



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:18 PM UTC

PDB ID : 7MTU / pdb_00007mtu
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from Bacillus anthracis in the complex with IMP and the inhibitor P221
Authors : Kim, Y.; Maltseva, N.; Makowska-Grzyska, M.; Gu, M.; Gollapalli, D.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2021-05-13
Resolution : 2.34 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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)

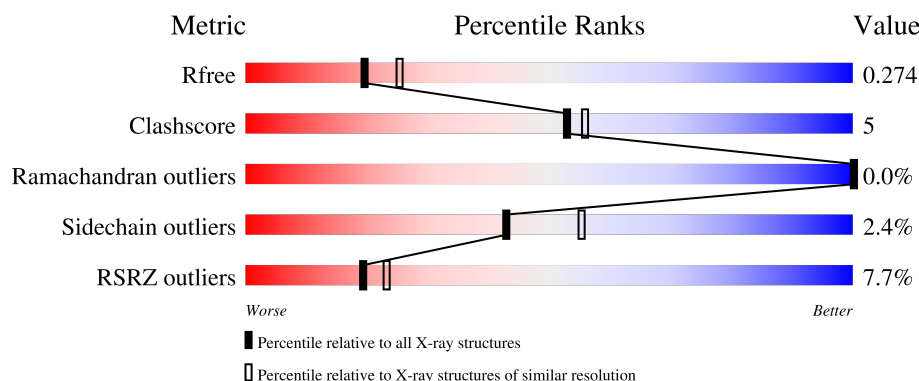
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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% 80% 10% 9%
1	B	384	5% 75% 15% 9%
1	C	384	3% 80% 11% 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	7% 79% 11% 9%
1	E	384	17% 72% 18% 10%
1	F	384	9% 80% 10% 9%
1	G	384	5% 79% 12% 9%
1	H	384	5% 77% 13% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21561 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

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

There are 208 discrepancies between the modelled and reference sequences:

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

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

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

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

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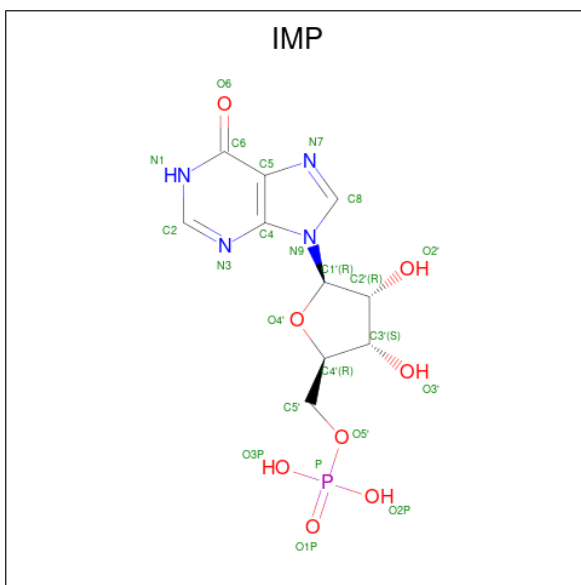
Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	GLY	-	expression tag	UNP A0A6H3A7R4
F	-13	VAL	-	expression tag	UNP A0A6H3A7R4
F	-12	ASP	-	expression tag	UNP A0A6H3A7R4
F	-11	LEU	-	expression tag	UNP A0A6H3A7R4
F	-10	GLY	-	expression tag	UNP A0A6H3A7R4
F	-9	THR	-	expression tag	UNP A0A6H3A7R4
F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

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

- Molecule 2 is INOSINIC ACID (CCD ID: IMP) (formula: C₁₀H₁₃N₄O₈P).



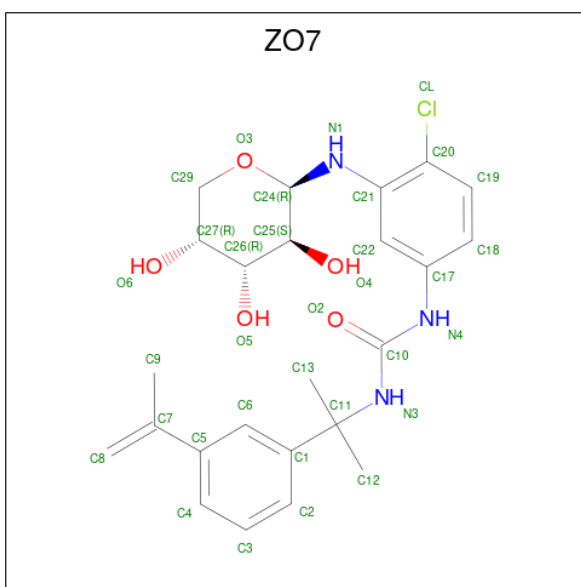
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	E	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	F	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	G	1	Total	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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is N-{2-chloro-5-[(2-[3-(prop-1-en-2-yl)phenyl]propan-2-yl}carbamoyl)amino]phenyl}-beta-D-arabinopyranosylamine (CCD ID: ZO7) (formula: C₂₄H₃₀ClN₃O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

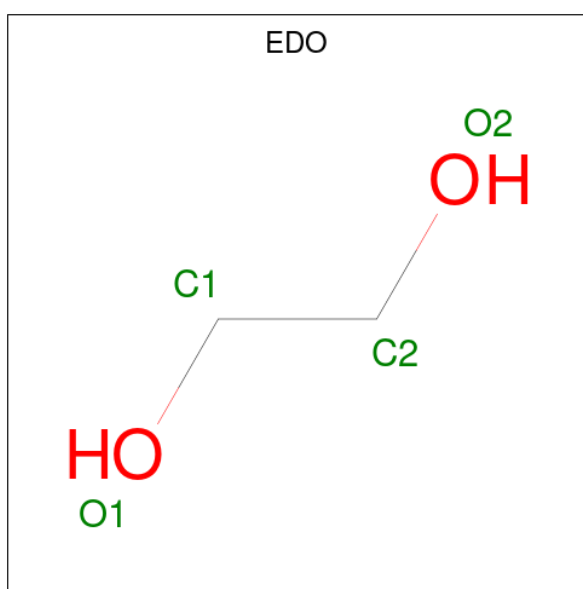
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		
5	C	1	Total	K	0	0
			1	1		
5	D	1	Total	K	0	0
			1	1		

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

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

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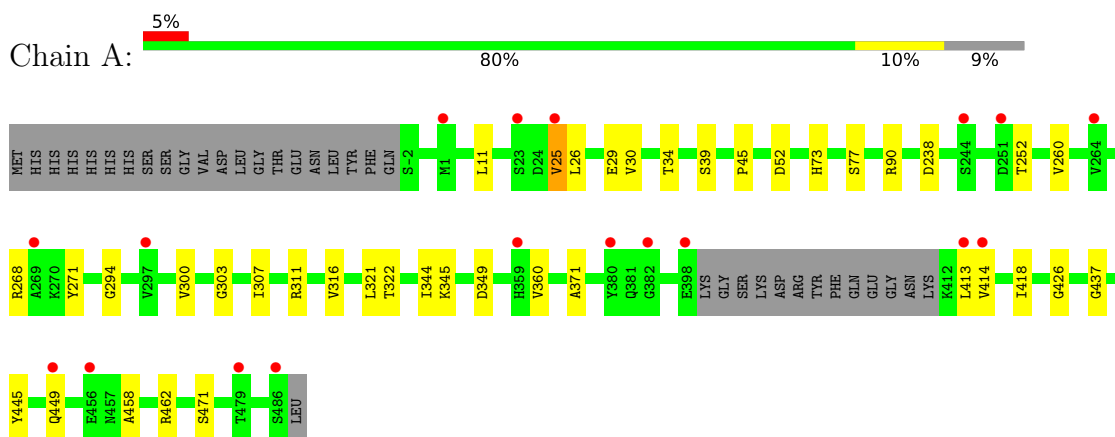
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	44	Total 44	O 44	0	0
7	F	40	Total 40	O 40	0	0
7	G	73	Total 73	O 73	0	0
7	H	66	Total 66	O 66	0	0

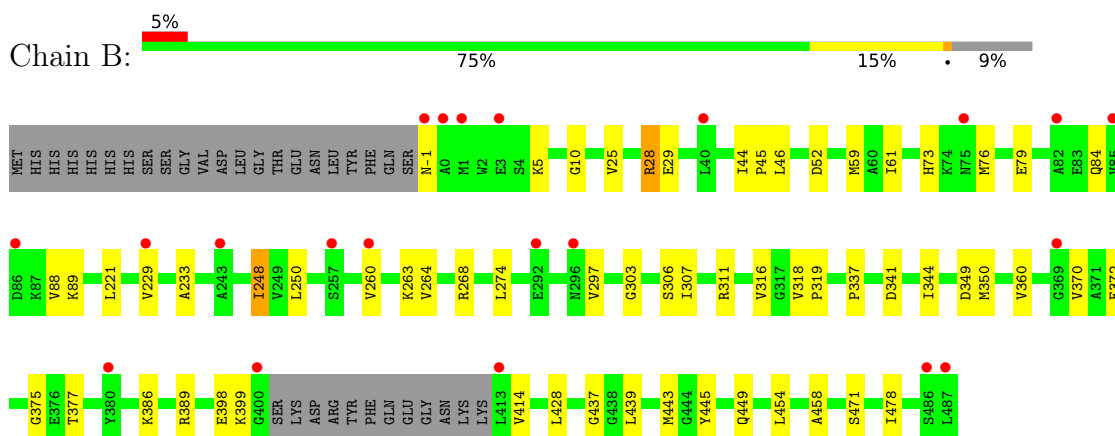
3 Residue-property plots

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.

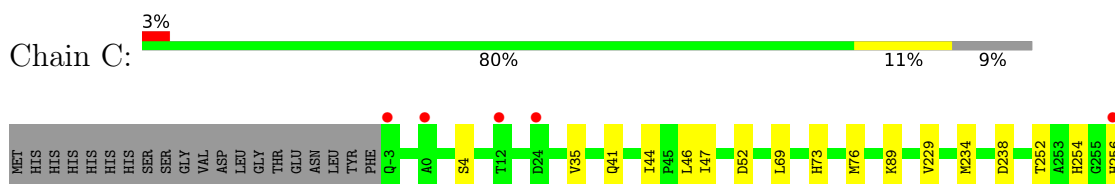
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

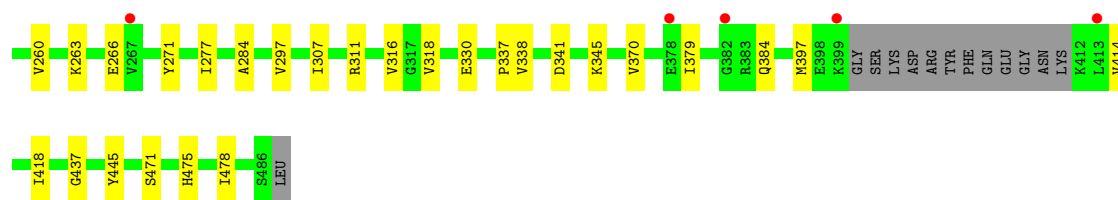


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

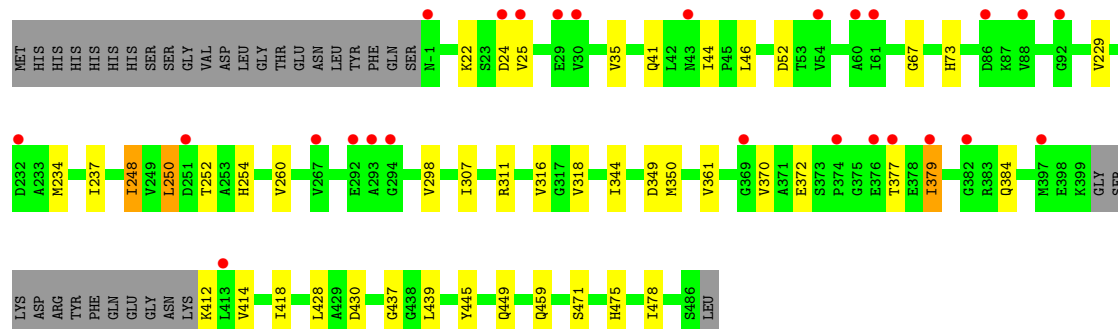
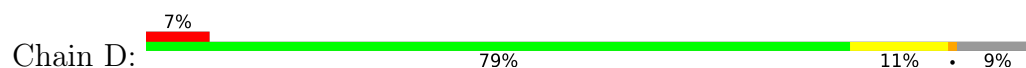


- Molecule 1: Inosine-5'-monophosphate dehydrogenase

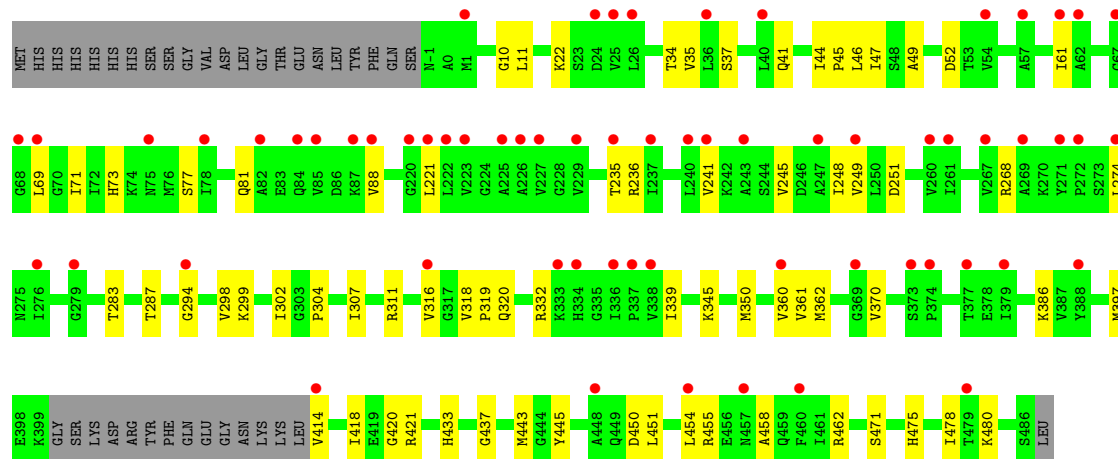




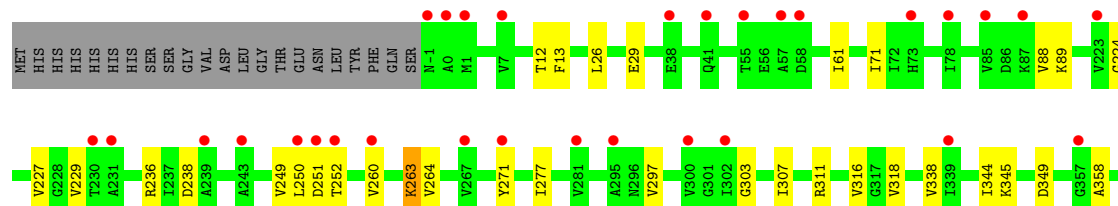
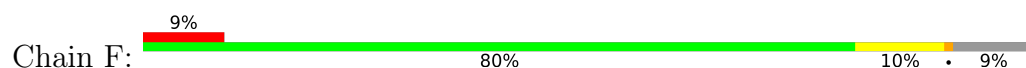
• Molecule 1: Inosine-5'-monophosphate dehydrogenase

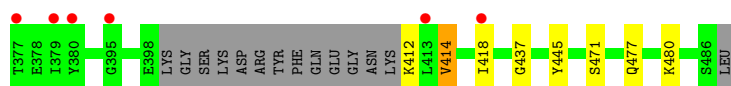


• Molecule 1: Inosine-5'-monophosphate dehydrogenase

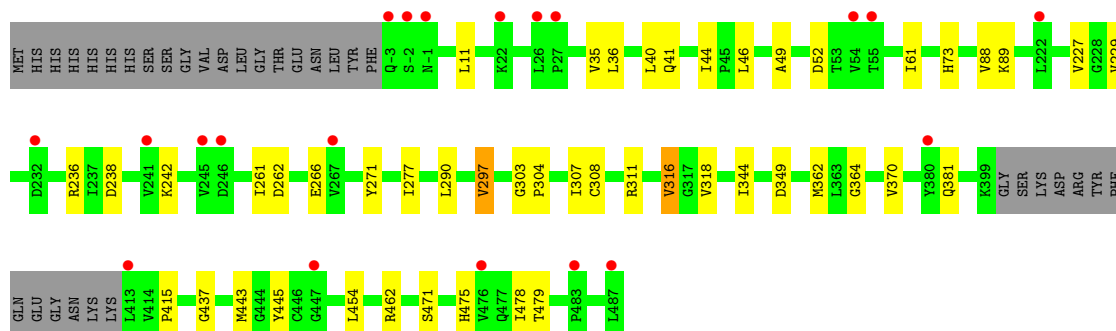
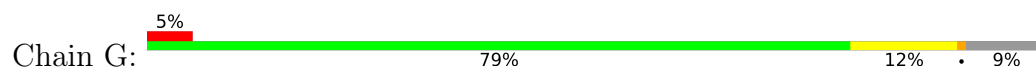


• Molecule 1: Inosine-5'-monophosphate dehydrogenase

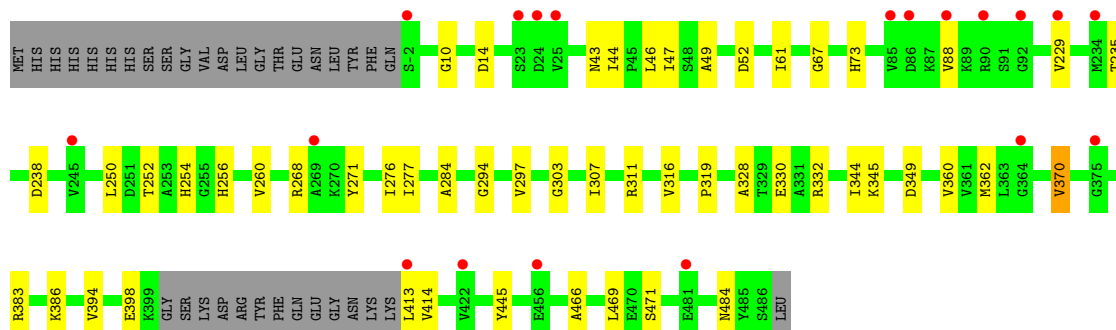
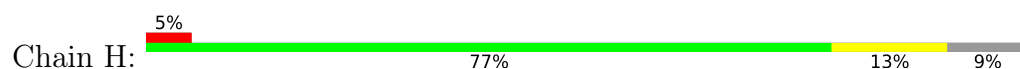




- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- 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	83.27Å 89.33Å 104.33Å 98.89° 90.40° 96.01°	Depositor
Resolution (Å)	41.68 – 2.34 41.68 – 2.34	Depositor EDS
% Data completeness (in resolution range)	75.9 (41.68-2.34) 75.9 (41.68-2.34)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.231 , 0.275 0.231 , 0.274	Depositor DCC
R_{free} test set	4636 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21561	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO, K, ZO7, 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	0.08	0/2605	0.23	0/3521
1	B	0.09	0/2617	0.25	0/3537
1	C	0.07	0/2612	0.23	0/3530
1	D	0.08	0/2597	0.24	0/3510
1	E	0.07	0/2580	0.23	0/3488
1	F	0.07	0/2599	0.22	0/3513
1	G	0.07	0/2611	0.24	0/3530
1	H	0.07	0/2594	0.23	0/3507
All	All	0.08	0/20815	0.23	0/28136

