



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:49 AM UTC

PDB ID : 4EAR / pdb\_00004ear  
Title : Crystal structure of purine nucleoside phosphorylase (W16Y, W94Y, W178Y, H257W) mutant from human complexed with DADMe-ImmG and phosphate  
Authors : Haapalainen, A.M.; Ho, M.C.; Suarez, J.J.; Almo, S.C.; Schramm, V.L.  
Deposited on : 2012-03-22  
Resolution : 1.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

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

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

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

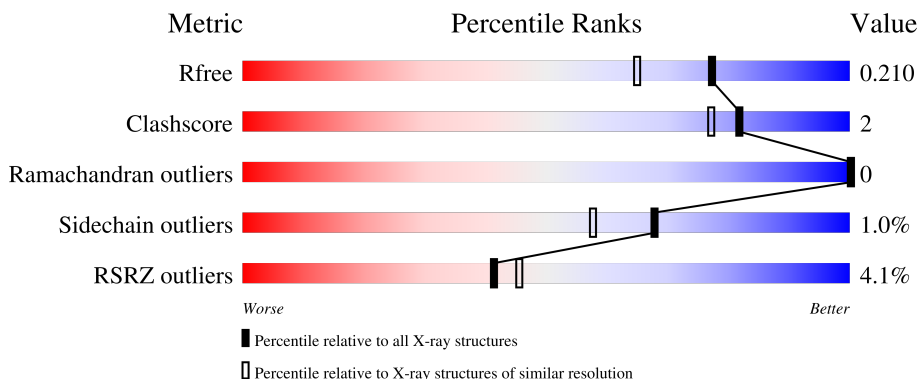
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	324	 3% 82% 5% 13%
1	B	324	 3% 84% 5% 11%
1	C	324	 5% 82% 5% 12%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7404 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	F	N	O	S			
1	A	283	2245	1428	1	392	408	16	0	6	0
1	B	287	2257	1434	1	392	415	15	0	3	0
1	C	285	2248	1431	1	389	411	16	0	5	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	expression tag	UNP P00491
A	-33	ARG	-	expression tag	UNP P00491
A	-32	GLY	-	expression tag	UNP P00491
A	-31	SER	-	expression tag	UNP P00491
A	-30	HIS	-	expression tag	UNP P00491
A	-29	HIS	-	expression tag	UNP P00491
A	-28	HIS	-	expression tag	UNP P00491
A	-27	HIS	-	expression tag	UNP P00491
A	-26	HIS	-	expression tag	UNP P00491
A	-25	HIS	-	expression tag	UNP P00491
A	-24	GLY	-	expression tag	UNP P00491
A	-23	MET	-	expression tag	UNP P00491
A	-22	ALA	-	expression tag	UNP P00491
A	-21	SER	-	expression tag	UNP P00491
A	-20	MET	-	expression tag	UNP P00491
A	-19	THR	-	expression tag	UNP P00491
A	-18	GLY	-	expression tag	UNP P00491
A	-17	GLY	-	expression tag	UNP P00491
A	-16	GLN	-	expression tag	UNP P00491
A	-15	GLN	-	expression tag	UNP P00491
A	-14	MET	-	expression tag	UNP P00491
A	-13	GLY	-	expression tag	UNP P00491
A	-12	ARG	-	expression tag	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	ASP	-	expression tag	UNP P00491
A	-10	LEU	-	expression tag	UNP P00491
A	-9	TYR	-	expression tag	UNP P00491
A	-8	ASP	-	expression tag	UNP P00491
A	-7	ASP	-	expression tag	UNP P00491
A	-6	ASP	-	expression tag	UNP P00491
A	-5	ASP	-	expression tag	UNP P00491
A	-4	LYS	-	expression tag	UNP P00491
A	-3	ASP	-	expression tag	UNP P00491
A	-2	PRO	-	expression tag	UNP P00491
A	-1	THR	-	expression tag	UNP P00491
A	0	LEU	-	expression tag	UNP P00491
A	16	TYR	TRP	engineered mutation	UNP P00491
A	51	SER	GLY	engineered mutation	UNP P00491
A	94	TYR	TRP	engineered mutation	UNP P00491
A	178	TYR	TRP	engineered mutation	UNP P00491
A	257	FT6	HIS	engineered mutation	UNP P00491
B	-34	MET	-	expression tag	UNP P00491
B	-33	ARG	-	expression tag	UNP P00491
B	-32	GLY	-	expression tag	UNP P00491
B	-31	SER	-	expression tag	UNP P00491
B	-30	HIS	-	expression tag	UNP P00491
B	-29	HIS	-	expression tag	UNP P00491
B	-28	HIS	-	expression tag	UNP P00491
B	-27	HIS	-	expression tag	UNP P00491
B	-26	HIS	-	expression tag	UNP P00491
B	-25	HIS	-	expression tag	UNP P00491
B	-24	GLY	-	expression tag	UNP P00491
B	-23	MET	-	expression tag	UNP P00491
B	-22	ALA	-	expression tag	UNP P00491
B	-21	SER	-	expression tag	UNP P00491
B	-20	MET	-	expression tag	UNP P00491
B	-19	THR	-	expression tag	UNP P00491
B	-18	GLY	-	expression tag	UNP P00491
B	-17	GLY	-	expression tag	UNP P00491
B	-16	GLN	-	expression tag	UNP P00491
B	-15	GLN	-	expression tag	UNP P00491
B	-14	MET	-	expression tag	UNP P00491
B	-13	GLY	-	expression tag	UNP P00491
B	-12	ARG	-	expression tag	UNP P00491
B	-11	ASP	-	expression tag	UNP P00491
B	-10	LEU	-	expression tag	UNP P00491

