



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:43 pm BST

PDB ID : 3PHB  
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.

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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

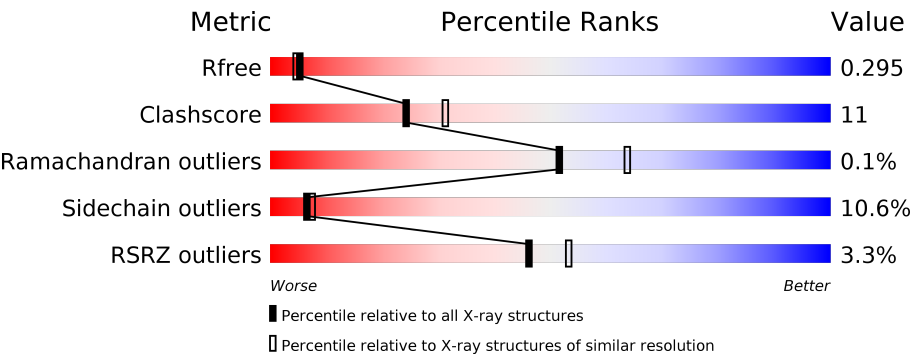
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	E	324	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>64%21%5%11%</div></div>
1	Q	324	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>62%22%••11%</div></div>
1	S	324	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>65%19%•12%</div></div>
1	T	324	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>69%16%•11%</div></div>
1	U	324	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>63%22%•12%</div></div>
1	Y	324	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>67%19%•12%</div></div>

## 2 Entry composition

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
1	E	288	Total	C	N	O	S	0	0	0
			2252	1433	393	410	16			
1	Q	287	Total	C	N	O	S	0	1	0
			2256	1434	396	410	16			
1	S	286	Total	C	N	O	S	0	0	0
			2238	1424	391	407	16			
1	T	287	Total	C	N	O	S	0	0	0
			2245	1428	392	409	16			
1	U	285	Total	C	N	O	S	0	1	0
			2241	1424	395	407	15			
1	Y	285	Total	C	N	O	S	0	0	0
			2230	1418	390	406	16			

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

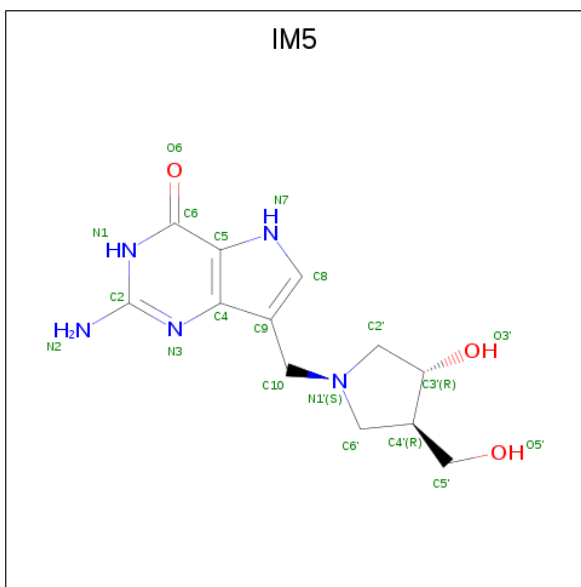
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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-29	HIS	-	EXPRESSION TAG	UNP P00491
Y	-28	HIS	-	EXPRESSION TAG	UNP P00491
Y	-27	HIS	-	EXPRESSION TAG	UNP P00491
Y	-26	HIS	-	EXPRESSION TAG	UNP P00491
Y	-25	HIS	-	EXPRESSION TAG	UNP P00491
Y	-24	GLY	-	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

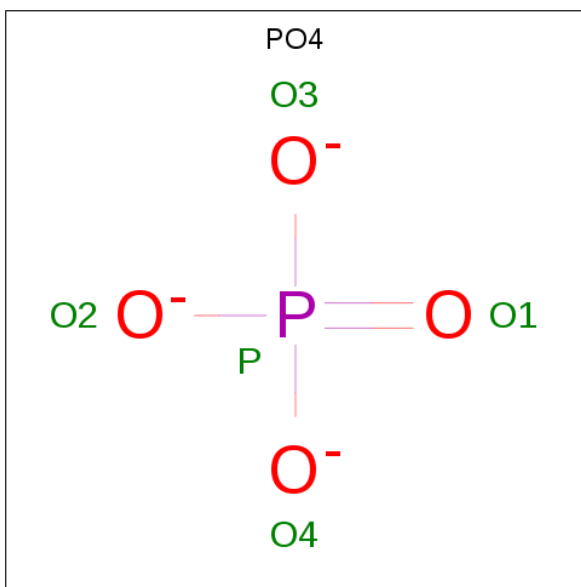
- Molecule 2 is 2-amino-7-{[(3R,4R)-3-hydroxy-4-(hydroxymethyl)pyrrolidin-1-yl]methyl}-3,5-dihydro-4H-pyrrolo[3,2-d]pyrimidin-4-one (three-letter code: IM5) (formula: C<sub>12</sub>H<sub>17</sub>N<sub>5</sub>O<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	S	1	Total	O	P	0	0
			5	4	1		
3	S	1	Total	O	P	0	0
			5	4	1		
3	T	1	Total	O	P	0	0
			5	4	1		
3	T	1	Total	O	P	0	0
			5	4	1		
3	U	1	Total	O	P	0	0
			5	4	1		
3	Y	1	Total	O	P	0	0
			5	4	1		
3	Y	1	Total	O	P	0	0
			5	4	1		
3	Y	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

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

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 ( $\text{RSRZ} > 2$ ). 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.

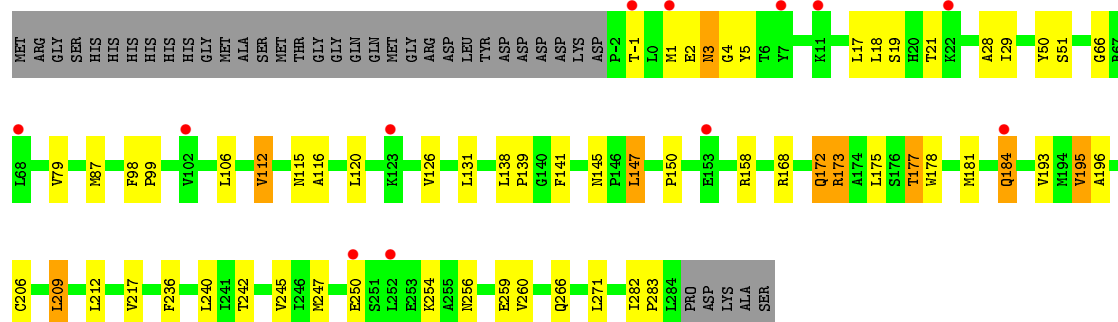
- Chain E:
- 
- Sequence logo for Chain E. The y-axis represents information content in bits (0.00 to 0.20). The x-axis lists amino acids. A color scale at the top indicates conservation levels: 2% (red), 64% (green), 21% (yellow), 5% (orange), and 11% (grey).
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1        | Met        | 0.00                       |
| 2        | Arg        | 0.00                       |
| 3        | Gly        | 0.00                       |
| 4        | Ser        | 0.00                       |
| 5        | His        | 0.00                       |
| 6        | His        | 0.00                       |
| 7        | His        | 0.00                       |
| 8        | His        | 0.00                       |
| 9        | His        | 0.00                       |
| 10       | His        | 0.00                       |
| 11       | His        | 0.00                       |
| 12       | His        | 0.00                       |
| 13       | His        | 0.00                       |
| 14       | His        | 0.00                       |
| 15       | Met        | 0.00                       |
| 16       | Met        | 0.00                       |
| 17       | Ala        | 0.00                       |
| 18       | Ser        | 0.00                       |
| 19       | Ser        | 0.00                       |
| 20       | Met        | 0.00                       |
| 21       | Thr        | 0.00                       |
| 22       | Gly        | 0.00                       |
| 23       | Gln        | 0.00                       |
| 24       | Gln        | 0.00                       |
| 25       | Met        | 0.00                       |
| 26       | Gly        | 0.00                       |
| 27       | Arg        | 0.00                       |
| 28       | Asp        | 0.00                       |
| 29       | Leu        | 0.00                       |
| 30       | Tyr        | 0.00                       |
| 31       | Asp        | 0.00                       |
| 32       | Asp        | 0.00                       |
| 33       | Asp        | 0.00                       |
| 34       | Lys        | 0.00                       |
| 35       | Asp        | 0.00                       |
| 36       | P-2        | 0.00                       |
| 37       | T-1        | 0.00                       |
| 38       | L0         | 0.00                       |
| 39       | M1         | 0.00                       |
| 40       | E2         | 0.00                       |
| 41       | N3         | 0.00                       |
| 42       | G4         | 0.00                       |
| 43       | Y5         | 0.00                       |
| 44       | T6         | 0.00                       |
| 45       | T7         | 0.00                       |
| 46       | E8         | 0.00                       |
| 47       | D9         | 0.00                       |
| 48       | E15        | 0.00                       |
| 49       | L18        | 0.00                       |
| 50       | S19        | 0.00                       |
| 51       | I29        | 0.00                       |
| 52       | G32        | 0.00                       |
| 53       | L38        | 0.00                       |
| 54       | L42        | 0.00                       |
| 55       | A45        | 0.00                       |
| 56       | G46        | 0.00                       |
| 57       | G47        | 0.00                       |
| 58       | L47        | 0.00                       |
| 59       | P150       | 0.00                       |
| 60       | H51        | 0.00                       |
| 61       | D52        | 0.00                       |
| 62       | E153       | 0.00                       |
| 63       | G156       | 0.00                       |
| 64       | D157       | 0.00                       |
| 65       | R158       | 0.00                       |
| 66       | F159       | 0.00                       |
| 67       | M170       | 0.00                       |
| 68       | L175       | 0.00                       |
| 69       | G176       | 0.00                       |
| 70       | T177       | 0.00                       |
| 71       | Q180       | 0.00                       |
| 72       | M181       | 0.00                       |
| 73       | G182       | 0.00                       |
| 74       | E183       | 0.00                       |
| 75       | Q184       | 0.00                       |
| 76       | L187       | 0.00                       |
| 77       | V193       | 0.00                       |
| 78       | E201       | 0.00                       |
| 79       | T202       | 0.00                       |
| 80       | E205       | 0.00                       |
| 81       | C206       | 0.00                       |
| 82       | R207       | 0.00                       |
| 83       | V208       | 0.00                       |
| 84       | L209       | 0.00                       |
| 85       | Q210       | 0.00                       |
| 86       | K211       | 0.00                       |
| 87       | L212       | 0.00                       |
| 88       | V217       | 0.00                       |
| 89       | G218       | 0.00                       |
| 90       | V227       | 0.00                       |
| 91       | F236       | 0.00                       |
| 92       | G237       | 0.00                       |
| 93       | F238       | 0.00                       |
| 94       | S239       | 0.00                       |
| 95       | K244       | 0.00                       |
| 96       | V245       | 0.00                       |
| 97       | D248       | 0.00                       |
| 98       | Y249       | 0.00                       |
| 99       | E250       | 0.00                       |
| 100      | N256       | 0.00                       |
| 101      | E257       | 0.00                       |
| 102      | E258       | 0.00                       |
| 103      | E259       | 0.00                       |
| 104      | V260       | 0.00                       |
| 105      | Q266       | 0.00                       |
| 106      | K269       | 0.00                       |
| 107      | K270       | 0.00                       |
| 108      | L271       | 0.00                       |
| 109      | E272       | 0.00                       |
| 110      | Q273       | 0.00                       |
| 111      | P285       | 0.00                       |
| 112      | ASP        | 0.00                       |
| 113      | LYS        | 0.00                       |
| 114      | ALA        | 0.00                       |
| 115      | PER        | 0.00                       |

