



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2024 – 09:54 AM EST

PDB ID : 3PHC
Title : Crystal Structure of Plasmodium falciparum purine nucleoside phosphorylase
in complex with DADMe-ImmG
Authors : Ho, M.; Edwards, A.A.; Almo, S.C.; Schramm, V.L.
Deposited on : 2010-11-03
Resolution : 2.00 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

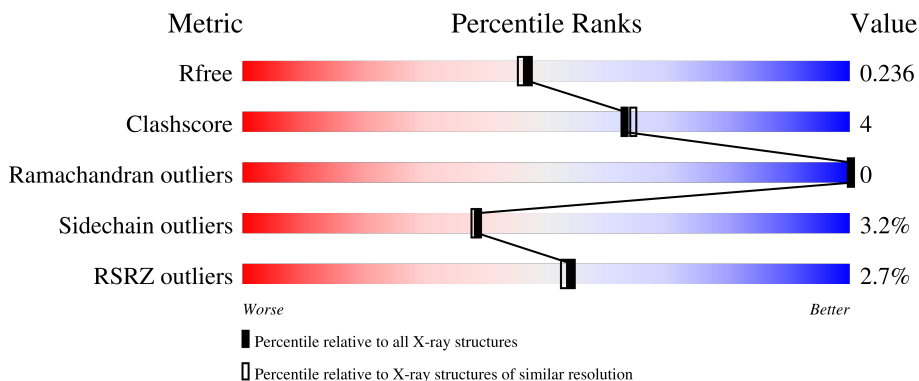
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	275	 3% 79% 7% • 12%
1	B	275	 3% 73% 14% • 12%
1	C	275	 3% 79% 10% • 12%
1	D	275	 % 80% 8% • 12%
1	E	275	 % 79% 8% • 12%

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Mol	Chain	Length	Quality of chain
1	F	275	 2% 78% 9% 12%

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
3	PO4	E	502	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11631 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 Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1861	1179	319	347	16	0	0	0
1	B	243	1861	1179	319	347	16	0	0	0
1	C	243	1861	1179	319	347	16	0	0	0
1	D	243	1861	1179	319	347	16	0	0	0
1	E	243	1861	1179	319	347	16	0	0	0
1	F	243	1861	1179	319	347	16	0	0	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	expression tag	UNP Q8T9Z7
A	246	LYS	-	expression tag	UNP Q8T9Z7
A	247	GLY	-	expression tag	UNP Q8T9Z7
A	248	GLU	-	expression tag	UNP Q8T9Z7
A	249	PHE	-	expression tag	UNP Q8T9Z7
A	250	GLU	-	expression tag	UNP Q8T9Z7
A	251	ALA	-	expression tag	UNP Q8T9Z7
A	252	TYR	-	expression tag	UNP Q8T9Z7
A	253	VAL	-	expression tag	UNP Q8T9Z7
A	254	GLU	-	expression tag	UNP Q8T9Z7
A	255	GLN	-	expression tag	UNP Q8T9Z7
A	256	LYS	-	expression tag	UNP Q8T9Z7
A	257	LEU	-	expression tag	UNP Q8T9Z7
A	258	ILE	-	expression tag	UNP Q8T9Z7
A	259	SER	-	expression tag	UNP Q8T9Z7
A	260	GLU	-	expression tag	UNP Q8T9Z7
A	261	GLU	-	expression tag	UNP Q8T9Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	262	ASP	-	expression tag	UNP Q8T9Z7
A	263	LEU	-	expression tag	UNP Q8T9Z7
A	264	ASN	-	expression tag	UNP Q8T9Z7
A	265	SER	-	expression tag	UNP Q8T9Z7
A	266	ALA	-	expression tag	UNP Q8T9Z7
A	267	VAL	-	expression tag	UNP Q8T9Z7
A	268	ASP	-	expression tag	UNP Q8T9Z7
A	269	HIS	-	expression tag	UNP Q8T9Z7
A	270	HIS	-	expression tag	UNP Q8T9Z7
A	271	HIS	-	expression tag	UNP Q8T9Z7
A	272	HIS	-	expression tag	UNP Q8T9Z7
A	273	HIS	-	expression tag	UNP Q8T9Z7
A	274	HIS	-	expression tag	UNP Q8T9Z7
B	1	LEU	-	expression tag	UNP Q8T9Z7
B	246	LYS	-	expression tag	UNP Q8T9Z7
B	247	GLY	-	expression tag	UNP Q8T9Z7
B	248	GLU	-	expression tag	UNP Q8T9Z7
B	249	PHE	-	expression tag	UNP Q8T9Z7
B	250	GLU	-	expression tag	UNP Q8T9Z7
B	251	ALA	-	expression tag	UNP Q8T9Z7
B	252	TYR	-	expression tag	UNP Q8T9Z7
B	253	VAL	-	expression tag	UNP Q8T9Z7
B	254	GLU	-	expression tag	UNP Q8T9Z7
B	255	GLN	-	expression tag	UNP Q8T9Z7
B	256	LYS	-	expression tag	UNP Q8T9Z7
B	257	LEU	-	expression tag	UNP Q8T9Z7
B	258	ILE	-	expression tag	UNP Q8T9Z7
B	259	SER	-	expression tag	UNP Q8T9Z7
B	260	GLU	-	expression tag	UNP Q8T9Z7
B	261	GLU	-	expression tag	UNP Q8T9Z7
B	262	ASP	-	expression tag	UNP Q8T9Z7
B	263	LEU	-	expression tag	UNP Q8T9Z7
B	264	ASN	-	expression tag	UNP Q8T9Z7
B	265	SER	-	expression tag	UNP Q8T9Z7
B	266	ALA	-	expression tag	UNP Q8T9Z7
B	267	VAL	-	expression tag	UNP Q8T9Z7
B	268	ASP	-	expression tag	UNP Q8T9Z7
B	269	HIS	-	expression tag	UNP Q8T9Z7
B	270	HIS	-	expression tag	UNP Q8T9Z7
B	271	HIS	-	expression tag	UNP Q8T9Z7
B	272	HIS	-	expression tag	UNP Q8T9Z7
B	273	HIS	-	expression tag	UNP Q8T9Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	274	HIS	-	expression tag	UNP Q8T9Z7
C	1	LEU	-	expression tag	UNP Q8T9Z7
C	246	LYS	-	expression tag	UNP Q8T9Z7
C	247	GLY	-	expression tag	UNP Q8T9Z7
C	248	GLU	-	expression tag	UNP Q8T9Z7
C	249	PHE	-	expression tag	UNP Q8T9Z7
C	250	GLU	-	expression tag	UNP Q8T9Z7
C	251	ALA	-	expression tag	UNP Q8T9Z7
C	252	TYR	-	expression tag	UNP Q8T9Z7
C	253	VAL	-	expression tag	UNP Q8T9Z7
C	254	GLU	-	expression tag	UNP Q8T9Z7
C	255	GLN	-	expression tag	UNP Q8T9Z7
C	256	LYS	-	expression tag	UNP Q8T9Z7
C	257	LEU	-	expression tag	UNP Q8T9Z7
C	258	ILE	-	expression tag	UNP Q8T9Z7
C	259	SER	-	expression tag	UNP Q8T9Z7
C	260	GLU	-	expression tag	UNP Q8T9Z7
C	261	GLU	-	expression tag	UNP Q8T9Z7
C	262	ASP	-	expression tag	UNP Q8T9Z7
C	263	LEU	-	expression tag	UNP Q8T9Z7
C	264	ASN	-	expression tag	UNP Q8T9Z7
C	265	SER	-	expression tag	UNP Q8T9Z7
C	266	ALA	-	expression tag	UNP Q8T9Z7
C	267	VAL	-	expression tag	UNP Q8T9Z7
C	268	ASP	-	expression tag	UNP Q8T9Z7
C	269	HIS	-	expression tag	UNP Q8T9Z7
C	270	HIS	-	expression tag	UNP Q8T9Z7
C	271	HIS	-	expression tag	UNP Q8T9Z7
C	272	HIS	-	expression tag	UNP Q8T9Z7
C	273	HIS	-	expression tag	UNP Q8T9Z7
C	274	HIS	-	expression tag	UNP Q8T9Z7
D	1	LEU	-	expression tag	UNP Q8T9Z7
D	246	LYS	-	expression tag	UNP Q8T9Z7
D	247	GLY	-	expression tag	UNP Q8T9Z7
D	248	GLU	-	expression tag	UNP Q8T9Z7
D	249	PHE	-	expression tag	UNP Q8T9Z7
D	250	GLU	-	expression tag	UNP Q8T9Z7
D	251	ALA	-	expression tag	UNP Q8T9Z7
D	252	TYR	-	expression tag	UNP Q8T9Z7
D	253	VAL	-	expression tag	UNP Q8T9Z7
D	254	GLU	-	expression tag	UNP Q8T9Z7
D	255	GLN	-	expression tag	UNP Q8T9Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	256	LYS	-	expression tag	UNP Q8T9Z7
D	257	LEU	-	expression tag	UNP Q8T9Z7
D	258	ILE	-	expression tag	UNP Q8T9Z7
D	259	SER	-	expression tag	UNP Q8T9Z7
D	260	GLU	-	expression tag	UNP Q8T9Z7
D	261	GLU	-	expression tag	UNP Q8T9Z7
D	262	ASP	-	expression tag	UNP Q8T9Z7
D	263	LEU	-	expression tag	UNP Q8T9Z7
D	264	ASN	-	expression tag	UNP Q8T9Z7
D	265	SER	-	expression tag	UNP Q8T9Z7
D	266	ALA	-	expression tag	UNP Q8T9Z7
D	267	VAL	-	expression tag	UNP Q8T9Z7
D	268	ASP	-	expression tag	UNP Q8T9Z7
D	269	HIS	-	expression tag	UNP Q8T9Z7
D	270	HIS	-	expression tag	UNP Q8T9Z7
D	271	HIS	-	expression tag	UNP Q8T9Z7
D	272	HIS	-	expression tag	UNP Q8T9Z7
D	273	HIS	-	expression tag	UNP Q8T9Z7
D	274	HIS	-	expression tag	UNP Q8T9Z7
E	1	LEU	-	expression tag	UNP Q8T9Z7
E	246	LYS	-	expression tag	UNP Q8T9Z7
E	247	GLY	-	expression tag	UNP Q8T9Z7
E	248	GLU	-	expression tag	UNP Q8T9Z7
E	249	PHE	-	expression tag	UNP Q8T9Z7
E	250	GLU	-	expression tag	UNP Q8T9Z7
E	251	ALA	-	expression tag	UNP Q8T9Z7
E	252	TYR	-	expression tag	UNP Q8T9Z7
E	253	VAL	-	expression tag	UNP Q8T9Z7
E	254	GLU	-	expression tag	UNP Q8T9Z7
E	255	GLN	-	expression tag	UNP Q8T9Z7
E	256	LYS	-	expression tag	UNP Q8T9Z7
E	257	LEU	-	expression tag	UNP Q8T9Z7
E	258	ILE	-	expression tag	UNP Q8T9Z7
E	259	SER	-	expression tag	UNP Q8T9Z7
E	260	GLU	-	expression tag	UNP Q8T9Z7
E	261	GLU	-	expression tag	UNP Q8T9Z7
E	262	ASP	-	expression tag	UNP Q8T9Z7
E	263	LEU	-	expression tag	UNP Q8T9Z7
E	264	ASN	-	expression tag	UNP Q8T9Z7
E	265	SER	-	expression tag	UNP Q8T9Z7
E	266	ALA	-	expression tag	UNP Q8T9Z7
E	267	VAL	-	expression tag	UNP Q8T9Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	268	ASP	-	expression tag	UNP Q8T9Z7
E	269	HIS	-	expression tag	UNP Q8T9Z7
E	270	HIS	-	expression tag	UNP Q8T9Z7
E	271	HIS	-	expression tag	UNP Q8T9Z7
E	272	HIS	-	expression tag	UNP Q8T9Z7
E	273	HIS	-	expression tag	UNP Q8T9Z7
E	274	HIS	-	expression tag	UNP Q8T9Z7
F	1	LEU	-	expression tag	UNP Q8T9Z7
F	246	LYS	-	expression tag	UNP Q8T9Z7
F	247	GLY	-	expression tag	UNP Q8T9Z7
F	248	GLU	-	expression tag	UNP Q8T9Z7
F	249	PHE	-	expression tag	UNP Q8T9Z7
F	250	GLU	-	expression tag	UNP Q8T9Z7
F	251	ALA	-	expression tag	UNP Q8T9Z7
F	252	TYR	-	expression tag	UNP Q8T9Z7
F	253	VAL	-	expression tag	UNP Q8T9Z7
F	254	GLU	-	expression tag	UNP Q8T9Z7
F	255	GLN	-	expression tag	UNP Q8T9Z7
F	256	LYS	-	expression tag	UNP Q8T9Z7
F	257	LEU	-	expression tag	UNP Q8T9Z7
F	258	ILE	-	expression tag	UNP Q8T9Z7
F	259	SER	-	expression tag	UNP Q8T9Z7
F	260	GLU	-	expression tag	UNP Q8T9Z7
F	261	GLU	-	expression tag	UNP Q8T9Z7
F	262	ASP	-	expression tag	UNP Q8T9Z7
F	263	LEU	-	expression tag	UNP Q8T9Z7
F	264	ASN	-	expression tag	UNP Q8T9Z7
F	265	SER	-	expression tag	UNP Q8T9Z7
F	266	ALA	-	expression tag	UNP Q8T9Z7
F	267	VAL	-	expression tag	UNP Q8T9Z7
F	268	ASP	-	expression tag	UNP Q8T9Z7
F	269	HIS	-	expression tag	UNP Q8T9Z7
F	270	HIS	-	expression tag	UNP Q8T9Z7
F	271	HIS	-	expression tag	UNP Q8T9Z7
F	272	HIS	-	expression tag	UNP Q8T9Z7
F	273	HIS	-	expression tag	UNP Q8T9Z7
F	274	HIS	-	expression tag	UNP Q8T9Z7

