



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:55 am BST

PDB ID : 5UQG
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from *Campylobacter jejuni* in the complex with inhibitor p200
Authors : Kim, Y.; Maltseva, N.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2017-02-08
Resolution : 2.03 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 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

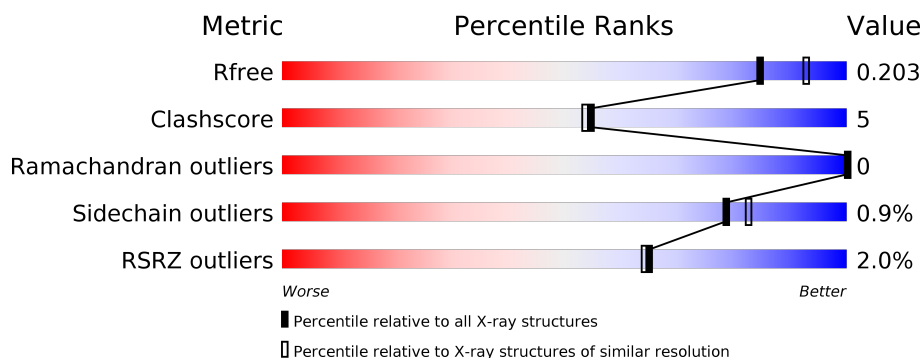
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	406	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>12%</div> </div> </div>
1	B	406	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>11%</div> </div> </div>
1	C	406	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>12%</div> </div> </div>
1	D	406	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>14%</div> </div> </div>
1	E	406	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>13%</div> </div> </div>
1	F	406	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	406	<div><div>%</div><div><div></div><div>74%</div><div>13%</div><div>13%</div></div></div>
1	H	406	<div><div>2%</div><div><div></div><div>80%</div><div>9%</div><div>10%</div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22396 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	356	Total	C	N	O	S	0	1	0
			2657	1669	471	503	14			
1	B	361	Total	C	N	O	S	0	0	0
			2687	1690	477	506	14			
1	C	356	Total	C	N	O	S	0	0	0
			2652	1668	470	500	14			
1	D	351	Total	C	N	O	S	0	3	0
			2621	1649	462	496	14			
1	E	354	Total	C	N	O	S	0	0	0
			2630	1656	464	496	14			
1	F	353	Total	C	N	O	S	0	3	0
			2645	1667	466	498	14			
1	G	353	Total	C	N	O	S	0	1	0
			2635	1656	467	498	14			
1	H	364	Total	C	N	O	S	0	0	0
			2708	1703	480	511	14			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
A	-22	HIS	-	expression tag	UNP A0A1B3XFT6
A	-21	HIS	-	expression tag	UNP A0A1B3XFT6
A	-20	HIS	-	expression tag	UNP A0A1B3XFT6
A	-19	HIS	-	expression tag	UNP A0A1B3XFT6
A	-18	HIS	-	expression tag	UNP A0A1B3XFT6
A	-17	HIS	-	expression tag	UNP A0A1B3XFT6
A	-16	SER	-	expression tag	UNP A0A1B3XFT6
A	-15	SER	-	expression tag	UNP A0A1B3XFT6
A	-14	GLY	-	expression tag	UNP A0A1B3XFT6
A	-13	VAL	-	expression tag	UNP A0A1B3XFT6
A	-12	ASP	-	expression tag	UNP A0A1B3XFT6
A	-11	LEU	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP A0A1B3XFT6
A	-9	THR	-	expression tag	UNP A0A1B3XFT6
A	-8	GLU	-	expression tag	UNP A0A1B3XFT6
A	-7	ASN	-	expression tag	UNP A0A1B3XFT6
A	-6	LEU	-	expression tag	UNP A0A1B3XFT6
A	-5	TYR	-	expression tag	UNP A0A1B3XFT6
A	-4	PHE	-	expression tag	UNP A0A1B3XFT6
A	-3	GLN	-	expression tag	UNP A0A1B3XFT6
A	-2	SER	-	expression tag	UNP A0A1B3XFT6
A	-1	ASN	-	expression tag	UNP A0A1B3XFT6
A	0	ALA	-	expression tag	UNP A0A1B3XFT6
A	195	GLY	-	linker	UNP A0A1B3XFT6
B	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
B	-22	HIS	-	expression tag	UNP A0A1B3XFT6
B	-21	HIS	-	expression tag	UNP A0A1B3XFT6
B	-20	HIS	-	expression tag	UNP A0A1B3XFT6
B	-19	HIS	-	expression tag	UNP A0A1B3XFT6
B	-18	HIS	-	expression tag	UNP A0A1B3XFT6
B	-17	HIS	-	expression tag	UNP A0A1B3XFT6
B	-16	SER	-	expression tag	UNP A0A1B3XFT6
B	-15	SER	-	expression tag	UNP A0A1B3XFT6
B	-14	GLY	-	expression tag	UNP A0A1B3XFT6
B	-13	VAL	-	expression tag	UNP A0A1B3XFT6
B	-12	ASP	-	expression tag	UNP A0A1B3XFT6
B	-11	LEU	-	expression tag	UNP A0A1B3XFT6
B	-10	GLY	-	expression tag	UNP A0A1B3XFT6
B	-9	THR	-	expression tag	UNP A0A1B3XFT6
B	-8	GLU	-	expression tag	UNP A0A1B3XFT6
B	-7	ASN	-	expression tag	UNP A0A1B3XFT6
B	-6	LEU	-	expression tag	UNP A0A1B3XFT6
B	-5	TYR	-	expression tag	UNP A0A1B3XFT6
B	-4	PHE	-	expression tag	UNP A0A1B3XFT6
B	-3	GLN	-	expression tag	UNP A0A1B3XFT6
B	-2	SER	-	expression tag	UNP A0A1B3XFT6
B	-1	ASN	-	expression tag	UNP A0A1B3XFT6
B	0	ALA	-	expression tag	UNP A0A1B3XFT6
B	195	GLY	-	linker	UNP A0A1B3XFT6
C	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
C	-22	HIS	-	expression tag	UNP A0A1B3XFT6
C	-21	HIS	-	expression tag	UNP A0A1B3XFT6
C	-20	HIS	-	expression tag	UNP A0A1B3XFT6
C	-19	HIS	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP A0A1B3XFT6
C	-17	HIS	-	expression tag	UNP A0A1B3XFT6
C	-16	SER	-	expression tag	UNP A0A1B3XFT6
C	-15	SER	-	expression tag	UNP A0A1B3XFT6
C	-14	GLY	-	expression tag	UNP A0A1B3XFT6
C	-13	VAL	-	expression tag	UNP A0A1B3XFT6
C	-12	ASP	-	expression tag	UNP A0A1B3XFT6
C	-11	LEU	-	expression tag	UNP A0A1B3XFT6
C	-10	GLY	-	expression tag	UNP A0A1B3XFT6
C	-9	THR	-	expression tag	UNP A0A1B3XFT6
C	-8	GLU	-	expression tag	UNP A0A1B3XFT6
C	-7	ASN	-	expression tag	UNP A0A1B3XFT6
C	-6	LEU	-	expression tag	UNP A0A1B3XFT6
C	-5	TYR	-	expression tag	UNP A0A1B3XFT6
C	-4	PHE	-	expression tag	UNP A0A1B3XFT6
C	-3	GLN	-	expression tag	UNP A0A1B3XFT6
C	-2	SER	-	expression tag	UNP A0A1B3XFT6
C	-1	ASN	-	expression tag	UNP A0A1B3XFT6
C	0	ALA	-	expression tag	UNP A0A1B3XFT6
C	195	GLY	-	linker	UNP A0A1B3XFT6
D	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
D	-22	HIS	-	expression tag	UNP A0A1B3XFT6
D	-21	HIS	-	expression tag	UNP A0A1B3XFT6
D	-20	HIS	-	expression tag	UNP A0A1B3XFT6
D	-19	HIS	-	expression tag	UNP A0A1B3XFT6
D	-18	HIS	-	expression tag	UNP A0A1B3XFT6
D	-17	HIS	-	expression tag	UNP A0A1B3XFT6
D	-16	SER	-	expression tag	UNP A0A1B3XFT6
D	-15	SER	-	expression tag	UNP A0A1B3XFT6
D	-14	GLY	-	expression tag	UNP A0A1B3XFT6
D	-13	VAL	-	expression tag	UNP A0A1B3XFT6
D	-12	ASP	-	expression tag	UNP A0A1B3XFT6
D	-11	LEU	-	expression tag	UNP A0A1B3XFT6
D	-10	GLY	-	expression tag	UNP A0A1B3XFT6
D	-9	THR	-	expression tag	UNP A0A1B3XFT6
D	-8	GLU	-	expression tag	UNP A0A1B3XFT6
D	-7	ASN	-	expression tag	UNP A0A1B3XFT6
D	-6	LEU	-	expression tag	UNP A0A1B3XFT6
D	-5	TYR	-	expression tag	UNP A0A1B3XFT6
D	-4	PHE	-	expression tag	UNP A0A1B3XFT6
D	-3	GLN	-	expression tag	UNP A0A1B3XFT6
D	-2	SER	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASN	-	expression tag	UNP A0A1B3XFT6
D	0	ALA	-	expression tag	UNP A0A1B3XFT6
D	195	GLY	-	linker	UNP A0A1B3XFT6
E	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
E	-22	HIS	-	expression tag	UNP A0A1B3XFT6
E	-21	HIS	-	expression tag	UNP A0A1B3XFT6
E	-20	HIS	-	expression tag	UNP A0A1B3XFT6
E	-19	HIS	-	expression tag	UNP A0A1B3XFT6
E	-18	HIS	-	expression tag	UNP A0A1B3XFT6
E	-17	HIS	-	expression tag	UNP A0A1B3XFT6
E	-16	SER	-	expression tag	UNP A0A1B3XFT6
E	-15	SER	-	expression tag	UNP A0A1B3XFT6
E	-14	GLY	-	expression tag	UNP A0A1B3XFT6
E	-13	VAL	-	expression tag	UNP A0A1B3XFT6
E	-12	ASP	-	expression tag	UNP A0A1B3XFT6
E	-11	LEU	-	expression tag	UNP A0A1B3XFT6
E	-10	GLY	-	expression tag	UNP A0A1B3XFT6
E	-9	THR	-	expression tag	UNP A0A1B3XFT6
E	-8	GLU	-	expression tag	UNP A0A1B3XFT6
E	-7	ASN	-	expression tag	UNP A0A1B3XFT6
E	-6	LEU	-	expression tag	UNP A0A1B3XFT6
E	-5	TYR	-	expression tag	UNP A0A1B3XFT6
E	-4	PHE	-	expression tag	UNP A0A1B3XFT6
E	-3	GLN	-	expression tag	UNP A0A1B3XFT6
E	-2	SER	-	expression tag	UNP A0A1B3XFT6
E	-1	ASN	-	expression tag	UNP A0A1B3XFT6
E	0	ALA	-	expression tag	UNP A0A1B3XFT6
E	195	GLY	-	linker	UNP A0A1B3XFT6
F	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
F	-22	HIS	-	expression tag	UNP A0A1B3XFT6
F	-21	HIS	-	expression tag	UNP A0A1B3XFT6
F	-20	HIS	-	expression tag	UNP A0A1B3XFT6
F	-19	HIS	-	expression tag	UNP A0A1B3XFT6
F	-18	HIS	-	expression tag	UNP A0A1B3XFT6
F	-17	HIS	-	expression tag	UNP A0A1B3XFT6
F	-16	SER	-	expression tag	UNP A0A1B3XFT6
F	-15	SER	-	expression tag	UNP A0A1B3XFT6
F	-14	GLY	-	expression tag	UNP A0A1B3XFT6
F	-13	VAL	-	expression tag	UNP A0A1B3XFT6
F	-12	ASP	-	expression tag	UNP A0A1B3XFT6
F	-11	LEU	-	expression tag	UNP A0A1B3XFT6
F	-10	GLY	-	expression tag	UNP A0A1B3XFT6

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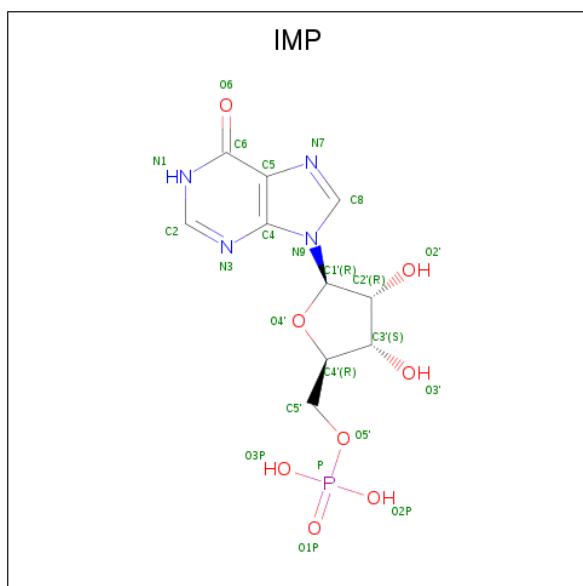
Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	THR	-	expression tag	UNP A0A1B3XFT6
F	-8	GLU	-	expression tag	UNP A0A1B3XFT6
F	-7	ASN	-	expression tag	UNP A0A1B3XFT6
F	-6	LEU	-	expression tag	UNP A0A1B3XFT6
F	-5	TYR	-	expression tag	UNP A0A1B3XFT6
F	-4	PHE	-	expression tag	UNP A0A1B3XFT6
F	-3	GLN	-	expression tag	UNP A0A1B3XFT6
F	-2	SER	-	expression tag	UNP A0A1B3XFT6
F	-1	ASN	-	expression tag	UNP A0A1B3XFT6
F	0	ALA	-	expression tag	UNP A0A1B3XFT6
F	195	GLY	-	linker	UNP A0A1B3XFT6
G	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
G	-22	HIS	-	expression tag	UNP A0A1B3XFT6
G	-21	HIS	-	expression tag	UNP A0A1B3XFT6
G	-20	HIS	-	expression tag	UNP A0A1B3XFT6
G	-19	HIS	-	expression tag	UNP A0A1B3XFT6
G	-18	HIS	-	expression tag	UNP A0A1B3XFT6
G	-17	HIS	-	expression tag	UNP A0A1B3XFT6
G	-16	SER	-	expression tag	UNP A0A1B3XFT6
G	-15	SER	-	expression tag	UNP A0A1B3XFT6
G	-14	GLY	-	expression tag	UNP A0A1B3XFT6
G	-13	VAL	-	expression tag	UNP A0A1B3XFT6
G	-12	ASP	-	expression tag	UNP A0A1B3XFT6
G	-11	LEU	-	expression tag	UNP A0A1B3XFT6
G	-10	GLY	-	expression tag	UNP A0A1B3XFT6
G	-9	THR	-	expression tag	UNP A0A1B3XFT6
G	-8	GLU	-	expression tag	UNP A0A1B3XFT6
G	-7	ASN	-	expression tag	UNP A0A1B3XFT6
G	-6	LEU	-	expression tag	UNP A0A1B3XFT6
G	-5	TYR	-	expression tag	UNP A0A1B3XFT6
G	-4	PHE	-	expression tag	UNP A0A1B3XFT6
G	-3	GLN	-	expression tag	UNP A0A1B3XFT6
G	-2	SER	-	expression tag	UNP A0A1B3XFT6
G	-1	ASN	-	expression tag	UNP A0A1B3XFT6
G	0	ALA	-	expression tag	UNP A0A1B3XFT6
G	195	GLY	-	linker	UNP A0A1B3XFT6
H	-23	MET	-	initiating methionine	UNP A0A1B3XFT6
H	-22	HIS	-	expression tag	UNP A0A1B3XFT6
H	-21	HIS	-	expression tag	UNP A0A1B3XFT6
H	-20	HIS	-	expression tag	UNP A0A1B3XFT6
H	-19	HIS	-	expression tag	UNP A0A1B3XFT6
H	-18	HIS	-	expression tag	UNP A0A1B3XFT6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	HIS	-	expression tag	UNP A0A1B3XFT6
H	-16	SER	-	expression tag	UNP A0A1B3XFT6
H	-15	SER	-	expression tag	UNP A0A1B3XFT6
H	-14	GLY	-	expression tag	UNP A0A1B3XFT6
H	-13	VAL	-	expression tag	UNP A0A1B3XFT6
H	-12	ASP	-	expression tag	UNP A0A1B3XFT6
H	-11	LEU	-	expression tag	UNP A0A1B3XFT6
H	-10	GLY	-	expression tag	UNP A0A1B3XFT6
H	-9	THR	-	expression tag	UNP A0A1B3XFT6
H	-8	GLU	-	expression tag	UNP A0A1B3XFT6
H	-7	ASN	-	expression tag	UNP A0A1B3XFT6
H	-6	LEU	-	expression tag	UNP A0A1B3XFT6
H	-5	TYR	-	expression tag	UNP A0A1B3XFT6
H	-4	PHE	-	expression tag	UNP A0A1B3XFT6
H	-3	GLN	-	expression tag	UNP A0A1B3XFT6
H	-2	SER	-	expression tag	UNP A0A1B3XFT6
H	-1	ASN	-	expression tag	UNP A0A1B3XFT6
H	0	ALA	-	expression tag	UNP A0A1B3XFT6
H	195	GLY	-	linker	UNP A0A1B3XFT6

- Molecule 2 is INOSINIC ACID (three-letter code: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



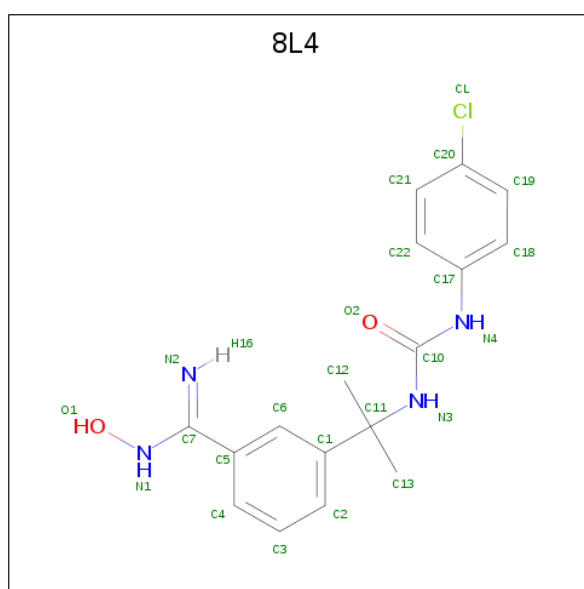
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 3-(2-{[(4-chlorophenyl)carbamoyl]amino}propan-2-yl)-N-hydroxybenzene-1-carboximidamide (three-letter code: 8L4) (formula: C₁₇H₁₉ClN₄O₂).