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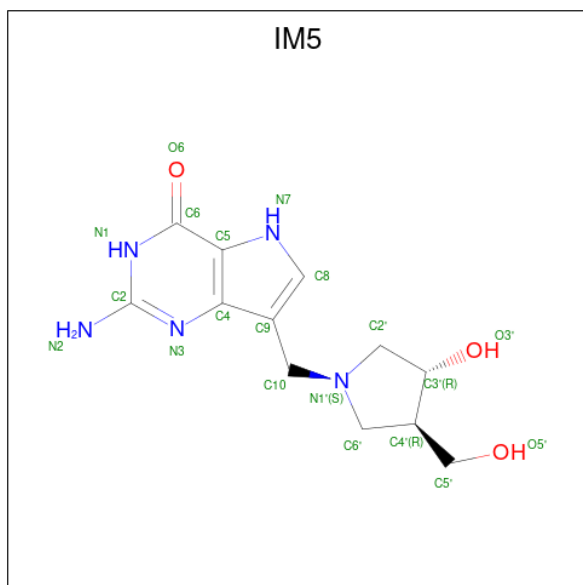
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	TYR	-	expression tag	UNP P00491
B	-8	ASP	-	expression tag	UNP P00491
B	-7	ASP	-	expression tag	UNP P00491
B	-6	ASP	-	expression tag	UNP P00491
B	-5	ASP	-	expression tag	UNP P00491
B	-4	LYS	-	expression tag	UNP P00491
B	-3	ASP	-	expression tag	UNP P00491
B	-2	PRO	-	expression tag	UNP P00491
B	-1	THR	-	expression tag	UNP P00491
B	0	LEU	-	expression tag	UNP P00491
B	16	TYR	TRP	engineered mutation	UNP P00491
B	51	SER	GLY	engineered mutation	UNP P00491
B	94	TYR	TRP	engineered mutation	UNP P00491
B	178	TYR	TRP	engineered mutation	UNP P00491
B	257	FT6	HIS	engineered mutation	UNP P00491
C	-34	MET	-	expression tag	UNP P00491
C	-33	ARG	-	expression tag	UNP P00491
C	-32	GLY	-	expression tag	UNP P00491
C	-31	SER	-	expression tag	UNP P00491
C	-30	HIS	-	expression tag	UNP P00491
C	-29	HIS	-	expression tag	UNP P00491
C	-28	HIS	-	expression tag	UNP P00491
C	-27	HIS	-	expression tag	UNP P00491
C	-26	HIS	-	expression tag	UNP P00491
C	-25	HIS	-	expression tag	UNP P00491
C	-24	GLY	-	expression tag	UNP P00491
C	-23	MET	-	expression tag	UNP P00491
C	-22	ALA	-	expression tag	UNP P00491
C	-21	SER	-	expression tag	UNP P00491
C	-20	MET	-	expression tag	UNP P00491
C	-19	THR	-	expression tag	UNP P00491
C	-18	GLY	-	expression tag	UNP P00491
C	-17	GLY	-	expression tag	UNP P00491
C	-16	GLN	-	expression tag	UNP P00491
C	-15	GLN	-	expression tag	UNP P00491
C	-14	MET	-	expression tag	UNP P00491
C	-13	GLY	-	expression tag	UNP P00491
C	-12	ARG	-	expression tag	UNP P00491
C	-11	ASP	-	expression tag	UNP P00491
C	-10	LEU	-	expression tag	UNP P00491
C	-9	TYR	-	expression tag	UNP P00491
C	-8	ASP	-	expression tag	UNP P00491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ASP	-	expression tag	UNP P00491
C	-6	ASP	-	expression tag	UNP P00491
C	-5	ASP	-	expression tag	UNP P00491
C	-4	LYS	-	expression tag	UNP P00491
C	-3	ASP	-	expression tag	UNP P00491
C	-2	PRO	-	expression tag	UNP P00491
C	-1	THR	-	expression tag	UNP P00491
C	0	LEU	-	expression tag	UNP P00491
C	16	TYR	TRP	engineered mutation	UNP P00491
C	51	SER	GLY	engineered mutation	UNP P00491
C	94	TYR	TRP	engineered mutation	UNP P00491
C	178	TYR	TRP	engineered mutation	UNP P00491
C	257	FT6	HIS	engineered mutation	UNP P00491

- Molecule 2 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 (CCD ID: IM5) (formula: C<sub>12</sub>H<sub>17</sub>N<sub>5</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
2	A	1	Total	C	N	O	0	0
			20	12	5	3		
2	B	1	Total	C	N	O	0	0
			20	12	5	3		
2	C	1	Total	C	N	O	0	0
			20	12	5	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

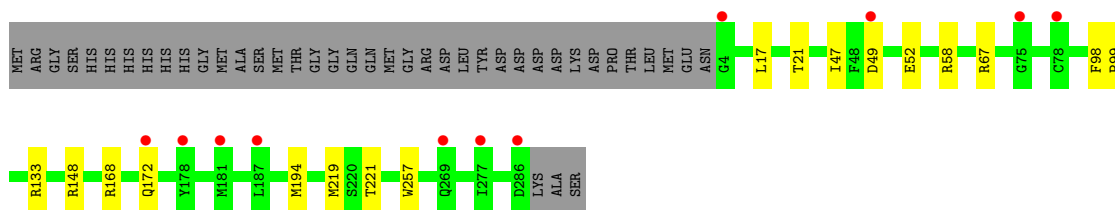
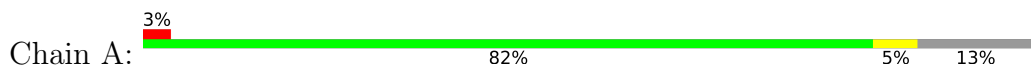
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	182	Total O 184 184	0	2
4	B	192	Total O 194 194	0	2
4	C	200	Total O 201 201	0	1