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

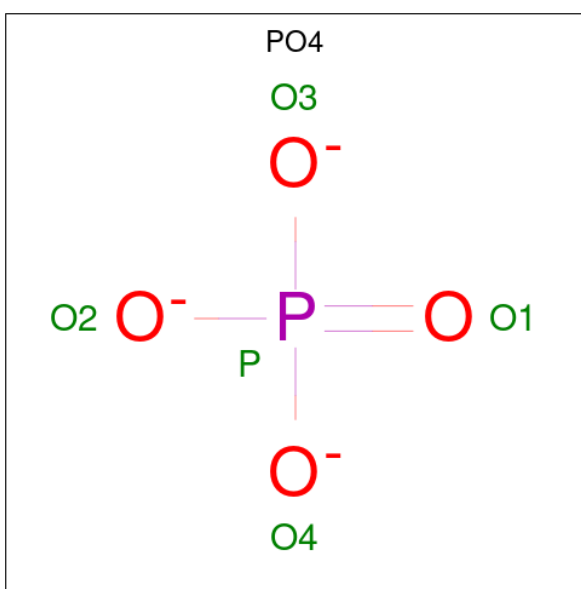
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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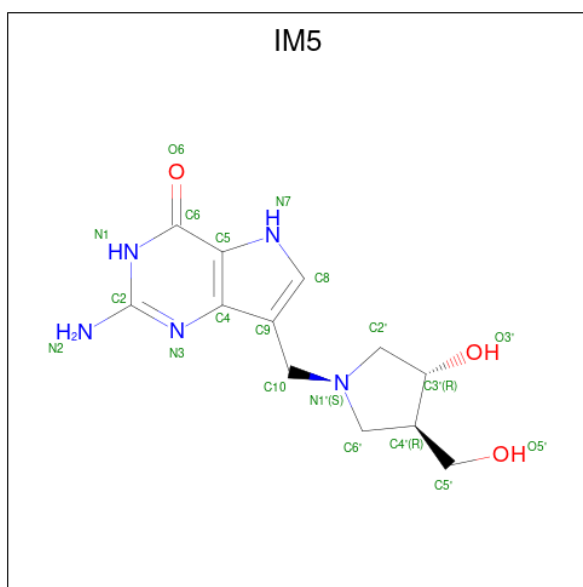
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0

- Molecule 4 is 2-amino-7-[[[(3R,4R)-3-hydroxy-4-(hydroxymethyl)pyrrolidin-1-yl]methyl]-3,5-dihydro-4H-pyrrolo[3,2-d]pyrimidin-4-one (three-letter code: IM5) (formula: C₁₂H₁₇N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	20	12	5	3	0	0
4	B	1	20	12	5	3	0	0
4	C	1	20	12	5	3	0	0
4	D	1	20	12	5	3	0	0
4	E	1	20	12	5	3	0	0
4	F	1	20	12	5	3	0	0

- Molecule 5 is water.

