



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:51 PM EDT

PDB ID : 7MTU  
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from Bacillus anthracis in the complex with IMP and the inhibitor P221  
Authors : Kim, Y.; Maltseva, N.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2021-05-13  
Resolution : 2.34 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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)

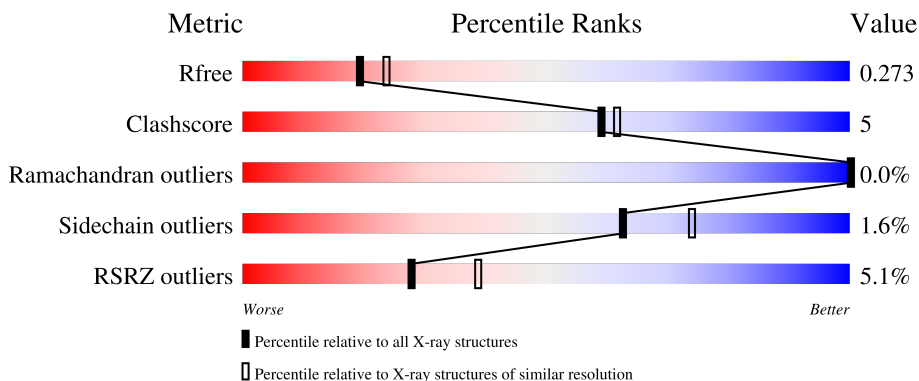
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


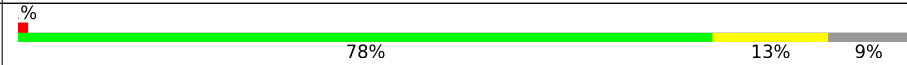
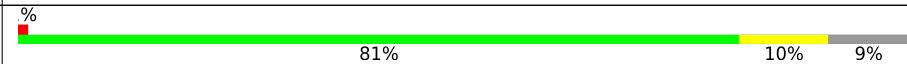
The reported resolution of this entry is 2.34 Å.

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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

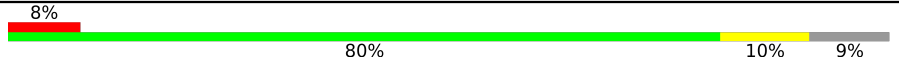
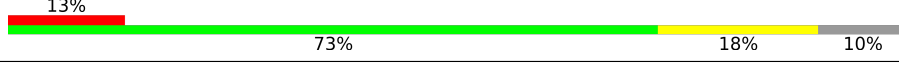
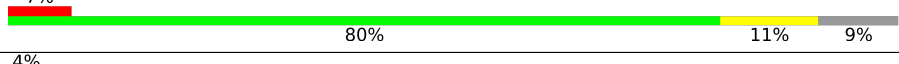


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	384	 2% 81% 10% 9%
1	B	384	 1% 78% 13% 9%
1	C	384	 1% 81% 10% 9%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.35.1

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Mol	Chain	Length	Quality of chain
1	D	384	 8% 80% 10% 9%
1	E	384	 13% 73% 18% 10%
1	F	384	 7% 80% 11% 9%
1	G	384	 4% 81% 10% 9%
1	H	384	 2% 79% 12% 9%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 21561 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	Total 2569	C 1612	N 452	O 489	S 16	0	1	0
1	B	350	Total 2581	C 1621	N 452	O 491	S 17	0	2	0
1	C	351	Total 2576	C 1617	N 452	O 491	S 16	0	0	0
1	D	349	Total 2561	C 1609	N 449	O 487	S 16	0	0	0
1	E	347	Total 2544	C 1597	N 446	O 485	S 16	0	0	0
1	F	348	Total 2563	C 1609	N 451	O 487	S 16	0	1	0
1	G	351	Total 2575	C 1617	N 451	O 491	S 16	0	0	0
1	H	349	Total 2558	C 1606	N 448	O 488	S 16	0	0	0

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A0A6H3A7R4
A	-22	HIS	-	expression tag	UNP A0A6H3A7R4
A	-21	HIS	-	expression tag	UNP A0A6H3A7R4
A	-20	HIS	-	expression tag	UNP A0A6H3A7R4
A	-19	HIS	-	expression tag	UNP A0A6H3A7R4
A	-18	HIS	-	expression tag	UNP A0A6H3A7R4
A	-17	HIS	-	expression tag	UNP A0A6H3A7R4
A	-16	SER	-	expression tag	UNP A0A6H3A7R4
A	-15	SER	-	expression tag	UNP A0A6H3A7R4
A	-14	GLY	-	expression tag	UNP A0A6H3A7R4
A	-13	VAL	-	expression tag	UNP A0A6H3A7R4
A	-12	ASP	-	expression tag	UNP A0A6H3A7R4
A	-11	LEU	-	expression tag	UNP A0A6H3A7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP A0A6H3A7R4
A	-9	THR	-	expression tag	UNP A0A6H3A7R4
A	-8	GLU	-	expression tag	UNP A0A6H3A7R4
A	-7	ASN	-	expression tag	UNP A0A6H3A7R4
A	-6	LEU	-	expression tag	UNP A0A6H3A7R4
A	-5	TYR	-	expression tag	UNP A0A6H3A7R4
A	-4	PHE	-	expression tag	UNP A0A6H3A7R4
A	-3	GLN	-	expression tag	UNP A0A6H3A7R4
A	-2	SER	-	expression tag	UNP A0A6H3A7R4
A	-1	ASN	-	expression tag	UNP A0A6H3A7R4
A	0	ALA	-	expression tag	UNP A0A6H3A7R4
A	92	GLY	-	linker	UNP A0A6H3A7R4
A	220	GLY	-	linker	UNP A0A6H3A7R4
B	-23	MET	-	initiating methionine	UNP A0A6H3A7R4
B	-22	HIS	-	expression tag	UNP A0A6H3A7R4
B	-21	HIS	-	expression tag	UNP A0A6H3A7R4
B	-20	HIS	-	expression tag	UNP A0A6H3A7R4
B	-19	HIS	-	expression tag	UNP A0A6H3A7R4
B	-18	HIS	-	expression tag	UNP A0A6H3A7R4
B	-17	HIS	-	expression tag	UNP A0A6H3A7R4
B	-16	SER	-	expression tag	UNP A0A6H3A7R4
B	-15	SER	-	expression tag	UNP A0A6H3A7R4
B	-14	GLY	-	expression tag	UNP A0A6H3A7R4
B	-13	VAL	-	expression tag	UNP A0A6H3A7R4
B	-12	ASP	-	expression tag	UNP A0A6H3A7R4
B	-11	LEU	-	expression tag	UNP A0A6H3A7R4
B	-10	GLY	-	expression tag	UNP A0A6H3A7R4
B	-9	THR	-	expression tag	UNP A0A6H3A7R4
B	-8	GLU	-	expression tag	UNP A0A6H3A7R4
B	-7	ASN	-	expression tag	UNP A0A6H3A7R4
B	-6	LEU	-	expression tag	UNP A0A6H3A7R4
B	-5	TYR	-	expression tag	UNP A0A6H3A7R4
B	-4	PHE	-	expression tag	UNP A0A6H3A7R4
B	-3	GLN	-	expression tag	UNP A0A6H3A7R4
B	-2	SER	-	expression tag	UNP A0A6H3A7R4
B	-1	ASN	-	expression tag	UNP A0A6H3A7R4
B	0	ALA	-	expression tag	UNP A0A6H3A7R4
B	92	GLY	-	linker	UNP A0A6H3A7R4
B	220	GLY	-	linker	UNP A0A6H3A7R4
C	-23	MET	-	initiating methionine	UNP A0A6H3A7R4
C	-22	HIS	-	expression tag	UNP A0A6H3A7R4
C	-21	HIS	-	expression tag	UNP A0A6H3A7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP A0A6H3A7R4
C	-19	HIS	-	expression tag	UNP A0A6H3A7R4
C	-18	HIS	-	expression tag	UNP A0A6H3A7R4
C	-17	HIS	-	expression tag	UNP A0A6H3A7R4
C	-16	SER	-	expression tag	UNP A0A6H3A7R4
C	-15	SER	-	expression tag	UNP A0A6H3A7R4
C	-14	GLY	-	expression tag	UNP A0A6H3A7R4
C	-13	VAL	-	expression tag	UNP A0A6H3A7R4
C	-12	ASP	-	expression tag	UNP A0A6H3A7R4
C	-11	LEU	-	expression tag	UNP A0A6H3A7R4
C	-10	GLY	-	expression tag	UNP A0A6H3A7R4
C	-9	THR	-	expression tag	UNP A0A6H3A7R4
C	-8	GLU	-	expression tag	UNP A0A6H3A7R4
C	-7	ASN	-	expression tag	UNP A0A6H3A7R4
C	-6	LEU	-	expression tag	UNP A0A6H3A7R4
C	-5	TYR	-	expression tag	UNP A0A6H3A7R4
C	-4	PHE	-	expression tag	UNP A0A6H3A7R4
C	-3	GLN	-	expression tag	UNP A0A6H3A7R4
C	-2	SER	-	expression tag	UNP A0A6H3A7R4
C	-1	ASN	-	expression tag	UNP A0A6H3A7R4
C	0	ALA	-	expression tag	UNP A0A6H3A7R4
C	92	GLY	-	linker	UNP A0A6H3A7R4
C	220	GLY	-	linker	UNP A0A6H3A7R4
D	-23	MET	-	initiating methionine	UNP A0A6H3A7R4
D	-22	HIS	-	expression tag	UNP A0A6H3A7R4
D	-21	HIS	-	expression tag	UNP A0A6H3A7R4
D	-20	HIS	-	expression tag	UNP A0A6H3A7R4
D	-19	HIS	-	expression tag	UNP A0A6H3A7R4
D	-18	HIS	-	expression tag	UNP A0A6H3A7R4
D	-17	HIS	-	expression tag	UNP A0A6H3A7R4
D	-16	SER	-	expression tag	UNP A0A6H3A7R4
D	-15	SER	-	expression tag	UNP A0A6H3A7R4
D	-14	GLY	-	expression tag	UNP A0A6H3A7R4
D	-13	VAL	-	expression tag	UNP A0A6H3A7R4
D	-12	ASP	-	expression tag	UNP A0A6H3A7R4
D	-11	LEU	-	expression tag	UNP A0A6H3A7R4
D	-10	GLY	-	expression tag	UNP A0A6H3A7R4
D	-9	THR	-	expression tag	UNP A0A6H3A7R4
D	-8	GLU	-	expression tag	UNP A0A6H3A7R4
D	-7	ASN	-	expression tag	UNP A0A6H3A7R4
D	-6	LEU	-	expression tag	UNP A0A6H3A7R4
D	-5	TYR	-	expression tag	UNP A0A6H3A7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	PHE	-	expression tag	UNP A0A6H3A7R4
D	-3	GLN	-	expression tag	UNP A0A6H3A7R4
D	-2	SER	-	expression tag	UNP A0A6H3A7R4
D	-1	ASN	-	expression tag	UNP A0A6H3A7R4
D	0	ALA	-	expression tag	UNP A0A6H3A7R4
D	92	GLY	-	linker	UNP A0A6H3A7R4
D	220	GLY	-	linker	UNP A0A6H3A7R4
E	-23	MET	-	initiating methionine	UNP A0A6H3A7R4
E	-22	HIS	-	expression tag	UNP A0A6H3A7R4
E	-21	HIS	-	expression tag	UNP A0A6H3A7R4
E	-20	HIS	-	expression tag	UNP A0A6H3A7R4
E	-19	HIS	-	expression tag	UNP A0A6H3A7R4
E	-18	HIS	-	expression tag	UNP A0A6H3A7R4
E	-17	HIS	-	expression tag	UNP A0A6H3A7R4
E	-16	SER	-	expression tag	UNP A0A6H3A7R4
E	-15	SER	-	expression tag	UNP A0A6H3A7R4
E	-14	GLY	-	expression tag	UNP A0A6H3A7R4
E	-13	VAL	-	expression tag	UNP A0A6H3A7R4
E	-12	ASP	-	expression tag	UNP A0A6H3A7R4
E	-11	LEU	-	expression tag	UNP A0A6H3A7R4
E	-10	GLY	-	expression tag	UNP A0A6H3A7R4
E	-9	THR	-	expression tag	UNP A0A6H3A7R4
E	-8	GLU	-	expression tag	UNP A0A6H3A7R4
E	-7	ASN	-	expression tag	UNP A0A6H3A7R4
E	-6	LEU	-	expression tag	UNP A0A6H3A7R4
E	-5	TYR	-	expression tag	UNP A0A6H3A7R4
E	-4	PHE	-	expression tag	UNP A0A6H3A7R4
E	-3	GLN	-	expression tag	UNP A0A6H3A7R4
E	-2	SER	-	expression tag	UNP A0A6H3A7R4
E	-1	ASN	-	expression tag	UNP A0A6H3A7R4
E	0	ALA	-	expression tag	UNP A0A6H3A7R4
E	92	GLY	-	linker	UNP A0A6H3A7R4
E	220	GLY	-	linker	UNP A0A6H3A7R4
F	-23	MET	-	initiating methionine	UNP A0A6H3A7R4
F	-22	HIS	-	expression tag	UNP A0A6H3A7R4
F	-21	HIS	-	expression tag	UNP A0A6H3A7R4
F	-20	HIS	-	expression tag	UNP A0A6H3A7R4
F	-19	HIS	-	expression tag	UNP A0A6H3A7R4
F	-18	HIS	-	expression tag	UNP A0A6H3A7R4
F	-17	HIS	-	expression tag	UNP A0A6H3A7R4
F	-16	SER	-	expression tag	UNP A0A6H3A7R4
F	-15	SER	-	expression tag	UNP A0A6H3A7R4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	GLY	-	expression tag	UNP A0A6H3A7R4
F	-13	VAL	-	expression tag	UNP A0A6H3A7R4
F	-12	ASP	-	expression tag	UNP A0A6H3A7R4
F	-11	LEU	-	expression tag	UNP A0A6H3A7R4
F	-10	GLY	-	expression tag	UNP A0A6H3A7R4
F	-9	THR	-	expression tag	UNP A0A6H3A7R4
F	-8	GLU	-	expression tag	UNP A0A6H3A7R4
F	-7	ASN	-	expression tag	UNP A0A6H3A7R4
F	-6	LEU	-	expression tag	UNP A0A6H3A7R4
F	-5	TYR	-	expression tag	UNP A0A6H3A7R4
F	-4	PHE	-	expression tag	UNP A0A6H3A7R4
F	-3	GLN	-	expression tag	UNP A0A6H3A7R4
F	-2	SER	-	expression tag	UNP A0A6H3A7R4
F	-1	ASN	-	expression tag	UNP A0A6H3A7R4
F	0	ALA	-	expression tag	UNP A0A6H3A7R4
F	92	GLY	-	linker	UNP A0A6H3A7R4
F	220	GLY	-	linker	UNP A0A6H3A7R4
G	-23	MET	-	initiating methionine	UNP A0A6H3A7R4
G	-22	HIS	-	expression tag	UNP A0A6H3A7R4
G	-21	HIS	-	expression tag	UNP A0A6H3A7R4
G	-20	HIS	-	expression tag	UNP A0A6H3A7R4
G	-19	HIS	-	expression tag	UNP A0A6H3A7R4
G	-18	HIS	-	expression tag	UNP A0A6H3A7R4
G	-17	HIS	-	expression tag	UNP A0A6H3A7R4
G	-16	SER	-	expression tag	UNP A0A6H3A7R4
G	-15	SER	-	expression tag	UNP A0A6H3A7R4
G	-14	GLY	-	expression tag	UNP A0A6H3A7R4
G	-13	VAL	-	expression tag	UNP A0A6H3A7R4
G	-12	ASP	-	expression tag	UNP A0A6H3A7R4
G	-11	LEU	-	expression tag	UNP A0A6H3A7R4
G	-10	GLY	-	expression tag	UNP A0A6H3A7R4
G	-9	THR	-	expression tag	UNP A0A6H3A7R4
G	-8	GLU	-	expression tag	UNP A0A6H3A7R4
G	-7	ASN	-	expression tag	UNP A0A6H3A7R4
G	-6	LEU	-	expression tag	UNP A0A6H3A7R4
G	-5	TYR	-	expression tag	UNP A0A6H3A7R4
G	-4	PHE	-	expression tag	UNP A0A6H3A7R4
G	-3	GLN	-	expression tag	UNP A0A6H3A7R4
G	-2	SER	-	expression tag	UNP A0A6H3A7R4
G	-1	ASN	-	expression tag	UNP A0A6H3A7R4
G	0	ALA	-	expression tag	UNP A0A6H3A7R4
G	92	GLY	-	linker	UNP A0A6H3A7R4

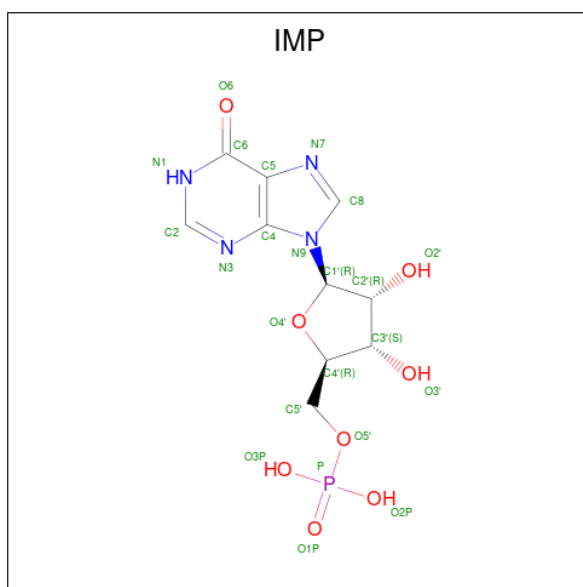
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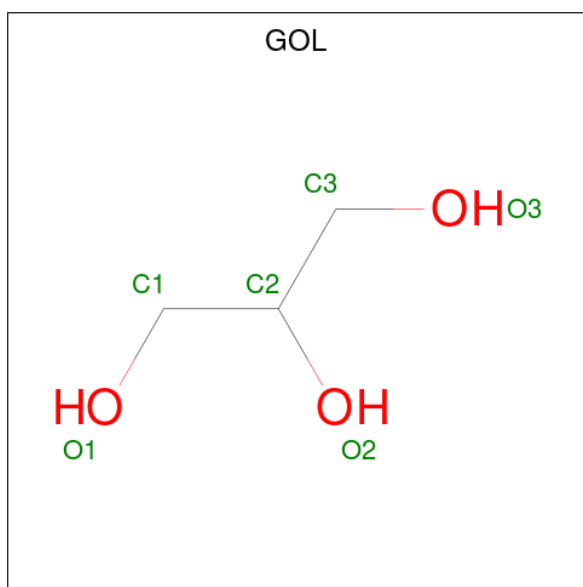
Chain	Residue	Modelled	Actual	Comment	Reference
G	220	GLY	-	linker	UNP A0A6H3A7R4
H	-23	MET	-	initiating methionine	UNP A0A6H3A7R4
H	-22	HIS	-	expression tag	UNP A0A6H3A7R4
H	-21	HIS	-	expression tag	UNP A0A6H3A7R4
H	-20	HIS	-	expression tag	UNP A0A6H3A7R4
H	-19	HIS	-	expression tag	UNP A0A6H3A7R4
H	-18	HIS	-	expression tag	UNP A0A6H3A7R4
H	-17	HIS	-	expression tag	UNP A0A6H3A7R4
H	-16	SER	-	expression tag	UNP A0A6H3A7R4
H	-15	SER	-	expression tag	UNP A0A6H3A7R4
H	-14	GLY	-	expression tag	UNP A0A6H3A7R4
H	-13	VAL	-	expression tag	UNP A0A6H3A7R4
H	-12	ASP	-	expression tag	UNP A0A6H3A7R4
H	-11	LEU	-	expression tag	UNP A0A6H3A7R4
H	-10	GLY	-	expression tag	UNP A0A6H3A7R4
H	-9	THR	-	expression tag	UNP A0A6H3A7R4
H	-8	GLU	-	expression tag	UNP A0A6H3A7R4
H	-7	ASN	-	expression tag	UNP A0A6H3A7R4
H	-6	LEU	-	expression tag	UNP A0A6H3A7R4
H	-5	TYR	-	expression tag	UNP A0A6H3A7R4
H	-4	PHE	-	expression tag	UNP A0A6H3A7R4
H	-3	GLN	-	expression tag	UNP A0A6H3A7R4
H	-2	SER	-	expression tag	UNP A0A6H3A7R4
H	-1	ASN	-	expression tag	UNP A0A6H3A7R4
H	0	ALA	-	expression tag	UNP A0A6H3A7R4
H	92	GLY	-	linker	UNP A0A6H3A7R4
H	220	GLY	-	linker	UNP A0A6H3A7R4