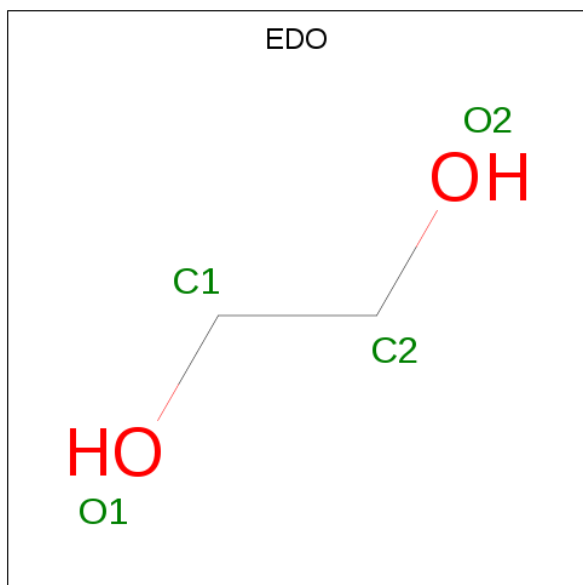
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	B	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	C	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	D	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	E	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	F	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		
3	H	1	Total	C	Cl	N	O	0	0
			24	17	1	4	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

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

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

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

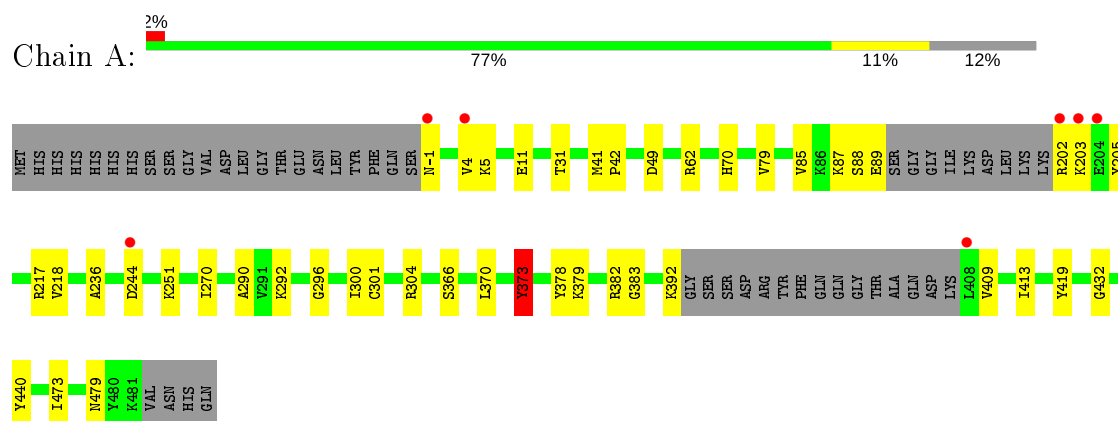
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	115	Total 115	O 115	0	0
6	B	115	Total 115	O 115	0	0
6	C	86	Total 86	O 86	0	0
6	D	92	Total 92	O 92	0	0
6	E	85	Total 85	O 85	0	0
6	F	84	Total 84	O 84	0	0
6	G	101	Total 101	O 101	0	0
6	H	91	Total 91	O 91	0	0

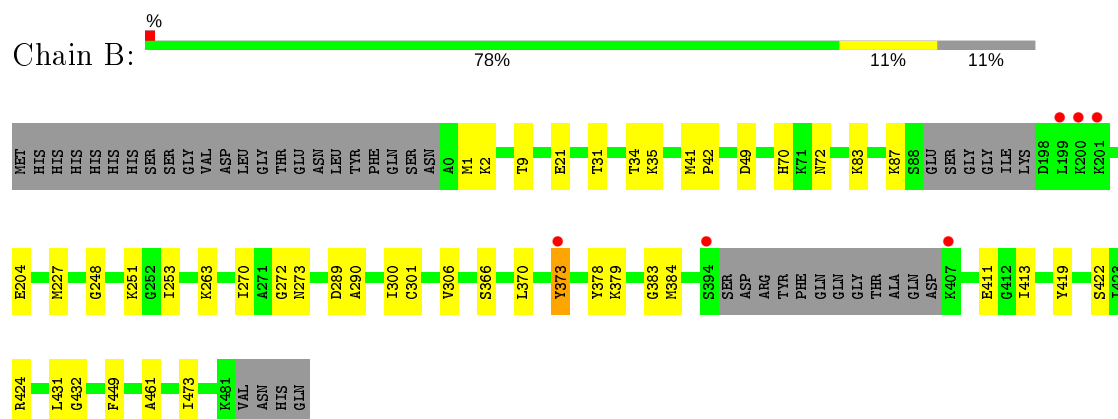
3 Residue-property plots [i](#)

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.

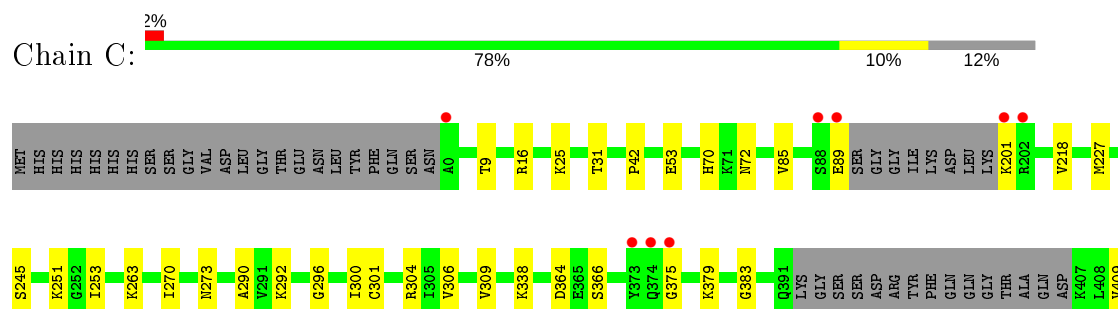
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase

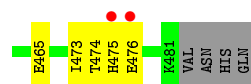
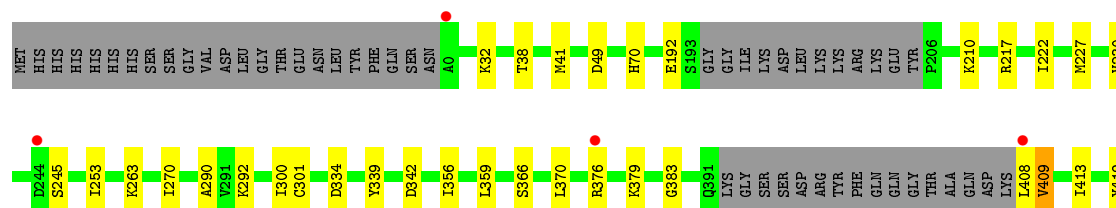
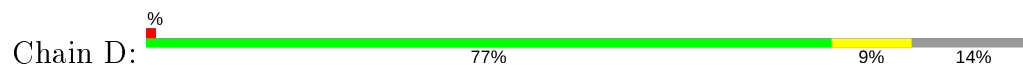


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

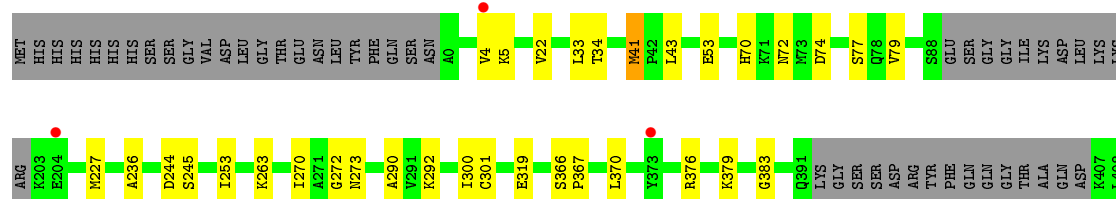
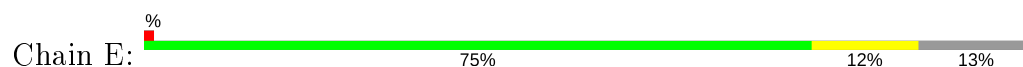




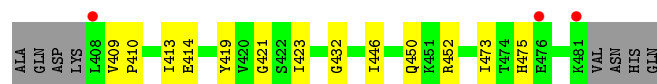
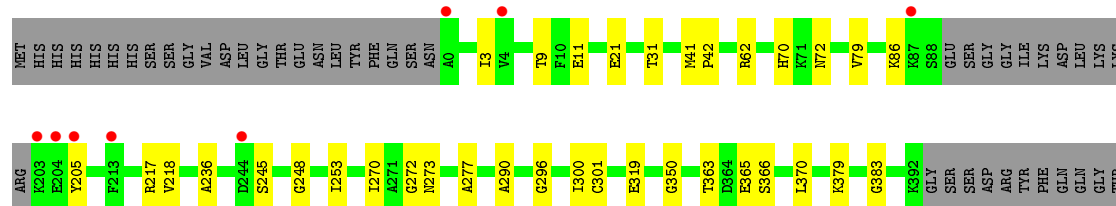
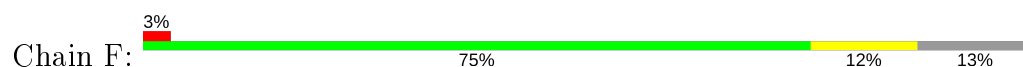
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



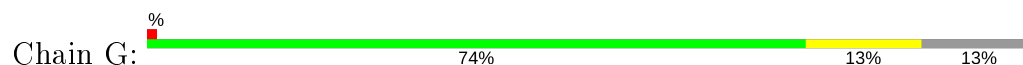
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

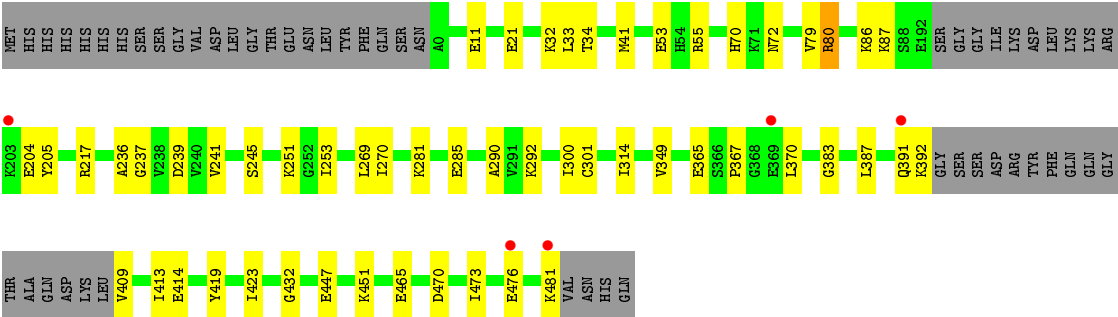


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

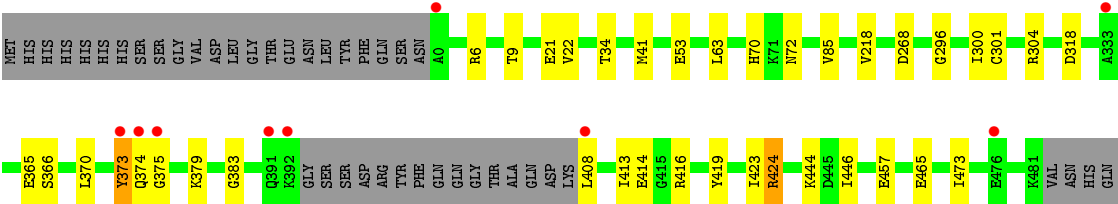
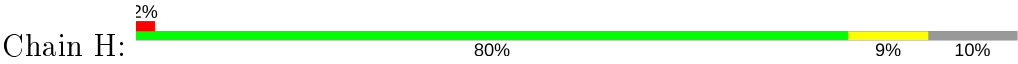


- Molecule 1: Inosine-5'-monophosphate dehydrogenase





● Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.89Å 137.96Å 116.55Å 90.00° 95.99° 90.00°	Depositor
Resolution (Å)	35.91 – 2.03 45.07 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.91-2.03) 99.2 (45.07-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.166 , 0.203 0.166 , 0.203	Depositor DCC
R_{free} test set	9632 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22396	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: IMP, K, 8L4, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/2691	0.81	4/3626 (0.1%)
1	B	0.40	0/2721	0.66	0/3663
1	C	0.40	0/2686	0.60	0/3618
1	D	0.45	0/2655	0.69	1/3581 (0.0%)
1	E	0.42	0/2664	0.65	2/3591 (0.1%)
1	F	0.42	0/2680	0.65	0/3614
1	G	0.44	0/2669	0.78	6/3596 (0.2%)
1	H	0.39	0/2743	0.64	1/3694 (0.0%)
All	All	0.42	0/21509	0.69	14/28983 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ARG	NE-CZ-NH2	-22.49	109.06	120.30
1	G	80	ARG	NE-CZ-NH2	-21.94	109.33	120.30
1	A	217	ARG	NE-CZ-NH1	13.09	126.84	120.30
1	G	80	ARG	CD-NE-CZ	12.04	140.45	123.60
1	G	80	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	E	41	MET	CG-SD-CE	-7.35	88.44	100.20
1	D	476	GLU	C-N-CA	6.60	138.21	121.70
1	A	373	TYR	CB-CG-CD2	-5.96	117.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	367	PRO	C-N-CA	-5.67	110.40	122.30
1	A	87	LYS	CA-CB-CG	5.42	125.33	113.40
1	H	41	MET	CA-CB-CG	-5.39	104.14	113.30
1	E	367	PRO	C-N-CA	-5.38	111.00	122.30
1	G	80	ARG	CG-CD-NE	-5.12	101.05	111.80
1	G	292	LYS	CD-CE-NZ	-5.07	100.05	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	80	ARG	Sidechain