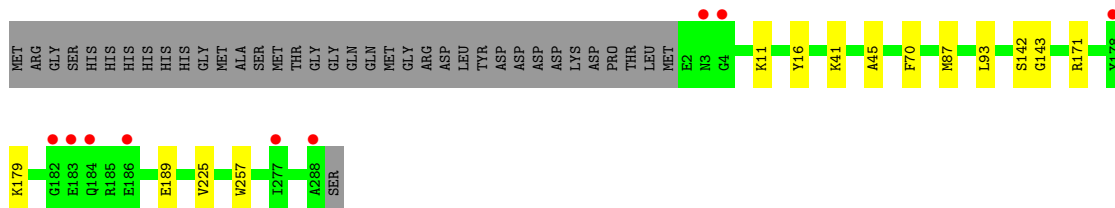
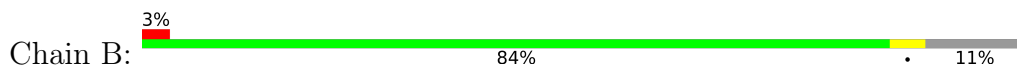
### 3 Residue-property plots [i](#)

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.

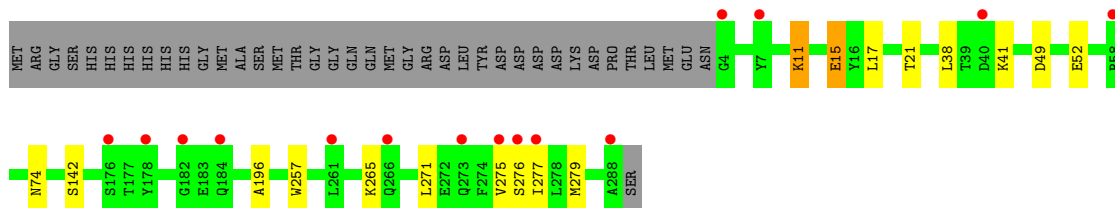
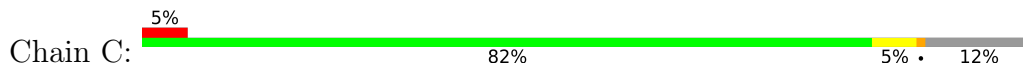
- Molecule 1: Purine nucleoside phosphorylase



- Molecule 1: Purine nucleoside phosphorylase



- Molecule 1: Purine nucleoside phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.92Å 131.10Å 137.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.24 – 1.70 41.24 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (41.24-1.70) 98.3 (41.24-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.175 , 0.203 0.184 , 0.210	Depositor DCC
$R_{free}$ test set	5592 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtrriage
Anisotropy	0.705	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.005 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IM5, FT6, PO4

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	0.74	0/2295	0.87	2/3099 (0.1%)
1	B	0.70	0/2298	0.85	1/3104 (0.0%)
1	C	0.72	0/2295	0.83	0/3099
All	All	0.72	0/6888	0.85	3/9302 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	VAL	N-CA-C	5.87	116.61	110.62
1	A	221	THR	CA-C-N	5.08	123.44	120.24
1	A	221	THR	C-N-CA	5.08	123.44	120.24

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	2245	0	2240	11	0
1	B	2257	0	2239	15	0
1	C	2248	0	2241	10	0
2	A	20	0	17	0	0
2	B	20	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	17	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	184	0	0	6	0
4	B	194	0	0	1	0
4	C	201	0	0	0	0
All	All	7404	0	6771	34	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (34) 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:B:171[B]:ARG:HH11	1:B:171[B]:ARG:HG2	1.20	1.06
1:B:171[B]:ARG:HH11	1:B:171[B]:ARG:CG	1.75	0.99
1:A:58[A]:ARG:HG2	4:A:419:HOH:O	1.77	0.83
1:B:87:MET:HE2	1:B:93:LEU:HD21	1.69	0.75
1:B:171[B]:ARG:HB3	1:B:171[B]:ARG:NH1	2.06	0.71
1:B:171[B]:ARG:HG2	1:B:171[B]:ARG:NH1	2.02	0.71
1:B:171[B]:ARG:CG	1:B:171[B]:ARG:NH1	2.46	0.68
1:B:171[B]:ARG:NH1	1:B:171[B]:ARG:CB	2.59	0.66
1:B:171[B]:ARG:HH11	1:B:171[B]:ARG:CB	2.11	0.62
1:C:275:VAL:O	1:C:279[B]:MET:HG2	2.08	0.54
1:B:142[B]:SER:HB2	1:C:142[B]:SER:OG	2.08	0.53
1:A:133[B]:ARG:NH1	4:A:480:HOH:O	2.43	0.51
1:A:168:ARG:NH2	4:A:539:HOH:O	2.41	0.50
1:C:74:ASN:OD1	1:C:276[B]:SER:HA	2.12	0.50
1:A:148[B]:ARG:CZ	4:A:552:HOH:O	2.59	0.50
1:A:168:ARG:O	1:A:172:GLN:HG3	2.11	0.49
1:C:38:LEU:HD22	1:C:275:VAL:HG21	1.96	0.48
1:B:171[B]:ARG:HH11	1:B:171[B]:ARG:HB3	1.74	0.48
1:C:38:LEU:HD21	1:C:271:LEU:HB3	1.98	0.46
1:C:74:ASN:OD1	1:C:276[A]:SER:HA	2.17	0.45
1:A:49:ASP:O	1:A:52:GLU:HG2	2.16	0.45
1:B:179:LYS:NZ	4:B:450:HOH:O	2.50	0.44
1:A:219:MET:HB2	4:A:409:HOH:O	2.18	0.43
1:A:47:ILE:HD13	1:A:67:ARG:HH21	1.83	0.43
1:B:143:GLY:HA2	1:C:196:ALA:CB	2.49	0.43
1:A:194:MET:SD	4:A:561:HOH:O	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:O	1:A:21:THR:HG22	2.19	0.42
1:C:17:LEU:O	1:C:21:THR:HG22	2.19	0.42
1:C:11:LYS:O	1:C:15:GLU:HG2	2.19	0.41
1:B:45:ALA:HA	1:B:70:PHE:O	2.20	0.41
1:C:49:ASP:O	1:C:52:GLU:HG2	2.21	0.41
1:A:98:PHE:HB3	1:A:99:PRO:HD3	2.03	0.40
1:B:16:TYR:CD2	1:B:16:TYR:C	2.99	0.40
1:B:171[B]:ARG:NH1	1:B:189:GLU:OE1	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	286/324 (88%)	282 (99%)	4 (1%)	0	100	100
1	B	287/324 (89%)	284 (99%)	3 (1%)	0	100	100
1	C	287/324 (89%)	283 (99%)	4 (1%)	0	100	100
All	All	860/972 (88%)	849 (99%)	11 (1%)	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	240/268 (90%)	240 (100%)	0	100	100
1	B	240/268 (90%)	238 (99%)	2 (1%)	73	65
1	C	240/268 (90%)	235 (98%)	5 (2%)	47	30
All	All	720/804 (90%)	713 (99%)	7 (1%)	68	58