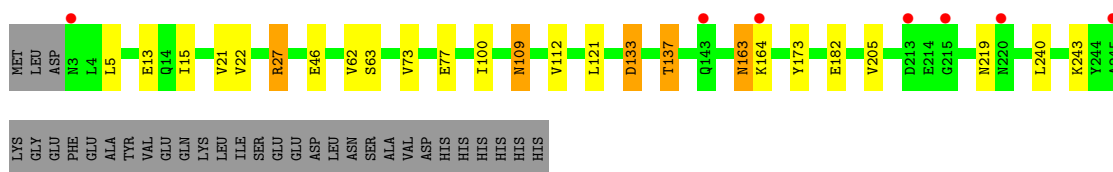
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	38	38	38	0	0
5	B	48	48	48	0	0
5	C	47	47	47	0	0
5	D	59	59	59	0	0
5	E	68	68	68	0	0
5	F	52	52	52	0	0

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.

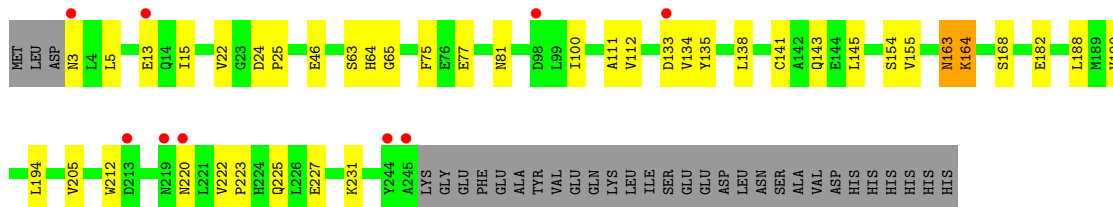
- Molecule 1: Purine nucleoside phosphorylase

Chain A: 




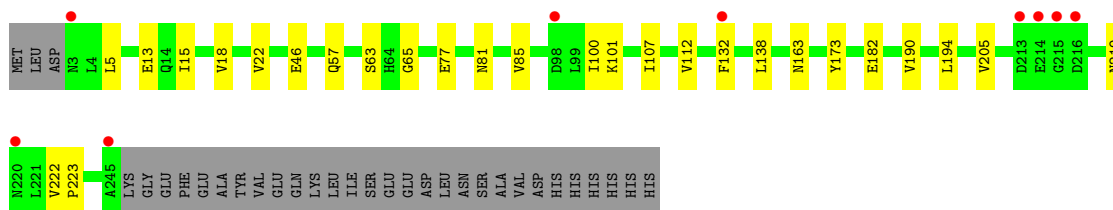
- Molecule 1: Purine nucleoside phosphorylase

Chain B: 




- Molecule 1: Purine nucleoside phosphorylase

Chain C: 



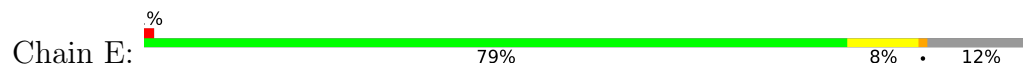
- Molecule 1: Purine nucleoside phosphorylase

Chain D: 



GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
ASN
ALA
VAL
ASP
HIS
HIS
HIS
HIS
HIS

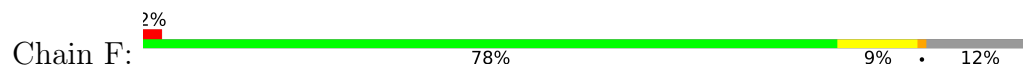
● Molecule 1: Purine nucleoside phosphorylase



MET LEU ASP N3 N4 L4 L5 I16 I18 V22 R27 V33 V38 E46 Y47 K48 Q57 K58 V62 S63 E77 N81 G90 R102 L121 M163 K164 F167 S168 E182 D216 V222 P223 A238 T242 A245 LYS GLU PHE GLU ALA TYR

VAL
GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
ASN
SER
ALA
VAL
ASP
HIS
HIS
HIS
HIS

● Molecule 1: Purine nucleoside phosphorylase



MET LEU ASP N3 N4 L4 L5 K12 E13 Q14 I15 V22 L41 E46 Q57 S63 H64 G65 E98 L99 I100 V112 V117 L121 F132 D133 S157 M163 S168 Y173 E182 M183 V205 C208 P209 D213 E214 V222 P223 A241

A245 LYS GLU PHE GLU ALA TYR VAL GLU LYS LEU ILE SER GLU ASP LEU ASN SER ALA VAL ASP HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.20Å 77.37Å 92.20Å 67.71° 73.62° 86.03°	Depositor
Resolution (Å)	20.00 – 2.00 19.92 – 1.99	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-2.00) 93.8 (19.92-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.99Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.235 0.198 , 0.236	Depositor DCC
R_{free} test set	4781 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11631	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, PO4, IM5

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	0.49	0/1893	0.59	1/2561 (0.0%)
1	B	0.51	0/1893	0.59	0/2561
1	C	0.51	0/1893	0.59	0/2561
1	D	0.53	0/1893	0.61	0/2561
1	E	0.54	0/1893	0.62	0/2561
1	F	0.49	0/1893	0.62	0/2561
All	All	0.51	0/11358	0.60	1/15366 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1861	0	1882	18	0
1	B	1861	0	1882	24	0
1	C	1861	0	1882	15	0
1	D	1861	0	1882	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1861	0	1882	17	0
1	F	1861	0	1882	16	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	2	0
3	F	5	0	0	0	0
4	A	20	0	17	0	0
4	B	20	0	17	1	0
4	C	20	0	17	0	0
4	D	20	0	17	0	0
4	E	20	0	17	0	0
4	F	20	0	17	0	0
5	A	38	0	0	2	0
5	B	48	0	0	0	0
5	C	47	0	0	2	0
5	D	59	0	0	1	0
5	E	68	0	0	2	0
5	F	52	0	0	0	0
All	All	11631	0	11394	97	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 4.

The worst 5 of 97 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:A:163:ASN:HD22	1:A:164:LYS:H	1.19	0.88
1:D:163:ASN:HD22	1:D:164:LYS:H	1.24	0.85
1:A:46:GLU:HB3	1:B:46:GLU:HB3	1.62	0.79
1:C:46:GLU:HB3	1:D:46:GLU:HB3	1.64	0.77
1:A:109:ASN:HD22	1:A:109:ASN:H	1.35	0.74

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	241/275 (88%)	233 (97%)	8 (3%)	0	100	100
1	B	241/275 (88%)	232 (96%)	9 (4%)	0	100	100
1	C	241/275 (88%)	234 (97%)	7 (3%)	0	100	100
1	D	241/275 (88%)	236 (98%)	5 (2%)	0	100	100
1	E	241/275 (88%)	235 (98%)	6 (2%)	0	100	100
1	F	241/275 (88%)	234 (97%)	7 (3%)	0	100	100
All	All	1446/1650 (88%)	1404 (97%)	42 (3%)	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	206/235 (88%)	199 (97%)	7 (3%)	37	36
1	B	206/235 (88%)	197 (96%)	9 (4%)	28	25
1	C	206/235 (88%)	202 (98%)	4 (2%)	57	61
1	D	206/235 (88%)	201 (98%)	5 (2%)	49	51
1	E	206/235 (88%)	201 (98%)	5 (2%)	49	51
1	F	206/235 (88%)	196 (95%)	10 (5%)	25	21
All	All	1236/1410 (88%)	1196 (97%)	40 (3%)	39	38

