wwPDB X-ray Structure Validation Summary Report (i)

Jan 25, 2022 – 10:13 AM EST

PDB ID	:	7MK5
Title	:	Crystal structure of Escherichia coli ClpP covalently inhibited by clipibicyclene
Authors	:	Culp, E.J.; Sychantha, D.; Hobson, C.; Pawlowski, A.J.; Prehna, G.; Wright, G.D.
Deposited on	:	2021-04-21
Resolution	:	2.95 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

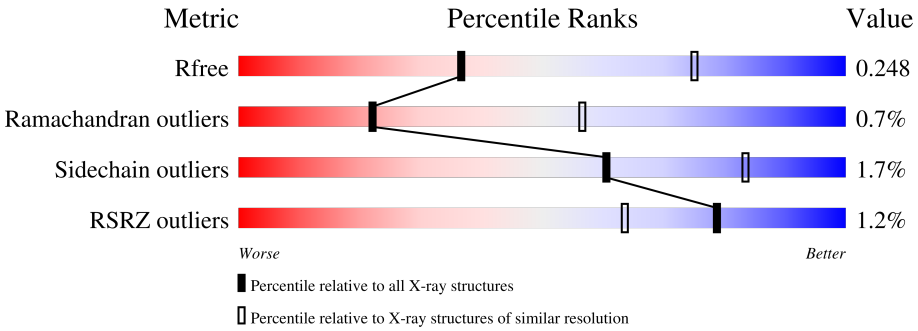
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	193	92% 6%
1	B	193	92% 6%
1	C	193	91% 7%
1	D	193	93% 6%
1	E	193	92% 6%
1	F	193	91% 7%

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Mol	Chain	Length	Quality of chain
1	G	193	90% 7%
1	H	193	90% 8%
1	I	193	92% 6%
1	J	193	91% 6%
1	K	193	90% 8%
1	L	193	92% 7%
1	M	193	91% 7%
1	N	193	92% 7%
1	O	193	91% 7%
1	P	193	91% 6%
1	Q	193	93% 6%
1	R	193	92% 6%
1	S	193	90% 6%
1	T	193	90% 7%
1	U	193	91% 7%
1	V	193	92% 6%
1	W	193	89% 10%
1	X	193	91% 7%
1	Y	193	91% 7%
1	Z	193	90% 7%
1	a	193	91% 8%
1	b	193	92% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZGV	I	302	-	-	-	X
4	ZGV	W	403	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 80695 atoms, of which 40496 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	182	Total	C	H	N	O	S	0	0	0
			2857	902	1434	244	265	12			
1	B	181	Total	C	H	N	O	S	0	0	0
			2830	892	1421	242	263	12			
1	C	179	Total	C	H	N	O	S	0	0	0
			2800	886	1404	237	261	12			
1	D	181	Total	C	H	N	O	S	0	0	0
			2843	898	1428	242	263	12			
1	E	182	Total	C	H	N	O	S	0	0	0
			2858	902	1435	244	265	12			
1	F	180	Total	C	H	N	O	S	0	0	0
			2808	888	1404	241	263	12			
1	G	179	Total	C	H	N	O	S	0	0	0
			2779	878	1391	237	261	12			
1	H	177	Total	C	H	N	O	S	0	0	0
			2776	876	1390	239	260	11			
1	I	181	Total	C	H	N	O	S	0	0	0
			2838	893	1426	243	264	12			
1	J	181	Total	C	H	N	O	S	0	0	0
			2824	893	1413	242	264	12			
1	K	178	Total	C	H	N	O	S	0	0	0
			2790	878	1401	239	260	12			
1	L	179	Total	C	H	N	O	S	0	0	0
			2806	883	1410	240	261	12			
1	M	179	Total	C	H	N	O	S	0	0	0
			2808	887	1408	240	261	12			
1	N	180	Total	C	H	N	O	S	0	0	0
			2825	892	1418	241	262	12			
1	O	179	Total	C	H	N	O	S	0	0	0
			2786	880	1397	236	261	12			
1	P	181	Total	C	H	N	O	S	0	0	0
			2846	898	1431	242	263	12			

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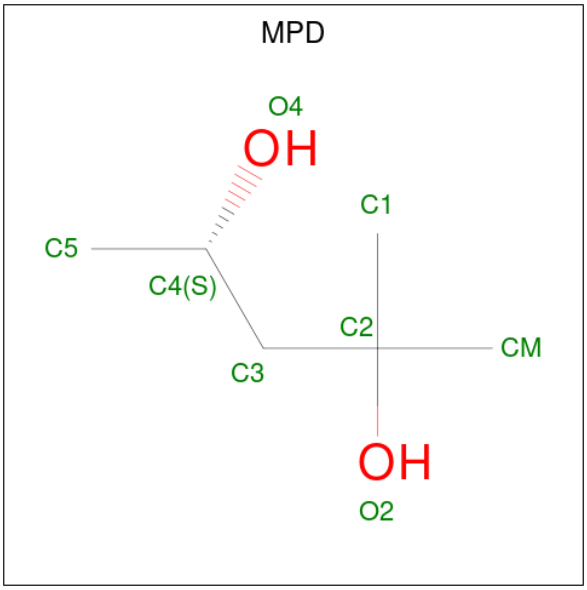
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	182	Total	C	H	N	O	S	0	0	0
			2859	903	1435	243	266	12			
1	R	181	Total	C	H	N	O	S	0	0	0
			2836	895	1423	242	264	12			
1	S	181	Total	C	H	N	O	S	0	0	0
			2840	896	1425	243	264	12			
1	T	179	Total	C	H	N	O	S	0	0	0
			2806	883	1410	240	261	12			
1	U	179	Total	C	H	N	O	S	0	0	0
			2809	884	1412	240	261	12			
1	V	181	Total	C	H	N	O	S	0	0	0
			2825	890	1416	243	264	12			
1	W	174	Total	C	H	N	O	S	0	0	0
			2718	856	1363	232	256	11			
1	X	179	Total	C	H	N	O	S	0	0	0
			2788	880	1398	237	261	12			
1	Y	179	Total	C	H	N	O	S	0	0	0
			2806	883	1410	240	261	12			
1	Z	179	Total	C	H	N	O	S	0	0	0
			2806	883	1410	240	261	12			
1	a	177	Total	C	H	N	O	S	0	0	0
			2766	872	1388	235	259	12			
1	b	180	Total	C	H	N	O	S	0	0	0
			2825	892	1418	241	262	12			

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	B	1	Total	C	H	O	0	0
			21	6	13	2		
2	B	1	Total	C	H	O	0	0
			22	6	14	2		
2	C	1	Total	C	H	O	0	0
			22	6	14	2		
2	D	1	Total	C	H	O	0	0
			22	6	14	2		
2	D	1	Total	C	H	O	0	0
			22	6	14	2		
2	D	1	Total	C	H	O	0	0
			22	6	14	2		
2	E	1	Total	C	H	O	0	0
			22	6	14	2		
2	F	1	Total	C	H	O	0	0
			22	6	14	2		
2	F	1	Total	C	H	O	0	0
			22	6	14	2		
2	F	1	Total	C	H	O	0	0
			22	6	14	2		
2	G	1	Total	C	H	O	0	0
			22	6	14	2		
2	H	1	Total	C	H	O	0	0
			22	6	14	2		
2	H	1	Total	C	H	O	0	0
			22	6	14	2		
2	I	1	Total	C	H	O	0	0
			22	6	14	2		
2	I	1	Total	C	H	O	0	0
			22	6	14	2		
2	J	1	Total	C	H	O	0	0
			22	6	14	2		
2	J	1	Total	C	H	O	0	0
			22	6	14	2		
2	K	1	Total	C	H	O	0	0
			22	6	14	2		
2	K	1	Total	C	H	O	0	0
			22	6	14	2		
2	L	1	Total	C	H	O	0	0
			22	6	14	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	H	O	0	0
			22	6	14	2		
2	N	1	Total	C	H	O	0	0
			22	6	14	2		
2	N	1	Total	C	H	O	0	0
			22	6	14	2		
2	O	1	Total	C	H	O	0	0
			22	6	14	2		
2	O	1	Total	C	H	O	0	0
			22	6	14	2		
2	P	1	Total	C	H	O	0	0
			22	6	14	2		
2	P	1	Total	C	H	O	0	0
			22	6	14	2		
2	Q	1	Total	C	H	O	0	0
			22	6	14	2		
2	Q	1	Total	C	H	O	0	0
			22	6	14	2		
2	Q	1	Total	C	H	O	0	0
			22	6	14	2		
2	R	1	Total	C	H	O	0	0
			22	6	14	2		
2	S	1	Total	C	H	O	0	0
			22	6	14	2		
2	S	1	Total	C	H	O	0	0
			22	6	14	2		
2	T	1	Total	C	H	O	0	0
			22	6	14	2		
2	T	1	Total	C	H	O	0	0
			22	6	14	2		
2	U	1	Total	C	H	O	0	0
			22	6	14	2		
2	V	1	Total	C	H	O	0	0
			22	6	14	2		
2	W	1	Total	C	H	O	0	0
			22	6	14	2		
2	W	1	Total	C	H	O	0	0
			22	6	14	2		
2	X	1	Total	C	H	O	0	0
			22	6	14	2		
2	Y	1	Total	C	H	O	0	0
			22	6	14	2		

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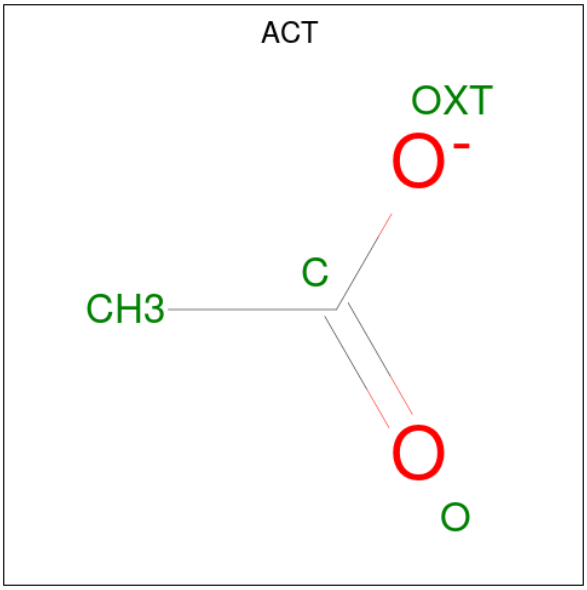
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Y	1	Total C H O 22 6 14 2	0	0
2	Z	1	Total C H O 22 6 14 2	0	0
2	Z	1	Total C H O 22 6 14 2	0	0
2	a	1	Total C H O 22 6 14 2	0	0
2	a	1	Total C H O 22 6 14 2	0	0
2	b	1	Total C H O 22 6 14 2	0	0
2	b	1	Total C H O 22 6 14 2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C H O 7 2 3 2	0	0
3	C	1	Total C H O 7 2 3 2	0	0
3	F	1	Total C H O 7 2 3 2	0	0

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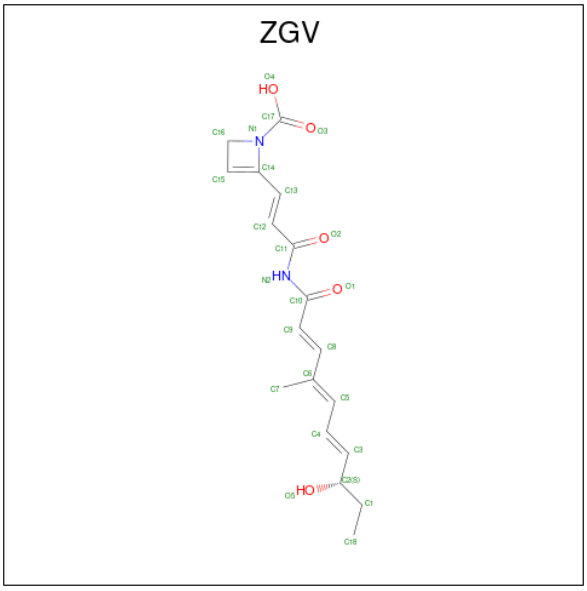
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	H	O	0	0
			7	2	3	2		
3	L	1	Total	C	H	O	0	0
			7	2	3	2		
3	P	1	Total	C	H	O	0	0
			7	2	3	2		
3	R	1	Total	C	H	O	0	0
			7	2	3	2		
3	X	1	Total	C	H	O	0	0
			7	2	3	2		
3	Z	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is 4-[(1E)-3-{[(2E,4E,6E,8S)-8-hydroxy-4-methyldeca-2,4,6-trienoyl]amino}-3-oxoprop-1-en-1-yl]azete-1(2H)-carboxylic acid (three-letter code: ZGV) (formula: $C_{18}H_{22}N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			45	18	21	2	4		
4	B	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	C	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	D	1	Total	C	H	N	O	0	0
			21	9	7	2	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	F	1	Total	C	H	N	O	0	0
			24	11	8	2	3		
4	G	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	H	1	Total	C	H	N	O	0	0
			24	11	8	2	3		
4	I	1	Total	C	H	N	O	0	0
			23	10	8	2	3		
4	J	1	Total	C	H	N	O	0	0
			24	11	8	2	3		
4	K	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	L	1	Total	C	H	N	O	0	0
			32	14	13	2	3		
4	M	1	Total	C	H	N	O	0	0
			30	13	12	2	3		
4	N	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	O	1	Total	C	H	N	O	0	0
			45	18	21	2	4		
4	P	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	Q	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	R	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	S	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	T	1	Total	C	H	N	O	0	0
			24	11	8	2	3		
4	U	1	Total	C	H	N	O	0	0
			21	9	7	2	3		
4	V	1	Total	C	H	N	O	0	0
			11	5	4	1	1		
4	W	1	Total	C	H	N	O	0	0
			45	18	21	2	4		
4	X	1	Total	C	H	N	O	0	0
			17	7	6	2	2		
4	Y	1	Total	C	H	N	O	0	0
			30	13	12	2	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	Z	1	Total	C	H	N	O	0	0
			11	5	4	1	1		
4	a	1	Total	C	H	N	O	0	0
			11	5	4	1	1		
4	b	1	Total	C	H	N	O	0	0
			17	7	6	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	4	Total	O	0	0
			4	4		
5	C	9	Total	O	0	0
			9	9		
5	D	4	Total	O	0	0
			4	4		
5	E	3	Total	O	0	0
			3	3		
5	F	3	Total	O	0	0
			3	3		
5	G	4	Total	O	0	0
			4	4		
5	H	5	Total	O	0	0
			5	5		
5	I	3	Total	O	0	0
			3	3		
5	J	5	Total	O	0	0
			5	5		
5	K	3	Total	O	0	0
			3	3		
5	L	4	Total	O	0	0
			4	4		
5	M	4	Total	O	0	0
			4	4		
5	N	3	Total	O	0	0
			3	3		
5	O	3	Total	O	0	0
			3	3		
5	P	2	Total	O	0	0
			2	2		

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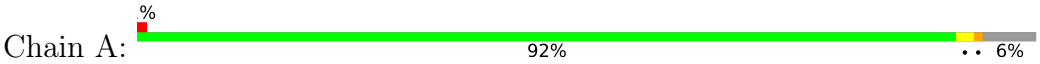
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Q	4	Total O 4 4	0	0
5	R	4	Total O 4 4	0	0
5	S	1	Total O 1 1	0	0
5	T	1	Total O 1 1	0	0
5	U	4	Total O 4 4	0	0
5	V	4	Total O 4 4	0	0
5	W	3	Total O 3 3	0	0
5	X	4	Total O 4 4	0	0
5	Y	4	Total O 4 4	0	0
5	Z	4	Total O 4 4	0	0
5	a	2	Total O 2 2	0	0
5	b	5	Total O 5 5	0	0

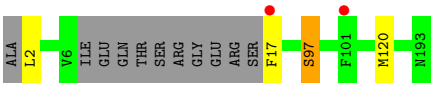
3 Residue-property plots (i)

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: ATP-dependent Clp protease proteolytic subunit

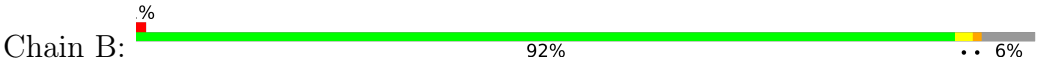
Chain A:





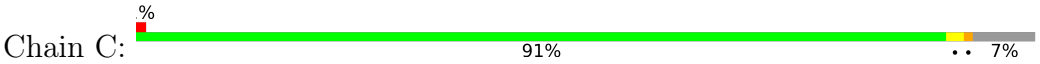
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

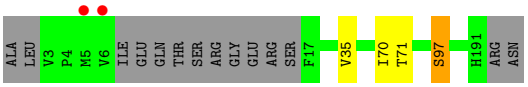
Chain B:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

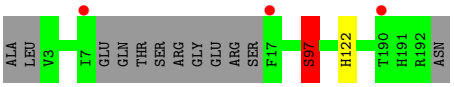
Chain C:





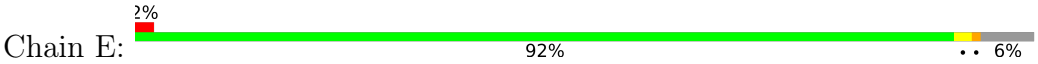
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



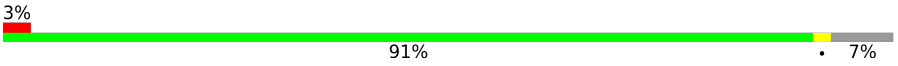
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

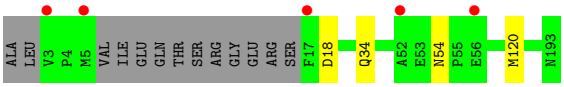
Chain E:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

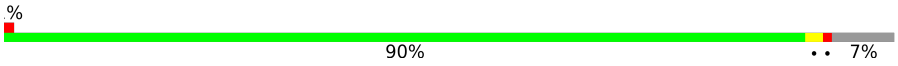
Chain F:

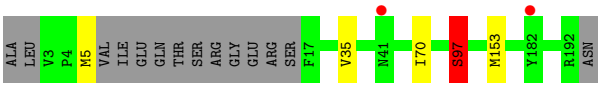




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

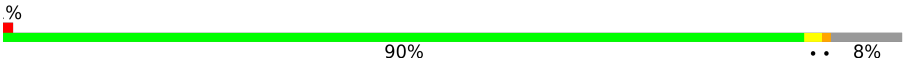
Chain G:





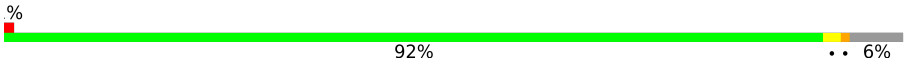
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

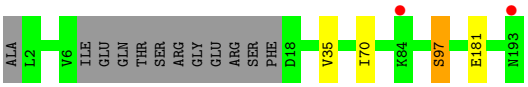
Chain H:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

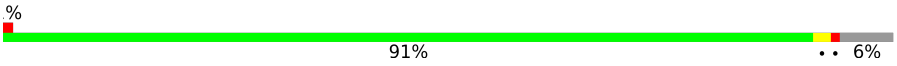
Chain I:

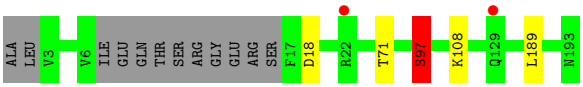




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

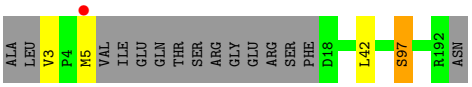
Chain J:





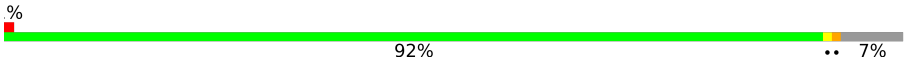
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

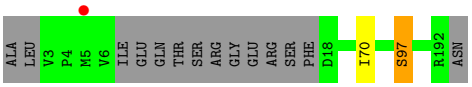
Chain K:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

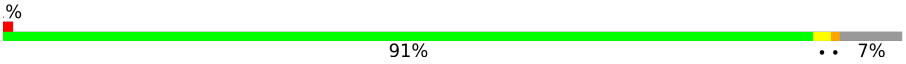
Chain L:

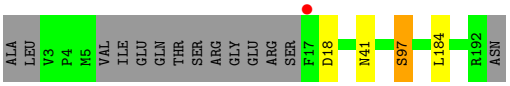




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

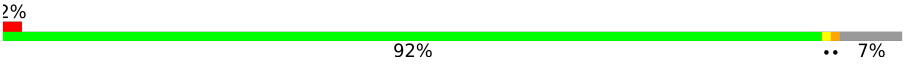
Chain M:





• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:

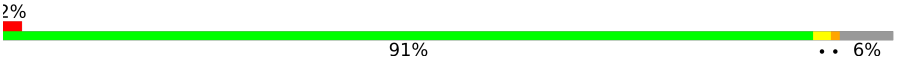


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain O:

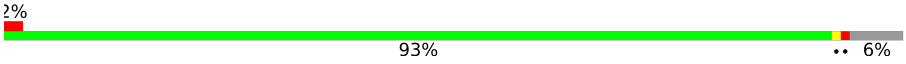
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

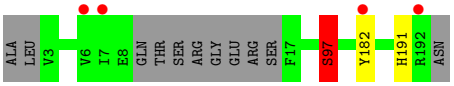
Chain P:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

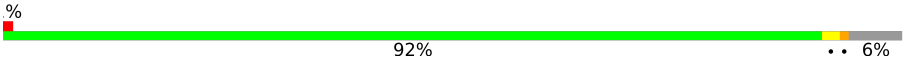
Chain Q:

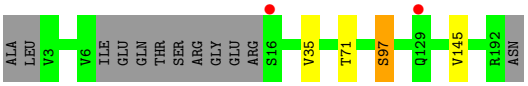




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

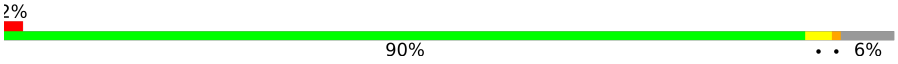
Chain R:

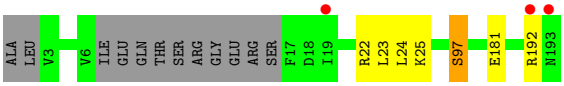




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

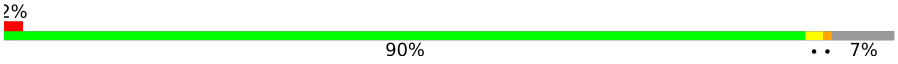
Chain S:

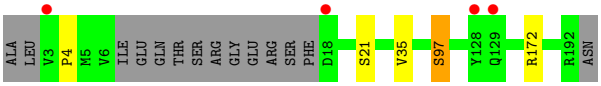




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

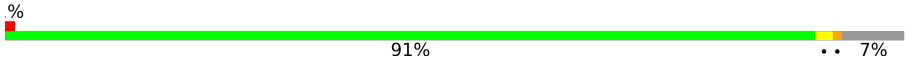
Chain T:

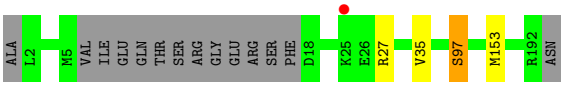




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

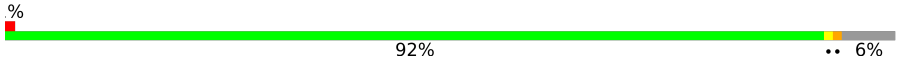
Chain U:

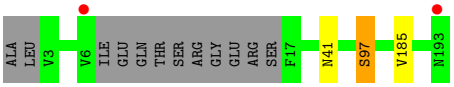




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

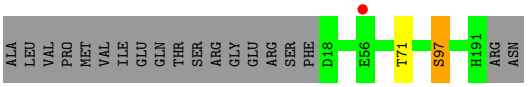
Chain V:





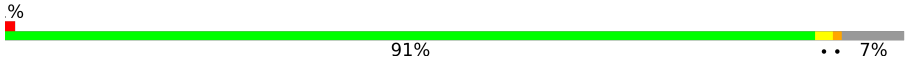
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

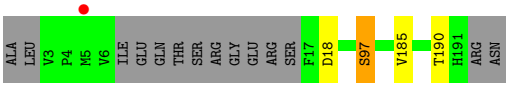
Chain W:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

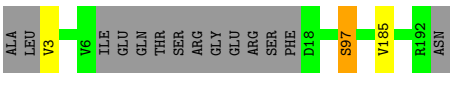
Chain X:





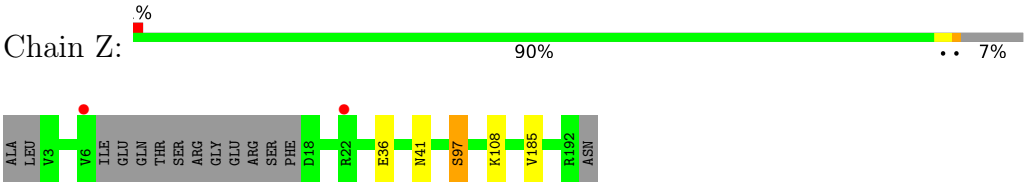
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Y:



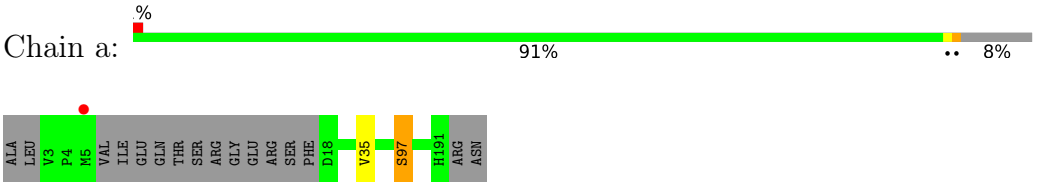
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain Z:



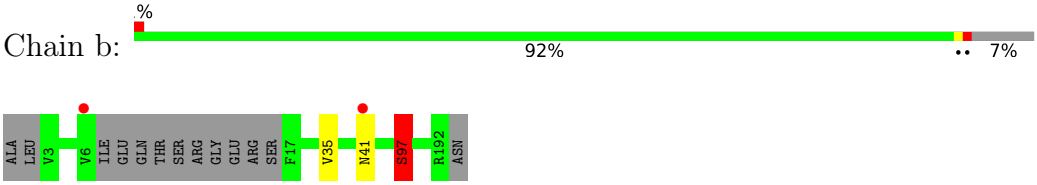
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain a:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.33Å 190.23Å 169.88Å 90.00° 93.61° 90.00°	Depositor
Resolution (Å)	45.41 – 2.95 47.07 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.41-2.95) 99.8 (47.07-2.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.211 , 0.248 0.210 , 0.248	Depositor DCC
R_{free} test set	6043 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	80695	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACT, MPD, ZGV

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	0.32	0/1446	0.54	1/1949 (0.1%)
1	B	0.30	0/1431	0.53	1/1929 (0.1%)
1	C	0.28	0/1419	0.53	1/1913 (0.1%)
1	D	0.30	0/1438	0.53	1/1938 (0.1%)
1	E	0.33	0/1446	0.56	1/1949 (0.1%)
1	F	0.52	0/1427	0.56	0/1924
1	G	0.29	0/1410	0.54	1/1901 (0.1%)
1	H	0.32	0/1409	0.55	1/1899 (0.1%)
1	I	0.28	0/1434	0.52	1/1933 (0.1%)
1	J	0.34	0/1434	0.55	1/1934 (0.1%)
1	K	0.33	0/1411	0.53	1/1901 (0.1%)
1	L	0.28	0/1418	0.54	1/1911 (0.1%)
1	M	0.28	0/1423	0.54	1/1917 (0.1%)
1	N	0.31	0/1430	0.52	1/1927 (0.1%)
1	O	0.29	0/1411	0.54	1/1904 (0.1%)
1	P	0.28	0/1438	0.57	1/1938 (0.1%)
1	Q	0.35	0/1447	0.55	1/1950 (0.1%)
1	R	0.28	0/1436	0.53	1/1935 (0.1%)
1	S	0.52	0/1438	0.60	0/1938
1	T	0.36	0/1418	0.59	2/1911 (0.1%)
1	U	0.38	0/1419	0.55	1/1912 (0.1%)
1	V	0.33	0/1431	0.54	1/1929 (0.1%)
1	W	0.32	0/1375	0.57	1/1852 (0.1%)
1	X	0.33	0/1412	0.54	1/1904 (0.1%)
1	Y	0.28	0/1418	0.54	1/1911 (0.1%)
1	Z	0.31	0/1418	0.57	2/1911 (0.1%)
1	a	0.34	0/1400	0.53	1/1887 (0.1%)
1	b	0.29	0/1430	0.53	1/1927 (0.1%)
All	All	0.33	0/39867	0.55	28/53734 (0.1%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	97	SER	N-CA-CB	-8.20	98.20	110.50
1	W	97	SER	N-CA-CB	-7.57	99.15	110.50
1	O	97	SER	N-CA-CB	-7.19	99.72	110.50
1	B	97	SER	N-CA-CB	-7.13	99.80	110.50
1	L	97	SER	N-CA-CB	-6.89	100.17	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/193 (92%)	172 (97%)	5 (3%)	1 (1%)	25	60
1	B	177/193 (92%)	173 (98%)	3 (2%)	1 (1%)	25	60
1	C	175/193 (91%)	170 (97%)	4 (2%)	1 (1%)	25	60
1	D	177/193 (92%)	170 (96%)	6 (3%)	1 (1%)	25	60
1	E	178/193 (92%)	174 (98%)	3 (2%)	1 (1%)	25	60
1	F	176/193 (91%)	170 (97%)	5 (3%)	1 (1%)	25	60
1	G	175/193 (91%)	169 (97%)	5 (3%)	1 (1%)	25	60
1	H	175/193 (91%)	170 (97%)	3 (2%)	2 (1%)	14	46
1	I	177/193 (92%)	172 (97%)	4 (2%)	1 (1%)	25	60
1	J	177/193 (92%)	170 (96%)	5 (3%)	2 (1%)	14	46
1	K	174/193 (90%)	169 (97%)	4 (2%)	1 (1%)	25	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	175/193 (91%)	171 (98%)	3 (2%)	1 (1%)	25	60
1	M	175/193 (91%)	170 (97%)	3 (2%)	2 (1%)	14	46
1	N	176/193 (91%)	169 (96%)	6 (3%)	1 (1%)	25	60
1	O	175/193 (91%)	171 (98%)	3 (2%)	1 (1%)	25	60
1	P	177/193 (92%)	170 (96%)	4 (2%)	3 (2%)	9	34
1	Q	178/193 (92%)	173 (97%)	4 (2%)	1 (1%)	25	60
1	R	177/193 (92%)	173 (98%)	3 (2%)	1 (1%)	25	60
1	S	177/193 (92%)	171 (97%)	4 (2%)	2 (1%)	14	46
1	T	175/193 (91%)	169 (97%)	4 (2%)	2 (1%)	14	46
1	U	175/193 (91%)	169 (97%)	5 (3%)	1 (1%)	25	60
1	V	177/193 (92%)	171 (97%)	5 (3%)	1 (1%)	25	60
1	W	172/193 (89%)	167 (97%)	4 (2%)	1 (1%)	25	60
1	X	175/193 (91%)	169 (97%)	4 (2%)	2 (1%)	14	46
1	Y	175/193 (91%)	171 (98%)	3 (2%)	1 (1%)	25	60
1	Z	175/193 (91%)	168 (96%)	6 (3%)	1 (1%)	25	60
1	a	173/193 (90%)	169 (98%)	3 (2%)	1 (1%)	25	60
1	b	176/193 (91%)	169 (96%)	6 (3%)	1 (1%)	25	60
All	All	4922/5404 (91%)	4769 (97%)	117 (2%)	36 (1%)	22	56

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	SER
1	G	97	SER
1	H	97	SER
1	I	97	SER
1	J	97	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/163 (94%)	151 (98%)	3 (2%)	57	81
1	B	152/163 (93%)	149 (98%)	3 (2%)	55	80
1	C	151/163 (93%)	148 (98%)	3 (2%)	55	80
1	D	153/163 (94%)	151 (99%)	2 (1%)	69	87
1	E	154/163 (94%)	150 (97%)	4 (3%)	46	75
1	F	151/163 (93%)	148 (98%)	3 (2%)	55	80
1	G	149/163 (91%)	144 (97%)	5 (3%)	37	69
1	H	149/163 (91%)	147 (99%)	2 (1%)	69	87
1	I	153/163 (94%)	150 (98%)	3 (2%)	55	80
1	J	152/163 (93%)	148 (97%)	4 (3%)	46	75
1	K	150/163 (92%)	147 (98%)	3 (2%)	55	80
1	L	151/163 (93%)	150 (99%)	1 (1%)	84	93
1	M	151/163 (93%)	149 (99%)	2 (1%)	69	87
1	N	152/163 (93%)	151 (99%)	1 (1%)	84	93
1	O	150/163 (92%)	148 (99%)	2 (1%)	69	87
1	P	153/163 (94%)	151 (99%)	2 (1%)	69	87
1	Q	154/163 (94%)	151 (98%)	3 (2%)	57	81
1	R	153/163 (94%)	150 (98%)	3 (2%)	55	80
1	S	153/163 (94%)	147 (96%)	6 (4%)	32	65
1	T	151/163 (93%)	149 (99%)	2 (1%)	69	87
1	U	151/163 (93%)	148 (98%)	3 (2%)	55	80
1	V	152/163 (93%)	150 (99%)	2 (1%)	69	87
1	W	145/163 (89%)	144 (99%)	1 (1%)	84	93
1	X	150/163 (92%)	148 (99%)	2 (1%)	69	87
1	Y	151/163 (93%)	149 (99%)	2 (1%)	69	87
1	Z	151/163 (93%)	148 (98%)	3 (2%)	55	80
1	a	149/163 (91%)	148 (99%)	1 (1%)	84	93
1	b	152/163 (93%)	149 (98%)	3 (2%)	55	80
All	All	4237/4564 (93%)	4163 (98%)	74 (2%)	60	83

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	27	ARG
1	b	35	VAL
1	U	153	MET
1	Y	3	VAL
1	H	70	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	R	41	ASN
1	W	41	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

88 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ZGV	S	203	1	11,14,25	0.84	1 (9%)	9,18,32	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACT	Z	303	-	1,3,3	5.19	1 (100%)	0,3,3	-	-
2	MPD	Q	301	-	7,7,7	0.94	1 (14%)	9,10,10	0.79	0
2	MPD	I	303	-	7,7,7	0.29	0	9,10,10	0.34	0
3	ACT	X	202	-	1,3,3	4.74	1 (100%)	0,3,3	-	-
2	MPD	O	302	-	7,7,7	0.30	0	9,10,10	0.31	0
2	MPD	I	301	-	7,7,7	0.26	0	9,10,10	0.32	0
2	MPD	B	301	-	7,7,7	0.98	0	9,10,10	0.79	0
3	ACT	P	204	-	1,3,3	4.30	1 (100%)	0,3,3	-	-
2	MPD	O	301	-	7,7,7	0.28	0	9,10,10	0.30	0
2	MPD	C	301	-	7,7,7	0.95	1 (14%)	9,10,10	1.01	0
4	ZGV	O	303	1	21,24,25	0.68	1 (4%)	22,30,32	0.53	0
4	ZGV	X	203	1	8,11,25	1.21	1 (12%)	6,14,32	0.68	0
2	MPD	V	301	-	7,7,7	0.81	0	9,10,10	0.75	0
2	MPD	A	301	-	7,7,7	0.29	0	9,10,10	0.29	0
2	MPD	X	201	-	7,7,7	0.28	0	9,10,10	0.40	0
4	ZGV	J	302	1	13,16,25	0.84	1 (7%)	12,20,32	1.51	1 (8%)
2	MPD	b	302	-	7,7,7	0.27	0	9,10,10	0.26	0
4	ZGV	P	203	1	11,14,25	0.73	0	9,18,32	0.55	0
2	MPD	P	202	-	7,7,7	0.27	0	9,10,10	0.44	0
4	ZGV	R	303	1	11,14,25	0.80	1 (9%)	9,18,32	0.38	0
4	ZGV	I	302	1	12,15,25	0.85	1 (8%)	11,19,32	1.33	1 (9%)
2	MPD	K	303	-	7,7,7	0.27	0	9,10,10	0.21	0
3	ACT	F	403	-	1,3,3	4.64	1 (100%)	0,3,3	-	-
2	MPD	Z	302	-	7,7,7	0.30	0	9,10,10	0.47	0
2	MPD	N	302	-	7,7,7	0.24	0	9,10,10	0.33	0
2	MPD	Q	304	-	7,7,7	0.28	0	9,10,10	0.37	0
3	ACT	B	303	-	1,3,3	4.69	1 (100%)	0,3,3	-	-
2	MPD	D	302	-	7,7,7	0.27	0	9,10,10	0.38	0
2	MPD	L	502	-	7,7,7	0.26	0	9,10,10	0.26	0
2	MPD	Y	303	-	7,7,7	0.27	0	9,10,10	0.26	0
2	MPD	N	301	-	7,7,7	0.27	0	9,10,10	0.28	0
4	ZGV	U	302	1	11,14,25	1.00	1 (9%)	9,18,32	0.35	0
4	ZGV	W	403	1	21,24,25	0.52	1 (4%)	22,30,32	0.43	0
2	MPD	F	404	-	7,7,7	0.32	0	9,10,10	0.59	0
2	MPD	G	301	-	7,7,7	0.20	0	9,10,10	0.32	0
2	MPD	E	301	-	7,7,7	0.26	0	9,10,10	0.65	0
2	MPD	H	303	-	7,7,7	0.28	0	9,10,10	0.30	0
4	ZGV	G	303	1	11,14,25	0.87	1 (9%)	9,18,32	0.31	0
4	ZGV	a	302	1	2,7,25	1.71	1 (50%)	1,9,32	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ZGV	A	304	1	21,24,25	0.38	0	22,30,32	0.49	0
2	MPD	T	202	-	7,7,7	0.30	0	9,10,10	0.54	0
3	ACT	L	501	-	1,3,3	4.71	1 (100%)	0,3,3	-	-
4	ZGV	K	302	1	11,14,25	1.05	1 (9%)	9,18,32	0.29	0
4	ZGV	Y	302	1	15,18,25	0.66	1 (6%)	14,23,32	0.51	0
2	MPD	S	201	-	7,7,7	0.28	0	9,10,10	0.26	0
2	MPD	U	301	-	7,7,7	0.18	0	9,10,10	0.65	0
2	MPD	a	301	-	7,7,7	0.28	0	9,10,10	0.60	0
2	MPD	Q	302	-	7,7,7	0.29	0	9,10,10	0.28	0
2	MPD	J	301	-	7,7,7	0.23	0	9,10,10	0.29	0
2	MPD	R	301	-	7,7,7	0.93	0	9,10,10	0.78	0
4	ZGV	B	304	1	11,14,25	0.89	1 (9%)	9,18,32	0.38	0
2	MPD	b	301	-	7,7,7	0.28	0	9,10,10	0.37	0
2	MPD	D	301	-	7,7,7	0.20	0	9,10,10	0.55	0
4	ZGV	Q	303	1	11,14,25	0.94	1 (9%)	9,18,32	0.29	0
2	MPD	T	201	-	7,7,7	0.25	0	9,10,10	0.27	0
4	ZGV	H	302	1	13,16,25	0.68	0	12,20,32	2.14	2 (16%)
4	ZGV	D	304	1	11,14,25	0.96	1 (9%)	9,18,32	0.32	0
2	MPD	M	301	-	7,7,7	0.32	0	9,10,10	0.27	0
3	ACT	C	303	-	1,3,3	4.14	1 (100%)	0,3,3	-	-
4	ZGV	T	203	1	13,16,25	0.96	1 (7%)	12,20,32	1.25	1 (8%)
4	ZGV	C	302	1	11,14,25	0.95	1 (9%)	9,18,32	0.31	0
4	ZGV	b	303	1	8,11,25	1.07	1 (12%)	6,14,32	0.72	0
2	MPD	a	303	-	7,7,7	0.22	0	9,10,10	0.38	0
2	MPD	Y	301	-	7,7,7	0.28	0	9,10,10	0.34	0
2	MPD	P	201	-	7,7,7	0.21	0	9,10,10	0.41	0
2	MPD	J	303	-	7,7,7	0.27	0	9,10,10	0.29	0
4	ZGV	E	302	1	11,14,25	0.95	1 (9%)	9,18,32	0.30	0
4	ZGV	M	302	1	15,18,25	0.75	1 (6%)	14,23,32	0.29	0
2	MPD	S	202	-	7,7,7	0.26	0	9,10,10	0.34	0
3	ACT	A	303	-	1,3,3	5.02	1 (100%)	0,3,3	-	-
4	ZGV	L	503	1	16,19,25	1.08	2 (12%)	16,24,32	0.68	0
3	ACT	R	302	-	1,3,3	4.41	1 (100%)	0,3,3	-	-
2	MPD	F	401	-	7,7,7	0.25	0	9,10,10	0.44	0
2	MPD	F	402	-	7,7,7	1.13	0	9,10,10	0.72	0
4	ZGV	N	303	1	11,14,25	0.97	1 (9%)	9,18,32	0.28	0
2	MPD	H	301	-	7,7,7	0.21	0	9,10,10	0.54	0
2	MPD	A	302	-	7,7,7	0.30	0	9,10,10	0.27	0
2	MPD	D	303	-	7,7,7	0.30	0	9,10,10	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ZGV	F	405	1	13,16,25	0.71	1 (7%)	12,20,32	1.43	1 (8%)
2	MPD	B	302	-	7,7,7	0.28	0	9,10,10	0.21	0
2	MPD	W	401	-	7,7,7	0.19	0	9,10,10	0.60	0
2	MPD	Z	301	-	7,7,7	0.30	0	9,10,10	0.24	0
2	MPD	K	301	-	7,7,7	0.27	0	9,10,10	0.47	0
4	ZGV	V	302	1	2,7,25	1.62	1 (50%)	1,9,32	0.16	0
4	ZGV	Z	304	1	2,7,25	1.69	1 (50%)	1,9,32	0.08	0
2	MPD	W	402	-	7,7,7	0.23	0	9,10,10	0.31	0
3	ACT	G	302	-	1,3,3	5.30	1 (100%)	0,3,3	-	-

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
4	ZGV	S	203	1	-	2/7/20/35	0/1/1/1
2	MPD	Q	301	-	-	2/5/5/5	-
2	MPD	I	303	-	-	0/5/5/5	-
2	MPD	O	302	-	-	0/5/5/5	-
2	MPD	I	301	-	-	1/5/5/5	-
2	MPD	B	301	-	-	2/5/5/5	-
2	MPD	O	301	-	-	1/5/5/5	-
2	MPD	C	301	-	-	1/5/5/5	-
4	ZGV	O	303	1	-	6/20/33/35	0/1/1/1
4	ZGV	X	203	1	-	0/3/16/35	0/1/1/1
2	MPD	V	301	-	-	1/5/5/5	-
2	MPD	A	301	-	-	0/5/5/5	-
2	MPD	X	201	-	-	3/5/5/5	-
4	ZGV	J	302	1	-	0/10/23/35	0/1/1/1
2	MPD	b	302	-	-	1/5/5/5	-
4	ZGV	P	203	1	-	2/7/20/35	0/1/1/1
2	MPD	P	202	-	-	1/5/5/5	-
4	ZGV	R	303	1	-	0/7/20/35	0/1/1/1
4	ZGV	I	302	1	-	2/9/22/35	0/1/1/1
2	MPD	K	303	-	-	4/5/5/5	-
2	MPD	Z	302	-	-	0/5/5/5	-
2	MPD	N	302	-	-	2/5/5/5	-
2	MPD	Q	304	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MPD	D	302	-	-	1/5/5/5	-
2	MPD	L	502	-	-	0/5/5/5	-
2	MPD	Y	303	-	-	3/5/5/5	-
2	MPD	N	301	-	-	5/5/5/5	-
4	ZGV	U	302	1	-	2/7/20/35	0/1/1/1
4	ZGV	W	403	1	-	4/20/33/35	0/1/1/1
2	MPD	F	404	-	-	3/5/5/5	-
2	MPD	G	301	-	-	0/5/5/5	-
2	MPD	E	301	-	-	2/5/5/5	-
2	MPD	H	303	-	-	1/5/5/5	-
4	ZGV	G	303	1	-	2/7/20/35	0/1/1/1
4	ZGV	a	302	1	-	0/0/11/35	0/1/1/1
4	ZGV	A	304	1	-	6/20/33/35	0/1/1/1
2	MPD	T	202	-	-	2/5/5/5	-
4	ZGV	K	302	1	-	0/7/20/35	0/1/1/1
4	ZGV	Y	302	1	-	2/12/25/35	0/1/1/1
2	MPD	S	201	-	-	1/5/5/5	-
2	MPD	U	301	-	-	4/5/5/5	-
2	MPD	a	301	-	-	4/5/5/5	-
2	MPD	Q	302	-	-	0/5/5/5	-
2	MPD	J	301	-	-	0/5/5/5	-
2	MPD	R	301	-	-	0/5/5/5	-
4	ZGV	B	304	1	-	2/7/20/35	0/1/1/1
2	MPD	b	301	-	-	4/5/5/5	-
2	MPD	D	301	-	-	1/5/5/5	-
4	ZGV	Q	303	1	-	2/7/20/35	0/1/1/1
2	MPD	T	201	-	-	2/5/5/5	-
4	ZGV	H	302	1	-	2/10/23/35	0/1/1/1
4	ZGV	D	304	1	-	0/7/20/35	0/1/1/1
2	MPD	M	301	-	-	2/5/5/5	-
4	ZGV	T	203	1	-	0/10/23/35	0/1/1/1
4	ZGV	C	302	1	-	2/7/20/35	0/1/1/1
4	ZGV	b	303	1	-	0/3/16/35	0/1/1/1
2	MPD	a	303	-	-	2/5/5/5	-
2	MPD	Y	301	-	-	2/5/5/5	-
2	MPD	P	201	-	-	5/5/5/5	-
2	MPD	J	303	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ZGV	E	302	1	-	2/7/20/35	0/1/1/1
4	ZGV	M	302	1	-	0/12/25/35	0/1/1/1
2	MPD	S	202	-	-	0/5/5/5	-
4	ZGV	L	503	1	-	2/14/27/35	0/1/1/1
2	MPD	F	401	-	-	3/5/5/5	-
2	MPD	F	402	-	-	2/5/5/5	-
4	ZGV	N	303	1	-	0/7/20/35	0/1/1/1
2	MPD	H	301	-	-	3/5/5/5	-
2	MPD	A	302	-	-	1/5/5/5	-
2	MPD	D	303	-	-	1/5/5/5	-
4	ZGV	F	405	1	-	0/10/23/35	0/1/1/1
2	MPD	B	302	-	-	0/5/5/5	-
2	MPD	W	401	-	-	5/5/5/5	-
2	MPD	Z	301	-	-	1/5/5/5	-
2	MPD	K	301	-	-	1/5/5/5	-
4	ZGV	V	302	1	-	0/0/11/35	0/1/1/1
4	ZGV	Z	304	1	-	0/0/11/35	0/1/1/1
2	MPD	W	402	-	-	5/5/5/5	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	ACT	CH3-C	5.30	1.55	1.48
3	Z	303	ACT	CH3-C	5.19	1.55	1.48
3	A	303	ACT	CH3-C	5.02	1.55	1.48
3	X	202	ACT	CH3-C	4.74	1.54	1.48
3	L	501	ACT	CH3-C	4.71	1.54	1.48

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	302	ZGV	C8-C9-C10	6.51	128.73	120.88
4	J	302	ZGV	C8-C9-C10	5.11	127.05	120.88
4	F	405	ZGV	C8-C9-C10	4.80	126.67	120.88
4	I	302	ZGV	C8-C9-C10	4.11	126.97	122.27
4	T	203	ZGV	C8-C9-C10	4.04	125.75	120.88

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

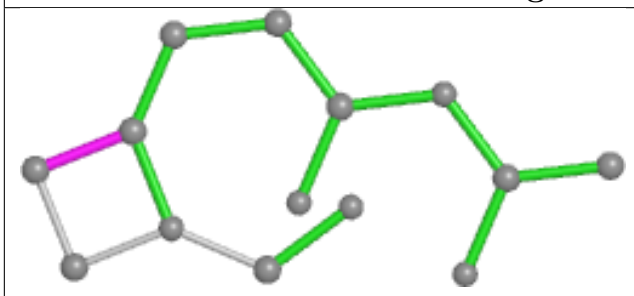
Mol	Chain	Res	Type	Atoms
2	B	301	MPD	C2-C3-C4-C5
2	F	404	MPD	C1-C2-C3-C4
2	F	404	MPD	O2-C2-C3-C4
2	H	301	MPD	C2-C3-C4-O4
2	K	301	MPD	C2-C3-C4-O4

There are no ring outliers.

