



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:48 AM UTC

PDB ID : 4MYX / pdb_00004myx
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 Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

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

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

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

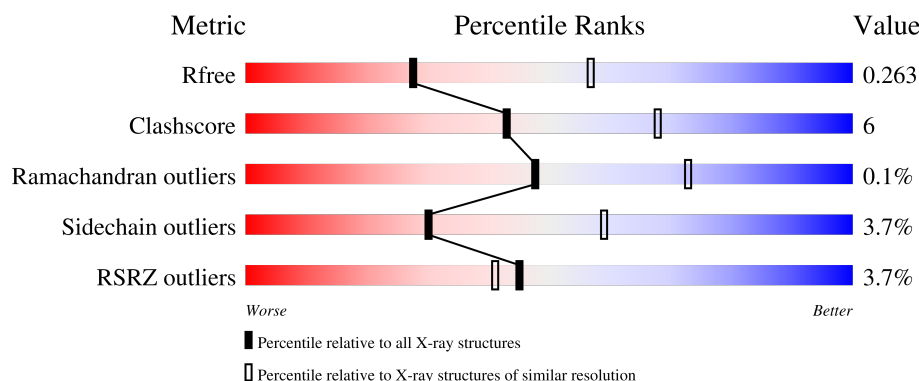
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of 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	5% 78% 14% 9%
1	B	384	4% 76% 15% 8%
1	C	384	2% 75% 15% 9%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	384	3% 77% 15% 8%
1	E	384	3% 77% 13% 8%
1	F	384	3% 78% 11% 9%
1	G	384	4% 78% 15% 7%
1	H	384	3% 72% 18% 9%

2 Entry composition

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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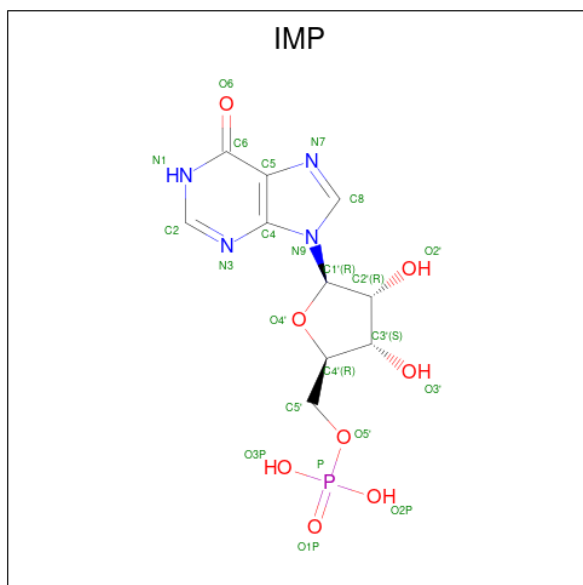
Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	GLY	-	expression tag	UNP Q81W29
F	-13	VAL	-	expression tag	UNP Q81W29
F	-12	ASP	-	expression tag	UNP Q81W29
F	-11	LEU	-	expression tag	UNP Q81W29
F	-10	GLY	-	expression tag	UNP Q81W29
F	-9	THR	-	expression tag	UNP Q81W29
F	-8	GLU	-	expression tag	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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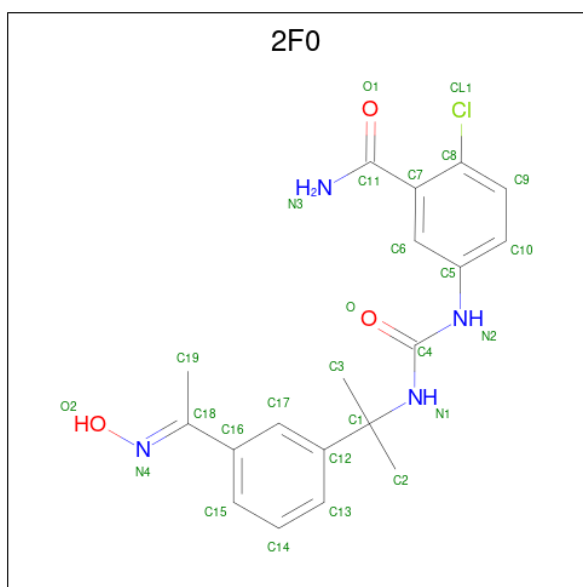
Chain	Residue	Modelled	Actual	Comment	Reference
G	220	GLY	-	linker	UNP Q81W29
H	-23	MET	-	expression tag	UNP Q81W29
H	-22	HIS	-	expression tag	UNP Q81W29
H	-21	HIS	-	expression tag	UNP Q81W29
H	-20	HIS	-	expression tag	UNP Q81W29
H	-19	HIS	-	expression tag	UNP Q81W29
H	-18	HIS	-	expression tag	UNP Q81W29
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 (CCD ID: IMP) (formula: C₁₀H₁₃N₄O₈P).



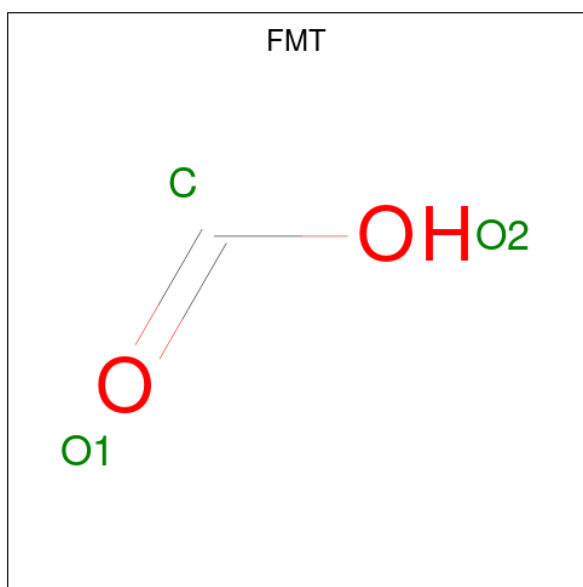
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	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 (CCD ID: 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 (CCD ID: FMT) (formula: CH₂O₂).



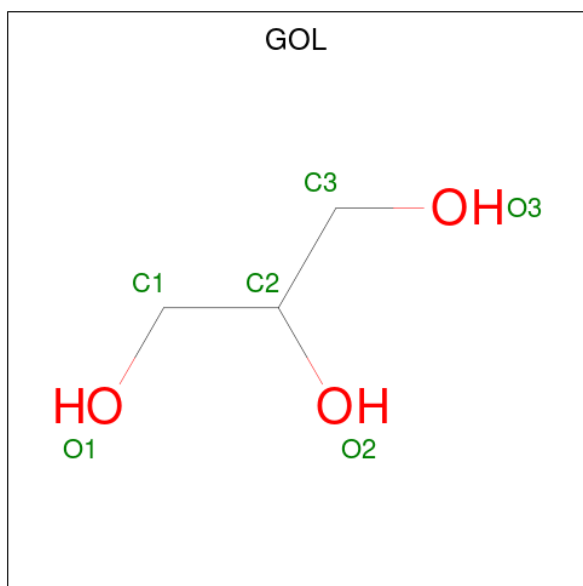
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total	C	O	0	0
			3	1	2		
4	E	1	Total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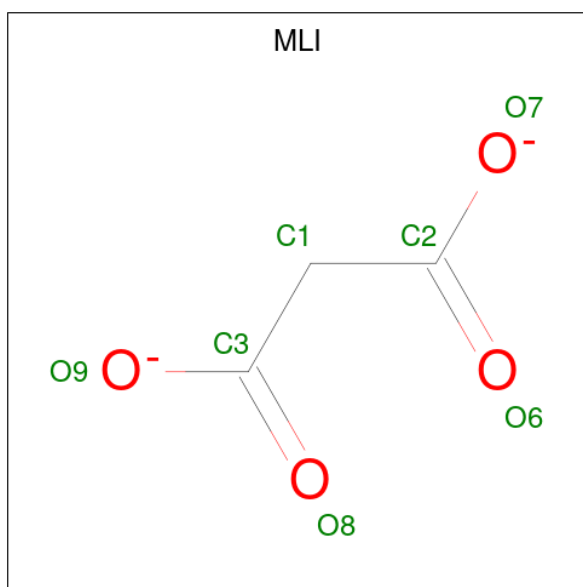
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



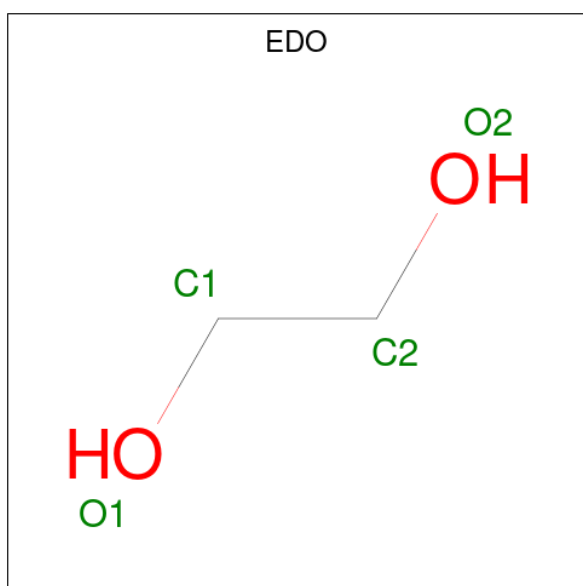
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is MALONATE ION (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



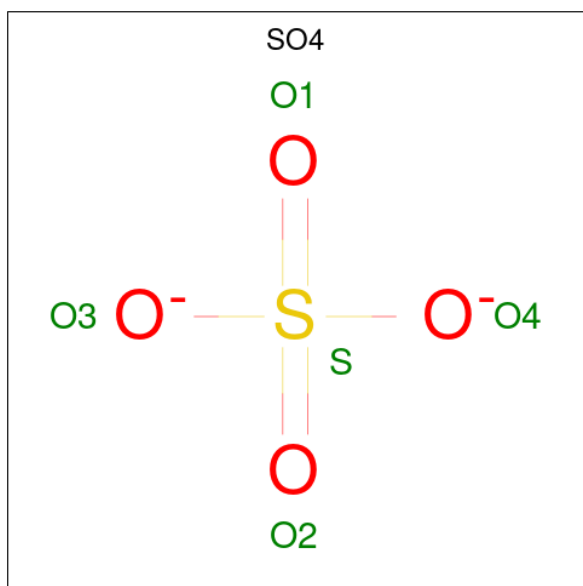
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	C	1	Total	C	O	0	0
			4	2	2		

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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 (CCD ID: 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

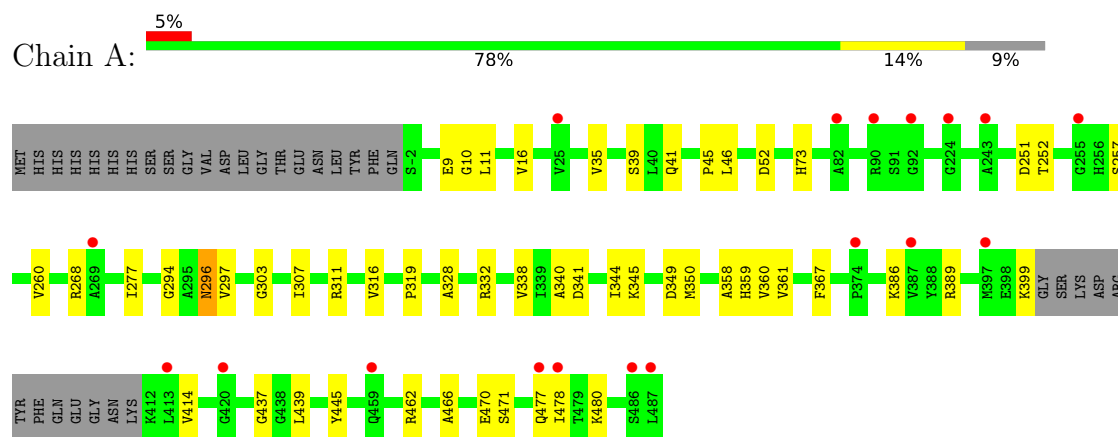
- Molecule 9 is water.

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

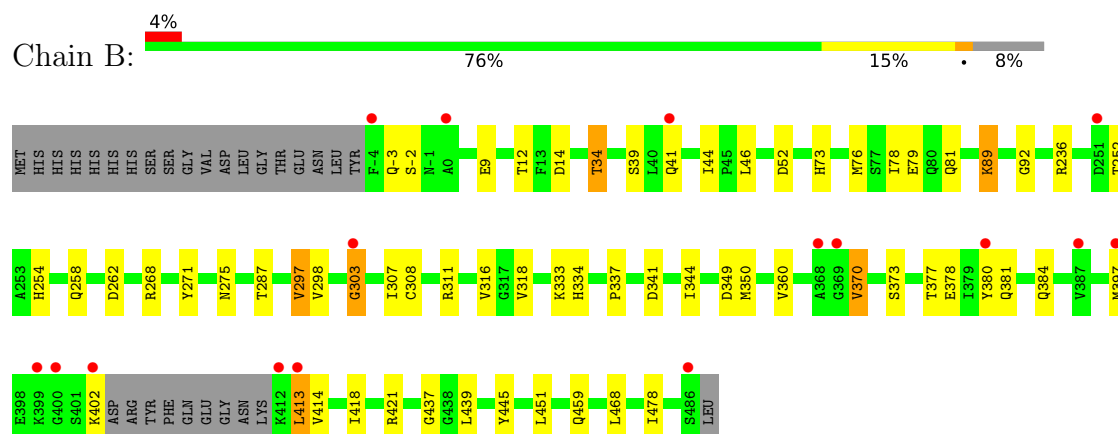
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

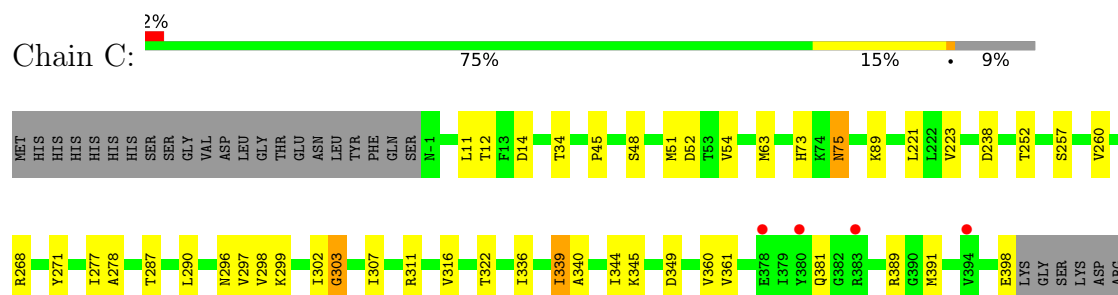
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase

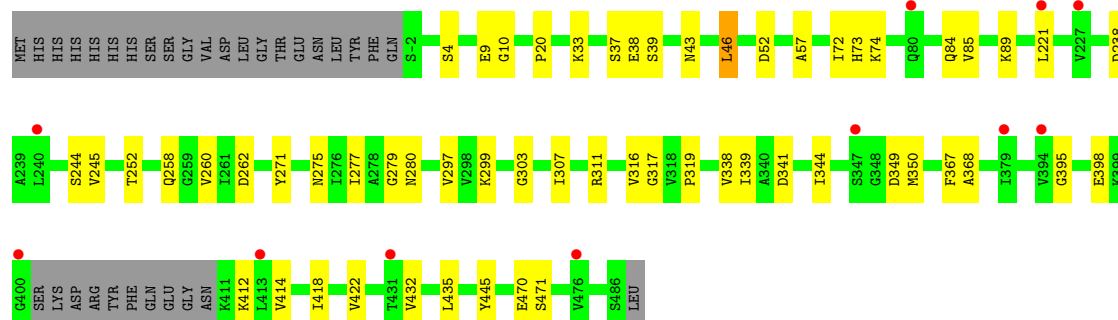
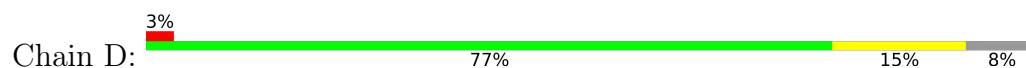


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

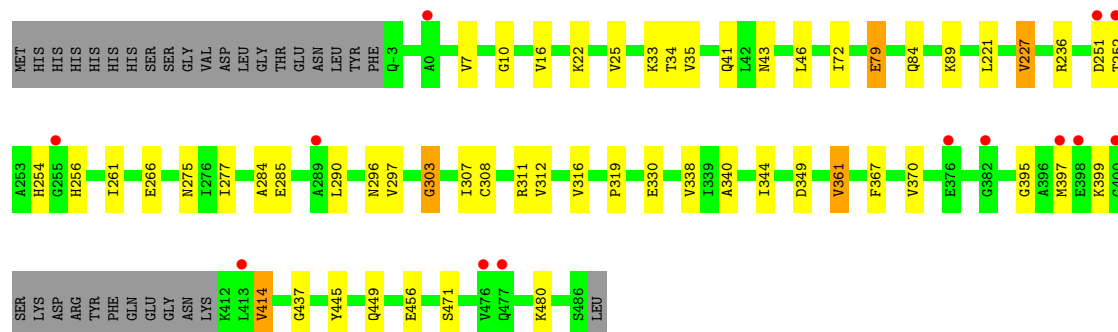
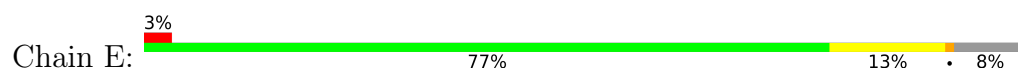




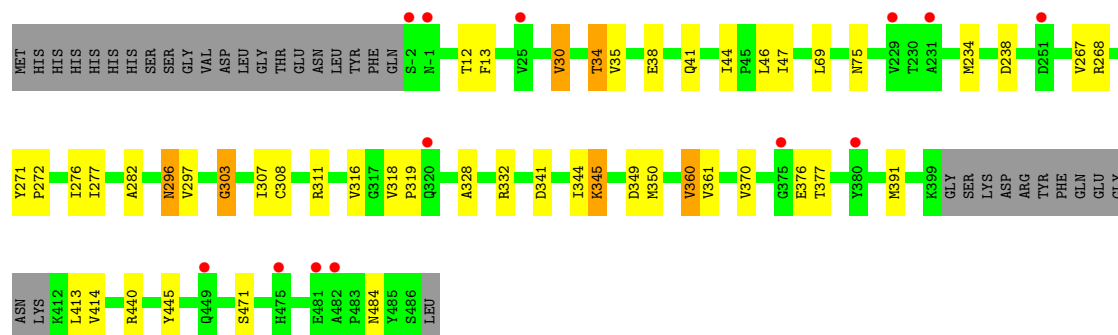
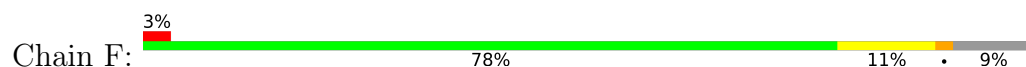
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



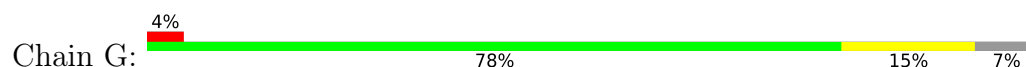
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