- Chain Q:
- 
- | Category | Percentage |
|----------|------------|
| Green    | 62%        |
| Yellow   | 22%        |
| Red      | 2%         |
| Grey     | 11%        |

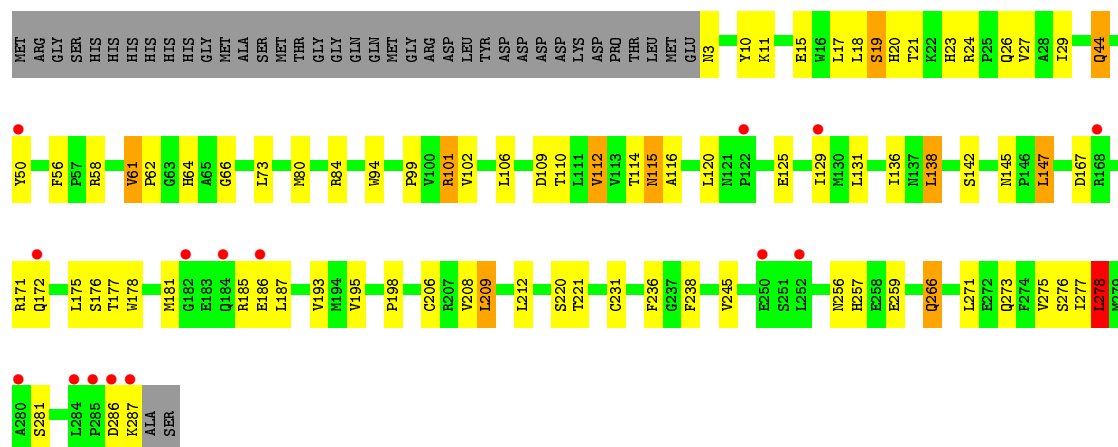
- Chain S:
- 
- | Category | Percentage |
|----------|------------|
| Green    | 65%        |
| Yellow   | 19%        |
| Red      | 4%         |
| Grey     | 12%        |
- Legend: MET, ARG, GLY, SER, HIS, THR, GLN, MET, ALA, SER, MET, THR, GLY, GLN, MET, ARG, ASP, LEU, TYR, ASP, ASP, ASP, LYS, ASP, PRO, THR, I47, R53, V69, L73, N74, G75, R76, M81, R84, M87, V102, L106, V112, V113, T114, M115, N121, P122, K123, D128, I136, N137, L138, P139, F141, S142, G143, Q144, N145, P146, L147, E153, A165, Y166, D167, M170, R171, L175, S176, T177, W178, K179, I180



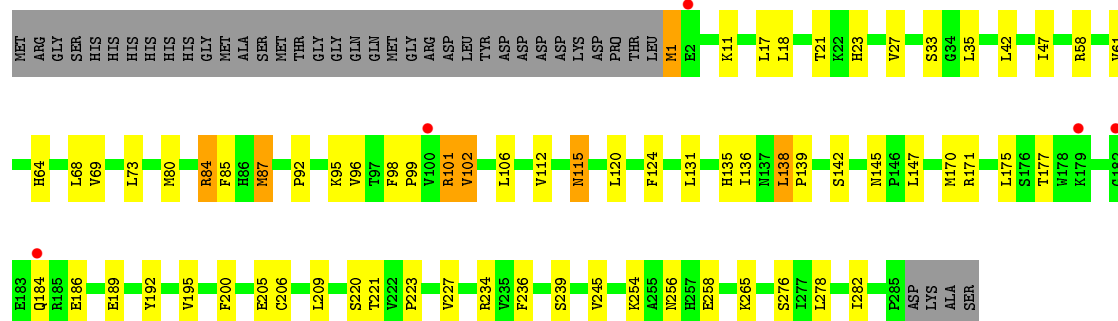
• Molecule 1: Purine nucleoside phosphorylase



• Molecule 1: Purine nucleoside phosphorylase



• Molecule 1: Purine nucleoside phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	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) 98.9 (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)	Xtriage
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	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.004 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage'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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	E	0.70	0/2305	0.77	1/3120 (0.0%)
1	Q	0.68	0/2308	0.77	2/3123 (0.1%)
1	S	0.64	0/2290	0.74	1/3099 (0.0%)
1	T	0.62	0/2297	0.72	0/3108
1	U	0.67	1/2293 (0.0%)	0.71	1/3102 (0.0%)
1	Y	0.65	0/2282	0.75	2/3088 (0.1%)
All	All	0.66	1/13775 (0.0%)	0.74	7/18640 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	231	CYS	CB-SG	-5.65	1.72	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	101	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	Q	101	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	Y	101	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	U	278	LEU	CA-CB-CG	5.45	127.84	115.30
1	Q	101	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	S	175	LEU	CA-CB-CG	5.37	127.66	115.30
1	E	63	GLY	N-CA-C	-5.04	100.51	113.10

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	62	0
1	Q	2256	0	2238	81	0
1	S	2238	0	2219	48	0
1	T	2245	0	2226	37	0
1	U	2241	0	2219	53	0
1	Y	2230	0	2208	45	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	298	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 11.

