Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2026 – 10:17 AM UTC

PDB ID	:	6DM8 / pdb_00006dm8
Title	:	Understanding the Species Selectivity of Myeloid cell leukemia-1 (Mcl-1) inhibitors
Authors	:	Zhao, B.
Deposited on	:	2018-06-04
Resolution	:	2.70 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

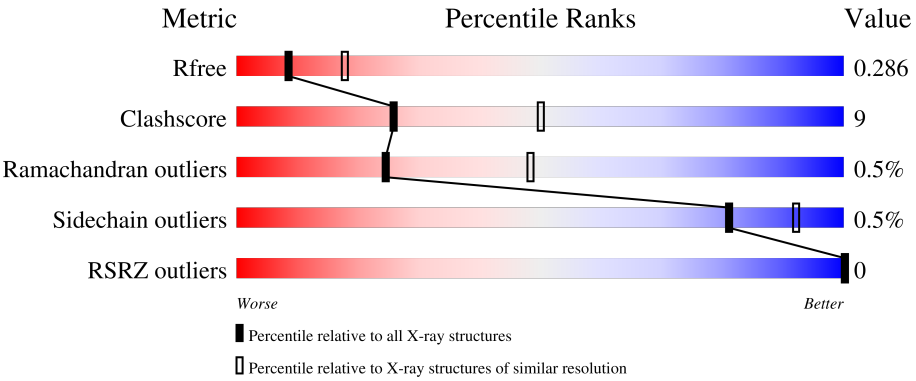
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	518	79% 19% ••
1	B	518	81% 17% ••
1	C	518	82% 15% •
1	D	518	78% 18% ••
1	E	518	77% 20% •

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Mol	Chain	Length	Quality of chain
1	F	518	76% 20%
1	G	518	78% 19%
1	H	518	79% 18%
2	I	2	50% 50%
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	50% 50%
2	M	2	50% 50%
2	N	2	50% 50%
2	O	2	50% 50%
2	P	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32595 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	1	0
			3910	2505	654	743	8			
1	B	507	Total	C	N	O	S	3	1	0
			3848	2470	645	725	8			
1	C	508	Total	C	N	O	S	3	1	0
			3872	2488	649	727	8			
1	D	504	Total	C	N	O	S	6	1	0
			3848	2476	639	725	8			
1	E	507	Total	C	N	O	S	0	0	0
			3860	2478	646	728	8			
1	F	504	Total	C	N	O	S	0	0	0
			3803	2447	626	722	8			
1	G	506	Total	C	N	O	S	0	1	0
			3814	2448	638	720	8			
1	H	501	Total	C	N	O	S	0	1	0
			3783	2430	627	718	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-215	GLY	-	expression tag	UNP P0AEX9
A	152	GLY	-	linker	UNP P0AEX9
A	153	SER	-	linker	UNP P0AEX9
B	-214	GLY	-	expression tag	UNP P0AEX9
B	152	GLY	-	linker	UNP P0AEX9
B	153	SER	-	linker	UNP P0AEX9
C	-214	GLY	-	expression tag	UNP P0AEX9
C	152	GLY	-	linker	UNP P0AEX9
C	153	SER	-	linker	UNP P0AEX9
D	-215	GLY	-	expression tag	UNP P0AEX9
D	152	GLY	-	linker	UNP P0AEX9
D	153	SER	-	linker	UNP P0AEX9

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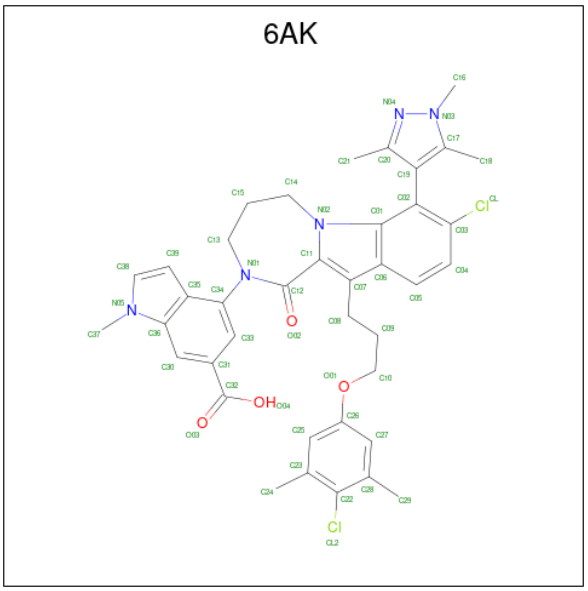
Chain	Residue	Modelled	Actual	Comment	Reference
E	-215	GLY	-	expression tag	UNP P0AEX9
E	152	GLY	-	linker	UNP P0AEX9
E	153	SER	-	linker	UNP P0AEX9
F	-215	GLY	-	expression tag	UNP P0AEX9
F	152	GLY	-	linker	UNP P0AEX9
F	153	SER	-	linker	UNP P0AEX9
G	-215	GLY	-	expression tag	UNP P0AEX9
G	152	GLY	-	linker	UNP P0AEX9
G	153	SER	-	linker	UNP P0AEX9
H	-214	GLY	-	expression tag	UNP P0AEX9
H	152	GLY	-	linker	UNP P0AEX9
H	153	SER	-	linker	UNP P0AEX9

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	N	2	Total	C	O	0	0	0
			23	12	11			
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	P	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is 4-{8-chloro-11-[3-(4-chloro-3,5-dimethylphenoxy)propyl]-1-oxo-7-(1,3,5-trimethyl-1H-pyrazol-4-yl)-4,5-dihydro-1H-[1,4]diazepino[1,2-a]indol-2(3H)-yl}-1-methyl-1H-indole-6-carboxylic acid (CCD ID: 6AK) (formula: $C_{39}H_{39}Cl_2N_5O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	A	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	A	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	B	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	B	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	C	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	C	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	C	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	C	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	D	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	D	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	E	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	E	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	F	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	F	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	F	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	G	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	G	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	G	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	H	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	H	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	H	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		
3	H	1	Total	C	Cl	N	O	0	0
			50	39	2	5	4		

- Molecule 4 is water.

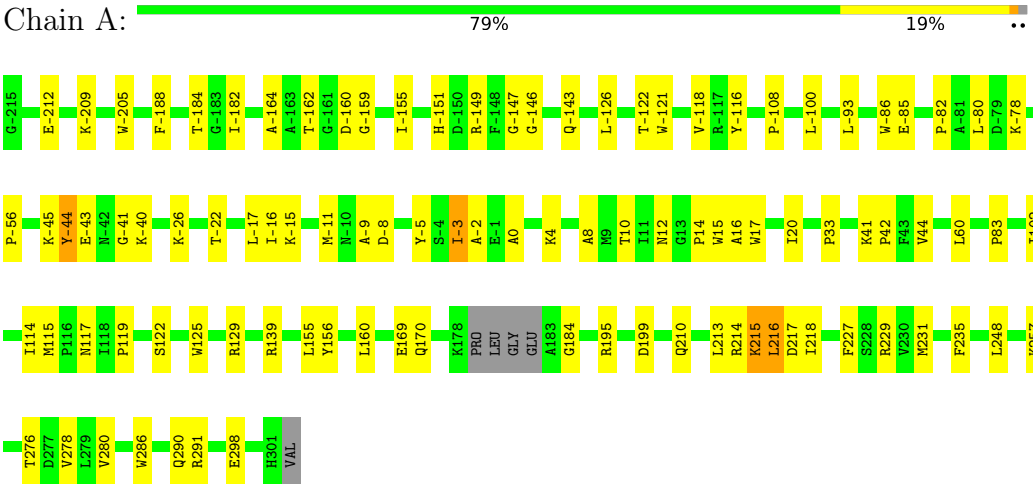
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	73	Total	O	0	0
			73	73		
4	C	58	Total	O	0	0
			58	58		
4	D	58	Total	O	0	0
			58	58		
4	E	45	Total	O	0	0
			45	45		
4	F	46	Total	O	0	0
			46	46		
4	G	73	Total	O	0	0
			73	73		
4	H	70	Total	O	0	0
			70	70		

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.

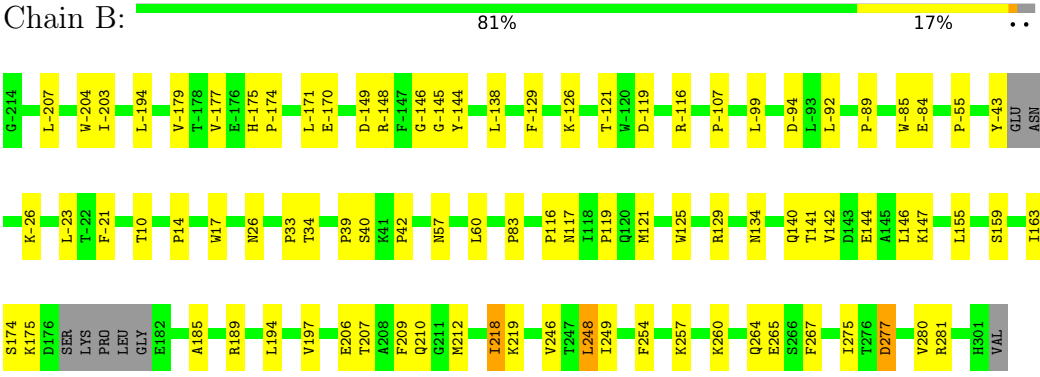
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera

Chain A:



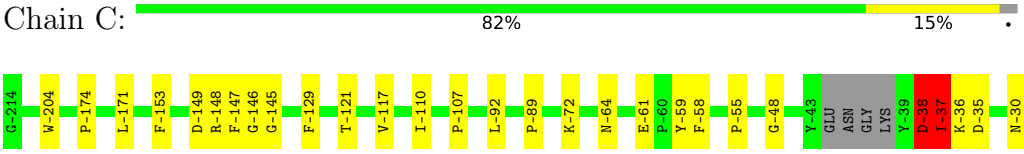
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera

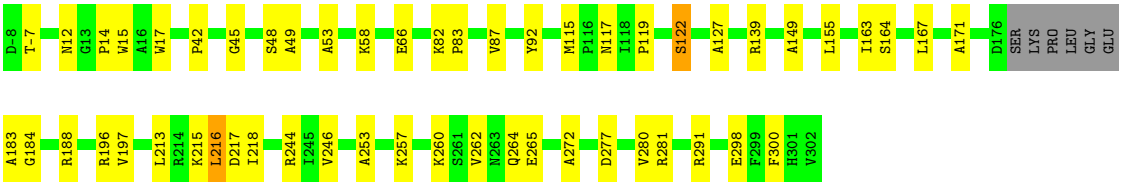
Chain B:



• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera

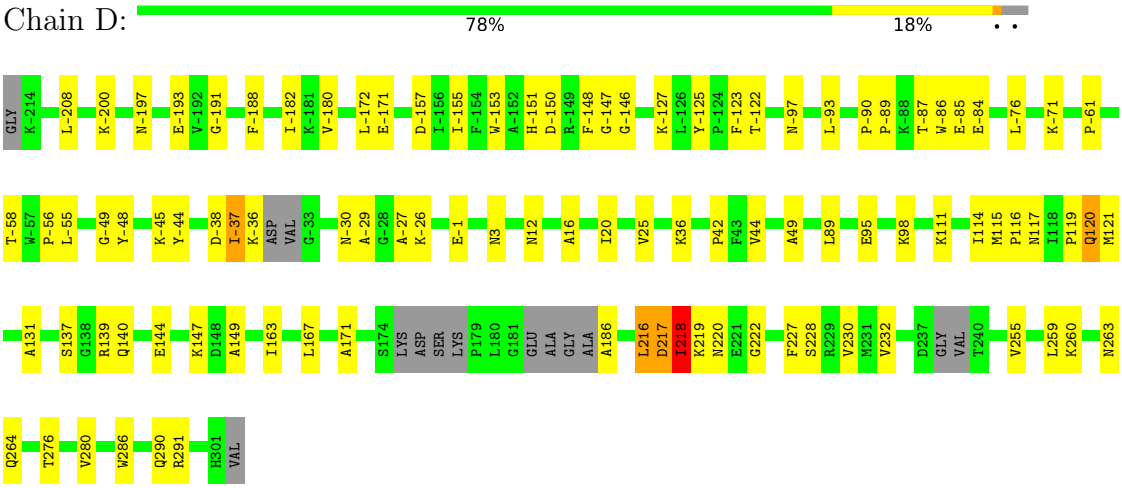
Chain C:





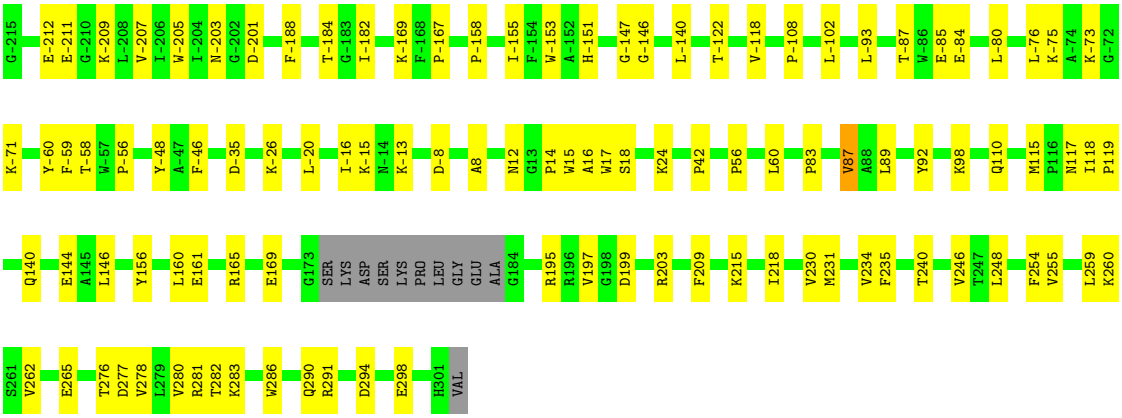
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera

Chain D:



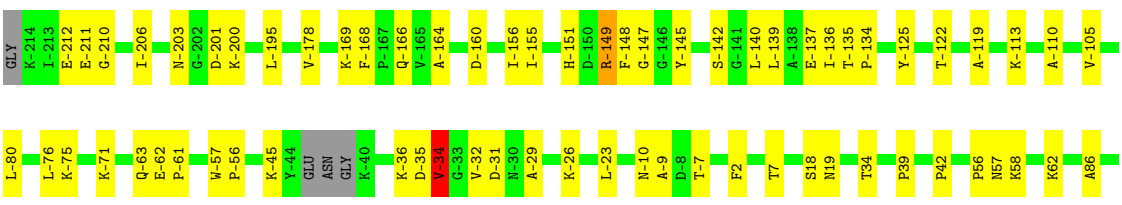
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera

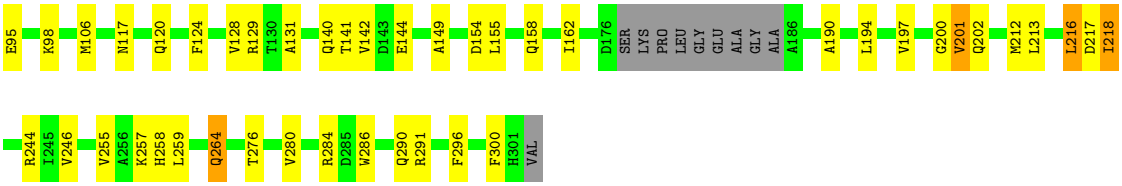
Chain E:



• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera

Chain F:

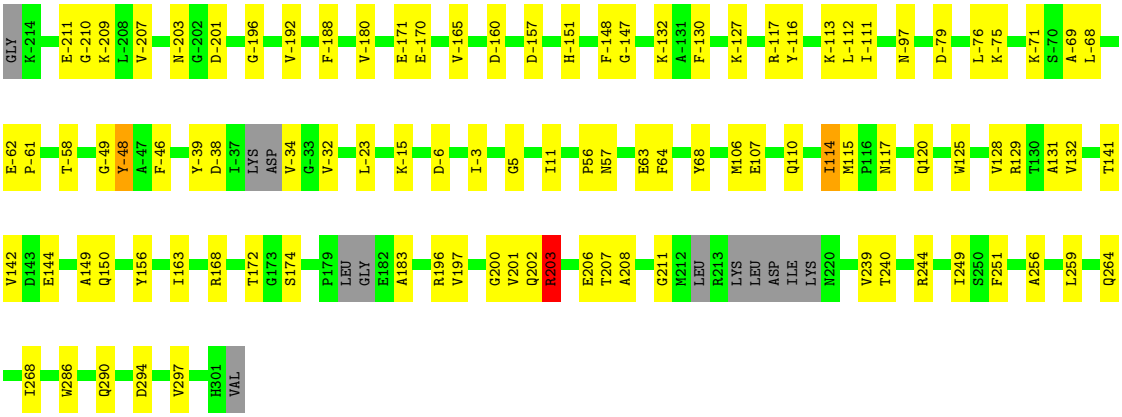




• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera

Chain G:

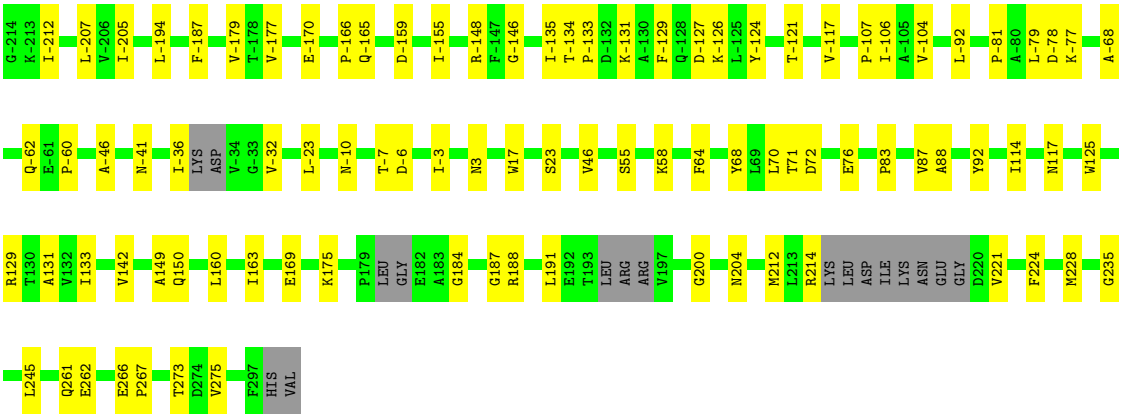




• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1 homolog - MBP chimera

Chain H:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:





• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.21Å 104.15Å 146.21Å 89.86° 89.80° 89.97°	Depositor
Resolution (Å)	29.97 – 2.70 29.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.97-2.70) 98.6 (29.97-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.68Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.245 , 0.288 0.249 , 0.286	Depositor DCC
R_{free} test set	1999 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 12.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.349 for h,-k,-l 0.458 for -h,k,-l 0.357 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	32595	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6AK, GLC