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	LYS
1	B	41	LYS
1	C	11	LYS
1	C	15	GLU
1	C	41	LYS
1	C	265	LYS
1	C	277	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	B	180	GLN
1	B	210	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](#)

3 non-standard protein/DNA/RNA residues 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
1	FT6	B	257	1	15,16,17	1.87	3 (20%)	17,22,24	1.95	4 (23%)
1	FT6	C	257	1	15,16,17	1.76	2 (13%)	17,22,24	2.00	4 (23%)
1	FT6	A	257	1	15,16,17	1.90	3 (20%)	17,22,24	1.85	4 (23%)

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
1	FT6	B	257	1	-	0/5/6/8	0/2/2/2
1	FT6	C	257	1	-	0/5/6/8	0/2/2/2
1	FT6	A	257	1	-	0/5/6/8	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	FT6	CD2-CE2	5.56	1.48	1.41
1	B	257	FT6	CD2-CE2	5.47	1.48	1.41
1	C	257	FT6	CD2-CE2	5.09	1.47	1.41
1	C	257	FT6	CD2-CG	2.66	1.48	1.44
1	A	257	FT6	CD2-CG	2.57	1.48	1.44
1	B	257	FT6	CD2-CG	2.26	1.47	1.44
1	B	257	FT6	CE2-NE1	-2.20	1.34	1.37
1	A	257	FT6	CE2-NE1	-2.01	1.34	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	FT6	CZ2-CE2-CD2	-5.50	118.13	122.52
1	B	257	FT6	CZ2-CE2-CD2	-5.44	118.18	122.52
1	A	257	FT6	CZ2-CE2-CD2	-5.02	118.51	122.52
1	B	257	FT6	CE3-CD2-CE2	3.34	122.30	118.84
1	C	257	FT6	CE3-CD2-CE2	3.32	122.28	118.84
1	C	257	FT6	CE2-CD2-CG	-2.98	104.16	107.17
1	A	257	FT6	CE3-CZ3-CH2	2.78	121.24	118.38
1	A	257	FT6	CE3-CD2-CE2	2.58	121.51	118.84
1	C	257	FT6	CE2-NE1-CD1	2.52	111.32	109.08
1	B	257	FT6	CE3-CZ3-CH2	2.46	120.91	118.38
1	A	257	FT6	CE2-CD2-CG	-2.20	104.95	107.17
1	B	257	FT6	CE2-CD2-CG	-2.07	105.08	107.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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	IM5	B	301	-	22,22,22	1.70	5 (22%)	25,32,32	2.11	10 (40%)
3	PO4	C	302	-	4,4,4	1.52	1 (25%)	6,6,6	1.46	2 (33%)
2	IM5	C	301	-	22,22,22	1.89	5 (22%)	25,32,32	1.86	7 (28%)
2	IM5	A	301	-	22,22,22	1.91	6 (27%)	25,32,32	1.77	6 (24%)
3	PO4	B	302	-	4,4,4	1.22	1 (25%)	6,6,6	0.91	0
3	PO4	A	302	-	4,4,4	1.34	1 (25%)	6,6,6	1.00	0

