



wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 02:19 am BST

PDB ID : 4MYX
Title : Crystal Structure of the Inosine 5'-monophosphate Dehydrogenase, with a Internal Deletion of CBS Domain from Bacillus anthracis str. Ame complexed with P32
Authors : Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Gorla, S.K.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; CSGID; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2013-09-28
Resolution : 2.70 Å(reported)

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

We welcome your comments at 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

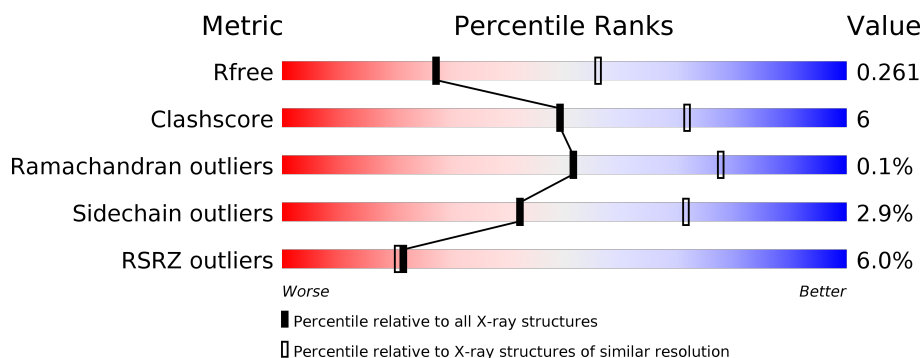
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>8%</div> <div>79% 13% 9%</div> </div>
1	B	384	<div> <div>2%</div> <div>77% 14% 8%</div> </div>
1	C	384	<div> <div>2%</div> <div>76% 15% 9%</div> </div>
1	D	384	<div> <div>7%</div> <div>78% 13% 8%</div> </div>
1	E	384	<div> <div>6%</div> <div>77% 13% 8%</div> </div>
1	F	384	<div> <div>8%</div> <div>79% 11% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	384	
1	H	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	G	502	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 21740 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
1	A	351	Total	C	N	O	S	0	7	0
			2637	1656	465	498	18			
1	B	355	Total	C	N	O	S	0	1	0
			2614	1641	458	499	16			
1	C	348	Total	C	N	O	S	0	4	0
			2587	1623	451	496	17			
1	D	352	Total	C	N	O	S	0	4	0
			2615	1639	459	501	16			
1	E	352	Total	C	N	O	S	0	2	0
			2597	1629	455	496	17			
1	F	350	Total	C	N	O	S	0	0	0
			2567	1612	450	489	16			
1	G	356	Total	C	N	O	S	0	2	0
			2627	1647	462	502	16			
1	H	350	Total	C	N	O	S	0	0	0
			2567	1612	450	489	16			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP Q81W29
A	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
A	-16	SER	-	EXPRESSION TAG	UNP Q81W29
A	-15	SER	-	EXPRESSION TAG	UNP Q81W29
A	-14	GLY	-	EXPRESSION TAG	UNP Q81W29
A	-13	VAL	-	EXPRESSION TAG	UNP Q81W29
A	-12	ASP	-	EXPRESSION TAG	UNP Q81W29
A	-11	LEU	-	EXPRESSION TAG	UNP Q81W29

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	EXPRESSION TAG	UNP Q81W29
A	-9	THR	-	EXPRESSION TAG	UNP Q81W29
A	-8	GLU	-	EXPRESSION TAG	UNP Q81W29
A	-7	ASN	-	EXPRESSION TAG	UNP Q81W29
A	-6	LEU	-	EXPRESSION TAG	UNP Q81W29
A	-5	TYR	-	EXPRESSION TAG	UNP Q81W29
A	-4	PHE	-	EXPRESSION TAG	UNP Q81W29
A	-3	GLN	-	EXPRESSION TAG	UNP Q81W29
A	-2	SER	-	EXPRESSION TAG	UNP Q81W29
A	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
A	0	ALA	-	EXPRESSION TAG	UNP Q81W29
A	92	GLY	-	LINKER	UNP Q81W29
A	220	GLY	-	LINKER	UNP Q81W29
B	-23	MET	-	EXPRESSION TAG	UNP Q81W29
B	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
B	-16	SER	-	EXPRESSION TAG	UNP Q81W29
B	-15	SER	-	EXPRESSION TAG	UNP Q81W29
B	-14	GLY	-	EXPRESSION TAG	UNP Q81W29
B	-13	VAL	-	EXPRESSION TAG	UNP Q81W29
B	-12	ASP	-	EXPRESSION TAG	UNP Q81W29
B	-11	LEU	-	EXPRESSION TAG	UNP Q81W29
B	-10	GLY	-	EXPRESSION TAG	UNP Q81W29
B	-9	THR	-	EXPRESSION TAG	UNP Q81W29
B	-8	GLU	-	EXPRESSION TAG	UNP Q81W29
B	-7	ASN	-	EXPRESSION TAG	UNP Q81W29
B	-6	LEU	-	EXPRESSION TAG	UNP Q81W29
B	-5	TYR	-	EXPRESSION TAG	UNP Q81W29
B	-4	PHE	-	EXPRESSION TAG	UNP Q81W29
B	-3	GLN	-	EXPRESSION TAG	UNP Q81W29
B	-2	SER	-	EXPRESSION TAG	UNP Q81W29
B	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
B	0	ALA	-	EXPRESSION TAG	UNP Q81W29
B	92	GLY	-	LINKER	UNP Q81W29
B	220	GLY	-	LINKER	UNP Q81W29
C	-23	MET	-	EXPRESSION TAG	UNP Q81W29
C	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
C	-21	HIS	-	EXPRESSION TAG	UNP Q81W29

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
C	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
C	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
C	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
C	-16	SER	-	EXPRESSION TAG	UNP Q81W29
C	-15	SER	-	EXPRESSION TAG	UNP Q81W29
C	-14	GLY	-	EXPRESSION TAG	UNP Q81W29
C	-13	VAL	-	EXPRESSION TAG	UNP Q81W29
C	-12	ASP	-	EXPRESSION TAG	UNP Q81W29
C	-11	LEU	-	EXPRESSION TAG	UNP Q81W29
C	-10	GLY	-	EXPRESSION TAG	UNP Q81W29
C	-9	THR	-	EXPRESSION TAG	UNP Q81W29
C	-8	GLU	-	EXPRESSION TAG	UNP Q81W29
C	-7	ASN	-	EXPRESSION TAG	UNP Q81W29
C	-6	LEU	-	EXPRESSION TAG	UNP Q81W29
C	-5	TYR	-	EXPRESSION TAG	UNP Q81W29
C	-4	PHE	-	EXPRESSION TAG	UNP Q81W29
C	-3	GLN	-	EXPRESSION TAG	UNP Q81W29
C	-2	SER	-	EXPRESSION TAG	UNP Q81W29
C	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
C	0	ALA	-	EXPRESSION TAG	UNP Q81W29
C	92	GLY	-	LINKER	UNP Q81W29
C	220	GLY	-	LINKER	UNP Q81W29
D	-23	MET	-	EXPRESSION TAG	UNP Q81W29
D	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
D	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
D	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
D	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
D	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
D	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
D	-16	SER	-	EXPRESSION TAG	UNP Q81W29
D	-15	SER	-	EXPRESSION TAG	UNP Q81W29
D	-14	GLY	-	EXPRESSION TAG	UNP Q81W29
D	-13	VAL	-	EXPRESSION TAG	UNP Q81W29
D	-12	ASP	-	EXPRESSION TAG	UNP Q81W29
D	-11	LEU	-	EXPRESSION TAG	UNP Q81W29
D	-10	GLY	-	EXPRESSION TAG	UNP Q81W29
D	-9	THR	-	EXPRESSION TAG	UNP Q81W29
D	-8	GLU	-	EXPRESSION TAG	UNP Q81W29
D	-7	ASN	-	EXPRESSION TAG	UNP Q81W29
D	-6	LEU	-	EXPRESSION TAG	UNP Q81W29
D	-5	TYR	-	EXPRESSION TAG	UNP Q81W29

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	PHE	-	EXPRESSION TAG	UNP Q81W29
D	-3	GLN	-	EXPRESSION TAG	UNP Q81W29
D	-2	SER	-	EXPRESSION TAG	UNP Q81W29
D	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
D	0	ALA	-	EXPRESSION TAG	UNP Q81W29
D	92	GLY	-	LINKER	UNP Q81W29
D	220	GLY	-	LINKER	UNP Q81W29
E	-23	MET	-	EXPRESSION TAG	UNP Q81W29
E	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
E	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
E	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
E	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
E	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
E	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
E	-16	SER	-	EXPRESSION TAG	UNP Q81W29
E	-15	SER	-	EXPRESSION TAG	UNP Q81W29
E	-14	GLY	-	EXPRESSION TAG	UNP Q81W29
E	-13	VAL	-	EXPRESSION TAG	UNP Q81W29
E	-12	ASP	-	EXPRESSION TAG	UNP Q81W29
E	-11	LEU	-	EXPRESSION TAG	UNP Q81W29
E	-10	GLY	-	EXPRESSION TAG	UNP Q81W29
E	-9	THR	-	EXPRESSION TAG	UNP Q81W29
E	-8	GLU	-	EXPRESSION TAG	UNP Q81W29
E	-7	ASN	-	EXPRESSION TAG	UNP Q81W29
E	-6	LEU	-	EXPRESSION TAG	UNP Q81W29
E	-5	TYR	-	EXPRESSION TAG	UNP Q81W29
E	-4	PHE	-	EXPRESSION TAG	UNP Q81W29
E	-3	GLN	-	EXPRESSION TAG	UNP Q81W29
E	-2	SER	-	EXPRESSION TAG	UNP Q81W29
E	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
E	0	ALA	-	EXPRESSION TAG	UNP Q81W29
E	92	GLY	-	LINKER	UNP Q81W29
E	220	GLY	-	LINKER	UNP Q81W29
F	-23	MET	-	EXPRESSION TAG	UNP Q81W29
F	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
F	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
F	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
F	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
F	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
F	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
F	-16	SER	-	EXPRESSION TAG	UNP Q81W29
F	-15	SER	-	EXPRESSION TAG	UNP Q81W29

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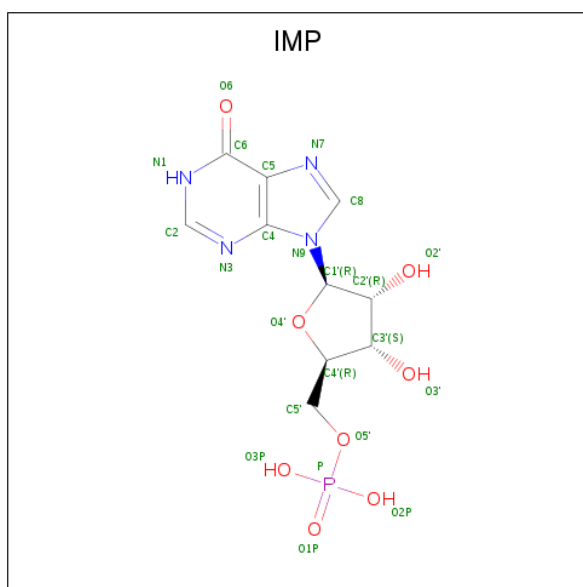
Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	GLY	-	EXPRESSION TAG	UNP Q81W29
F	-13	VAL	-	EXPRESSION TAG	UNP Q81W29
F	-12	ASP	-	EXPRESSION TAG	UNP Q81W29
F	-11	LEU	-	EXPRESSION TAG	UNP Q81W29
F	-10	GLY	-	EXPRESSION TAG	UNP Q81W29
F	-9	THR	-	EXPRESSION TAG	UNP Q81W29
F	-8	GLU	-	EXPRESSION TAG	UNP Q81W29
F	-7	ASN	-	EXPRESSION TAG	UNP Q81W29
F	-6	LEU	-	EXPRESSION TAG	UNP Q81W29
F	-5	TYR	-	EXPRESSION TAG	UNP Q81W29
F	-4	PHE	-	EXPRESSION TAG	UNP Q81W29
F	-3	GLN	-	EXPRESSION TAG	UNP Q81W29
F	-2	SER	-	EXPRESSION TAG	UNP Q81W29
F	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
F	0	ALA	-	EXPRESSION TAG	UNP Q81W29
F	92	GLY	-	LINKER	UNP Q81W29
F	220	GLY	-	LINKER	UNP Q81W29
G	-23	MET	-	EXPRESSION TAG	UNP Q81W29
G	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
G	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
G	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
G	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
G	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
G	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
G	-16	SER	-	EXPRESSION TAG	UNP Q81W29
G	-15	SER	-	EXPRESSION TAG	UNP Q81W29
G	-14	GLY	-	EXPRESSION TAG	UNP Q81W29
G	-13	VAL	-	EXPRESSION TAG	UNP Q81W29
G	-12	ASP	-	EXPRESSION TAG	UNP Q81W29
G	-11	LEU	-	EXPRESSION TAG	UNP Q81W29
G	-10	GLY	-	EXPRESSION TAG	UNP Q81W29
G	-9	THR	-	EXPRESSION TAG	UNP Q81W29
G	-8	GLU	-	EXPRESSION TAG	UNP Q81W29
G	-7	ASN	-	EXPRESSION TAG	UNP Q81W29
G	-6	LEU	-	EXPRESSION TAG	UNP Q81W29
G	-5	TYR	-	EXPRESSION TAG	UNP Q81W29
G	-4	PHE	-	EXPRESSION TAG	UNP Q81W29
G	-3	GLN	-	EXPRESSION TAG	UNP Q81W29
G	-2	SER	-	EXPRESSION TAG	UNP Q81W29
G	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
G	0	ALA	-	EXPRESSION TAG	UNP Q81W29
G	92	GLY	-	LINKER	UNP Q81W29

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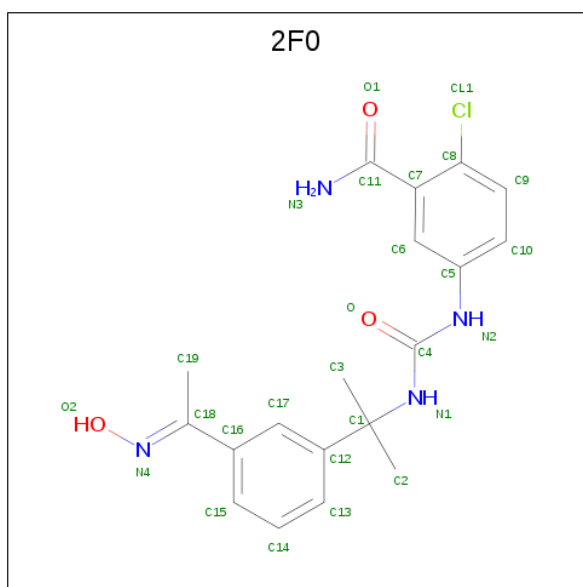
Chain	Residue	Modelled	Actual	Comment	Reference
G	220	GLY	-	LINKER	UNP Q81W29
H	-23	MET	-	EXPRESSION TAG	UNP Q81W29
H	-22	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-21	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-20	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-19	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-18	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-17	HIS	-	EXPRESSION TAG	UNP Q81W29
H	-16	SER	-	EXPRESSION TAG	UNP Q81W29
H	-15	SER	-	EXPRESSION TAG	UNP Q81W29
H	-14	GLY	-	EXPRESSION TAG	UNP Q81W29
H	-13	VAL	-	EXPRESSION TAG	UNP Q81W29
H	-12	ASP	-	EXPRESSION TAG	UNP Q81W29
H	-11	LEU	-	EXPRESSION TAG	UNP Q81W29
H	-10	GLY	-	EXPRESSION TAG	UNP Q81W29
H	-9	THR	-	EXPRESSION TAG	UNP Q81W29
H	-8	GLU	-	EXPRESSION TAG	UNP Q81W29
H	-7	ASN	-	EXPRESSION TAG	UNP Q81W29
H	-6	LEU	-	EXPRESSION TAG	UNP Q81W29
H	-5	TYR	-	EXPRESSION TAG	UNP Q81W29
H	-4	PHE	-	EXPRESSION TAG	UNP Q81W29
H	-3	GLN	-	EXPRESSION TAG	UNP Q81W29
H	-2	SER	-	EXPRESSION TAG	UNP Q81W29
H	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
H	0	ALA	-	EXPRESSION TAG	UNP Q81W29
H	92	GLY	-	LINKER	UNP Q81W29
H	220	GLY	-	LINKER	UNP Q81W29