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	0.31	1/4002 (0.0%)	0.39	2/5440 (0.0%)
1	B	0.12	0/3939	0.30	0/5356
1	C	0.25	0/3964	0.39	2/5390 (0.0%)
1	D	0.28	1/3939 (0.0%)	0.45	0/5348
1	E	0.11	0/3949	0.32	1/5368 (0.0%)
1	F	0.33	3/3892 (0.1%)	0.48	5/5300 (0.1%)
1	G	0.18	0/3905	0.42	0/5313
1	H	0.15	0/3873	0.34	0/5270
All	All	0.23	5/31463 (0.0%)	0.39	10/42785 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	217	ASP	CA-C	-7.71	1.44	1.52
1	F	-34	VAL	C-O	-5.68	1.17	1.24
1	F	-149	ARG	C-O	-5.18	1.17	1.24
1	A	218	ILE	C-O	-5.17	1.18	1.24
1	D	-37	ILE	C-O	-5.17	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	216	LEU	N-CA-C	-8.77	97.87	110.59
1	A	-43	GLU	N-CA-C	-8.39	98.07	110.48
1	C	-38	ASP	N-CA-C	8.35	122.76	107.73
1	F	264	GLN	N-CA-C	-8.29	100.27	110.88
1	A	-44	TYR	N-CA-C	8.22	123.03	112.92
1	F	218	ILE	N-CA-C	6.01	121.83	109.34
1	E	262	VAL	N-CA-C	-5.83	106.81	112.29
1	F	-75	LYS	N-CA-C	-5.75	105.02	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	-37	ILE	N-CA-CB	-5.70	101.82	111.23
1	F	-36	LYS	N-CA-C	5.04	117.81	109.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3910	0	3760	77	0
1	B	3848	0	3696	69	0
1	C	3872	0	3738	56	0
1	D	3848	0	3690	83	0
1	E	3860	0	3717	68	0
1	F	3803	0	3612	82	0
1	G	3814	0	3626	80	0
1	H	3783	0	3613	71	0
2	I	23	0	21	2	0
2	J	23	0	21	1	0
2	K	23	0	21	2	0
2	L	23	0	21	2	0
2	M	23	0	21	1	0
2	N	23	0	21	2	0
2	O	23	0	21	1	0
2	P	23	0	21	0	0
3	A	150	0	0	3	0
3	B	100	0	0	4	0
3	C	200	0	0	4	0
3	D	100	0	0	1	0
3	E	100	0	0	3	0
3	F	200	0	0	7	0
3	G	150	0	0	5	0
3	H	200	0	0	5	0
4	A	50	0	0	3	0
4	B	73	0	0	7	0
4	C	58	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	58	0	0	4	0
4	E	45	0	0	3	0
4	F	46	0	0	5	0
4	G	73	0	0	5	0
4	H	70	0	0	9	0
All	All	32595	0	29620	585	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (585) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:C	1:B:248:LEU:HD23	1.71	1.16
1:D:116:PRO:HD2	1:D:121:MET:CE	1.83	1.08
3:A:404:6AK:C16	1:G:114:ILE:HB	1.85	1.05
3:H:301:6AK:CL2	4:H:467:HOH:O	2.20	0.95
1:D:116:PRO:HD2	1:D:121:MET:HE2	1.50	0.91
3:C:405:6AK:C16	1:D:114:ILE:HG22	2.00	0.91
1:D:116:PRO:HD2	1:D:121:MET:HE1	1.50	0.91
1:D:-45:LYS:HG3	1:D:-36:LYS:HB3	1.61	0.83
1:G:168:ARG:HH21	1:G:172:THR:HG21	1.43	0.83
1:A:-143:GLN:HB2	4:A:501:HOH:O	1.79	0.81
1:E:-212:GLU:HG2	1:E:-209:LYS:HE2	1.63	0.81
1:C:213:LEU:HD12	1:C:216:LEU:HD11	1.62	0.79
1:A:-44:TYR:CE1	1:A:-40:LYS:HA	2.17	0.79
1:G:-61:PRO:HA	1:G:-58:THR:HG22	1.65	0.78
1:A:262:VAL:HG13	1:A:264:GLN:HG3	1.68	0.75
1:E:-75:LYS:NZ	1:E:-13:LYS:O	2.20	0.75
1:F:-136:ILE:HD11	1:F:-110:ALA:CA	2.16	0.74
1:F:-136:ILE:HD11	1:F:-110:ALA:C	2.12	0.74
1:B:209:PHE:HA	1:B:212:MET:HB3	1.68	0.74
1:H:200:GLY:O	1:H:204:ASN:N	2.20	0.74
1:G:141:THR:HG23	1:G:144:GLU:H	1.52	0.74
1:F:154:ASP:HB3	1:F:158:GLN:HG3	1.68	0.73
1:A:115:MET:HE3	1:A:125:TRP:HZ2	1.54	0.73
1:F:-135:THR:O	1:F:62:LYS:NZ	2.21	0.73
1:F:58:LYS:NZ	4:F:503:HOH:O	2.20	0.72
1:H:-135:ILE:HG22	1:H:-133:PRO:HD3	1.72	0.71
1:B:163:ILE:HD12	1:B:249:ILE:HG12	1.73	0.71
1:B:248:LEU:HD23	1:B:249:ILE:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:PRO:HB2	1:F:291:ARG:HH22	1.53	0.71
1:A:-205:TRP:HB2	1:A:-155:ILE:HD12	1.72	0.70
1:H:72:ASP:O	1:H:76:GLU:HG3	1.91	0.70
1:C:-204:TRP:HB3	1:C:-171:LEU:HD11	1.73	0.70
1:A:235:PHE:CZ	1:A:248:LEU:HD13	2.27	0.70
1:D:12:ASN:ND2	4:D:502:HOH:O	2.25	0.69
1:G:64:PHE:O	1:G:68:TYR:HB2	1.91	0.69
1:B:248:LEU:HD21	1:B:275:ILE:HG23	1.73	0.69
1:F:19:ASN:N	4:F:501:HOH:O	2.20	0.68
1:E:-184:THR:HG23	1:E:-182:ILE:H	1.57	0.68
1:H:-23:LEU:HD23	1:H:142:VAL:HG13	1.75	0.68
1:D:-146:GLY:HA2	1:D:119:PRO:HB3	1.76	0.68
1:D:147:LYS:HZ3	1:D:291:ARG:HB3	1.57	0.68
1:E:12:ASN:HD21	1:E:15:TRP:NE1	1.92	0.68
1:H:-165:GLN:N	1:H:-165:GLN:OE1	2.27	0.68
1:A:-188:PHE:O	1:A:-184:THR:HB	1.94	0.67
1:E:282:THR:HG23	1:E:283:LYS:HG2	1.74	0.67
1:D:-76:LEU:HB3	1:D:-71:LYS:HB2	1.77	0.67
1:G:-203:ASN:ND2	1:G:-201:ASP:OD1	2.27	0.67
1:G:64:PHE:HA	1:G:68:TYR:HD2	1.60	0.67
1:D:-172:LEU:HD11	1:D:-155:ILE:HD11	1.76	0.67
1:G:256:ALA:HB1	1:G:268:ILE:HD11	1.76	0.67
1:F:194:LEU:HA	1:F:197:VAL:HG22	1.78	0.66
1:G:168:ARG:HD3	1:G:172:THR:HG21	1.76	0.66
1:H:163:ILE:HD12	1:H:273:THR:HG22	1.76	0.66
1:F:-136:ILE:HG22	1:F:-134:PRO:HD3	1.78	0.66
1:H:160:LEU:HA	1:H:273:THR:HG21	1.78	0.66
1:E:110:GLN:NE2	4:E:503:HOH:O	2.29	0.66
1:F:259:LEU:O	1:F:264:GLN:N	2.27	0.65
1:B:-207:LEU:HB2	1:B:-179:VAL:HG22	1.78	0.65
1:E:260:LYS:HD2	1:E:265:GLU:HG3	1.79	0.65
1:G:-58:THR:HG21	1:G:132:VAL:HG11	1.77	0.65
1:G:208:ALA:HB1	3:G:401:6AK:CL	2.34	0.64
1:F:200:GLY:O	1:F:202:GLN:N	2.28	0.64
1:G:64:PHE:HA	1:G:68:TYR:CD2	2.33	0.64
1:D:218:ILE:HD11	1:D:227:PHE:HE2	1.63	0.64
1:E:-93:LEU:HD23	1:E:8:ALA:HB1	1.80	0.63
3:C:405:6AK:C16	1:D:114:ILE:CG2	2.75	0.63
1:D:186:ALA:N	4:D:511:HOH:O	2.32	0.63
1:B:-170:GLU:HB2	1:B:-148:ARG:HE	1.64	0.63
1:A:17:TRP:HB2	1:A:83:PRO:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:TRP:O	1:G:290:GLN:HG2	1.98	0.63
1:A:-78:LYS:HD3	1:D:263:ASN:HB2	1.81	0.63
1:E:-26:LYS:HD3	1:E:146:LEU:HD12	1.80	0.63
1:E:87:VAL:HG21	1:E:92:TYR:HB3	1.80	0.63
1:G:-171:GLU:HG2	1:G:-170:GLU:HG2	1.81	0.62
1:F:-142:SER:HB2	1:F:-140:LEU:HD11	1.80	0.62
1:F:-62:GLU:CD	1:F:129:ARG:NH2	2.57	0.62
1:B:172:THR:HG22	1:B:174:SER:H	1.64	0.62
1:D:-125:TYR:O	1:D:-122:THR:HG22	2.00	0.62
1:A:139:ARG:HH22	1:C:139:ARG:HB3	1.64	0.61
1:A:129:ARG:HH21	2:I:2:GLC:H62	1.64	0.61
1:G:259:LEU:O	1:G:264:GLN:N	2.33	0.61
1:B:248:LEU:HD23	1:B:248:LEU:O	1.99	0.61
1:G:-32:VAL:N	1:G:150:GLN:OE1	2.34	0.61
1:G:63:GLU:HG3	1:G:68:TYR:HE2	1.66	0.61
1:G:115:MET:HE3	1:G:125:TRP:HZ2	1.66	0.61
1:G:202:GLN:O	1:G:206:GLU:N	2.34	0.60
1:G:-23:LEU:HD23	1:G:142:VAL:HG13	1.83	0.60
1:A:-41:GLY:O	1:A:-40:LYS:HG3	2.01	0.60
1:D:16:ALA:O	1:D:20:ILE:HG13	2.01	0.60
1:H:169:GLU:HG2	1:H:175:LYS:HA	1.83	0.60
1:G:168:ARG:O	1:G:172:THR:HG22	2.02	0.60
1:H:187:GLY:O	1:H:191:LEU:N	2.28	0.60
1:A:156:TYR:HD2	1:A:280:VAL:HG21	1.66	0.59
1:A:235:PHE:HE1	3:A:401:6AK:C09	2.15	0.59
1:D:230:VAL:HA	3:E:403:6AK:CL2	2.39	0.59
1:G:-39:TYR:CE2	1:G:114:ILE:HG22	2.37	0.59
1:D:216:LEU:O	1:D:217:ASP:CB	2.48	0.59
1:F:-62:GLU:OE2	1:F:129:ARG:NH2	2.35	0.59
1:H:-212:ILE:CD1	1:H:-159:ASP:HA	2.31	0.59
1:H:188:ARG:HA	1:H:191:LEU:HB2	1.84	0.59
1:H:-6:ASP:H	1:H:-3:ILE:HD12	1.67	0.59
1:D:-61:PRO:HA	1:D:-58:THR:OG1	2.02	0.59
1:D:111:LYS:HD2	4:D:507:HOH:O	2.03	0.59
1:D:116:PRO:CD	1:D:121:MET:HE2	2.28	0.59
1:F:141:THR:OG1	1:F:144:GLU:HB2	2.02	0.59
1:A:235:PHE:HZ	1:A:248:LEU:HB2	1.68	0.58
1:B:-85:TRP:HB3	1:B:-21:PHE:HE2	1.67	0.58
1:B:254:PHE:HA	1:B:257:LYS:HE2	1.84	0.58
1:C:53:ALA:O	1:C:58:LYS:NZ	2.36	0.58
1:H:-131:LYS:HE3	1:H:-127:ASP:OD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LYS:NZ	1:D:291:ARG:HB3	2.19	0.58
1:A:-93:LEU:HD22	1:A:-80:LEU:HD21	1.85	0.58
1:F:162:ILE:HD13	1:F:190:ALA:HB3	1.84	0.58
1:F:257:LYS:NZ	4:F:507:HOH:O	2.36	0.58
1:G:-62:GLU:HG3	1:G:129:ARG:HE	1.69	0.58
1:C:-38:ASP:O	1:C:-36:LYS:N	2.37	0.58
1:E:-93:LEU:HD22	1:E:-80:LEU:HD21	1.85	0.58
1:D:218:ILE:CD1	1:D:227:PHE:HE2	2.17	0.58
1:H:71:THR:N	4:H:413:HOH:O	2.36	0.58
1:H:221:VAL:HA	1:H:224:PHE:CE2	2.39	0.58
1:C:-174:PRO:HD2	1:C:-171:LEU:HD13	1.85	0.58
1:A:-93:LEU:HD23	1:A:8:ALA:HB1	1.86	0.57
1:D:-171:GLU:HG2	1:D:-153:TRP:CZ2	2.39	0.57
1:H:-170:GLU:HB2	1:H:-148:ARG:HD2	1.86	0.57
1:D:228:SER:O	1:D:232:VAL:HG23	2.04	0.57
1:A:227:PHE:HB3	1:A:231:MET:HE2	1.87	0.57
1:D:259:LEU:HD22	1:D:264:GLN:HB2	1.87	0.57
1:G:196:ARG:O	1:G:200:GLY:N	2.37	0.57
1:H:-187:PHE:CD1	1:H:68:TYR:HE2	2.23	0.57
1:D:-200[A]:LYS:NZ	2:L:1:GLC:O2	2.34	0.57
1:F:158:GLN:O	1:F:162:ILE:HG13	2.05	0.57
1:H:-32:VAL:H	1:H:150:GLN:NE2	2.03	0.57
1:C:281:ARG:NH2	4:C:506:HOH:O	2.38	0.57
1:E:-188:PHE:O	1:E:-184:THR:HG22	2.04	0.57
1:C:183:ALA:N	4:C:507:HOH:O	2.38	0.56
1:B:248:LEU:HD22	1:B:249:ILE:HD12	1.88	0.56
1:H:-148:ARG:NH1	4:H:412:HOH:O	2.35	0.56
1:H:68:TYR:C	4:H:413:HOH:O	2.48	0.56
1:B:-55:PRO:HG3	1:B:42:PRO:HA	1.87	0.56
1:F:155:LEU:HD22	1:F:280:VAL:HG22	1.87	0.56
1:G:206:GLU:CD	1:G:207:THR:H	2.13	0.56
1:B:-204:TRP:HB3	1:B:-171:LEU:HD11	1.87	0.56
1:C:-38:ASP:C	1:C:-36:LYS:H	2.14	0.56
1:E:17:TRP:HB2	1:E:83:PRO:HG2	1.87	0.56
1:F:-10:ASN:OD1	1:F:-7:THR:OG1	2.24	0.55
1:D:216:LEU:O	1:D:217:ASP:CG	2.49	0.55
1:A:-184:THR:HG22	1:A:-182:ILE:H	1.71	0.55
1:G:244:ARG:NH1	4:G:513:HOH:O	2.38	0.55
1:B:248:LEU:HG	3:B:403:6AK:C10	2.36	0.55
1:F:-56:PRO:HG3	1:F:42:PRO:HA	1.88	0.55
1:F:2:PHE:HA	1:F:7:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:GLN:HG2	3:G:404:6AK:C25	2.36	0.55
1:H:-129:PHE:HA	1:H:-126:LYS:HD2	1.89	0.55
1:D:-56:PRO:HG3	1:D:42:PRO:HA	1.88	0.55
1:G:-210:GLY:O	1:G:-209:LYS:HD3	2.06	0.55
1:B:-174:PRO:HD2	1:B:-171:LEU:HD13	1.89	0.55
1:D:-171:GLU:HG2	1:D:-153:TRP:CH2	2.41	0.55
1:G:114:ILE:HD11	3:G:403:6AK:C24	2.37	0.55
1:C:291:ARG:HH21	1:C:298:GLU:CD	2.13	0.54
3:F:405:6AK:C19	3:F:405:6AK:C14	2.86	0.54
1:B:248:LEU:CG	3:B:403:6AK:C10	2.85	0.54
1:F:-136:ILE:CD1	1:F:-110:ALA:C	2.80	0.54
1:E:140:GLN:HB3	1:E:144:GLU:HG3	1.90	0.54
1:E:56:PRO:HB2	1:F:291:ARG:NH2	2.22	0.54
1:G:239:VAL:HG12	1:G:240:THR:N	2.22	0.54
1:A:235:PHE:CZ	1:A:248:LEU:HB2	2.42	0.54
1:C:197:VAL:HG12	1:C:246:VAL:HG11	1.90	0.54
1:E:-182:ILE:HD13	1:E:60:LEU:HD13	1.90	0.54
1:F:255:VAL:O	1:F:259:LEU:HG	2.08	0.54
1:F:-76:LEU:HB3	1:F:-71:LYS:HB2	1.90	0.54
1:D:-30:ASN:OD1	1:D:-27:ALA:N	2.36	0.54
1:F:276:THR:O	1:F:280:VAL:HG23	2.08	0.53
1:E:-76:LEU:HB3	1:E:-71:LYS:HB2	1.90	0.53
1:E:-58:THR:HG21	1:E:-20:LEU:HD22	1.89	0.53
1:E:197:VAL:HG12	1:E:246:VAL:HG11	1.91	0.53
1:G:115:MET:HE3	1:G:125:TRP:CZ2	2.43	0.53
1:E:231:MET:HB3	1:E:278:VAL:HG11	1.89	0.53
1:F:-125:TYR:O	1:F:-122:THR:OG1	2.25	0.53
1:G:-34:VAL:HG12	1:G:150:GLN:HE22	1.73	0.53
1:E:-118:VAL:HG21	1:E:-108:PRO:HD3	1.89	0.53
1:E:294:ASP:O	1:E:298:GLU:HG3	2.08	0.53
1:B:-149:ASP:OD2	1:B:-149:ASP:N	2.42	0.53
1:C:216:LEU:HB3	1:C:218:ILE:HG22	1.90	0.53
1:D:218:ILE:CD1	1:D:227:PHE:CE2	2.92	0.53
1:B:134:ASN:HB3	1:B:140:GLN:HB2	1.91	0.53
1:E:169:GLU:OE1	1:E:195:ARG:NE	2.36	0.53
3:F:405:6AK:C14	3:F:405:6AK:C20	2.86	0.52
1:H:-212:ILE:HD13	1:H:-159:ASP:HA	1.89	0.52
1:C:265:GLU:H	1:C:265:GLU:CD	2.18	0.52
1:B:147:LYS:N	4:B:502:HOH:O	2.41	0.52
1:E:255:VAL:O	1:E:259:LEU:HG	2.10	0.52
1:F:140:GLN:NE2	1:F:144:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:-62:GLN:HA	1:H:133:ILE:HD11	1.92	0.52
1:A:-147:GLY:HA3	1:A:117:ASN:O	2.09	0.52
1:B:-92:LEU:HD21	1:B:-89:PRO:HA	1.91	0.52
1:F:-136:ILE:HD11	1:F:-110:ALA:N	2.23	0.52
1:G:-165:VAL:HG22	1:G:-160:ASP:HB3	1.92	0.52
1:H:-32:VAL:HB	1:H:150:GLN:HE21	1.75	0.52
1:A:169:GLU:OE2	1:A:195:ARG:NE	2.36	0.52
1:G:-211:GLU:HG2	1:G:56:PRO:HG3	1.92	0.52
1:A:-8:ASP:OD2	1:C:139:ARG:NE	2.43	0.52
1:F:-147:GLY:HA3	1:F:117:ASN:O	2.10	0.52
1:H:-41:ASN:N	4:H:405:HOH:O	2.43	0.52
1:A:-149:ARG:NH1	1:A:122:SER:OG	2.42	0.52
1:A:210:GLN:HB3	1:A:214:ARG:HH21	1.75	0.52
1:D:120:GLN:O	1:D:120:GLN:HG2	2.09	0.52
1:H:-121:THR:HG21	1:H:88:ALA:HB1	1.92	0.52
1:E:277:ASP:OD1	1:E:281:ARG:HD3	2.10	0.52
1:F:259:LEU:HB3	1:F:264:GLN:HB2	1.91	0.51
1:E:14:PRO:HA	1:E:17:TRP:CE2	2.45	0.51
1:B:257:LYS:HA	1:B:260:LYS:HB2	1.93	0.51
1:D:216:LEU:C	1:D:217:ASP:CG	2.75	0.51
1:F:-105:VAL:HB	1:F:86:ALA:HB3	1.91	0.51
1:H:-207:LEU:HD12	1:H:-187:PHE:HE2	1.75	0.51
1:B:-148:ARG:HH12	1:B:125:TRP:CD1	2.28	0.51
1:H:114:ILE:HD13	3:H:305:6AK:C23	2.41	0.51
1:A:229:ARG:NH1	3:A:404:6AK:O02	2.43	0.51
1:F:-195:LEU:HD23	1:F:-178:VAL:HG11	1.91	0.51
1:D:218:ILE:HD11	1:D:227:PHE:CE2	2.43	0.51
1:E:87:VAL:HG23	1:E:89:LEU:H	1.75	0.51
1:F:-200:LYS:NZ	2:N:1:GLC:O2	2.44	0.51
1:F:-142:SER:HB2	1:F:-140:LEU:CD1	2.41	0.51
1:H:266:GLU:HG2	1:H:267:PRO:HD3	1.93	0.51
1:B:129:ARG:NH1	4:B:517:HOH:O	2.43	0.51
1:D:217:ASP:OD1	1:D:218:ILE:N	2.36	0.51
1:H:-81:PRO:HG2	4:H:439:HOH:O	2.11	0.51
1:A:115:MET:HE3	1:A:125:TRP:CZ2	2.42	0.51
1:F:-168:PHE:CG	1:F:-155:ILE:HD12	2.45	0.51
1:F:-61:PRO:HD3	1:F:129:ARG:HG2	1.91	0.51
1:G:163:ILE:HG23	1:G:249:ILE:HG23	1.93	0.51
1:G:131:ALA:HB2	1:G:149:ALA:HB2	1.93	0.51
1:B:129:ARG:HH21	2:J:2:GLC:H62	1.75	0.50
1:B:185:ALA:HB1	1:B:189:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-87:THR:HG22	1:D:-85:GLU:H	1.76	0.50
1:E:-146:GLY:HA2	1:E:119:PRO:HB3	1.92	0.50
1:E:-102:LEU:HD21	1:E:-60:TYR:HE2	1.75	0.50
1:F:213:LEU:HD11	1:F:258:HIS:CG	2.46	0.50
1:G:-49:GLY:O	1:G:-48:TYR:HB2	2.11	0.50
1:E:-201:ASP:OD2	2:M:1:GLC:O1	2.27	0.50
1:G:-211:GLU:HG2	1:G:56:PRO:CG	2.40	0.50
1:G:-113:LYS:HE3	1:G:-111:ILE:HG22	1.94	0.50
1:B:-84:GLU:OE1	1:B:-84:GLU:N	2.42	0.50
1:F:131:ALA:HB2	1:F:149:ALA:HB2	1.93	0.50
1:G:-130:PHE:O	1:G:-127:LYS:HB2	2.11	0.50
1:D:-172:LEU:HD11	1:D:-155:ILE:CD1	2.42	0.50
1:E:-85:GLU:N	1:E:-85:GLU:OE1	2.45	0.50
1:F:-29:ALA:HA	1:F:-26:LYS:HD2	1.93	0.50
1:H:-205:ILE:HB	1:H:-177:VAL:HG22	1.94	0.50
1:A:-205:TRP:CB	1:A:-155:ILE:HD12	2.40	0.50
1:H:17:TRP:HB2	1:H:83:PRO:HG2	1.94	0.50
1:D:-123:PHE:HB2	3:D:403:6AK:C26	2.42	0.50
1:B:218:ILE:N	4:B:516:HOH:O	2.43	0.49
1:B:248:LEU:C	1:B:248:LEU:CD2	2.50	0.49
1:D:-147:GLY:HA3	1:D:117:ASN:O	2.12	0.49
1:E:-147:GLY:HA3	1:E:117:ASN:O	2.11	0.49
1:E:24:LYS:NZ	4:E:507:HOH:O	2.44	0.49
1:A:-85:GLU:OE1	1:A:-85:GLU:N	2.43	0.49
1:E:-205:TRP:HB2	1:E:-155:ILE:HD12	1.94	0.49
1:F:-145:TYR:HB2	1:F:-139:LEU:HD11	1.94	0.49
1:H:3:ASN:O	1:H:23:SER:OG	2.29	0.49
1:D:44:VAL:HB	1:D:114:ILE:HA	1.94	0.49
1:F:-203:ASN:ND2	1:F:-201:ASP:OD1	2.45	0.49
1:A:-82:PRO:HG3	1:A:-17:LEU:HD21	1.93	0.49
1:C:-129:PHE:CZ	1:C:66:GLU:HG2	2.48	0.49
1:H:-60:PRO:HD3	1:H:129:ARG:HG3	1.95	0.49
1:A:44:VAL:HB	1:A:114:ILE:HA	1.95	0.49
1:B:-26:LYS:HG2	1:B:146:LEU:HD12	1.94	0.49
1:E:-87:THR:HG23	1:E:-84:GLU:H	1.78	0.49
1:F:213:LEU:HD23	1:F:255:VAL:HG22	1.93	0.49
1:G:-117:ARG:HG3	1:G:-112:LEU:HD23	1.94	0.49
1:D:95:GLU:HA	1:D:98:LYS:HE3	1.95	0.49
1:B:248:LEU:HB2	3:B:403:6AK:C10	2.42	0.49
1:H:131:ALA:HB2	1:H:149:ALA:HB2	1.94	0.49
1:A:-160:ASP:OD1	1:A:-159:GLY:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-29:ALA:HA	1:D:-26:LYS:HD2	1.94	0.49
1:F:201:VAL:HG11	1:F:246:VAL:HG12	1.94	0.49
