



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 03:31 AM EDT

PDB ID : 9AUW / pdb_00009auw
Title : Crystal structure of A. baumannii GuaB dCBS with inhibitor GNE9979
Authors : Harris, S.F.; Wu, P.
Deposited on : 2024-03-01
Resolution : 2.30 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:

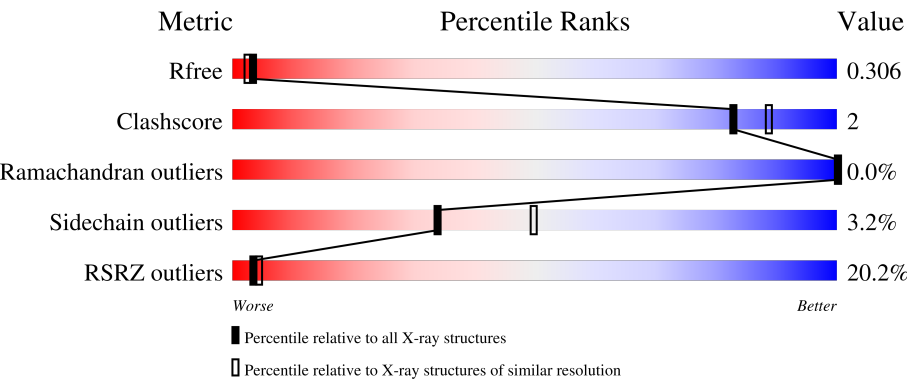
MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	395	<div><div>19%</div><div><div></div><div>77%</div><div>8%</div><div>15%</div></div></div>
1	B	395	<div><div>17%</div><div><div></div><div>77%</div><div>7%</div><div>15%</div></div></div>
1	C	395	<div><div>14%</div><div><div></div><div>77%</div><div>8%</div><div>15%</div></div></div>
1	D	395	<div><div>17%</div><div><div></div><div>78%</div><div>6%</div><div>15%</div></div></div>
1	E	395	<div><div>17%</div><div><div></div><div>79%</div><div>6%</div><div>15%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	395	
1	G	395	
1	H	395	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20734 atoms, of which 104 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	336	Total	C	N	O	S	0	4	0
			2476	1553	438	469	16			
1	B	336	Total	C	N	O	S	0	4	0
			2473	1551	436	470	16			
1	C	336	Total	C	N	O	S	0	1	0
			2452	1539	432	465	16			
1	D	337	Total	C	N	O	S	0	4	0
			2482	1556	438	472	16			
1	E	337	Total	C	N	O	S	0	2	0
			2464	1545	434	469	16			
1	F	338	Total	C	N	O	S	0	3	0
			2480	1556	437	471	16			
1	G	336	Total	C	N	O	S	0	4	0
			2475	1551	438	470	16			
1	H	336	Total	C	N	O	S	0	4	0
			2475	1551	438	470	16			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P31002
A	-14	HIS	-	expression tag	UNP P31002
A	-13	HIS	-	expression tag	UNP P31002
A	-12	HIS	-	expression tag	UNP P31002
A	-11	HIS	-	expression tag	UNP P31002
A	-10	HIS	-	expression tag	UNP P31002
A	-9	HIS	-	expression tag	UNP P31002
A	-8	GLY	-	expression tag	UNP P31002
A	-7	GLU	-	expression tag	UNP P31002
A	-6	ASN	-	expression tag	UNP P31002
A	-5	LEU	-	expression tag	UNP P31002
A	-4	TYR	-	expression tag	UNP P31002
A	-3	PHE	-	expression tag	UNP P31002

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	expression tag	UNP P31002
A	-1	GLY	-	expression tag	UNP P31002
A	0	SER	-	expression tag	UNP P31002
B	-15	MET	-	initiating methionine	UNP P31002
B	-14	HIS	-	expression tag	UNP P31002
B	-13	HIS	-	expression tag	UNP P31002
B	-12	HIS	-	expression tag	UNP P31002
B	-11	HIS	-	expression tag	UNP P31002
B	-10	HIS	-	expression tag	UNP P31002
B	-9	HIS	-	expression tag	UNP P31002
B	-8	GLY	-	expression tag	UNP P31002
B	-7	GLU	-	expression tag	UNP P31002
B	-6	ASN	-	expression tag	UNP P31002
B	-5	LEU	-	expression tag	UNP P31002
B	-4	TYR	-	expression tag	UNP P31002
B	-3	PHE	-	expression tag	UNP P31002
B	-2	GLN	-	expression tag	UNP P31002
B	-1	GLY	-	expression tag	UNP P31002
B	0	SER	-	expression tag	UNP P31002
C	-15	MET	-	initiating methionine	UNP P31002
C	-14	HIS	-	expression tag	UNP P31002
C	-13	HIS	-	expression tag	UNP P31002
C	-12	HIS	-	expression tag	UNP P31002
C	-11	HIS	-	expression tag	UNP P31002
C	-10	HIS	-	expression tag	UNP P31002
C	-9	HIS	-	expression tag	UNP P31002
C	-8	GLY	-	expression tag	UNP P31002
C	-7	GLU	-	expression tag	UNP P31002
C	-6	ASN	-	expression tag	UNP P31002
C	-5	LEU	-	expression tag	UNP P31002
C	-4	TYR	-	expression tag	UNP P31002
C	-3	PHE	-	expression tag	UNP P31002
C	-2	GLN	-	expression tag	UNP P31002
C	-1	GLY	-	expression tag	UNP P31002
C	0	SER	-	expression tag	UNP P31002
D	-15	MET	-	initiating methionine	UNP P31002
D	-14	HIS	-	expression tag	UNP P31002
D	-13	HIS	-	expression tag	UNP P31002
D	-12	HIS	-	expression tag	UNP P31002
D	-11	HIS	-	expression tag	UNP P31002
D	-10	HIS	-	expression tag	UNP P31002
D	-9	HIS	-	expression tag	UNP P31002

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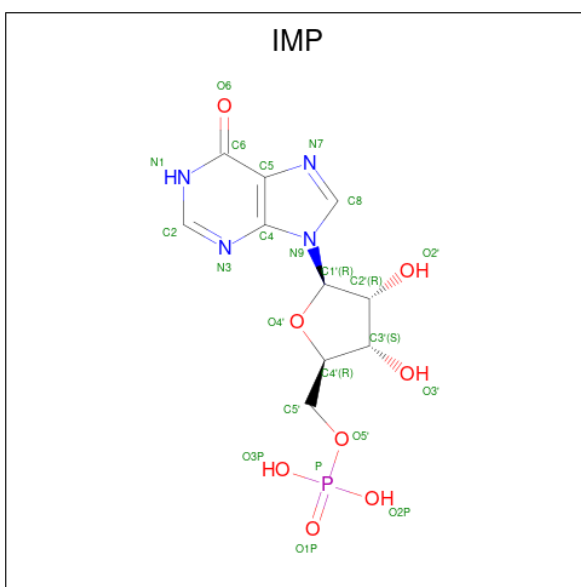
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	expression tag	UNP P31002
D	-7	GLU	-	expression tag	UNP P31002
D	-6	ASN	-	expression tag	UNP P31002
D	-5	LEU	-	expression tag	UNP P31002
D	-4	TYR	-	expression tag	UNP P31002
D	-3	PHE	-	expression tag	UNP P31002
D	-2	GLN	-	expression tag	UNP P31002
D	-1	GLY	-	expression tag	UNP P31002
D	0	SER	-	expression tag	UNP P31002
E	-15	MET	-	initiating methionine	UNP P31002
E	-14	HIS	-	expression tag	UNP P31002
E	-13	HIS	-	expression tag	UNP P31002
E	-12	HIS	-	expression tag	UNP P31002
E	-11	HIS	-	expression tag	UNP P31002
E	-10	HIS	-	expression tag	UNP P31002
E	-9	HIS	-	expression tag	UNP P31002
E	-8	GLY	-	expression tag	UNP P31002
E	-7	GLU	-	expression tag	UNP P31002
E	-6	ASN	-	expression tag	UNP P31002
E	-5	LEU	-	expression tag	UNP P31002
E	-4	TYR	-	expression tag	UNP P31002
E	-3	PHE	-	expression tag	UNP P31002
E	-2	GLN	-	expression tag	UNP P31002
E	-1	GLY	-	expression tag	UNP P31002
E	0	SER	-	expression tag	UNP P31002
F	-15	MET	-	initiating methionine	UNP P31002
F	-14	HIS	-	expression tag	UNP P31002
F	-13	HIS	-	expression tag	UNP P31002
F	-12	HIS	-	expression tag	UNP P31002
F	-11	HIS	-	expression tag	UNP P31002
F	-10	HIS	-	expression tag	UNP P31002
F	-9	HIS	-	expression tag	UNP P31002
F	-8	GLY	-	expression tag	UNP P31002
F	-7	GLU	-	expression tag	UNP P31002
F	-6	ASN	-	expression tag	UNP P31002
F	-5	LEU	-	expression tag	UNP P31002
F	-4	TYR	-	expression tag	UNP P31002
F	-3	PHE	-	expression tag	UNP P31002
F	-2	GLN	-	expression tag	UNP P31002
F	-1	GLY	-	expression tag	UNP P31002
F	0	SER	-	expression tag	UNP P31002
G	-15	MET	-	initiating methionine	UNP P31002

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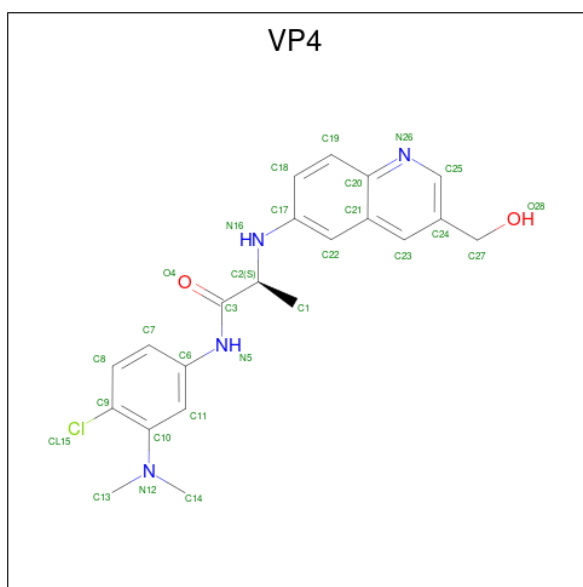
Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP P31002
G	-13	HIS	-	expression tag	UNP P31002
G	-12	HIS	-	expression tag	UNP P31002
G	-11	HIS	-	expression tag	UNP P31002
G	-10	HIS	-	expression tag	UNP P31002
G	-9	HIS	-	expression tag	UNP P31002
G	-8	GLY	-	expression tag	UNP P31002
G	-7	GLU	-	expression tag	UNP P31002
G	-6	ASN	-	expression tag	UNP P31002
G	-5	LEU	-	expression tag	UNP P31002
G	-4	TYR	-	expression tag	UNP P31002
G	-3	PHE	-	expression tag	UNP P31002
G	-2	GLN	-	expression tag	UNP P31002
G	-1	GLY	-	expression tag	UNP P31002
G	0	SER	-	expression tag	UNP P31002
H	-15	MET	-	initiating methionine	UNP P31002
H	-14	HIS	-	expression tag	UNP P31002
H	-13	HIS	-	expression tag	UNP P31002
H	-12	HIS	-	expression tag	UNP P31002
H	-11	HIS	-	expression tag	UNP P31002
H	-10	HIS	-	expression tag	UNP P31002
H	-9	HIS	-	expression tag	UNP P31002
H	-8	GLY	-	expression tag	UNP P31002
H	-7	GLU	-	expression tag	UNP P31002
H	-6	ASN	-	expression tag	UNP P31002
H	-5	LEU	-	expression tag	UNP P31002
H	-4	TYR	-	expression tag	UNP P31002
H	-3	PHE	-	expression tag	UNP P31002
H	-2	GLN	-	expression tag	UNP P31002
H	-1	GLY	-	expression tag	UNP P31002
H	0	SER	-	expression tag	UNP P31002

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	C	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	D	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	E	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	F	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	G	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		
2	H	1	Total	C	H	N	O	P	0	0
			36	10	13	4	8	1		

- Molecule 3 is N-[4-chloro-3-(dimethylamino)phenyl]-N 2 -[3-(hydroxymethyl)quinolin-6-yl]-L-alaninamide (CCD ID: VP4) (formula: C₂₁H₂₃ClN₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	B	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	C	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	D	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	E	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	F	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	G	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		
3	H	1	Total	C	Cl	N	O	0	0
			28	21	1	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	62	Total	O	0	0
			62	62		
4	C	69	Total	O	0	0
			69	69		
4	D	41	Total	O	0	0
			41	41		

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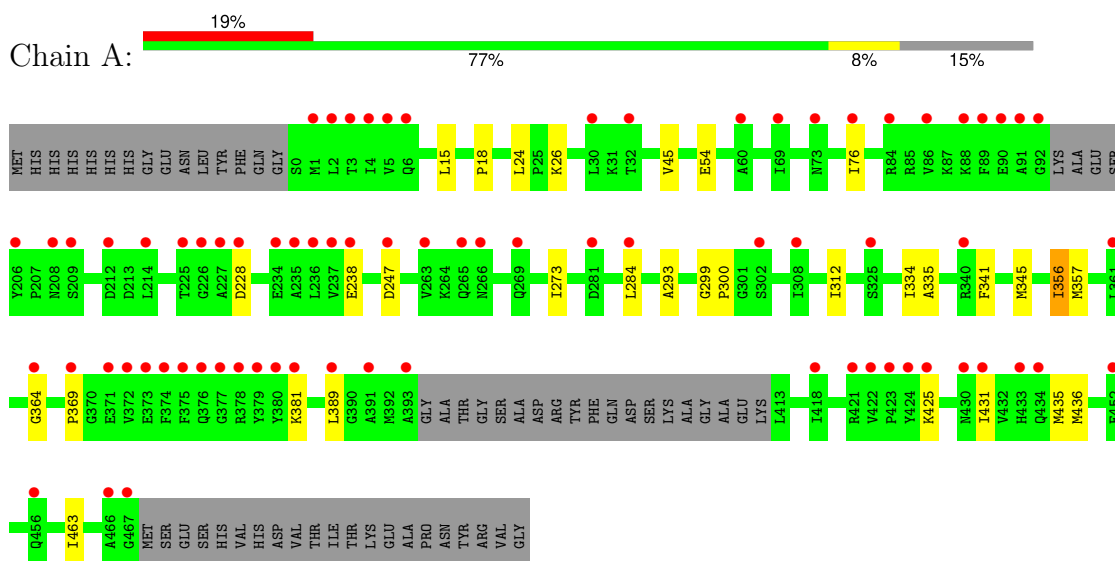
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	48	Total 48	O 48	0	0
4	F	52	Total 52	O 52	0	0
4	G	53	Total 53	O 53	0	0
4	H	60	Total 60	O 60	0	0

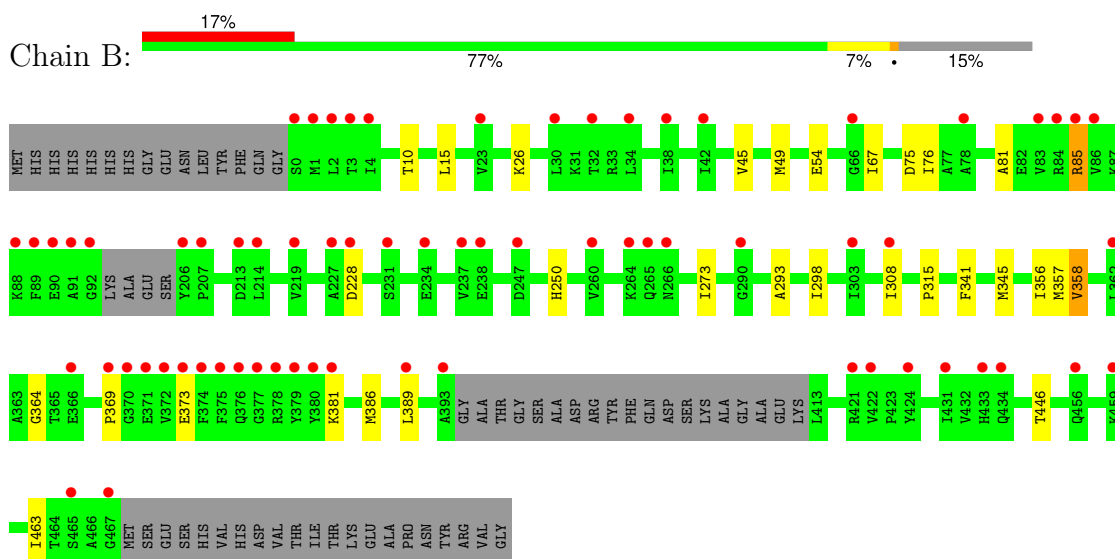
3 Residue-property plots [i](#)

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

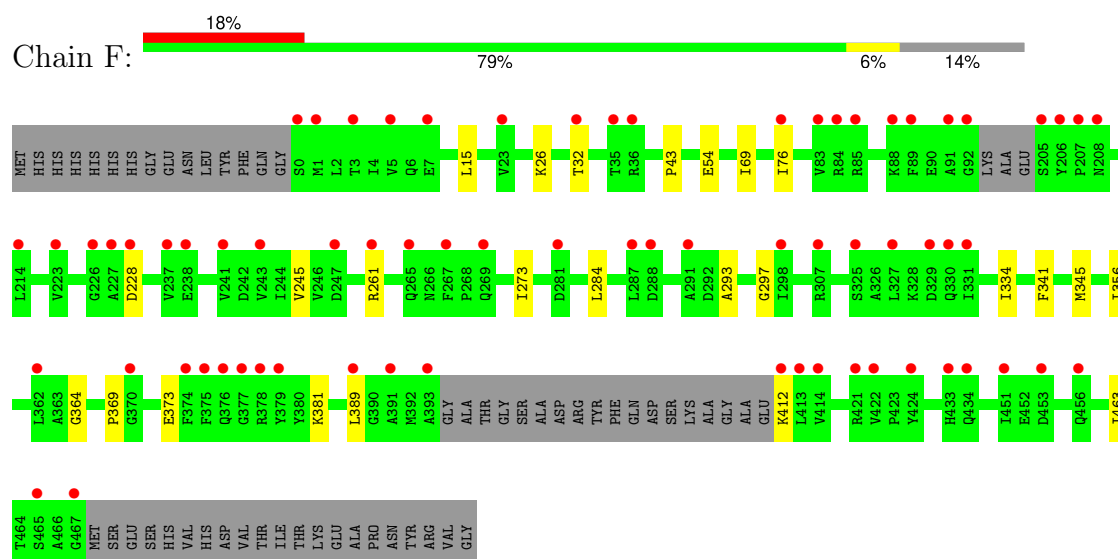
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