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
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 2-chloro-5-[[[(2-{3-[(1E)-N-hydroxyethanimidoyl]phenyl}propan-2-yl)carbamoyl]amino]benzamide (three-letter code: 2F0) (formula: C₁₉H₂₁ClN₄O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	B	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	C	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	D	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	E	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	E	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	F	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		
3	H	1	Total	C	Cl	N	O	0	0
			27	19	1	4	3		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



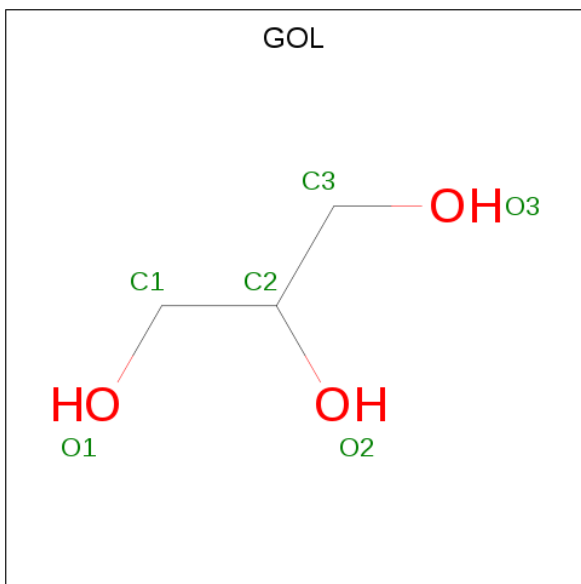
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	F	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total	C	O	0	0
			3	1	2		
4	H	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	E	1	Total	C	O	0	0
			7	3	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	D	1	Total C O 4 2 2	0	0
7	E	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0
8	G	1	Total O S 5 4 1	0	0

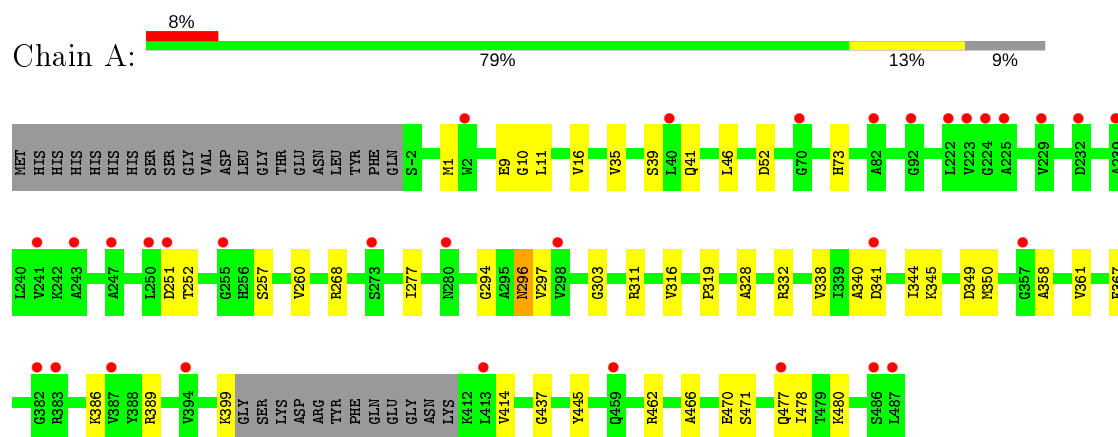
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	53	Total 53	O 53	0	0
9	B	62	Total 62	O 62	0	0
9	C	52	Total 52	O 52	0	0
9	D	49	Total 49	O 49	0	0
9	E	48	Total 48	O 48	0	0
9	F	37	Total 37	O 37	0	0
9	G	48	Total 48	O 48	0	0
9	H	54	Total 54	O 54	0	0

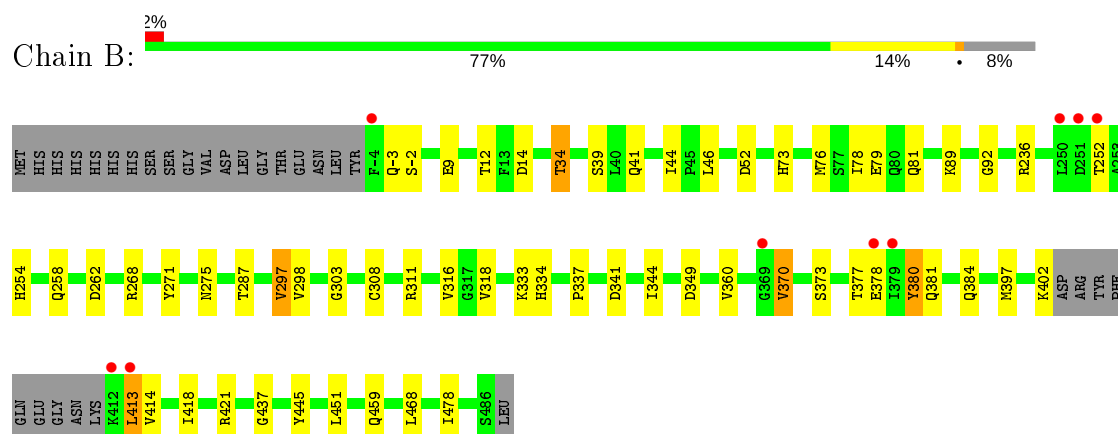
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

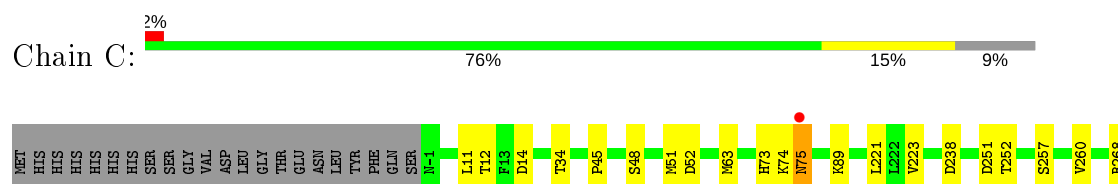
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

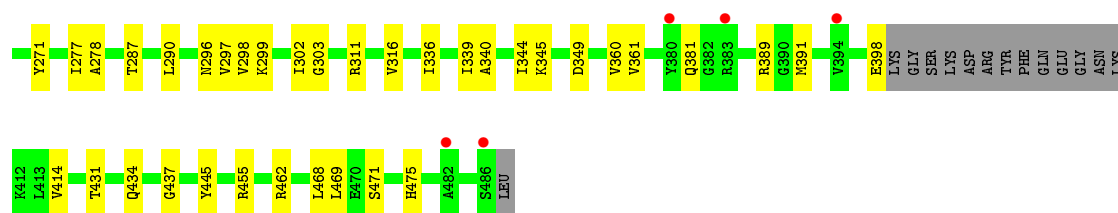


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

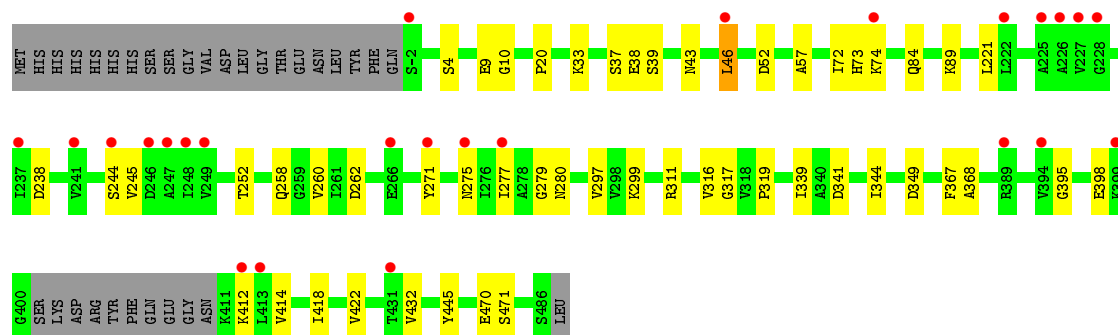
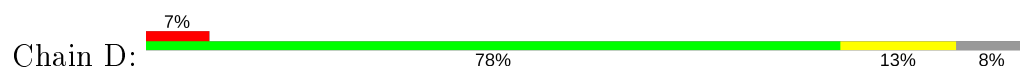


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

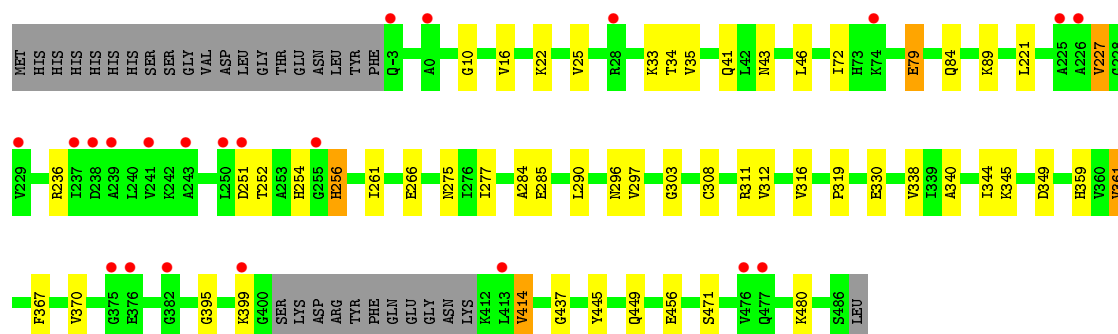
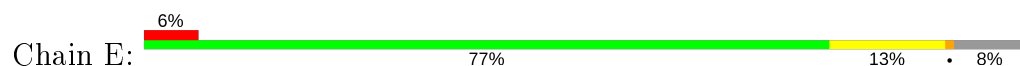




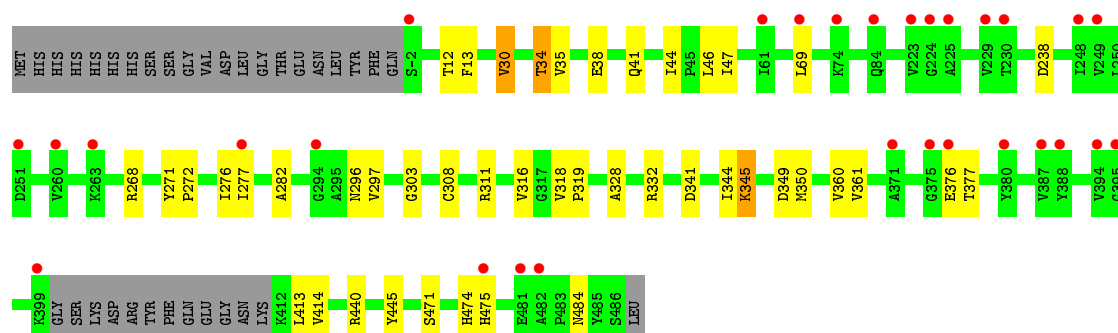
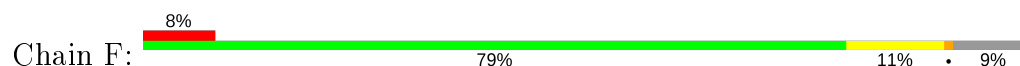
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



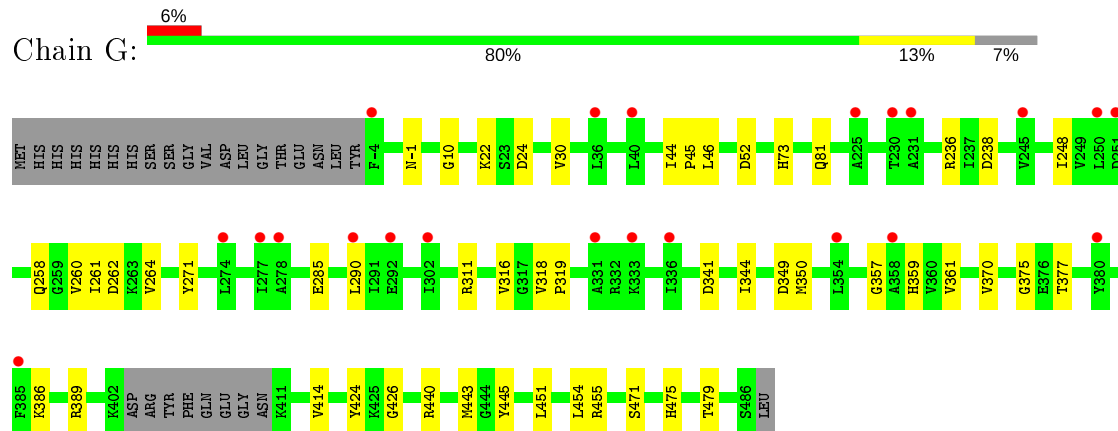
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



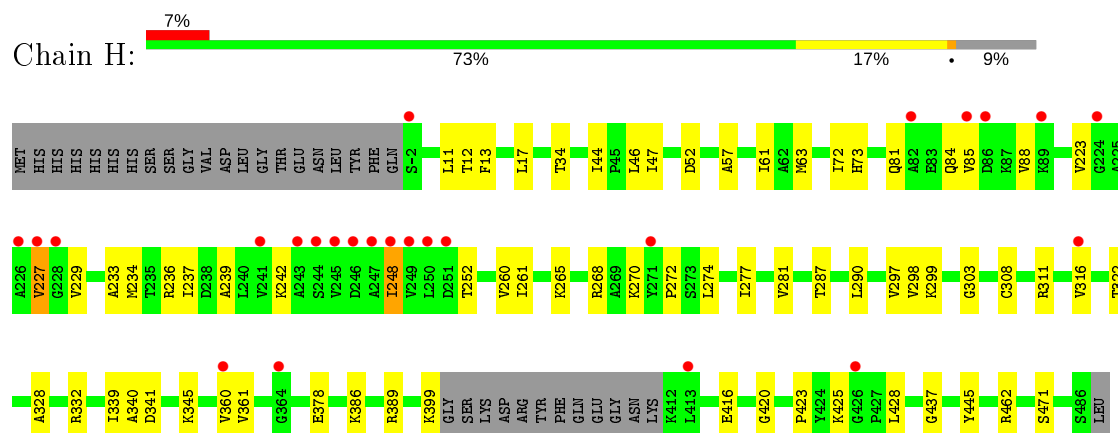
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• 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, α , β , γ	85.36Å 89.82Å 104.50Å 81.41° 90.42° 83.50°	Depositor
Resolution (Å)	41.90 – 2.70 48.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.90-2.70) 98.1 (48.17-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, R_{free}	0.218 , 0.260 0.219 , 0.261	Depositor DCC
R_{free} test set	4101 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21740	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 2F0, FMT, MLI, EDO, IMP, SO4

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	0.20	0/2673	0.39	0/3610
1	B	0.21	0/2651	0.41	0/3581
1	C	0.20	0/2623	0.40	0/3545
1	D	0.21	0/2651	0.40	0/3581
1	E	0.21	0/2633	0.39	0/3557
1	F	0.21	0/2603	0.39	0/3518
1	G	0.20	0/2663	0.38	0/3596
1	H	0.20	0/2603	0.39	0/3518
All	All	0.21	0/21100	0.39	0/28506

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	2637	0	2702	35	0
1	B	2614	0	2667	41	0
1	C	2587	0	2631	36	0
1	D	2615	0	2664	29	0
1	E	2597	0	2651	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2567	0	2626	26	0
1	G	2627	0	2682	32	0
1	H	2567	0	2626	44	0
2	A	23	0	11	1	0
2	B	23	0	11	2	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
2	E	23	0	11	0	0
2	F	23	0	11	1	0
2	G	23	0	11	1	0
2	H	23	0	11	1	0
3	A	27	0	21	3	0
3	B	27	0	21	2	0
3	C	27	0	21	1	0
3	D	27	0	21	3	0
3	E	54	0	42	6	0
3	F	27	0	21	2	0
3	H	27	0	21	4	0
4	A	6	0	2	0	0
4	B	3	0	1	0	0
4	C	3	0	1	0	0
4	D	6	0	2	0	0
4	E	9	0	3	0	0
4	F	6	0	2	0	0
4	H	12	0	4	0	0
5	A	6	0	8	0	0
5	E	6	0	8	0	0
6	A	7	0	2	0	0
6	E	7	0	2	0	0
7	B	4	0	6	0	0
7	C	8	0	12	4	0
7	D	12	0	18	0	0
7	E	4	0	6	0	0
7	F	12	0	18	2	0
8	C	5	0	0	0	0
8	G	10	0	0	0	0
9	A	53	0	0	0	0
9	B	62	0	0	1	0
9	C	52	0	0	0	0
9	D	49	0	0	0	0
9	E	48	0	0	0	0
9	F	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	48	0	0	1	0
9	H	54	0	0	1	0
All	All	21740	0	21600	253	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 6.