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2569	0	2625	25	0
1	B	2581	0	2637	36	0
1	C	2576	0	2634	30	0
1	D	2561	0	2621	33	0
1	E	2544	0	2597	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2563	0	2620	28	0
1	G	2575	0	2632	28	0
1	H	2558	0	2613	31	0
2	A	23	0	11	0	0
2	B	23	0	11	2	0
2	C	23	0	11	1	0
2	D	23	0	11	0	0
2	E	23	0	11	0	0
2	F	23	0	11	0	0
2	G	23	0	11	0	0
2	H	23	0	11	0	0
3	A	18	0	24	0	0
3	C	6	0	8	0	0
3	H	12	0	16	0	0
4	A	33	0	0	0	0
4	B	33	0	0	0	0
4	C	33	0	0	0	0
4	D	33	0	0	0	0
4	E	33	0	0	0	0
4	F	33	0	0	0	0
4	G	33	0	0	0	0
4	H	33	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	F	4	0	6	0	0
7	A	86	0	0	0	0
7	B	88	0	0	0	0
7	C	86	0	0	0	0
7	D	54	0	0	0	0
7	E	44	0	0	1	0
7	F	40	0	0	0	0
7	G	73	0	0	1	0
7	H	66	0	0	2	0
All	All	21561	0	21121	211	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 (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:GLY:HA3	1:H:414:VAL:HG21	1.76	0.67
1:E:414:VAL:HG21	1:G:437:GLY:HA3	1.78	0.65
1:E:316:VAL:HG11	1:G:445:TYR:HB3	1.81	0.63
1:H:229:VAL:HG21	1:H:260:VAL:HG22	1.82	0.61
1:C:311:ARG:HD2	1:D:471:SER:HA	1.83	0.60
1:C:44:ILE:HD12	1:C:46:LEU:HD12	1.83	0.60
1:E:49:ALA:HA	1:E:362:MET:HE2	1.82	0.60
1:G:344:ILE:HG23	1:G:349:ASP:HB2	1.83	0.60
1:C:234:MET:HE2	1:C:266:GLU:HG2	1.82	0.60
1:B:248:ILE:HG12	1:B:274:LEU:HD21	1.83	0.60
1:G:311:ARG:HD2	1:H:471:SER:HA	1.83	0.59
1:E:61:ILE:HG12	1:E:88:VAL:HG13	1.85	0.59
1:C:229:VAL:HG21	1:C:260:VAL:HG22	1.84	0.58
1:A:437:GLY:HA3	1:B:414:VAL:HG21	1.85	0.58
1:F:229:VAL:HG13	1:F:263:LYS:HD2	1.84	0.58
1:H:44:ILE:HD12	1:H:46:LEU:HD12	1.85	0.58
1:A:316:VAL:HG11	1:C:445:TYR:HB3	1.85	0.58
1:E:287:THR:HG23	1:E:298:VAL:HG21	1.86	0.58
1:F:311:ARG:NH2	1:F:318:VAL:O	2.37	0.57
1:E:71:ILE:HG12	1:E:249:VAL:HG21	1.86	0.57
1:H:344:ILE:HG23	1:H:349:ASP:HB2	1.86	0.57
1:A:238:ASP:OD1	1:A:271:TYR:OH	2.21	0.57
1:B:344:ILE:HG23	1:B:349:ASP:HB2	1.87	0.57
1:E:311:ARG:NH2	1:E:318:VAL:O	2.38	0.57
1:E:44:ILE:HD12	1:E:46:LEU:HD12	1.87	0.56
1:F:338:VAL:HG23	1:F:358:ALA:HA	1.87	0.56
1:A:252:THR:HG21	1:A:260:VAL:HG21	1.85	0.56
1:B:445:TYR:HB3	1:D:316:VAL:HG11	1.87	0.56
1:E:11:LEU:HD11	1:E:462:ARG:HD3	1.88	0.56
1:E:437:GLY:HA3	1:F:414:VAL:HG11	1.88	0.56
1:A:303:GLY:HA3	1:A:311:ARG:HE	1.70	0.56
1:A:471:SER:HA	1:B:311:ARG:HD2	1.88	0.55
1:G:415:PRO:O	1:H:484:ASN:ND2	2.37	0.55
1:E:451:LEU:HB3	1:E:455:ARG:HH12	1.72	0.55
1:A:414:VAL:HG21	1:C:437:GLY:HA3	1.88	0.55
1:A:311:ARG:HD2	1:C:471:SER:HA	1.89	0.54
1:F:277:ILE:HG12	1:F:297:VAL:HB	1.89	0.54
1:H:49:ALA:HA	1:H:362:MET:HE3	1.89	0.54
1:E:370:VAL:O	1:E:386:LYS:NZ	2.40	0.54
1:E:420:GLY:HA2	1:G:479:THR:HG23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:ASP:OD2	2:C:502:IMP:O2'	2.26	0.54
1:D:237:ILE:HG12	1:D:248:ILE:HG12	1.89	0.54
1:E:311:ARG:HD2	1:G:471:SER:HA	1.90	0.53
1:E:268:ARG:HD2	1:E:294:GLY:HA3	1.91	0.53
1:B:370:VAL:HG12	1:B:372:GLU:H	1.74	0.53
1:D:22:LYS:NZ	1:D:24:ASP:OD1	2.41	0.53
1:E:445:TYR:CG	1:F:316:VAL:HG21	2.44	0.53
1:G:11:LEU:HD11	1:G:462:ARG:HD3	1.90	0.53
1:C:297:VAL:HG22	1:C:337:PRO:HG2	1.91	0.53
1:E:471:SER:HA	1:F:311:ARG:HD2	1.91	0.53
1:B:389:ARG:HH12	1:B:399:LYS:HD3	1.74	0.53
1:D:370:VAL:HG12	1:D:372:GLU:H	1.74	0.52
1:B:437:GLY:HA3	1:D:414:VAL:HG21	1.90	0.52
1:C:418:ILE:HD13	1:D:478:ILE:HG12	1.91	0.52
1:F:303:GLY:HA3	1:F:311:ARG:HE	1.73	0.52
1:G:311:ARG:NH2	1:G:318:VAL:O	2.42	0.52
1:A:418:ILE:HD13	1:C:478:ILE:HG12	1.92	0.52
1:E:450:ASP:N	1:E:450:ASP:OD1	2.43	0.52
1:D:25:VAL:HG11	1:D:449:GLN:HG2	1.92	0.51
1:H:303:GLY:HA3	1:H:311:ARG:HE	1.74	0.51
1:E:418:ILE:HD13	1:G:478:ILE:HG12	1.93	0.51
1:C:316:VAL:HG21	1:D:445:TYR:CD2	2.45	0.51
1:C:345:LYS:HD2	1:D:475:HIS:CE1	2.46	0.51
1:E:475:HIS:CE1	1:F:345:LYS:HD2	2.46	0.51
1:H:14:ASP:OD2	1:H:345:LYS:NZ	2.44	0.51
1:F:445:TYR:HB3	1:H:316:VAL:HG11	1.92	0.51
1:G:316:VAL:HG21	1:H:445:TYR:CG	2.46	0.51
1:A:445:TYR:HB3	1:B:316:VAL:HG11	1.92	0.50
1:B:44:ILE:HD12	1:B:46:LEU:HD12	1.93	0.50
1:E:339:ILE:HG12	1:E:360:VAL:HG13	1.92	0.50
1:A:345:LYS:HD2	1:C:475:HIS:CE1	2.46	0.50
1:B:311:ARG:NH2	1:B:318:VAL:O	2.44	0.50
1:F:471:SER:HA	1:H:311:ARG:HD2	1.94	0.50
1:G:35:VAL:HG13	1:G:41:GLN:HG2	1.93	0.50
1:D:311:ARG:NH2	1:D:318:VAL:O	2.44	0.50
1:C:47:ILE:HG12	1:C:69:LEU:HB3	1.93	0.50
1:C:311:ARG:NH2	1:C:318:VAL:O	2.45	0.50
1:D:229:VAL:HG21	1:D:260:VAL:HG22	1.93	0.49
1:D:350:MET:HG3	1:D:361:VAL:HG21	1.94	0.49
1:A:458:ALA:O	1:B:5:LYS:NZ	2.43	0.49
1:B:268:ARG:NH2	1:B:274:LEU:O	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HG13	1:B:88:VAL:HG22	1.94	0.49
1:B:76:MET:HE1	1:B:84:GLN:HE22	1.78	0.49
1:B:478:ILE:HG12	1:D:418:ILE:HD13	1.94	0.49
1:B:28:ARG:HG2	1:B:29:GLU:HG3	1.94	0.49
1:G:238:ASP:OD1	1:G:271:TYR:OH	2.30	0.49
1:F:238:ASP:OD1	1:F:271:TYR:OH	2.31	0.49
1:D:44:ILE:HD12	1:D:46:LEU:HD12	1.93	0.49
1:E:35:VAL:HG12	1:E:41:GLN:HG2	1.94	0.48
1:C:4:SER:O	1:D:459:GLN:NE2	2.44	0.48
1:F:303:GLY:HA3	1:F:311:ARG:NE	2.28	0.48
1:B:471:SER:HA	1:D:311:ARG:HD2	1.96	0.48
1:H:284:ALA:HB1	1:H:330:GLU:HB2	1.95	0.48
1:E:52:ASP:HA	1:E:73:HIS:CD2	2.49	0.48
1:E:248:ILE:HG13	1:E:274:LEU:HD21	1.95	0.48
1:H:61:ILE:HG13	1:H:88:VAL:HG22	1.95	0.48
1:A:25:VAL:HG12	1:A:29:GLU:HG3	1.95	0.48
1:B:229:VAL:HG11	1:B:260:VAL:HG22	1.95	0.47
1:G:44:ILE:HD12	1:G:46:LEU:HD12	1.95	0.47
1:G:227:VAL:HG13	1:G:236:ARG:HD2	1.97	0.47
1:G:443:MET:HG2	1:G:454:LEU:HD22	1.97	0.47
1:H:252:THR:HG21	1:H:260:VAL:HG21	1.97	0.47
1:B:250:LEU:HD12	1:B:264:VAL:HG12	1.97	0.47
1:H:52:ASP:HA	1:H:73:HIS:CD2	2.50	0.47
1:H:370:VAL:O	1:H:386:LYS:NZ	2.45	0.47
1:E:45:PRO:C	1:E:360:VAL:HG23	2.40	0.47
1:G:261:ILE:HD13	1:G:290:LEU:HD23	1.97	0.47
1:C:52:ASP:HA	1:C:73:HIS:CD2	2.50	0.47
1:G:52:ASP:HA	1:G:73:HIS:CD2	2.50	0.47
1:B:25:VAL:HG11	1:B:449:GLN:HG2	1.97	0.46
1:D:252:THR:HG22	1:D:254:HIS:H	1.80	0.46
1:G:36:LEU:HD12	1:G:40:LEU:HD22	1.97	0.46
1:D:52:ASP:HA	1:D:73:HIS:CD2	2.51	0.46
1:D:412:LYS:HD2	1:D:412:LYS:HA	1.76	0.46
1:A:268:ARG:NH2	1:A:294:GLY:O	2.41	0.46
1:F:61:ILE:HG13	1:F:88:VAL:HG22	1.97	0.46
1:A:26:LEU:O	1:A:30:VAL:HG23	2.16	0.45
1:C:238:ASP:OD1	1:C:271:TYR:OH	2.29	0.45
1:A:11:LEU:HD11	1:A:462:ARG:HD3	1.99	0.45
1:E:47:ILE:HG12	1:E:69:LEU:HB3	1.97	0.45
1:F:227:VAL:HG23	1:F:236:ARG:HD2	1.99	0.45
1:B:341:ASP:OD2	2:B:501:IMP:O2'	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LYS:HE3	1:B:221:LEU:O	2.17	0.45
1:A:25:VAL:HG21	1:A:449:GLN:HB2	1.99	0.45
1:B:350:MET:HE3	1:B:439:LEU:HB2	1.99	0.45
1:F:250:LEU:HD22	1:F:264:VAL:HG22	1.98	0.45
1:D:377:THR:HG21	1:D:384:GLN:HB3	1.99	0.45
1:C:256:HIS:CD2	1:D:22:LYS:HD3	2.51	0.45
1:D:229:VAL:HG22	1:D:250:LEU:HD12	1.98	0.45
1:E:304:PRO:HB3	1:E:320:GLN:HB2	1.99	0.44
1:H:238:ASP:OD1	1:H:271:TYR:OH	2.29	0.44
1:H:268:ARG:NH2	1:H:294:GLY:O	2.50	0.44
1:C:316:VAL:HG21	1:D:445:TYR:CG	2.53	0.44
1:B:73:HIS:CE1	1:B:76:MET:HE3	2.52	0.44
1:B:443:MET:HG2	1:B:454:LEU:HD22	1.99	0.44
1:G:303:GLY:HA2	1:G:308:CYS:SG	2.58	0.44
1:C:229:VAL:HG13	1:C:263:LYS:HD2	1.99	0.44
1:F:344:ILE:HG23	1:F:349:ASP:HB2	1.98	0.44
1:C:414:VAL:HG21	1:D:437:GLY:HA3	1.99	0.44
1:A:344:ILE:HG23	1:A:349:ASP:HB2	1.99	0.44
1:H:277:ILE:HG12	1:H:297:VAL:HB	1.99	0.44
1:A:321:LEU:HD12	1:A:321:LEU:HA	1.86	0.44
1:E:350:MET:HG3	1:E:361:VAL:HG21	2.00	0.44
1:B:45:PRO:C	1:B:360:VAL:HG23	2.43	0.43
1:C:252:THR:HG22	1:C:254:HIS:H	1.83	0.43
1:H:10:GLY:HA3	1:H:319:PRO:HG2	2.00	0.43
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.53	0.43
1:D:44:ILE:HG12	1:D:67:GLY:C	2.43	0.43
1:D:350:MET:HE2	1:D:350:MET:HB3	1.92	0.43
1:D:379:ILE:H	1:D:379:ILE:HG13	1.60	0.43
1:E:433:HIS:NE2	1:F:412:LYS:O	2.41	0.43
1:H:303:GLY:HA3	1:H:311:ARG:NE	2.33	0.43
1:G:277:ILE:HG12	1:G:297:VAL:HB	1.99	0.43
1:H:47:ILE:HG13	1:H:360:VAL:HG11	1.99	0.43
1:E:443:MET:HG2	1:E:454:LEU:HD22	1.99	0.43
1:C:35:VAL:HG13	1:C:41:GLN:HG2	2.00	0.43
1:E:88:VAL:HG12	1:E:221:LEU:HB2	1.99	0.43
1:E:10:GLY:HA3	1:E:319:PRO:HG2	1.98	0.43
1:E:421:ARG:NH2	7:E:604:HOH:O	2.45	0.43
1:E:81:GLN:OE1	1:E:236:ARG:NE	2.52	0.43
1:B:303:GLY:HA3	1:B:311:ARG:HG3	2.01	0.43
1:F:26:LEU:HB2	1:F:29:GLU:HG2	2.01	0.43
1:E:251:ASP:OD1	1:E:299:LYS:NZ	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:SER:OG	2:B:501:IMP:O2P	2.32	0.42
1:D:430:ASP:N	1:D:430:ASP:OD1	2.52	0.42
1:G:49:ALA:HA	1:G:362:MET:HE3	2.01	0.42
1:B:10:GLY:HA3	1:B:319:PRO:HG2	2.00	0.42
1:D:344:ILE:HG23	1:D:349:ASP:HB2	2.00	0.42
1:A:303:GLY:HA3	1:A:311:ARG:NE	2.34	0.42
1:D:370:VAL:HG11	1:D:428:LEU:HB2	2.01	0.42
1:G:316:VAL:HG11	1:H:445:TYR:HB2	2.01	0.42
1:H:383:ARG:NH2	7:H:602:HOH:O	2.39	0.42
1:F:480:LYS:HB3	1:F:480:LYS:HE2	1.83	0.42
1:B:52:ASP:HA	1:B:73:HIS:CD2	2.54	0.42
1:G:262:ASP:O	1:G:266:GLU:HG2	2.20	0.42
1:B:375:GLY:O	1:B:386:LYS:NZ	2.48	0.42
1:G:61:ILE:HG13	1:G:88:VAL:HG22	2.02	0.42
1:A:371:ALA:N	1:A:426:GLY:O	2.50	0.42
1:A:45:PRO:C	1:A:360:VAL:HG23	2.45	0.42
1:A:316:VAL:HG21	1:C:445:TYR:HB2	2.02	0.42
1:H:250:LEU:HD13	1:H:276:ILE:HG23	2.02	0.42
1:E:241:VAL:HA	1:E:245:VAL:HG12	2.02	0.41
1:G:381:GLN:NE2	7:G:611:HOH:O	2.52	0.41
1:C:284:ALA:HB1	1:C:330:GLU:HB2	2.02	0.41
1:E:454:LEU:HD12	1:E:458:ALA:HB2	2.01	0.41
1:E:478:ILE:HG12	1:F:418:ILE:HD12	2.02	0.41
1:F:12:THR:OG1	1:F:13:PHE:N	2.53	0.41
1:F:477:GLN:NE2	7:H:602:HOH:O	2.51	0.41
1:B:59:MET:HE1	1:B:428:LEU:HD13	2.01	0.41
1:A:11:LEU:N	1:A:322:THR:OG1	2.47	0.41
1:B:454:LEU:HD12	1:B:458:ALA:HB2	2.02	0.41
1:E:22:LYS:HE2	1:E:22:LYS:HB2	1.81	0.41
1:F:249:VAL:HG12	1:F:251:ASP:HB2	2.02	0.41
1:G:303:GLY:N	1:G:304:PRO:CD	2.84	0.41
1:H:43:ASN:HB2	1:H:67:GLY:HA3	2.02	0.41
1:B:233:ALA:HB3	1:B:263:LYS:HE2	2.02	0.41
1:C:89:LYS:HD3	1:C:89:LYS:HA	1.90	0.41
1:E:345:LYS:HD2	1:G:475:HIS:CE1	2.56	0.41
1:F:71:ILE:HD13	1:F:224:GLY:HA3	2.03	0.41
1:H:328:ALA:O	1:H:332:ARG:HB2	2.20	0.41
1:H:466:ALA:HA	1:H:469:LEU:HD12	2.01	0.41
1:F:260:VAL:O	1:F:264:VAL:HG23	2.20	0.40
1:H:394:VAL:O	1:H:398:GLU:HG2	2.21	0.40
1:E:480:LYS:HE2	1:E:480:LYS:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:VAL:HG22	1:F:277:ILE:HB	2.02	0.40
1:H:254:HIS:CE1	1:H:256:HIS:HB3	2.57	0.40
1:C:277:ILE:HG12	1:C:297:VAL:HB	2.02	0.40
1:C:379:ILE:HG12	1:C:384:GLN:HG2	2.03	0.40
1:D:234:MET:HE3	1:D:234:MET:HA	2.03	0.40
1:D:350:MET:HE3	1:D:439:LEU:HB2	2.03	0.40
1:B:297:VAL:HG22	1:B:337:PRO:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	346/384 (90%)	337 (97%)	9 (3%)	0	100	100
1	B	348/384 (91%)	342 (98%)	6 (2%)	0	100	100
1	C	347/384 (90%)	338 (97%)	9 (3%)	0	100	100
1	D	345/384 (90%)	337 (98%)	8 (2%)	0	100	100
1	E	343/384 (89%)	334 (97%)	9 (3%)	0	100	100
1	F	345/384 (90%)	336 (97%)	9 (3%)	0	100	100
1	G	347/384 (90%)	339 (98%)	7 (2%)	1 (0%)	36	41
1	H	345/384 (90%)	336 (97%)	9 (3%)	0	100	100
All	All	2766/3072 (90%)	2699 (98%)	66 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	364	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/298 (90%)	259 (97%)	9 (3%)	32	42
1	B	269/298 (90%)	262 (97%)	7 (3%)	40	53
1	C	269/298 (90%)	264 (98%)	5 (2%)	50	63
1	D	267/298 (90%)	260 (97%)	7 (3%)	40	53
1	E	265/298 (89%)	256 (97%)	9 (3%)	32	42
1	F	267/298 (90%)	262 (98%)	5 (2%)	50	63
1	G	269/298 (90%)	262 (97%)	7 (3%)	40	53
1	H	267/298 (90%)	263 (98%)	4 (2%)	57	69
All	All	2141/2384 (90%)	2088 (98%)	53 (2%)	43	54