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	IM5	C	301	-	-	1/6/18/18	0/3/3/3
2	IM5	B	301	-	-	1/6/18/18	0/3/3/3
2	IM5	A	301	-	-	1/6/18/18	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	IM5	C4-C9	-4.75	1.34	1.45
2	C	301	IM5	C4-C9	-4.71	1.34	1.45
2	A	301	IM5	C4-C9	-4.06	1.35	1.45
2	A	301	IM5	C6'-C4'	3.87	1.58	1.53
2	C	301	IM5	C8-C9	-3.64	1.33	1.38
2	C	301	IM5	C5-N7	-3.07	1.33	1.38
2	B	301	IM5	C10-C9	2.99	1.54	1.51
2	A	301	IM5	C10-C9	2.89	1.54	1.51
2	A	301	IM5	C8-C9	-2.83	1.34	1.38
2	A	301	IM5	C2'-C3'	2.82	1.56	1.52
2	B	301	IM5	C2-N1	2.71	1.44	1.37
2	C	301	IM5	C2'-C3'	2.67	1.56	1.52
2	A	301	IM5	C10-N1'	2.37	1.52	1.47
2	B	301	IM5	O3'-C3'	2.34	1.48	1.43
3	C	302	PO4	P-O4	-2.22	1.48	1.54
2	B	301	IM5	C5-C6	-2.22	1.35	1.41
2	C	301	IM5	C10-N1'	2.19	1.51	1.47
3	B	302	PO4	P-O2	-2.08	1.48	1.54
3	A	302	PO4	P-O2	-2.05	1.48	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	IM5	C5-C4-N3	-4.76	120.50	124.86
2	A	301	IM5	C5-C4-N3	-4.75	120.52	124.86
2	C	301	IM5	C9-C10-N1'	4.46	119.63	113.38
2	B	301	IM5	C2-N1-C6	-4.02	117.82	125.11
2	C	301	IM5	C3'-C2'-N1'	-3.75	97.55	104.47
2	C	301	IM5	C5-C4-N3	-3.59	121.58	124.86
2	B	301	IM5	C5-C6-N1	3.11	120.68	112.13
2	A	301	IM5	C3'-C2'-N1'	-3.07	98.80	104.47
2	A	301	IM5	C2-N1-C6	-2.97	119.73	125.11
2	B	301	IM5	O6-C6-N1	-2.89	114.68	120.11
2	B	301	IM5	C4-N3-C2	2.81	121.04	116.63
3	C	302	PO4	O4-P-O2	2.58	115.92	107.91
2	C	301	IM5	C10-N1'-C6'	-2.56	108.48	113.39
2	B	301	IM5	O5'-C5'-C4'	-2.44	105.70	111.26
3	C	302	PO4	O3-P-O1	-2.43	102.36	110.95
2	A	301	IM5	C5-C6-N1	2.38	118.65	112.13
2	C	301	IM5	C2-N1-C6	-2.37	120.82	125.11
2	B	301	IM5	C5-C4-C9	2.10	108.00	105.75
2	C	301	IM5	N1-C2-N3	-2.10	119.48	123.32
2	C	301	IM5	C5-C6-N1	2.09	117.88	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	IM5	C6'-C4'-C5'	-2.07	109.86	112.71
2	B	301	IM5	C9-C10-N1'	2.07	116.27	113.38
2	B	301	IM5	N2-C2-N3	2.03	123.63	119.67
2	B	301	IM5	C3'-C2'-N1'	-2.01	100.75	104.47
2	A	301	IM5	C5-C4-C9	2.01	107.90	105.75

There are no chirality outliers.

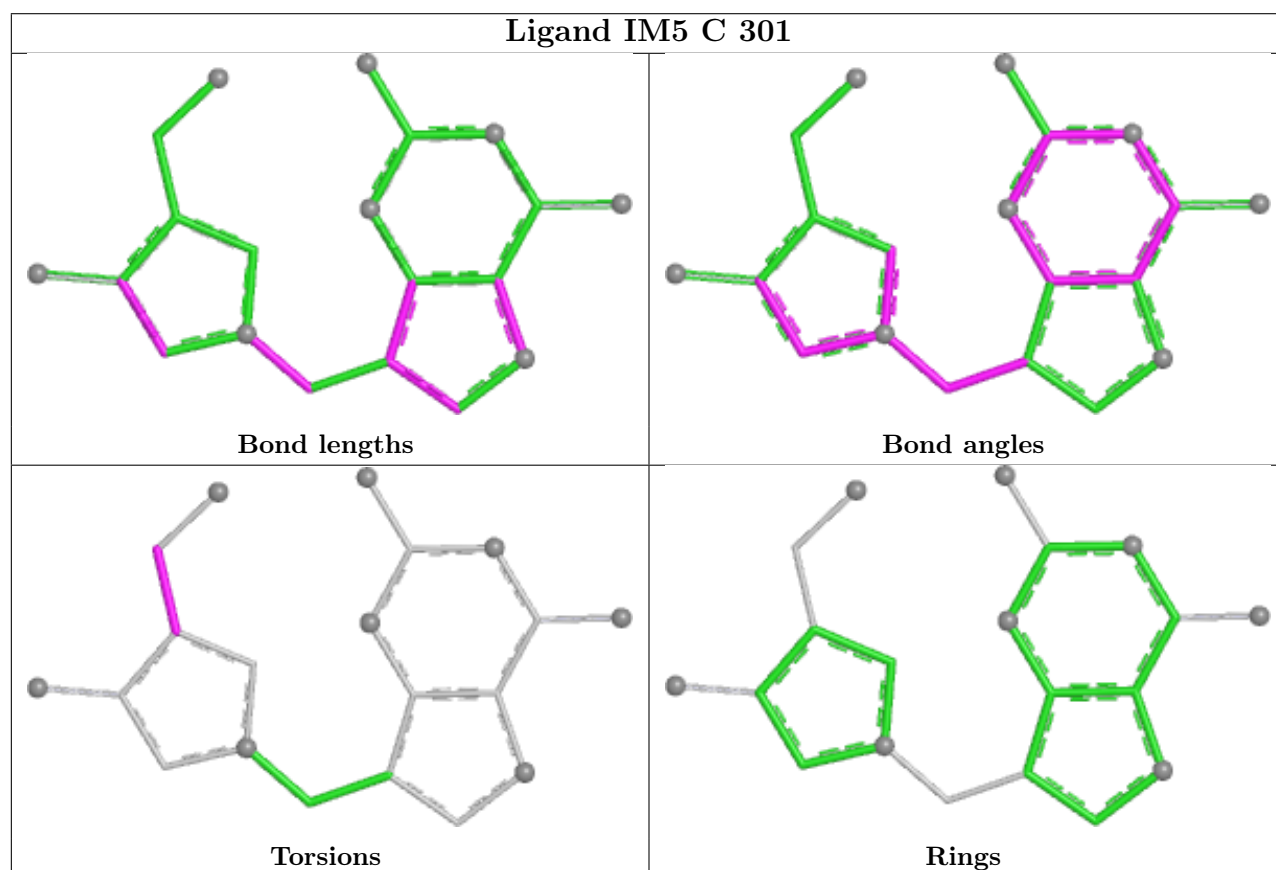
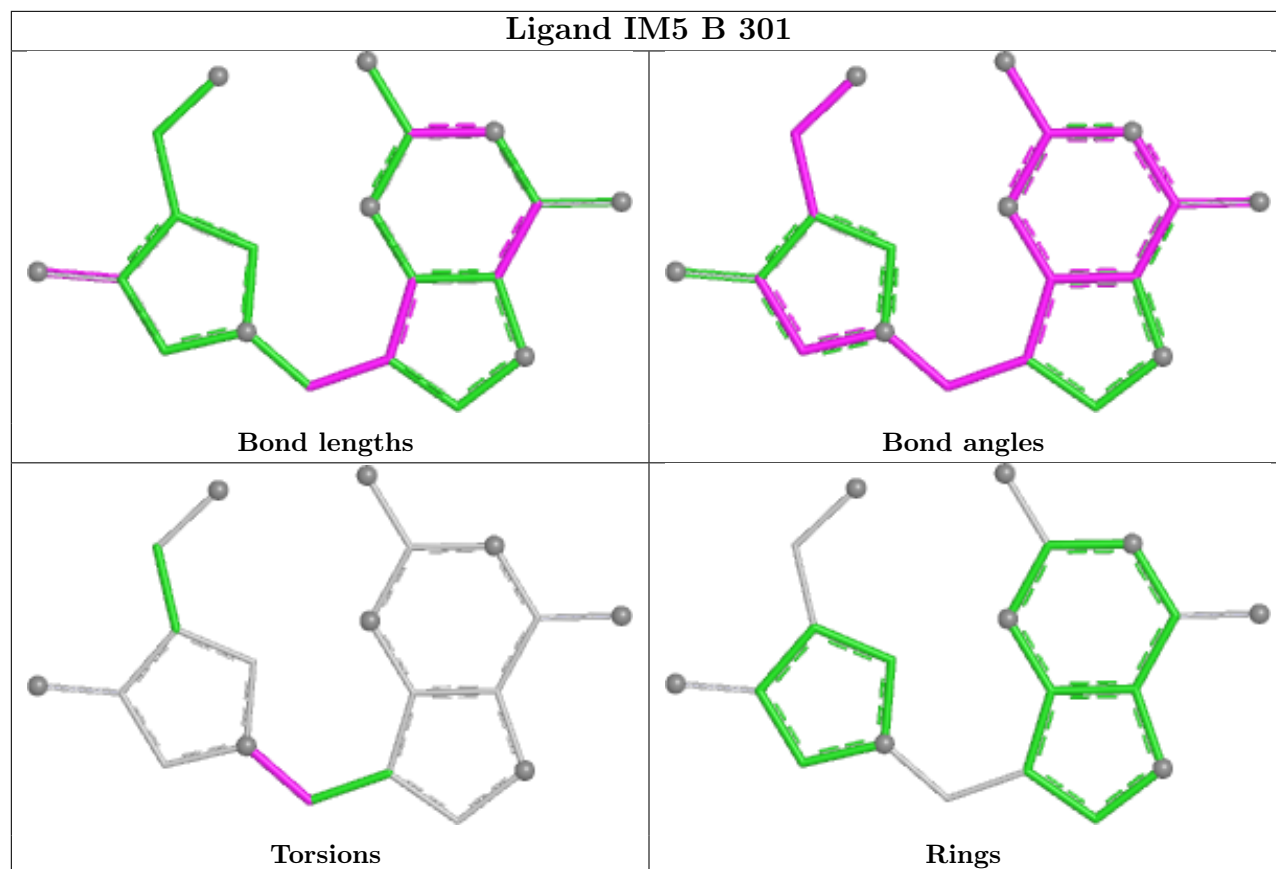
All (3) torsion outliers are listed below:

