



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:47 pm BST

PDB ID : 1QK4  
Title : TOXOPLASMA GONDII HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE IMP COMPLEX  
Authors : Heroux, A.; White, E.L.; Ross, L.J.; Borhani, D.W.  
Deposited on : 1999-07-09  
Resolution : 1.90 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](mailto: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.

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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 : 2.11  
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

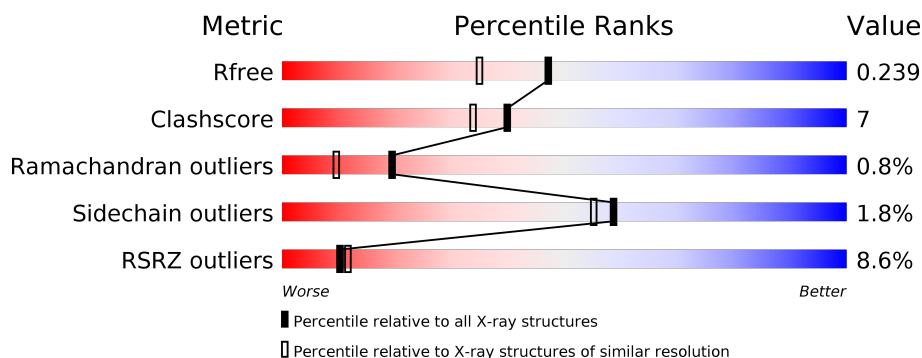
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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  $\geq 3$ , 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	233	<div> <div>7%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	233	<div> <div>12%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• •</div> </div> </div>
1	C	233	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>• • 9%</div> </div> </div>
1	D	233	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7683 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.

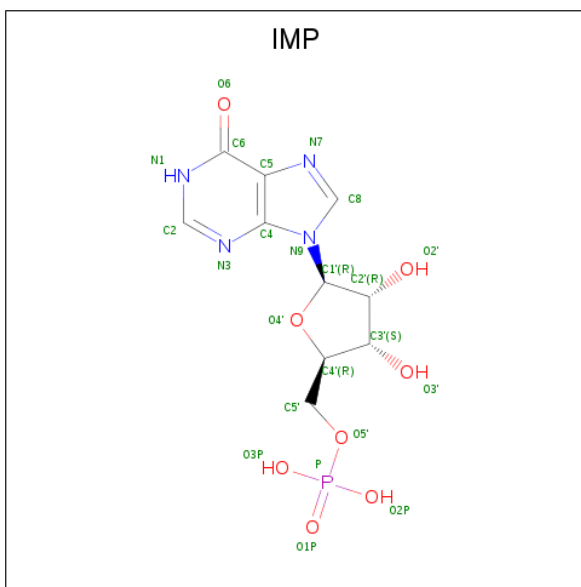
- Molecule 1 is a protein called HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1815	1173	301	333	8			
1	B	224	Total	C	N	O	S	0	2	0
			1807	1168	300	330	9			
1	C	213	Total	C	N	O	S	0	5	0
			1725	1117	282	319	7			
1	D	219	Total	C	N	O	S	0	3	0
			1759	1144	286	320	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0A	GLY	-	cloning artifact	UNP Q26997
A	0B	SER	-	cloning artifact	UNP Q26997
A	0C	HIS	-	cloning artifact	UNP Q26997
B	0A	GLY	-	cloning artifact	UNP Q26997
B	0B	SER	-	cloning artifact	UNP Q26997
B	0C	HIS	-	cloning artifact	UNP Q26997
C	0A	GLY	-	cloning artifact	UNP Q26997
C	0B	SER	-	cloning artifact	UNP Q26997
C	0C	HIS	-	cloning artifact	UNP Q26997
D	0A	GLY	-	cloning artifact	UNP Q26997
D	0B	SER	-	cloning artifact	UNP Q26997
D	0C	HIS	-	cloning artifact	UNP Q26997

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>4</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

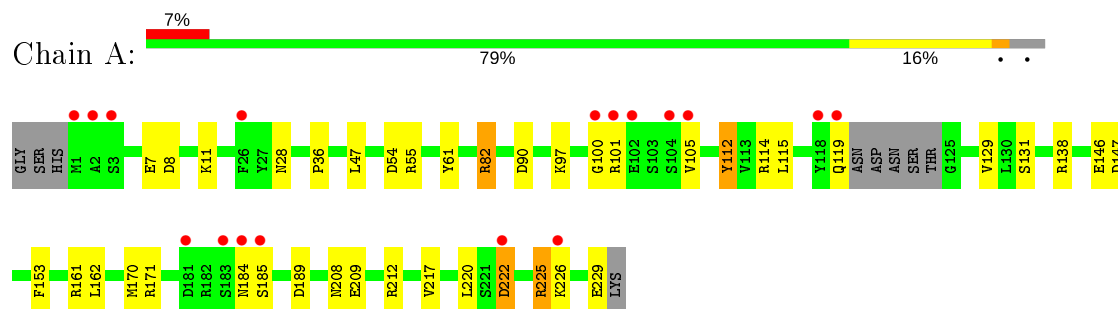
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	105	Total	O	0	0
			105	105		
3	C	135	Total	O	0	0
			135	135		
3	D	121	Total	O	0	0
			121	121		

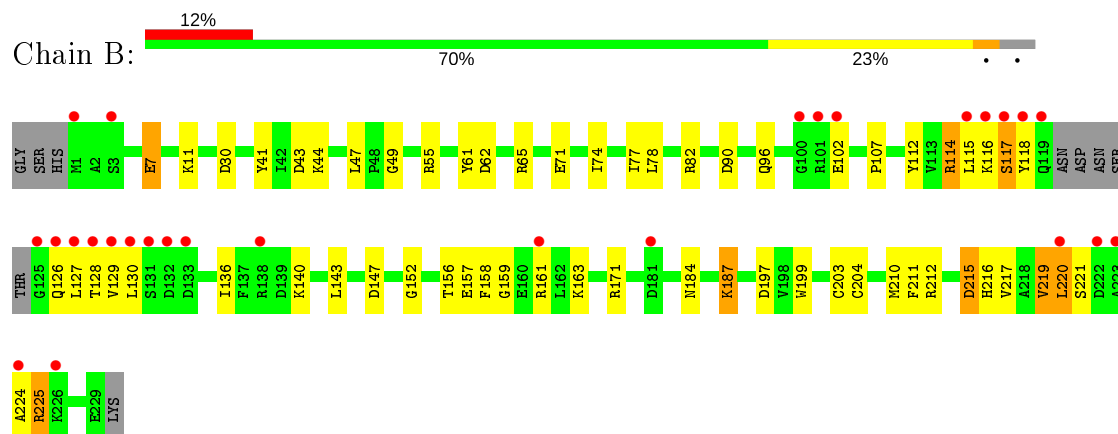
### 3 Residue-property plots [i](#)

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.