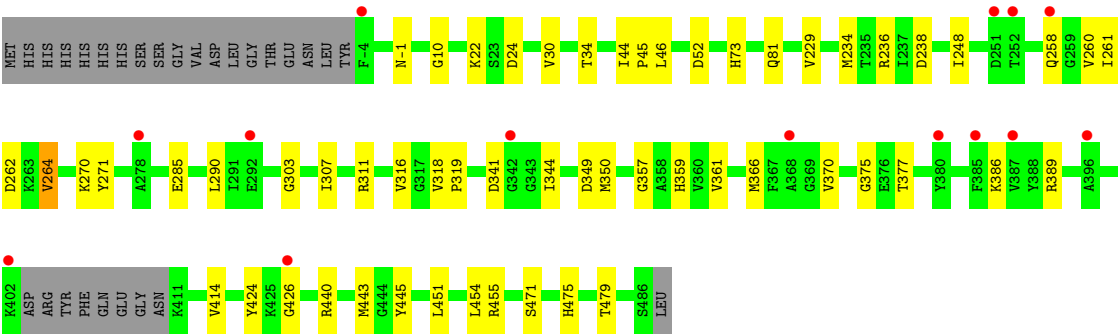


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

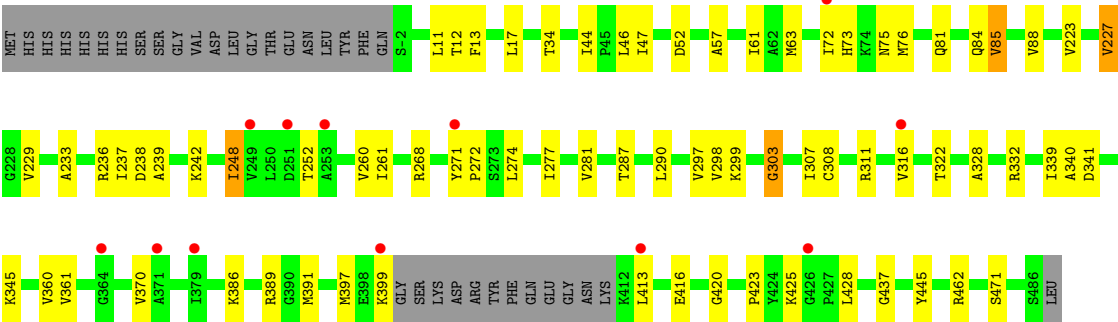


- Molecule 1: Inosine-5'-monophosphate dehydrogenase





● Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.36Å 89.82Å 104.50Å 81.41° 90.42° 83.50°	Depositor
Resolution (Å)	41.90 – 2.70 41.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.90-2.70) 98.1 (41.90-2.70)	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 0.221 , 0.263	Depositor DCC
R_{free} test set	4101 reflections (4.90%)	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)	0.31 , 37.5	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, 2F0, FMT, EDO, MLI, IMP

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	0.27	0/2673	0.72	0/3610
1	B	0.28	0/2651	0.75	2/3581 (0.1%)
1	C	0.28	0/2623	0.75	2/3545 (0.1%)
1	D	0.28	0/2651	0.77	2/3581 (0.1%)
1	E	0.29	0/2633	0.74	2/3557 (0.1%)
1	F	0.28	0/2603	0.73	2/3518 (0.1%)
1	G	0.28	0/2663	0.74	2/3596 (0.1%)
1	H	0.28	0/2603	0.76	2/3518 (0.1%)
All	All	0.28	0/21100	0.74	14/28506 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	303	GLY	CA-C-N	-7.33	112.62	120.47
1	H	303	GLY	C-N-CA	-7.33	112.62	120.47
1	G	303	GLY	CA-C-N	-6.89	112.55	120.89
1	G	303	GLY	C-N-CA	-6.89	112.55	120.89
1	D	303	GLY	CA-C-N	-6.84	112.61	120.89
1	D	303	GLY	C-N-CA	-6.84	112.61	120.89
1	C	303	GLY	CA-C-N	-6.76	112.74	120.04
1	C	303	GLY	C-N-CA	-6.76	112.74	120.04
1	B	303	GLY	CA-C-N	-6.75	112.72	120.89
1	B	303	GLY	C-N-CA	-6.75	112.72	120.89
1	E	303	GLY	CA-C-N	-6.63	113.09	120.45
1	E	303	GLY	C-N-CA	-6.63	113.09	120.45
1	F	303	GLY	CA-C-N	-6.25	113.29	120.04
1	F	303	GLY	C-N-CA	-6.25	113.29	120.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2637	0	2702	38	0
1	B	2614	0	2667	42	0
1	C	2587	0	2631	37	0
1	D	2615	0	2664	30	0
1	E	2597	0	2651	34	0
1	F	2567	0	2626	27	0
1	G	2627	0	2682	35	0
1	H	2567	0	2626	46	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
9	G	48	0	0	1	0
9	H	54	0	0	0	0
All	All	21740	0	21600	266	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.

All (266) 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:O	3:A:502:2F0:H13	1.93	0.68
1:E:344:ILE:HG23	1:E:349:ASP:HB2	1.75	0.68
1:A:340:ALA:HB3	1:A:361:VAL:HG12	1.76	0.68
1:A:268[A]:ARG:NH2	1:A:296:ASN:OD1	2.28	0.67
1:B:297:VAL:HG13	1:B:337:PRO:HG2	1.77	0.66
1:A:389:ARG:HH22	1:A:399:LYS:HD2	1.60	0.66
3:E:502:2F0:O	3:E:502:2F0:H13	1.95	0.66
1:D:57:ALA:HB2	1:D:84:GLN:HB2	1.78	0.65
1:C:278:ALA:HB3	1:C:290:LEU:HD21	1.79	0.65
1:G:375:GLY:O	1:G:386:LYS:NZ	2.31	0.63
1:A:344[A]:ILE:HG23	1:A:349:ASP:HB2	1.79	0.63
1:H:389:ARG:HH22	1:H:399:LYS:HD2	1.63	0.63
1:B:459:GLN:NE2	1:D:4:SER:O	2.31	0.62
1:A:437:GLY:HA3	1:B:414:VAL:HG21	1.82	0.62
1:E:72:ILE:HD13	1:E:84:GLN:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ARG:NH1	1:B:9:GLU:OE1	2.33	0.61
1:D:258:GLN:NE2	1:D:262:ASP:OD2	2.32	0.61
1:C:51:MET:HE3	1:C:54:VAL:HG21	1.81	0.61
1:H:227:VAL:HG12	1:H:236:ARG:HD2	1.81	0.61
1:E:456:GLU:OE1	1:G:-1:ASN:ND2	2.33	0.61
1:H:239:ALA:HA	1:H:242:LYS:HE3	1.82	0.61
1:B:258:GLN:NE2	1:B:262:ASP:OD1	2.31	0.60
1:C:299:LYS:HG3	1:C:339:ILE:HB	1.82	0.60
1:A:277:ILE:HG13	1:A:297:VAL:HB	1.83	0.60
1:A:341:ASP:OD2	2:A:501:IMP:O2'	2.20	0.58
1:C:51:MET:SD	2:C:502:IMP:H8	2.43	0.58
1:D:311:ARG:HD3	1:D:317:GLY:HA3	1.84	0.58
1:G:359:HIS:ND1	9:G:628:HOH:O	2.32	0.58
1:E:437:GLY:HA3	1:G:414:VAL:HG21	1.86	0.58
1:E:46:LEU:HD23	1:E:367:PHE:HZ	1.69	0.58
3:D:501:2F0:O	3:D:501:2F0:H13	2.04	0.57
1:F:277:ILE:HG12	1:F:297:VAL:HB	1.87	0.57
1:H:340:ALA:HB3	1:H:361:VAL:HG12	1.86	0.57
1:C:455:ARG:HH12	7:C:504:EDO:H22	1.69	0.57
1:B:380:TYR:HD2	1:B:381:GLN:H	1.52	0.56
1:F:34:THR:HG21	1:F:360:VAL:HG23	1.87	0.56
1:H:11:LEU:HD11	1:H:462:ARG:HD3	1.88	0.56
1:A:471:SER:HA	1:B:311:ARG:HD2	1.85	0.56
1:E:312:VAL:HG22	7:F:506:EDO:H12	1.87	0.56
1:H:281:VAL:HG11	1:H:290:LEU:HD11	1.86	0.56
1:B:44:ILE:HD12	1:B:46:LEU:HD12	1.87	0.55
1:F:35:VAL:HG13	1:F:41:GLN:HG2	1.88	0.55
1:G:30:VAL:O	1:G:440:ARG:NH1	2.40	0.55
1:H:277:ILE:HG12	1:H:297:VAL:HB	1.87	0.55
1:H:341:ASP:OD2	2:H:504:IMP:O2'	2.25	0.55
3:A:502:2F0:O	3:A:502:2F0:H3	2.06	0.55
1:B:344:ILE:HG23	1:B:349:ASP:HB2	1.88	0.55
1:C:316:VAL:HG11	1:D:445:TYR:HB3	1.89	0.55
1:E:10:GLY:HA3	1:E:319:PRO:HG2	1.89	0.55
1:H:423:PRO:HB2	1:H:425:LYS:HE3	1.89	0.55
1:B:341:ASP:OD2	2:B:500:IMP:O2'	2.24	0.54
1:D:277:ILE:HG12	1:D:297:VAL:HB	1.89	0.54
1:B:437:GLY:HA3	1:D:414:VAL:HG21	1.89	0.54
1:D:39:SER:HB2	1:D:275:ASN:HD21	1.71	0.54
1:G:81:GLN:OE1	1:G:236:ARG:NH1	2.35	0.54
1:B:380:TYR:CD2	1:B:381:GLN:N	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:ARG:HD2	1:F:471:SER:HA	1.89	0.54
1:F:47:ILE:HG12	1:F:69:LEU:HB3	1.90	0.54
1:H:299:LYS:HG3	1:H:339:ILE:HB	1.89	0.54
1:A:350:MET:HE3	1:A:439:LEU:HB2	1.89	0.54
1:G:238:ASP:OD1	1:G:271:TYR:OH	2.25	0.53
1:C:431:THR:HG23	7:C:506:EDO:H22	1.91	0.53
1:A:11:LEU:HD11	1:A:462:ARG:HD3	1.91	0.53
1:E:22:LYS:NZ	1:G:285:GLU:OE1	2.41	0.53
1:D:72:ILE:HG23	1:D:84:GLN:HE21	1.74	0.53
1:F:341:ASP:OD2	2:F:501:IMP:O2'	2.26	0.53
1:H:44:ILE:HD12	1:H:46:LEU:HD12	1.91	0.53
1:B:397:MET:SD	3:B:501:2F0:H21	2.49	0.53
1:E:277:ILE:HG12	1:E:297:VAL:HB	1.91	0.53
1:G:341:ASP:OD2	2:G:501:IMP:O2'	2.25	0.53
1:A:46[B]:LEU:HD23	1:A:367:PHE:HZ	1.74	0.52
1:C:268:ARG:NH2	1:C:296:ASN:OD1	2.42	0.52
1:H:72:ILE:HD13	1:H:84:GLN:HB3	1.92	0.52
1:E:227:VAL:HG13	1:E:236:ARG:HD2	1.92	0.52
1:F:234:MET:HE1	1:F:267:VAL:HA	1.91	0.52
1:G:445:TYR:HB3	1:H:316:VAL:HG11	1.91	0.52
1:C:252:THR:HG21	1:C:260:VAL:HG22	1.92	0.52
3:C:503:2F0:O	3:C:503:2F0:H3	2.09	0.52
1:F:311:ARG:HD2	1:H:471:SER:HA	1.92	0.51
1:E:445:TYR:HB2	1:G:316:VAL:HG21	1.92	0.51
1:B:76:MET:O	1:B:236:ARG:NH1	2.42	0.51
1:A:296:ASN:OD1	1:A:296:ASN:N	2.42	0.51
1:C:238:ASP:OD1	1:C:271:TYR:OH	2.26	0.51
1:F:44:ILE:HD12	1:F:46:LEU:HD12	1.93	0.51
1:A:9:GLU:OE2	1:C:462:ARG:NH1	2.45	0.50
1:F:12:THR:OG1	1:F:13:PHE:N	2.41	0.50
1:D:252:THR:HG21	1:D:260:VAL:HG21	1.93	0.50
1:G:10:GLY:HA3	1:G:319:PRO:HG2	1.92	0.50
1:B:333:LYS:HB2	1:B:334:HIS:HD2	1.76	0.50
3:E:502:2F0:O	3:E:502:2F0:H3	2.10	0.50
3:E:502:2F0:O1	3:E:502:2F0:CL1	2.66	0.50
3:E:509:2F0:O	3:E:509:2F0:H13	2.11	0.50
1:G:443:MET:HG2	1:G:454:LEU:HD22	1.94	0.50
1:B:478:ILE:HG12	1:D:418:ILE:HD13	1.94	0.50
3:B:501:2F0:H3	3:B:501:2F0:O	2.11	0.50
1:C:277:ILE:HG12	1:C:297:VAL:HB	1.94	0.50
1:C:302:ILE:HD12	1:D:20:PRO:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:ARG:NH2	1:G:318:VAL:O	2.44	0.50
1:B:445:TYR:HB3	1:D:316:VAL:HG11	1.94	0.50
1:E:35:VAL:HG13	1:E:41:GLN:HG2	1.94	0.50
3:E:502:2F0:O	3:E:502:2F0:C3	2.59	0.50
1:F:350:MET:HG3	1:F:361:VAL:HG21	1.94	0.50
3:H:505:2F0:O	3:H:505:2F0:H13	2.11	0.50
1:H:61:ILE:HD11	1:H:88:VAL:HA	1.93	0.49
1:A:252:THR:HG21	1:A:260:VAL:HG21	1.94	0.49
1:D:341:ASP:OD2	2:D:504:IMP:O2'	2.30	0.49
1:G:234:MET:HE2	1:G:270:LYS:HD3	1.93	0.49
1:C:381:GLN:HG2	1:E:25:VAL:HG12	1.94	0.49
1:A:478:ILE:HG12	1:B:418:ILE:HD12	1.94	0.49
1:E:252:THR:HG22	1:E:254:HIS:H	1.77	0.49
1:E:25:VAL:HG11	1:E:449:GLN:HG2	1.95	0.49
1:G:475:HIS:NE2	1:H:345:LYS:HD2	2.27	0.49
1:B:377:THR:CG2	1:B:384:GLN:HB3	2.43	0.49
1:D:52:ASP:HA	1:D:73:HIS:CD2	2.46	0.49
1:H:397:MET:HE3	1:H:413:LEU:HD13	1.96	0.48
1:F:316:VAL:HG11	1:H:445:TYR:HB3	1.95	0.48
1:D:46:LEU:HD12	1:D:367:PHE:HZ	1.78	0.48
1:F:38:GLU:CD	1:F:38:GLU:H	2.21	0.48
1:G:471:SER:HA	1:H:311:ARG:HD2	1.95	0.48
1:H:75:ASN:HB2	1:H:391:MET:HE1	1.95	0.48
1:A:257:SER:HB3	1:A:260:VAL:HG23	1.95	0.48
1:C:311:ARG:HD2	1:D:471:SER:HA	1.96	0.48
1:B:303:GLY:HA2	1:B:308:CYS:SG	2.53	0.48
1:B:268:ARG:NH1	1:B:271:TYR:O	2.47	0.47
1:E:79:GLU:H	1:E:79:GLU:CD	2.22	0.47
1:H:229:VAL:HG11	1:H:260:VAL:HA	1.96	0.47
1:H:88:VAL:HG11	1:H:223:VAL:HB	1.96	0.47
1:A:303:GLY:HA3	1:A:311:ARG:HE	1.79	0.47
1:A:311:ARG:HD2	1:C:471:SER:HA	1.96	0.47
1:F:344:ILE:HG23	1:F:349:ASP:HB2	1.95	0.47
3:F:502:2F0:O	3:F:502:2F0:C6	2.54	0.47
1:H:328:ALA:O	1:H:332:ARG:HB2	2.14	0.47
1:E:33:LYS:HG2	1:E:43:ASN:HD22	1.80	0.47
1:G:260:VAL:O	1:G:264:VAL:HG12	2.14	0.47
1:C:11:LEU:HD11	1:C:462:ARG:HD3	1.96	0.47
1:C:340:ALA:HB3	1:C:361:VAL:HG12	1.96	0.47
1:G:424:TYR:CZ	1:G:426:GLY:HA2	2.49	0.47
1:E:275:ASN:HA	1:E:296:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ILE:HG13	1:H:360:VAL:HG11	1.97	0.47
1:C:339:ILE:HD13	1:C:360:VAL:HG13	1.96	0.47
1:H:416:GLU:OE1	3:H:505:2F0:N2	2.32	0.47
1:E:471:SER:HA	1:G:311:ARG:HD2	1.96	0.46
1:F:238:ASP:OD1	1:F:271:TYR:OH	2.27	0.46
1:H:11:LEU:N	1:H:322:THR:OG1	2.39	0.46
1:C:45:PRO:C	1:C:360:VAL:HG23	2.40	0.46
1:F:30:VAL:O	1:F:440:ARG:NH1	2.48	0.46
1:A:345:LYS:HD2	1:C:475:HIS:CD2	2.50	0.46
1:D:299:LYS:HG3	1:D:339:ILE:HB	1.98	0.46
1:F:328:ALA:O	1:F:332:ARG:HB2	2.15	0.46
1:A:303:GLY:HA3	1:A:311:ARG:NE	2.31	0.46
1:A:445:TYR:HB3	1:B:316:VAL:HG11	1.98	0.46
3:A:502:2F0:O	3:A:502:2F0:C3	2.56	0.46
1:A:350:MET:HG3	1:A:361:VAL:HG21	1.98	0.46
1:C:34:THR:HA	7:C:504:EDO:H21	1.98	0.45
1:G:261:ILE:HD13	1:G:290:LEU:HD23	1.97	0.45
1:D:238:ASP:OD1	1:D:271:TYR:OH	2.27	0.45
1:G:52:ASP:HA	1:G:73:HIS:CD2	2.52	0.45
1:B:377:THR:HG21	1:B:384:GLN:HB3	1.98	0.45
1:C:75:ASN:HB2	1:C:391:MET:HE1	1.99	0.45
3:D:501:2F0:O	3:D:501:2F0:H3	2.16	0.45
1:E:311:ARG:O	7:F:506:EDO:O2	2.33	0.45
1:B:252:THR:HG22	1:B:254:HIS:H	1.80	0.45
1:F:319:PRO:HD3	1:H:17:LEU:HD12	1.97	0.45
1:A:344[B]:ILE:HB	1:A:349:ASP:HB2	1.99	0.45
1:E:316:VAL:HG11	1:F:445:TYR:HB3	1.99	0.45
1:H:52:ASP:HA	1:H:73:HIS:CD2	2.52	0.45
1:H:238:ASP:OD1	1:H:271:TYR:OH	2.32	0.45
1:B:81:GLN:OE1	1:B:236:ARG:NE	2.48	0.45
1:B:52:ASP:HA	1:B:73:HIS:CD2	2.52	0.45
1:B:350:MET:HE3	1:B:439:LEU:HB2	1.99	0.45
1:B:413:LEU:O	9:B:645:HOH:O	2.20	0.45
1:F:303:GLY:HA2	1:F:308:CYS:SG	2.56	0.45
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.52	0.45
1:G:45:PRO:HG3	1:G:451:LEU:HD11	1.99	0.44
1:C:52:ASP:HA	1:C:73:HIS:CD2	2.51	0.44
1:C:434:GLN:HB2	7:C:506:EDO:H12	2.00	0.44
1:H:248:ILE:HD12	1:H:274:LEU:HD21	1.99	0.44
1:D:344:ILE:HG23	1:D:349:ASP:HB2	2.00	0.44
3:D:501:2F0:O	3:D:501:2F0:C3	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:GLY:HA2	1:E:308:CYS:SG	2.57	0.44
1:A:328:ALA:O	1:A:332:ARG:N	2.46	0.44
1:D:89:LYS:HD2	1:D:244:SER:O	2.17	0.44
1:F:414:VAL:HG21	1:H:437:GLY:HA3	1.98	0.44
1:H:81:GLN:O	1:H:85:VAL:HG12	2.17	0.44
1:B:378:GLU:OE1	1:B:421:ARG:NH2	2.50	0.44
3:H:505:2F0:O1	3:H:505:2F0:CL1	2.72	0.44
1:F:276:ILE:H	1:F:296:ASN:HB2	1.83	0.44
1:H:268:ARG:HD3	1:H:272:PRO:HA	1.99	0.43
1:E:285:GLU:OE1	1:E:285:GLU:N	2.47	0.43
1:E:395:GLY:O	1:E:399:LYS:HD3	2.18	0.43
1:E:480:LYS:HE3	1:E:480:LYS:HB2	1.73	0.43
1:H:57:ALA:O	1:H:61:ILE:HG12	2.17	0.43
1:G:258[B]:GLN:NE2	1:G:262:ASP:OD1	2.43	0.43
1:H:303:GLY:HA2	1:H:308:CYS:SG	2.58	0.43
1:B:308:CYS:SG	2:B:500:IMP:H2	2.59	0.43
1:D:10:GLY:HA3	1:D:319:PRO:HG2	1.99	0.43
1:G:44:ILE:HD12	1:G:46:LEU:HD12	1.99	0.43
1:G:350:MET:HE2	1:G:350:MET:HB3	1.87	0.43
1:B:39:SER:OG	1:B:275:ASN:ND2	2.52	0.43
1:E:414:VAL:HG23	1:F:484:ASN:HD22	1.84	0.43
1:F:268:ARG:NH1	1:F:272:PRO:O	2.52	0.43
1:H:233:ALA:O	1:H:237:ILE:HG12	2.18	0.43
1:E:284:ALA:HB1	1:E:330:GLU:HB2	2.01	0.43
1:C:48:SER:HB2	1:C:63:MET:HG3	2.01	0.42
1:G:344:ILE:HG23	1:G:349:ASP:HB2	2.00	0.42
1:B:34:THR:HG23	1:B:451:LEU:HD12	2.01	0.42
1:C:12:THR:OG1	1:D:470:GLU:OE1	2.34	0.42
1:C:344:ILE:HG23	1:C:349:ASP:HB2	2.01	0.42
1:D:37:SER:OG	1:D:38:GLU:N	2.53	0.42
1:B:311:ARG:NH2	1:B:318:VAL:O	2.53	0.42
1:E:340:ALA:HB3	1:E:361:VAL:HG22	2.01	0.42
1:G:479:THR:HG23	1:H:420:GLY:HA2	2.01	0.42
1:H:237:ILE:HG23	1:H:248:ILE:HD13	2.02	0.42
1:A:45:PRO:C	1:A:360:VAL:HG23	2.45	0.42
1:H:287:THR:HG23	1:H:298:VAL:HG11	2.02	0.42
1:D:395:GLY:O	1:D:398[A]:GLU:HG2	2.20	0.42
1:D:33:LYS:HG2	1:D:43:ASN:HA	2.02	0.42
1:H:12:THR:OG1	1:H:13:PHE:N	2.51	0.42
1:E:445:TYR:HB3	1:G:316:VAL:HG11	2.00	0.42
1:G:357:GLY:HA2	1:G:455:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:HA3	1:A:319:PRO:HG2	2.02	0.42
1:A:345:LYS:HD2	1:C:475:HIS:NE2	2.34	0.42
1:E:89:LYS:HD3	1:E:89:LYS:HA	1.88	0.42
1:G:344:ILE:HG22	1:G:366:MET:HE1	2.01	0.42
1:G:445:TYR:HB2	1:H:316:VAL:HG21	2.02	0.42
1:H:61:ILE:HD13	1:H:88:VAL:HG13	2.01	0.42
1:A:466:ALA:HB1	1:B:14:ASP:HB2	2.02	0.41
1:A:470:GLU:OE1	1:B:12:THR:OG1	2.32	0.41
3:E:509:2F0:O	3:E:509:2F0:H3	2.20	0.41
1:C:14:ASP:HB3	1:C:468:LEU:HD22	2.02	0.41
1:F:282:ALA:HB1	1:F:318:VAL:HB	2.01	0.41
1:H:34:THR:HG21	1:H:360:VAL:HG22	2.01	0.41
1:A:35:VAL:HG13	1:A:41:GLN:HG2	2.02	0.41
1:B:78:ILE:H	1:B:78:ILE:HD12	1.85	0.41
1:G:22:LYS:HE2	1:H:261:ILE:HD12	2.02	0.41
1:A:345:LYS:HE2	1:A:345:LYS:HB2	1.89	0.41
1:E:254:HIS:CE1	1:E:256:HIS:HB3	2.55	0.41
1:F:345:LYS:H	1:F:345:LYS:HG3	1.71	0.41
1:D:368:ALA:HB3	1:D:422:VAL:HG21	2.02	0.41
1:H:63:MET:SD	1:H:428:LEU:HD21	2.60	0.41
1:C:89:LYS:HE3	1:C:221:LEU:O	2.21	0.41
1:D:279:GLY:HA3	1:D:280:ASN:HA	1.92	0.41
1:G:24:ASP:OD1	1:G:24:ASP:N	2.53	0.41
1:A:338:VAL:HG23	1:A:358:ALA:HA	2.01	0.41
1:B:14:ASP:HB3	1:B:468:LEU:HD22	2.03	0.41
1:C:296:ASN:O	1:C:336:ILE:HG23	2.21	0.41
1:A:268[A]:ARG:NH2	1:A:294:GLY:O	2.54	0.41
1:A:316:VAL:HG11	1:C:445:TYR:HB3	2.03	0.40
1:C:287:THR:HG23	1:C:298:VAL:HG21	2.03	0.40
1:G:350:MET:HG3	1:G:361:VAL:HG21	2.03	0.40
1:B:370:VAL:O	1:B:373:SER:HB3	2.22	0.40
1:C:303:GLY:HA3	1:C:311:ARG:HG3	2.03	0.40
1:E:261:ILE:HD13	1:E:290:LEU:HD23	2.03	0.40
1:E:397[A]:MET:HA	1:E:397[A]:MET:HE2	2.03	0.40
1:F:75:ASN:HB2	1:F:391:MET:HE1	2.03	0.40
1:H:73:HIS:CE1	1:H:76:MET:HE2	2.55	0.40
1:B:89:LYS:HD2	1:B:89:LYS:HA	1.76	0.40
1:B:445:TYR:HB2	1:D:316:VAL:HG21	2.04	0.40
1:B:451:LEU:HD23	1:B:451:LEU:HA	1.94	0.40
1:A:45:PRO:C	1:A:46[B]:LEU:HD12	2.46	0.40
1:B:287:THR:HG23	1:B:298:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:SER:OG	1:C:260:VAL:HG23	2.22	0.40
1:D:350:MET:HE1	1:D:435:LEU:HB3	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	354/384 (92%)	342 (97%)	12 (3%)	0	100	100
1	B	352/384 (92%)	343 (97%)	8 (2%)	1 (0%)	36	60
1	C	348/384 (91%)	338 (97%)	10 (3%)	0	100	100
1	D	352/384 (92%)	340 (97%)	11 (3%)	1 (0%)	36	60
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
All	All	2802/3072 (91%)	2728 (97%)	72 (3%)	2 (0%)	48	73