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	34	THR
1	A	39	SER
1	A	77	SER
1	A	90[A]	ARG
1	A	90[B]	ARG
1	A	300	VAL
1	A	307	ILE
1	A	413	LEU
1	B	-1	ASN
1	B	28	ARG
1	B	79	GLU
1	B	248	ILE
1	B	307	ILE
1	B	377	THR
1	B	398	GLU
1	C	76	MET
1	C	307	ILE
1	C	338	VAL

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Mol	Chain	Res	Type
1	C	370	VAL
1	C	397	MET
1	D	35	VAL
1	D	41	GLN
1	D	248	ILE
1	D	250	LEU
1	D	298	VAL
1	D	307	ILE
1	D	379	ILE
1	E	34	THR
1	E	37	SER
1	E	77	SER
1	E	235	THR
1	E	283	THR
1	E	302	ILE
1	E	307	ILE
1	E	332	ARG
1	E	397	MET
1	F	89	LYS
1	F	252	THR
1	F	263	LYS
1	F	307	ILE
1	F	414	VAL
1	G	89	LYS
1	G	229	VAL
1	G	242	LYS
1	G	297	VAL
1	G	307	ILE
1	G	316	VAL
1	G	370	VAL
1	H	235	THR
1	H	307	ILE
1	H	370	VAL
1	H	413	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	433	HIS
1	A	474	HIS
1	B	433	HIS
1	B	457	ASN

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Mol	Chain	Res	Type
1	B	474	HIS
1	D	359	HIS
1	D	449	GLN
1	D	459	GLN
1	D	475	HIS
1	E	258	GLN
1	E	359	HIS
1	E	475	HIS
1	F	256	HIS
1	G	275	ASN
1	G	359	HIS
1	H	41	GLN
1	H	334	HIS
1	H	381	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	F	504	-	3,3,3	0.44	0	2,2,2	0.31	0
2	IMP	G	502	-	25,25,25	1.12	1 (4%)	37,38,38	2.04	10 (27%)
4	ZO7	A	504	-	35,35,35	1.05	5 (14%)	51,51,51	1.25	3 (5%)
4	ZO7	E	502	-	35,35,35	1.06	5 (14%)	51,51,51	1.35	4 (7%)
2	IMP	A	501	-	25,25,25	1.13	1 (4%)	37,38,38	2.06	10 (27%)
3	GOL	A	502	-	5,5,5	0.93	0	5,5,5	1.09	0
3	GOL	A	503	-	5,5,5	0.93	0	5,5,5	1.06	0
4	ZO7	B	502	-	35,35,35	1.08	5 (14%)	51,51,51	1.23	2 (3%)
3	GOL	A	506	-	5,5,5	0.93	0	5,5,5	1.08	0
4	ZO7	C	504	-	35,35,35	1.07	5 (14%)	51,51,51	1.33	4 (7%)
4	ZO7	F	502	-	35,35,35	1.09	5 (14%)	51,51,51	1.48	6 (11%)
4	ZO7	H	506	-	35,35,35	1.04	5 (14%)	51,51,51	1.26	3 (5%)
2	IMP	D	502	-	25,25,25	1.12	1 (4%)	37,38,38	2.09	10 (27%)
3	GOL	C	503	-	5,5,5	0.93	0	5,5,5	1.09	0
3	GOL	H	504	-	5,5,5	0.93	0	5,5,5	1.09	0
2	IMP	B	501	-	25,25,25	1.12	1 (4%)	37,38,38	2.10	10 (27%)
2	IMP	C	502	-	25,25,25	1.11	1 (4%)	37,38,38	2.07	10 (27%)
2	IMP	E	501	-	25,25,25	1.13	1 (4%)	37,38,38	2.09	10 (27%)
4	ZO7	G	503	-	35,35,35	1.08	5 (14%)	51,51,51	1.38	5 (9%)
4	ZO7	D	503	-	35,35,35	1.07	5 (14%)	51,51,51	1.51	6 (11%)
3	GOL	H	503	-	5,5,5	0.94	0	5,5,5	1.09	0
2	IMP	F	501	-	25,25,25	1.12	1 (4%)	37,38,38	2.06	10 (27%)
2	IMP	H	502	-	25,25,25	1.11	1 (4%)	37,38,38	2.05	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
6	EDO	F	504	-	-	0/1/1/1	-
2	IMP	G	502	-	-	3/10/26/26	0/3/3/3
4	ZO7	A	504	-	-	0/23/40/40	0/3/3/3
4	ZO7	E	502	-	-	0/23/40/40	0/3/3/3
2	IMP	A	501	-	-	2/10/26/26	0/3/3/3
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
4	ZO7	B	502	-	-	0/23/40/40	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	506	-	-	3/4/4/4	-
4	ZO7	C	504	-	-	0/23/40/40	0/3/3/3
4	ZO7	F	502	-	-	0/23/40/40	0/3/3/3
4	ZO7	H	506	-	-	1/23/40/40	0/3/3/3
2	IMP	D	502	-	-	4/10/26/26	0/3/3/3
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	H	504	-	-	2/4/4/4	-
2	IMP	B	501	-	-	3/10/26/26	0/3/3/3
2	IMP	C	502	-	-	4/10/26/26	0/3/3/3
2	IMP	E	501	-	-	2/10/26/26	0/3/3/3
4	ZO7	G	503	-	-	0/23/40/40	0/3/3/3
4	ZO7	D	503	-	-	0/23/40/40	0/3/3/3
3	GOL	H	503	-	-	2/4/4/4	-
2	IMP	F	501	-	-	5/10/26/26	0/3/3/3
2	IMP	H	502	-	-	3/10/26/26	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	IMP	C2-N3	4.54	1.38	1.30
2	E	501	IMP	C2-N3	4.51	1.38	1.30
2	B	501	IMP	C2-N3	4.51	1.38	1.30
2	D	502	IMP	C2-N3	4.49	1.38	1.30
2	G	502	IMP	C2-N3	4.48	1.38	1.30
2	H	502	IMP	C2-N3	4.46	1.38	1.30
2	F	501	IMP	C2-N3	4.45	1.38	1.30
2	C	502	IMP	C2-N3	4.42	1.38	1.30
4	E	502	ZO7	C9-C7	-2.87	1.32	1.46
4	D	503	ZO7	C9-C7	-2.87	1.32	1.46
4	F	502	ZO7	C9-C7	-2.87	1.32	1.46
4	H	506	ZO7	C9-C7	-2.87	1.32	1.46
4	C	504	ZO7	C9-C7	-2.87	1.32	1.46
4	G	503	ZO7	C9-C7	-2.87	1.32	1.46
4	A	504	ZO7	C9-C7	-2.86	1.32	1.46
4	B	502	ZO7	C9-C7	-2.86	1.32	1.46
4	G	503	ZO7	C11-C1	-2.75	1.50	1.53
4	C	504	ZO7	C20-CL	2.71	1.80	1.73
4	B	502	ZO7	C11-C1	-2.71	1.50	1.53
4	D	503	ZO7	C11-C1	-2.70	1.50	1.53
4	F	502	ZO7	C11-C1	-2.68	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	502	ZO7	C20-CL	2.67	1.79	1.73
4	E	502	ZO7	C11-C1	-2.67	1.50	1.53
4	E	502	ZO7	C20-CL	2.67	1.79	1.73
4	B	502	ZO7	C20-CL	2.66	1.79	1.73
4	H	506	ZO7	C11-C1	-2.66	1.50	1.53
4	D	503	ZO7	C20-CL	2.65	1.79	1.73
4	A	504	ZO7	C11-C1	-2.64	1.50	1.53
4	A	504	ZO7	C20-CL	2.64	1.79	1.73
4	G	503	ZO7	C20-CL	2.64	1.79	1.73
4	C	504	ZO7	C11-C1	-2.63	1.50	1.53
4	H	506	ZO7	C20-CL	2.62	1.79	1.73
4	B	502	ZO7	C24-N1	2.43	1.46	1.42
4	F	502	ZO7	C24-N1	2.40	1.46	1.42
4	G	503	ZO7	C24-N1	2.37	1.46	1.42
4	F	502	ZO7	C17-N4	-2.37	1.36	1.41
4	B	502	ZO7	C17-N4	-2.37	1.36	1.41
4	C	504	ZO7	C24-N1	2.36	1.46	1.42
4	C	504	ZO7	C17-N4	-2.36	1.36	1.41
4	D	503	ZO7	C24-N1	2.36	1.46	1.42
4	A	504	ZO7	C17-N4	-2.34	1.36	1.41
4	G	503	ZO7	C17-N4	-2.33	1.36	1.41
4	D	503	ZO7	C17-N4	-2.33	1.37	1.41
4	H	506	ZO7	C17-N4	-2.31	1.37	1.41
4	E	502	ZO7	C24-N1	2.31	1.46	1.42
4	E	502	ZO7	C17-N4	-2.28	1.37	1.41
4	A	504	ZO7	C24-N1	2.22	1.46	1.42
4	H	506	ZO7	C24-N1	2.03	1.45	1.42

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	503	ZO7	C25-C24-N1	-6.72	104.47	110.67
4	H	506	ZO7	C25-C24-N1	-6.23	104.92	110.67
4	C	504	ZO7	C25-C24-N1	-6.22	104.92	110.67
4	A	504	ZO7	C25-C24-N1	-6.21	104.94	110.67
4	F	502	ZO7	C25-C24-N1	-6.16	104.99	110.67
2	A	501	IMP	C5-C6-N1	6.14	119.61	110.78
4	E	502	ZO7	C25-C24-N1	-6.07	105.06	110.67
2	C	502	IMP	C5-C6-N1	6.02	119.44	110.78
2	B	501	IMP	C5-C6-N1	6.02	119.43	110.78
4	G	503	ZO7	C25-C24-N1	-6.02	105.11	110.67
2	D	502	IMP	C5-C6-N1	5.99	119.39	110.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	IMP	C5-C6-N1	5.91	119.28	110.78
2	H	502	IMP	C5-C6-N1	5.85	119.18	110.78
2	F	501	IMP	C5-C6-N1	5.82	119.14	110.78
2	G	502	IMP	C5-C6-N1	5.72	119.00	110.78
4	B	502	ZO7	C25-C24-N1	-5.53	105.57	110.67
2	A	501	IMP	C2-N3-C4	4.91	120.16	111.53
2	E	501	IMP	C2-N3-C4	4.88	120.11	111.53
2	D	502	IMP	C2-N3-C4	4.86	120.07	111.53
2	H	502	IMP	C2-N3-C4	4.85	120.06	111.53
2	B	501	IMP	C2-N3-C4	4.84	120.04	111.53
2	F	501	IMP	C2-N3-C4	4.84	120.04	111.53
2	A	501	IMP	C5-C4-N3	-4.82	120.18	127.27
2	G	502	IMP	C2-N3-C4	4.80	119.98	111.53
2	H	502	IMP	C5-C4-N3	-4.78	120.24	127.27
2	E	501	IMP	C5-C4-N3	-4.72	120.32	127.27
2	D	502	IMP	C5-C4-N3	-4.72	120.32	127.27
2	C	502	IMP	C2-N3-C4	4.70	119.80	111.53
2	B	501	IMP	C5-C4-N3	-4.68	120.38	127.27
2	G	502	IMP	C5-C4-N3	-4.65	120.43	127.27
4	F	502	ZO7	C20-C21-N1	-4.64	118.06	120.43
2	F	501	IMP	C5-C4-N3	-4.61	120.48	127.27
2	C	502	IMP	C5-C4-N3	-4.50	120.65	127.27
2	F	501	IMP	N1-C2-N3	-4.46	120.36	125.50
2	E	501	IMP	N1-C2-N3	-4.45	120.37	125.50
2	G	502	IMP	N1-C2-N3	-4.45	120.38	125.50
2	B	501	IMP	N1-C2-N3	-4.39	120.45	125.50
2	D	502	IMP	N1-C2-N3	-4.32	120.52	125.50
2	H	502	IMP	N1-C2-N3	-4.29	120.56	125.50
2	C	502	IMP	N1-C2-N3	-4.29	120.56	125.50
2	A	501	IMP	N1-C2-N3	-4.28	120.57	125.50
2	A	501	IMP	C2-N1-C6	-4.01	119.59	125.09
2	C	502	IMP	C2-N1-C6	-3.88	119.78	125.09
2	B	501	IMP	C2-N1-C6	-3.84	119.83	125.09
2	D	502	IMP	C2-N1-C6	-3.84	119.83	125.09
2	H	502	IMP	C2-N1-C6	-3.79	119.90	125.09
2	E	501	IMP	C2-N1-C6	-3.75	119.95	125.09
2	F	501	IMP	C2-N1-C6	-3.66	120.07	125.09
2	G	502	IMP	C2-N1-C6	-3.61	120.14	125.09
4	G	503	ZO7	C20-C21-N1	-3.40	118.69	120.43
4	D	503	ZO7	C29-O3-C24	3.21	116.38	111.97
2	G	502	IMP	O6-C6-C5	-3.00	118.62	126.53
2	B	501	IMP	O3P-P-O2P	2.96	118.89	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	502	ZO7	C26-C25-C24	2.95	114.19	109.86
2	D	502	IMP	O3P-P-O2P	2.93	118.78	107.80
4	D	503	ZO7	C26-C25-C24	2.92	114.15	109.86
2	C	502	IMP	O3P-P-O2P	2.91	118.73	107.80
2	E	501	IMP	O3P-P-O2P	2.89	118.63	107.80
4	G	503	ZO7	C26-C25-C24	2.89	114.10	109.86
2	F	501	IMP	O3P-P-O2P	2.88	118.62	107.80
4	D	503	ZO7	C20-C21-N1	-2.84	118.97	120.43
4	H	506	ZO7	C20-C21-N1	-2.80	119.00	120.43
2	C	502	IMP	O6-C6-C5	-2.80	119.15	126.53
4	E	502	ZO7	C20-C21-N1	-2.79	119.00	120.43
2	B	501	IMP	O6-C6-C5	-2.77	119.21	126.53
2	E	501	IMP	O6-C6-C5	-2.75	119.28	126.53
4	B	502	ZO7	C21-N1-C24	-2.70	120.50	123.18
4	C	504	ZO7	C20-C21-N1	-2.69	119.05	120.43
4	D	503	ZO7	O3-C24-C25	2.68	113.63	110.05
2	H	502	IMP	O6-C6-C5	-2.67	119.49	126.53
2	C	502	IMP	N9-C8-N7	-2.66	108.46	113.40
2	D	502	IMP	O6-C6-C5	-2.62	119.62	126.53
2	G	502	IMP	N9-C8-N7	-2.62	108.55	113.40
2	B	501	IMP	N9-C8-N7	-2.62	108.55	113.40
2	F	501	IMP	O6-C6-C5	-2.60	119.66	126.53
2	H	502	IMP	C8-N7-C5	2.60	108.89	104.26
2	H	502	IMP	N9-C8-N7	-2.60	108.59	113.40
2	D	502	IMP	N9-C8-N7	-2.59	108.59	113.40
2	E	501	IMP	N9-C8-N7	-2.57	108.64	113.40
2	F	501	IMP	N9-C8-N7	-2.56	108.65	113.40
2	D	502	IMP	C8-N7-C5	2.55	108.80	104.26
2	E	501	IMP	C8-N7-C5	2.53	108.77	104.26
2	G	502	IMP	C8-N7-C5	2.52	108.75	104.26
2	F	501	IMP	C8-N7-C5	2.51	108.74	104.26
2	B	501	IMP	C8-N7-C5	2.50	108.72	104.26
4	E	502	ZO7	C26-C25-C24	2.49	113.52	109.86
2	C	502	IMP	C8-N7-C5	2.46	108.65	104.26
4	H	506	ZO7	C21-N1-C24	-2.46	120.74	123.18
2	A	501	IMP	N9-C8-N7	-2.46	108.85	113.40
2	A	501	IMP	C8-N7-C5	2.45	108.62	104.26
2	A	501	IMP	N9-C4-N3	2.40	132.37	126.90
2	A	501	IMP	O6-C6-C5	-2.39	120.21	126.53
2	B	501	IMP	N9-C4-N3	2.38	132.33	126.90
4	F	502	ZO7	C29-O3-C24	2.37	115.23	111.97
2	H	502	IMP	N9-C4-N3	2.36	132.28	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	502	IMP	N9-C4-N3	2.35	132.24	126.90
2	E	501	IMP	N9-C4-N3	2.34	132.24	126.90
4	A	504	ZO7	C21-N1-C24	-2.33	120.87	123.18
2	D	502	IMP	N9-C4-N3	2.30	132.14	126.90
4	E	502	ZO7	C29-O3-C24	2.29	115.12	111.97
2	C	502	IMP	N9-C4-N3	2.28	132.09	126.90
4	G	503	ZO7	C29-O3-C24	2.28	115.10	111.97
4	D	503	ZO7	O3-C24-N1	2.27	113.07	109.38
2	F	501	IMP	N9-C4-N3	2.25	132.03	126.90
4	A	504	ZO7	C20-C21-N1	-2.25	119.28	120.43
4	G	503	ZO7	O3-C24-C25	2.23	113.04	110.05
4	F	502	ZO7	O3-C24-N1	2.16	112.89	109.38
4	F	502	ZO7	O3-C24-C25	2.12	112.89	110.05
4	C	504	ZO7	C29-O3-C24	2.12	114.89	111.97
2	G	502	IMP	O2P-P-O1P	2.03	118.75	110.83
2	A	501	IMP	O2P-P-O1P	2.03	118.74	110.83
4	C	504	ZO7	C11-N3-C10	2.01	128.19	124.01

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	IMP	C5'-O5'-P-O1P
2	B	501	IMP	C5'-O5'-P-O1P
2	B	501	IMP	C5'-O5'-P-O2P
2	B	501	IMP	C5'-O5'-P-O3P
2	C	502	IMP	C5'-O5'-P-O2P
2	D	502	IMP	C5'-O5'-P-O2P
2	D	502	IMP	C5'-O5'-P-O3P
2	E	501	IMP	C5'-O5'-P-O2P
2	F	501	IMP	C5'-O5'-P-O1P
2	F	501	IMP	C5'-O5'-P-O2P
2	F	501	IMP	C5'-O5'-P-O3P
2	G	502	IMP	C5'-O5'-P-O1P
2	G	502	IMP	C5'-O5'-P-O2P
2	G	502	IMP	C5'-O5'-P-O3P
2	H	502	IMP	C5'-O5'-P-O2P
2	H	502	IMP	C5'-O5'-P-O3P
3	A	503	GOL	O1-C1-C2-C3
2	F	501	IMP	C3'-C4'-C5'-O5'
2	F	501	IMP	O4'-C4'-C5'-O5'
3	A	503	GOL	C1-C2-C3-O3