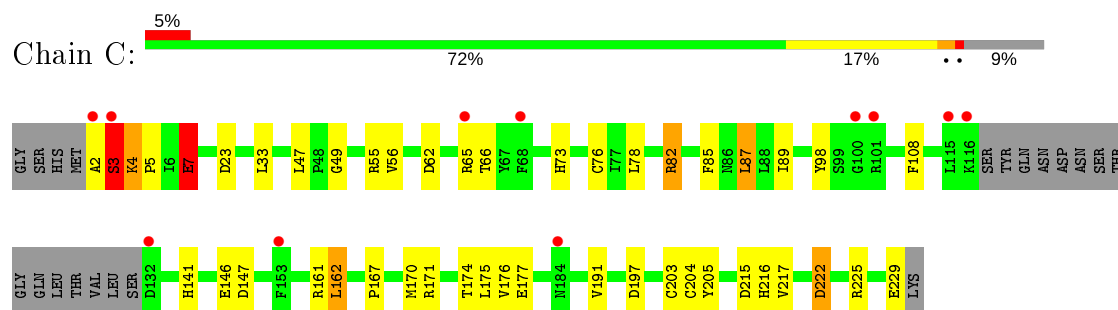
#### • Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE



#### • Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE

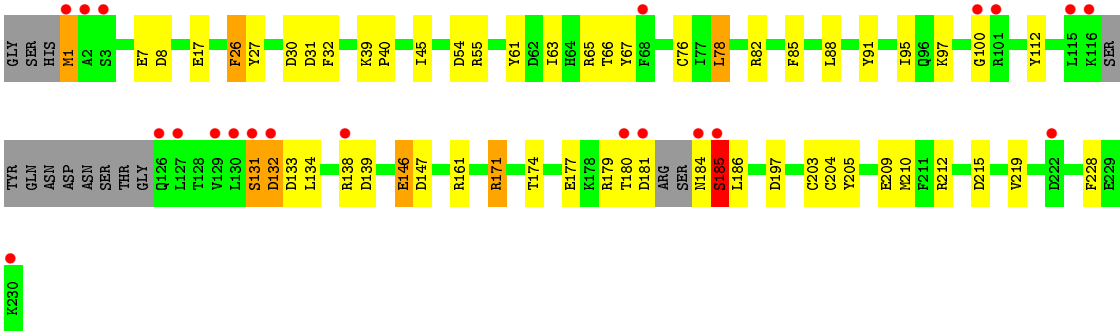


#### • Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE



#### • Molecule 1: HYPOXANTHINE-GUANINE PHOSPHORIBOSYLTRANSFERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.54Å 102.44Å 108.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.50 – 1.90 12.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (12.50-1.90) 100.0 (12.44-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.189 , 0.238 0.190 , 0.239	Depositor DCC
$R_{free}$ test set	3778 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 60.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IMP

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	0.71	0/1858	1.51	22/2505 (0.9%)
1	B	0.66	0/1860	1.64	30/2510 (1.2%)
1	C	0.75	0/1792	1.55	25/2422 (1.0%)
1	D	0.73	0/1818	1.60	38/2453 (1.5%)
All	All	0.71	0/7328	1.58	115/9890 (1.2%)

There are no bond length outliers.

