,52	1.67	6 (20%)
2	ITT	C	1001	3	25,33,33	1.62	5 (20%)	29,52,52	1.74	4 (13%)
2	ITT	E	1001	3	25,33,33	1.62	5 (20%)	29,52,52	1.70	6 (20%)
5	IMP	D	1001	-	21,25,25	1.63	4 (19%)	23,38,38	1.79	5 (21%)
2	ITT	G	1001	3	25,33,33	1.62	5 (20%)	29,52,52	1.81	7 (24%)
4	POP	D	1000	3	6,8,8	0.70	0	13,13,13	1.54	1 (7%)

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	ITT	H	1001	3	-	4/18/38/38	0/3/3/3
2	ITT	B	1001	3	-	7/18/38/38	0/3/3/3
2	ITT	F	1001	3	-	5/18/38/38	0/3/3/3
2	ITT	A	1001	3	-	2/18/38/38	0/3/3/3
2	ITT	C	1001	3	-	3/18/38/38	0/3/3/3
2	ITT	E	1001	3	-	5/18/38/38	0/3/3/3
5	IMP	D	1001	-	-	4/6/26/26	0/3/3/3
2	ITT	G	1001	3	-	6/18/38/38	0/3/3/3
4	POP	D	1000	3	-	0/6/6/6	-

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1001	IMP	C6-N1	4.21	1.40	1.33
2	B	1001	ITT	C2-N1	3.57	1.40	1.33
2	E	1001	ITT	C2-N1	3.55	1.40	1.33
2	C	1001	ITT	C2-N1	3.53	1.40	1.33
5	D	1001	IMP	C2-N1	3.52	1.40	1.33

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1001	ITT	N3-C2-N1	-5.93	119.41	128.68
5	D	1001	IMP	N3-C2-N1	-5.65	119.84	128.68
2	C	1001	ITT	N3-C2-N1	-5.60	119.92	128.68
2	B	1001	ITT	N3-C2-N1	-5.56	119.99	128.68
2	F	1001	ITT	N3-C2-N1	-5.46	120.15	128.68

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1001	ITT	C5'-O5'-PA-O1A
2	B	1001	ITT	PB-O3B-PG-O3G
2	B	1001	ITT	C5'-O5'-PA-O1A
2	F	1001	ITT	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	D	1001	IMP	C5'-O5'-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ITT	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 then 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 ITT H 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ITT B 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ITT F 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ITT A 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ITT C 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ITT E 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand IMP D 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand ITT G 1001

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	184/196 (93%)	0.06	7 (3%)	40	30	27, 30, 33, 35	0
1	B	194/196 (98%)	-0.19	4 (2%)	63	54	25, 29, 32, 34	0
1	C	194/196 (98%)	-0.21	1 (0%)	91	88	25, 29, 32, 33	0
1	D	195/196 (99%)	-0.31	5 (2%)	56	46	24, 29, 33, 35	0
1	E	190/196 (96%)	-0.25	3 (1%)	72	66	25, 29, 32, 35	0
1	F	194/196 (98%)	-0.31	1 (0%)	91	88	22, 29, 33, 35	0
1	G	186/196 (94%)	-0.13	4 (2%)	62	52	25, 29, 33, 36	0
1	H	184/196 (93%)	0.01	7 (3%)	40	30	27, 30, 33, 34	0
All	All	1521/1568 (97%)	-0.17	32 (2%)	63	54	22, 29, 33, 36	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	65	GLN	3.8
1	D	194	ALA	3.6
1	H	69	LEU	3.6
1	G	65	GLN	3.3
1	D	65	GLN	3.2