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	168	SER
1	F	117	VAL
1	E	182	GLU
1	F	15	ILE
1	F	133	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	163	ASN
1	E	151	ASN
1	E	57	GLN
1	E	163	ASN
1	B	57	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IM5	D	501	-	18,22,22	0.92	1 (5%)	18,32,32	2.08	3 (16%)
4	IM5	F	501	-	18,22,22	0.81	0	18,32,32	1.81	4 (22%)
4	IM5	C	501	-	18,22,22	0.88	0	18,32,32	1.98	4 (22%)
3	PO4	D	502	-	4,4,4	0.80	0	6,6,6	0.73	0
4	IM5	E	501	-	18,22,22	0.82	0	18,32,32	1.98	5 (27%)
3	PO4	C	502	-	4,4,4	0.83	0	6,6,6	0.51	0
3	PO4	E	502	-	4,4,4	0.77	0	6,6,6	0.69	0
3	PO4	A	502	-	4,4,4	0.82	0	6,6,6	0.52	0
3	PO4	B	502	-	4,4,4	0.83	0	6,6,6	0.47	0
3	PO4	F	502	-	4,4,4	0.76	0	6,6,6	0.38	0
4	IM5	B	501	-	18,22,22	0.77	0	18,32,32	1.91	5 (27%)
4	IM5	A	501	-	18,22,22	0.83	0	18,32,32	1.94	3 (16%)

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
4	IM5	D	501	-	-	2/5/18/18	0/3/3/3
4	IM5	F	501	-	-	2/5/18/18	0/3/3/3
4	IM5	C	501	-	-	4/5/18/18	0/3/3/3
4	IM5	E	501	-	-	2/5/18/18	0/3/3/3
4	IM5	B	501	-	-	2/5/18/18	0/3/3/3
4	IM5	A	501	-	-	2/5/18/18	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	IM5	C6-N1	-2.28	1.34	1.37

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	IM5	C9-C10-N1'	6.00	123.25	112.75
4	E	501	IM5	C9-C10-N1'	5.48	122.34	112.75
4	A	501	IM5	C9-C10-N1'	5.14	121.75	112.75
4	C	501	IM5	C9-C10-N1'	5.09	121.66	112.75
4	B	501	IM5	C9-C10-N1'	4.79	121.14	112.75

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

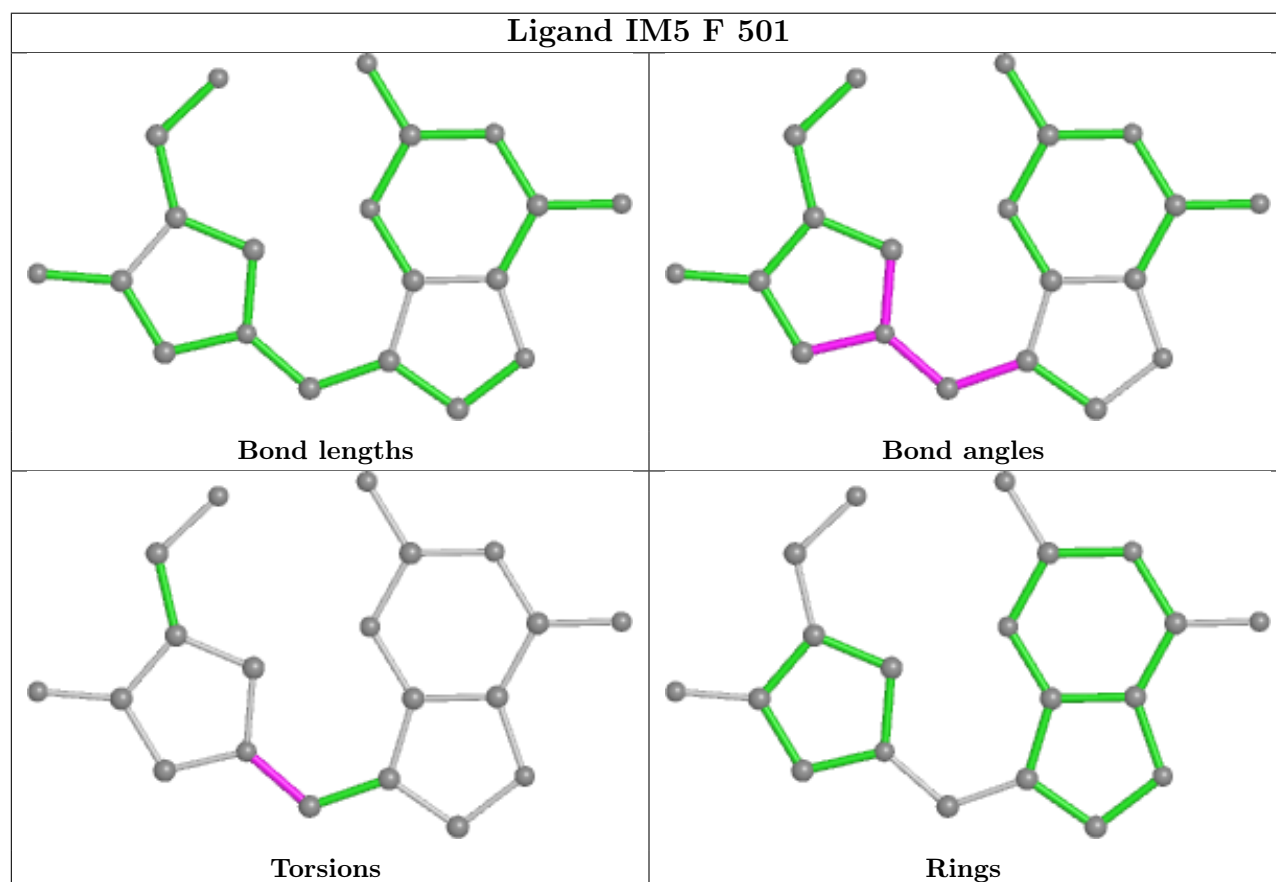
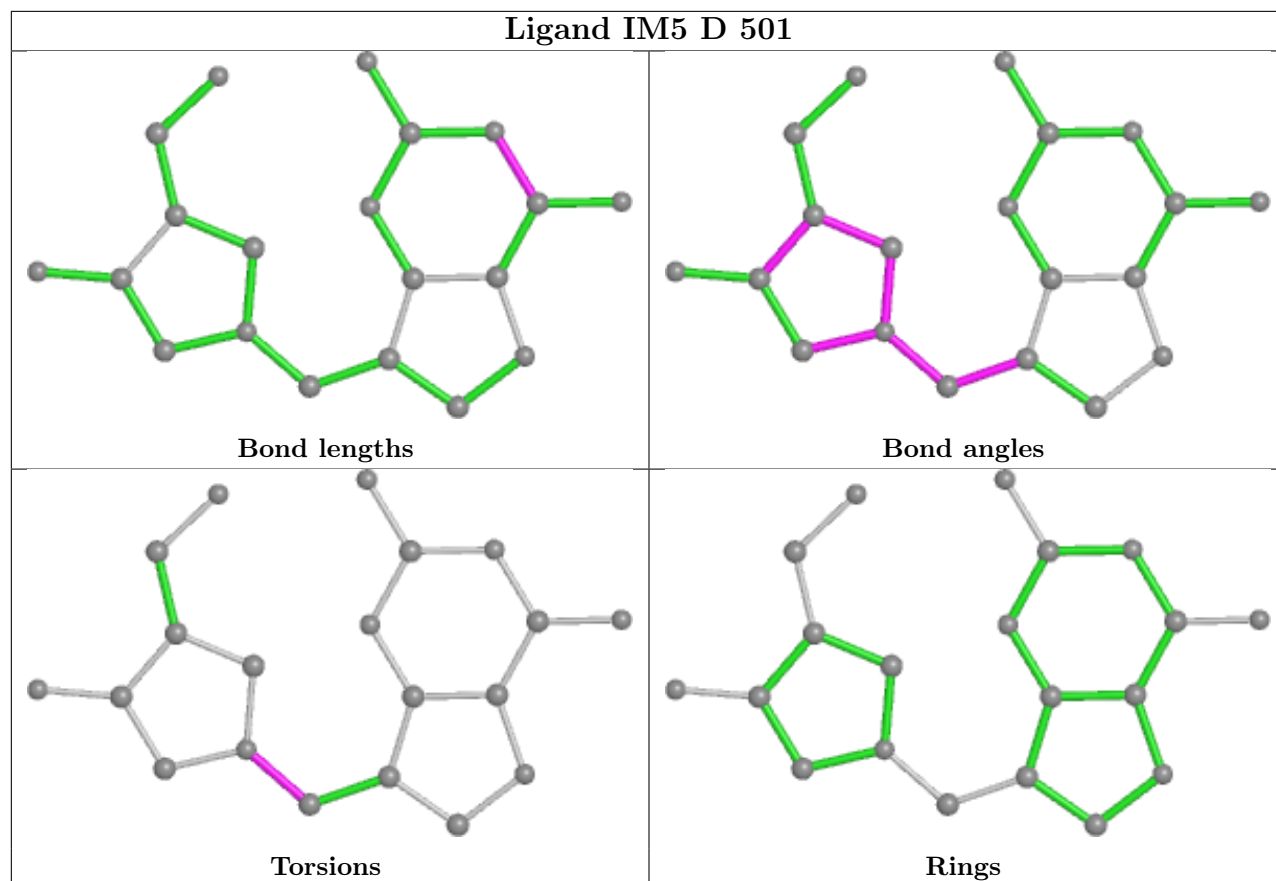
Mol	Chain	Res	Type	Atoms
4	A	501	IM5	C9-C10-N1'-C6'
4	B	501	IM5	C9-C10-N1'-C6'
4	C	501	IM5	C9-C10-N1'-C6'
4	C	501	IM5	C3'-C4'-C5'-O5'
4	C	501	IM5	C6'-C4'-C5'-O5'