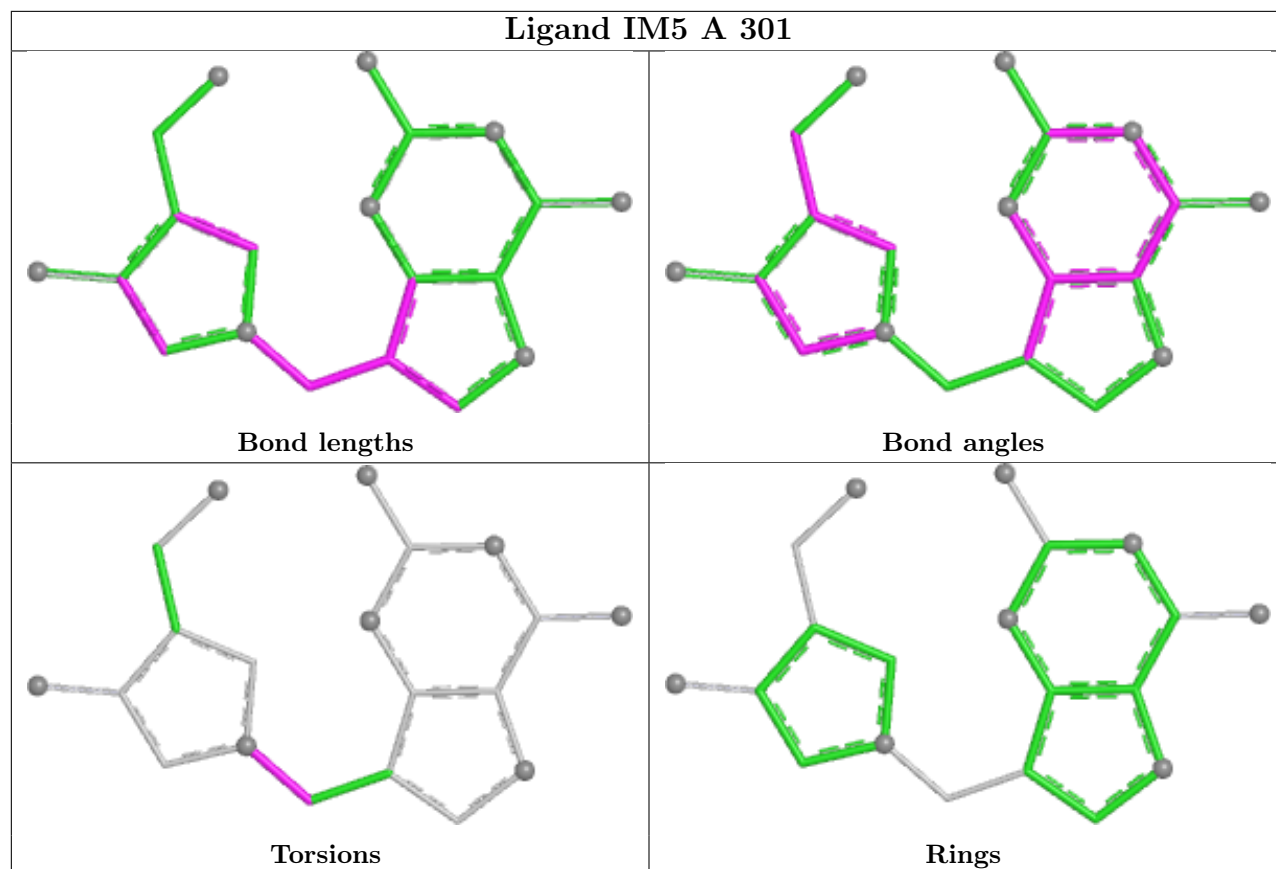
Mol	Chain	Res	Type	Atoms
2	A	301	IM5	C9-C10-N1'-C6'
2	B	301	IM5	C9-C10-N1'-C6'
2	C	301	IM5	C3'-C4'-C5'-O5'

