



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 3PHB / pdb\_00003phb  
Title : Crystal Structure of human purine nucleoside phosphorylase in complex with DADMe-ImmG  
Authors : Ho, M.; Cassera, M.B.; Murkin, A.S.; Almo, S.C.; Schramm, V.L.  
Deposited on : 2010-11-03  
Resolution : 2.30 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

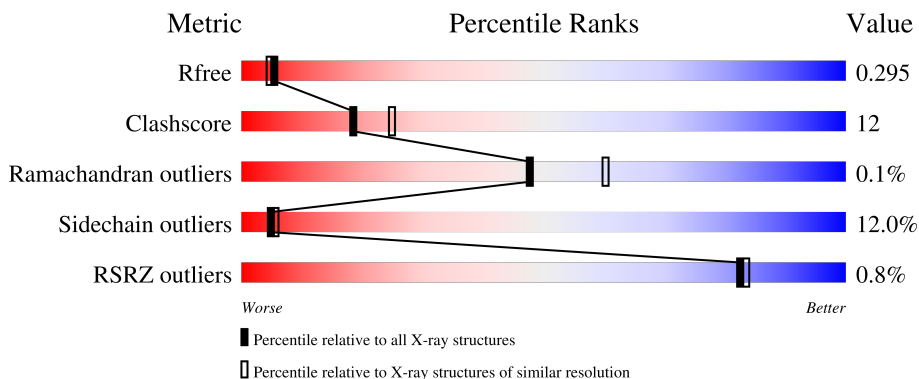
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	E	324	
1	Q	324	
1	S	324	
1	T	324	
1	U	324	

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Mol	Chain	Length	Quality of chain
1	Y	324	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a green segment on the left labeled '65%', a yellow segment in the middle labeled '20%', and a grey segment on the right labeled '12%'. The segments are separated by thin black lines.</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13732 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	E	288	2252	1433	393	410	16	0	0	0
1	Q	287	2256	1434	396	410	16	0	1	0
1	S	286	2238	1424	391	407	16	0	0	0
1	T	287	2245	1428	392	409	16	0	0	0
1	U	285	2241	1424	395	407	15	0	1	0
1	Y	285	2230	1418	390	406	16	0	0	0

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-34	MET	-	expression tag	UNP P00491
E	-33	ARG	-	expression tag	UNP P00491
E	-32	GLY	-	expression tag	UNP P00491
E	-31	SER	-	expression tag	UNP P00491
E	-30	HIS	-	expression tag	UNP P00491
E	-29	HIS	-	expression tag	UNP P00491
E	-28	HIS	-	expression tag	UNP P00491
E	-27	HIS	-	expression tag	UNP P00491
E	-26	HIS	-	expression tag	UNP P00491
E	-25	HIS	-	expression tag	UNP P00491
E	-24	GLY	-	expression tag	UNP P00491
E	-23	MET	-	expression tag	UNP P00491
E	-22	ALA	-	expression tag	UNP P00491
E	-21	SER	-	expression tag	UNP P00491
E	-20	MET	-	expression tag	UNP P00491
E	-19	THR	-	expression tag	UNP P00491
E	-18	GLY	-	expression tag	UNP P00491

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

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

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

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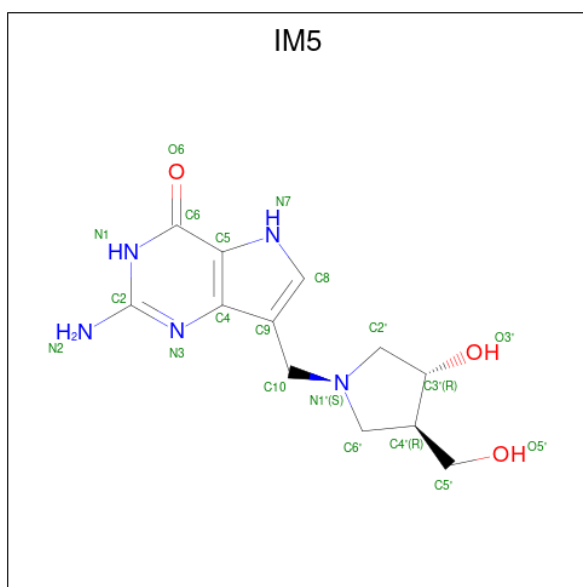
Chain	Residue	Modelled	Actual	Comment	Reference
T	51	SER	GLY	conflict	UNP P00491
U	-34	MET	-	expression tag	UNP P00491
U	-33	ARG	-	expression tag	UNP P00491
U	-32	GLY	-	expression tag	UNP P00491
U	-31	SER	-	expression tag	UNP P00491
U	-30	HIS	-	expression tag	UNP P00491
U	-29	HIS	-	expression tag	UNP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

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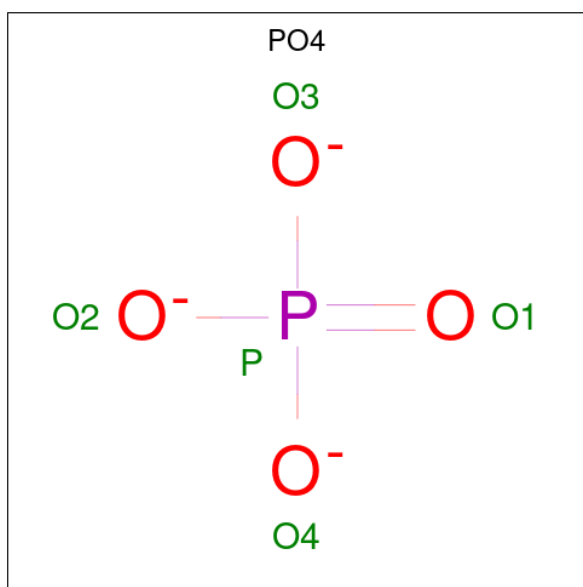
Chain	Residue	Modelled	Actual	Comment	Reference
Y	-29	HIS	-	expression tag	UNP P00491
Y	-28	HIS	-	expression tag	UNP P00491
Y	-27	HIS	-	expression tag	UNP P00491
Y	-26	HIS	-	expression tag	UNP P00491
Y	-25	HIS	-	expression tag	UNP P00491
Y	-24	GLY	-	expression tag	UNP P00491
Y	-23	MET	-	expression tag	UNP P00491
Y	-22	ALA	-	expression tag	UNP P00491
Y	-21	SER	-	expression tag	UNP P00491
Y	-20	MET	-	expression tag	UNP P00491
Y	-19	THR	-	expression tag	UNP P00491
Y	-18	GLY	-	expression tag	UNP P00491
Y	-17	GLY	-	expression tag	UNP P00491
Y	-16	GLN	-	expression tag	UNP P00491
Y	-15	GLN	-	expression tag	UNP P00491
Y	-14	MET	-	expression tag	UNP P00491
Y	-13	GLY	-	expression tag	UNP P00491
Y	-12	ARG	-	expression tag	UNP P00491
Y	-11	ASP	-	expression tag	UNP P00491
Y	-10	LEU	-	expression tag	UNP P00491
Y	-9	TYR	-	expression tag	UNP P00491
Y	-8	ASP	-	expression tag	UNP P00491
Y	-7	ASP	-	expression tag	UNP P00491
Y	-6	ASP	-	expression tag	UNP P00491
Y	-5	ASP	-	expression tag	UNP P00491
Y	-4	LYS	-	expression tag	UNP P00491
Y	-3	ASP	-	expression tag	UNP P00491
Y	-2	PRO	-	expression tag	UNP P00491
Y	-1	THR	-	expression tag	UNP P00491
Y	0	LEU	-	expression tag	UNP P00491
Y	51	SER	GLY	conflict	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	E	1	Total	C	N	O	0	0
			20	12	5	3		
2	Q	1	Total	C	N	O	0	0
			20	12	5	3		
2	S	1	Total	C	N	O	0	0
			20	12	5	3		
2	T	1	Total	C	N	O	0	0
			20	12	5	3		
2	U	1	Total	C	N	O	0	0
			20	12	5	3		
2	Y	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	E	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	Q	1	Total O P 5 4 1	0	0
3	Q	1	Total O P 5 4 1	0	0
3	S	1	Total O P 5 4 1	0	0
3	S	1	Total O P 5 4 1	0	0
3	T	1	Total O P 5 4 1	0	0
3	T	1	Total O P 5 4 1	0	0
3	U	1	Total O P 5 4 1	0	0
3	Y	1	Total O P 5 4 1	0	0
3	Y	1	Total O P 5 4 1	0	0
3	Y	1	Total O P 5 4 1	0	0

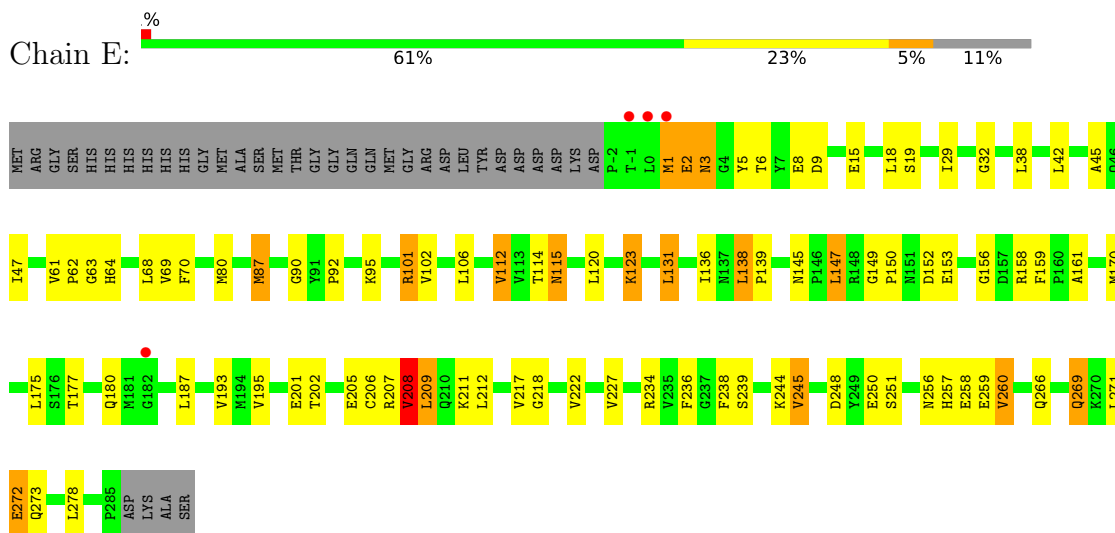
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	16	Total O 16 16	0	0
4	Q	18	Total O 18 18	0	0
4	S	15	Total O 15 15	0	0
4	T	10	Total O 10 10	0	0
4	U	13	Total O 13 13	0	0
4	Y	18	Total O 18 18	0	0

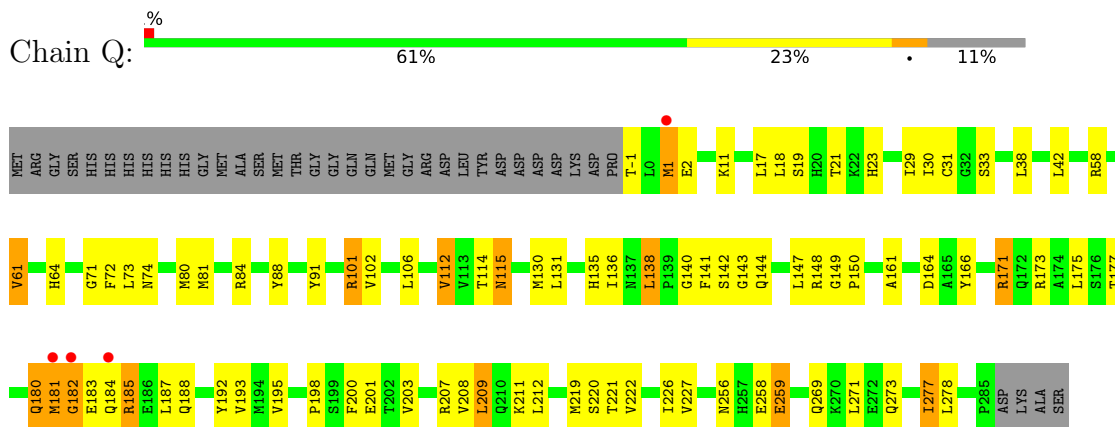
### 3 Residue-property plots i

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.