All (298) 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:HG3	1:Q:171[A]:ARG:HH21	1.13	1.07
1:T:184:GLN:HE21	1:T:184:GLN:H	1.02	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:Q:171[B]:ARG:HG3	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:HG22	1:U:177:THR:O	1.86	0.76
1:T:131:LEU:HD21	1:T:236:PHE:CZ	2.20	0.75
1:T:184:GLN:NE2	1:T:184:GLN:H	1.81	0.75
1:Y:73:LEU:HD22	1:Y:80:MET:HE1	1.70	0.74
1:E:269:GLN:HA	1:E:269:GLN:HE21	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:N	1:T:184:GLN:HE21	1.85	0.72
1:Q:195:VAL:CG1	4:Q:293:HOH:O	2.39	0.70
1:E:153:GLU:HA	1:E:156:GLY:O	1.91	0.69
1:U:177:THR:O	1:U:177:THR:CG2	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:U:256:ASN:ND2	1:U:259:GLU:H	1.93	0.67
1:E:145:ASN:OD1	1:E:147:LEU:HB2	1.95	0.66
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:E:115:ASN:HD22	1:E:115:ASN:C	2.00	0.65
1:Q:142:SER:CB	1:Y:139:PRO:HA	2.26	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:S:87:MET:HE2	1:S:194:MET:HE1	1.78	0.64
1:Q:181:MET:HG2	1:Q:273:GLN:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:125:GLU:HB2	1:U:185:ARG:HH12	1.62	0.64
1:Q:143:GLY:HA2	1:Y:87:MET:HE2	1.79	0.63
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: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:Q:182:GLY:C	1:Q:183:GLU:HG2	2.20	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:Q:73:LEU:HD22	1:Q:80:MET:HE1	1.85	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
1:E:170:MET:HE3	1:E:236:PHE:HB2	1.85	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:171[B]:ARG:HH11	1:Q:171[B]:ARG:CB	2.20	0.55
1:Q:171[B]:ARG:CB	1:Q:171[B]:ARG:NH1	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:Q:166:TYR:CB	1:Q:171[B]:ARG:NH2	2.70	0.54
1:U:266:GLN:HA	1:U:266:GLN:HE21	1.71	0.54
1:Y:135:HIS:HA	1:Y:192:TYR:O	2.07	0.54
1:U:73:LEU:HD22	1:U:80:MET:HE1	1.89	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: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:101:ARG:HH11	1:Y:101:ARG:HG2	1.73	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: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
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: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:171[A]:ARG:CG	1:Q:171[A]:ARG:HH21	1.99	0.51
1:Q:61:VAL:HG13	4:Q:296:HOH:O	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:201:GLU:H	1:E:201:GLU:CD	2.14	0.51
1:Q:171[B]:ARG:HB2	1:Q:171[B]:ARG:CZ	2.41	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:E:6:THR:O	1:E:9:ASP:HB2	2.11	0.50
1:S:258:GLU:CD	1:S:258:GLU:H	2.15	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: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:115:ASN:ND2	1:E:115:ASN:C	2.65	0.49
1:Q:195:VAL:HG12	4:Q:293:HOH:O	2.10	0.49
1:U:23:HIS:O	1:U:24:ARG:HD3	2.12	0.49
1:E:90:GLY:O	1:Y:1:MET:HA	2.13	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:E:258:GLU:H	1:E:258:GLU:CD	2.17	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:T:1:MET:CG	3:T:290:PO4:O4	2.62	0.48
1:Q:141:PHE:CZ	1:Y:205:GLU:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:CYS:SG	1:S:245:VAL:HG22	2.53	0.47
1:S:30:ILE:HG12	1:S:81:MET:SD	2.54	0.47
1:U:167:ASP:O	1:U:171:ARG:HG3	2.13	0.47
1:U:62:PRO:O	1:U:257:HIS:NE2	2.34	0.47
1:Y:131:LEU:HD22	1:Y:236:PHE:CZ	2.49	0.47
1:Q:-1:THR:HG21	1:Y:95:LYS:NZ	2.29	0.47
1:E:38:LEU:HD21	1:E:271:LEU:HB3	1.96	0.47
1:Q:38:LEU:HD21	1:Q:271:LEU:HB3	1.97	0.47
1:Q:30:ILE:HG12	1:Q:81:MET:SD	2.54	0.47
1:E:3:ASN:ND2	1:E:5:TYR:HB2	2.30	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:Q:182:GLY:C	1:Q:183:GLU:CG	2.84	0.47
1:S:115:ASN:HD22	1:S:115:ASN:C	2.18	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
1:Q:33:SER:OG	1:Q:64:HIS:CE1	2.57	0.46
1:T:131:LEU:HD23	1:T:131:LEU:HA	1.70	0.46
1:S:139:PRO:HA	1:U:142:SER:HB2	1.98	0.46
1:U:185:ARG:HH11	1:U:185:ARG:HG3	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: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:S:87:MET:HE2	1:S:194:MET:CE	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:29:ILE:HG12	1:Q:112:VAL:HG13	1.98	0.45
1:Q:23:HIS:CE1	1:Q:71:GLY:HA2	2.51	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:E:8:GLU:CD	1:E:8:GLU:H	2.21	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
1:Q:31:CYS:HA	1:Q:114:THR:OG1	2.19	0.43
1:Y:256:ASN:HD22	1:Y:258:GLU:HB2	1.83	0.43
1:Q:136:ILE:HG22	1:Q:138:LEU:HD13	2.01	0.43
1:Q:64:HIS:HD2	1:Q:84:ARG:N	1.97	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:NH1	1:Q:171[B]:ARG:CG	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:E:248:ASP:OD1	1:E:250:GLU:HB2	2.19	0.43
1:E:158:ARG:NH2	1:Q:198:PRO:HG3	2.28	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:171:ARG:HG2	1:S:236:PHE:CE1	2.53	0.42
1:S:32:GLY:H	1:S:35:LEU:HD12	1.84	0.42
1:T:168:ARG:O	1:T:172:GLN:HG3	2.19	0.42
1:S:29:ILE:HG23	1:S:112:VAL:HG22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:175:LEU:HD12	1:U:187:LEU:HD23	2.01	0.42
1:U:115:ASN:HD22	1:U:115:ASN:C	2.23	0.42
1:E:123:LYS:CE	1:E:123:LYS:HA	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: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:T:3:ASN:HD22	1:T:4:GLY:N	2.18	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:Q:166:TYR:C	1:Q:171[B]:ARG:HH22	2.24	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:193:VAL:HG11	1:Q:209:LEU:HG	2.01	0.41
1:Q:115:ASN:C	1:Q:115:ASN:HD22	2.23	0.41
1:T:282:ILE:HG22	1:T:283:PRO:O	2.19	0.41
1:S:177:THR:HG22	1:S:181:MET:CE	2.51	0.41
1:U:10:TYR:CD1	1:U:101:ARG:HB2	2.56	0.41
1:Q:131:LEU:HD11	1:Q:187:LEU:HD23	2.03	0.41
1:Q:1:MET:HG2	1:Q:148:ARG:CD	2.43	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: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:E:269:GLN:HE21	1:E:269:GLN:CA	2.20	0.41
1:E:170:MET:CE	1:E:236:PHE:HB2	2.50	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:T:87:MET:HB3	1:T:87:MET:HE2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:T:2:GLU:CB	1:T:150:PRO:HD2	2.51	0.40
1:E:152:ASP:C	1:E:152:ASP:OD1	2.59	0.40
1:Q:183:GLU:HB2	1:Q:185:ARG:H	1.86	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

### 5.3.1 Protein backbone

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%)	41	50
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%)	34	42
1	Y	283/324 (87%)	276 (98%)	7 (2%)	0	100	100
All	All	1708/1944 (88%)	1646 (96%)	60 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

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



### 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	E	240/269 (89%)	212 (88%)	28 (12%)	5	6
1	Q	240/269 (89%)	210 (88%)	30 (12%)	4	5
1	S	238/269 (88%)	212 (89%)	26 (11%)	6	7
1	T	239/269 (89%)	216 (90%)	23 (10%)	8	10
1	U	238/269 (88%)	213 (90%)	25 (10%)	7	8
1	Y	237/269 (88%)	216 (91%)	21 (9%)	9	11
All	All	1432/1614 (89%)	1279 (89%)	153 (11%)	6	7

All (153) 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	56	PHE
1	E	61	VAL
1	E	87	MET
1	E	101	ARG
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	175	LEU
1	E	208	VAL
1	E	209	LEU
1	E	212	LEU
1	E	227	VAL
1	E	244	LYS

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Mol	Chain	Res	Type
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	Q	1	MET
1	Q	18	LEU
1	Q	19	SER
1	Q	22	LYS
1	Q	58	ARG
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	175	LEU
1	Q	180	GLN
1	Q	181	MET
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	250	GLU
1	Q	259	GLU
1	Q	269	GLN
1	Q	273	GLN
1	Q	277	ILE
1	Q	278	LEU
1	S	1	MET
1	S	18	LEU
1	S	22	LYS
1	S	44	GLN
1	S	74	ASN
1	S	84	ARG

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Mol	Chain	Res	Type
1	S	102	VAL
1	S	106	LEU
1	S	112	VAL
1	S	115	ASN
1	S	138	LEU
1	S	147	LEU
1	S	175	LEU
1	S	177	THR
1	S	180	GLN
1	S	185	ARG
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	273	GLN
1	S	278	LEU
1	T	-1	THR
1	T	3	ASN
1	T	18	LEU
1	T	19	SER
1	T	51	SER
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	209	LEU
1	T	212	LEU
1	T	247	MET
1	T	250	GLU
1	T	254	LYS