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



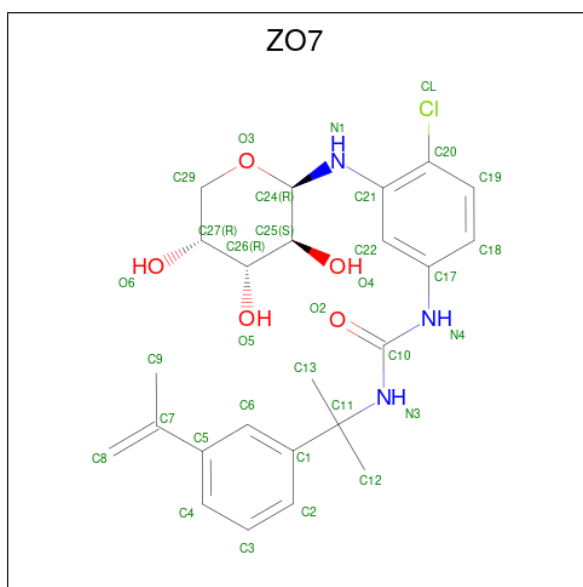
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is N-{2-chloro-5-[(2-[3-(prop-1-en-2-yl)phenyl]propan-2-yl)carbamoyl]amino]phenyl}-beta-D-arabinopyranosylamine (three-letter code: ZO7) (formula: C<sub>24</sub>H<sub>30</sub>ClN<sub>3</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
4	A	1	Total 33	C 24	Cl 1	N 3	O 5	0	0
4	B	1	Total 33	C 24	Cl 1	N 3	O 5	0	0
4	C	1	Total 33	C 24	Cl 1	N 3	O 5	0	0
4	D	1	Total 33	C 24	Cl 1	N 3	O 5	0	0
4	E	1	Total 33	C 24	Cl 1	N 3	O 5	0	0
4	F	1	Total 33	C 24	Cl 1	N 3	O 5	0	0
4	G	1	Total 33	C 24	Cl 1	N 3	O 5	0	0
4	H	1	Total 33	C 24	Cl 1	N 3	O 5	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

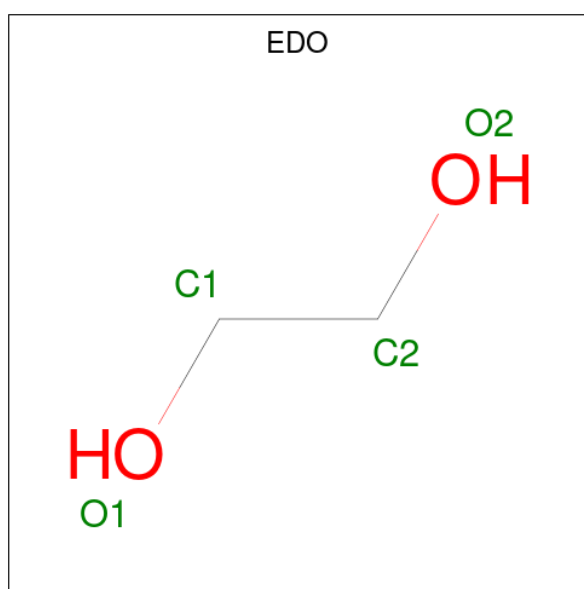
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total 1 K 1	0	0
5	B	1	Total 1 K 1	0	0
5	C	1	Total 1 K 1	0	0
5	D	1	Total 1 K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0
5	G	1	Total K 1 1	0	0
5	H	2	Total K 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	86	Total O 86 86	0	0
7	B	88	Total O 88 88	0	0
7	C	86	Total O 86 86	0	0
7	D	54	Total O 54 54	0	0

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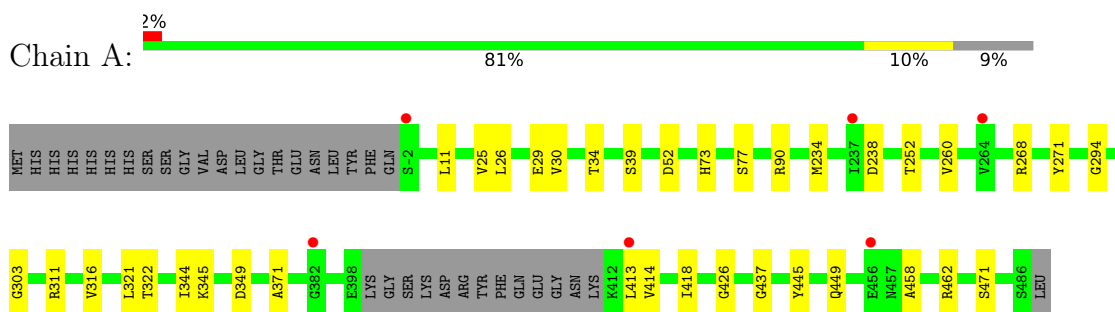
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
7	E	44	Total O 44 44	0	0
7	F	40	Total O 40 40	0	0
7	G	73	Total O 73 73	0	0
7	H	66	Total O 66 66	0	0

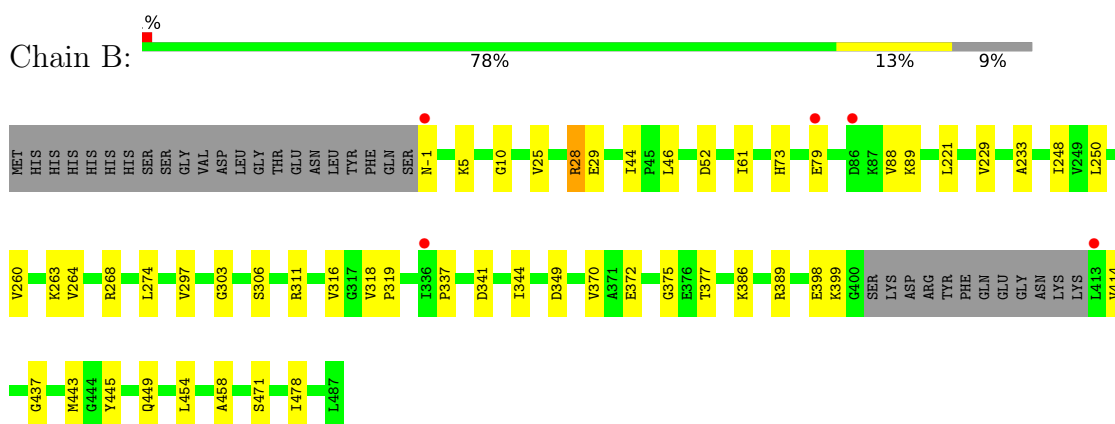
### 3 Residue-property plots [i](#)

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.

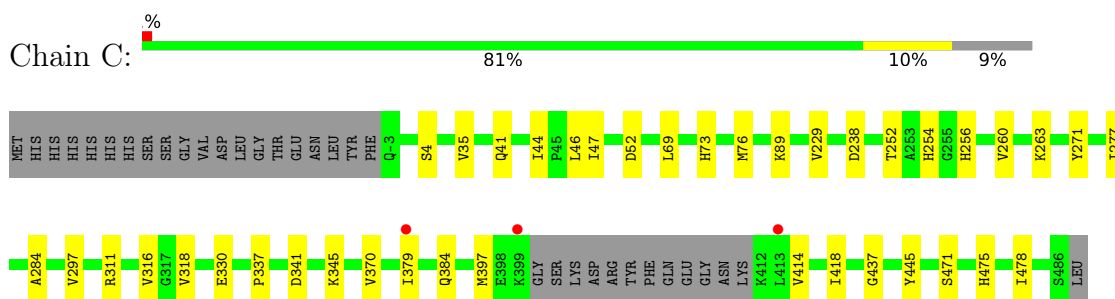
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



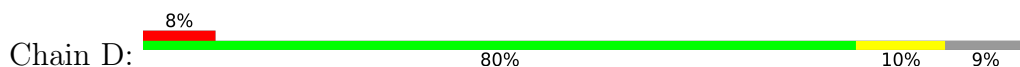
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

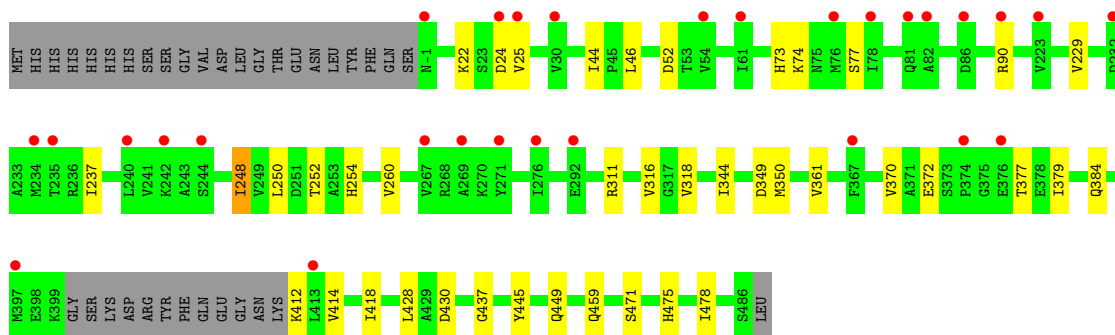


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

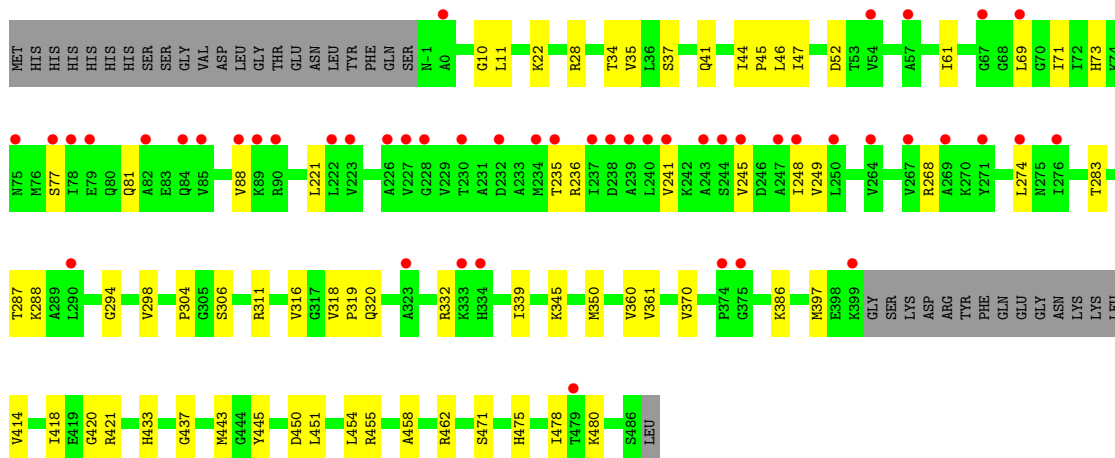


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

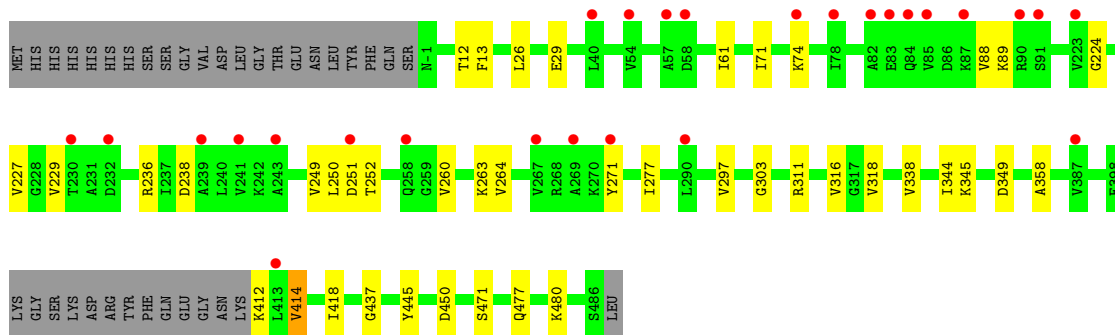
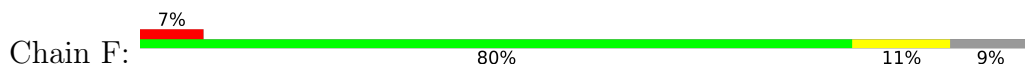




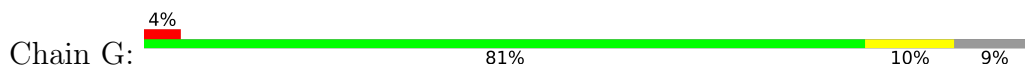
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



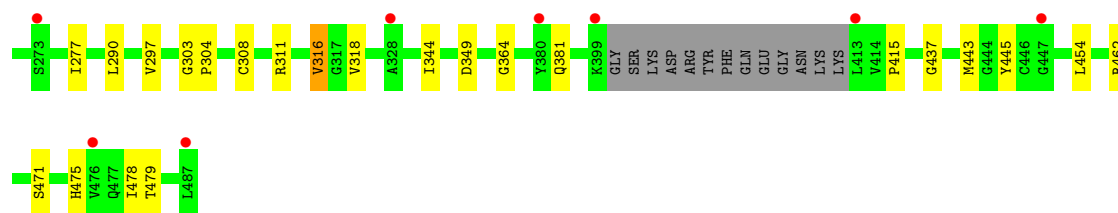
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



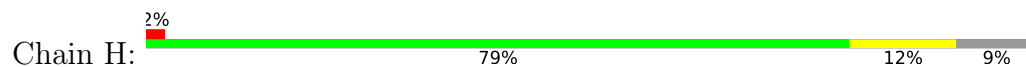
• Molecule 1: Inosine-5'-monophosphate dehydrogenase







● Molecule 1: Inosine-5'-monophosphate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.27Å 89.33Å 104.33Å 98.89° 90.40° 96.01°	Depositor
Resolution (Å)	41.68 – 2.34 47.81 – 2.34	Depositor EDS
% Data completeness (in resolution range)	75.9 (41.68-2.34) 75.9 (47.81-2.34)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.231 , 0.275 0.231 , 0.273	Depositor DCC
$R_{free}$ test set	4636 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.7	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	21561	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.95% 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: GOL, ZO7, K, IMP, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/2605	0.46	0/3521
1	B	0.24	0/2617	0.46	0/3537
1	C	0.24	0/2612	0.45	0/3530
1	D	0.24	0/2597	0.45	0/3510
1	E	0.24	0/2580	0.45	0/3488
1	F	0.24	0/2599	0.45	0/3513
1	G	0.24	0/2611	0.45	0/3530
1	H	0.24	0/2594	0.45	0/3507
All	All	0.24	0/20815	0.45	0/28136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2569	0	2625	24	0
1	B	2581	0	2637	31	0
1	C	2576	0	2634	29	0
1	D	2561	0	2621	29	0
1	E	2544	0	2597	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2563	0	2620	29	0
1	G	2575	0	2632	26	0
1	H	2558	0	2613	29	0
2	A	23	0	11	0	0
2	B	23	0	11	2	0
2	C	23	0	11	1	0
2	D	23	0	11	0	0
2	E	23	0	11	1	0
2	F	23	0	11	0	0
2	G	23	0	11	0	0
2	H	23	0	11	0	0
3	A	18	0	24	0	0
3	C	6	0	8	0	0
3	H	12	0	16	0	0
4	A	33	0	0	0	0
4	B	33	0	0	0	0
4	C	33	0	0	0	0
4	D	33	0	0	0	0
4	E	33	0	0	0	0
4	F	33	0	0	0	0
4	G	33	0	0	0	0
4	H	33	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	F	4	0	6	0	0
7	A	86	0	0	0	0
7	B	88	0	0	0	0
7	C	86	0	0	0	0
7	D	54	0	0	0	0
7	E	44	0	0	2	0
7	F	40	0	0	0	0
7	G	73	0	0	1	0
7	H	66	0	0	2	0
All	All	21561	0	21121	197	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 5.