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 [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, 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	282/324 (87%)	0.48	11 (3%) 43 47	18, 34, 62, 120	6 (2%)
1	B	286/324 (88%)	0.49	9 (3%) 51 55	19, 37, 60, 95	3 (1%)
1	C	284/324 (87%)	0.41	15 (5%) 32 35	18, 34, 58, 94	5 (1%)
All	All	852/972 (87%)	0.46	35 (4%) 41 45	18, 35, 62, 120	14 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	MET	4.5
1	C	273	GLN	4.5
1	A	178	TYR	4.4
1	C	178	TYR	3.8
1	C	288	ALA	3.7
1	A	75	GLY	3.6
1	C	184	GLN	3.3
1	A	286	ASP	3.2
1	C	182	GLY	3.1
1	C	275	VAL	2.9
1	C	277	ILE	2.8
1	B	184	GLN	2.8
1	B	288	ALA	2.8
1	B	3	ASN	2.8
1	B	4	GLY	2.7
1	A	4	GLY	2.6
1	B	277	ILE	2.6
1	C	266	GLN	2.5
1	B	182	GLY	2.5
1	A	49	ASP	2.4
1	A	78	CYS	2.4
1	C	176	SER	2.4
1	B	186	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	276[A]	SER	2.3
1	C	40	ASP	2.3
1	C	58	ARG	2.3
1	A	172	GLN	2.3
1	A	187	LEU	2.3
1	B	178	TYR	2.3
1	C	7	TYR	2.2
1	A	277	ILE	2.2
1	A	269	GLN	2.1
1	C	261	LEU	2.1
1	C	4	GLY	2.0
1	B	183	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	FT6	A	257	15/16	0.91	0.11	37,51,59,66	0
1	FT6	B	257	15/16	0.92	0.12	33,43,51,55	0
1	FT6	C	257	15/16	0.92	0.10	27,36,42,53	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

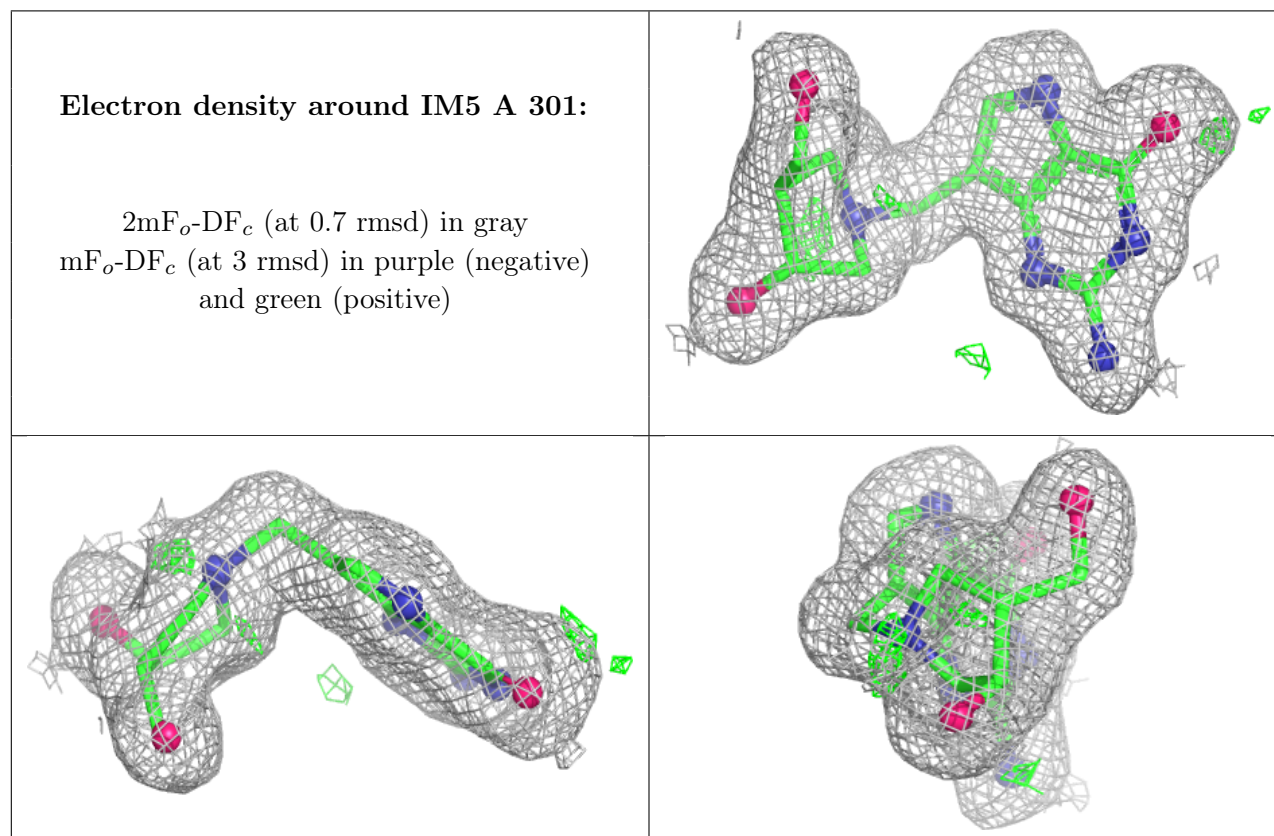
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	IM5	A	301	20/20	0.95	0.07	25,26,29,32	0
2	IM5	B	301	20/20	0.96	0.06	22,26,29,32	0
2	IM5	C	301	20/20	0.97	0.05	22,23,26,29	0