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Mol	Chain	Res	Type
1	T	266	GLN
1	U	11	LYS
1	U	18	LEU
1	U	19	SER
1	U	44	GLN
1	U	56	PHE
1	U	58	ARG
1	U	61	VAL
1	U	84	ARG
1	U	101	ARG
1	U	106	LEU
1	U	112	VAL
1	U	115	ASN
1	U	138	LEU
1	U	147	LEU
1	U	176	SER
1	U	186	GLU
1	U	208	VAL
1	U	209	LEU
1	U	212	LEU
1	U	266	GLN
1	U	276	SER
1	U	278	LEU
1	U	281	SER
1	U	286	ASP
1	U	287	LYS
1	Y	1	MET
1	Y	11	LYS
1	Y	18	LEU
1	Y	35	LEU
1	Y	58	ARG
1	Y	84	ARG
1	Y	87	MET
1	Y	102	VAL
1	Y	106	LEU
1	Y	112	VAL
1	Y	115	ASN
1	Y	138	LEU
1	Y	175	LEU
1	Y	177	THR
1	Y	184	GLN
1	Y	186	GLU

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Mol	Chain	Res	Type
1	Y	195	VAL
1	Y	209	LEU
1	Y	265	LYS
1	Y	276	SER
1	Y	278	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	3	ASN
1	E	44	GLN
1	E	115	ASN
1	E	151	ASN
1	E	256	ASN
1	E	266	GLN
1	E	269	GLN
1	E	273	GLN
1	Q	64	HIS
1	Q	115	ASN
1	Q	180	GLN
1	Q	184	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	115	ASN
1	T	172	GLN
1	T	180	GLN
1	T	184	GLN
1	T	256	ASN
1	U	3	ASN
1	U	115	ASN
1	U	172	GLN
1	U	256	ASN
1	U	266	GLN
1	U	273	GLN
1	Y	64	HIS
1	Y	115	ASN

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Mol	Chain	Res	Type
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 carbohydrates 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	Y	292	-	19,22,22	1.22	1 (5%)	17,32,32	2.71	6 (35%)
3	PO4	Y	291	-	4,4,4	0.87	0	6,6,6	0.53	0
2	IM5	T	291	-	19,22,22	1.19	1 (5%)	17,32,32	2.51	7 (41%)
3	PO4	T	292	-	4,4,4	1.15	0	6,6,6	0.57	0
3	PO4	E	291	-	4,4,4	0.91	0	6,6,6	0.60	0
3	PO4	Y	293	-	4,4,4	0.92	0	6,6,6	0.90	0
2	IM5	E	290	-	19,22,22	1.03	1 (5%)	17,32,32	2.60	6 (35%)
3	PO4	Y	290	-	4,4,4	0.90	0	6,6,6	0.89	0
3	PO4	T	290	-	4,4,4	0.90	0	6,6,6	0.82	0
3	PO4	S	290	-	4,4,4	1.33	1 (25%)	6,6,6	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	Q	292	-	4,4,4	1.11	0	6,6,6	0.49	0
3	PO4	S	292	-	4,4,4	0.79	0	6,6,6	1.11	0
3	PO4	U	291	-	4,4,4	0.82	0	6,6,6	0.89	0
2	IM5	Q	290	-	19,22,22	1.28	1 (5%)	17,32,32	2.29	4 (23%)
3	PO4	Q	291	-	4,4,4	1.25	0	6,6,6	0.66	0
2	IM5	U	290	-	19,22,22	1.08	1 (5%)	17,32,32	2.45	5 (29%)
2	IM5	S	291	-	19,22,22	1.11	1 (5%)	17,32,32	2.41	4 (23%)
3	PO4	E	292	-	4,4,4	0.93	0	6,6,6	0.34	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	Y	292	-	-	2/5/18/18	0/3/3/3
2	IM5	T	291	-	-	3/5/18/18	0/3/3/3
2	IM5	E	290	-	-	1/5/18/18	0/3/3/3
2	IM5	Q	290	-	-	0/5/18/18	0/3/3/3
2	IM5	S	291	-	-	3/5/18/18	0/3/3/3
2	IM5	U	290	-	-	0/5/18/18	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	291	IM5	C6-C5	4.48	1.49	1.41
2	Y	292	IM5	C6-C5	4.38	1.48	1.41
2	Q	290	IM5	C6-C5	4.23	1.48	1.41
2	U	290	IM5	C6-C5	4.01	1.48	1.41
2	S	291	IM5	C6-C5	3.85	1.48	1.41
2	E	290	IM5	C6-C5	3.81	1.47	1.41
3	S	290	PO4	P-O2	-2.09	1.48	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	292	IM5	C6-C5-C4	-6.68	114.42	120.80
2	E	290	IM5	C6-C5-C4	-6.16	114.92	120.80
2	U	290	IM5	C6-C5-C4	-6.04	115.03	120.80
2	S	291	IM5	C6-C5-C4	-5.98	115.08	120.80
2	Q	290	IM5	C6-C5-C4	-5.43	115.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	291	IM5	C5-C6-N1	-5.30	116.19	123.43
2	T	291	IM5	C6-C5-C4	-5.13	115.90	120.80
2	E	290	IM5	C6-N1-C2	5.02	123.91	115.93
2	T	291	IM5	C6-N1-C2	4.86	123.65	115.93
2	U	290	IM5	C6-N1-C2	4.72	123.42	115.93
2	Y	292	IM5	C6-N1-C2	4.70	123.40	115.93
2	Y	292	IM5	C5-C6-N1	-4.57	117.18	123.43
2	E	290	IM5	C5-C6-N1	-4.56	117.20	123.43
2	S	291	IM5	C6-N1-C2	4.36	122.85	115.93
2	U	290	IM5	C5-C6-N1	-4.22	117.66	123.43
2	Q	290	IM5	C6-N1-C2	3.97	122.23	115.93
2	S	291	IM5	C5-C6-N1	-3.78	118.27	123.43
2	Q	290	IM5	N3-C2-N1	-3.66	122.35	127.22
2	S	291	IM5	N3-C2-N1	-3.53	122.52	127.22
2	Q	290	IM5	C5-C6-N1	-3.46	118.70	123.43
2	E	290	IM5	N3-C2-N1	-3.22	122.92	127.22
2	Y	292	IM5	N3-C2-N1	-3.11	123.07	127.22
2	U	290	IM5	N3-C2-N1	-3.04	123.17	127.22
2	U	290	IM5	C3'-C2'-N1'	-2.86	98.98	104.44
2	T	291	IM5	N3-C2-N1	-2.69	123.63	127.22
2	Y	292	IM5	C6'-N1'-C2'	2.29	107.59	104.19
2	Y	292	IM5	C10-N1'-C2'	-2.25	109.45	113.27
2	T	291	IM5	C10-N1'-C2'	-2.23	109.49	113.27
2	E	290	IM5	C6'-N1'-C2'	2.23	107.50	104.19
2	E	290	IM5	O5'-C5'-C4'	-2.06	106.63	111.36
2	T	291	IM5	C9-C10-N1'	2.05	117.07	114.14
2	T	291	IM5	C3'-C2'-N1'	-2.05	100.53	104.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Y	292	IM5	C9-C10-N1'-C6'
2	T	291	IM5	C3'-C4'-C5'-O5'
2	T	291	IM5	C6'-C4'-C5'-O5'
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	S	291	IM5	C9-C10-N1'-C6'
2	E	290	IM5	C9-C10-N1'-C6'
2	Y	292	IM5	C9-C10-N1'-C2'