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

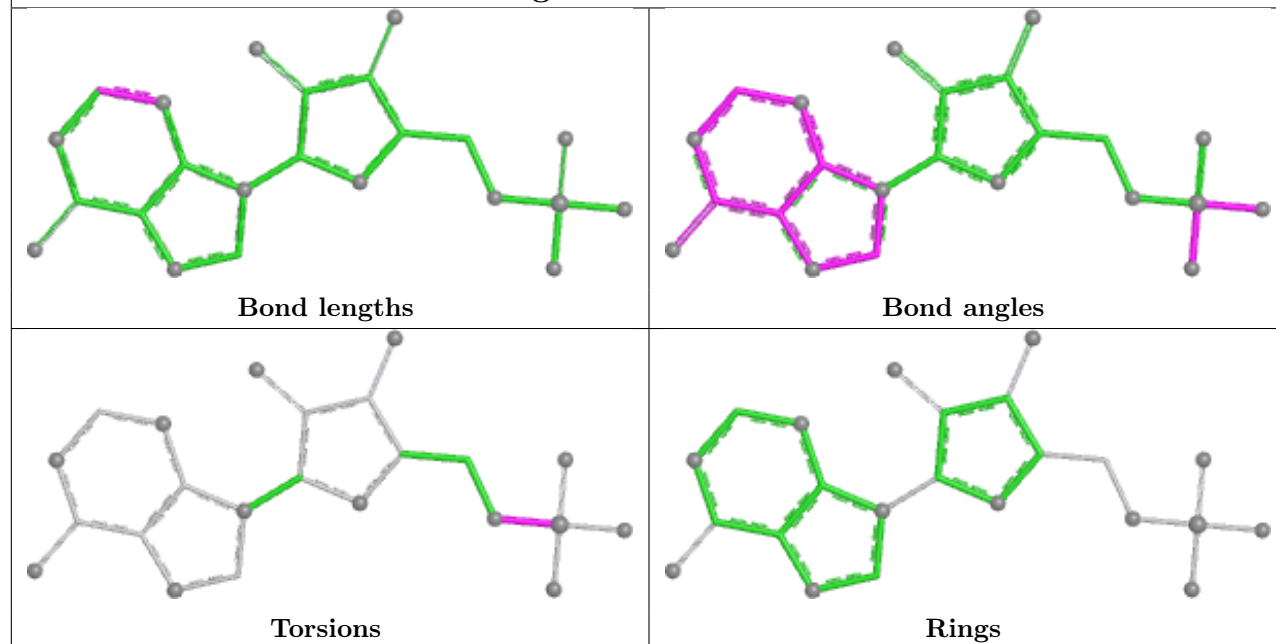
There are no ring outliers.

2 monomers are involved in 3 short contacts:

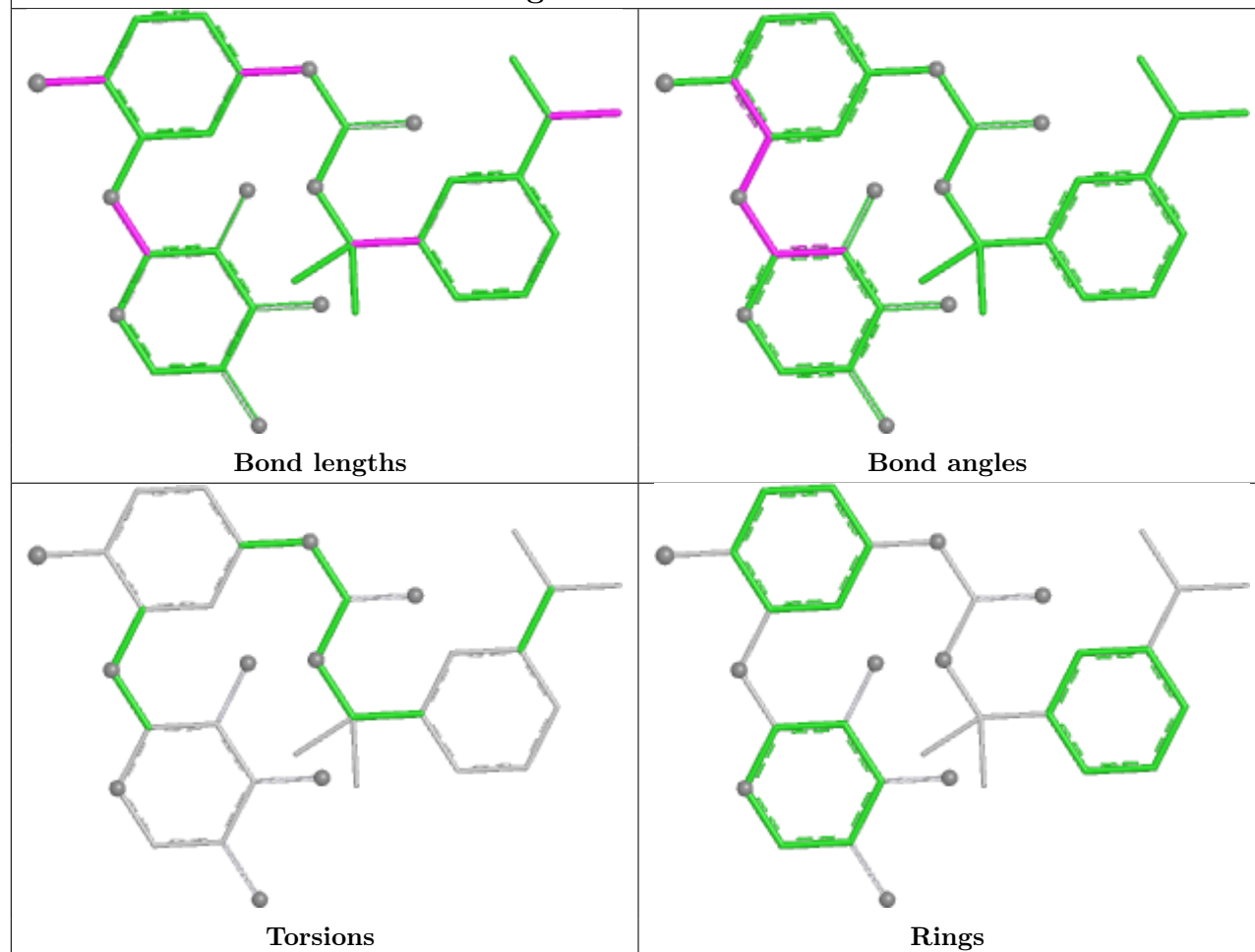
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	IMP	2	0
2	C	502	IMP	1	0

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

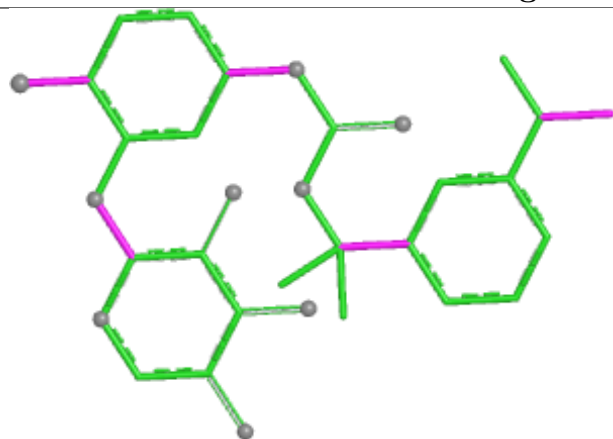
Ligand IMP G 502



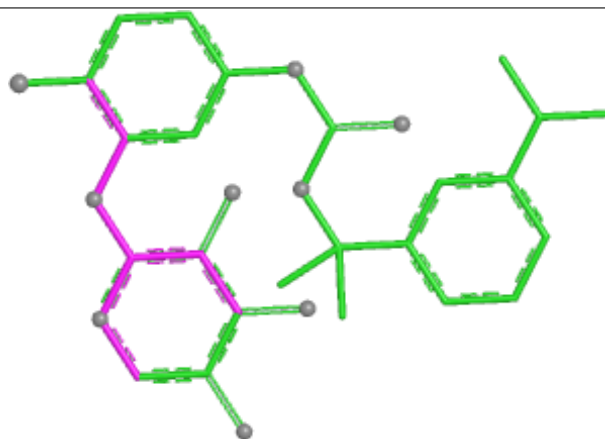
Ligand ZO7 A 504



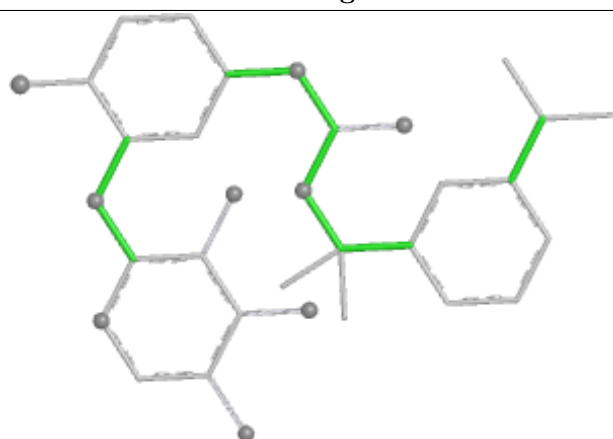
Ligand ZO7 E 502



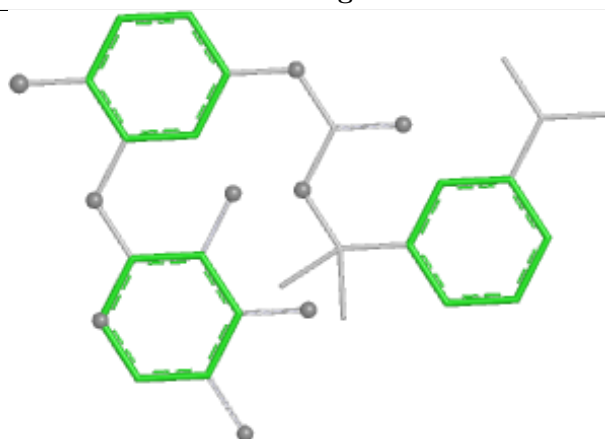
Bond lengths



Bond angles

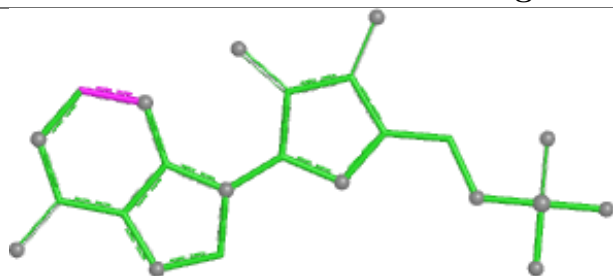


Torsions

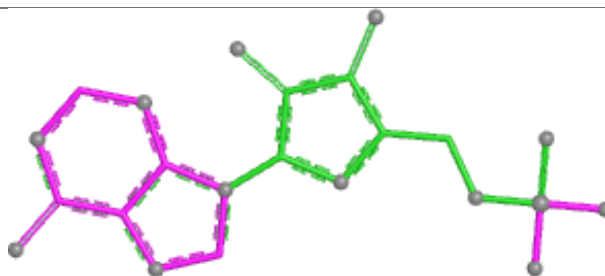


Rings

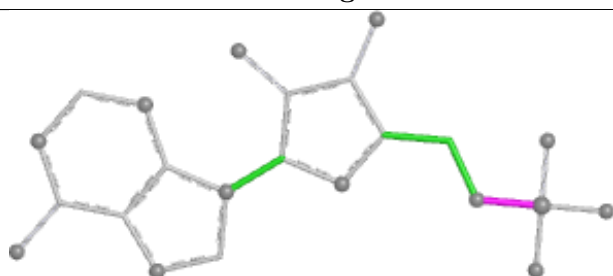
Ligand IMP A 501



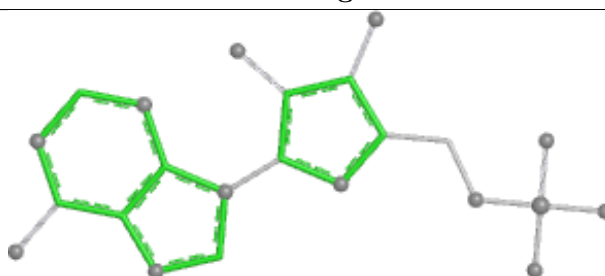
Bond lengths



Bond angles

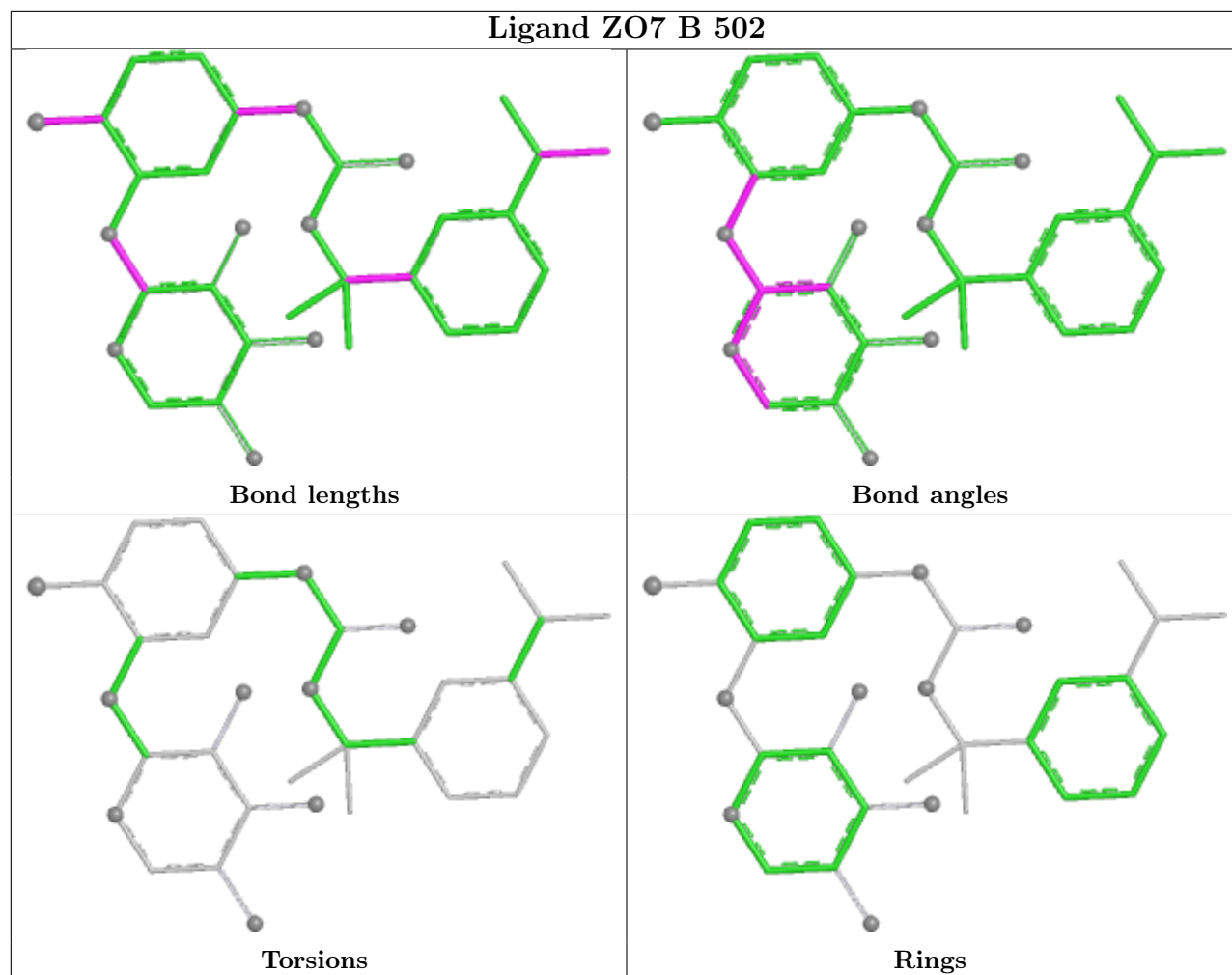


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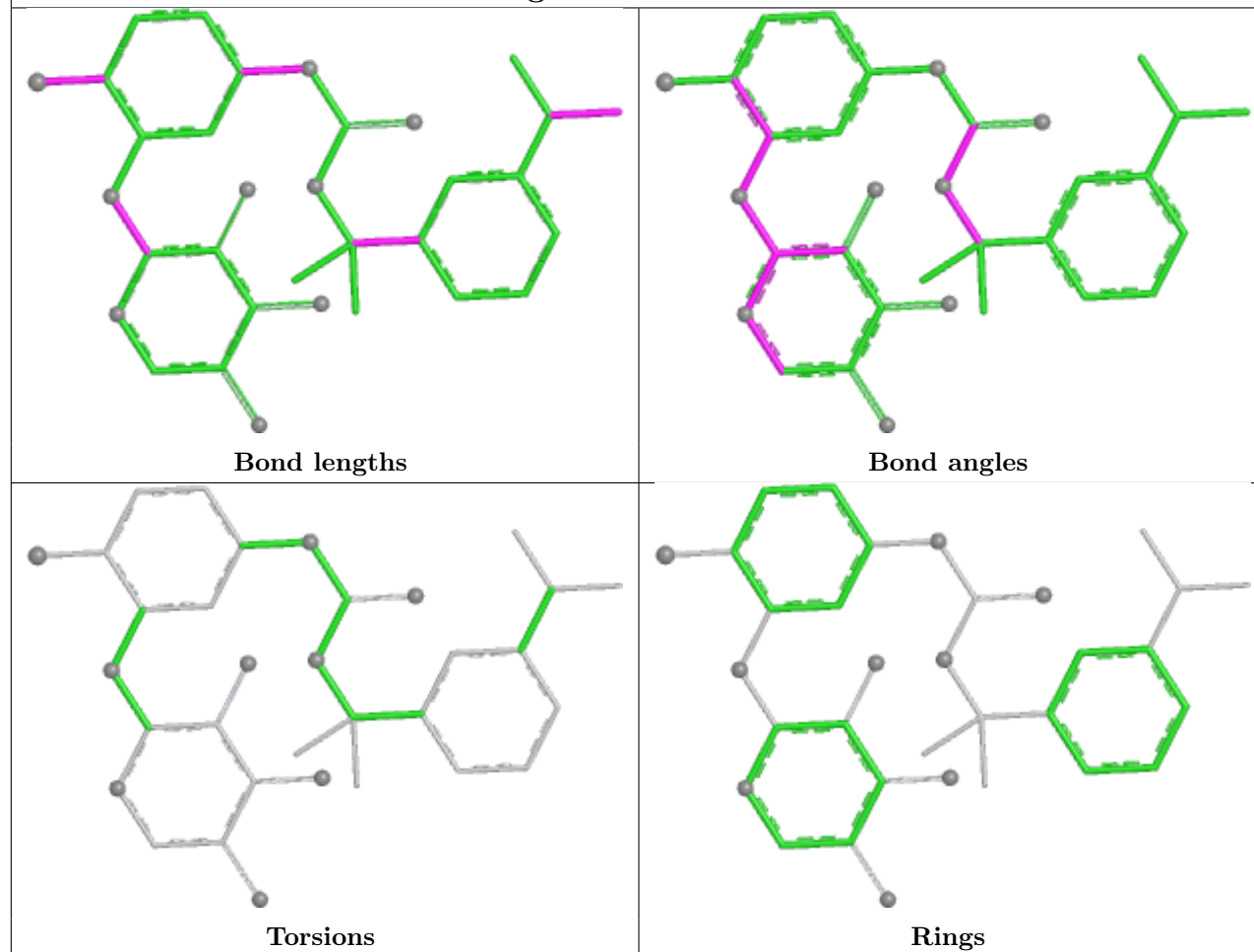