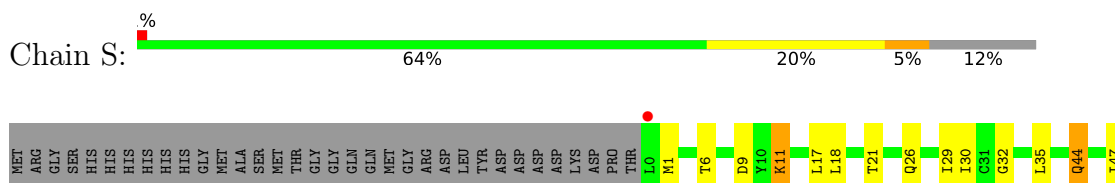
- Molecule 1: Purine nucleoside phosphorylase



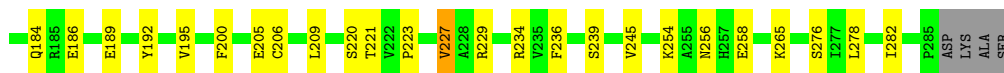
- Molecule 1: Purine nucleoside phosphorylase



- Molecule 1: Purine nucleoside phosphorylase







## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	269.27Å 52.63Å 128.12Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	19.91 – 2.30 19.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.91-2.30) 98.7 (19.91-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.30Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.230 , 0.295 0.230 , 0.295	Depositor DCC
$R_{free}$ test set	3982 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.004 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, 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	E	0.84	3/2305 (0.1%)	1.06	3/3120 (0.1%)
1	Q	0.79	0/2308	1.04	5/3123 (0.2%)
1	S	0.78	0/2290	1.03	0/3099
1	T	0.75	0/2297	1.00	2/3108 (0.1%)
1	U	0.78	2/2293 (0.1%)	0.97	0/3102
1	Y	0.76	0/2282	1.02	3/3088 (0.1%)
All	All	0.78	5/13775 (0.0%)	1.02	13/18640 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	222	VAL	CA-CB	6.03	1.57	1.54
1	E	208	VAL	CA-CB	5.25	1.60	1.54
1	U	227	VAL	CA-CB	5.18	1.61	1.54
1	U	61	VAL	CA-CB	5.06	1.60	1.54
1	E	161	ALA	N-CA	5.02	1.52	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	GLY	CA-C-N	6.73	126.71	119.78
1	E	149	GLY	C-N-CA	6.73	126.71	119.78
1	Q	182	GLY	N-CA-C	-6.36	103.50	112.60
1	T	190	GLY	N-CA-C	6.17	119.76	110.75
1	Q	91	TYR	CA-C-N	5.78	125.71	119.76
1	Q	91	TYR	C-N-CA	5.78	125.71	119.76
1	T	89	GLU	N-CA-C	-5.62	106.39	113.18
1	Y	145	ASN	CA-C-N	5.47	125.14	119.56
1	Y	145	ASN	C-N-CA	5.47	125.14	119.56
1	Q	149	GLY	CA-C-N	5.30	125.61	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	149	GLY	C-N-CA	5.30	125.61	119.93
1	Y	165	ALA	N-CA-C	5.26	117.02	111.28
1	E	64	HIS	N-CA-C	-5.10	99.09	108.02

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	E	2252	0	2233	66	0
1	Q	2256	0	2238	87	0
1	S	2238	0	2219	51	0
1	T	2245	0	2226	39	0
1	U	2241	0	2219	57	0
1	Y	2230	0	2208	54	0
2	E	20	0	17	1	0
2	Q	20	0	17	0	0
2	S	20	0	17	0	0
2	T	20	0	17	0	0
2	U	20	0	17	1	0
2	Y	20	0	17	0	0
3	E	10	0	0	0	0
3	Q	10	0	0	0	0
3	S	10	0	0	0	0
3	T	10	0	0	1	0
3	U	5	0	0	0	0
3	Y	15	0	0	0	0
4	E	16	0	0	1	0
4	Q	18	0	0	6	0
4	S	15	0	0	0	0
4	T	10	0	0	0	0
4	U	13	0	0	1	0
4	Y	18	0	0	1	0
All	All	13732	0	13445	324	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 12.