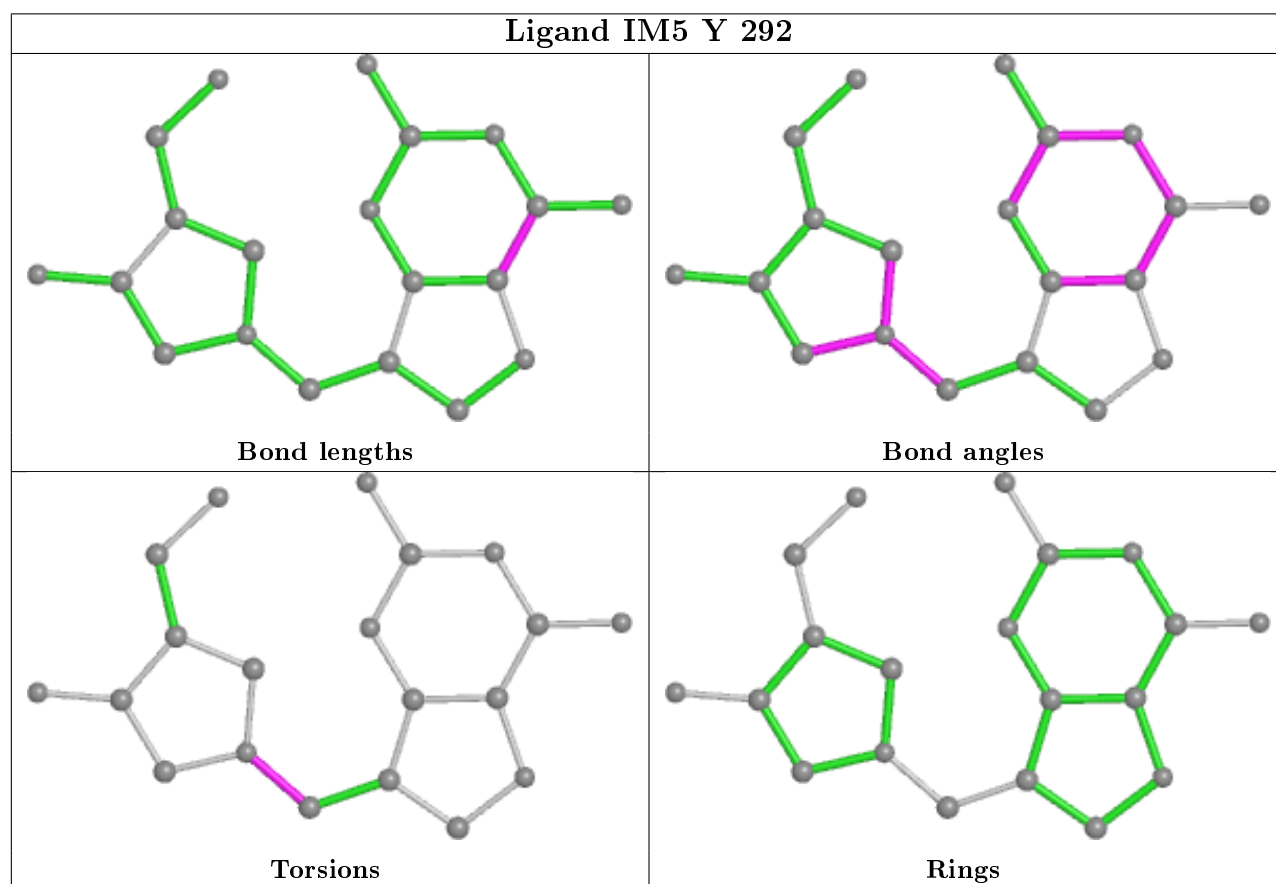


There are no ring outliers.

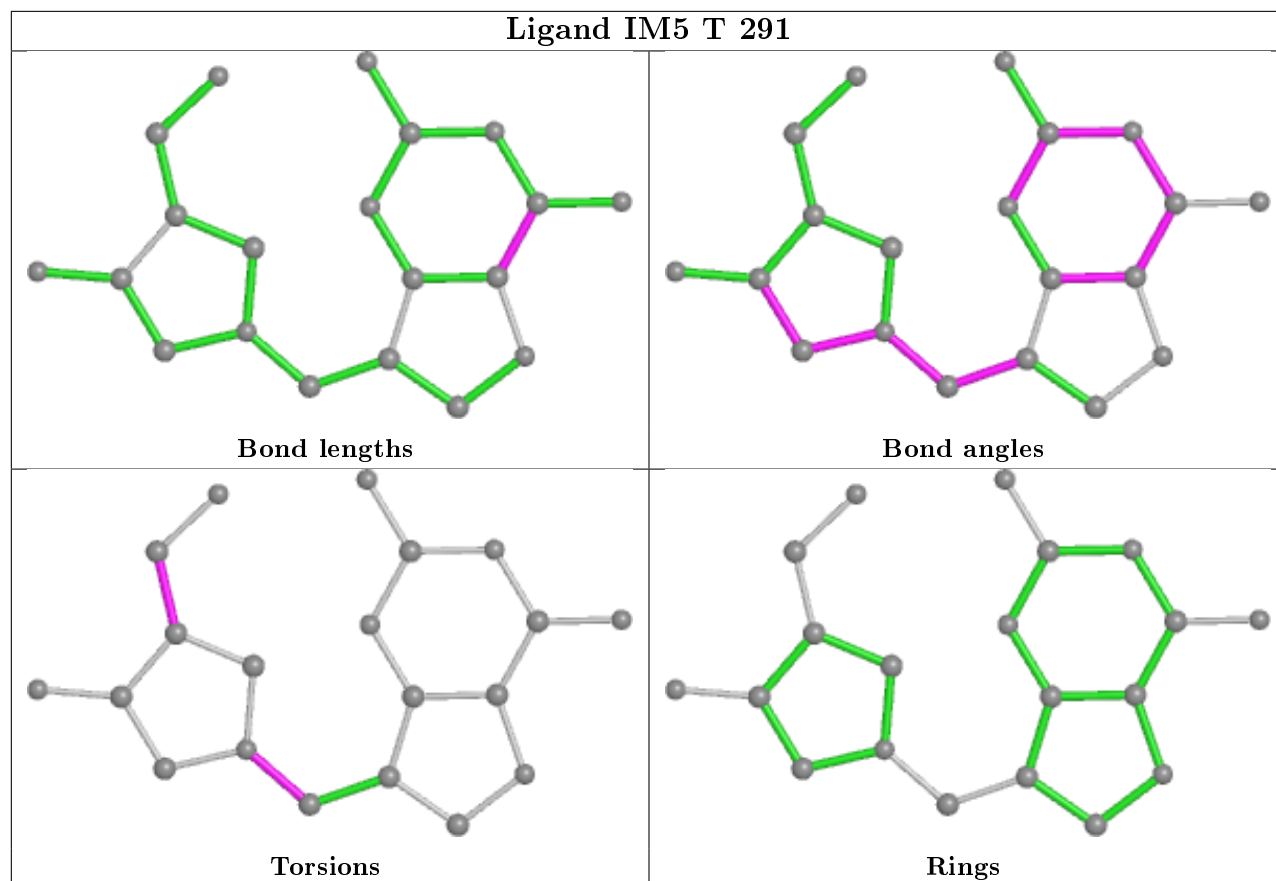
3 monomers are involved in 3 short contacts:

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

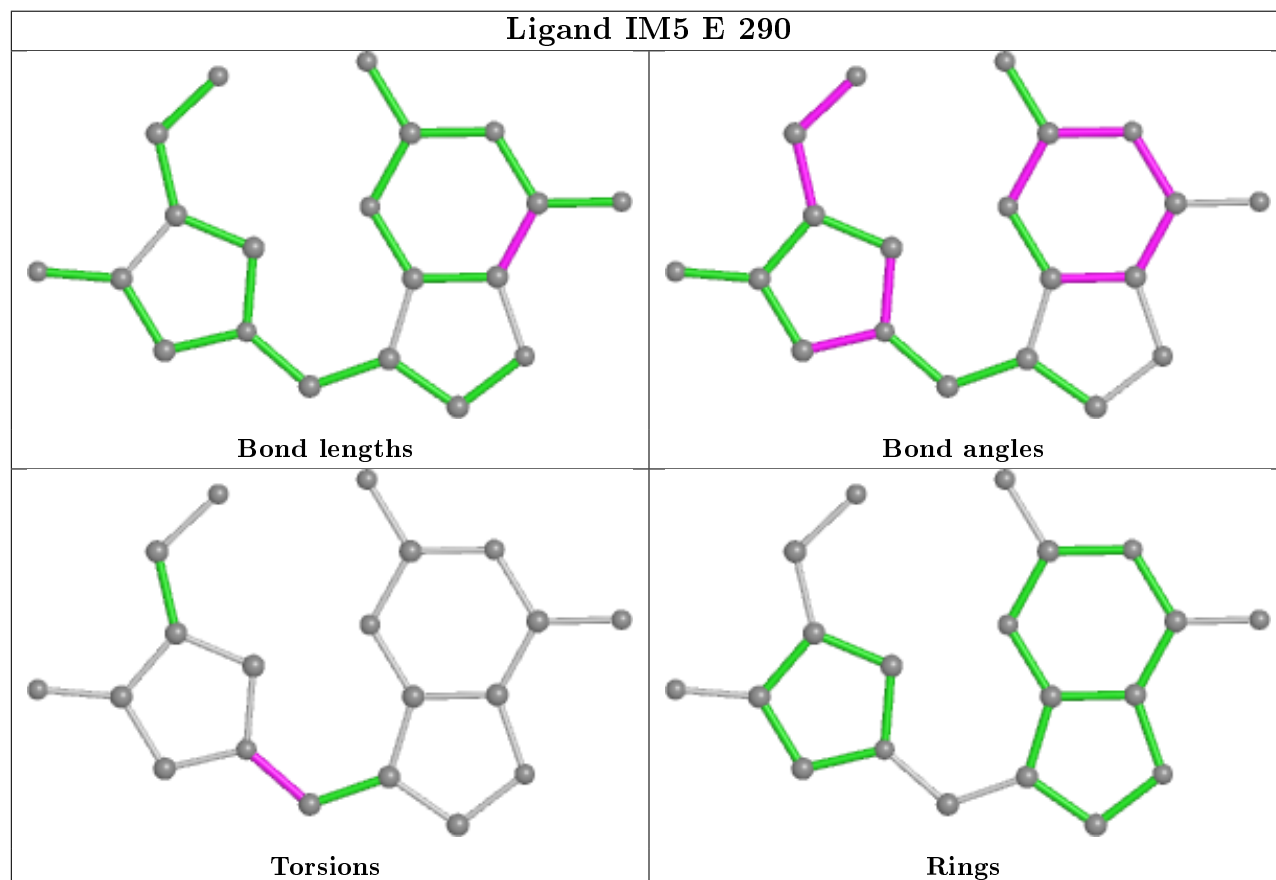
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