All (2) Ramachandran outliers are listed below:

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

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	276/298 (93%)	267 (97%)	9 (3%)	33	63
1	B	273/298 (92%)	261 (96%)	12 (4%)	25	53
1	C	270/298 (91%)	259 (96%)	11 (4%)	27	56
1	D	273/298 (92%)	264 (97%)	9 (3%)	33	63
1	E	271/298 (91%)	258 (95%)	13 (5%)	23	50
1	F	268/298 (90%)	258 (96%)	10 (4%)	30	59
1	G	274/298 (92%)	266 (97%)	8 (3%)	37	67
1	H	268/298 (90%)	261 (97%)	7 (3%)	40	70
All	All	2173/2384 (91%)	2094 (96%)	79 (4%)	30	60

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	39	SER
1	A	251	ASP
1	A	296	ASN
1	A	307	ILE
1	A	359	HIS
1	A	386	LYS
1	A	477	GLN
1	A	480	LYS
1	B	-3	GLN
1	B	-2	SER
1	B	34	THR
1	B	41	GLN
1	B	79	GLU
1	B	89	LYS
1	B	297	VAL
1	B	307	ILE
1	B	360	VAL
1	B	370	VAL
1	B	402	LYS
1	B	413	LEU
1	C	75	ASN
1	C	223	VAL
1	C	307	ILE

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Mol	Chain	Res	Type
1	C	322	THR
1	C	339	ILE
1	C	345	LYS
1	C	389	ARG
1	C	398	GLU
1	C	414	VAL
1	C	418	ILE
1	C	469	LEU
1	D	9	GLU
1	D	46	LEU
1	D	74	LYS
1	D	85	VAL
1	D	221	LEU
1	D	245	VAL
1	D	307	ILE
1	D	338	VAL
1	D	432	VAL
1	E	7	VAL
1	E	16	VAL
1	E	34	THR
1	E	79	GLU
1	E	221	LEU
1	E	227	VAL
1	E	251	ASP
1	E	266	GLU
1	E	307	ILE
1	E	338	VAL
1	E	361	VAL
1	E	370	VAL
1	E	414	VAL
1	F	30	VAL
1	F	34	THR
1	F	296	ASN
1	F	307	ILE
1	F	345	LYS
1	F	360	VAL
1	F	370	VAL
1	F	376	GLU
1	F	377	THR
1	F	413	LEU
1	G	34	THR
1	G	229	VAL

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Mol	Chain	Res	Type
1	G	248	ILE
1	G	264	VAL
1	G	307	ILE
1	G	370	VAL
1	G	377	THR
1	G	389	ARG
1	H	85	VAL
1	H	227	VAL
1	H	248	ILE
1	H	252	THR
1	H	307	ILE
1	H	370	VAL
1	H	386	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	GLN
1	A	434	GLN
1	A	474	HIS
1	B	275	ASN
1	B	334	HIS
1	B	474	HIS
1	C	359	HIS
1	C	475	HIS
1	D	84	GLN
1	D	474	HIS
1	E	43	ASN
1	E	73	HIS
1	E	359	HIS
1	E	474	HIS
1	E	477	GLN
1	F	258	GLN
1	F	275	ASN
1	F	474	HIS
1	G	359	HIS
1	G	459	GLN
1	G	472	HIS
1	G	474	HIS
1	H	41	GLN
1	H	434	GLN
1	H	457	ASN

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Mol	Chain	Res	Type
1	H	475	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 oligosaccharides 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	$\# Z > 2$
2	IMP	G	501	-	25,25,25	1.12	1 (4%)	37,38,38	2.05	9 (24%)
4	FMT	H	502	-	2,2,2	0.74	0	1,1,1	0.24	0
3	2F0	E	502	-	28,28,28	1.65	6 (21%)	40,40,40	1.27	5 (12%)
4	FMT	B	503	-	2,2,2	0.76	0	1,1,1	0.22	0
4	FMT	H	506	-	2,2,2	0.74	0	1,1,1	0.22	0
2	IMP	C	502	-	25,25,25	1.12	1 (4%)	37,38,38	2.05	9 (24%)
3	2F0	C	503	-	28,28,28	1.68	5 (17%)	40,40,40	1.30	3 (7%)
7	EDO	D	505	-	3,3,3	0.44	0	2,2,2	0.37	0
7	EDO	C	506	-	3,3,3	0.42	0	2,2,2	0.31	0
8	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.07	0
7	EDO	D	502	-	3,3,3	0.43	0	2,2,2	0.37	0
2	IMP	A	501	-	25,25,25	1.19	1 (4%)	37,38,38	2.10	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2F0	F	502	-	28,28,28	1.65	5 (17%)	40,40,40	1.52	4 (10%)
4	FMT	E	503	-	2,2,2	0.74	0	1,1,1	0.23	0
4	FMT	F	507	-	2,2,2	0.74	0	1,1,1	0.23	0
8	SO4	G	502	-	4,4,4	0.24	0	6,6,6	0.08	0
4	FMT	H	503	-	2,2,2	0.76	0	1,1,1	0.24	0
3	2F0	E	509	-	28,28,28	1.82	5 (17%)	40,40,40	1.20	2 (5%)
7	EDO	C	504	-	3,3,3	0.43	0	2,2,2	0.37	0
4	FMT	A	503	-	2,2,2	0.74	0	1,1,1	0.23	0
4	FMT	F	503	-	2,2,2	0.74	0	1,1,1	0.23	0
6	MLI	E	508	-	6,6,6	1.23	0	7,7,7	1.31	0
7	EDO	E	505	-	3,3,3	0.43	0	2,2,2	0.37	0
3	2F0	D	501	-	28,28,28	1.49	5 (17%)	40,40,40	1.68	7 (17%)
7	EDO	F	505	-	3,3,3	0.43	0	2,2,2	0.37	0
7	EDO	B	502	-	3,3,3	0.42	0	2,2,2	0.41	0
2	IMP	H	504	-	25,25,25	1.12	1 (4%)	37,38,38	2.01	9 (24%)
2	IMP	D	504	-	25,25,25	1.12	1 (4%)	37,38,38	2.03	9 (24%)
2	IMP	E	501	-	25,25,25	1.12	1 (4%)	37,38,38	2.05	9 (24%)
6	MLI	A	506	-	6,6,6	1.22	0	7,7,7	1.32	0
4	FMT	D	506	-	2,2,2	0.73	0	1,1,1	0.23	0
7	EDO	F	506	-	3,3,3	0.42	0	2,2,2	0.36	0
5	GOL	E	506	-	5,5,5	0.39	0	5,5,5	0.24	0
2	IMP	F	501	-	25,25,25	1.12	1 (4%)	37,38,38	2.08	9 (24%)
4	FMT	E	507	-	2,2,2	0.75	0	1,1,1	0.25	0
4	FMT	E	504	-	2,2,2	0.74	0	1,1,1	0.23	0
3	2F0	A	502	-	28,28,28	1.76	6 (21%)	40,40,40	1.16	4 (10%)
4	FMT	C	501	-	2,2,2	0.74	0	1,1,1	0.24	0
4	FMT	H	501	-	2,2,2	0.75	0	1,1,1	0.24	0
5	GOL	A	505	-	5,5,5	0.37	0	5,5,5	0.36	0
3	2F0	B	501	-	28,28,28	1.83	4 (14%)	40,40,40	1.15	2 (5%)
3	2F0	H	505	-	28,28,28	1.55	3 (10%)	40,40,40	1.54	6 (15%)
7	EDO	D	503	-	3,3,3	0.44	0	2,2,2	0.36	0
7	EDO	F	504	-	3,3,3	0.44	0	2,2,2	0.37	0
4	FMT	D	507	-	2,2,2	0.74	0	1,1,1	0.23	0
8	SO4	G	503	-	4,4,4	0.24	0	6,6,6	0.08	0
4	FMT	A	504	-	2,2,2	0.75	0	1,1,1	0.23	0
2	IMP	B	500	-	25,25,25	1.10	1 (4%)	37,38,38	2.04	9 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	G	501	-	-	0/10/26/26	0/3/3/3
3	2F0	E	502	-	-	3/25/25/25	0/2/2/2
2	IMP	C	502	-	-	0/10/26/26	0/3/3/3
3	2F0	C	503	-	-	4/25/25/25	0/2/2/2
7	EDO	D	505	-	-	0/1/1/1	-
7	EDO	C	506	-	-	0/1/1/1	-
7	EDO	D	502	-	-	0/1/1/1	-
2	IMP	A	501	-	-	0/10/26/26	0/3/3/3
3	2F0	F	502	-	-	4/25/25/25	0/2/2/2
3	2F0	E	509	-	-	5/25/25/25	0/2/2/2
7	EDO	C	504	-	-	0/1/1/1	-
6	MLI	E	508	-	-	4/4/4/4	-
7	EDO	E	505	-	-	0/1/1/1	-
3	2F0	D	501	-	-	3/25/25/25	0/2/2/2
7	EDO	F	505	-	-	0/1/1/1	-
7	EDO	B	502	-	-	0/1/1/1	-
2	IMP	H	504	-	-	0/10/26/26	0/3/3/3
2	IMP	D	504	-	-	0/10/26/26	0/3/3/3
2	IMP	E	501	-	-	0/10/26/26	0/3/3/3
6	MLI	A	506	-	-	0/4/4/4	-
7	EDO	F	506	-	-	0/1/1/1	-
5	GOL	E	506	-	-	2/4/4/4	-
2	IMP	F	501	-	-	0/10/26/26	0/3/3/3
3	2F0	A	502	-	-	3/25/25/25	0/2/2/2
5	GOL	A	505	-	-	2/4/4/4	-
3	2F0	B	501	-	-	4/25/25/25	0/2/2/2
3	2F0	H	505	-	-	0/25/25/25	0/2/2/2
7	EDO	D	503	-	-	0/1/1/1	-
7	EDO	F	504	-	-	0/1/1/1	-
2	IMP	B	500	-	-	0/10/26/26	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	2F0	C1-C12	-5.41	1.47	1.53
3	E	509	2F0	C1-C12	-5.38	1.47	1.53
3	C	503	2F0	C1-C12	-5.20	1.47	1.53
3	F	502	2F0	C1-C12	-5.20	1.47	1.53
2	A	501	IMP	C2-N3	4.91	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	2F0	C1-C12	-4.85	1.48	1.53
2	F	501	IMP	C2-N3	4.52	1.38	1.30
2	G	501	IMP	C2-N3	4.51	1.38	1.30
2	C	502	IMP	C2-N3	4.50	1.38	1.30
2	E	501	IMP	C2-N3	4.47	1.38	1.30
2	D	504	IMP	C2-N3	4.46	1.38	1.30
2	H	504	IMP	C2-N3	4.44	1.38	1.30
2	B	500	IMP	C2-N3	4.41	1.38	1.30
3	A	502	2F0	C1-N1	-4.28	1.43	1.47
3	E	509	2F0	C1-N1	-4.26	1.43	1.47
3	E	502	2F0	C1-C12	-4.24	1.48	1.53
3	H	505	2F0	C1-C12	-4.10	1.49	1.53
3	D	501	2F0	C1-C12	-4.10	1.49	1.53
3	B	501	2F0	C1-N1	-4.05	1.43	1.47
3	E	502	2F0	C1-N1	-3.72	1.43	1.47
3	C	503	2F0	C1-N1	-3.44	1.43	1.47
3	H	505	2F0	C1-N1	-3.42	1.44	1.47
3	B	501	2F0	C18-N4	-3.20	1.23	1.28
3	F	502	2F0	C1-N1	-2.86	1.44	1.47
3	F	502	2F0	C4-N2	-2.83	1.31	1.37
3	E	509	2F0	C18-N4	-2.60	1.24	1.28
3	B	501	2F0	C4-N2	-2.58	1.31	1.37
3	D	501	2F0	C1-N1	-2.54	1.44	1.47
3	C	503	2F0	C4-N2	-2.49	1.32	1.37
3	E	509	2F0	C4-N2	-2.43	1.32	1.37
3	A	502	2F0	C18-N4	-2.43	1.24	1.28
3	E	502	2F0	C4-N2	-2.39	1.32	1.37
3	H	505	2F0	C4-N2	-2.38	1.32	1.37
3	A	502	2F0	C4-N2	-2.35	1.32	1.37
3	E	502	2F0	C18-N4	-2.34	1.24	1.28
3	C	503	2F0	C2-C1	-2.30	1.50	1.53
3	C	503	2F0	C18-N4	-2.23	1.24	1.28
3	F	502	2F0	C2-C1	-2.21	1.50	1.53
3	A	502	2F0	C2-C1	-2.21	1.50	1.53
3	E	502	2F0	C4-N1	-2.20	1.31	1.35
3	F	502	2F0	C18-N4	-2.17	1.24	1.28
3	A	502	2F0	C4-N1	-2.15	1.31	1.35
3	D	501	2F0	C18-N4	-2.09	1.25	1.28
3	D	501	2F0	C2-C1	-2.06	1.51	1.53
3	E	509	2F0	C4-N1	-2.04	1.31	1.35
3	D	501	2F0	C4-N2	-2.03	1.33	1.37
3	E	502	2F0	O1-C11	-2.02	1.20	1.24