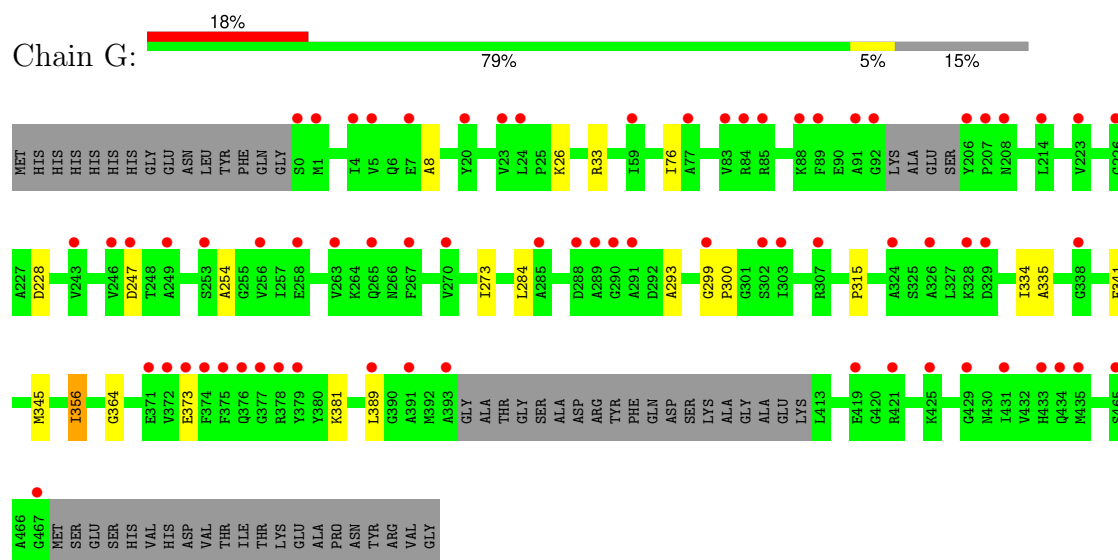
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



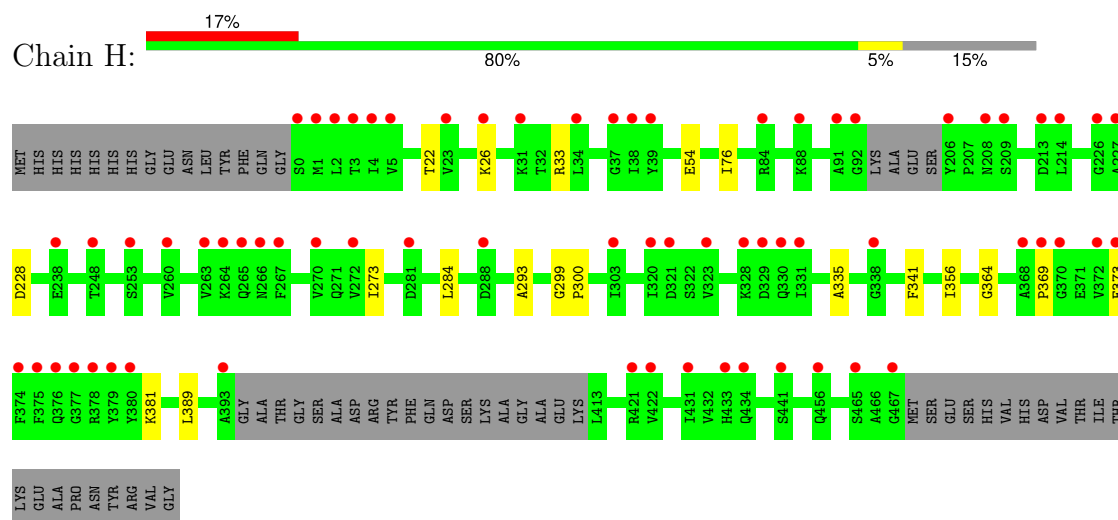
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.72Å 127.30Å 127.48Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	46.00 – 2.30 46.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.00-2.30) 99.0 (46.00-2.30)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.244 , 0.265 0.282 , 0.306	Depositor DCC
R_{free} test set	8032 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.2	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	0.85	EDS
Total number of atoms	20734	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.39% 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: VP4, 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	0.44	0/2508	0.65	0/3389
1	B	0.45	0/2505	0.66	0/3386
1	C	0.44	0/2484	0.65	0/3357
1	D	0.44	0/2514	0.65	0/3396
1	E	0.43	0/2496	0.64	0/3373
1	F	0.44	0/2512	0.64	0/3394
1	G	0.45	0/2507	0.65	0/3387
1	H	0.44	0/2507	0.65	0/3387
All	All	0.44	0/20033	0.65	0/27069

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	2476	0	2534	15	0
1	B	2473	0	2527	15	0
1	C	2452	0	2510	18	0
1	D	2482	0	2538	12	0
1	E	2464	0	2519	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2480	0	2540	10	0
1	G	2475	0	2530	10	0
1	H	2475	0	2530	7	0
2	A	23	13	11	0	0
2	B	23	13	11	0	0
2	C	23	13	11	0	0
2	D	23	13	11	1	0
2	E	23	13	11	0	0
2	F	23	13	11	0	0
2	G	23	13	11	0	0
2	H	23	13	11	0	0
3	A	28	0	0	0	0
3	B	28	0	0	0	0
3	C	28	0	0	0	0
3	D	28	0	0	0	0
3	E	28	0	0	0	0
3	F	28	0	0	0	0
3	G	28	0	0	0	0
3	H	28	0	0	0	0
4	A	60	0	0	0	0
4	B	62	0	0	2	0
4	C	69	0	0	6	0
4	D	41	0	0	0	0
4	E	48	0	0	0	0
4	F	52	0	0	1	0
4	G	53	0	0	2	0
4	H	60	0	0	0	0
All	All	20630	104	20316	93	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 2.

All (93) 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:C:347:LYS:HD2	4:C:904:HOH:O	1.79	0.83
1:F:69:ILE:HD13	4:F:905:HOH:O	1.81	0.81
1:C:344:ASP:HA	4:C:904:HOH:O	1.83	0.77
1:G:293:ALA:HB1	4:G:913:HOH:O	1.84	0.76
1:C:30:LEU:HD22	4:C:969:HOH:O	1.93	0.68
1:C:11:PHE:HB3	4:C:904:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:ILE:HD12	1:C:439:LEU:HD21	1.82	0.59
1:B:250:HIS:HD2	4:B:951:HOH:O	1.84	0.59
1:C:431:ILE:O	1:C:435:MET:HG2	2.03	0.59
1:B:358:VAL:HG22	4:B:903:HOH:O	2.03	0.58
1:A:345:MET:HG2	1:A:356:ILE:HG21	1.85	0.58
1:G:273:ILE:HG12	1:G:293:ALA:HB3	1.85	0.58
1:F:273:ILE:HG12	1:F:293:ALA:HB3	1.86	0.58
1:H:273:ILE:HG12	1:H:293:ALA:HB3	1.85	0.58
1:E:273:ILE:HD13	1:E:334:ILE:HD11	1.85	0.58
1:C:273:ILE:HG12	1:C:293:ALA:HB3	1.86	0.56
1:D:273:ILE:HG12	1:D:293:ALA:HB3	1.87	0.56
1:E:273:ILE:HG12	1:E:293:ALA:HB3	1.86	0.56
1:E:335:ALA:HB3	1:E:356:ILE:HG13	1.88	0.55
1:G:335:ALA:HB3	1:G:356:ILE:HG13	1.87	0.55
1:B:273:ILE:HG12	1:B:293:ALA:HB3	1.87	0.54
1:E:364:GLY:HA2	1:E:381:LYS:HB2	1.89	0.54
1:H:335:ALA:HB3	1:H:356:ILE:HG13	1.90	0.54
1:C:364:GLY:HA2	1:C:381:LYS:HB2	1.90	0.54
4:C:963:HOH:O	1:D:18:PRO:HD2	2.08	0.54
1:B:45:VAL:O	1:B:357:MET:HA	2.08	0.54
1:A:273:ILE:HG12	1:A:293:ALA:HB3	1.88	0.53
1:B:364:GLY:HA2	1:B:381:LYS:HB2	1.91	0.53
1:H:364:GLY:HA2	1:H:381:LYS:HB2	1.91	0.53
1:F:364:GLY:HA2	1:F:381:LYS:HB2	1.91	0.52
1:A:364:GLY:HA2	1:A:381:LYS:HB2	1.89	0.52
1:G:364:GLY:HA2	1:G:381:LYS:HB2	1.90	0.51
1:D:364:GLY:HA2	1:D:381:LYS:HB2	1.92	0.51
1:C:335:ALA:HB3	1:C:356:ILE:HG13	1.93	0.50
1:G:76:ILE:HD11	1:G:228:ASP:HB2	1.96	0.48
1:C:76:ILE:HD11	1:C:228:ASP:HB2	1.95	0.48
1:D:299:GLY:N	1:D:300:PRO:HD3	2.29	0.47
1:F:76:ILE:HD11	1:F:228:ASP:HB2	1.96	0.47
1:B:81:ALA:HB1	1:B:85:ARG:HH21	1.80	0.47
1:B:49:MET:HG2	1:B:386:MET:HG2	1.95	0.47
1:D:76:ILE:HD11	1:D:228:ASP:HB2	1.97	0.47
1:A:335:ALA:HB3	1:A:356:ILE:HG13	1.96	0.47
1:E:76:ILE:HD11	1:E:228:ASP:HB2	1.97	0.47
1:G:334:ILE:HG13	4:G:913:HOH:O	2.14	0.46
1:A:299:GLY:N	1:A:300:PRO:HD3	2.31	0.46
1:H:76:ILE:HD11	1:H:228:ASP:HB2	1.96	0.46
1:A:76:ILE:HD11	1:A:228:ASP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:GLY:N	1:C:300:PRO:HD3	2.31	0.45
1:B:76:ILE:HD11	1:B:228:ASP:HB2	1.97	0.45
1:D:345:MET:HG2	1:D:356:ILE:HG21	1.98	0.45
1:D:335:ALA:HB3	1:D:356:ILE:HG13	1.98	0.44
1:C:439:LEU:HD12	1:C:439:LEU:O	2.17	0.44
1:E:299:GLY:N	1:E:300:PRO:HD3	2.32	0.44
1:B:54:GLU:HB2	1:B:369:PRO:HG3	1.99	0.44
1:D:54:GLU:HB2	1:D:369:PRO:HG3	2.00	0.44
1:C:431:ILE:HD12	1:C:431:ILE:H	1.83	0.43
1:D:304:CYS:HB2	2:D:801:IMP:C2	2.48	0.43
1:E:345:MET:HG2	1:E:356:ILE:HG21	1.99	0.43
1:F:345:MET:HG2	1:F:356:ILE:HG21	2.00	0.43
1:B:10:THR:HB	1:B:315:PRO:HB3	1.99	0.43
1:A:54:GLU:HB2	1:A:369:PRO:HG3	2.00	0.42
1:A:312:ILE:HD11	1:B:446:THR:HG23	2.01	0.42
1:F:273:ILE:HD13	1:F:334:ILE:HD11	2.01	0.42
1:D:45:VAL:O	1:D:357:MET:HA	2.20	0.42
1:A:431:ILE:H	1:A:431:ILE:HD12	1.85	0.42
1:C:439:LEU:HG	4:C:969:HOH:O	2.20	0.42
1:A:425:LYS:HB3	1:A:431:ILE:HD11	2.02	0.42
1:G:299:GLY:N	1:G:300:PRO:HD3	2.34	0.42
1:H:299:GLY:N	1:H:300:PRO:HD3	2.34	0.42
1:C:54:GLU:HB2	1:C:369:PRO:HG3	2.02	0.41
1:D:342:SER:HB3	1:D:435:MET:HA	2.02	0.41
1:B:298:ILE:HG21	1:C:18:PRO:HG3	2.03	0.41
1:E:425:LYS:HB3	1:E:431:ILE:HD11	2.01	0.41
1:B:345:MET:HG2	1:B:356:ILE:HG21	2.02	0.41
1:A:45:VAL:O	1:A:357:MET:HA	2.21	0.41
1:E:46:SER:HB3	1:E:362:LEU:HD13	2.02	0.41
1:C:345:MET:HG2	1:C:356:ILE:HG21	2.03	0.41
1:F:69:ILE:HD12	1:F:245:VAL:HG21	2.03	0.41
1:A:273:ILE:HD13	1:A:334:ILE:HD11	2.03	0.41
1:F:54:GLU:HB2	1:F:369:PRO:HG3	2.02	0.41
1:B:15:LEU:HD12	1:B:463:ILE:HG21	2.02	0.41
1:B:45:VAL:HG13	1:B:67:ILE:HG23	2.03	0.41
1:G:345:MET:HG2	1:G:356:ILE:HG21	2.02	0.41
1:A:15:LEU:HD12	1:A:463:ILE:HG21	2.03	0.40
1:A:18:PRO:HG3	1:D:298:ILE:HG21	2.03	0.40
1:E:15:LEU:HD12	1:E:463:ILE:HG21	2.03	0.40
1:F:15:LEU:HD12	1:F:463:ILE:HG21	2.03	0.40
1:C:273:ILE:HD13	1:C:334:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:THR:HG21	1:F:43:PRO:HB3	2.04	0.40
1:A:431:ILE:O	1:A:435:MET:HG2	2.22	0.40
1:G:8:ALA:CB	1:G:315:PRO:HD2	2.52	0.40
1:G:254:ALA:HB2	1:H:22:THR:HG22	2.03	0.40
1:H:54:GLU:HB2	1:H:369:PRO:HG3	2.03	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	334/395 (85%)	328 (98%)	6 (2%)	0	100	100
1	B	334/395 (85%)	322 (96%)	12 (4%)	0	100	100
1	C	331/395 (84%)	324 (98%)	7 (2%)	0	100	100
1	D	335/395 (85%)	327 (98%)	8 (2%)	0	100	100
1	E	333/395 (84%)	328 (98%)	5 (2%)	0	100	100
1	F	335/395 (85%)	327 (98%)	7 (2%)	1 (0%)	37	47
1	G	334/395 (85%)	327 (98%)	7 (2%)	0	100	100
1	H	334/395 (85%)	326 (98%)	8 (2%)	0	100	100
All	All	2670/3160 (84%)	2609 (98%)	60 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	297	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	255/298 (86%)	246 (96%)	9 (4%)	31	46
1	B	255/298 (86%)	247 (97%)	8 (3%)	35	51
1	C	252/298 (85%)	241 (96%)	11 (4%)	24	35
1	D	256/298 (86%)	247 (96%)	9 (4%)	31	46
1	E	254/298 (85%)	248 (98%)	6 (2%)	44	61
1	F	256/298 (86%)	249 (97%)	7 (3%)	40	57
1	G	255/298 (86%)	247 (97%)	8 (3%)	35	51
1	H	255/298 (86%)	249 (98%)	6 (2%)	44	61
All	All	2038/2384 (86%)	1974 (97%)	64 (3%)	34	51

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	26	LYS
1	A	238	GLU
1	A	247	ASP
1	A	284	LEU
1	A	341	PHE
1	A	356	ILE
1	A	389	LEU
1	A	436	MET
1	B	26	LYS
1	B	75	ASP
1	B	85	ARG
1	B	308	ILE
1	B	341	PHE
1	B	358	VAL
1	B	373	GLU
1	B	389	LEU
1	C	23	VAL
1	C	24	LEU

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Mol	Chain	Res	Type
1	C	26	LYS
1	C	261	ARG
1	C	284	LEU
1	C	341	PHE
1	C	356	ILE
1	C	373	GLU
1	C	378	ARG
1	C	389	LEU
1	C	439	LEU
1	D	26	LYS
1	D	284	LEU
1	D	304	CYS
1	D	307	ARG
1	D	308	ILE
1	D	341	PHE
1	D	356	ILE
1	D	373	GLU
1	D	389	LEU
1	E	26	LYS
1	E	284	LEU
1	E	341	PHE
1	E	356	ILE
1	E	373	GLU
1	E	389	LEU
1	F	26	LYS
1	F	261	ARG
1	F	284	LEU
1	F	341	PHE
1	F	373	GLU
1	F	389	LEU
1	F	412	LYS
1	G	26	LYS
1	G	33	ARG
1	G	247	ASP
1	G	284	LEU
1	G	341	PHE
1	G	356	ILE
1	G	373	GLU
1	G	389	LEU
1	H	26	LYS
1	H	33	ARG
1	H	284	LEU