All (324) 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:U:177:THR:HG21	1:U:277:ILE:CG2	1.80	1.10
1:Q:171[A]:ARG:HH21	1:Q:171[A]:ARG:HG3	1.13	1.07
1:T:184:GLN:H	1:T:184:GLN:HE21	1.02	0.97
1:U:177:THR:CG2	1:U:277:ILE:HG21	1.98	0.93
1:U:177:THR:HG21	1:U:277:ILE:HG23	1.52	0.92
1:U:177:THR:CG2	1:U:277:ILE:CG2	2.50	0.90
1:U:29:ILE:HG23	1:U:112:VAL:HG22	1.52	0.90
1:Q:64:HIS:HD2	1:Q:84:ARG:H	1.15	0.89
1:E:159:PHE:HB3	1:Q:200:PHE:CE2	2.09	0.88
1:Q:171[A]:ARG:HG3	1:Q:171[A]:ARG:NH2	1.89	0.84
1:S:207:ARG:HA	1:S:210:GLN:HE21	1.43	0.83
1:Q:171[B]:ARG:HG3	1:Q:171[B]:ARG:HH11	1.44	0.82
1:Q:33:SER:OG	1:Q:64:HIS:HE1	1.65	0.80
1:Q:1:MET:HG2	1:Q:148:ARG:HD3	1.62	0.79
1:Y:120:LEU:HD23	1:Y:245:VAL:HG21	1.63	0.79
1:E:101:ARG:HD3	4:E:307:HOH:O	1.83	0.77
1:Y:33:SER:OG	1:Y:64:HIS:HE1	1.68	0.76
1:Q:171[B]:ARG:HH11	1:Q:171[B]:ARG:CG	1.97	0.76
1:U:177:THR:O	1:U:177:THR:HG22	1.86	0.76
1:T:131:LEU:HD21	1:T:236:PHE:CZ	2.20	0.75
1:T:184:GLN:H	1:T:184:GLN:NE2	1.81	0.75
1:E:269:GLN:HE21	1:E:269:GLN:HA	1.52	0.73
1:E:2:GLU:HB3	1:E:150:PRO:HD2	1.71	0.72
1:Q:171[B]:ARG:NH1	1:Q:171[B]:ARG:HB2	2.04	0.72
1:T:184:GLN:HE21	1:T:184:GLN:N	1.85	0.72
1:Q:195:VAL:CG1	4:Q:293:HOH:O	2.39	0.70
1:E:115:ASN:C	1:E:115:ASN:HD22	2.00	0.69
1:E:153:GLU:HA	1:E:156:GLY:O	1.91	0.69
1:U:177:THR:CG2	1:U:177:THR:O	2.40	0.69
1:E:158:ARG:HH21	1:Q:198:PRO:HG3	1.57	0.69
1:E:2:GLU:CB	1:E:150:PRO:HD2	2.23	0.68
1:Y:206:CYS:SG	1:Y:245:VAL:HG23	2.34	0.68
1:E:3:ASN:HD22	1:E:5:TYR:H	1.43	0.67
1:Q:143:GLY:CA	1:Y:87:MET:HE1	2.24	0.67
1:U:256:ASN:ND2	1:U:259:GLU:H	1.93	0.67
1:S:87:MET:HE2	1:S:194:MET:HE1	1.77	0.67
1:E:145:ASN:OD1	1:E:147:LEU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:PHE:HB3	1:Q:200:PHE:HE2	1.57	0.66
1:U:177:THR:HG22	1:U:277:ILE:HG21	1.75	0.65
1:Q:64:HIS:CD2	1:Q:84:ARG:H	2.06	0.65
1:Q:143:GLY:HA2	1:Y:87:MET:HE1	1.78	0.65
1:U:42:LEU:HD21	1:U:80:MET:HE3	1.79	0.65
1:Q:142:SER:CB	1:Y:139:PRO:HA	2.26	0.65
1:Q:182:GLY:C	1:Q:183:GLU:HG2	2.20	0.65
1:T:120:LEU:HD23	1:T:245:VAL:HG21	1.79	0.65
1:Q:2:GLU:HG3	1:Q:150:PRO:HD2	1.80	0.64
1:Q:181:MET:HG2	1:Q:273:GLN:HG3	1.79	0.64
1:U:125:GLU:HB2	1:U:185:ARG:HH12	1.62	0.64
1:Q:203:VAL:O	1:Q:207:ARG:HG2	1.99	0.63
1:U:61:VAL:HG22	1:U:64:HIS:CD2	2.34	0.63
1:E:139:PRO:HA	1:Y:142:SER:HB3	1.81	0.63
1:Q:72:PHE:CZ	1:S:180:GLN:HG3	2.34	0.63
1:T:3:ASN:ND2	1:T:5:TYR:H	1.96	0.63
1:T:29:ILE:HG23	1:T:112:VAL:HG22	1.81	0.62
1:Y:73:LEU:HD22	1:Y:80:MET:HE1	1.82	0.62
1:E:206:CYS:SG	1:E:245:VAL:HG22	2.40	0.62
1:U:145:ASN:OD1	1:U:147:LEU:HB2	2.00	0.62
1:U:19:SER:HB3	1:U:20:HIS:ND1	2.16	0.61
1:Q:220:SER:HB2	4:Q:303:HOH:O	1.99	0.61
1:Q:72:PHE:HZ	1:S:180:GLN:HG3	1.64	0.61
1:E:139:PRO:HA	1:Y:142:SER:CB	2.30	0.61
1:E:115:ASN:ND2	1:E:239:SER:OG	2.31	0.61
1:S:136:ILE:HB	1:S:193:VAL:HG23	1.83	0.61
1:S:177:THR:O	1:S:181:MET:HG2	2.02	0.60
1:Y:115:ASN:ND2	1:Y:239:SER:OG	2.27	0.60
1:E:177:THR:O	1:E:180:GLN:HB2	2.02	0.60
1:Y:33:SER:OG	1:Y:64:HIS:CE1	2.53	0.60
1:E:136:ILE:HG22	1:E:138:LEU:HD13	1.84	0.59
1:T:131:LEU:HD21	1:T:236:PHE:HZ	1.68	0.59
1:S:6:THR:O	1:S:9:ASP:HB2	2.02	0.59
1:Q:142:SER:HB2	1:Y:139:PRO:HA	1.84	0.58
1:E:131:LEU:HD11	1:E:236:PHE:CE1	2.37	0.58
1:Y:64:HIS:HD2	1:Y:84:ARG:H	1.50	0.58
1:Q:1:MET:CG	1:Q:148:ARG:HD3	2.34	0.58
1:Y:145:ASN:OD1	1:Y:147:LEU:HB2	2.03	0.58
1:U:116:ALA:O	2:U:290:IM5:H10A	2.04	0.58
1:E:131:LEU:HD21	1:E:236:PHE:HZ	1.69	0.57
1:U:181:MET:HA	1:U:273:GLN:HE21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:166:TYR:HB3	1:Q:171[B]:ARG:HH22	1.69	0.57
1:Y:73:LEU:HD22	1:Y:80:MET:CE	2.34	0.57
1:E:131:LEU:HD11	1:E:236:PHE:HE1	1.68	0.57
1:E:32:GLY:HA3	1:E:115:ASN:HA	1.85	0.57
1:Y:99:PRO:HA	1:Y:102:VAL:HG13	1.86	0.57
1:E:257:HIS:HA	1:E:260:VAL:HG13	1.87	0.57
1:E:272:GLU:HG2	1:E:273:GLN:N	2.20	0.56
1:E:207:ARG:O	1:E:211:LYS:HG3	2.05	0.56
1:Q:166:TYR:CB	1:Q:171[B]:ARG:HH22	2.19	0.56
1:T:256:ASN:ND2	1:T:259:GLU:H	2.02	0.56
1:S:170:MET:CE	1:S:234:ARG:HG2	2.35	0.56
1:Q:182:GLY:O	1:Q:183:GLU:HG2	2.05	0.56
1:U:206:CYS:SG	1:U:245:VAL:HG23	2.45	0.56
1:Q:220:SER:O	1:Q:221:THR:HB	2.06	0.56
1:E:201:GLU:CD	1:E:201:GLU:H	2.14	0.55
1:Q:171[B]:ARG:HH11	1:Q:171[B]:ARG:CB	2.20	0.55
1:Q:171[B]:ARG:NH1	1:Q:171[B]:ARG:CB	2.69	0.55
1:Y:47:ILE:HG12	1:Y:69:VAL:HG13	1.87	0.55
1:Q:73:LEU:HD22	1:Q:80:MET:CE	2.36	0.55
1:Y:170:MET:HE2	1:Y:234:ARG:HG2	1.87	0.55
1:S:258:GLU:CD	1:S:258:GLU:H	2.15	0.55
1:Q:166:TYR:CB	1:Q:171[B]:ARG:NH2	2.70	0.54
1:U:266:GLN:HE21	1:U:266:GLN:HA	1.71	0.54
1:Y:135:HIS:HA	1:Y:192:TYR:O	2.07	0.54
1:S:236:PHE:CD2	1:S:278:LEU:HD21	2.43	0.54
1:Q:17:LEU:O	1:Q:21:THR:HG22	2.09	0.53
1:Y:220:SER:O	1:Y:221:THR:HB	2.07	0.53
1:Y:42:LEU:HD21	1:Y:80:MET:HE3	1.90	0.53
1:E:258:GLU:CD	1:E:258:GLU:H	2.17	0.53
1:Q:180:GLN:HB3	1:S:44:GLN:OE1	2.08	0.53
1:E:62:PRO:O	1:E:257:HIS:NE2	2.34	0.53
1:S:26:GLN:OE1	1:S:76:ARG:HD2	2.09	0.53
1:T:173:ARG:O	1:T:177:THR:OG1	2.25	0.53
1:Q:166:TYR:HB3	1:Q:171[B]:ARG:NH2	2.24	0.53
1:Y:42:LEU:HD11	1:Y:80:MET:HG3	1.90	0.53
1:Y:61:VAL:HG22	1:Y:64:HIS:ND1	2.23	0.53
1:Y:101:ARG:HG2	1:Y:101:ARG:HH11	1.73	0.53
1:S:47:ILE:HG23	1:S:69:VAL:HG22	1.90	0.53
1:U:136:ILE:HG22	1:U:138:LEU:HD13	1.91	0.53
1:Q:143:GLY:HA2	1:Y:87:MET:CE	2.39	0.52
1:S:11:LYS:HB3	1:S:11:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:VAL:HA	1:E:211:LYS:HD2	1.90	0.52
1:Y:27:VAL:HG21	1:Y:282:ILE:HD13	1.90	0.52
1:E:256:ASN:O	1:E:260:VAL:HG12	2.09	0.52
1:E:123:LYS:HE2	1:E:123:LYS:HA	1.90	0.51
1:S:114:THR:HG22	1:S:238:PHE:CE1	2.44	0.51
1:S:115:ASN:C	1:S:115:ASN:HD22	2.18	0.51
1:Q:29:ILE:HD12	1:Q:80:MET:HE2	1.91	0.51
1:Q:256:ASN:HD22	1:Q:258:GLU:HB3	1.75	0.51
1:S:207:ARG:HA	1:S:210:GLN:NE2	2.20	0.51
1:Q:61:VAL:HG13	4:Q:296:HOH:O	2.10	0.51
1:Q:171[A]:ARG:HH21	1:Q:171[A]:ARG:CG	1.99	0.51
1:T:158:ARG:HH21	1:U:198:PRO:HG3	1.75	0.51
1:U:26:GLN:HG2	1:U:109:ASP:OD1	2.11	0.51
1:U:50:TYR:CE2	1:U:66:GLY:HA2	2.46	0.51
1:Y:171:ARG:NH1	1:Y:189:GLU:OE1	2.43	0.51
1:T:2:GLU:HB2	1:T:150:PRO:HD2	1.93	0.51
1:U:61:VAL:HG22	1:U:64:HIS:HD2	1.75	0.51
1:U:112:VAL:HA	1:U:236:PHE:O	2.10	0.51
1:Q:171[B]:ARG:HB2	1:Q:171[B]:ARG:CZ	2.41	0.51
1:Q:182:GLY:C	1:Q:183:GLU:CG	2.84	0.51
1:U:177:THR:CG2	1:U:277:ILE:HG23	2.29	0.51
1:Y:170:MET:CE	1:Y:234:ARG:HG2	2.41	0.50
1:E:131:LEU:HD21	1:E:236:PHE:CZ	2.46	0.50
1:S:273:GLN:O	1:S:277:ILE:HD13	2.11	0.50
1:E:269:GLN:HA	1:E:269:GLN:NE2	2.23	0.50
1:U:3:ASN:ND2	1:U:94:TRP:HB2	2.26	0.50
1:E:131:LEU:HD23	1:E:187:LEU:HD21	1.94	0.50
1:S:177:THR:HG22	1:S:181:MET:HE2	1.93	0.50
1:U:279:MET:HE2	1:U:282:ILE:HD11	1.93	0.50
1:E:6:THR:O	1:E:9:ASP:HB2	2.11	0.50
1:U:120:LEU:HD23	1:U:245:VAL:HG21	1.93	0.50
1:T:193:VAL:HG13	1:T:217:VAL:HG23	1.93	0.50
1:Q:256:ASN:ND2	1:Q:259:GLU:H	2.10	0.50
1:E:114:THR:HG22	1:E:238:PHE:CE2	2.47	0.49
1:T:50:TYR:CE2	1:T:66:GLY:HA2	2.47	0.49
1:Y:23:HIS:HB3	4:Y:300:HOH:O	2.12	0.49
1:E:8:GLU:CD	1:E:8:GLU:H	2.21	0.49
1:T:141:PHE:HA	1:U:195:VAL:HG13	1.94	0.49
1:T:193:VAL:HG11	1:T:209:LEU:HG	1.94	0.49
1:E:90:GLY:O	1:Y:1:MET:HA	2.13	0.49
1:Q:195:VAL:HG12	4:Q:293:HOH:O	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:23:HIS:O	1:U:24:ARG:HD3	2.12	0.49
1:Y:206:CYS:SG	1:Y:245:VAL:CG2	3.01	0.48
1:U:27:VAL:HG22	1:U:110:THR:HB	1.95	0.48
1:E:193:VAL:HG11	1:E:209:LEU:HG	1.94	0.48
1:Q:222:VAL:O	1:Q:226:ILE:HG13	2.14	0.48
1:S:171:ARG:HG2	1:S:236:PHE:HE1	1.78	0.48
1:T:116:ALA:HB1	1:T:242:THR:HG21	1.96	0.48
1:U:61:VAL:HG13	4:U:294:HOH:O	2.14	0.48
1:Q:142:SER:HB3	1:Y:139:PRO:HA	1.96	0.48
1:S:195:VAL:O	1:S:219:MET:HA	2.14	0.48
1:U:17:LEU:O	1:U:21:THR:HG22	2.14	0.48
1:Q:141:PHE:CZ	1:Y:205:GLU:HG2	2.48	0.48
1:T:1:MET:CG	3:T:290:PO4:O4	2.62	0.48
1:Q:143:GLY:HA3	1:Y:87:MET:HE1	1.95	0.47
1:Q:177:THR:HG21	1:Q:277:ILE:HG23	1.95	0.47
1:S:165:ALA:O	1:S:229:ARG:HD3	2.14	0.47
1:T:145:ASN:OD1	1:T:147:LEU:HB2	2.14	0.47
1:U:181:MET:HA	1:U:273:GLN:NE2	2.28	0.47
1:E:29:ILE:HG23	1:E:112:VAL:HG22	1.96	0.47
1:S:30:ILE:HG12	1:S:81:MET:SD	2.54	0.47
1:S:206:CYS:SG	1:S:245:VAL:HG22	2.53	0.47
1:U:167:ASP:O	1:U:171:ARG:HG3	2.13	0.47
1:E:115:ASN:C	1:E:115:ASN:ND2	2.65	0.47
1:U:62:PRO:O	1:U:257:HIS:NE2	2.34	0.47
1:Q:-1:THR:HG21	1:Y:95:LYS:NZ	2.29	0.47
1:Y:131:LEU:HD22	1:Y:236:PHE:CZ	2.49	0.47
1:E:38:LEU:HD21	1:E:271:LEU:HB3	1.96	0.47
1:E:3:ASN:ND2	1:E:5:TYR:HB2	2.30	0.47
1:Q:30:ILE:HG12	1:Q:81:MET:SD	2.54	0.47
1:Q:38:LEU:HD21	1:Q:271:LEU:HB3	1.97	0.47
1:Q:42:LEU:HD21	1:Q:80:MET:HE3	1.97	0.47
1:Q:115:ASN:C	1:Q:115:ASN:HD22	2.23	0.47
1:U:115:ASN:C	1:U:115:ASN:HD22	2.23	0.47
1:U:178:TRP:CE3	1:U:181:MET:HG3	2.50	0.47
1:U:193:VAL:HG11	1:U:209:LEU:HG	1.97	0.47
1:S:143:GLY:HA2	1:T:196:ALA:CB	2.44	0.47
1:Y:120:LEU:HD23	1:Y:245:VAL:CG2	2.40	0.47
1:T:98:PHE:HB3	1:T:99:PRO:HD3	1.97	0.47
1:S:175:LEU:HD13	1:S:187:LEU:HD23	1.96	0.46
1:S:136:ILE:HG22	1:S:138:LEU:HD13	1.98	0.46
1:E:120:LEU:HD11	1:E:217:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:33:SER:OG	1:Q:64:HIS:CE1	2.57	0.46
1:S:11:LYS:HB3	1:S:11:LYS:HZ3	1.79	0.46
1:S:87:MET:HE2	1:S:194:MET:CE	2.42	0.46
1:T:131:LEU:HD23	1:T:131:LEU:HA	1.70	0.46
1:Q:166:TYR:C	1:Q:171[B]:ARG:HH22	2.24	0.46
1:S:139:PRO:HA	1:U:142:SER:HB2	1.98	0.46
1:U:185:ARG:HG3	1:U:185:ARG:HH11	1.81	0.46
1:Q:177:THR:CG2	1:Q:277:ILE:HG23	2.46	0.46
1:T:240:LEU:HD22	1:T:271:LEU:HD11	1.98	0.46
1:E:47:ILE:HG12	1:E:69:VAL:HG22	1.97	0.46
1:Q:164:ASP:OD1	1:Y:254:LYS:NZ	2.39	0.46
1:Y:136:ILE:HG22	1:Y:138:LEU:HD13	1.98	0.46
1:T:170:MET:HE2	1:T:234:ARG:CD	2.46	0.46
1:U:275:VAL:O	1:U:278:LEU:HB3	2.16	0.45
1:S:17:LEU:O	1:S:21:THR:HG22	2.16	0.45
1:T:28:ALA:HA	1:T:79:VAL:O	2.15	0.45
1:T:58:ARG:O	1:T:91:TYR:OH	2.30	0.45
1:Y:64:HIS:CD2	1:Y:84:ARG:H	2.32	0.45
1:E:42:LEU:HD11	1:E:80:MET:HG3	1.97	0.45
1:E:2:GLU:HB2	1:E:150:PRO:HD2	1.95	0.45
1:E:45:ALA:HA	1:E:70:PHE:O	2.16	0.45
1:T:5:TYR:CE2	1:T:98:PHE:HB2	2.52	0.45
1:E:170:MET:HE2	1:E:234:ARG:HD2	1.98	0.45
1:Q:23:HIS:CE1	1:Q:71:GLY:HA2	2.51	0.45
1:Q:29:ILE:HG12	1:Q:112:VAL:HG13	1.98	0.45
1:E:152:ASP:OD1	1:E:152:ASP:C	2.59	0.45
1:Q:130:MET:HA	1:Q:188:GLN:HB2	1.99	0.45
1:S:142:SER:HB2	1:T:139:PRO:HA	1.99	0.45
1:S:167:ASP:O	1:S:171:ARG:HG3	2.17	0.45
1:E:92:PRO:HD2	1:E:95:LYS:HG3	1.99	0.44
1:Q:195:VAL:O	1:Q:219:MET:HA	2.17	0.44
1:E:68:LEU:HD12	1:E:80:MET:O	2.17	0.44
1:T:87:MET:HE2	1:T:87:MET:HB3	1.82	0.44
1:U:29:ILE:HG12	1:U:112:VAL:HG13	1.98	0.44
1:E:202:THR:OG1	1:E:205:GLU:HG3	2.16	0.44
1:S:193:VAL:HG11	1:S:209:LEU:HG	1.98	0.44
1:Q:101:ARG:HD3	4:Q:297:HOH:O	2.18	0.44
1:T:206:CYS:SG	1:T:245:VAL:HG23	2.57	0.44
1:S:139:PRO:HA	1:U:142:SER:CB	2.47	0.44
1:T:242:THR:HG21	1:T:260:VAL:HG13	1.99	0.43
1:Y:17:LEU:O	1:Y:21:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:31:CYS:HA	1:Q:114:THR:OG1	2.19	0.43
1:Y:205:GLU:O	1:Y:206:CYS:C	2.62	0.43
1:Y:256:ASN:HD22	1:Y:258:GLU:HB2	1.83	0.43
1:Q:64:HIS:HD2	1:Q:84:ARG:N	1.97	0.43
1:Q:136:ILE:HG22	1:Q:138:LEU:HD13	2.01	0.43
1:Q:177:THR:O	1:Q:180:GLN:HG3	2.18	0.43
1:S:145:ASN:OD1	1:S:147:LEU:HB2	2.19	0.43
1:Y:85:PHE:O	1:Y:96:VAL:HG13	2.18	0.43
1:Q:171[B]:ARG:CG	1:Q:171[B]:ARG:NH1	2.64	0.43
1:Q:180:GLN:CB	1:S:44:GLN:OE1	2.67	0.43
1:U:15:GLU:O	1:U:19:SER:HB2	2.19	0.43
1:Q:195:VAL:HG13	4:Q:293:HOH:O	2.15	0.43
1:U:210:GLN:HE22	1:U:247:MET:HE2	1.84	0.43
1:E:158:ARG:NH2	1:Q:198:PRO:HG3	2.28	0.43
1:E:248:ASP:OD1	1:E:250:GLU:HB2	2.19	0.43
1:S:206:CYS:HB2	1:S:245:VAL:CG2	2.49	0.43
1:U:206:CYS:SG	1:U:245:VAL:CG2	3.06	0.43
1:S:32:GLY:H	1:S:35:LEU:HD12	1.84	0.42
1:S:171:ARG:HG2	1:S:236:PHE:CE1	2.53	0.42
1:T:168:ARG:O	1:T:172:GLN:HG3	2.19	0.42
1:U:170:MET:HE2	1:U:234:ARG:HD2	2.01	0.42
1:S:29:ILE:HG23	1:S:112:VAL:HG22	2.01	0.42
1:E:250:GLU:O	1:E:251:SER:C	2.60	0.42
1:S:128:ASP:OD1	1:S:185:ARG:HD3	2.18	0.42
1:Q:61:VAL:HG22	1:Q:64:HIS:ND1	2.34	0.42
1:S:114:THR:HG22	1:S:238:PHE:CZ	2.54	0.42
1:U:175:LEU:HD12	1:U:187:LEU:HD23	2.01	0.42
1:Y:164:ASP:CG	1:Y:229:ARG:HH21	2.27	0.42
1:E:123:LYS:HA	1:E:123:LYS:CE	2.50	0.42
1:E:211:LYS:O	1:Q:211:LYS:HE3	2.19	0.42
1:Q:140:GLY:HA2	1:Q:144:GLN:O	2.20	0.42
1:Q:161:ALA:HA	1:Y:200:PHE:HB2	2.02	0.42
1:S:141:PHE:HA	1:T:195:VAL:HG22	2.00	0.42
1:Y:98:PHE:HB3	1:Y:99:PRO:HD3	2.01	0.42
1:Q:88:TYR:HB2	1:Q:198:PRO:HD3	2.01	0.42
1:S:29:ILE:HD12	1:S:80:MET:HE2	2.01	0.42
1:U:129:ILE:HD11	1:U:271:LEU:HD23	2.02	0.42
1:Y:68:LEU:HD12	1:Y:80:MET:O	2.18	0.42
1:Y:92:PRO:HD2	1:Y:95:LYS:HG3	2.02	0.42
1:E:218:GLY:HA2	2:E:290:IM5:N3	2.35	0.42
1:E:87:MET:HB3	1:E:87:MET:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3:ASN:HD22	1:T:4:GLY:N	2.18	0.41
1:U:162:MET:HE1	1:U:229:ARG:HB2	2.01	0.41
1:E:170:MET:HE3	1:E:236:PHE:HB2	2.01	0.41
1:E:269:GLN:HA	1:E:272:GLU:OE2	2.20	0.41
1:Q:181:MET:CG	1:Q:273:GLN:HG3	2.49	0.41
1:S:121:ASN:HA	1:S:122:PRO:HD2	1.84	0.41
1:S:201:GLU:H	1:S:201:GLU:CD	2.27	0.41
1:S:73:LEU:HD21	1:S:275:VAL:HG12	2.03	0.41
1:E:29:ILE:HG12	1:E:112:VAL:HG13	2.02	0.41
1:Q:73:LEU:HD22	1:Q:80:MET:HE2	2.01	0.41
1:Q:193:VAL:HG11	1:Q:209:LEU:HG	2.01	0.41
1:T:282:ILE:HG22	1:T:283:PRO:O	2.19	0.41
1:U:10:TYR:CD1	1:U:101:ARG:HB2	2.56	0.41
1:Y:109:ASP:OD1	1:Y:109:ASP:C	2.63	0.41
1:E:170:MET:CE	1:E:236:PHE:HB2	2.50	0.41
1:Q:1:MET:HG2	1:Q:148:ARG:CD	2.43	0.41
1:Q:131:LEU:HD11	1:Q:187:LEU:HD23	2.03	0.41
1:U:220:SER:O	1:U:221:THR:HB	2.20	0.41
1:Y:223:PRO:O	1:Y:227:VAL:HG13	2.21	0.41
1:E:269:GLN:HE21	1:E:269:GLN:CA	2.20	0.41
1:Q:11:LYS:HB3	1:Q:11:LYS:HE2	1.86	0.41
1:S:178:TRP:CD2	1:S:187:LEU:HD13	2.55	0.41
1:U:172:GLN:HE21	1:U:172:GLN:HB2	1.77	0.41
1:Y:135:HIS:CD2	1:Y:135:HIS:C	2.99	0.41
1:Q:201:GLU:N	1:Q:201:GLU:CD	2.79	0.41
1:S:87:MET:CE	1:S:194:MET:CE	2.98	0.41
1:U:114:THR:HG22	1:U:238:PHE:CZ	2.56	0.41
1:Y:124:PHE:N	1:Y:124:PHE:CD1	2.89	0.41
1:E:62:PRO:HA	1:E:63:GLY:HA2	1.89	0.40
1:T:172:GLN:HE21	1:T:172:GLN:HB2	1.69	0.40
1:T:178:TRP:CE3	1:T:181:MET:HG3	2.56	0.40
1:U:131:LEU:HG	1:U:187:LEU:HD21	2.04	0.40
1:Q:135:HIS:HA	1:Q:192:TYR:O	2.21	0.40
1:S:147:LEU:HD22	1:S:226:ILE:CG2	2.51	0.40
1:Y:115:ASN:HD22	1:Y:115:ASN:C	2.30	0.40
1:T:2:GLU:CB	1:T:150:PRO:HD2	2.51	0.40
1:E:1:MET:HE3	1:E:1:MET:HB3	1.97	0.40
1:Q:183:GLU:HB2	1:Q:185:ARG:H	1.86	0.40
1:Q:201:GLU:CD	1:Q:201:GLU:H	2.30	0.40
1:T:17:LEU:O	1:T:21:THR:HG22	2.21	0.40
1:U:99:PRO:HA	1:U:102:VAL:HG13	2.04	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	E	286/324 (88%)	274 (96%)	12 (4%)	0	100	100
1	Q	286/324 (88%)	275 (96%)	10 (4%)	1 (0%)	36	46
1	S	284/324 (88%)	274 (96%)	10 (4%)	0	100	100
1	T	285/324 (88%)	274 (96%)	11 (4%)	0	100	100
1	U	284/324 (88%)	273 (96%)	10 (4%)	1 (0%)	30	38
1	Y	283/324 (87%)	276 (98%)	7 (2%)	0	100	100
All	All	1708/1944 (88%)	1646 (96%)	60 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	181	MET
1	U	44	GLN