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	ARG	NE-CZ-NH1	21.27	130.93	120.30
1	B	212	ARG	NE-CZ-NH2	17.26	128.93	120.30
1	C	3	SER	C-N-CA	15.26	159.85	121.70
1	C	161	ARG	NE-CZ-NH2	-14.05	113.28	120.30
1	B	55	ARG	NE-CZ-NH2	-13.43	113.58	120.30
1	B	65	ARG	CD-NE-CZ	13.03	141.84	123.60
1	A	138	ARG	NE-CZ-NH2	12.44	126.52	120.30
1	D	212	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	D	82	ARG	CD-NE-CZ	11.26	139.37	123.60
1	A	114	ARG	NE-CZ-NH2	-11.23	114.68	120.30
1	A	212	ARG	NE-CZ-NH2	10.61	125.61	120.30
1	A	222	ASP	CB-CG-OD1	10.57	127.81	118.30
1	D	161	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	55	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	138	ARG	NE-CZ-NH1	-9.79	115.41	120.30
1	D	138	ARG	CD-NE-CZ	9.70	137.18	123.60
1	B	55	ARG	CD-NE-CZ	9.68	137.15	123.60
1	D	55	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	55	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	D	65	ARG	NE-CZ-NH1	9.55	125.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ARG	CD-NE-CZ	9.54	136.96	123.60
1	D	205	TYR	CB-CG-CD1	8.87	126.32	121.00
1	A	114	ARG	NH1-CZ-NH2	8.60	128.86	119.40
1	B	90	ASP	CB-CG-OD1	8.41	125.87	118.30
1	C	147	ASP	CB-CG-OD1	8.27	125.74	118.30
1	D	146	GLU	OE1-CD-OE2	-8.13	113.54	123.30
1	D	205	TYR	CB-CG-CD2	-8.08	116.15	121.00
1	D	78	LEU	O-C-N	-8.06	109.80	122.70
1	B	78	LEU	O-C-N	-8.04	109.83	122.70
1	C	171	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	C	146	GLU	OE1-CD-OE2	7.81	132.67	123.30
1	A	114	ARG	NE-CZ-NH1	-7.69	116.45	120.30
1	A	82	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	D	55	ARG	CG-CD-NE	-7.52	96.01	111.80
1	D	185	SER	N-CA-C	7.50	131.26	111.00
1	B	65	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	62	ASP	CB-CG-OD1	7.37	124.93	118.30
1	C	205	TYR	CB-CG-CD1	-7.36	116.58	121.00
1	B	171	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	D	139	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	78	LEU	CA-C-N	7.25	133.16	117.20
1	B	225	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	26[A]	PHE	CB-CG-CD2	-7.23	115.74	120.80
1	D	26[B]	PHE	CB-CG-CD2	-7.23	115.74	120.80
1	A	112	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	A	147	ASP	CB-CG-OD2	7.07	124.66	118.30
1	C	4	LYS	N-CA-C	7.06	130.06	111.00
1	C	171	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	215	ASP	CB-CG-OD2	7.05	124.64	118.30
1	B	55	ARG	NH1-CZ-NH2	6.96	127.05	119.40
1	C	177	GLU	OE1-CD-OE2	6.89	131.57	123.30
1	B	171	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	147	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	171	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	55	ARG	CG-CD-NE	-6.52	98.10	111.80
1	C	4	LYS	N-CA-CB	-6.51	98.87	110.60
1	B	71	GLU	OE1-CD-OE2	6.38	130.96	123.30
1	A	171	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	30	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	D	17	GLU	OE1-CD-OE2	-6.28	115.76	123.30
1	B	65	ARG	NH1-CZ-NH2	-6.26	112.52	119.40
1	D	138	ARG	NE-CZ-NH1	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	179	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	C	98	TYR	CB-CG-CD2	6.23	124.74	121.00
1	A	55	ARG	CG-CD-NE	-6.19	98.81	111.80
1	B	212	ARG	NH1-CZ-NH2	-6.12	112.67	119.40
1	D	8	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	B	77	ILE	O-C-N	6.10	132.46	122.70
1	A	54	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	90	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	222	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	C	229	GLU	CA-C-O	-6.03	107.43	120.10
1	D	131	SER	N-CA-CB	-6.03	101.46	110.50
1	B	30	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	3	SER	O-C-N	-5.98	113.14	122.70
1	D	31	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	61	TYR	CB-CG-CD1	-5.91	117.45	121.00
1	D	185	SER	CA-C-O	5.88	132.44	120.10
1	D	27	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	A	82	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	C	7	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	B	114	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	C	3	SER	CA-C-O	5.81	132.29	120.10
1	A	61	TYR	CB-CG-CD1	-5.78	117.53	121.00
1	D	78	LEU	CA-C-N	5.78	129.90	117.20
1	D	65	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	215	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	C	222	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	197	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	147	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	209	GLU	OE1-CD-OE2	-5.52	116.67	123.30
1	B	197	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	C	82	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	26[A]	PHE	CB-CG-CD1	5.48	124.64	120.80
1	D	26[B]	PHE	CB-CG-CD1	5.48	124.64	120.80
1	D	215	ASP	CB-CG-OD1	-5.43	113.42	118.30
1	C	55	ARG	CG-CD-NE	-5.36	100.55	111.80
1	A	225	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	30	ASP	CB-CG-OD1	5.34	123.10	118.30
1	C	225	ARG	CD-NE-CZ	5.31	131.04	123.60
1	D	61	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	B	43	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	C	23	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	161	ARG	NH1-CZ-NH2	5.23	125.15	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	VAL	CA-CB-CG1	-5.22	103.07	110.90
1	D	65	ARG	CD-NE-CZ	5.21	130.89	123.60
1	A	189	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	D	54	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	82	ARG	CG-CD-NE	-5.12	101.05	111.80
1	C	62	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	176	VAL	CG1-CB-CG2	-5.10	102.74	110.90
1	A	212	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	B	90	ASP	OD1-CG-OD2	-5.06	113.69	123.30
1	C	73	HIS	CA-CB-CG	-5.05	105.01	113.60
1	C	161	ARG	NH1-CZ-NH2	5.04	124.94	119.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1815	0	1802	26	0
1	B	1807	0	1789	44	0
1	C	1725	0	1690	19	0
1	D	1759	0	1726	28	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	0	0
2	D	23	0	11	0	0
3	A	124	0	0	2	0
3	B	105	0	0	2	0
3	C	135	0	0	0	0
3	D	121	0	0	2	0
All	All	7683	0	7051	104	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 7.