1:G:-210:GLY:H	1:G:57:ASN:HD21	1.61	0.49
1:C:167:LEU:HD23	1:C:253:ALA:HA	1.94	0.48
1:D:-208:LEU:O	1:D:-180:VAL:HA	2.13	0.48
1:F:-57:TRP:CH2	1:F:-32:VAL:HG13	2.48	0.48
1:C:-48:GLY:HA2	1:C:-30:ASN:HD21	1.78	0.48
1:E:291:ARG:HH12	1:E:298:GLU:CD	2.21	0.48
1:H:-134:THR:O	1:H:-134:THR:OG1	2.29	0.48
1:A:-182:ILE:HD13	1:A:60:LEU:HD13	1.96	0.48
1:B:141:THR:OG1	1:B:144:GLU:HG3	2.14	0.48
1:B:277:ASP:O	1:B:281:ARG:HG3	2.13	0.48
1:D:-208:LEU:HD12	1:D:-188:PHE:HE2	1.78	0.48
1:E:-75:LYS:HG3	1:E:-71:LYS:O	2.13	0.48
1:E:286:TRP:O	1:E:290:GLN:HG2	2.13	0.48
1:B:159:SER:O	1:B:163:ILE:HG12	2.14	0.48
1:C:45:GLY:HA2	1:C:115:MET:HE2	1.95	0.48
1:C:215:LYS:CD	3:C:405:6AK:C29	2.91	0.48
1:E:-203:ASN:HD22	1:E:-153:TRP:HZ3	1.61	0.48
1:H:76:GLU:HG2	1:H:92:TYR:CZ	2.49	0.48
1:A:-151:HIS:NE2	1:A:115:MET:O	2.35	0.48
1:H:228:MET:HG3	1:H:275:VAL:HG11	1.96	0.48
1:A:210:GLN:O	1:A:214:ARG:N	2.47	0.48
1:C:-72:LYS:O	1:C:-72:LYS:HD3	2.13	0.48
1:B:14:PRO:HA	1:B:17:TRP:CE2	2.49	0.48
1:E:230:VAL:O	1:E:234:VAL:HG13	2.14	0.48
1:F:-169:LYS:O	1:F:-166:GLN:HB2	2.14	0.48
1:F:-149:ARG:NE	2:N:2:GLC:O3	2.43	0.48
1:A:41:LYS:NZ	1:A:111:LYS:O	2.31	0.48
1:G:239:VAL:HG12	1:G:240:THR:H	1.79	0.48
1:A:290:GLN:O	1:A:291:ARG:HB2	2.14	0.48
1:B:-145:GLY:HA2	1:B:119:PRO:HB3	1.95	0.48
1:C:184:GLY:O	1:C:188:ARG:HG2	2.13	0.48
1:D:-1:GLU:O	1:D:3:ASN:ND2	2.47	0.47
1:B:-121:THR:HB	1:B:-107:PRO:HB2	1.96	0.47
1:D:259:LEU:O	1:D:264:GLN:N	2.26	0.47
1:H:-212:ILE:HD11	1:H:-159:ASP:HA	1.96	0.47
1:H:235:GLY:HA3	3:H:301:6AK:O04	2.14	0.47
1:E:-16:ILE:HG22	1:E:-15:LYS:HE2	1.96	0.47
1:H:-187:PHE:CD1	1:H:68:TYR:CE2	3.02	0.47
1:H:-166:PRO:HG2	1:H:-165:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:PHE:O	1:H:68:TYR:HB2	2.14	0.47
1:C:163:ILE:HG13	1:C:164:SER:N	2.29	0.47
1:D:-155:ILE:O	1:D:49:ALA:HA	2.15	0.47
1:E:-8:ASP:HB2	4:E:525:HOH:O	2.15	0.47
1:F:-206:ILE:HG12	1:F:-156:ILE:HB	1.96	0.47
1:F:-164:ALA:HA	1:F:-160:ASP:O	2.14	0.47
1:G:172:THR:HG23	1:G:174:SER:H	1.79	0.47
1:A:-122:THR:HB	1:A:-108:PRO:HB2	1.97	0.47
1:A:210:GLN:HA	1:A:213:LEU:HB3	1.96	0.47
1:H:-6:ASP:CG	1:H:-3:ILE:HD12	2.39	0.47
1:B:-43:TYR:OH	1:B:116:PRO:HB3	2.15	0.47
1:C:-153:PHE:CE1	1:C:49:ALA:HB2	2.50	0.47
1:H:71:THR:HG23	4:H:413:HOH:O	2.13	0.47
1:A:-44:TYR:CD2	1:A:-44:TYR:O	2.68	0.47
1:A:-16:ILE:HG21	1:A:-9:ALA:HB2	1.96	0.47
1:B:-94:ASP:OD1	1:B:26:ASN:HB3	2.14	0.47
1:B:-85:TRP:CD1	1:B:33:PRO:HB2	2.50	0.47
1:B:-23:LEU:HD23	1:B:142:VAL:HG13	1.97	0.47
1:G:-39:TYR:HE2	1:G:114:ILE:HG22	1.78	0.47
1:D:-93:LEU:HD21	1:D:-90:PRO:HA	1.97	0.47
1:G:-79:ASP:OD1	1:G:-75:LYS:HE3	2.15	0.47
1:C:-92:LEU:HD21	1:C:-89:PRO:HA	1.96	0.47
1:E:161:GLU:OE2	1:E:165:ARG:NH1	2.48	0.47
1:E:234:VAL:HG23	1:E:235:PHE:HD1	1.80	0.47
1:A:-44:TYR:O	1:A:-44:TYR:CG	2.68	0.47
1:B:-170:GLU:HB2	1:B:-148:ARG:NE	2.27	0.47
1:C:-10:ASN:O	1:C:-7:THR:HG22	2.15	0.47
1:D:-87:THR:HG22	1:D:-85:GLU:N	2.29	0.47
1:D:36:LYS:NZ	4:D:508:HOH:O	2.31	0.47
1:E:12:ASN:HD22	1:E:16:ALA:HB2	1.79	0.47
1:A:-26:LYS:O	1:A:-22:THR:OG1	2.27	0.46
1:F:-211:GLU:HG2	1:F:56:PRO:HB2	1.96	0.46
1:C:262:VAL:HG13	1:C:264:GLN:HG3	1.97	0.46
1:D:-93:LEU:HD21	1:D:-89:PRO:HD3	1.96	0.46
1:F:-119:ALA:HB2	3:F:403:6AK:C24	2.45	0.46
1:A:-86:TRP:CD1	1:A:33:PRO:HB2	2.50	0.46
1:C:-55:PRO:HG3	1:C:42:PRO:HA	1.97	0.46
1:C:-38:ASP:C	1:C:-36:LYS:N	2.72	0.46
1:C:215:LYS:O	1:C:217:ASP:N	2.49	0.46
1:F:18:SER:HB2	4:F:501:HOH:O	2.15	0.46
1:G:-147:GLY:HA3	1:G:117:ASN:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HB3	1:A:257:LYS:HE3	1.98	0.46
1:C:155:LEU:HD23	1:C:280:VAL:HG13	1.96	0.46
1:H:-10:ASN:O	1:H:-7:THR:HG22	2.14	0.46
1:A:14:PRO:HA	1:A:17:TRP:CE2	2.51	0.46
1:C:87:VAL:HG21	1:C:92:TYR:HB3	1.98	0.46
1:F:-210:GLY:N	1:F:57:ASN:OD1	2.44	0.46
1:H:-194:LEU:HG	1:H:-177:VAL:HG21	1.97	0.46
1:A:210:GLN:HB3	1:A:214:ARG:NH2	2.31	0.46
1:D:216:LEU:O	1:D:217:ASP:HB3	2.15	0.46
1:H:-187:PHE:HD2	1:H:-179:VAL:HG21	1.79	0.46
1:D:220:ASN:HD22	1:D:222:GLY:H	1.64	0.46
1:B:171:ALA:HB1	1:B:260:LYS:CG	2.46	0.46
1:D:-191:GLY:HA3	1:D:-180:VAL:HG11	1.98	0.46
1:D:137:SER:OG	1:D:139:ARG:HB3	2.16	0.46
1:G:-61:PRO:HG3	1:G:128:VAL:HG23	1.97	0.46
1:A:-212:GLU:CD	1:A:-209:LYS:HD3	2.41	0.46
1:D:-127:LYS:HB3	1:D:89:LEU:HD23	1.97	0.46
1:D:163:ILE:O	1:D:167:LEU:HG	2.15	0.46
1:G:-188:PHE:HD2	1:G:-180:VAL:CG2	2.29	0.46
1:H:-205:ILE:HG12	1:H:-155:ILE:HB	1.97	0.46
1:D:-151:HIS:HA	1:D:-148:PHE:HD2	1.80	0.46
1:G:-6:ASP:OD1	1:G:-3:ILE:HD12	2.16	0.46
1:G:-116:TYR:O	1:G:-113:LYS:HB3	2.15	0.45
1:H:-92:LEU:HD21	1:H:-79:LEU:HD21	1.98	0.45
1:A:-116:TYR:OH	4:A:501:HOH:O	2.20	0.45
1:G:-196:GLY:O	1:G:-192:VAL:HG23	2.16	0.45
1:G:-79:ASP:O	1:G:-75:LYS:HG3	2.16	0.45
1:G:-6:ASP:HB2	4:G:566:HOH:O	2.17	0.45
1:B:17:TRP:HB2	1:B:83:PRO:HG2	1.98	0.45
1:C:127:ALA:HB1	1:C:149:ALA:HA	1.98	0.45
1:F:162:ILE:HG21	1:F:190:ALA:HB3	1.98	0.45
1:A:102:ILE:O	1:A:106:MET:HG2	2.16	0.45
1:A:235:PHE:CE1	1:A:248:LEU:HD13	2.51	0.45
1:B:57:ASN:HB3	1:B:60:LEU:HB2	1.99	0.45
1:C:244:ARG:HD2	3:C:401:6AK:C36	2.46	0.45
1:D:230:VAL:HG22	3:E:403:6AK:C29	2.47	0.45
1:A:-212:GLU:H	1:A:-212:GLU:HG2	1.57	0.45
1:A:-146:GLY:HA2	1:A:119:PRO:HB3	1.99	0.45
1:A:291:ARG:HH12	1:A:298:GLU:HB3	1.81	0.45
1:D:-87:THR:HB	1:D:-84:GLU:OE1	2.17	0.45
1:D:-45:LYS:HE3	1:D:-45:LYS:HB2	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:261:GLN:NE2	4:H:417:HOH:O	2.45	0.45
1:G:-188:PHE:HD2	1:G:-180:VAL:HG21	1.81	0.45
1:B:265:GLU:O	4:B:501:HOH:O	2.20	0.45
1:C:17:TRP:HB2	1:C:83:PRO:HG2	1.99	0.45
1:F:-63:GLN:NE2	1:F:-9:ALA:O	2.41	0.45
1:F:-31:ASP:OD1	1:F:-26:LYS:HE3	2.17	0.45
1:D:171:ALA:O	1:D:260:LYS:HD3	2.17	0.45
1:G:-71:LYS:HE3	1:G:5:GLY:O	2.17	0.45
1:H:-146:GLY:HA3	1:H:117:ASN:O	2.17	0.45
1:C:-30:ASN:O	1:C:-26:LYS:HG3	2.17	0.45
1:D:131:ALA:HB2	1:D:149:ALA:HB2	1.99	0.45
1:E:-48:TYR:OH	1:E:-35:ASP:OD1	2.26	0.45
1:A:-126:LEU:HD12	1:A:-121:TRP:CZ2	2.52	0.45
1:F:244:ARG:HG2	3:F:401:6AK:C35	2.47	0.45
1:B:206:GLU:O	1:B:210:GLN:N	2.50	0.44
1:E:-211:GLU:OE2	1:E:-211:GLU:N	2.50	0.44
1:E:-122:THR:HB	1:E:-108:PRO:HB2	1.99	0.44
1:C:82:LYS:NZ	4:C:502:HOH:O	2.21	0.44
1:D:-191:GLY:CA	1:D:-180:VAL:HG11	2.47	0.44
1:B:248:LEU:CB	3:B:403:6AK:C10	2.95	0.44
1:D:-150:ASP:OD1	2:L:2:GLC:O3	2.34	0.44
1:G:-148:PHE:HB3	1:G:-111:ILE:HD12	1.99	0.44
1:B:-99:LEU:HD12	1:B:10:THR:O	2.17	0.44
1:F:95:GLU:HA	1:F:98:LYS:HE3	1.99	0.44
3:F:405:6AK:C12	3:F:405:6AK:C09	2.96	0.44
1:H:-78:ASP:HA	1:H:-68:ALA:HB2	2.00	0.44
1:H:55:SER:O	1:H:58:LYS:NZ	2.43	0.44
1:H:87:VAL:HG21	1:H:92:TYR:CD2	2.52	0.44
1:A:115:MET:HE1	2:I:2:GLC:H2	2.00	0.44
1:B:207:THR:N	4:B:525:HOH:O	2.49	0.44
1:C:-64:ASN:O	1:C:-58:PHE:HB2	2.17	0.44
1:G:-132:LYS:H	1:G:-132:LYS:HG2	1.59	0.44
1:G:207:THR:O	1:G:211:GLY:N	2.36	0.44
1:C:163:ILE:HD11	1:C:272:ALA:O	2.18	0.44
1:G:-76:LEU:HB3	1:G:-71:LYS:HB2	1.99	0.44
1:G:294:ASP:O	1:G:297:VAL:HG22	2.17	0.44
1:D:-97:ASN:HD21	1:D:25:VAL:HG21	1.83	0.43
1:D:-49:GLY:O	1:D:-48:TYR:HB2	2.18	0.43
1:F:-137:GLU:OE2	1:F:-113:LYS:HG2	2.18	0.43
1:B:197:VAL:HG12	1:B:246:VAL:HG11	2.00	0.43
1:D:230:VAL:CG2	3:E:403:6AK:C29	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:GLN:NE2	1:G:156:TYR:HB3	2.33	0.43
1:B:116:PRO:HD2	1:B:121:MET:HE2	2.00	0.43
1:F:124:PHE:O	1:F:128:VAL:HG23	2.18	0.43
1:A:-100:LEU:HD13	1:A:33:PRO:HD3	2.00	0.43
1:A:-15:LYS:HA	1:A:-15:LYS:HD3	1.62	0.43
1:B:-144:TYR:HB3	1:B:-138:LEU:HD13	2.01	0.43
1:C:-149:ASP:HB3	1:C:115:MET:HE3	2.00	0.43
1:D:276:THR:O	1:D:280:VAL:HG22	2.18	0.43
1:E:-151:HIS:NE2	1:E:115:MET:O	2.48	0.43
1:B:207:THR:HA	1:B:210:GLN:HB2	2.00	0.43
1:E:-87:THR:HG22	1:E:-84:GLU:OE1	2.19	0.43
1:E:-59:PHE:HE2	1:E:12:ASN:OD1	2.01	0.43
1:H:184:GLY:O	1:H:188:ARG:N	2.44	0.43
1:C:-61:GLU:HB3	2:K:2:GLC:O6	2.18	0.43
1:G:-68:LEU:HD11	1:G:11:ILE:HD12	2.01	0.43
1:A:119:PRO:O	4:A:502:HOH:O	2.21	0.43
1:C:14:PRO:HA	1:C:17:TRP:CE2	2.54	0.43
1:F:-80:LEU:O	1:F:-76:LEU:HD12	2.19	0.43
1:C:277:ASP:O	1:C:281:ARG:HG3	2.19	0.43
1:D:286:TRP:CZ2	1:D:290:GLN:HG3	2.53	0.43
1:E:-169:LYS:HA	1:E:-169:LYS:HD3	1.80	0.43
1:F:-62:GLU:CD	1:F:129:ARG:HH22	2.26	0.43
1:F:154:ASP:HB3	1:F:158:GLN:CG	2.43	0.43
1:G:-79:ASP:HA	1:G:-69:ALA:HB2	1.99	0.43
1:A:286:TRP:CZ3	1:A:290:GLN:HG3	2.54	0.43
1:C:-121:THR:HB	1:C:-107:PRO:HB2	1.99	0.43
1:D:-38:ASP:OD1	1:D:-37:ILE:N	2.46	0.43
1:A:-164:ALA:HA	1:A:-160:ASP:O	2.19	0.42
1:A:215:LYS:HB2	1:A:216:LEU:H	1.65	0.42
1:B:194:LEU:HD21	1:B:249:ILE:HG21	2.00	0.42
1:E:-76:LEU:HD23	1:E:-73:LYS:HZ3	1.83	0.42
1:E:160:LEU:HB2	1:E:276:THR:HG21	2.01	0.42
1:F:34:THR:HG22	1:F:39:PRO:HA	2.00	0.42
1:B:-203:ILE:O	1:B:-175:HIS:HA	2.19	0.42
1:B:-194:LEU:HD23	1:B:-177:VAL:HG11	2.02	0.42
1:C:291:ARG:NH2	1:C:298:GLU:OE1	2.52	0.42
1:D:-197:ASN:O	1:D:-193:GLU:HG3	2.20	0.42
1:H:228:MET:HE2	3:H:301:6AK:CL2	2.57	0.42
1:A:12:ASN:ND2	1:A:16:ALA:HB2	2.33	0.42
1:B:175:LYS:N	4:B:527:HOH:O	2.52	0.42
1:C:-147:PHE:CE2	1:C:48:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:LYS:H	1:E:98:LYS:HD2	1.84	0.42
1:H:212:MET:C	1:H:214:ARG:H	2.27	0.42
1:D:140:GLN:NE2	1:D:144:GLU:HB3	2.34	0.42
1:F:212:MET:O	1:F:216:LEU:HG	2.19	0.42
1:G:107:GLU:HG3	4:G:518:HOH:O	2.18	0.42
1:H:-32:VAL:HB	1:H:150:GLN:NE2	2.35	0.42
1:B:-119:ASP:OD1	1:B:-116:ARG:NH1	2.42	0.42
1:C:-59:TYR:HB2	2:K:2:GLC:O5	2.18	0.42
1:F:-23:LEU:HD23	1:F:142:VAL:HG13	2.00	0.42
1:F:286:TRP:O	1:F:290:GLN:HG2	2.20	0.42
1:H:-106:ILE:HD13	1:H:70:LEU:HD21	2.02	0.42
1:H:-104:VAL:HG22	1:H:46:VAL:HG22	2.00	0.42
1:E:-46:PHE:CD2	1:E:118:ILE:HD11	2.55	0.42
1:G:125:TRP:CE3	2:O:2:GLC:H61	2.55	0.42
1:G:244:ARG:HD2	4:G:513:HOH:O	2.20	0.42
1:G:251:PHE:HD2	3:G:401:6AK:C22	2.32	0.42
1:A:-5:TYR:HH	1:A:15:TRP:CD1	2.38	0.42
1:A:16:ALA:O	1:A:20:ILE:HG13	2.19	0.42
1:D:-86:TRP:CE2	1:D:-55:LEU:HD13	2.55	0.42
1:E:-207:VAL:HG23	1:E:-158:PRO:HA	2.01	0.42
1:E:199:ASP:HB3	1:E:203:ARG:HH11	1.85	0.42
1:A:155:LEU:CD1	1:A:280:VAL:HB	2.50	0.42
1:B:-85:TRP:HB3	1:B:-21:PHE:CE2	2.52	0.42
1:E:240:THR:OG1	1:E:283:LYS:NZ	2.48	0.42
1:F:-212:GLU:O	1:F:57:ASN:ND2	2.46	0.42
1:F:-45:LYS:NZ	4:F:509:HOH:O	2.40	0.42
1:A:160:LEU:HB2	1:A:276:THR:HG21	2.01	0.42
1:B:155:LEU:HD23	1:B:280:VAL:HG13	2.02	0.42
1:H:245:LEU:HD12	3:H:301:6AK:C25	2.50	0.42
1:D:-188:PHE:CE2	1:D:-182:ILE:HG21	2.55	0.42
1:F:-151:HIS:HA	1:F:-148:PHE:HD2	1.85	0.42
1:F:280:VAL:O	1:F:284:ARG:HB2	2.20	0.42
1:H:-187:PHE:HD1	1:H:68:TYR:HE2	1.68	0.42
1:H:221:VAL:HA	1:H:224:PHE:CZ	2.54	0.42
1:C:-9:ALA:O	4:C:501:HOH:O	2.21	0.41
1:D:-171:GLU:H	1:D:-171:GLU:HG3	1.52	0.41
1:F:-35:ASP:O	1:F:-34:VAL:CB	2.67	0.41
1:F:213:LEU:HD11	1:F:258:HIS:CD2	2.55	0.41
1:D:-208:LEU:HA	1:D:-157:ASP:OD2	2.21	0.41
1:F:-168:PHE:CD1	1:F:-155:ILE:HD12	2.55	0.41
1:G:-97:ASN:ND2	4:G:521:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:-46:PHE:HA	1:G:-38:ASP:O	2.20	0.41
1:A:-118:VAL:HG21	1:A:-108:PRO:HD3	2.03	0.41
1:A:-56:PRO:HG3	1:A:42:PRO:HA	2.01	0.41
1:B:-129:PHE:CD1	1:B:-126:LYS:HD2	2.56	0.41
1:G:-151:HIS:HA	1:G:-148:PHE:HD2	1.85	0.41
1:G:-15:LYS:HD3	1:G:-15:LYS:HA	1.82	0.41
1:H:-117:VAL:HG21	1:H:-107:PRO:HD3	2.02	0.41
1:H:70:LEU:N	4:H:413:HOH:O	2.53	0.41
1:B:264:GLN:HE21	1:B:267:PHE:HD2	1.69	0.41
1:C:-146:GLY:HA3	1:C:117:ASN:O	2.20	0.41
1:C:12:ASN:OD1	1:C:15:TRP:NE1	2.52	0.41
1:C:196:ARG:NH2	1:C:300:PHE:O	2.38	0.41
1:E:-167:PRO:HA	1:E:-140:LEU:HD13	2.03	0.41
1:F:162:ILE:HG13	1:F:162:ILE:H	1.72	0.41
1:G:202:GLN:O	1:G:203:ARG:C	2.63	0.41
1:D:-44:TYR:O	1:D:-44:TYR:CG	2.73	0.41
1:H:125:TRP:O	1:H:129:ARG:HB2	2.20	0.41
1:E:87:VAL:HG23	1:E:89:LEU:N	2.35	0.41
1:E:209:PHE:HB3	1:E:254:PHE:CD2	2.54	0.41
1:E:235:PHE:CZ	1:E:248:LEU:HB2	2.56	0.41
1:F:120:GLN:HE21	1:F:120:GLN:HB2	1.73	0.41
1:G:106:MET:HE3	3:G:404:6AK:C24	2.50	0.41
1:C:-145:GLY:HA2	1:C:119:PRO:HB3	2.02	0.41
1:C:171:ALA:HB1	1:C:260:LYS:HB2	2.03	0.41
1:D:-188:PHE:CZ	1:D:-182:ILE:HG21	2.55	0.41
1:E:-15:LYS:HA	1:E:-15:LYS:HD3	1.80	0.41
1:G:-207:VAL:O	1:G:-157:ASP:N	2.53	0.41
1:B:34:THR:HG22	1:B:39:PRO:HA	2.03	0.41
1:F:-206:ILE:HA	1:F:-156:ILE:O	2.21	0.41
1:F:162:ILE:HD13	1:F:190:ALA:CB	2.48	0.41
1:G:-39:TYR:HE2	1:G:114:ILE:CG2	2.32	0.41
1:G:197:VAL:O	1:G:201:VAL:HG12	2.21	0.41
1:C:-148:ARG:NH1	1:C:122[B]:SER:OG	2.54	0.41
1:C:-117:VAL:HG21	1:C:-107:PRO:HD3	2.03	0.41
1:C:253:ALA:O	1:C:257:LYS:HG3	2.20	0.41
1:F:106:MET:HE3	3:F:404:6AK:C24	2.51	0.41
1:G:-34:VAL:HG12	1:G:150:GLN:NE2	2.36	0.41
1:B:146:LEU:HB2	4:B:502:HOH:O	2.21	0.41
1:B:219:LYS:O	1:H:-77:LYS:NZ	2.44	0.41
1:E:-56:PRO:HG3	1:E:42:PRO:HA	2.02	0.41
1:H:-124:TYR:O	1:H:-121:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-64:LEU:HD11	1:A:-11:MET:HE3	2.03	0.40
1:A:0:ALA:HB1	1:A:4:LYS:NZ	2.36	0.40
1:A:170:GLN:NE2	1:A:199:ASP:OD1	2.51	0.40
1:A:231:MET:HB3	1:A:278:VAL:HG11	2.03	0.40
1:A:286:TRP:O	1:A:290:GLN:HG2	2.21	0.40
1:B:33:PRO:O	1:B:40:SER:OG	2.32	0.40
1:E:18:SER:OG	1:E:83:PRO:HD3	2.21	0.40
1:A:-162:THR:HG22	1:A:-162:THR:O	2.21	0.40
1:E:156:TYR:HD2	1:E:280:VAL:HG21	1.85	0.40
1:G:-39:TYR:CE2	1:G:114:ILE:CG2	3.04	0.40
1:A:-67:MET:O	1:A:10:THR:OG1	2.37	0.40
1:A:-3:ILE:HG13	1:A:-2:ALA:N	2.35	0.40
1:D:-146:GLY:HA2	1:D:119:PRO:CB	2.46	0.40
1:D:115:MET:HE3	1:D:115:MET:HB2	1.94	0.40
1:F:-61:PRO:HD3	1:F:129:ARG:CG	2.51	0.40
1:F:296:PHE:CE1	1:F:300:PHE:HE2	2.39	0.40
3:F:405:6AK:C09	3:F:405:6AK:O02	2.69	0.40
1:H:187:GLY:C	1:H:191:LEU:HD23	2.46	0.40
1:B:207:THR:HA	1:B:210:GLN:CB	2.51	0.40
1:C:-37:ILE:HD13	1:C:-37:ILE:HG21	1.86	0.40
1:B:-146:GLY:HA3	1:B:117:ASN:O	2.22	0.40
1:D:255:VAL:O	1:D:259:LEU:HG	2.21	0.40
1:G:239:VAL:CG1	1:G:240:THR:N	2.85	0.40
1:H:-92:LEU:CD2	1:H:-79:LEU:HD21	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	510/518 (98%)	489 (96%)	18 (4%)	3 (1%)	21 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	502/518 (97%)	488 (97%)	13 (3%)	1 (0%)	43	68
1	C	503/518 (97%)	489 (97%)	12 (2%)	2 (0%)	30	54
1	D	495/518 (96%)	475 (96%)	16 (3%)	4 (1%)	16	37
1	E	503/518 (97%)	486 (97%)	15 (3%)	2 (0%)	30	54
1	F	498/518 (96%)	481 (97%)	14 (3%)	3 (1%)	21	44
1	G	499/518 (96%)	473 (95%)	23 (5%)	3 (1%)	21	44
1	H	492/518 (95%)	469 (95%)	21 (4%)	2 (0%)	30	54
All	All	4002/4144 (97%)	3850 (96%)	132 (3%)	20 (0%)	24	48