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	2F0	O2-N4-C18	6.42	121.61	112.65
2	F	501	IMP	C5-C6-N1	6.15	119.63	110.78
2	A	501	IMP	C5-C6-N1	6.13	119.60	110.78
3	F	502	2F0	O2-N4-C18	6.03	121.06	112.65
2	E	501	IMP	C5-C6-N1	6.00	119.40	110.78
2	C	502	IMP	C5-C6-N1	5.98	119.38	110.78
2	B	500	IMP	C5-C6-N1	5.96	119.35	110.78
2	G	501	IMP	C5-C6-N1	5.91	119.27	110.78
2	D	504	IMP	C5-C6-N1	5.89	119.25	110.78
2	H	504	IMP	C5-C6-N1	5.73	119.02	110.78
3	H	505	2F0	O2-N4-C18	5.10	119.77	112.65
2	A	501	IMP	C5-C4-N3	-5.05	119.84	127.27
2	A	501	IMP	C2-N3-C4	5.01	120.33	111.53
2	F	501	IMP	C2-N3-C4	4.96	120.26	111.53
2	G	501	IMP	C2-N3-C4	4.95	120.24	111.53
2	E	501	IMP	C2-N3-C4	4.92	120.18	111.53
2	C	502	IMP	C2-N3-C4	4.91	120.16	111.53
2	D	504	IMP	C2-N3-C4	4.86	120.09	111.53
2	B	500	IMP	C2-N3-C4	4.75	119.89	111.53
2	G	501	IMP	C5-C4-N3	-4.75	120.28	127.27
2	H	504	IMP	C2-N3-C4	4.74	119.87	111.53
2	E	501	IMP	C5-C4-N3	-4.73	120.30	127.27
2	F	501	IMP	C5-C4-N3	-4.72	120.32	127.27
2	C	502	IMP	C5-C4-N3	-4.70	120.35	127.27
2	B	500	IMP	C5-C4-N3	-4.66	120.41	127.27
3	A	502	2F0	O2-N4-C18	4.66	119.15	112.65
2	D	504	IMP	C5-C4-N3	-4.65	120.42	127.27
2	A	501	IMP	N1-C2-N3	-4.61	120.19	125.50
2	G	501	IMP	N1-C2-N3	-4.52	120.30	125.50
2	C	502	IMP	N1-C2-N3	-4.49	120.32	125.50
2	F	501	IMP	N1-C2-N3	-4.48	120.34	125.50
2	H	504	IMP	C5-C4-N3	-4.48	120.68	127.27
2	H	504	IMP	N1-C2-N3	-4.46	120.36	125.50
2	E	501	IMP	N1-C2-N3	-4.42	120.41	125.50
2	D	504	IMP	N1-C2-N3	-4.41	120.42	125.50
3	E	502	2F0	O2-N4-C18	4.22	118.54	112.65
3	D	501	2F0	C17-C16-C18	-4.14	114.82	120.53
2	B	500	IMP	N1-C2-N3	-4.08	120.80	125.50
3	H	505	2F0	C8-C7-C11	-4.07	116.09	122.58
3	C	503	2F0	O2-N4-C18	4.06	118.32	112.65
2	B	500	IMP	C2-N1-C6	-3.96	119.66	125.09
2	F	501	IMP	C2-N1-C6	-3.90	119.75	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	IMP	C2-N1-C6	-3.88	119.77	125.09
2	E	501	IMP	C2-N1-C6	-3.85	119.81	125.09
3	E	509	2F0	O2-N4-C18	3.83	117.99	112.65
2	C	502	IMP	C2-N1-C6	-3.78	119.91	125.09
2	D	504	IMP	C2-N1-C6	-3.74	119.97	125.09
2	G	501	IMP	C2-N1-C6	-3.71	120.00	125.09
2	H	504	IMP	C2-N1-C6	-3.60	120.16	125.09
2	H	504	IMP	O6-C6-C5	-2.86	118.97	126.53
3	H	505	2F0	C17-C16-C18	-2.84	116.61	120.53
3	B	501	2F0	C19-C18-N4	-2.83	115.72	123.59
2	A	501	IMP	O6-C6-C5	-2.82	119.08	126.53
3	B	501	2F0	C19-C18-C16	2.82	124.05	119.48
3	D	501	2F0	C19-C18-C16	2.72	123.88	119.48
2	C	502	IMP	O6-C6-C5	-2.70	119.40	126.53
3	F	502	2F0	C1-N1-C4	2.64	129.49	124.01
2	H	504	IMP	N9-C8-N7	-2.64	108.51	113.40
2	B	500	IMP	N9-C8-N7	-2.63	108.52	113.40
2	G	501	IMP	O6-C6-C5	-2.63	119.59	126.53
2	B	500	IMP	C8-N7-C5	2.62	108.93	104.26
2	F	501	IMP	N9-C8-N7	-2.60	108.57	113.40
2	D	504	IMP	N9-C8-N7	-2.57	108.64	113.40
2	D	504	IMP	C8-N7-C5	2.55	108.80	104.26
3	H	505	2F0	C6-C7-C8	2.54	120.65	117.84
2	A	501	IMP	N9-C4-N3	2.54	132.69	126.90
2	E	501	IMP	N9-C8-N7	-2.54	108.69	113.40
2	F	501	IMP	C8-N7-C5	2.53	108.78	104.26
2	B	500	IMP	O6-C6-C5	-2.53	119.86	126.53
3	E	502	2F0	C8-C7-C11	-2.52	118.55	122.58
2	H	504	IMP	C8-N7-C5	2.52	108.75	104.26
2	G	501	IMP	N9-C8-N7	-2.52	108.72	113.40
2	G	501	IMP	C8-N7-C5	2.52	108.75	104.26
2	D	504	IMP	O6-C6-C5	-2.52	119.88	126.53
2	E	501	IMP	C8-N7-C5	2.49	108.70	104.26
2	F	501	IMP	O6-C6-C5	-2.47	120.01	126.53
2	E	501	IMP	O6-C6-C5	-2.45	120.05	126.53
2	C	502	IMP	N9-C8-N7	-2.44	108.87	113.40
2	C	502	IMP	C8-N7-C5	2.40	108.54	104.26
3	C	503	2F0	C1-N1-C4	2.37	128.92	124.01
2	C	502	IMP	N9-C4-N3	2.35	132.25	126.90
2	G	501	IMP	N9-C4-N3	2.34	132.22	126.90
2	F	501	IMP	N9-C4-N3	2.32	132.19	126.90
2	E	501	IMP	N9-C4-N3	2.32	132.19	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	509	2F0	C6-C7-C8	2.31	120.39	117.84
3	D	501	2F0	C8-C7-C11	-2.29	118.92	122.58
3	D	501	2F0	C6-C7-C8	2.28	120.36	117.84
2	A	501	IMP	N9-C8-N7	-2.26	109.20	113.40
3	D	501	2F0	C15-C16-C18	2.25	123.94	121.27
2	B	500	IMP	N9-C4-N3	2.24	132.00	126.90
2	D	504	IMP	N9-C4-N3	2.24	132.00	126.90
3	D	501	2F0	C17-C12-C1	-2.23	117.14	120.63
2	A	501	IMP	C8-N7-C5	2.22	108.21	104.26
3	E	502	2F0	C19-C18-N4	-2.22	117.43	123.59
2	H	504	IMP	N9-C4-N3	2.22	131.95	126.90
3	E	502	2F0	C19-C18-C16	2.20	123.05	119.48
3	E	502	2F0	C6-C7-C8	2.15	120.22	117.84
3	H	505	2F0	C15-C16-C17	2.15	121.74	119.25
3	C	503	2F0	C8-C7-C11	-2.14	119.17	122.58
3	F	502	2F0	O1-C11-N3	-2.09	119.59	122.62
3	A	502	2F0	C19-C18-N4	-2.05	117.88	123.59
3	A	502	2F0	C19-C18-C16	2.05	122.80	119.48
3	F	502	2F0	C3-C1-N1	2.04	113.17	107.88
3	A	502	2F0	C17-C16-C18	-2.03	117.73	120.53
3	H	505	2F0	C7-C8-CL1	-2.02	118.03	121.01

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	2F0	N3-C11-C7-C8
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
3	F	502	2F0	O1-C11-C7-C6
5	A	505	GOL	O1-C1-C2-C3
3	A	502	2F0	C3-C1-N1-C4
5	E	506	GOL	O1-C1-C2-O2
3	C	503	2F0	O1-C11-C7-C8
3	C	503	2F0	N3-C11-C7-C6
3	A	502	2F0	C2-C1-N1-C4
3	D	501	2F0	C3-C1-N1-C4
3	E	502	2F0	C2-C1-N1-C4
3	E	502	2F0	C3-C1-N1-C4
3	E	509	2F0	C3-C1-N1-C4

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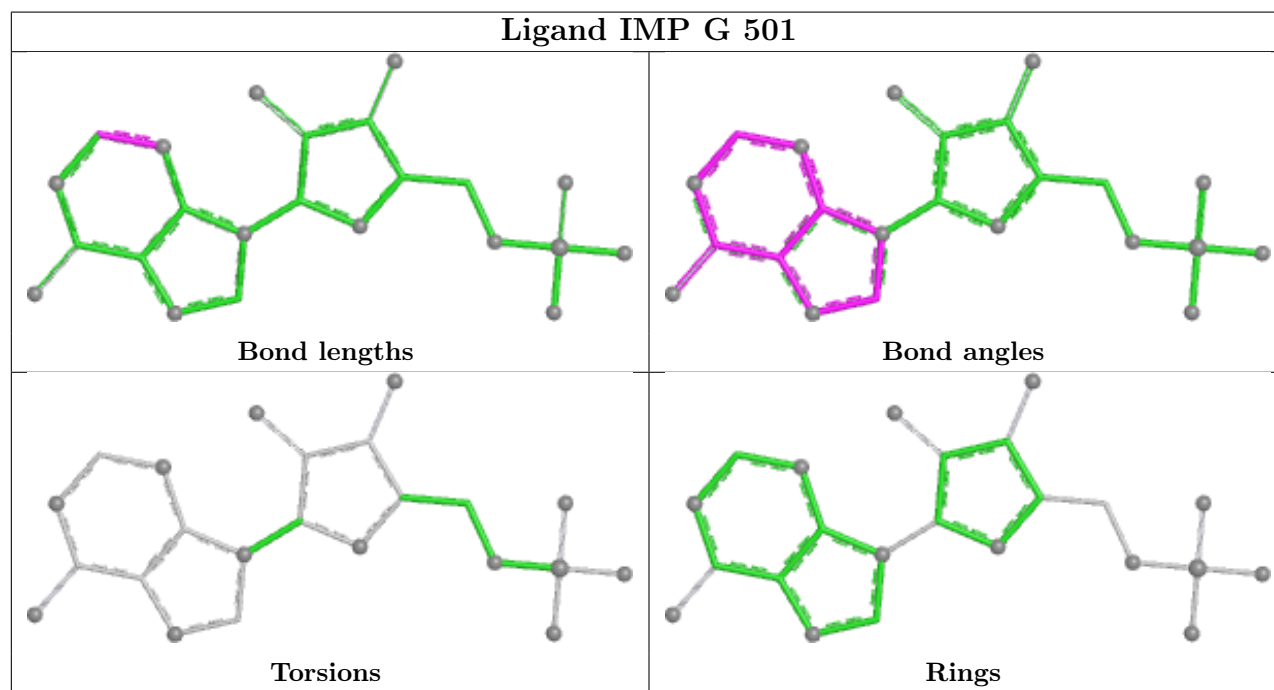
Mol	Chain	Res	Type	Atoms
3	C	503	2F0	O1-C11-C7-C6
3	B	501	2F0	O1-C11-C7-C8
3	B	501	2F0	N3-C11-C7-C8
3	E	509	2F0	O1-C11-C7-C8
3	E	509	2F0	N3-C11-C7-C8
3	E	509	2F0	C2-C1-N1-C4
5	A	505	GOL	O1-C1-C2-O2
3	A	502	2F0	C12-C1-N1-C4
3	E	502	2F0	C12-C1-N1-C4
3	E	509	2F0	C12-C1-N1-C4
6	E	508	MLI	C2-C1-C3-O8
3	D	501	2F0	C2-C1-N1-C4
3	B	501	2F0	N3-C11-C7-C6
6	E	508	MLI	C3-C1-C2-O6
6	E	508	MLI	C3-C1-C2-O7
6	E	508	MLI	C2-C1-C3-O9
3	B	501	2F0	O1-C11-C7-C6
3	D	501	2F0	N3-C11-C7-C8

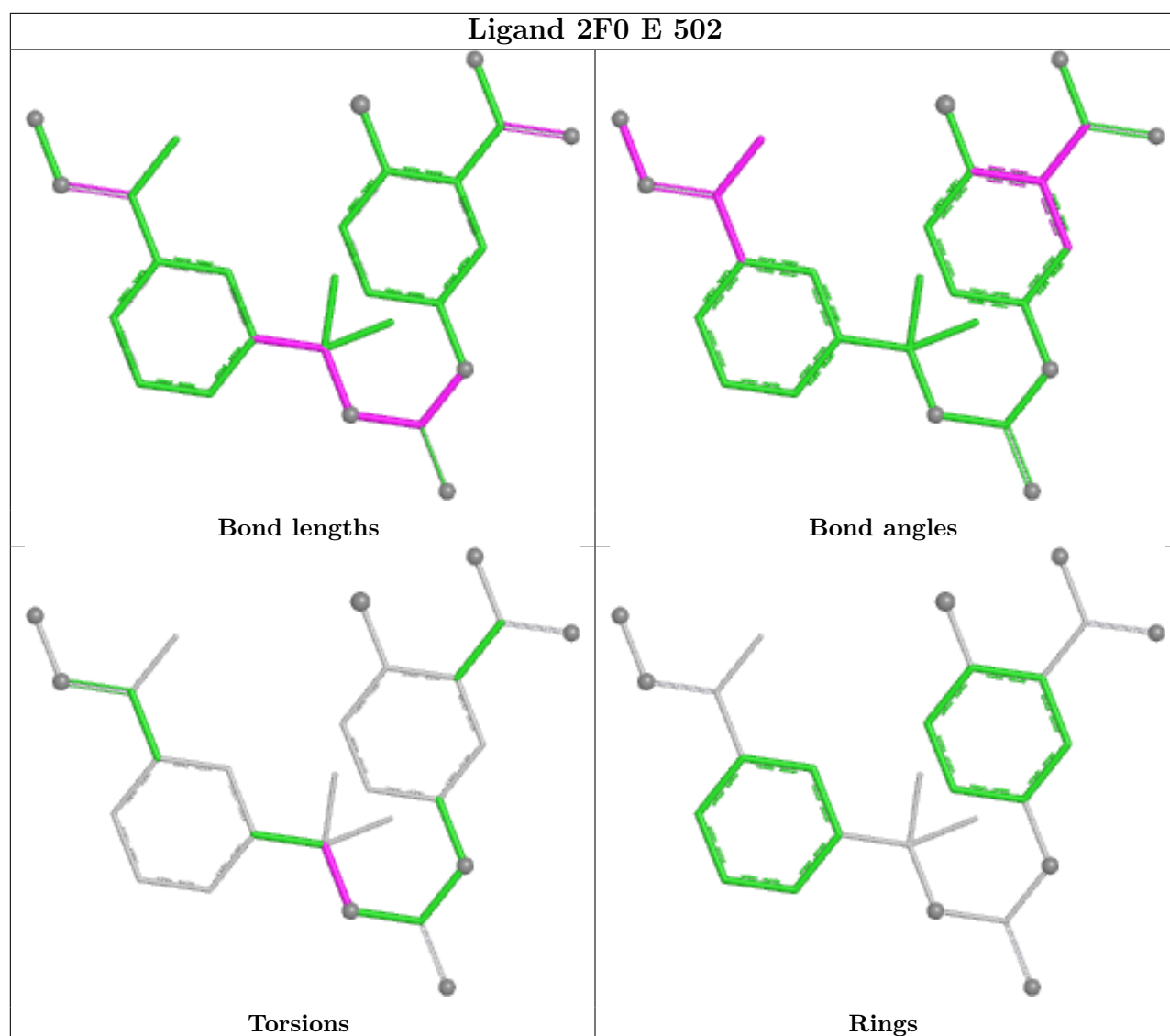
There are no ring outliers.

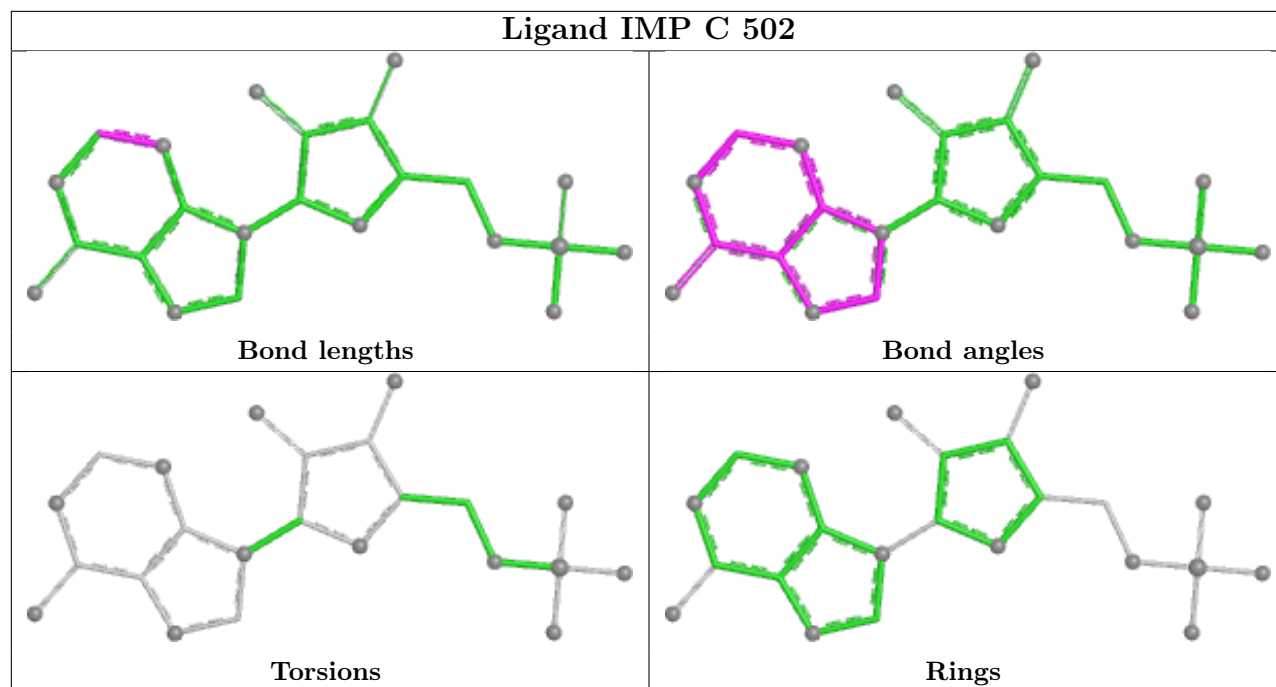
18 monomers are involved in 35 short contacts:

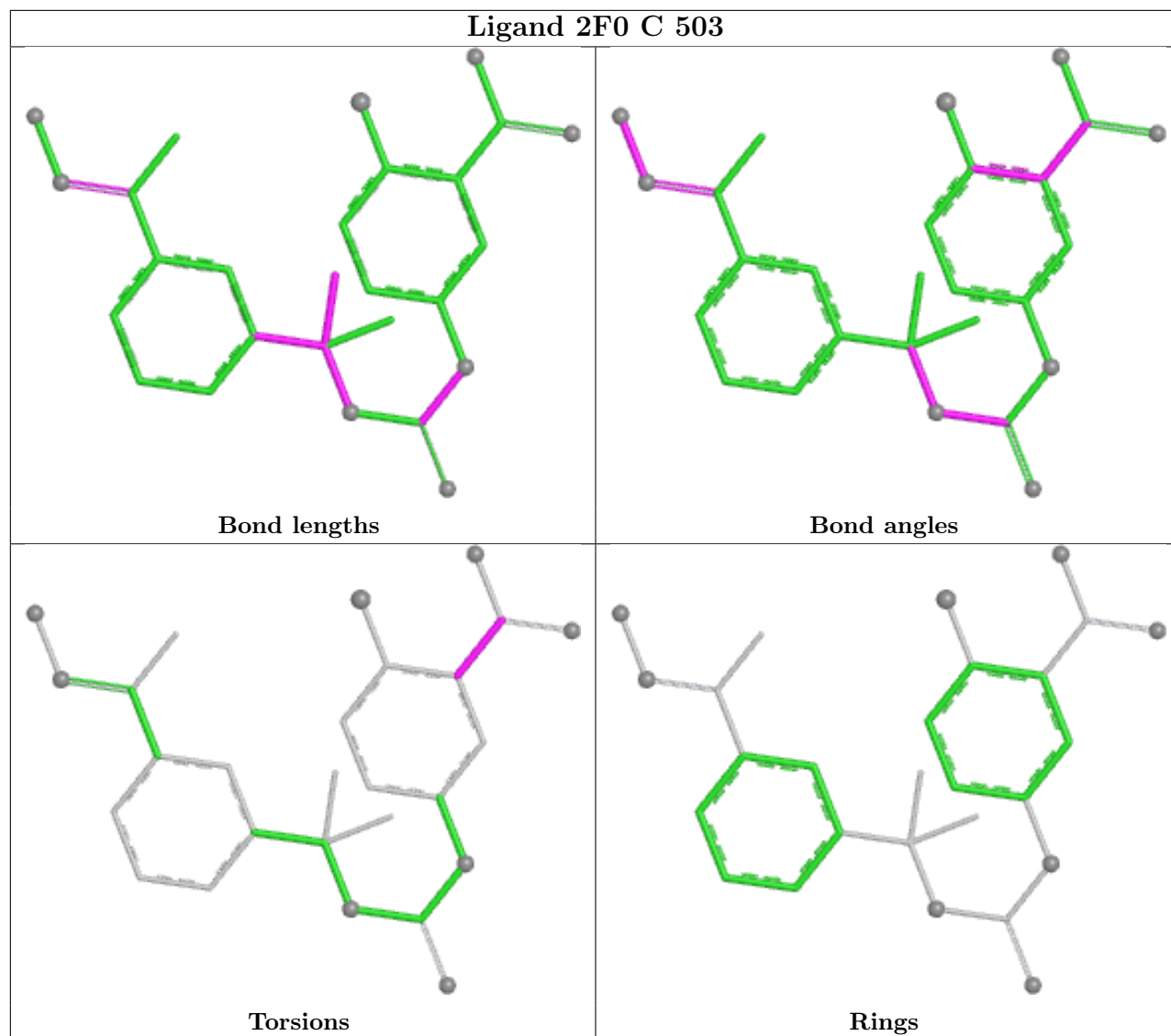
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	IMP	1	0
3	E	502	2F0	4	0
2	C	502	IMP	1	0
3	C	503	2F0	1	0
7	C	506	EDO	2	0
2	A	501	IMP	1	0
3	F	502	2F0	2	0
3	E	509	2F0	2	0
7	C	504	EDO	2	0
3	D	501	2F0	3	0
2	H	504	IMP	1	0
2	D	504	IMP	1	0
7	F	506	EDO	2	0
2	F	501	IMP	1	0
3	A	502	2F0	3	0
3	B	501	2F0	2	0
3	H	505	2F0	4	0
2	B	500	IMP	2	0