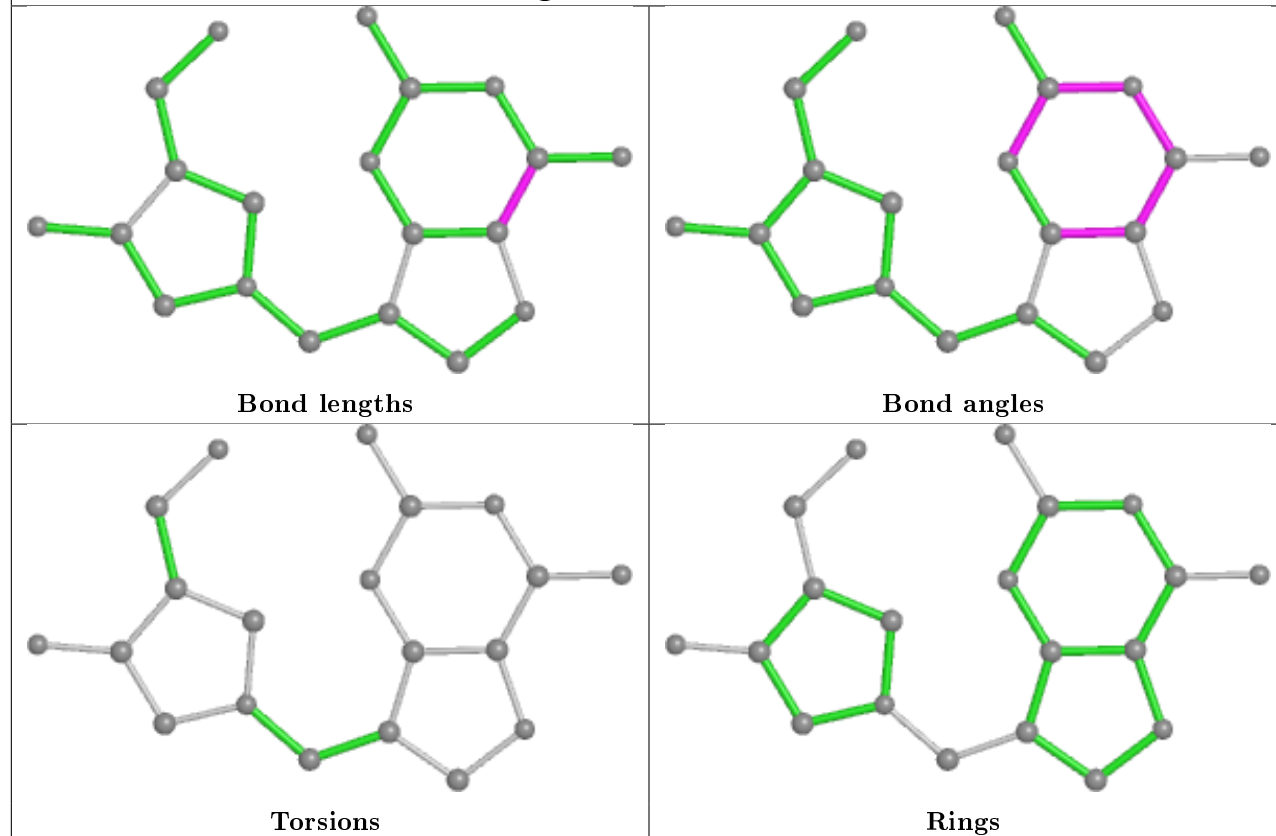
## Ligand IM5 T 291



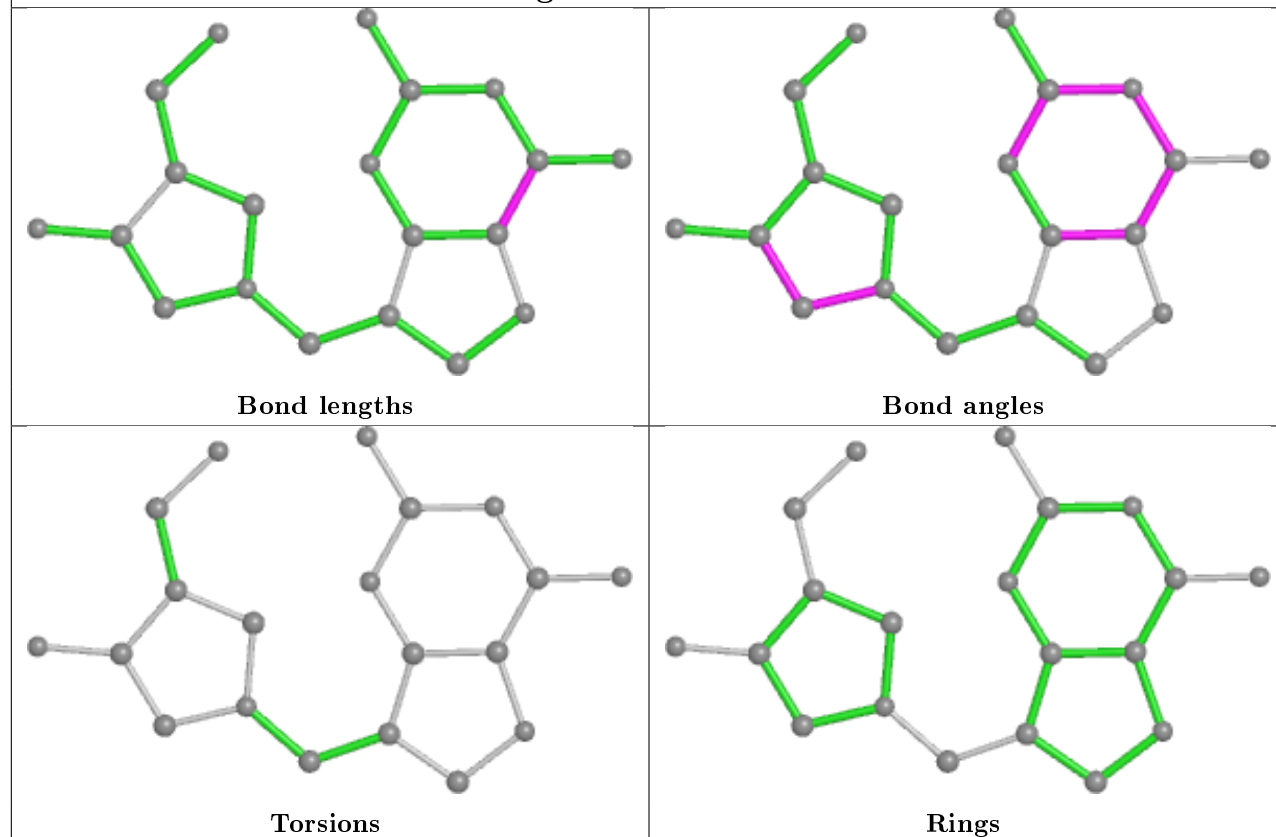
## Ligand IM5 E 290

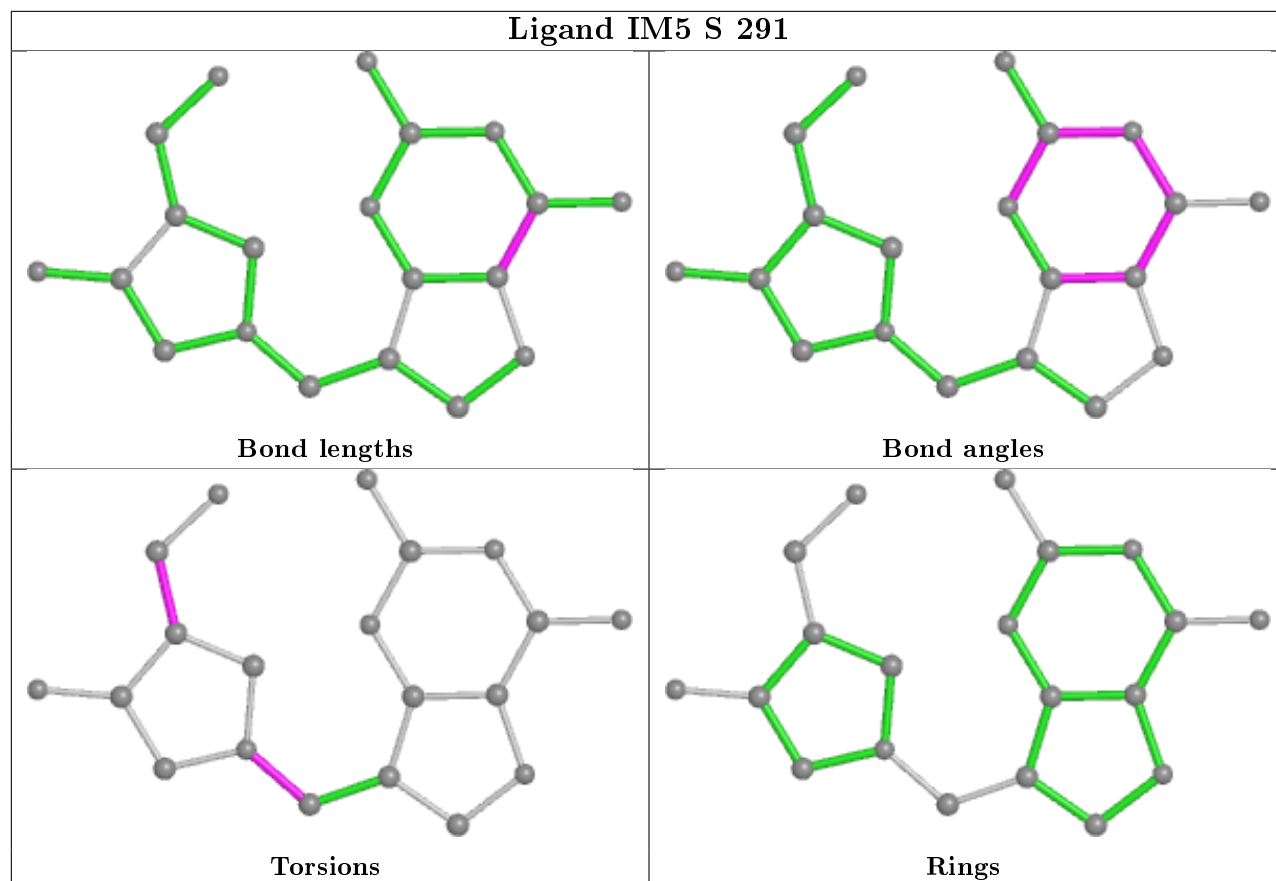


## Ligand IM5 Q 290



## Ligand IM5 U 290





## 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	E	288/324 (88%)	0.12	6 (2%) 63 70	20, 45, 67, 80	0
1	Q	287/324 (88%)	-0.01	6 (2%) 63 70	25, 42, 62, 81	0
1	S	286/324 (88%)	0.02	13 (4%) 33 40	27, 44, 65, 86	0
1	T	287/324 (88%)	0.19	12 (4%) 36 43	28, 51, 65, 77	0
1	U	285/324 (87%)	0.22	15 (5%) 26 33	23, 48, 72, 83	0
1	Y	285/324 (87%)	0.03	5 (1%) 68 74	31, 42, 63, 72	0
All	All	1718/1944 (88%)	0.09	57 (3%) 46 53	20, 45, 68, 86	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	182	GLY	6.9
1	Q	181	MET	6.1
1	S	184	GLN	5.7
1	Q	184	GLN	5.6
1	S	180	GLN	4.7
1	U	182	GLY	4.7
1	S	252	LEU	4.2
1	E	-1	THR	4.0
1	T	22	LYS	3.9
1	Q	182	GLY	3.9
1	S	182	GLY	3.8
1	U	287	LYS	3.7
1	E	-2	PRO	3.7
1	E	184	GLN	3.6
1	T	184	GLN	3.4
1	S	269	GLN	3.0
1	T	1	MET	3.0
1	S	179	LYS	3.0
1	T	102	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	0	LEU	2.9
1	U	286	ASP	2.8
1	Y	184	GLN	2.8
1	S	183	GLU	2.7
1	Q	58	ARG	2.5
1	U	168	ARG	2.5
1	T	252	LEU	2.5
1	U	284	LEU	2.4
1	U	186	GLU	2.4
1	T	123	LYS	2.4
1	Q	-1	THR	2.4
1	Q	1	MET	2.4
1	S	285	PRO	2.3
1	S	0	LEU	2.3
1	Y	182	GLY	2.3
1	T	153	GLU	2.3
1	U	184	GLN	2.3
1	S	181	MET	2.2
1	Y	179	LYS	2.2
1	U	122	PRO	2.2
1	Y	2	GLU	2.1
1	U	252	LEU	2.1
1	S	153	GLU	2.1
1	U	280	ALA	2.1