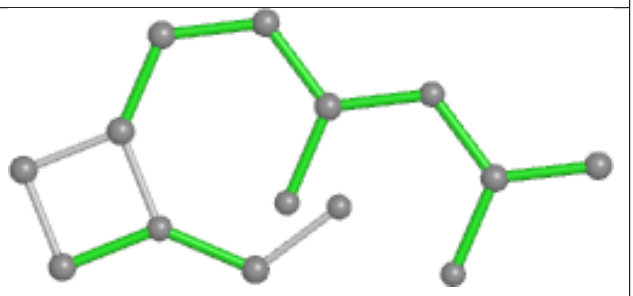
No monomer is involved in short contacts.

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 then 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.

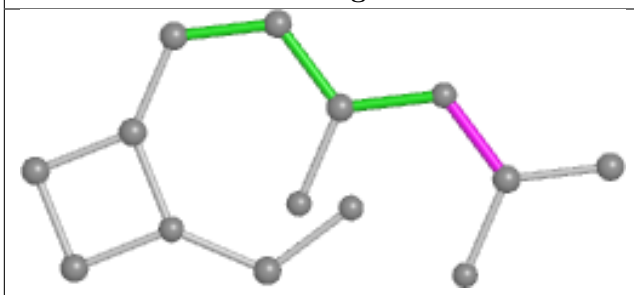
Ligand ZGV S 203



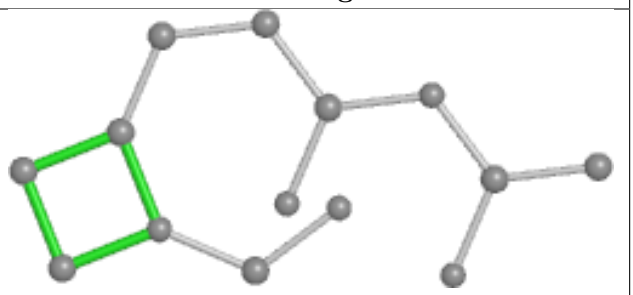
Bond lengths



Bond angles

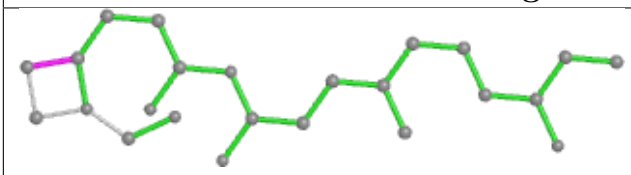


Torsions



Rings

Ligand ZGV O 303



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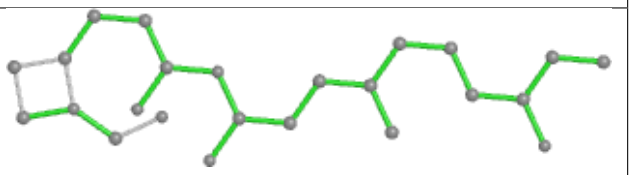
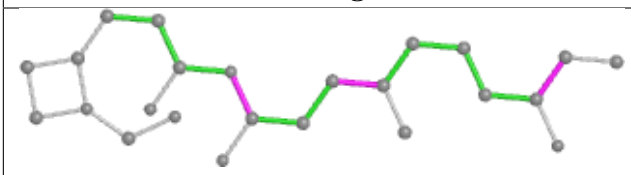
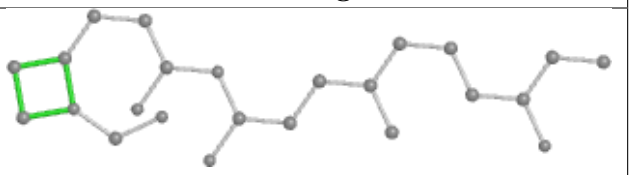


Bond angles

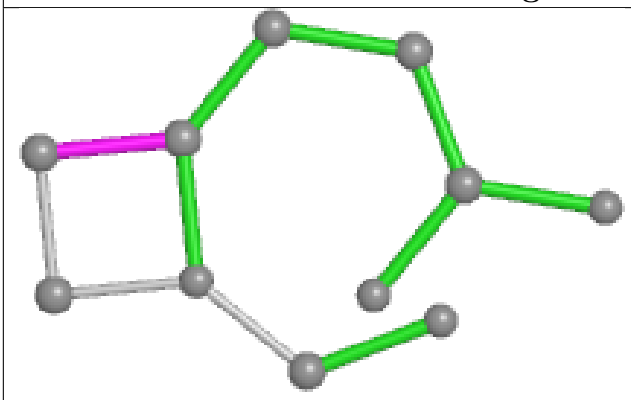


Torsions



Rings

Ligand ZGV X 203



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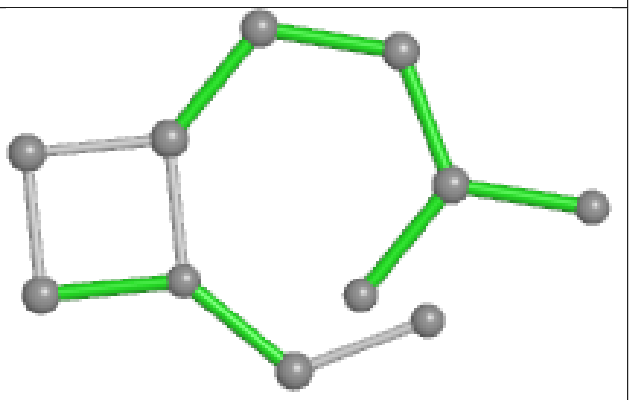

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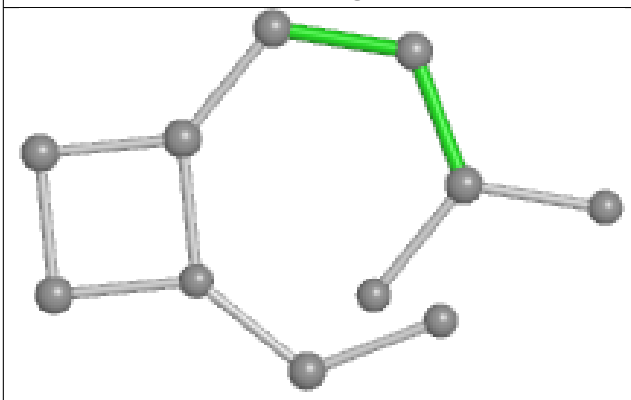

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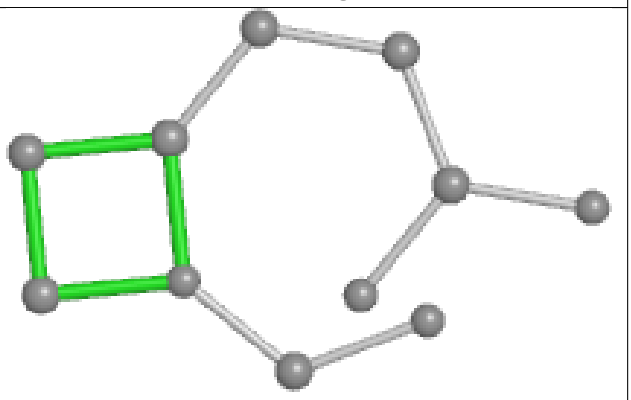
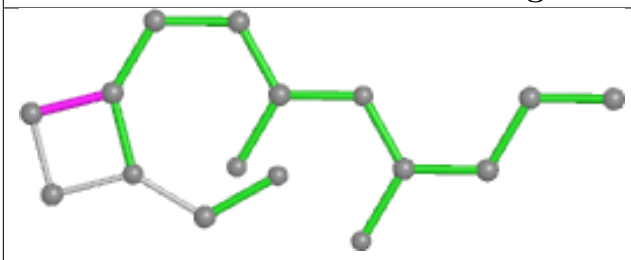


Rings

Ligand ZGV J 302



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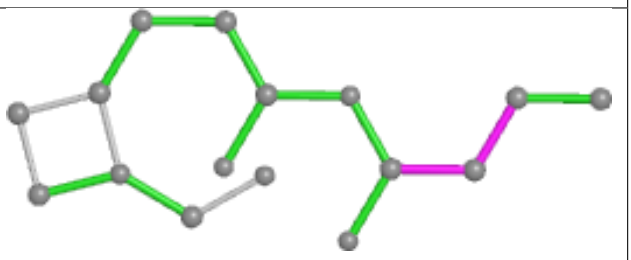

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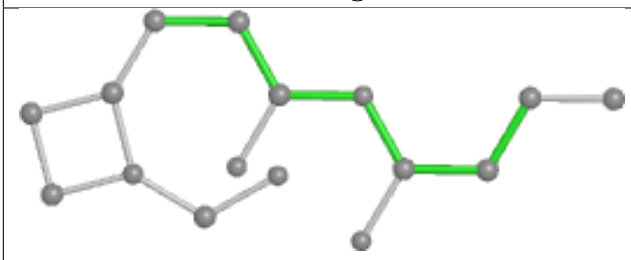

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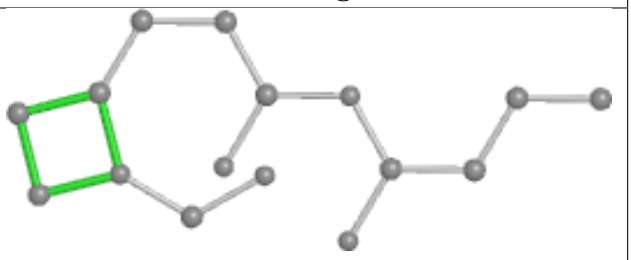
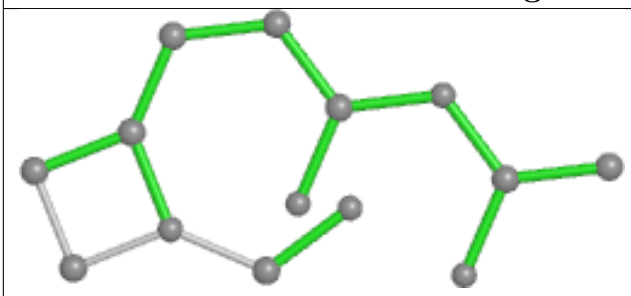


Rings

Ligand ZGV P 203



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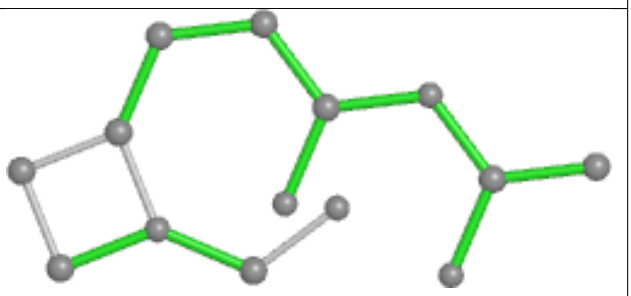

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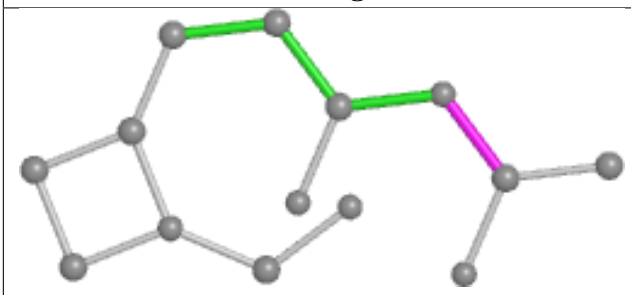

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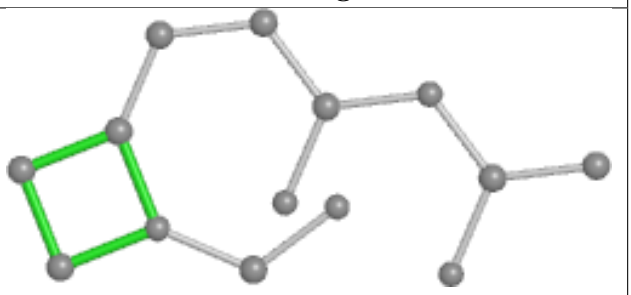
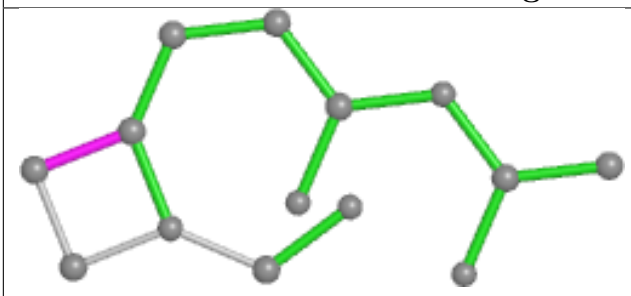


Rings

Ligand ZGV R 303



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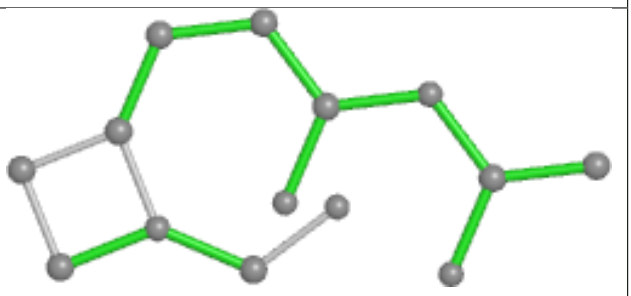

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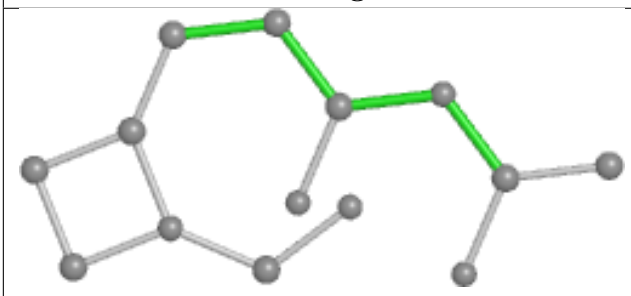

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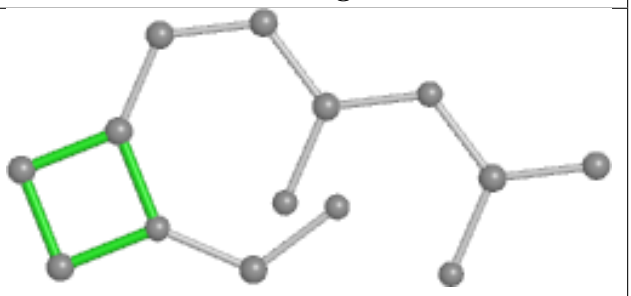
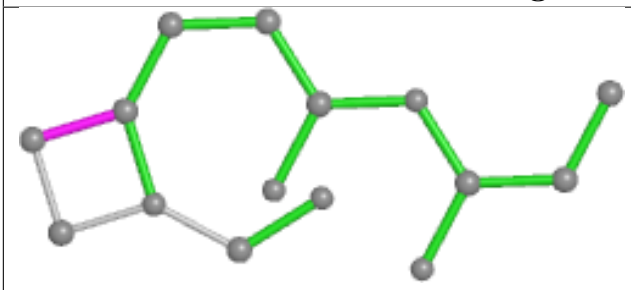


Rings

Ligand ZGV I 302



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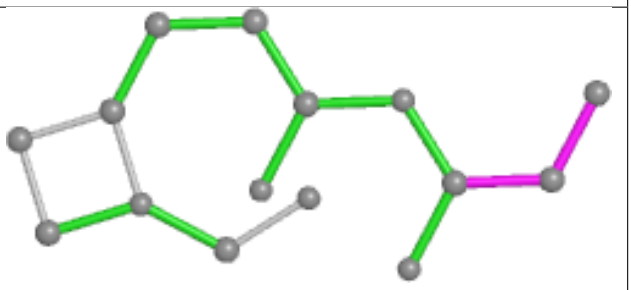

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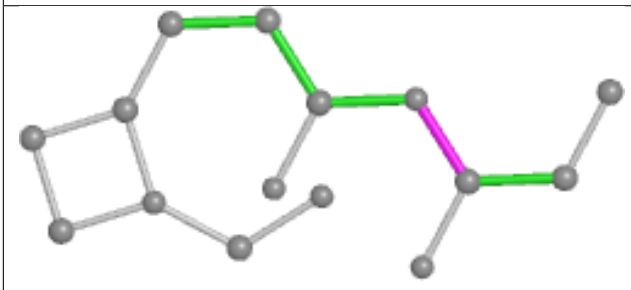

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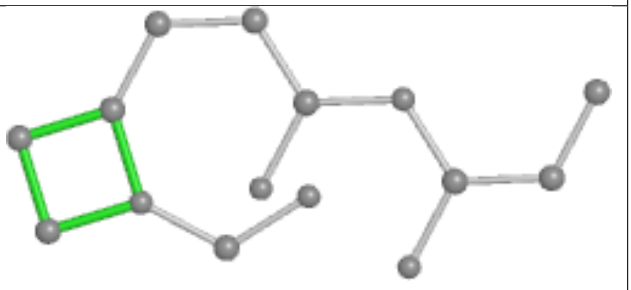
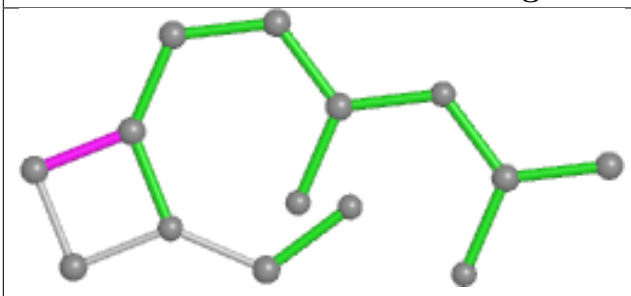


Rings

Ligand ZGV U 302



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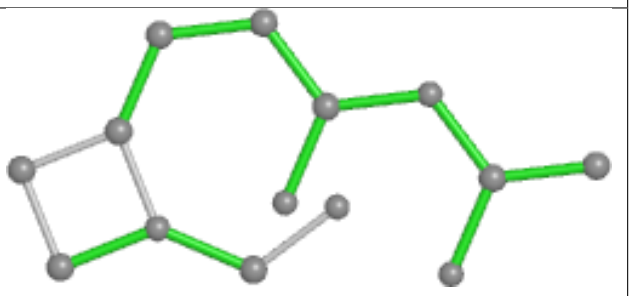

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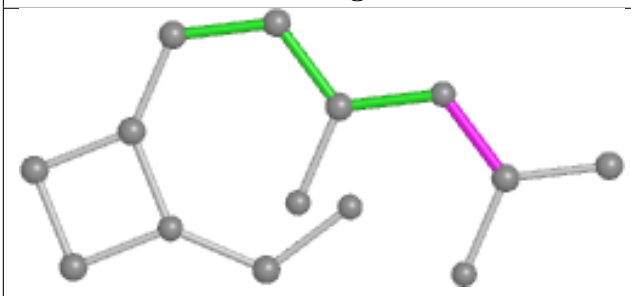

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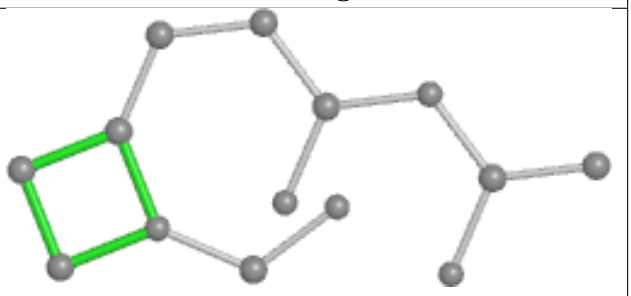
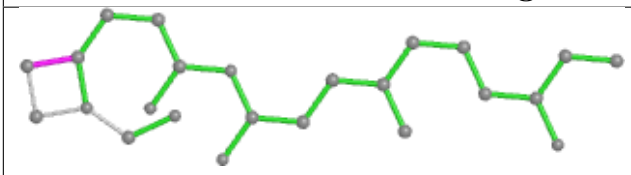


Rings

Ligand ZGV W 403



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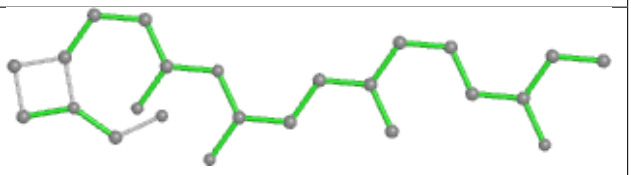
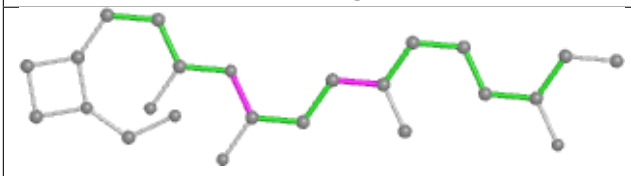


Bond angles



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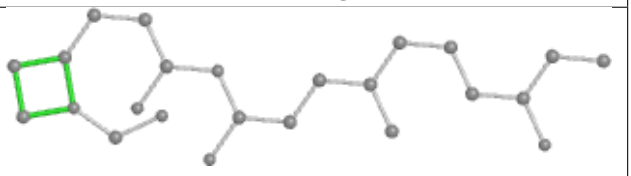
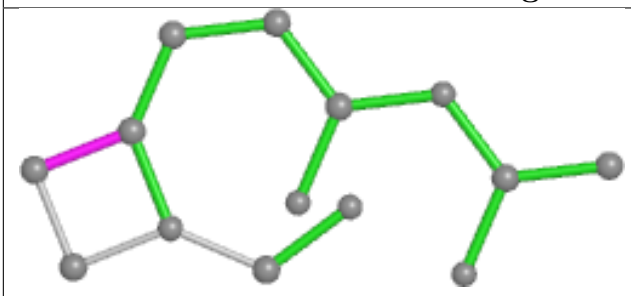