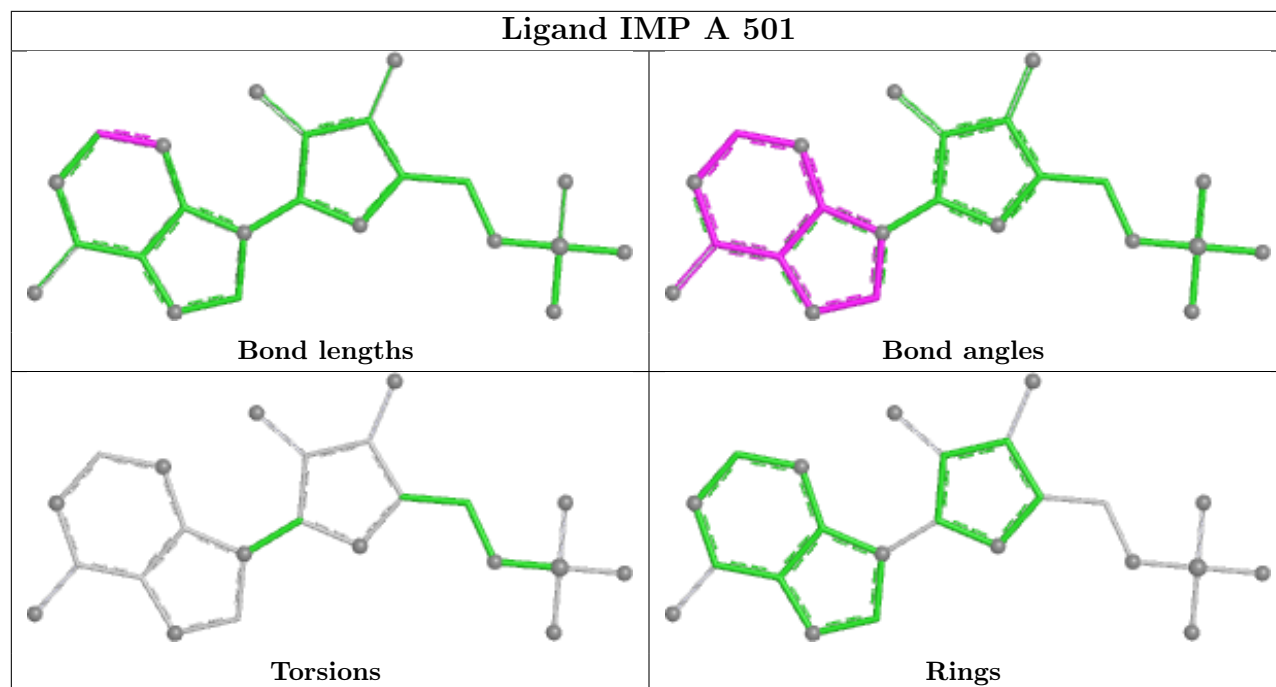
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