Rings

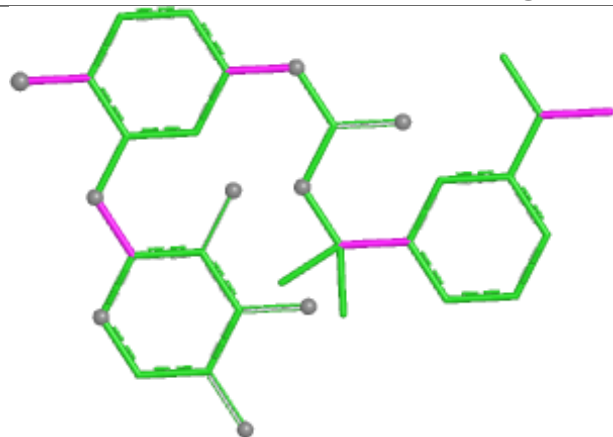
Ligand ZO7 B 502



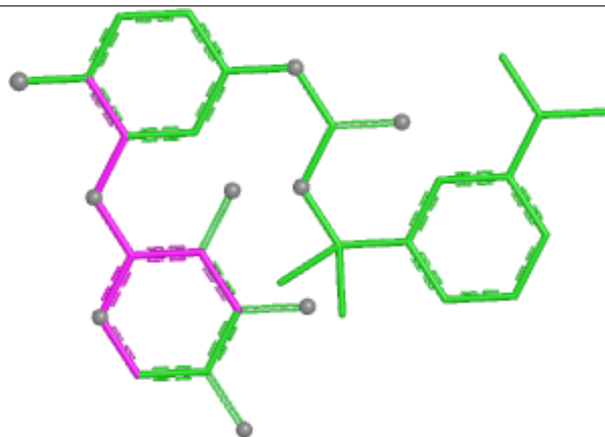
Ligand ZO7 C 504



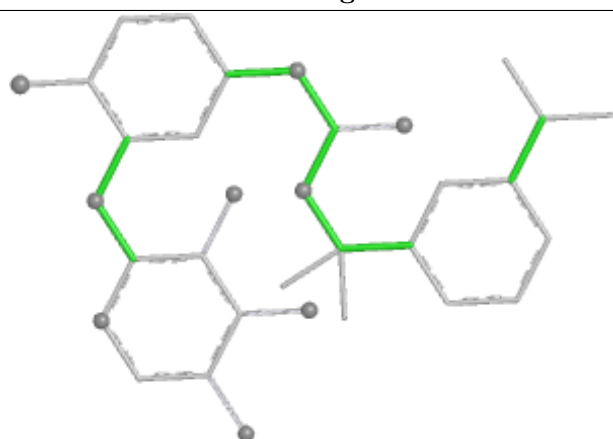
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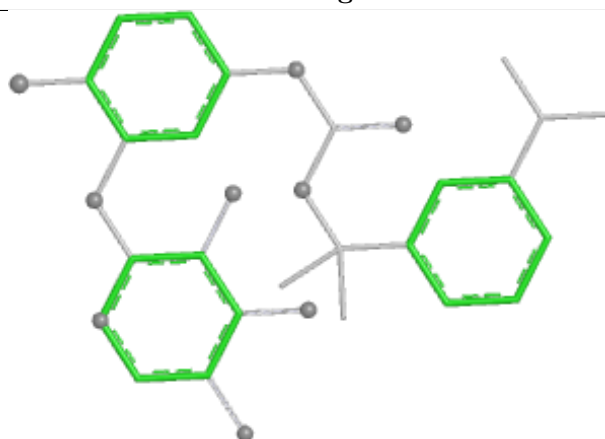
Bond lengths