All (197) 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:F:437:GLY:HA3	1:H:414:VAL:HG21	1.76	0.67
1:E:414:VAL:HG21	1:G:437:GLY:HA3	1.78	0.65
1:E:316:VAL:HG11	1:G:445:TYR:HB3	1.81	0.63
1:H:229:VAL:HG21	1:H:260:VAL:HG22	1.82	0.61
1:C:311:ARG:HD2	1:D:471:SER:HA	1.83	0.60
1:C:44:ILE:HD12	1:C:46:LEU:HD12	1.83	0.60
1:G:344:ILE:HG23	1:G:349:ASP:HB2	1.83	0.60
1:B:248:ILE:HG12	1:B:274:LEU:HD21	1.83	0.60
1:G:311:ARG:HD2	1:H:471:SER:HA	1.83	0.59
1:E:61:ILE:HG12	1:E:88:VAL:HG13	1.85	0.59
1:C:229:VAL:HG21	1:C:260:VAL:HG22	1.84	0.58
1:A:437:GLY:HA3	1:B:414:VAL:HG21	1.85	0.58
1:F:229:VAL:HG13	1:F:263:LYS:HD2	1.84	0.58
1:H:44:ILE:HD12	1:H:46:LEU:HD12	1.85	0.58
1:A:316:VAL:HG11	1:C:445:TYR:HB3	1.85	0.58
1:E:287:THR:HG23	1:E:298:VAL:HG21	1.86	0.58
1:F:311:ARG:NH2	1:F:318:VAL:O	2.37	0.57
1:E:71:ILE:HG12	1:E:249:VAL:HG21	1.86	0.57
1:H:344:ILE:HG23	1:H:349:ASP:HB2	1.86	0.57
1:A:238:ASP:OD1	1:A:271:TYR:OH	2.21	0.57
1:B:344:ILE:HG23	1:B:349:ASP:HB2	1.87	0.57
1:E:311:ARG:NH2	1:E:318:VAL:O	2.38	0.57
1:E:44:ILE:HD12	1:E:46:LEU:HD12	1.87	0.56
1:F:338:VAL:HG23	1:F:358:ALA:HA	1.87	0.56
1:A:252:THR:HG21	1:A:260:VAL:HG21	1.85	0.56
1:B:445:TYR:HB3	1:D:316:VAL:HG11	1.87	0.56
1:E:11:LEU:HD11	1:E:462:ARG:HD3	1.88	0.56
1:E:437:GLY:HA3	1:F:414:VAL:HG11	1.88	0.56
1:A:303:GLY:HA3	1:A:311:ARG:HE	1.70	0.56
1:A:471:SER:HA	1:B:311:ARG:HD2	1.88	0.55
1:G:415:PRO:O	1:H:484:ASN:ND2	2.37	0.55
1:E:451:LEU:HB3	1:E:455:ARG:HH12	1.72	0.55
1:A:414:VAL:HG21	1:C:437:GLY:HA3	1.88	0.55
1:A:311:ARG:HD2	1:C:471:SER:HA	1.89	0.54
1:F:277:ILE:HG12	1:F:297:VAL:HB	1.89	0.54
1:E:370:VAL:O	1:E:386:LYS:NZ	2.40	0.54
1:E:420:GLY:HA2	1:G:479:THR:HG23	1.90	0.54
1:C:341:ASP:OD2	2:C:502:IMP:O2'	2.26	0.54
1:D:237:ILE:HG12	1:D:248:ILE:HG12	1.89	0.54
1:E:311:ARG:HD2	1:G:471:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:ARG:HD2	1:E:294:GLY:HA3	1.91	0.53
1:B:370:VAL:HG12	1:B:372:GLU:H	1.74	0.53
1:D:22:LYS:NZ	1:D:24:ASP:OD1	2.41	0.53
1:E:445:TYR:CG	1:F:316:VAL:HG21	2.44	0.53
1:G:11:LEU:HD11	1:G:462:ARG:HD3	1.90	0.53
1:C:297:VAL:HG22	1:C:337:PRO:HG2	1.91	0.53
1:E:471:SER:HA	1:F:311:ARG:HD2	1.91	0.53
1:B:389:ARG:HH12	1:B:399:LYS:HD3	1.74	0.53
1:D:370:VAL:HG12	1:D:372:GLU:H	1.74	0.52
1:B:437:GLY:HA3	1:D:414:VAL:HG21	1.90	0.52
1:C:418:ILE:HD13	1:D:478:ILE:HG12	1.91	0.52
1:F:303:GLY:HA3	1:F:311:ARG:HE	1.73	0.52
1:G:311:ARG:NH2	1:G:318:VAL:O	2.42	0.52
1:A:418:ILE:HD13	1:C:478:ILE:HG12	1.92	0.52
1:E:450:ASP:N	1:E:450:ASP:OD1	2.43	0.52
1:D:25:VAL:HG11	1:D:449:GLN:HG2	1.92	0.51
1:H:303:GLY:HA3	1:H:311:ARG:HE	1.74	0.51
1:E:418:ILE:HD13	1:G:478:ILE:HG12	1.93	0.51
1:C:316:VAL:HG21	1:D:445:TYR:CD2	2.45	0.51
1:C:345:LYS:HD2	1:D:475:HIS:CE1	2.46	0.51
1:E:475:HIS:CE1	1:F:345:LYS:HD2	2.46	0.51
1:F:445:TYR:HB3	1:H:316:VAL:HG11	1.92	0.51
1:G:316:VAL:HG21	1:H:445:TYR:CG	2.46	0.51
1:H:14:ASP:OD2	1:H:345:LYS:NZ	2.44	0.51
1:A:445:TYR:HB3	1:B:316:VAL:HG11	1.92	0.50
1:B:44:ILE:HD12	1:B:46:LEU:HD12	1.93	0.50
1:E:339:ILE:HG12	1:E:360:VAL:HG13	1.92	0.50
1:A:345:LYS:HD2	1:C:475:HIS:CE1	2.46	0.50
1:B:311:ARG:NH2	1:B:318:VAL:O	2.44	0.50
1:F:471:SER:HA	1:H:311:ARG:HD2	1.94	0.50
1:G:35:VAL:HG13	1:G:41:GLN:HG2	1.93	0.50
1:D:311:ARG:NH2	1:D:318:VAL:O	2.44	0.50
1:C:47:ILE:HG12	1:C:69:LEU:HB3	1.93	0.50
1:C:311:ARG:NH2	1:C:318:VAL:O	2.45	0.50
1:D:229:VAL:HG21	1:D:260:VAL:HG22	1.93	0.49
1:D:350:MET:HG3	1:D:361:VAL:HG21	1.94	0.49
1:A:458:ALA:O	1:B:5:LYS:NZ	2.43	0.49
1:B:268:ARG:NH2	1:B:274:LEU:O	2.39	0.49
1:B:61:ILE:HG13	1:B:88:VAL:HG22	1.94	0.49
1:B:478:ILE:HG12	1:D:418:ILE:HD13	1.94	0.49
1:B:28:ARG:HG2	1:B:29:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:ASP:OD1	1:F:271:TYR:OH	2.31	0.49
1:D:44:ILE:HD12	1:D:46:LEU:HD12	1.93	0.49
1:E:35:VAL:HG12	1:E:41:GLN:HG2	1.94	0.48
1:C:4:SER:O	1:D:459:GLN:NE2	2.44	0.48
1:F:303:GLY:HA3	1:F:311:ARG:NE	2.28	0.48
1:B:471:SER:HA	1:D:311:ARG:HD2	1.96	0.48
1:H:284:ALA:HB1	1:H:330:GLU:HB2	1.95	0.48
1:E:52:ASP:HA	1:E:73:HIS:CD2	2.49	0.48
1:E:248:ILE:HG13	1:E:274:LEU:HD21	1.95	0.48
1:H:61:ILE:HG13	1:H:88:VAL:HG22	1.95	0.48
1:A:25:VAL:HG12	1:A:29:GLU:HG3	1.95	0.48
1:B:229:VAL:HG11	1:B:260:VAL:HG22	1.95	0.47
1:G:44:ILE:HD12	1:G:46:LEU:HD12	1.95	0.47
1:G:227:VAL:HG13	1:G:236:ARG:HD2	1.97	0.47
1:G:443:MET:HG2	1:G:454:LEU:HD22	1.97	0.47
1:H:252:THR:HG21	1:H:260:VAL:HG21	1.97	0.47
1:B:250:LEU:HD12	1:B:264:VAL:HG12	1.97	0.47
1:H:52:ASP:HA	1:H:73:HIS:CD2	2.50	0.47
1:H:370:VAL:O	1:H:386:LYS:NZ	2.45	0.47
1:G:261:ILE:HD13	1:G:290:LEU:HD23	1.97	0.47
1:C:52:ASP:HA	1:C:73:HIS:CD2	2.50	0.47
1:G:52:ASP:HA	1:G:73:HIS:CD2	2.50	0.47
1:B:25:VAL:HG11	1:B:449:GLN:HG2	1.97	0.46
1:D:252:THR:HG22	1:D:254:HIS:H	1.80	0.46
1:G:36:LEU:HD12	1:G:40:LEU:HD22	1.97	0.46
1:D:52:ASP:HA	1:D:73:HIS:CD2	2.51	0.46
1:D:412:LYS:HA	1:D:412:LYS:HD2	1.76	0.46
1:A:268:ARG:NH2	1:A:294:GLY:O	2.41	0.46
1:E:288:LYS:NZ	7:E:605:HOH:O	2.49	0.46
1:F:61:ILE:HG13	1:F:88:VAL:HG22	1.97	0.46
1:A:26:LEU:O	1:A:30:VAL:HG23	2.16	0.45
1:C:238:ASP:OD1	1:C:271:TYR:OH	2.29	0.45
1:A:11:LEU:HD11	1:A:462:ARG:HD3	1.99	0.45
1:E:47:ILE:HG12	1:E:69:LEU:HB3	1.97	0.45
1:F:227:VAL:HG23	1:F:236:ARG:HD2	1.99	0.45
1:B:341:ASP:OD2	2:B:501:IMP:O2'	2.29	0.45
1:B:89:LYS:HE3	1:B:221:LEU:O	2.17	0.45
1:A:25:VAL:HG21	1:A:449:GLN:HB2	1.99	0.45
1:F:250:LEU:HD22	1:F:264:VAL:HG22	1.98	0.45
1:D:377:THR:HG21	1:D:384:GLN:HB3	1.99	0.45
1:C:256:HIS:CD2	1:D:22:LYS:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:VAL:HG22	1:D:250:LEU:HD12	1.98	0.45
1:E:304:PRO:HB3	1:E:320:GLN:HB2	1.99	0.44
1:H:268:ARG:NH2	1:H:294:GLY:O	2.50	0.44
1:C:316:VAL:HG21	1:D:445:TYR:CG	2.53	0.44
1:B:443:MET:HG2	1:B:454:LEU:HD22	1.99	0.44
1:G:303:GLY:HA2	1:G:308:CYS:SG	2.58	0.44
1:C:229:VAL:HG13	1:C:263:LYS:HD2	1.99	0.44
1:F:344:ILE:HG23	1:F:349:ASP:HB2	1.98	0.44
1:C:414:VAL:HG21	1:D:437:GLY:HA3	1.99	0.44
1:A:344:ILE:HG23	1:A:349:ASP:HB2	1.99	0.44
1:H:277:ILE:HG12	1:H:297:VAL:HB	1.99	0.44
1:A:321:LEU:HD12	1:A:321:LEU:HA	1.86	0.44
1:E:350:MET:HG3	1:E:361:VAL:HG21	2.00	0.44
1:C:252:THR:HG22	1:C:254:HIS:H	1.83	0.43
1:H:10:GLY:HA3	1:H:319:PRO:HG2	2.00	0.43
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.53	0.43
1:D:379:ILE:H	1:D:379:ILE:HG13	1.60	0.43
1:E:433:HIS:NE2	1:F:412:LYS:O	2.41	0.43
1:H:303:GLY:HA3	1:H:311:ARG:NE	2.33	0.43
1:G:277:ILE:HG12	1:G:297:VAL:HB	1.99	0.43
1:H:47:ILE:HG13	1:H:360:VAL:HG11	1.99	0.43
1:E:443:MET:HG2	1:E:454:LEU:HD22	1.99	0.43
1:C:35:VAL:HG13	1:C:41:GLN:HG2	2.00	0.43
1:E:88:VAL:HG12	1:E:221:LEU:HB2	1.99	0.43
1:E:10:GLY:HA3	1:E:319:PRO:HG2	1.98	0.43
1:E:421:ARG:NH2	7:E:604:HOH:O	2.45	0.43
1:E:81:GLN:OE1	1:E:236:ARG:NE	2.52	0.43
1:B:303:GLY:HA3	1:B:311:ARG:HG3	2.01	0.43
1:F:26:LEU:HB2	1:F:29:GLU:HG2	2.01	0.43
1:B:306:SER:OG	2:B:501:IMP:O2P	2.32	0.42
1:D:430:ASP:N	1:D:430:ASP:OD1	2.52	0.42
1:B:10:GLY:HA3	1:B:319:PRO:HG2	2.00	0.42
1:D:344:ILE:HG23	1:D:349:ASP:HB2	2.00	0.42
1:A:303:GLY:HA3	1:A:311:ARG:NE	2.34	0.42
1:D:370:VAL:HG11	1:D:428:LEU:HB2	2.01	0.42
1:G:316:VAL:HG11	1:H:445:TYR:HB2	2.01	0.42
1:H:383:ARG:NH2	7:H:602:HOH:O	2.39	0.42
1:F:480:LYS:HB3	1:F:480:LYS:HE2	1.83	0.42
1:B:52:ASP:HA	1:B:73:HIS:CD2	2.54	0.42
1:E:45:PRO:C	1:E:360:VAL:HG23	2.40	0.42
1:G:262:ASP:O	1:G:266:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:GLY:O	1:B:386:LYS:NZ	2.48	0.42
1:G:61:ILE:HG13	1:G:88:VAL:HG22	2.02	0.42
1:A:371:ALA:N	1:A:426:GLY:O	2.50	0.42
1:A:316:VAL:HG21	1:C:445:TYR:HB2	2.02	0.42
1:H:250:LEU:HD13	1:H:276:ILE:HG23	2.02	0.42
1:E:241:VAL:HA	1:E:245:VAL:HG12	2.02	0.41
1:G:381:GLN:NE2	7:G:611:HOH:O	2.52	0.41
1:C:284:ALA:HB1	1:C:330:GLU:HB2	2.02	0.41
1:E:454:LEU:HD12	1:E:458:ALA:HB2	2.01	0.41
1:E:478:ILE:HG12	1:F:418:ILE:HD12	2.02	0.41
1:F:12:THR:OG1	1:F:13:PHE:N	2.53	0.41
1:F:477:GLN:NE2	7:H:602:HOH:O	2.51	0.41
1:F:450:ASP:N	1:F:450:ASP:OD1	2.54	0.41
1:A:11:LEU:N	1:A:322:THR:OG1	2.47	0.41
1:B:454:LEU:HD12	1:B:458:ALA:HB2	2.02	0.41
1:E:22:LYS:HE2	1:E:22:LYS:HB2	1.81	0.41
1:F:249:VAL:HG12	1:F:251:ASP:HB2	2.02	0.41
1:G:303:GLY:N	1:G:304:PRO:CD	2.84	0.41
1:H:43:ASN:HB2	1:H:67:GLY:HA3	2.02	0.41
1:B:233:ALA:HB3	1:B:263:LYS:HE2	2.02	0.41
1:C:89:LYS:HD3	1:C:89:LYS:HA	1.90	0.41
1:E:345:LYS:HD2	1:G:475:HIS:CE1	2.56	0.41
1:F:71:ILE:HD13	1:F:224:GLY:HA3	2.03	0.41
1:H:328:ALA:O	1:H:332:ARG:HB2	2.20	0.41
1:H:466:ALA:HA	1:H:469:LEU:HD12	2.01	0.41
1:F:260:VAL:O	1:F:264:VAL:HG23	2.20	0.40
1:H:394:VAL:O	1:H:398:GLU:HG2	2.21	0.40
1:E:480:LYS:HE2	1:E:480:LYS:HB3	1.86	0.40
1:F:249:VAL:HG22	1:F:277:ILE:HB	2.02	0.40
1:H:254:HIS:CE1	1:H:256:HIS:HB3	2.57	0.40
1:C:277:ILE:HG12	1:C:297:VAL:HB	2.02	0.40
1:C:379:ILE:HG12	1:C:384:GLN:HG2	2.03	0.40
1:E:306:SER:OG	2:E:501:IMP:O2P	2.31	0.40
1:B:297:VAL:HG22	1:B:337:PRO:HG2	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	A	346/384 (90%)	337 (97%)	9 (3%)	0	100	100
1	B	348/384 (91%)	342 (98%)	6 (2%)	0	100	100
1	C	347/384 (90%)	338 (97%)	9 (3%)	0	100	100
1	D	345/384 (90%)	337 (98%)	8 (2%)	0	100	100
1	E	343/384 (89%)	334 (97%)	9 (3%)	0	100	100
1	F	345/384 (90%)	336 (97%)	9 (3%)	0	100	100
1	G	347/384 (90%)	339 (98%)	7 (2%)	1 (0%)	41	47
1	H	345/384 (90%)	336 (97%)	9 (3%)	0	100	100
All	All	2766/3072 (90%)	2699 (98%)	66 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	364	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/298 (90%)	261 (97%)	7 (3%)	46	56
1	B	269/298 (90%)	264 (98%)	5 (2%)	57	68
1	C	269/298 (90%)	266 (99%)	3 (1%)	73	83
1	D	267/298 (90%)	263 (98%)	4 (2%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	265/298 (89%)	257 (97%)	8 (3%)	41	50
1	F	267/298 (90%)	263 (98%)	4 (2%)	65	76
1	G	269/298 (90%)	266 (99%)	3 (1%)	73	83
1	H	267/298 (90%)	265 (99%)	2 (1%)	84	90
All	All	2141/2384 (90%)	2105 (98%)	36 (2%)	62	72

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	39	SER
1	A	77	SER
1	A	90[A]	ARG
1	A	90[B]	ARG
1	A	234	MET
1	A	413	LEU
1	B	-1	ASN
1	B	28	ARG
1	B	79	GLU
1	B	377	THR
1	B	398	GLU
1	C	76	MET
1	C	370	VAL
1	C	397	MET
1	D	74	LYS
1	D	77	SER
1	D	90	ARG
1	D	248	ILE
1	E	28	ARG
1	E	34	THR
1	E	37	SER
1	E	77	SER
1	E	235	THR
1	E	283	THR
1	E	332	ARG
1	E	397	MET
1	F	74	LYS
1	F	89	LYS
1	F	252	THR
1	F	414	VAL
1	G	89	LYS

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Mol	Chain	Res	Type
1	G	229	VAL
1	G	316	VAL
1	H	235	THR
1	H	449	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	381	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

Of 32 ligands modelled in this entry, 9 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	EDO	F	504	-	3,3,3	0.47	0	2,2,2	0.26	0
4	ZO7	G	503	-	35,35,35	1.07	5 (14%)	50,51,51	1.42	5 (10%)
3	GOL	H	504	-	5,5,5	0.91	0	5,5,5	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	IMP	B	501	-	21,25,25	1.48	2 (9%)	24,38,38	1.41	5 (20%)
2	IMP	E	501	-	21,25,25	1.48	2 (9%)	24,38,38	1.39	5 (20%)
4	ZO7	H	506	-	35,35,35	1.03	5 (14%)	50,51,51	1.29	3 (6%)
2	IMP	A	501	-	21,25,25	1.48	2 (9%)	24,38,38	1.26	5 (20%)
3	GOL	C	503	-	5,5,5	0.90	0	5,5,5	1.02	0
3	GOL	H	503	-	5,5,5	0.91	0	5,5,5	1.01	0
3	GOL	A	503	-	5,5,5	0.91	0	5,5,5	0.98	0
2	IMP	F	501	-	21,25,25	1.47	2 (9%)	24,38,38	1.35	5 (20%)
4	ZO7	B	502	-	35,35,35	1.07	5 (14%)	50,51,51	1.25	2 (4%)
3	GOL	A	502	-	5,5,5	0.91	0	5,5,5	1.01	0
2	IMP	G	502	-	21,25,25	1.48	2 (9%)	24,38,38	1.34	5 (20%)
2	IMP	D	502	-	21,25,25	1.46	2 (9%)	24,38,38	1.38	5 (20%)
2	IMP	H	502	-	21,25,25	1.46	2 (9%)	24,38,38	1.29	4 (16%)
4	ZO7	D	503	-	35,35,35	1.07	5 (14%)	50,51,51	1.54	6 (12%)
2	IMP	C	502	-	21,25,25	1.48	2 (9%)	24,38,38	1.39	5 (20%)
4	ZO7	F	502	-	35,35,35	1.08	5 (14%)	50,51,51	1.53	6 (12%)
4	ZO7	E	502	-	35,35,35	1.06	5 (14%)	50,51,51	1.39	5 (10%)
3	GOL	A	506	-	5,5,5	0.90	0	5,5,5	1.00	0
4	ZO7	A	504	-	35,35,35	1.04	5 (14%)	50,51,51	1.28	3 (6%)
4	ZO7	C	504	-	35,35,35	1.06	5 (14%)	50,51,51	1.35	3 (6%)

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
6	EDO	F	504	-	-	0/1/1/1	-
4	ZO7	G	503	-	-	2/23/40/40	0/3/3/3
3	GOL	H	504	-	-	2/4/4/4	-
2	IMP	B	501	-	-	3/6/26/26	0/3/3/3
2	IMP	E	501	-	-	2/6/26/26	0/3/3/3
4	ZO7	H	506	-	-	3/23/40/40	0/3/3/3
2	IMP	A	501	-	-	2/6/26/26	0/3/3/3
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	H	503	-	-	2/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	F	501	-	-	5/6/26/26	0/3/3/3
4	ZO7	B	502	-	-	2/23/40/40	0/3/3/3
3	GOL	A	502	-	-	0/4/4/4	-
2	IMP	G	502	-	-	3/6/26/26	0/3/3/3
2	IMP	D	502	-	-	4/6/26/26	0/3/3/3
2	IMP	H	502	-	-	3/6/26/26	0/3/3/3
4	ZO7	D	503	-	-	2/23/40/40	0/3/3/3
2	IMP	C	502	-	-	4/6/26/26	0/3/3/3
4	ZO7	F	502	-	-	2/23/40/40	0/3/3/3
4	ZO7	E	502	-	-	2/23/40/40	0/3/3/3
3	GOL	A	506	-	-	3/4/4/4	-
4	ZO7	A	504	-	-	2/23/40/40	0/3/3/3
4	ZO7	C	504	-	-	2/23/40/40	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IMP	C2-N3	4.79	1.38	1.29
2	E	501	IMP	C2-N3	4.75	1.38	1.29
2	B	501	IMP	C2-N3	4.75	1.38	1.29
2	D	502	IMP	C2-N3	4.73	1.38	1.29
2	G	502	IMP	C2-N3	4.72	1.38	1.29
2	H	502	IMP	C2-N3	4.70	1.38	1.29
2	F	501	IMP	C2-N3	4.69	1.38	1.29
2	C	502	IMP	C2-N3	4.66	1.38	1.29
2	C	502	IMP	C5-C6	-4.09	1.39	1.47
2	B	501	IMP	C5-C6	-4.00	1.39	1.47
2	G	502	IMP	C5-C6	-3.97	1.39	1.47
2	E	501	IMP	C5-C6	-3.94	1.39	1.47
2	A	501	IMP	C5-C6	-3.94	1.39	1.47
2	F	501	IMP	C5-C6	-3.92	1.39	1.47
2	H	502	IMP	C5-C6	-3.89	1.39	1.47
2	D	502	IMP	C5-C6	-3.87	1.39	1.47
4	E	502	ZO7	C9-C7	-2.86	1.32	1.46
4	D	503	ZO7	C9-C7	-2.86	1.32	1.46
4	F	502	ZO7	C9-C7	-2.86	1.32	1.46
4	H	506	ZO7	C9-C7	-2.86	1.32	1.46
4	C	504	ZO7	C9-C7	-2.85	1.32	1.46
4	G	503	ZO7	C9-C7	-2.85	1.32	1.46
4	A	504	ZO7	C9-C7	-2.85	1.32	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	ZO7	C9-C7	-2.85	1.32	1.46
4	C	504	ZO7	C20-CL	2.69	1.80	1.73
4	F	502	ZO7	C20-CL	2.66	1.79	1.73
4	E	502	ZO7	C20-CL	2.65	1.79	1.73
4	B	502	ZO7	C20-CL	2.64	1.79	1.73
4	D	503	ZO7	C20-CL	2.63	1.79	1.73
4	A	504	ZO7	C20-CL	2.62	1.79	1.73
4	G	503	ZO7	C20-CL	2.62	1.79	1.73
4	H	506	ZO7	C20-CL	2.60	1.79	1.73
4	G	503	ZO7	C11-C1	-2.55	1.50	1.53
4	B	502	ZO7	C24-N1	2.53	1.46	1.42
4	B	502	ZO7	C11-C1	-2.51	1.50	1.53
4	F	502	ZO7	C24-N1	2.51	1.46	1.42
4	D	503	ZO7	C11-C1	-2.50	1.50	1.53
4	F	502	ZO7	C11-C1	-2.48	1.50	1.53
4	G	503	ZO7	C24-N1	2.48	1.46	1.42
4	E	502	ZO7	C11-C1	-2.48	1.50	1.53
4	C	504	ZO7	C24-N1	2.47	1.46	1.42
4	H	506	ZO7	C11-C1	-2.46	1.50	1.53
4	D	503	ZO7	C24-N1	2.46	1.46	1.42
4	A	504	ZO7	C11-C1	-2.45	1.50	1.53
4	C	504	ZO7	C11-C1	-2.44	1.50	1.53
4	E	502	ZO7	C24-N1	2.41	1.46	1.42
4	B	502	ZO7	C17-N4	-2.36	1.36	1.41
4	F	502	ZO7	C17-N4	-2.36	1.36	1.41
4	C	504	ZO7	C17-N4	-2.35	1.36	1.41
4	A	504	ZO7	C17-N4	-2.33	1.36	1.41
4	G	503	ZO7	C17-N4	-2.32	1.36	1.41
4	D	503	ZO7	C17-N4	-2.32	1.37	1.41
4	H	506	ZO7	C17-N4	-2.31	1.37	1.41
4	A	504	ZO7	C24-N1	2.30	1.46	1.42
4	E	502	ZO7	C17-N4	-2.28	1.37	1.41
4	H	506	ZO7	C24-N1	2.09	1.45	1.42