### 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	E	240/269 (89%)	209 (87%)	31 (13%)	4	4
1	Q	240/269 (89%)	212 (88%)	28 (12%)	5	6
1	S	238/269 (88%)	205 (86%)	33 (14%)	3	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	239/269 (89%)	209 (87%)	30 (13%)	4	5
1	U	238/269 (88%)	211 (89%)	27 (11%)	5	7
1	Y	237/269 (88%)	214 (90%)	23 (10%)	8	10
All	All	1432/1614 (89%)	1260 (88%)	172 (12%)	5	5

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	MET
1	E	2	GLU
1	E	3	ASN
1	E	15	GLU
1	E	18	LEU
1	E	19	SER
1	E	61	VAL
1	E	87	MET
1	E	101	ARG
1	E	102	VAL
1	E	106	LEU
1	E	112	VAL
1	E	115	ASN
1	E	123	LYS
1	E	131	LEU
1	E	138	LEU
1	E	147	LEU
1	E	175	LEU
1	E	195	VAL
1	E	208	VAL
1	E	209	LEU
1	E	212	LEU
1	E	227	VAL
1	E	244	LYS
1	E	245	VAL
1	E	259	GLU
1	E	260	VAL
1	E	266	GLN
1	E	269	GLN
1	E	272	GLU
1	E	278	LEU
1	Q	1	MET
1	Q	18	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Q	19	SER
1	Q	58	ARG
1	Q	61	VAL
1	Q	74	ASN
1	Q	101	ARG
1	Q	102	VAL
1	Q	106	LEU
1	Q	112	VAL
1	Q	115	ASN
1	Q	138	LEU
1	Q	147	LEU
1	Q	171[A]	ARG
1	Q	171[B]	ARG
1	Q	173	ARG
1	Q	175	LEU
1	Q	180	GLN
1	Q	184	GLN
1	Q	185	ARG
1	Q	208	VAL
1	Q	209	LEU
1	Q	212	LEU
1	Q	227	VAL
1	Q	259	GLU
1	Q	269	GLN
1	Q	277	ILE
1	Q	278	LEU
1	S	1	MET
1	S	11	LYS
1	S	18	LEU
1	S	44	GLN
1	S	69	VAL
1	S	74	ASN
1	S	102	VAL
1	S	106	LEU
1	S	112	VAL
1	S	115	ASN
1	S	126	VAL
1	S	138	LEU
1	S	147	LEU
1	S	163	SER
1	S	168	ARG
1	S	173	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	S	175	LEU
1	S	177	THR
1	S	180	GLN
1	S	185	ARG
1	S	195	VAL
1	S	208	VAL
1	S	209	LEU
1	S	227	VAL
1	S	245	VAL
1	S	247	MET
1	S	250	GLU
1	S	265	LYS
1	S	269	GLN
1	S	270	LYS
1	S	273	GLN
1	S	278	LEU
1	S	279	MET
1	T	-1	THR
1	T	18	LEU
1	T	19	SER
1	T	51	SER
1	T	73	LEU
1	T	101	ARG
1	T	102	VAL
1	T	106	LEU
1	T	112	VAL
1	T	115	ASN
1	T	126	VAL
1	T	138	LEU
1	T	147	LEU
1	T	172	GLN
1	T	173	ARG
1	T	175	LEU
1	T	177	THR
1	T	184	GLN
1	T	195	VAL
1	T	208	VAL
1	T	209	LEU
1	T	210	GLN
1	T	212	LEU
1	T	227	VAL
1	T	247	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	T	250	GLU
1	T	254	LYS
1	T	266	GLN
1	T	277	ILE
1	T	278	LEU
1	U	11	LYS
1	U	18	LEU
1	U	19	SER
1	U	44	GLN
1	U	58	ARG
1	U	61	VAL
1	U	84	ARG
1	U	102	VAL
1	U	106	LEU
1	U	112	VAL
1	U	115	ASN
1	U	131	LEU
1	U	138	LEU
1	U	147	LEU
1	U	176	SER
1	U	208	VAL
1	U	209	LEU
1	U	212	LEU
1	U	226	ILE
1	U	227	VAL
1	U	247	MET
1	U	266	GLN
1	U	276	SER
1	U	277	ILE
1	U	278	LEU
1	U	281	SER
1	U	286	ASP
1	Y	1	MET
1	Y	11	LYS
1	Y	18	LEU
1	Y	58	ARG
1	Y	61	VAL
1	Y	69	VAL
1	Y	102	VAL
1	Y	106	LEU
1	Y	112	VAL
1	Y	115	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Y	138	LEU
1	Y	172	GLN
1	Y	173	ARG
1	Y	175	LEU
1	Y	177	THR
1	Y	184	GLN
1	Y	186	GLU
1	Y	195	VAL
1	Y	209	LEU
1	Y	227	VAL
1	Y	265	LYS
1	Y	276	SER
1	Y	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	3	ASN
1	E	44	GLN
1	E	115	ASN
1	E	151	ASN
1	E	188	GLN
1	E	256	ASN
1	E	266	GLN
1	E	269	GLN
1	Q	64	HIS
1	Q	115	ASN
1	Q	180	GLN
1	Q	184	GLN
1	Q	188	GLN
1	Q	210	GLN
1	Q	256	ASN
1	S	172	GLN
1	S	180	GLN
1	S	210	GLN
1	S	266	GLN
1	S	273	GLN
1	T	3	ASN
1	T	44	GLN
1	T	55	ASN
1	T	172	GLN
1	T	180	GLN