The worst 5 of 253 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)
3:H:505:2F0:H3	3:H:505:2F0:O	1.89	0.72
3:F:502:2F0:H3	3:F:502:2F0:O	1.89	0.72
1:A:414:VAL:HG21	1:C:437:GLY:HA3	1.72	0.71
3:A:502:2F0:H13	3:A:502:2F0:O	1.93	0.68
1:E:344:ILE:HG23	1:E:349:ASP:HB2	1.75	0.68

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	354/384 (92%)	342 (97%)	12 (3%)	0	100	100
1	B	352/384 (92%)	343 (97%)	8 (2%)	1 (0%)	41	66
1	C	348/384 (91%)	338 (97%)	10 (3%)	0	100	100
1	D	352/384 (92%)	340 (97%)	11 (3%)	1 (0%)	41	66
1	E	350/384 (91%)	342 (98%)	8 (2%)	0	100	100
1	F	346/384 (90%)	336 (97%)	10 (3%)	0	100	100
1	G	354/384 (92%)	350 (99%)	4 (1%)	0	100	100
1	H	346/384 (90%)	337 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2802/3072 (91%)	2728 (97%)	72 (3%)	2 (0%)	51 78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	92	GLY
1	D	412	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	276/298 (93%)	268 (97%)	8 (3%)	42 71
1	B	273/298 (92%)	262 (96%)	11 (4%)	31 60
1	C	270/298 (91%)	261 (97%)	9 (3%)	38 67
1	D	273/298 (92%)	267 (98%)	6 (2%)	52 79
1	E	271/298 (91%)	258 (95%)	13 (5%)	25 53
1	F	268/298 (90%)	261 (97%)	7 (3%)	46 75
1	G	274/298 (92%)	270 (98%)	4 (2%)	65 86
1	H	268/298 (90%)	263 (98%)	5 (2%)	57 82
All	All	2173/2384 (91%)	2110 (97%)	63 (3%)	42 71

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	9	GLU
1	E	34	THR
1	H	227	VAL
1	D	46	LEU
1	D	221	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	43	ASN
1	E	474	HIS
1	G	459	GLN
1	D	84	GLN
1	F	474	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

48 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	$\# Z > 2$
4	FMT	D	507	-	0,2,2	0.00	-	0,1,1	0.00	-
3	2F0	B	501	-	28,28,28	1.73	4 (14%)	40,40,40	1.11	2 (5%)
4	FMT	H	501	-	0,2,2	0.00	-	0,1,1	0.00	-
2	IMP	H	504	-	21,25,25	1.30	3 (14%)	23,38,38	1.44	2 (8%)
7	EDO	F	504	-	3,3,3	0.47	0	2,2,2	0.33	0
4	FMT	F	507	-	0,2,2	0.00	-	0,1,1	0.00	-
7	EDO	F	505	-	3,3,3	0.46	0	2,2,2	0.32	0
4	FMT	A	504	-	0,2,2	0.00	-	0,1,1	0.00	-
7	EDO	D	505	-	3,3,3	0.47	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	E	504	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	D	506	-	0,2,2	0.00	-	0,1,1	0.00	-
8	SO4	G	502	-	4,4,4	0.14	0	6,6,6	0.06	0
7	EDO	D	503	-	3,3,3	0.47	0	2,2,2	0.31	0
5	GOL	A	505	-	5,5,5	0.36	0	5,5,5	0.33	0
4	FMT	E	503	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	503	-	0,2,2	0.00	-	0,1,1	0.00	-
7	EDO	C	504	-	3,3,3	0.46	0	2,2,2	0.33	0
2	IMP	C	502	-	21,25,25	1.30	3 (14%)	23,38,38	1.42	2 (8%)
2	IMP	E	501	-	21,25,25	1.29	3 (14%)	23,38,38	1.42	2 (8%)
3	2F0	A	502	-	28,28,28	1.67	6 (21%)	40,40,40	1.13	2 (5%)
2	IMP	F	501	-	21,25,25	1.29	3 (14%)	23,38,38	1.43	2 (8%)
8	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	G	503	-	4,4,4	0.14	0	6,6,6	0.05	0
6	MLI	E	508	-	0,6,6	0.00	-	0,7,7	0.00	-
3	2F0	F	502	-	28,28,28	1.57	5 (17%)	40,40,40	1.48	3 (7%)
4	FMT	F	503	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	E	506	-	5,5,5	0.39	0	5,5,5	0.21	0
4	FMT	H	503	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	E	507	-	0,2,2	0.00	-	0,1,1	0.00	-
3	2F0	C	503	-	28,28,28	1.59	5 (17%)	40,40,40	1.26	3 (7%)
6	MLI	A	506	-	0,6,6	0.00	-	0,7,7	0.00	-
4	FMT	H	506	-	0,2,2	0.00	-	0,1,1	0.00	-
3	2F0	E	509	-	28,28,28	1.73	4 (14%)	40,40,40	1.18	2 (5%)
2	IMP	B	500	-	21,25,25	1.27	3 (14%)	23,38,38	1.38	2 (8%)
3	2F0	E	502	-	28,28,28	1.58	5 (17%)	40,40,40	1.23	5 (12%)
7	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.37	0
3	2F0	D	501	-	28,28,28	1.42	4 (14%)	40,40,40	1.64	7 (17%)
2	IMP	G	501	-	21,25,25	1.31	3 (14%)	23,38,38	1.43	2 (8%)
2	IMP	A	501	-	21,25,25	1.36	3 (14%)	23,38,38	1.44	2 (8%)
4	FMT	C	501	-	0,2,2	0.00	-	0,1,1	0.00	-
7	EDO	D	502	-	3,3,3	0.46	0	2,2,2	0.33	0
7	EDO	C	506	-	3,3,3	0.46	0	2,2,2	0.27	0
7	EDO	E	505	-	3,3,3	0.47	0	2,2,2	0.32	0
4	FMT	A	503	-	0,2,2	0.00	-	0,1,1	0.00	-
3	2F0	H	505	-	28,28,28	1.48	3 (10%)	40,40,40	1.50	6 (15%)
2	IMP	D	504	-	21,25,25	1.29	3 (14%)	23,38,38	1.42	2 (8%)
7	EDO	F	506	-	3,3,3	0.45	0	2,2,2	0.31	0
4	FMT	H	502	-	0,2,2	0.00	-	0,1,1	0.00	-

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
3	2F0	B	501	-	-	4/25/25/25	0/2/2/2
2	IMP	H	504	-	-	0/6/26/26	0/3/3/3
7	EDO	F	504	-	-	0/1/1/1	-
7	EDO	F	505	-	-	0/1/1/1	-
7	EDO	D	505	-	-	0/1/1/1	-
7	EDO	D	503	-	-	0/1/1/1	-
7	EDO	C	504	-	-	0/1/1/1	-
2	IMP	C	502	-	-	0/6/26/26	0/3/3/3
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
3	2F0	A	502	-	-	3/25/25/25	0/2/2/2
2	IMP	F	501	-	-	0/6/26/26	0/3/3/3
6	MLI	E	508	-	-	0/0/4/4	-
3	2F0	F	502	-	-	4/25/25/25	0/2/2/2
5	GOL	A	505	-	-	2/4/4/4	-
5	GOL	E	506	-	-	2/4/4/4	-
3	2F0	C	503	-	-	4/25/25/25	0/2/2/2
6	MLI	A	506	-	-	0/0/4/4	-
3	2F0	E	509	-	-	5/25/25/25	0/2/2/2
2	IMP	B	500	-	-	0/6/26/26	0/3/3/3
3	2F0	E	502	-	-	3/25/25/25	0/2/2/2
7	EDO	B	502	-	-	0/1/1/1	-
3	2F0	D	501	-	-	3/25/25/25	0/2/2/2
2	IMP	G	501	-	-	0/6/26/26	0/3/3/3
2	IMP	A	501	-	-	0/6/26/26	0/3/3/3
7	EDO	D	502	-	-	0/1/1/1	-
7	EDO	C	506	-	-	0/1/1/1	-
7	EDO	E	505	-	-	0/1/1/1	-
3	2F0	H	505	-	-	0/25/25/25	0/2/2/2
2	IMP	D	504	-	-	0/6/26/26	0/3/3/3
7	EDO	F	506	-	-	0/1/1/1	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	2F0	C1-C12	-4.97	1.47	1.53
3	E	509	2F0	C1-C12	-4.94	1.47	1.53
3	C	503	2F0	C1-C12	-4.78	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	2F0	C1-C12	-4.78	1.47	1.53
3	A	502	2F0	C1-C12	-4.46	1.48	1.53

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	2F0	O2-N4-C18	6.23	121.61	112.68
3	F	502	2F0	O2-N4-C18	5.85	121.06	112.68
2	A	501	IMP	N3-C2-N1	-5.43	120.19	128.68
2	G	501	IMP	N3-C2-N1	-5.36	120.30	128.68
2	C	502	IMP	N3-C2-N1	-5.35	120.32	128.68

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	GOL	O1-C1-C2-C3
3	F	502	2F0	O1-C11-C7-C8
3	F	502	2F0	N3-C11-C7-C6
3	F	502	2F0	N3-C11-C7-C8
5	E	506	GOL	O1-C1-C2-C3

There are no ring outliers.

18 monomers are involved in 35 short contacts:

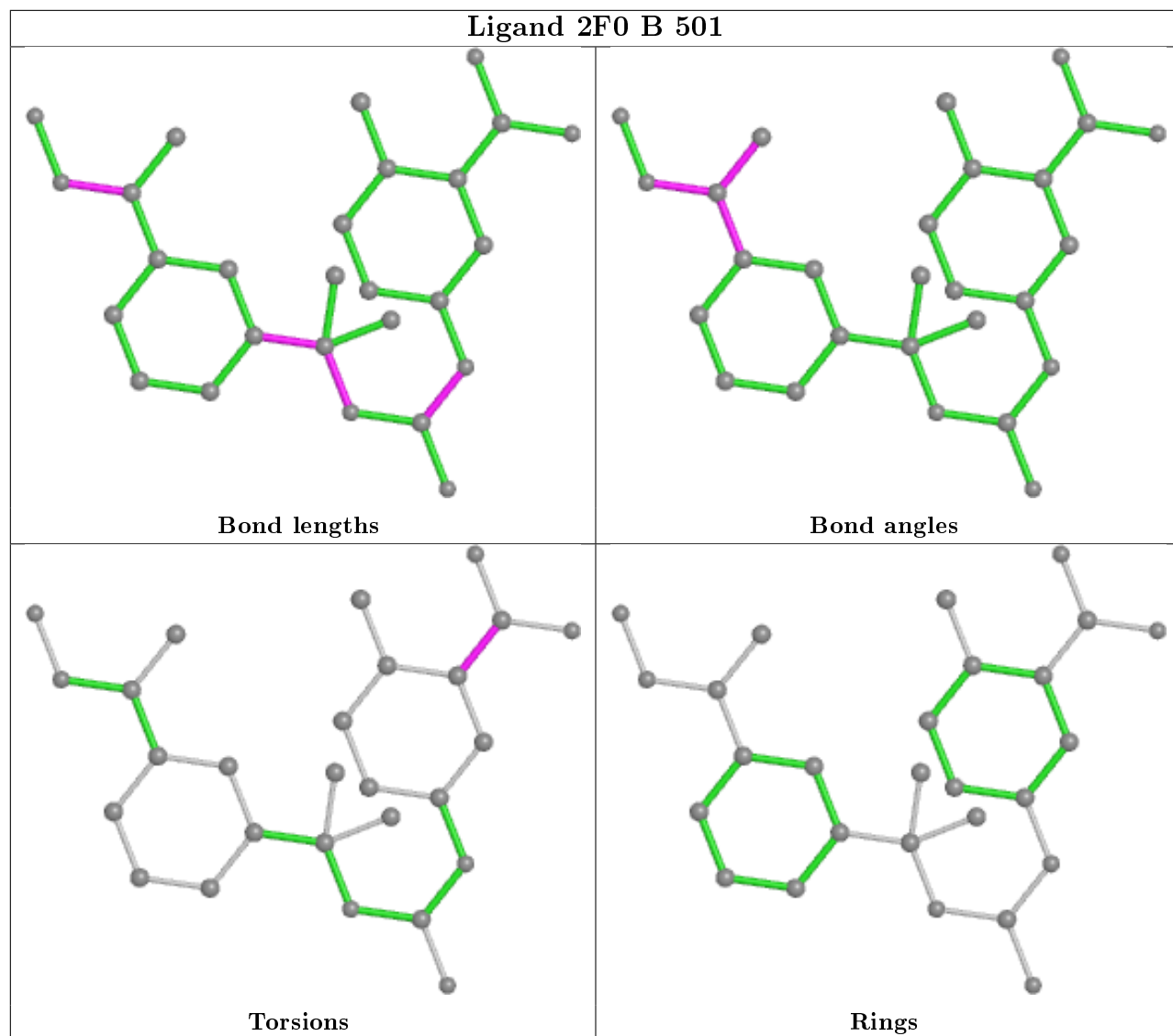
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	2F0	2	0
2	H	504	IMP	1	0
7	C	504	EDO	2	0
2	C	502	IMP	1	0
3	A	502	2F0	3	0
2	F	501	IMP	1	0
3	F	502	2F0	2	0
3	C	503	2F0	1	0
3	E	509	2F0	2	0
2	B	500	IMP	2	0
3	E	502	2F0	4	0
3	D	501	2F0	3	0
2	G	501	IMP	1	0
2	A	501	IMP	1	0
7	C	506	EDO	2	0

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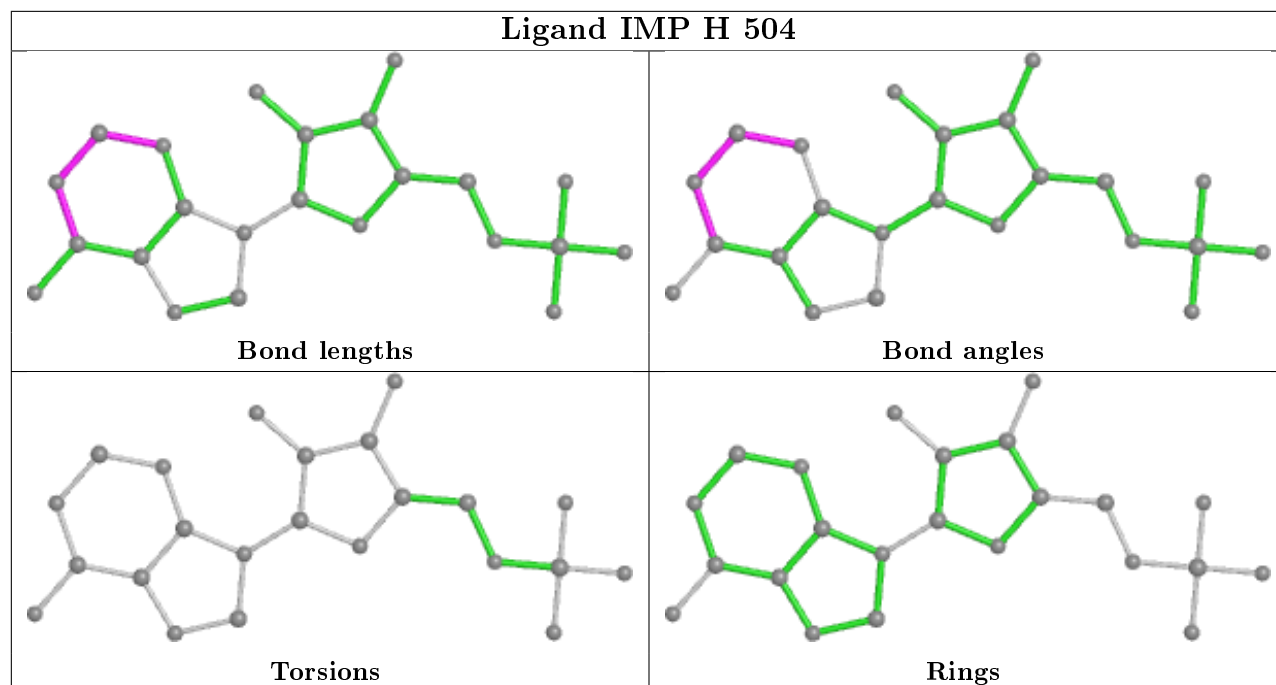
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	505	2F0	4	0
2	D	504	IMP	1	0
7	F	506	EDO	2	0