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	2657	0	2742	31	0
1	B	2687	0	2788	33	0
1	C	2652	0	2745	28	0
1	D	2621	0	2708	27	0
1	E	2630	0	2722	40	0
1	F	2645	0	2738	34	0
1	G	2635	0	2720	37	0
1	H	2708	0	2809	31	0
2	A	23	0	11	2	0
2	B	23	0	11	1	0
2	C	23	0	11	1	0
2	D	23	0	11	2	0
2	E	23	0	11	1	0
2	F	23	0	11	1	0
2	G	23	0	11	1	0
2	H	23	0	11	1	0
3	A	24	0	0	0	0
3	B	24	0	0	0	0
3	C	24	0	0	0	0
3	D	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	24	0	0	0	0
3	F	48	0	0	0	0
3	H	24	0	0	0	0
4	A	4	0	6	0	0
4	E	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	115	0	0	1	0
6	B	115	0	0	1	0
6	C	86	0	0	1	0
6	D	92	0	0	2	0
6	E	85	0	0	0	0
6	F	84	0	0	2	0
6	G	101	0	0	2	0
6	H	91	0	0	2	0
All	All	22396	0	22072	227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASP:OD2	1:A:292:LYS:NZ	2.09	0.85
1:B:41:MET:HG3	1:B:431:LEU:HD11	1.56	0.84
1:F:245:SER:HB2	1:F:253:ILE:HD11	1.72	0.72
1:E:432:GLY:HA3	1:F:409[A]:VAL:HG21	1.72	0.71
1:A:382:ARG:HH22	1:A:392:LYS:HE3	1.60	0.67
1:B:366:SER:OG	1:B:379:LYS:HE2	1.94	0.67
1:E:41:MET:CE	1:E:431:LEU:HD21	2.24	0.67
1:G:245:SER:HB2	1:G:253:ILE:HD11	1.76	0.66
1:E:455:PHE:HB2	1:F:3:ILE:HD13	1.76	0.66
1:B:413:ILE:HD13	1:H:473:ILE:HG12	1.77	0.66
1:E:473:ILE:HD12	1:E:482:VAL:CG2	2.25	0.66
1:C:446:ILE:O	1:C:450:GLN:HG3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:SER:OG	1:A:379:LYS:HE2	1.97	0.65
1:D:245:SER:HB2	1:D:253:ILE:HD11	1.78	0.65
1:F:270:ILE:HG12	1:F:290:ALA:HB3	1.79	0.65
1:F:300:ILE:HD13	1:F:383:GLY:HA2	1.79	0.64
1:F:446:ILE:O	1:F:450:GLN:HG3	1.97	0.64
1:D:192:GLU:OE2	1:D:210:LYS:NZ	2.28	0.64
1:B:41:MET:HG3	1:B:431:LEU:CD1	2.28	0.63
1:F:70:HIS:HD2	1:F:72:ASN:H	1.47	0.62
1:H:70:HIS:HD2	1:H:72:ASN:H	1.46	0.62
1:E:270:ILE:HG12	1:E:290:ALA:HB3	1.81	0.62
1:C:273:ASN:OD1	1:C:292:LYS:HE3	2.01	0.61
1:G:281:LYS:O	1:G:285:GLU:HG3	2.00	0.61
1:E:70:HIS:HD2	1:E:72:ASN:H	1.47	0.61
1:C:409:VAL:HG21	1:G:432:GLY:HA3	1.82	0.61
1:H:366:SER:OG	1:H:379:LYS:HE2	2.01	0.61
1:F:79:VAL:HG13	1:F:236:ALA:HB2	1.81	0.61
1:A:370:LEU:HD21	1:A:419:TYR:CD1	2.36	0.61
1:C:89:GLU:HG2	1:C:201:LYS:HD2	1.84	0.60
1:A:432:GLY:HA3	1:D:409[B]:VAL:HG21	1.83	0.60
1:F:370:LEU:HD21	1:F:419:TYR:CD1	2.35	0.60
1:D:300:ILE:HD13	1:D:383:GLY:HA2	1.81	0.59
1:C:338:LYS:HE2	1:G:470:ASP:OD2	2.02	0.59
1:D:270:ILE:HG12	1:D:290:ALA:HB3	1.83	0.59
1:B:83:LYS:O	1:B:87:LYS:HG2	2.01	0.59
1:A:413:ILE:HD13	1:B:473:ILE:HG12	1.85	0.58
1:C:70:HIS:HD2	1:C:72:ASN:H	1.49	0.58
1:D:376:ARG:NH1	6:D:602:HOH:O	2.35	0.58
1:A:382:ARG:HH22	1:A:392:LYS:CE	2.16	0.58
1:D:301:CYS:SG	2:D:500:IMP:H2	2.44	0.58
1:E:41:MET:HE3	1:E:431:LEU:HD21	1.85	0.57
1:E:473:ILE:HD12	1:E:482:VAL:HG22	1.86	0.57
1:E:74:ASP:OD1	1:E:77:SER:N	2.31	0.57
1:C:366:SER:OG	1:C:379:LYS:HE2	2.05	0.57
1:E:22:VAL:HG11	1:E:444:LYS:HG2	1.86	0.57
1:G:70:HIS:HD2	1:G:72:ASN:H	1.51	0.56
1:A:301:CYS:SG	2:A:501:IMP:H2	2.45	0.56
1:G:55[A]:ARG:HD3	1:G:365:GLU:HG3	1.87	0.56
1:B:31:THR:HG21	1:B:42:PRO:HB3	1.88	0.56
1:D:32:LYS:HD2	1:D:38:THR:HG22	1.88	0.56
1:E:446:ILE:O	1:E:450:GLN:HG3	2.06	0.56
1:B:373:TYR:C	1:B:373:TYR:HD1	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ILE:HD13	1:G:473:ILE:HG12	1.88	0.55
1:A:251:LYS:HB2	1:B:21:GLU:HG2	1.89	0.55
1:B:370:LEU:HD21	1:B:419:TYR:CD1	2.41	0.55
1:E:300:ILE:HD13	1:E:383:GLY:HA2	1.89	0.55
1:F:473:ILE:HG12	1:G:413:ILE:HD13	1.88	0.55
1:H:53:GLU:OE1	1:H:70:HIS:HE1	1.89	0.55
1:G:241:VAL:HG23	1:G:269:LEU:CD1	2.37	0.55
1:B:306:VAL:HG21	1:B:411:GLU:HG2	1.88	0.54
1:E:41:MET:HG3	1:E:41:MET:O	2.05	0.54
1:H:300:ILE:HD13	1:H:383:GLY:HA2	1.90	0.54
1:F:452:ARG:NH1	6:F:602:HOH:O	2.41	0.54
1:F:475:HIS:HB2	1:G:414:GLU:HB2	1.89	0.54
1:G:387:LEU:O	1:G:391:GLN:HG2	2.08	0.54
1:A:409:VAL:HG21	1:B:432:GLY:HA3	1.88	0.54
1:G:301:CYS:SG	2:G:502:IMP:H2	2.48	0.54
1:D:370:LEU:HD21	1:D:419:TYR:CD1	2.43	0.54
1:H:22:VAL:HG11	1:H:444:LYS:HG2	1.90	0.54
1:E:41:MET:HE1	1:E:431:LEU:HD21	1.89	0.54
1:D:339:TYR:O	1:D:342:ASP:HB2	2.08	0.53
1:A:382:ARG:HH12	1:A:392:LYS:HE2	1.73	0.53
1:A:88:SER:O	1:A:89:GLU:HG3	2.08	0.53
1:E:227:MET:HE3	1:E:263:LYS:HD3	1.91	0.53
1:C:301:CYS:SG	2:C:500:IMP:H2	2.48	0.53
1:A:300:ILE:HD13	1:A:383:GLY:HA2	1.90	0.53
1:G:370:LEU:HD21	1:G:419:TYR:CD1	2.43	0.53
1:D:227:MET:HE3	1:D:263:LYS:HD3	1.91	0.53
1:H:301:CYS:SG	2:H:502:IMP:H2	2.48	0.53
1:E:366:SER:OG	1:E:379:LYS:HE2	2.09	0.53
1:F:432:GLY:HA3	1:G:409:VAL:HG21	1.91	0.53
1:D:49:ASP:HA	1:D:70:HIS:CD2	2.44	0.53
1:A:62:ARG:HD3	1:A:205:TYR:CE2	2.44	0.52
1:C:300:ILE:HD13	1:C:383:GLY:HA2	1.91	0.52
1:E:70:HIS:CD2	1:E:72:ASN:H	2.27	0.52
1:B:373:TYR:C	1:B:373:TYR:CD1	2.83	0.52
1:D:227:MET:CE	1:D:263:LYS:HD3	2.39	0.52
1:G:72:ASN:ND2	1:G:392:LYS:HE2	2.25	0.52
1:D:465:GLU:OE2	1:H:9:THR:OG1	2.26	0.52
1:H:370:LEU:HD21	1:H:419:TYR:CD1	2.44	0.52
1:D:300:ILE:HD13	1:D:383:GLY:CA	2.41	0.51
1:B:301:CYS:SG	2:B:502:IMP:H2	2.51	0.51
1:D:292:LYS:HE3	1:D:334:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLU:CG	1:B:424:ARG:HH22	2.24	0.51
1:G:270:ILE:HG12	1:G:290:ALA:HB3	1.92	0.51
1:G:204:GLU:HG3	1:G:205:TYR:CD2	2.47	0.50
1:H:373:TYR:CD2	1:H:374:GLN:HG3	2.46	0.50
1:A:379:LYS:NZ	6:A:603:HOH:O	2.44	0.50
1:E:41:MET:HE1	1:E:43:LEU:HD12	1.93	0.50
1:H:6:ARG:HH22	1:H:457:GLU:CD	2.15	0.50
1:C:245:SER:HB2	1:C:253:ILE:HD11	1.94	0.49
1:E:33:LEU:HG	1:E:34:THR:HG23	1.95	0.49
1:A:479:ASN:ND2	1:D:409[A]:VAL:HG13	2.27	0.49
1:D:473:ILE:HG12	1:H:413:ILE:HD13	1.94	0.49
1:B:204:GLU:HG2	1:B:424:ARG:HH22	1.77	0.49
1:B:300:ILE:HD13	1:B:383:GLY:HA2	1.95	0.49
1:F:366:SER:OG	1:F:379:LYS:HE2	2.12	0.49
1:A:49:ASP:HA	1:A:70:HIS:CD2	2.47	0.49
1:E:245:SER:HB2	1:E:253:ILE:HD11	1.95	0.49
1:E:244:ASP:OD1	1:E:292:LYS:NZ	2.34	0.49
1:F:300:ILE:HD13	1:F:383:GLY:CA	2.41	0.49
1:C:473:ILE:HG12	1:E:413:ILE:HD13	1.95	0.49
1:B:248:GLY:HA2	1:B:253:ILE:HG13	1.95	0.48
1:B:49:ASP:HA	1:B:70:HIS:CD2	2.47	0.48
1:F:217:ARG:HD2	6:F:638:HOH:O	2.13	0.48
1:E:41:MET:HB2	1:E:41:MET:HE3	1.50	0.48
1:G:33:LEU:HG	1:G:34:THR:HG23	1.96	0.48
1:H:6:ARG:NH2	1:H:457:GLU:OE2	2.46	0.48
1:B:72:ASN:HB2	1:B:384:MET:HE3	1.95	0.48
1:E:465:GLU:OE2	1:F:9:THR:OG1	2.30	0.48
1:G:53:GLU:OE2	1:G:70:HIS:HE1	1.97	0.48
1:C:25:LYS:HG2	6:C:655:HOH:O	2.13	0.48
1:E:5:LYS:NZ	1:E:319:GLU:OE1	2.39	0.47
1:A:11:GLU:HB2	1:B:461:ALA:HB1	1.96	0.47
1:E:475:HIS:HB2	1:F:414:GLU:HB2	1.96	0.47
1:H:373:TYR:CE2	1:H:374:GLN:HG3	2.48	0.47
1:C:9:THR:OG1	1:G:465:GLU:OE2	2.30	0.47
1:C:85:VAL:HG11	1:C:218:VAL:HB	1.95	0.47
1:A:79:VAL:HG13	1:A:236:ALA:HB2	1.96	0.47
1:C:16:ARG:HD2	1:E:4:VAL:HG21	1.97	0.47
1:F:409[B]:VAL:HG13	1:F:410[B]:PRO:HD2	1.97	0.47
1:H:34:THR:OG1	1:H:268:ASP:OD2	2.21	0.47
1:A:31:THR:HG21	1:A:42:PRO:HB3	1.97	0.47
1:E:227:MET:CE	1:E:263:LYS:HD3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:CYS:SG	2:E:501:IMP:H2	2.55	0.47
1:B:72:ASN:HB2	1:B:384:MET:CE	2.44	0.47
1:F:296:GLY:HA2	1:F:301:CYS:SG	2.54	0.47
1:A:85:VAL:HG11	1:A:218:VAL:HB	1.97	0.46
1:B:270:ILE:HG12	1:B:290:ALA:HB3	1.98	0.46
1:C:251:LYS:HB2	1:G:21:GLU:HG2	1.97	0.46
1:G:365:GLU:HB2	1:G:423:ILE:HD12	1.96	0.46
1:G:476:GLU:HG2	1:G:481:LYS:HE2	1.98	0.46
1:E:53:GLU:OE2	1:E:70:HIS:HE1	1.99	0.46
1:F:21:GLU:HG2	1:G:251:LYS:HB2	1.98	0.46
1:B:227:MET:CE	1:B:263:LYS:HD3	2.46	0.46
1:B:251:LYS:HB2	1:H:21:GLU:HG2	1.96	0.46
1:G:241:VAL:HG23	1:G:269:LEU:HD12	1.97	0.46
1:G:300:ILE:HD13	1:G:383:GLY:HA2	1.97	0.45
1:H:296:GLY:HA3	1:H:304:ARG:HG3	1.98	0.45
1:D:300:ILE:HG13	1:D:300:ILE:H	1.49	0.45
1:F:300:ILE:H	1:F:300:ILE:HG13	1.44	0.45
1:E:370:LEU:HD21	1:E:419:TYR:CD1	2.52	0.45
1:B:422:SER:HB2	6:B:607:HOH:O	2.16	0.45
1:G:447:GLU:HG2	1:G:451:LYS:HE3	1.99	0.45
1:H:408:LEU:N	6:H:604:HOH:O	2.50	0.45
1:G:241:VAL:HG23	1:G:269:LEU:HD13	1.98	0.45
1:B:1:MET:N	1:H:318:ASP:OD1	2.50	0.45
1:C:53:GLU:OE2	1:C:70:HIS:HE1	2.00	0.45
1:C:70:HIS:CD2	1:C:72:ASN:H	2.32	0.45
1:G:11:GLU:HG3	6:G:657:HOH:O	2.17	0.44
1:G:32:LYS:HE3	1:G:34:THR:O	2.17	0.44
1:B:9:THR:OG1	1:H:465:GLU:OE2	2.28	0.44
1:A:88:SER:C	1:A:89:GLU:HG3	2.38	0.44
1:A:373:TYR:CD1	1:A:373:TYR:C	2.91	0.44
1:C:306:VAL:HG13	6:G:639:HOH:O	2.17	0.44
1:C:296:GLY:HA3	1:C:304:ARG:HE	1.82	0.44
1:A:296:GLY:HA3	1:A:304:ARG:HG3	2.00	0.44
1:F:301:CYS:SG	2:F:501:IMP:H2	2.58	0.44
1:E:41:MET:CE	1:E:43:LEU:HG	2.48	0.43
1:E:461:ALA:HB1	1:F:11:GLU:HB2	2.00	0.43
1:F:31:THR:HG21	1:F:42:PRO:HB3	1.99	0.43
1:G:86:LYS:HE2	1:G:237:GLY:O	2.18	0.43
1:D:301:CYS:SG	2:D:500:IMP:C2	3.06	0.43
1:F:272:GLY:HA3	1:F:273:ASN:HA	1.90	0.43
1:H:446:ILE:HG12	6:H:623:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:MET:HE3	1:B:263:LYS:HD3	1.99	0.43
1:D:475:HIS:HB2	1:H:414:GLU:HB2	1.99	0.43
1:H:373:TYR:HD2	1:H:374:GLN:N	2.17	0.43
1:B:34:THR:HB	1:B:289:ASP:HB3	2.01	0.43
1:E:79:VAL:HG13	1:E:236:ALA:HB2	2.00	0.43
1:E:300:ILE:HD13	1:E:383:GLY:CA	2.49	0.43
1:H:85:VAL:HG11	1:H:218:VAL:HB	2.00	0.43
1:A:89:GLU:HG2	1:A:202:ARG:HD2	2.01	0.43
1:H:296:GLY:HA2	1:H:301:CYS:SG	2.59	0.43
1:D:356:ILE:HG21	1:D:359:LEU:HB2	2.00	0.43
1:C:270:ILE:HG12	1:C:290:ALA:HB3	2.01	0.42
1:A:270:ILE:HG12	1:A:290:ALA:HB3	2.01	0.42
1:D:222:ILE:HD13	1:D:230:VAL:HG22	2.02	0.42
1:H:63:LEU:HD21	1:H:424:ARG:HD2	2.01	0.42
1:E:272:GLY:HA3	1:E:273:ASN:HA	1.92	0.42
1:C:375:GLY:HA2	1:H:375:GLY:O	2.20	0.42
1:C:227:MET:CE	1:C:263:LYS:HD3	2.49	0.42
1:F:365:GLU:HB2	1:F:423:ILE:HD12	2.00	0.42
1:G:300:ILE:HD13	1:G:383:GLY:CA	2.50	0.42
1:C:31:THR:HG21	1:C:42:PRO:HB3	2.01	0.42
1:F:248:GLY:HA2	1:F:253:ILE:HG13	2.02	0.42
1:H:300:ILE:HD13	1:H:383:GLY:CA	2.49	0.42
1:B:272:GLY:HA3	1:B:273:ASN:HA	1.93	0.42
1:C:432:GLY:HA3	1:E:409:VAL:HG21	2.01	0.42
1:A:4:VAL:HG23	1:A:5:LYS:HG2	2.01	0.41
1:F:277:ALA:HB2	1:F:319:GLU:HG2	2.02	0.41
1:G:70:HIS:CD2	1:G:72:ASN:H	2.33	0.41
1:A:373:TYR:HD1	1:A:373:TYR:C	2.24	0.41
1:F:62:ARG:HB3	1:F:205:TYR:CD1	2.55	0.41
1:H:365:GLU:HB2	1:H:423:ILE:HD12	2.01	0.41
1:B:35:LYS:HE3	1:B:35:LYS:HB3	1.78	0.41
1:F:350:GLY:HA2	1:F:450:GLN:OE1	2.20	0.41
1:C:300:ILE:HD13	1:C:383:GLY:CA	2.50	0.41
1:E:300:ILE:HG13	1:E:300:ILE:H	1.62	0.41
1:B:300:ILE:HD13	1:B:383:GLY:CA	2.51	0.41
1:A:473:ILE:HG12	1:D:413:ILE:HD13	2.01	0.41
1:F:363:THR:HA	1:F:421:GLY:O	2.21	0.41
1:C:304:ARG:HG2	1:C:309:VAL:O	2.21	0.41
1:D:366:SER:OG	1:D:379:LYS:HE2	2.20	0.41
1:D:474:THR:HG22	1:H:416:ARG:NH1	2.36	0.41
1:F:86:LYS:HD3	1:F:218:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:ILE:HG12	1:F:413:ILE:HD13	2.02	0.41
1:G:79:VAL:HG13	1:G:236:ALA:HB2	2.03	0.41
1:A:301:CYS:SG	2:A:501:IMP:C2	3.09	0.41
1:G:300:ILE:HG13	1:G:300:ILE:H	1.54	0.41
1:G:217:ARG:HA	1:G:239:ASP:OD2	2.21	0.40
1:D:217:ARG:HD2	6:D:614:HOH:O	2.20	0.40
1:E:376:ARG:HH22	1:E:481:LYS:NZ	2.19	0.40
1:G:314:ILE:HD12	1:G:349:VAL:HG21	2.03	0.40
1:A:300:ILE:HD13	1:A:383:GLY:CA	2.50	0.40
1:H:300:ILE:H	1:H:300:ILE:HG13	1.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	351/406 (86%)	344 (98%)	7 (2%)	0	100	100
1	B	355/406 (87%)	348 (98%)	7 (2%)	0	100	100
1	C	350/406 (86%)	343 (98%)	7 (2%)	0	100	100
1	D	347/406 (86%)	338 (97%)	9 (3%)	0	100	100
1	E	348/406 (86%)	341 (98%)	7 (2%)	0	100	100
1	F	349/406 (86%)	343 (98%)	6 (2%)	0	100	100
1	G	348/406 (86%)	339 (97%)	9 (3%)	0	100	100
1	H	360/406 (89%)	353 (98%)	7 (2%)	0	100	100
All	All	2808/3248 (86%)	2749 (98%)	59 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	281/323 (87%)	275 (98%)	6 (2%)	53	55
1	B	284/323 (88%)	280 (99%)	4 (1%)	67	70
1	C	280/323 (87%)	278 (99%)	2 (1%)	84	87
1	D	278/323 (86%)	273 (98%)	5 (2%)	59	61
1	E	278/323 (86%)	278 (100%)	0	100	100
1	F	280/323 (87%)	279 (100%)	1 (0%)	91	93
1	G	278/323 (86%)	276 (99%)	2 (1%)	84	87
1	H	286/323 (88%)	284 (99%)	2 (1%)	84	87
All	All	2245/2584 (87%)	2223 (99%)	22 (1%)	78	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	41	MET
1	A	203	LYS
1	A	373	TYR
1	A	378	TYR
1	A	440	TYR
1	B	2	LYS
1	B	373	TYR
1	B	378	TYR
1	B	449	PHE
1	C	364	ASP
1	C	419	TYR
1	D	41	MET
1	D	408[A]	LEU
1	D	408[B]	LEU
1	D	409[A]	VAL
1	D	409[B]	VAL
1	F	41	MET
1	G	41	MET