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	ZO7	C25-C24-N1	-6.89	104.46	110.71
4	H	506	ZO7	C25-C24-N1	-6.39	104.92	110.71
4	C	504	ZO7	C25-C24-N1	-6.38	104.92	110.71
4	A	504	ZO7	C25-C24-N1	-6.36	104.94	110.71
4	F	502	ZO7	C25-C24-N1	-6.31	104.99	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	502	ZO7	C25-C24-N1	-6.23	105.06	110.71
4	G	503	ZO7	C25-C24-N1	-6.18	105.11	110.71
4	B	502	ZO7	C25-C24-N1	-5.67	105.57	110.71
4	F	502	ZO7	C20-C21-N1	-4.98	118.06	120.43
4	G	503	ZO7	C20-C21-N1	-3.64	118.69	120.43
2	A	501	IMP	C5-C6-N1	3.20	119.61	113.95
4	D	503	ZO7	C29-O3-C24	3.18	116.39	111.98
2	C	502	IMP	C5-C6-N1	3.11	119.44	113.95
2	B	501	IMP	C5-C6-N1	3.10	119.43	113.95
2	H	502	IMP	C8-N7-C5	3.10	108.89	102.99
2	D	502	IMP	C5-C6-N1	3.07	119.38	113.95
4	D	503	ZO7	C20-C21-N1	-3.05	118.97	120.43
2	D	502	IMP	C8-N7-C5	3.05	108.80	102.99
2	E	501	IMP	C8-N7-C5	3.04	108.77	102.99
2	G	502	IMP	C8-N7-C5	3.03	108.76	102.99
2	E	501	IMP	C5-C6-N1	3.02	119.28	113.95
2	F	501	IMP	C8-N7-C5	3.02	108.74	102.99
4	H	506	ZO7	C20-C21-N1	-3.01	119.00	120.43
2	B	501	IMP	C8-N7-C5	3.01	108.72	102.99
4	E	502	ZO7	C20-C21-N1	-3.00	119.00	120.43
2	C	502	IMP	C8-N7-C5	2.97	108.65	102.99
2	H	502	IMP	C5-C6-N1	2.96	119.19	113.95
2	A	501	IMP	C8-N7-C5	2.95	108.62	102.99
2	G	502	IMP	O6-C6-C5	-2.95	118.62	124.37
2	B	501	IMP	O3P-P-O2P	2.95	118.89	107.64
2	F	501	IMP	C5-C6-N1	2.94	119.14	113.95
4	F	502	ZO7	C26-C25-C24	2.92	114.19	109.94
2	D	502	IMP	O3P-P-O2P	2.91	118.77	107.64
4	C	504	ZO7	C20-C21-N1	-2.90	119.05	120.43
2	C	502	IMP	O3P-P-O2P	2.90	118.73	107.64
4	D	503	ZO7	C26-C25-C24	2.89	114.15	109.94
2	E	501	IMP	O3P-P-O2P	2.88	118.63	107.64
2	F	501	IMP	O3P-P-O2P	2.87	118.62	107.64
2	G	502	IMP	C5-C6-N1	2.86	119.00	113.95
4	G	503	ZO7	C26-C25-C24	2.85	114.10	109.94
4	D	503	ZO7	O3-C24-C25	2.78	113.63	109.99
2	C	502	IMP	O6-C6-C5	-2.67	119.15	124.37
2	B	501	IMP	O6-C6-C5	-2.64	119.21	124.37
2	E	501	IMP	O6-C6-C5	-2.61	119.28	124.37
4	B	502	ZO7	C21-N1-C24	-2.59	120.51	123.16
2	H	502	IMP	O6-C6-C5	-2.50	119.50	124.37
4	E	502	ZO7	C26-C25-C24	2.46	113.52	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	IMP	O6-C6-C5	-2.43	119.62	124.37
4	A	504	ZO7	C20-C21-N1	-2.42	119.28	120.43
2	F	501	IMP	O6-C6-C5	-2.41	119.66	124.37
4	H	506	ZO7	C21-N1-C24	-2.37	120.74	123.16
4	F	502	ZO7	C29-O3-C24	2.35	115.23	111.98
4	G	503	ZO7	O3-C24-C25	2.32	113.03	109.99
4	E	502	ZO7	C29-O3-C24	2.26	115.12	111.98
4	G	503	ZO7	C29-O3-C24	2.26	115.10	111.98
4	D	503	ZO7	O3-C24-N1	2.25	113.06	109.46
4	A	504	ZO7	C21-N1-C24	-2.24	120.87	123.16
4	F	502	ZO7	O3-C24-C25	2.21	112.89	109.99
4	F	502	ZO7	O3-C24-N1	2.14	112.89	109.46
2	A	501	IMP	O6-C6-C5	-2.13	120.21	124.37
2	F	501	IMP	N1-C2-N3	-2.11	120.36	125.87
2	E	501	IMP	N1-C2-N3	-2.11	120.37	125.87
2	G	502	IMP	N1-C2-N3	-2.10	120.38	125.87
4	C	504	ZO7	C29-O3-C24	2.10	114.89	111.98
4	E	502	ZO7	O3-C24-C25	2.08	112.72	109.99
2	B	501	IMP	N1-C2-N3	-2.08	120.45	125.87
2	G	502	IMP	O2P-P-O1P	2.06	118.75	110.68
2	A	501	IMP	O2P-P-O1P	2.06	118.74	110.68
2	D	502	IMP	N1-C2-N3	-2.05	120.52	125.87
2	H	502	IMP	N1-C2-N3	-2.04	120.56	125.87
2	C	502	IMP	N1-C2-N3	-2.04	120.56	125.87
2	A	501	IMP	N1-C2-N3	-2.03	120.58	125.87

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	IMP	C5'-O5'-P-O1P
2	B	501	IMP	C5'-O5'-P-O1P
2	B	501	IMP	C5'-O5'-P-O2P
2	B	501	IMP	C5'-O5'-P-O3P
2	C	502	IMP	C5'-O5'-P-O2P
2	D	502	IMP	C5'-O5'-P-O2P
2	D	502	IMP	C5'-O5'-P-O3P
2	E	501	IMP	C5'-O5'-P-O2P
2	F	501	IMP	C5'-O5'-P-O1P
2	F	501	IMP	C5'-O5'-P-O2P
2	F	501	IMP	C5'-O5'-P-O3P
2	G	502	IMP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
2	G	502	IMP	C5'-O5'-P-O2P
2	G	502	IMP	C5'-O5'-P-O3P
2	H	502	IMP	C5'-O5'-P-O2P
2	H	502	IMP	C5'-O5'-P-O3P
3	A	503	GOL	O1-C1-C2-C3
2	F	501	IMP	C3'-C4'-C5'-O5'
2	F	501	IMP	O4'-C4'-C5'-O5'
3	A	503	GOL	C1-C2-C3-O3
3	A	506	GOL	O1-C1-C2-C3
3	C	503	GOL	O1-C1-C2-C3
3	H	504	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-O2
2	D	502	IMP	C5'-O5'-P-O1P
3	A	503	GOL	O2-C2-C3-O3
3	A	506	GOL	O2-C2-C3-O3
3	H	503	GOL	O1-C1-C2-C3
4	B	502	ZO7	C4-C5-C7-C9
2	C	502	IMP	C5'-O5'-P-O1P
2	E	501	IMP	C5'-O5'-P-O1P
4	B	502	ZO7	C6-C5-C7-C9
4	F	502	ZO7	C6-C5-C7-C9
4	H	506	ZO7	O3-C24-N1-C21
4	E	502	ZO7	C6-C5-C7-C9
4	E	502	ZO7	C4-C5-C7-C9
4	G	503	ZO7	C6-C5-C7-C9
4	D	503	ZO7	C6-C5-C7-C9
3	H	503	GOL	O1-C1-C2-O2
3	H	504	GOL	O1-C1-C2-O2
2	C	502	IMP	C3'-C4'-C5'-O5'
2	A	501	IMP	C5'-O5'-P-O3P
2	C	502	IMP	C5'-O5'-P-O3P
4	A	504	ZO7	C6-C5-C7-C9
4	C	504	ZO7	C6-C5-C7-C9
4	G	503	ZO7	C4-C5-C7-C9
4	H	506	ZO7	C6-C5-C7-C9
2	H	502	IMP	C5'-O5'-P-O1P
4	F	502	ZO7	C4-C5-C7-C9
3	A	506	GOL	O1-C1-C2-O2
3	C	503	GOL	O1-C1-C2-O2
4	A	504	ZO7	C4-C5-C7-C9
4	C	504	ZO7	C4-C5-C7-C9
4	D	503	ZO7	C4-C5-C7-C9

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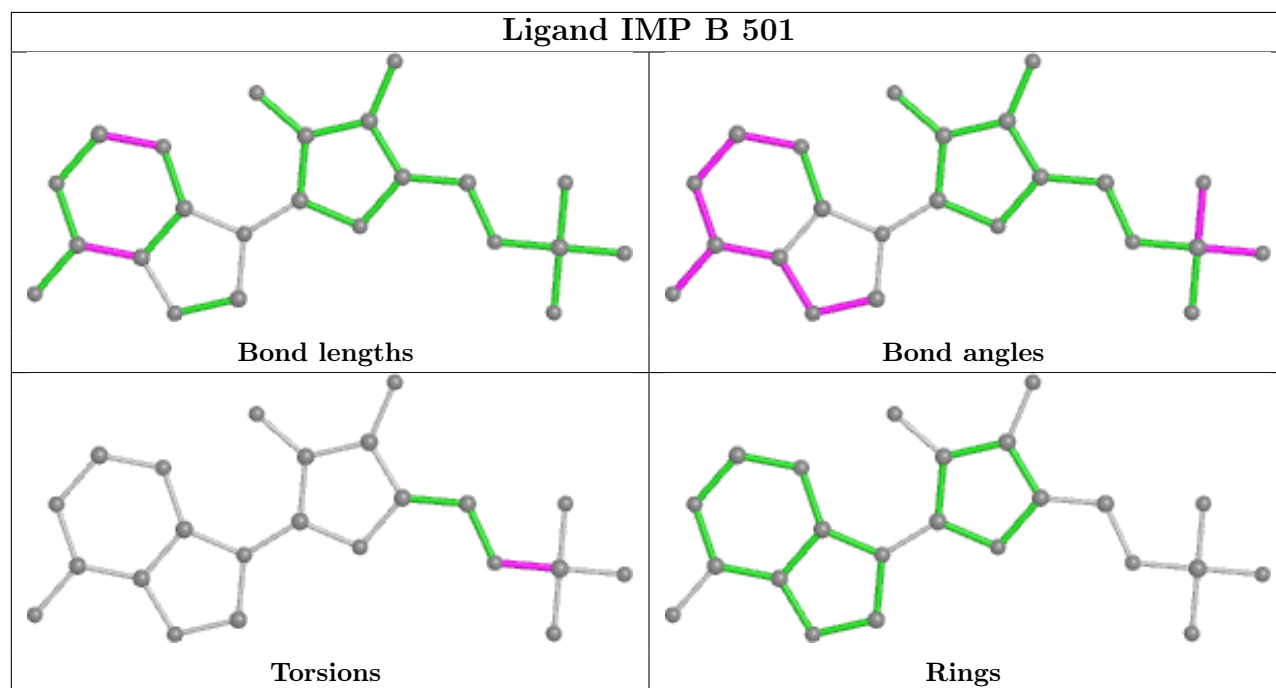
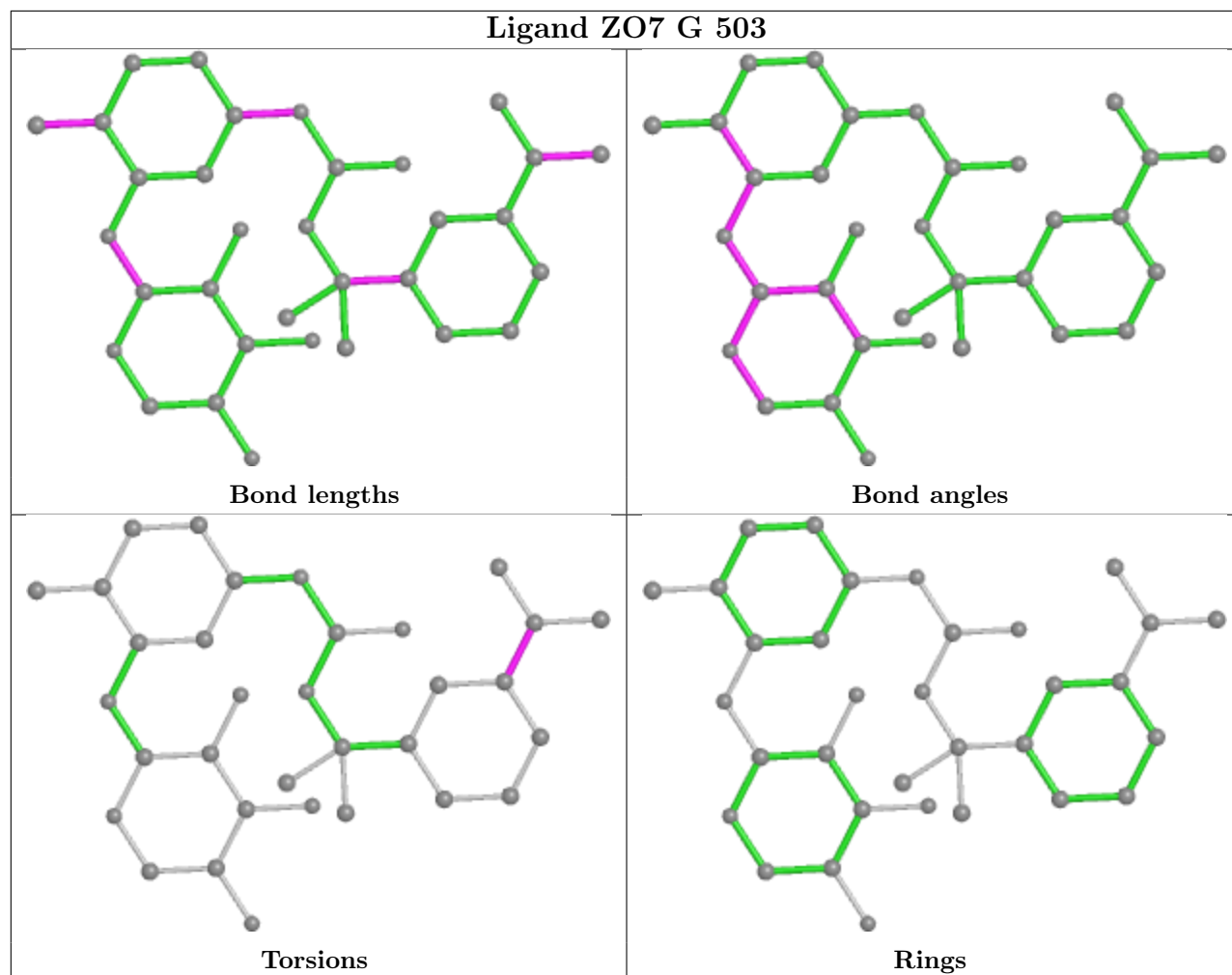
Mol	Chain	Res	Type	Atoms
4	H	506	ZO7	C4-C5-C7-C9
2	D	502	IMP	C3'-C4'-C5'-O5'

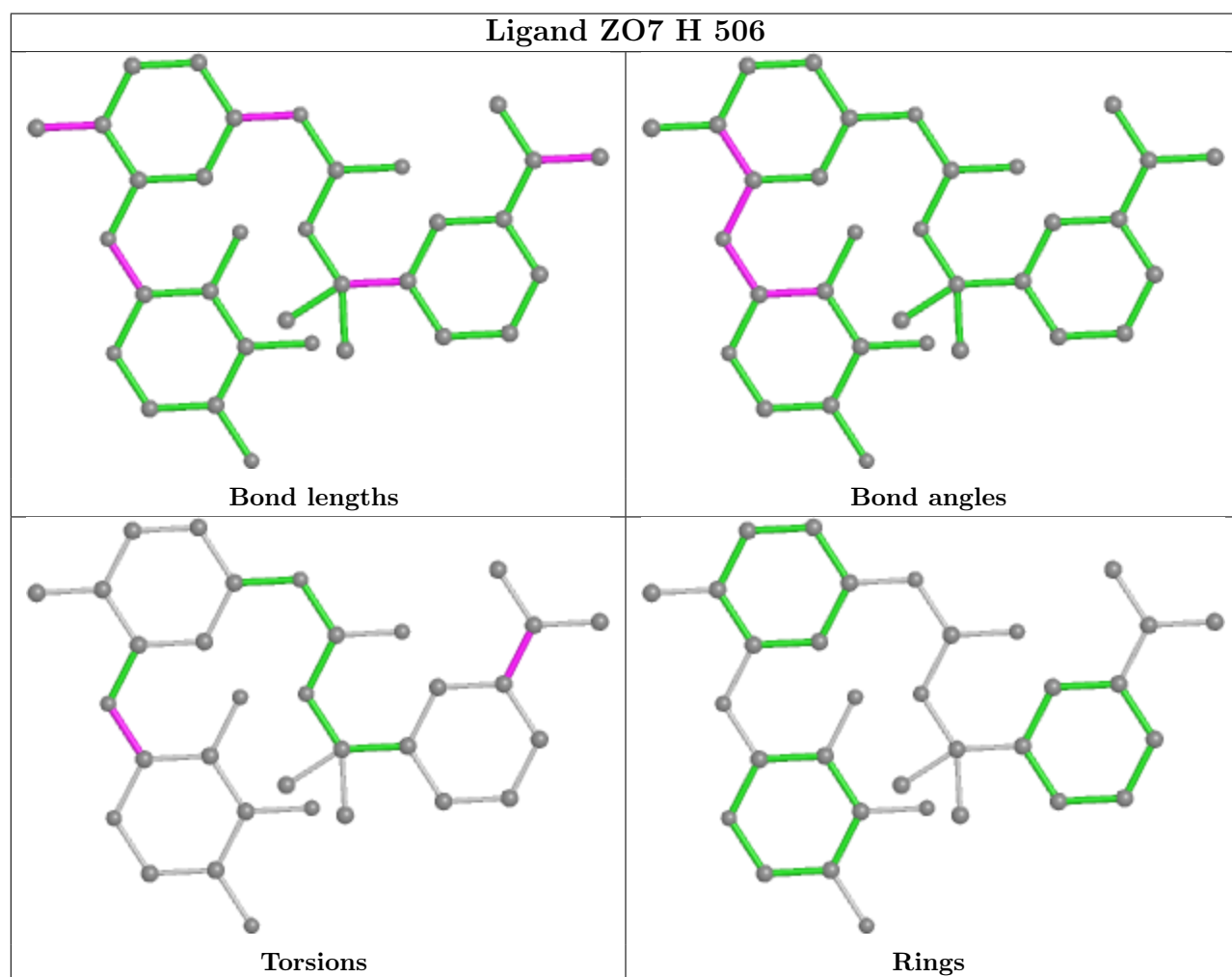
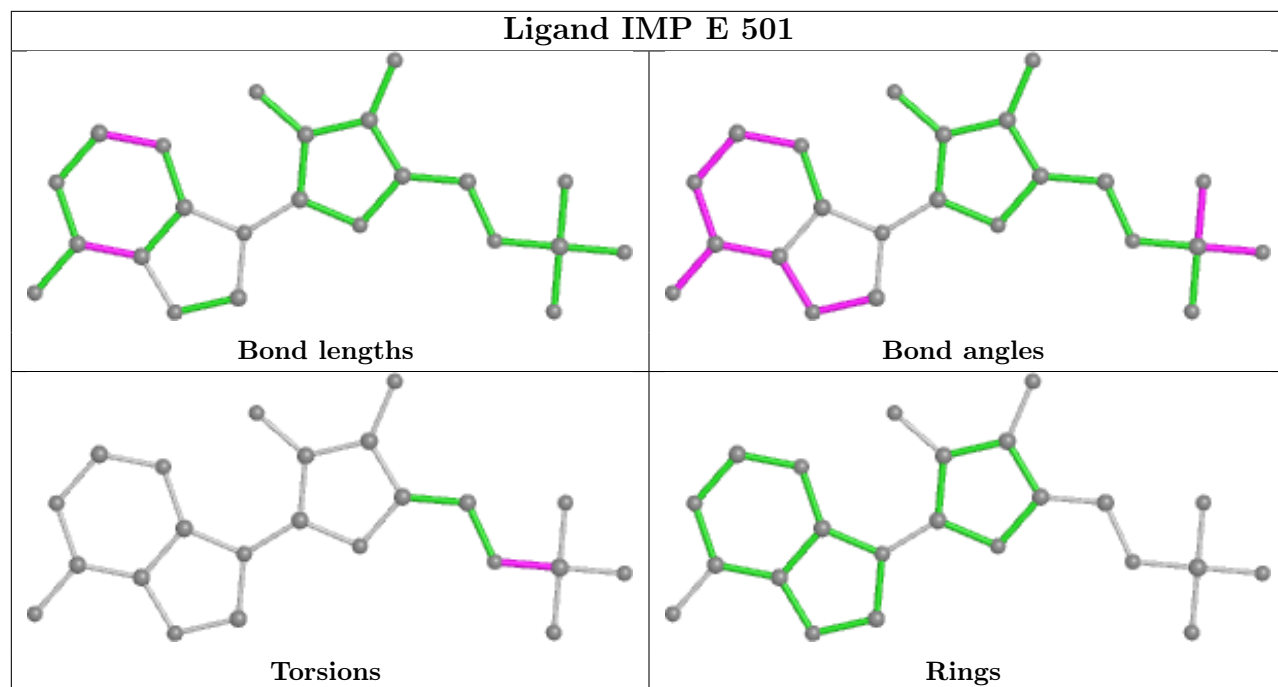
There are no ring outliers.