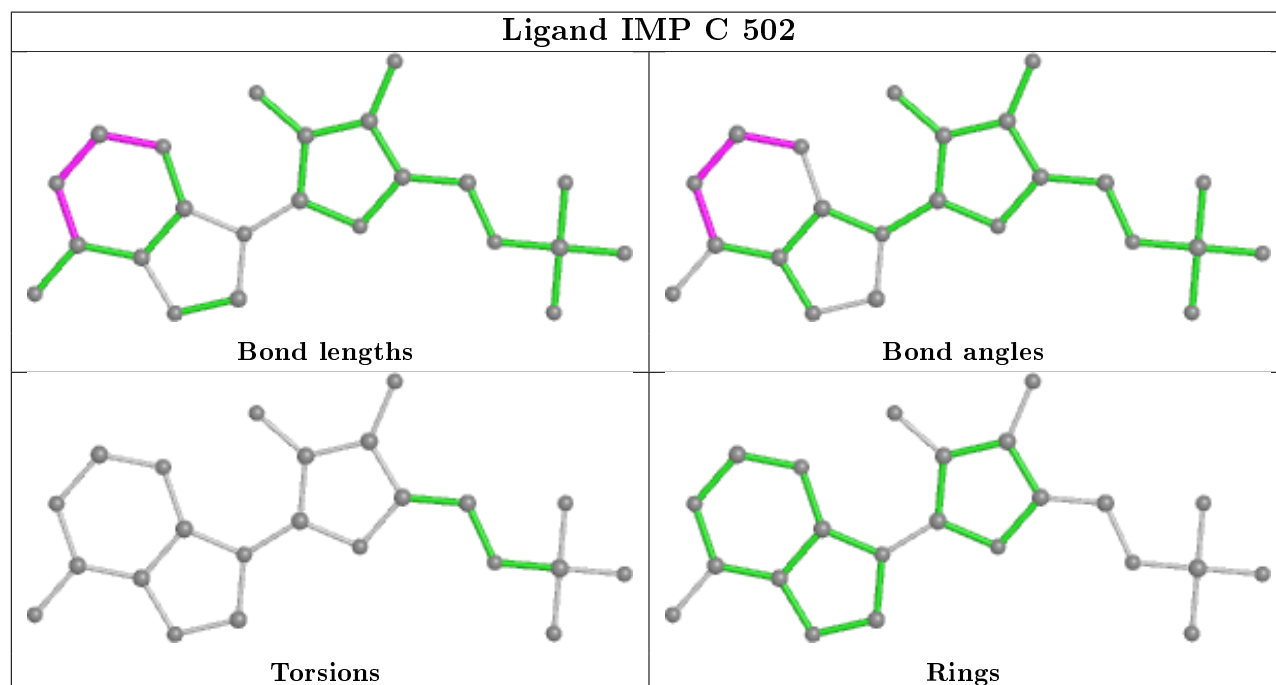
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