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Mol	Chain	Res	Type
1	H	341	PHE
1	H	373	GLU
1	H	389	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	GLN
1	B	250	HIS
1	C	330	GLN
1	D	330	GLN
1	F	250	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	VP4	E	802	-	30,30,30	0.78	0	42,42,42	1.20	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IMP	G	801	-	21,25,25	0.84	1 (4%)	22,38,38	0.69	0
2	IMP	C	801	-	21,25,25	0.85	1 (4%)	22,38,38	0.66	0
2	IMP	B	801	-	21,25,25	0.85	1 (4%)	22,38,38	0.71	0
2	IMP	H	801	-	21,25,25	0.83	1 (4%)	22,38,38	0.70	0
3	VP4	C	802	-	30,30,30	0.73	0	42,42,42	1.36	4 (9%)
2	IMP	A	801	-	21,25,25	0.85	1 (4%)	22,38,38	0.67	0
3	VP4	D	802	-	30,30,30	0.73	0	42,42,42	1.30	4 (9%)
3	VP4	F	802	-	30,30,30	0.70	0	42,42,42	1.34	4 (9%)
3	VP4	B	802	-	30,30,30	0.73	0	42,42,42	1.36	4 (9%)
2	IMP	E	801	-	21,25,25	0.84	0	22,38,38	0.69	0
3	VP4	A	802	-	30,30,30	0.63	0	42,42,42	1.32	3 (7%)
2	IMP	D	801	-	21,25,25	0.81	1 (4%)	22,38,38	0.69	0
2	IMP	F	801	-	21,25,25	0.81	1 (4%)	22,38,38	0.69	0
3	VP4	H	802	-	30,30,30	0.71	0	42,42,42	1.28	3 (7%)
3	VP4	G	802	-	30,30,30	0.74	0	42,42,42	1.26	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VP4	E	802	-	-	1/18/18/18	0/3/3/3
2	IMP	G	801	-	-	1/6/26/26	0/3/3/3
2	IMP	C	801	-	-	1/6/26/26	0/3/3/3
2	IMP	B	801	-	-	1/6/26/26	0/3/3/3
2	IMP	H	801	-	-	1/6/26/26	0/3/3/3
3	VP4	C	802	-	-	3/18/18/18	0/3/3/3
2	IMP	A	801	-	-	1/6/26/26	0/3/3/3
3	VP4	D	802	-	-	0/18/18/18	0/3/3/3
3	VP4	F	802	-	-	2/18/18/18	0/3/3/3
3	VP4	B	802	-	-	3/18/18/18	0/3/3/3
2	IMP	E	801	-	-	1/6/26/26	0/3/3/3
3	VP4	A	802	-	-	2/18/18/18	0/3/3/3
2	IMP	D	801	-	-	1/6/26/26	0/3/3/3
2	IMP	F	801	-	-	1/6/26/26	0/3/3/3
3	VP4	H	802	-	-	1/18/18/18	0/3/3/3
3	VP4	G	802	-	-	2/18/18/18	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	IMP	C8-N7	-2.33	1.31	1.34
2	G	801	IMP	C8-N7	-2.31	1.31	1.34
2	H	801	IMP	C8-N7	-2.26	1.31	1.34
2	A	801	IMP	C8-N7	-2.24	1.31	1.34
2	C	801	IMP	C8-N7	-2.17	1.31	1.34
2	F	801	IMP	C8-N7	-2.08	1.31	1.34
2	D	801	IMP	C8-N7	-2.06	1.31	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	802	VP4	C25-N26-C20	4.64	122.33	116.96
3	A	802	VP4	C25-N26-C20	4.56	122.23	116.96
3	B	802	VP4	C25-N26-C20	4.33	121.97	116.96
3	H	802	VP4	C25-N26-C20	4.29	121.92	116.96
3	D	802	VP4	C25-N26-C20	4.27	121.90	116.96
3	C	802	VP4	C25-N26-C20	4.19	121.81	116.96
3	G	802	VP4	C25-N26-C20	4.18	121.80	116.96
3	E	802	VP4	C25-N26-C20	4.16	121.78	116.96
3	H	802	VP4	C23-C24-C25	3.59	120.07	116.88
3	B	802	VP4	C23-C24-C25	3.53	120.02	116.88
3	B	802	VP4	C17-N16-C2	3.21	128.11	122.60
3	C	802	VP4	C17-N16-C2	3.10	127.93	122.60
3	F	802	VP4	C23-C24-C25	3.04	119.58	116.88
3	C	802	VP4	C23-C24-C25	3.04	119.58	116.88
3	D	802	VP4	C23-C24-C25	2.81	119.37	116.88
3	E	802	VP4	C23-C24-C25	2.79	119.36	116.88
3	A	802	VP4	C17-N16-C2	2.79	127.40	122.60
3	G	802	VP4	C23-C24-C25	2.75	119.32	116.88
3	A	802	VP4	C23-C24-C25	2.70	119.27	116.88
3	F	802	VP4	C10-C9-CL15	2.52	123.02	120.24
3	D	802	VP4	C10-C9-CL15	2.49	122.98	120.24
3	G	802	VP4	C17-N16-C2	2.47	126.85	122.60
3	G	802	VP4	C10-C9-CL15	2.38	122.87	120.24
3	C	802	VP4	C10-C9-CL15	2.31	122.79	120.24
3	F	802	VP4	C17-N16-C2	2.21	126.40	122.60
3	B	802	VP4	C10-C9-CL15	2.20	122.67	120.24
3	H	802	VP4	C17-N16-C2	2.06	126.14	122.60
3	E	802	VP4	C21-C20-N26	-2.05	119.21	122.03
3	E	802	VP4	C17-N16-C2	2.02	126.07	122.60
3	D	802	VP4	C17-N16-C2	2.02	126.07	122.60

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	802	VP4	C9-C10-N12-C13
3	A	802	VP4	C9-C10-N12-C13
3	B	802	VP4	C9-C10-N12-C13
3	F	802	VP4	C9-C10-N12-C13
3	G	802	VP4	C9-C10-N12-C13
3	B	802	VP4	C9-C10-N12-C14
3	E	802	VP4	C9-C10-N12-C13
3	G	802	VP4	C9-C10-N12-C14
3	A	802	VP4	C9-C10-N12-C14
3	F	802	VP4	C9-C10-N12-C14
3	C	802	VP4	C9-C10-N12-C13
2	E	801	IMP	C3'-C4'-C5'-O5'
2	F	801	IMP	C3'-C4'-C5'-O5'
3	C	802	VP4	C9-C10-N12-C14
3	B	802	VP4	C3-C2-N16-C17
2	A	801	IMP	C3'-C4'-C5'-O5'
2	D	801	IMP	C3'-C4'-C5'-O5'
2	H	801	IMP	C3'-C4'-C5'-O5'
2	G	801	IMP	C3'-C4'-C5'-O5'
2	C	801	IMP	C3'-C4'-C5'-O5'
2	B	801	IMP	C3'-C4'-C5'-O5'
3	C	802	VP4	C3-C2-N16-C17

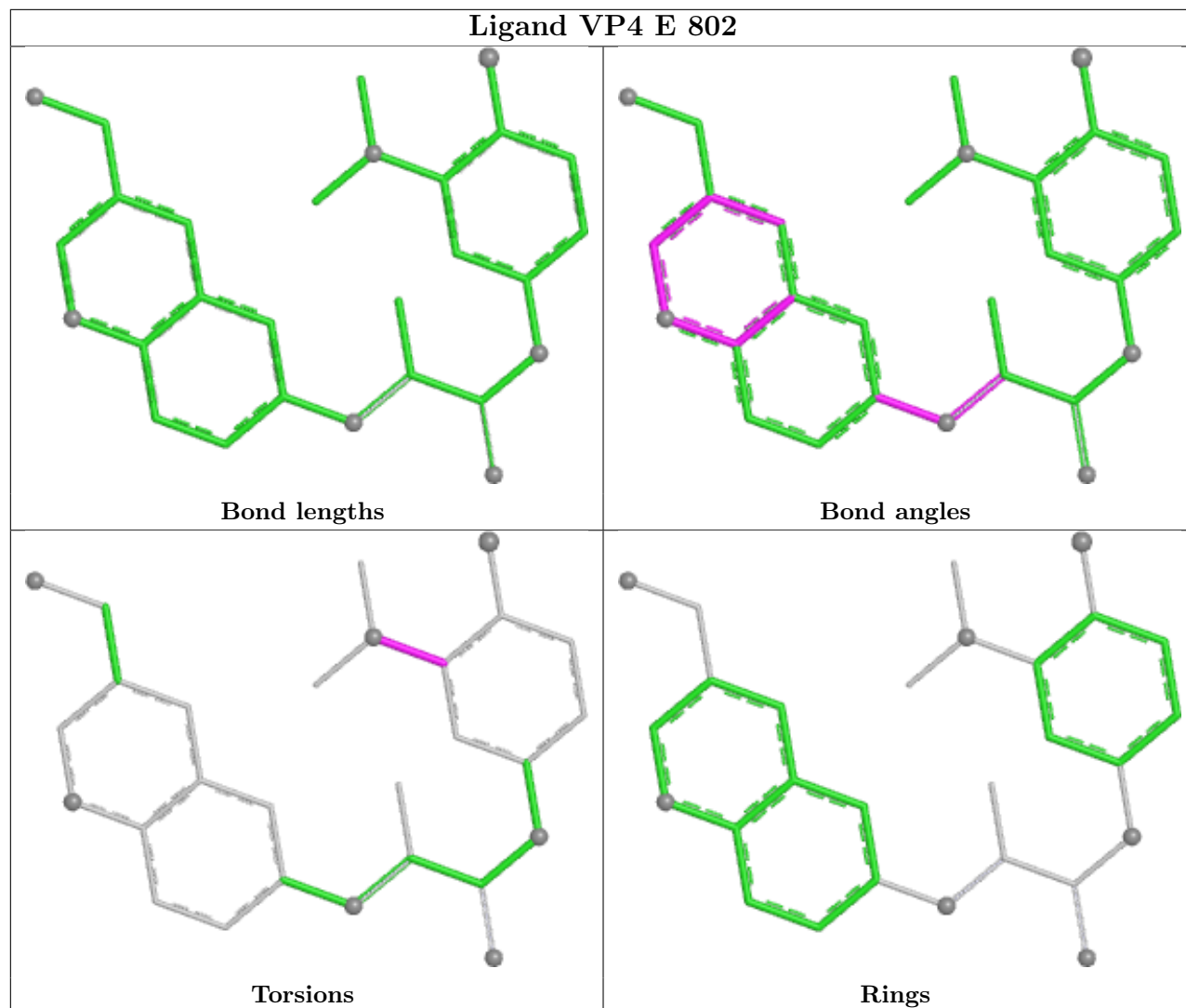
There are no ring outliers.

1 monomer is involved in 1 short contact:

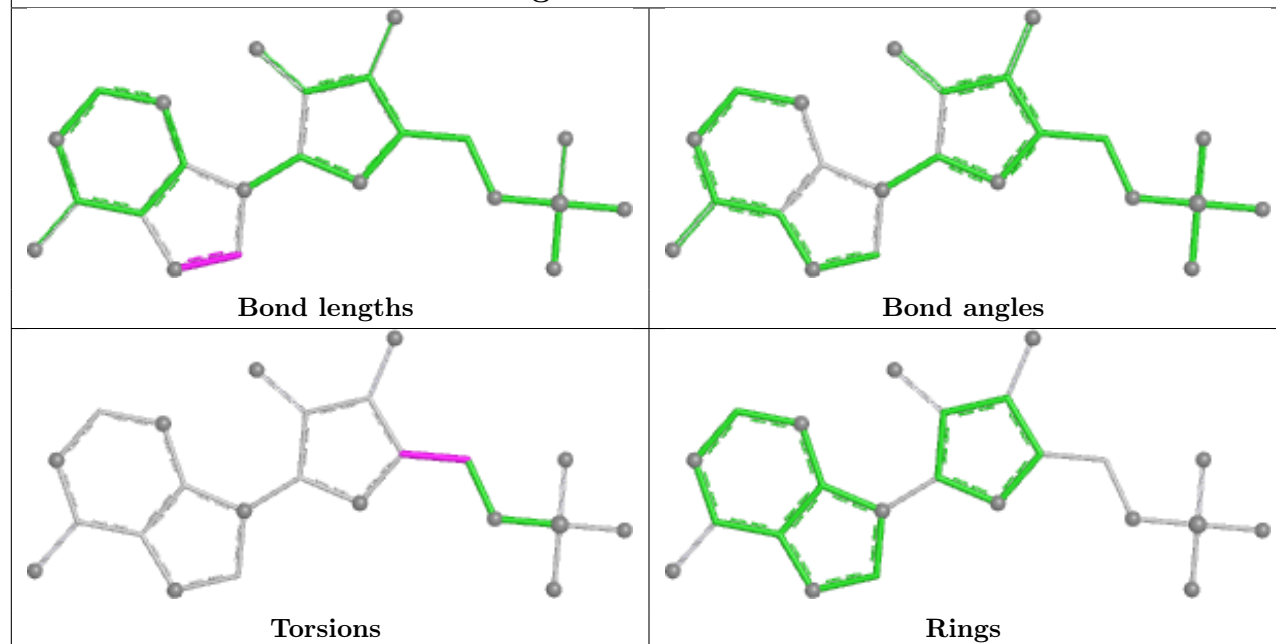
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	IMP	1	0

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

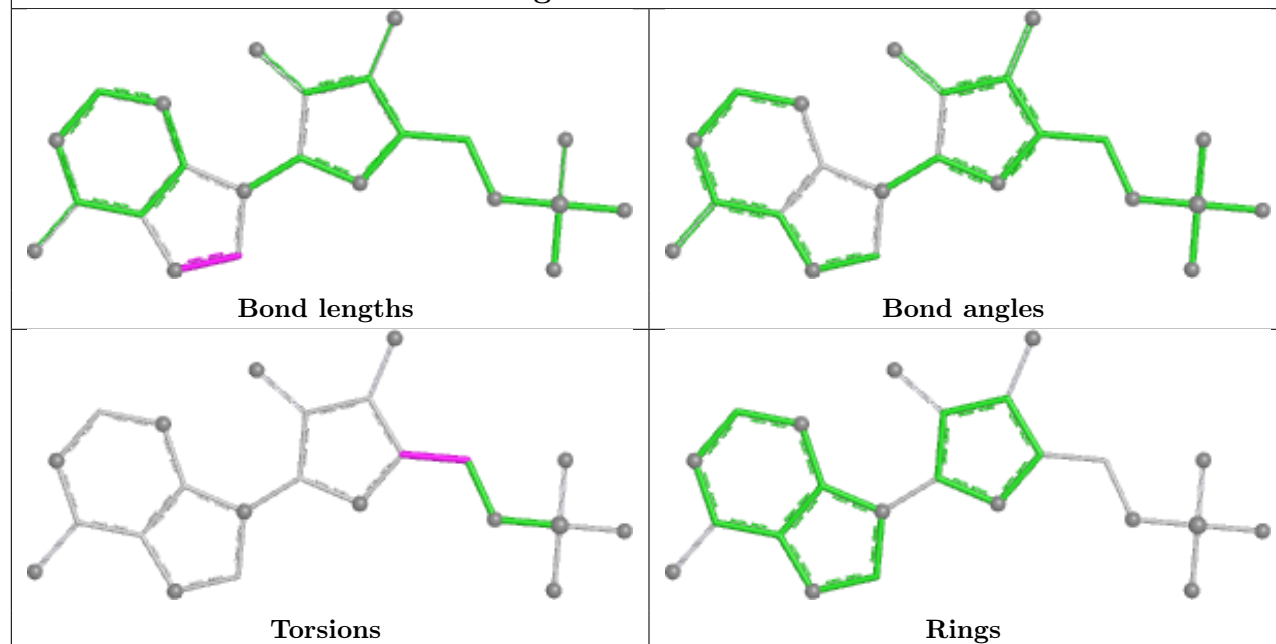
equivalents in the CSD to analyse the geometry.