Bond angles

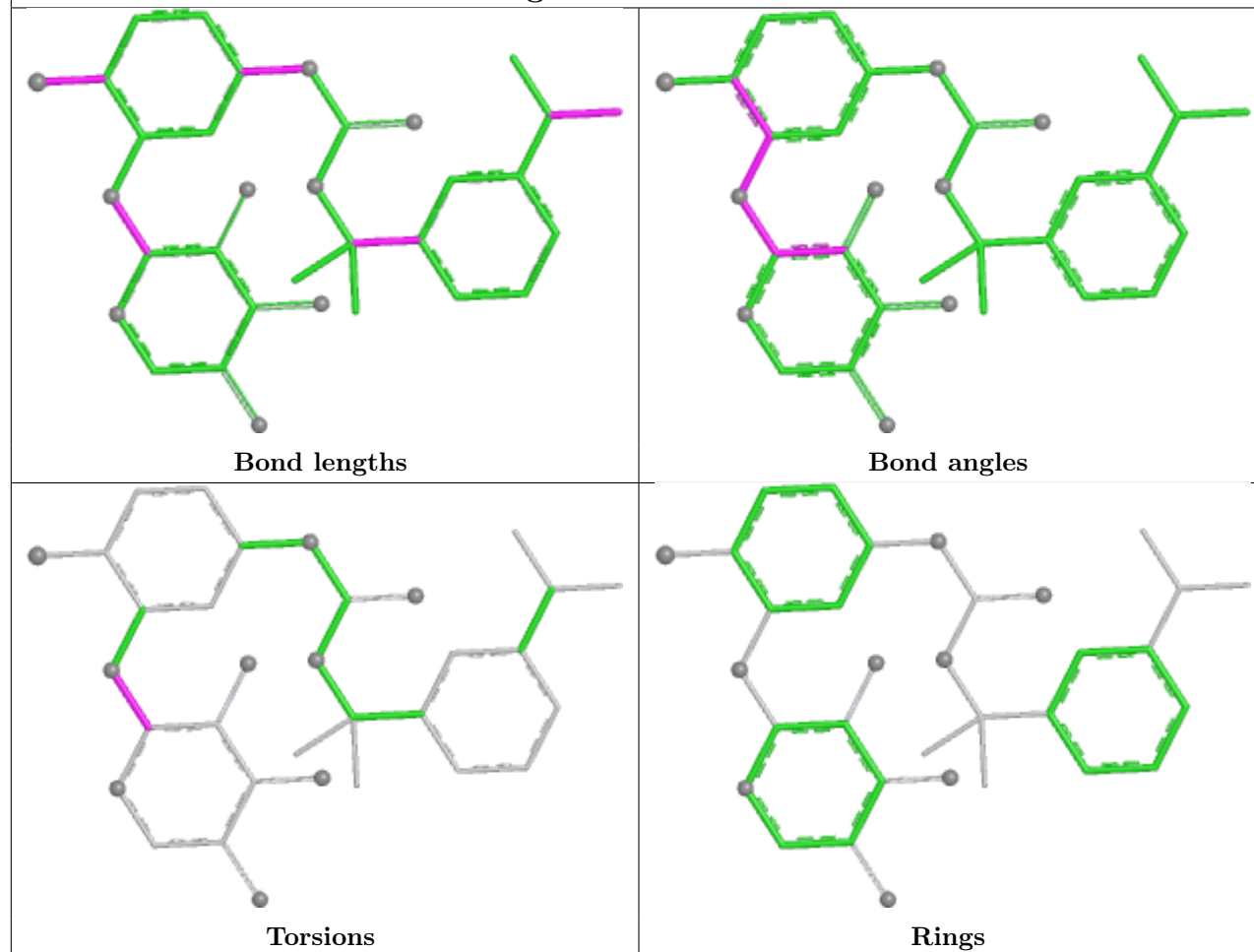


Torsions

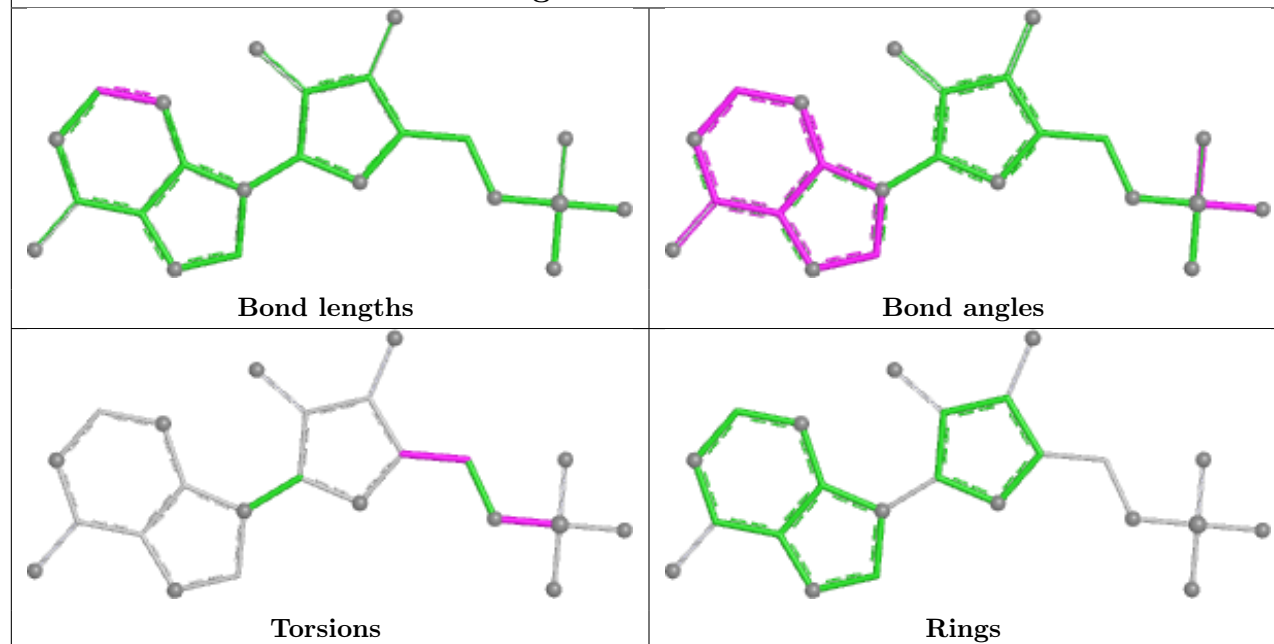


Rings

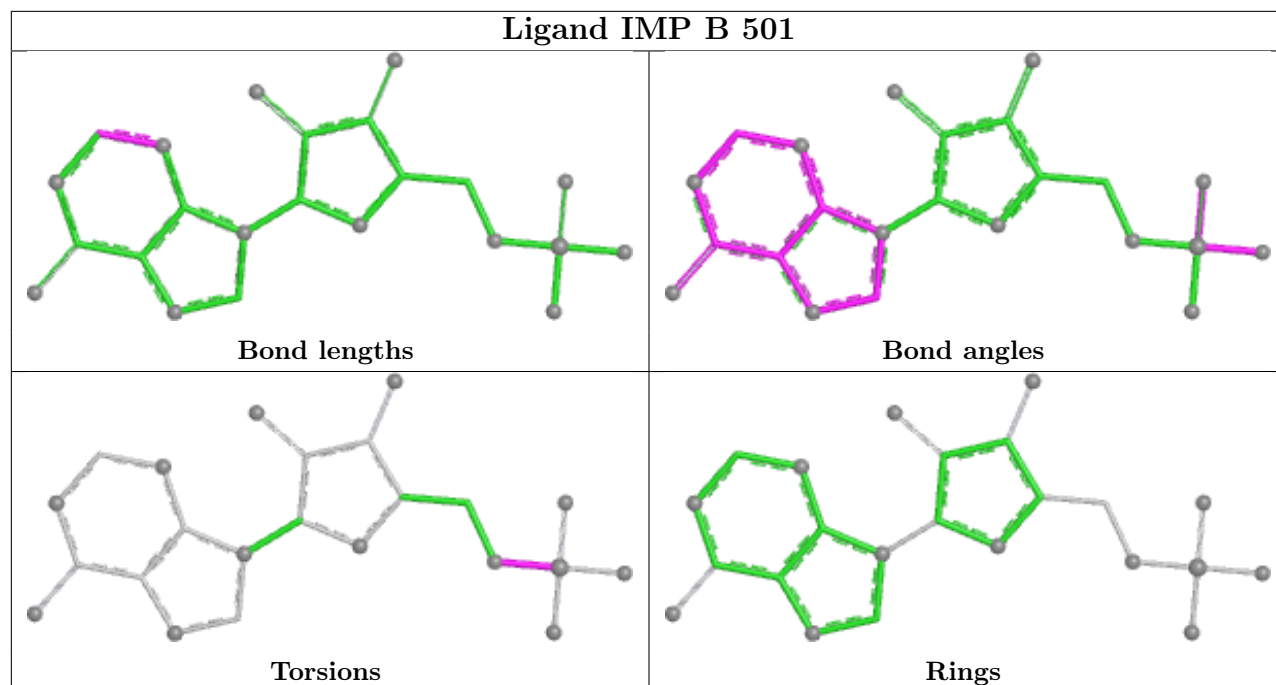
Ligand ZO7 H 506



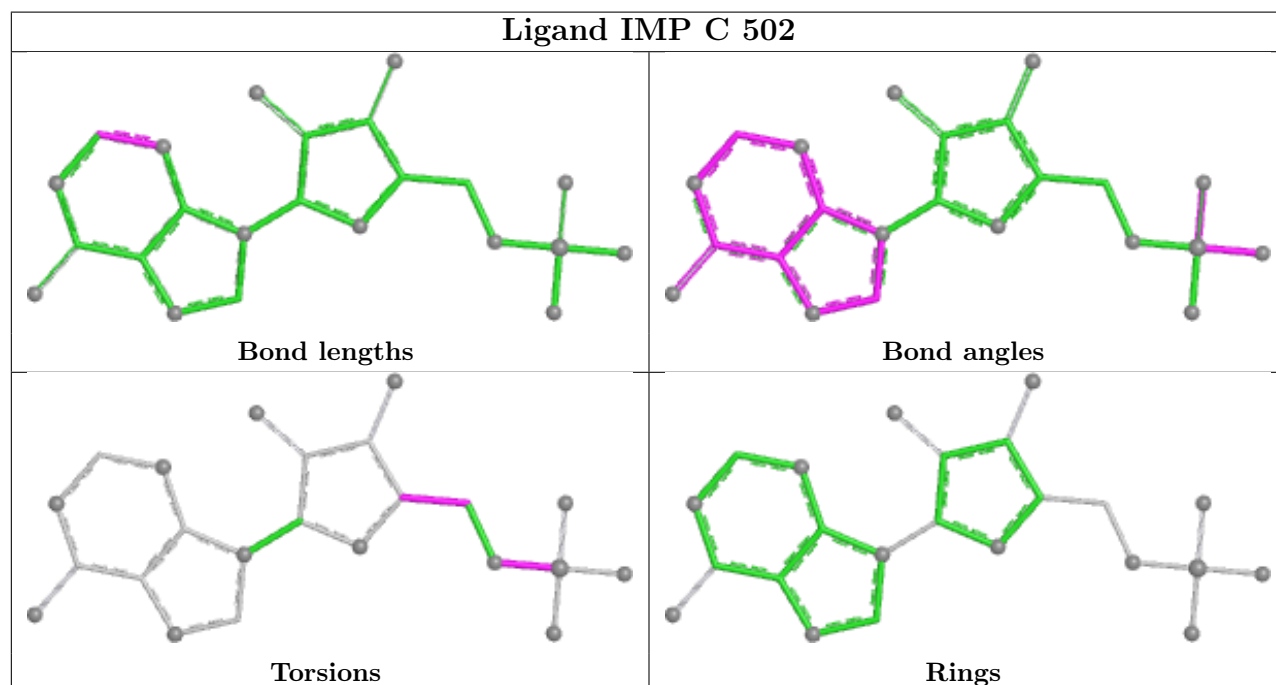
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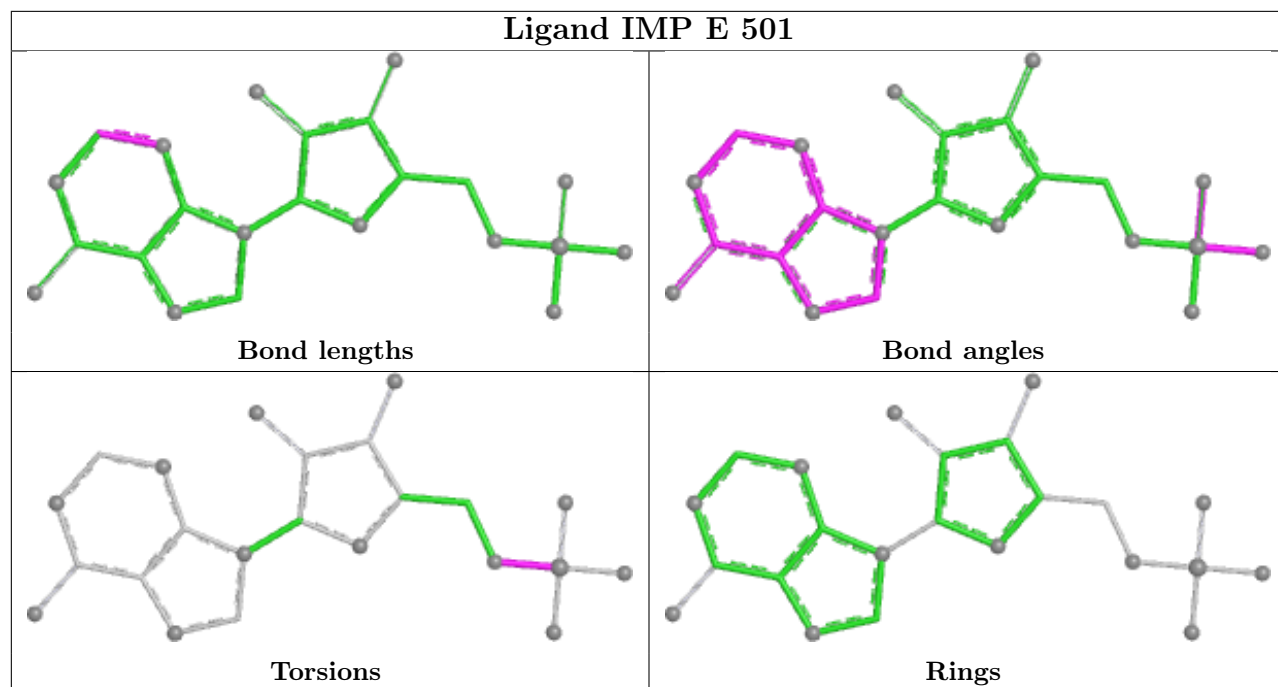
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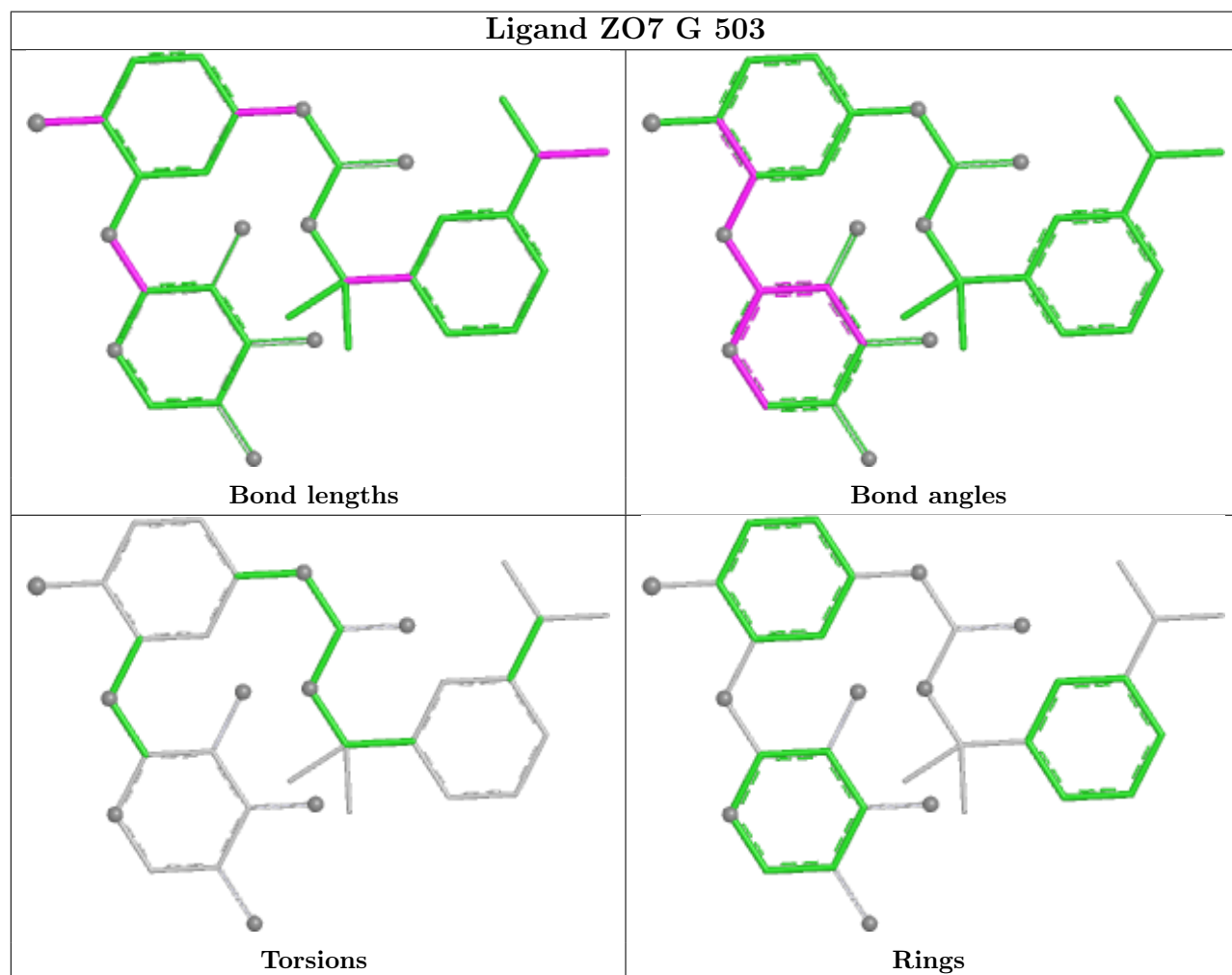
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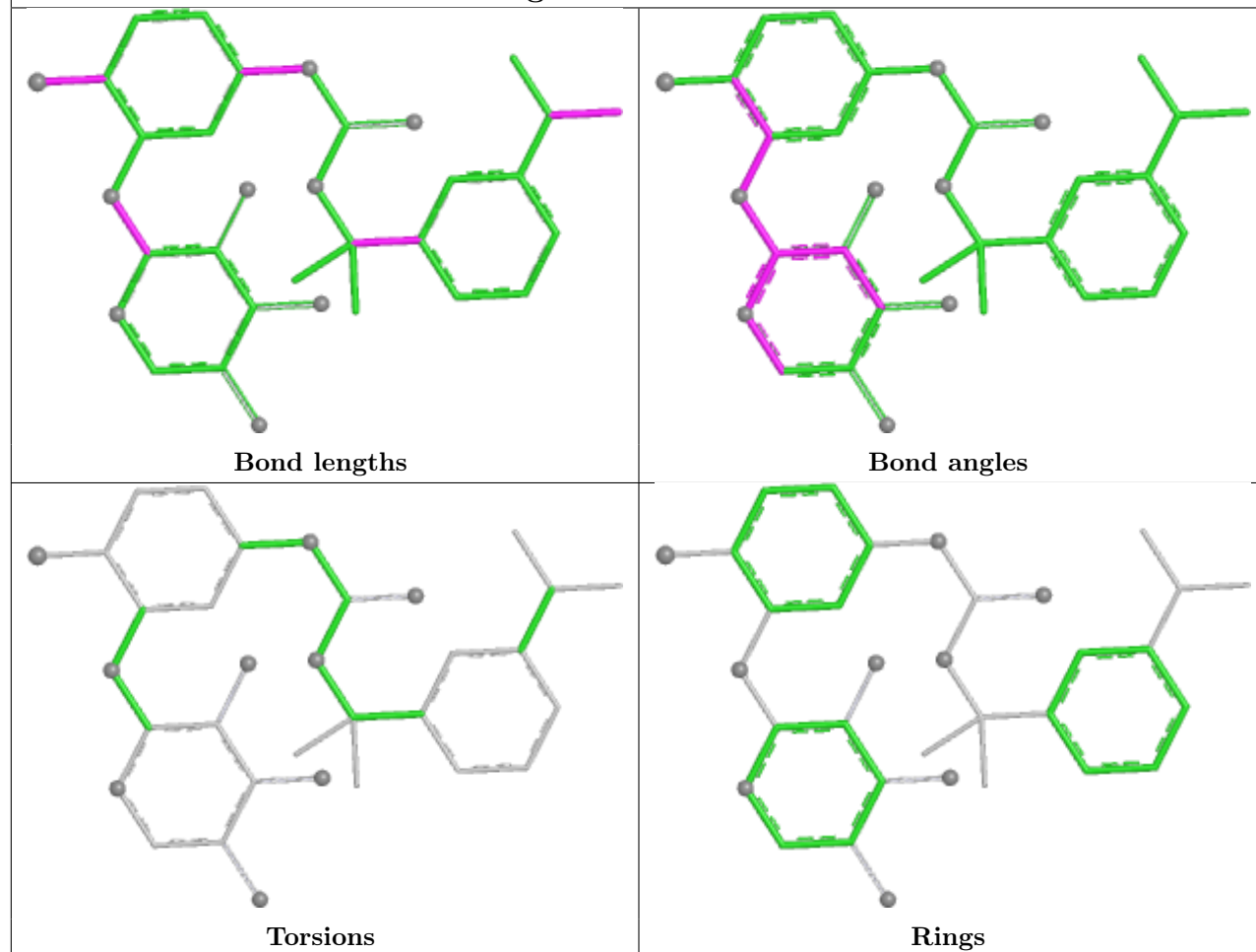
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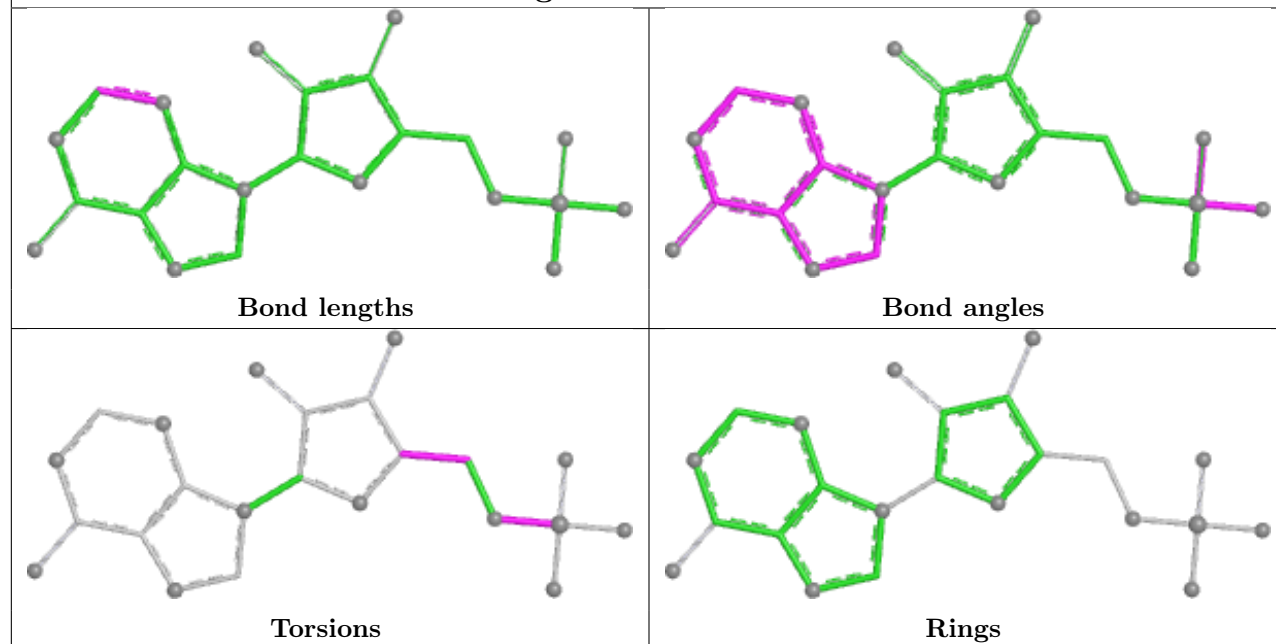
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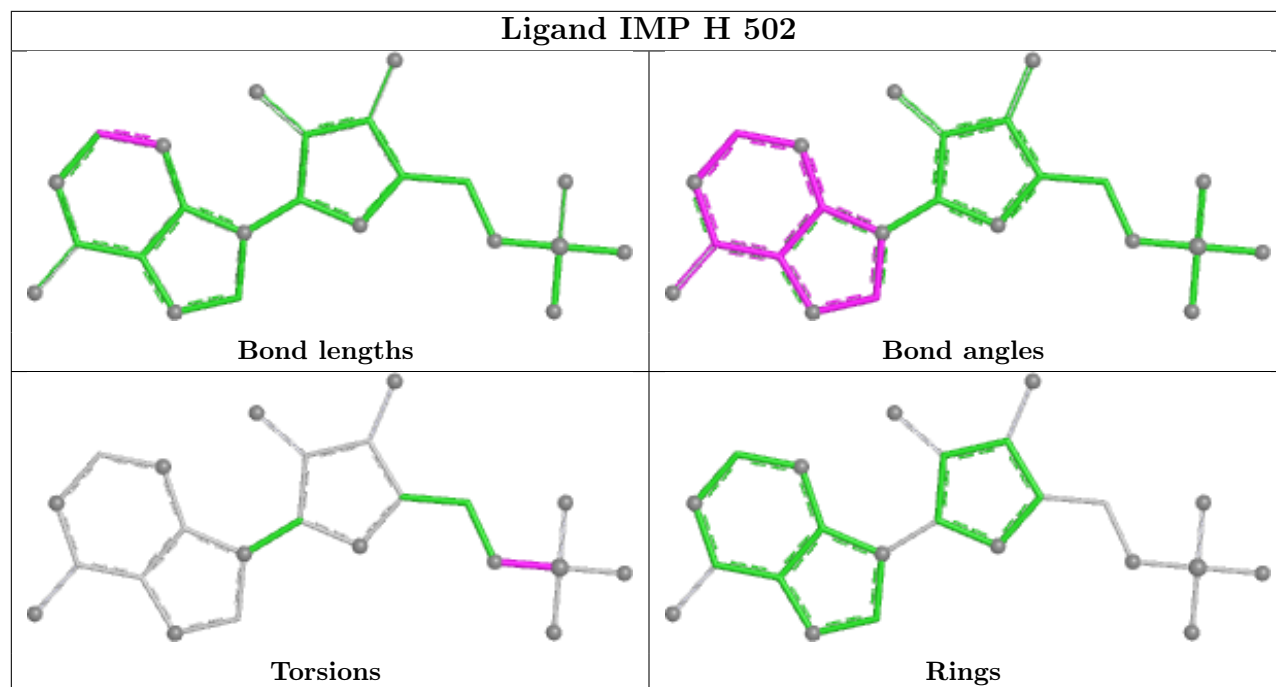


Ligand ZO7 D 503



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	349/384 (90%)	0.59	18 (5%)	33	39	18, 31, 54, 79	1 (0%)
1	B	350/384 (91%)	0.59	21 (6%)	27	32	18, 32, 54, 87	2 (0%)
1	C	351/384 (91%)	0.53	10 (2%)	55	61	20, 32, 54, 75	0
1	D	349/384 (90%)	0.83	26 (7%)	20	25	20, 42, 65, 86	0
1	E	347/384 (90%)	1.28	64 (18%)	3	4	28, 54, 84, 97	0
1	F	348/384 (90%)	0.96	36 (10%)	12	14	23, 44, 74, 104	1 (0%)
1	G	351/384 (91%)	0.75	20 (5%)	29	34	21, 39, 62, 86	0
1	H	349/384 (90%)	0.68	19 (5%)	31	37	21, 35, 61, 93	0
All	All	2794/3072 (90%)	0.78	214 (7%)	19	23	18, 38, 71, 104	4 (0%)

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	223	VAL	5.5
1	A	382	GLY	5.3
1	F	243	ALA	4.8
1	E	88	VAL	4.7
1	E	226	ALA	4.6
1	E	479	THR	4.5
1	A	413	LEU	4.3
1	B	413	LEU	4.2
1	G	476	VAL	4.1
1	B	86	ASP	4.0
1	D	-1	ASN	4.0
1	E	25	VAL	3.9
1	G	413	LEU	3.9
1	E	272	PRO	3.9
1	E	448	ALA	3.9
1	E	334	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	374	PRO	3.7
1	E	57	ALA	3.5
1	G	487	LEU	3.5
1	F	231	ALA	3.5
1	D	54	VAL	3.5
1	E	67	GLY	3.5
1	G	447	GLY	3.4
1	D	61	ILE	3.3
1	F	413	LEU	3.3
1	D	25	VAL	3.3
1	B	-1	ASN	3.3
1	C	413	LEU	3.3
1	D	379	ILE	3.3
1	E	243	ALA	3.2
1	E	276	ILE	3.2
1	G	-1	ASN	3.2
1	F	251	ASP	3.1
1	F	267	VAL	3.1
1	E	261	ILE	3.1
1	A	456	GLU	3.1
1	E	247	ALA	3.1
1	F	7	VAL	3.1
1	E	84	GLN	3.1
1	F	-1	ASN	3.1
1	D	293	ALA	3.1
1	E	62	ALA	3.1
1	F	281	VAL	3.1
1	H	23	SER	3.0
1	E	225	ALA	3.0
1	E	454	LEU	2.9
1	F	260	VAL	2.9
1	F	41	GLN	2.9
1	H	481	GLU	2.9
1	A	269	ALA	2.9
1	G	245	VAL	2.9
1	F	377	THR	2.9
1	B	0	ALA	2.9
1	B	82	ALA	2.9
1	D	30	VAL	2.9
1	D	413	LEU	2.9
1	A	25	VAL	2.9
1	B	400	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	333	LYS	2.8
1	B	257	SER	2.8
1	A	398	GLU	2.8
1	G	267	VAL	2.8
1	D	24	ASP	2.8
1	D	43	ASN	2.8
1	D	294	GLY	2.8
1	F	0	ALA	2.8
1	E	379	ILE	2.7
1	F	78	ILE	2.7
1	D	369	GLY	2.7
1	E	338	VAL	2.7
1	H	25	VAL	2.7
1	E	269	ALA	2.7
1	F	295	ALA	2.7
1	E	78	ILE	2.7
1	E	274	LEU	2.7
1	H	85	VAL	2.7
1	H	375	GLY	2.7
1	F	223	VAL	2.6
1	G	54	VAL	2.6
1	H	86	ASP	2.6
1	C	12	THR	2.6
1	H	364	GLY	2.6
1	H	-2	SER	2.6
1	H	456	GLU	2.6
1	H	92	GLY	2.6
1	E	40	LEU	2.6
1	D	397	MET	2.6
1	H	422	VAL	2.6
1	E	373	SER	2.6
1	G	-2	SER	2.6
1	F	87	LYS	2.6
1	E	369	GLY	2.6
1	E	237	ILE	2.6
1	F	339	ILE	2.6
1	F	239	ALA	2.5
1	D	374	PRO	2.5
1	E	54	VAL	2.5
1	G	241	VAL	2.5
1	B	380	TYR	2.5
1	E	271	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLU	2.5
1	E	75	ASN	2.5
1	E	260	VAL	2.5
1	B	243	ALA	2.5
1	D	267	VAL	2.5
1	E	222	LEU	2.5
1	B	369	GLY	2.5
1	E	68	GLY	2.5
1	A	479	THR	2.4
1	A	264	VAL	2.4
1	E	360	VAL	2.4
1	E	26	LEU	2.4
1	F	395	GLY	2.4
1	H	229	VAL	2.4
1	G	246	ASP	2.4
1	D	382	GLY	2.4
1	E	460	PHE	2.4
1	D	376	GLU	2.4
1	F	357	GLY	2.4
1	E	377	THR	2.4
1	F	230	THR	2.4
1	H	88	VAL	2.4
1	H	234	MET	2.4
1	E	240	LEU	2.4
1	G	-3	GLN	2.4
1	D	232	ASP	2.3
1	E	279	GLY	2.3
1	B	260	VAL	2.3
1	F	85	VAL	2.3
1	E	221	LEU	2.3
1	A	380	TYR	2.3
1	E	1	MET	2.3
1	G	55	THR	2.3
1	F	73	HIS	2.3
1	F	250	LEU	2.3
1	C	24	ASP	2.3
1	E	227	VAL	2.3
1	F	300	VAL	2.3
1	G	232	ASP	2.3
1	F	1	MET	2.3
1	E	388	TYR	2.3
1	D	377	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	3	GLU	2.3
1	F	379	ILE	2.3
1	C	267	VAL	2.3
1	E	241	VAL	2.3
1	B	296	ASN	2.2
1	C	382	GLY	2.2
1	D	60	ALA	2.2
1	A	414	VAL	2.2
1	B	40	LEU	2.2
1	B	229	VAL	2.2
1	D	88	VAL	2.2
1	E	36	LEU	2.2
1	E	85	VAL	2.2
1	E	267	VAL	2.2
1	H	245	VAL	2.2
1	D	86	ASP	2.2
1	E	337	PRO	2.2
1	A	359	HIS	2.2
1	D	29	GLU	2.2
1	C	-3	GLN	2.2
1	E	82	ALA	2.2
1	B	486	SER	2.2
1	F	302	ILE	2.2
1	E	24	ASP	2.2
1	E	457	ASN	2.2
1	D	92	GLY	2.2
1	C	0	ALA	2.2
1	F	57	ALA	2.2
1	F	380	TYR	2.2
1	F	418	ILE	2.2
1	H	90	ARG	2.2
1	B	75	ASN	2.2
1	G	380	TYR	2.1
1	E	69	LEU	2.1
1	H	413	LEU	2.1
1	A	297	VAL	2.1
1	D	251	ASP	2.1
1	E	229	VAL	2.1
1	E	414	VAL	2.1
1	F	58	ASP	2.1
1	F	38	GLU	2.1
1	G	483	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	22	LYS	2.1
1	B	292	GLU	2.1
1	H	24	ASP	2.1
1	A	449	GLN	2.1
1	B	85	VAL	2.1
1	G	27	PRO	2.1
1	E	220	GLY	2.1
1	C	256	HIS	2.1
1	E	336	ILE	2.1
1	F	271	TYR	2.1
1	E	316	VAL	2.1
1	E	235	THR	2.0
1	F	252	THR	2.0
1	A	1	MET	2.0
1	H	269	ALA	2.0
1	A	251	ASP	2.0
1	B	487	LEU	2.0
1	E	61	ILE	2.0
1	E	249	VAL	2.0
1	E	294	GLY	2.0
1	E	87	LYS	2.0
1	B	1[A]	MET	2.0
1	A	23	SER	2.0
1	A	244	SER	2.0
1	A	486	SER	2.0
1	C	378	GLU	2.0
1	F	55	THR	2.0
1	G	26	LEU	2.0
1	G	222	LEU	2.0
1	C	399	LYS	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