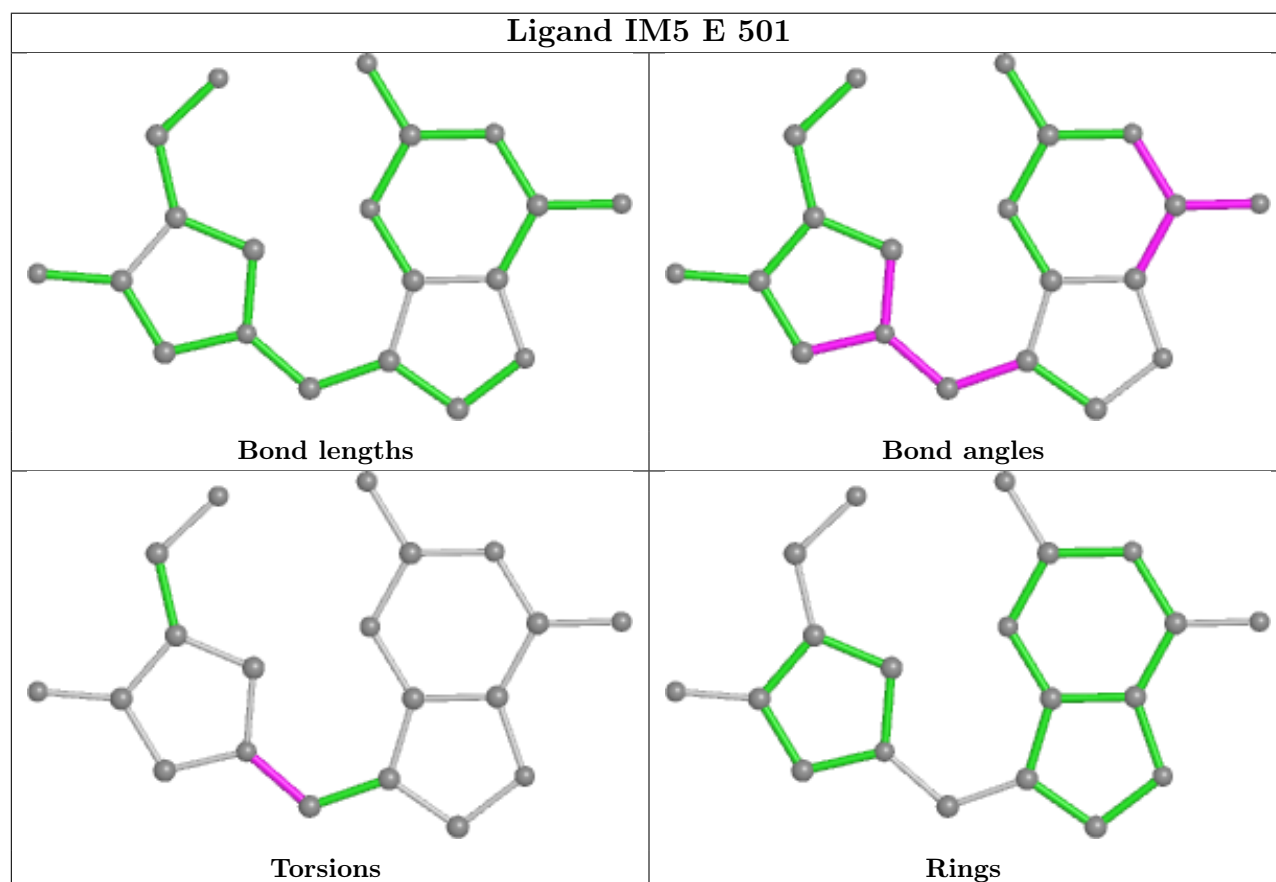
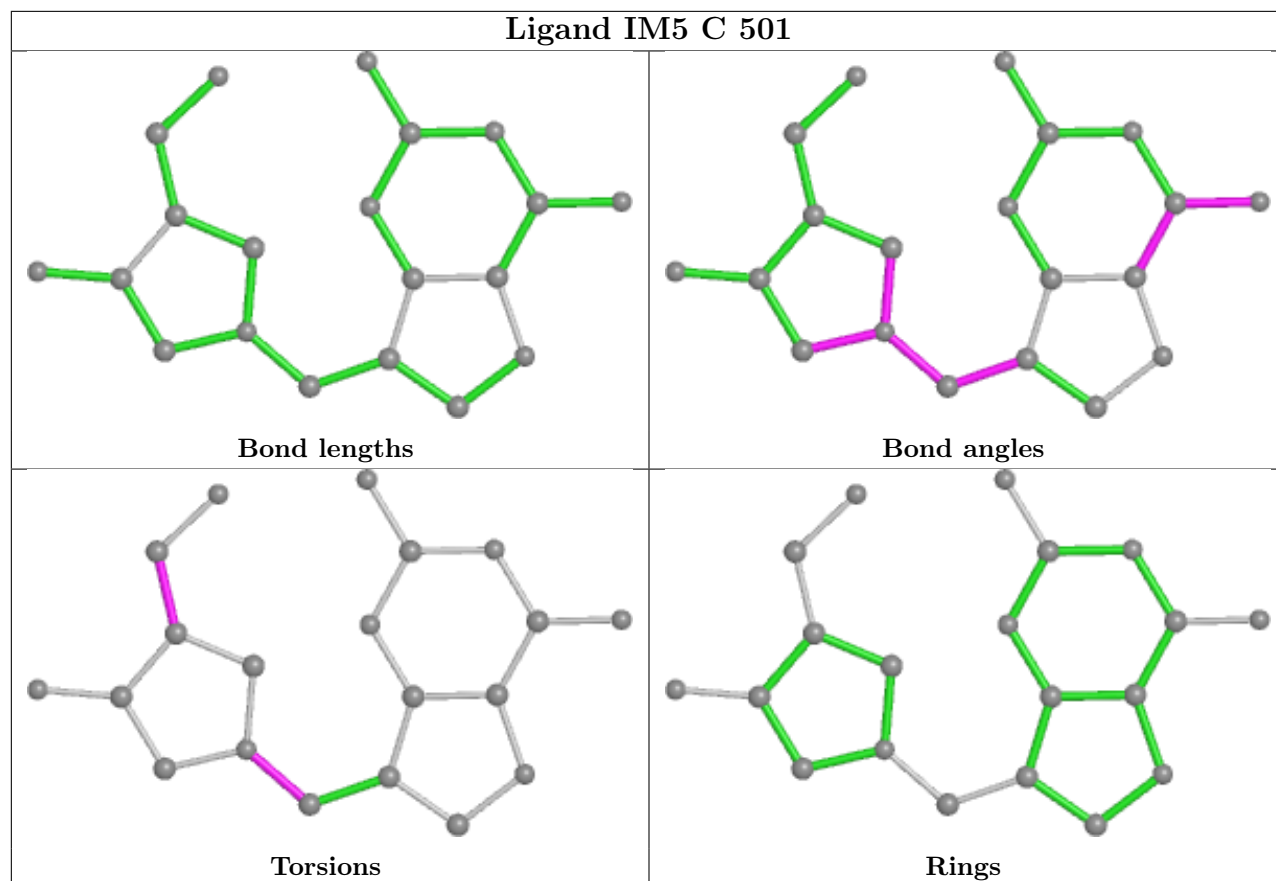
There are no ring outliers.