All (104) 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:49:GLY:H	1:C:216:HIS:HD2	1.07	0.98
1:B:156[A]:THR:HG21	1:B:184:ASN:HD21	1.25	0.97
1:B:49:GLY:H	1:B:216:HIS:HD2	1.16	0.91
1:D:184:ASN:O	1:D:185:SER:HB2	1.72	0.90
1:B:220:LEU:HD23	1:B:225:ARG:HG2	1.55	0.86
1:B:156[A]:THR:HG21	1:B:184:ASN:ND2	1.90	0.86
1:C:49:GLY:H	1:C:216:HIS:CD2	1.93	0.83
1:D:210[A]:MET:HG3	1:D:228:PHE:CD2	2.18	0.79
1:B:49:GLY:H	1:B:216:HIS:CD2	2.01	0.78
1:B:156[A]:THR:CG2	1:B:184:ASN:HD21	1.97	0.78
1:C:7:GLU:H	1:C:7:GLU:CD	1.90	0.75
1:B:199:TRP:HD1	1:B:220:LEU:HD11	1.50	0.73
1:A:184:ASN:O	1:A:185:SER:HB2	1.91	0.70
1:D:180:THR:HG22	1:D:197:ASP:CG	2.12	0.69
1:B:127:LEU:HD23	1:B:161:ARG:HH22	1.58	0.69
1:A:100:GLY:H	1:D:100:GLY:H	1.39	0.68
1:D:131:SER:HB2	1:D:134:LEU:HD21	1.78	0.65
1:A:131:SER:HA	1:B:130:LEU:HD21	1.80	0.64
1:B:114:ARG:HB3	1:B:130:LEU:HB3	1.81	0.63
1:B:118:TYR:HB2	1:B:126:GLN:HG2	1.81	0.63
1:A:36:PRO:HG2	1:B:102:GLU:HB2	1.81	0.62
1:B:152:GLY:O	1:B:156[A]:THR:HG23	1.99	0.62
1:C:203:CYS:O	1:C:204:CYS:HB2	1.99	0.61
1:D:26[A]:PHE:CE2	1:D:219:VAL:HG21	2.36	0.61
1:B:158:PHE:HD1	1:B:161:ARG:HH21	1.48	0.59
1:B:115:LEU:HD22	1:B:127:LEU:HD21	1.84	0.59
1:C:76:CYS:HB2	1:C:85:PHE:CD1	2.39	0.58
1:B:117:SER:HA	1:B:127:LEU:HD12	1.85	0.58
1:B:136:ILE:O	1:B:140:LYS:HD2	2.05	0.57
1:B:161:ARG:HD3	3:B:2065:HOH:O	2.04	0.56
1:A:28:ASN:HB3	3:A:2020:HOH:O	2.06	0.55
1:B:115:LEU:CD2	1:B:129:VAL:HG22	2.37	0.55
1:D:177:GLU:HG3	3:D:2098:HOH:O	2.08	0.54
1:D:76:CYS:HB2	1:D:85:PHE:CD1	2.43	0.54
1:B:102:GLU:HB3	3:B:2050:HOH:O	2.06	0.54
1:A:184:ASN:O	1:A:185:SER:CB	2.57	0.53
1:B:74:ILE:HD12	1:B:143:LEU:HD23	1.90	0.52
1:C:82:ARG:HG3	1:D:112:TYR:OH	2.10	0.52
1:D:63:ILE:HD12	1:D:88:LEU:HD11	1.90	0.52
1:C:49:GLY:N	1:C:216:HIS:HD2	1.90	0.52
1:C:56:VAL:HG11	1:C:87:LEU:HB3	1.92	0.52
1:B:41:TYR:HB3	1:B:224:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162[B]:LEU:HD23	1:C:170:MET:HE3	1.92	0.50
1:A:131:SER:CA	1:B:130:LEU:HD21	2.41	0.50
1:B:199:TRP:O	1:B:220:LEU:HD13	2.12	0.50
1:B:11:LYS:O	1:B:187:LYS:HE3	2.12	0.49
1:A:7:GLU:H	1:A:7:GLU:CD	2.16	0.49
1:B:115:LEU:HD22	1:B:127:LEU:CD2	2.42	0.49
1:D:180:THR:HG22	1:D:197:ASP:OD2	2.12	0.49
1:D:32:PHE:CD2	1:D:45[B]:ILE:HD12	2.48	0.49
1:A:105:VAL:HG13	3:A:2040:HOH:O	2.13	0.48
1:A:82:ARG:HG3	1:B:112:TYR:OH	2.12	0.48
1:C:162[A]:LEU:HD12	1:C:167:PRO:HG3	1.95	0.48
1:A:119:GLN:NE2	1:A:153:PHE:HB2	2.29	0.48
1:A:208:ASN:O	1:A:209:GLU:HB2	2.14	0.48
1:C:3:SER:HG	1:C:141:HIS:CE1	2.31	0.47
1:B:47:LEU:HB2	1:B:217:VAL:HB	1.95	0.47
1:D:203:CYS:O	1:D:204:CYS:HB2	2.14	0.47
1:B:96:GLN:OE1	1:B:107:PRO:HD3	2.15	0.46
1:D:180:THR:O	1:D:181:ASP:C	2.53	0.46
1:A:119:GLN:HE21	1:A:153:PHE:HB2	1.81	0.45
1:A:8:ASP:HA	1:A:11:LYS:HD2	1.98	0.45
1:B:44:LYS:HB2	1:B:219:VAL:HG22	1.98	0.45
1:C:78:LEU:HD11	1:D:78:LEU:HD11	1.99	0.45
1:D:67:TYR:OH	1:D:171:ARG:HD2	2.17	0.45
1:B:115:LEU:HD23	1:B:129:VAL:HG22	1.99	0.45
1:A:112:TYR:OH	1:B:82:ARG:HG3	2.18	0.44
1:B:220:LEU:HD23	1:B:225:ARG:CG	2.37	0.44
1:D:76:CYS:HB2	1:D:85:PHE:CG	2.53	0.44
1:B:127:LEU:HD23	1:B:161:ARG:NH2	2.28	0.44
1:A:115:LEU:CD2	1:A:129:VAL:HG22	2.48	0.44
1:A:225:ARG:O	1:A:229:GLU:N	2.51	0.43
1:D:131:SER:O	1:D:132:ASP:C	2.57	0.43
1:B:210:MET:HG3	1:B:211:PHE:CD2	2.52	0.43
1:C:89:ILE:HB	1:C:108:PHE:CZ	2.53	0.43
1:C:47:LEU:HB2	1:C:217:VAL:HB	2.00	0.43
1:A:161:ARG:HH11	1:A:161:ARG:HG3	1.83	0.43
1:D:180:THR:HG21	3:D:2077:HOH:O	2.19	0.43
1:A:36:PRO:CG	1:B:102:GLU:HB2	2.47	0.43
1:D:186:LEU:HD23	1:D:186:LEU:C	2.39	0.43
1:C:215:ASP:OD1	1:D:97:LYS:NZ	2.47	0.42
1:B:7:GLU:H	1:B:7:GLU:HG3	1.41	0.42
1:C:2:ALA:HA	1:C:66:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:O	1:A:226:LYS:HG3	2.20	0.42
1:A:97:LYS:NZ	1:B:215:ASP:OD1	2.38	0.42
1:C:4:LYS:HA	1:C:5:PRO:HD3	1.88	0.42
1:A:220:LEU:HD21	1:A:225:ARG:HG2	2.02	0.42
1:B:116:LYS:HB2	1:B:128:THR:HB	2.01	0.42
1:D:1:MET:HB3	1:D:66:THR:O	2.19	0.42
1:C:174:THR:O	1:C:191:VAL:HA	2.21	0.41
1:A:47:LEU:HB2	1:A:217:VAL:HB	2.03	0.41
1:B:203:CYS:O	1:B:204[A]:CYS:HB2	2.21	0.41
1:B:199:TRP:CD1	1:B:220:LEU:HD11	2.41	0.41
1:D:91:TYR:O	1:D:95:ILE:HG13	2.21	0.41
1:A:162:LEU:HB3	1:A:170:MET:HE1	2.03	0.41
1:B:159:GLY:O	1:B:163:LYS:HG3	2.21	0.41
1:D:146:GLU:O	1:D:174:THR:HA	2.21	0.41
1:D:39:LYS:HB2	1:D:40:PRO:HD3	2.03	0.41
1:A:100:GLY:H	1:D:100:GLY:N	2.14	0.40
1:A:100:GLY:N	1:D:100:GLY:H	2.13	0.40
1:D:7:GLU:H	1:D:7:GLU:CD	2.23	0.40
1:B:129:VAL:HG23	1:B:161:ARG:NH1	2.37	0.40
1:C:76:CYS:HB2	1:C:85:PHE:CG	2.55	0.40
1:B:219:VAL:O	1:B:220:LEU:C	2.60	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	220/233 (94%)	212 (96%)	7 (3%)	1 (0%)	29	18
1	B	222/233 (95%)	213 (96%)	7 (3%)	2 (1%)	17	7
1	C	214/233 (92%)	211 (99%)	2 (1%)	1 (0%)	29	18
1	D	216/233 (93%)	210 (97%)	3 (1%)	3 (1%)	11	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	872/932 (94%)	846 (97%)	19 (2%)	7 (1%)	19	9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	220	LEU
1	B	221	SER
1	C	3	SER
1	D	132	ASP
1	D	133	ASP
1	D	185	SER
1	A	101	ARG