1	U	129	ILE	2.1
1	U	250	GLU	2.1
1	Y	100	VAL	2.1
1	S	58	ARG	2.1
1	T	250	GLU	2.1
1	T	7	TYR	2.1
1	U	285	PRO	2.1
1	E	269	GLN	2.1
1	U	50	TYR	2.1
1	U	172	GLN	2.0
1	T	11	LYS	2.0
1	T	68	LEU	2.0
1	S	123	LYS	2.0
1	T	-1	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

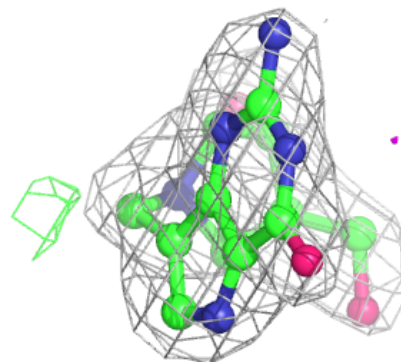
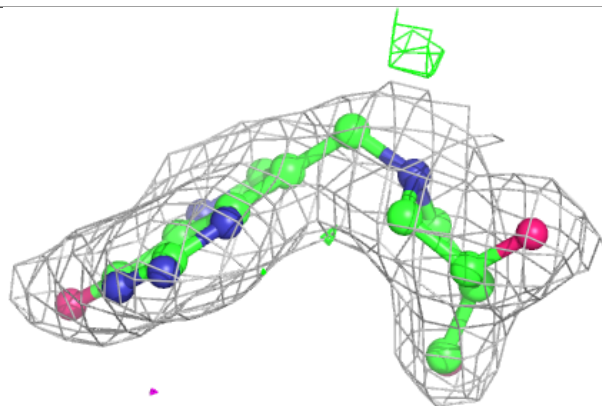
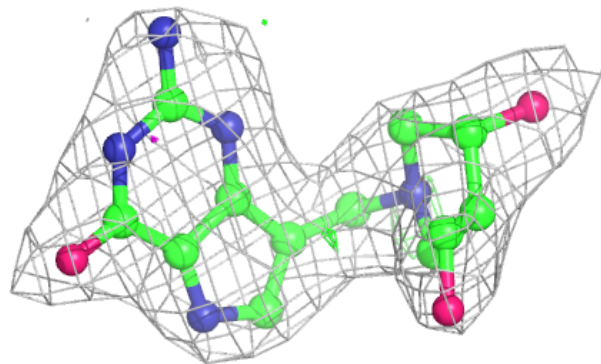
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	E	292	5/5	0.94	0.18	64,64,66,67	0
2	IM5	E	290	20/20	0.95	0.16	33,38,42,45	0
2	IM5	U	290	20/20	0.95	0.14	32,36,39,41	0
3	PO4	Y	291	5/5	0.95	0.33	95,95,95,95	0
3	PO4	Q	292	5/5	0.96	0.20	67,67,68,68	0
2	IM5	T	291	20/20	0.96	0.18	29,33,38,43	0
2	IM5	Y	292	20/20	0.96	0.17	34,36,39,41	0
3	PO4	S	290	5/5	0.97	0.17	48,49,49,50	0
2	IM5	Q	290	20/20	0.97	0.10	26,30,37,37	0
2	IM5	S	291	20/20	0.97	0.13	32,36,39,42	0
3	PO4	T	290	5/5	0.97	0.18	66,66,66,67	0
3	PO4	Y	290	5/5	0.97	0.10	62,62,62,63	0
3	PO4	S	292	5/5	0.98	0.13	39,39,41,42	0
3	PO4	T	292	5/5	0.98	0.12	42,44,46,47	0
3	PO4	U	291	5/5	0.98	0.13	42,42,44,44	0
3	PO4	E	291	5/5	0.99	0.13	36,37,38,41	0
3	PO4	Q	291	5/5	0.99	0.12	35,36,37,40	0
3	PO4	Y	293	5/5	0.99	0.10	35,35,36,36	0

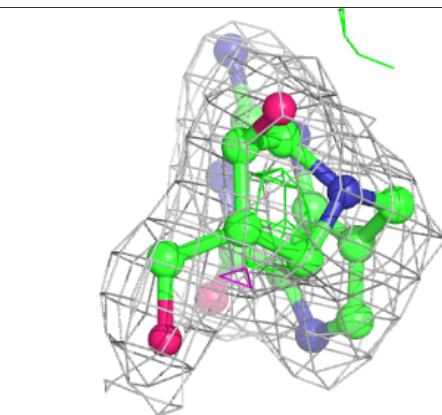
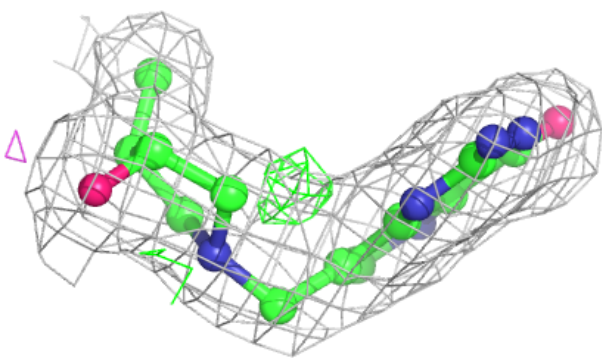
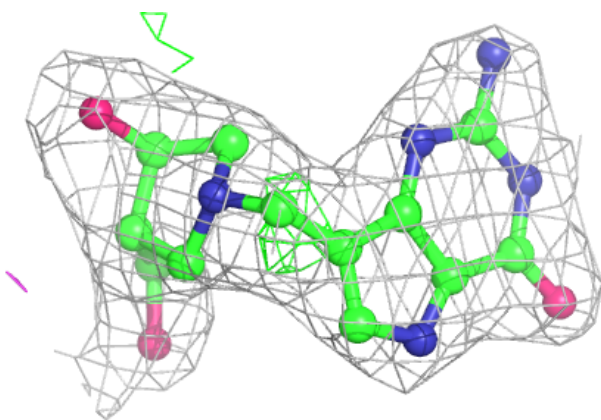
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around IM5 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 U 290:**