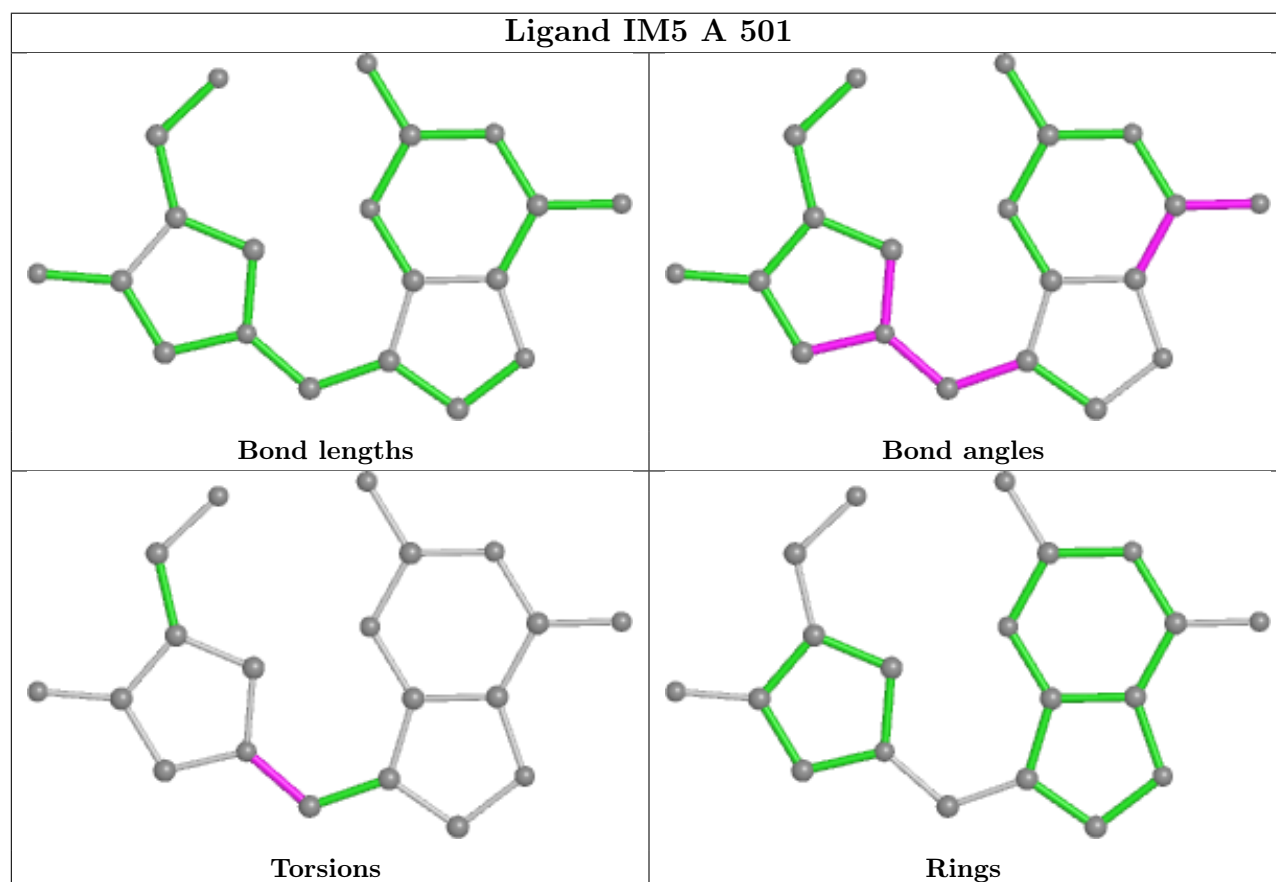
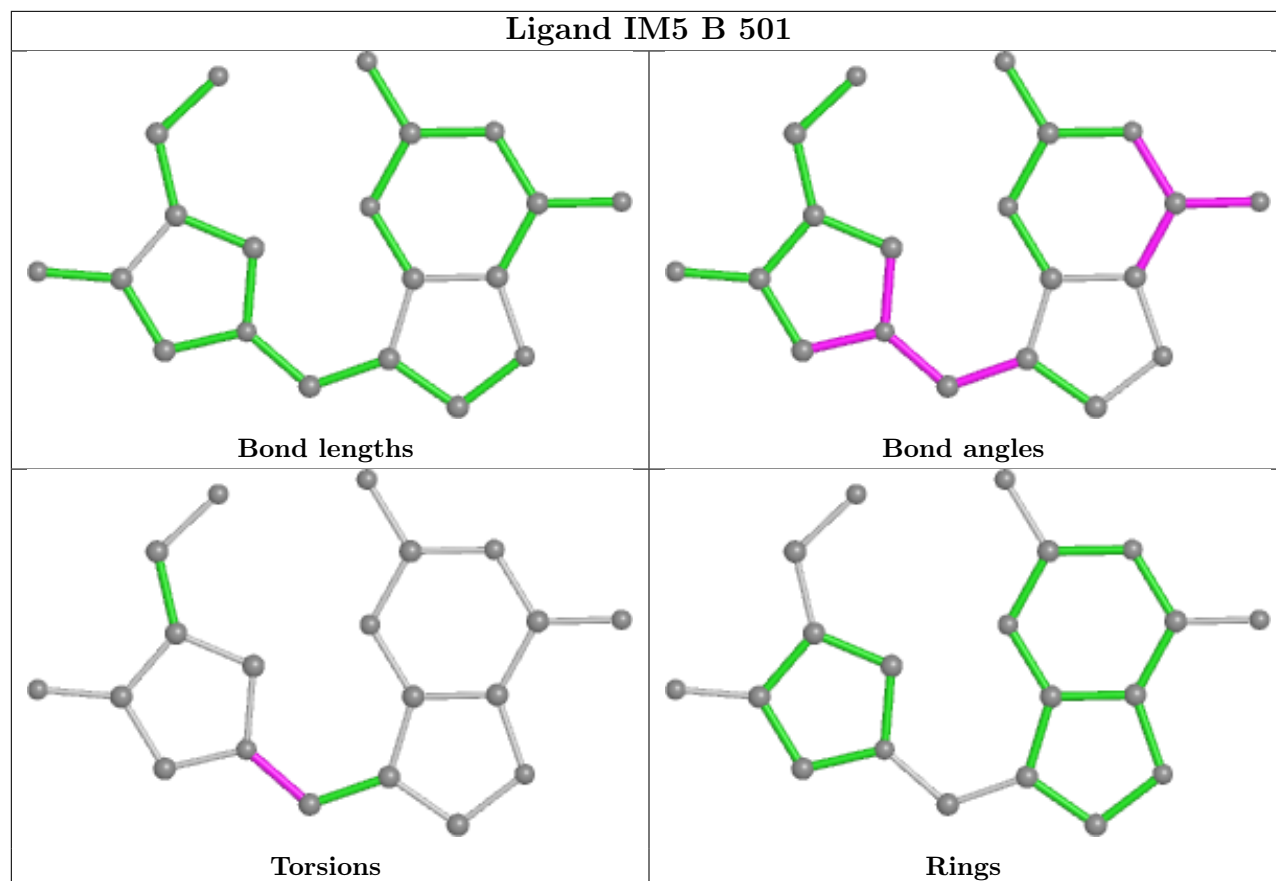
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	PO4	2	0
3	A	502	PO4	1	0
4	B	501	IM5	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.