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/207 (96%)	198 (100%)	1 (0%)	88	89
1	B	198/207 (96%)	194 (98%)	4 (2%)	55	51
1	C	190/207 (92%)	182 (96%)	8 (4%)	30	20
1	D	191/207 (92%)	189 (99%)	2 (1%)	76	76
All	All	778/828 (94%)	763 (98%)	15 (2%)	59	53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	B	7	GLU
1	B	117	SER
1	B	157	GLU
1	B	187	LYS
1	C	7	GLU
1	C	33	LEU
1	C	65	ARG

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Mol	Chain	Res	Type
1	C	87	LEU
1	C	162[A]	LEU
1	C	162[B]	LEU
1	C	175	LEU
1	C	222	ASP
1	D	1	MET
1	D	185	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	B	216	HIS
1	C	24	ASN
1	C	96	GLN
1	C	184	ASN
1	C	216	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	IMP	A	300	-	21,25,25	1.58	3 (14%)	23,38,38	1.66	5 (21%)
2	IMP	B	300	-	21,25,25	1.58	3 (14%)	23,38,38	1.80	5 (21%)
2	IMP	C	300	-	21,25,25	1.42	4 (19%)	23,38,38	1.76	6 (26%)
2	IMP	D	300	-	21,25,25	1.48	3 (14%)	23,38,38	1.53	4 (17%)

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	IMP	A	300	-	-	3/6/26/26	0/3/3/3
2	IMP	B	300	-	-	2/6/26/26	0/3/3/3
2	IMP	C	300	-	-	0/6/26/26	0/3/3/3
2	IMP	D	300	-	-	5/6/26/26	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	IMP	C6-N1	5.23	1.42	1.33
2	C	300	IMP	C6-N1	3.96	1.39	1.33
2	D	300	IMP	C6-N1	3.94	1.39	1.33
2	B	300	IMP	C2-N1	3.90	1.41	1.33
2	B	300	IMP	C6-N1	3.62	1.39	1.33
2	C	300	IMP	C2-N1	3.16	1.39	1.33
2	D	300	IMP	O4'-C1'	3.06	1.45	1.41
2	B	300	IMP	O4'-C1'	3.06	1.45	1.41
2	D	300	IMP	C2-N1	2.79	1.39	1.33
2	A	300	IMP	C2-N1	2.68	1.38	1.33
2	A	300	IMP	C8-N7	-2.39	1.30	1.34
2	C	300	IMP	O4'-C1'	2.39	1.44	1.41
2	C	300	IMP	P-O2P	-2.01	1.47	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	IMP	C2-N1-C6	4.32	123.12	115.88
2	D	300	IMP	C2-N1-C6	4.31	123.10	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	IMP	C2-N1-C6	4.26	123.01	115.88
2	A	300	IMP	C2-N1-C6	4.15	122.83	115.88
2	A	300	IMP	N3-C2-N1	-3.36	123.42	128.68
2	B	300	IMP	N3-C2-N1	-3.12	123.80	128.68
2	B	300	IMP	O3P-P-O5'	-3.05	98.62	106.73
2	C	300	IMP	O4'-C1'-C2'	2.74	110.93	106.93
2	B	300	IMP	O3'-C3'-C2'	2.68	120.48	111.82
2	C	300	IMP	O5'-P-O1P	-2.50	99.47	106.47
2	D	300	IMP	O2'-C2'-C1'	2.50	120.08	110.85
2	C	300	IMP	C3'-C2'-C1'	2.36	104.53	100.98
2	C	300	IMP	C2'-C3'-C4'	2.32	107.16	102.64
2	D	300	IMP	C5'-C4'-C3'	-2.32	106.49	115.18
2	A	300	IMP	C1'-N9-C4	-2.26	122.67	126.64
2	C	300	IMP	O2'-C2'-C1'	2.21	119.03	110.85
2	A	300	IMP	C6-C5-C4	-2.17	118.73	120.80
2	B	300	IMP	C5'-C4'-C3'	-2.12	107.25	115.18
2	D	300	IMP	O4'-C4'-C5'	2.06	116.16	109.37
2	A	300	IMP	O4'-C4'-C5'	-2.05	102.62	109.37

There are no chirality outliers.

All (10) torsion outliers are listed below:

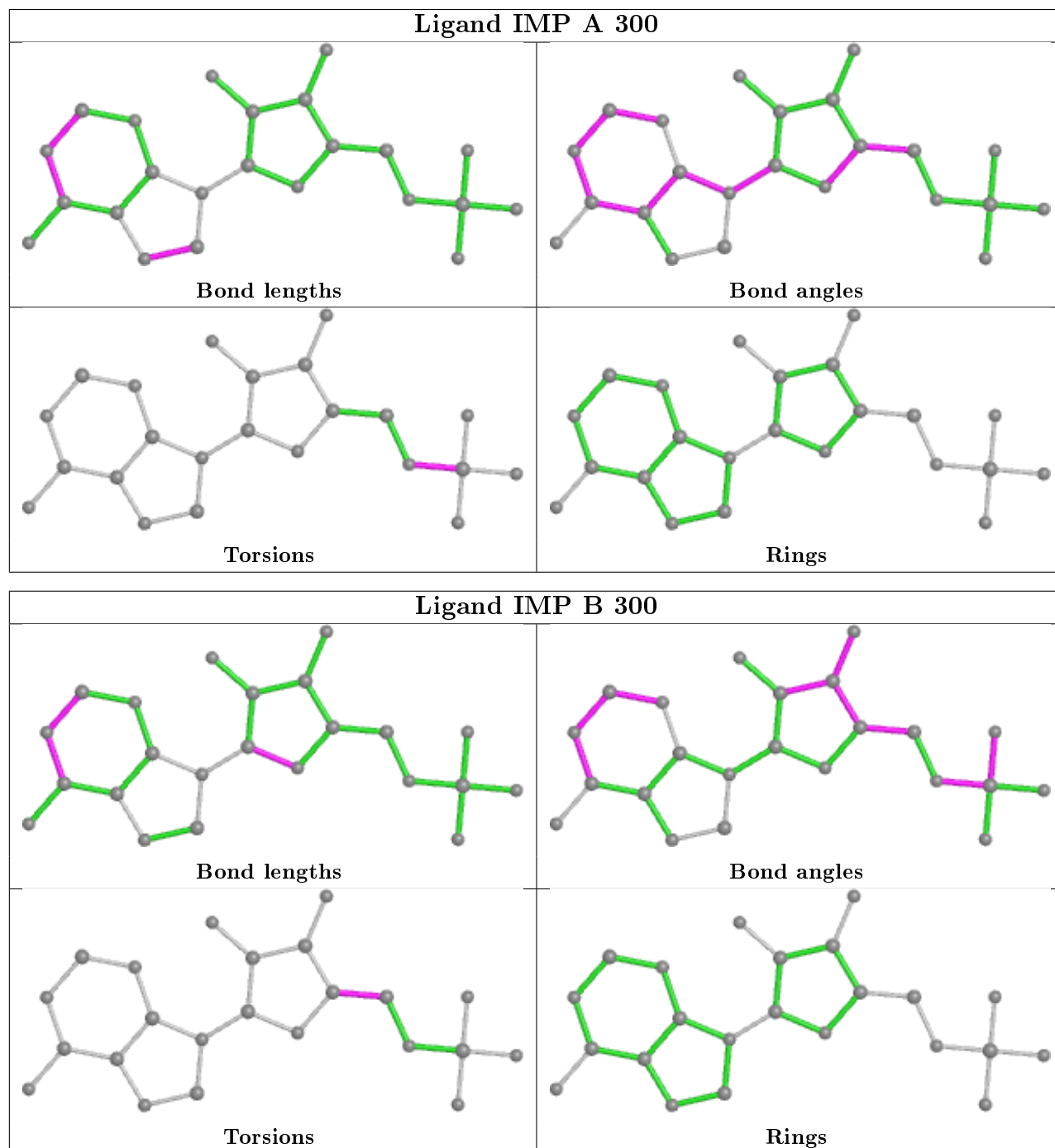
Mol	Chain	Res	Type	Atoms
2	A	300	IMP	C5'-O5'-P-O2P
2	A	300	IMP	C5'-O5'-P-O3P
2	B	300	IMP	O4'-C4'-C5'-O5'
2	B	300	IMP	C3'-C4'-C5'-O5'
2	D	300	IMP	C5'-O5'-P-O2P
2	D	300	IMP	C5'-O5'-P-O3P
2	D	300	IMP	O4'-C4'-C5'-O5'
2	D	300	IMP	C3'-C4'-C5'-O5'
2	A	300	IMP	C5'-O5'-P-O1P
2	D	300	IMP	C5'-O5'-P-O1P