Rings

Ligand ZGV G 303



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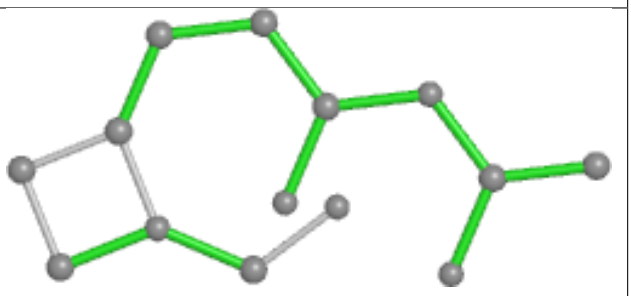
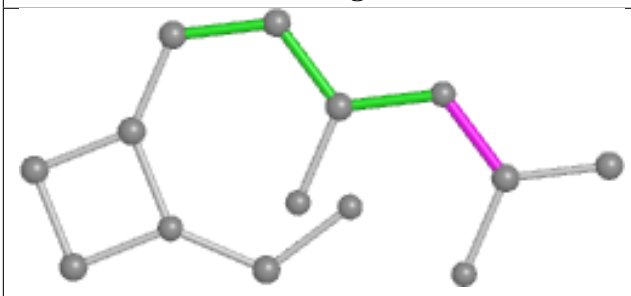


Bond angles



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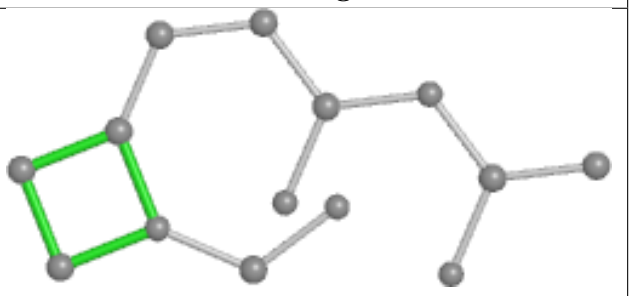
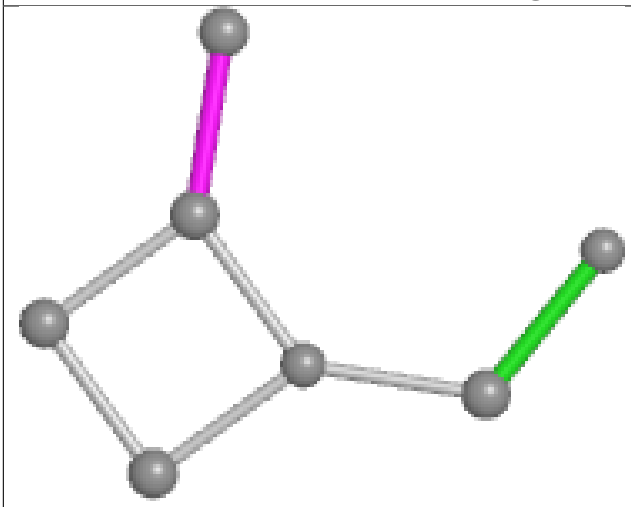


Rings

Ligand ZGV a 302



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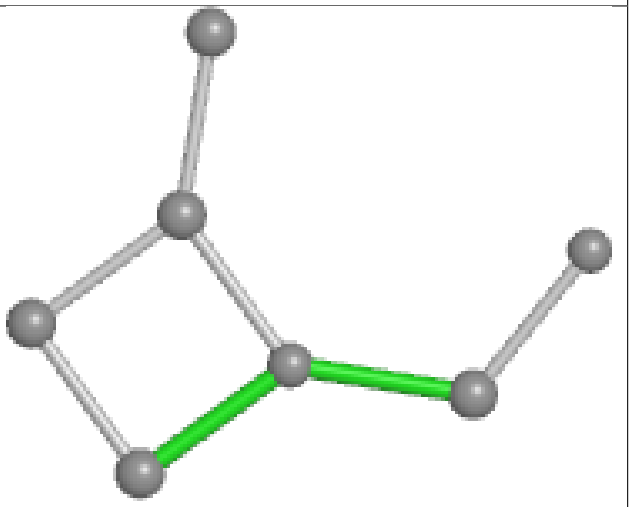
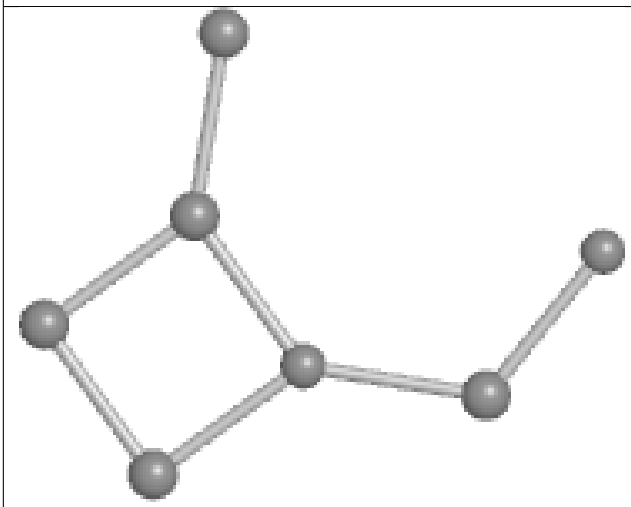


Bond angles



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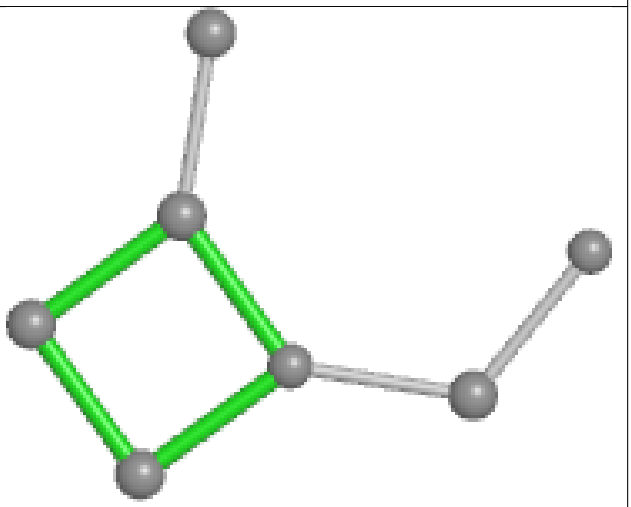
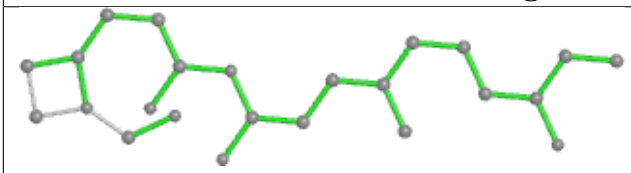


Rings

Ligand ZGV A 304



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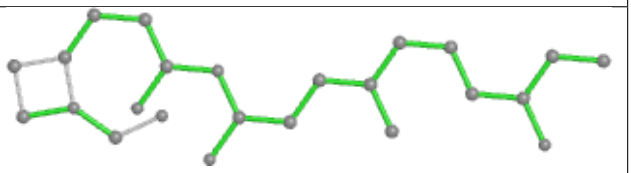

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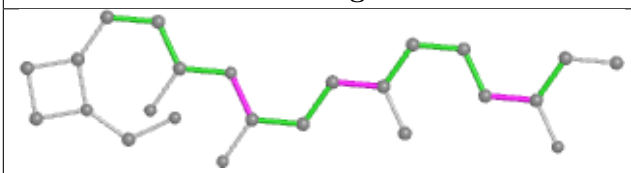

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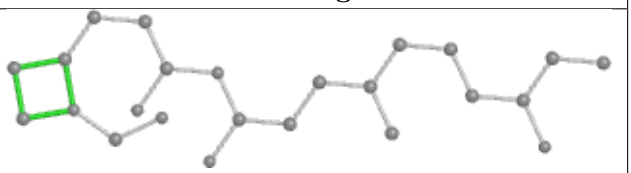
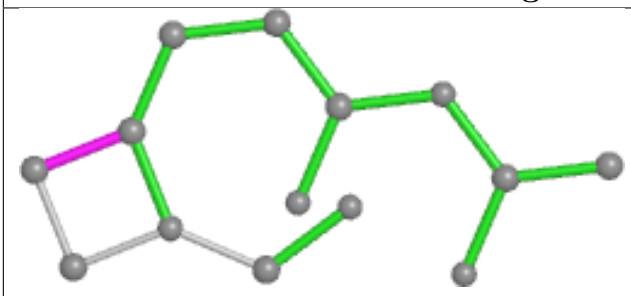


Rings

Ligand ZGV K 302



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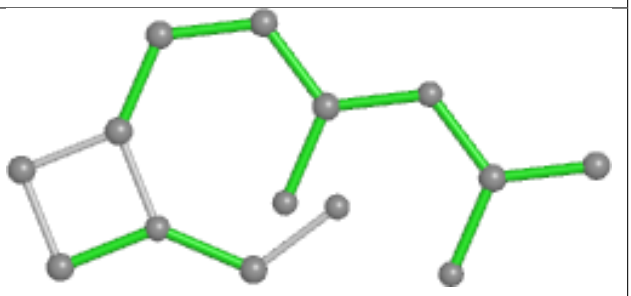

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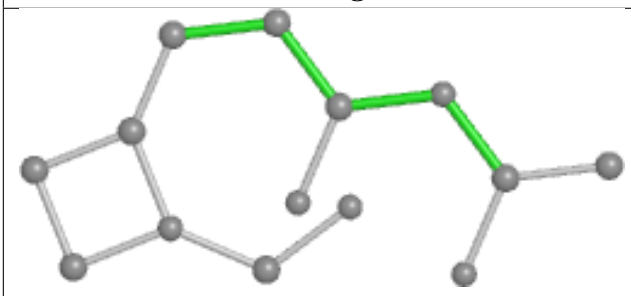

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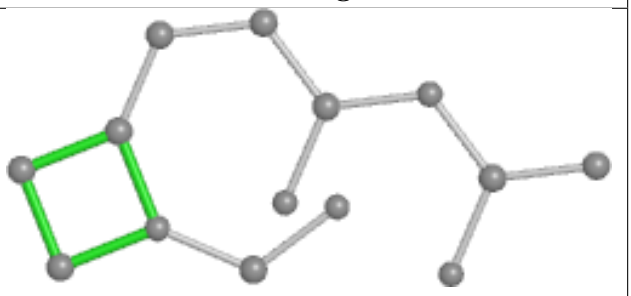
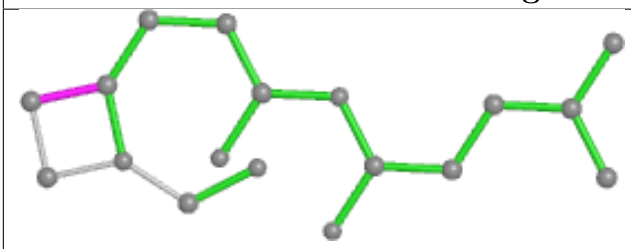


Rings

Ligand ZGV Y 302



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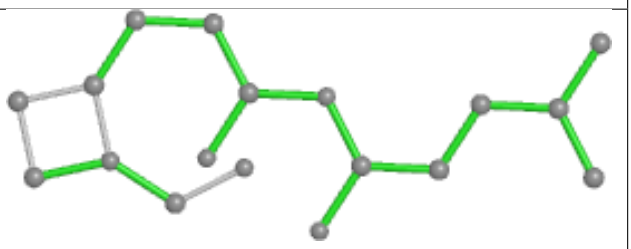
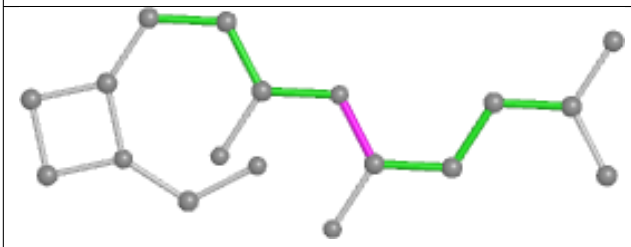


Bond angles



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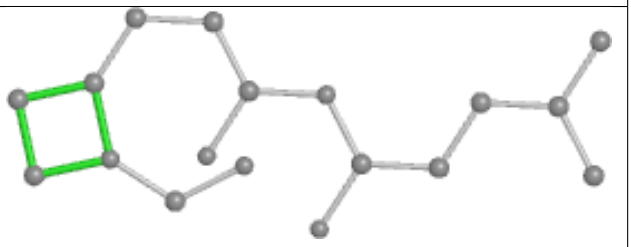
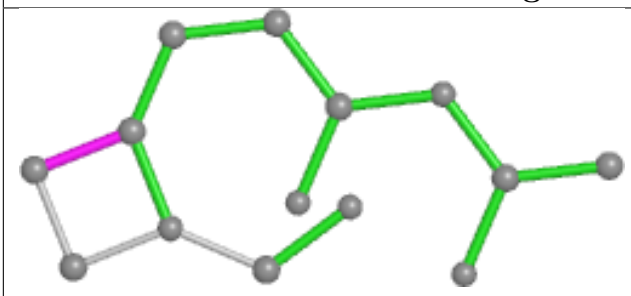


Rings

Ligand ZGV B 304



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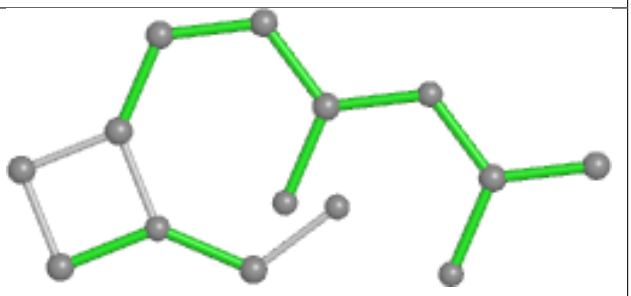
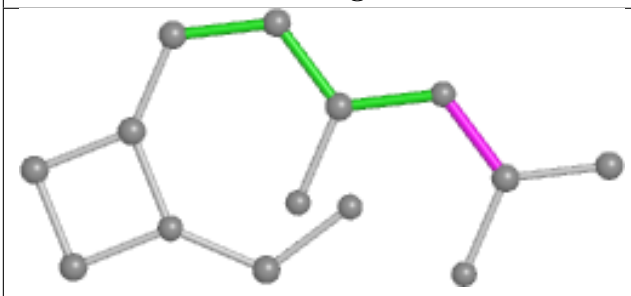
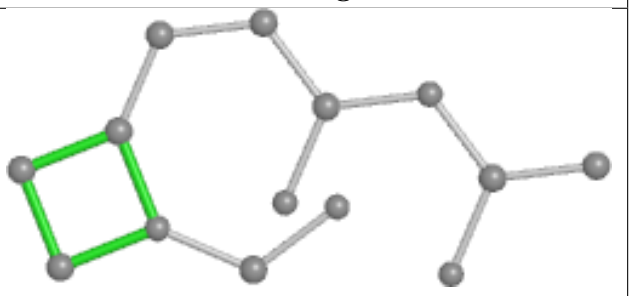


Bond angles

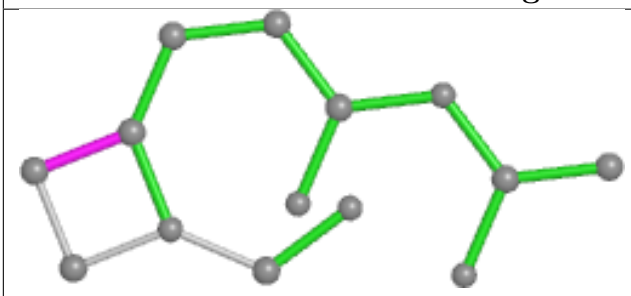


Torsions



Rings

Ligand ZGV Q 303



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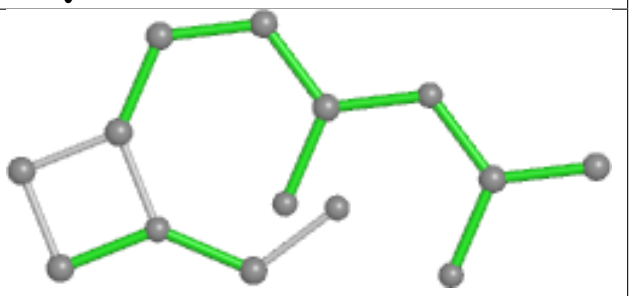
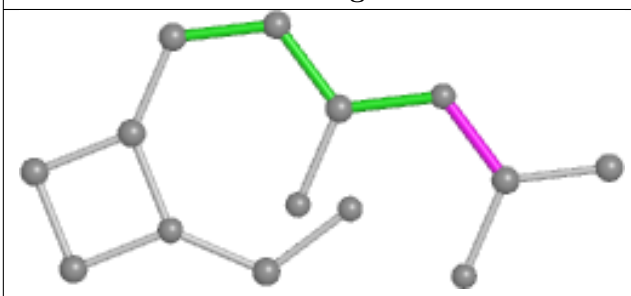
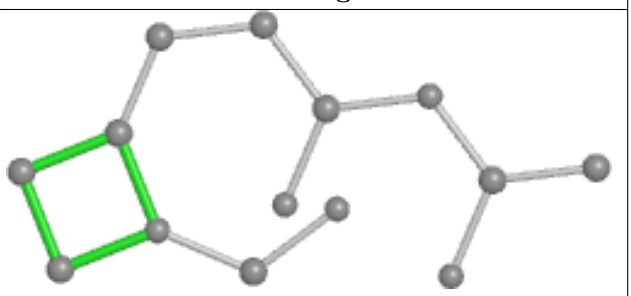


Bond angles

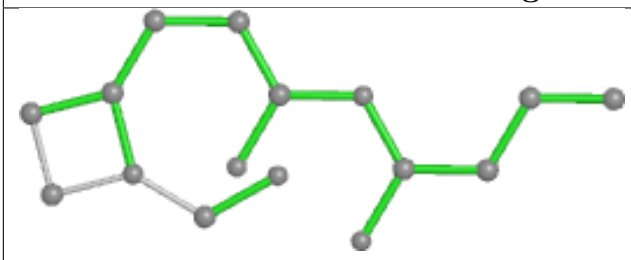


Torsions



Rings

Ligand ZGV H 302



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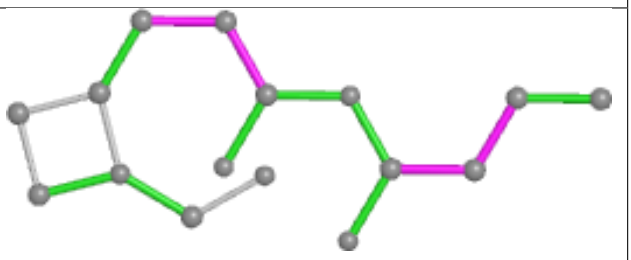
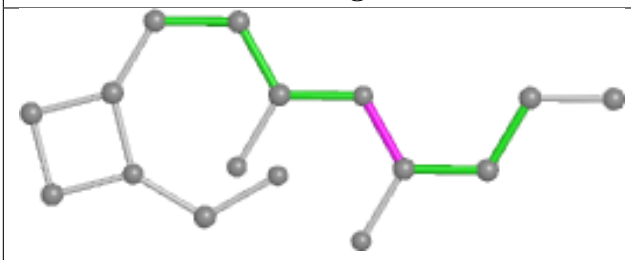
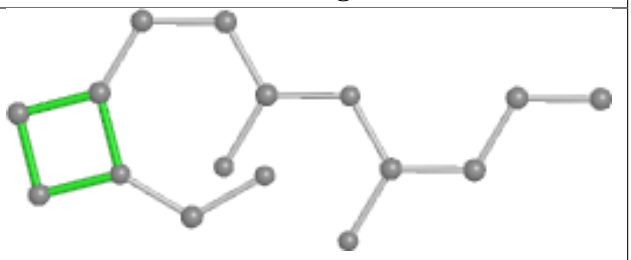


Bond angles

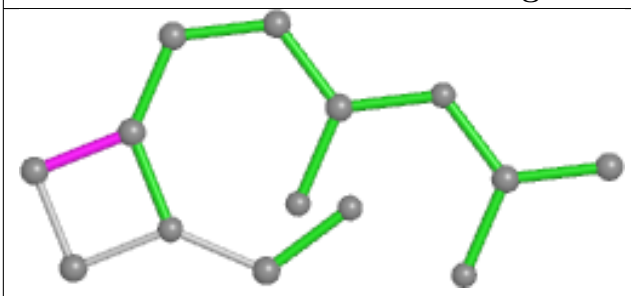


Torsions



Rings

Ligand ZGV D 304



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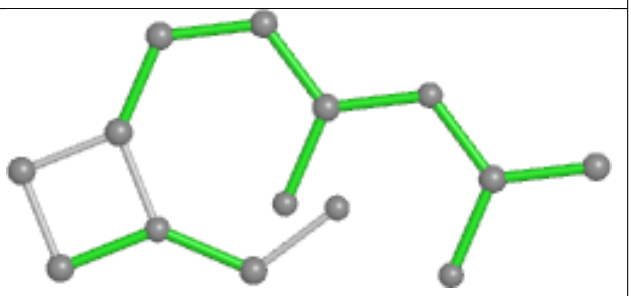
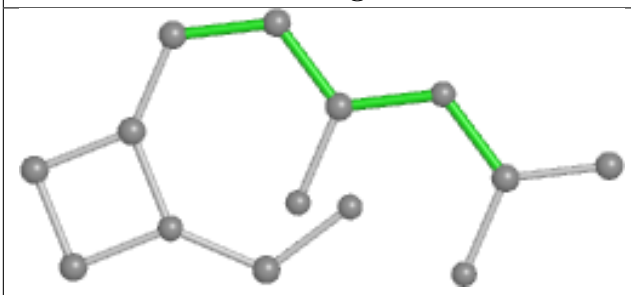
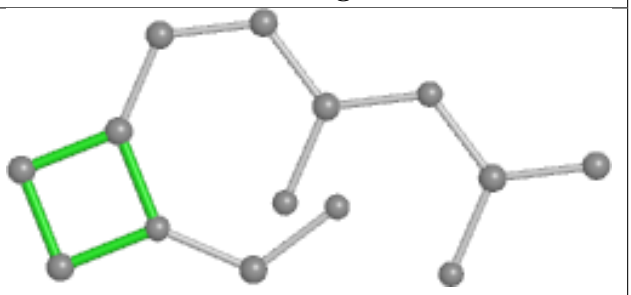