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Mol	Chain	Res	Type
1	T	184	GLN
1	T	256	ASN
1	U	3	ASN
1	U	46	GLN
1	U	115	ASN
1	U	172	GLN
1	U	256	ASN
1	U	266	GLN
1	U	273	GLN
1	Y	46	GLN
1	Y	64	HIS
1	Y	115	ASN
1	Y	172	GLN
1	Y	210	GLN
1	Y	256	ASN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

18 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	Q	290	-	22,22,22	2.12	4 (18%)	25,32,32	2.19	6 (24%)
2	IM5	T	291	-	22,22,22	2.19	4 (18%)	25,32,32	2.13	9 (36%)
3	PO4	Q	291	-	4,4,4	1.30	0	6,6,6	0.69	0
3	PO4	S	292	-	4,4,4	0.83	0	6,6,6	1.16	0
2	IM5	U	290	-	22,22,22	2.02	4 (18%)	25,32,32	2.07	7 (28%)
2	IM5	Y	292	-	22,22,22	2.11	3 (13%)	25,32,32	2.24	5 (20%)
3	PO4	T	290	-	4,4,4	0.94	0	6,6,6	0.86	0
3	PO4	E	292	-	4,4,4	0.98	0	6,6,6	0.36	0
3	PO4	Q	292	-	4,4,4	1.17	0	6,6,6	0.51	0
3	PO4	S	290	-	4,4,4	1.39	1 (25%)	6,6,6	0.81	0
3	PO4	Y	293	-	4,4,4	0.97	0	6,6,6	0.95	0
3	PO4	U	291	-	4,4,4	0.86	0	6,6,6	0.93	0
3	PO4	Y	290	-	4,4,4	0.95	0	6,6,6	0.93	0
3	PO4	Y	291	-	4,4,4	0.91	0	6,6,6	0.56	0
2	IM5	E	290	-	22,22,22	2.07	4 (18%)	25,32,32	2.22	7 (28%)
2	IM5	S	291	-	22,22,22	2.13	3 (13%)	25,32,32	2.16	7 (28%)
3	PO4	E	291	-	4,4,4	0.94	0	6,6,6	0.63	0
3	PO4	T	292	-	4,4,4	1.21	0	6,6,6	0.59	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	Q	290	-	-	1/6/18/18	0/3/3/3
2	IM5	T	291	-	-	3/6/18/18	0/3/3/3
2	IM5	U	290	-	-	0/6/18/18	0/3/3/3
2	IM5	Y	292	-	-	1/6/18/18	0/3/3/3
2	IM5	E	290	-	-	1/6/18/18	0/3/3/3
2	IM5	S	291	-	-	3/6/18/18	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	291	IM5	C5-C4	8.86	1.47	1.38
2	T	291	IM5	C5-C4	8.79	1.47	1.38
2	Y	292	IM5	C5-C4	8.69	1.46	1.38
2	E	290	IM5	C5-C4	8.32	1.46	1.38
2	Q	290	IM5	C5-C4	8.19	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	290	IM5	C5-C4	8.18	1.46	1.38
2	T	291	IM5	C5-N7	-3.09	1.33	1.38
2	E	290	IM5	C5-N7	-2.95	1.33	1.38
2	Q	290	IM5	C6-N1	-2.67	1.33	1.38
2	S	291	IM5	C5-N7	-2.49	1.34	1.38
2	E	290	IM5	C6-N1	-2.48	1.34	1.38
2	T	291	IM5	C5-C6	2.41	1.49	1.41
2	U	290	IM5	C5-N7	-2.38	1.34	1.38
2	Y	292	IM5	C5-C6	2.35	1.48	1.41
2	Y	292	IM5	C5-N7	-2.30	1.34	1.38
2	Q	290	IM5	C5-C6	2.27	1.48	1.41
2	T	291	IM5	C6-N1	-2.25	1.34	1.38
2	Q	290	IM5	C5-N7	-2.24	1.34	1.38
2	U	290	IM5	C6-N1	-2.18	1.34	1.38
3	S	290	PO4	P-O2	-2.17	1.48	1.54
2	U	290	IM5	C5-C6	2.14	1.48	1.41
2	S	291	IM5	C5-C6	2.04	1.48	1.41
2	E	290	IM5	C5-C6	2.02	1.47	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	292	IM5	C4-C5-C6	-7.94	114.42	121.41
2	E	290	IM5	C4-C5-C6	-7.38	114.92	121.41
2	U	290	IM5	C4-C5-C6	-7.26	115.03	121.41
2	S	291	IM5	C4-C5-C6	-7.19	115.08	121.41
2	Q	290	IM5	C4-C5-C6	-6.59	115.61	121.41
2	T	291	IM5	C4-C5-C6	-6.27	115.90	121.41
2	Q	290	IM5	C5-C4-N3	-4.50	120.74	124.86
2	Y	292	IM5	C6-C5-N7	4.14	139.05	131.14
2	T	291	IM5	C6-C5-N7	4.00	138.78	131.14
2	E	290	IM5	C6'-C4'-C5'	-3.74	107.57	112.71
2	E	290	IM5	C6-C5-N7	3.62	138.06	131.14
2	U	290	IM5	C6-C5-N7	3.44	137.71	131.14
2	S	291	IM5	O6-C6-C5	-3.35	119.18	127.26
2	Q	290	IM5	C6-C5-N7	3.34	137.52	131.14
2	S	291	IM5	C6-C5-N7	3.06	136.98	131.14
2	U	290	IM5	C3'-C2'-N1'	-2.97	98.98	104.47
2	T	291	IM5	C5-C4-N3	-2.90	122.21	124.86
2	S	291	IM5	C5-C4-N3	-2.68	122.41	124.86
2	T	291	IM5	C9-C10-N1'	2.64	117.07	113.38
2	U	290	IM5	O6-C6-C5	-2.59	121.01	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	290	IM5	O6-C6-C5	-2.59	121.02	127.26
2	T	291	IM5	C5-C4-C9	2.43	108.35	105.75
2	Q	290	IM5	C5-C6-N1	2.39	118.70	112.13
2	Y	292	IM5	C6'-N1'-C2'	2.39	107.59	104.12
2	Q	290	IM5	C4-N3-C2	2.36	120.33	116.63
2	S	291	IM5	C9-C10-N1'	2.35	116.67	113.38
2	E	290	IM5	O6-C6-C5	-2.35	121.61	127.26
2	E	290	IM5	C6'-N1'-C2'	2.33	107.50	104.12
2	U	290	IM5	O3'-C3'-C4'	-2.27	105.15	111.76
2	S	291	IM5	C9-C8-N7	2.26	112.14	109.22
2	T	291	IM5	C9-C8-N7	2.26	112.14	109.22
2	S	291	IM5	C5-C6-N1	2.24	118.27	112.13
2	Y	292	IM5	C9-C10-N1'	2.20	116.46	113.38
2	U	290	IM5	C5-C4-N3	-2.17	122.87	124.86
2	T	291	IM5	C3'-C2'-N1'	-2.13	100.53	104.47
2	T	291	IM5	C6'-C4'-C5'	2.07	115.55	112.71
2	Y	292	IM5	C10-N1'-C2'	-2.06	109.45	113.39
2	T	291	IM5	C10-N1'-C2'	-2.04	109.49	113.39
2	E	290	IM5	O5'-C5'-C4'	-2.03	106.63	111.26
2	U	290	IM5	C5-C6-N1	2.01	117.66	112.13
2	E	290	IM5	C3'-C2'-N1'	-2.00	100.77	104.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	290	IM5	C9-C10-N1'-C6'
2	Q	290	IM5	C9-C10-N1'-C6'
2	S	291	IM5	C9-C10-N1'-C6'
2	S	291	IM5	C3'-C4'-C5'-O5'
2	S	291	IM5	C6'-C4'-C5'-O5'
2	T	291	IM5	C9-C10-N1'-C6'
2	T	291	IM5	C3'-C4'-C5'-O5'
2	T	291	IM5	C6'-C4'-C5'-O5'
2	Y	292	IM5	C9-C10-N1'-C6'

There are no ring outliers.

3 monomers are involved in 3 short contacts:

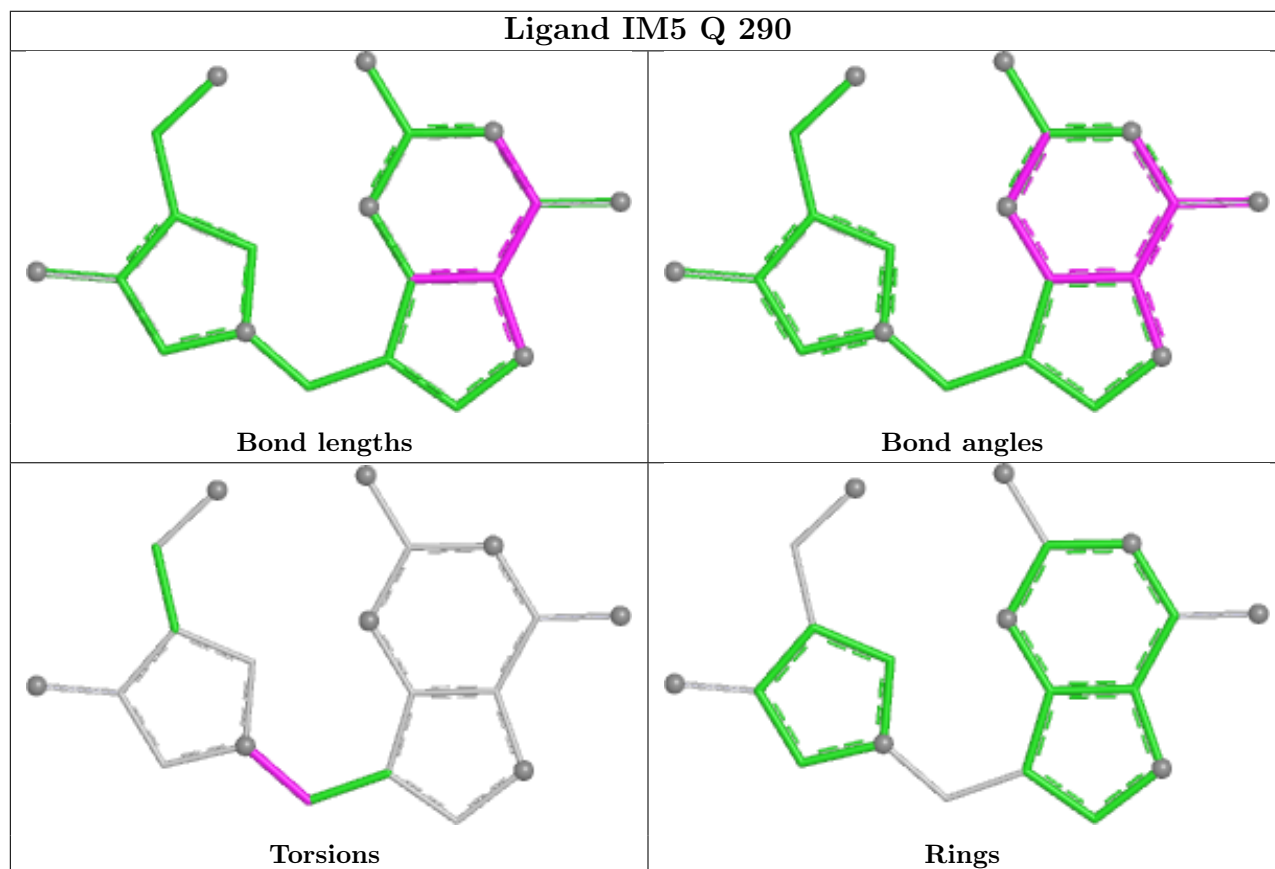
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	U	290	IM5	1	0