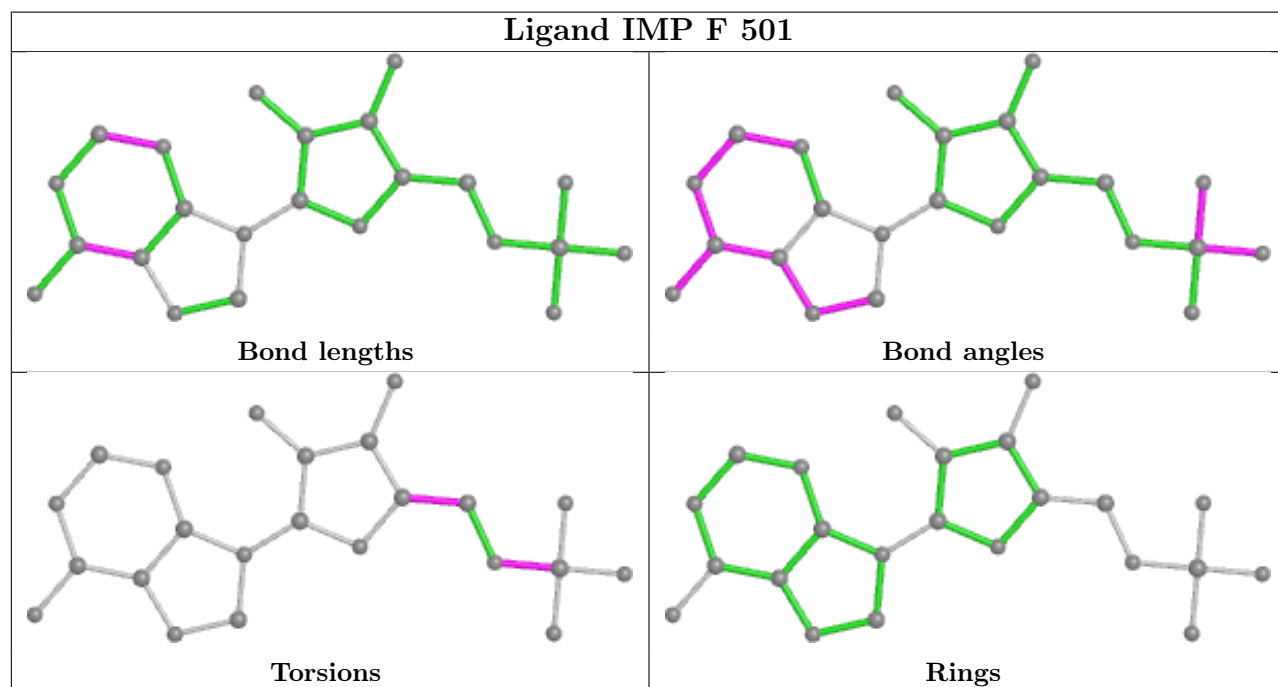
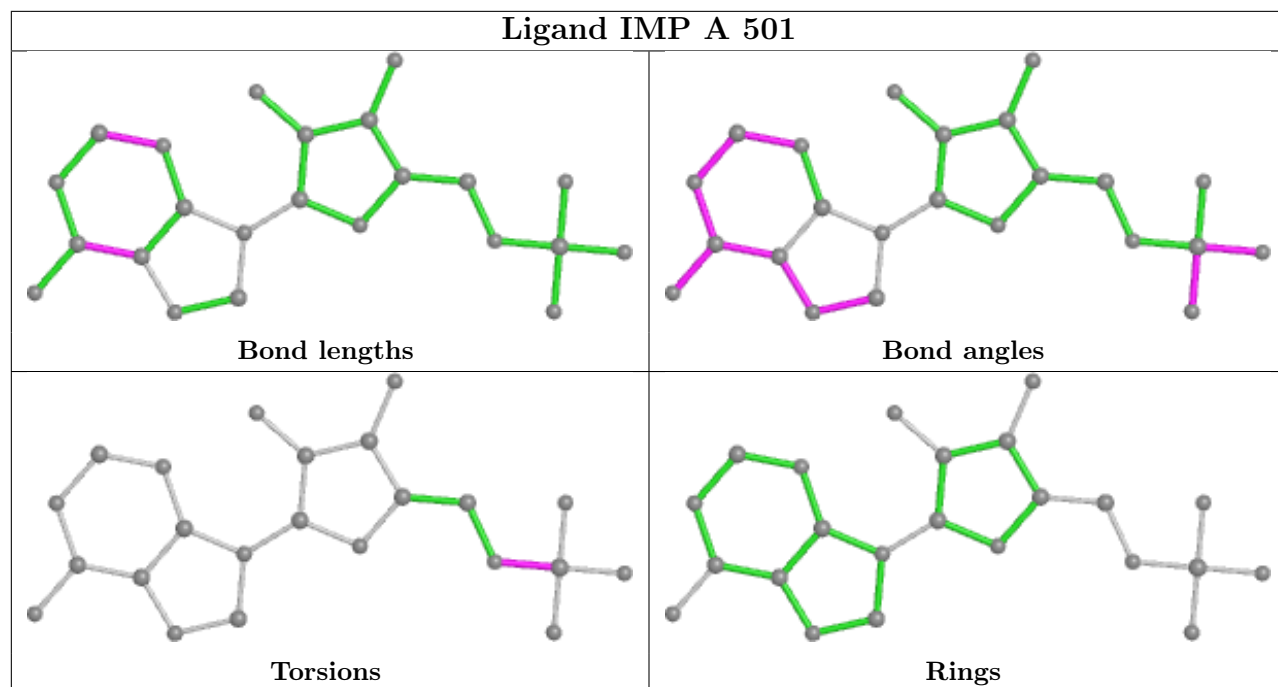
3 monomers are involved in 4 short contacts:

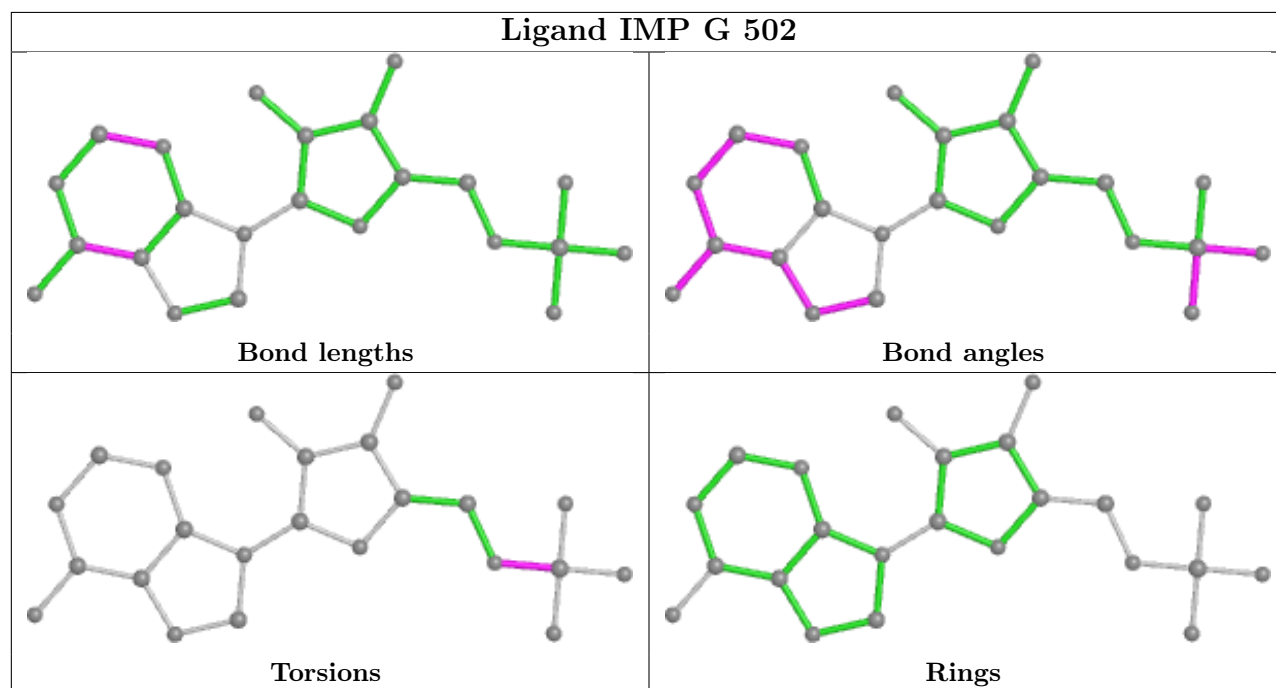
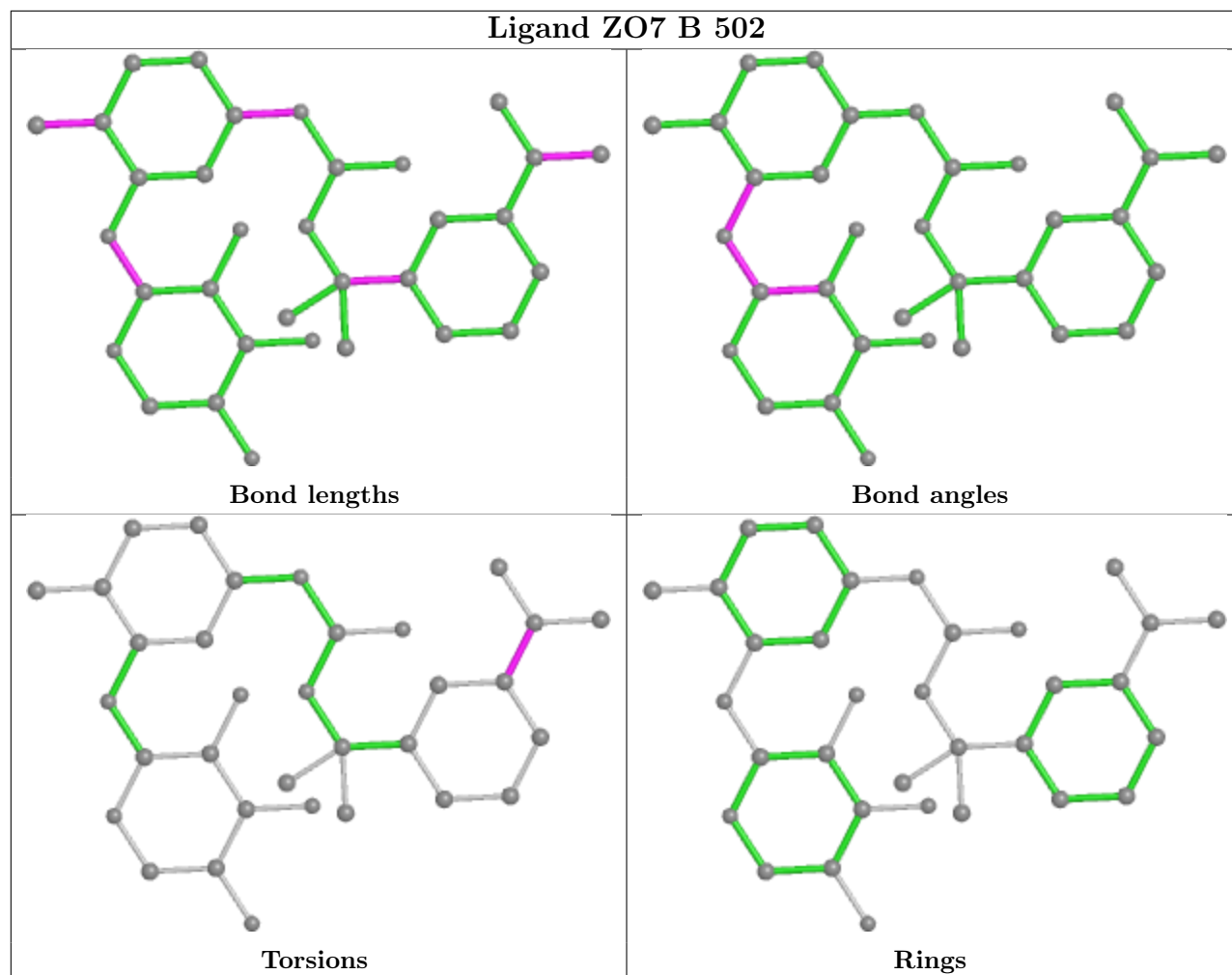
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	IMP	2	0
2	E	501	IMP	1	0
2	C	502	IMP	1	0

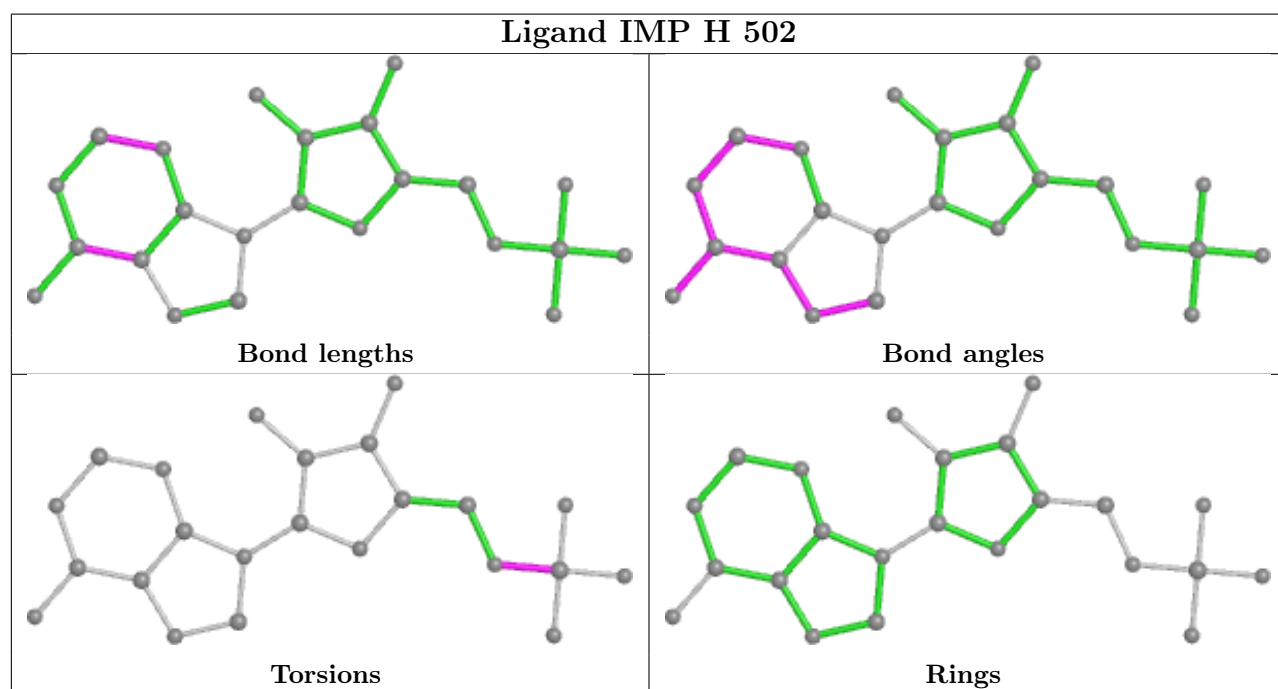
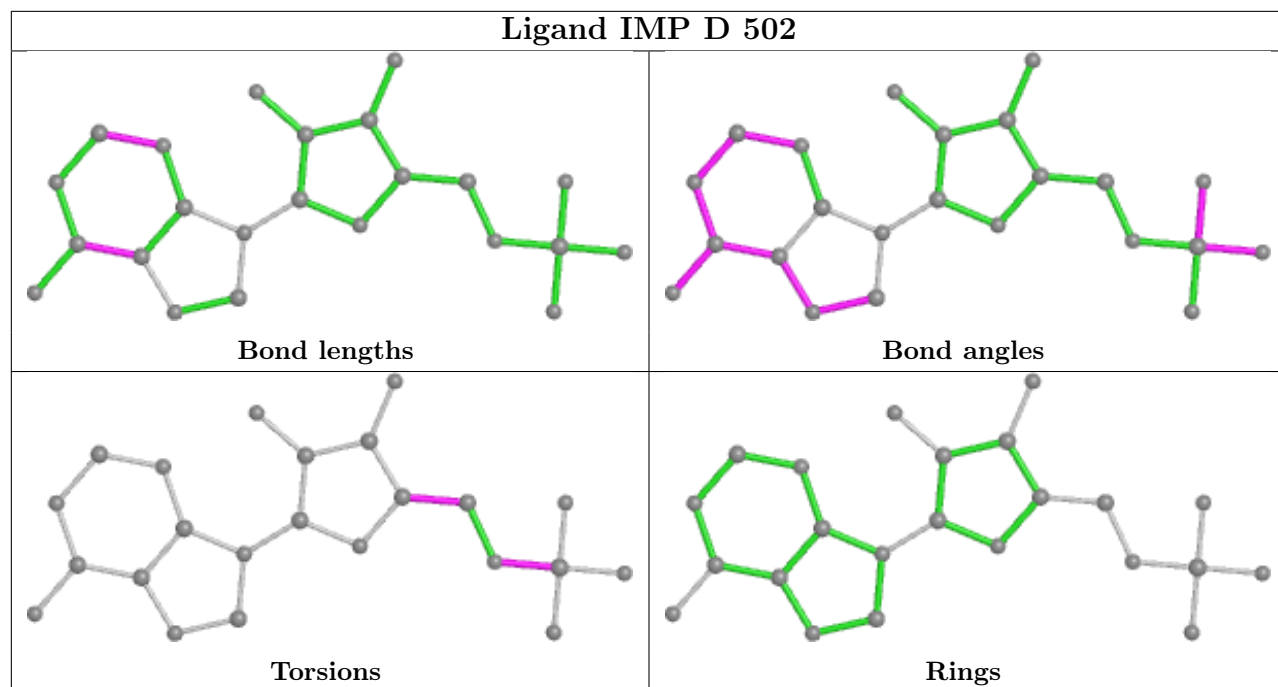
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