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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	MG	E	1002	1/1	0.69	0.15	73,73,73,73	0
3	MG	B	1002	1/1	0.82	0.12	45,45,45,45	0
3	MG	G	1002	1/1	0.87	0.14	64,64,64,64	0
3	MG	C	1002	1/1	0.90	0.15	55,55,55,55	0
3	MG	F	1002	1/1	0.91	0.11	31,31,31,31	0
2	ITT	G	1001	31/31	0.91	0.17	39,44,53,54	0
2	ITT	E	1001	31/31	0.92	0.17	33,41,50,51	0
2	ITT	B	1001	31/31	0.94	0.14	40,44,51,52	0
2	ITT	C	1001	31/31	0.94	0.14	37,42,52,53	0
2	ITT	F	1001	31/31	0.94	0.15	35,39,48,49	0
5	IMP	D	1001	23/23	0.95	0.12	32,35,41,42	0
2	ITT	H	1001	31/31	0.95	0.14	39,42,51,51	0
3	MG	D	1002	1/1	0.95	0.14	40,40,40,40	0
2	ITT	A	1001	31/31	0.96	0.13	46,49,57,57	0
3	MG	H	1002	1/1	0.97	0.25	77,77,77,77	0
3	MG	A	1002	1/1	0.97	0.12	60,60,60,60	0
4	POP	D	1000	9/9	0.97	0.13	30,31,32,33	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 ITT G 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
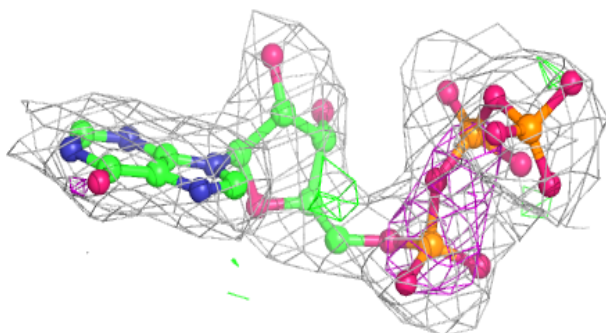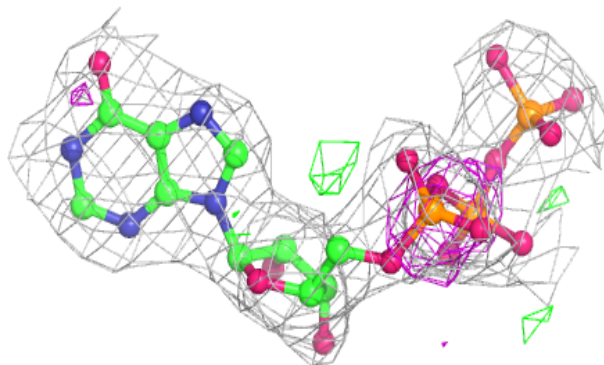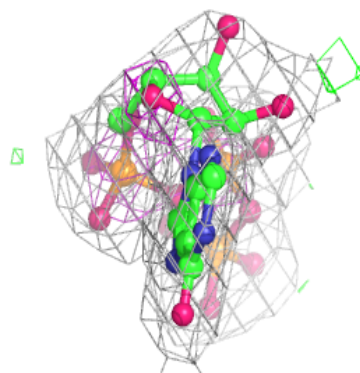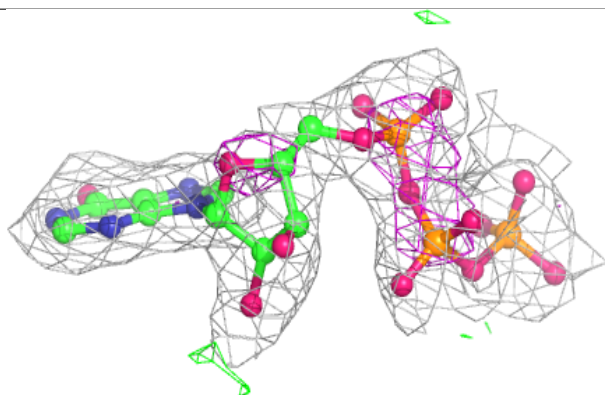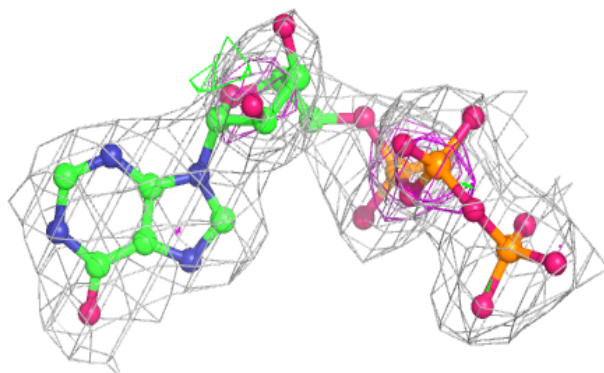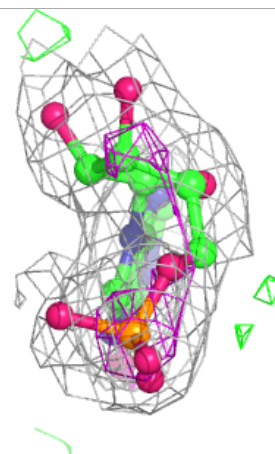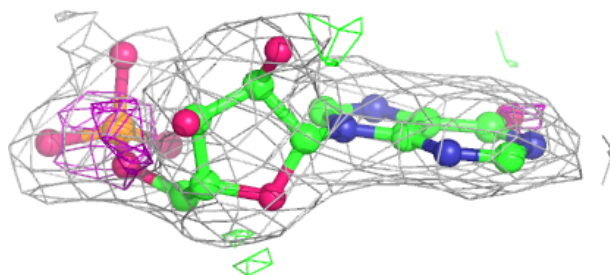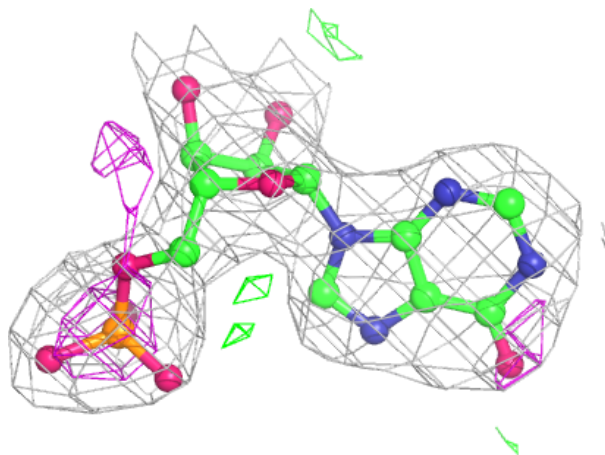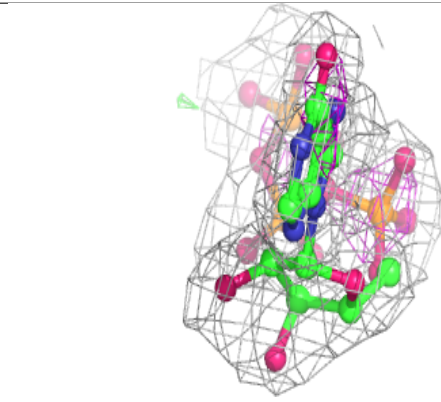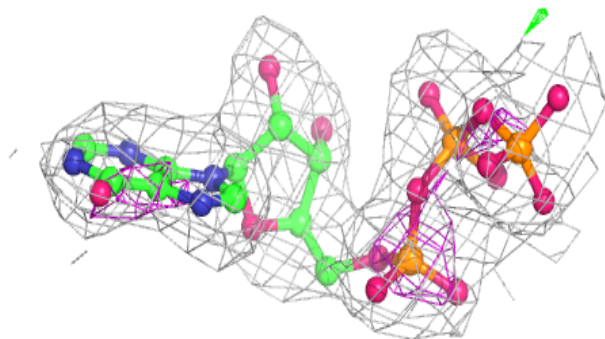mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