Bond angles

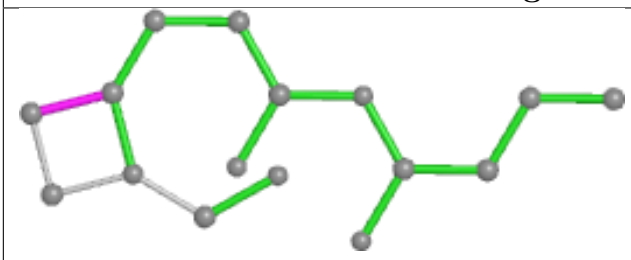


Torsions



Rings

Ligand ZGV T 203



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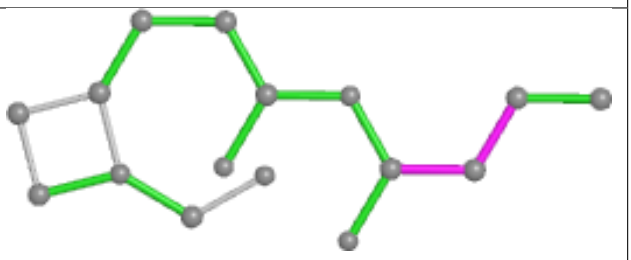
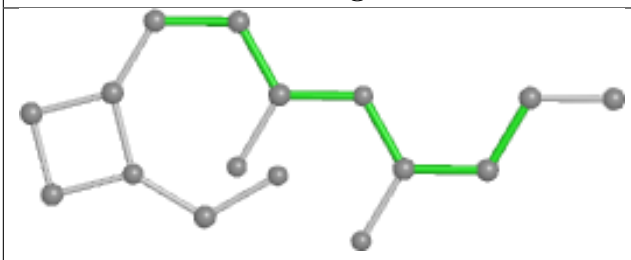


Bond angles



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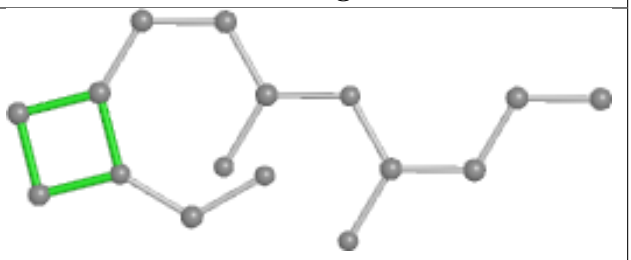
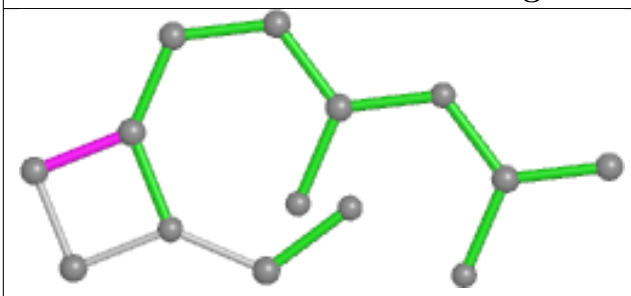
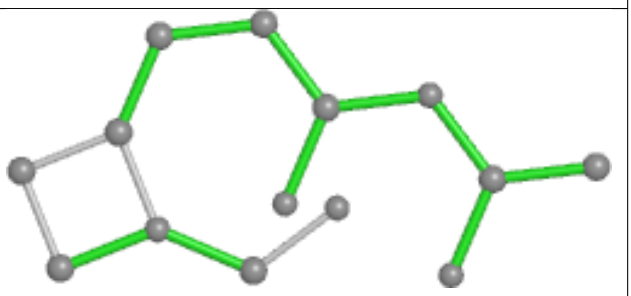


Rings

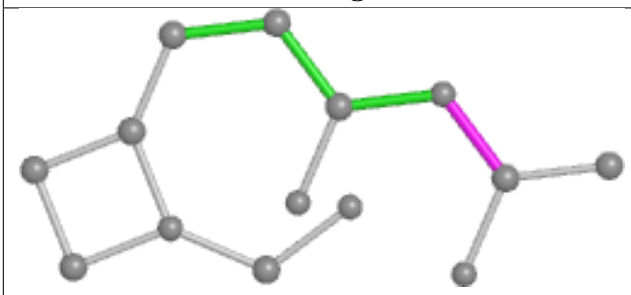
Ligand ZGV C 302



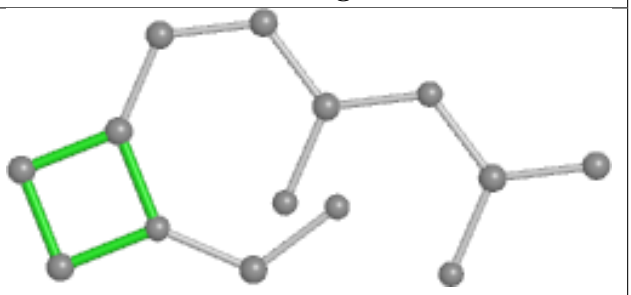
Bond lengths



Bond angles

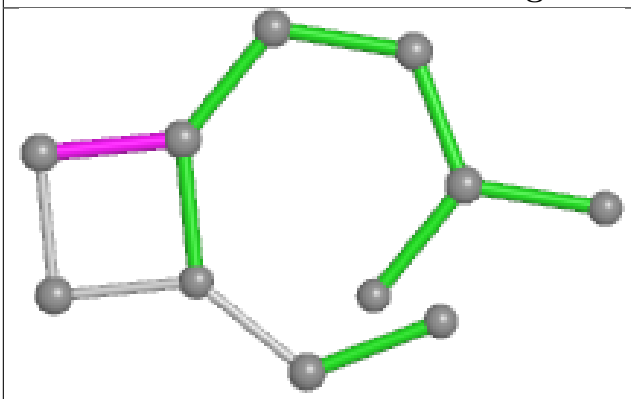


Torsions

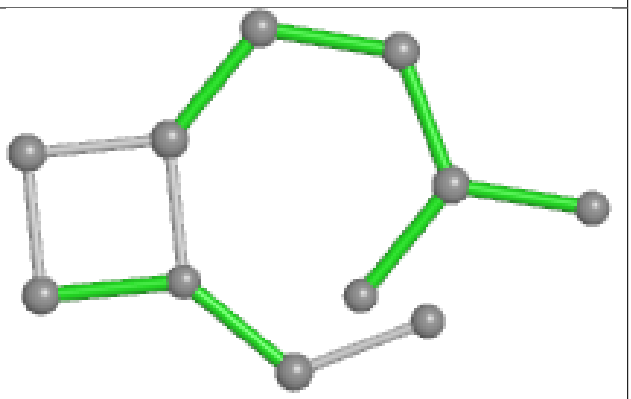


Rings

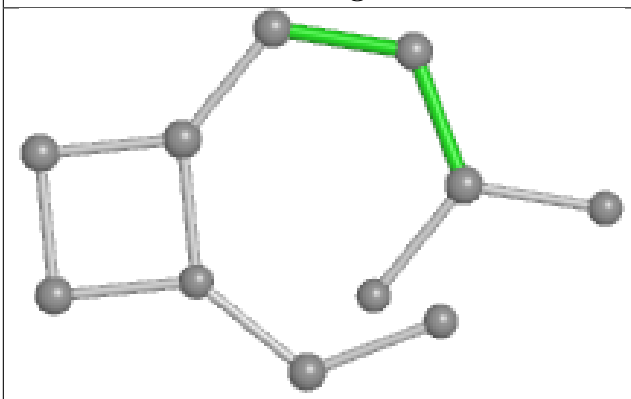
Ligand ZGV b 303



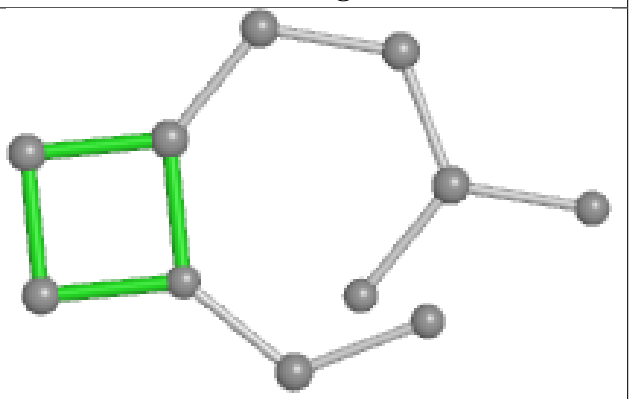
Bond lengths



Bond angles

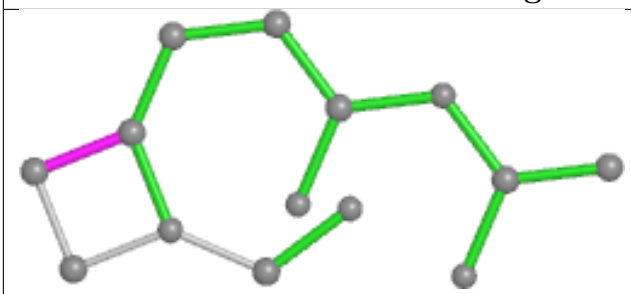


Torsions



Rings

Ligand ZGV E 302



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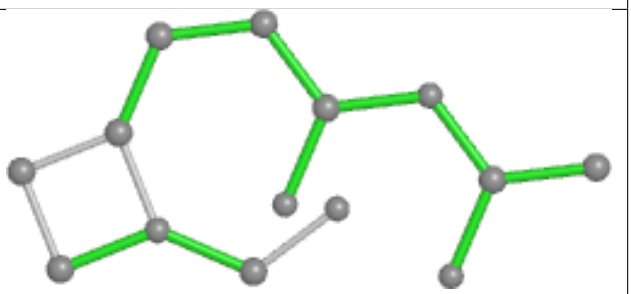
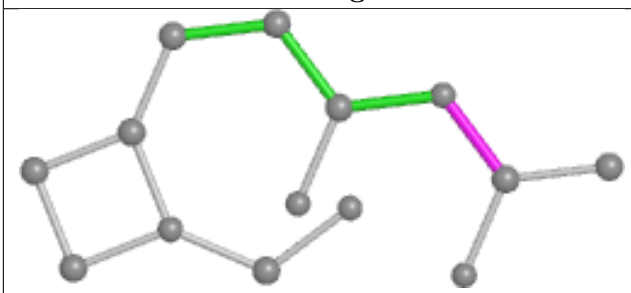
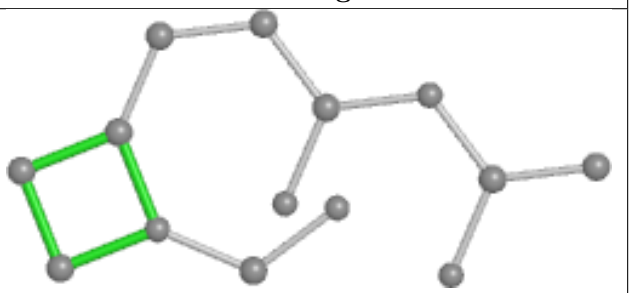


Bond angles

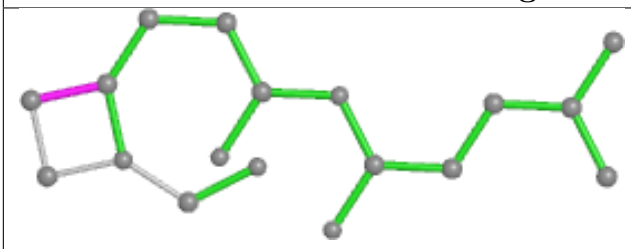


Torsions

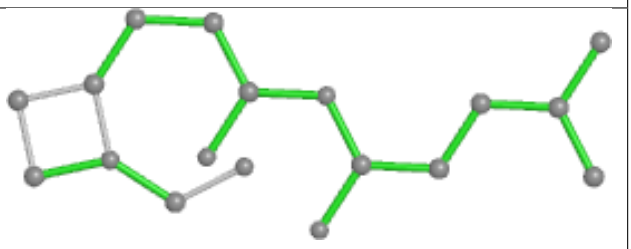


Rings

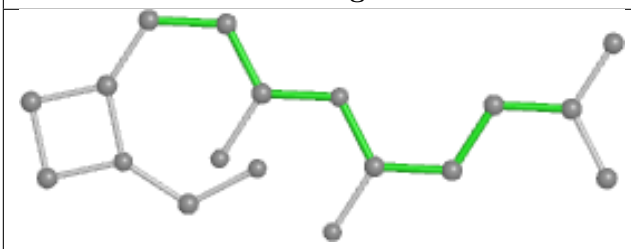
Ligand ZGV M 302



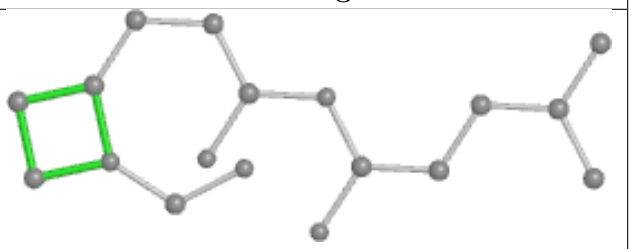
Bond lengths



Bond angles

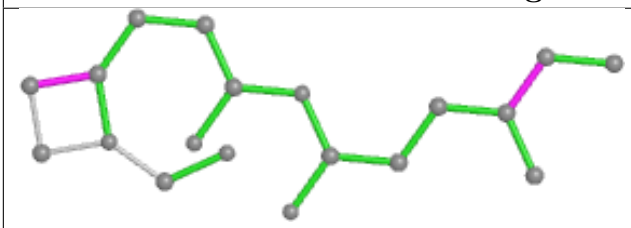


Torsions

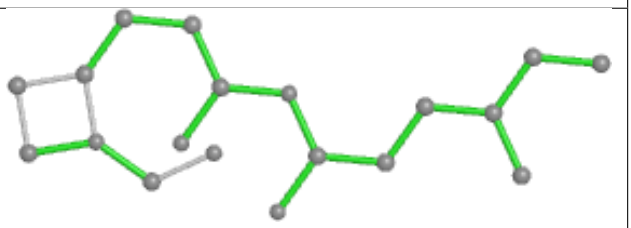


Rings

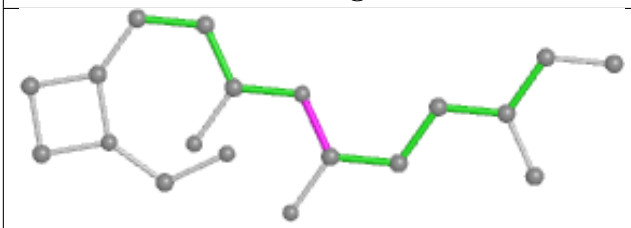
Ligand ZGV L 503



Bond lengths



Bond angles



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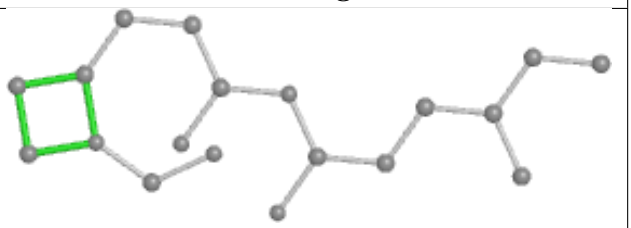
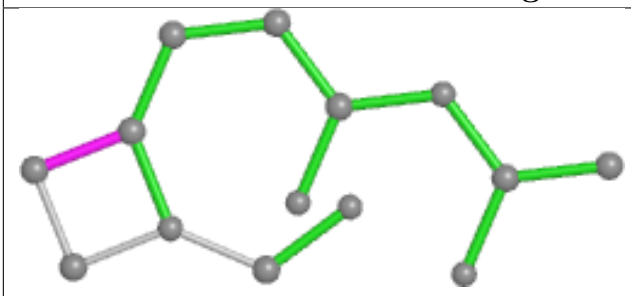


Rings

Ligand ZGV N 303



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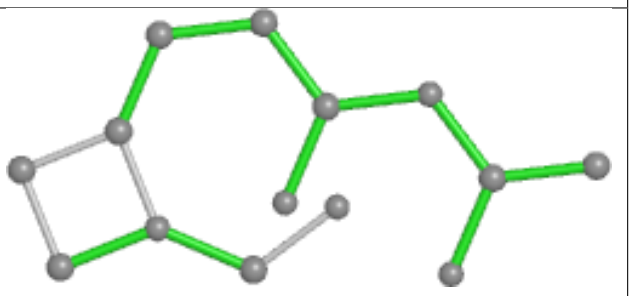
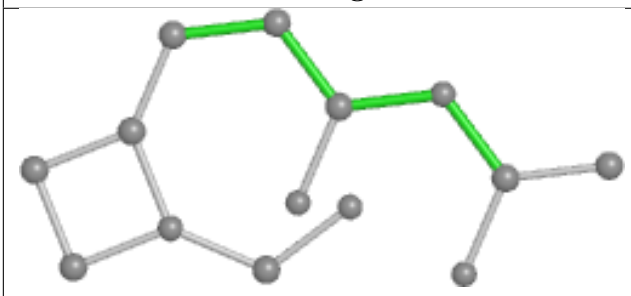
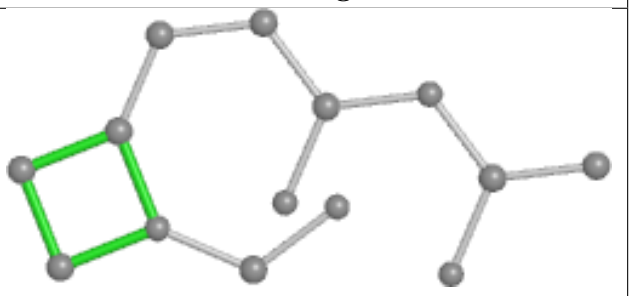