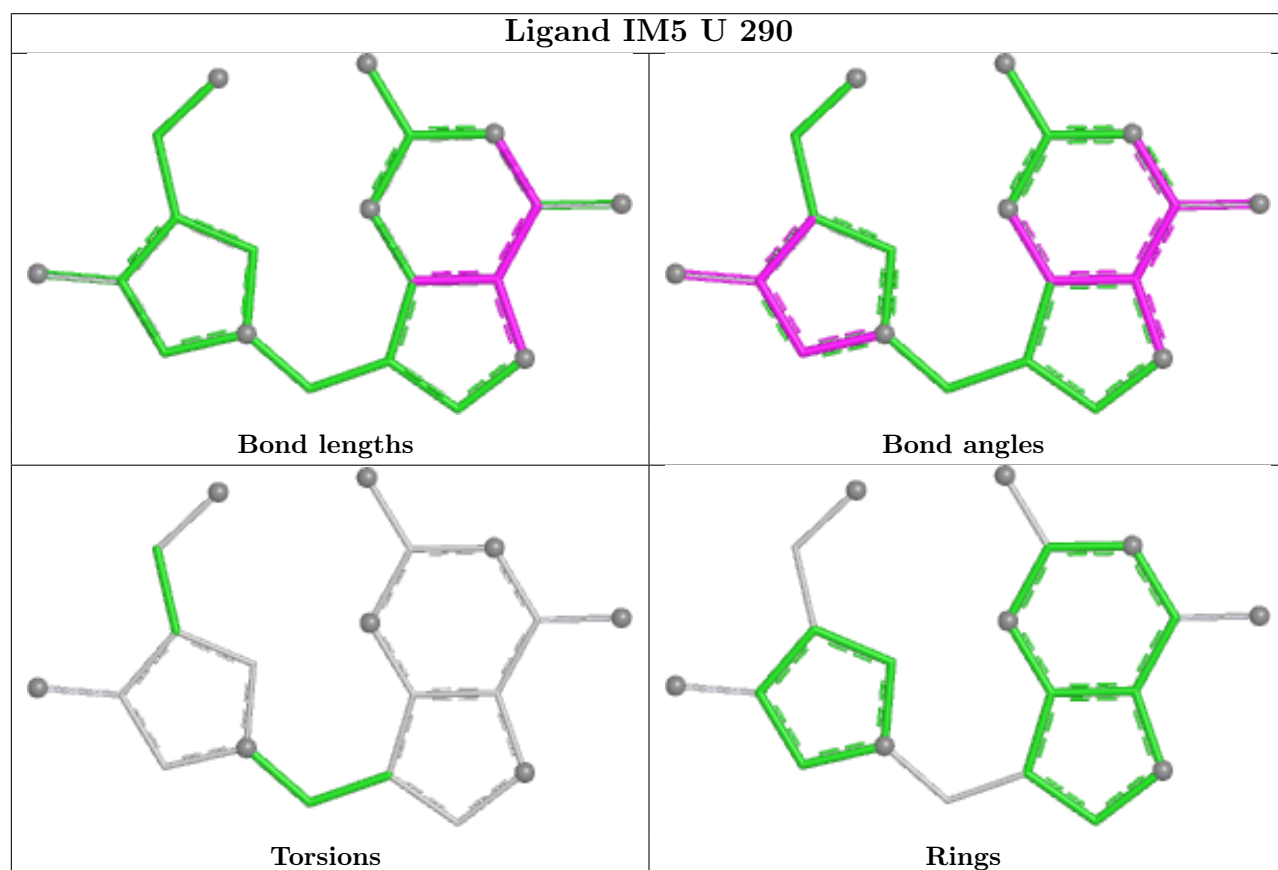
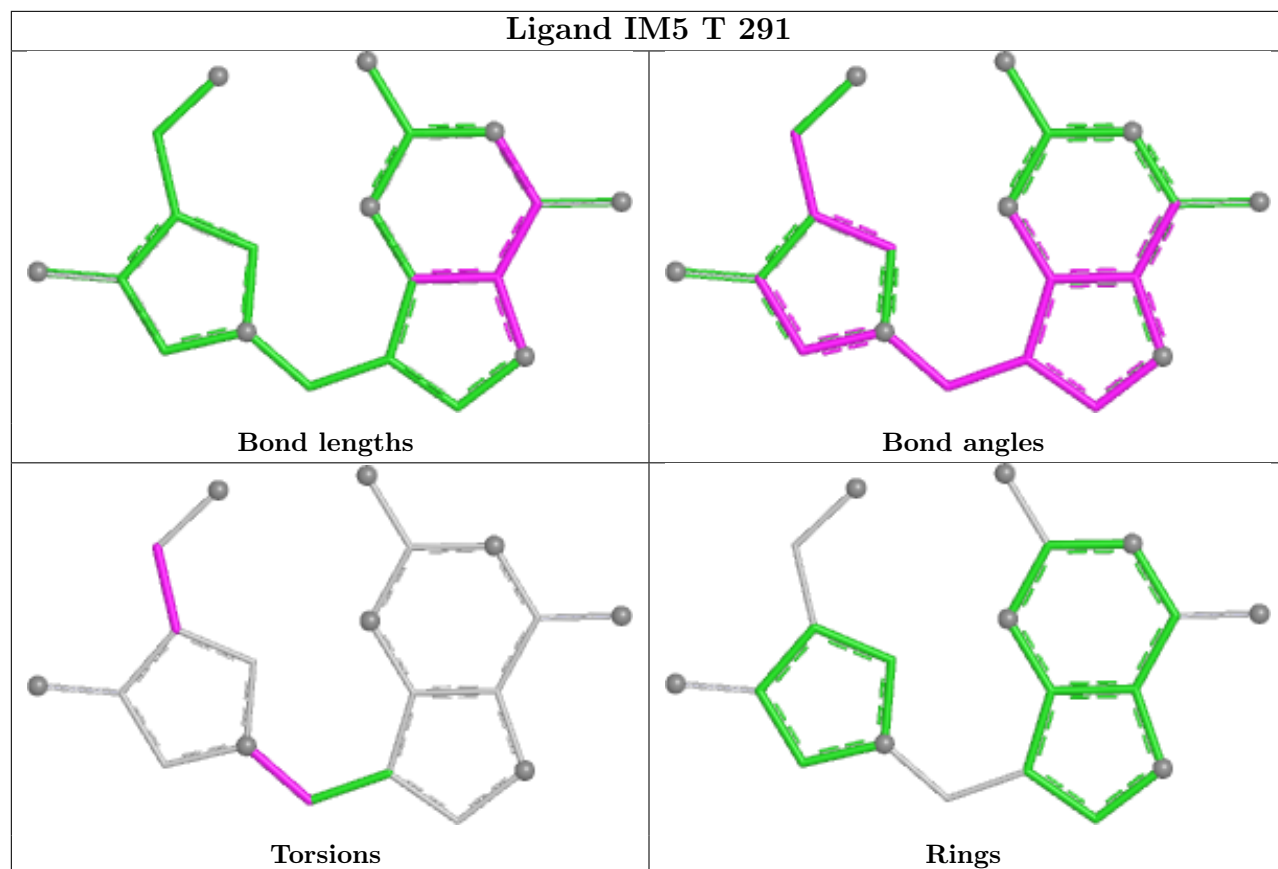
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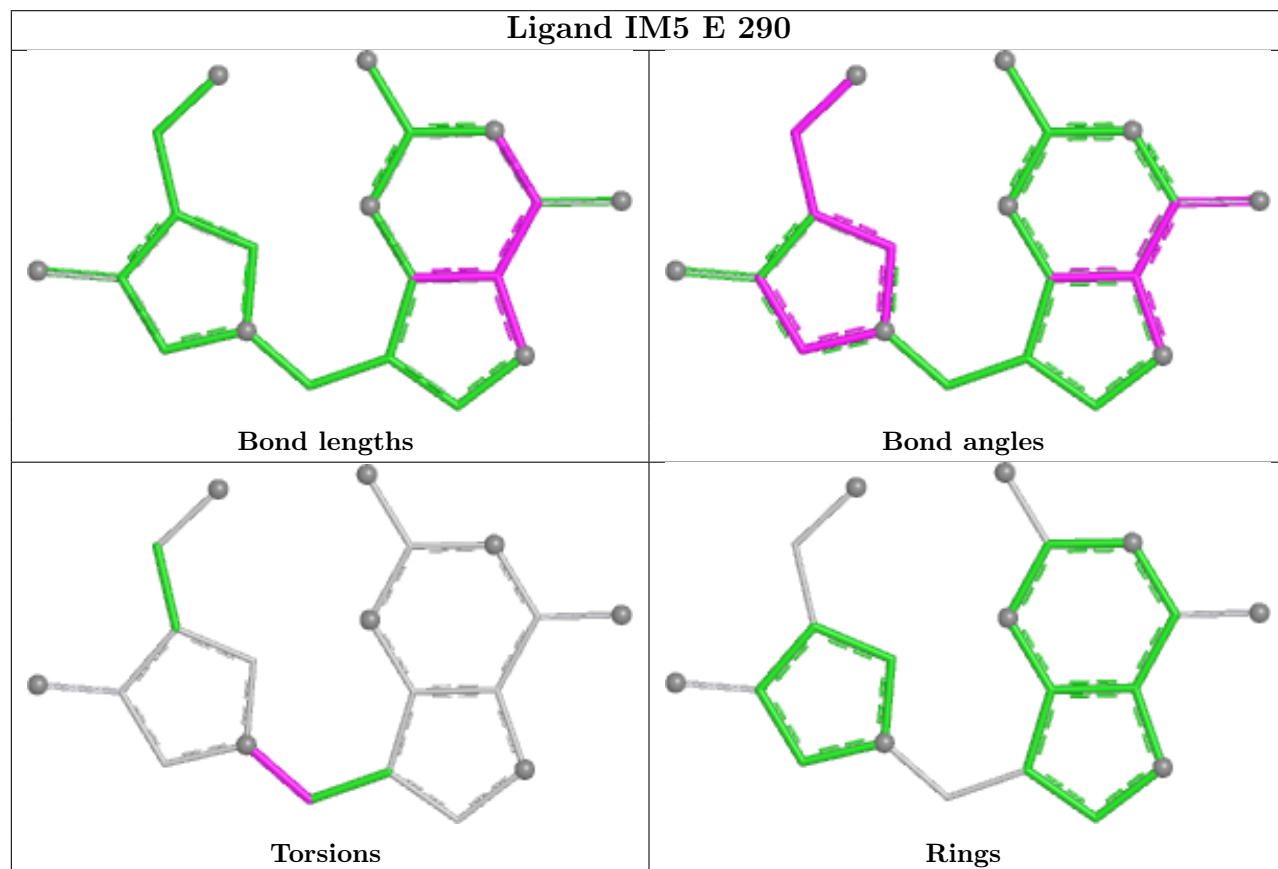
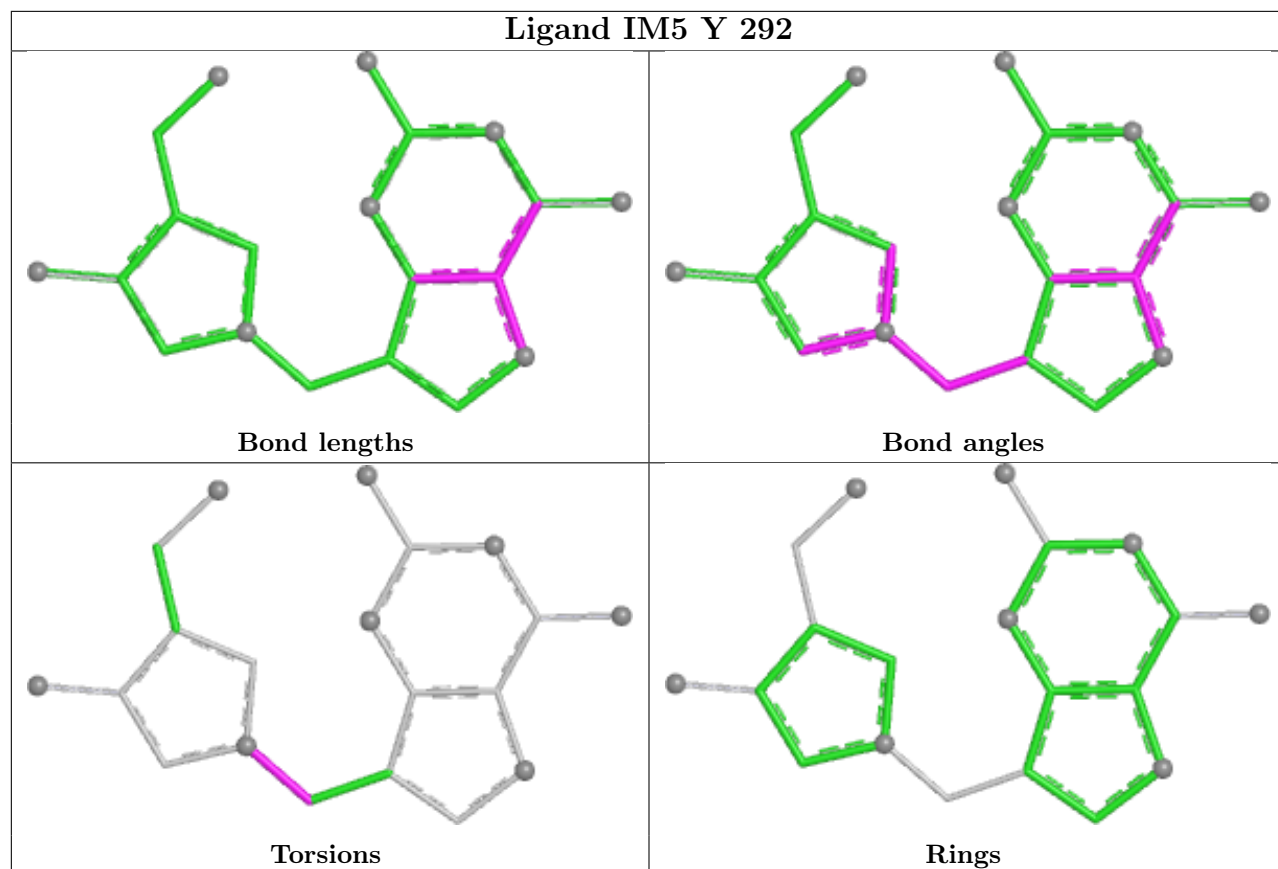
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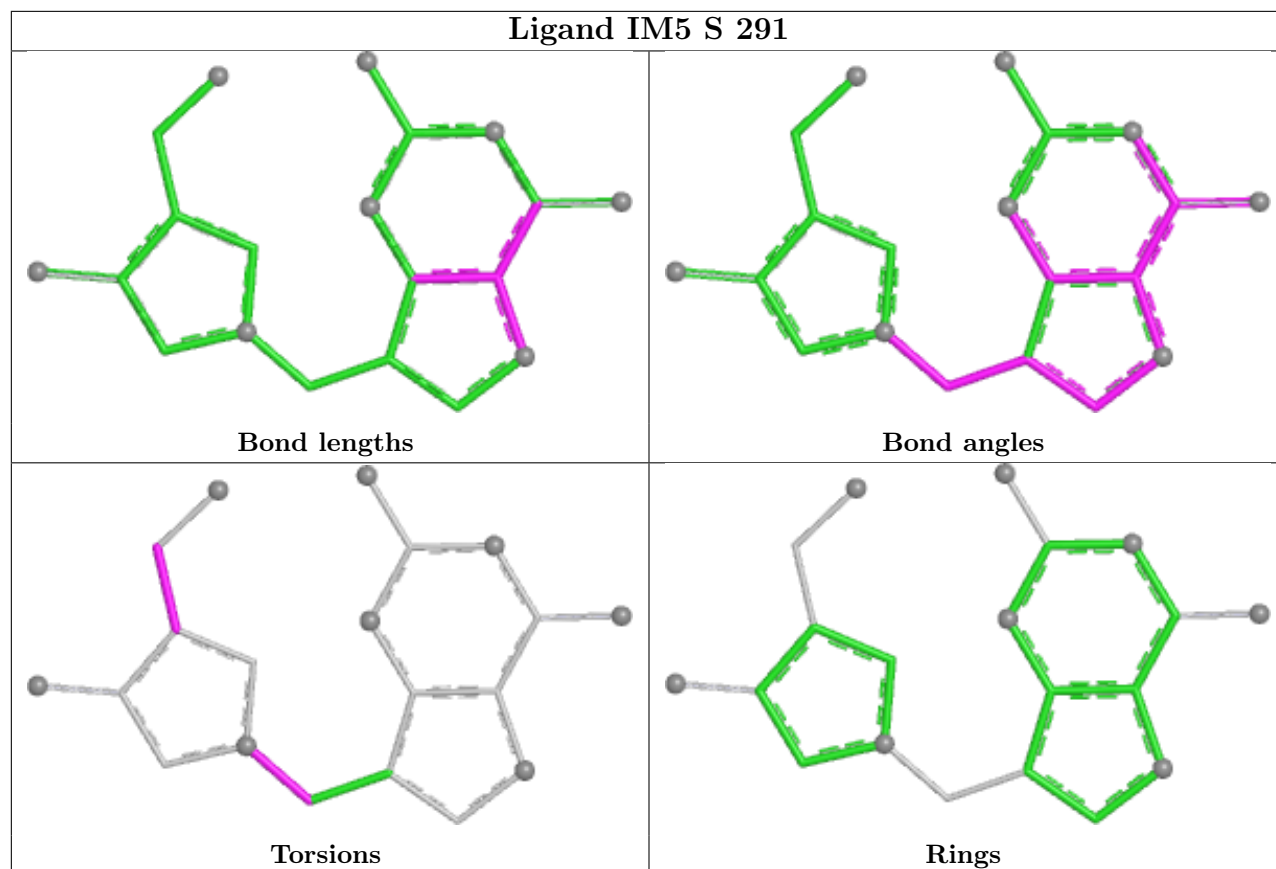
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	290	PO4	1	0
2	E	290	IM5	1	0