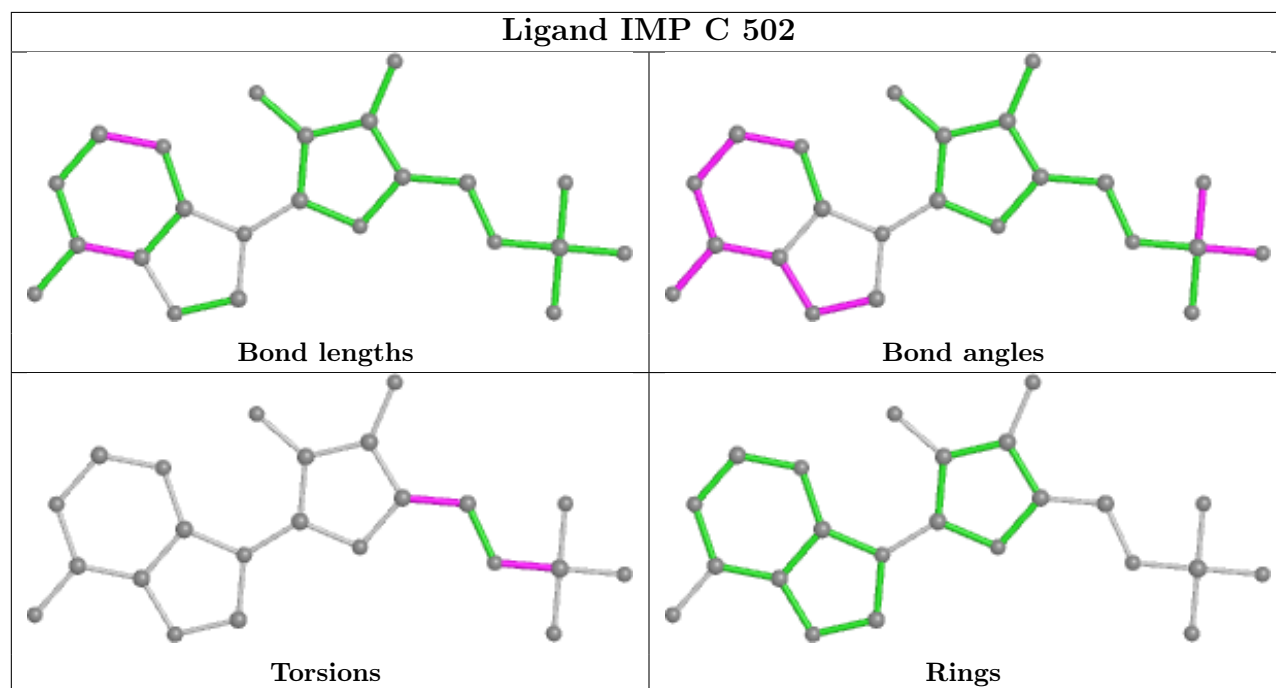
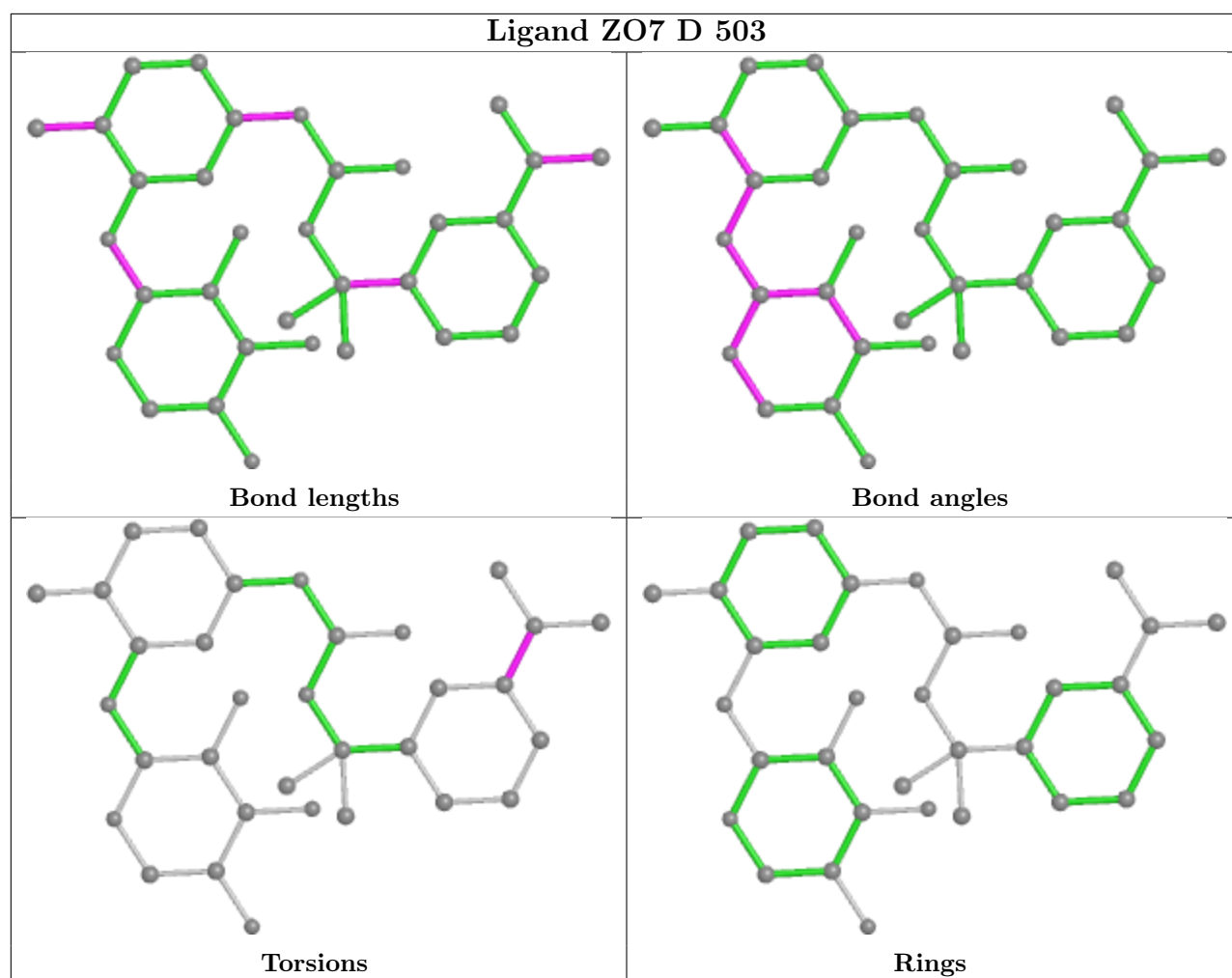