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-37	ILE
1	C	216	LEU
1	D	216	LEU
1	D	217	ASP
1	D	218	ILE
1	F	-34	VAL
1	F	218	ILE
1	G	-48	TYR
1	G	203	ARG
1	H	262	GLU
1	E	215	LYS
1	E	218	ILE
1	A	184	GLY
1	A	215	LYS
1	H	-46	ALA
1	A	216	LEU
1	G	183	ALA
1	D	219	LYS
1	B	218	ILE
1	F	201	VAL

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	387/421 (92%)	384 (99%)	3 (1%)	73 88
1	B	378/421 (90%)	376 (100%)	2 (0%)	81 92
1	C	383/421 (91%)	378 (99%)	5 (1%)	61 83
1	D	378/421 (90%)	376 (100%)	2 (0%)	81 92
1	E	383/421 (91%)	382 (100%)	1 (0%)	86 94
1	F	371/421 (88%)	371 (100%)	0	100 100
1	G	370/421 (88%)	368 (100%)	2 (0%)	81 92
1	H	373/421 (89%)	372 (100%)	1 (0%)	86 94
All	All	3023/3368 (90%)	3007 (100%)	16 (0%)	81 92

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-45	LYS
1	A	-3	ILE
1	A	217	ASP
1	B	248	LEU
1	B	277	ASP
1	C	-110	ILE
1	C	-38	ASP
1	C	-35	ASP
1	C	122[A]	SER
1	C	122[B]	SER
1	D	120	GLN
1	D	218	ILE
1	E	87	VAL
1	G	114	ILE
1	G	203	ARG
1	H	-36	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	B	67	ASN
1	B	233	HIS
1	B	264	GLN

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Mol	Chain	Res	Type
1	C	-142	GLN
1	C	-96	ASN
1	C	-14	ASN
1	C	264	GLN
1	D	-166	GLN
1	D	3	ASN
1	D	170	GLN
1	D	220	ASN
1	E	-203	ASN
1	E	12	ASN
1	E	233	HIS
1	E	258	HIS
1	F	26	ASN
1	F	120	GLN
1	F	205	HIS
1	G	57	ASN
1	G	233	HIS
1	H	-142	GLN
1	H	255	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

16 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	I	1	2	12,12,12	0.97	0	17,17,17	0.85	1 (5%)
2	GLC	I	2	2	11,11,12	1.02	1 (9%)	15,15,17	0.95	1 (6%)
2	GLC	J	1	2	12,12,12	0.97	0	17,17,17	0.75	0
2	GLC	J	2	2	11,11,12	1.03	1 (9%)	15,15,17	1.09	1 (6%)
2	GLC	K	1	2	12,12,12	0.96	0	17,17,17	0.81	0
2	GLC	K	2	2	11,11,12	1.02	1 (9%)	15,15,17	1.05	1 (6%)
2	GLC	L	1	2	12,12,12	0.97	0	17,17,17	0.77	0
2	GLC	L	2	2	11,11,12	1.04	1 (9%)	15,15,17	1.42	2 (13%)
2	GLC	M	1	2	12,12,12	1.05	1 (8%)	17,17,17	1.56	3 (17%)
2	GLC	M	2	2	11,11,12	1.03	1 (9%)	15,15,17	0.91	1 (6%)
2	GLC	N	1	2	12,12,12	0.98	0	17,17,17	0.68	0
2	GLC	N	2	2	11,11,12	1.08	1 (9%)	15,15,17	1.30	1 (6%)
2	GLC	O	1	2	12,12,12	0.99	0	17,17,17	0.87	1 (5%)
2	GLC	O	2	2	11,11,12	0.94	1 (9%)	15,15,17	1.38	1 (6%)
2	GLC	P	1	2	12,12,12	0.98	0	17,17,17	0.74	0
2	GLC	P	2	2	11,11,12	1.02	1 (9%)	15,15,17	1.01	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	GLC	L	1	2	-	0/2/22/22	0/1/1/1
2	GLC	L	2	2	-	1/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GLC	M	2	2	-	2/2/19/22	0/1/1/1
2	GLC	N	1	2	-	0/2/22/22	0/1/1/1
2	GLC	N	2	2	-	2/2/19/22	0/1/1/1
2	GLC	O	1	2	-	2/2/22/22	0/1/1/1
2	GLC	O	2	2	-	0/2/19/22	0/1/1/1
2	GLC	P	1	2	-	1/2/22/22	0/1/1/1
2	GLC	P	2	2	-	0/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	2	GLC	O5-C5	2.54	1.48	1.43
2	N	2	GLC	O5-C5	2.46	1.48	1.43
2	K	2	GLC	O5-C5	2.36	1.48	1.43
2	O	2	GLC	O5-C5	2.34	1.48	1.43
2	J	2	GLC	O5-C5	2.33	1.48	1.43
2	P	2	GLC	O5-C5	2.31	1.47	1.43
2	M	2	GLC	O5-C5	2.30	1.47	1.43
2	I	2	GLC	O5-C5	2.12	1.47	1.43
2	M	1	GLC	C1-C2	2.11	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	2	GLC	C1-O5-C5	4.25	117.88	112.19
2	L	2	GLC	C1-O5-C5	3.97	117.50	112.19
2	O	2	GLC	C1-O5-C5	3.83	117.32	112.19
2	J	2	GLC	C1-O5-C5	3.57	116.98	112.19
2	K	2	GLC	C1-O5-C5	3.45	116.81	112.19
2	M	1	GLC	O5-C5-C4	-3.29	103.76	109.70
2	M	1	GLC	C1-C2-C3	3.22	116.93	110.36
2	P	2	GLC	C1-O5-C5	3.15	116.40	112.19
2	M	1	GLC	C4-C3-C2	2.88	115.89	110.83
2	M	2	GLC	C1-O5-C5	2.72	115.83	112.19
2	L	2	GLC	C1-C2-C3	-2.52	105.97	109.64
2	I	2	GLC	C1-O5-C5	2.34	115.32	112.19
2	O	1	GLC	C1-O5-C5	2.25	118.01	113.65
2	I	1	GLC	C1-O5-C5	2.00	117.53	113.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	2	GLC	C4-C5-C6-O6
2	N	2	GLC	O5-C5-C6-O6
2	O	1	GLC	C4-C5-C6-O6
2	O	1	GLC	O5-C5-C6-O6
2	M	2	GLC	C4-C5-C6-O6
2	L	2	GLC	O5-C5-C6-O6
2	M	2	GLC	O5-C5-C6-O6
2	P	1	GLC	O5-C5-C6-O6

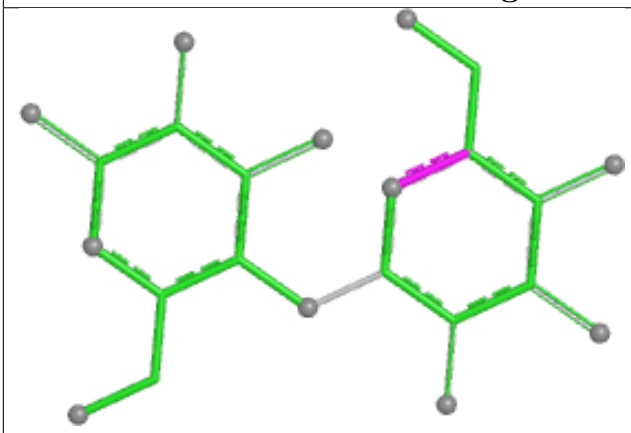
There are no ring outliers.

9 monomers are involved in 11 short contacts:

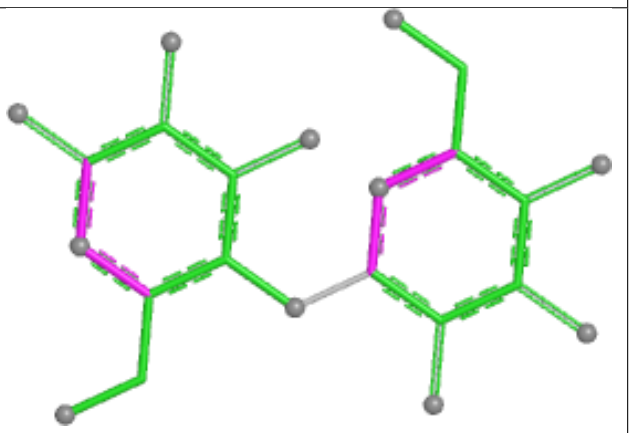
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	1	GLC	1	0
2	L	1	GLC	1	0
2	N	2	GLC	1	0
2	L	2	GLC	1	0
2	M	1	GLC	1	0
2	O	2	GLC	1	0
2	K	2	GLC	2	0
2	I	2	GLC	2	0
2	J	2	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