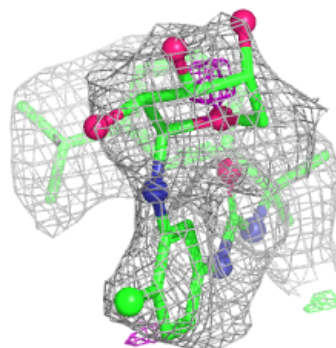
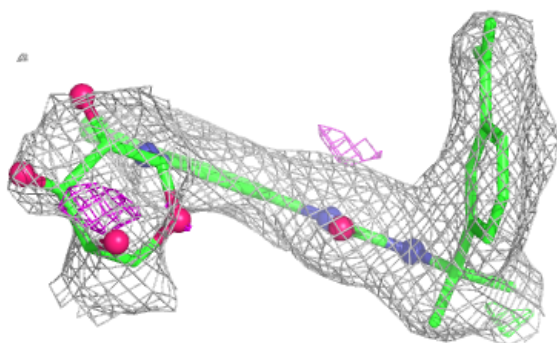
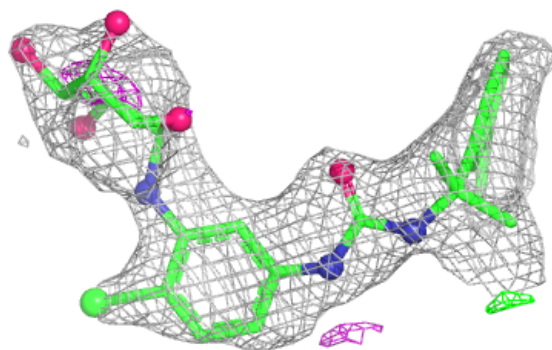
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	506	6/6	0.74	0.12	37,44,47,50	0
3	GOL	H	504	6/6	0.79	0.13	37,42,43,45	0
3	GOL	A	503	6/6	0.80	0.11	36,38,39,41	0
3	GOL	C	503	6/6	0.81	0.13	32,37,44,45	0
4	ZO7	F	502	33/33	0.81	0.12	38,47,67,71	1
4	ZO7	C	504	33/33	0.82	0.12	30,37,55,60	1
4	ZO7	E	502	33/33	0.82	0.13	40,46,71,75	1
3	GOL	H	503	6/6	0.82	0.11	39,40,47,52	0
4	ZO7	D	503	33/33	0.83	0.12	34,40,59,64	0
4	ZO7	H	506	33/33	0.83	0.13	22,37,55,59	1
3	GOL	A	502	6/6	0.84	0.13	27,37,40,43	0
6	EDO	F	504	4/4	0.86	0.10	33,46,47,51	0
4	ZO7	G	503	33/33	0.87	0.11	25,32,53,56	1
4	ZO7	A	504	33/33	0.87	0.11	24,31,51,55	1
4	ZO7	B	502	33/33	0.87	0.11	18,31,50,51	1
5	K	H	505	1/1	0.91	0.07	58,58,58,58	0
5	K	G	501	1/1	0.92	0.06	37,37,37,37	0
2	IMP	F	501	23/23	0.93	0.10	25,33,37,40	0
2	IMP	G	502	23/23	0.93	0.10	19,29,34,38	0
2	IMP	H	502	23/23	0.93	0.10	17,23,26,32	0
2	IMP	E	501	23/23	0.93	0.10	36,38,42,45	0
2	IMP	C	502	23/23	0.94	0.09	13,24,30,31	0
2	IMP	B	501	23/23	0.95	0.08	18,23,25,27	0
2	IMP	A	501	23/23	0.95	0.07	18,22,25,26	0
2	IMP	D	502	23/23	0.95	0.08	24,31,35,37	0
5	K	C	501	1/1	0.96	0.16	22,22,22,22	0
5	K	B	503	1/1	0.97	0.14	29,29,29,29	0
5	K	H	501	1/1	0.98	0.07	29,29,29,29	0
5	K	E	503	1/1	0.98	0.06	37,37,37,37	0
5	K	D	501	1/1	0.98	0.07	23,23,23,23	0
5	K	A	505	1/1	0.99	0.05	17,17,17,17	0
5	K	F	503	1/1	0.99	0.06	20,20,20,20	0

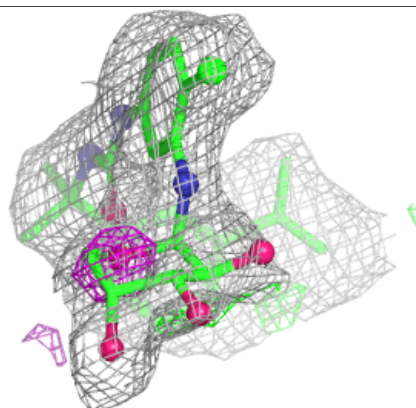
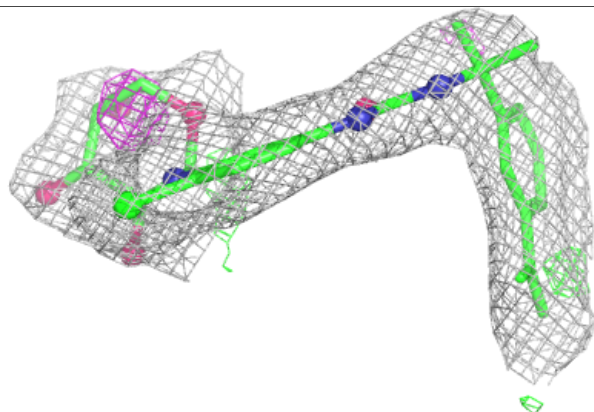
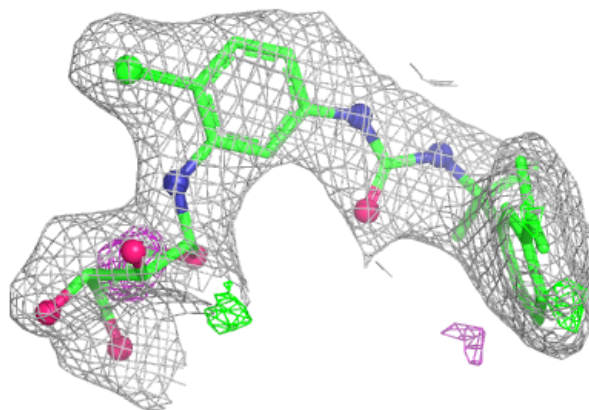
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZO7 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)

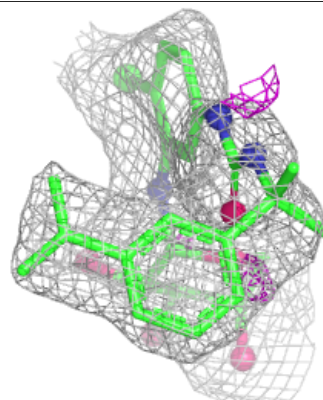
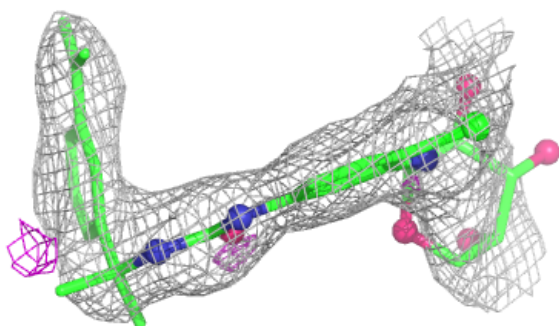
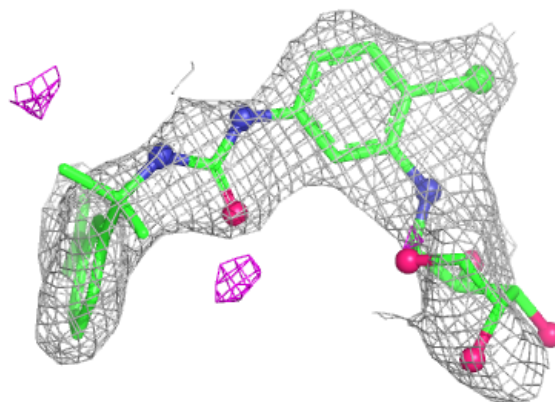
**Electron density around ZO7 C 504:**

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

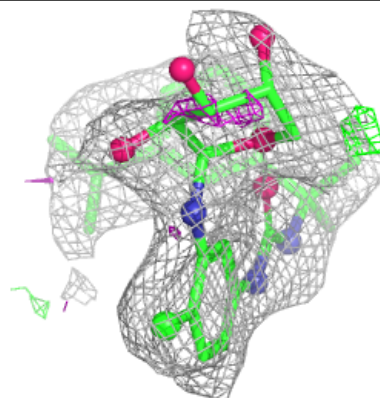
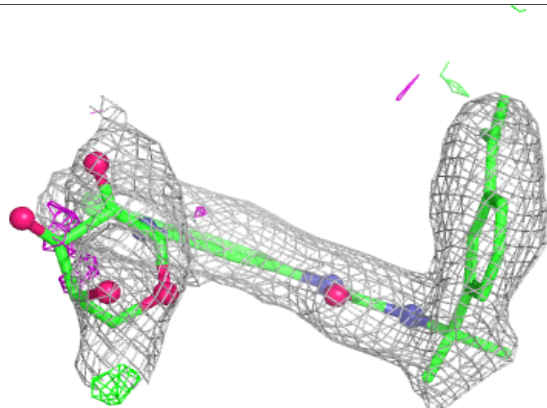
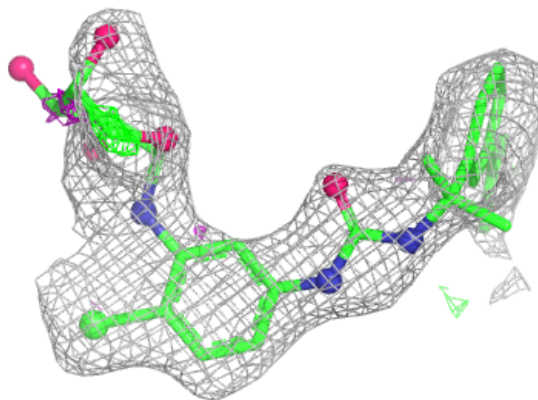


Electron density around ZO7 E 502:

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

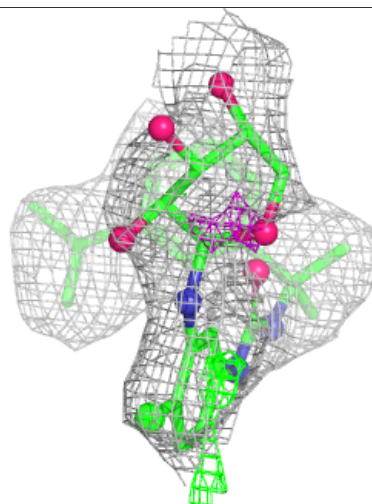
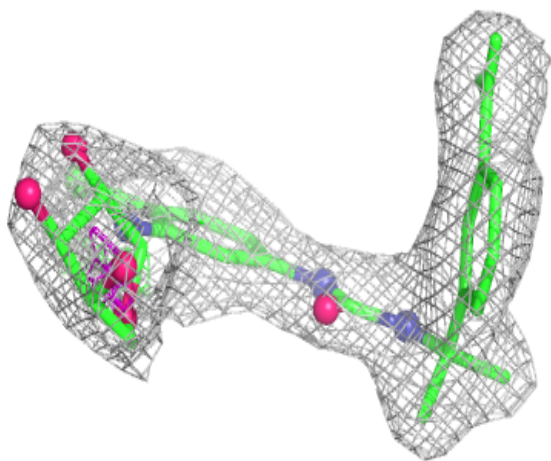
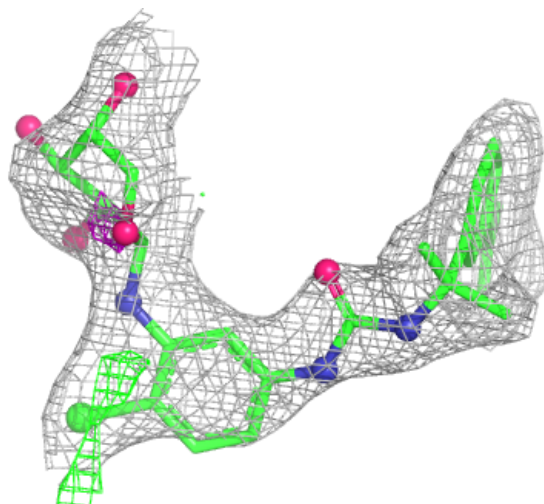
**Electron density around ZO7 D 503:**

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



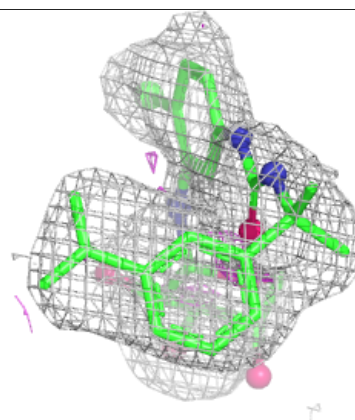
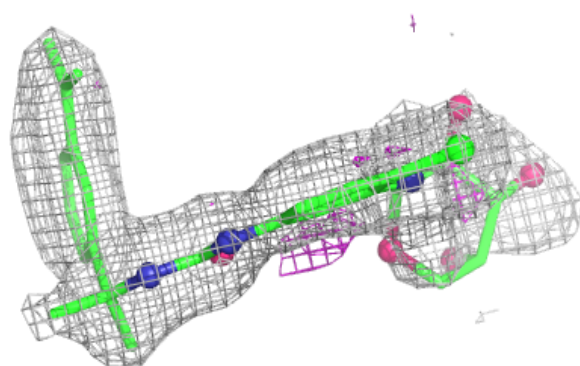
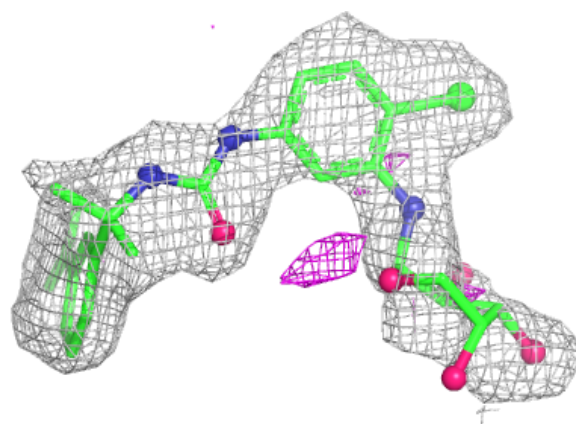
Electron density around ZO7 H 506:

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

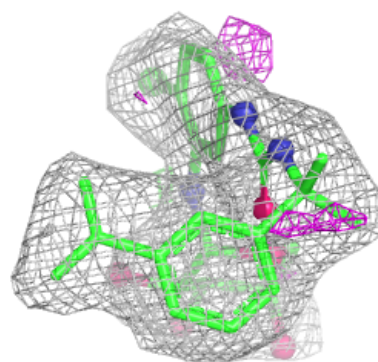
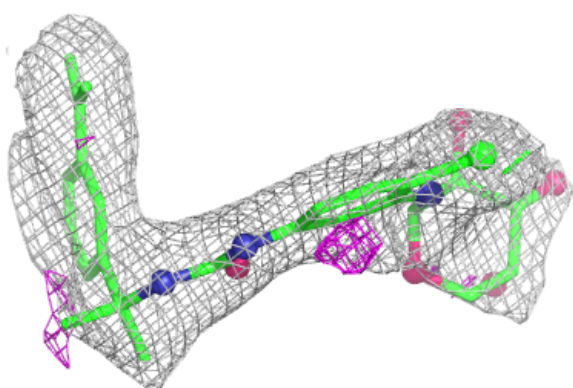
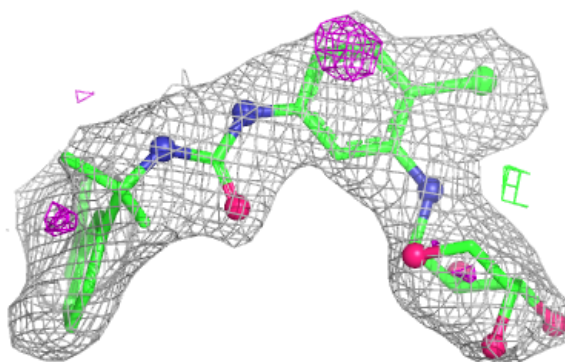


Electron density around ZO7 G 503:

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

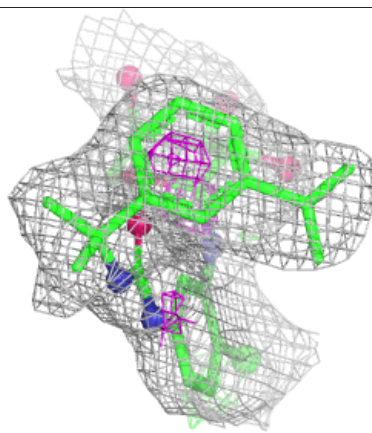
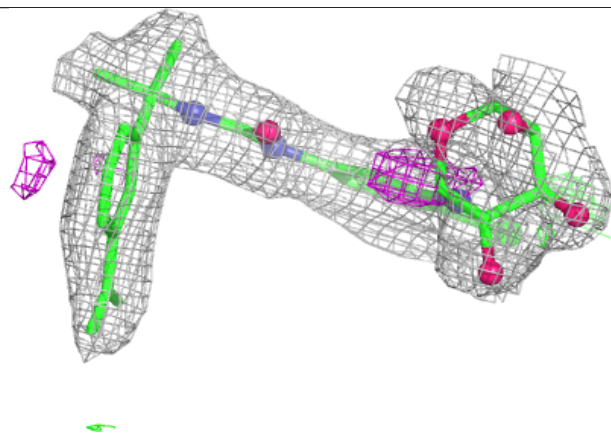
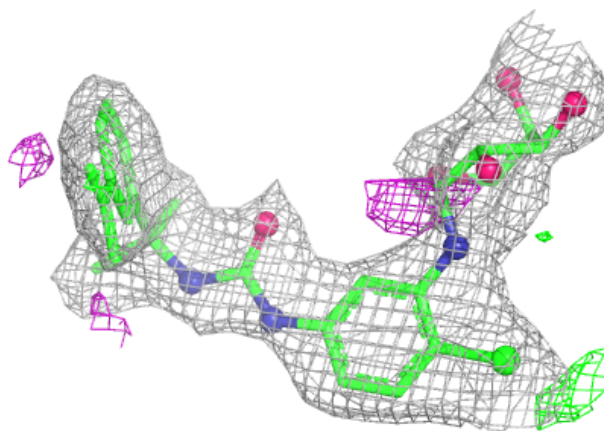
**Electron density around ZO7 A 504:**