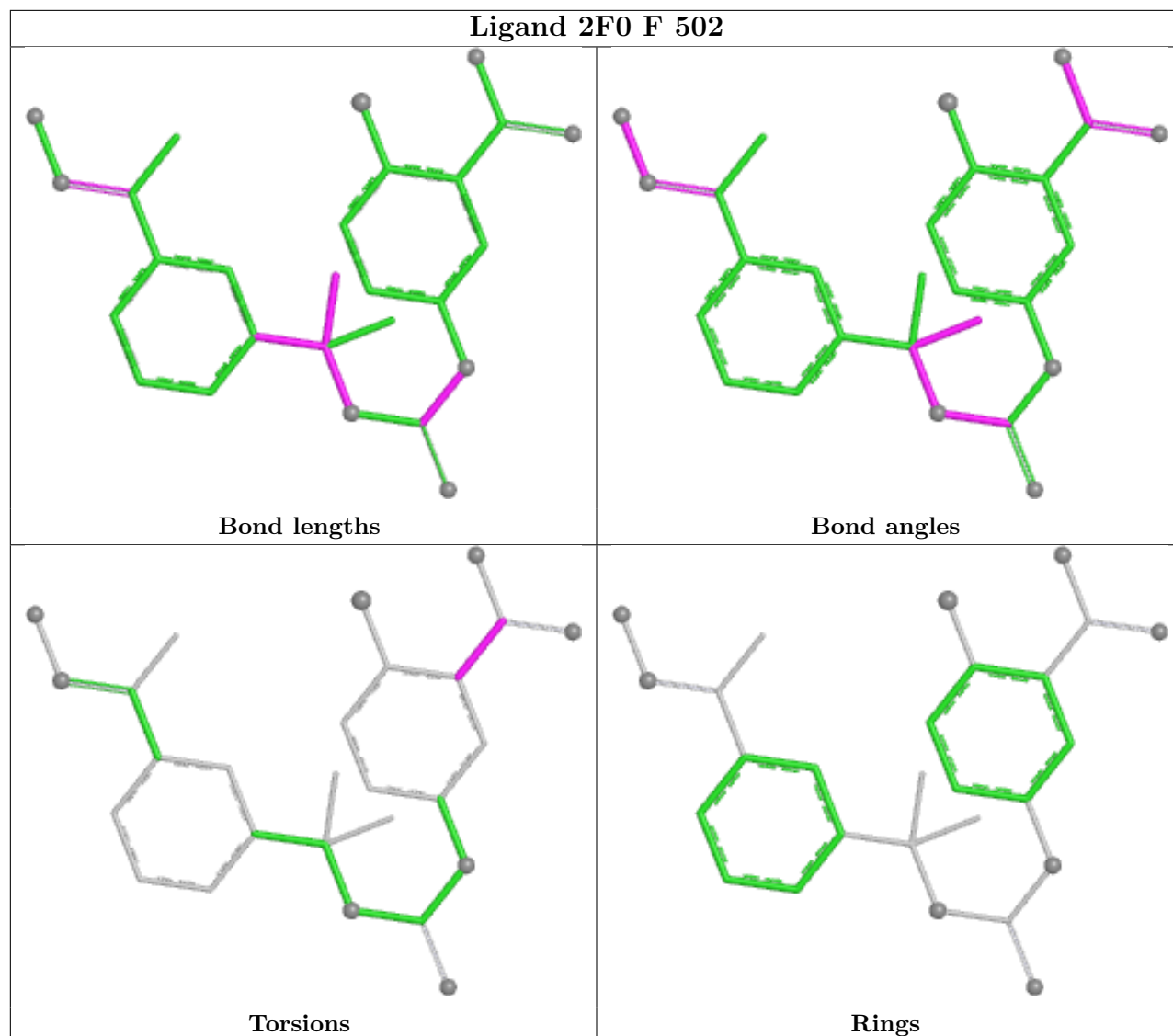


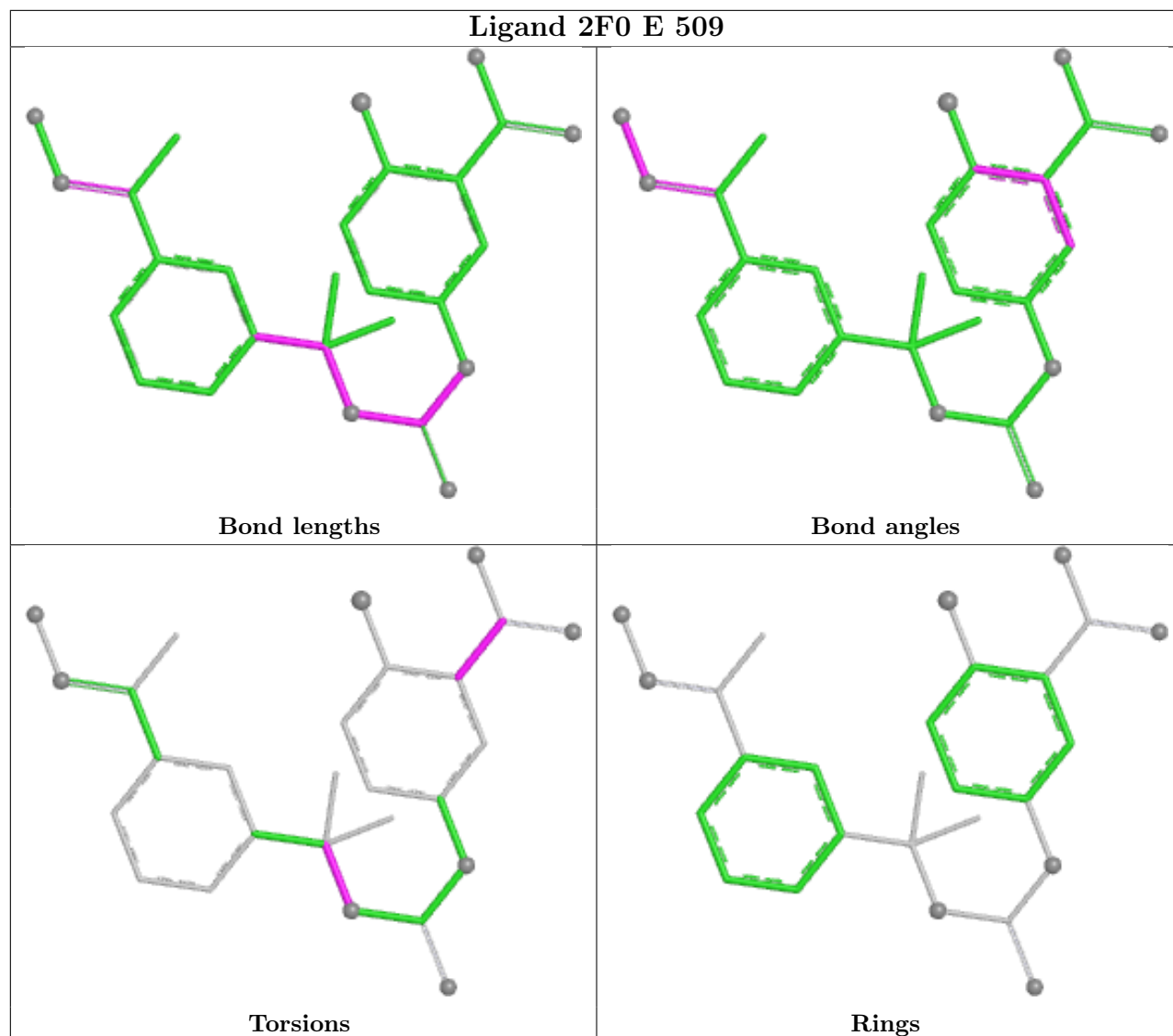


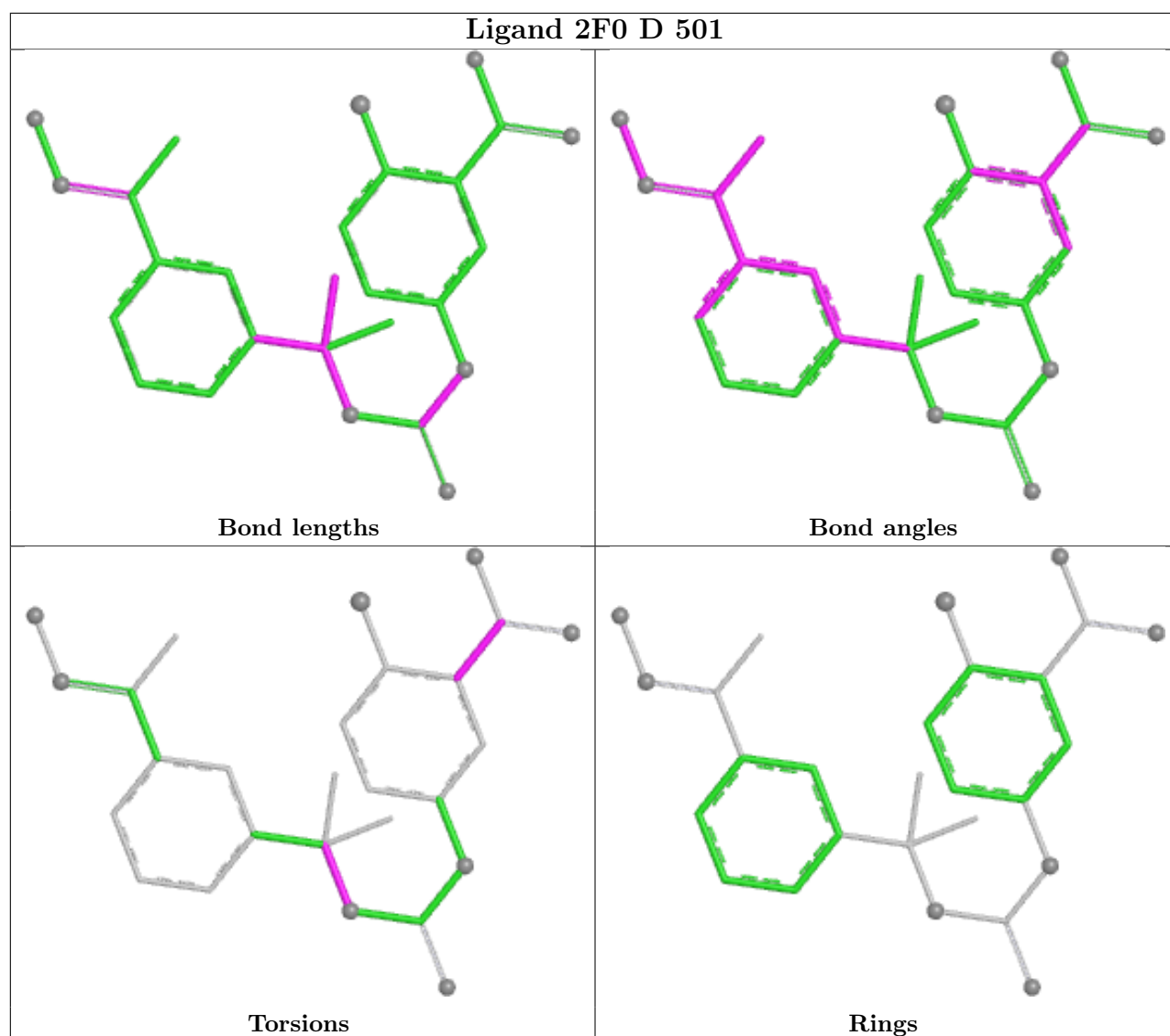




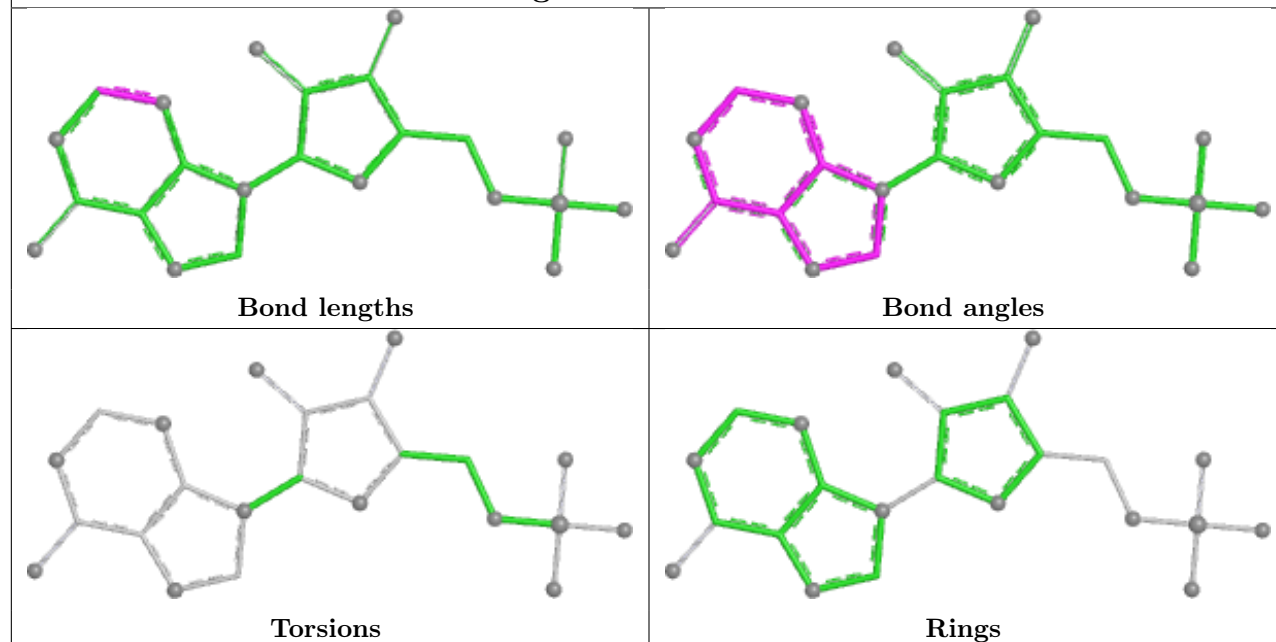




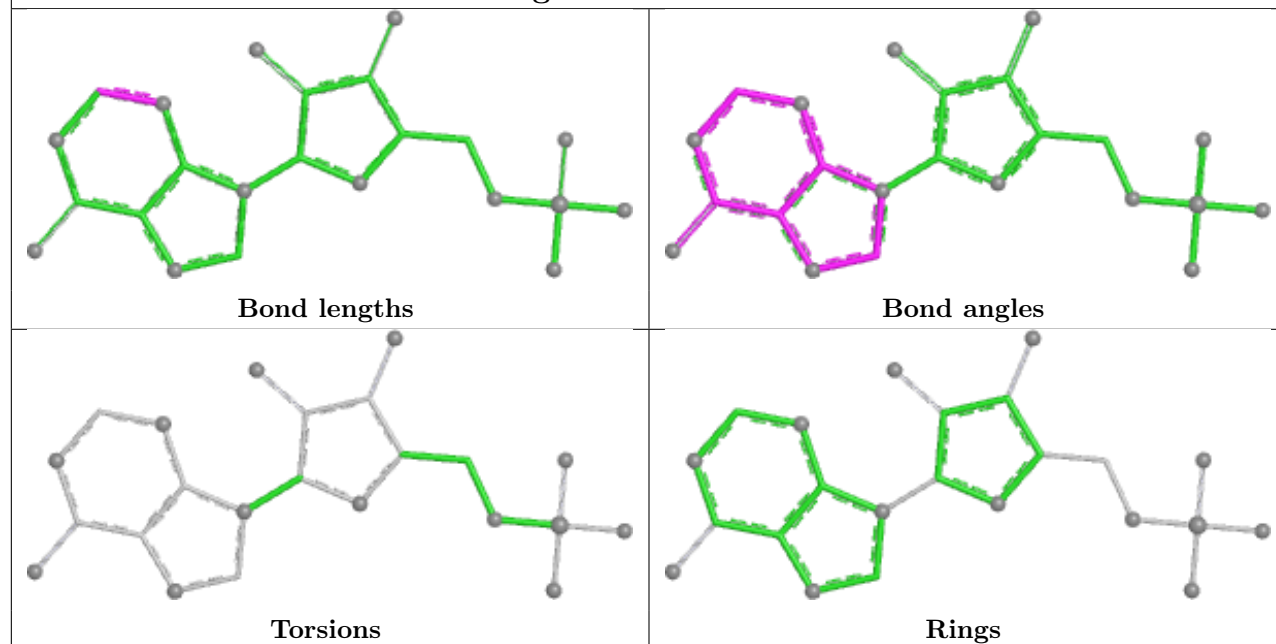




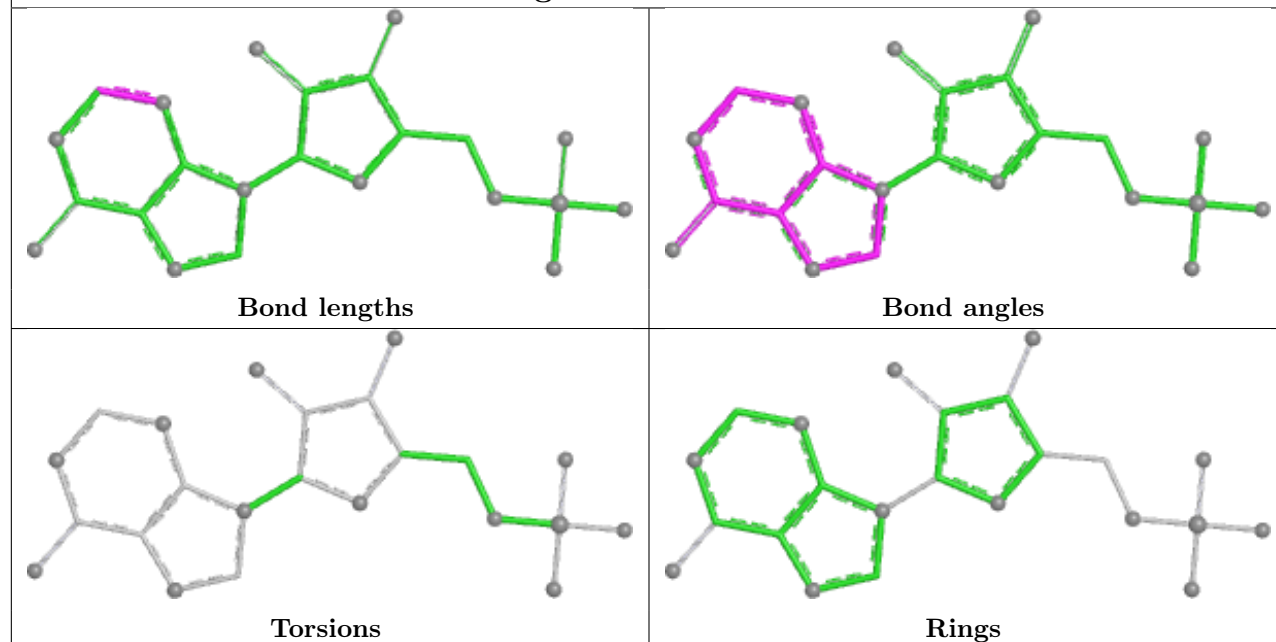
Ligand IMP H 504



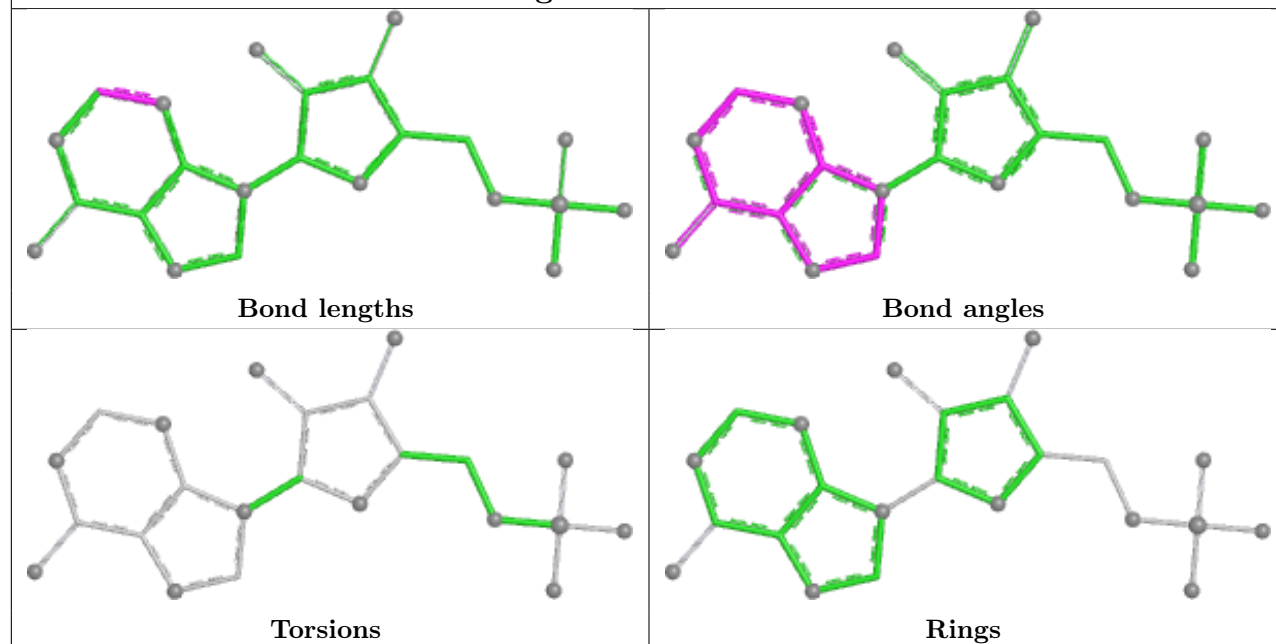
Ligand IMP D 504

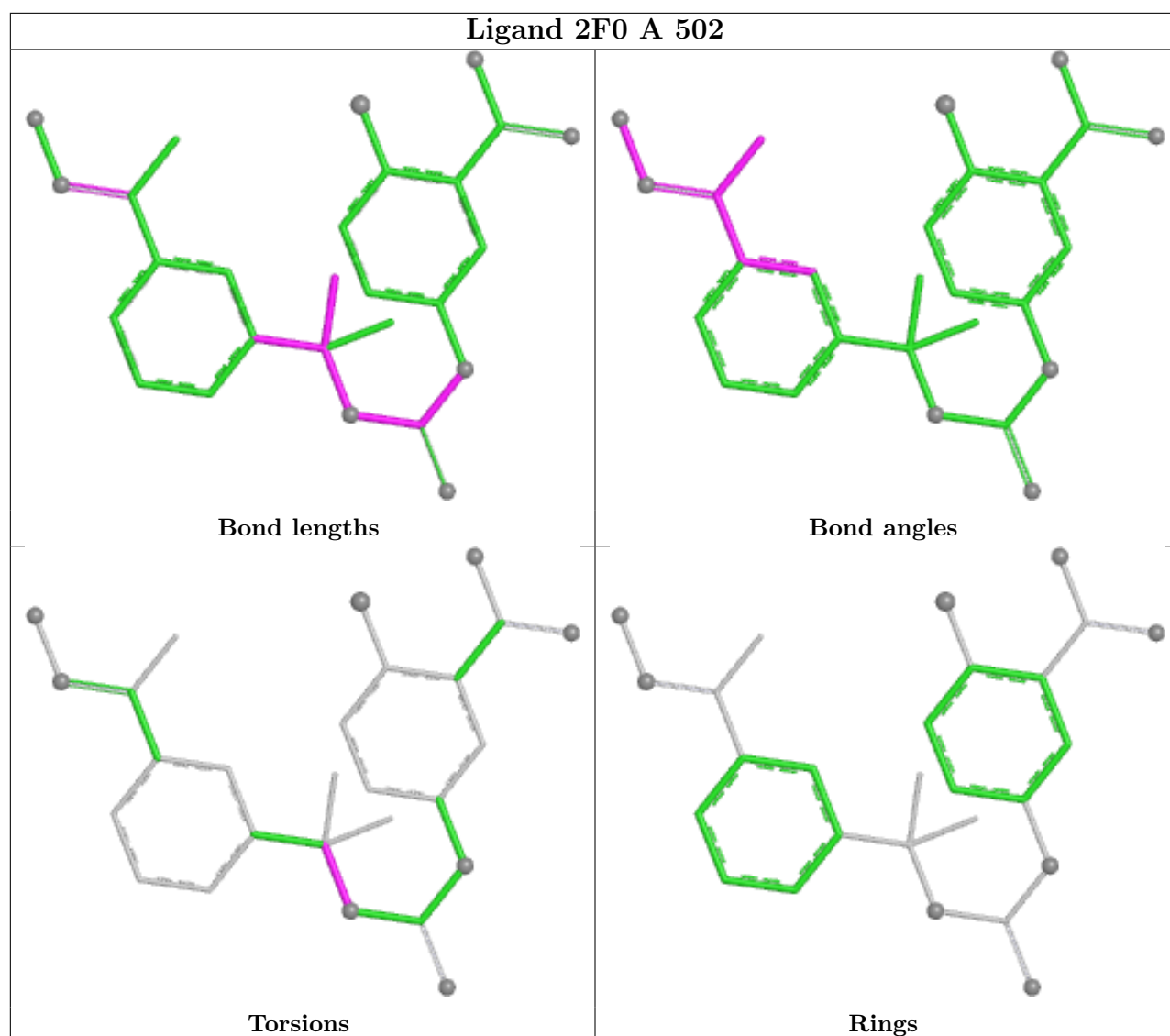


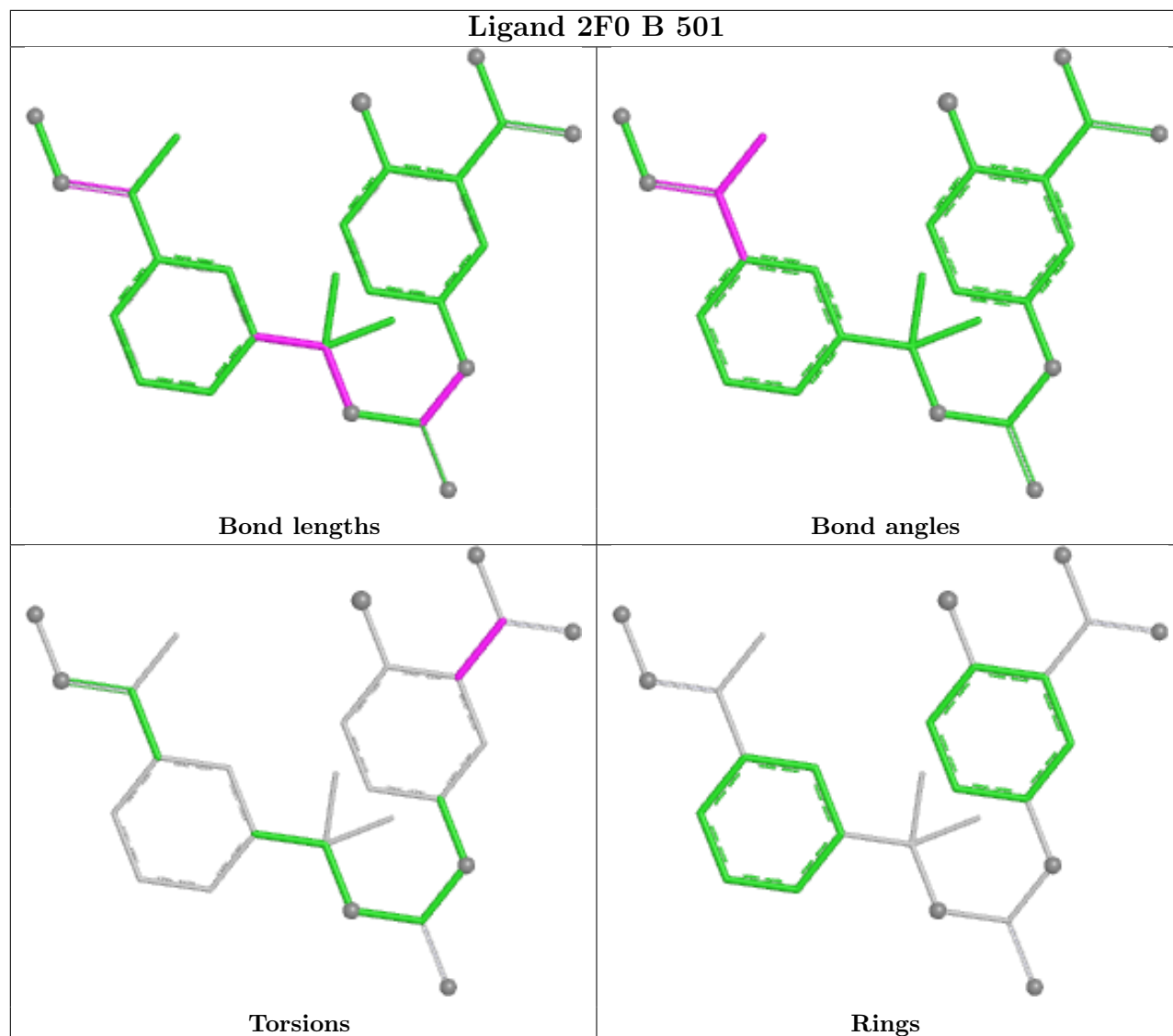
Ligand IMP E 501

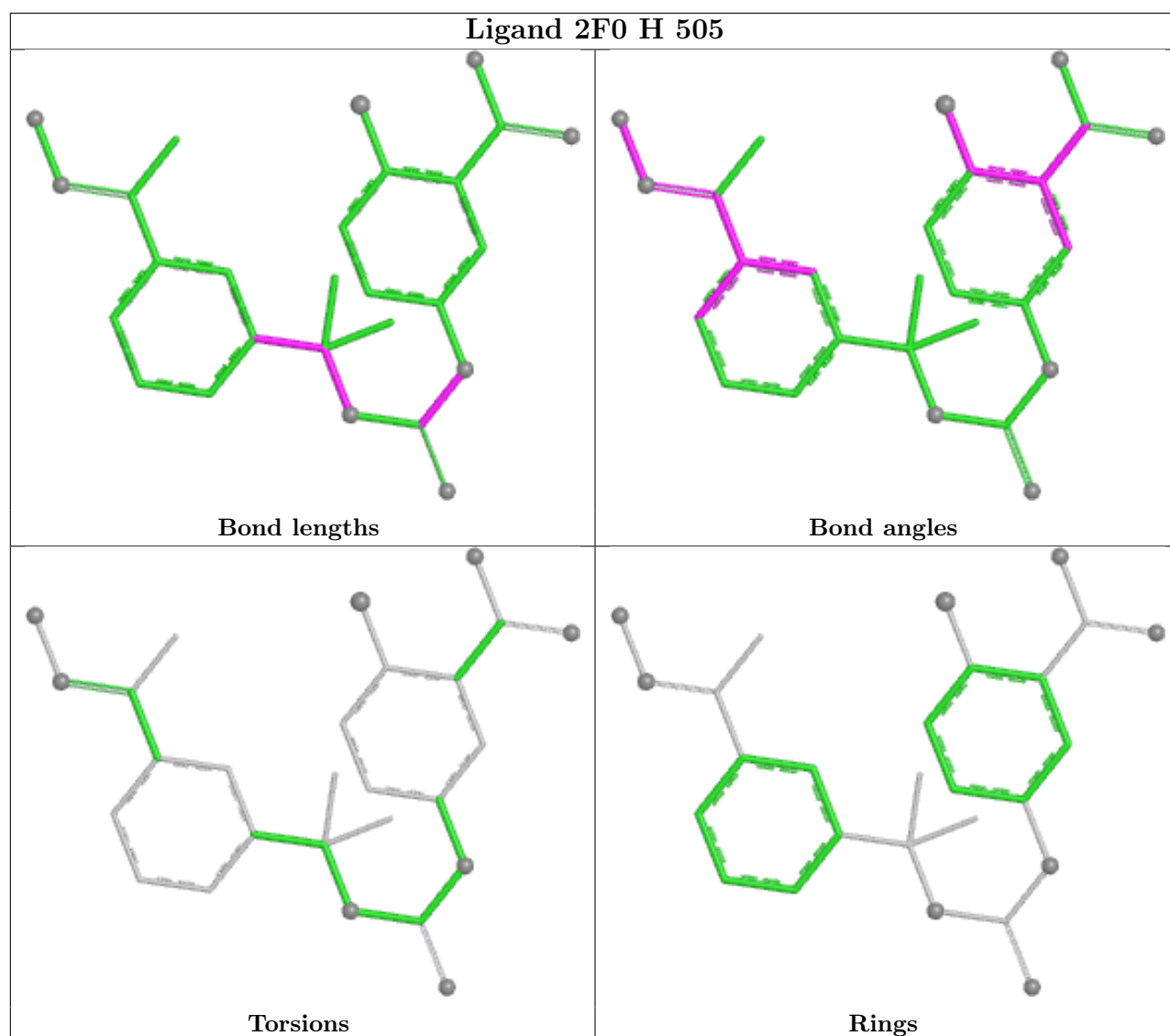


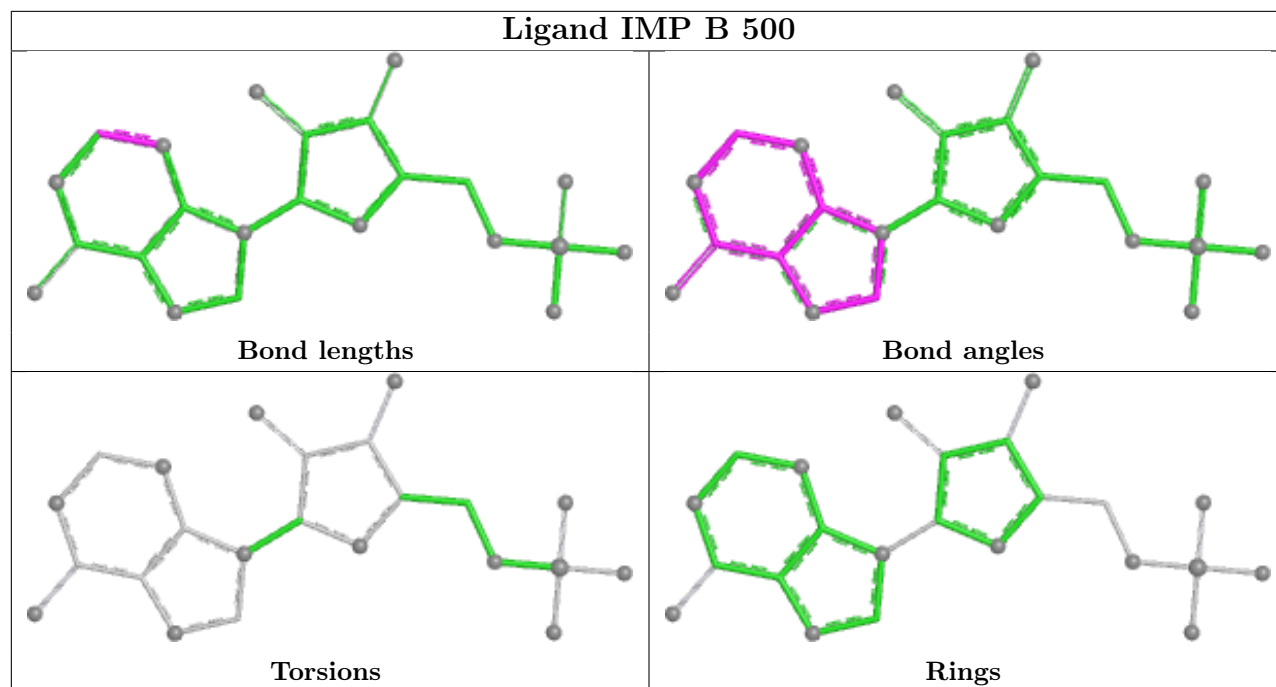
Ligand IMP F 501











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 ⓘ

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, 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%)	0.53	18 (5%)	33	29	17, 46, 70, 84	8 (2%)
1	B	355/384 (92%)	0.51	16 (4%)	38	34	25, 45, 68, 102	3 (0%)
1	C	348/384 (90%)	0.36	7 (2%)	65	62	22, 45, 64, 74	4 (1%)
1	D	352/384 (91%)	0.55	11 (3%)	51	48	23, 47, 68, 97	4 (1%)
1	E	352/384 (91%)	0.55	13 (3%)	45	41	29, 46, 72, 89	3 (0%)
1	F	350/384 (91%)	0.45	13 (3%)	45	41	34, 50, 70, 85	1 (0%)
1	G	356/384 (92%)	0.56	14 (3%)	43	39	25, 49, 67, 87	3 (0%)
1	H	350/384 (91%)	0.56	12 (3%)	48	44	33, 51, 70, 80	1 (0%)
All	All	2814/3072 (91%)	0.51	104 (3%)	45	41	17, 48, 70, 102	27 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	258[A]	GLN	5.1
1	F	482	ALA	4.5
1	E	413	LEU	4.3
1	A	90[A]	ARG	4.3
1	C	482	ALA	4.2
1	A	413	LEU	4.1
1	B	-4	PHE	4.0
1	D	400	GLY	3.9
1	A	224	GLY	3.9
1	H	426	GLY	3.8
1	A	487	LEU	3.6
1	E	397[A]	MET	3.5
1	E	476	VAL	3.4
1	D	413	LEU	3.3
1	E	400	GLY	3.3
1	D	240	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	426	GLY	3.2
1	C	486	SER	3.2
1	G	278	ALA	3.2
1	F	475	HIS	3.1
1	F	-2	SER	3.1
1	H	316	VAL	3.1
1	A	477	GLN	3.1
1	A	374	PRO	3.0
1	F	251	ASP	3.0
1	B	369	GLY	3.0
1	B	251	ASP	2.9
1	B	399	LYS	2.9
1	E	398[A]	GLU	2.8
1	D	347	SER	2.8
1	A	255	GLY	2.8
1	F	25	VAL	2.8
1	G	-4	PHE	2.8
1	D	379	ILE	2.8
1	G	385	PHE	2.7
1	F	380	TYR	2.7
1	G	380	TYR	2.7
1	G	252	THR	2.7
1	A	486	SER	2.7
1	F	481	GLU	2.7
1	B	397	MET	2.6
1	H	371	ALA	2.6
1	B	380	TYR	2.5
1	F	231	ALA	2.5
1	C	413	LEU	2.5
1	E	382	GLY	2.5
1	H	364	GLY	2.5
1	H	413	LEU	2.4
1	D	80[A]	GLN	2.4
1	H	253	ALA	2.4
1	G	292	GLU	2.4
1	G	402	LYS	2.4
1	A	420	GLY	2.4
1	F	229	VAL	2.4
1	E	376	GLU	2.3
1	D	476	VAL	2.3
1	D	431	THR	2.3
1	C	394	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	249	VAL	2.3
1	C	378	GLU	2.3
1	E	477	GLN	2.3
1	A	387	VAL	2.3
1	B	413	LEU	2.3
1	E	252	THR	2.2
1	A	243	ALA	2.2
1	E	0	ALA	2.2
1	G	368	ALA	2.2
1	A	459	GLN	2.2
1	B	41	GLN	2.2
1	B	486	SER	2.2
1	E	251	ASP	2.2
1	H	271	TYR	2.2
1	E	255	GLY	2.2
1	H	251	ASP	2.2
1	H	379	ILE	2.2
1	G	396	ALA	2.1
1	C	383	ARG	2.1
1	B	402	LYS	2.1
1	F	-1	ASN	2.1
1	G	387	VAL	2.1
1	A	82	ALA	2.1
1	B	412	LYS	2.1
1	D	221	LEU	2.1
1	A	92	GLY	2.1
1	D	227	VAL	2.1
1	H	72	ILE	2.1
1	B	303	GLY	2.1
1	C	380	TYR	2.1
1	G	342	GLY	2.1
1	B	387	VAL	2.1
1	G	251	ASP	2.1
1	A	269	ALA	2.1
1	B	0	ALA	2.1
1	B	368	ALA	2.1
1	A	397[A]	MET	2.1
1	A	478	ILE	2.1
1	F	320	GLN	2.0
1	F	449	GLN	2.0
1	A	25	VAL	2.0
1	D	394	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	289	ALA	2.0
1	H	399	LYS	2.0
1	B	400	GLY	2.0
1	F	375	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
4	FMT	F	507	3/3	0.46	0.22	69,69,70,70	0
8	SO4	G	502	5/5	0.59	0.19	127,128,128,128	0