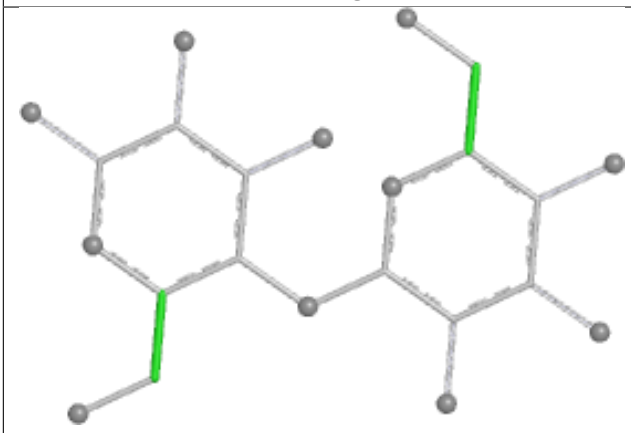
Oligosaccharide Chain I



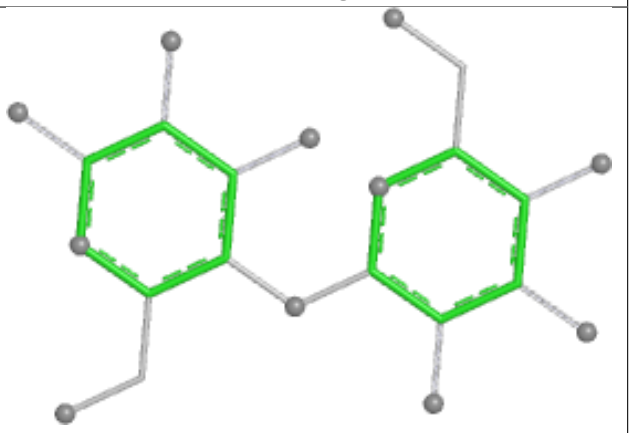
Bond lengths



Bond angles

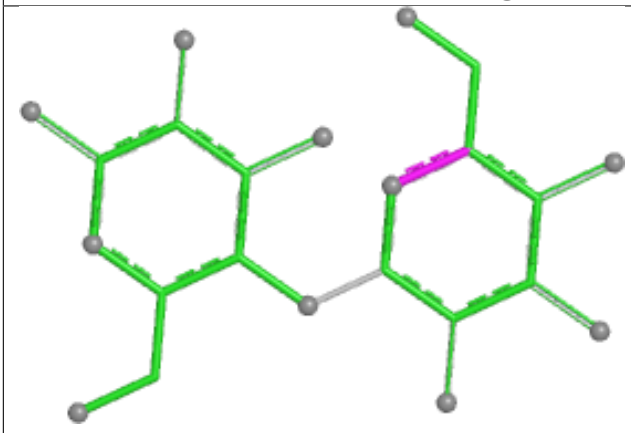


Torsions

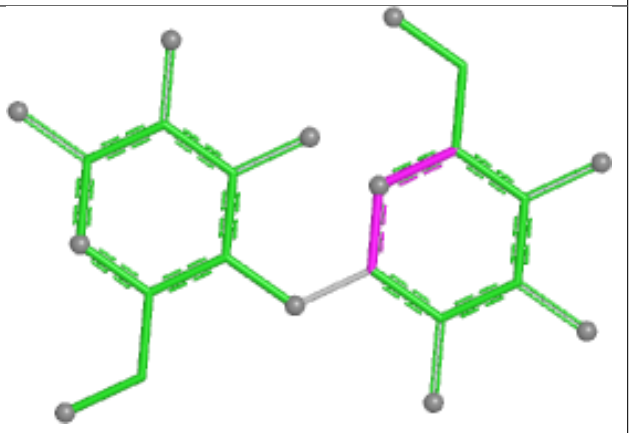


Rings

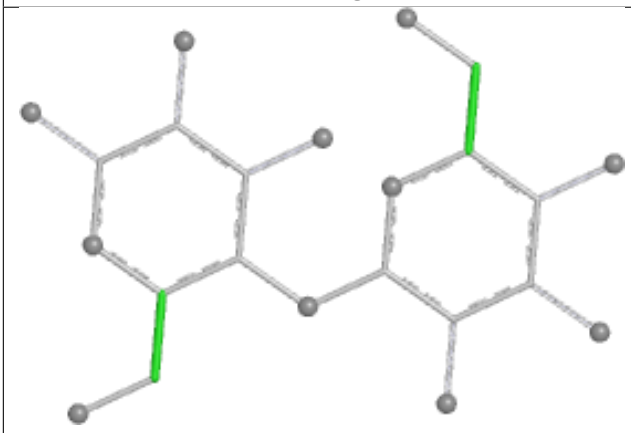
Oligosaccharide Chain J



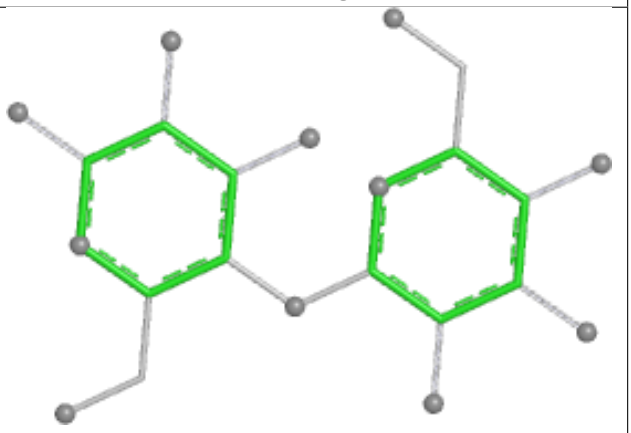
Bond lengths



Bond angles

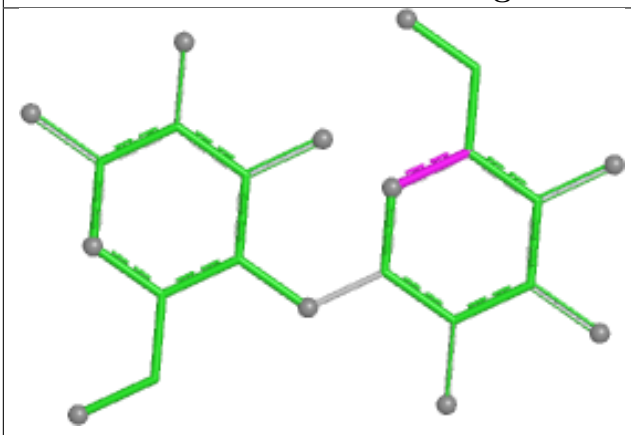


Torsions

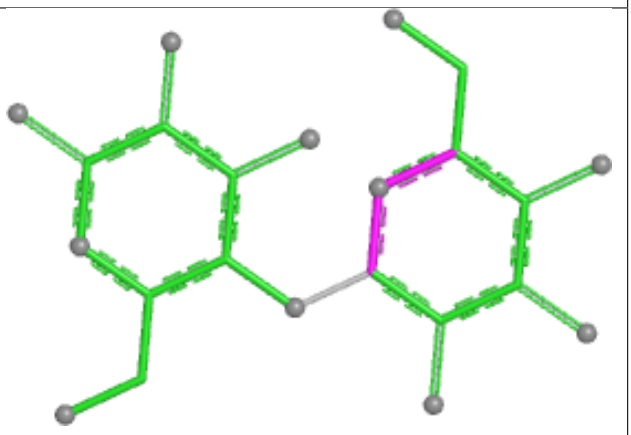


Rings

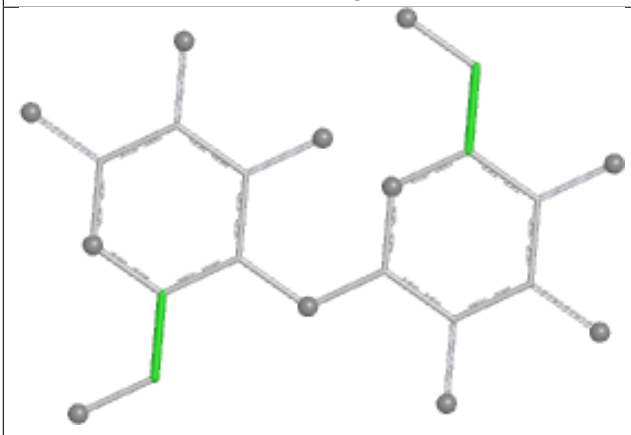
Oligosaccharide Chain K



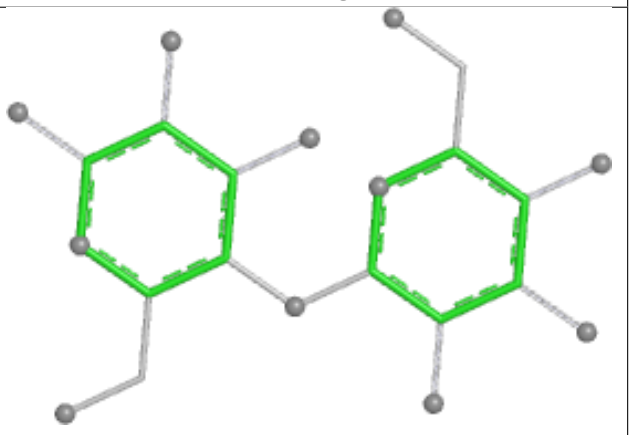
Bond lengths



Bond angles

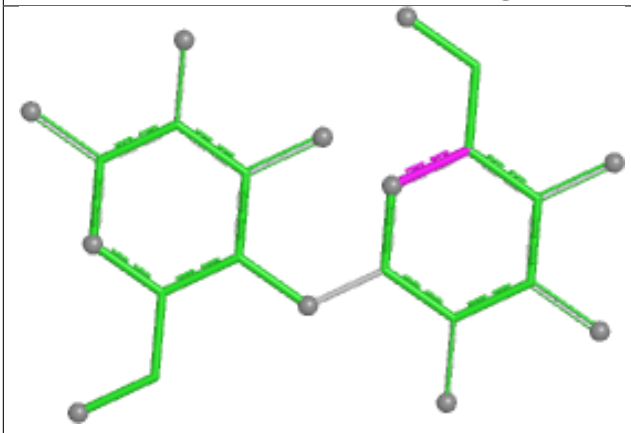


Torsions

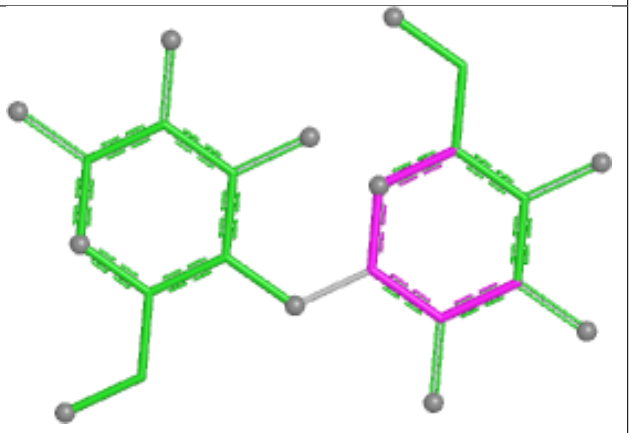


Rings

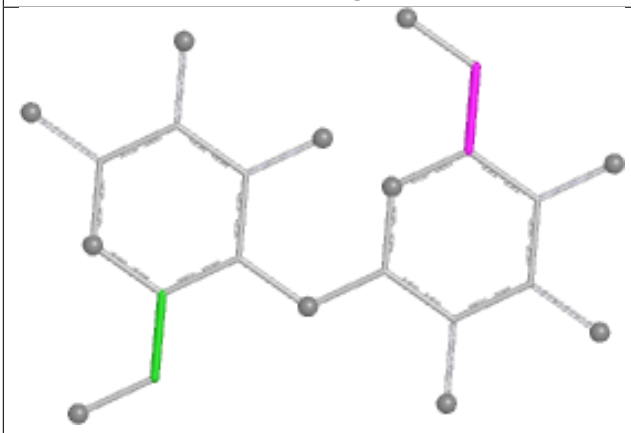
Oligosaccharide Chain L



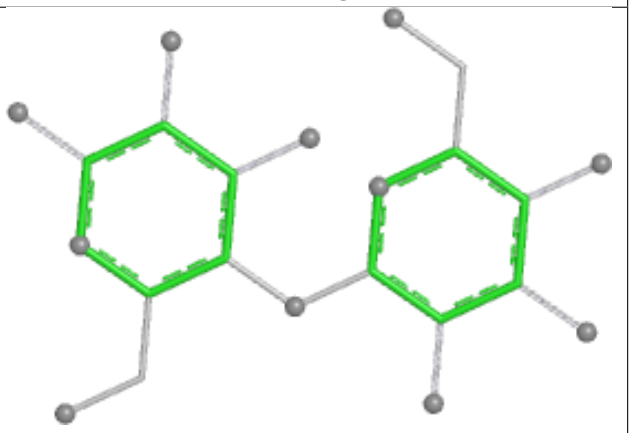
Bond lengths



Bond angles

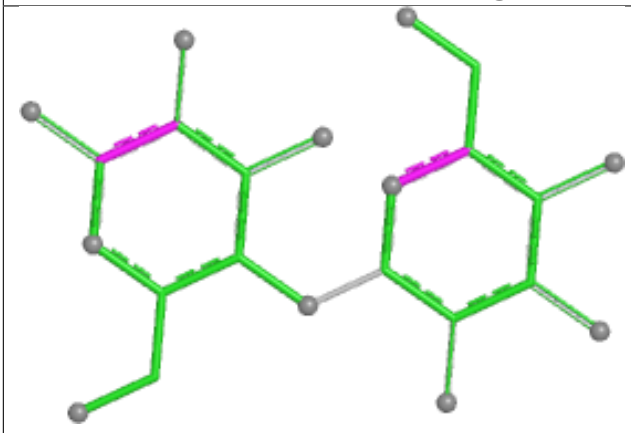


Torsions

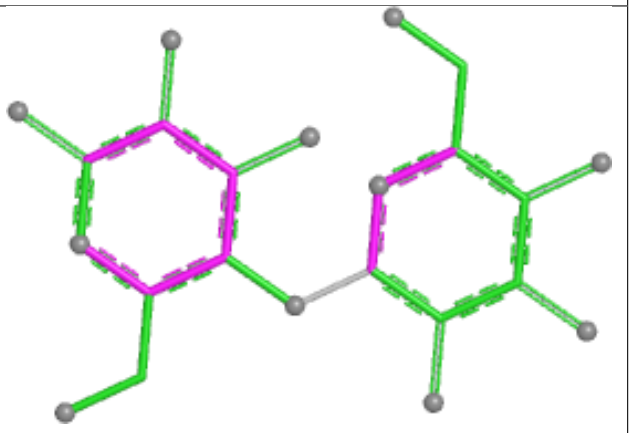


Rings

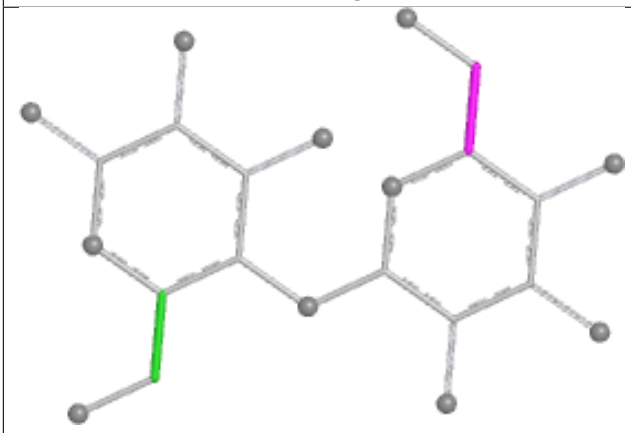
Oligosaccharide Chain M



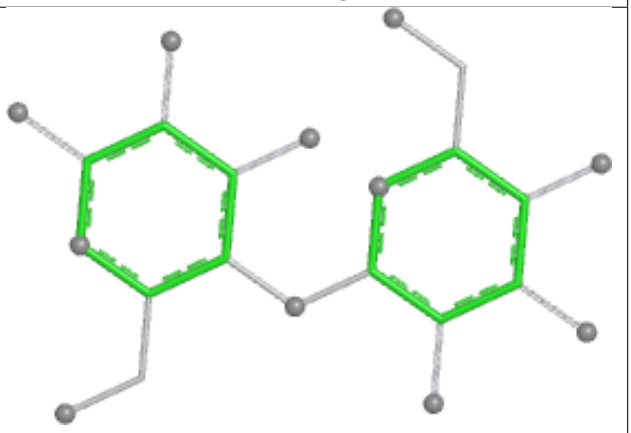
Bond lengths



Bond angles

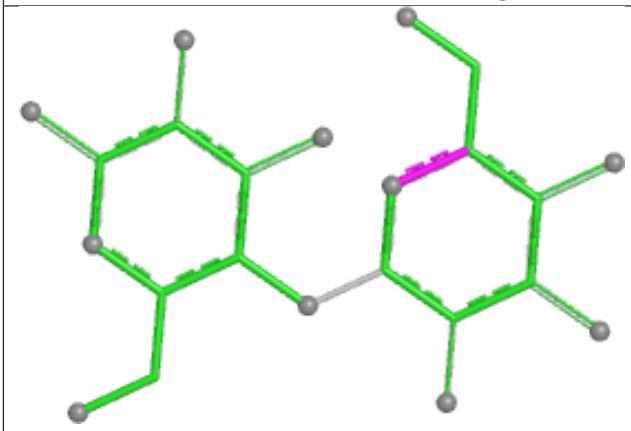


Torsions

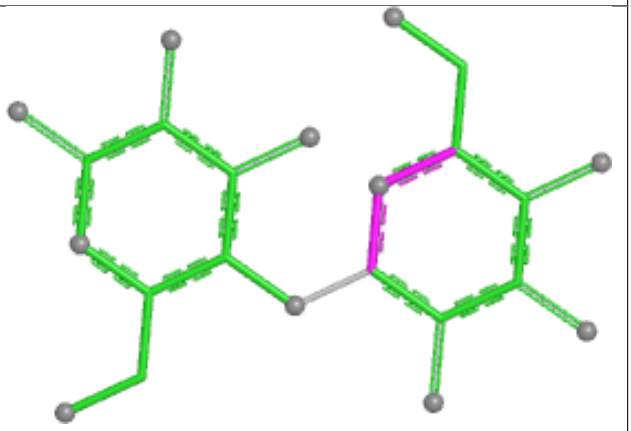


Rings

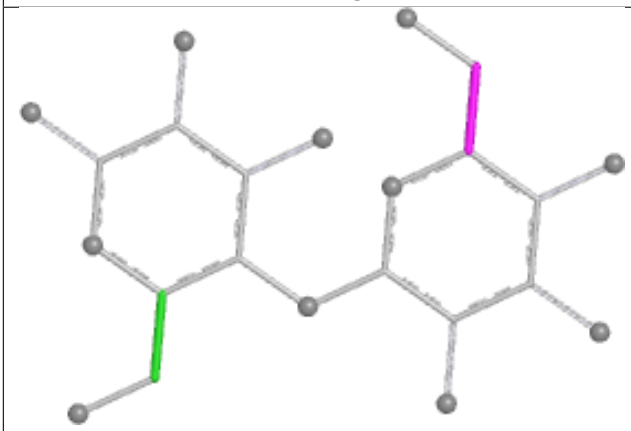
Oligosaccharide Chain N



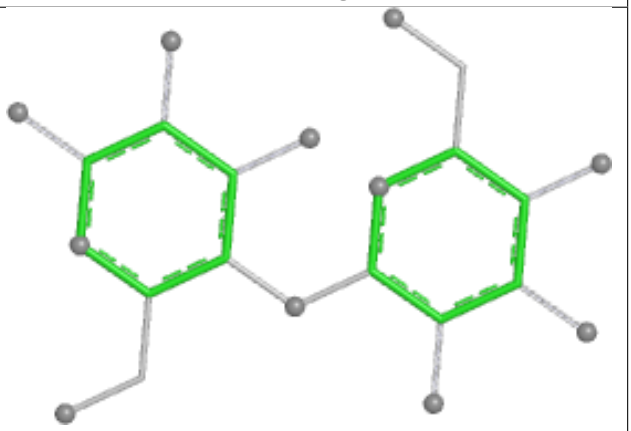
Bond lengths



Bond angles

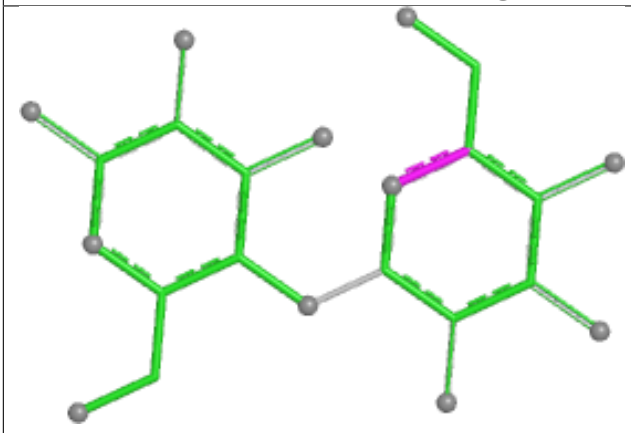


Torsions

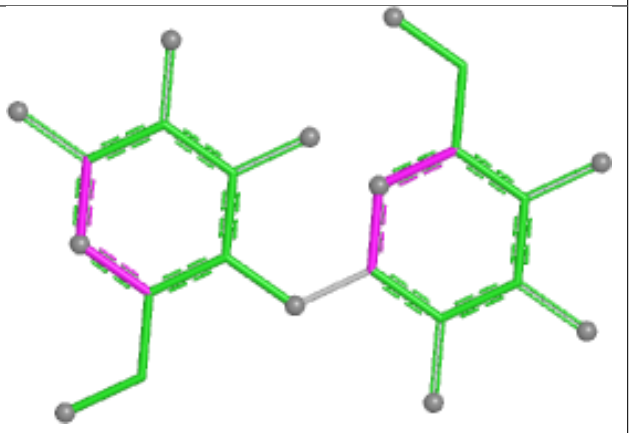


Rings

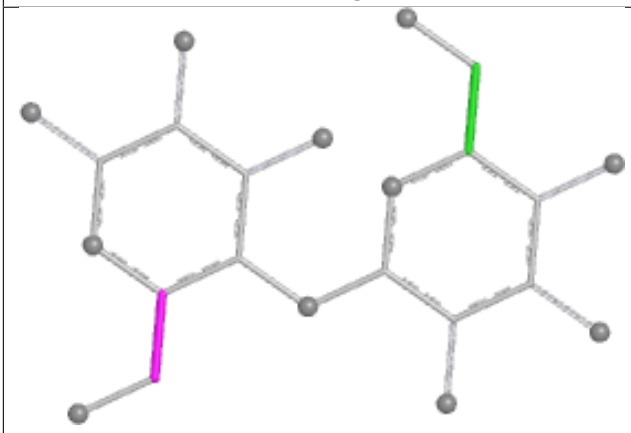
Oligosaccharide Chain O



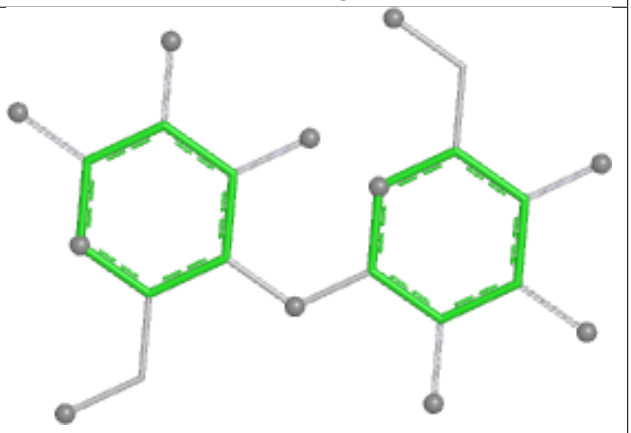
Bond lengths



Bond angles

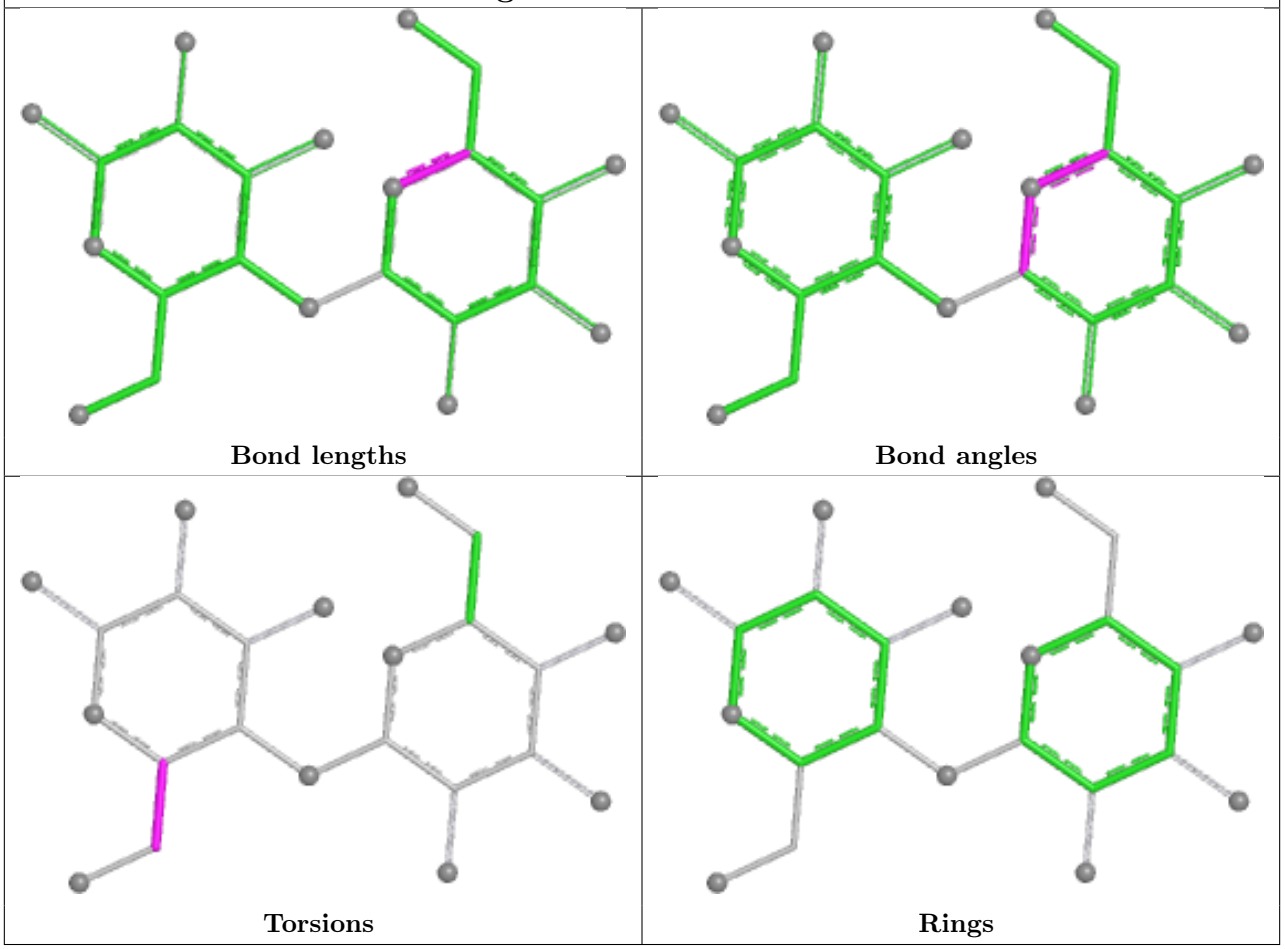


Torsions



Rings

Oligosaccharide Chain P



5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	6AK	G	404	-	55,56,56	0.90	2 (3%)	70,85,85	1.82	13 (18%)
3	6AK	G	403	-	55,56,56	0.87	1 (1%)	70,85,85	1.69	13 (18%)
3	6AK	E	401	-	55,56,56	0.86	1 (1%)	70,85,85	1.63	11 (15%)
3	6AK	A	404	-	55,56,56	0.89	0	70,85,85	1.78	13 (18%)
3	6AK	H	304	-	55,56,56	0.88	1 (1%)	70,85,85	1.78	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	6AK	D	401	-	55,56,56	0.87	1 (1%)	70,85,85	1.68	12 (17%)
3	6AK	A	403	-	55,56,56	0.88	1 (1%)	70,85,85	1.53	10 (14%)
3	6AK	C	405	-	55,56,56	0.90	1 (1%)	70,85,85	1.90	16 (22%)
3	6AK	H	303	-	55,56,56	0.97	2 (3%)	70,85,85	1.75	13 (18%)
3	6AK	F	404	-	55,56,56	0.88	1 (1%)	70,85,85	1.86	12 (17%)
3	6AK	F	403	-	55,56,56	0.90	1 (1%)	70,85,85	1.71	13 (18%)
3	6AK	G	401	-	55,56,56	0.90	1 (1%)	70,85,85	1.75	14 (20%)
3	6AK	F	405	-	55,56,56	2.42	17 (30%)	70,85,85	1.84	18 (25%)
3	6AK	D	403	-	55,56,56	0.85	1 (1%)	70,85,85	1.65	14 (20%)
3	6AK	C	403	-	55,56,56	0.89	1 (1%)	70,85,85	1.53	11 (15%)
3	6AK	B	403	-	55,56,56	0.89	2 (3%)	70,85,85	1.82	16 (22%)
3	6AK	F	401	-	55,56,56	0.89	1 (1%)	70,85,85	1.75	13 (18%)
3	6AK	H	301	-	55,56,56	0.90	1 (1%)	70,85,85	1.69	11 (15%)
3	6AK	B	402	-	55,56,56	0.91	1 (1%)	70,85,85	1.57	10 (14%)
3	6AK	C	404	-	55,56,56	0.89	2 (3%)	70,85,85	1.82	13 (18%)
3	6AK	E	403	-	55,56,56	0.89	1 (1%)	70,85,85	1.49	9 (12%)
3	6AK	A	401	-	55,56,56	0.86	1 (1%)	70,85,85	1.67	12 (17%)
3	6AK	H	305	-	55,56,56	0.88	1 (1%)	70,85,85	1.64	10 (14%)
3	6AK	C	401	-	55,56,56	0.86	2 (3%)	70,85,85	1.67	11 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6AK	G	404	-	-	11/19/33/33	0/6/7/7
3	6AK	G	403	-	-	10/19/33/33	0/6/7/7
3	6AK	E	401	-	-	5/19/33/33	0/6/7/7
3	6AK	A	404	-	-	10/19/33/33	0/6/7/7
3	6AK	H	304	-	-	7/19/33/33	0/6/7/7
3	6AK	D	401	-	-	3/19/33/33	0/6/7/7
3	6AK	A	403	-	-	5/19/33/33	0/6/7/7
3	6AK	C	405	-	-	2/19/33/33	0/6/7/7
3	6AK	H	303	-	-	5/19/33/33	0/6/7/7
3	6AK	F	404	-	-	5/19/33/33	0/6/7/7

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6AK	F	403	-	-	11/19/33/33	0/6/7/7
3	6AK	G	401	-	-	6/19/33/33	0/6/7/7
3	6AK	F	405	-	-	6/19/33/33	0/6/7/7
3	6AK	D	403	-	-	1/19/33/33	0/6/7/7
3	6AK	C	403	-	-	3/19/33/33	0/6/7/7
3	6AK	B	403	-	-	4/19/33/33	0/6/7/7
3	6AK	F	401	-	-	5/19/33/33	0/6/7/7
3	6AK	H	301	-	-	6/19/33/33	0/6/7/7
3	6AK	B	402	-	-	2/19/33/33	0/6/7/7
3	6AK	C	404	-	-	5/19/33/33	0/6/7/7
3	6AK	E	403	-	-	4/19/33/33	0/6/7/7
3	6AK	A	401	-	-	4/19/33/33	0/6/7/7
3	6AK	H	305	-	-	11/19/33/33	0/6/7/7
3	6AK	C	401	-	-	4/19/33/33	0/6/7/7

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	405	6AK	C34-N01	-6.72	1.35	1.44
3	F	405	6AK	C35-C34	-6.61	1.35	1.41
3	F	405	6AK	C35-C36	-6.43	1.35	1.41
3	F	405	6AK	C11-N02	-4.08	1.34	1.39
3	F	405	6AK	C01-N02	-4.06	1.32	1.40
3	F	405	6AK	C38-N05	-3.90	1.34	1.37
3	F	405	6AK	C03-CL	-3.39	1.65	1.73
3	F	405	6AK	C33-C31	-3.22	1.34	1.39
3	F	405	6AK	C06-C01	-3.13	1.36	1.41
3	F	405	6AK	C13-N01	-3.12	1.41	1.48
3	F	405	6AK	N03-N04	-2.97	1.31	1.36
3	F	405	6AK	C37-N05	-2.95	1.41	1.46
3	F	405	6AK	C02-C19	-2.86	1.44	1.50
3	F	405	6AK	C06-C07	-2.80	1.39	1.44
3	F	405	6AK	C08-C07	-2.68	1.47	1.51
3	H	303	6AK	C02-C19	-2.63	1.45	1.50
3	F	405	6AK	C22-CL2	-2.44	1.67	1.72
3	F	404	6AK	C02-C19	-2.43	1.45	1.50
3	F	403	6AK	C02-C19	-2.42	1.45	1.50
3	A	401	6AK	C02-C19	-2.42	1.45	1.50
3	D	401	6AK	C02-C19	-2.40	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	6AK	C02-C19	-2.40	1.45	1.50
3	F	405	6AK	C16-N03	-2.35	1.42	1.46
3	C	403	6AK	C02-C19	-2.33	1.45	1.50
3	C	404	6AK	C02-C19	-2.33	1.45	1.50
3	F	401	6AK	C02-C19	-2.33	1.45	1.50
3	A	403	6AK	C02-C19	-2.31	1.45	1.50
3	E	403	6AK	C02-C19	-2.30	1.45	1.50
3	G	403	6AK	C02-C19	-2.29	1.45	1.50
3	C	401	6AK	C02-C19	-2.29	1.45	1.50
3	H	305	6AK	C02-C19	-2.27	1.45	1.50
3	B	402	6AK	C02-C19	-2.26	1.45	1.50
3	D	403	6AK	C02-C19	-2.24	1.45	1.50
3	B	403	6AK	C02-C19	-2.23	1.45	1.50
3	G	404	6AK	C02-C19	-2.23	1.45	1.50
3	G	401	6AK	C02-C19	-2.23	1.45	1.50
3	H	301	6AK	C02-C19	-2.23	1.45	1.50
3	H	303	6AK	C11-C07	2.17	1.40	1.37
3	C	405	6AK	C02-C19	-2.15	1.45	1.50
3	H	304	6AK	C02-C19	-2.11	1.46	1.50
3	B	403	6AK	C35-C34	2.10	1.43	1.41
3	G	404	6AK	C35-C34	2.06	1.43	1.41
3	C	404	6AK	C35-C34	2.05	1.43	1.41
3	C	401	6AK	C35-C34	2.00	1.43	1.41