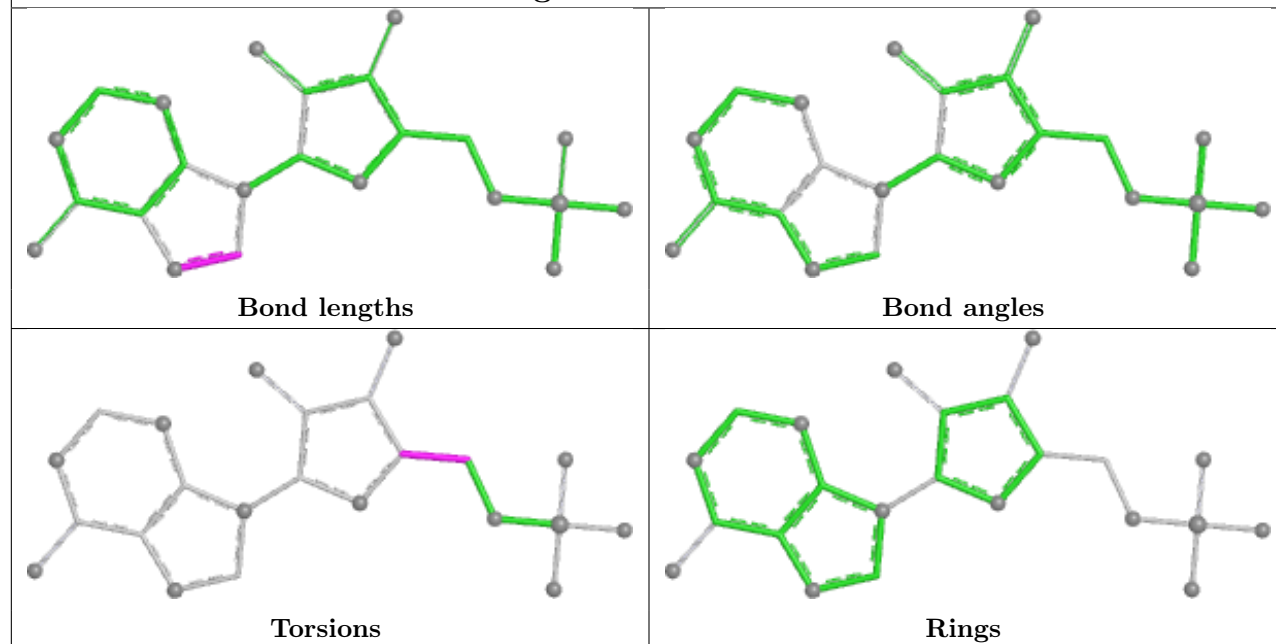
Ligand IMP G 801



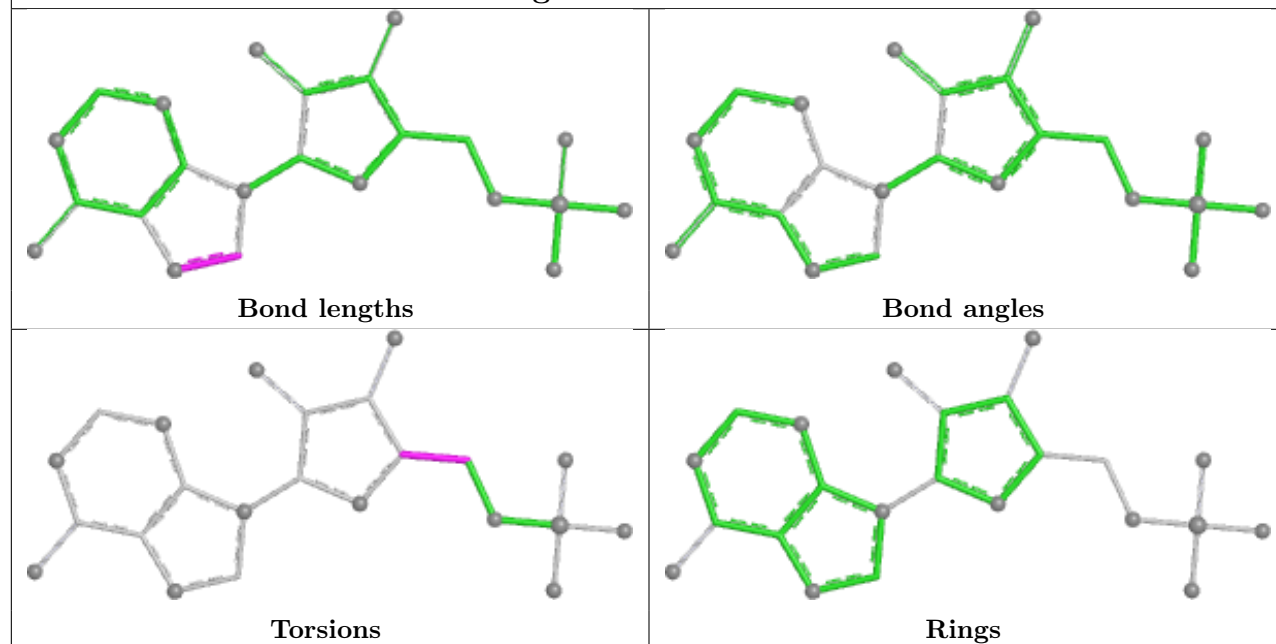
Ligand IMP C 801



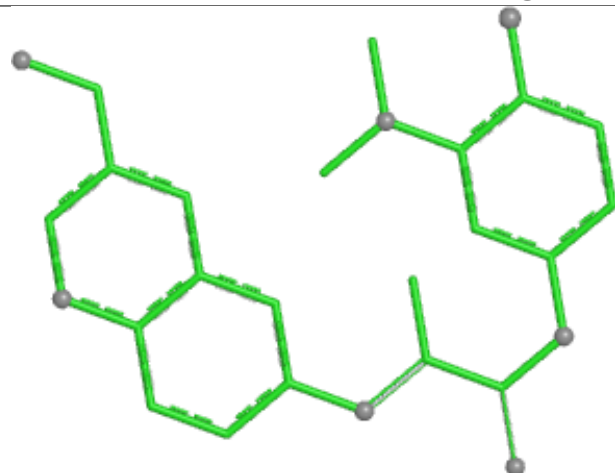
Ligand IMP B 801



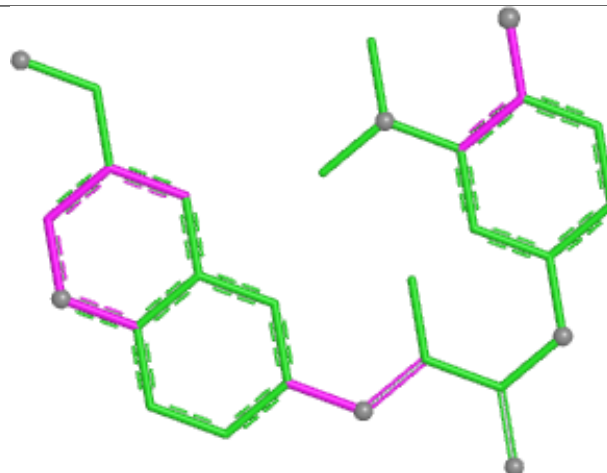
Ligand IMP H 801



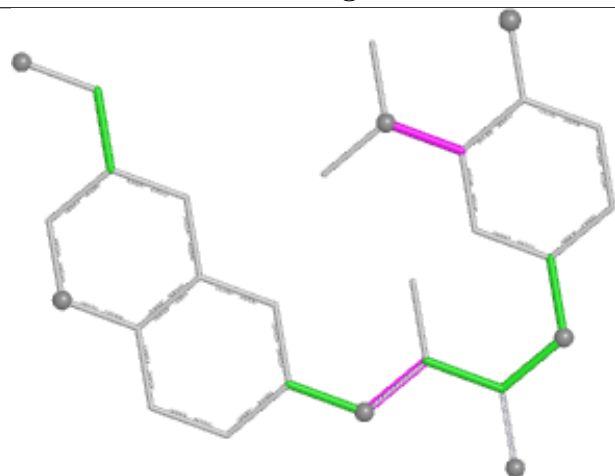
Ligand VP4 C 802



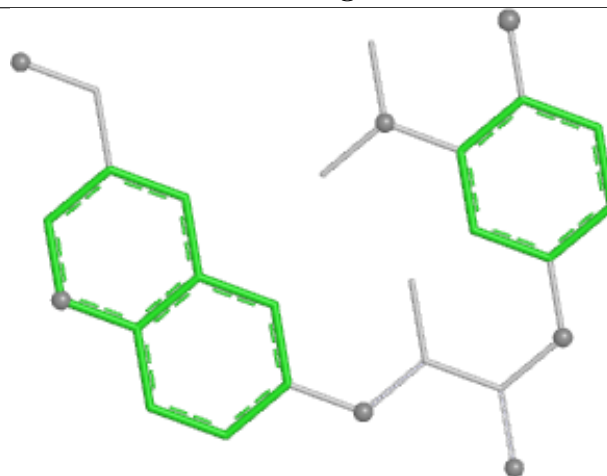
Bond lengths



Bond angles

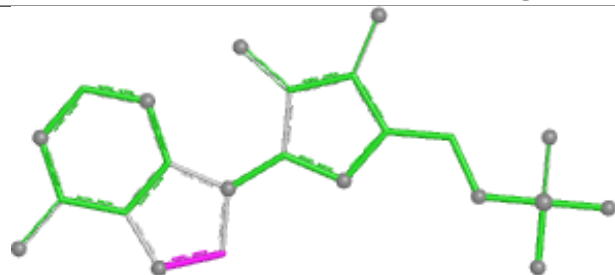


Torsions

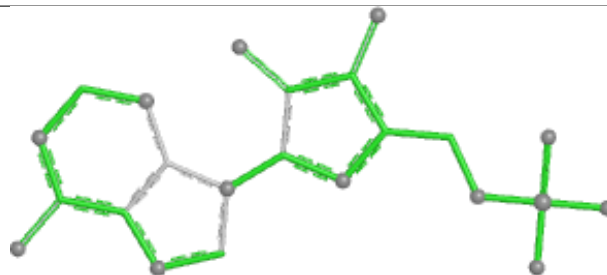


Rings

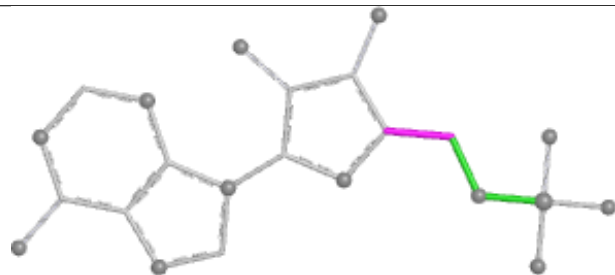
Ligand IMP A 801



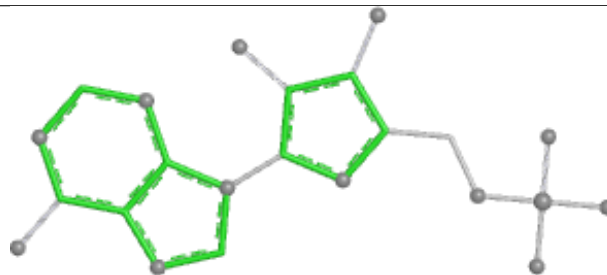
Bond lengths



Bond angles

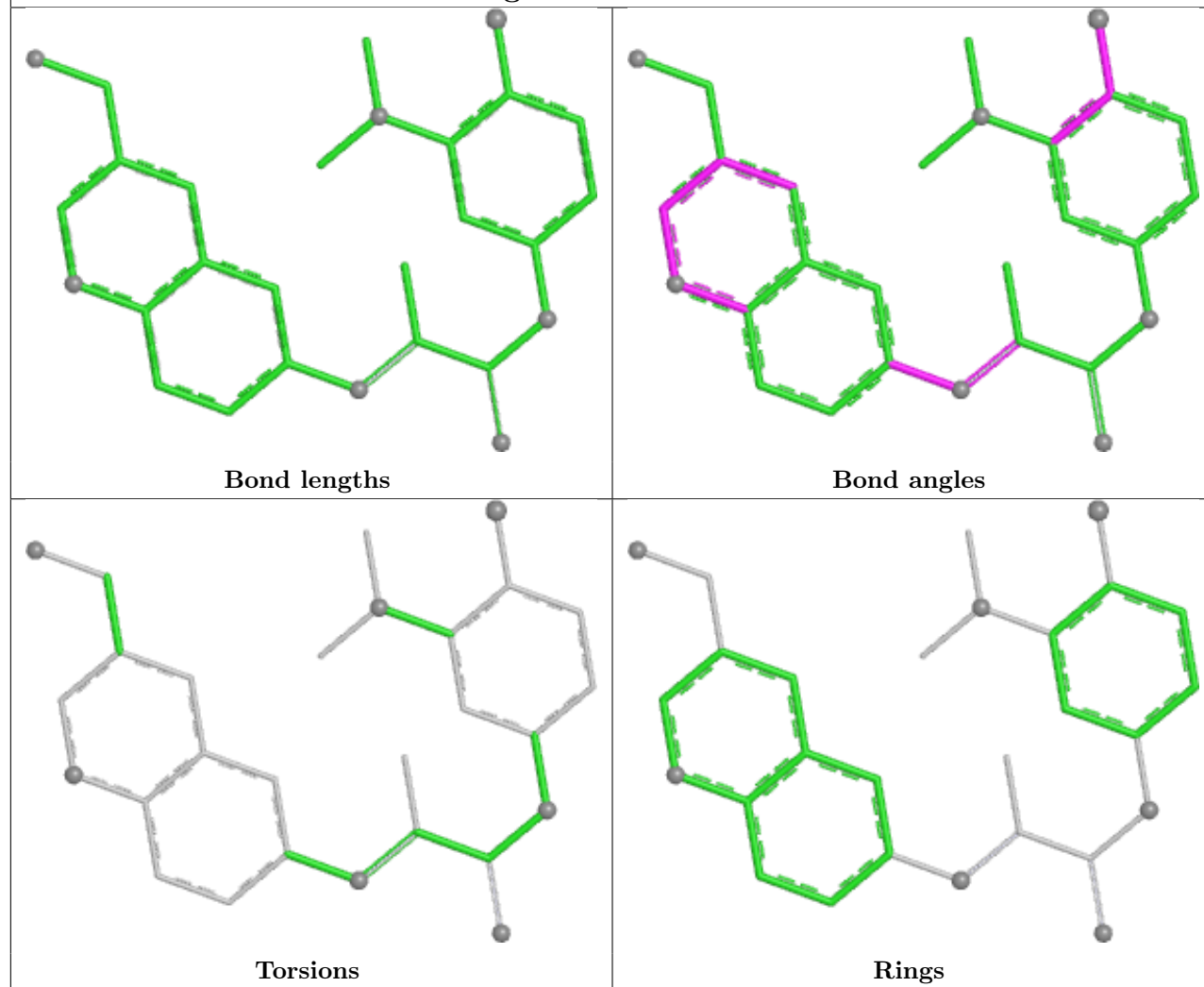


Torsions

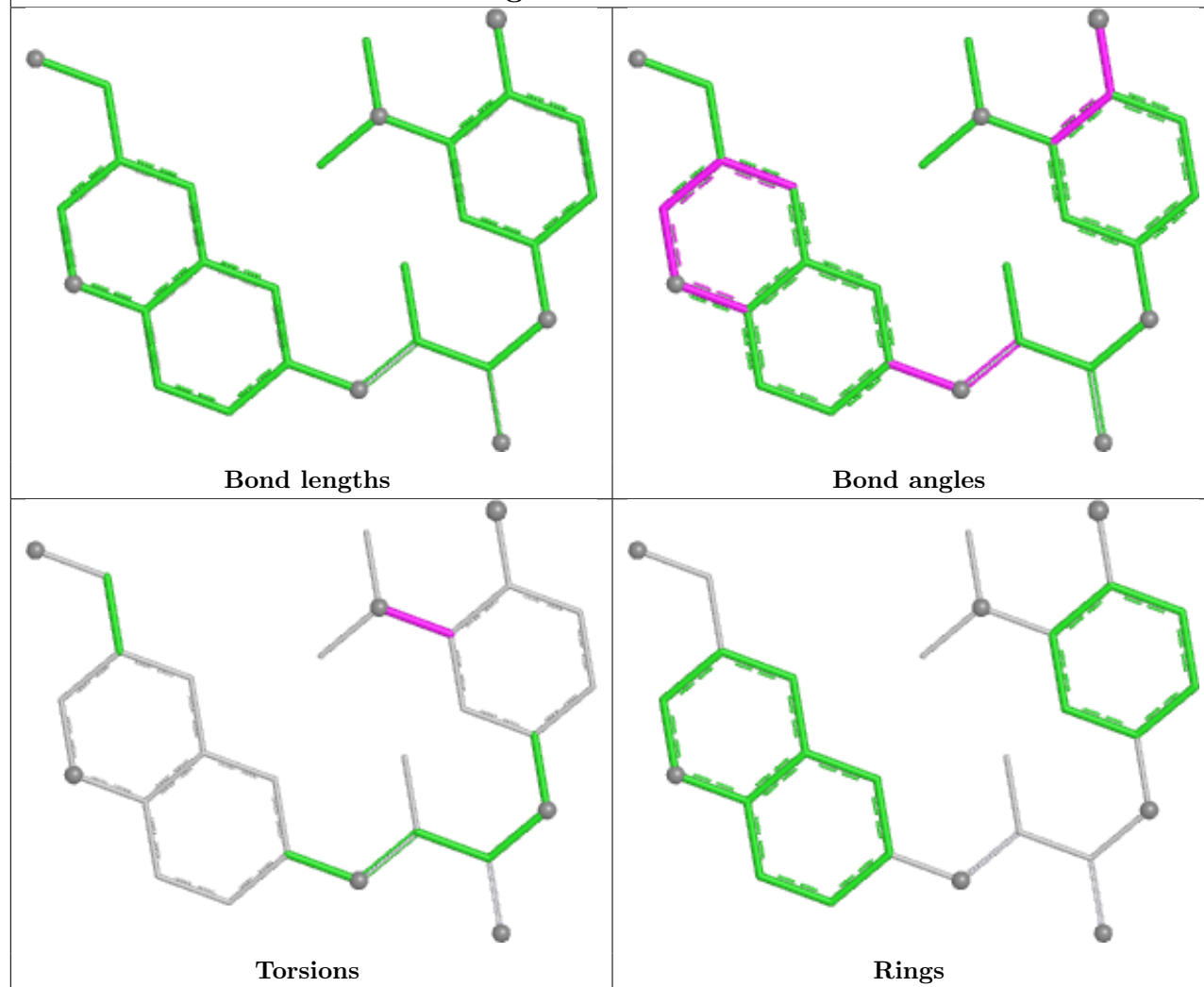


Rings

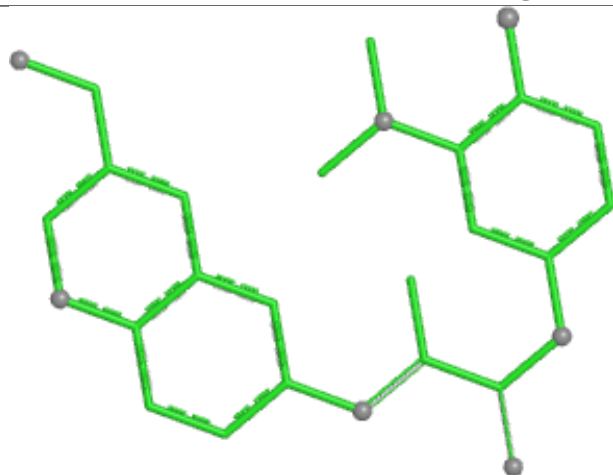
Ligand VP4 D 802



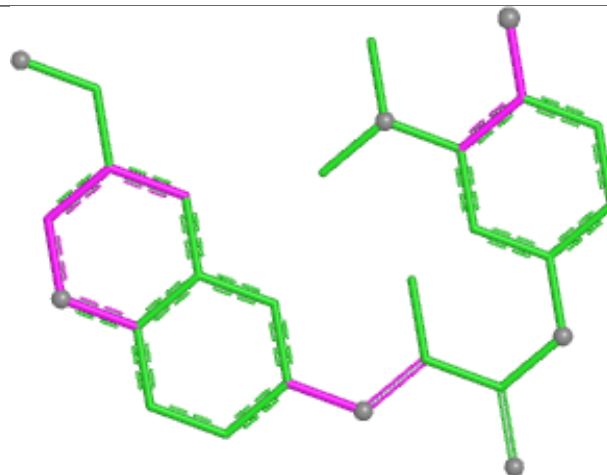
Ligand VP4 F 802



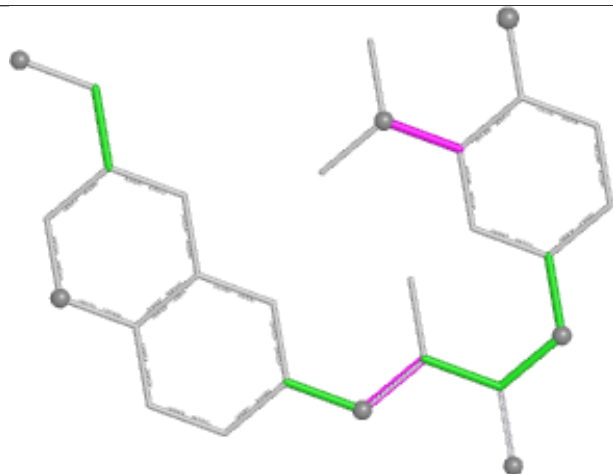
Ligand VP4 B 802



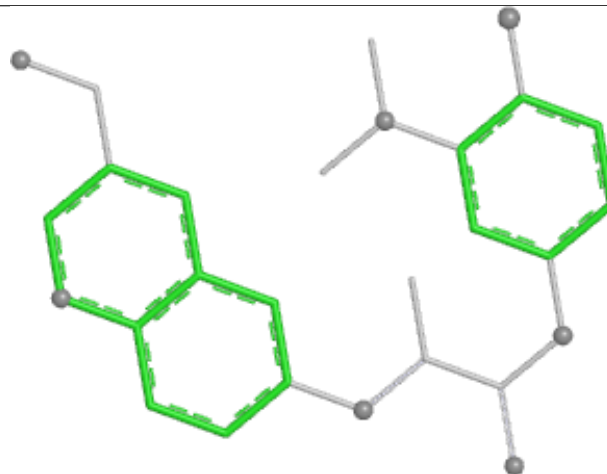
Bond lengths



Bond angles

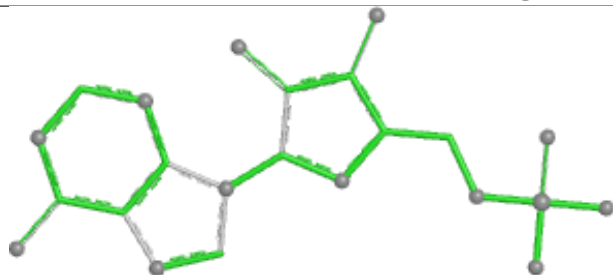


Torsions

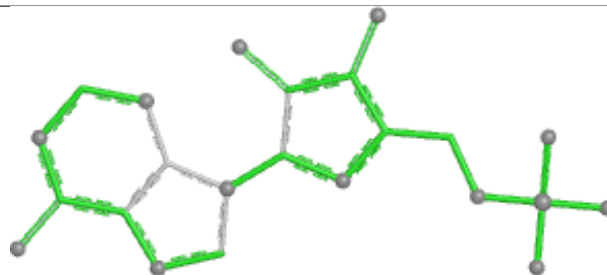


Rings

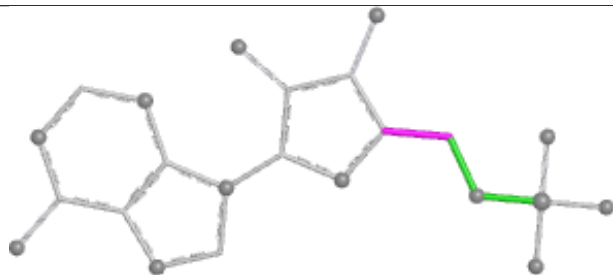
Ligand IMP E 801



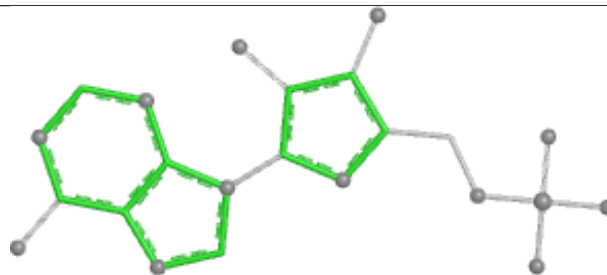
Bond lengths



Bond angles