7	EDO	D	502	4/4	0.62	0.15	59,60,60,60	0
8	SO4	G	503	5/5	0.62	0.14	144,144,145,145	0
7	EDO	F	505	4/4	0.66	0.22	56,58,59,59	0
4	FMT	D	507	3/3	0.67	0.20	62,62,63,64	0
7	EDO	F	504	4/4	0.69	0.17	66,67,69,69	0
6	MLI	A	506	7/7	0.71	0.14	87,88,91,91	0
5	GOL	E	506	6/6	0.71	0.16	50,52,53,54	0
7	EDO	C	506	4/4	0.73	0.23	54,56,58,59	0
5	GOL	A	505	6/6	0.73	0.15	48,51,51,52	0
4	FMT	H	506	3/3	0.74	0.15	65,65,65,65	0
7	EDO	E	505	4/4	0.74	0.15	41,43,45,46	0
4	FMT	H	501	3/3	0.76	0.11	62,62,63,63	0
4	FMT	E	503	3/3	0.78	0.16	74,74,74,75	0
4	FMT	A	504	3/3	0.79	0.10	62,62,63,64	0
8	SO4	C	505	5/5	0.80	0.09	119,119,119,119	0
6	MLI	E	508	7/7	0.82	0.10	64,65,67,68	0
7	EDO	D	503	4/4	0.82	0.17	51,53,55,56	0

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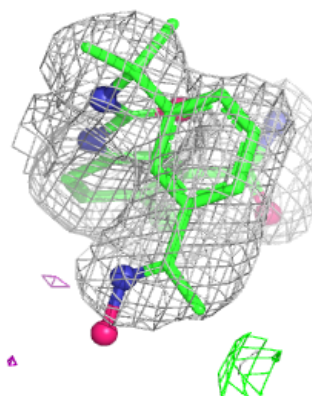
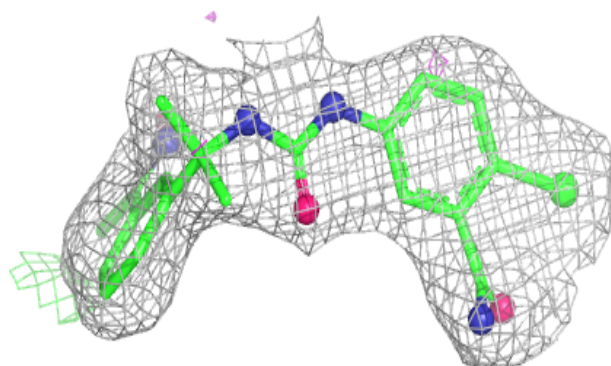
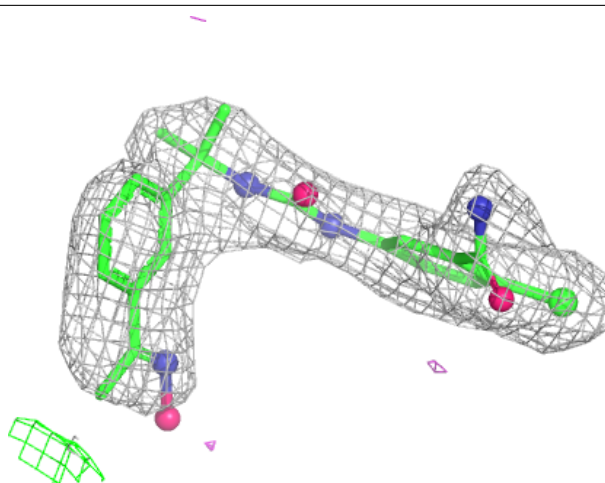
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FMT	E	504	3/3	0.84	0.10	53,53,53,53	0
4	FMT	A	503	3/3	0.84	0.15	48,48,48,49	0
7	EDO	B	502	4/4	0.84	0.18	71,71,71,72	0
4	FMT	D	506	3/3	0.85	0.11	43,43,46,47	0
4	FMT	C	501	3/3	0.85	0.15	69,69,70,71	0
4	FMT	H	503	3/3	0.85	0.11	66,66,67,67	0
7	EDO	D	505	4/4	0.85	0.13	55,56,57,57	0
7	EDO	C	504	4/4	0.85	0.13	53,54,54,54	0
4	FMT	B	503	3/3	0.87	0.14	46,46,47,49	0
3	2F0	H	505	27/27	0.87	0.12	47,53,59,63	0
4	FMT	F	503	3/3	0.88	0.10	42,42,43,44	0
3	2F0	E	502	27/27	0.88	0.11	38,43,52,54	0
3	2F0	A	502	27/27	0.88	0.12	37,45,50,58	0
3	2F0	F	502	27/27	0.89	0.10	42,49,54,67	0
3	2F0	C	503	27/27	0.90	0.11	43,50,54,56	0
2	IMP	E	501	23/23	0.90	0.10	31,35,43,44	0
3	2F0	B	501	27/27	0.90	0.12	41,50,56,61	0
3	2F0	D	501	27/27	0.91	0.10	34,42,57,61	0
3	2F0	E	509	27/27	0.91	0.11	39,51,55,57	0
4	FMT	E	507	3/3	0.91	0.09	37,37,37,37	0
2	IMP	H	504	23/23	0.92	0.10	37,41,47,48	0
4	FMT	H	502	3/3	0.92	0.13	68,68,68,68	0
2	IMP	D	504	23/23	0.93	0.09	36,41,45,49	0
2	IMP	A	501	23/23	0.93	0.08	35,40,44,45	0
7	EDO	F	506	4/4	0.94	0.09	39,39,39,40	0
2	IMP	F	501	23/23	0.94	0.10	37,44,47,48	0
2	IMP	G	501	23/23	0.94	0.09	36,39,41,42	0
2	IMP	B	500	23/23	0.94	0.09	33,36,38,39	0
2	IMP	C	502	23/23	0.95	0.08	32,41,44,46	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.

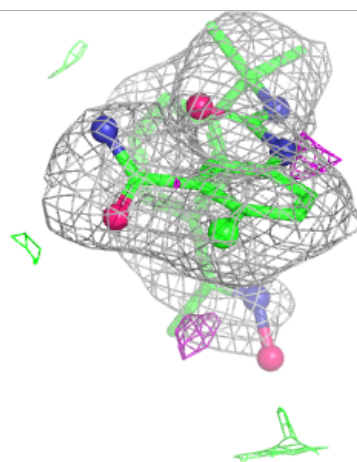
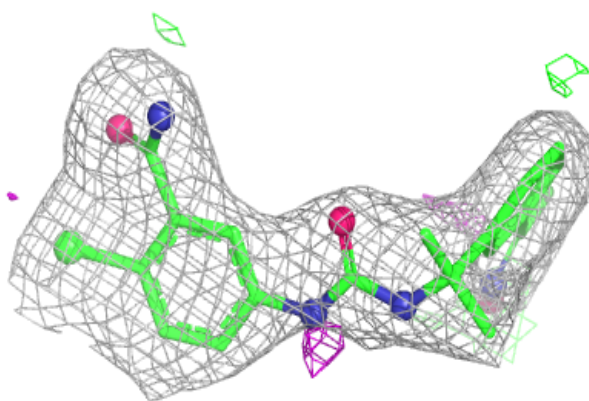
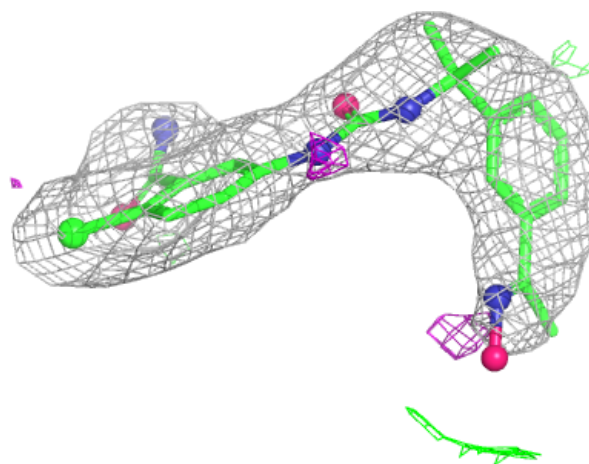
Electron density around 2F0 H 505:

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



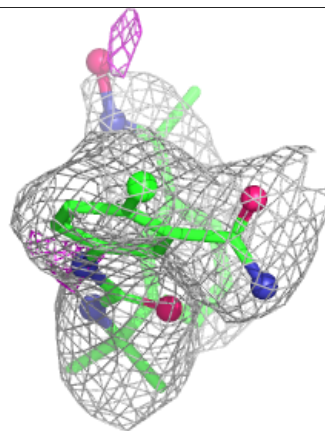
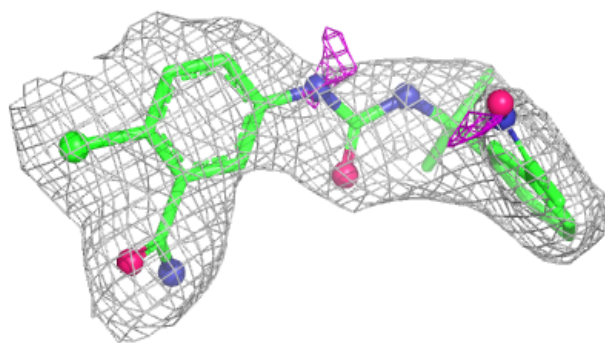
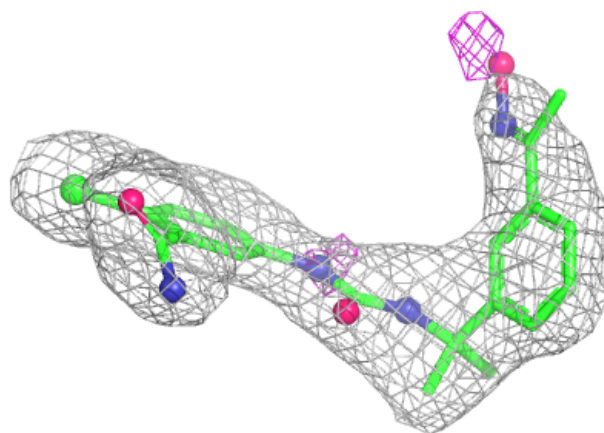
Electron density around 2F0 E 502:

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



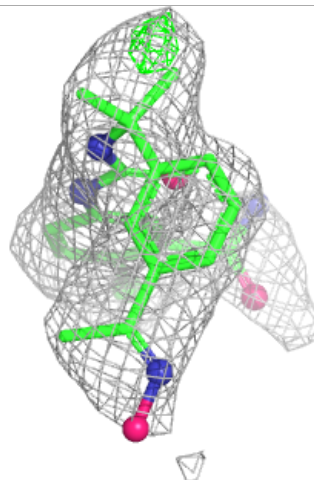
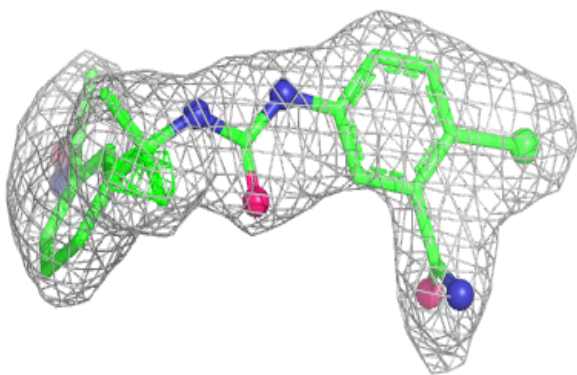
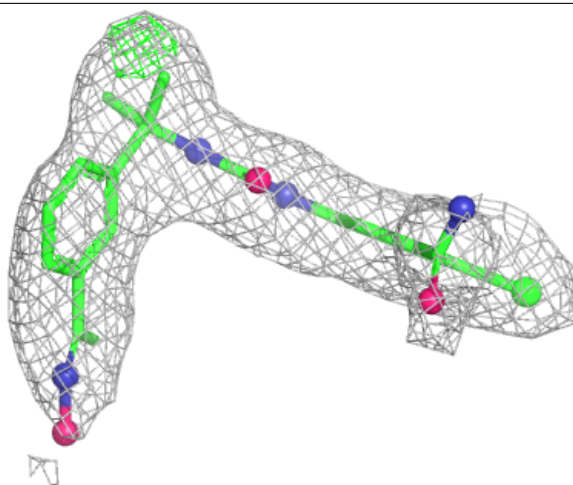
Electron density around 2F0 A 502:

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



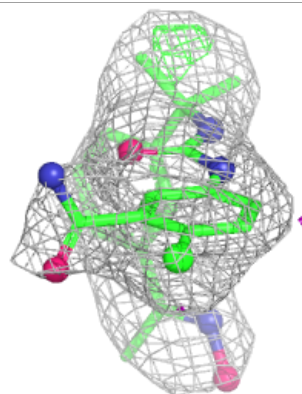
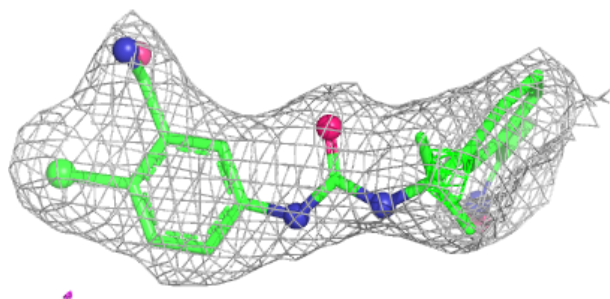
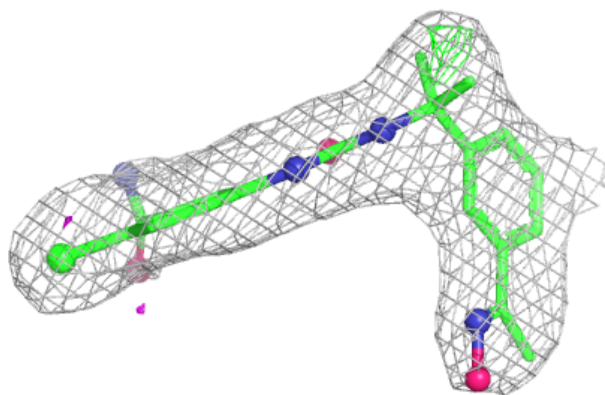
Electron density around 2F0 F 502:

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

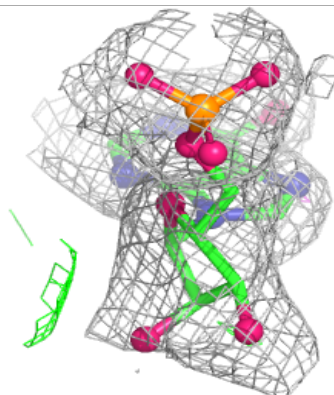
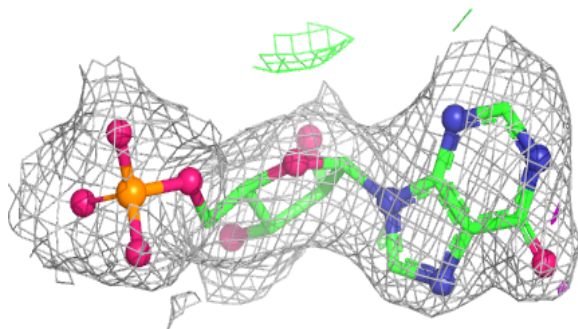
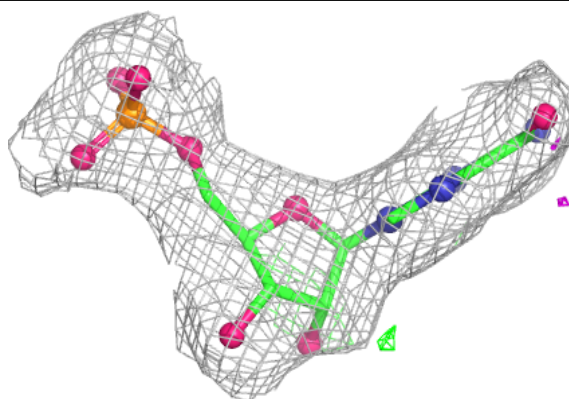


Electron density around 2F0 C 503:

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

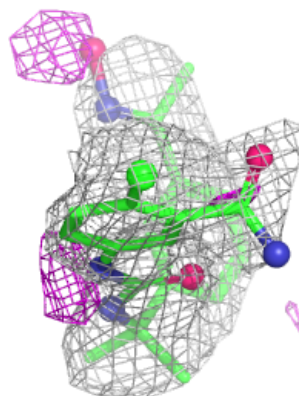
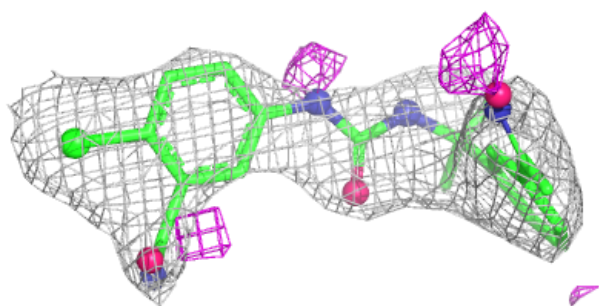
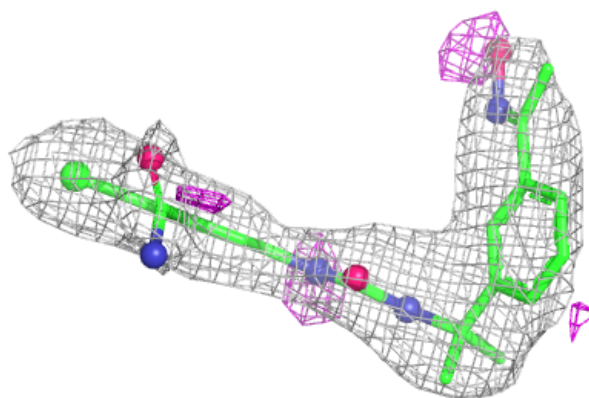
**Electron density around IMP E 501:**

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

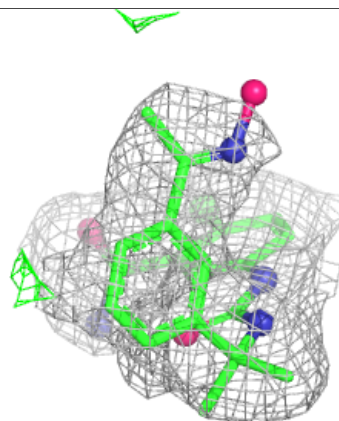
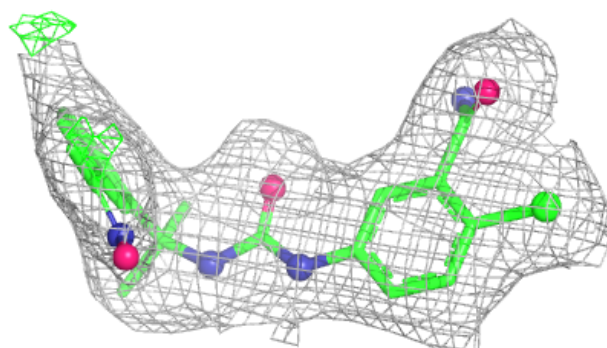
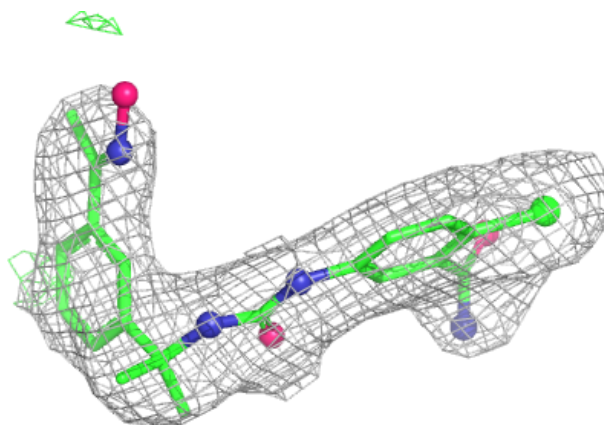


Electron density around 2F0 B 501:

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

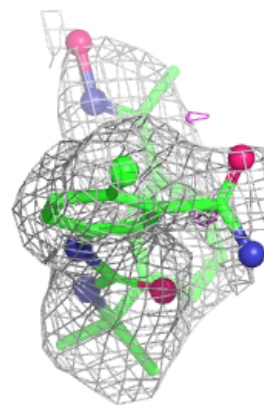
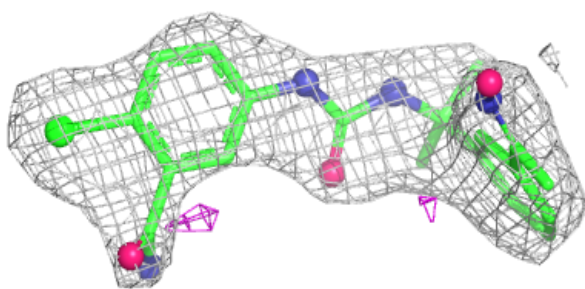
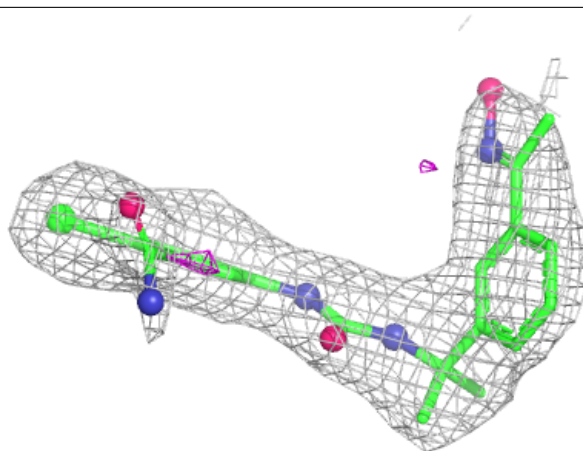
**Electron density around 2F0 D 501:**

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



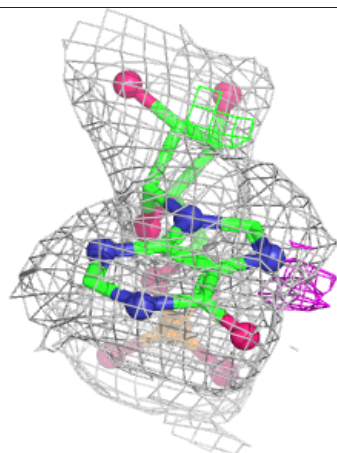
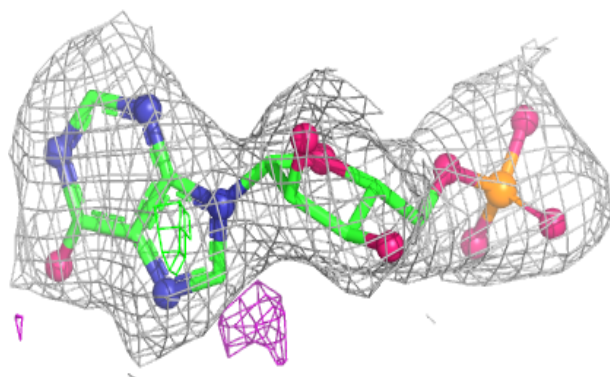
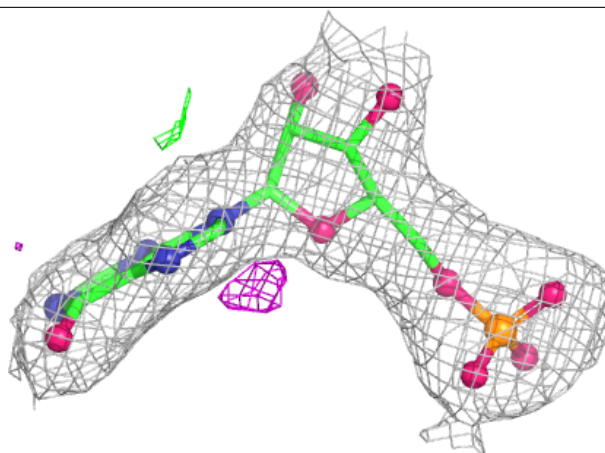
Electron density around 2F0 E 509:

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

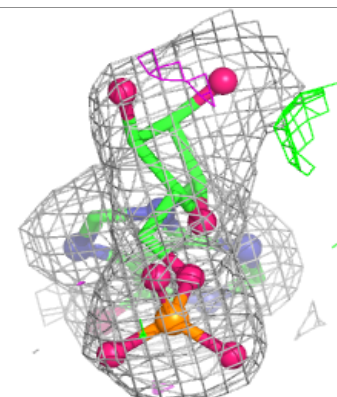
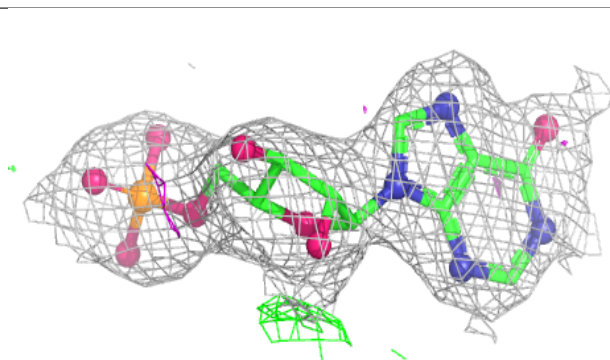
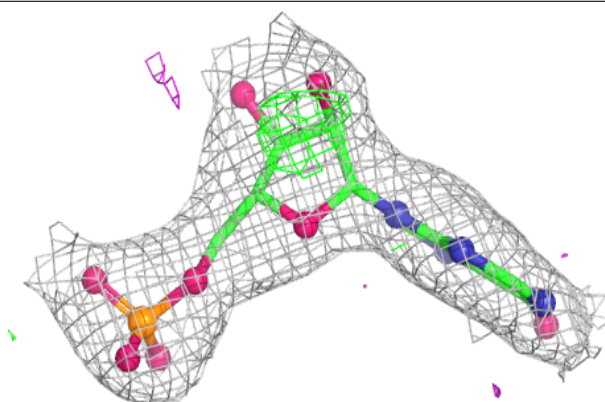


Electron density around IMP H 504:

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

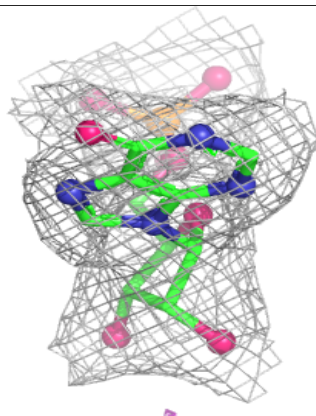
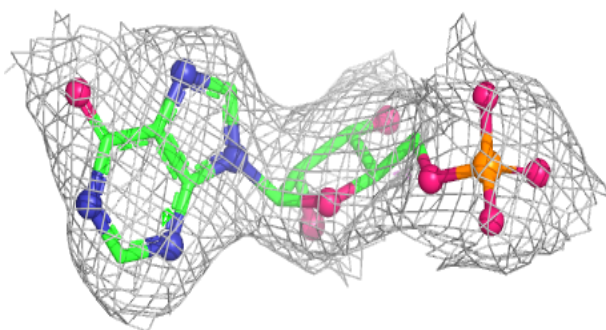
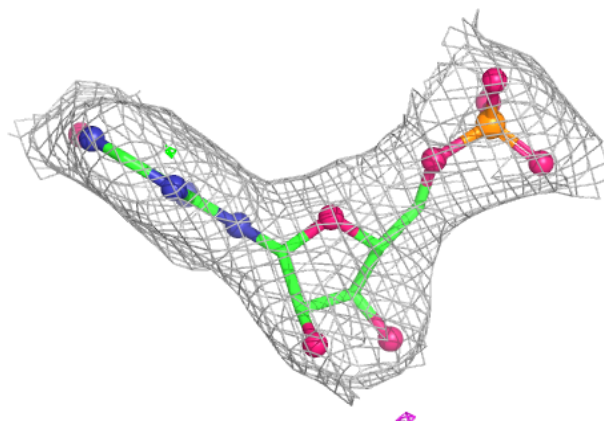
**Electron density around IMP D 504:**

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

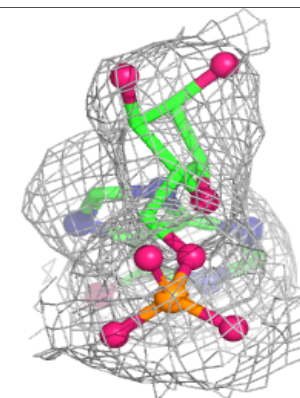
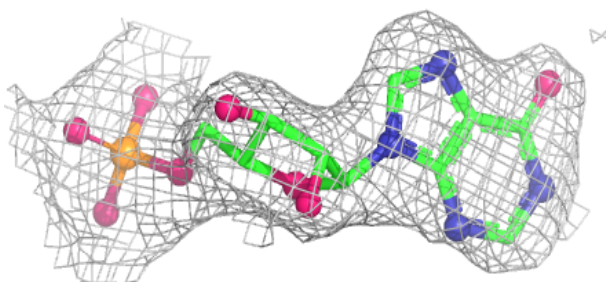
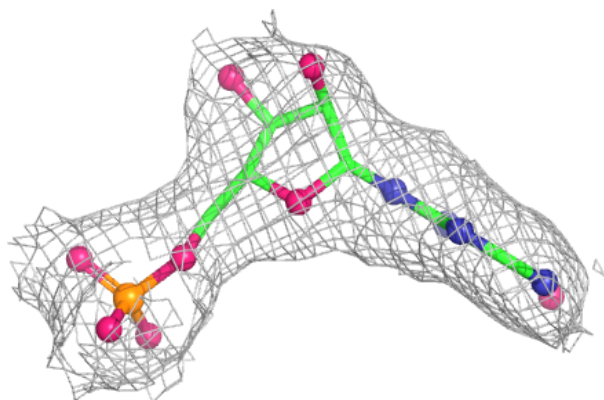


Electron density around IMP A 501:

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

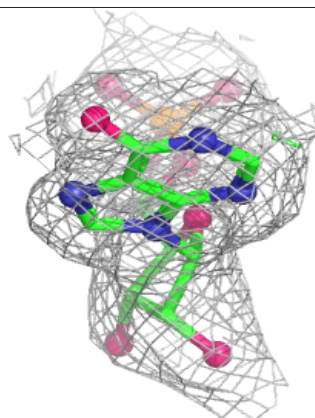
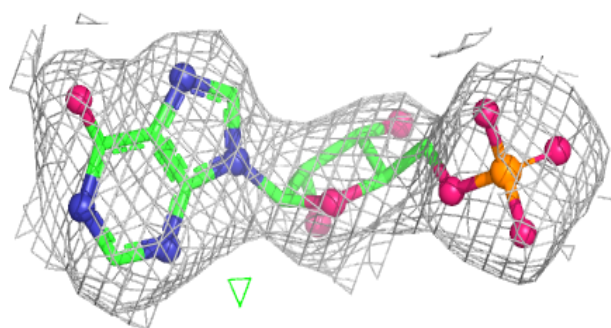
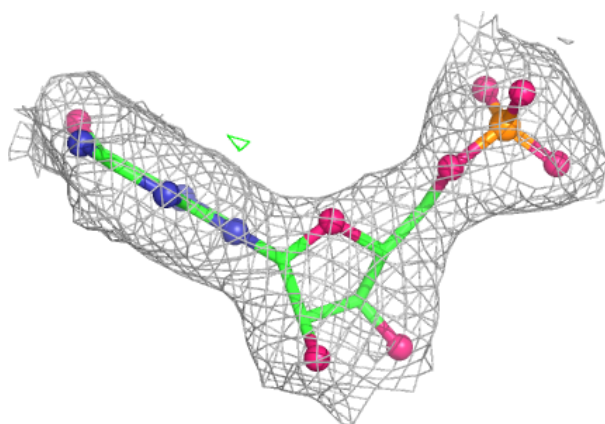
**Electron density around IMP F 501:**

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

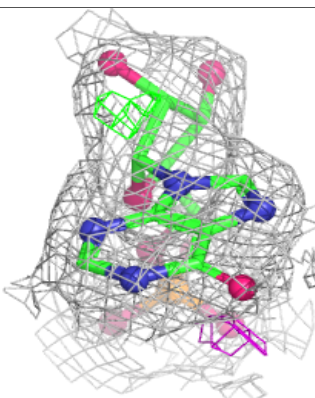
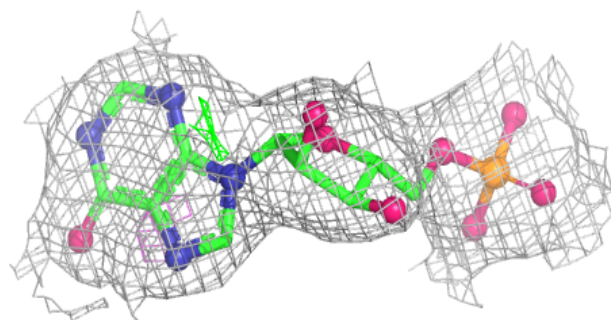
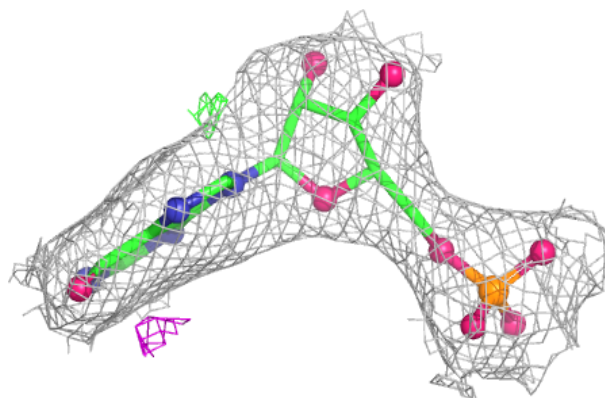


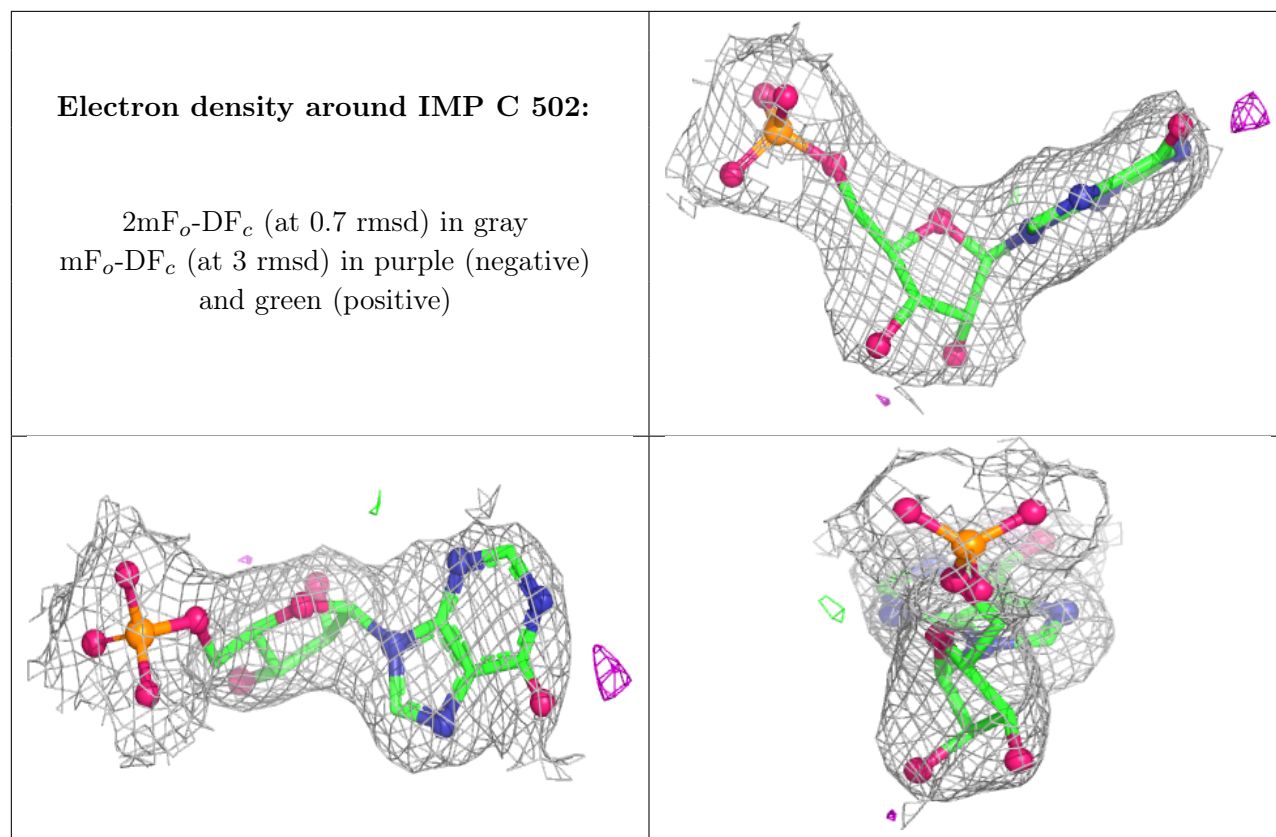
Electron density around IMP G 501:

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

**Electron density around IMP 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.