All (302) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	404	6AK	C35-C34-N01	8.19	130.50	121.01
3	C	404	6AK	C35-C34-N01	7.61	129.83	121.01
3	G	404	6AK	C35-C34-N01	7.18	129.33	121.01
3	H	304	6AK	C35-C34-N01	6.68	128.75	121.01
3	C	401	6AK	C35-C34-N01	6.48	128.52	121.01
3	C	405	6AK	C35-C34-N01	6.47	128.51	121.01
3	A	404	6AK	C08-C07-C11	-6.34	122.16	127.46
3	H	301	6AK	C36-N05-C38	6.25	112.27	108.35
3	F	401	6AK	C35-C34-N01	6.23	128.24	121.01
3	G	401	6AK	C36-N05-C38	6.20	112.23	108.35
3	B	403	6AK	C35-C34-N01	6.15	128.14	121.01
3	H	303	6AK	C13-C15-C14	-5.91	100.15	113.99
3	D	401	6AK	C35-C34-N01	5.63	127.54	121.01
3	F	403	6AK	C36-N05-C38	5.50	111.80	108.35
3	D	403	6AK	C36-N05-C38	5.29	111.66	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	305	6AK	C36-N05-C38	5.21	111.61	108.35
3	E	403	6AK	C36-N05-C38	5.20	111.61	108.35
3	G	403	6AK	C35-C34-N01	5.17	127.00	121.01
3	G	403	6AK	C36-N05-C38	5.15	111.57	108.35
3	C	403	6AK	C36-N05-C38	5.14	111.57	108.35
3	F	404	6AK	C36-N05-C38	5.12	111.56	108.35
3	E	401	6AK	C36-N05-C38	5.12	111.56	108.35
3	B	402	6AK	C36-N05-C38	5.10	111.55	108.35
3	F	405	6AK	C36-N05-C38	5.08	111.53	108.35
3	A	403	6AK	C36-N05-C38	5.05	111.51	108.35
3	C	405	6AK	C36-N05-C38	5.04	111.51	108.35
3	A	401	6AK	C36-N05-C38	5.04	111.51	108.35
3	F	401	6AK	C36-N05-C38	5.04	111.51	108.35
3	D	401	6AK	C36-N05-C38	5.03	111.50	108.35
3	C	401	6AK	C36-N05-C38	5.01	111.49	108.35
3	C	404	6AK	C36-N05-C38	5.00	111.48	108.35
3	A	401	6AK	C35-C34-N01	5.00	126.80	121.01
3	G	404	6AK	C36-N05-C38	4.99	111.47	108.35
3	B	403	6AK	C36-N05-C38	4.98	111.47	108.35
3	H	304	6AK	C36-N05-C38	4.97	111.46	108.35
3	H	303	6AK	C36-N05-C38	4.95	111.45	108.35
3	A	404	6AK	C36-N05-C38	4.86	111.39	108.35
3	H	301	6AK	C35-C34-N01	4.81	126.58	121.01
3	A	404	6AK	C13-C15-C14	-4.77	102.81	113.99
3	F	403	6AK	C35-C34-N01	4.76	126.53	121.01
3	G	401	6AK	C13-C15-C14	-4.74	102.87	113.99
3	B	402	6AK	C13-C15-C14	-4.64	103.10	113.99
3	C	403	6AK	C13-C15-C14	-4.63	103.14	113.99
3	H	301	6AK	C39-C38-N05	-4.62	106.02	110.39
3	G	401	6AK	C39-C38-N05	-4.55	106.10	110.39
3	F	405	6AK	C03-C02-C19	4.53	128.41	121.67
3	E	401	6AK	C39-C38-N05	-4.52	106.12	110.39
3	A	403	6AK	C39-C38-N05	-4.51	106.13	110.39
3	C	403	6AK	C39-C38-N05	-4.50	106.14	110.39
3	G	403	6AK	C39-C38-N05	-4.49	106.15	110.39
3	D	403	6AK	C39-C38-N05	-4.47	106.17	110.39
3	F	401	6AK	C39-C38-N05	-4.45	106.19	110.39
3	A	401	6AK	C39-C38-N05	-4.44	106.20	110.39
3	B	402	6AK	C39-C38-N05	-4.44	106.20	110.39
3	E	403	6AK	C39-C38-N05	-4.44	106.20	110.39
3	F	403	6AK	C39-C38-N05	-4.43	106.21	110.39
3	H	303	6AK	C39-C38-N05	-4.42	106.22	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	401	6AK	C35-C34-N01	4.40	126.11	121.01
3	H	305	6AK	C39-C38-N05	-4.38	106.26	110.39
3	D	401	6AK	C39-C38-N05	-4.37	106.27	110.39
3	B	403	6AK	C39-C38-N05	-4.36	106.27	110.39
3	C	401	6AK	C39-C38-N05	-4.35	106.28	110.39
3	H	304	6AK	C39-C38-N05	-4.35	106.28	110.39
3	G	404	6AK	C39-C38-N05	-4.35	106.28	110.39
3	F	405	6AK	C13-C15-C14	-4.34	103.81	113.99
3	C	404	6AK	C39-C38-N05	-4.33	106.30	110.39
3	F	404	6AK	C39-C38-N05	-4.33	106.30	110.39
3	C	405	6AK	C13-C15-C14	-4.31	103.87	113.99
3	H	305	6AK	C35-C34-N01	4.25	125.94	121.01
3	A	404	6AK	C39-C38-N05	-4.24	106.38	110.39
3	C	405	6AK	C39-C38-N05	-4.20	106.42	110.39
3	E	403	6AK	C13-C15-C14	-4.12	104.34	113.99
3	H	305	6AK	C01-N02-C11	4.10	111.26	107.21
3	F	403	6AK	C13-C15-C14	-4.08	104.43	113.99
3	A	404	6AK	C09-C08-C07	4.07	119.71	113.30
3	F	404	6AK	C33-C34-N01	-4.06	110.76	119.17
3	C	405	6AK	C08-C07-C11	-4.05	124.08	127.46
3	H	304	6AK	C13-C15-C14	-4.01	104.58	113.99
3	D	403	6AK	C35-C34-N01	4.01	125.66	121.01
3	B	403	6AK	C01-N02-C11	3.98	111.14	107.21
3	F	401	6AK	C13-C15-C14	-3.92	104.80	113.99
3	F	401	6AK	C01-N02-C11	3.92	111.08	107.21
3	G	403	6AK	C01-N02-C11	3.92	111.07	107.21
3	F	404	6AK	C13-C15-C14	-3.89	104.86	113.99
3	A	403	6AK	C13-C15-C14	-3.89	104.88	113.99
3	F	405	6AK	C15-C14-N02	3.89	124.33	113.33
3	H	301	6AK	C13-C15-C14	-3.86	104.94	113.99
3	D	401	6AK	C01-N02-C11	3.85	111.00	107.21
3	G	404	6AK	C13-C15-C14	-3.82	105.02	113.99
3	F	403	6AK	C01-N02-C11	3.80	110.96	107.21
3	H	305	6AK	C13-C15-C14	-3.79	105.10	113.99
3	C	404	6AK	C13-C15-C14	-3.75	105.20	113.99
3	B	403	6AK	C13-C15-C14	-3.73	105.25	113.99
3	G	401	6AK	C35-C34-N01	3.69	125.29	121.01
3	C	404	6AK	C33-C34-N01	-3.69	111.54	119.17
3	F	405	6AK	C39-C38-N05	-3.61	106.98	110.39
3	E	401	6AK	C01-N02-C11	3.60	110.76	107.21
3	F	405	6AK	C16-N03-C17	-3.57	124.83	128.09
3	F	401	6AK	C37-N05-C36	-3.52	122.42	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	404	6AK	C06-C07-C11	-3.50	104.23	106.99
3	D	403	6AK	C03-C02-C19	-3.49	116.46	121.67
3	C	401	6AK	C13-C15-C14	-3.49	105.80	113.99
3	H	301	6AK	C01-N02-C11	3.49	110.65	107.21
3	F	405	6AK	C14-N02-C01	-3.44	116.77	124.99
3	C	405	6AK	C06-C07-C11	-3.43	104.28	106.99
3	D	401	6AK	C13-C15-C14	-3.42	105.98	113.99
3	G	404	6AK	C37-N05-C36	-3.40	122.53	125.69
3	C	405	6AK	C33-C34-N01	-3.37	112.20	119.17
3	F	405	6AK	C13-N01-C34	-3.35	109.13	115.88
3	D	403	6AK	C01-N02-C11	3.34	110.51	107.21
3	G	404	6AK	C33-C34-N01	-3.34	112.25	119.17
3	G	401	6AK	C01-N02-C11	3.31	110.48	107.21
3	E	403	6AK	C01-N02-C11	3.29	110.46	107.21
3	E	401	6AK	C37-N05-C36	-3.23	122.69	125.69
3	C	403	6AK	C01-N02-C11	3.21	110.38	107.21
3	B	402	6AK	C01-N02-C11	3.21	110.37	107.21
3	G	404	6AK	C01-N02-C11	3.20	110.36	107.21
3	H	303	6AK	C19-C17-N03	-3.19	104.31	106.61
3	A	403	6AK	C35-C34-N01	3.18	124.70	121.01
3	C	401	6AK	C01-N02-C11	3.18	110.34	107.21
3	H	304	6AK	C33-C34-N01	-3.15	112.64	119.17
3	C	404	6AK	C01-N02-C11	3.14	110.31	107.21
3	A	401	6AK	C13-C15-C14	-3.11	106.69	113.99
3	H	303	6AK	C35-C34-N01	3.11	124.62	121.01
3	C	405	6AK	C10-O01-C26	3.11	126.01	117.93
3	A	401	6AK	C01-N02-C11	3.10	110.27	107.21
3	H	304	6AK	C06-C07-C11	-3.09	104.55	106.99
3	A	401	6AK	C35-C39-C38	3.07	109.65	107.01
3	C	401	6AK	C33-C34-N01	-3.07	112.81	119.17
3	F	404	6AK	C01-N02-C11	3.06	110.23	107.21
3	H	303	6AK	C35-C39-C38	3.06	109.64	107.01
3	G	403	6AK	C35-C39-C38	3.06	109.64	107.01
3	E	401	6AK	C35-C39-C38	3.05	109.64	107.01
3	H	303	6AK	C14-N02-C01	-3.04	117.72	124.99
3	B	403	6AK	C37-N05-C36	-3.04	122.87	125.69
3	H	303	6AK	C06-C07-C11	-3.03	104.60	106.99
3	B	403	6AK	C35-C39-C38	3.01	109.59	107.01
3	C	404	6AK	C37-N05-C36	-3.01	122.90	125.69
3	C	401	6AK	C37-N05-C36	-3.00	122.91	125.69
3	C	405	6AK	C06-C01-N02	-2.98	104.89	109.78
3	B	403	6AK	C03-C02-C19	-2.98	117.23	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	404	6AK	C35-C39-C38	2.97	109.57	107.01
3	H	304	6AK	C37-N05-C36	-2.97	122.93	125.69
3	A	403	6AK	C35-C39-C38	2.96	109.56	107.01
3	D	403	6AK	C35-C39-C38	2.96	109.56	107.01
3	B	402	6AK	C10-O01-C26	2.96	125.62	117.93
3	D	401	6AK	C35-C39-C38	2.95	109.54	107.01
3	C	401	6AK	C35-C39-C38	2.95	109.54	107.01
3	C	403	6AK	C35-C39-C38	2.95	109.54	107.01
3	G	404	6AK	C35-C39-C38	2.94	109.53	107.01
3	H	304	6AK	C35-C39-C38	2.93	109.53	107.01
3	F	401	6AK	C35-C39-C38	2.92	109.52	107.01
3	F	401	6AK	C33-C34-N01	-2.92	113.12	119.17
3	F	403	6AK	C37-N05-C36	-2.91	122.99	125.69
3	F	404	6AK	C37-N05-C36	-2.91	122.99	125.69
3	C	405	6AK	C16-N03-C17	-2.90	125.44	128.09
3	F	404	6AK	C35-C39-C38	2.90	109.50	107.01
3	G	403	6AK	C03-C02-C19	-2.90	117.36	121.67
3	E	401	6AK	C13-C15-C14	-2.89	107.20	113.99
3	G	401	6AK	C06-C01-N02	-2.89	105.05	109.78
3	H	304	6AK	C06-C01-N02	-2.88	105.05	109.78
3	B	402	6AK	C35-C39-C38	2.88	109.49	107.01
3	C	405	6AK	C37-N05-C36	-2.87	123.02	125.69
3	A	401	6AK	C37-N05-C36	-2.87	123.03	125.69
3	E	403	6AK	C35-C39-C38	2.87	109.47	107.01
3	D	401	6AK	C37-N05-C36	-2.86	123.03	125.69
3	G	403	6AK	C06-C01-N02	-2.83	105.14	109.78
3	H	305	6AK	C37-N05-C36	-2.82	123.07	125.69
3	H	305	6AK	C35-C39-C38	2.82	109.43	107.01
3	G	403	6AK	C37-N05-C36	-2.79	123.10	125.69
3	F	405	6AK	C33-C34-C35	2.79	123.89	120.83
3	F	403	6AK	C16-N03-C17	-2.78	125.56	128.09
3	C	403	6AK	C37-N05-C36	-2.76	123.12	125.69
3	B	402	6AK	C35-C34-N01	2.76	124.21	121.01
3	A	404	6AK	C01-N02-C11	2.76	109.93	107.21
3	B	403	6AK	C33-C34-N01	-2.75	113.47	119.17
3	E	401	6AK	C03-C02-C19	-2.75	117.57	121.67
3	B	402	6AK	C37-N05-C36	-2.75	123.14	125.69
3	A	401	6AK	C06-C01-N02	-2.75	105.27	109.78
3	D	403	6AK	C06-C01-N02	-2.73	105.30	109.78
3	F	405	6AK	C18-C17-C19	2.72	135.12	130.30
3	A	401	6AK	C03-C02-C19	-2.71	117.63	121.67
3	H	301	6AK	C35-C39-C38	2.71	109.34	107.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	305	6AK	C16-N03-C17	-2.71	125.62	128.09
3	G	401	6AK	C01-C02-C19	2.70	127.22	122.91
3	F	405	6AK	C01-C02-C19	-2.69	118.61	122.91
3	A	403	6AK	C37-N05-C36	-2.69	123.19	125.69
3	D	401	6AK	C33-C34-N01	-2.66	113.66	119.17
3	B	403	6AK	C10-O01-C26	2.64	124.80	117.93
3	B	403	6AK	C06-C01-N02	-2.64	105.46	109.78
3	D	403	6AK	C01-C02-C19	2.64	127.12	122.91
3	A	404	6AK	C35-C39-C38	2.64	109.27	107.01
3	C	404	6AK	C06-C01-N02	-2.63	105.47	109.78
3	F	403	6AK	C35-C39-C38	2.63	109.27	107.01
3	G	401	6AK	C35-C39-C38	2.62	109.27	107.01
3	F	404	6AK	C16-N03-C17	-2.62	125.70	128.09
3	E	401	6AK	C06-C01-N02	-2.62	105.49	109.78
3	H	303	6AK	C16-N03-C17	-2.61	125.70	128.09
3	D	403	6AK	C37-N05-C36	-2.61	123.27	125.69
3	G	404	6AK	C06-C01-N02	-2.60	105.51	109.78
3	H	303	6AK	C37-N05-C36	-2.60	123.28	125.69
3	H	305	6AK	C06-C01-N02	-2.58	105.55	109.78
3	C	405	6AK	C35-C39-C38	2.58	109.23	107.01
3	E	403	6AK	C37-N05-C36	-2.58	123.30	125.69
3	F	405	6AK	C08-C07-C11	-2.56	125.33	127.46
3	F	403	6AK	C03-C02-C19	-2.55	117.86	121.67
3	D	401	6AK	C06-C01-N02	-2.55	105.60	109.78
3	A	403	6AK	C01-N02-C11	2.55	109.72	107.21
3	H	301	6AK	C16-N03-C17	-2.55	125.77	128.09
3	E	403	6AK	C35-C34-N01	2.54	123.96	121.01
3	H	301	6AK	C06-C01-N02	-2.53	105.63	109.78
3	E	401	6AK	C16-N03-C17	-2.53	125.78	128.09
3	A	404	6AK	C06-C01-N02	-2.51	105.67	109.78
3	F	401	6AK	C06-C01-N02	-2.50	105.68	109.78
3	C	404	6AK	C16-N03-C17	-2.49	125.81	128.09
3	G	401	6AK	C16-N03-C17	-2.48	125.83	128.09
3	F	404	6AK	C03-C02-C19	-2.47	117.99	121.67
3	C	403	6AK	C35-C34-N01	2.46	123.86	121.01
3	F	403	6AK	C06-C01-N02	-2.46	105.75	109.78
3	H	305	6AK	C08-C07-C11	2.46	129.51	127.46
3	H	304	6AK	C01-N02-C11	2.46	109.63	107.21
3	H	304	6AK	C16-N03-C17	-2.46	125.85	128.09
3	F	401	6AK	C16-N03-C17	-2.46	125.85	128.09
3	B	403	6AK	C16-N03-C17	-2.45	125.85	128.09
3	A	404	6AK	C35-C34-N01	2.45	123.85	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	6AK	C16-N03-C17	-2.44	125.87	128.09
3	F	405	6AK	O01-C10-C09	-2.42	99.39	108.30
3	A	401	6AK	C16-N03-C17	-2.42	125.88	128.09
3	C	405	6AK	C03-C02-C19	-2.41	118.07	121.67
3	D	401	6AK	C16-N03-C17	-2.41	125.89	128.09
3	A	403	6AK	C16-N03-C17	-2.41	125.89	128.09
3	F	403	6AK	C33-C34-N01	-2.41	114.19	119.17
3	G	404	6AK	C16-N03-C17	-2.39	125.91	128.09
3	G	401	6AK	C03-C02-C19	-2.39	118.11	121.67
3	C	405	6AK	C01-N02-C11	2.38	109.56	107.21
3	B	403	6AK	C01-C02-C19	2.37	126.69	122.91
3	D	403	6AK	C13-C15-C14	-2.37	108.43	113.99
3	A	403	6AK	C06-C01-N02	-2.36	105.92	109.78
3	H	301	6AK	C33-C34-N01	-2.36	114.29	119.17
3	G	404	6AK	C31-C33-C34	2.35	123.19	118.69
3	B	402	6AK	C16-N03-C17	-2.35	125.95	128.09
3	E	403	6AK	C06-C01-N02	-2.35	105.93	109.78
3	E	403	6AK	C16-N03-C17	-2.33	125.96	128.09
3	C	403	6AK	C16-N03-C17	-2.33	125.97	128.09
3	C	401	6AK	C06-C01-N02	-2.32	105.98	109.78
3	C	403	6AK	C08-C07-C11	2.31	129.39	127.46
3	F	404	6AK	C31-C33-C34	2.28	123.05	118.69
3	F	404	6AK	C06-C01-N02	-2.27	106.07	109.78
3	G	404	6AK	C33-C34-C35	-2.27	118.35	120.83
3	H	303	6AK	C18-C17-C19	2.26	134.31	130.30
3	D	403	6AK	C15-C14-N02	2.26	119.74	113.33
3	G	403	6AK	C33-C34-N01	-2.26	114.49	119.17
3	A	404	6AK	C01-C06-C07	2.26	109.76	106.22
3	H	304	6AK	C03-C02-C19	-2.26	118.31	121.67
3	B	403	6AK	C33-C34-C35	-2.25	118.37	120.83
3	A	404	6AK	C29-C28-C27	-2.25	115.61	119.57
3	F	403	6AK	C10-O01-C26	2.25	123.77	117.93
3	F	405	6AK	C06-C07-C11	-2.25	105.22	106.99
3	F	403	6AK	C18-C17-C19	2.24	134.27	130.30
3	G	404	6AK	C03-C02-C19	-2.23	118.34	121.67
3	D	403	6AK	C16-N03-C17	-2.23	126.05	128.09
3	C	404	6AK	C31-C33-C34	2.23	122.95	118.69
3	A	404	6AK	C37-N05-C36	-2.22	123.63	125.69
3	G	401	6AK	C05-C06-C07	-2.22	129.95	133.73
3	A	401	6AK	C33-C34-N01	-2.21	114.59	119.17
3	G	403	6AK	C13-C15-C14	-2.20	108.82	113.99
3	F	405	6AK	C04-C03-C02	2.20	124.81	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	401	6AK	C01-C06-C07	2.20	109.67	106.22
3	C	405	6AK	C26-C25-C23	2.18	122.90	120.61
3	C	404	6AK	C03-C02-C19	-2.17	118.44	121.67
3	G	401	6AK	C33-C34-N01	-2.14	114.74	119.17
3	F	405	6AK	C18-C17-N03	-2.13	119.60	122.97
3	G	403	6AK	C33-C34-C35	-2.13	118.50	120.83
3	C	403	6AK	C19-C17-N03	-2.12	105.08	106.61
3	F	401	6AK	C03-C02-C19	-2.12	118.51	121.67
3	F	405	6AK	C29-C28-C27	2.12	123.30	119.57
3	G	403	6AK	C01-C02-C19	2.11	126.28	122.91
3	H	304	6AK	C31-C33-C34	2.11	122.72	118.69
3	C	401	6AK	C31-C33-C34	2.11	122.72	118.69
3	D	401	6AK	C03-C02-C19	-2.10	118.55	121.67
3	F	405	6AK	C20-N04-N03	-2.09	103.21	105.55
3	B	403	6AK	C31-C33-C34	2.08	122.67	118.69
3	H	303	6AK	C24-C23-C25	2.08	123.24	119.57
3	C	405	6AK	C01-C02-C19	2.07	126.22	122.91
3	H	304	6AK	C33-C34-C35	-2.07	118.56	120.83
3	H	301	6AK	C08-C07-C11	2.06	129.18	127.46
3	H	303	6AK	C06-C01-N02	-2.05	106.42	109.78
3	D	403	6AK	C19-C17-N03	-2.05	105.13	106.61
3	H	301	6AK	C37-N05-C36	-2.05	123.79	125.69
3	F	401	6AK	C31-C33-C34	2.05	122.60	118.69
3	C	404	6AK	C33-C34-C35	-2.04	118.60	120.83
3	E	401	6AK	C36-C35-C39	-2.04	105.30	106.92
3	D	401	6AK	O03-C32-C31	2.04	126.80	121.46
3	A	401	6AK	C33-C34-C35	-2.03	118.60	120.83
3	A	403	6AK	C19-C17-N03	-2.03	105.14	106.61
3	B	403	6AK	C36-C35-C39	-2.03	105.31	106.92
3	F	401	6AK	C33-C34-C35	-2.02	118.61	120.83
3	B	402	6AK	C06-C01-N02	-2.02	106.47	109.78
3	C	403	6AK	C06-C01-N02	-2.01	106.49	109.78
3	D	403	6AK	C18-C17-C19	2.01	133.85	130.30
3	G	401	6AK	C06-C07-C11	-2.00	105.41	106.99
3	G	403	6AK	C16-N03-C17	-2.00	126.26	128.09

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	6AK	C07-C08-C09-C10
3	A	403	6AK	C30-C31-C32-O04

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Mol	Chain	Res	Type	Atoms
3	A	404	6AK	C07-C08-C09-C10
3	B	403	6AK	C07-C08-C09-C10
3	C	401	6AK	C07-C08-C09-C10
3	D	401	6AK	C07-C08-C09-C10
3	E	401	6AK	C07-C08-C09-C10
3	F	401	6AK	C07-C08-C09-C10
3	F	403	6AK	C06-C07-C08-C09
3	F	403	6AK	C07-C08-C09-C10
3	F	405	6AK	C06-C07-C08-C09
3	G	401	6AK	C06-C07-C08-C09
3	G	401	6AK	C35-C34-N01-C12
3	G	403	6AK	C06-C07-C08-C09
3	G	403	6AK	C07-C08-C09-C10
3	G	404	6AK	C35-C34-N01-C12
3	H	303	6AK	C06-C07-C08-C09
3	H	303	6AK	C07-C08-C09-C10
3	H	304	6AK	C07-C08-C09-C10
3	H	305	6AK	C11-C07-C08-C09
3	H	305	6AK	C06-C07-C08-C09
3	H	305	6AK	C07-C08-C09-C10
3	A	403	6AK	C33-C31-C32-O03
3	A	403	6AK	C33-C31-C32-O04
3	A	403	6AK	C30-C31-C32-O03
3	F	404	6AK	C33-C31-C32-O03
3	F	404	6AK	C33-C31-C32-O04
3	F	404	6AK	C30-C31-C32-O03
3	H	304	6AK	C30-C31-C32-O03
3	F	404	6AK	C30-C31-C32-O04
3	H	304	6AK	C33-C31-C32-O03
3	H	304	6AK	C33-C31-C32-O04
3	H	304	6AK	C30-C31-C32-O04
3	F	405	6AK	C11-C07-C08-C09
3	C	404	6AK	C33-C31-C32-O04
3	C	404	6AK	C33-C31-C32-O03
3	C	403	6AK	C25-C26-O01-C10
3	C	403	6AK	C27-C26-O01-C10
3	E	403	6AK	C25-C26-O01-C10
3	C	404	6AK	C30-C31-C32-O04
3	E	403	6AK	C27-C26-O01-C10
3	H	301	6AK	C25-C26-O01-C10
3	H	305	6AK	C27-C26-O01-C10
3	H	301	6AK	C08-C09-C10-O01

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Mol	Chain	Res	Type	Atoms
3	A	404	6AK	C25-C26-O01-C10
3	A	404	6AK	C27-C26-O01-C10
3	H	301	6AK	C27-C26-O01-C10
3	H	305	6AK	C25-C26-O01-C10
3	C	404	6AK	C30-C31-C32-O03
3	A	404	6AK	C33-C31-C32-O04
3	D	401	6AK	C27-C26-O01-C10
3	F	401	6AK	C27-C26-O01-C10
3	D	401	6AK	C25-C26-O01-C10
3	A	404	6AK	C33-C31-C32-O03
3	A	404	6AK	C30-C31-C32-O04
3	F	401	6AK	C25-C26-O01-C10
3	F	403	6AK	C08-C09-C10-O01
3	A	404	6AK	C30-C31-C32-O03
3	G	404	6AK	C08-C09-C10-O01
3	H	304	6AK	C08-C09-C10-O01
3	G	403	6AK	C08-C09-C10-O01
3	C	405	6AK	C08-C09-C10-O01
3	C	401	6AK	C27-C26-O01-C10
3	F	403	6AK	C27-C26-O01-C10
3	F	405	6AK	C25-C26-O01-C10
3	H	305	6AK	C33-C31-C32-O04
3	G	403	6AK	C27-C26-O01-C10
3	B	403	6AK	C27-C26-O01-C10
3	F	403	6AK	C25-C26-O01-C10
3	G	401	6AK	C27-C26-O01-C10
3	F	405	6AK	C27-C26-O01-C10
3	H	305	6AK	C33-C31-C32-O03
3	C	401	6AK	C25-C26-O01-C10
3	F	403	6AK	C11-C07-C08-C09
3	B	403	6AK	C25-C26-O01-C10
3	G	403	6AK	C25-C26-O01-C10
3	H	305	6AK	C30-C31-C32-O04
3	G	401	6AK	C25-C26-O01-C10
3	H	305	6AK	C30-C31-C32-O03
3	G	404	6AK	C25-C26-O01-C10
3	H	301	6AK	C06-C07-C08-C09
3	E	403	6AK	C09-C10-O01-C26
3	G	404	6AK	C27-C26-O01-C10
3	A	404	6AK	C09-C10-O01-C26
3	H	303	6AK	C09-C10-O01-C26
3	C	403	6AK	C09-C10-O01-C26

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Mol	Chain	Res	Type	Atoms
3	H	305	6AK	C08-C09-C10-O01
3	F	401	6AK	C08-C09-C10-O01
3	G	403	6AK	C33-C31-C32-O04
3	H	305	6AK	C09-C10-O01-C26
3	E	401	6AK	C27-C26-O01-C10
3	G	403	6AK	C33-C31-C32-O03
3	B	402	6AK	C25-C26-O01-C10
3	F	405	6AK	C07-C08-C09-C10
3	G	401	6AK	C07-C08-C09-C10
3	G	404	6AK	C07-C08-C09-C10
3	H	301	6AK	C07-C08-C09-C10
3	G	403	6AK	C30-C31-C32-O04
3	H	303	6AK	C08-C09-C10-O01
3	G	403	6AK	C30-C31-C32-O03
3	B	402	6AK	C27-C26-O01-C10
3	G	401	6AK	C08-C09-C10-O01
3	E	401	6AK	C25-C26-O01-C10
3	C	405	6AK	C09-C10-O01-C26
3	A	401	6AK	C08-C09-C10-O01
3	A	401	6AK	C35-C34-N01-C12
3	A	404	6AK	C35-C34-N01-C12
3	B	403	6AK	C35-C34-N01-C12
3	H	301	6AK	C35-C34-N01-C12
3	H	303	6AK	C35-C34-N01-C12
3	G	404	6AK	C33-C34-N01-C12
3	D	403	6AK	C11-C07-C08-C09
3	F	403	6AK	C33-C31-C32-O04
3	A	404	6AK	C11-C07-C08-C09
3	F	403	6AK	C33-C31-C32-O03
3	F	403	6AK	C30-C31-C32-O04
3	G	403	6AK	C09-C10-O01-C26
3	F	403	6AK	C30-C31-C32-O03
3	A	403	6AK	C08-C09-C10-O01
3	E	401	6AK	C08-C09-C10-O01
3	F	403	6AK	C09-C10-O01-C26
3	G	404	6AK	C33-C31-C32-O04
3	G	404	6AK	C30-C31-C32-O04
3	G	404	6AK	C33-C31-C32-O03
3	C	401	6AK	C35-C34-N01-C12
3	C	404	6AK	C35-C34-N01-C12
3	E	401	6AK	C35-C34-N01-C12
3	E	403	6AK	C35-C34-N01-C12

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Mol	Chain	Res	Type	Atoms
3	F	401	6AK	C35-C34-N01-C12
3	F	404	6AK	C35-C34-N01-C12
3	H	304	6AK	C35-C34-N01-C12
3	A	401	6AK	C27-C26-O01-C10
3	G	404	6AK	C30-C31-C32-O03
3	G	404	6AK	C35-C34-N01-C13
3	F	405	6AK	C09-C10-O01-C26

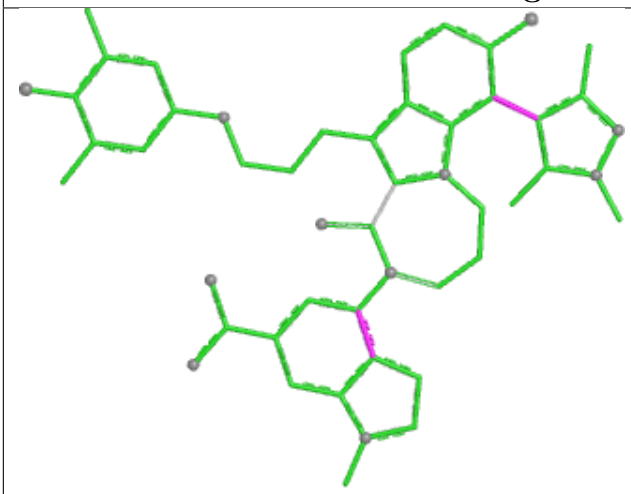
There are no ring outliers.