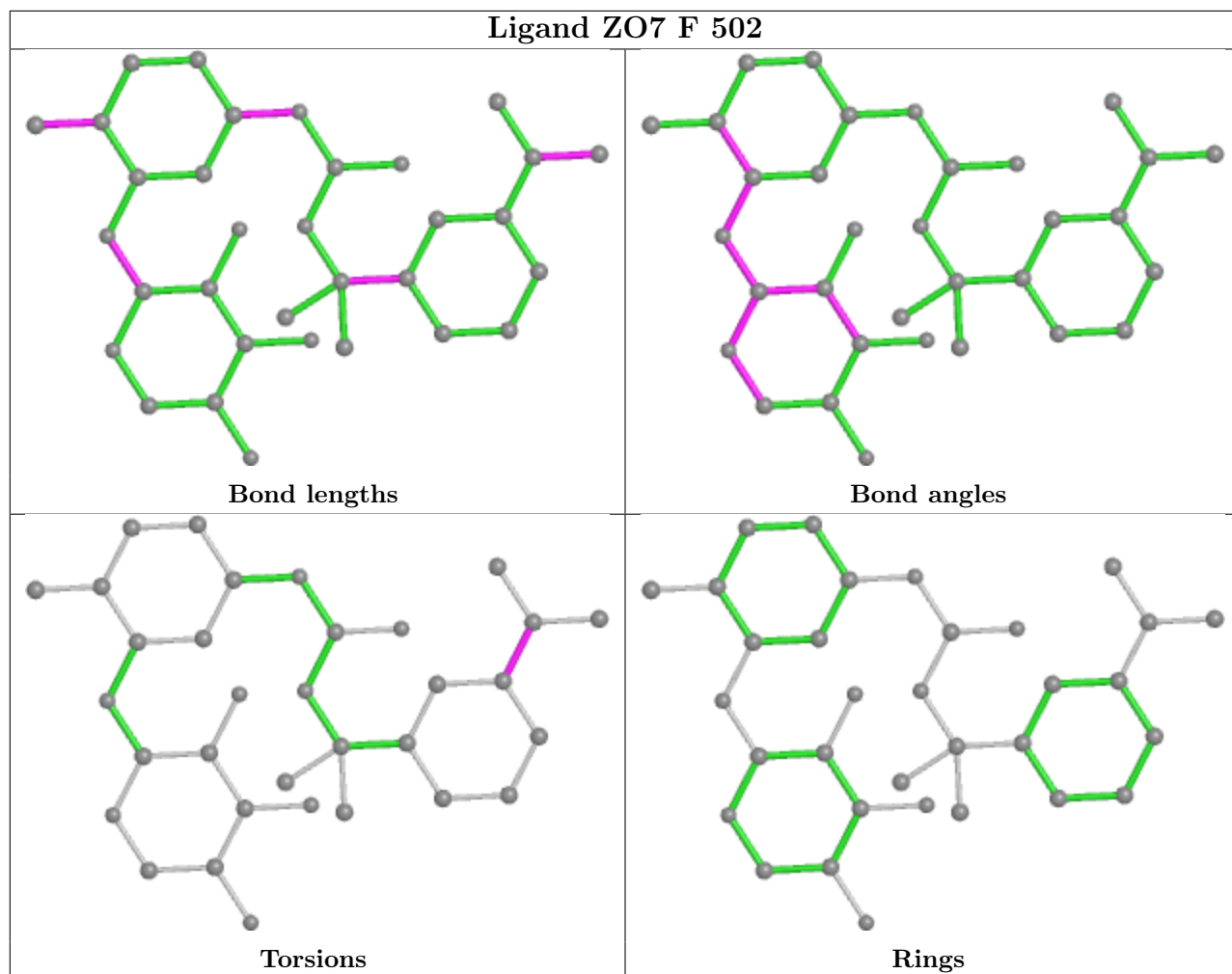


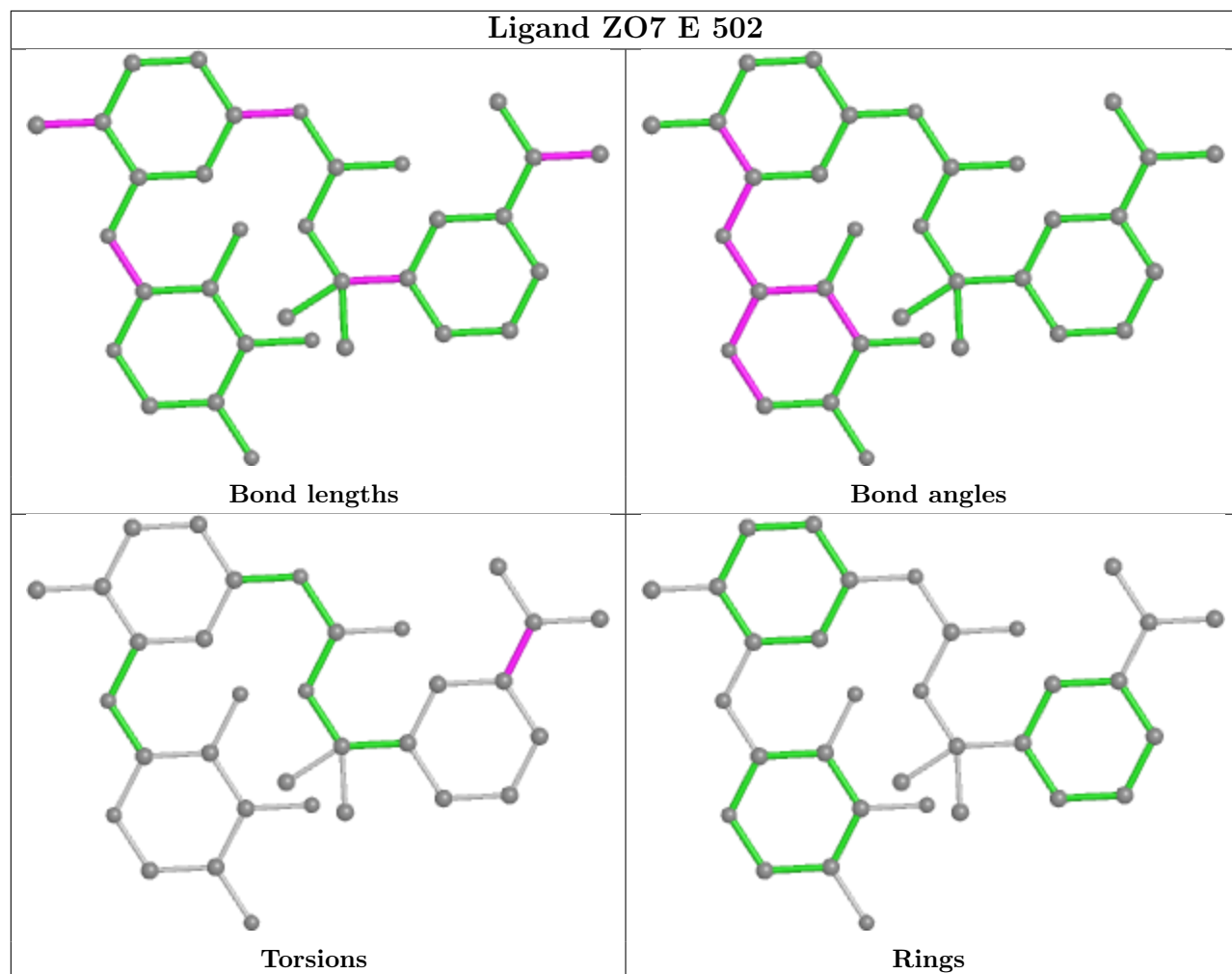


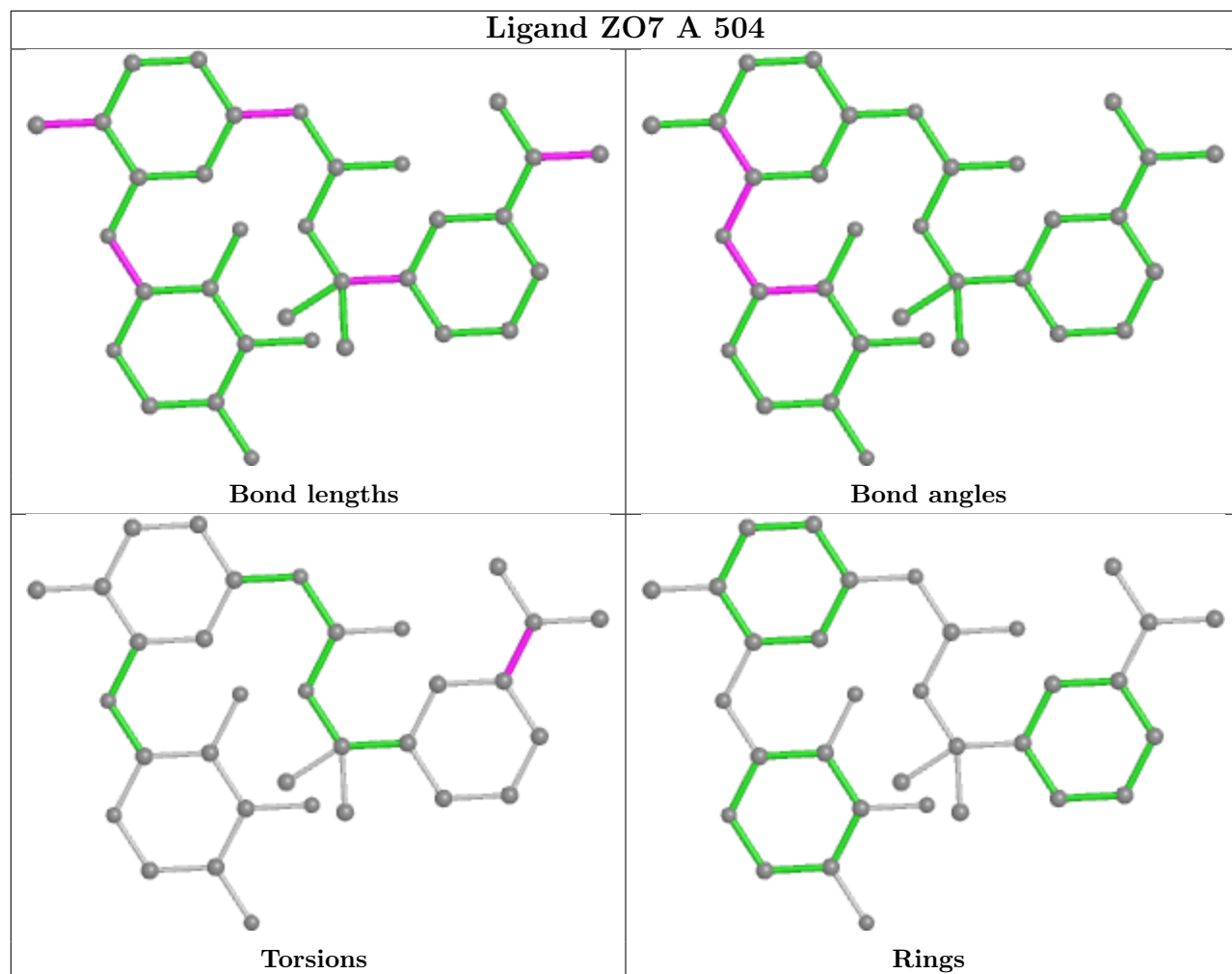


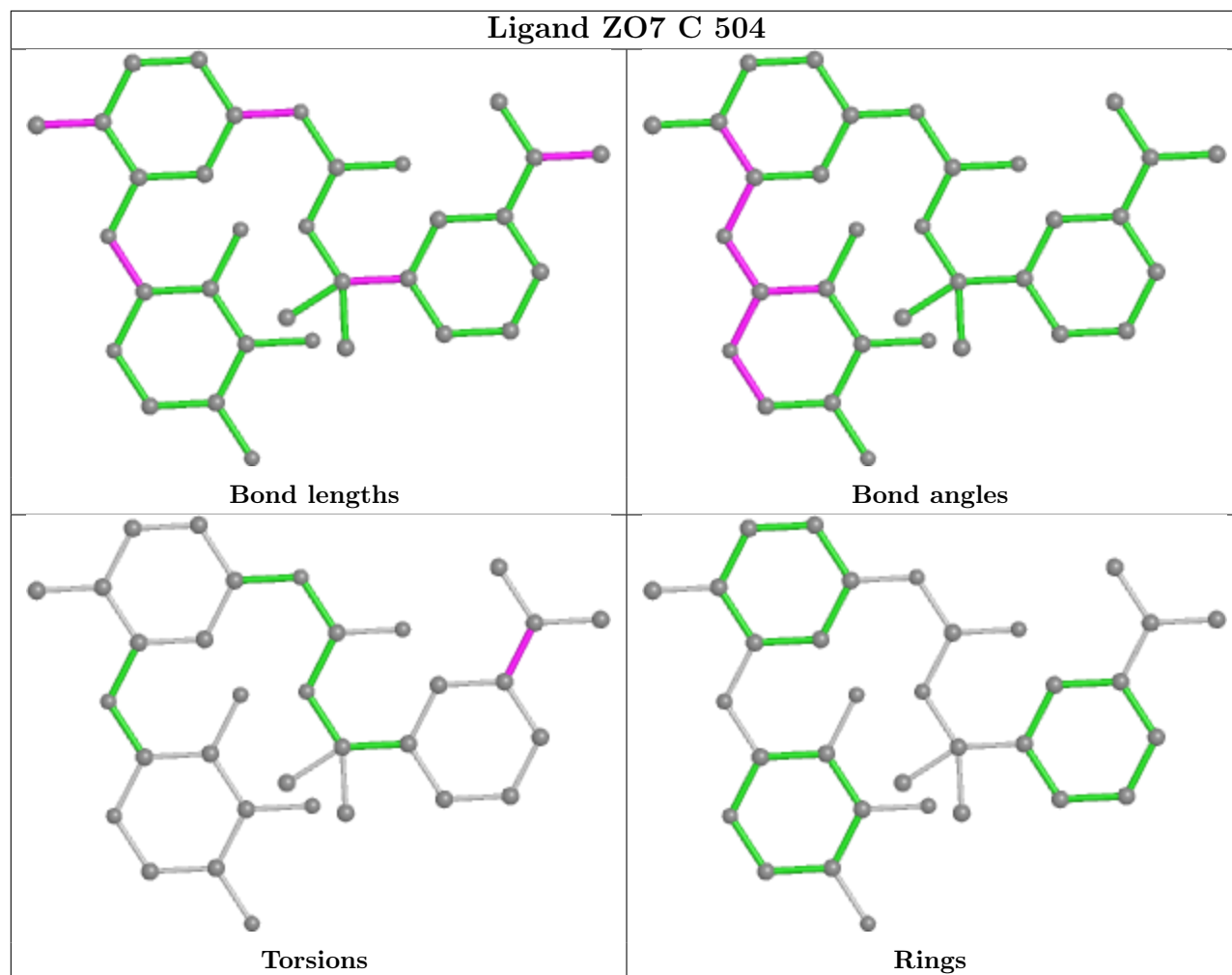












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	349/384 (90%)	0.20	6 (1%) 70 78	18, 31, 54, 79	0
1	B	350/384 (91%)	0.29	5 (1%) 75 82	18, 32, 54, 87	0
1	C	351/384 (91%)	0.24	3 (0%) 84 89	20, 32, 54, 75	0
1	D	349/384 (90%)	0.58	29 (8%) 11 17	20, 42, 65, 86	0
1	E	347/384 (90%)	0.86	49 (14%) 2 4	28, 54, 84, 97	0
1	F	348/384 (90%)	0.65	27 (7%) 13 19	23, 44, 74, 104	0
1	G	351/384 (91%)	0.40	15 (4%) 35 46	21, 39, 62, 86	0
1	H	349/384 (90%)	0.31	8 (2%) 60 69	21, 35, 61, 93	0
All	All	2794/3072 (90%)	0.44	142 (5%) 28 39	18, 38, 71, 104	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	223	VAL	6.2
1	E	234	MET	4.8
1	A	382	GLY	4.8
1	F	243	ALA	4.7
1	E	334	HIS	4.5
1	C	413	LEU	4.3
1	D	397	MET	4.2
1	E	240	LEU	4.2
1	E	69	LEU	4.1
1	D	374	PRO	3.9
1	G	273	SER	3.9
1	D	376	GLU	3.8
1	D	413	LEU	3.8
1	E	222	LEU	3.8
1	E	82	ALA	3.7
1	B	413	LEU	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	234	MET	3.7
1	D	86	ASP	3.7
1	E	235	THR	3.6
1	F	241	VAL	3.6
1	D	-1	ASN	3.6
1	E	78	ILE	3.6
1	E	79	GLU	3.5
1	E	57	ALA	3.5
1	D	240	LEU	3.5
1	E	239	ALA	3.5
1	E	375	GLY	3.5
1	E	479	THR	3.4
1	E	75	ASN	3.4
1	G	476	VAL	3.4
1	G	250	LEU	3.4
1	F	54	VAL	3.4
1	E	230	THR	3.3
1	D	269	ALA	3.3
1	E	226	ALA	3.3
1	G	487	LEU	3.3
1	E	374	PRO	3.3
1	E	250	LEU	3.3
1	F	413	LEU	3.3
1	E	399	LYS	3.2
1	E	90	ARG	3.2
1	F	74	LYS	3.2
1	E	227	VAL	3.1
1	F	57	ALA	3.1
1	F	85	VAL	3.1
1	E	67	GLY	3.1
1	F	223	VAL	3.1
1	D	61	ILE	3.1
1	A	413	LEU	3.0
1	E	276	ILE	3.0
1	G	267	VAL	3.0
1	D	81	GLN	3.0
1	E	247	ALA	2.9
1	E	88	VAL	2.9
1	G	413	LEU	2.9
1	G	328	ALA	2.9
1	D	223	VAL	2.8
1	F	230	THR	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	232	ASP	2.8
1	F	58	ASP	2.8
1	F	90	ARG	2.8
1	G	-2	SER	2.8
1	A	237	ILE	2.8
1	D	292	GLU	2.7
1	F	83	GLU	2.7
1	D	90	ARG	2.7
1	H	232	ASP	2.7
1	E	333	LYS	2.7
1	F	87	LYS	2.7
1	E	248	ILE	2.7
1	E	271	TYR	2.6
1	E	245	VAL	2.6
1	E	244	SER	2.6
1	D	242	LYS	2.6
1	E	237	ILE	2.6
1	A	456	GLU	2.6
1	D	244	SER	2.6
1	F	239	ALA	2.6
1	D	235	THR	2.5
1	E	84	GLN	2.5
1	E	241	VAL	2.5
1	E	274	LEU	2.5
1	H	88	VAL	2.5
1	F	258	GLN	2.5
1	D	76	MET	2.5
1	G	380	TYR	2.5
1	C	399	LYS	2.5
1	E	290	LEU	2.5
1	F	290	LEU	2.5
1	E	77	SER	2.4
1	D	82	ALA	2.4
1	E	85	VAL	2.4
1	F	78	ILE	2.4
1	D	54	VAL	2.4
1	D	25	VAL	2.4
1	G	399	LYS	2.4
1	C	379	ILE	2.4
1	F	267	VAL	2.4
1	G	-1	ASN	2.4
1	F	269	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	271	TYR	2.3
1	E	0	ALA	2.3
1	D	267	VAL	2.3
1	E	267	VAL	2.3
1	D	276	ILE	2.3
1	B	79	GLU	2.3
1	E	238	ASP	2.3
1	H	234	MET	2.3
1	H	230	THR	2.3
1	E	228	GLY	2.3
1	E	232	ASP	2.3
1	F	84	GLN	2.3
1	B	-1	ASN	2.2
1	H	229	VAL	2.2
1	E	264	VAL	2.2
1	A	-2	SER	2.2
1	D	78	ILE	2.2
1	G	241	VAL	2.2
1	H	394	VAL	2.2
1	E	269	ALA	2.2
1	F	82	ALA	2.2
1	H	481	GLU	2.2
1	B	86	ASP	2.2
1	D	24	ASP	2.2
1	E	89	LYS	2.1
1	A	264	VAL	2.1
1	G	35	VAL	2.1
1	F	232	ASP	2.1
1	E	54	VAL	2.1
1	F	387	VAL	2.1
1	B	336	ILE	2.1
1	H	382	GLY	2.1
1	F	251	ASP	2.1
1	D	271	TYR	2.1
1	F	91	SER	2.1
1	G	-3	GLN	2.0
1	F	40	LEU	2.0
1	E	243	ALA	2.0
1	D	30	VAL	2.0
1	E	323	ALA	2.0
1	D	367	PHE	2.0
1	G	447	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 monosaccharides 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.

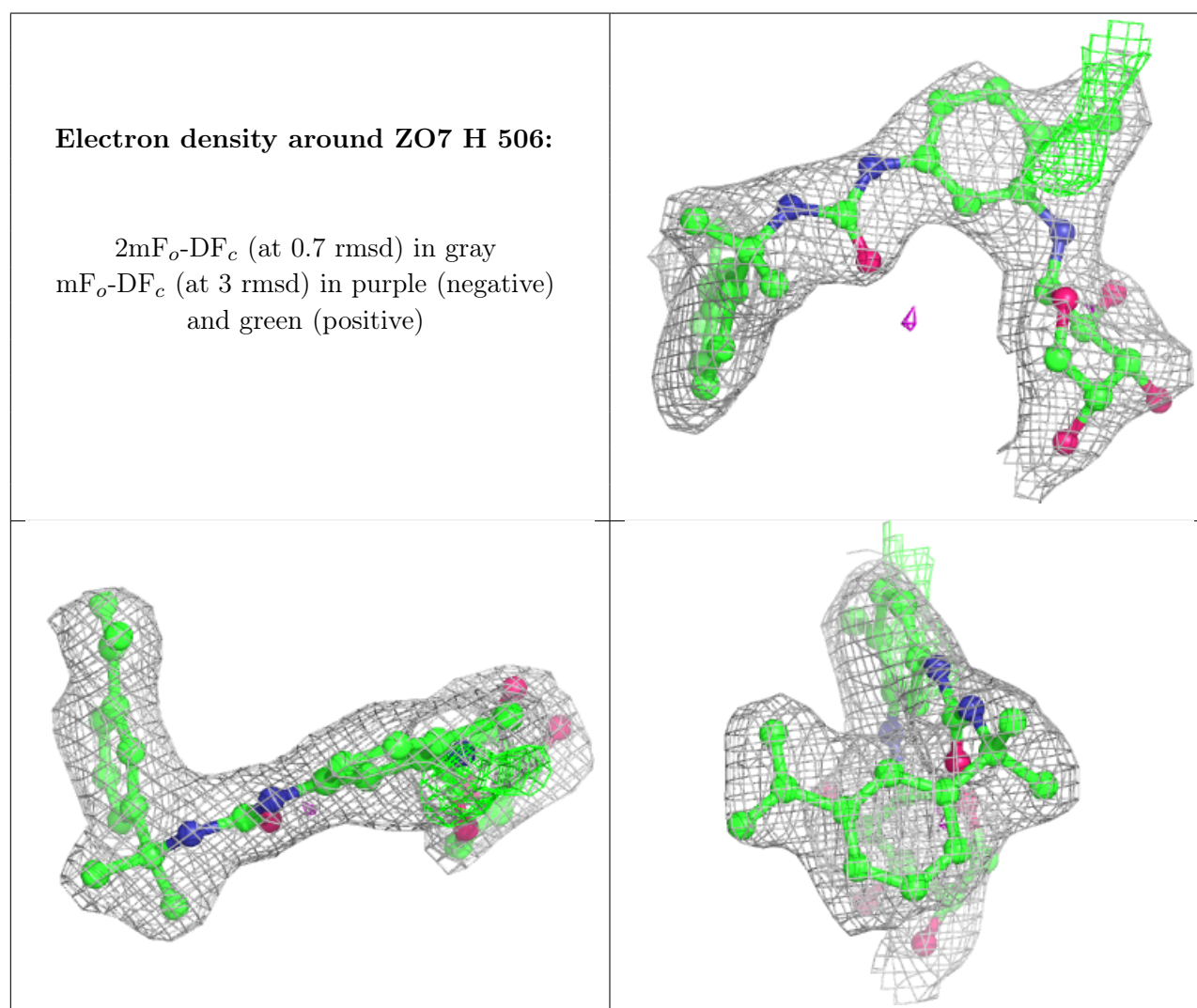
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	H	503	6/6	0.84	0.21	39,40,47,52	0
6	EDO	F	504	4/4	0.84	0.26	33,46,47,51	0
3	GOL	C	503	6/6	0.85	0.17	32,37,44,45	0
4	ZO7	H	506	33/33	0.87	0.19	22,37,55,59	1
4	ZO7	D	503	33/33	0.89	0.22	34,40,59,64	0
4	ZO7	E	502	33/33	0.89	0.25	40,46,71,75	1
4	ZO7	F	502	33/33	0.89	0.26	38,47,67,71	1
3	GOL	A	503	6/6	0.89	0.18	36,38,39,41	0
4	ZO7	C	504	33/33	0.89	0.17	30,37,55,60	1
4	ZO7	G	503	33/33	0.90	0.19	25,32,53,56	1
3	GOL	A	506	6/6	0.90	0.19	37,44,47,50	0
3	GOL	H	504	6/6	0.90	0.12	37,42,43,45	0
4	ZO7	B	502	33/33	0.91	0.16	18,31,50,51	1
5	K	G	501	1/1	0.91	0.10	37,37,37,37	0
4	ZO7	A	504	33/33	0.91	0.19	24,31,51,55	1
5	K	H	505	1/1	0.93	0.07	58,58,58,58	0
3	GOL	A	502	6/6	0.93	0.09	27,37,40,43	0
2	IMP	H	502	23/23	0.94	0.16	17,23,26,32	0
2	IMP	F	501	23/23	0.94	0.14	25,33,37,40	0
2	IMP	E	501	23/23	0.95	0.13	36,38,42,45	0
2	IMP	C	502	23/23	0.95	0.15	13,24,30,31	0
2	IMP	G	502	23/23	0.95	0.14	19,29,34,38	0
2	IMP	A	501	23/23	0.96	0.12	18,22,25,26	0
2	IMP	B	501	23/23	0.96	0.14	18,23,25,27	0
5	K	E	503	1/1	0.97	0.04	37,37,37,37	0
2	IMP	D	502	23/23	0.97	0.12	24,31,35,37	0
5	K	A	505	1/1	0.98	0.07	17,17,17,17	0

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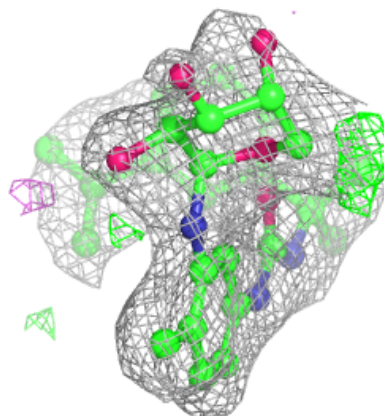
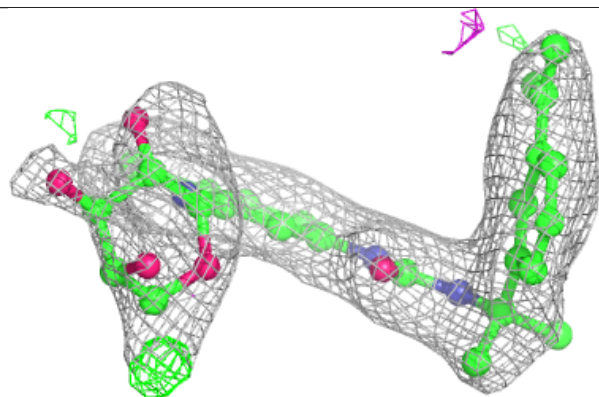
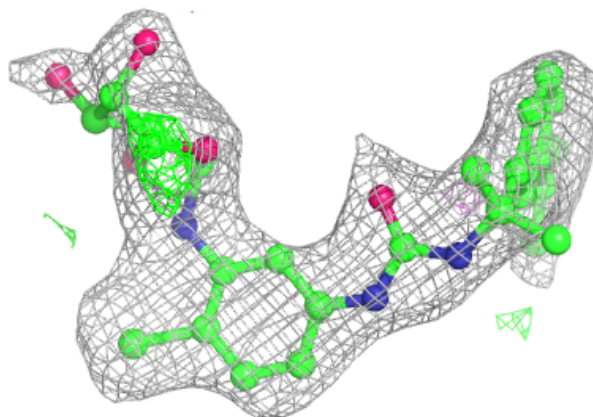
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	K	C	501	1/1	0.99	0.04	22,22,22,22	0
5	K	H	501	1/1	0.99	0.05	29,29,29,29	0
5	K	B	503	1/1	0.99	0.05	29,29,29,29	0
5	K	F	503	1/1	0.99	0.05	20,20,20,20	0
5	K	D	501	1/1	1.00	0.04	23,23,23,23	0

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.



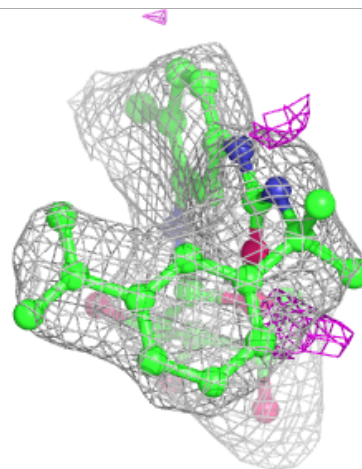
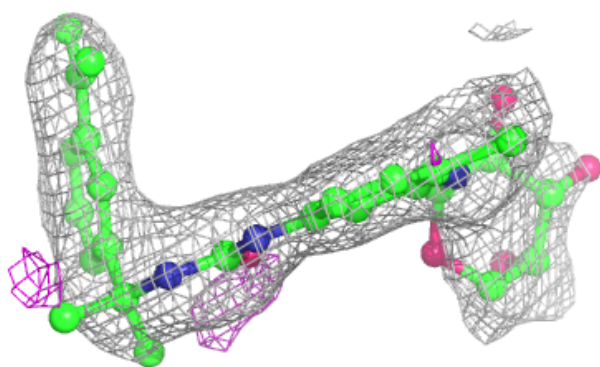
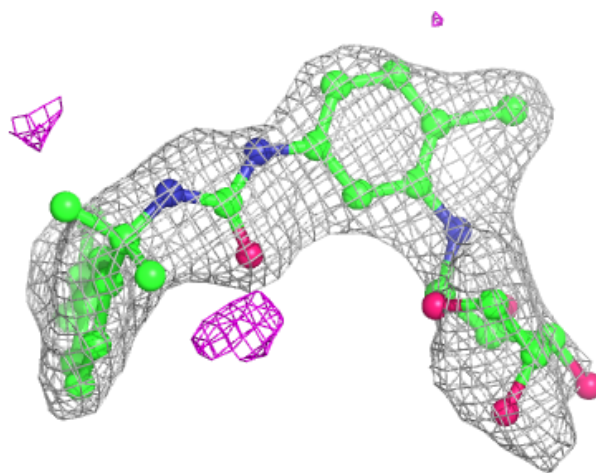
**Electron density around ZO7 D 503:**

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



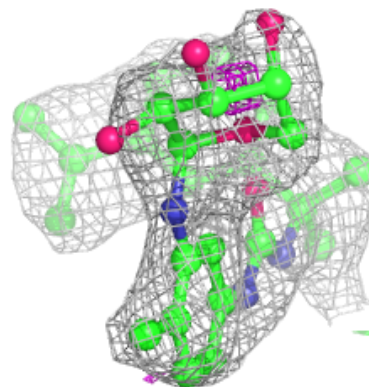
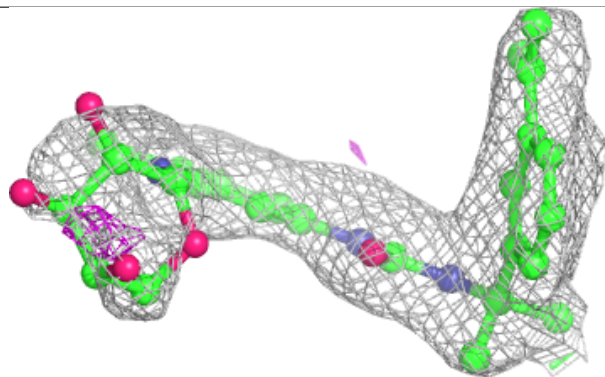
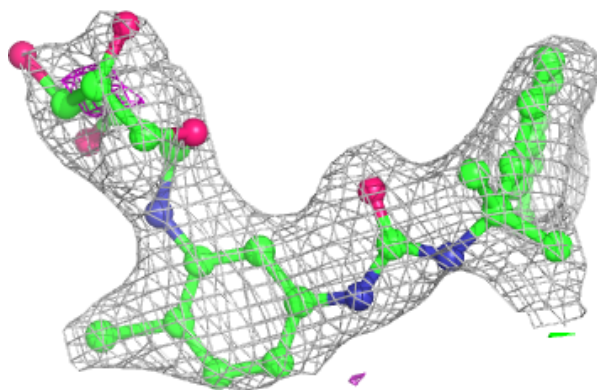
**Electron density around ZO7 E 502:**

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



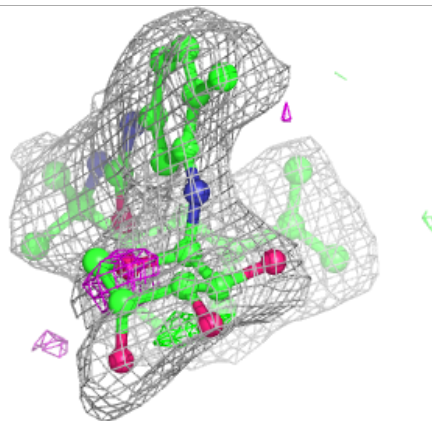
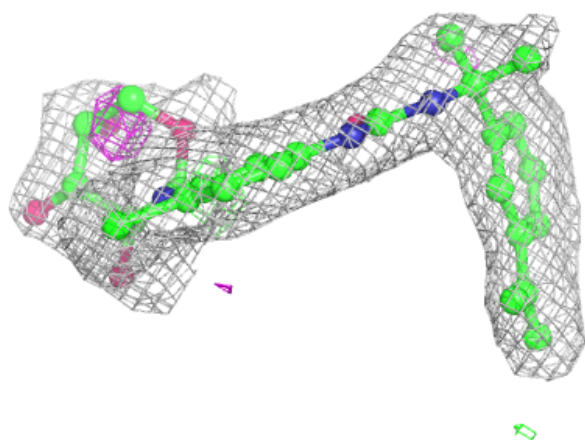
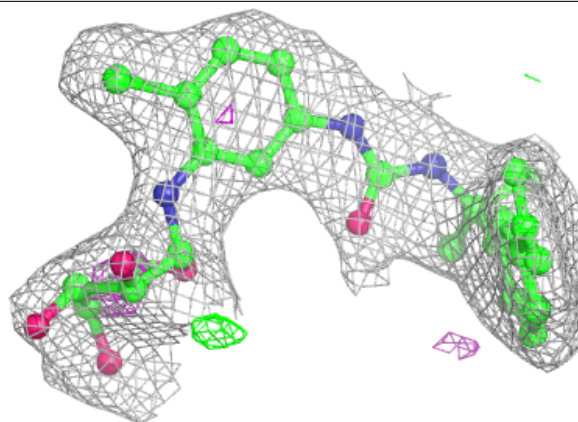
**Electron density around ZO7 F 502:**