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Mol	Chain	Res	Type
1	G	87	LYS
1	H	373	TYR
1	H	424	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	70	HIS
1	E	70	HIS
1	F	70	HIS
1	F	209	ASN
1	G	70	HIS
1	G	391	GLN
1	H	70	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IMP	H	502	-	21,25,25	1.12	3 (14%)	23,38,38	1.57	4 (17%)
3	8L4	D	501	-	25,25,25	1.51	6 (24%)	32,35,35	1.22	2 (6%)
3	8L4	F	502	-	25,25,25	1.08	3 (12%)	32,35,35	1.12	4 (12%)
3	8L4	H	503	-	25,25,25	1.15	3 (12%)	32,35,35	1.29	3 (9%)
3	8L4	C	501	-	25,25,25	1.39	3 (12%)	32,35,35	1.31	3 (9%)
3	8L4	B	503	-	25,25,25	1.59	6 (24%)	32,35,35	1.00	0
2	IMP	D	500	-	21,25,25	1.17	2 (9%)	23,38,38	1.50	3 (13%)
3	8L4	F	503	-	25,25,25	1.64	5 (20%)	32,35,35	1.33	1 (3%)
2	IMP	G	502	-	21,25,25	1.27	3 (14%)	23,38,38	1.53	4 (17%)
2	IMP	A	501	-	21,25,25	1.37	3 (14%)	23,38,38	1.39	2 (8%)
2	IMP	E	501	-	21,25,25	1.20	3 (14%)	23,38,38	1.46	4 (17%)
2	IMP	B	502	-	21,25,25	1.20	3 (14%)	23,38,38	1.52	4 (17%)
2	IMP	F	501	-	21,25,25	1.33	3 (14%)	23,38,38	1.32	2 (8%)
4	EDO	E	503	-	3,3,3	0.33	0	2,2,2	0.40	0
3	8L4	E	502	-	25,25,25	1.12	3 (12%)	32,35,35	1.02	2 (6%)
2	IMP	C	500	-	21,25,25	1.18	3 (14%)	23,38,38	1.75	4 (17%)
4	EDO	A	503	-	3,3,3	0.55	0	2,2,2	0.14	0
3	8L4	A	502	-	25,25,25	1.54	4 (16%)	32,35,35	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	H	502	-	-	0/6/26/26	0/3/3/3
3	8L4	D	501	-	-	3/19/21/21	0/2/2/2
3	8L4	F	502	-	-	0/19/21/21	0/2/2/2
3	8L4	H	503	-	-	2/19/21/21	0/2/2/2
3	8L4	C	501	-	-	2/19/21/21	0/2/2/2
3	8L4	B	503	-	-	0/19/21/21	0/2/2/2
2	IMP	D	500	-	-	0/6/26/26	0/3/3/3
3	8L4	F	503	-	-	2/19/21/21	0/2/2/2
2	IMP	G	502	-	-	0/6/26/26	0/3/3/3
2	IMP	A	501	-	-	0/6/26/26	0/3/3/3
2	IMP	E	501	-	-	0/6/26/26	0/3/3/3
2	IMP	B	502	-	-	0/6/26/26	0/3/3/3
2	IMP	F	501	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	503	-	-	0/1/1/1	-
3	8L4	E	502	-	-	2/19/21/21	0/2/2/2
2	IMP	C	500	-	-	0/6/26/26	0/3/3/3
4	EDO	A	503	-	-	0/1/1/1	-
3	8L4	A	502	-	-	2/19/21/21	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	IMP	C2-N3	4.15	1.38	1.32
2	A	501	IMP	C2-N3	3.99	1.38	1.32
3	F	503	8L4	C17-N4	-3.80	1.33	1.41
3	A	502	8L4	C11-C1	-3.79	1.49	1.53
2	E	501	IMP	C2-N3	3.78	1.38	1.32
3	B	503	8L4	C11-C1	-3.77	1.49	1.53
2	G	502	IMP	C2-N3	3.75	1.38	1.32
3	B	503	8L4	C17-N4	-3.70	1.34	1.41
3	D	501	8L4	C17-N4	-3.65	1.34	1.41
2	B	502	IMP	C2-N3	3.59	1.37	1.32
2	D	500	IMP	C2-N3	3.51	1.37	1.32
2	C	500	IMP	C2-N3	3.32	1.37	1.32
3	F	503	8L4	C11-C1	-3.32	1.49	1.53
3	C	501	8L4	C17-N4	-3.30	1.35	1.41
2	H	502	IMP	C2-N3	3.23	1.37	1.32
3	F	502	8L4	C11-C1	-3.19	1.49	1.53
3	H	503	8L4	C11-C1	-3.07	1.49	1.53
2	C	500	IMP	C6-N1	3.01	1.38	1.33
3	A	502	8L4	C17-N4	-2.96	1.35	1.41
3	D	501	8L4	C11-C1	-2.94	1.50	1.53
2	G	502	IMP	C6-N1	2.90	1.38	1.33
2	F	501	IMP	C2-N1	2.89	1.39	1.33
3	F	503	8L4	C11-N3	-2.87	1.44	1.47
2	B	502	IMP	C6-N1	2.86	1.38	1.33
2	A	501	IMP	C6-N1	2.82	1.37	1.33
2	D	500	IMP	C6-N1	2.81	1.37	1.33
2	A	501	IMP	C2-N1	2.81	1.39	1.33
2	F	501	IMP	C6-N1	2.73	1.37	1.33
3	H	503	8L4	C20-CL	2.71	1.80	1.74
3	E	502	8L4	C11-C1	-2.68	1.50	1.53
3	A	502	8L4	C11-N3	-2.64	1.44	1.47
2	E	501	IMP	C6-N1	2.61	1.37	1.33
3	F	503	8L4	C10-N4	-2.55	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	8L4	C10-N4	-2.53	1.32	1.37
3	E	502	8L4	C20-CL	2.51	1.80	1.74
2	H	502	IMP	C6-N1	2.47	1.37	1.33
3	A	502	8L4	C10-N4	-2.41	1.32	1.37
2	G	502	IMP	C2-N1	2.38	1.38	1.33
3	B	503	8L4	C11-N3	-2.37	1.44	1.47
2	E	501	IMP	C2-N1	2.36	1.38	1.33
3	C	501	8L4	C10-N4	-2.36	1.32	1.37
2	H	502	IMP	C2-N1	2.34	1.38	1.33
3	B	503	8L4	C20-CL	2.33	1.79	1.74
3	F	503	8L4	C20-CL	2.33	1.79	1.74
3	F	502	8L4	C20-CL	2.30	1.79	1.74
3	E	502	8L4	C17-N4	-2.28	1.37	1.41
2	B	502	IMP	C2-N1	2.25	1.38	1.33
3	C	501	8L4	C11-C1	-2.14	1.51	1.53
2	C	500	IMP	C2-N1	2.14	1.37	1.33
3	F	502	8L4	C17-N4	-2.11	1.37	1.41
3	D	501	8L4	C20-CL	2.08	1.79	1.74
3	H	503	8L4	C17-N4	-2.07	1.37	1.41
3	B	503	8L4	C10-N4	-2.05	1.33	1.37
3	D	501	8L4	C7-N1	-2.03	1.31	1.35
3	D	501	8L4	C10-N3	-2.03	1.31	1.35
3	B	503	8L4	C7-N1	-2.02	1.31	1.35

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	503	8L4	C5-C7-N1	5.47	123.17	114.69
2	C	500	IMP	N3-C2-N1	-5.19	120.56	128.68
3	C	501	8L4	C5-C7-N1	5.06	122.54	114.69
3	D	501	8L4	C5-C7-N1	4.94	122.34	114.69
2	G	502	IMP	N3-C2-N1	-4.80	121.18	128.68
2	H	502	IMP	N3-C2-N1	-4.73	121.28	128.68
2	A	501	IMP	N3-C2-N1	-4.56	121.56	128.68
2	D	500	IMP	N3-C2-N1	-4.51	121.63	128.68
2	F	501	IMP	N3-C2-N1	-4.26	122.02	128.68
2	B	502	IMP	N3-C2-N1	-4.23	122.07	128.68
2	E	501	IMP	N3-C2-N1	-4.18	122.14	128.68
3	H	503	8L4	C5-C7-N1	3.30	119.80	114.69
3	H	503	8L4	C12-C11-C13	-3.16	105.76	109.55
2	C	500	IMP	C1'-N9-C4	-3.15	121.11	126.64
2	H	502	IMP	C2-N1-C6	2.97	120.86	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	502	IMP	C2-N1-C6	2.94	120.81	115.88
2	C	500	IMP	C2-N1-C6	2.90	120.73	115.88
2	D	500	IMP	C2-N1-C6	2.89	120.72	115.88
3	E	502	8L4	C12-C11-N3	2.74	115.26	107.89
2	D	500	IMP	C4-C5-N7	-2.64	106.64	109.40
2	B	502	IMP	C2-N1-C6	2.61	120.25	115.88
2	G	502	IMP	O3P-P-O2P	2.60	117.56	107.64
2	C	500	IMP	C4-C5-N7	-2.59	106.70	109.40
2	A	501	IMP	C2-N1-C6	2.57	120.18	115.88
2	H	502	IMP	C4-C5-N7	-2.56	106.73	109.40
2	B	502	IMP	C4-C5-N7	-2.55	106.74	109.40
2	E	501	IMP	C2-N1-C6	2.55	120.15	115.88
3	C	501	8L4	C12-C11-N3	2.50	114.62	107.89
3	E	502	8L4	C5-C7-N1	2.49	118.54	114.69
3	C	501	8L4	C12-C11-C13	-2.36	106.72	109.55
3	H	503	8L4	C12-C11-N3	2.28	114.02	107.89
2	G	502	IMP	C1'-N9-C4	-2.28	122.64	126.64
3	F	502	8L4	C12-C11-N3	2.26	113.97	107.89
3	F	502	8L4	C12-C11-C13	-2.22	106.89	109.55
2	H	502	IMP	C1'-N9-C4	-2.14	122.88	126.64
2	E	501	IMP	C4-C5-N7	-2.14	107.17	109.40
2	E	501	IMP	C1'-N9-C4	-2.13	122.90	126.64
2	B	502	IMP	C1'-N9-C4	-2.12	122.91	126.64
3	D	501	8L4	C6-C5-C7	-2.07	116.79	120.30
2	F	501	IMP	C2-N1-C6	2.05	119.31	115.88
3	F	502	8L4	C5-C7-N1	2.01	117.80	114.69
3	F	502	8L4	C6-C1-C11	-2.00	117.50	120.70

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	502	8L4	C4-C5-C7-N1
3	E	502	8L4	C6-C5-C7-N1
3	D	501	8L4	C6-C5-C7-N1
3	H	503	8L4	C4-C5-C7-N1
3	H	503	8L4	C6-C5-C7-N1
3	F	503	8L4	C4-C5-C7-N1
3	F	503	8L4	C6-C5-C7-N1
3	D	501	8L4	C12-C11-N3-C10
3	D	501	8L4	C4-C5-C7-N1
3	A	502	8L4	C4-C5-C7-N1

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Mol	Chain	Res	Type	Atoms
3	C	501	8L4	C4-C5-C7-N1
3	A	502	8L4	C6-C5-C7-N1
3	C	501	8L4	C6-C5-C7-N1

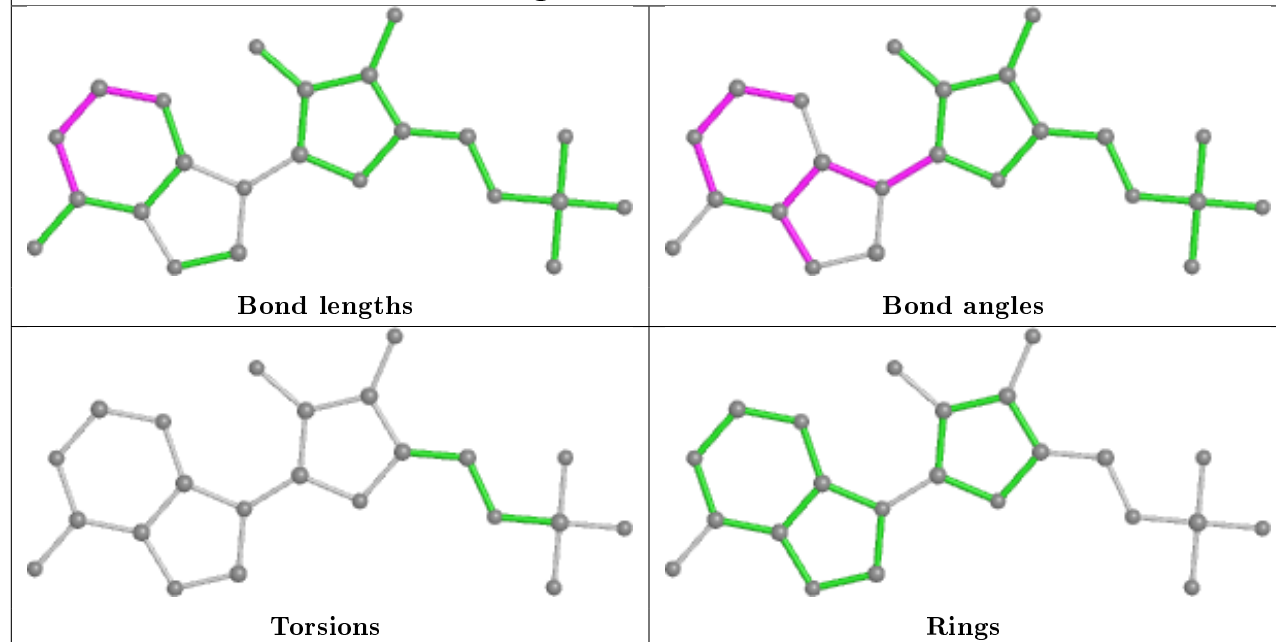
There are no ring outliers.

8 monomers are involved in 10 short contacts:

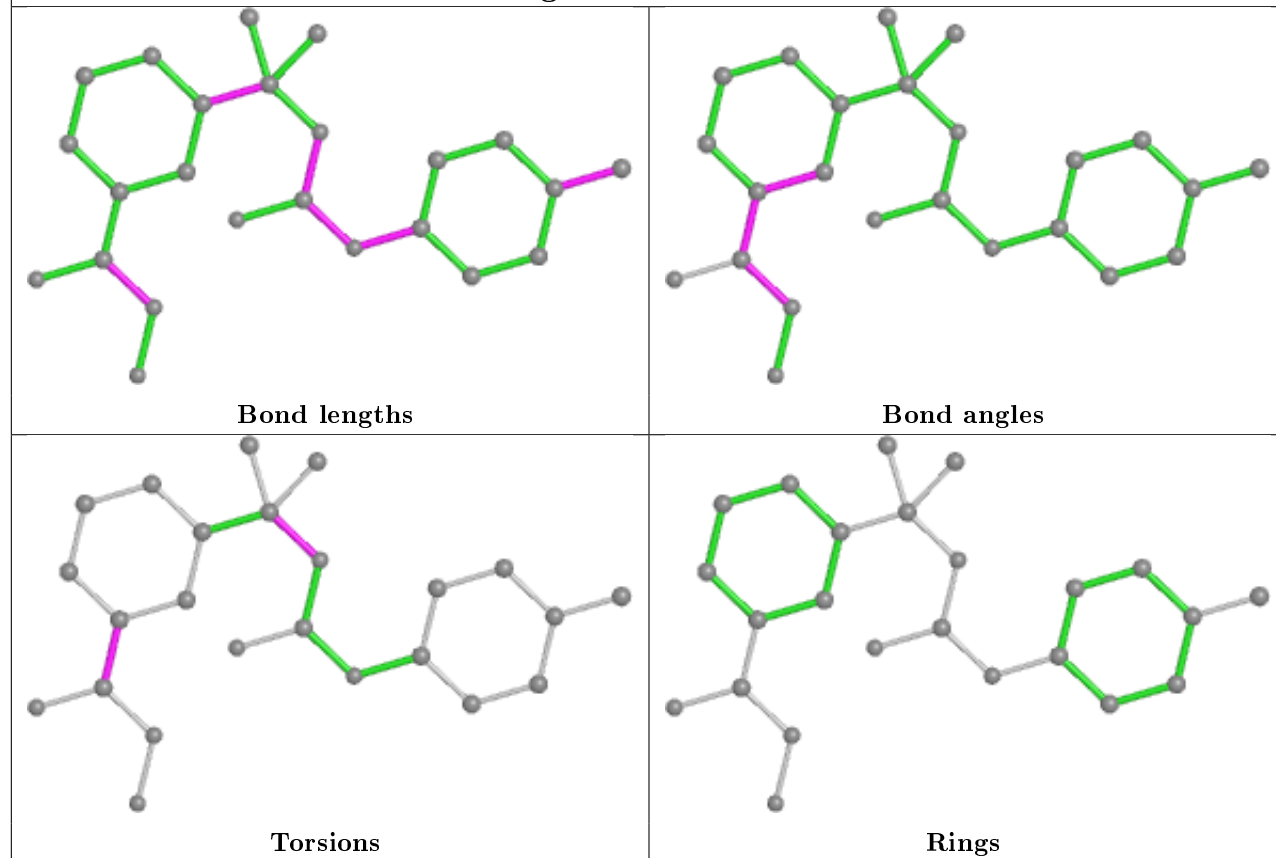
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	502	IMP	1	0
2	D	500	IMP	2	0
2	G	502	IMP	1	0
2	A	501	IMP	2	0
2	E	501	IMP	1	0
2	B	502	IMP	1	0
2	F	501	IMP	1	0
2	C	500	IMP	1	0

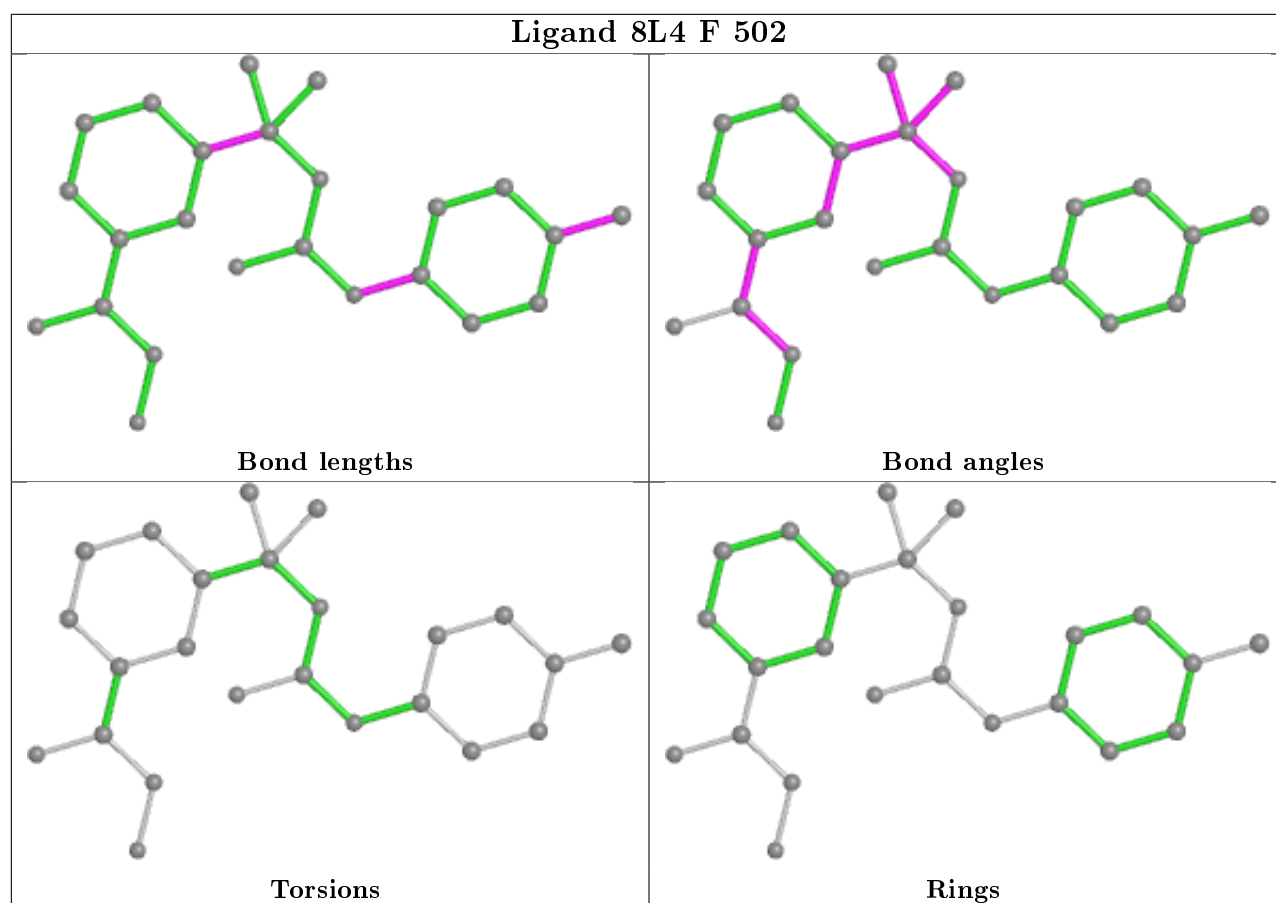
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IMP H 502