16 monomers are involved in 32 short contacts:

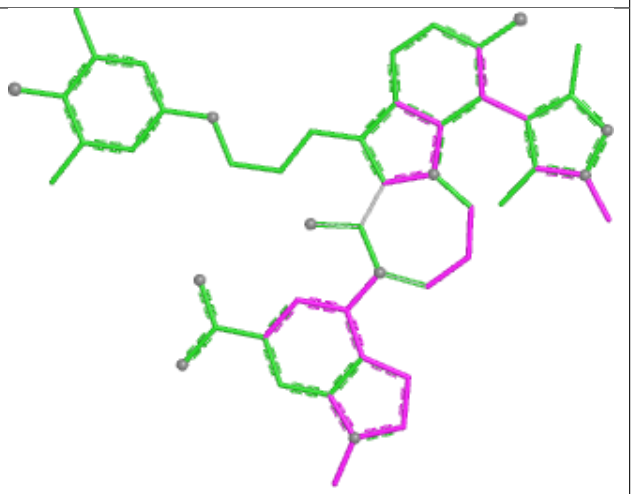
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	404	6AK	2	0
3	G	403	6AK	1	0
3	A	404	6AK	2	0
3	C	405	6AK	3	0
3	F	404	6AK	1	0
3	F	403	6AK	1	0
3	G	401	6AK	2	0
3	F	405	6AK	4	0
3	D	403	6AK	1	0
3	B	403	6AK	4	0
3	F	401	6AK	1	0
3	H	301	6AK	4	0
3	E	403	6AK	3	0
3	A	401	6AK	1	0
3	H	305	6AK	1	0
3	C	401	6AK	1	0

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

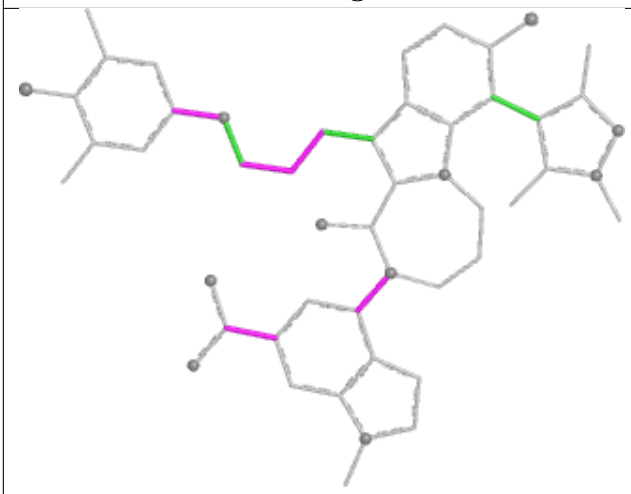
Ligand 6AK G 404



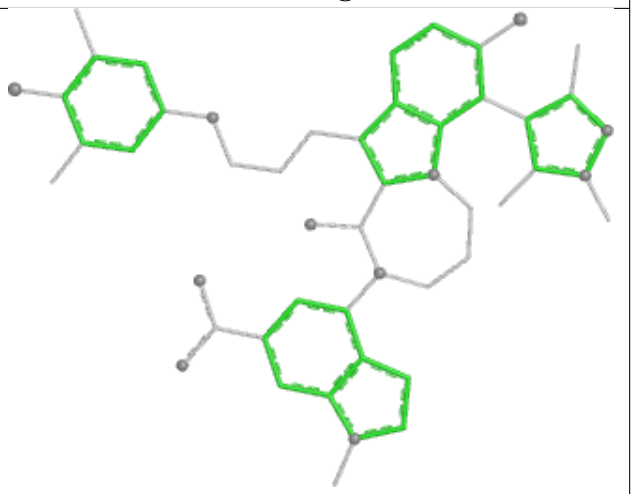
Bond lengths



Bond angles

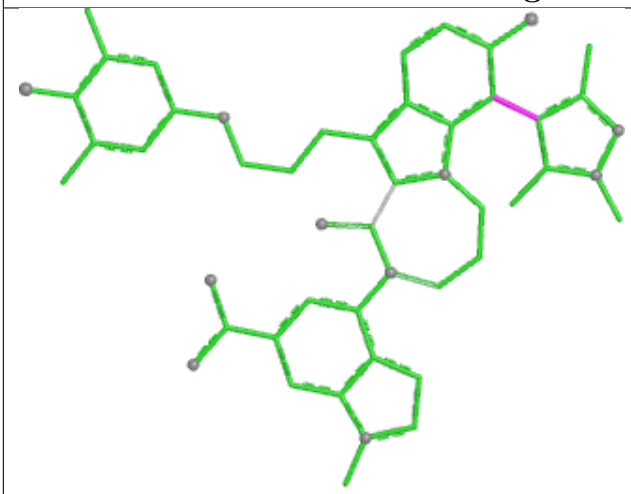


Torsions



Rings

Ligand 6AK G 403



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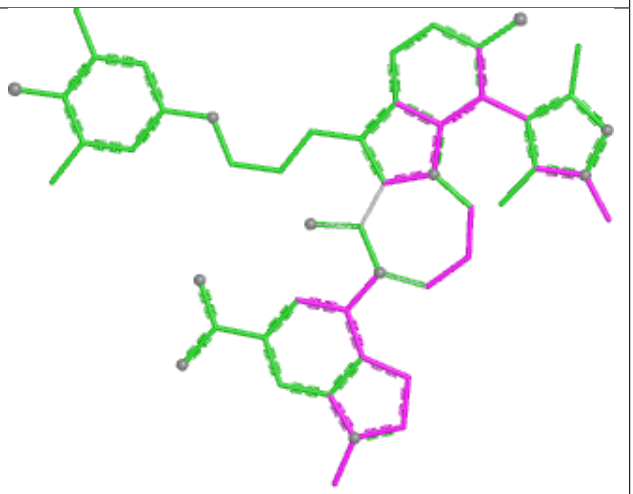
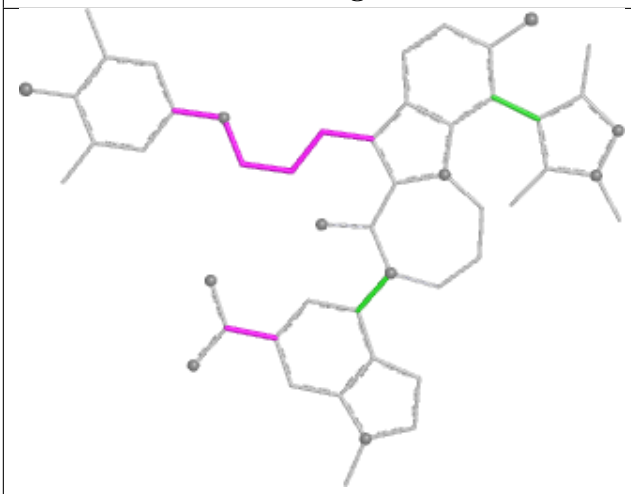


Bond angles



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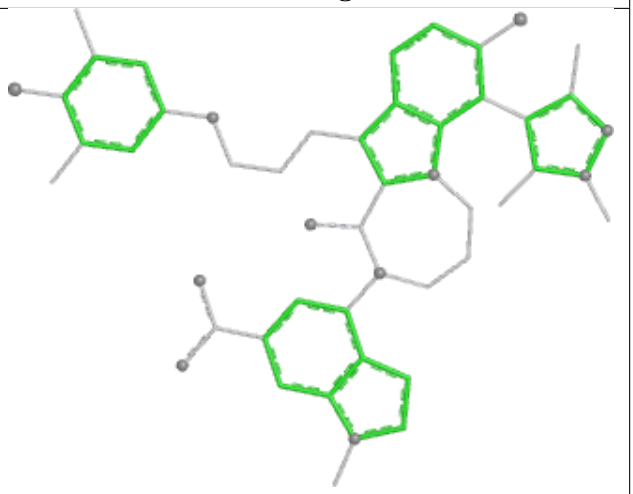
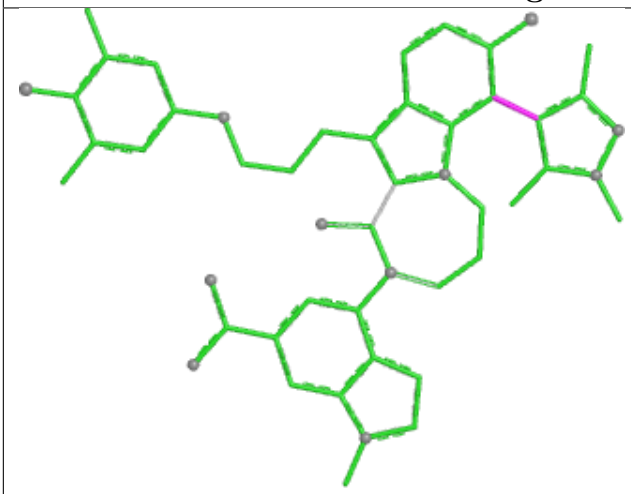


Rings

Ligand 6AK E 401



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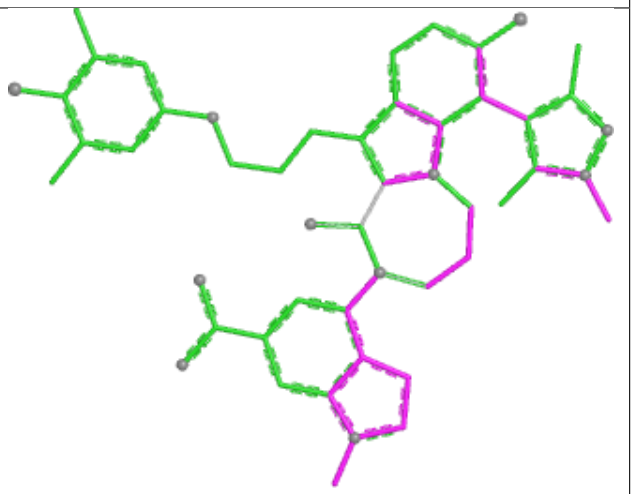
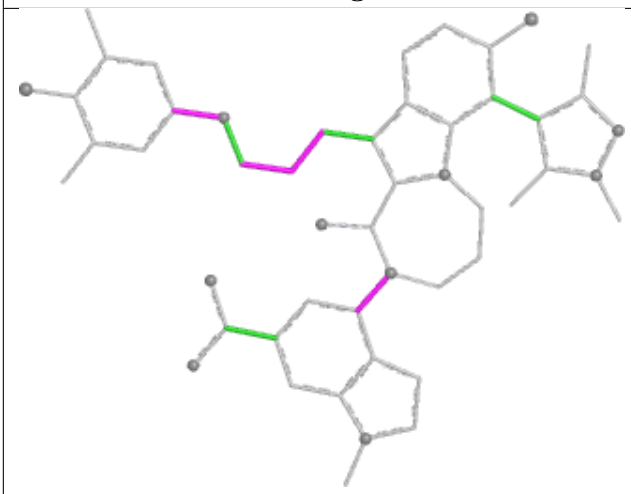


Bond angles



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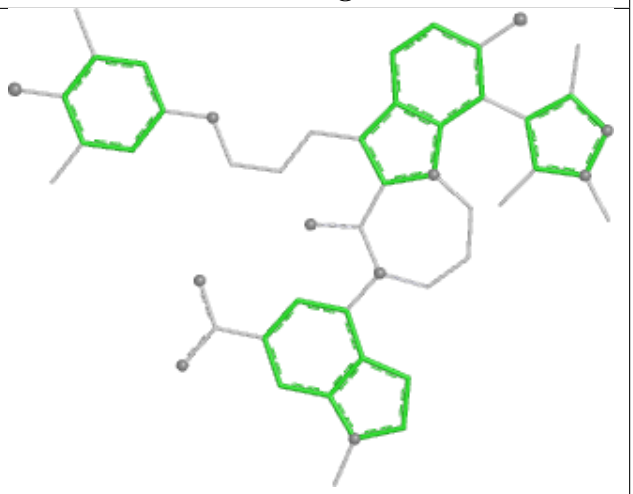
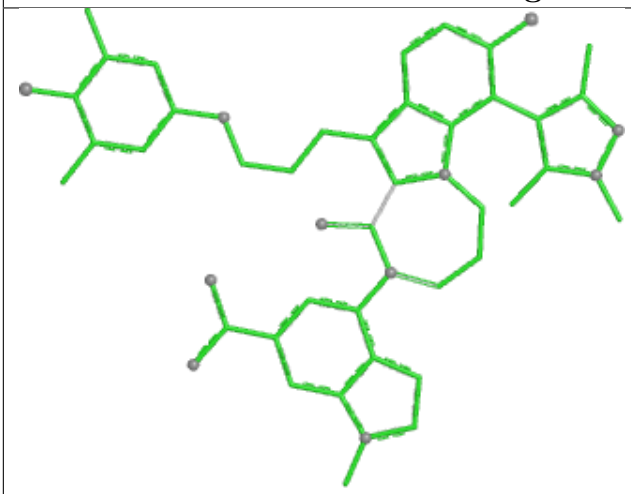


Rings

Ligand 6AK A 404



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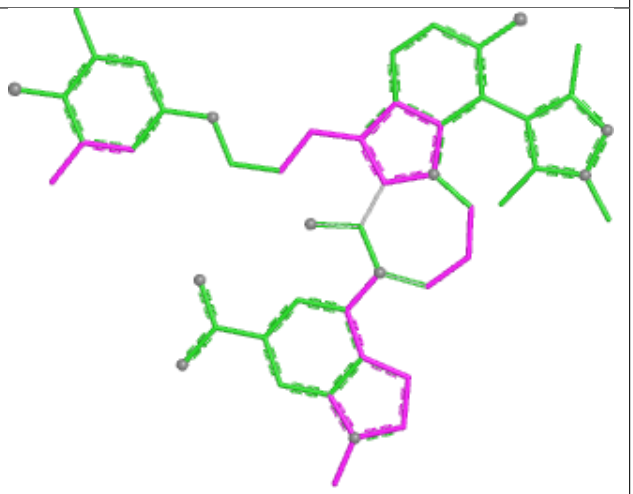
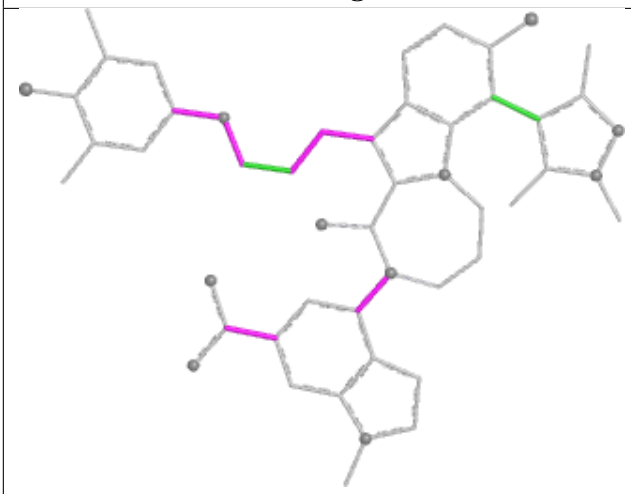
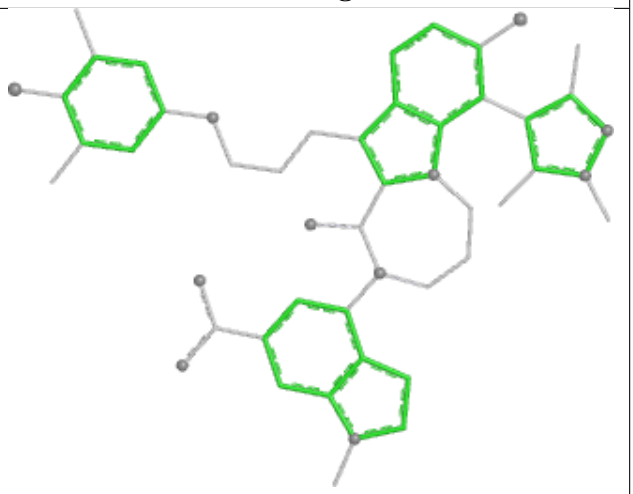


Bond angles

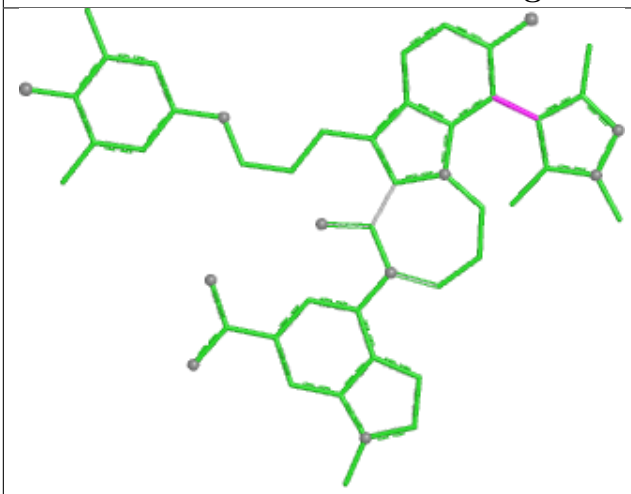


Torsions

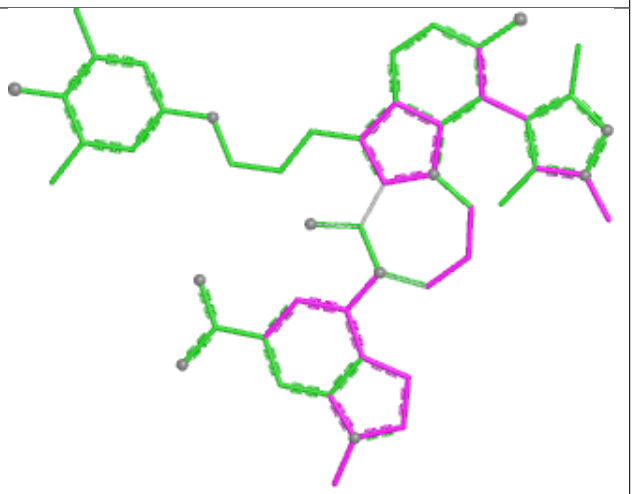


Rings

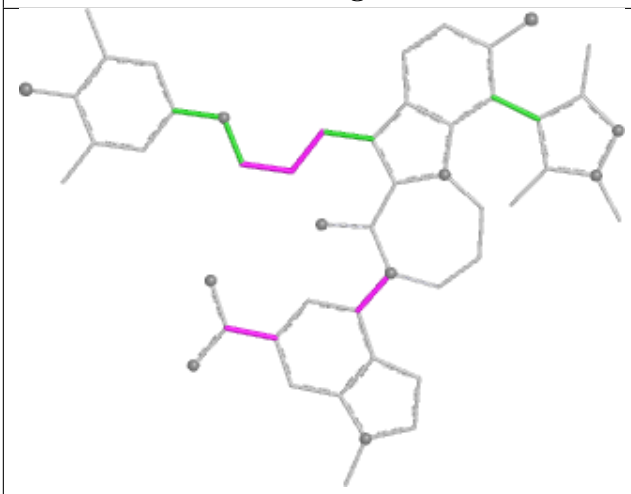
Ligand 6AK H 304



Bond lengths



Bond angles



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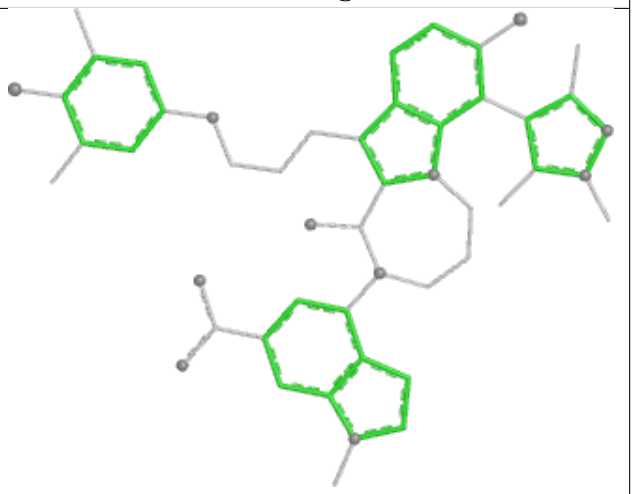
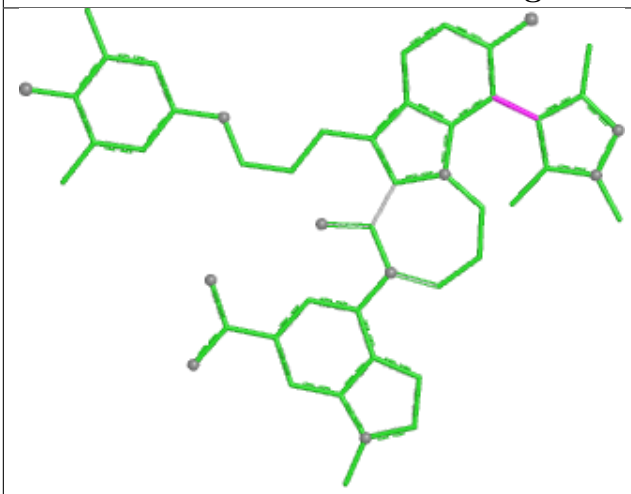


Rings

Ligand 6AK D 401



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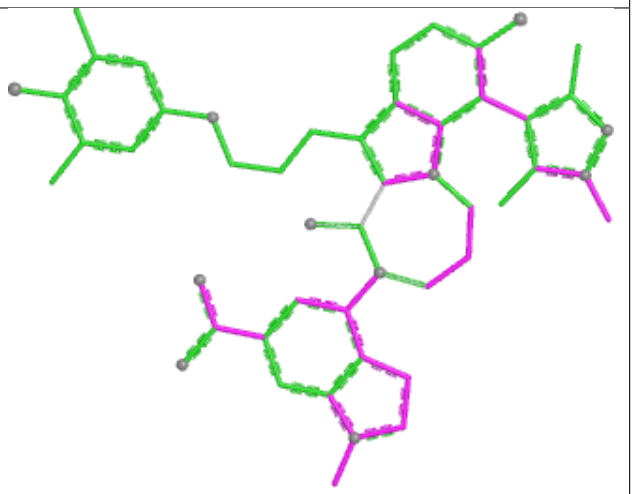
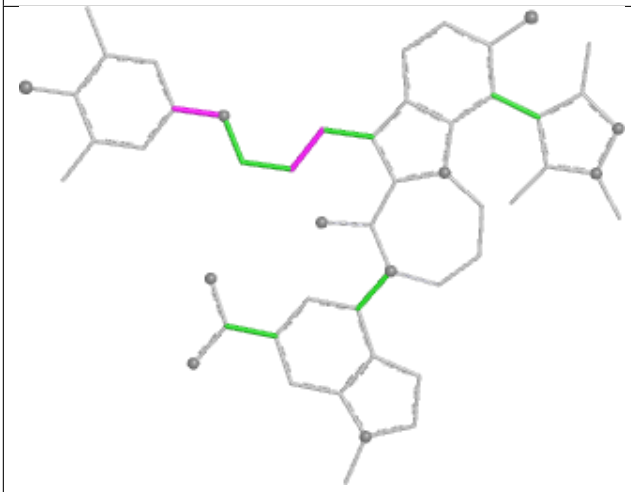