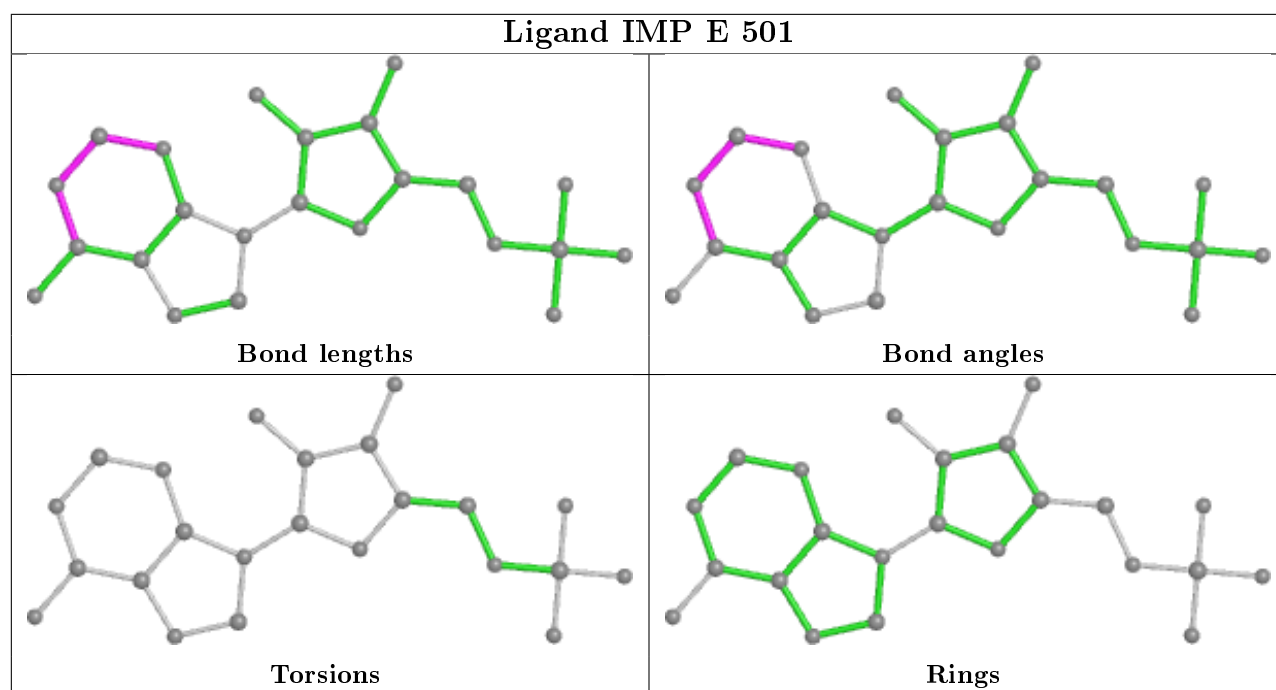


Ligand IMP H 504

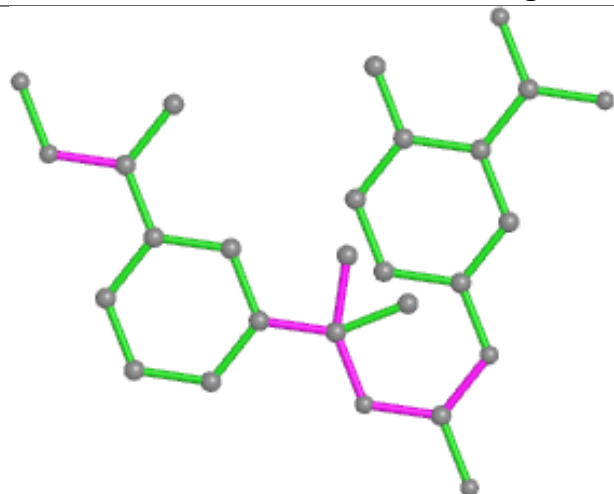


Ligand IMP C 502

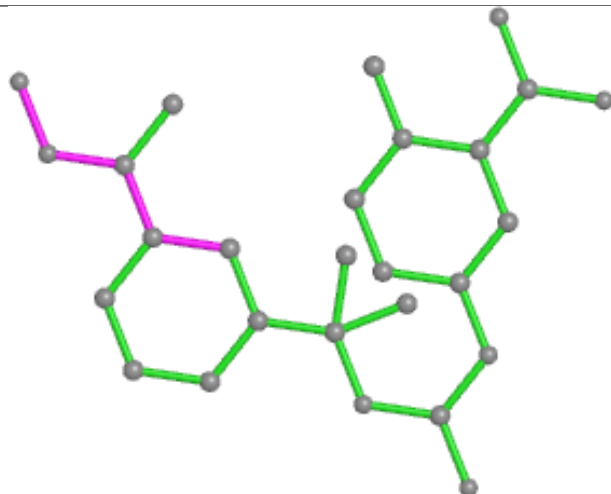




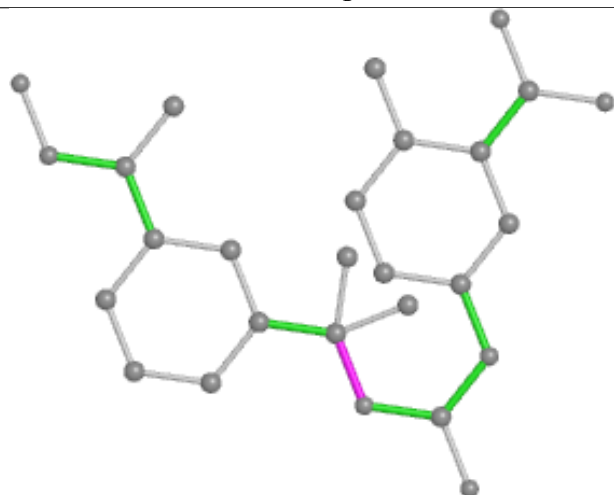
Ligand 2F0 A 502



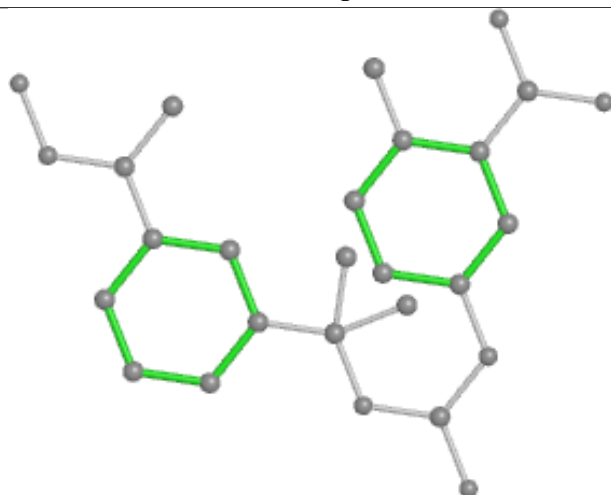
Bond lengths



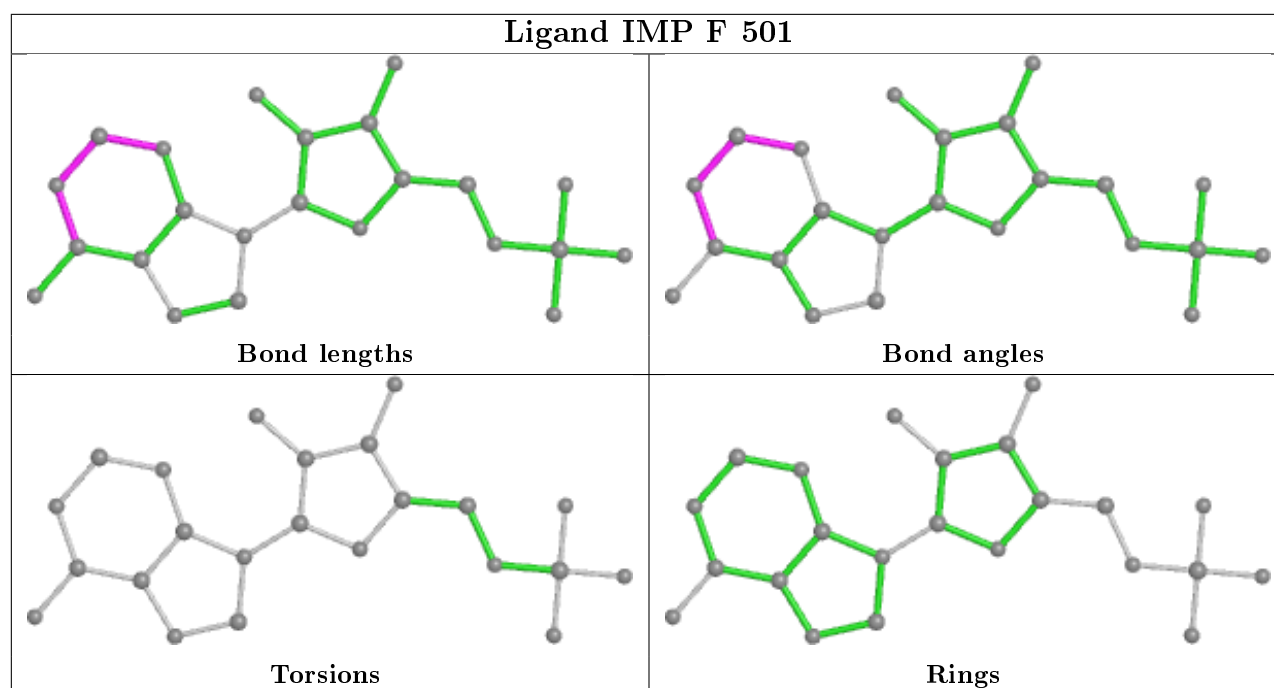
Bond angles

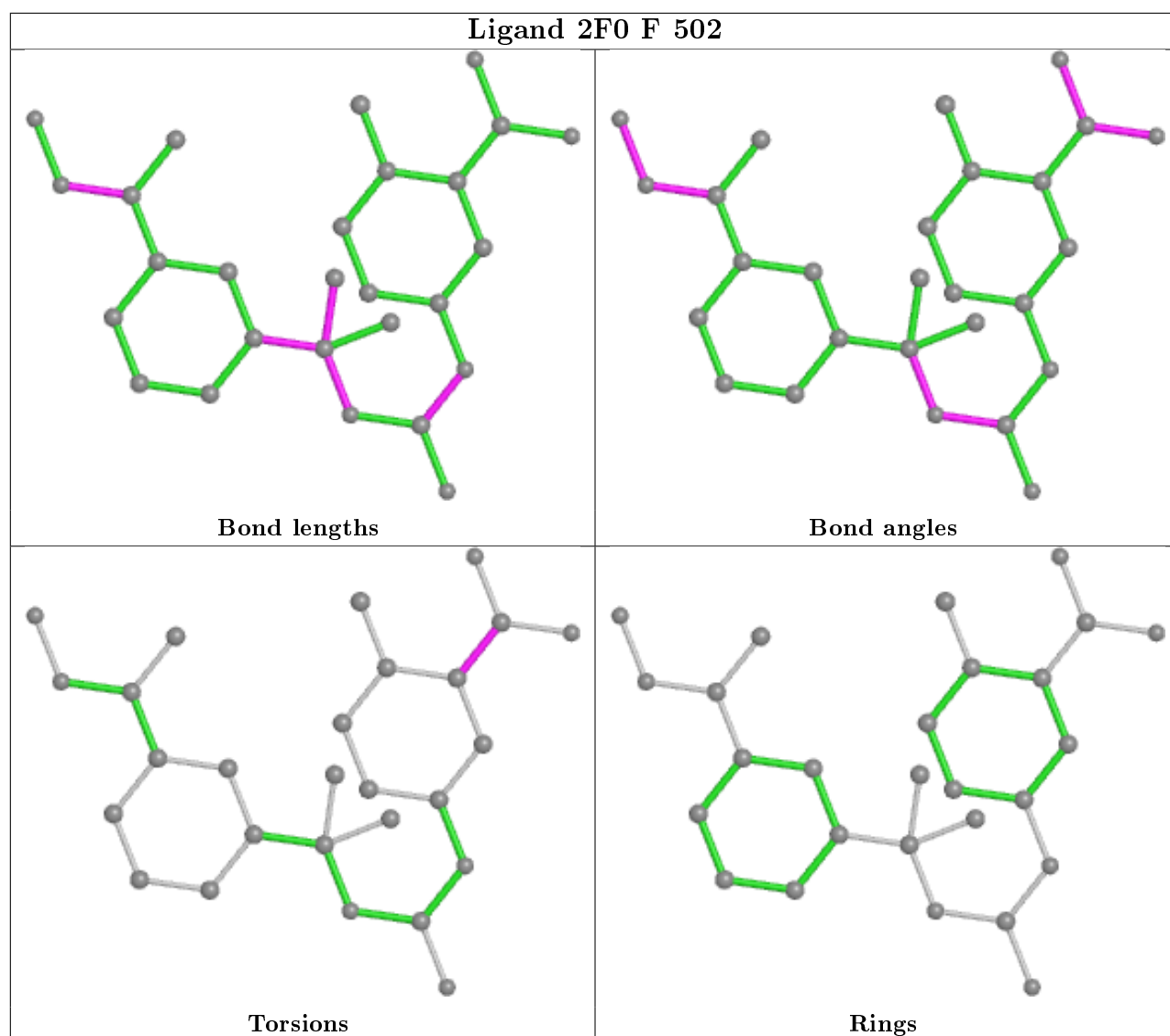


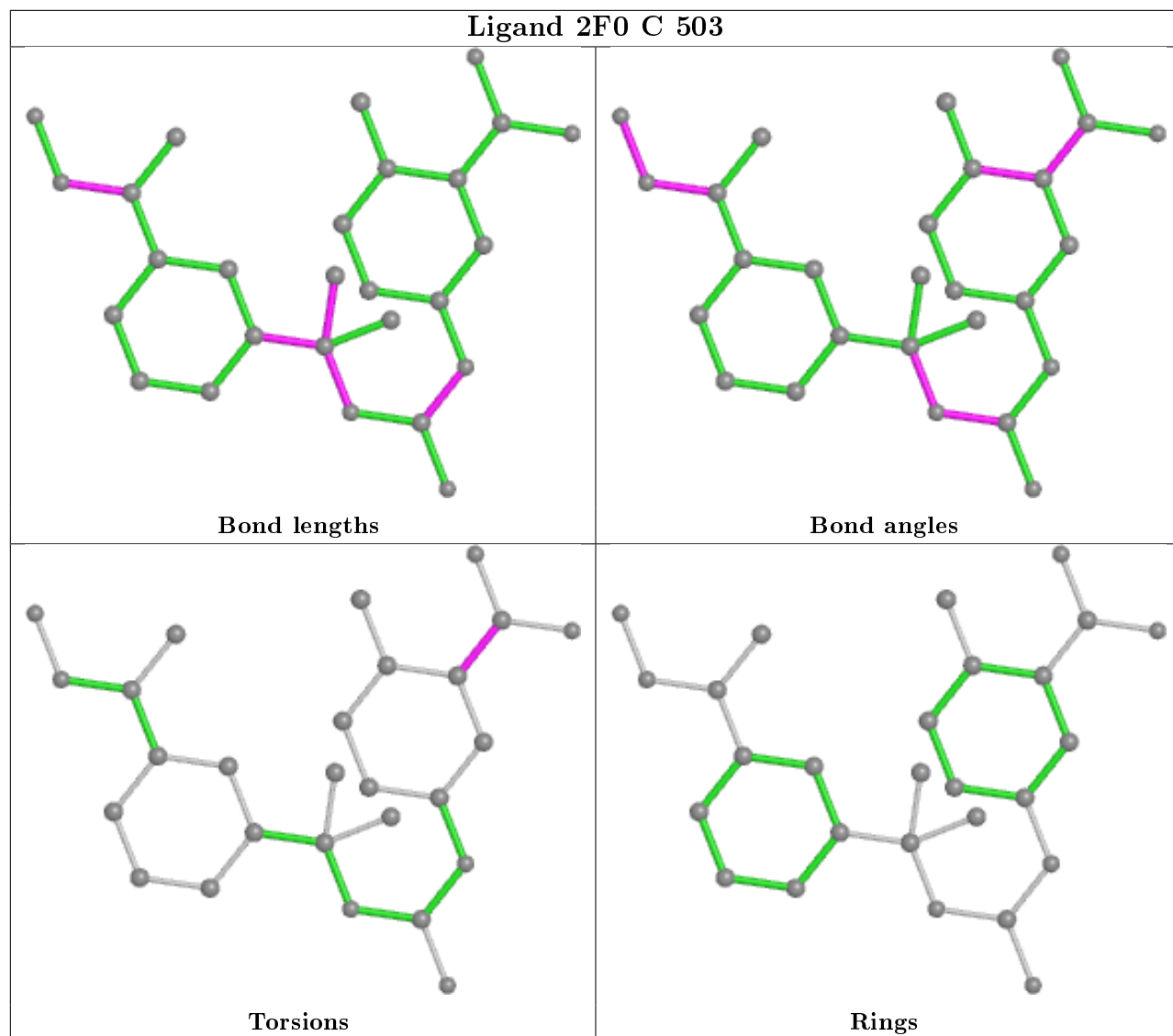
Torsions



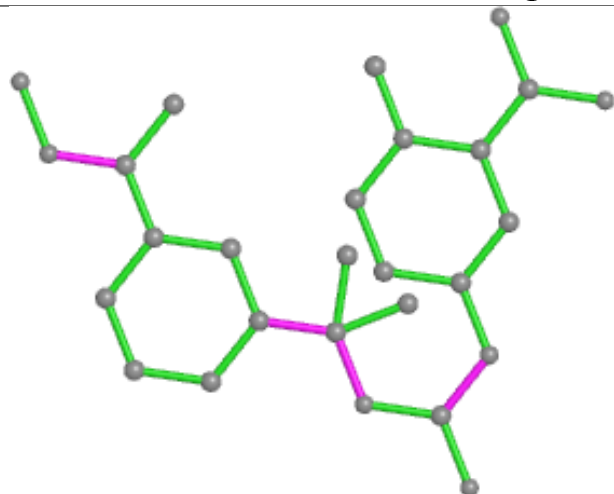
Rings



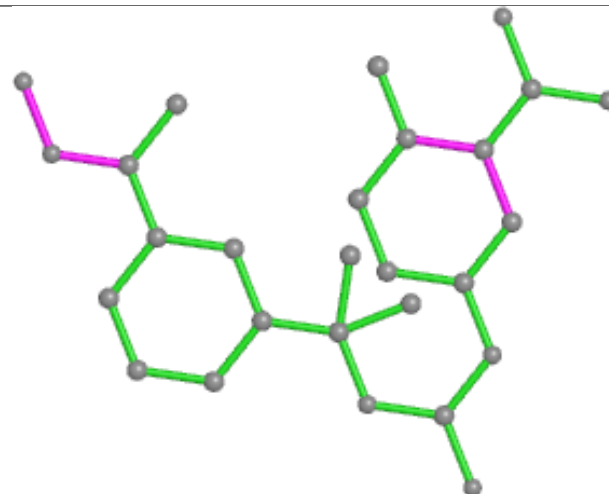




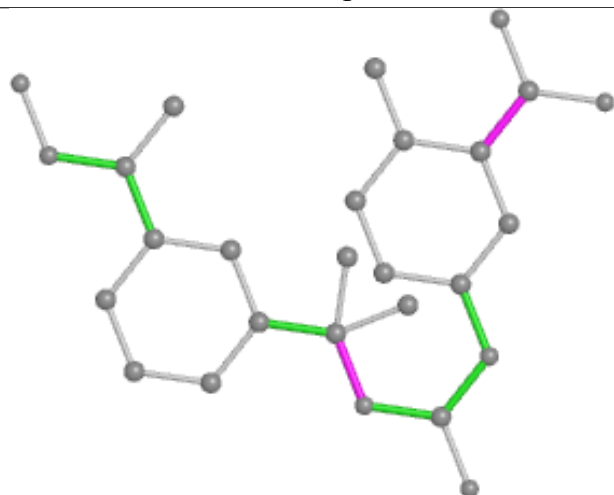
Ligand 2F0 E 509



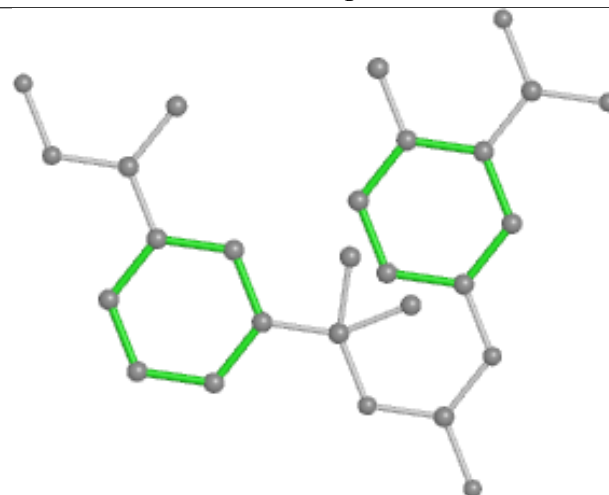
Bond lengths



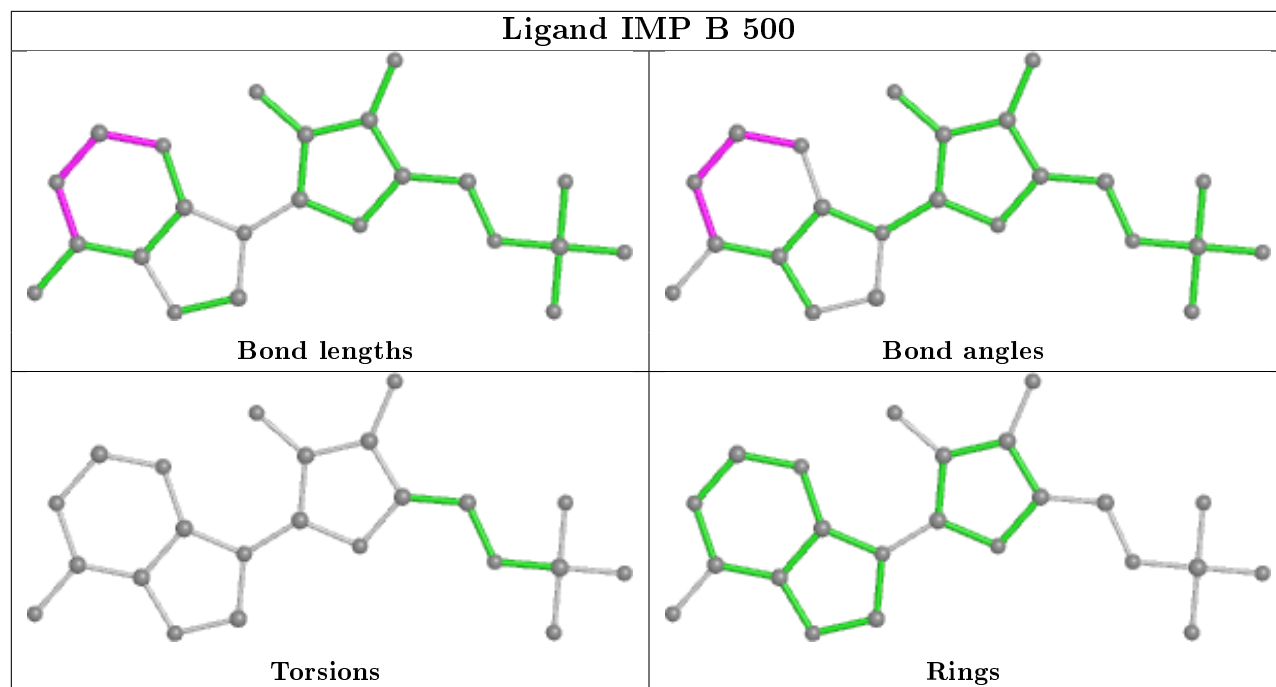
Bond angles

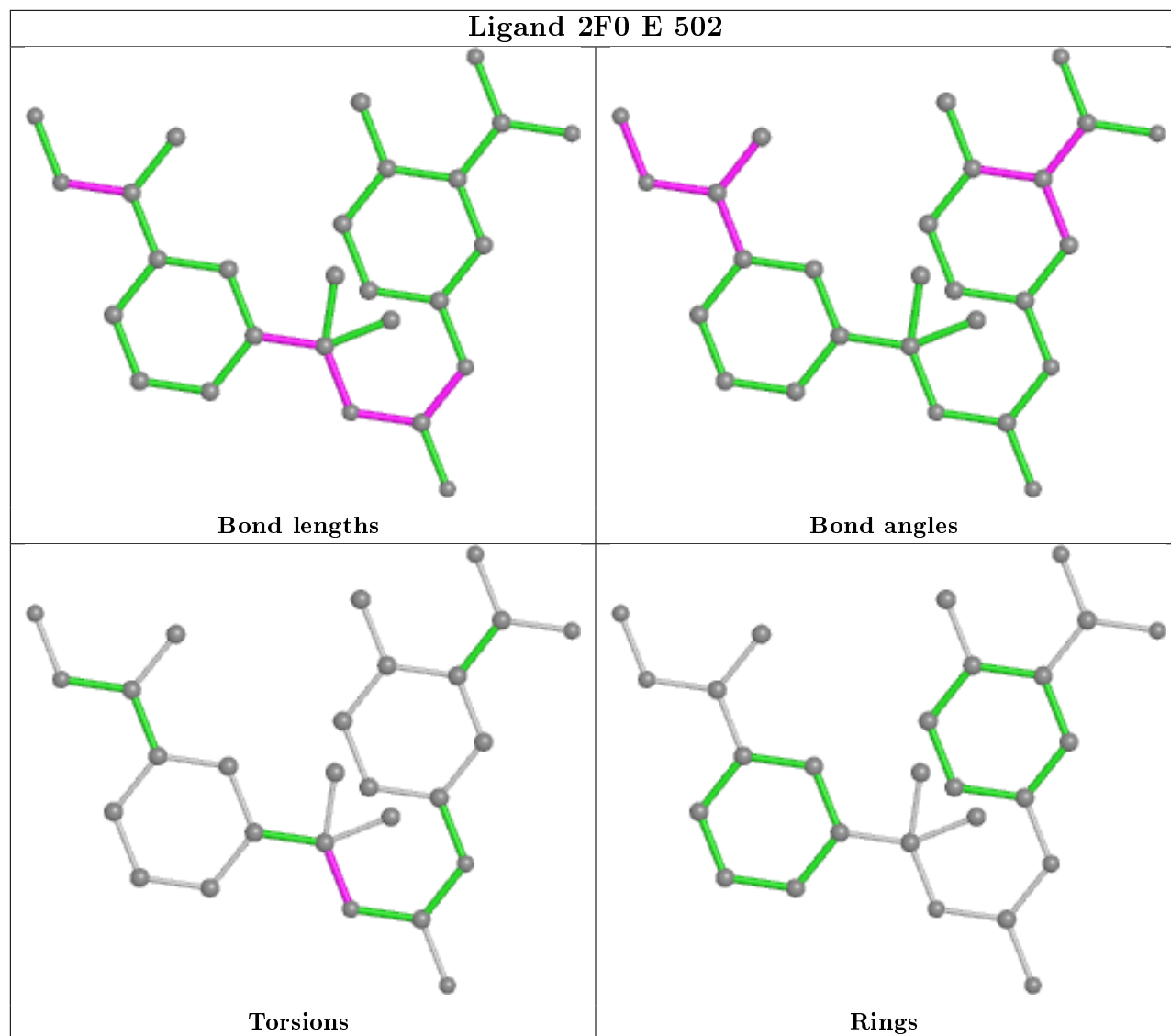


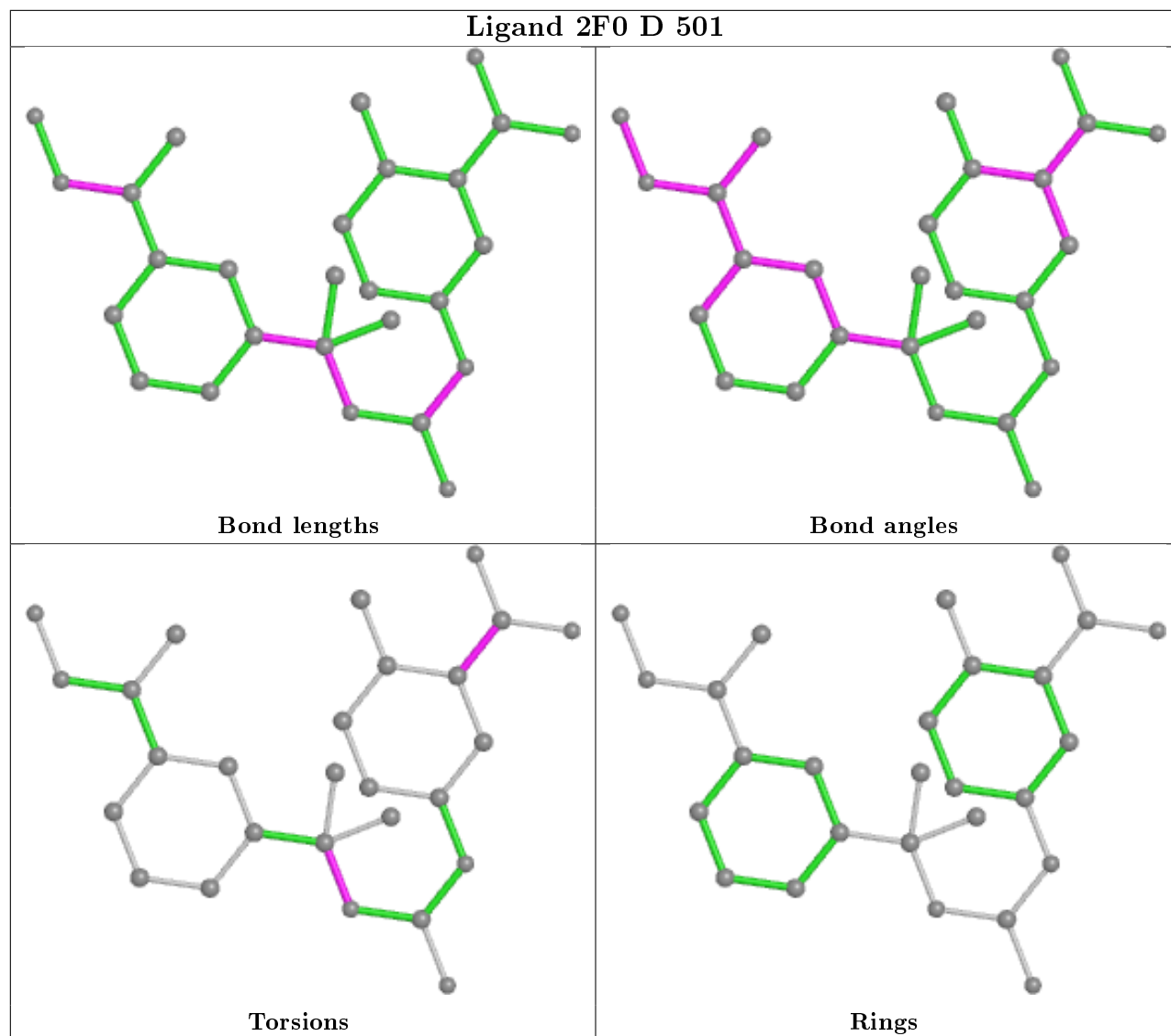
Torsions



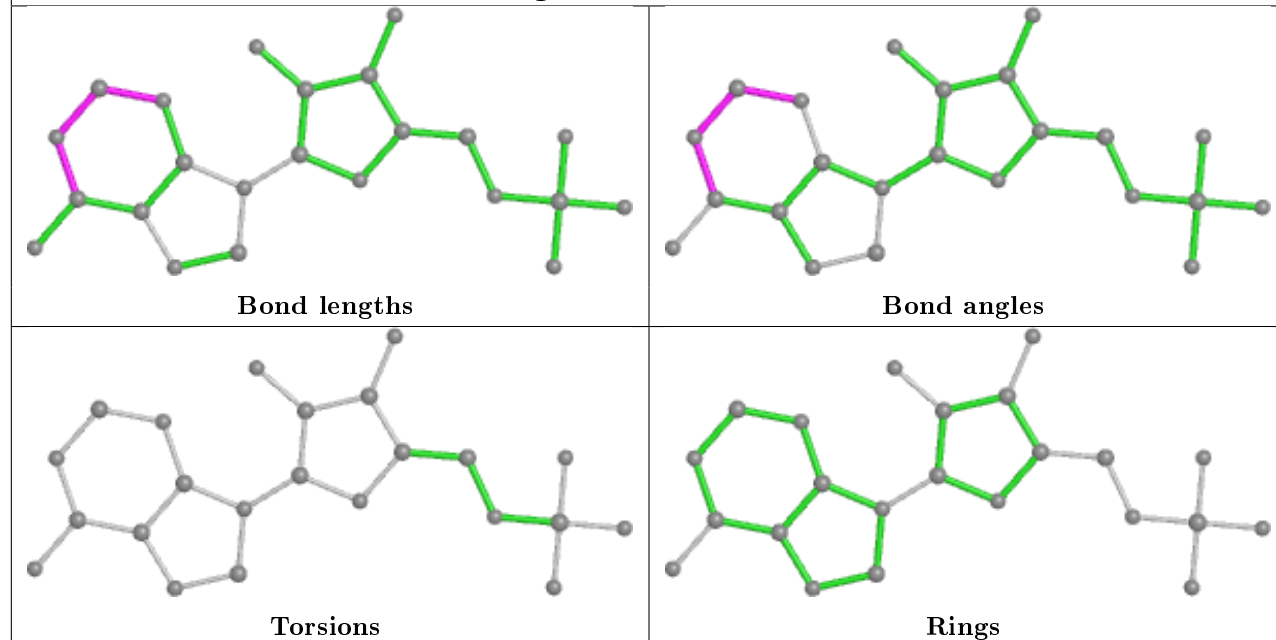
Rings



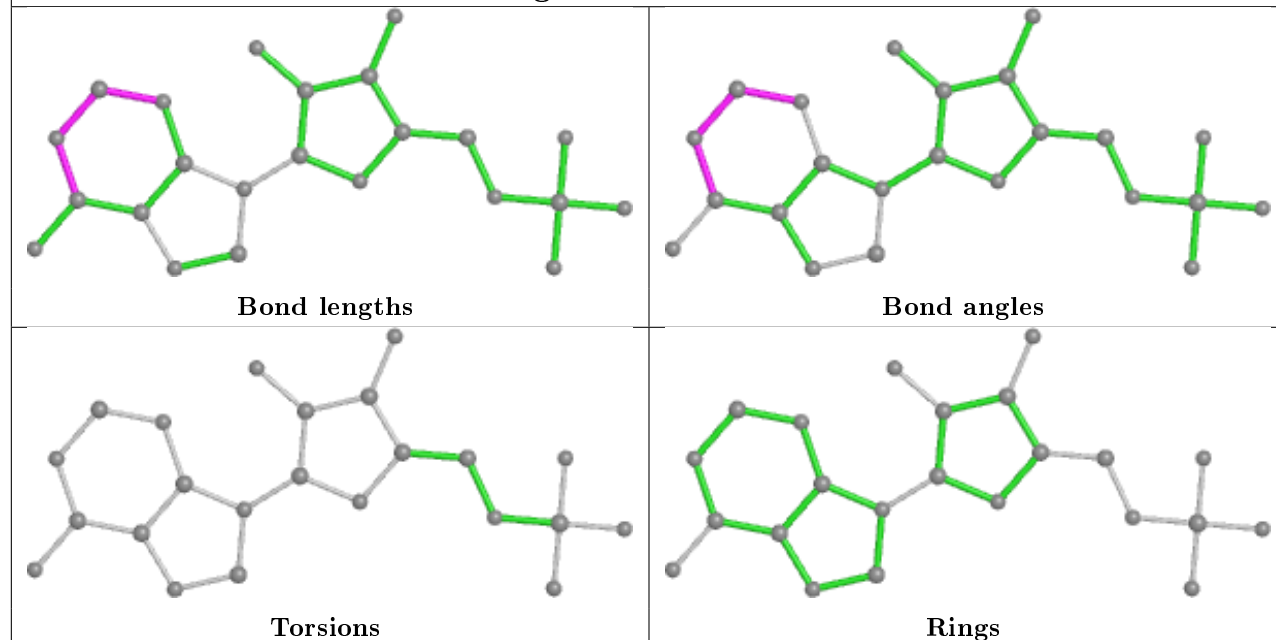


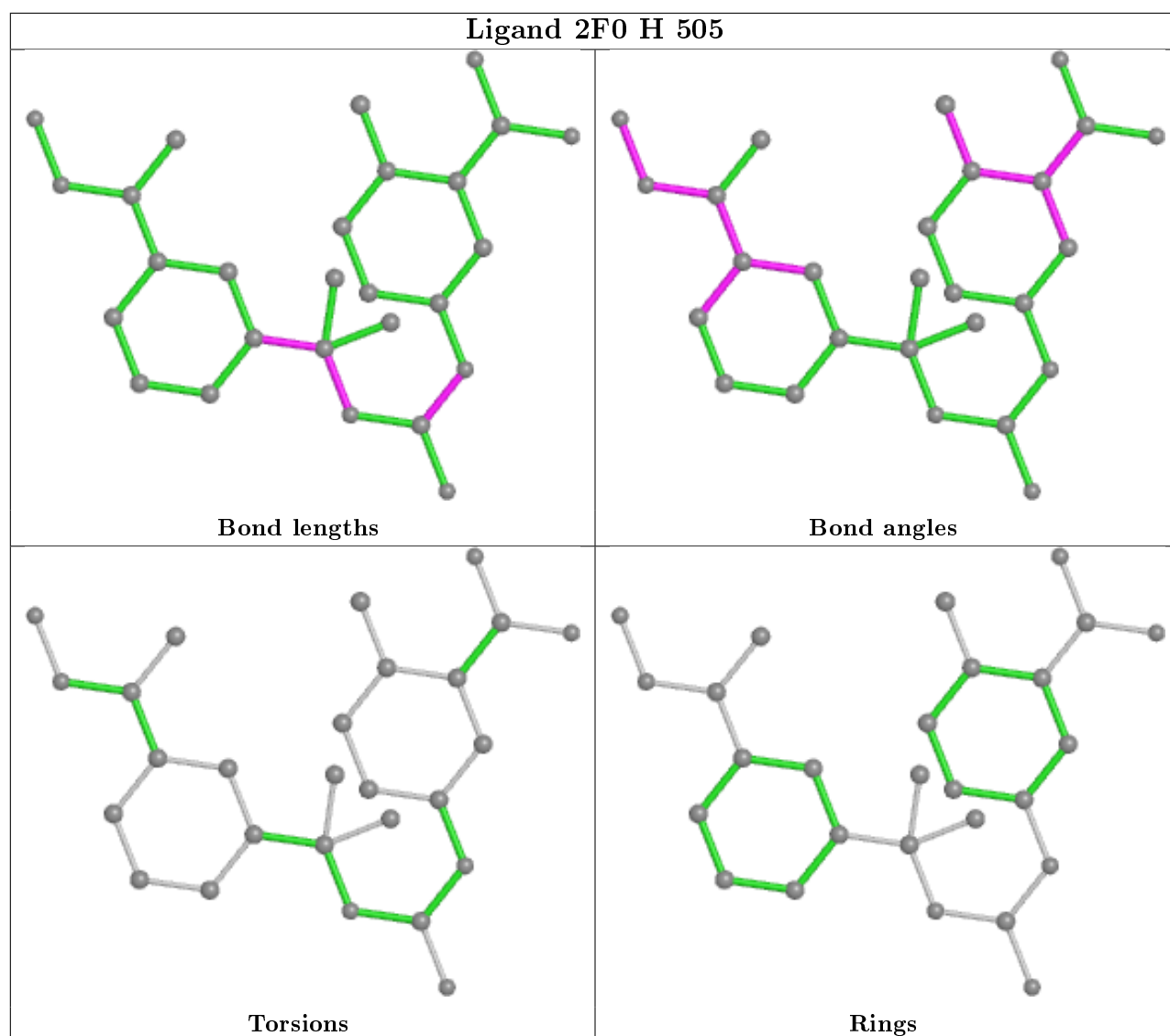


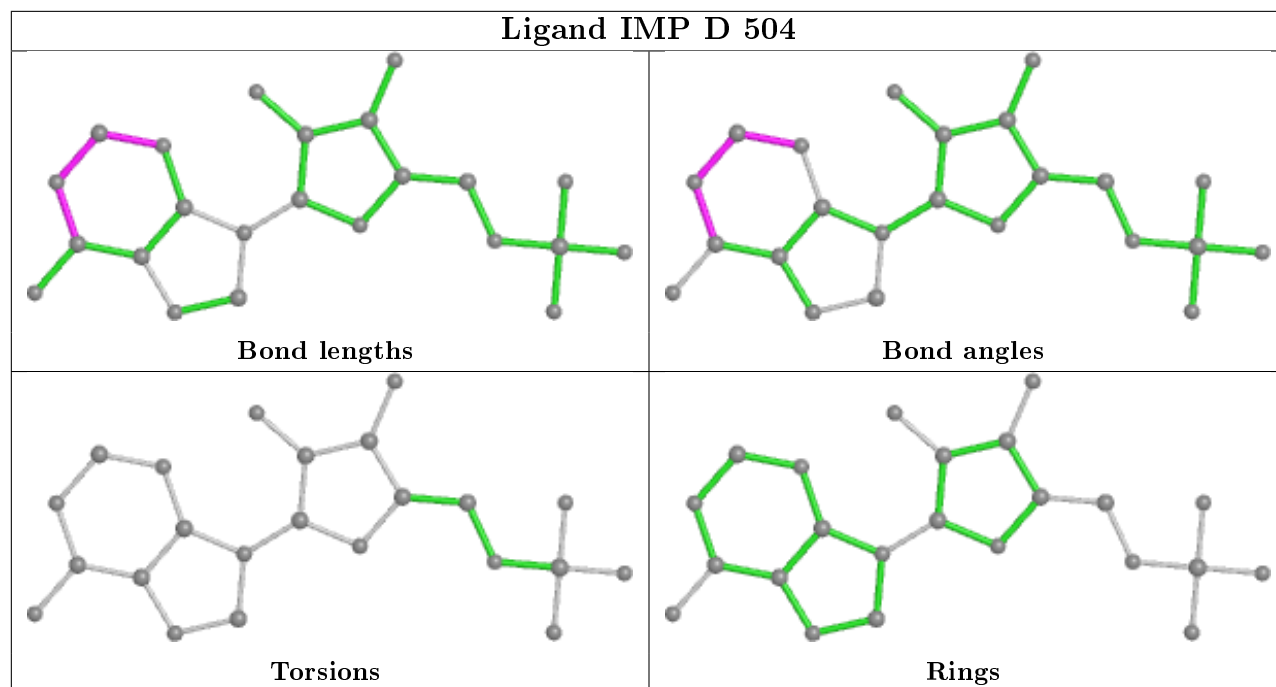
Ligand IMP G 501



Ligand IMP A 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	351/384 (91%)	0.49	32 (9%) 9 7	27, 47, 70, 84	1 (0%)
1	B	355/384 (92%)	0.35	9 (2%) 57 59	25, 45, 68, 102	2 (0%)
1	C	348/384 (90%)	0.27	6 (1%) 70 72	32, 45, 64, 74	0
1	D	352/384 (91%)	0.56	25 (7%) 16 14	30, 48, 68, 97	0
1	E	352/384 (91%)	0.46	22 (6%) 20 19	31, 46, 73, 89	1 (0%)
1	F	350/384 (91%)	0.59	29 (8%) 11 9	34, 50, 70, 85	1 (0%)
1	G	356/384 (92%)	0.50	22 (6%) 20 19	31, 49, 67, 87	1 (0%)
1	H	350/384 (91%)	0.57	25 (7%) 16 14	33, 51, 71, 80	1 (0%)
All	All	2814/3072 (91%)	0.47	170 (6%) 21 20	25, 48, 70, 102	7 (0%)

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	226	ALA	7.3