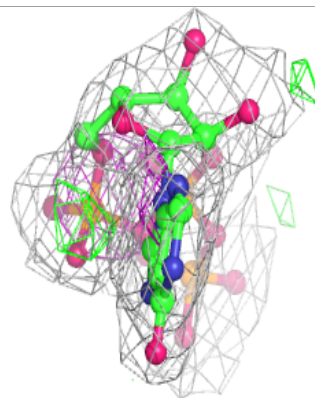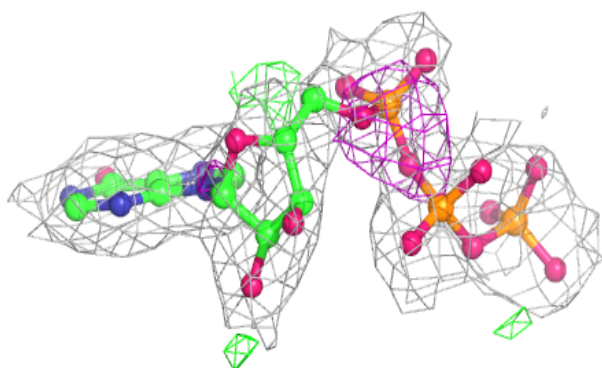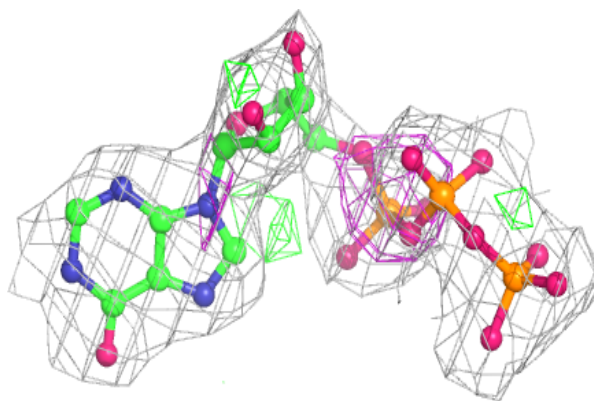
Electron density around ITT E 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
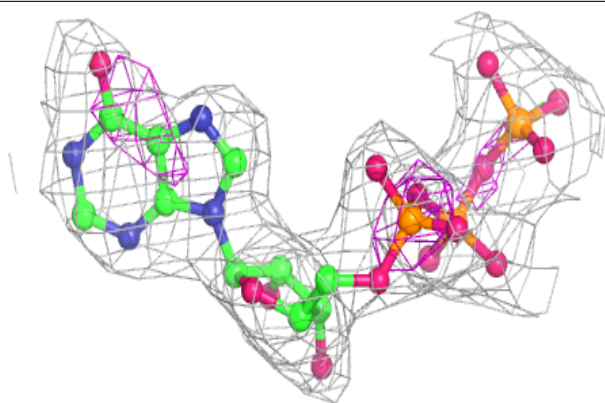and green (positive)
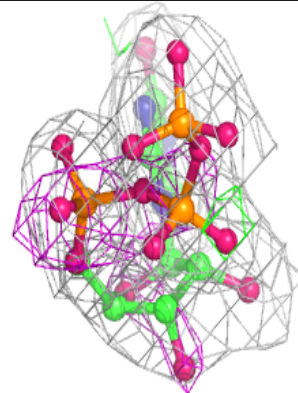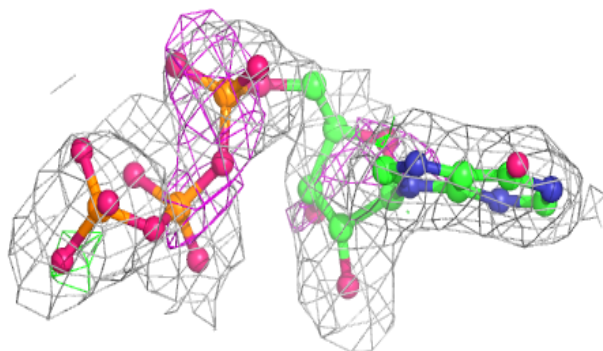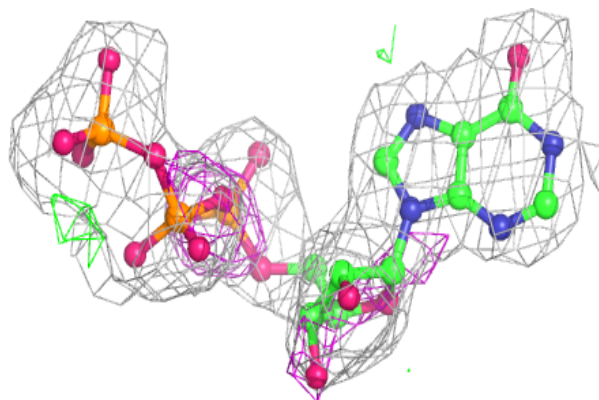
Electron density around ITT B 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
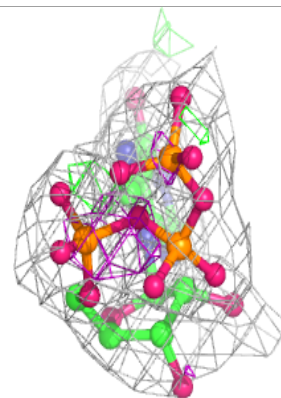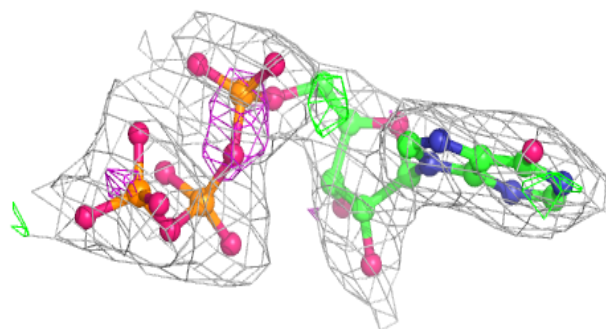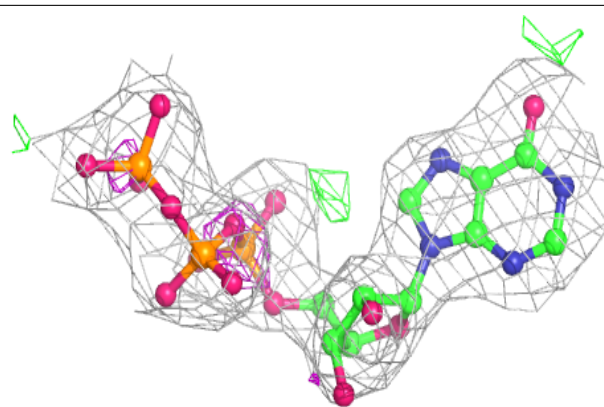