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, 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	E	288/324 (88%)	0.05	4 (1%) 73 75	20, 45, 67, 80	0
1	Q	287/324 (88%)	-0.09	4 (1%) 73 75	24, 42, 62, 81	1 (0%)
1	S	286/324 (88%)	-0.09	2 (0%) 84 85	27, 44, 65, 86	0
1	T	287/324 (88%)	0.12	2 (0%) 84 85	28, 51, 65, 77	0
1	U	285/324 (87%)	0.09	1 (0%) 88 89	23, 48, 72, 83	1 (0%)
1	Y	285/324 (87%)	-0.06	1 (0%) 88 89	31, 42, 63, 72	0
All	All	1718/1944 (88%)	0.00	14 (0%) 82 83	20, 45, 68, 86	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	182	GLY	3.1
1	Q	181	MET	3.1
1	S	0	LEU	2.7
1	Q	1	MET	2.5
1	E	0	LEU	2.5
1	E	1	MET	2.5
1	S	180	GLN	2.4
1	T	-2	PRO	2.3
1	Q	182	GLY	2.3
1	Y	1	MET	2.3
1	T	252	LEU	2.2
1	E	-1	THR	2.2
1	Q	184	GLN	2.1
1	U	182	GLY	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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

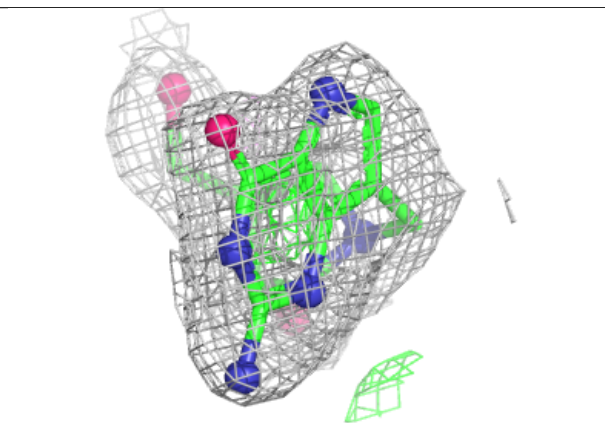
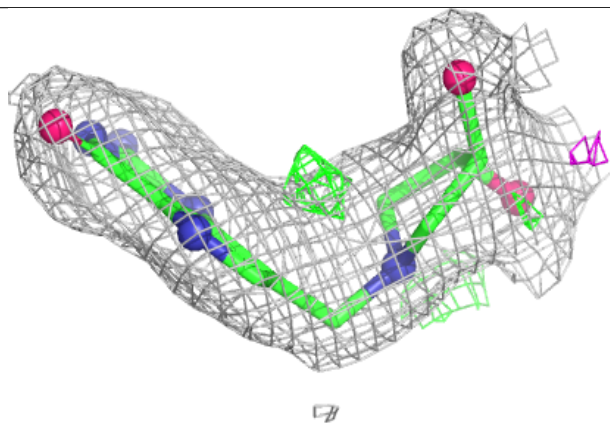
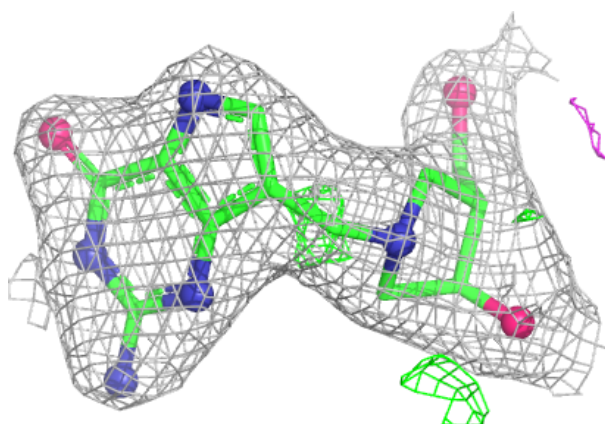
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	PO4	Y	291	5/5	0.74	0.13	95,95,95,95	0
3	PO4	Q	292	5/5	0.89	0.14	67,67,68,68	0
3	PO4	E	292	5/5	0.89	0.14	64,64,66,67	0
3	PO4	Y	290	5/5	0.91	0.09	62,62,62,63	0
2	IM5	U	290	20/20	0.92	0.07	32,36,39,41	0
2	IM5	E	290	20/20	0.93	0.08	33,38,42,45	0
3	PO4	T	290	5/5	0.93	0.12	66,66,66,67	0
3	PO4	S	290	5/5	0.94	0.11	48,49,49,50	0
2	IM5	T	291	20/20	0.95	0.07	29,33,38,43	0
3	PO4	T	292	5/5	0.95	0.07	42,44,46,47	0
3	PO4	U	291	5/5	0.95	0.07	42,42,44,44	0
2	IM5	S	291	20/20	0.95	0.06	32,36,39,42	0
2	IM5	Y	292	20/20	0.95	0.07	34,36,39,41	0
2	IM5	Q	290	20/20	0.96	0.05	26,30,37,37	0
3	PO4	S	292	5/5	0.97	0.05	39,39,41,42	0
3	PO4	E	291	5/5	0.97	0.05	36,37,38,41	0
3	PO4	Y	293	5/5	0.97	0.05	35,35,36,36	0
3	PO4	Q	291	5/5	0.98	0.04	35,36,37,40	0