Bond angles

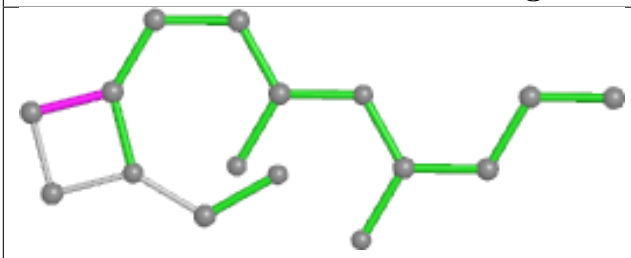


Torsions

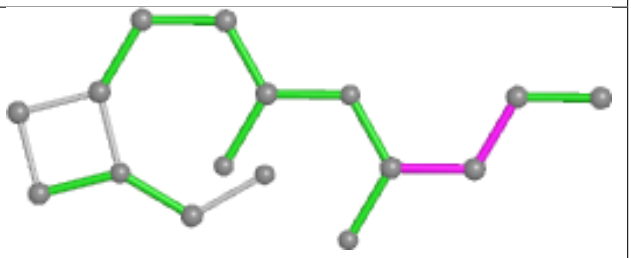


Rings

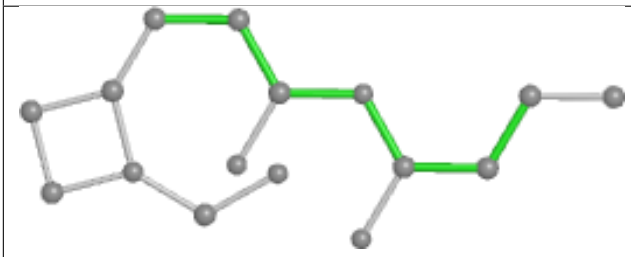
Ligand ZGV F 405



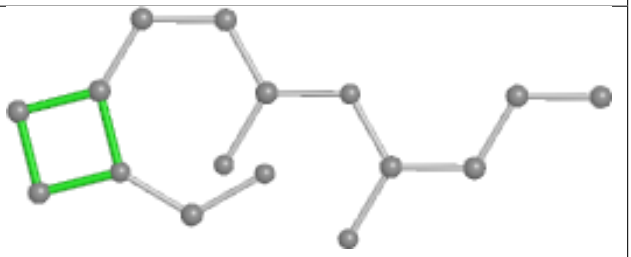
Bond lengths



Bond angles

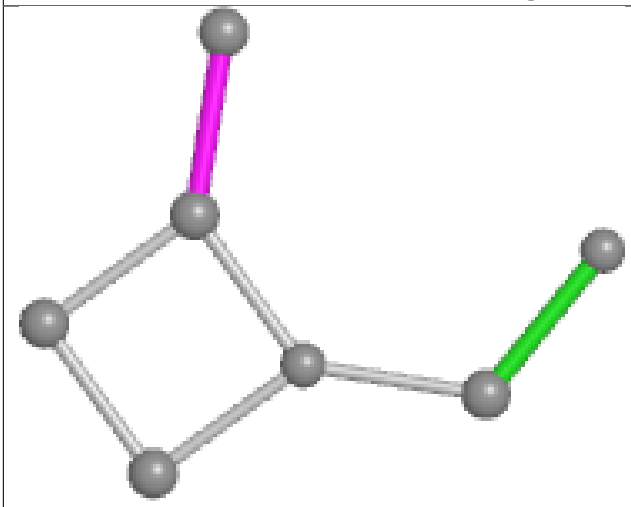


Torsions

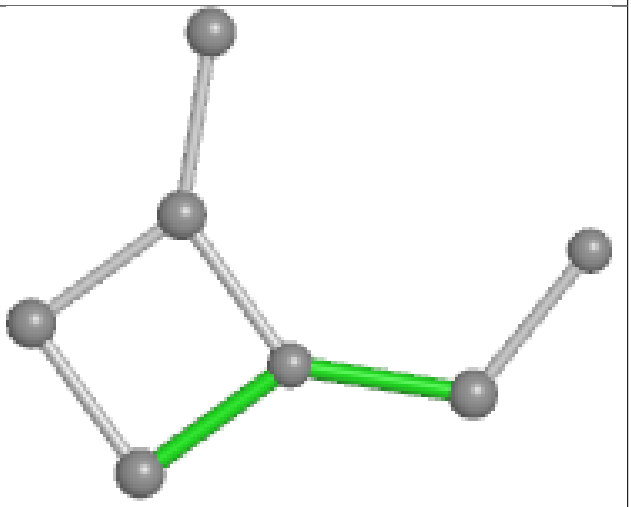


Rings

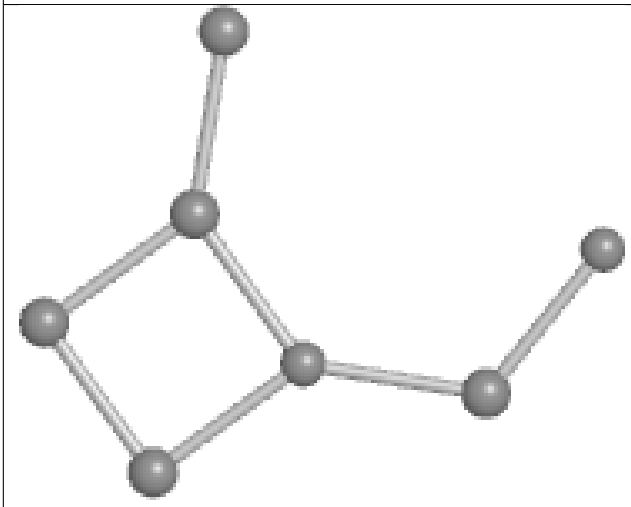
Ligand ZGV V 302



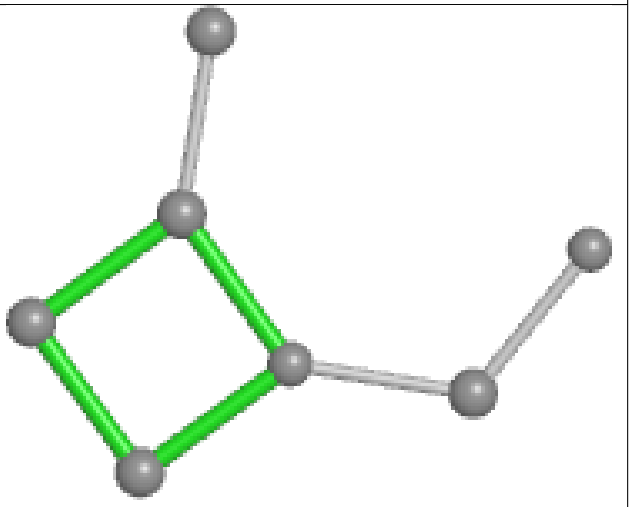
Bond lengths



Bond angles

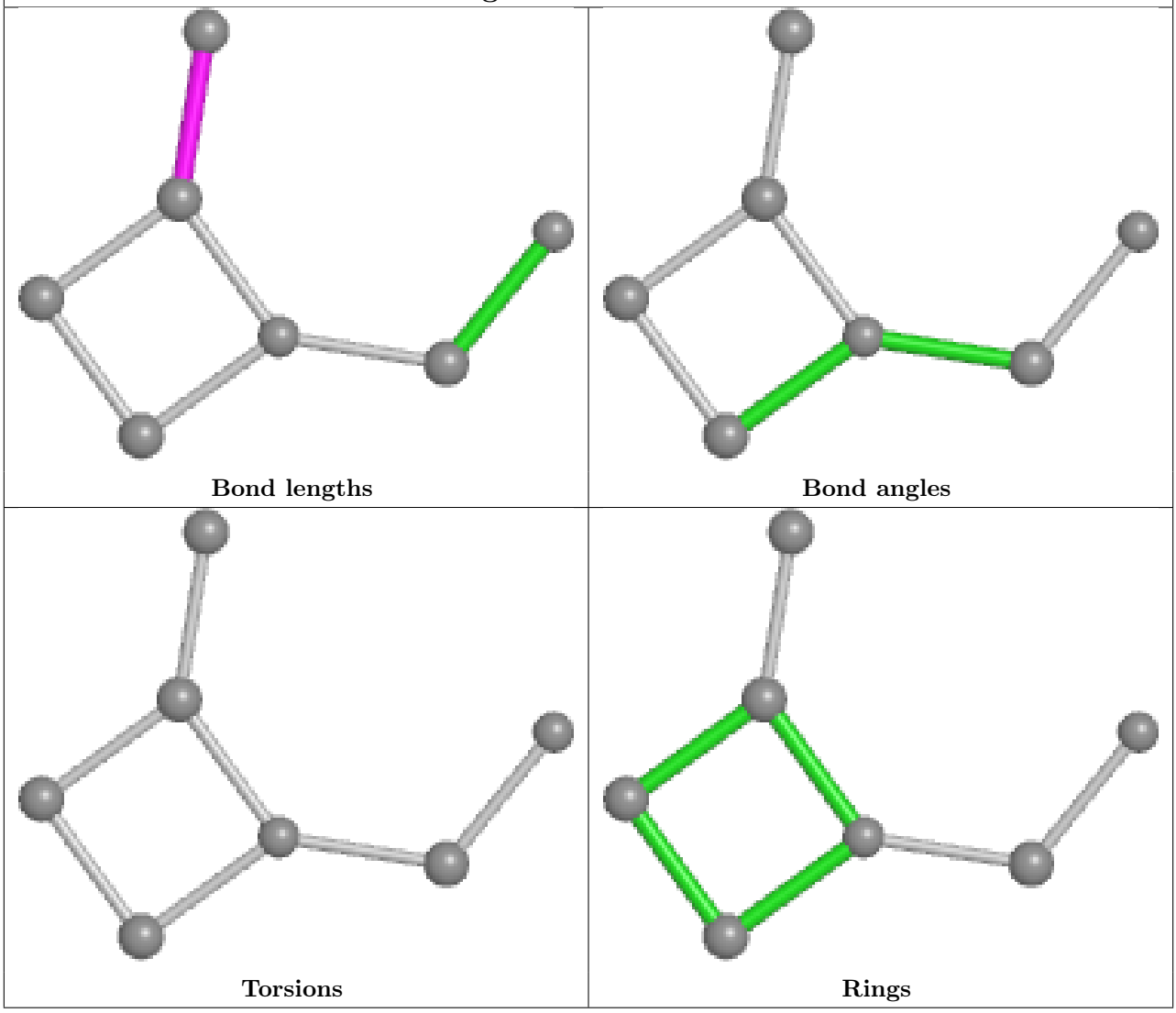


Torsions



Rings

Ligand ZGV Z 304



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, 95^{th} 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	182/193 (94%)	0.04	2 (1%)	80	65	47, 58, 79, 102	0
1	B	181/193 (93%)	-0.01	1 (0%)	89	78	47, 55, 76, 86	0
1	C	179/193 (92%)	0.00	2 (1%)	80	65	42, 51, 79, 124	0
1	D	181/193 (93%)	0.07	3 (1%)	70	53	43, 53, 73, 121	0
1	E	182/193 (94%)	0.07	4 (2%)	62	45	43, 53, 75, 141	0
1	F	180/193 (93%)	0.05	5 (2%)	53	36	42, 53, 82, 120	0
1	G	179/193 (92%)	0.22	2 (1%)	80	65	47, 56, 82, 101	0
1	H	177/193 (91%)	0.13	2 (1%)	80	65	45, 57, 73, 120	0
1	I	181/193 (93%)	0.13	2 (1%)	80	65	45, 55, 82, 118	0
1	J	181/193 (93%)	0.01	2 (1%)	80	65	42, 52, 76, 105	0
1	K	178/193 (92%)	0.09	1 (0%)	89	78	41, 53, 76, 117	0
1	L	179/193 (92%)	0.07	1 (0%)	89	78	44, 52, 81, 136	0
1	M	179/193 (92%)	0.19	1 (0%)	89	78	44, 54, 77, 129	0
1	N	180/193 (93%)	0.13	3 (1%)	70	53	43, 55, 78, 102	0
1	O	179/193 (92%)	0.12	0	100	100	40, 52, 76, 99	0
1	P	181/193 (93%)	0.01	4 (2%)	62	45	39, 49, 69, 103	0
1	Q	182/193 (94%)	0.12	4 (2%)	62	45	40, 52, 76, 113	0
1	R	181/193 (93%)	0.13	2 (1%)	80	65	43, 54, 74, 115	0
1	S	181/193 (93%)	0.02	3 (1%)	70	53	42, 52, 73, 135	0
1	T	179/193 (92%)	0.11	4 (2%)	62	45	44, 55, 80, 114	0
1	U	179/193 (92%)	0.02	1 (0%)	89	78	43, 54, 78, 105	0
1	V	181/193 (93%)	0.04	2 (1%)	80	65	40, 50, 72, 100	0
1	W	174/193 (90%)	-0.00	1 (0%)	89	78	41, 50, 71, 85	0
1	X	179/193 (92%)	0.01	1 (0%)	89	78	42, 53, 75, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	Y	179/193 (92%)	-0.03	0 100 100	41, 50, 75, 115	0
1	Z	179/193 (92%)	0.01	2 (1%) 80 65	42, 56, 82, 118	0
1	a	177/193 (91%)	0.18	1 (0%) 89 78	47, 57, 83, 110	0
1	b	180/193 (93%)	0.03	2 (1%) 80 65	43, 52, 77, 96	0
All	All	5030/5404 (93%)	0.07	58 (1%) 79 63	39, 53, 78, 141	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	5	MET	4.9
1	E	17	PHE	4.7
1	H	17	PHE	4.7
1	M	17	PHE	4.4
1	X	5	MET	4.1

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(Å^2)	Q<0.9
4	ZGV	U	302	14/25	0.65	0.36	67,77,87,93	0
4	ZGV	C	302	14/25	0.69	0.31	55,67,79,85	0
4	ZGV	R	303	14/25	0.72	0.32	55,67,79,90	0
4	ZGV	F	405	16/25	0.72	0.29	62,74,89,92	0
4	ZGV	W	403	24/25	0.73	0.43	61,81,104,105	0
4	ZGV	I	302	15/25	0.74	0.41	64,72,85,87	0
4	ZGV	G	303	14/25	0.74	0.32	61,70,83,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZGV	S	203	14/25	0.75	0.27	58,71,81,89	0
4	ZGV	L	503	19/25	0.77	0.36	54,72,90,93	0
3	ACT	Z	303	4/4	0.78	0.27	54,59,66,66	0
3	ACT	B	303	4/4	0.78	0.26	54,59,65,65	0
4	ZGV	D	304	14/25	0.78	0.31	61,73,82,88	0
4	ZGV	E	302	14/25	0.78	0.31	58,64,74,78	0
4	ZGV	A	304	24/25	0.80	0.36	66,81,98,102	0
4	ZGV	T	203	16/25	0.80	0.26	56,66,77,80	0
4	ZGV	N	303	14/25	0.80	0.34	53,65,77,82	0
4	ZGV	J	302	16/25	0.80	0.28	55,66,76,81	0
4	ZGV	O	303	24/25	0.81	0.35	56,75,91,100	0
4	ZGV	X	203	11/25	0.81	0.30	48,57,69,81	0
4	ZGV	Y	302	18/25	0.81	0.28	49,61,74,75	0
4	ZGV	M	302	18/25	0.82	0.36	66,79,89,93	0
4	ZGV	K	302	14/25	0.83	0.24	61,68,80,82	0
2	MPD	D	303	8/8	0.83	0.38	57,69,73,74	0
4	ZGV	B	304	14/25	0.83	0.25	54,68,81,86	0
2	MPD	H	301	8/8	0.83	0.32	53,64,66,72	0
4	ZGV	P	203	14/25	0.84	0.26	51,61,71,79	0
4	ZGV	H	302	16/25	0.84	0.27	52,67,83,84	0
2	MPD	S	202	8/8	0.85	0.37	52,63,67,73	0
4	ZGV	b	303	11/25	0.85	0.23	52,61,74,80	0
2	MPD	Z	302	8/8	0.86	0.33	56,67,72,72	0
4	ZGV	Q	303	14/25	0.86	0.26	52,63,73,77	0
2	MPD	D	302	8/8	0.86	0.37	54,66,68,69	0
4	ZGV	V	302	7/25	0.86	0.25	48,51,62,62	0
2	MPD	Q	304	8/8	0.87	0.28	55,67,73,80	0
2	MPD	S	201	8/8	0.88	0.35	48,58,60,62	0
2	MPD	Q	302	8/8	0.88	0.24	55,66,71,72	0
2	MPD	H	303	8/8	0.88	0.31	59,71,76,79	0
2	MPD	b	302	8/8	0.88	0.35	50,64,67,68	0
2	MPD	D	301	8/8	0.89	0.43	54,66,71,71	0
2	MPD	W	402	8/8	0.89	0.29	49,59,64,68	0
2	MPD	F	404	8/8	0.89	0.32	50,60,64,68	0
2	MPD	P	201	8/8	0.89	0.29	47,57,60,71	0
3	ACT	R	302	4/4	0.90	0.17	55,61,67,67	0
2	MPD	I	303	8/8	0.90	0.23	51,62,65,71	0
2	MPD	A	302	8/8	0.90	0.26	53,64,67,71	0
2	MPD	a	303	8/8	0.90	0.22	49,59,68,68	0
2	MPD	B	302	8/8	0.90	0.25	56,68,72,75	0
2	MPD	U	301	8/8	0.90	0.37	56,68,72,73	0
3	ACT	G	302	4/4	0.90	0.16	56,58,69,69	0

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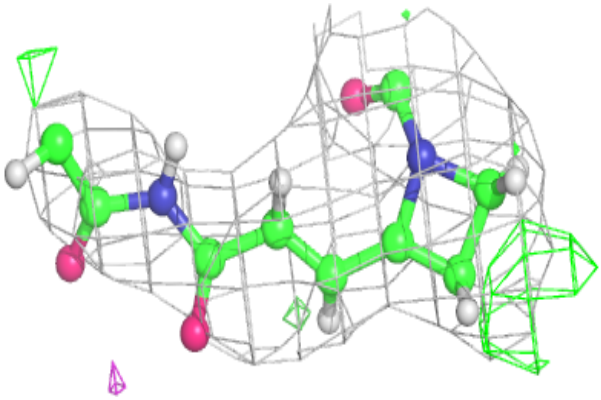
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MPD	a	301	8/8	0.91	0.37	53,65,68,69	0
2	MPD	P	202	8/8	0.91	0.23	50,61,65,65	0
2	MPD	I	301	8/8	0.91	0.32	53,64,69,70	0
2	MPD	F	401	8/8	0.91	0.26	48,61,66,66	0
2	MPD	K	301	8/8	0.91	0.36	54,65,70,70	0
2	MPD	K	303	8/8	0.91	0.21	51,62,65,67	0
2	MPD	T	201	8/8	0.91	0.27	50,61,63,64	0
2	MPD	M	301	8/8	0.91	0.31	49,61,63,66	0
2	MPD	N	302	8/8	0.91	0.26	54,65,68,68	0
2	MPD	Y	303	8/8	0.91	0.26	47,57,63,63	0
4	ZGV	Z	304	7/25	0.91	0.23	51,56,64,68	0
2	MPD	G	301	8/8	0.91	0.27	53,64,71,72	0
2	MPD	C	301	8/8	0.92	0.20	49,60,63,63	0
2	MPD	L	502	8/8	0.92	0.27	51,62,66,67	0
2	MPD	R	301	8/8	0.92	0.30	49,60,67,67	0
3	ACT	A	303	4/4	0.92	0.20	55,58,66,66	0
2	MPD	T	202	8/8	0.92	0.28	53,64,66,66	0
2	MPD	X	201	8/8	0.93	0.30	50,60,68,68	0
2	MPD	O	302	8/8	0.93	0.27	49,59,64,64	0
2	MPD	Z	301	8/8	0.93	0.24	53,65,69,69	0
2	MPD	J	301	8/8	0.93	0.31	48,58,62,65	0
2	MPD	E	301	8/8	0.93	0.28	51,61,65,68	0
2	MPD	N	301	8/8	0.93	0.39	50,61,64,65	0
2	MPD	F	402	8/8	0.93	0.34	49,61,65,67	0
2	MPD	V	301	8/8	0.93	0.23	52,64,65,65	0
2	MPD	O	301	8/8	0.93	0.34	50,61,68,68	0
3	ACT	F	403	4/4	0.93	0.24	55,59,66,66	0
2	MPD	Y	301	8/8	0.94	0.26	48,58,59,60	0
3	ACT	C	303	4/4	0.94	0.25	49,57,59,60	0
2	MPD	W	401	8/8	0.94	0.20	53,64,68,68	0
2	MPD	J	303	8/8	0.94	0.26	50,60,66,66	0
3	ACT	L	501	4/4	0.94	0.15	56,62,68,68	0
2	MPD	B	301	8/8	0.94	0.29	53,66,67,67	0
4	ZGV	a	302	7/25	0.94	0.18	50,52,63,63	0
3	ACT	X	202	4/4	0.94	0.15	56,58,71,71	0
2	MPD	A	301	8/8	0.95	0.35	57,68,75,75	0
2	MPD	Q	301	8/8	0.96	0.30	48,60,62,62	0
3	ACT	P	204	4/4	0.96	0.13	49,55,59,59	0
2	MPD	b	301	8/8	0.96	0.22	49,60,64,64	0

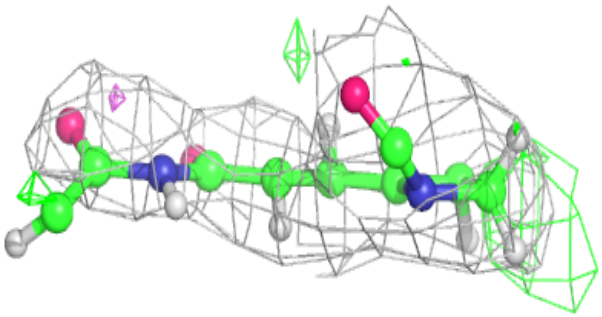
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

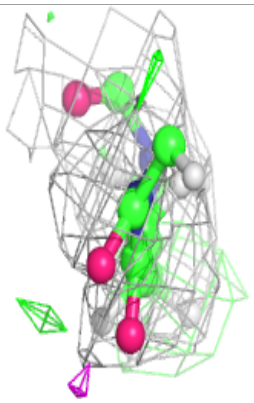
orientation to approximate a three-dimensional view.

Electron density around ZGV U 302:

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

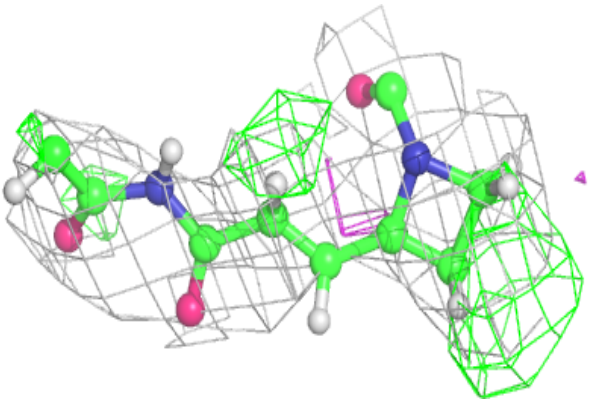


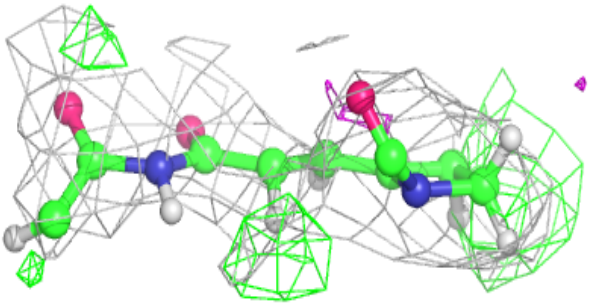


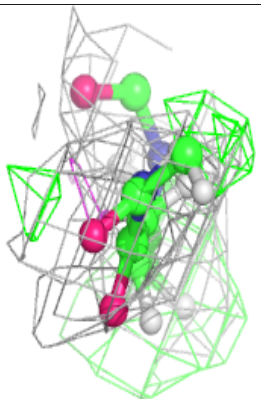


Electron density around ZGV C 302:

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

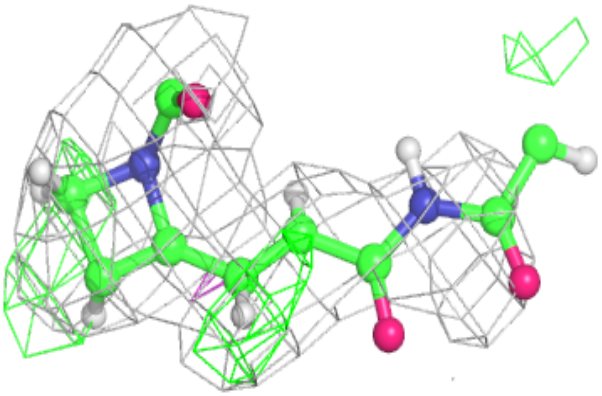


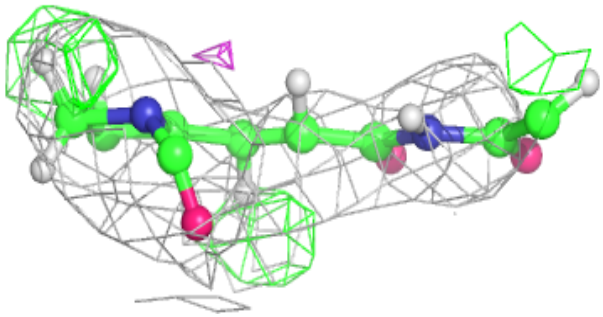


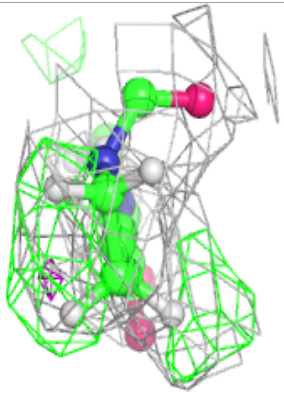


Electron density around ZGV R 303:

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

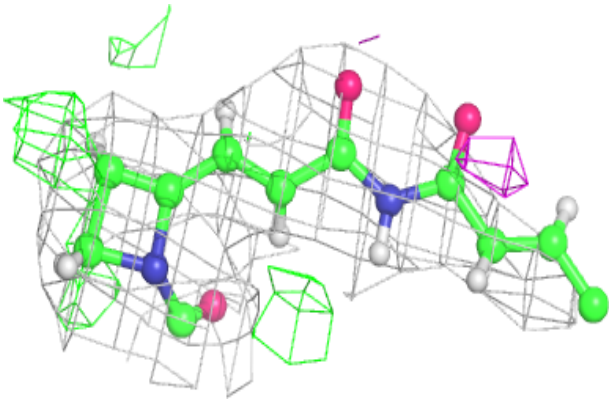


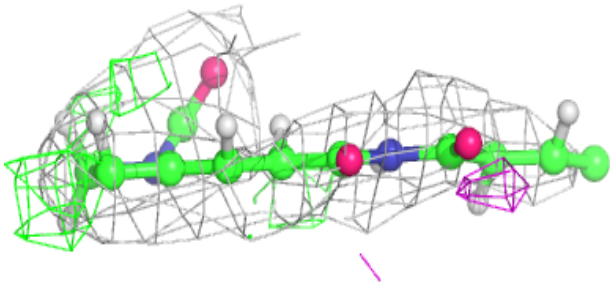


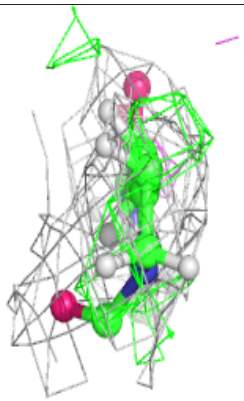


Electron density around ZGV F 405:

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

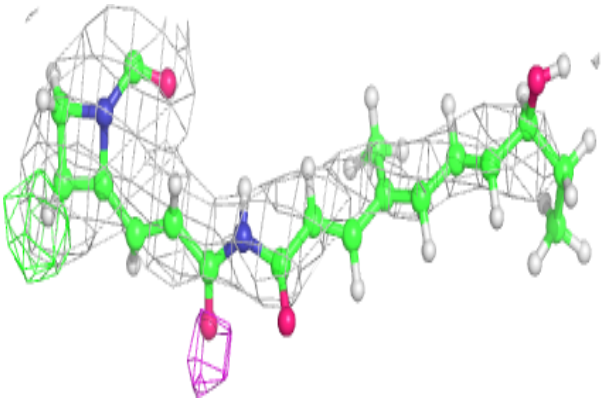


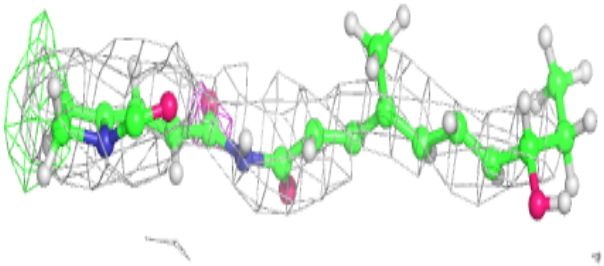


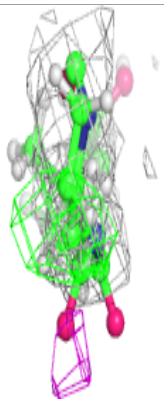


Electron density around ZGV W 403:

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

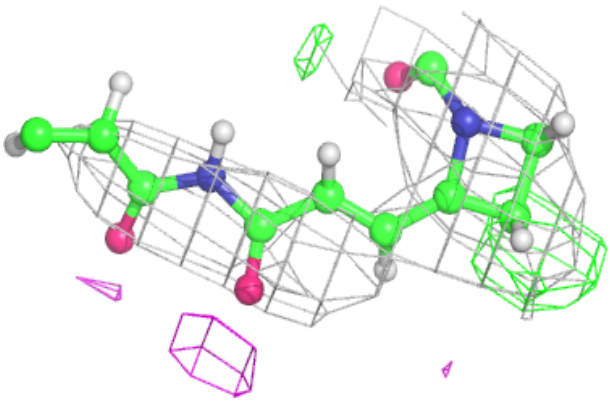


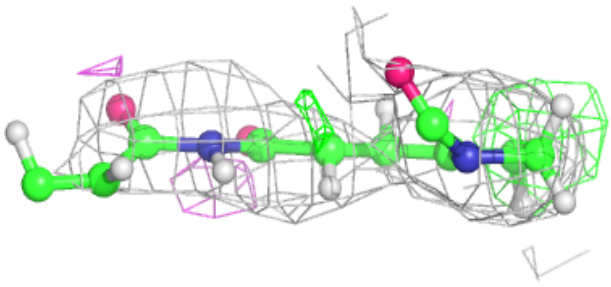


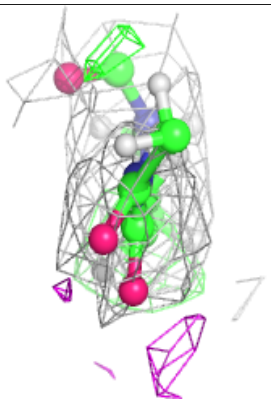


Electron density around ZGV I 302:

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

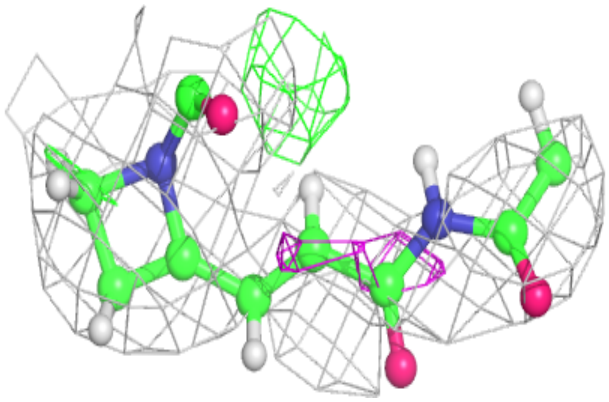


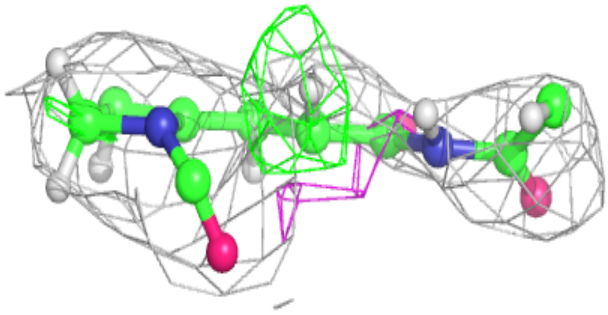


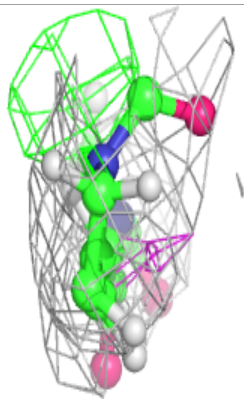


Electron density around ZGV G 303:

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

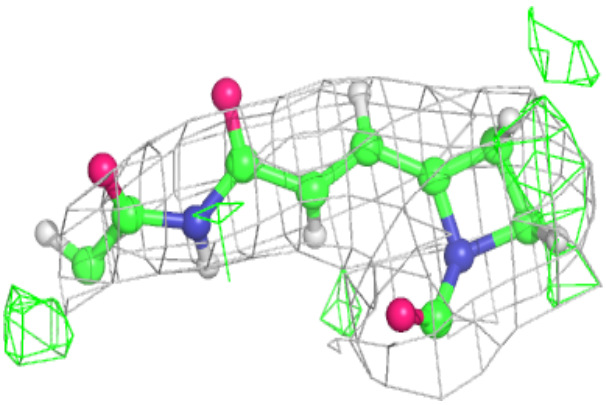


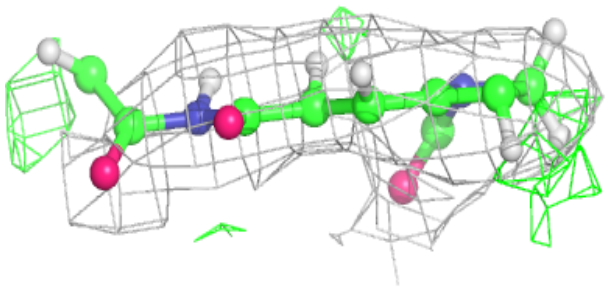


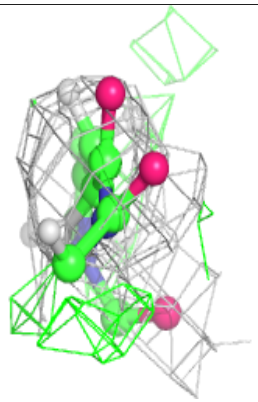


Electron density around ZGV S 203:

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

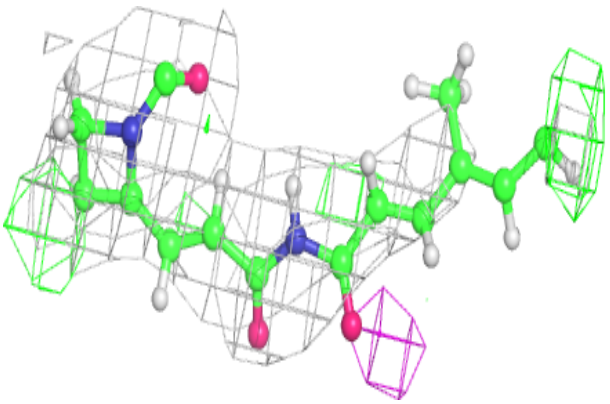


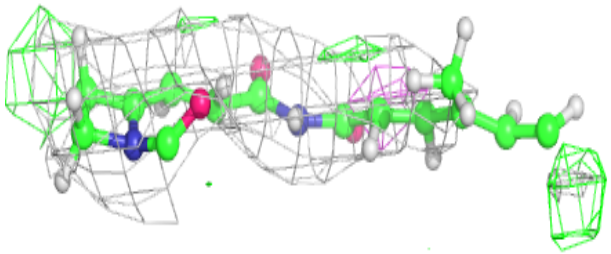




Electron density around ZGV L 503:

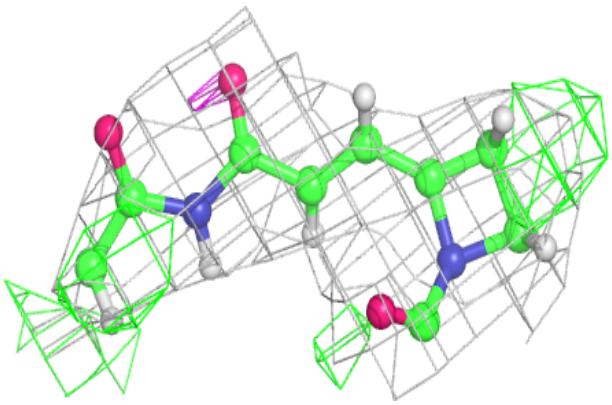
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

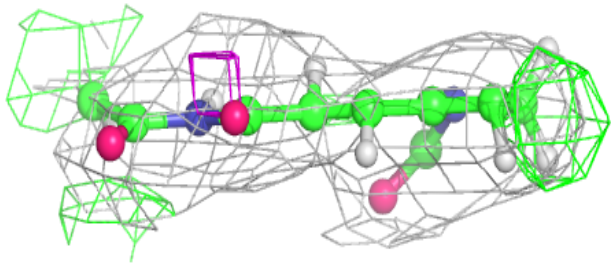


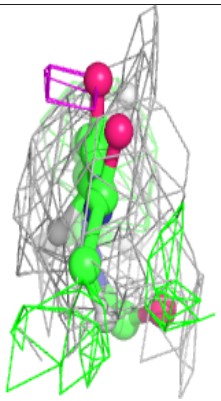


Electron density around ZGV D 304:

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

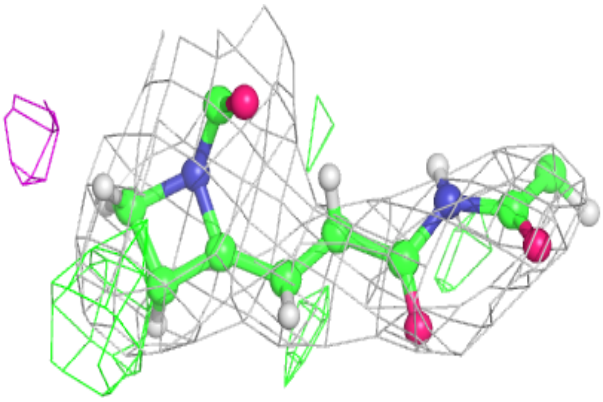


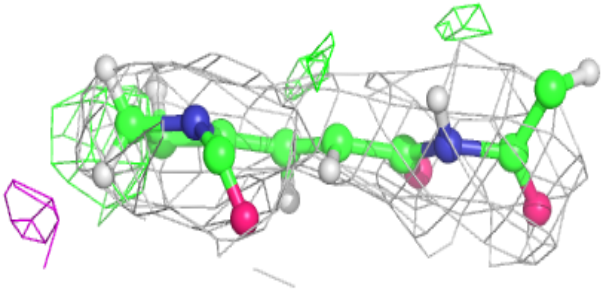




Electron density around ZGV E 302:

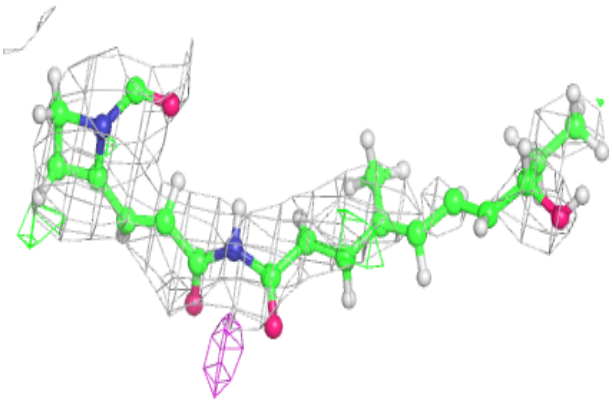
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

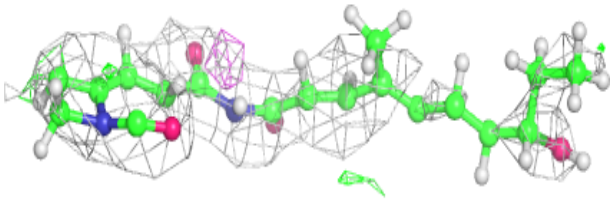


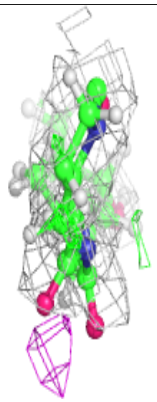


Electron density around ZGV A 304:

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

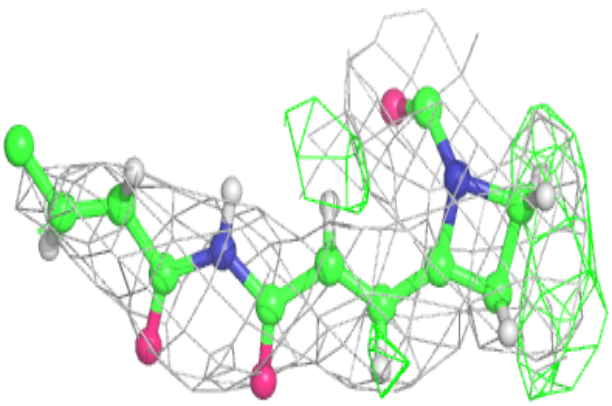


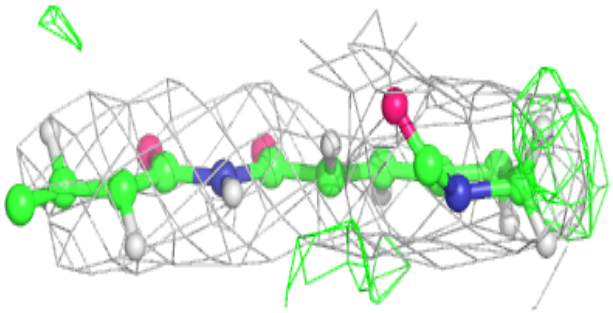


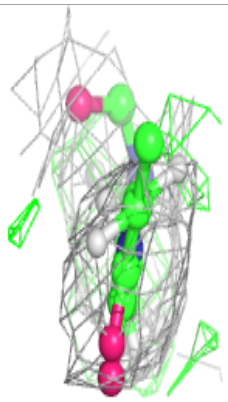


Electron density around ZGV T 203:

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

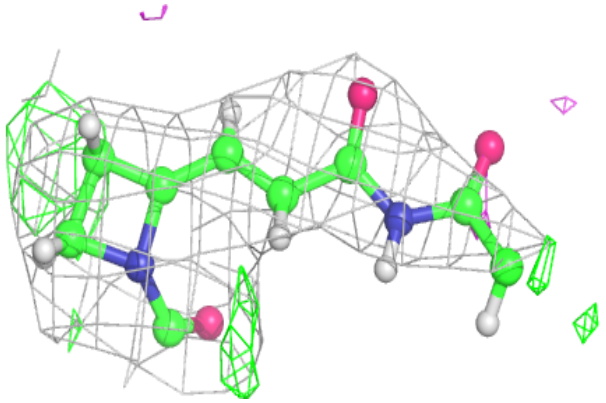


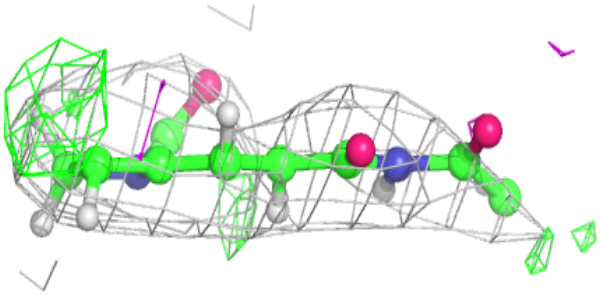


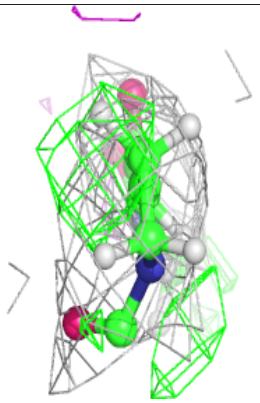


Electron density around ZGV N 303:

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

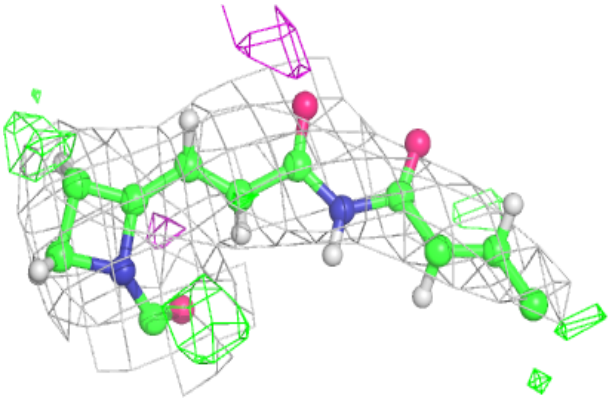


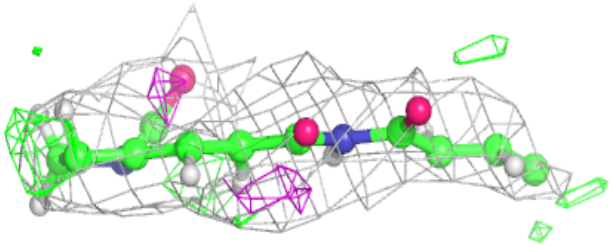


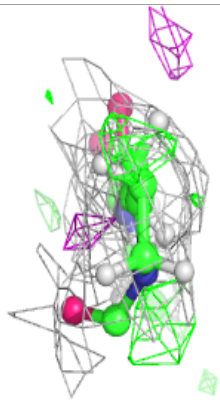


Electron density around ZGV J 302:

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

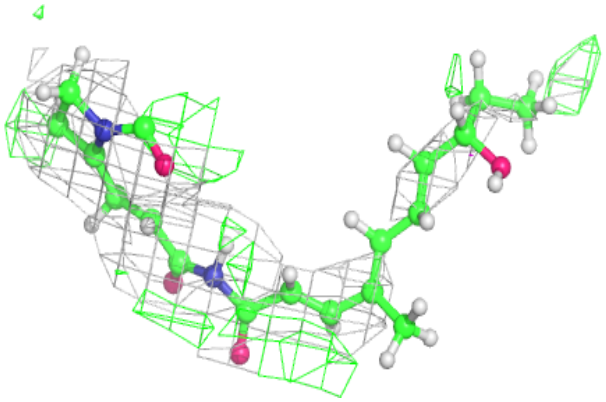


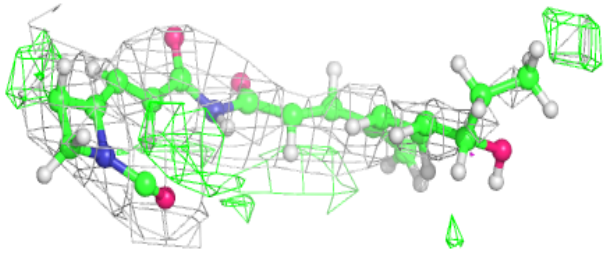


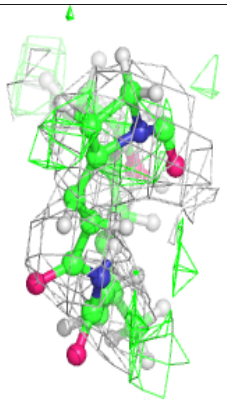


Electron density around ZGV O 303:

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

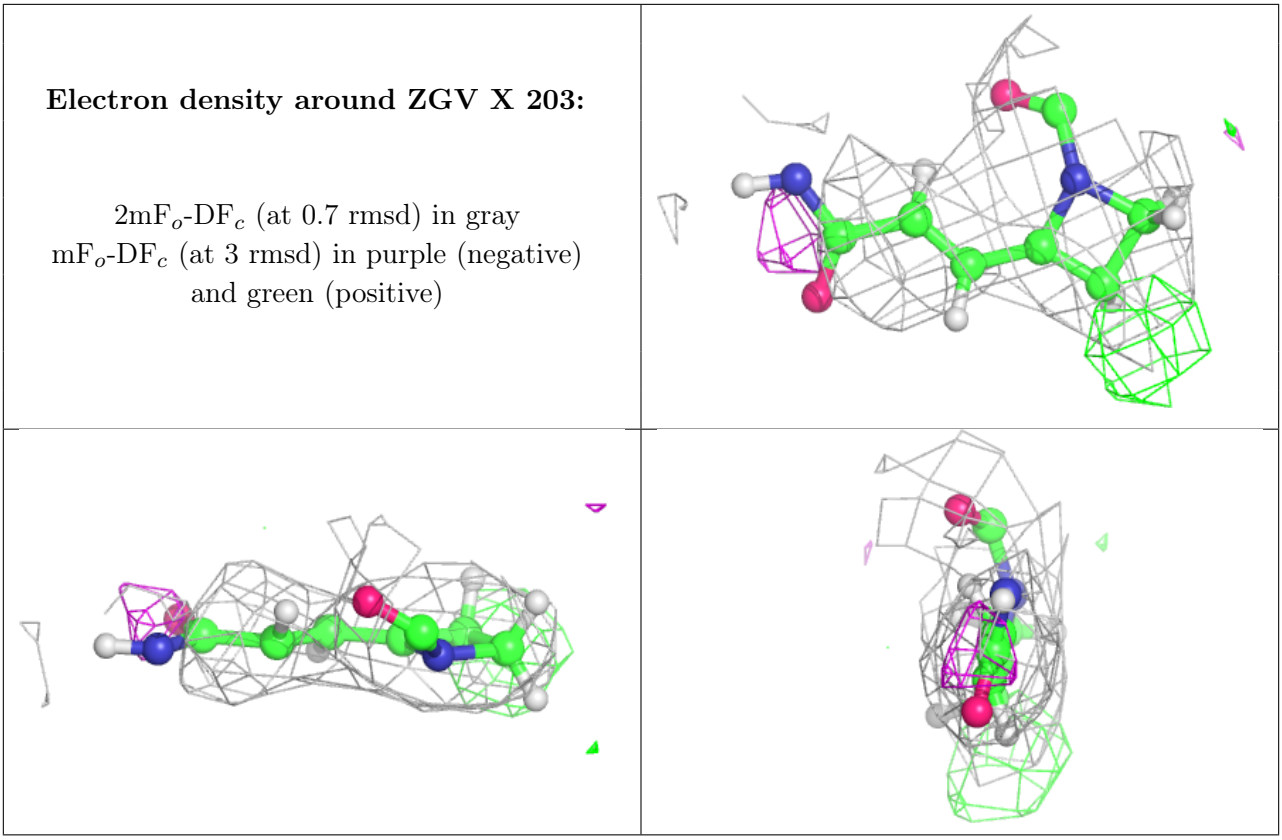






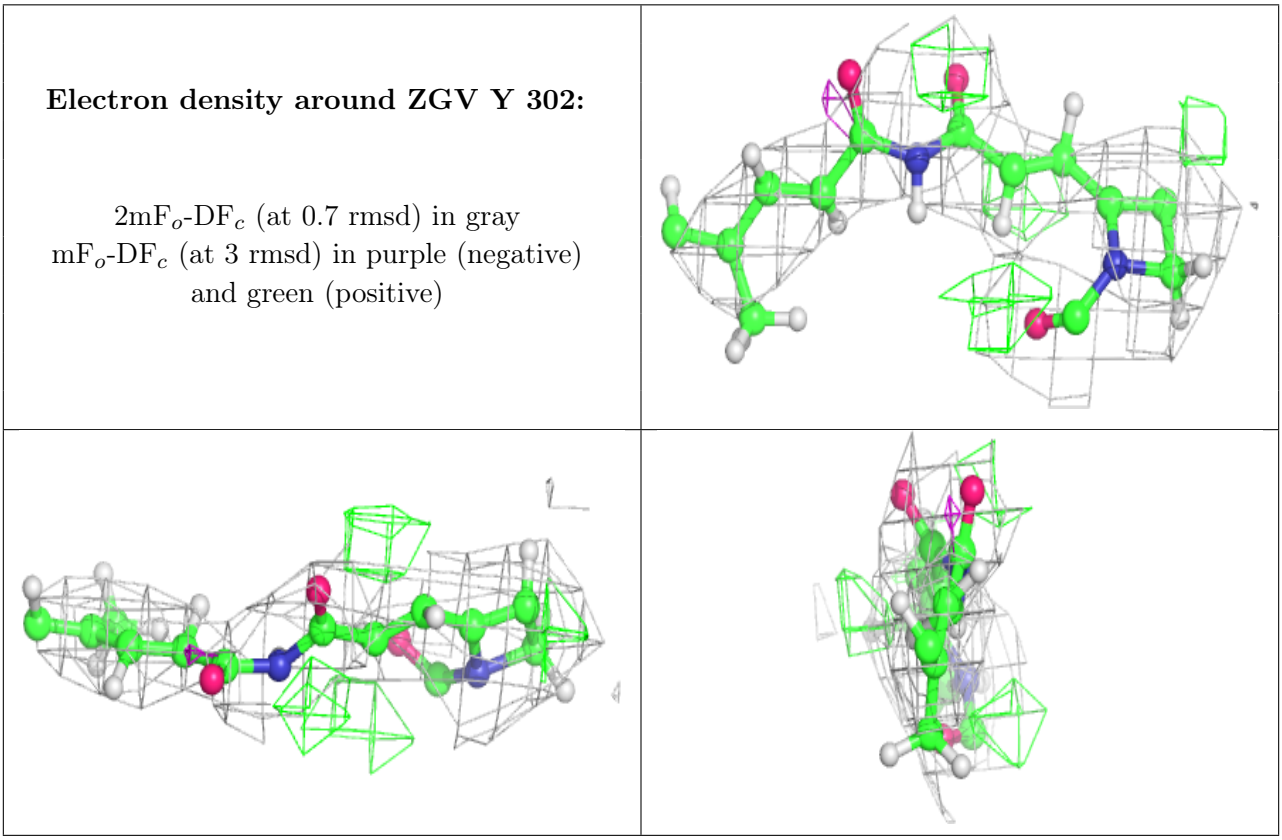
Electron density around ZGV X 203:

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



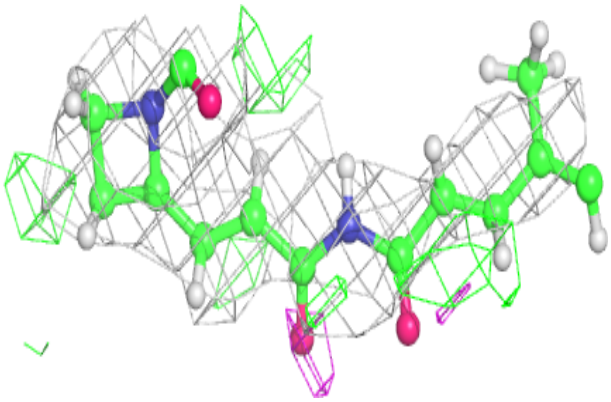
Electron density around ZGV Y 302:

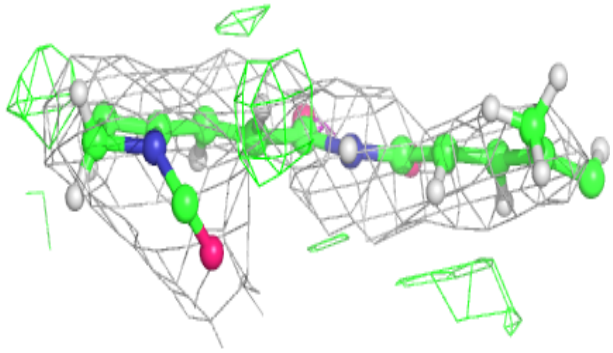
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

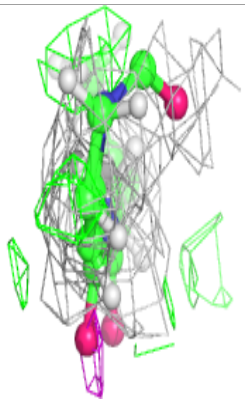


Electron density around ZGV M 302:

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

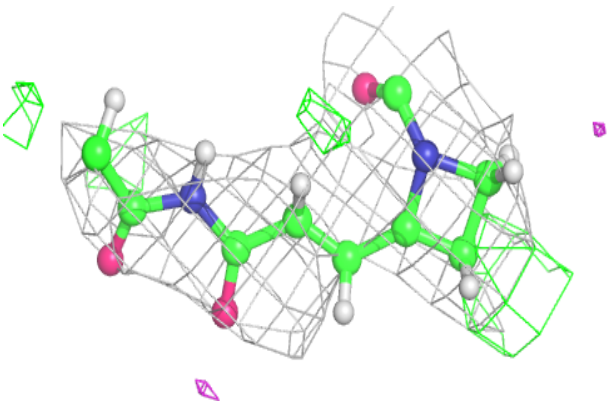


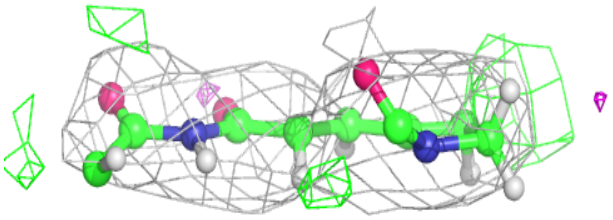


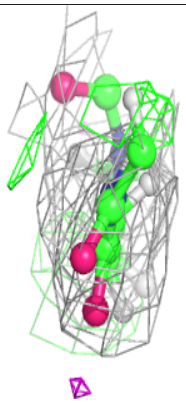


Electron density around ZGV K 302:

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

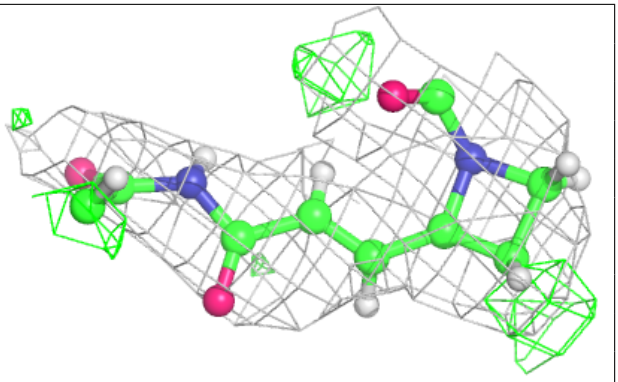


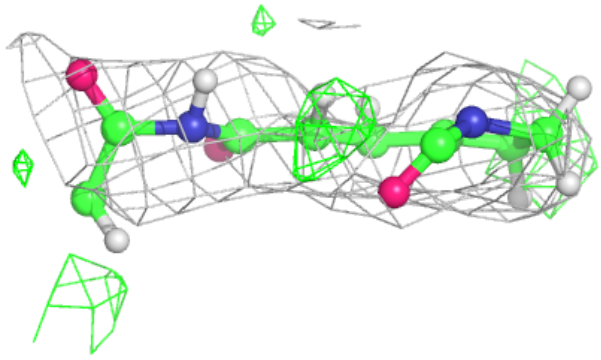


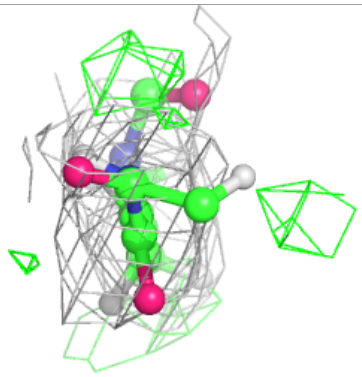


Electron density around ZGV B 304:

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

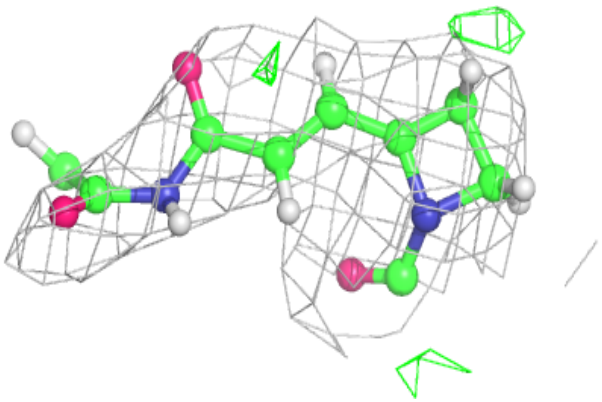


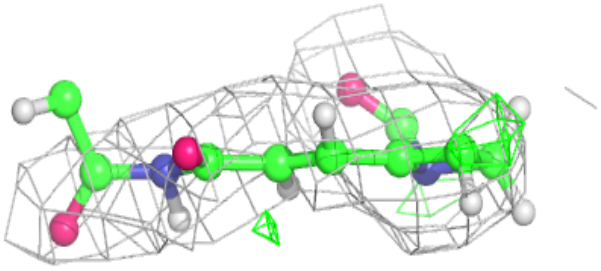


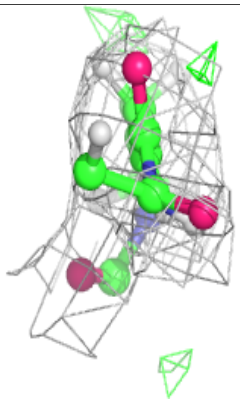


Electron density around ZGV P 203:

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

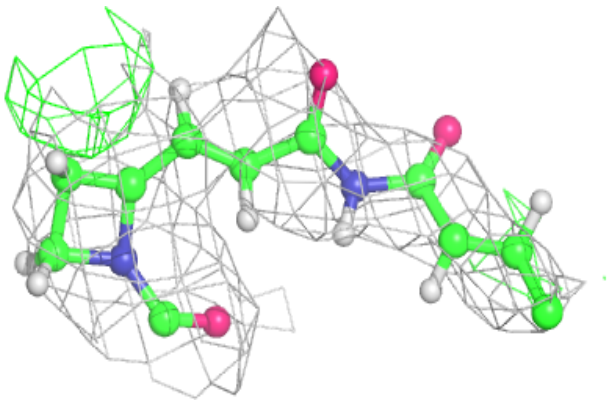


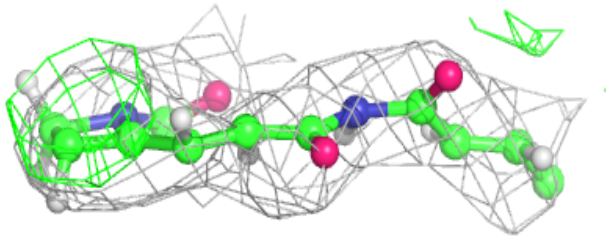


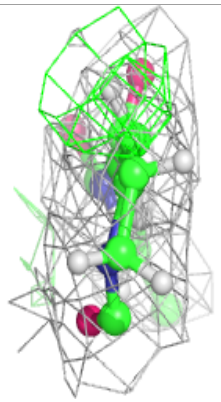


Electron density around ZGV H 302:

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

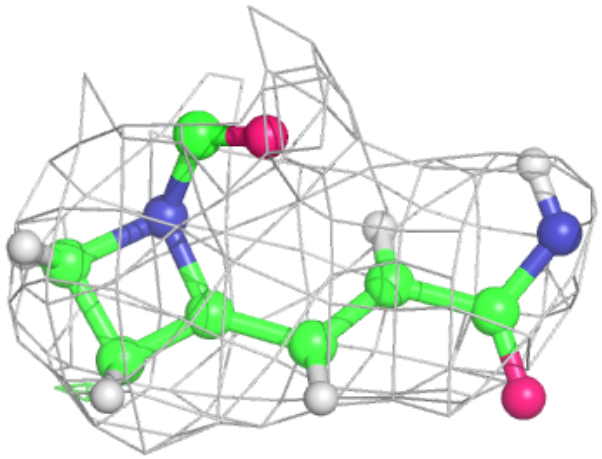


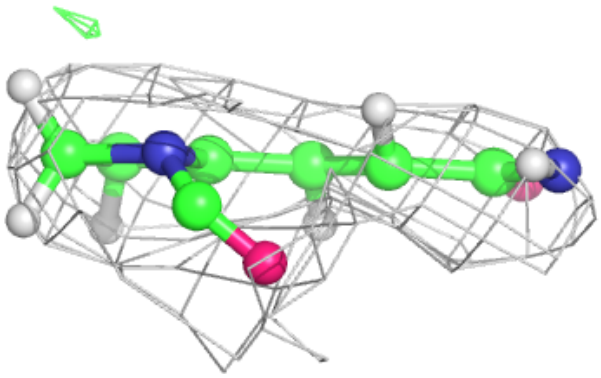


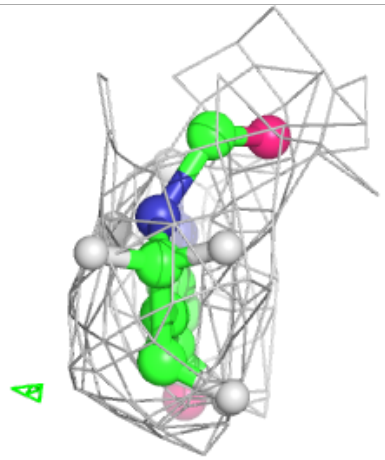


Electron density around ZGV b 303:

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

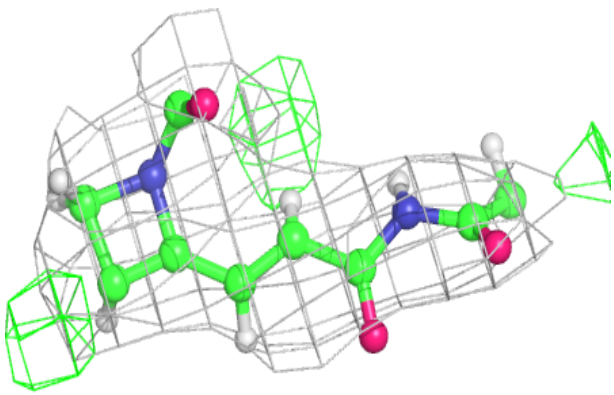


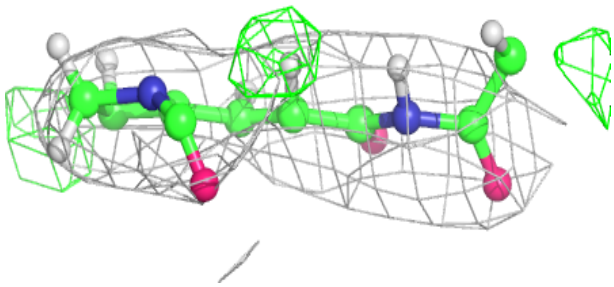


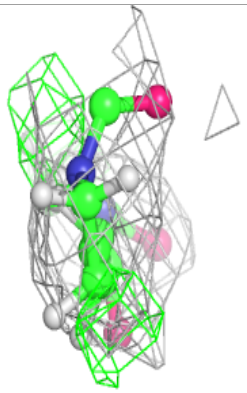


Electron density around ZGV Q 303:

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

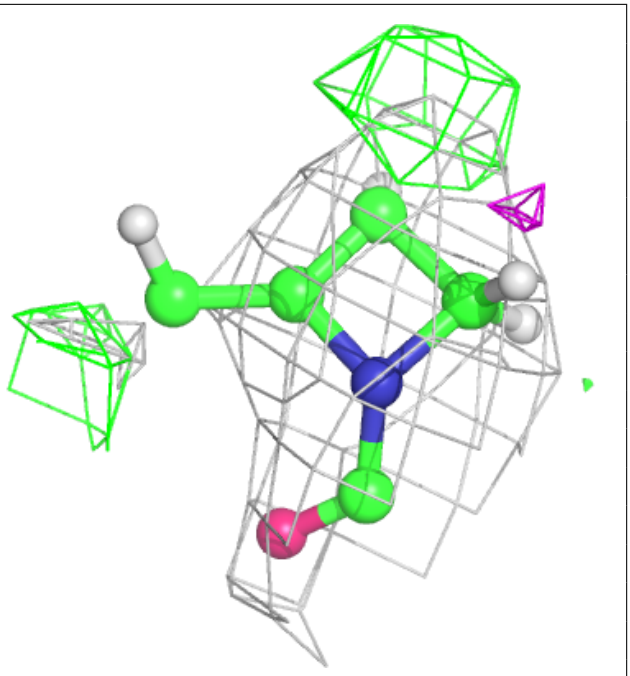


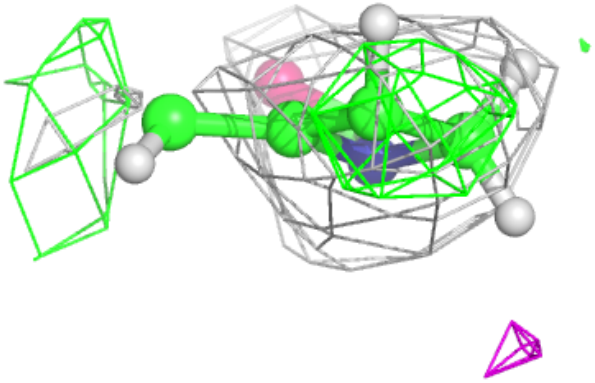


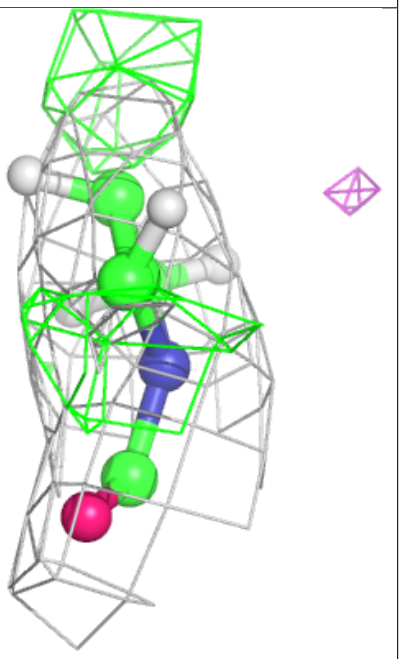


Electron density around ZGV V 302:

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

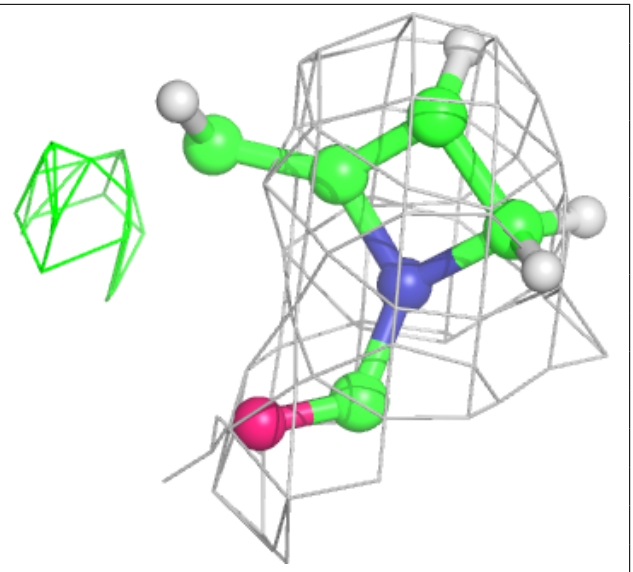


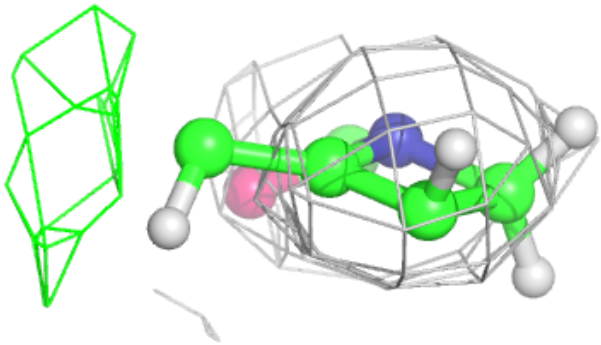


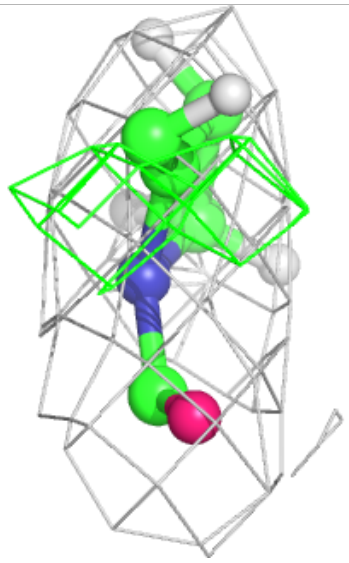


Electron density around ZGV Z 304:

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

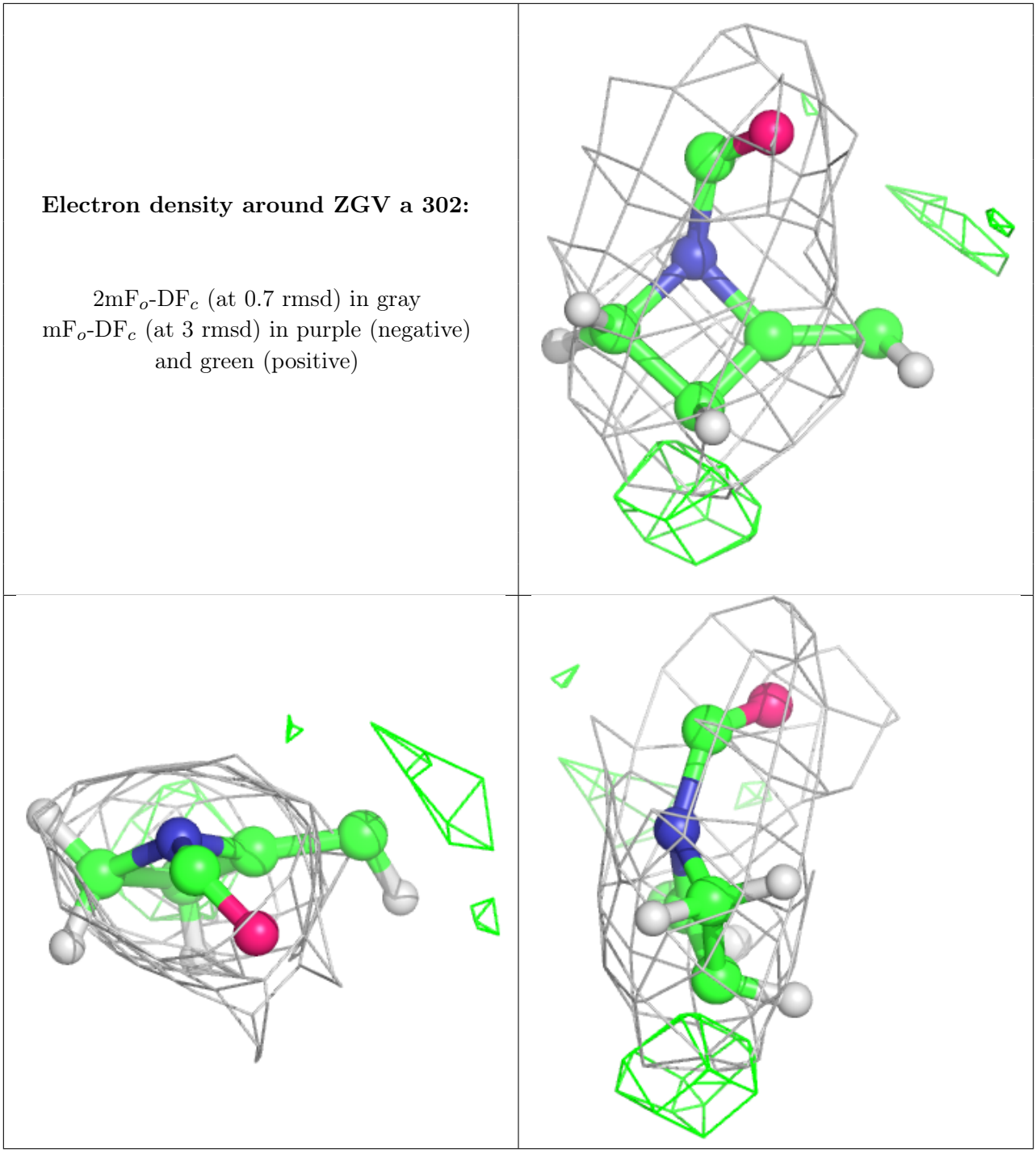






Electron density around ZGV a 302:

$2mF_o$-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.