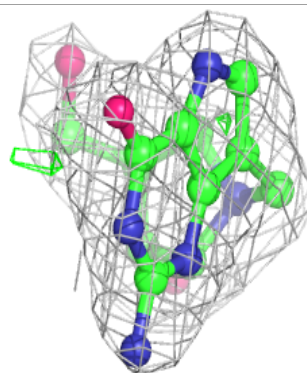
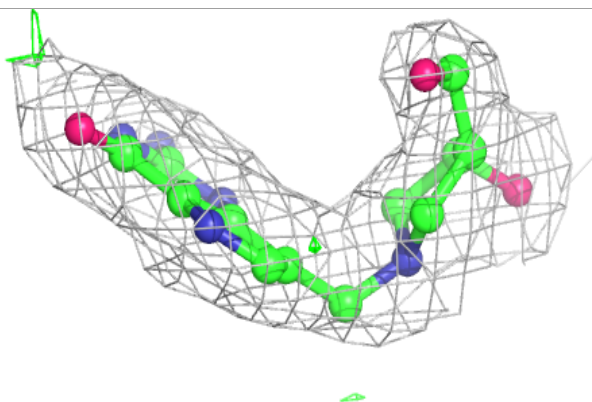
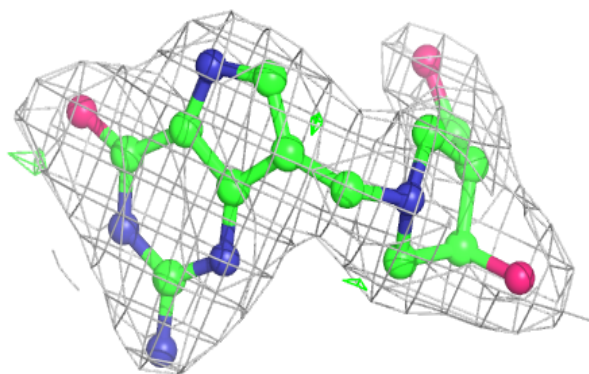
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



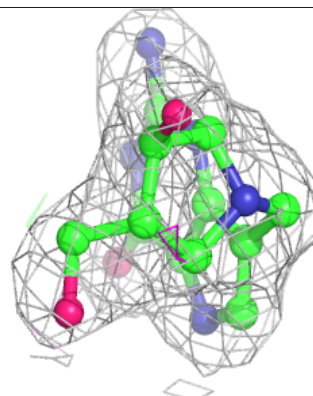
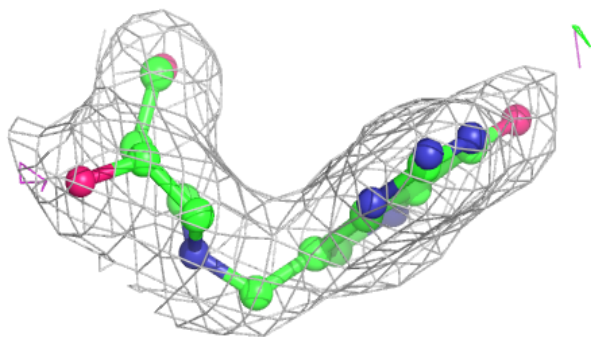
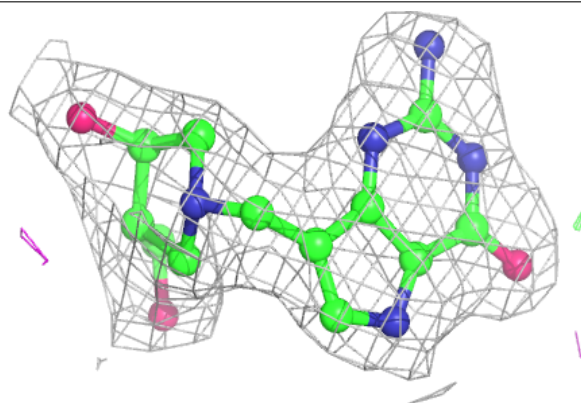


**Electron density around IM5 T 291:**

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

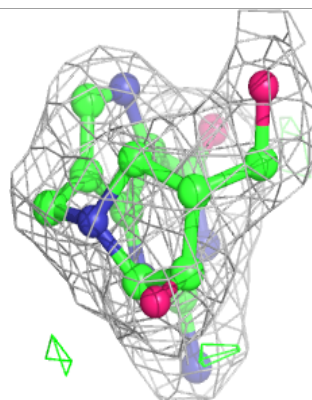
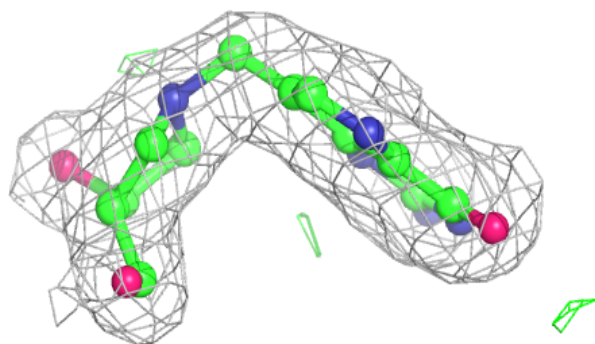
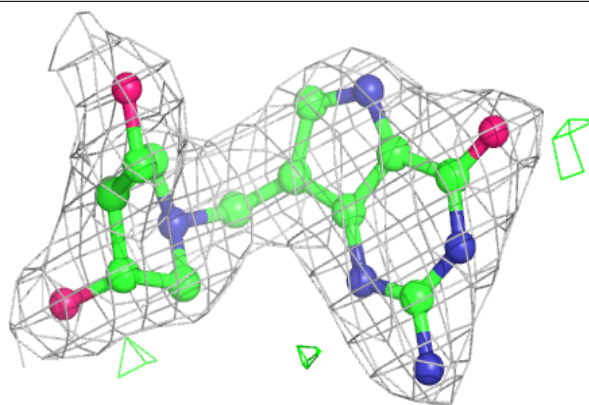
**Electron density around IM5 Y 292:**

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

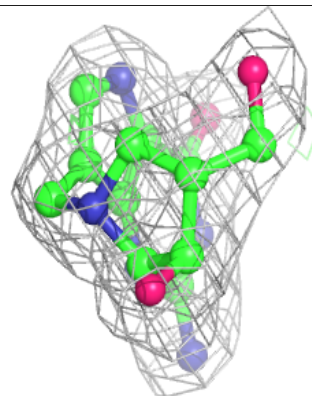
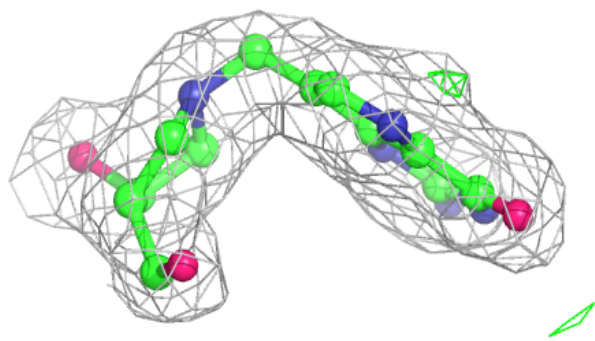
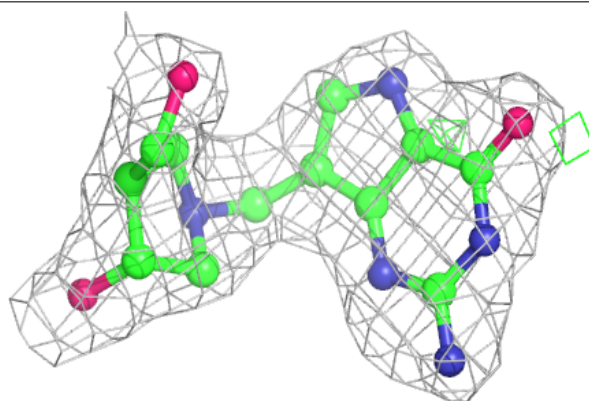


**Electron density around IM5 Q 290:**

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

**Electron density around IM5 S 291:**

$2mF_o-DF_c$  (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.