Electron density around ITT C 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
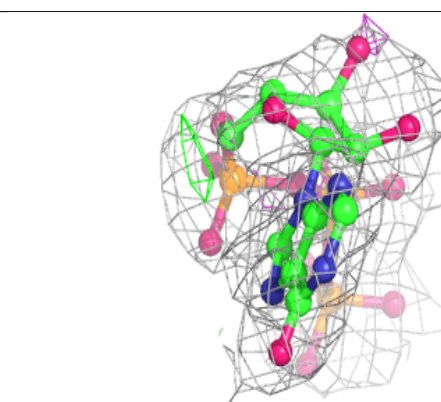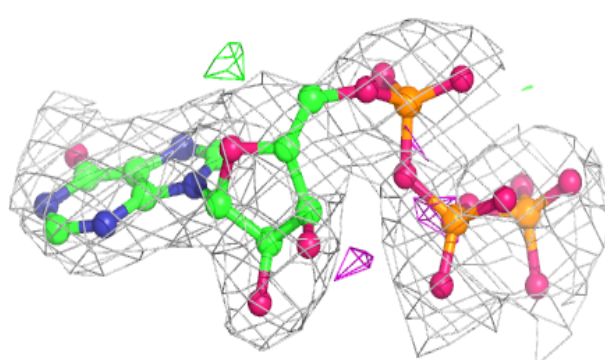and green (positive)
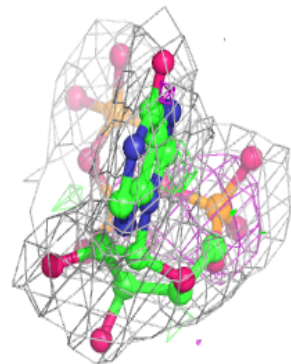
Electron density around ITT F 1001:

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

Electron density around IMP D 1001:

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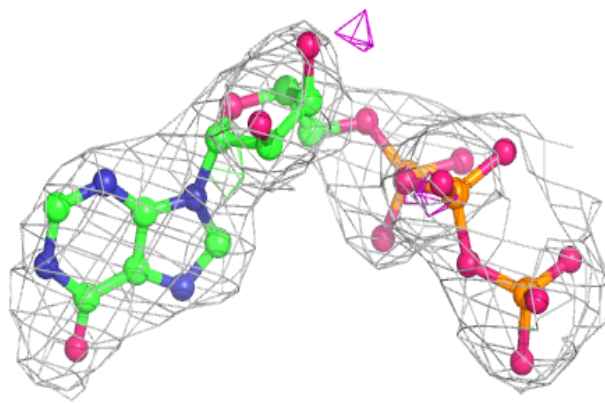and green (positive)

Electron density around ITT H 1001:

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

Electron density around ITT A 1001:

$2mF_o$-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.