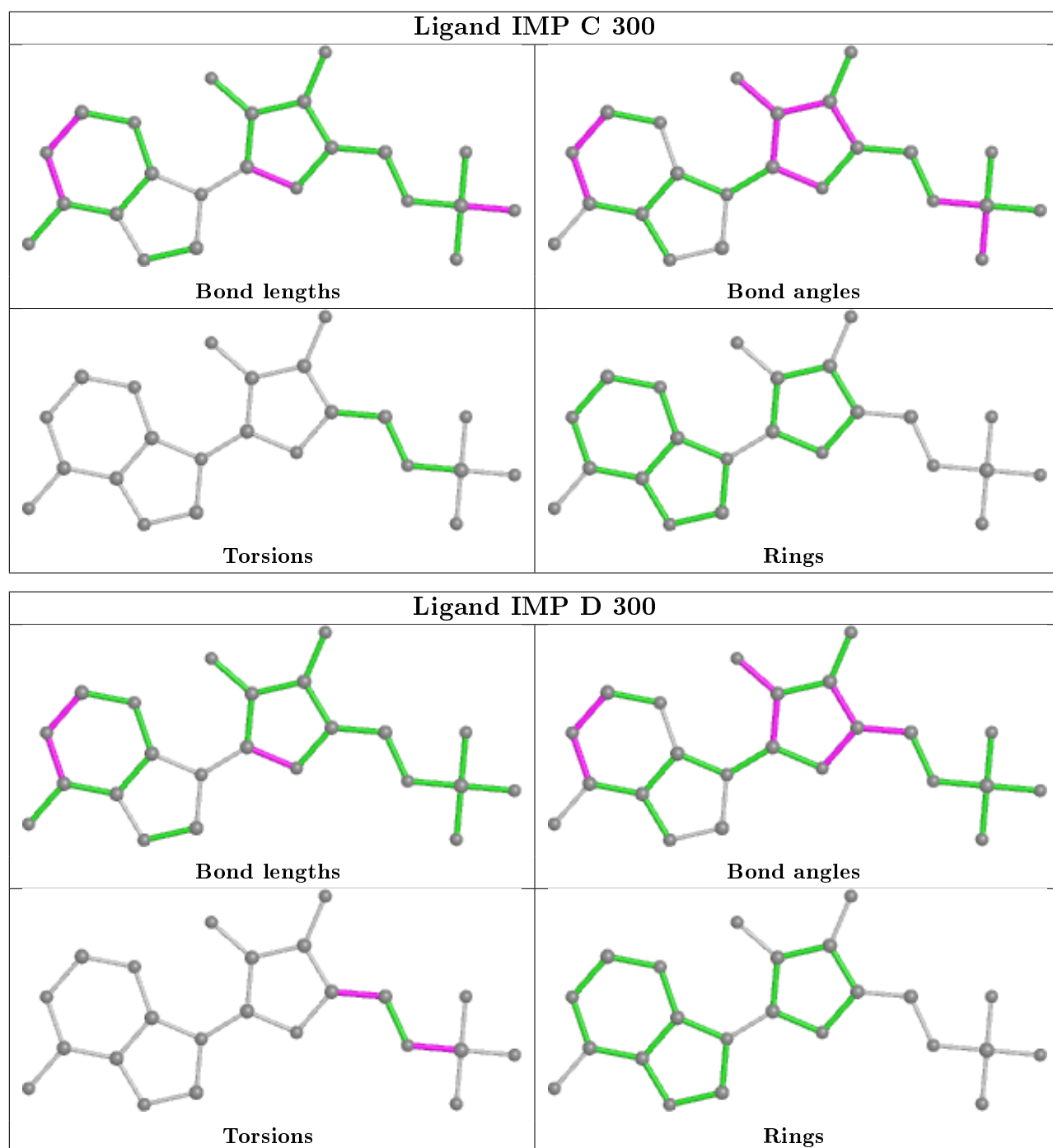
There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	224/233 (96%)	0.21	17 (7%) 13 15	11, 19, 46, 69	0
1	B	224/233 (96%)	0.51	27 (12%) 4 4	10, 22, 60, 72	0
1	C	213/233 (91%)	-0.04	11 (5%) 27 30	8, 16, 37, 63	0
1	D	219/233 (93%)	0.25	21 (9%) 8 9	10, 18, 45, 61	0
All	All	880/932 (94%)	0.24	76 (8%) 10 12	8, 19, 48, 72	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	ASN	14.3
1	B	118	TYR	7.9
1	B	223	ALA	7.4
1	B	130	LEU	7.1
1	C	115	LEU	6.6
1	B	127	LEU	6.4
1	A	1	MET	6.3
1	B	126	GLN	6.0
1	D	1	MET	5.8
1	B	100	GLY	5.7
1	B	132	ASP	5.3
1	A	118	TYR	5.2
1	B	119	GLN	5.1
1	A	183	SER	4.9
1	B	128	THR	4.8
1	B	131	SER	4.8
1	A	3	SER	4.8
1	A	184	ASN	4.6
1	B	129	VAL	4.6
1	A	101	ARG	4.6
1	D	116	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.1
1	D	101	ARG	4.0
1	C	3	SER	4.0
1	C	100	GLY	3.9
1	C	116	LYS	3.8
1	B	220	LEU	3.7
1	B	222	ASP	3.6
1	D	132	ASP	3.5
1	D	115	LEU	3.5
1	D	130	LEU	3.5
1	D	185	SER	3.5
1	D	2	ALA	3.5
1	A	181	ASP	3.4
1	A	185	SER	3.4
1	B	116	LYS	3.4
1	A	100	GLY	3.4
1	D	68	PHE	3.3
1	A	105	VAL	3.3
1	C	101	ARG	3.3
1	C	2	ALA	3.3
1	D	181	ASP	3.2
1	D	131	SER	3.2
1	B	117	SER	3.1
1	A	104	SER	3.1
1	B	133	ASP	3.0
1	D	3	SER	3.0
1	B	101	ARG	2.9
1	A	26	PHE	2.9
1	C	132	ASP	2.8
1	D	230	LYS	2.8
1	B	181	ASP	2.7
1	D	222	ASP	2.7
1	B	125	GLY	2.7
1	A	2	ALA	2.7
1	D	126	GLN	2.6
1	A	119	GLN	2.6
1	B	224	ALA	2.6
1	A	102	GLU	2.6
1	B	115	LEU	2.5
1	C	65	ARG	2.5
1	A	222	ASP	2.4
1	B	161	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	153	PHE	2.4
1	B	102	GLU	2.4
1	D	127	LEU	2.4
1	C	68	PHE	2.3
1	D	180	THR	2.3
1	A	226	LYS	2.2
1	C	184	ASN	2.2
1	B	3	SER	2.2
1	D	138	ARG	2.2
1	D	100	GLY	2.1
1	D	129	VAL	2.1
1	B	226	LYS	2.1
1	B	138	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

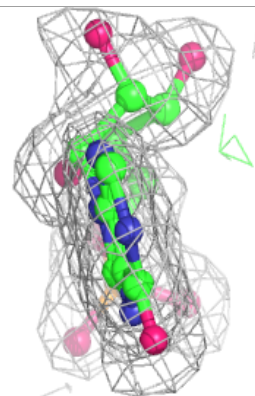
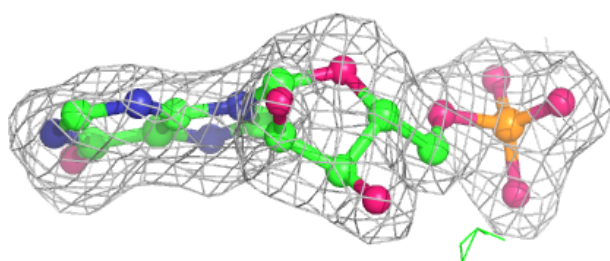
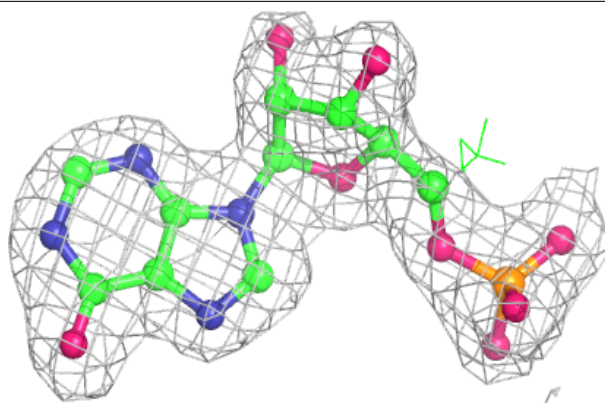
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	IMP	B	300	23/23	0.95	0.11	16,23,27,33	0
2	IMP	D	300	23/23	0.96	0.11	13,20,27,28	0
2	IMP	C	300	23/23	0.97	0.08	12,16,24,30	0
2	IMP	A	300	23/23	0.97	0.10	15,18,25,25	0