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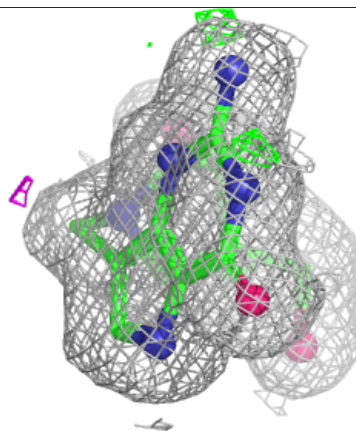
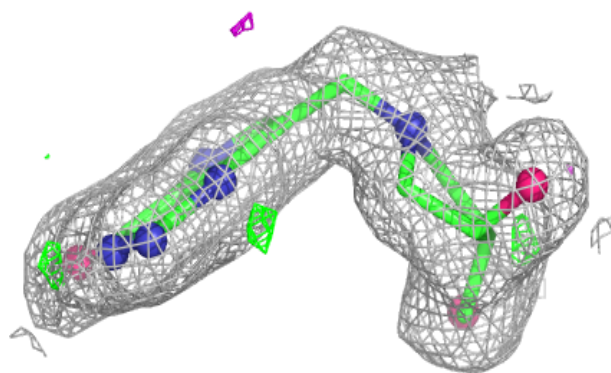
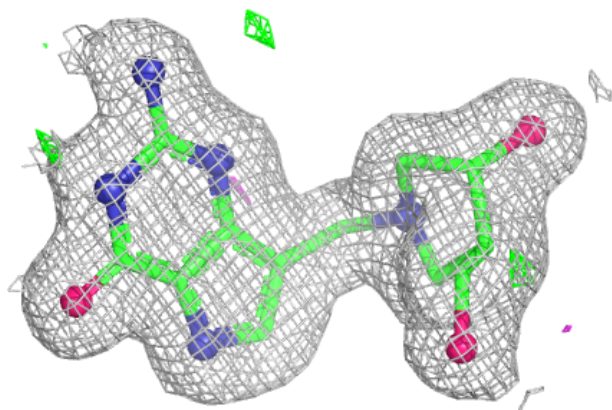
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	A	302	5/5	0.98	0.05	26,26,27,27	0
3	PO4	B	302	5/5	0.98	0.05	25,26,27,27	0
3	PO4	C	302	5/5	0.99	0.04	23,24,25,25	0

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.

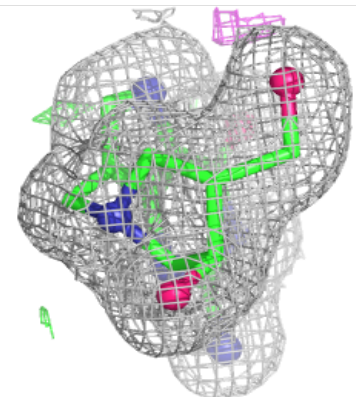
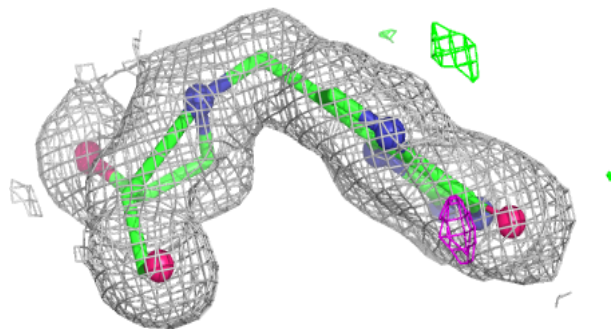
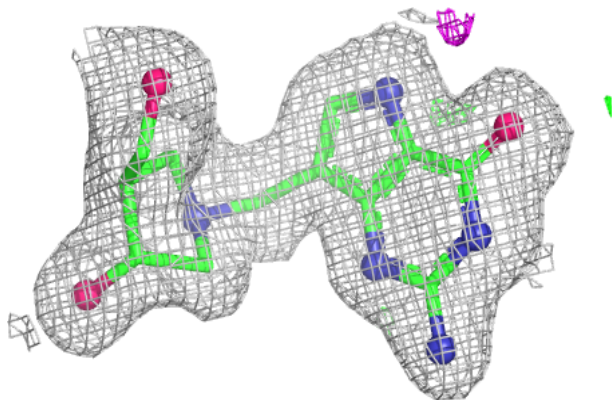


**Electron density around IM5 B 301:**

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

**Electron density around IM5 C 301:**

$2mF_o-DF_c$  (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.