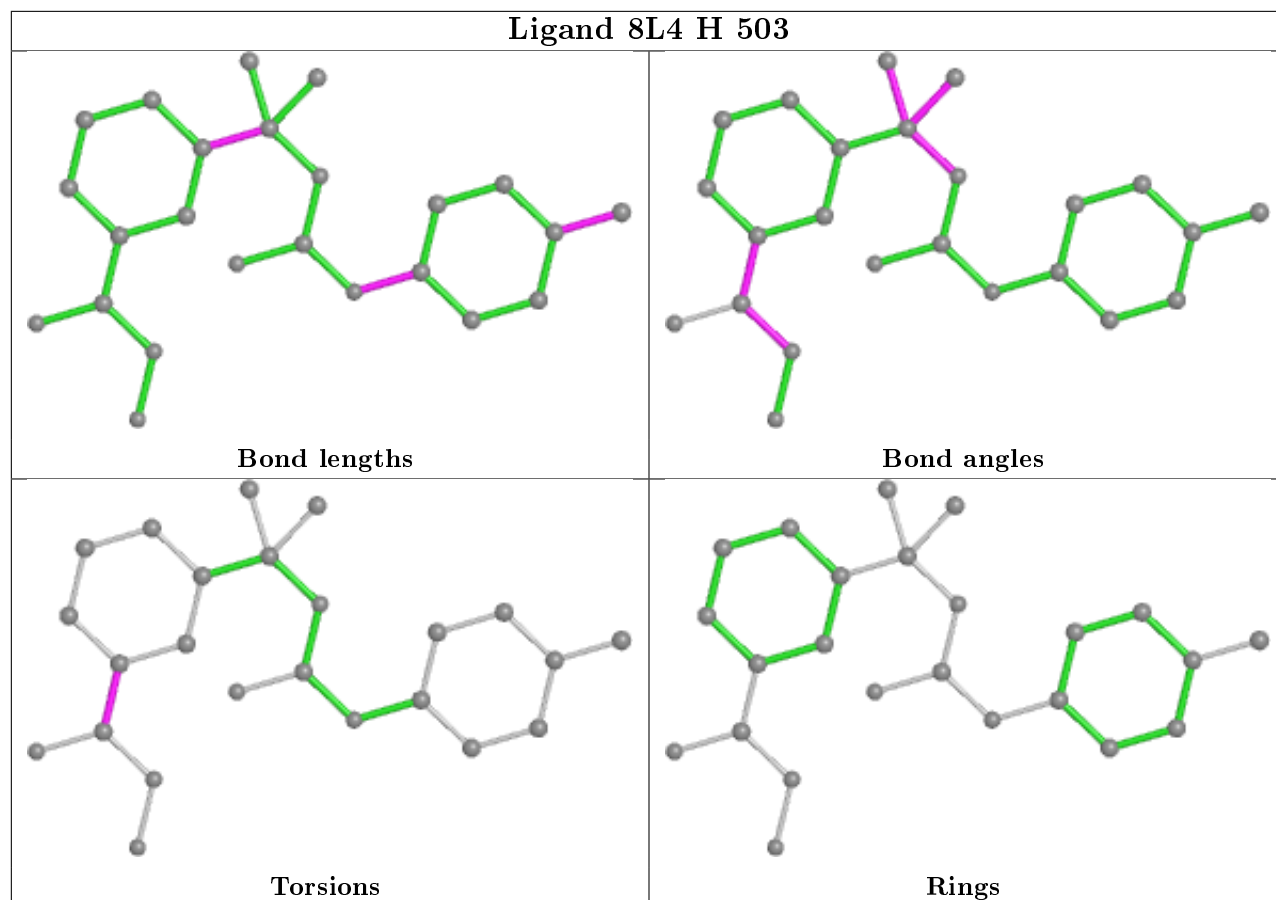


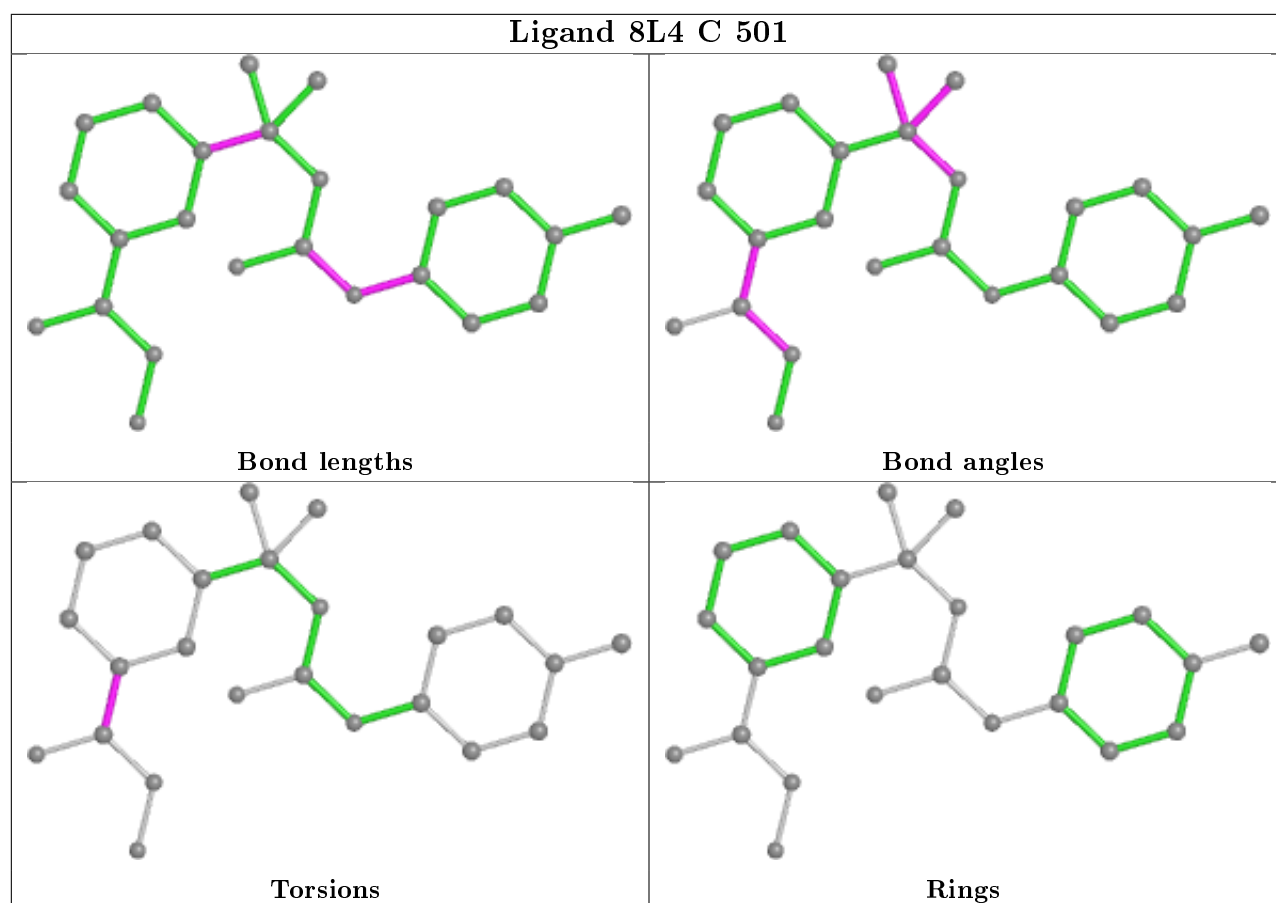
Ligand 8L4 D 501



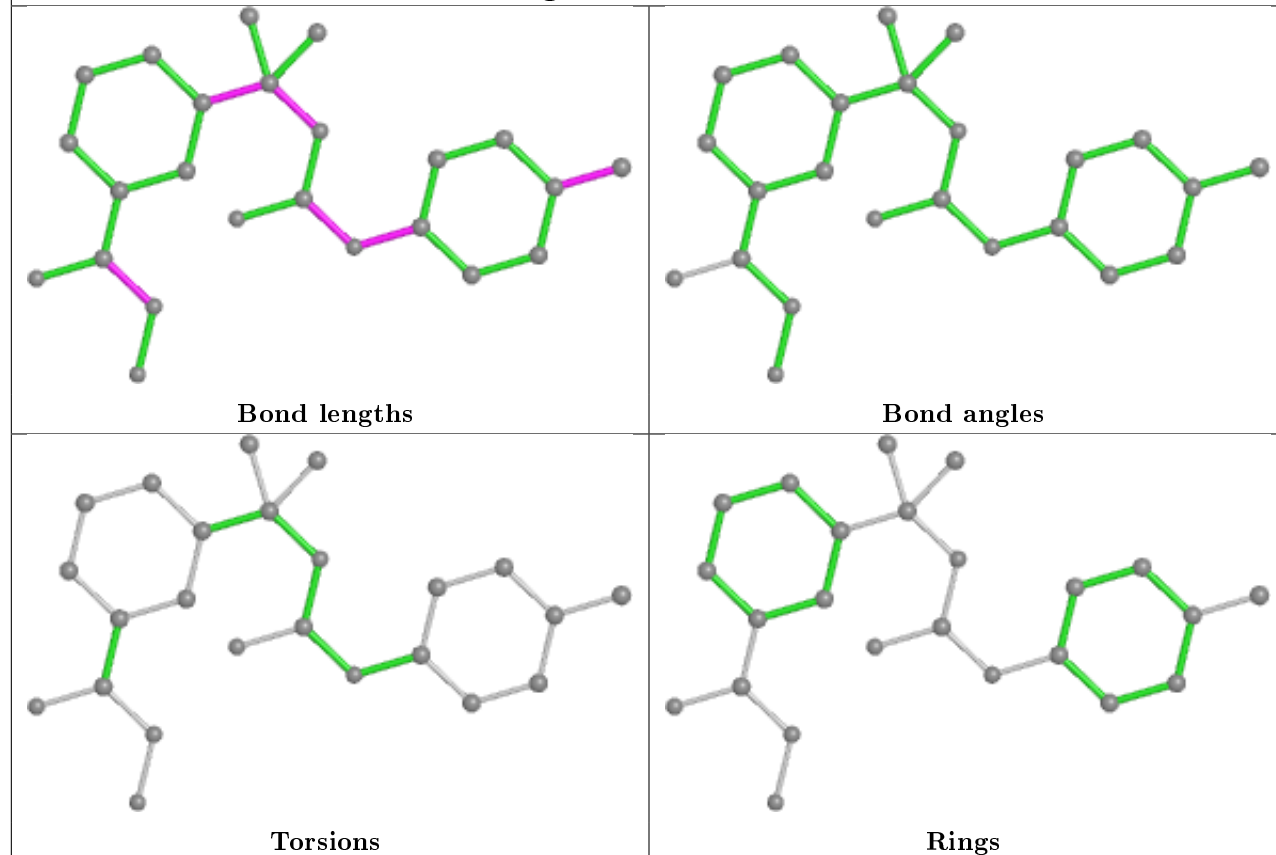


Ligand 8L4 H 503

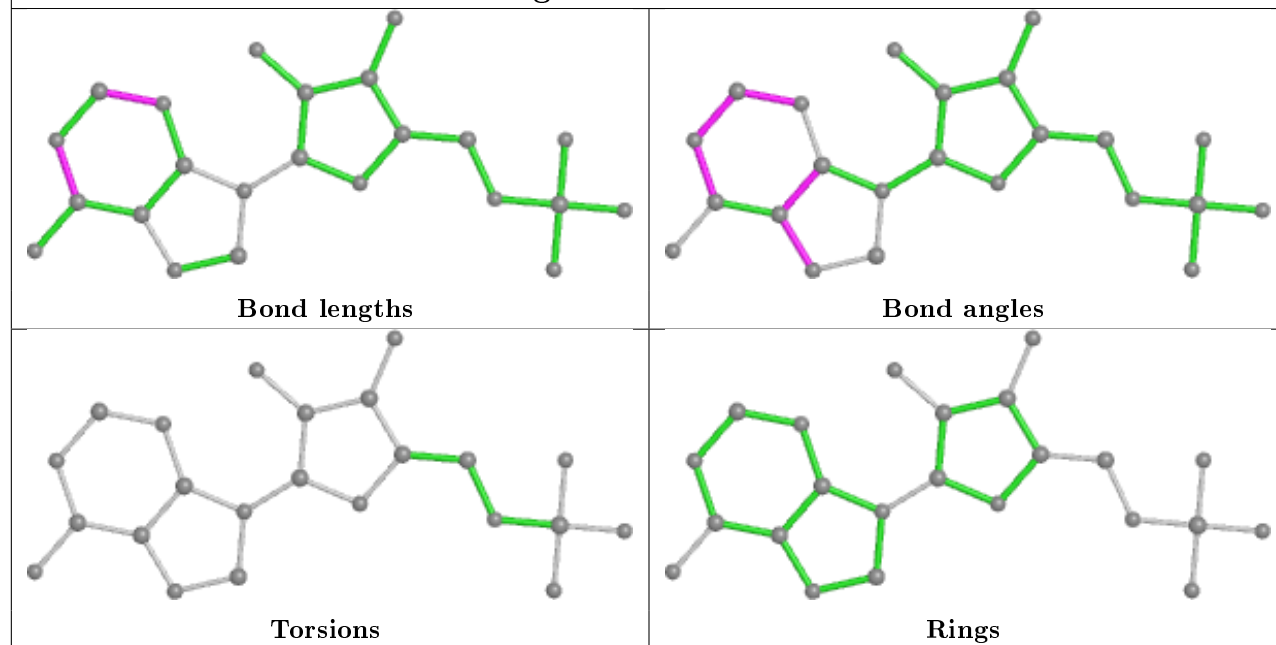




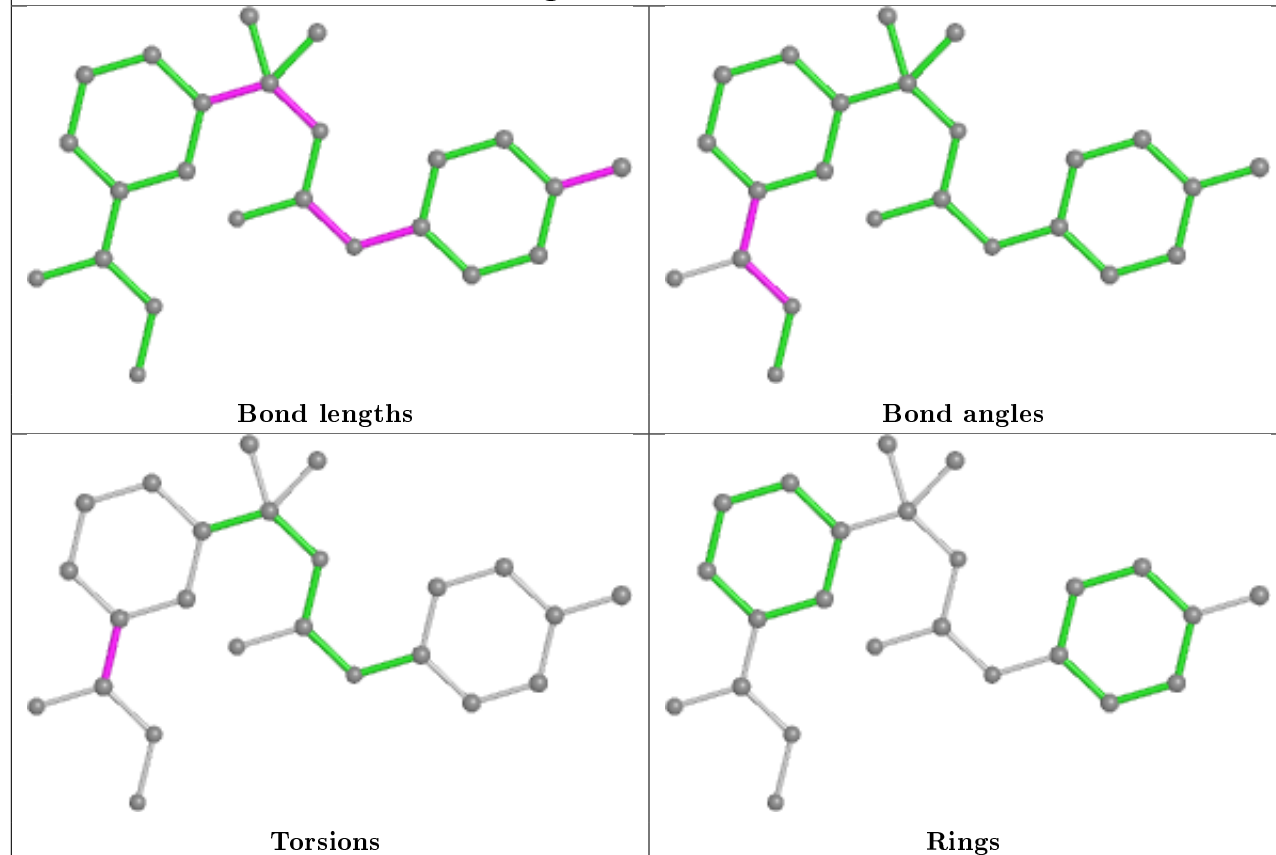
Ligand 8L4 B 503



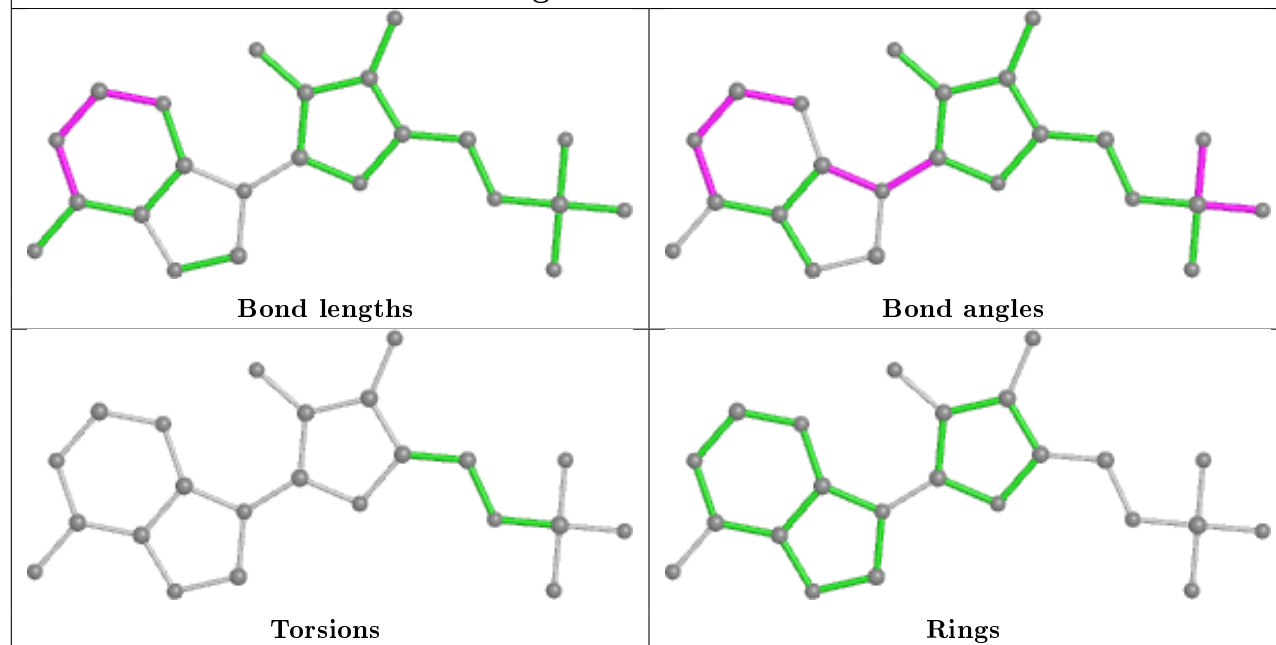
Ligand IMP D 500



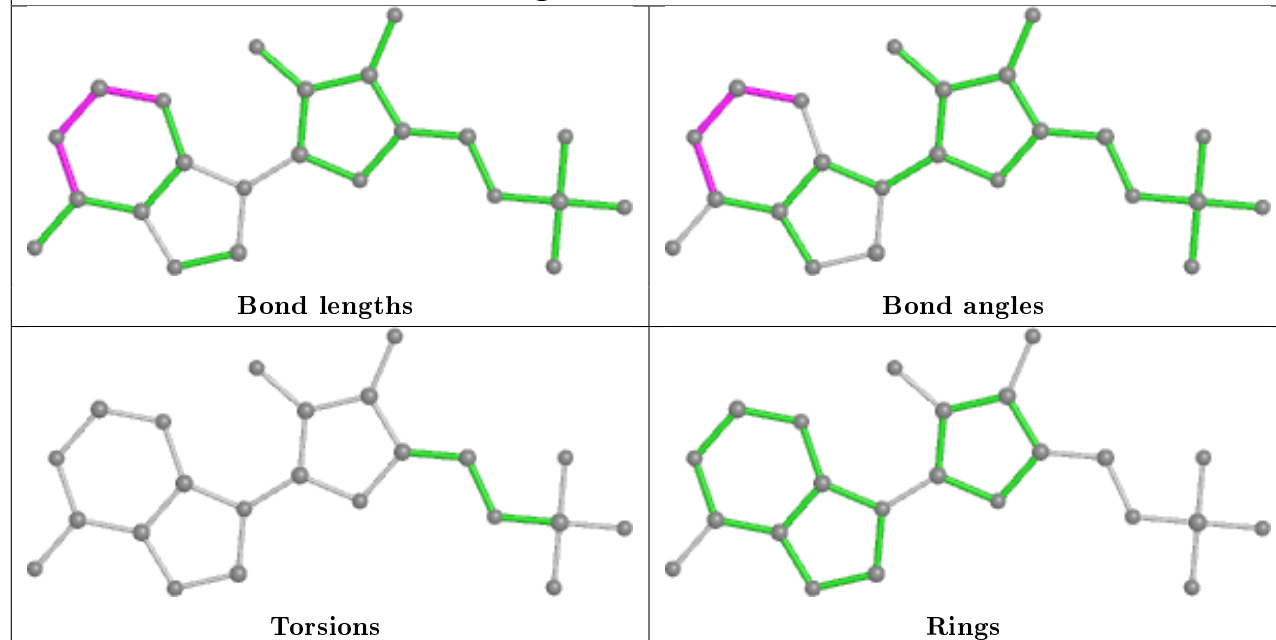
Ligand 8L4 F 503



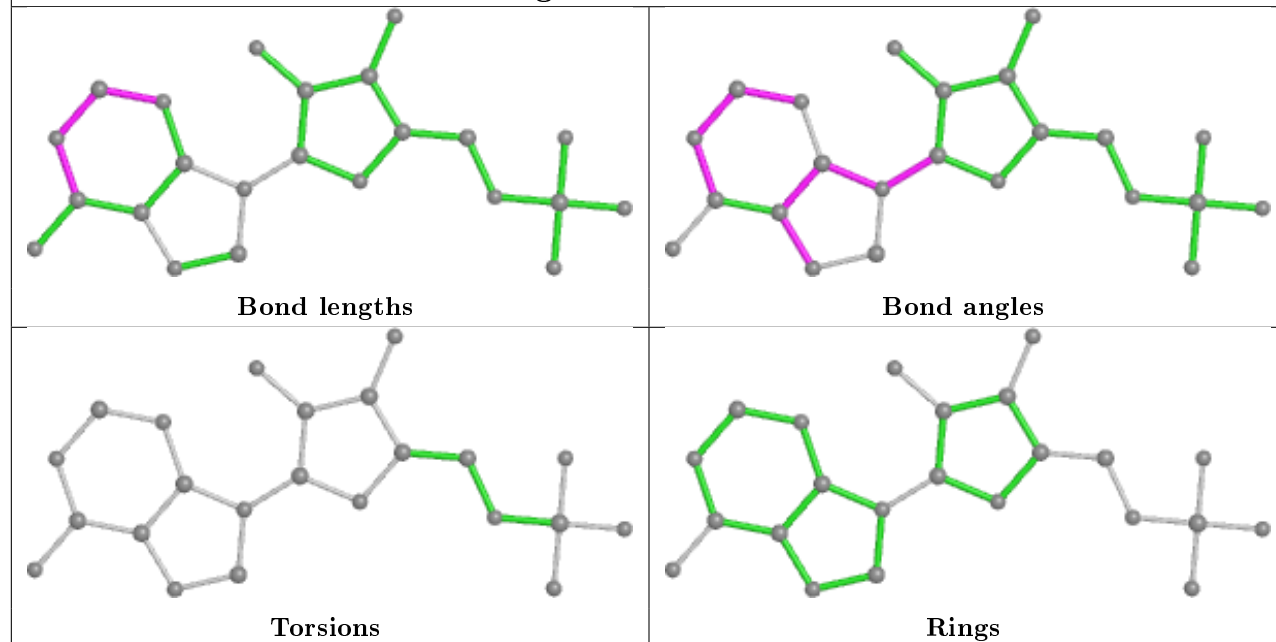
Ligand IMP G 502



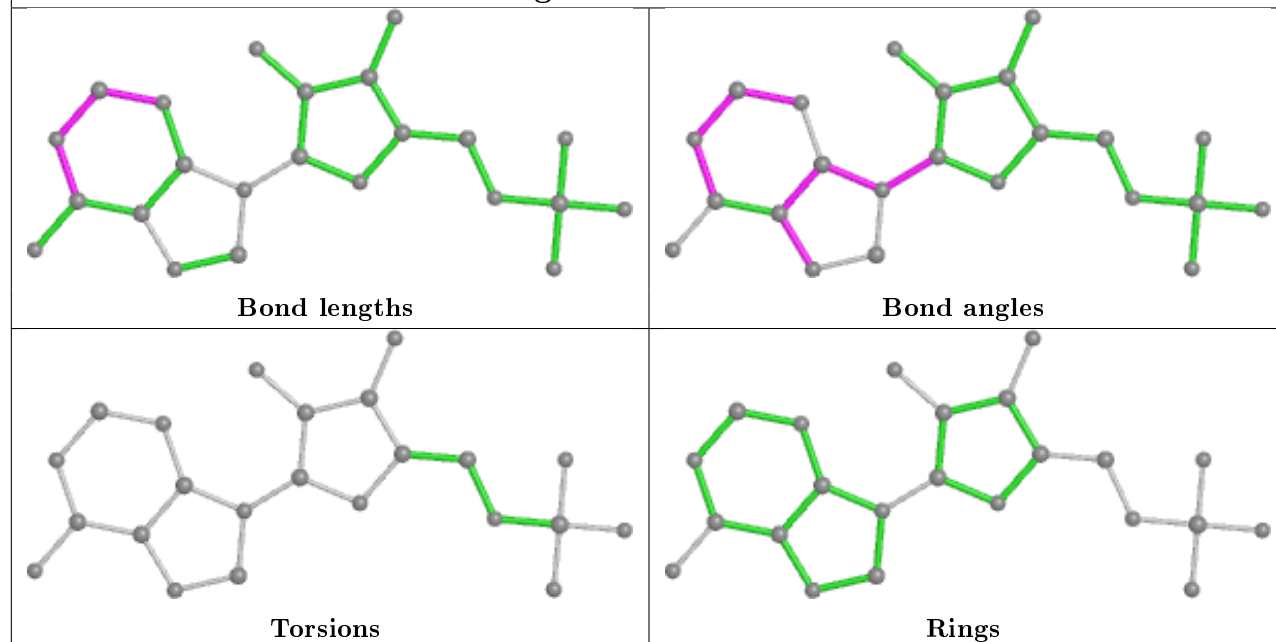
Ligand IMP A 501



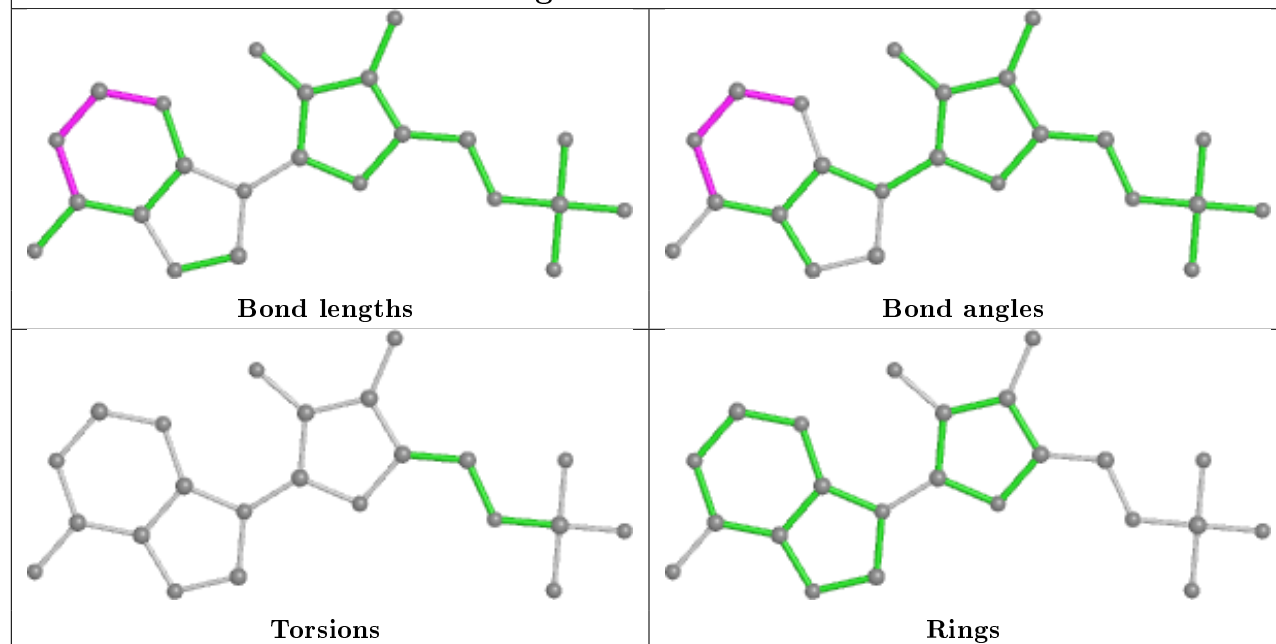
Ligand IMP E 501



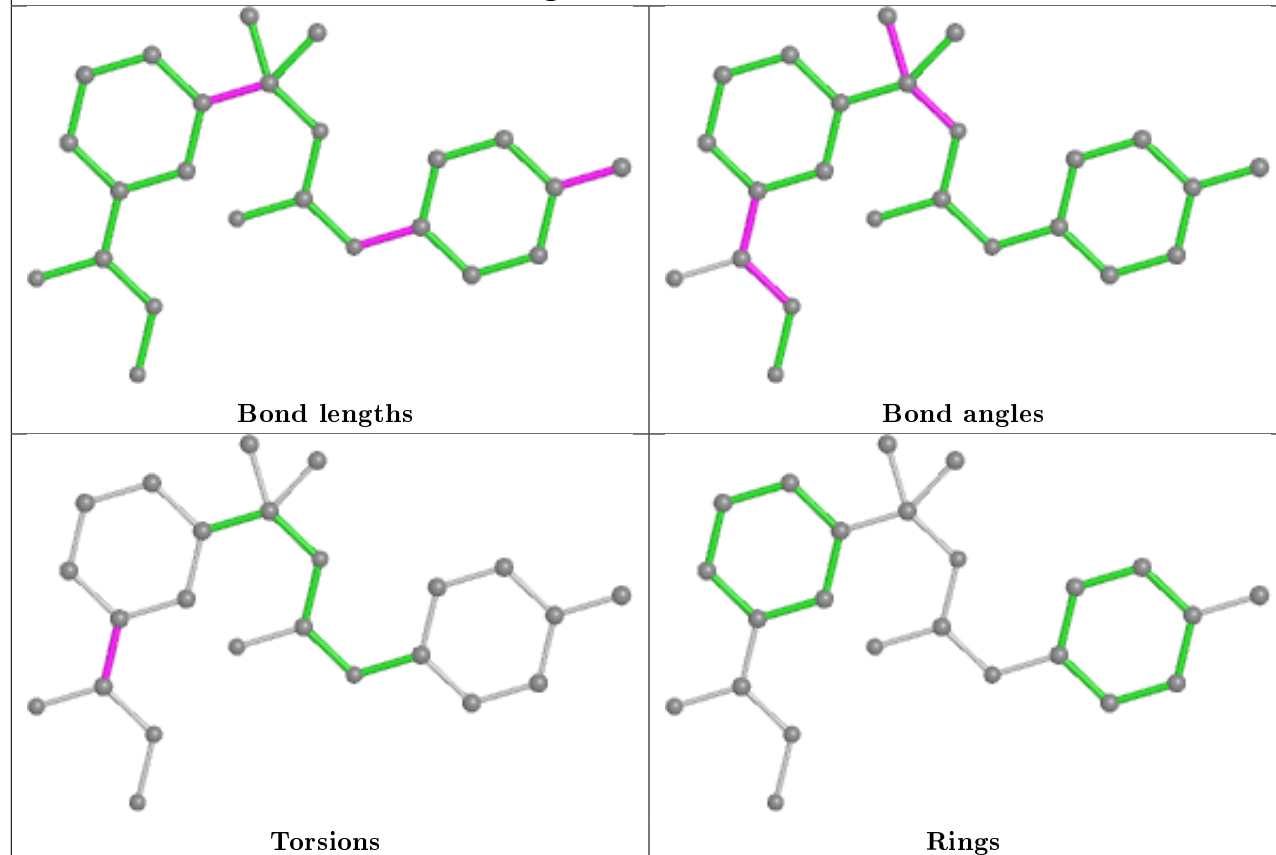
Ligand IMP B 502



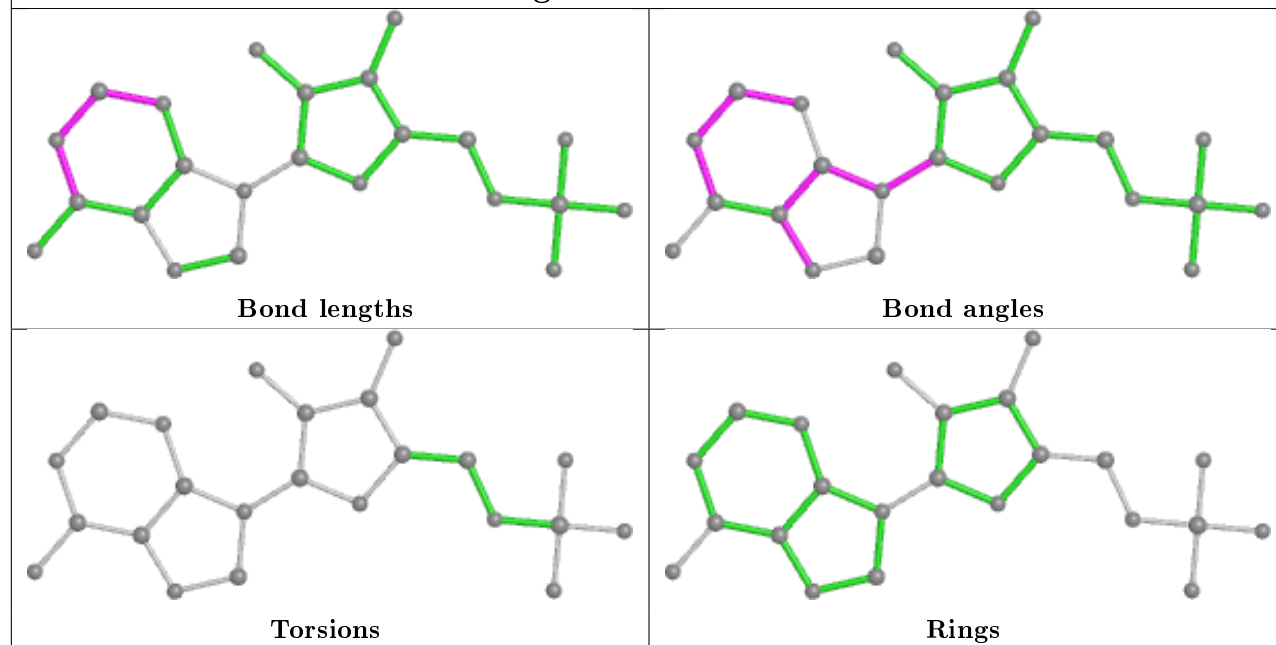
Ligand IMP F 501

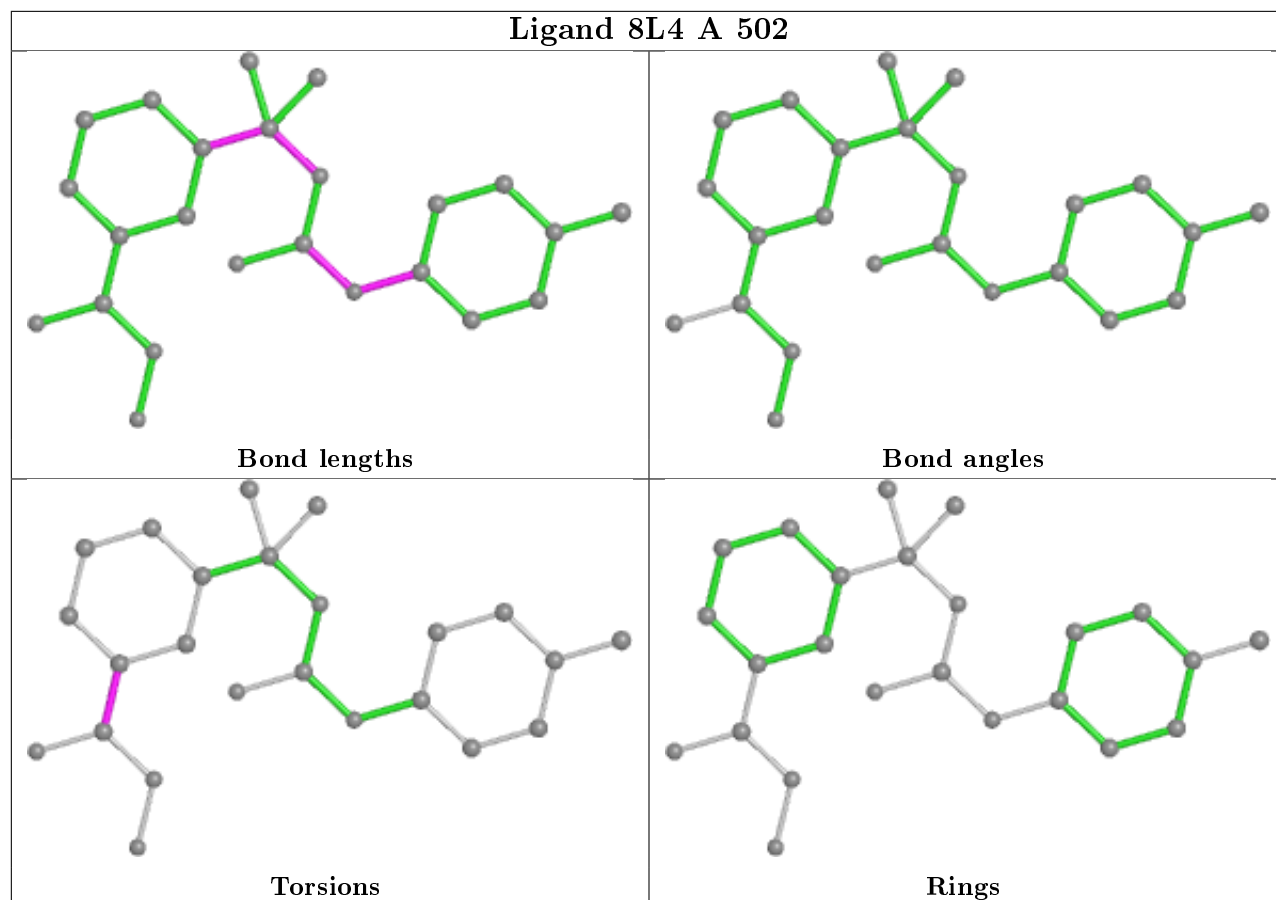


Ligand 8L4 E 502



Ligand IMP C 500





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	356/406 (87%)	-0.31	7 (1%) 65 64	17, 26, 44, 95	0
1	B	361/406 (88%)	-0.21	6 (1%) 70 69	17, 25, 48, 79	0
1	C	356/406 (87%)	-0.17	9 (2%) 57 57	19, 27, 52, 101	0
1	D	351/406 (86%)	-0.22	6 (1%) 70 69	18, 26, 45, 75	0
1	E	354/406 (87%)	-0.19	4 (1%) 80 80	20, 28, 48, 75	0
1	F	353/406 (86%)	-0.08	11 (3%) 49 48	19, 29, 48, 76	0
1	G	353/406 (86%)	-0.24	5 (1%) 75 74	20, 28, 46, 80	0
1	H	364/406 (89%)	0.04	9 (2%) 57 57	19, 28, 49, 81	0
All	All	2848/3248 (87%)	-0.17	57 (2%) 65 64	17, 27, 48, 101	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	373	TYR	5.1
1	B	199	LEU	4.8
1	F	408[A]	LEU	4.8
1	A	202	ARG	4.6
1	B	200	LYS	4.4
1	E	4	VAL	3.9
1	D	0	ALA	3.8
1	F	204	GLU	3.8
1	A	203	LYS	3.7
1	F	205	TYR	3.7
1	C	0	ALA	3.6
1	C	88	SER	3.3