1	H	-2	SER	6.5
1	H	226	ALA	6.0
1	E	413	LEU	5.5
1	H	250	LEU	5.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
7	EDO	F	504	4/4	0.62	0.39	66,67,69,69	0
4	FMT	F	507	3/3	0.66	0.37	69,69,70,70	0
8	SO4	G	502	5/5	0.66	0.53	127,128,128,128	0
5	GOL	A	505	6/6	0.67	0.30	48,51,51,52	0
5	GOL	E	506	6/6	0.70	0.30	50,52,53,54	0
6	MLI	A	506	7/7	0.70	0.40	87,88,91,91	0
7	EDO	D	502	4/4	0.71	0.25	59,60,60,60	0
7	EDO	D	503	4/4	0.72	0.30	51,53,55,56	0
8	SO4	G	503	5/5	0.73	0.34	144,144,145,145	0
4	FMT	D	507	3/3	0.77	0.28	62,62,63,64	0
4	FMT	H	502	3/3	0.79	0.31	68,68,68,68	0
4	FMT	E	504	3/3	0.80	0.19	53,53,53,53	0
4	FMT	H	506	3/3	0.81	0.24	65,65,65,65	0
7	EDO	C	506	4/4	0.81	0.38	54,56,58,59	0
7	EDO	F	505	4/4	0.81	0.13	56,58,59,59	0
4	FMT	B	503	3/3	0.82	0.35	46,46,47,49	0
4	FMT	D	506	3/3	0.83	0.14	43,43,46,47	0
4	FMT	E	503	3/3	0.84	0.24	74,74,74,75	0
7	EDO	C	504	4/4	0.85	0.19	53,54,54,54	0
4	FMT	H	501	3/3	0.85	0.19	62,62,63,63	0
4	FMT	A	504	3/3	0.86	0.37	62,62,63,64	0
4	FMT	H	503	3/3	0.86	0.16	66,66,67,67	0
7	EDO	E	505	4/4	0.86	0.14	41,43,45,46	0
7	EDO	D	505	4/4	0.86	0.24	55,56,57,57	0
8	SO4	C	505	5/5	0.88	0.24	119,119,119,119	0
6	MLI	E	508	7/7	0.88	0.25	64,65,67,68	0
3	2F0	F	502	27/27	0.89	0.24	42,49,54,67	0
7	EDO	B	502	4/4	0.89	0.38	71,71,71,72	0
3	2F0	H	505	27/27	0.90	0.24	47,53,59,63	0
3	2F0	D	501	27/27	0.91	0.22	34,42,57,61	0
4	FMT	A	503	3/3	0.91	0.31	48,48,48,49	0
3	2F0	E	509	27/27	0.91	0.26	39,51,55,57	0
3	2F0	B	501	27/27	0.91	0.30	41,50,56,61	0
3	2F0	E	502	27/27	0.92	0.23	38,43,52,54	0
3	2F0	C	503	27/27	0.92	0.25	43,50,54,56	0
3	2F0	A	502	27/27	0.92	0.29	37,45,50,58	0
4	FMT	C	501	3/3	0.92	0.33	69,69,70,71	0