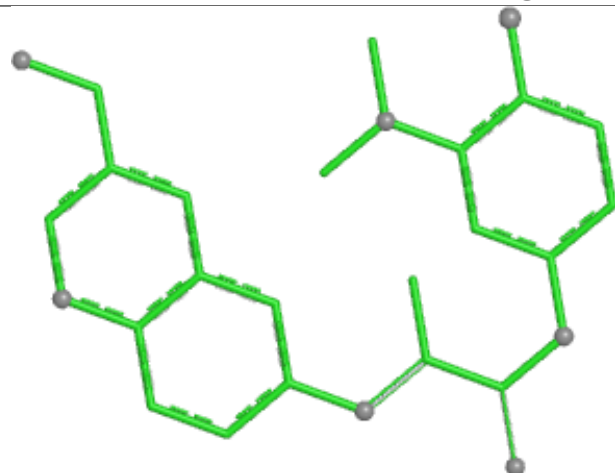


Torsions

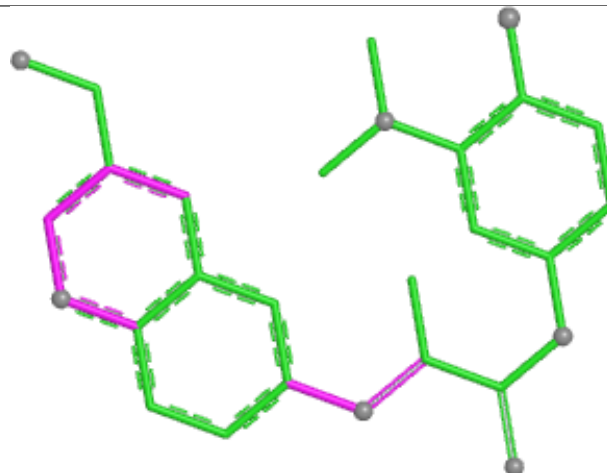


Rings

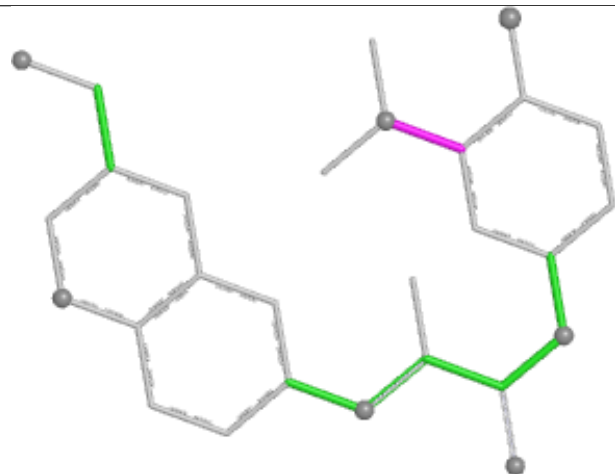
Ligand VP4 A 802



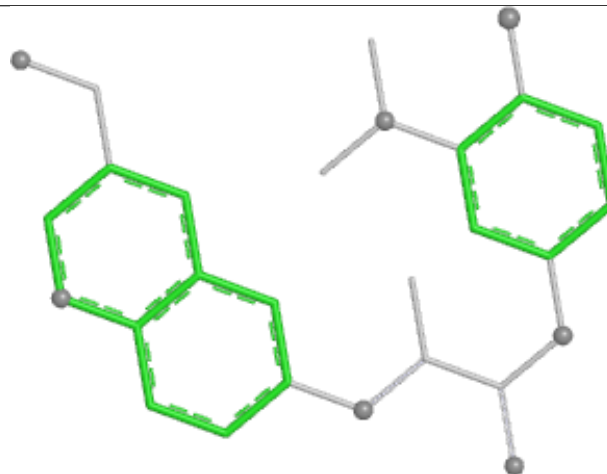
Bond lengths



Bond angles

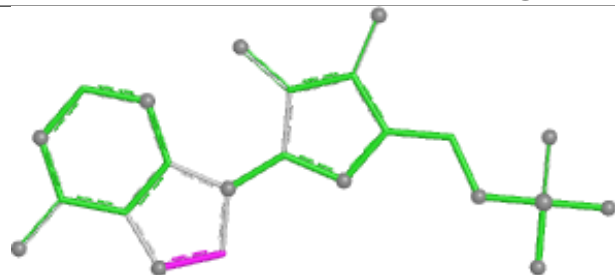


Torsions

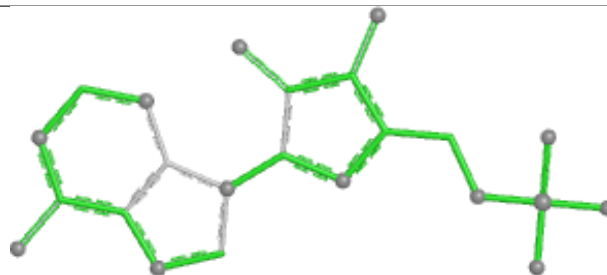


Rings

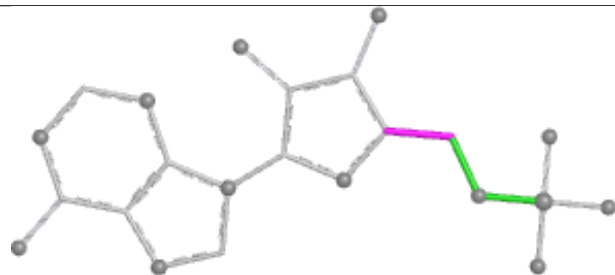
Ligand IMP D 801



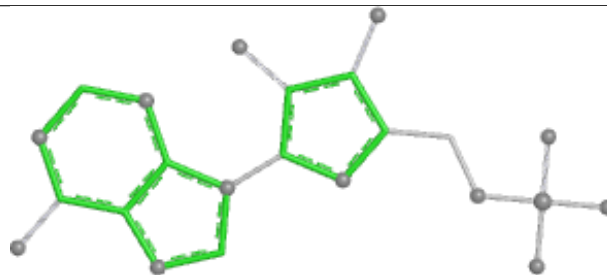
Bond lengths



Bond angles

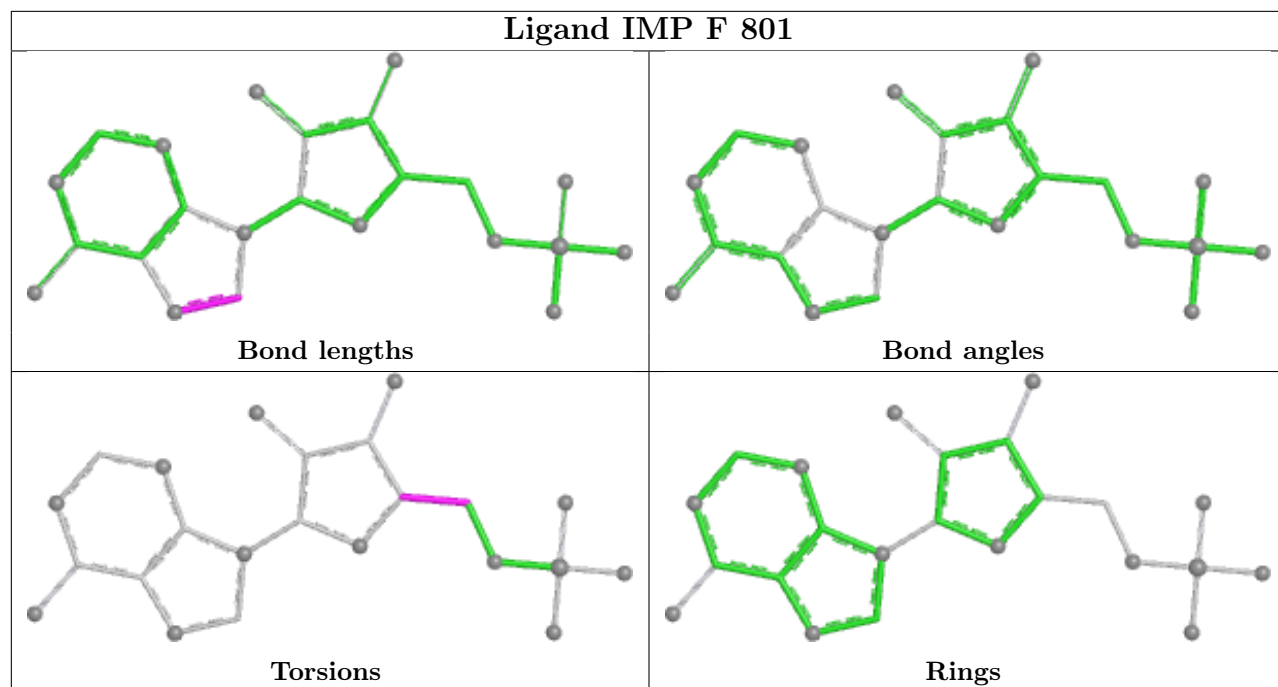


Torsions

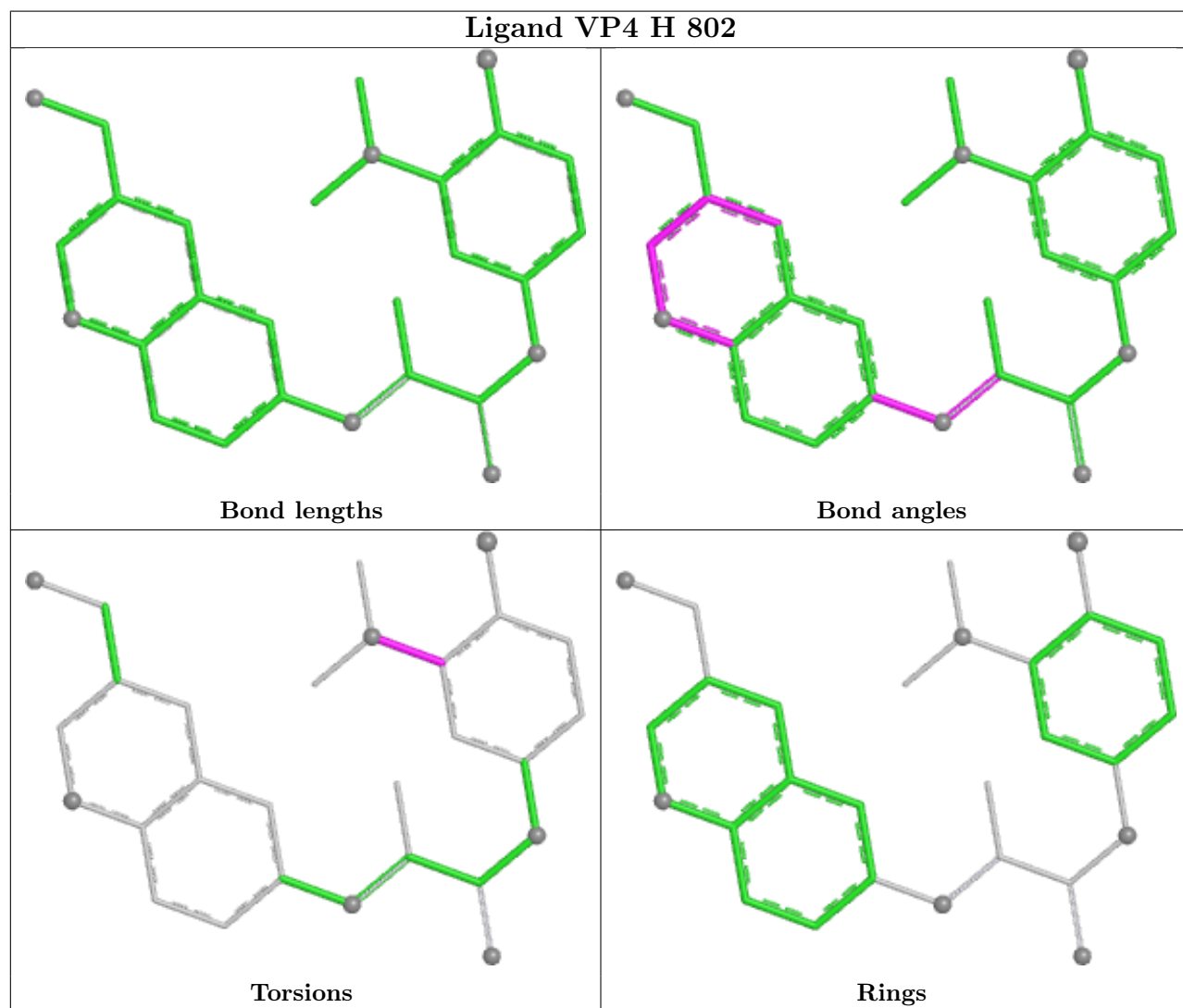


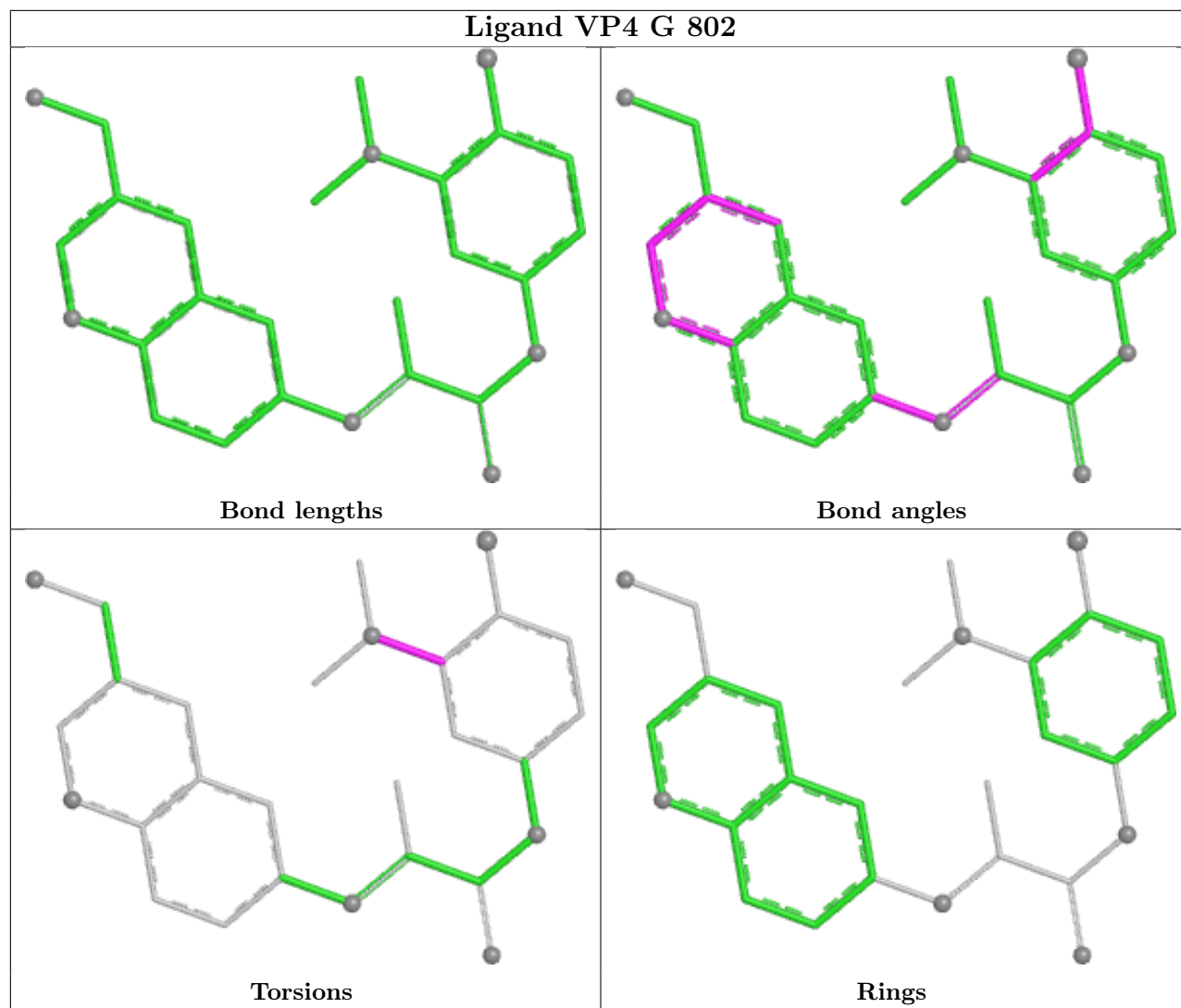
Rings

Ligand IMP F 801



Ligand VP4 H 802





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	336/395 (85%)	1.29	75 (22%) 3 3	10, 24, 48, 94	4 (1%)
1	B	336/395 (85%)	1.24	68 (20%) 3 4	9, 23, 50, 94	4 (1%)
1	C	336/395 (85%)	1.25	55 (16%) 5 6	11, 24, 49, 84	1 (0%)
1	D	337/395 (85%)	1.29	69 (20%) 3 4	7, 24, 48, 96	4 (1%)
1	E	337/395 (85%)	1.34	69 (20%) 3 4	9, 25, 48, 68	2 (0%)
1	F	338/395 (85%)	1.37	70 (20%) 3 4	10, 25, 47, 77	3 (0%)
1	G	336/395 (85%)	1.36	70 (20%) 3 4	11, 25, 49, 72	4 (1%)
1	H	336/395 (85%)	1.29	68 (20%) 3 4	11, 25, 47, 71	4 (1%)
All	All	2692/3160 (85%)	1.30	544 (20%) 3 4	7, 24, 49, 96	26 (0%)