1	D	476	GLU	3.3
1	A	-1	ASN	3.2
1	B	407	LYS	3.2
1	G	476	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	374	GLN	3.2
1	D	376	ARG	3.2
1	D	408[A]	LEU	3.2
1	G	481	LYS	3.2
1	F	0	ALA	3.1
1	A	244	ASP	3.1
1	F	203	LYS	3.0
1	C	373	TYR	2.8
1	C	375	GLY	2.8
1	F	476	GLU	2.7
1	C	89	GLU	2.7
1	F	213	PHE	2.7
1	E	204	GLU	2.6
1	G	203	LYS	2.6
1	H	392	LYS	2.6
1	E	373	TYR	2.6
1	H	375	GLY	2.6
1	A	408	LEU	2.6
1	B	373	TYR	2.6
1	F	481	LYS	2.5
1	C	201	LYS	2.5
1	G	391	GLN	2.5
1	H	391	GLN	2.5
1	C	202	ARG	2.4
1	C	476	GLU	2.4
1	H	408	LEU	2.4
1	A	204	GLU	2.4
1	B	394	SER	2.4
1	F	4	VAL	2.3
1	F	244	ASP	2.3
1	E	482	VAL	2.2
1	H	0	ALA	2.2
1	H	476	GLU	2.2
1	D	475	HIS	2.1
1	A	4	VAL	2.1
1	F	87	LYS	2.1
1	C	374	GLN	2.1
1	B	201	LYS	2.1
1	D	244	ASP	2.0
1	G	369	GLU	2.0
1	H	333	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

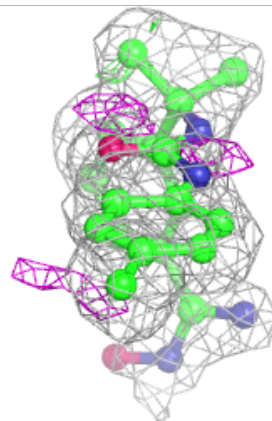
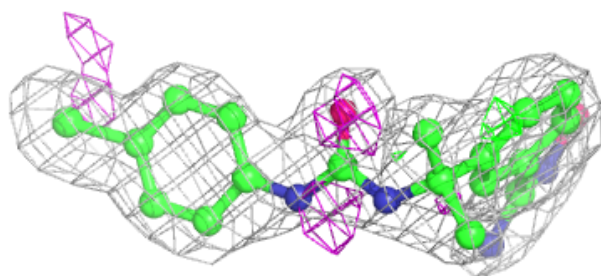
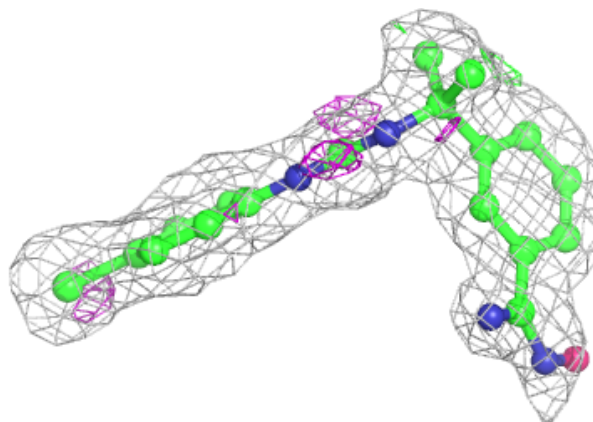
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	E	503	4/4	0.85	0.19	45,48,48,49	0
3	8L4	F	503	24/24	0.89	0.15	24,33,41,55	0
3	8L4	E	502	24/24	0.93	0.14	27,29,39,52	0
3	8L4	D	501	24/24	0.93	0.12	22,28,34,55	0
3	8L4	F	502	24/24	0.93	0.12	22,26,35,50	0
3	8L4	A	502	24/24	0.93	0.12	21,27,35,51	0
3	8L4	H	503	24/24	0.94	0.10	24,30,40,54	0
3	8L4	C	501	24/24	0.94	0.14	20,32,37,59	0
3	8L4	B	503	24/24	0.94	0.13	21,25,31,46	0
4	EDO	A	503	4/4	0.95	0.08	23,31,37,41	0
2	IMP	G	502	23/23	0.97	0.09	18,23,28,29	0
2	IMP	B	502	23/23	0.97	0.10	16,20,23,25	0
2	IMP	F	501	23/23	0.97	0.10	18,24,26,27	0
2	IMP	E	501	23/23	0.97	0.10	18,25,27,32	0