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



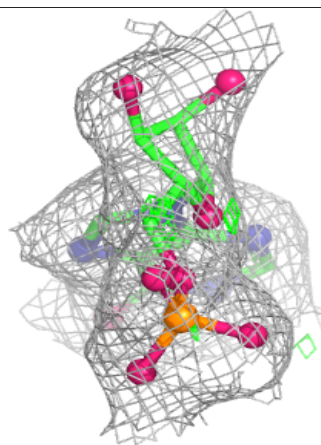
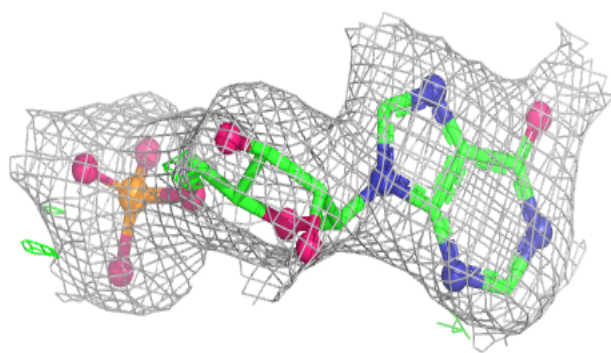
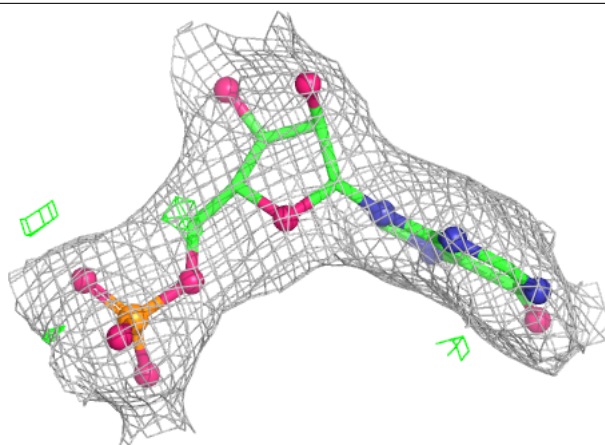
Electron density around ZO7 B 502:

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



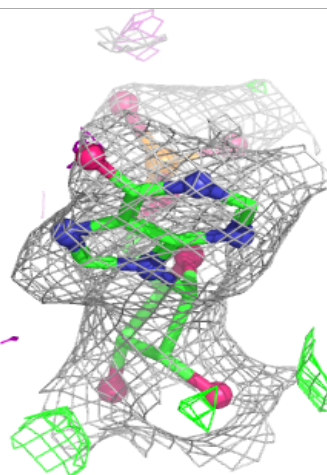
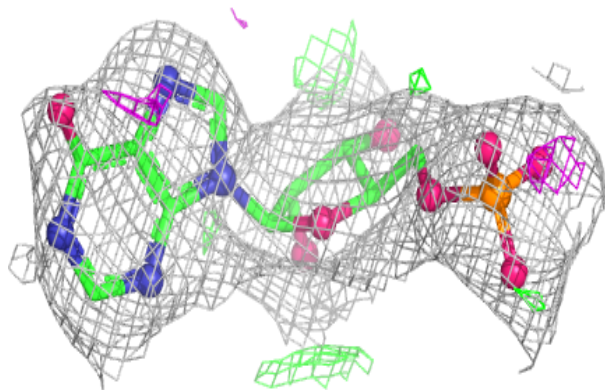
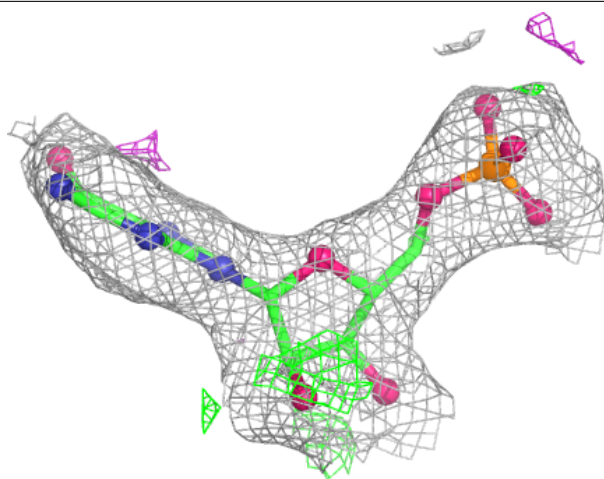
Electron density around IMP F 501:

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



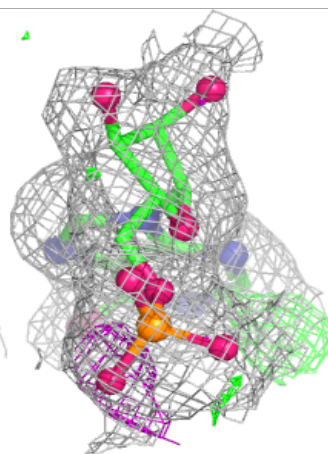
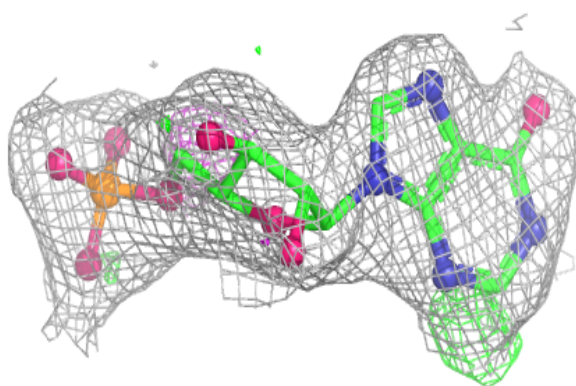
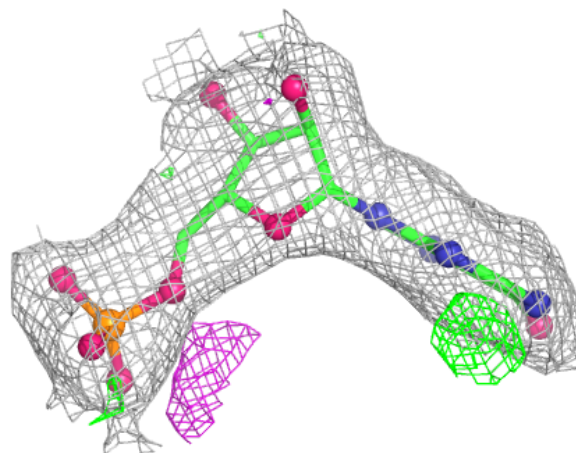
Electron density around IMP G 502:

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



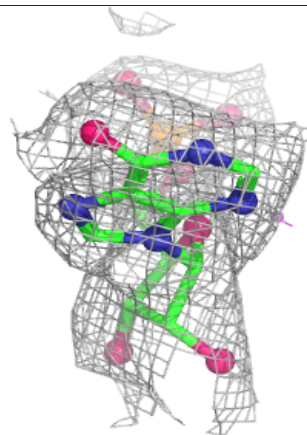
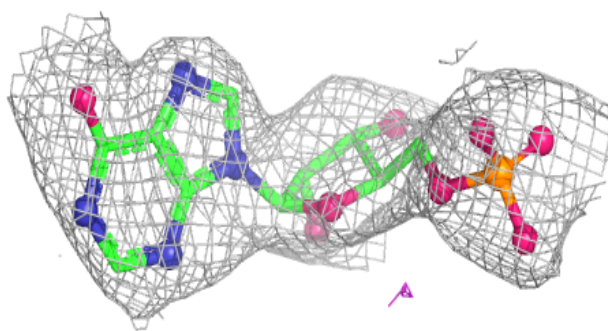
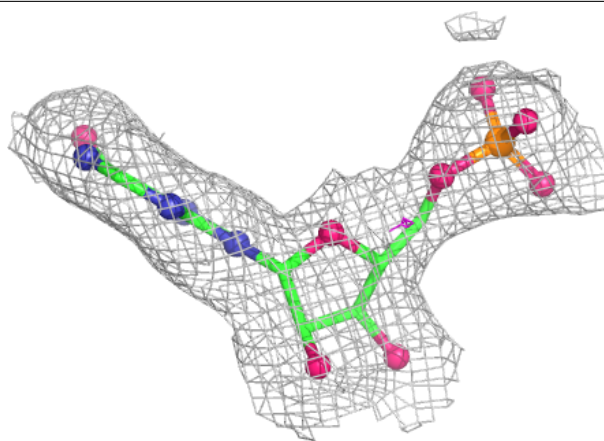
Electron density around IMP H 502:

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



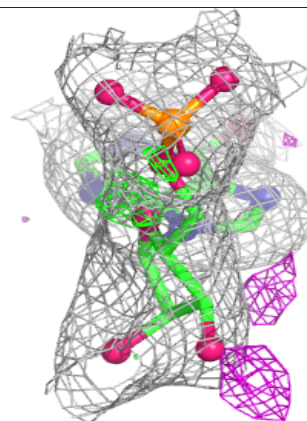
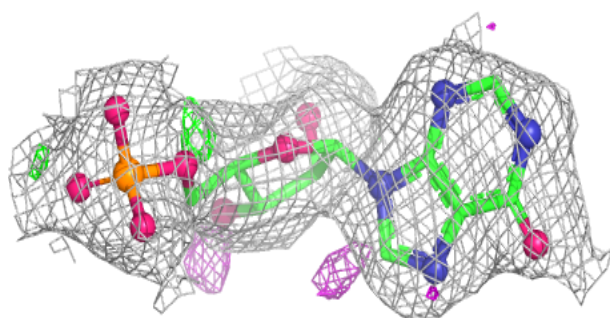
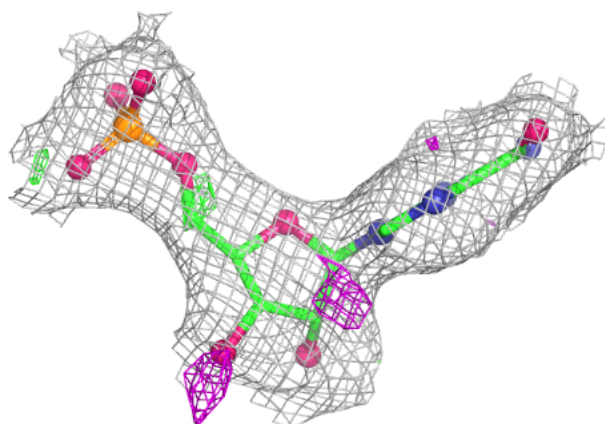
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



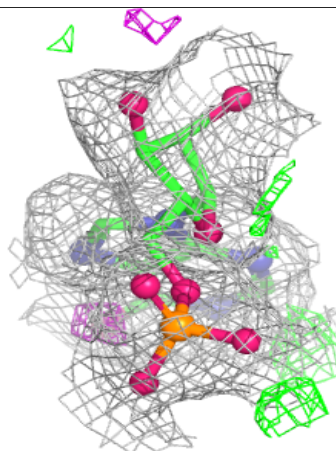
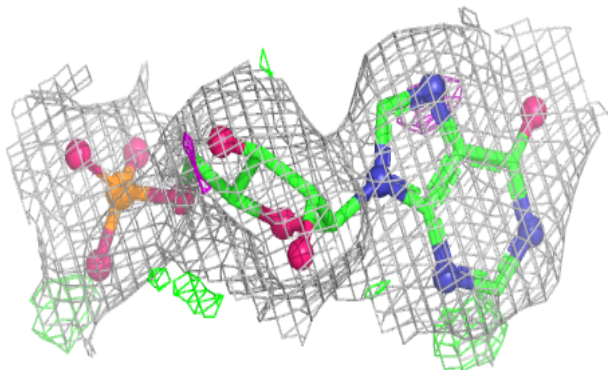
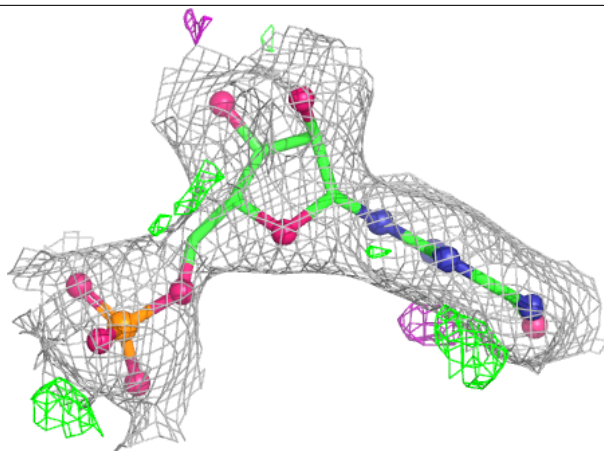
Electron density around IMP C 502:

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

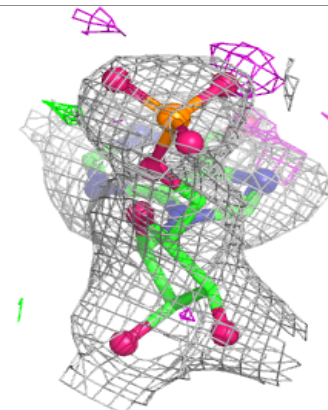
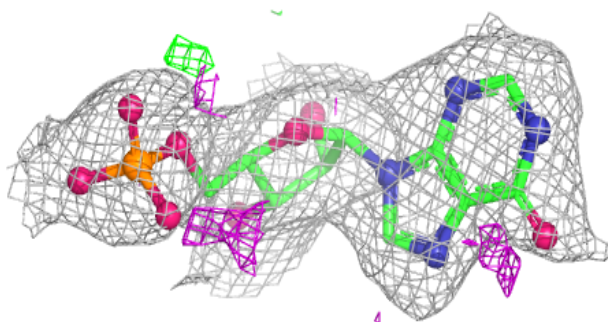
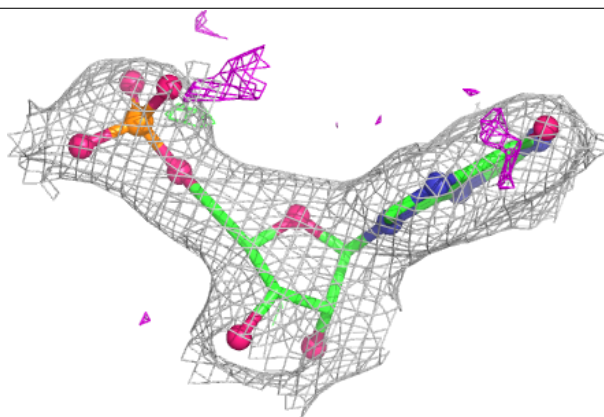


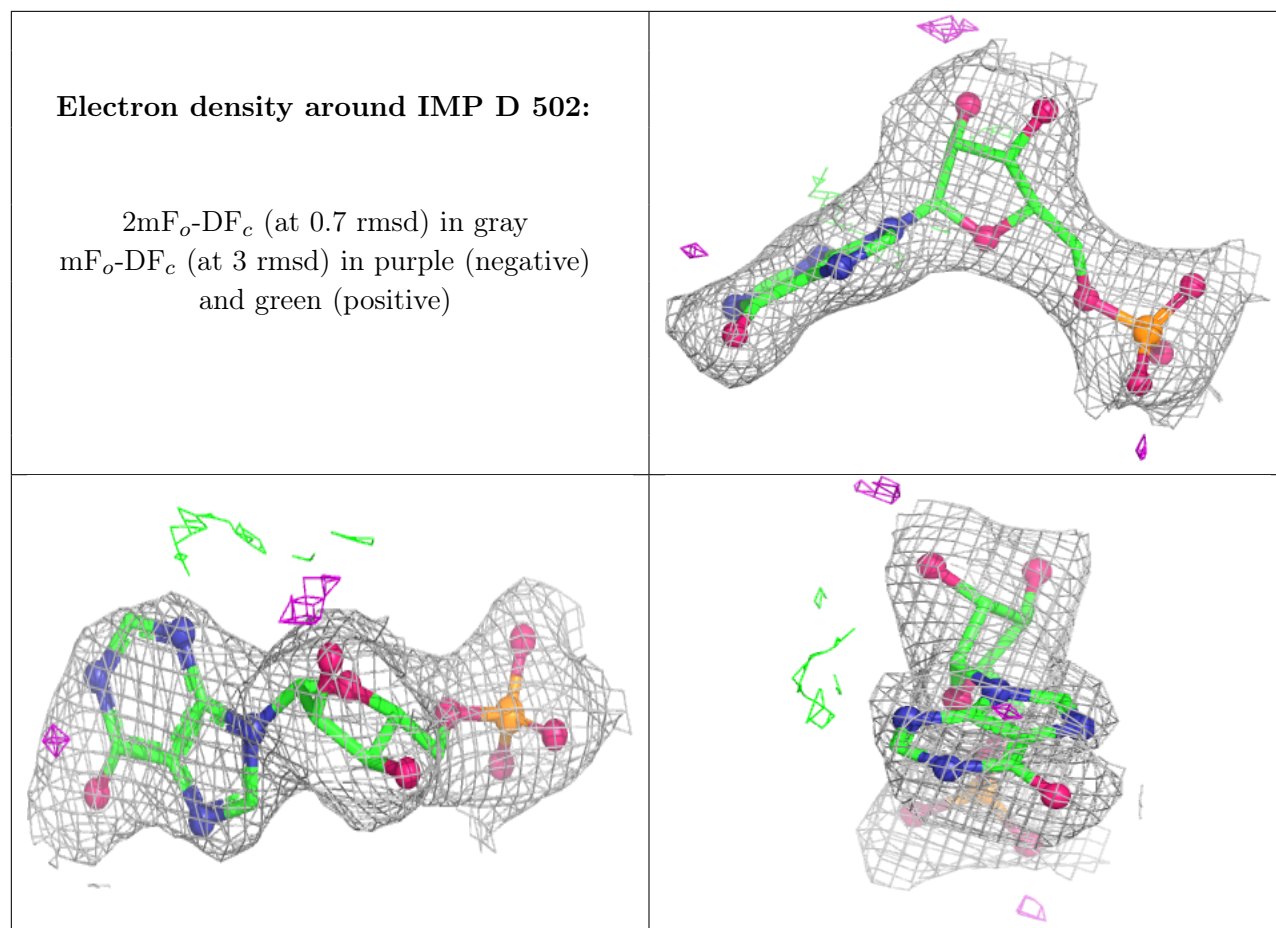
Electron density around IMP B 501:

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

**Electron density around IMP A 501:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.