All (544) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	92	GLY	9.2
1	A	92	GLY	8.5
1	B	92	GLY	8.1
1	A	373	GLU	7.4
1	C	91	ALA	7.4
1	C	92	GLY	7.3
1	H	92	GLY	7.3
1	H	91	ALA	7.0
1	B	467	GLY	6.9
1	F	92	GLY	6.8
1	E	92	GLY	6.5
1	F	393	ALA	6.4
1	H	393	ALA	6.4
1	F	91	ALA	6.3
1	G	91	ALA	6.3
1	G	393	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	F	1	MET	6.0
1	D	374	PHE	6.0
1	D	91	ALA	5.9
1	F	467	GLY	5.9
1	E	91	ALA	5.9
1	A	374	PHE	5.9
1	C	393	ALA	5.9
1	A	227	ALA	5.7
1	A	375	PHE	5.5
1	C	467	GLY	5.4
1	C	376	GLN	5.4
1	F	375	PHE	5.4
1	B	374	PHE	5.2
1	A	467	GLY	5.2
1	H	2	LEU	5.1
1	E	5	VAL	5.0
1	E	88	LYS	5.0
1	H	467	GLY	4.9
1	F	421	ARG	4.9
1	G	378	ARG	4.9
1	D	467	GLY	4.9
1	E	393	ALA	4.9
1	C	373	GLU	4.9
1	E	433[A]	HIS	4.9
1	D	373	GLU	4.9
1	G	375	PHE	4.8
1	A	372	VAL	4.7
1	G	328	LYS	4.6
1	A	377	GLY	4.5
1	E	378	ARG	4.5
1	D	393	ALA	4.5
1	G	467	GLY	4.5
1	A	91	ALA	4.4
1	A	393	ALA	4.4
1	B	378	ARG	4.4
1	F	88	LYS	4.4
1	H	206	TYR	4.3
1	G	92	GLY	4.3
1	D	375	PHE	4.3
1	B	85	ARG	4.3
1	E	376	GLN	4.3
1	E	288	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	376	GLN	4.2
1	A	376	GLN	4.2
1	G	88	LYS	4.2
1	D	433[A]	HIS	4.2
1	F	84	ARG	4.2
1	H	288	ASP	4.2
1	D	378	ARG	4.2
1	D	466	ALA	4.2
1	G	247	ASP	4.2
1	B	376	GLN	4.1
1	C	208	ASN	4.1
1	A	88	LYS	4.1
1	C	372	VAL	4.1
1	G	23	VAL	4.1
1	H	465	SER	4.1
1	H	209	SER	4.1
1	C	421	ARG	4.1
1	F	0	SER	4.0
1	E	375	PHE	4.0
1	B	372	VAL	4.0
1	F	23[A]	VAL	4.0
1	H	456	GLN	4.0
1	D	376	GLN	4.0
1	G	431	ILE	4.0
1	G	372	VAL	3.9
1	G	7	GLU	3.9
1	H	328	LYS	3.9
1	F	281	ASP	3.9
1	H	265	GLN	3.9
1	E	0	SER	3.9
1	F	208	ASN	3.9
1	G	206	TYR	3.9
1	D	377	GLY	3.9
1	E	1	MET	3.8
1	C	375	PHE	3.8
1	E	374	PHE	3.8
1	C	266	ASN	3.8
1	C	374	PHE	3.8
1	E	328	LYS	3.8
1	F	378	ARG	3.8
1	F	389	LEU	3.8
1	H	374	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	393	ALA	3.8
1	D	330	GLN	3.8
1	B	90	GLU	3.8
1	E	372	VAL	3.8
1	F	5	VAL	3.7
1	H	372	VAL	3.7
1	G	421	ARG	3.7
1	D	231	SER	3.7
1	E	2	LEU	3.7
1	G	389	LEU	3.7
1	D	1	MET	3.7
1	H	330	GLN	3.7
1	B	2	LEU	3.7
1	G	373	GLU	3.6
1	H	238	GLU	3.6
1	A	423	PRO	3.6
1	B	91	ALA	3.6
1	C	228	ASP	3.6
1	A	421	ARG	3.6
1	C	424	TYR	3.6
1	B	228	ASP	3.6
1	H	38	ILE	3.6
1	A	1	MET	3.6
1	H	370	GLY	3.5
1	G	288	ASP	3.5
1	B	3	THR	3.5
1	A	2	LEU	3.5
1	H	267	PHE	3.5
1	H	0	SER	3.5
1	D	227	ALA	3.5
1	E	289	ALA	3.5
1	B	377	GLY	3.5
1	A	228	ASP	3.5
1	H	375	PHE	3.5
1	H	421	ARG	3.5
1	G	265	GLN	3.5
1	B	371	GLU	3.5
1	A	424	TYR	3.5
1	B	88	LYS	3.5
1	C	371	GLU	3.4
1	E	467	GLY	3.4
1	G	465	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	370	GLY	3.4
1	D	371	GLU	3.4
1	B	424	TYR	3.4
1	H	379	TYR	3.4
1	G	433[A]	HIS	3.4
1	B	373	GLU	3.4
1	E	4	ILE	3.3
1	B	375	PHE	3.3
1	D	265[A]	GLN	3.3
1	F	456	GLN	3.3
1	A	379	TYR	3.3
1	F	237	VAL	3.3
1	H	214	LEU	3.3
1	H	26	LYS	3.3
1	C	1	MET	3.3
1	A	247	ASP	3.3
1	C	75	ASP	3.3
1	B	431	ILE	3.3
1	H	433[A]	HIS	3.3
1	E	379	TYR	3.3
1	H	373	GLU	3.3
1	B	1	MET	3.3
1	G	377	GLY	3.3
1	H	1	MET	3.3
1	D	434	GLN	3.3
1	E	267	PHE	3.3
1	E	457	ASN	3.3
1	D	3	THR	3.2
1	G	374	PHE	3.2
1	H	23	VAL	3.2
1	C	390	GLY	3.2
1	C	420	GLY	3.2
1	G	379	TYR	3.2
1	A	466	ALA	3.2
1	B	227	ALA	3.2
1	G	84[A]	ARG	3.2
1	B	264	LYS	3.2
1	G	258	GLU	3.2
1	F	374	PHE	3.2
1	C	265	GLN	3.2
1	B	379	TYR	3.2
1	B	389	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	5	VAL	3.1
1	A	389	LEU	3.1
1	F	265	GLN	3.1
1	A	32	THR	3.1
1	C	459	LYS	3.1
1	F	414	VAL	3.1
1	C	238	GLU	3.1
1	B	84	ARG	3.1
1	D	412	LYS	3.1
1	G	1	MET	3.1
1	E	423	PRO	3.1
1	C	236	LEU	3.0
1	E	226	GLY	3.0
1	B	421	ARG	3.0
1	D	206	TYR	3.0
1	A	269	GLN	3.0
1	F	451	ILE	3.0
1	C	466	ALA	3.0
1	H	39	TYR	3.0
1	D	372	VAL	3.0
1	G	243	VAL	3.0
1	C	229	THR	3.0
1	F	206	TYR	3.0
1	B	0	SER	3.0
1	B	89	PHE	3.0
1	B	381	LYS	3.0
1	D	75	ASP	3.0
1	H	227	ALA	3.0
1	F	7	GLU	2.9
1	B	214	LEU	2.9
1	F	205	SER	2.9
1	D	85	ARG	2.9
1	A	422	VAL	2.9
1	H	329	ASP	2.9
1	B	234	GLU	2.9
1	B	4	ILE	2.9
1	B	290	GLY	2.9
1	E	349	ILE	2.9
1	E	243	VAL	2.9
1	F	227	ALA	2.9
1	A	238	GLU	2.9
1	D	88	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	265	GLN	2.9
1	G	434	GLN	2.9
1	A	371	GLU	2.9
1	F	207	PRO	2.8
1	E	290	GLY	2.8
1	D	214	LEU	2.8
1	D	389	LEU	2.8
1	B	247	ASP	2.8
1	F	267	PHE	2.8
1	G	270	VAL	2.8
1	F	377	GLY	2.8
1	H	4	ILE	2.8
1	A	434	GLN	2.8
1	D	456	GLN	2.8
1	F	434	GLN	2.8
1	G	207	PRO	2.8
1	C	263	VAL	2.8
1	D	392	MET	2.8
1	C	85	ARG	2.8
1	D	37	GLY	2.8
1	H	377	GLY	2.8
1	A	214	LEU	2.8
1	F	413	LEU	2.8
1	A	433[A]	HIS	2.8
1	H	376	GLN	2.8
1	H	88	LYS	2.8
1	D	380	TYR	2.8
1	C	378	ARG	2.8
1	H	378	ARG	2.8
1	A	225	THR	2.8
1	F	433[A]	HIS	2.8
1	E	205	SER	2.7
1	D	7	GLU	2.7
1	F	36	ARG	2.7
1	E	424	TYR	2.7
1	G	83	VAL	2.7
1	G	208	ASN	2.7
1	C	307	ARG	2.7
1	E	452	GLU	2.7
1	C	247	ASP	2.7
1	F	89	PHE	2.7
1	B	219	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	389	LEU	2.7
1	B	238	GLU	2.7
1	E	7	GLU	2.7
1	A	302	SER	2.7
1	A	89	PHE	2.7
1	A	380	TYR	2.7
1	C	422	VAL	2.7
1	B	456	GLN	2.7
1	G	326	ALA	2.7
1	C	72	LYS	2.7
1	A	378	ARG	2.7
1	G	435	MET	2.7
1	G	329	ASP	2.7
1	C	83	VAL	2.7
1	H	5	VAL	2.7
1	G	285	ALA	2.7
1	B	66	GLY	2.6
1	A	452	GLU	2.6
1	C	419	GLU	2.6
1	H	431	ILE	2.6
1	D	207	PRO	2.6
1	B	433[A]	HIS	2.6
1	E	456	GLN	2.6
1	C	77	ALA	2.6
1	E	391	ALA	2.6
1	E	373	GLU	2.6
1	E	331	ILE	2.6
1	B	207	PRO	2.6
1	F	412	LYS	2.6
1	C	389	LEU	2.6
1	E	454	LEU	2.6
1	B	83	VAL	2.5
1	F	223	VAL	2.5
1	F	291	ALA	2.5
1	F	422	VAL	2.5
1	G	391	ALA	2.5
1	H	422	VAL	2.5
1	H	213	ASP	2.5
1	F	226	GLY	2.5
1	H	37	GLY	2.5
1	A	86	VAL	2.5
1	G	291	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	368	ALA	2.5
1	A	73	ASN	2.5
1	B	380	TYR	2.5
1	A	265	GLN	2.5
1	H	434	GLN	2.5
1	G	4	ILE	2.5
1	E	465	SER	2.5
1	F	329	ASP	2.5
1	E	37	GLY	2.5
1	A	5	VAL	2.5
1	D	233	VAL	2.5
1	A	361	LEU	2.5
1	A	226	GLY	2.5
1	H	226	GLY	2.5
1	D	381	LYS	2.5
1	A	391	ALA	2.5
1	B	237	VAL	2.5
1	D	86	VAL	2.5
1	E	227	ALA	2.5
1	G	89	PHE	2.5
1	F	327	LEU	2.5
1	D	208	ASN	2.5
1	D	248	THR	2.5
1	C	423	PRO	2.5
1	D	42	ILE	2.4
1	G	425	LYS	2.4
1	H	264	LYS	2.4
1	C	319	ALA	2.4
1	C	433[A]	HIS	2.4
1	D	5	VAL	2.4
1	A	206	TYR	2.4
1	A	325	SER	2.4
1	A	418	ILE	2.4
1	B	465	SER	2.4
1	D	76	ILE	2.4
1	D	325	SER	2.4
1	C	288	ASP	2.4
1	D	228	ASP	2.4
1	E	329	ASP	2.4
1	B	86	VAL	2.4
1	E	434	GLN	2.4
1	F	391	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	260	VAL	2.4
1	B	38	ILE	2.4
1	G	253	SER	2.4
1	D	379	TYR	2.4
1	F	379	TYR	2.4
1	B	30	LEU	2.4
1	B	23	VAL	2.4
1	B	260	VAL	2.4
1	F	32	THR	2.4
1	E	371	GLU	2.4
1	F	298	ILE	2.4
1	E	352	GLY	2.4
1	E	438	GLY	2.4
1	G	429	GLY	2.4
1	B	434	GLN	2.4
1	A	60	ALA	2.4
1	A	430	ASN	2.4
1	C	78	ALA	2.4
1	A	237	VAL	2.3
1	A	90	GLU	2.3
1	E	419	GLU	2.3
1	D	425	LYS	2.3
1	D	0	SER	2.3
1	E	247	ASP	2.3
1	H	303	ILE	2.3
1	D	84	ARG	2.3
1	G	307	ARG	2.3
1	G	299	GLY	2.3
1	H	266	ASN	2.3
1	C	89	PHE	2.3
1	E	459	LYS	2.3
1	A	281	ASP	2.3
1	E	463	ILE	2.3
1	F	307	ARG	2.3
1	F	465	SER	2.3
1	H	253	SER	2.3
1	H	338	GLY	2.3
1	H	34	LEU	2.3
1	A	425	LYS	2.3
1	G	371	GLU	2.3
1	C	86	VAL	2.3
1	E	3	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	84[A]	ARG	2.3
1	A	431	ILE	2.3
1	H	441	SER	2.3
1	A	6	GLN	2.3
1	F	269	GLN	2.3
1	G	376	GLN	2.3
1	F	370	GLY	2.3
1	H	380	TYR	2.3
1	B	459	LYS	2.3
1	E	425	LYS	2.3
1	G	77	ALA	2.3
1	A	3	THR	2.3
1	E	422	VAL	2.3
1	F	3	THR	2.3
1	F	243	VAL	2.3
1	H	369	PRO	2.3
1	G	267	PHE	2.3
1	C	4	ILE	2.3
1	C	434	GLN	2.3
1	D	4	ILE	2.3
1	F	288	ASP	2.3
1	F	453	ASP	2.3
1	E	68	GLY	2.3
1	C	380	TYR	2.2
1	E	285	ALA	2.2
1	G	324	ALA	2.2
1	E	207	PRO	2.2
1	D	36	ARG	2.2
1	D	89	PHE	2.2
1	A	69	ILE	2.2
1	A	209	SER	2.2
1	A	308	ILE	2.2
1	G	302	SER	2.2
1	H	321	ASP	2.2
1	E	72	LYS	2.2
1	A	266	ASN	2.2
1	C	206	TYR	2.2
1	E	361	LEU	2.2
1	G	20	TYR	2.2
1	A	235	ALA	2.2
1	A	340	ARG	2.2
1	D	391	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	272	VAL	2.2
1	H	323	VAL	2.2
1	A	456	GLN	2.2
1	G	0	SER	2.2
1	A	76	ILE	2.2
1	H	331	ILE	2.2
1	A	236	LEU	2.2
1	B	266	ASN	2.2
1	F	85	ARG	2.2
1	G	24	LEU	2.2
1	E	206	TYR	2.2
1	B	369	PRO	2.2
1	H	3	THR	2.2
1	D	263	VAL	2.2
1	F	247	ASP	2.2
1	G	214	LEU	2.2
1	E	268	PRO	2.2
1	B	206	TYR	2.2
1	E	81	ALA	2.2
1	G	246	VAL	2.2
1	D	264	LYS	2.2
1	D	341	PHE	2.2
1	A	234	GLU	2.1
1	B	231	SER	2.1
1	C	377	GLY	2.1
1	D	215	GLY	2.1
1	F	238	GLU	2.1
1	C	84	ARG	2.1
1	C	457	ASN	2.1
1	D	361	LEU	2.1
1	F	214	LEU	2.1
1	F	287	LEU	2.1
1	F	362	LEU	2.1
1	G	249	ALA	2.1
1	A	381	LYS	2.1
1	F	35	THR	2.1
1	A	263	VAL	2.1
1	D	213	ASP	2.1
1	D	366	GLU	2.1
1	F	228	ASP	2.1
1	H	281	ASP	2.1
1	G	338	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	84	ARG	2.1
1	C	257	ILE	2.1
1	E	38	ILE	2.1
1	F	76	ILE	2.1
1	H	320	ILE	2.1
1	C	287	LEU	2.1
1	D	2	LEU	2.1
1	C	330	GLN	2.1
1	H	31	LYS	2.1
1	E	326	ALA	2.1
1	F	424	TYR	2.1
1	E	260	VAL	2.1
1	G	256	VAL	2.1
1	D	90	GLU	2.1
1	A	364	GLY	2.1
1	F	325	SER	2.1
1	G	85	ARG	2.1
1	F	331	ILE	2.1
1	A	30	LEU	2.1
1	A	284	LEU	2.1
1	D	269	GLN	2.1
1	B	32	THR	2.1
1	D	78	ALA	2.1
1	H	248	THR	2.1
1	D	237	VAL	2.1
1	F	241	VAL	2.1
1	G	419	GLU	2.1
1	H	270	VAL	2.1
1	D	247	ASP	2.1
1	G	226	GLY	2.1
1	A	208	ASN	2.1
1	B	265	GLN	2.1
1	B	362	LEU	2.1
1	D	266	ASN	2.1
1	H	208	ASN	2.1
1	B	78	ALA	2.1
1	D	305	THR	2.1
1	B	366	GLU	2.0
1	B	422	VAL	2.0
1	G	223	VAL	2.0
1	G	263	VAL	2.0
1	A	212	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	370	GLY	2.0
1	D	390	GLY	2.0
1	E	370	GLY	2.0
1	E	360	SER	2.0
1	A	4	ILE	2.0
1	B	42	ILE	2.0
1	B	308	ILE	2.0
1	F	330	GLN	2.0
1	A	369	PRO	2.0
1	C	2	LEU	2.0
1	C	90	GLU	2.0
1	E	353	ALA	2.0
1	F	261	ARG	2.0
1	G	289	ALA	2.0
1	E	450	VAL	2.0
1	F	83	VAL	2.0
1	H	263	VAL	2.0
1	B	213	ASP	2.0
1	G	290	GLY	2.0
1	B	303	ILE	2.0
1	G	59	ILE	2.0
1	G	303	ILE	2.0
1	B	34	LEU	2.0
1	E	315	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