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	243/275 (88%)	-0.01	7 (2%) 51 50	20, 31, 44, 50	0
1	B	243/275 (88%)	0.04	9 (3%) 41 41	19, 32, 46, 53	0
1	C	243/275 (88%)	-0.03	9 (3%) 41 41	20, 29, 44, 52	0
1	D	243/275 (88%)	-0.18	4 (1%) 72 70	18, 26, 38, 46	0
1	E	243/275 (88%)	-0.22	4 (1%) 72 70	18, 25, 35, 44	0
1	F	243/275 (88%)	-0.07	6 (2%) 57 56	19, 28, 42, 47	0
All	All	1458/1650 (88%)	-0.08	39 (2%) 54 53	18, 28, 43, 53	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	245	ALA	6.7
1	A	3	ASN	6.2
1	B	245	ALA	4.8
1	F	245	ALA	4.5
1	E	245	ALA	4.4

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

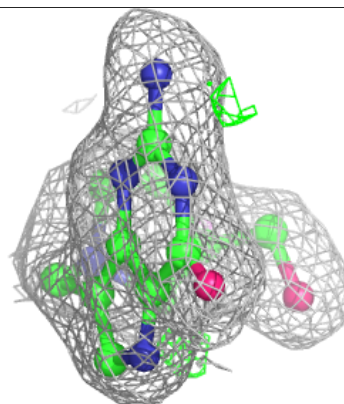
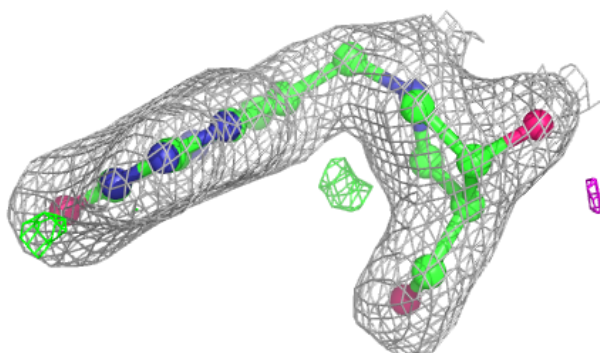
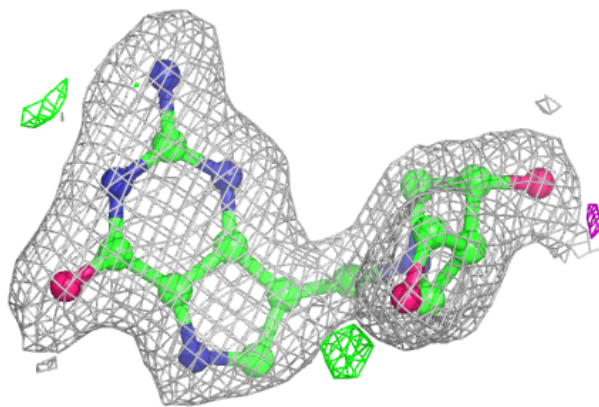
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IM5	A	501	20/20	0.92	0.10	27,31,32,32	0
4	IM5	B	501	20/20	0.92	0.10	29,32,35,37	0
4	IM5	C	501	20/20	0.92	0.12	26,28,31,32	0
4	IM5	D	501	20/20	0.93	0.12	25,28,31,32	0
4	IM5	E	501	20/20	0.93	0.12	20,22,25,28	0
4	IM5	F	501	20/20	0.93	0.12	25,28,29,30	0
3	PO4	A	502	5/5	0.97	0.08	33,34,35,36	0
3	PO4	C	502	5/5	0.97	0.08	30,31,33,33	0
3	PO4	E	502	5/5	0.98	0.07	22,22,23,24	0
3	PO4	F	502	5/5	0.98	0.07	28,29,31,32	0
3	PO4	B	502	5/5	0.98	0.06	37,38,39,39	0
3	PO4	D	502	5/5	0.98	0.07	27,28,29,29	0
2	K	A	275	1/1	0.99	0.03	29,29,29,29	0
2	K	E	275	1/1	0.99	0.04	24,24,24,24	0
2	K	C	275	1/1	1.00	0.02	28,28,28,28	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.

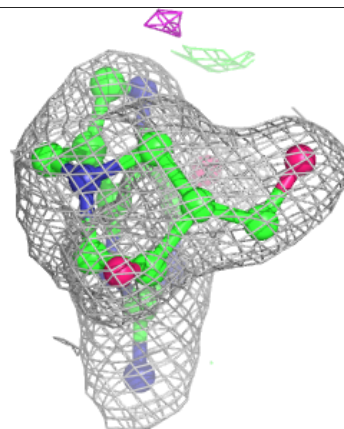
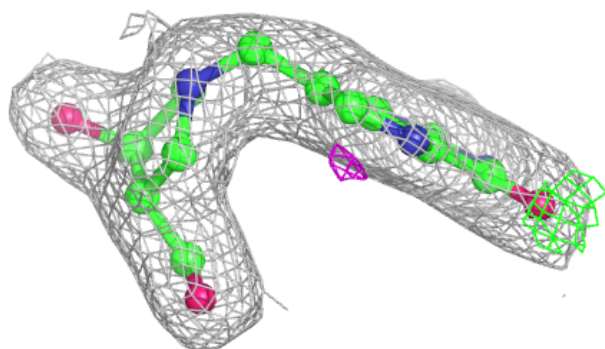
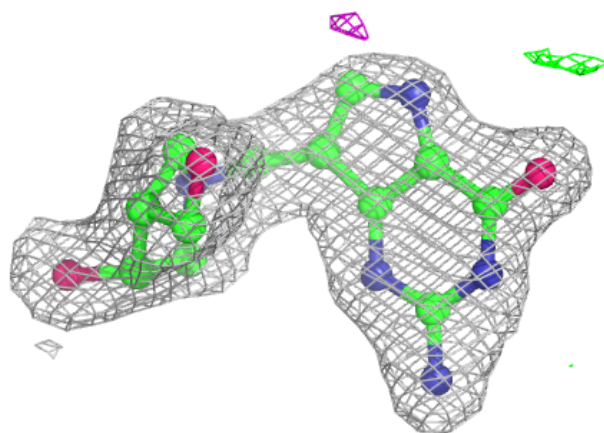
Electron density around IM5 A 501:

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



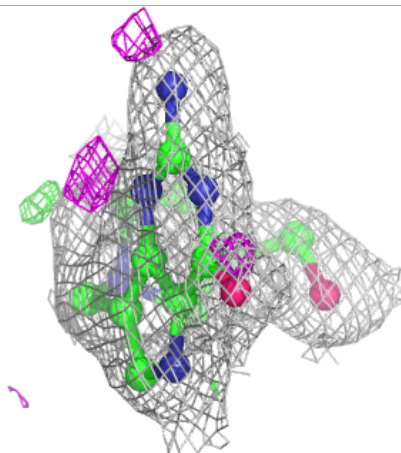
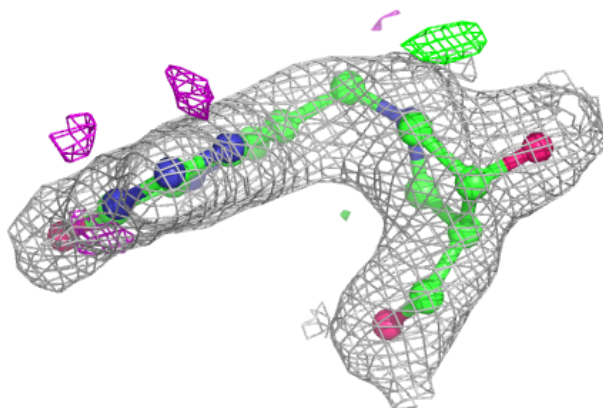
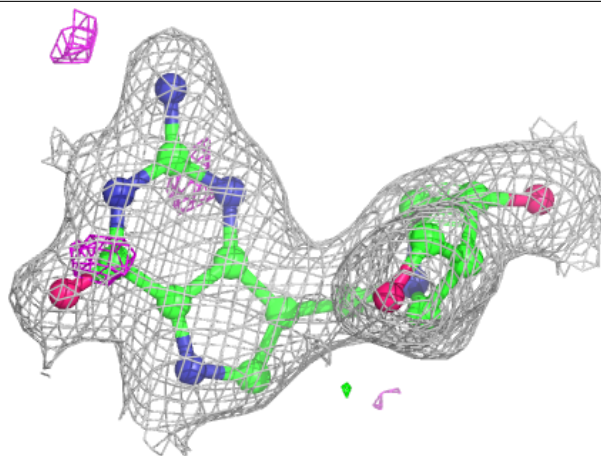
Electron density around IM5 B 501:

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



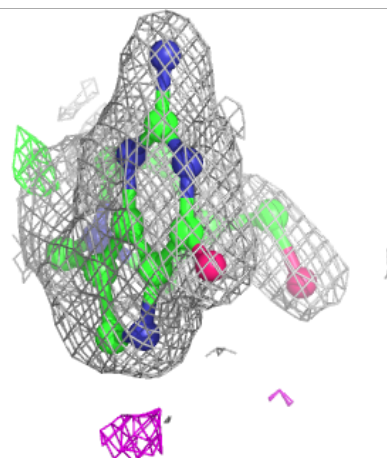
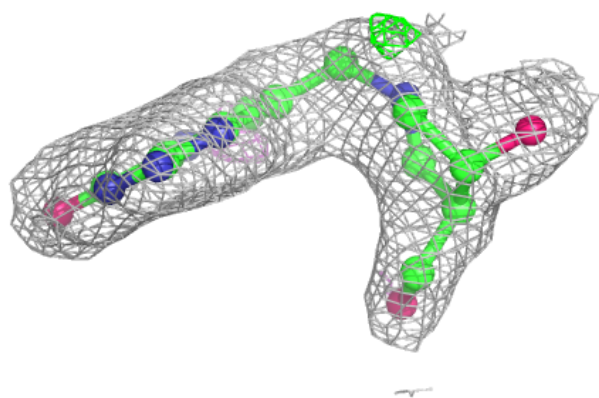
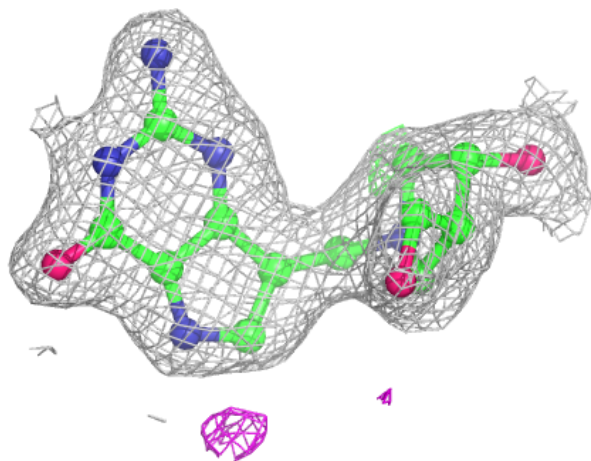
Electron density around IM5 C 501:

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



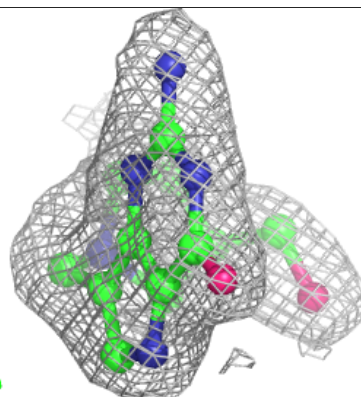
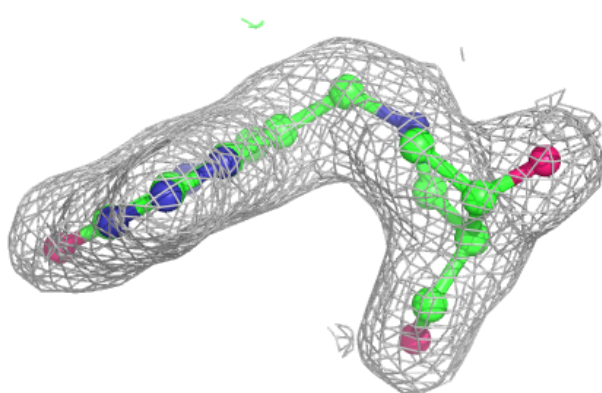
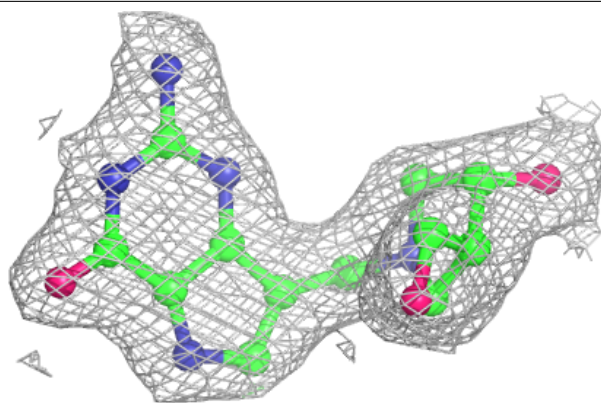
Electron density around IM5 D 501:

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

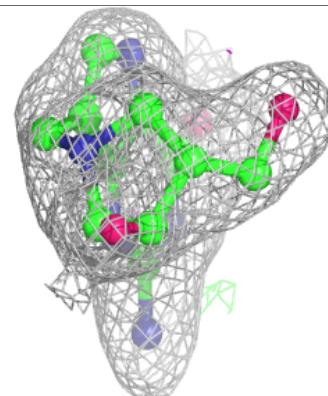
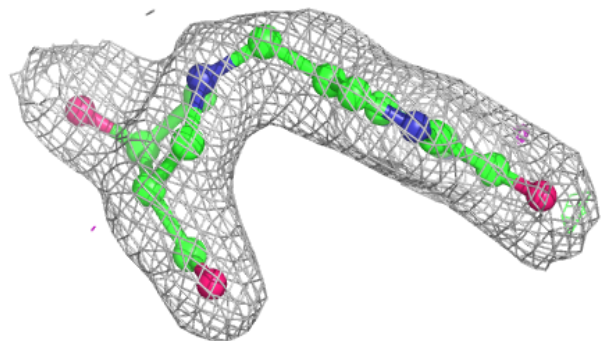
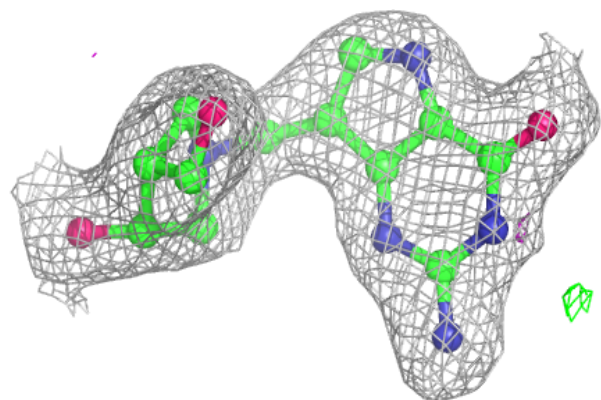


Electron density around IM5 E 501:

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

**Electron density around IM5 F 501:**

$2mF_o-DF_c$ (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.