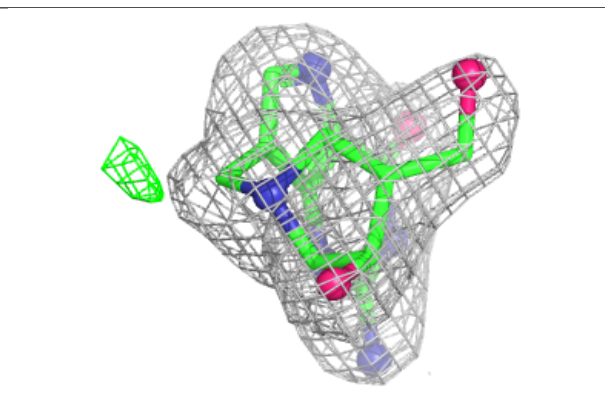
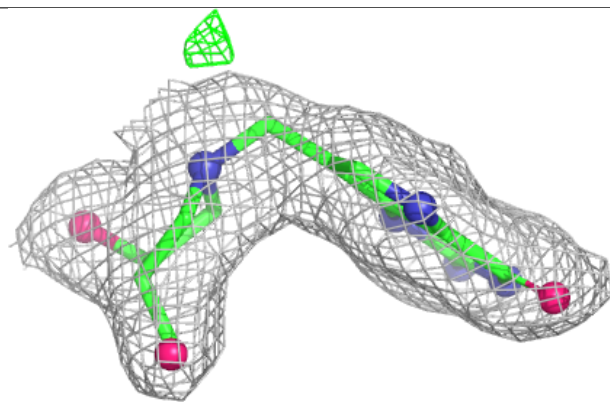
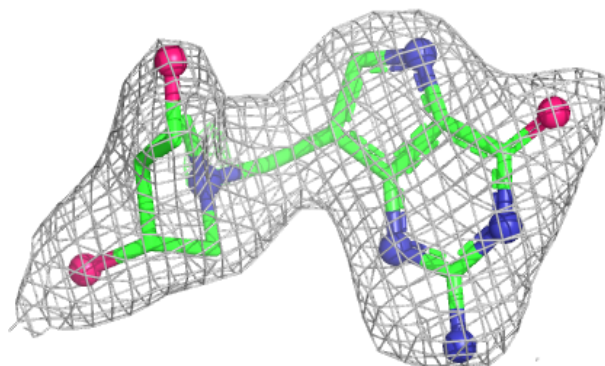
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around IM5 U 290:**

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

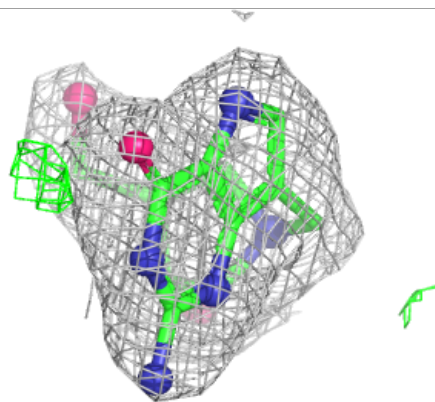
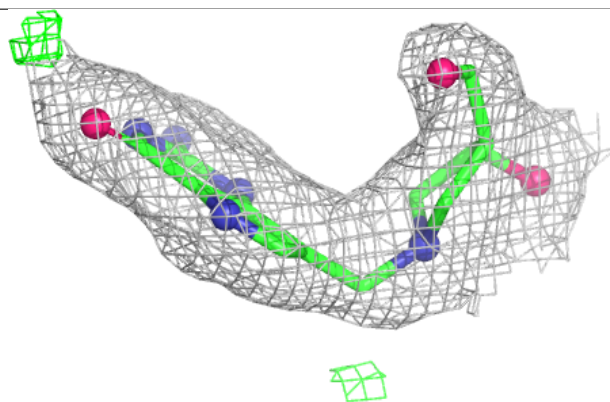
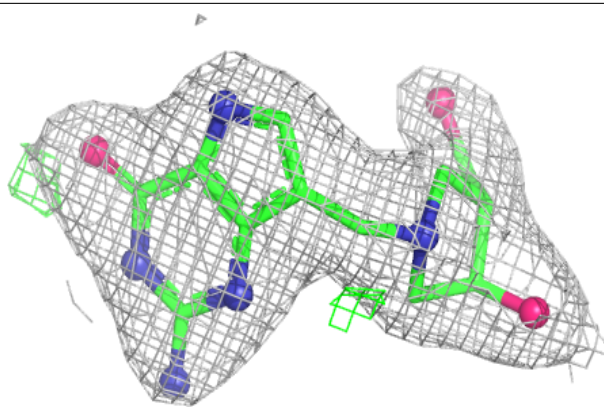
**Electron density around IM5 E 290:**

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

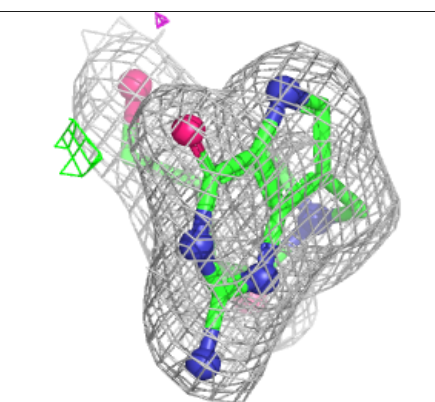
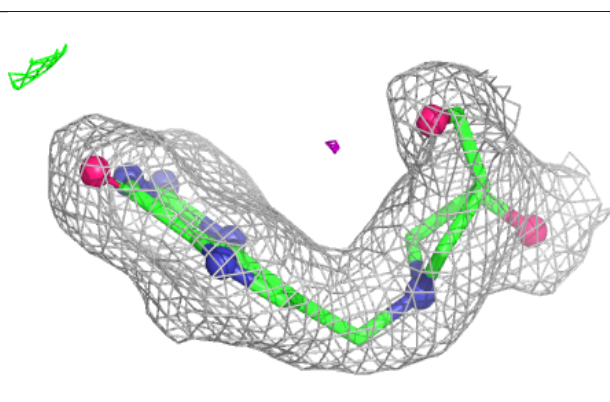
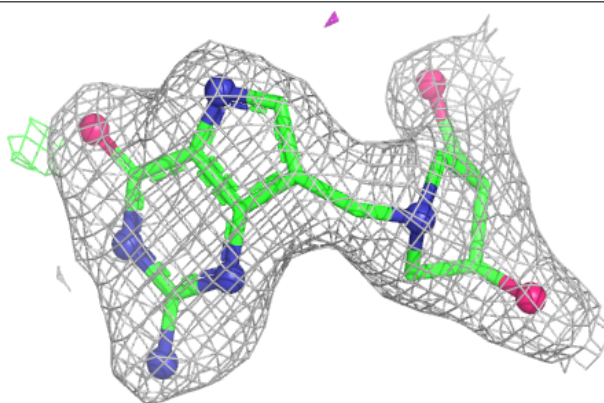


**Electron density around IM5 T 291:**

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

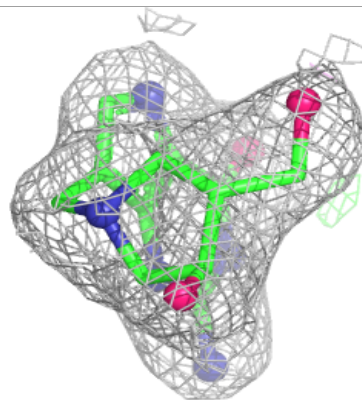
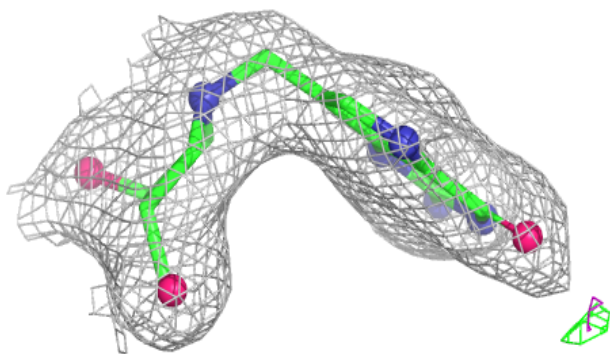
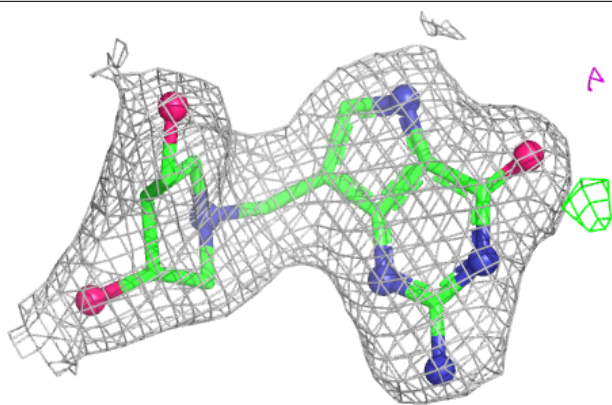
**Electron density around IM5 S 291:**

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

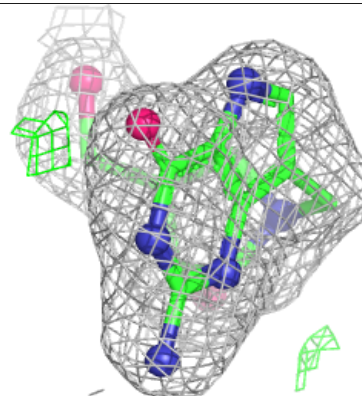
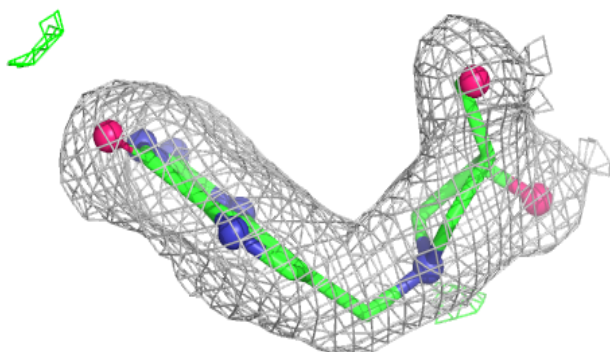
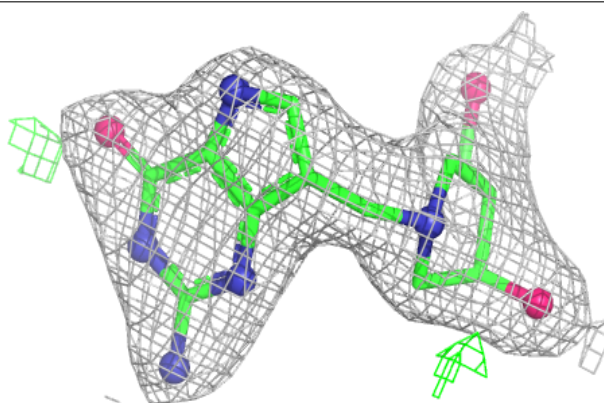


**Electron density around IM5 Y 292:**

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

**Electron density around IM5 Q 290:**

$2mF_o-DF_c$  (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.