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



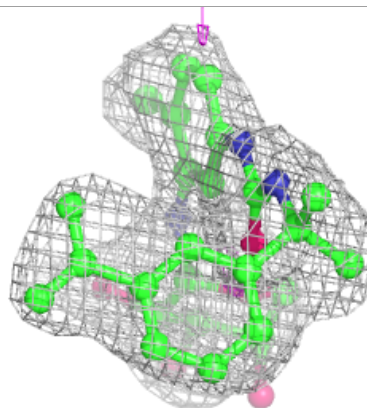
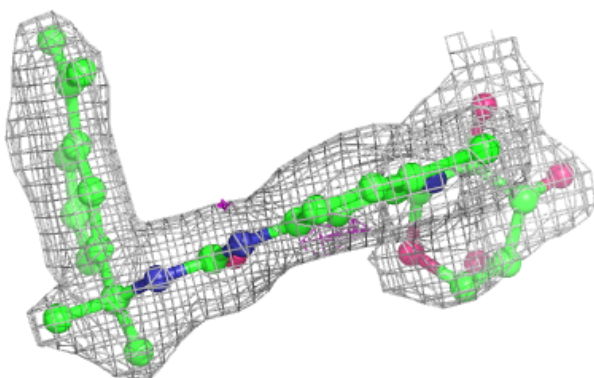
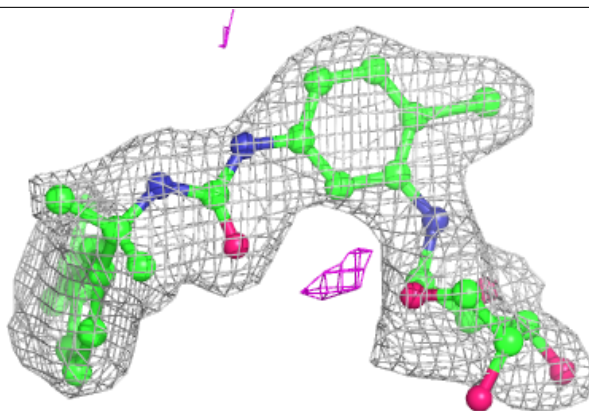
**Electron density around ZO7 C 504:**

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



**Electron density around ZO7 G 503:**

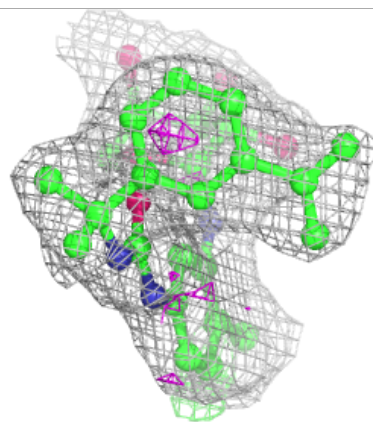
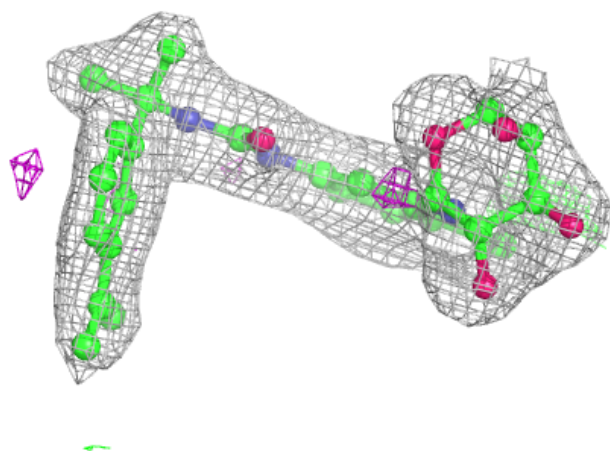
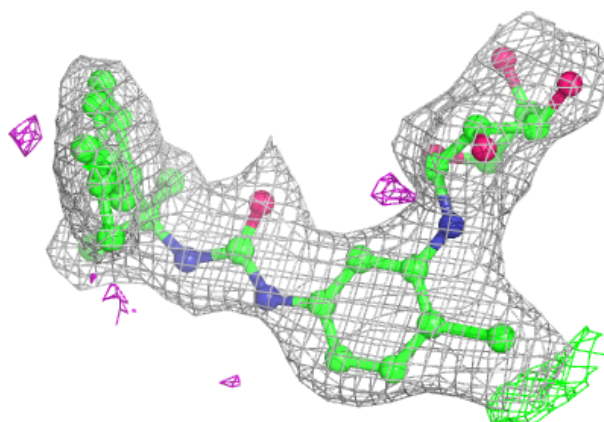
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





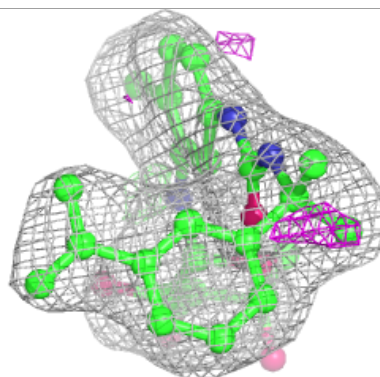
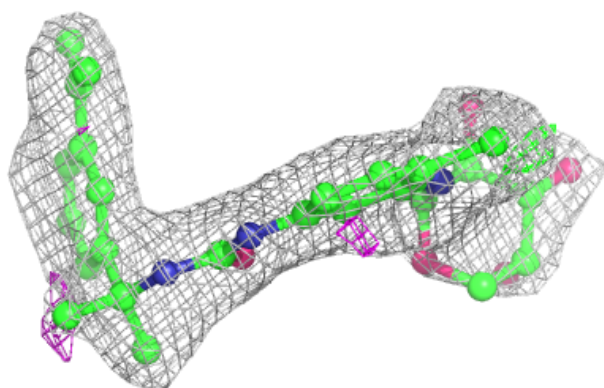
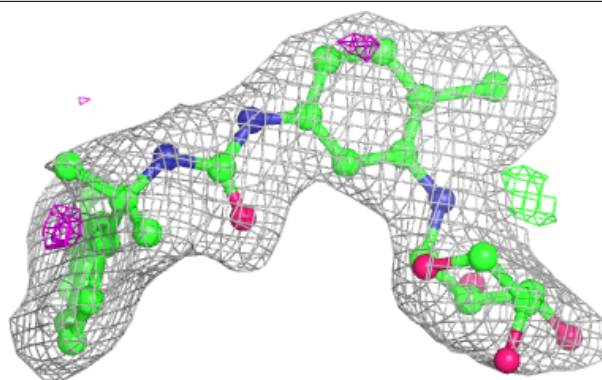
**Electron density around ZO7 B 502:**

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

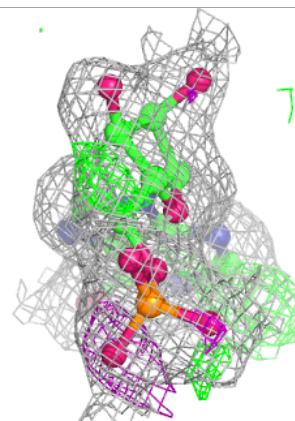
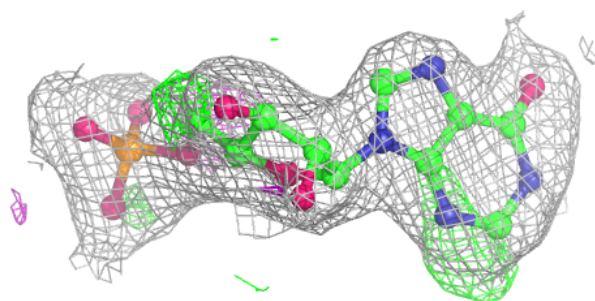
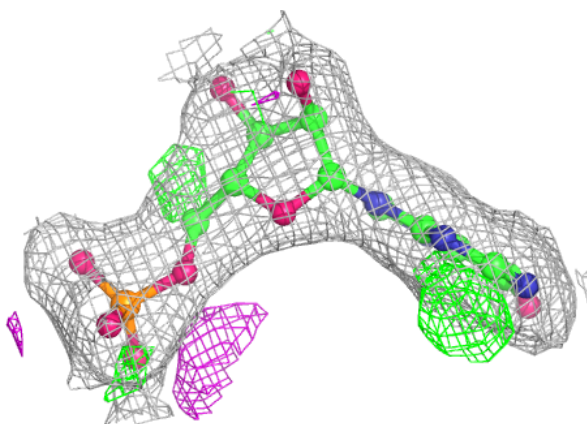


**Electron density around ZO7 A 504:**

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

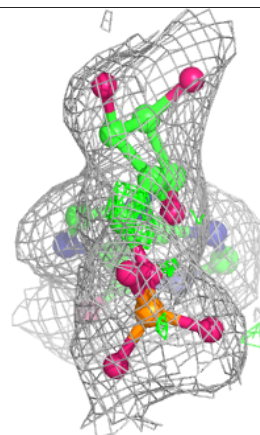
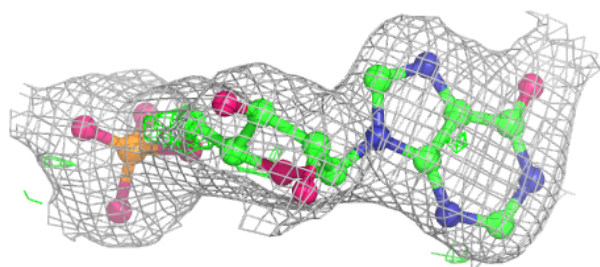
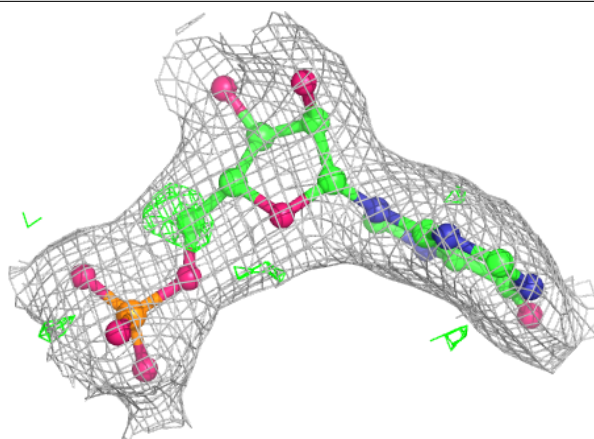
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and green (positive)



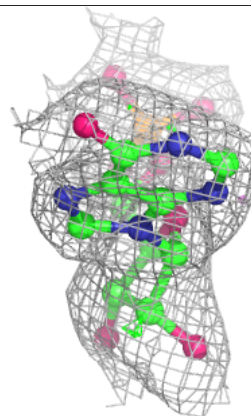
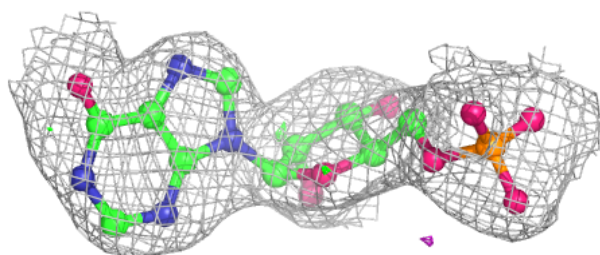
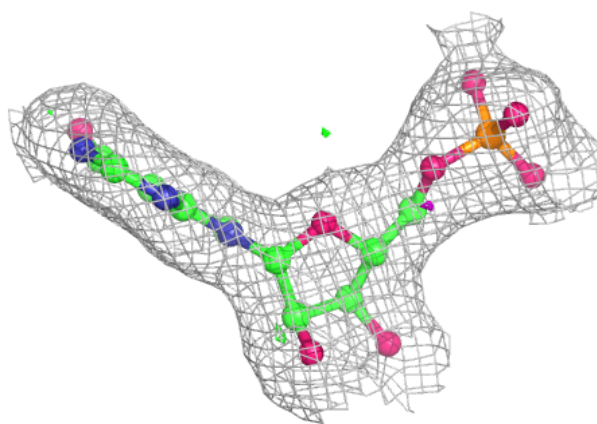
**Electron density around IMP F 501:**

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

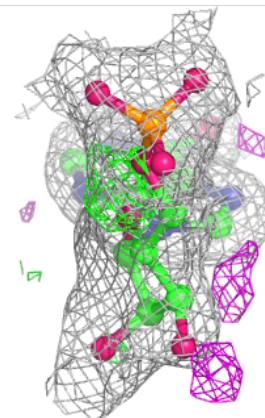
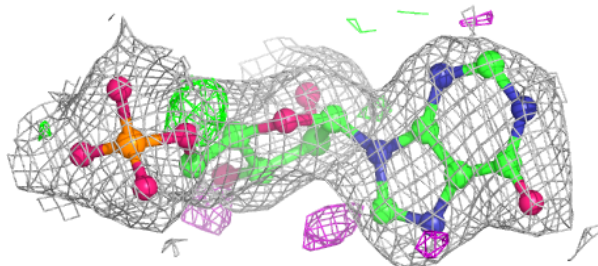
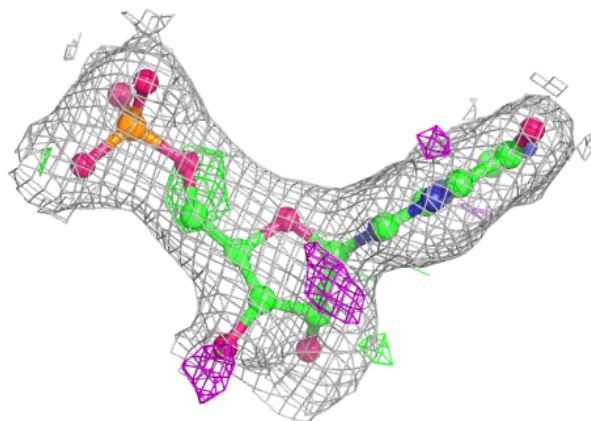


**Electron density around IMP E 501:**

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and green (positive)

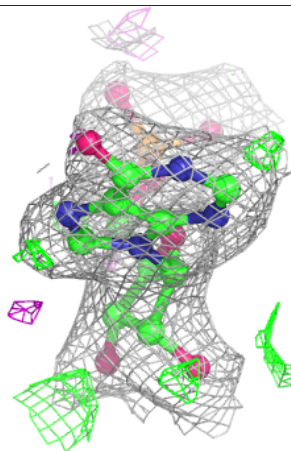
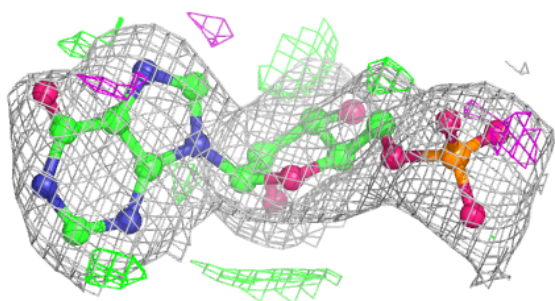
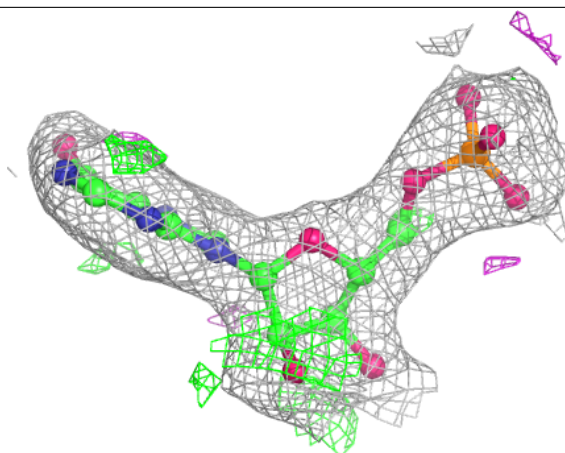
**Electron density around IMP C 502:**

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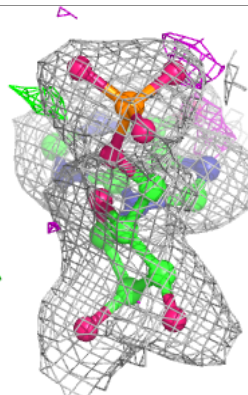
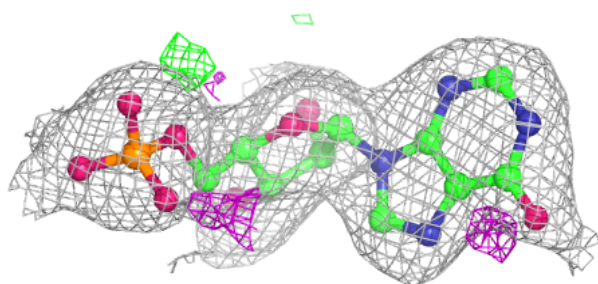
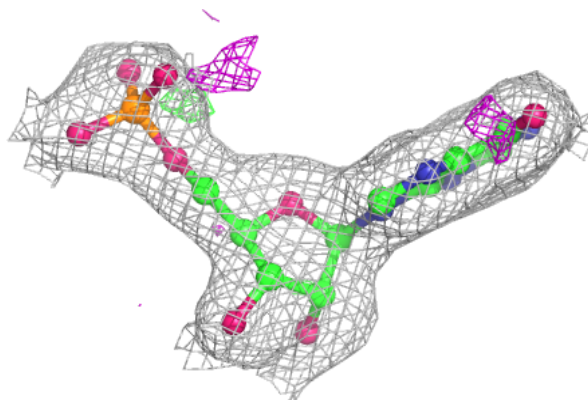


**Electron density around IMP G 502:**

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

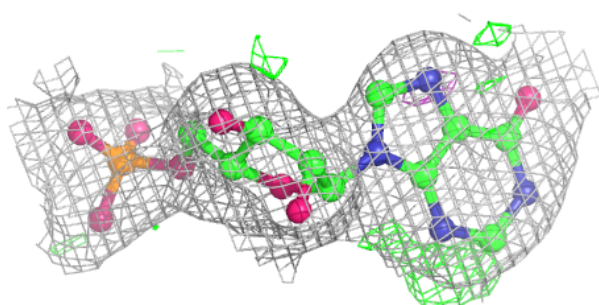
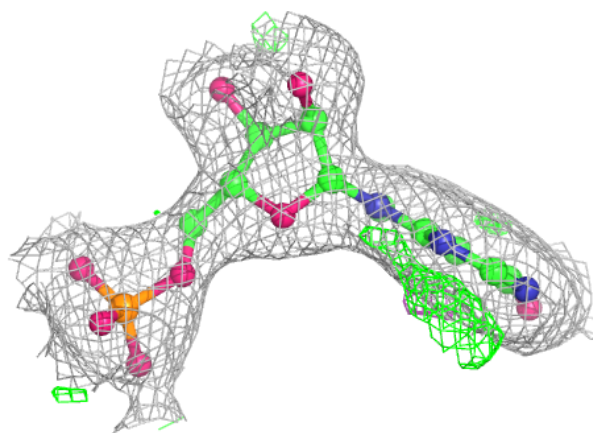
**Electron density around IMP A 501:**

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

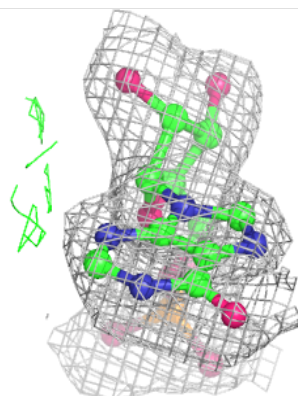
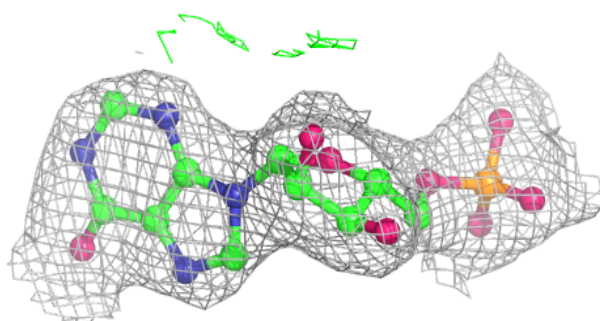
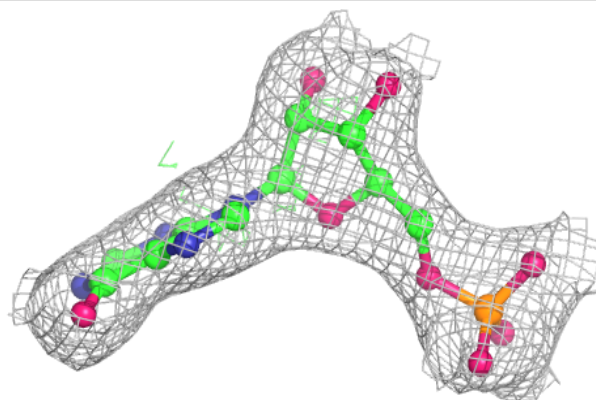


**Electron density around IMP B 501:**

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

**Electron density around IMP D 502:**

$2mF_o-DF_c$  (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.