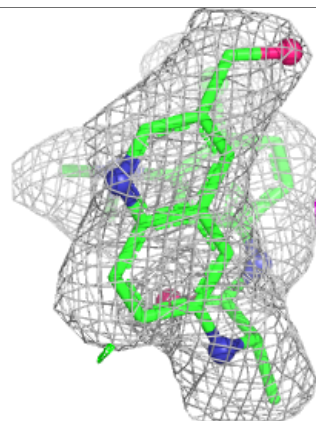
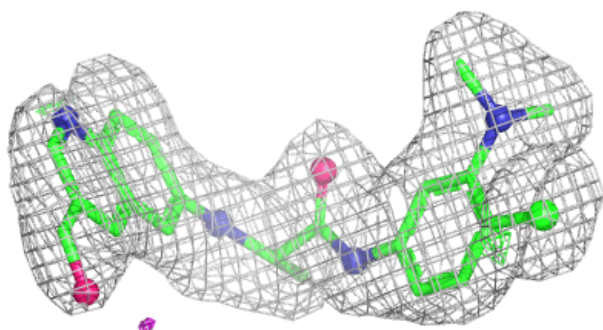
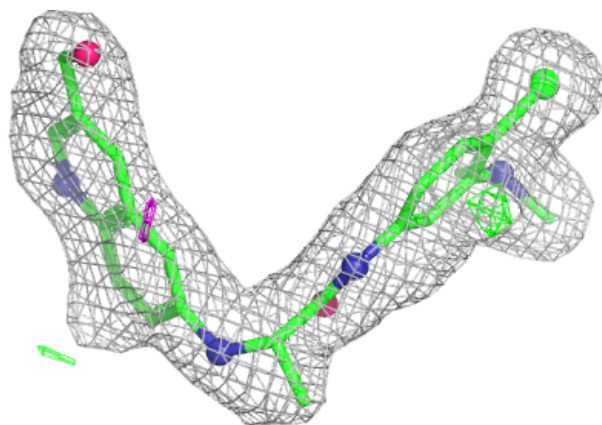
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	VP4	F	802	28/28	0.86	0.14	23,28,32,34	0
3	VP4	B	802	28/28	0.88	0.11	14,19,27,28	0
3	VP4	D	802	28/28	0.88	0.12	16,22,29,30	0
3	VP4	A	802	28/28	0.88	0.12	12,18,24,30	0
3	VP4	H	802	28/28	0.88	0.11	26,30,33,35	0
3	VP4	G	802	28/28	0.89	0.12	16,24,33,33	0
3	VP4	C	802	28/28	0.89	0.12	14,22,26,27	0
2	IMP	E	801	23/23	0.93	0.10	13,21,25,26	0
2	IMP	F	801	23/23	0.93	0.10	19,22,25,25	0
3	VP4	E	802	28/28	0.93	0.10	14,24,33,34	0
2	IMP	H	801	23/23	0.94	0.09	15,23,25,26	0
2	IMP	B	801	23/23	0.94	0.09	14,19,26,26	0
2	IMP	D	801	23/23	0.94	0.09	14,23,26,27	0
2	IMP	G	801	23/23	0.95	0.09	10,21,23,23	0
2	IMP	A	801	23/23	0.95	0.09	14,19,21,22	0
2	IMP	C	801	23/23	0.96	0.09	11,20,25,26	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.

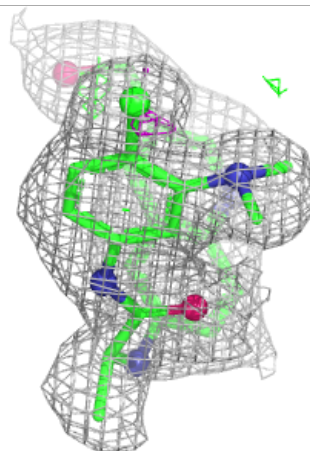
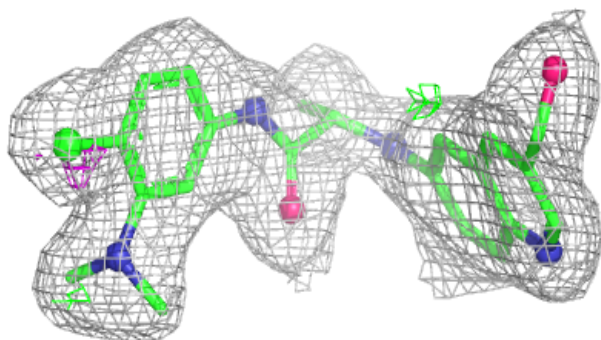
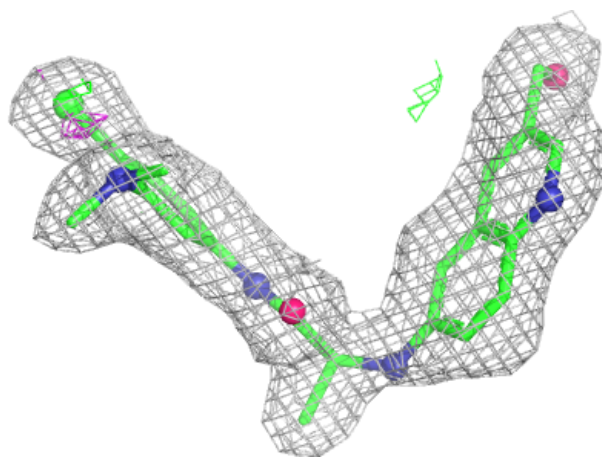
Electron density around VP4 F 802:

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



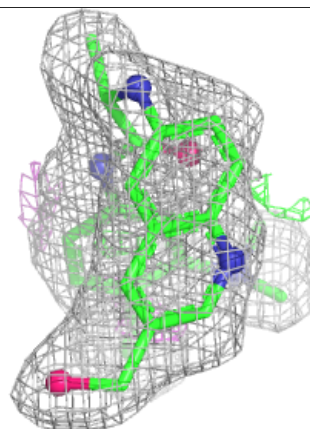
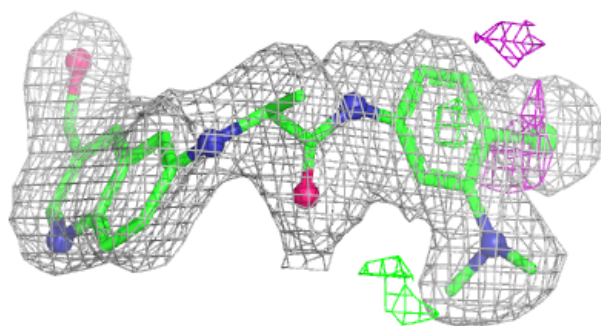
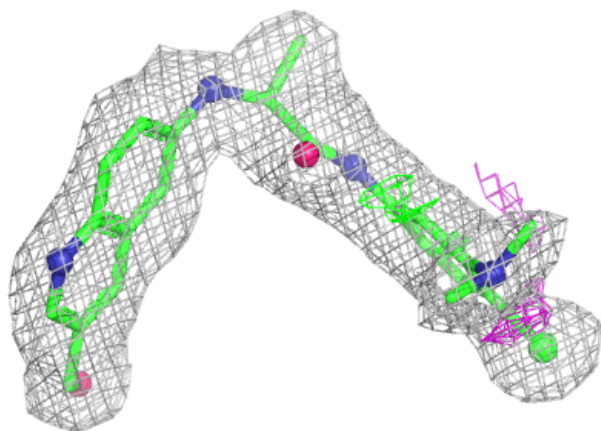
Electron density around VP4 B 802:

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



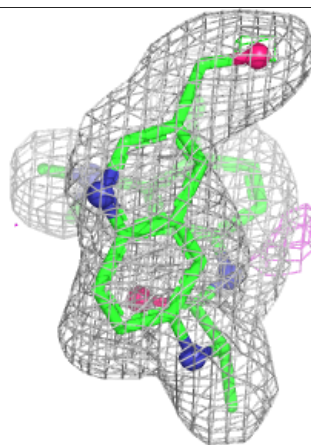
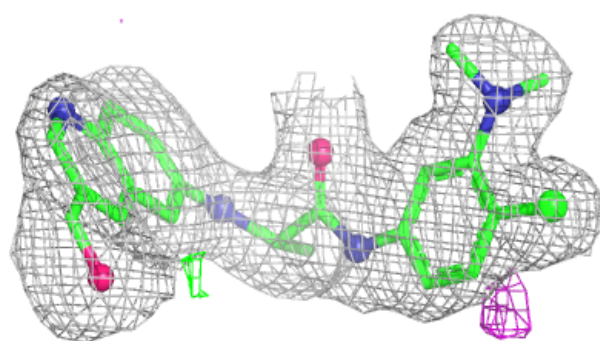
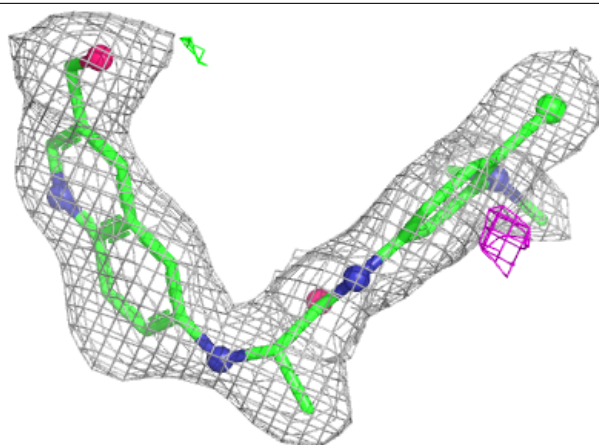
Electron density around VP4 D 802:

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



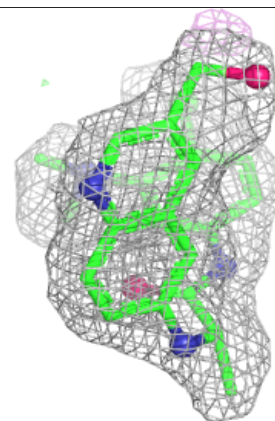
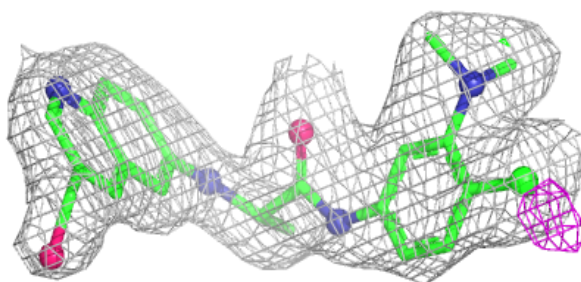
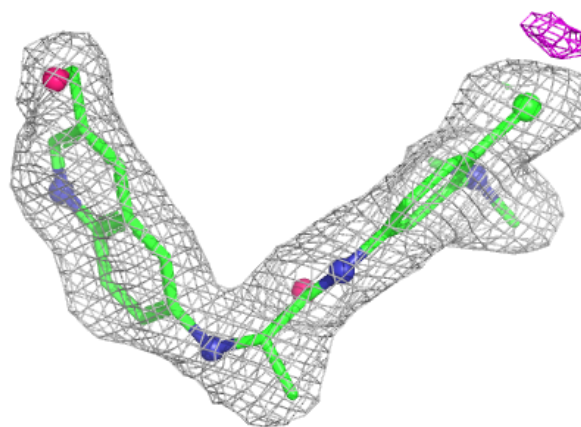
Electron density around VP4 A 802:

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



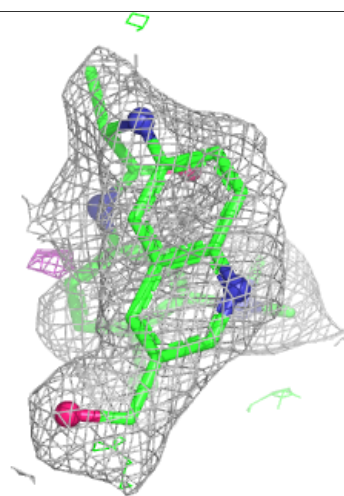
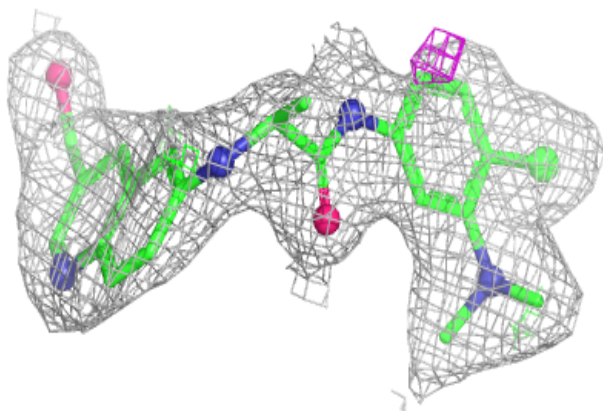
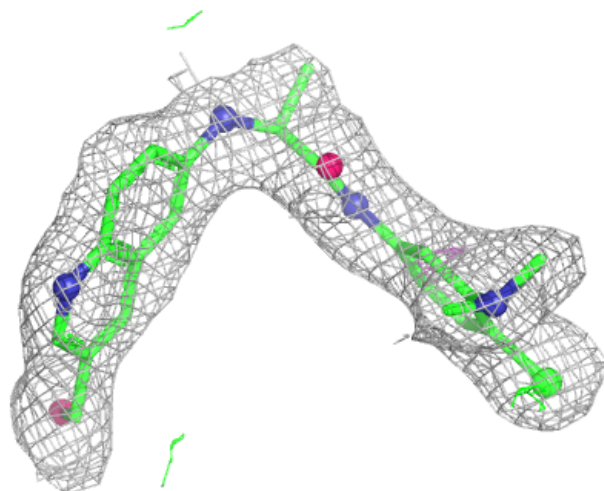
Electron density around VP4 H 802:

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



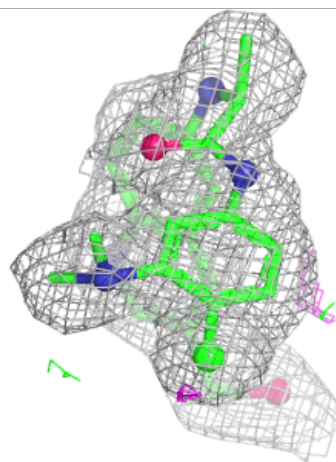
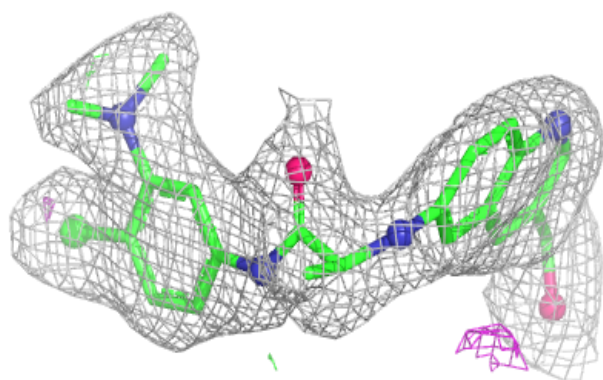
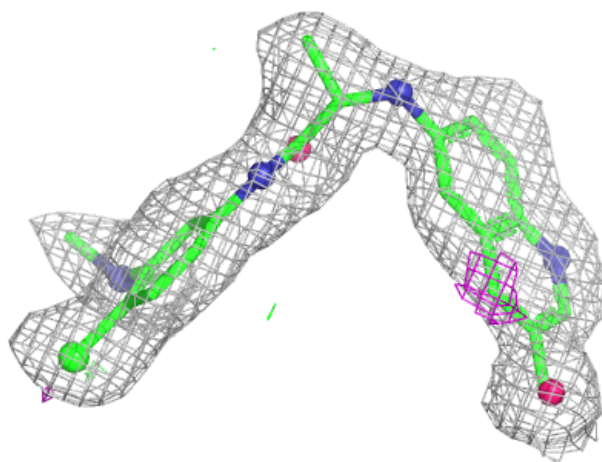
Electron density around VP4 G 802:

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



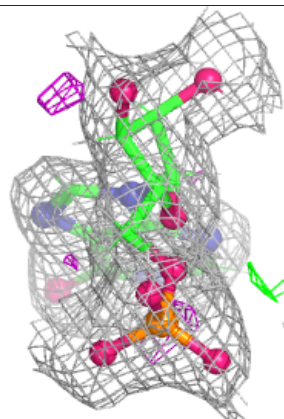
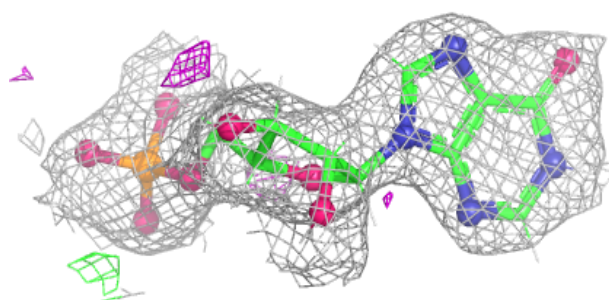
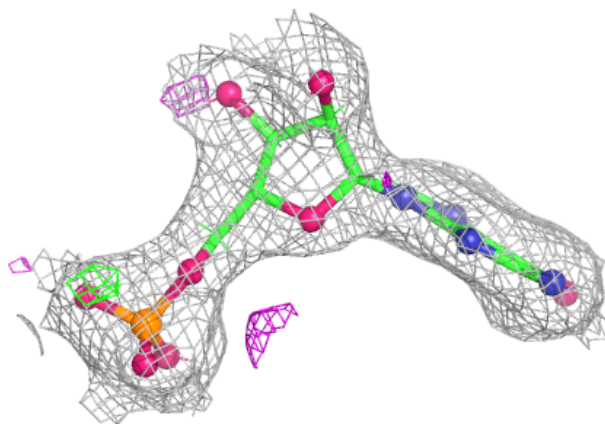
Electron density around VP4 C 802:

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

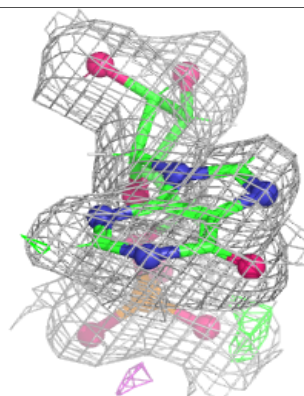
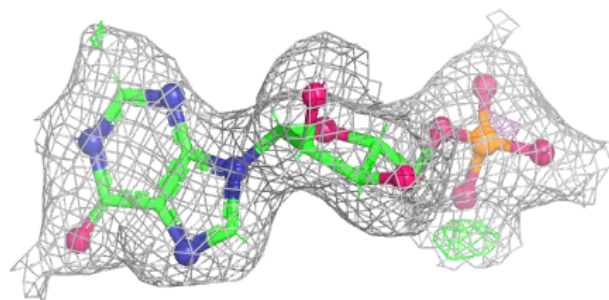
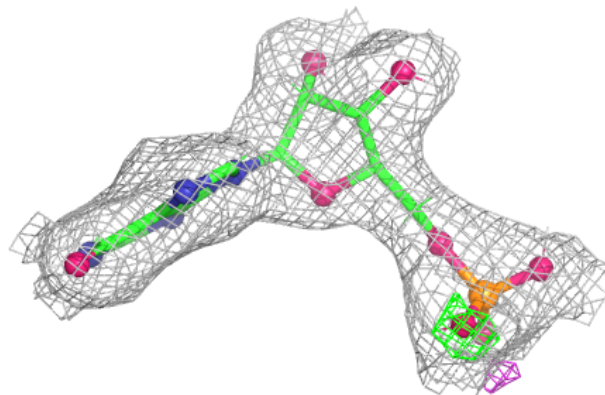


Electron density around IMP E 801:

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

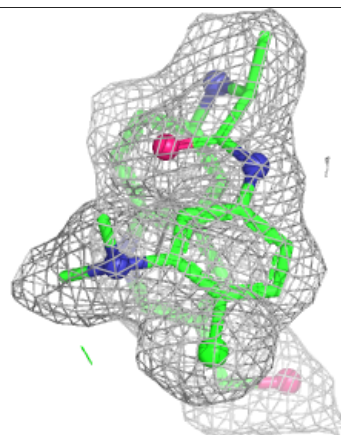
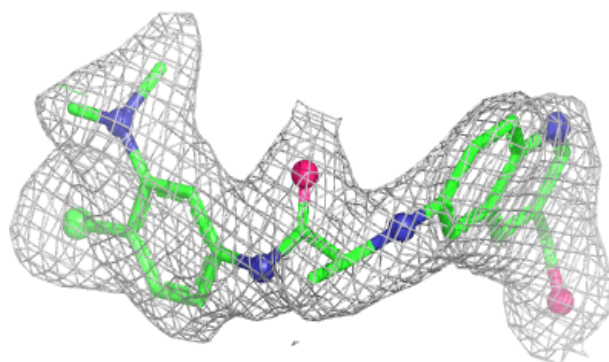
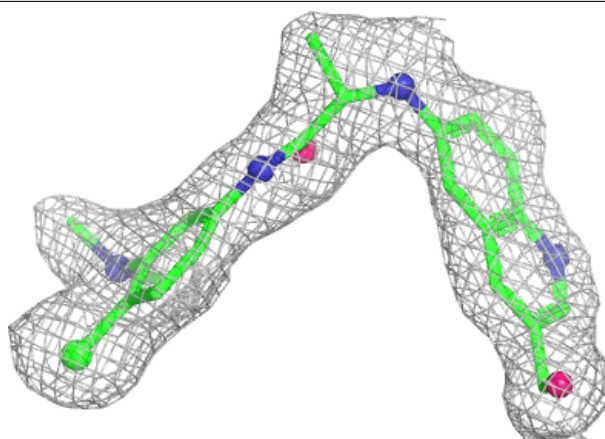
**Electron density around IMP F 801:**

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

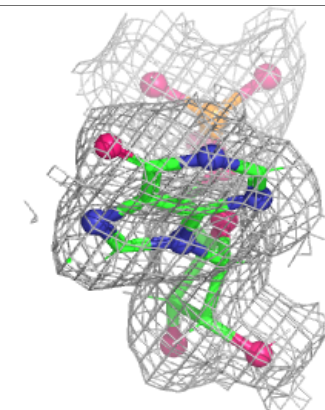
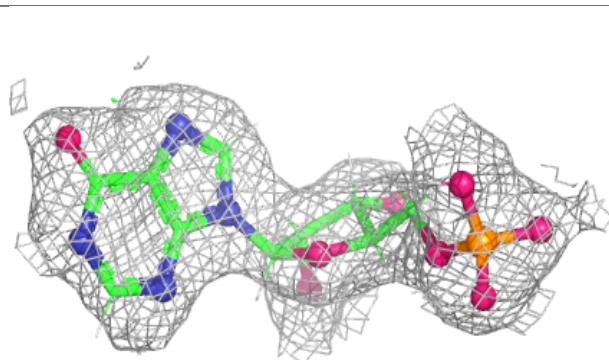
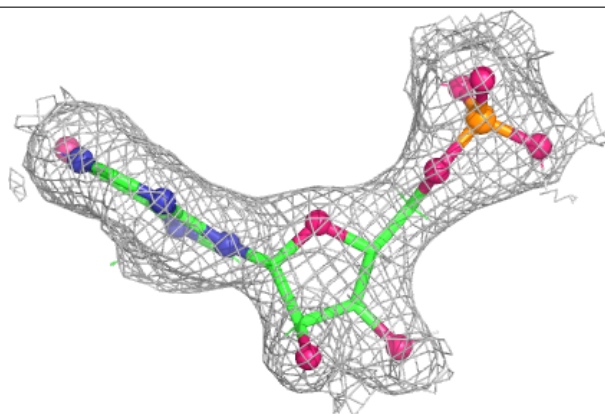


Electron density around VP4 E 802:

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

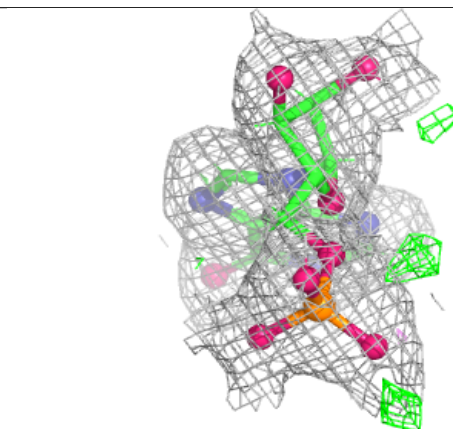
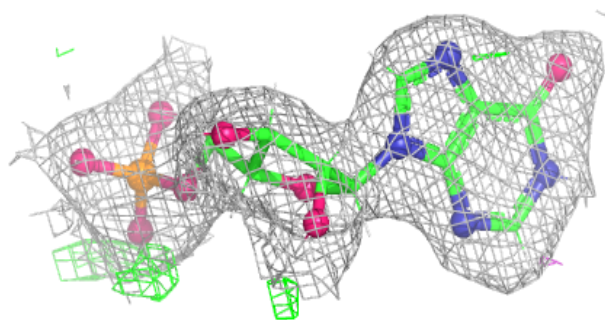
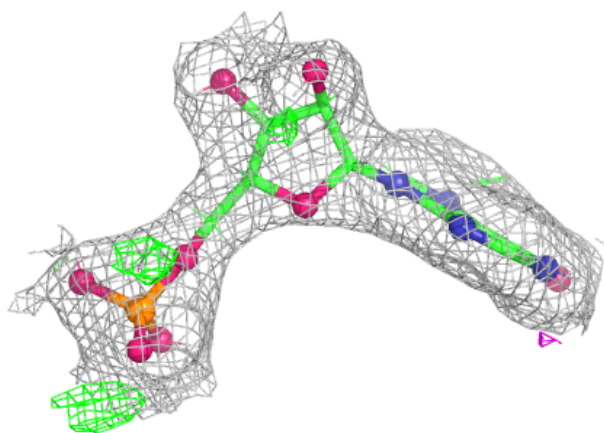
**Electron density around IMP H 801:**

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

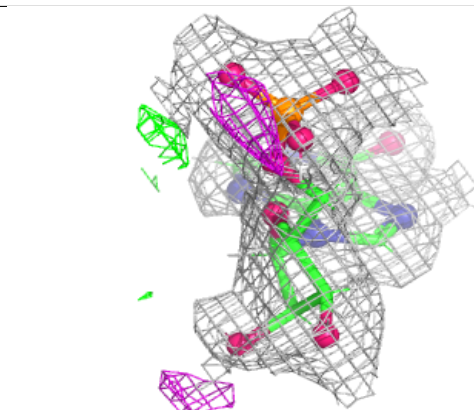
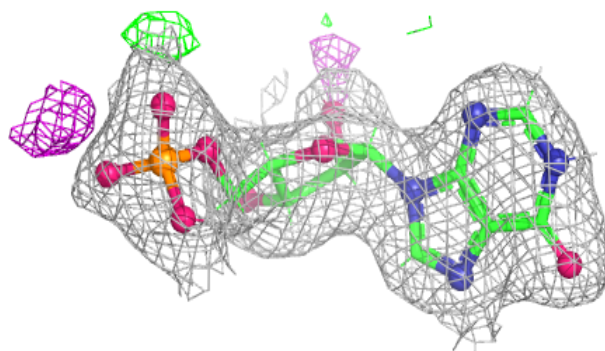
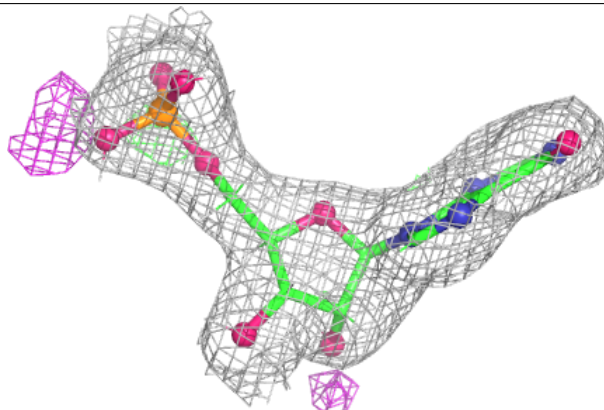


Electron density around IMP B 801:

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

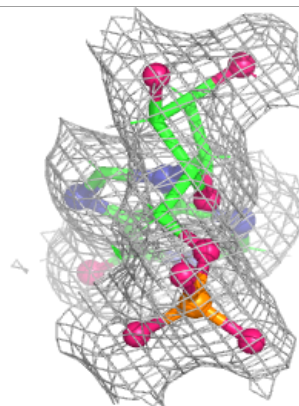
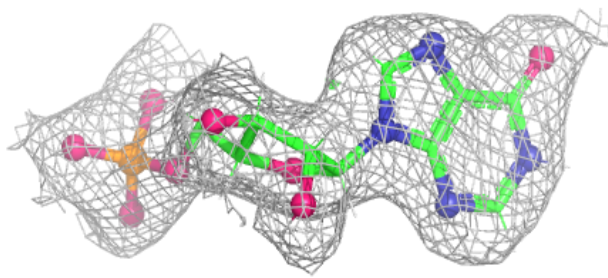
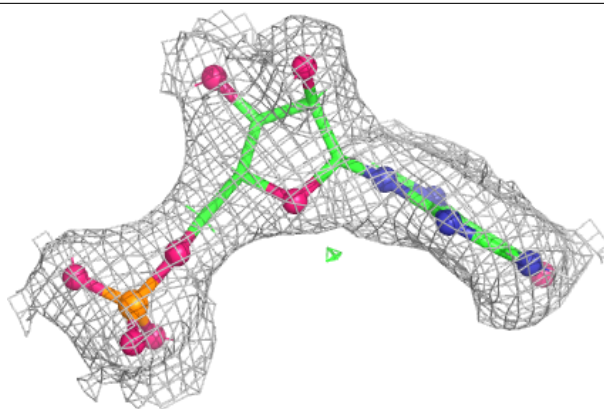
**Electron density around IMP D 801:**

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

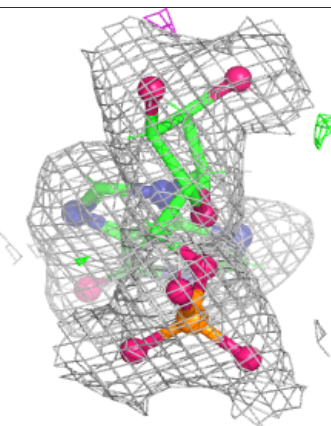
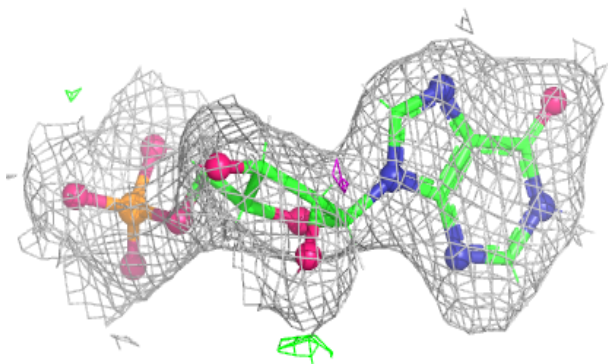
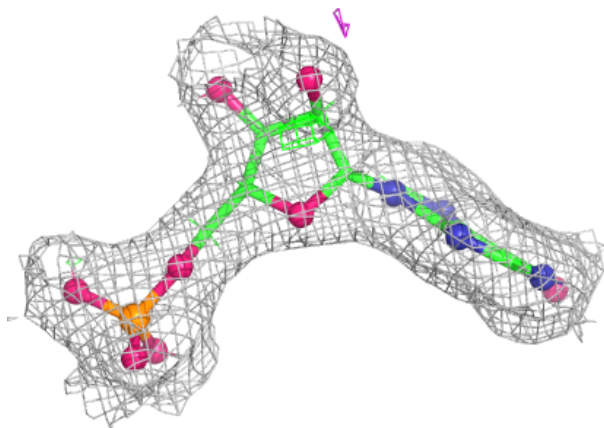


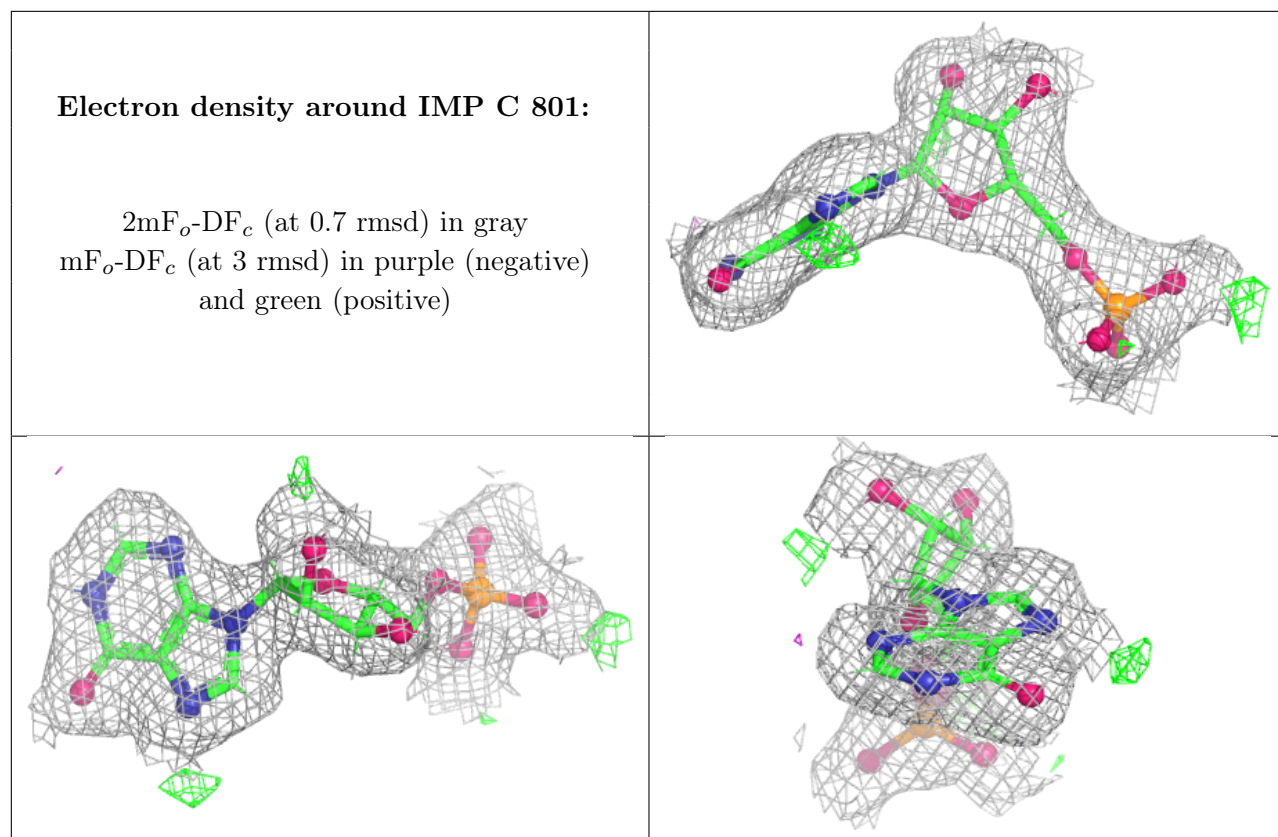
Electron density around IMP G 801:

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

**Electron density around IMP A 801:**

$2mF_o-DF_c$ (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.