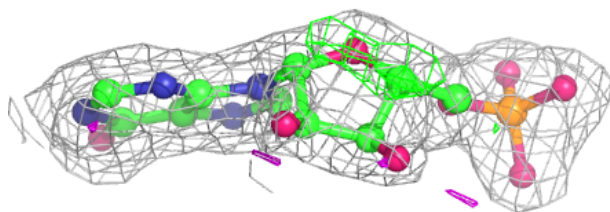
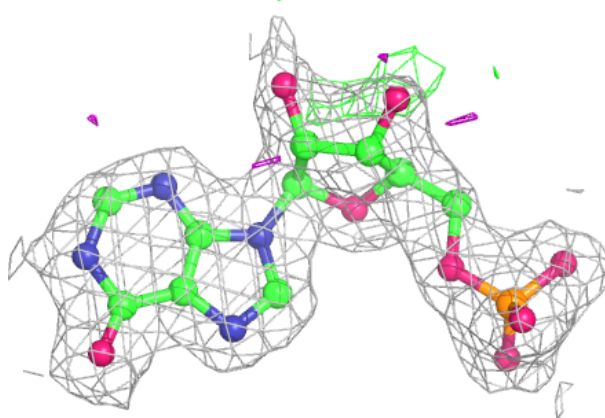
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around IMP B 300:**

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

**Electron density around IMP D 300:**

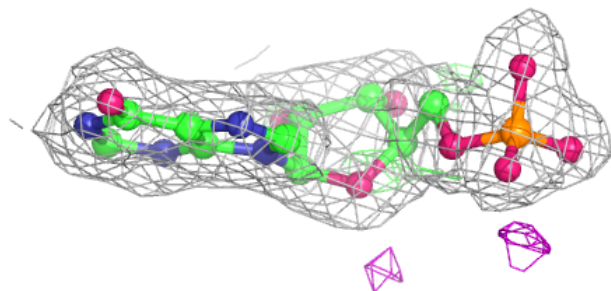
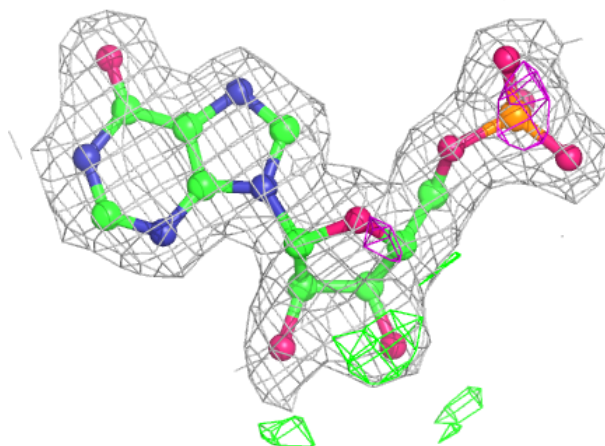
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

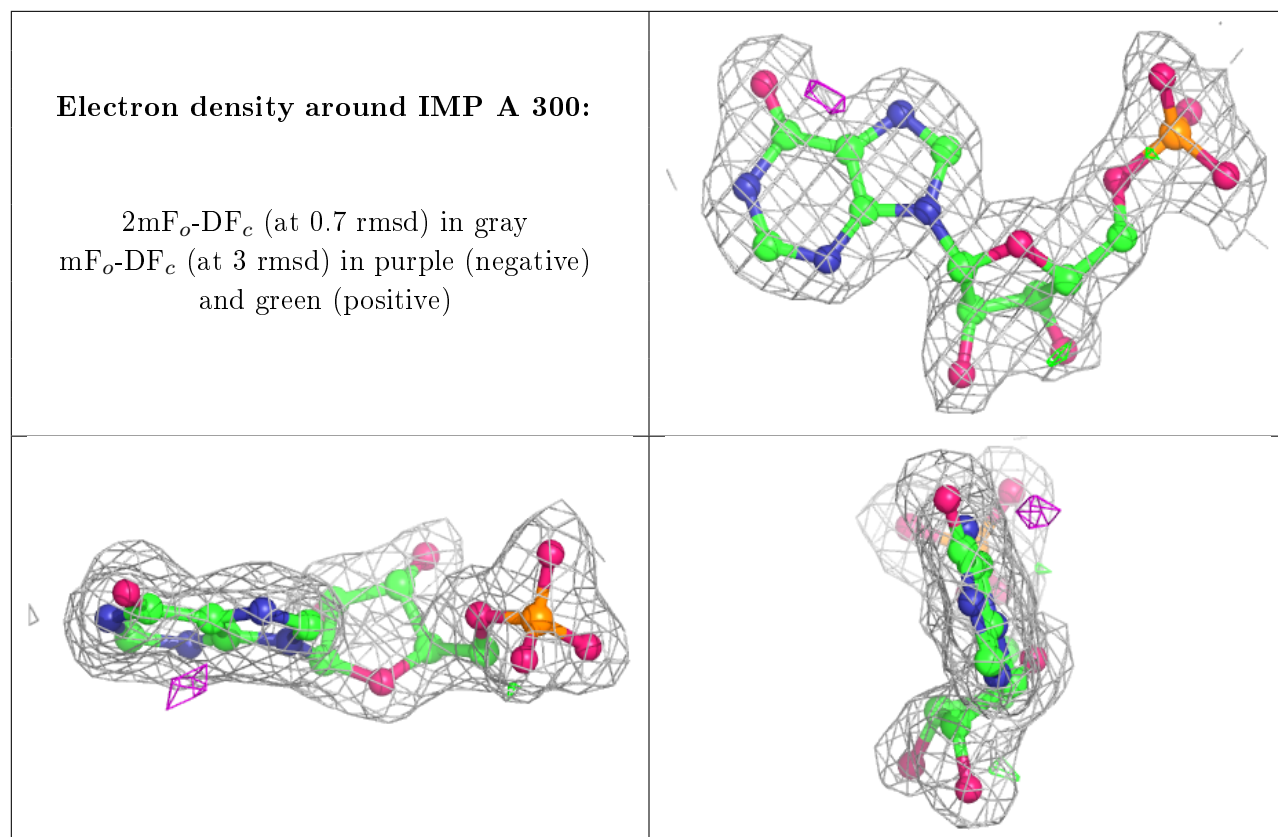




**Electron density around IMP C 300:**

$2mF_o-DF_c$  (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.