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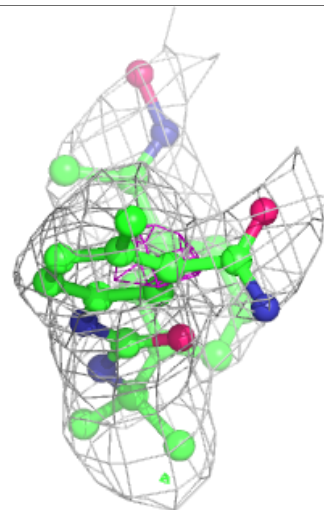
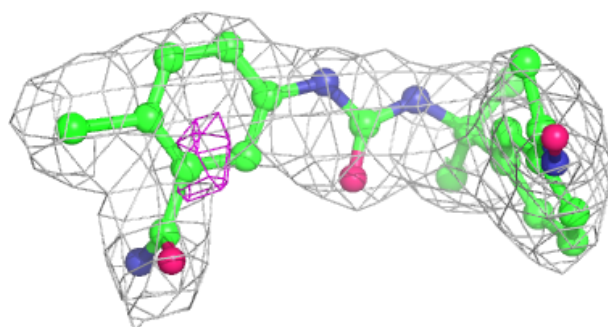
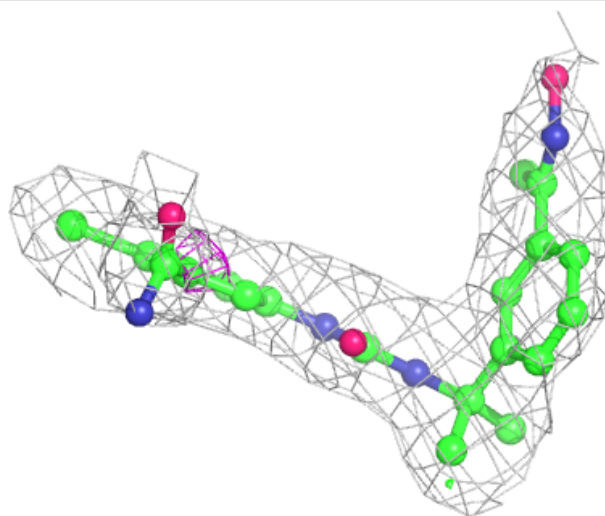
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IMP	E	501	23/23	0.92	0.19	31,35,43,44	0
4	FMT	F	503	3/3	0.93	0.16	42,42,43,44	0
2	IMP	F	501	23/23	0.94	0.20	37,44,47,48	0
2	IMP	A	501	23/23	0.95	0.15	35,40,44,45	0
2	IMP	H	504	23/23	0.95	0.18	37,41,47,48	0
4	FMT	E	507	3/3	0.95	0.17	37,37,37,37	0
2	IMP	D	504	23/23	0.95	0.24	36,41,45,49	0
7	EDO	F	506	4/4	0.95	0.20	39,39,39,40	0
2	IMP	G	501	23/23	0.95	0.16	36,39,41,42	0
2	IMP	C	502	23/23	0.96	0.17	32,41,44,46	0
2	IMP	B	500	23/23	0.96	0.16	33,36,38,39	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.

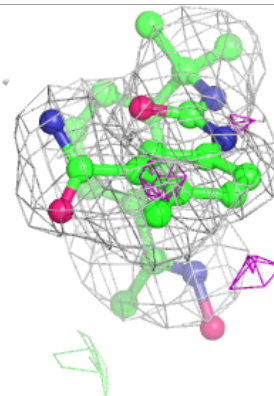
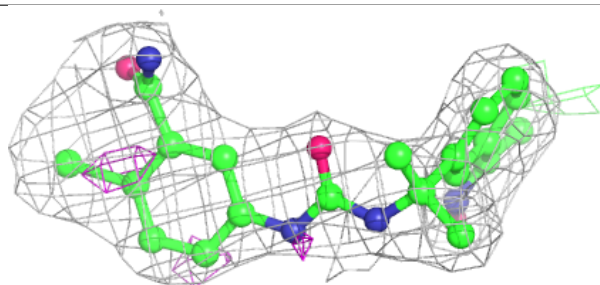
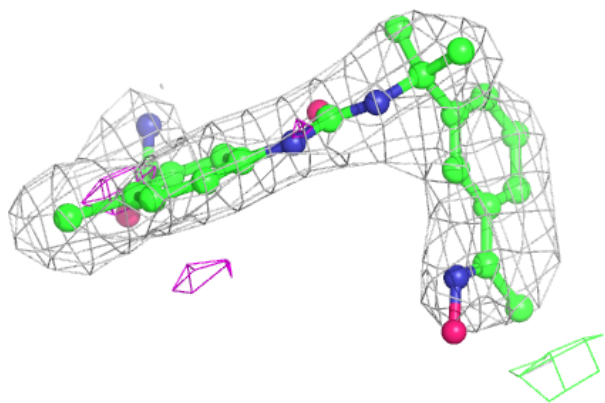
Electron density around 2F0 F 502:

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

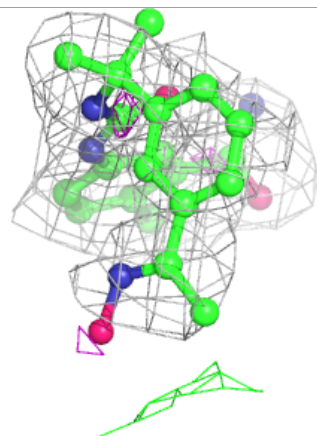
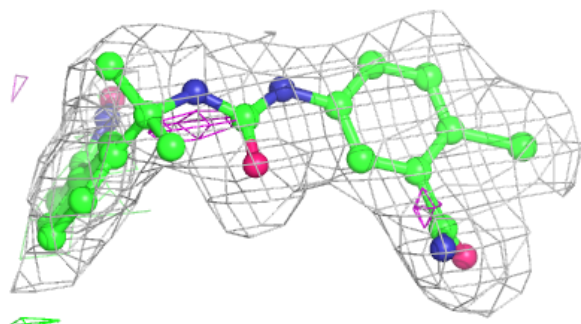
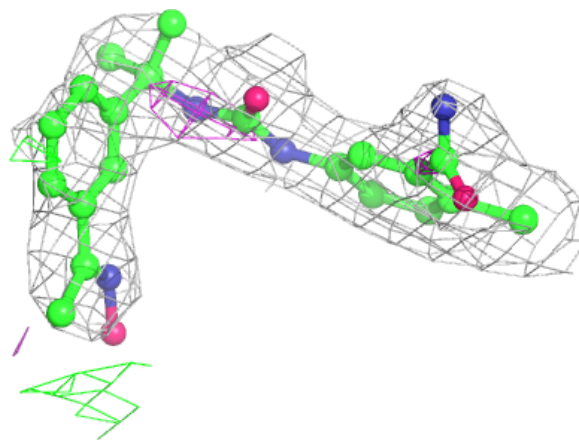


Electron density around 2F0 H 505:

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and green (positive)

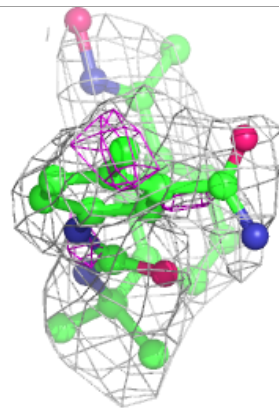
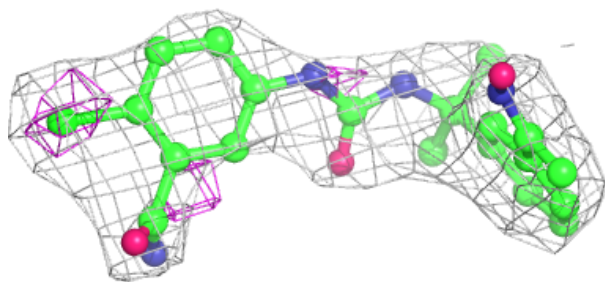
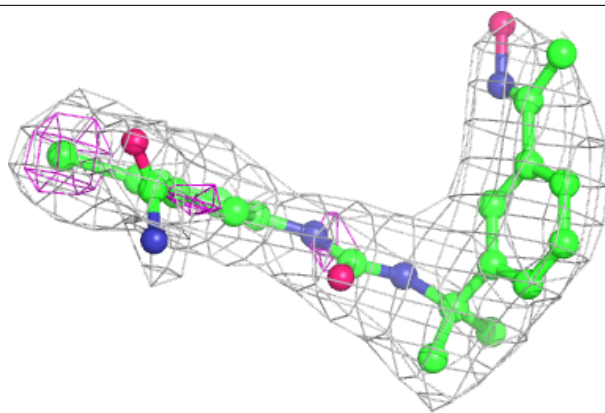
**Electron density around 2F0 D 501:**

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and green (positive)



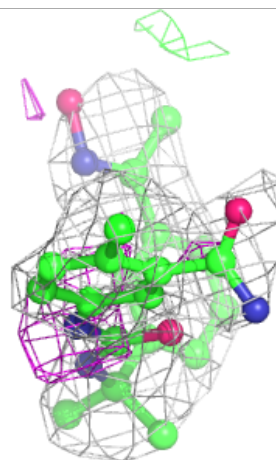
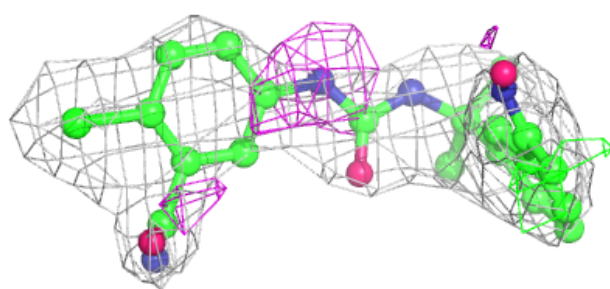
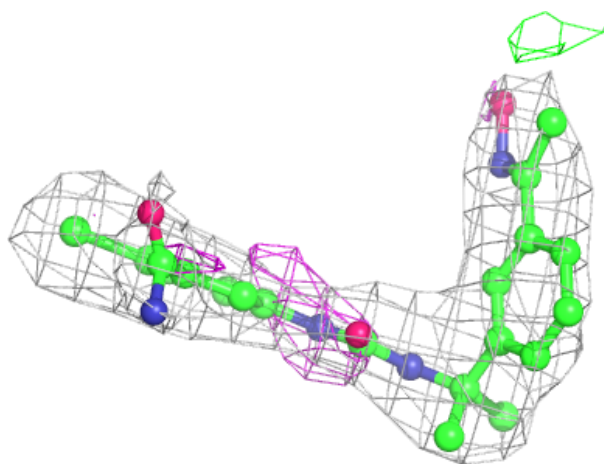
Electron density around 2F0 E 509:

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



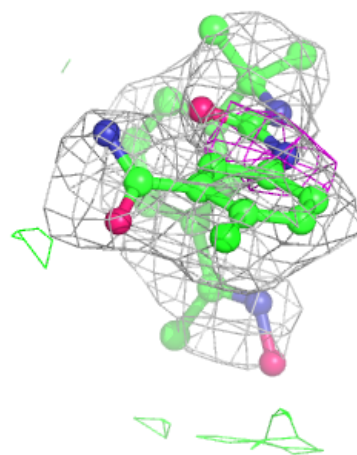
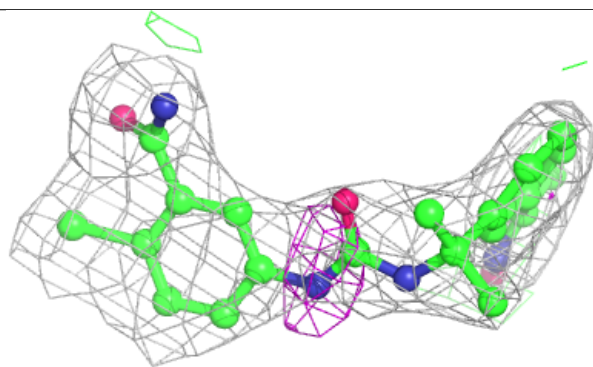
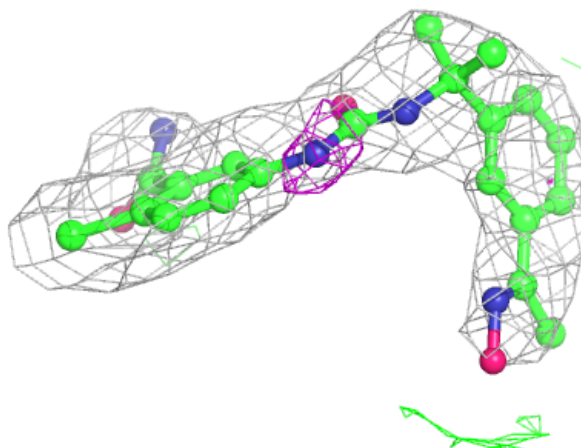
Electron density around 2F0 B 501:

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



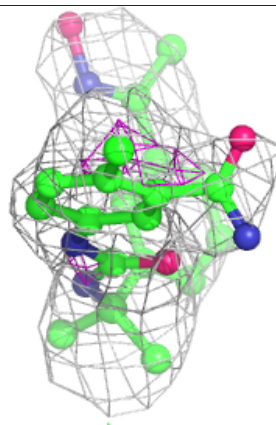
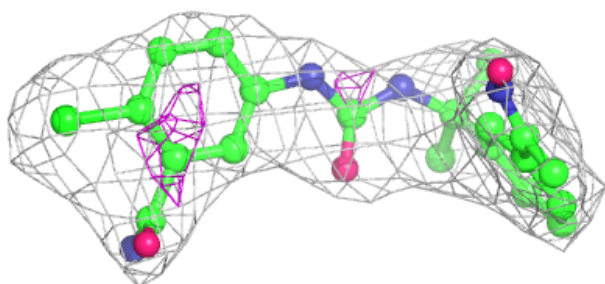
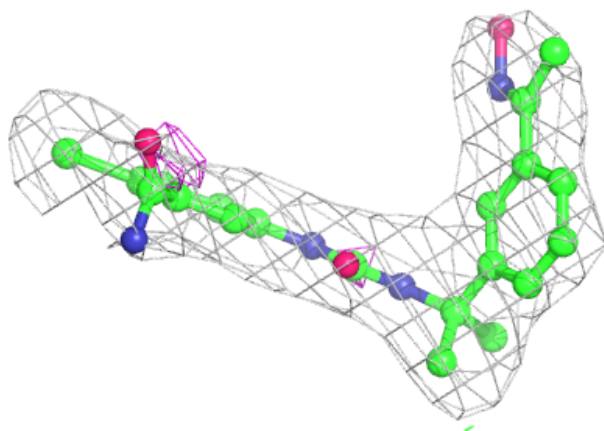
Electron density around 2F0 E 502:

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

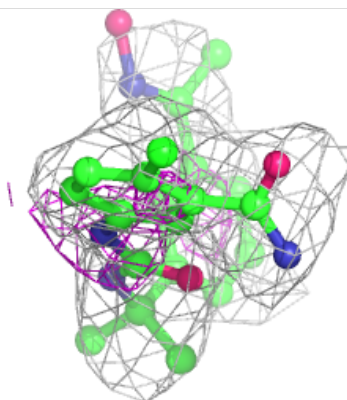
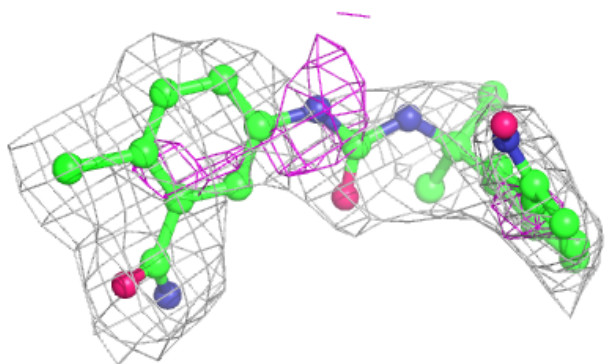
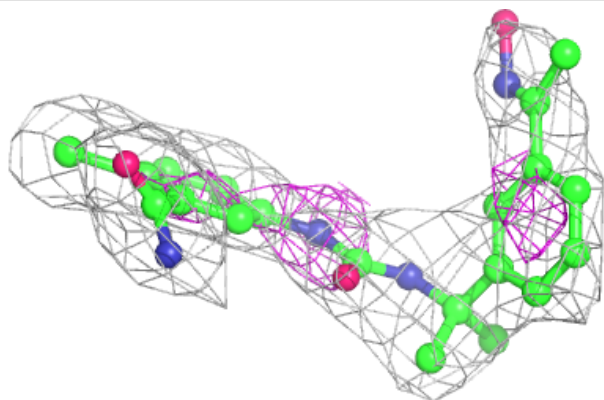


Electron density around 2F0 C 503:

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

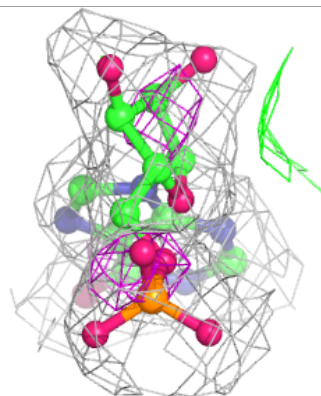
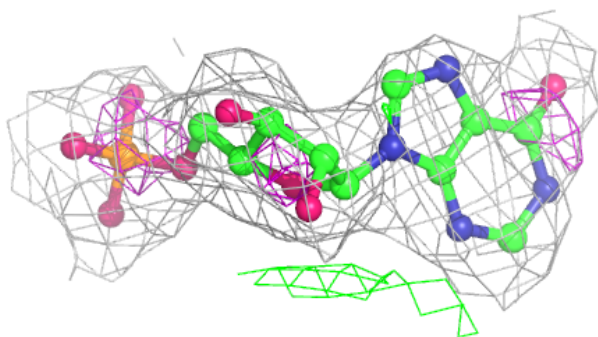
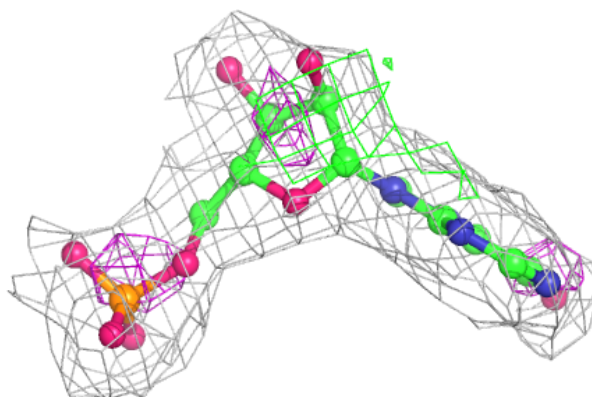
**Electron density around 2F0 A 502:**

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

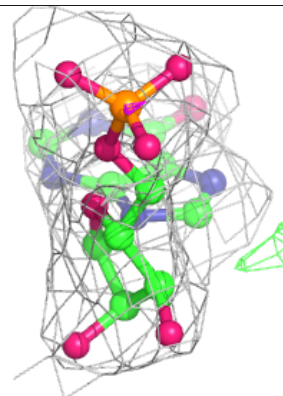
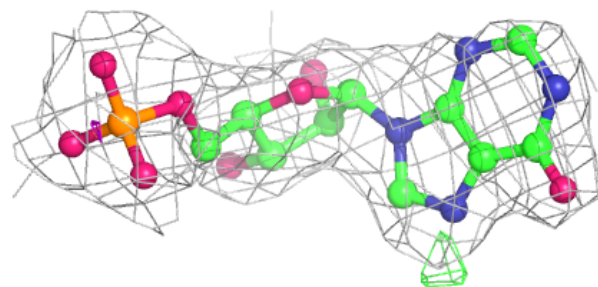
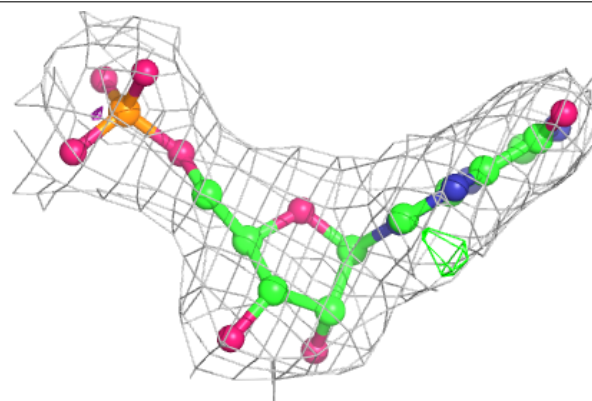


Electron density around IMP E 501:

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

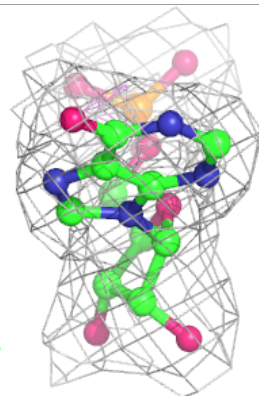
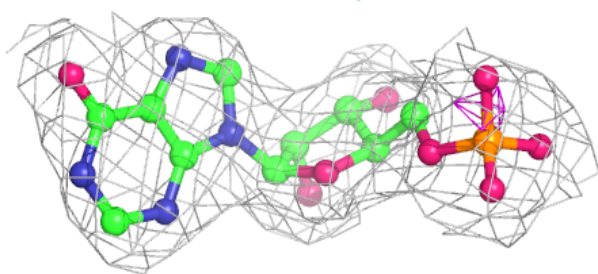
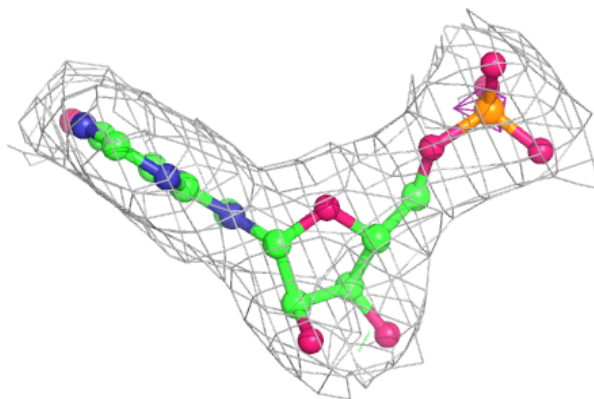
**Electron density around IMP F 501:**

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

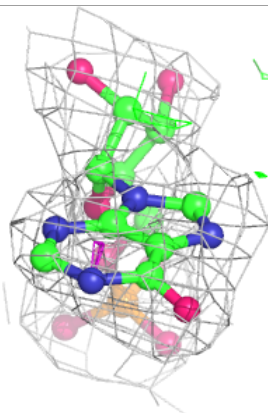
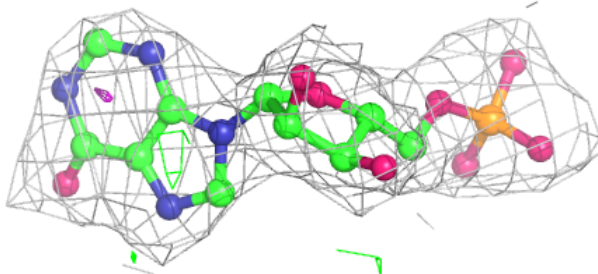
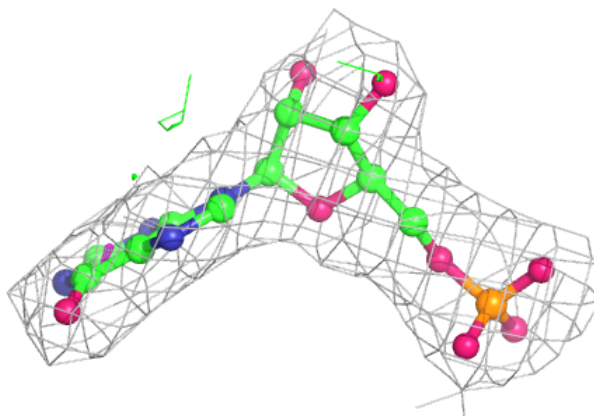


Electron density around IMP A 501:

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

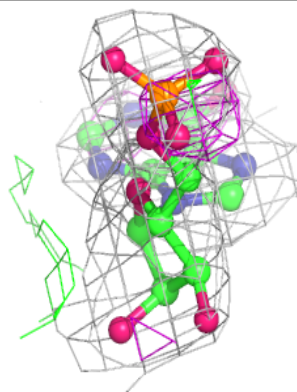
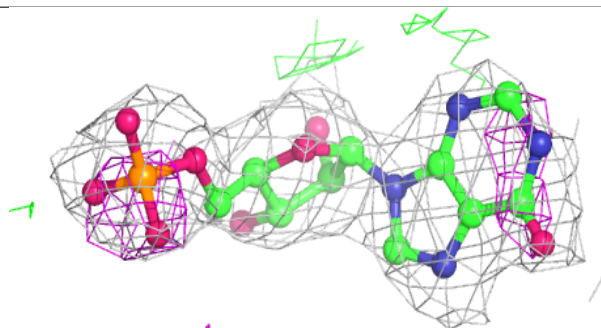
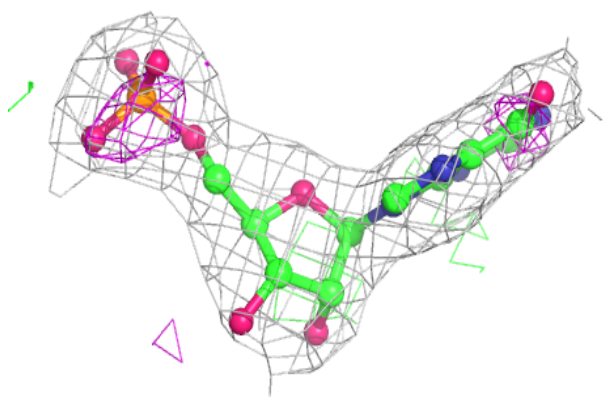
**Electron density around IMP H 504:**

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

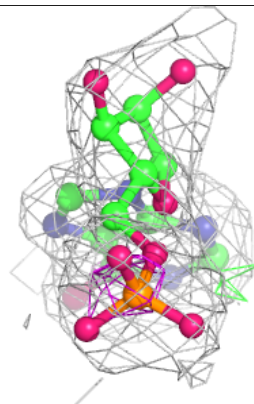
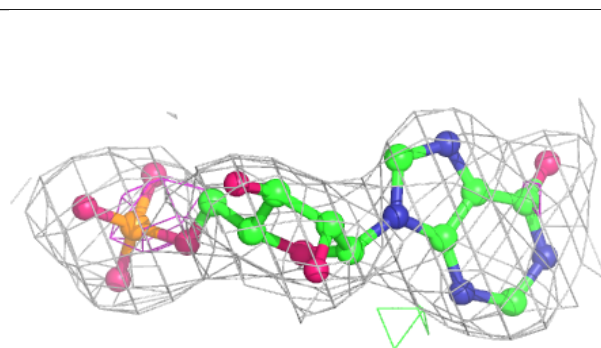
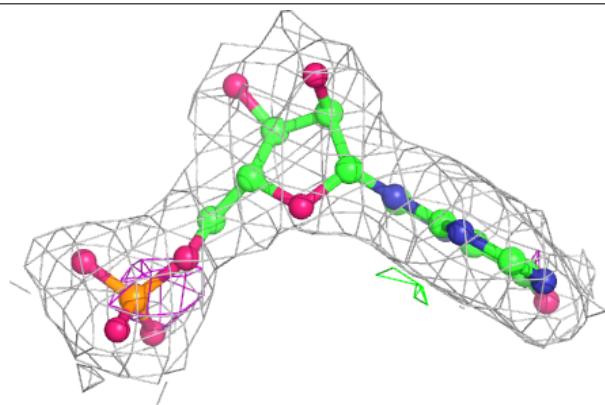


Electron density around IMP D 504:

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

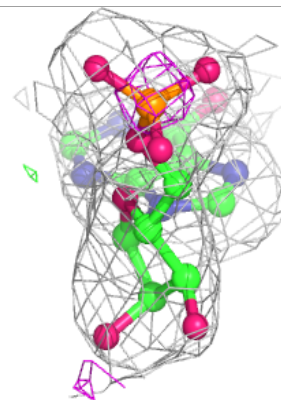
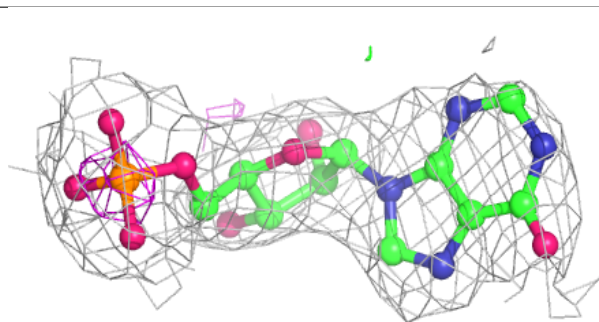
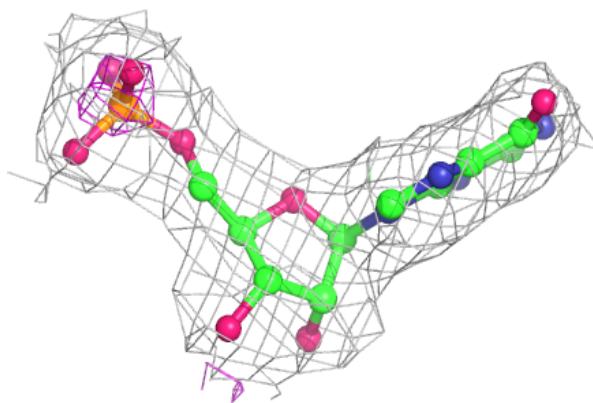
**Electron density around IMP G 501:**

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

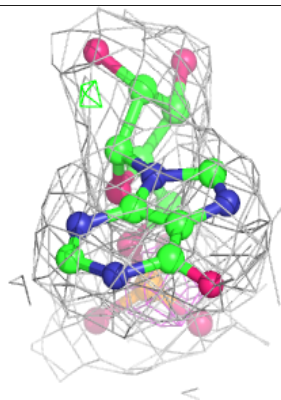
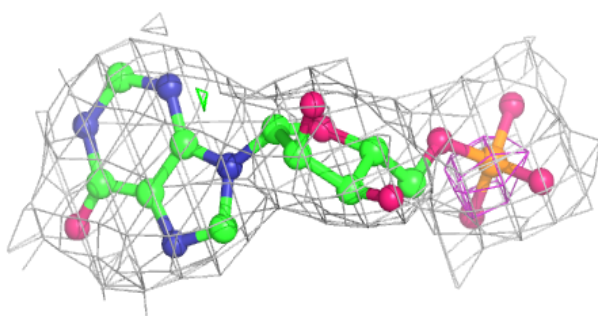
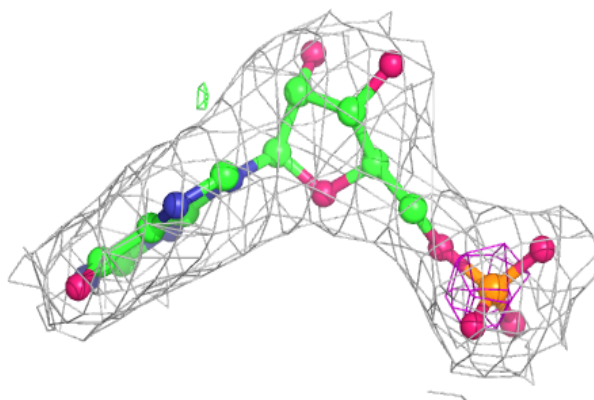


Electron density around IMP C 502:

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

**Electron density around IMP B 500:**

$2mF_o-DF_c$ (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.