2	IMP	D	500	23/23	0.98	0.10	16,20,22,24	0
2	IMP	H	502	23/23	0.98	0.15	20,25,29,32	0
2	IMP	C	500	23/23	0.98	0.09	21,23,28,29	0
2	IMP	A	501	23/23	0.98	0.10	16,20,23,23	0
5	K	H	501	1/1	0.99	0.07	25,25,25,25	0
5	K	G	501	1/1	0.99	0.05	26,26,26,26	0
5	K	B	501	1/1	0.99	0.09	20,20,20,20	0
5	K	E	504	1/1	0.99	0.10	23,23,23,23	0
5	K	C	502	1/1	0.99	0.10	24,24,24,24	0
5	K	D	502	1/1	1.00	0.08	25,25,25,25	0
5	K	F	504	1/1	1.00	0.06	25,25,25,25	0
5	K	A	504	1/1	1.00	0.06	25,25,25,25	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.

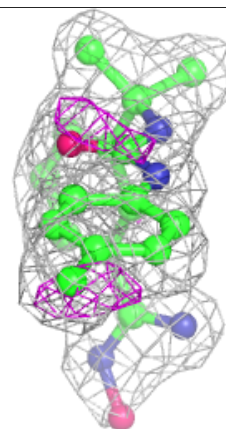
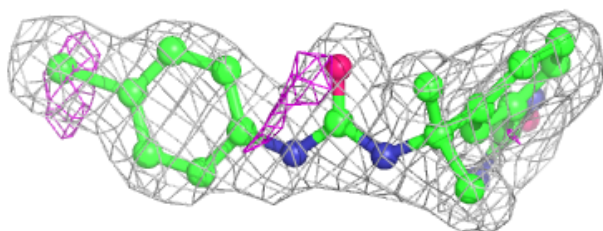
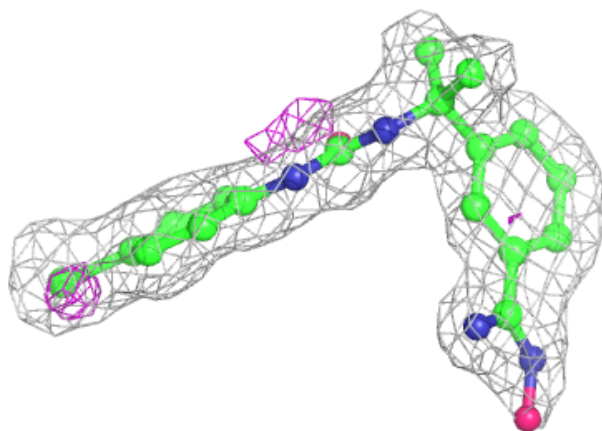
Electron density around 8L4 F 503:

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

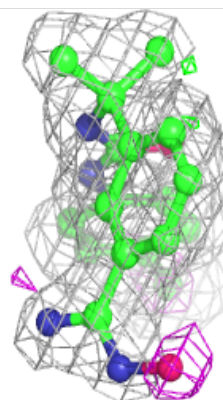
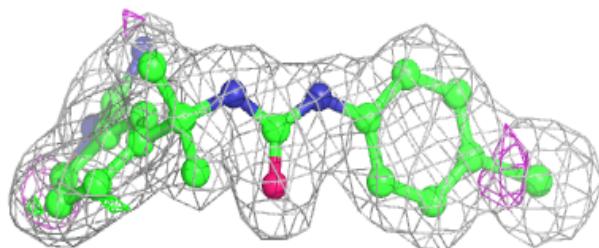
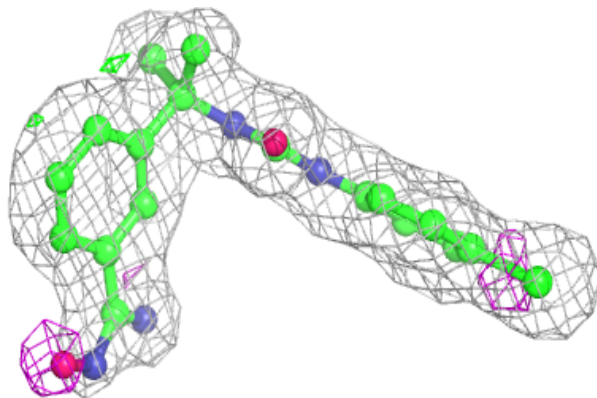


Electron density around 8L4 E 502:

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

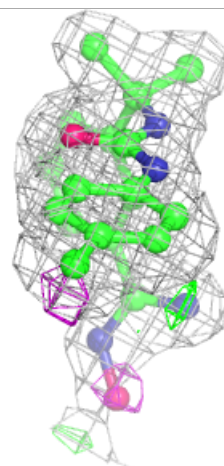
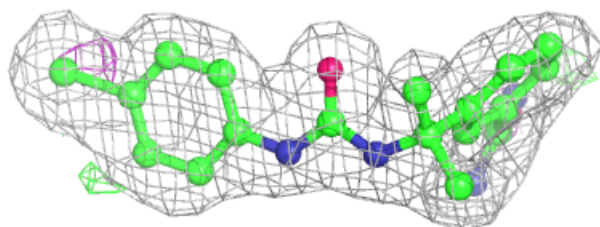
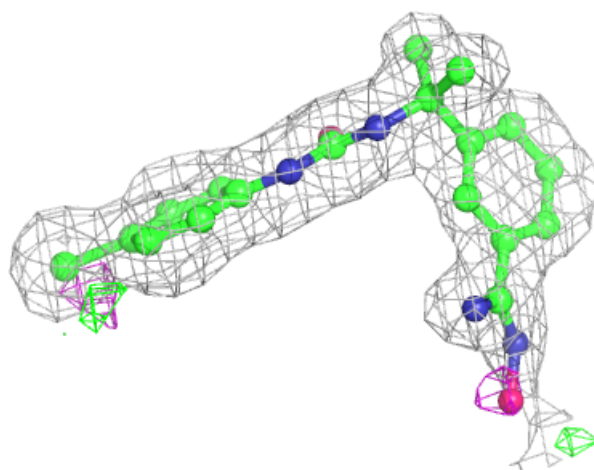
**Electron density around 8L4 D 501:**

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



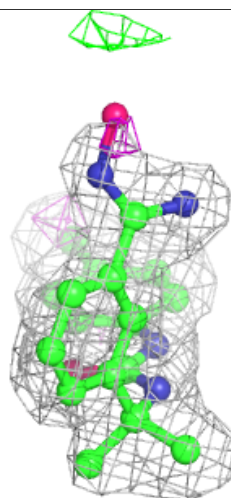
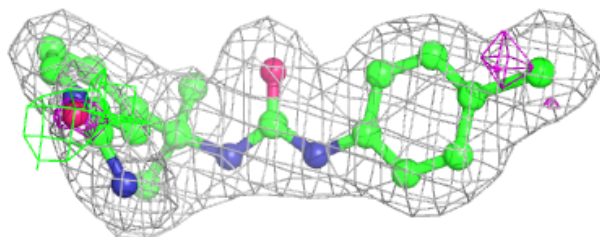
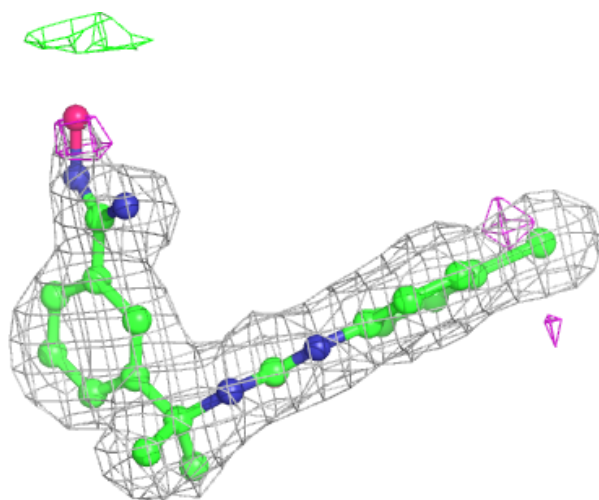
Electron density around 8L4 F 502:

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



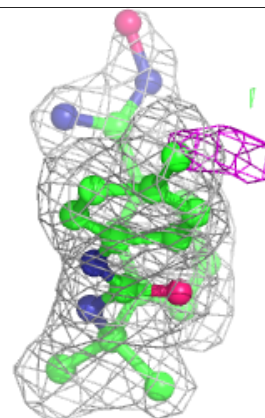
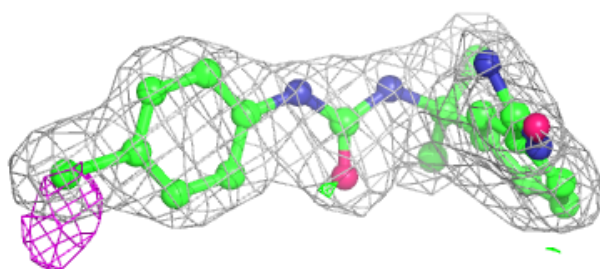
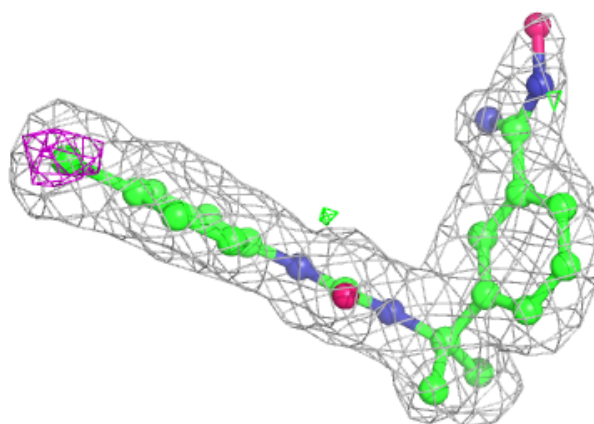
Electron density around 8L4 A 502:

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

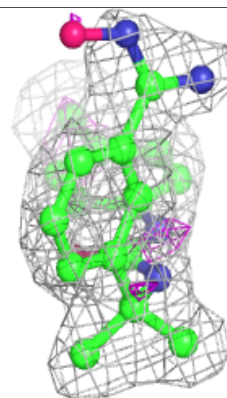
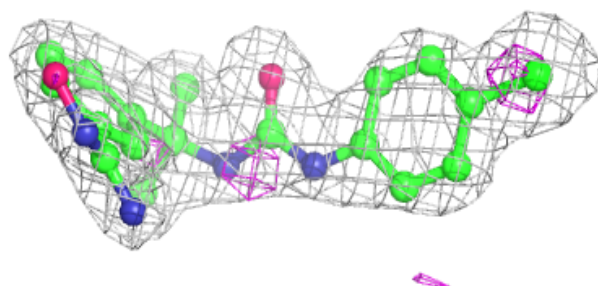
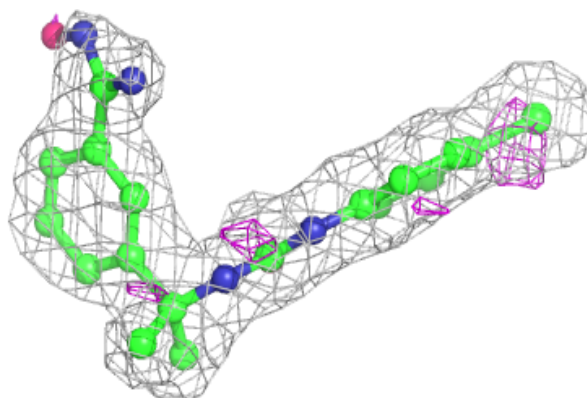


Electron density around 8L4 H 503:

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

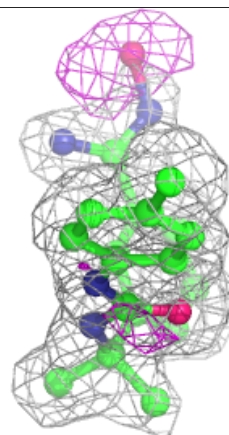
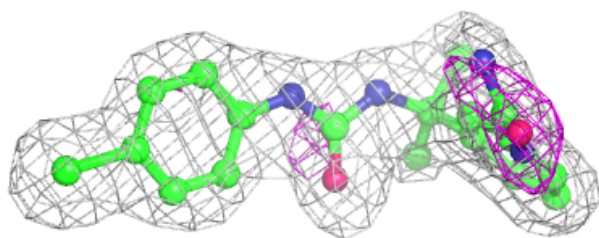
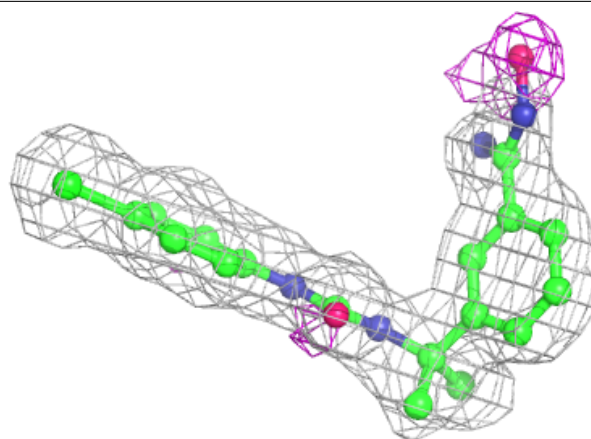
**Electron density around 8L4 C 501:**

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

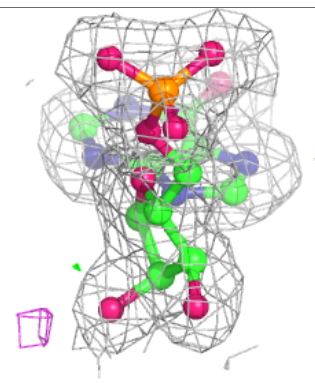
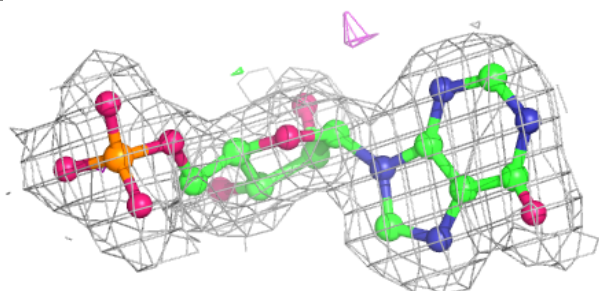
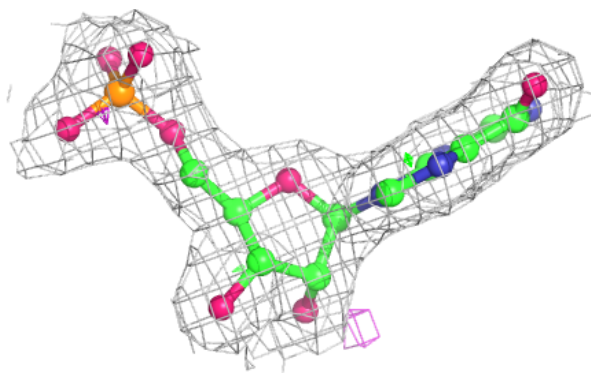


Electron density around 8L4 B 503:

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

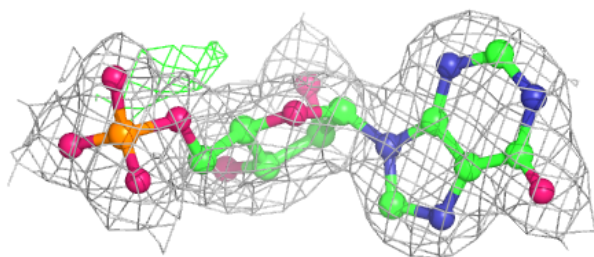
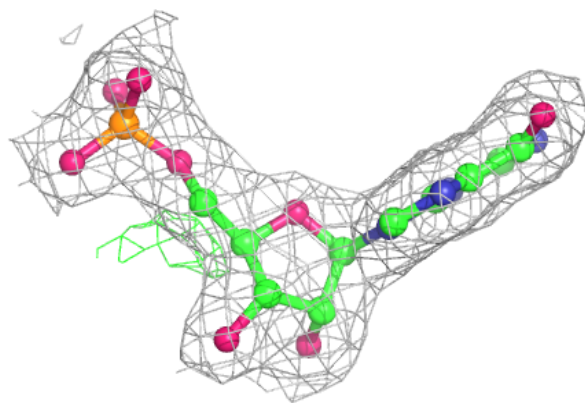
**Electron density around IMP G 502:**

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

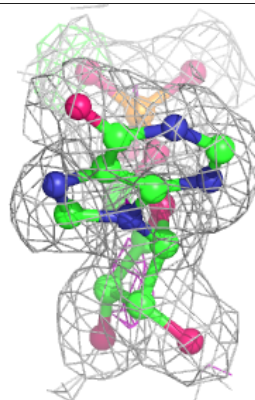
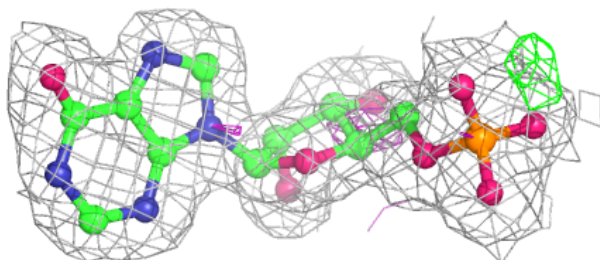
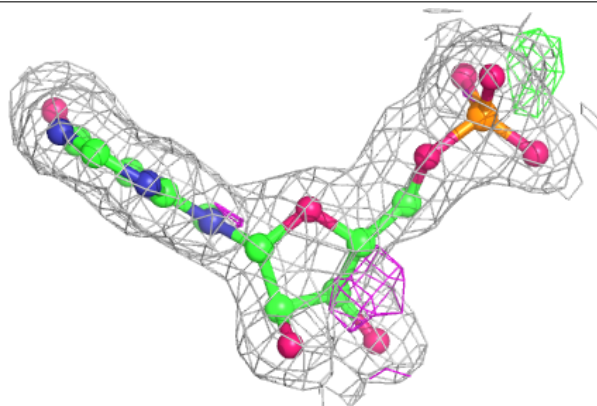


Electron density around IMP B 502:

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

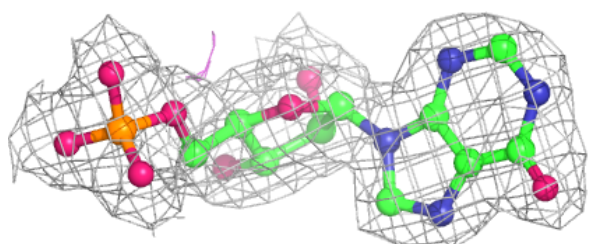
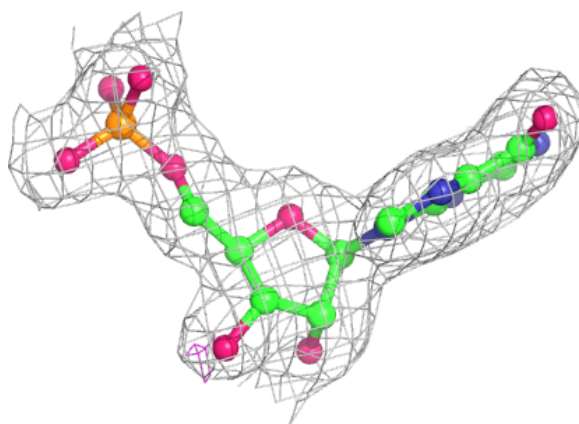
**Electron density around IMP F 501:**

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

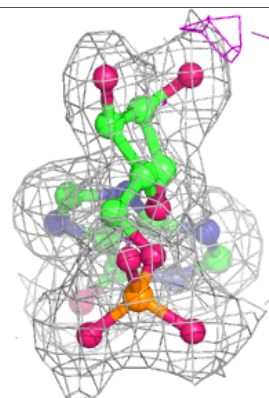
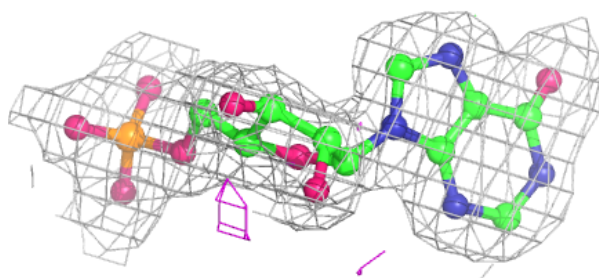
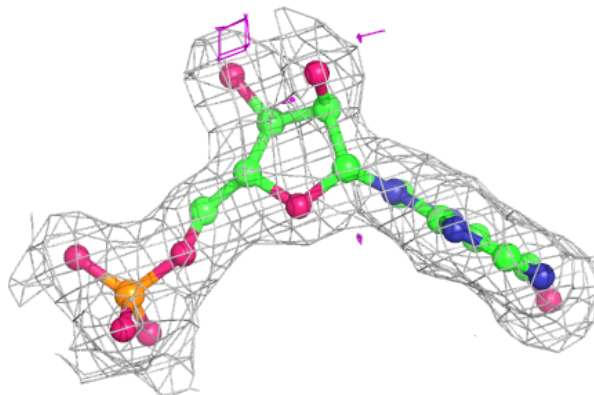


Electron density around IMP E 501:

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

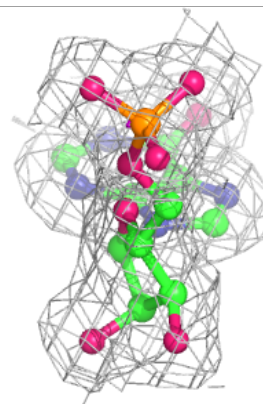
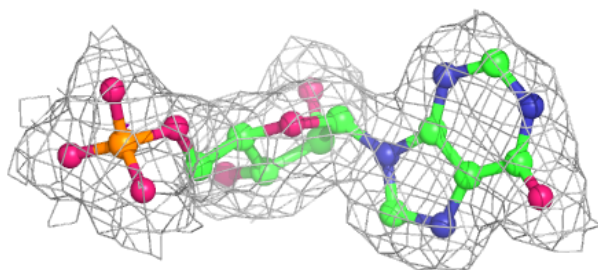
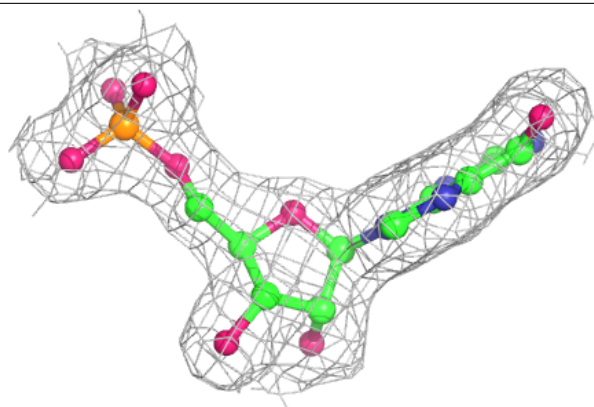
**Electron density around IMP D 500:**

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

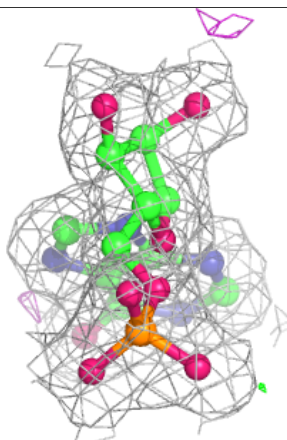
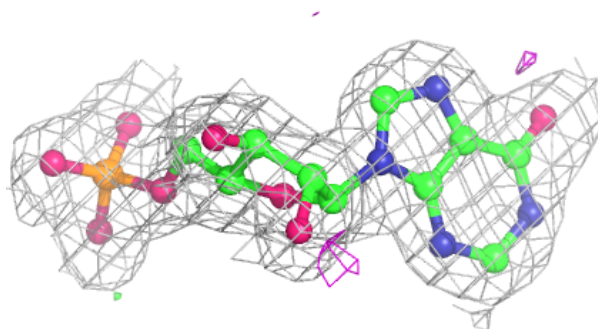
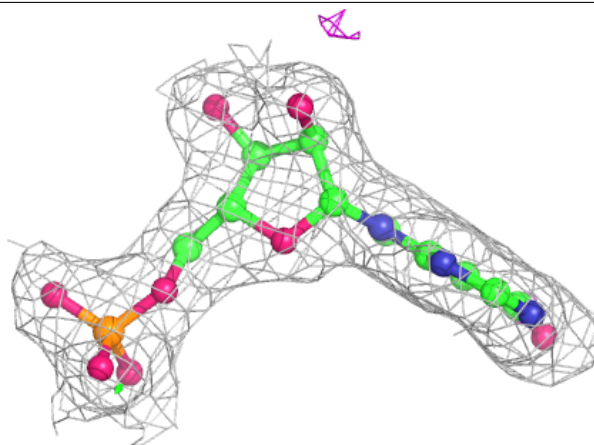


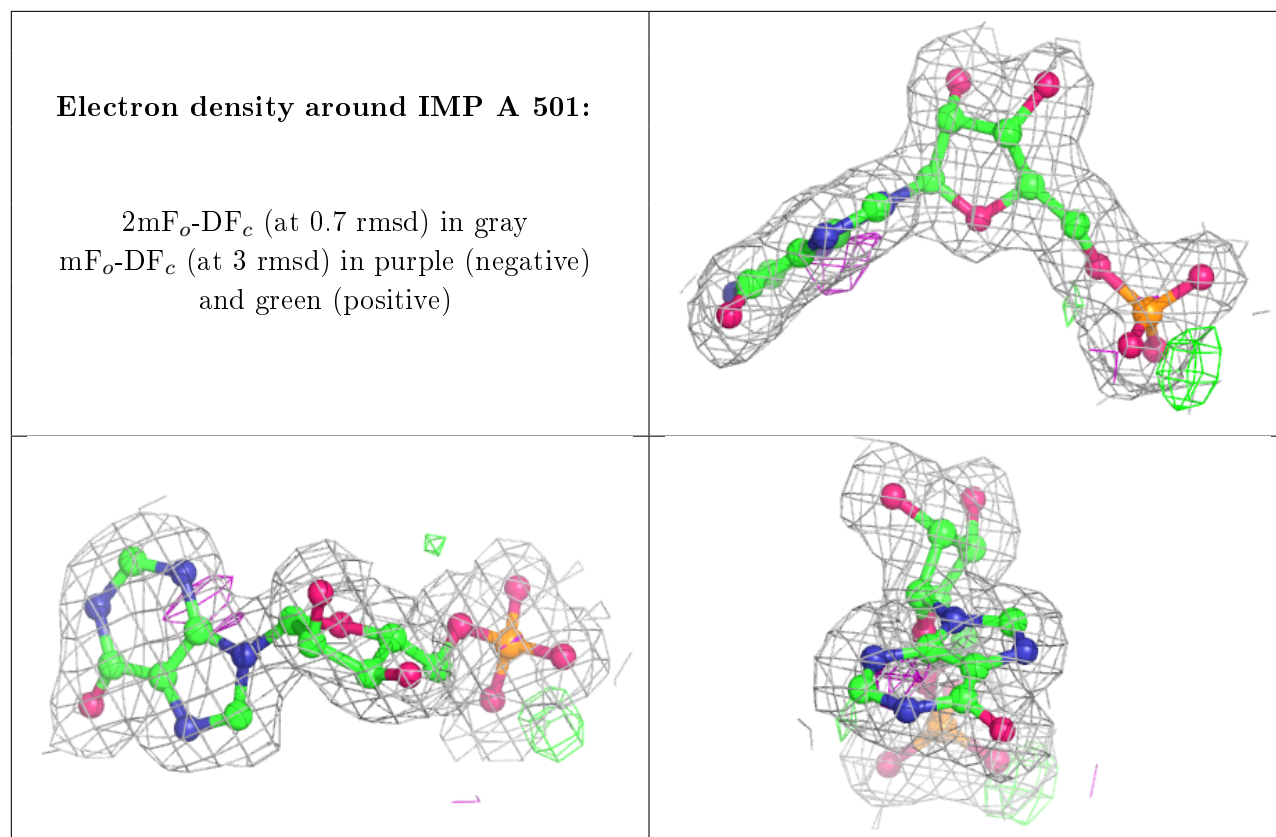
Electron density around IMP H 502:

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

**Electron density around IMP C 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.