Bond angles



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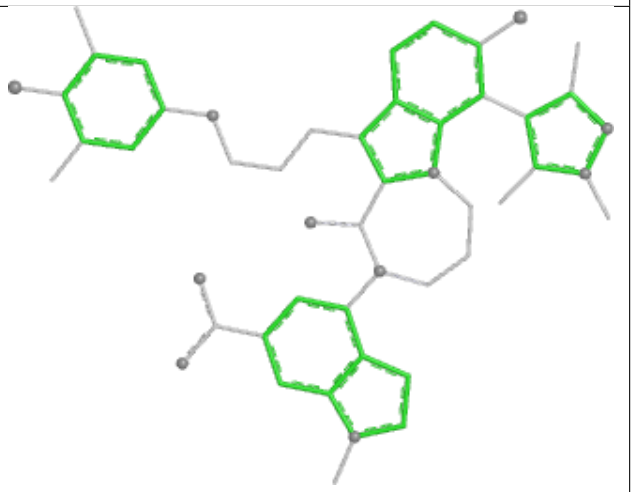
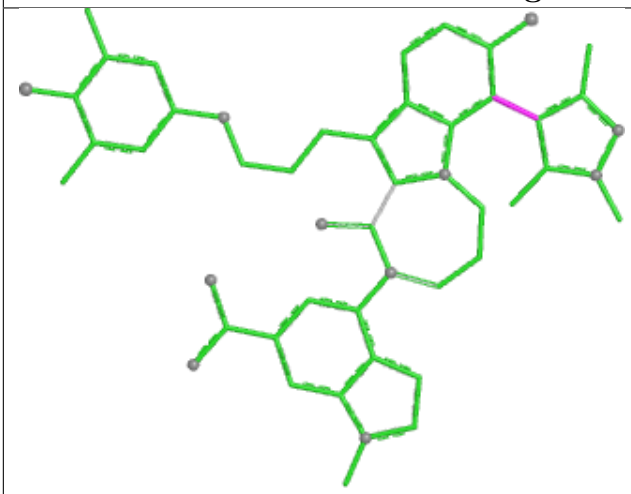


Rings

Ligand 6AK A 403



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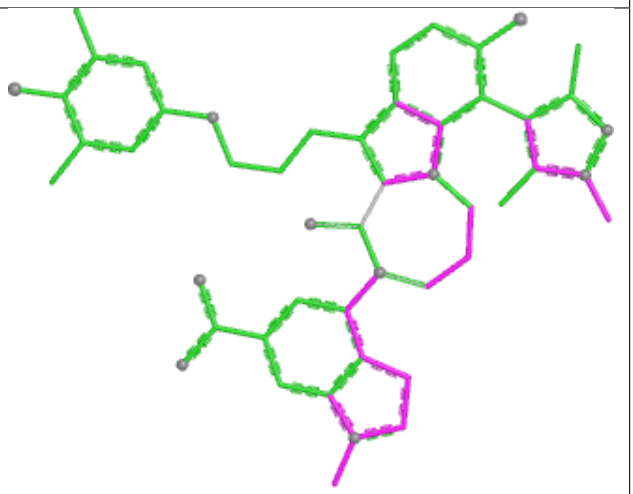
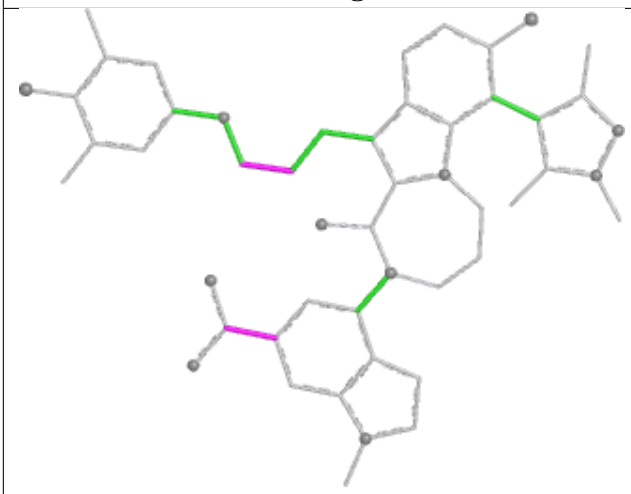


Bond angles



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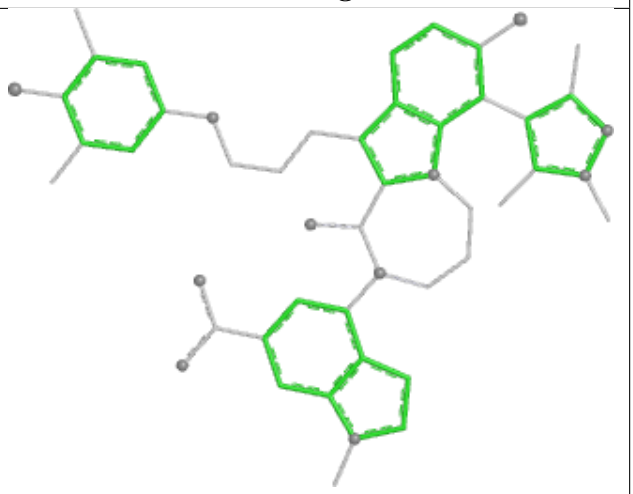
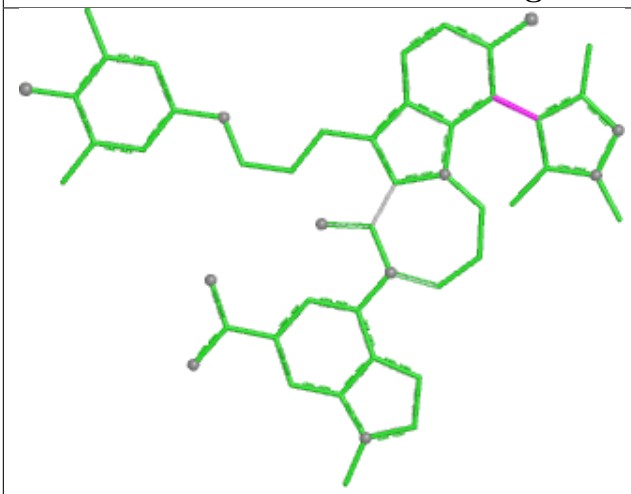


Rings

Ligand 6AK C 405



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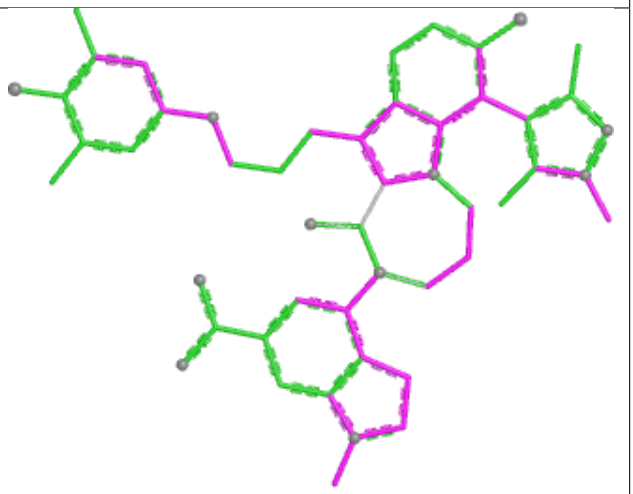

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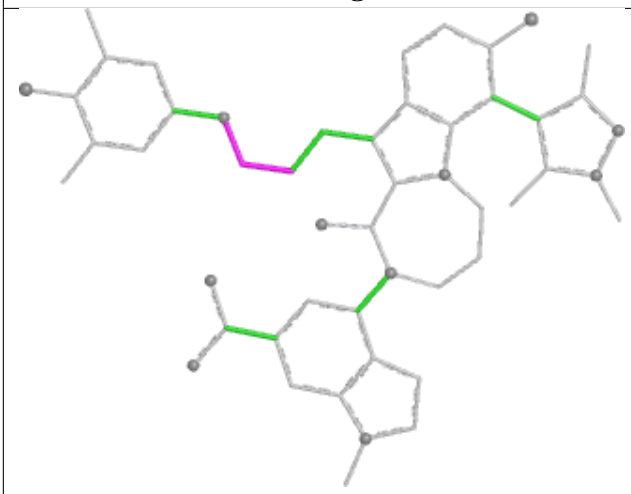
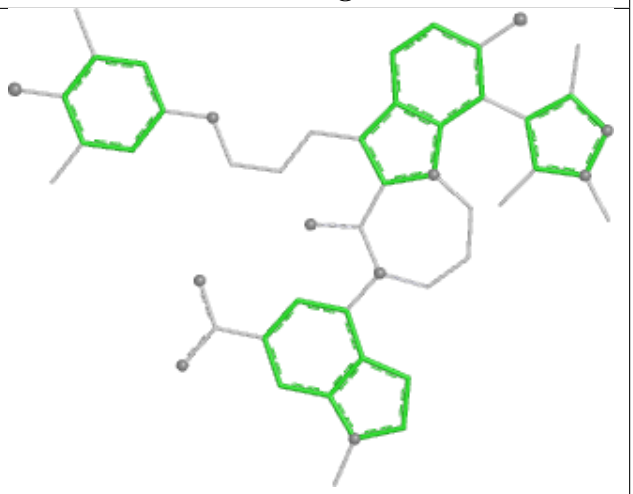
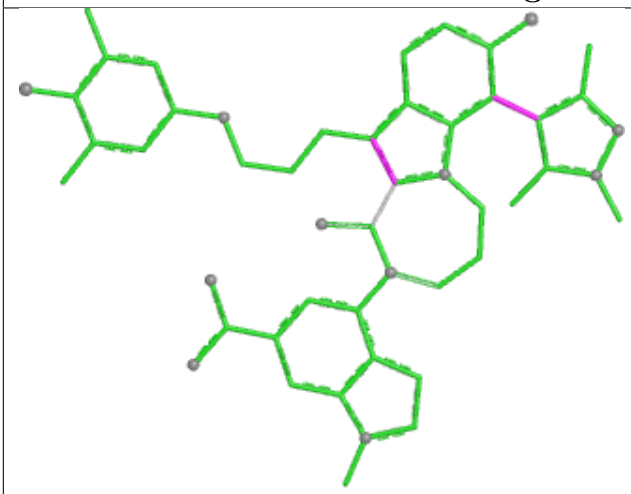


Torsions



Rings

Ligand 6AK H 303



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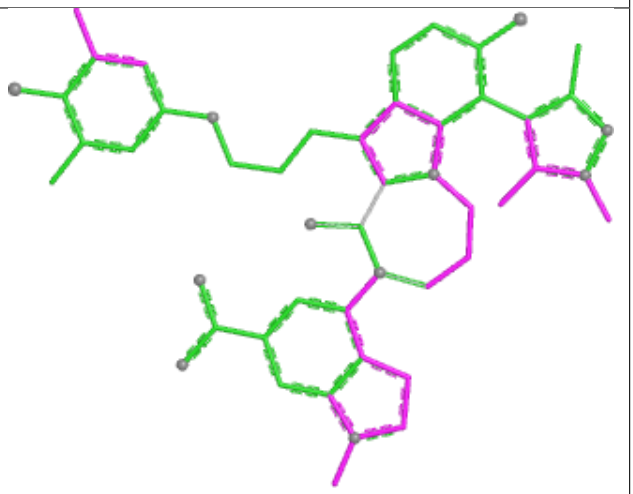
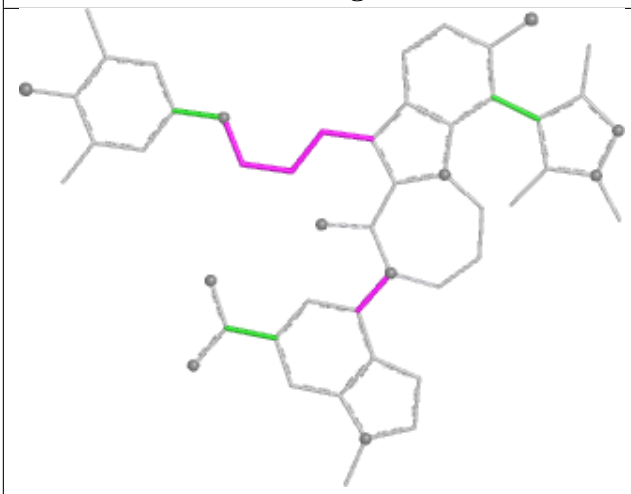


Bond angles



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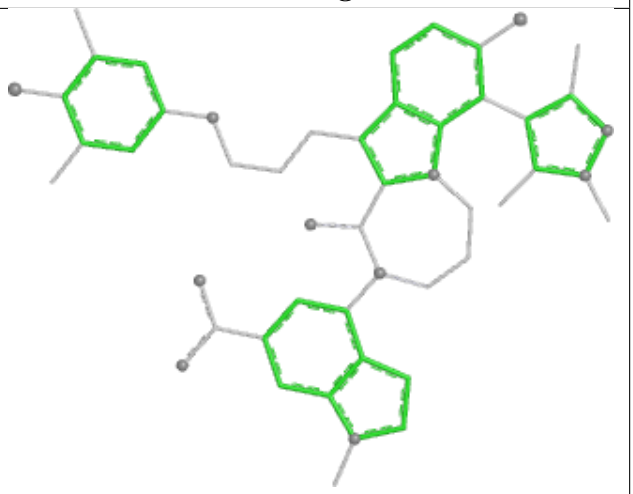
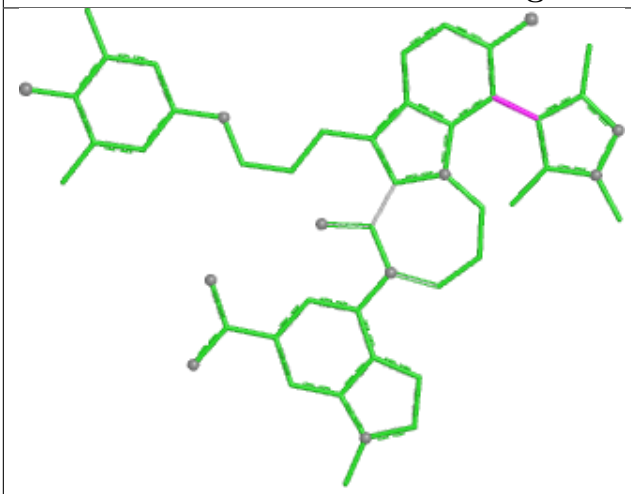


Rings

Ligand 6AK F 404



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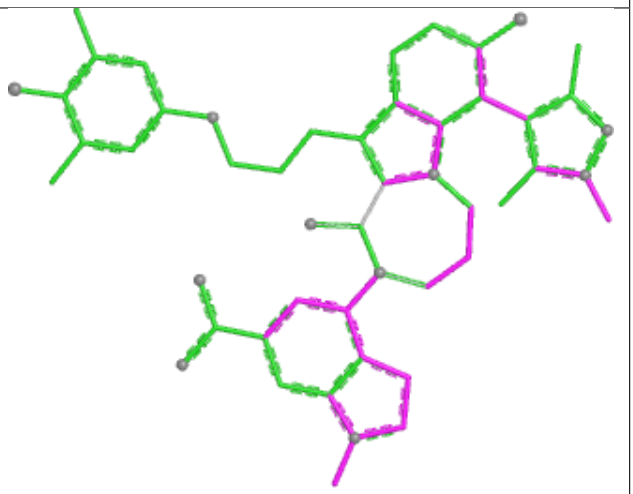

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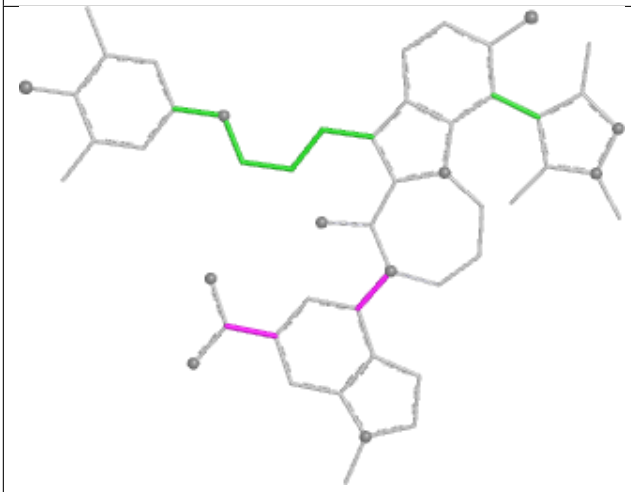

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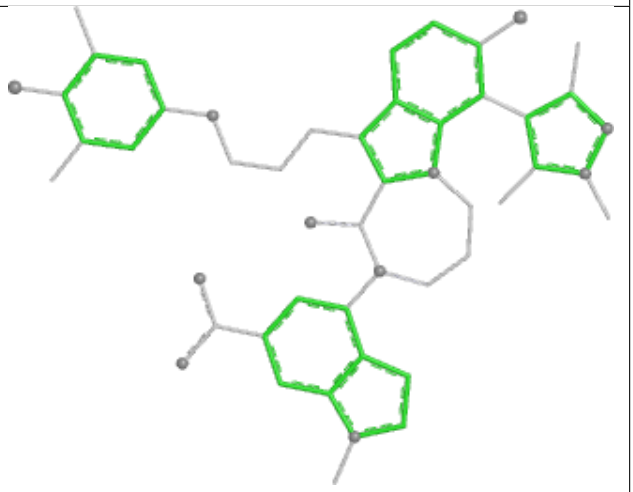

Rings

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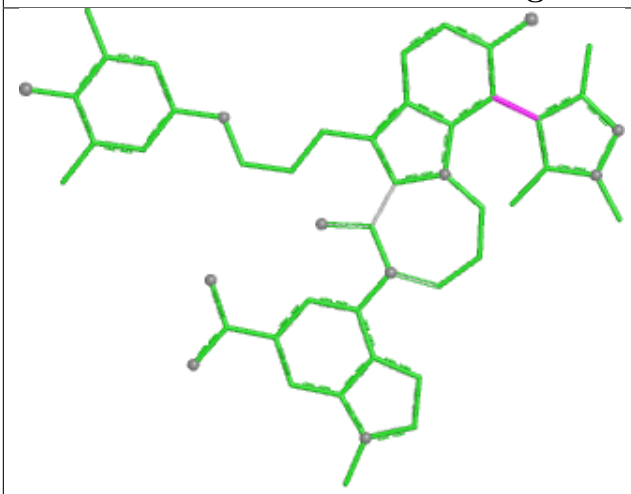

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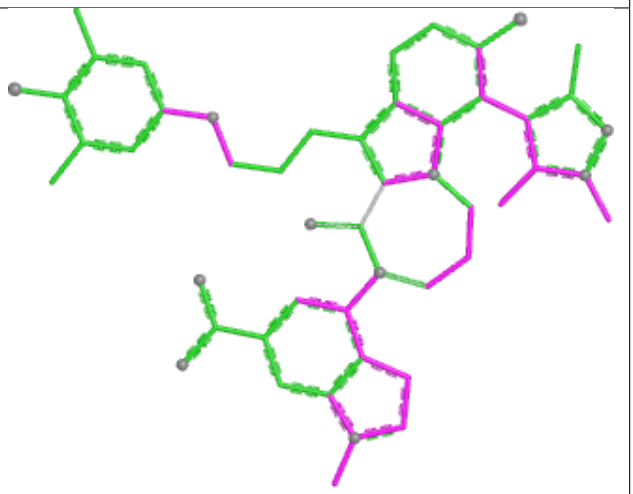

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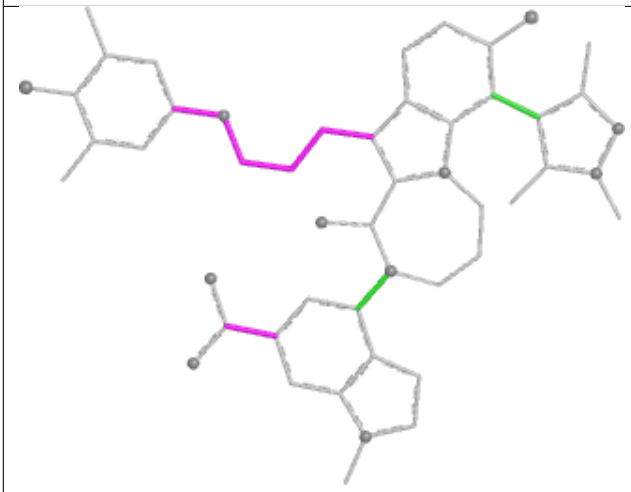

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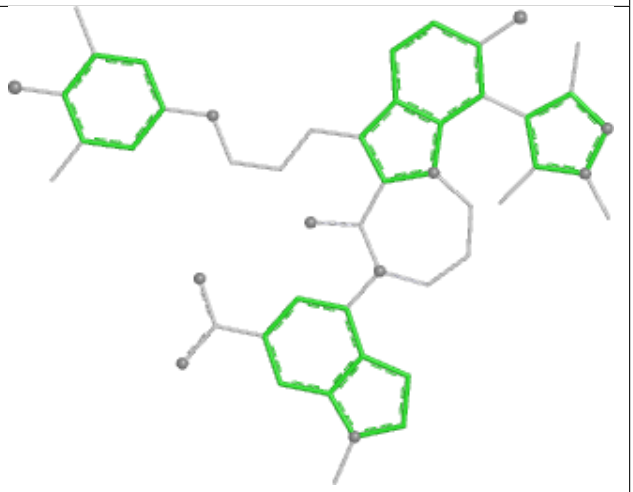
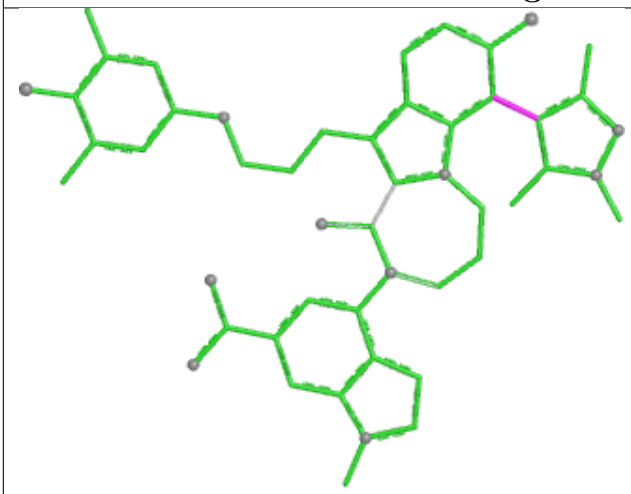


Rings

Ligand 6AK G 401



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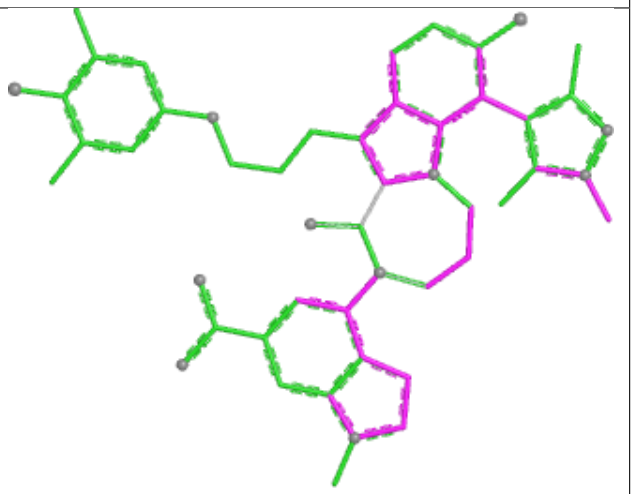

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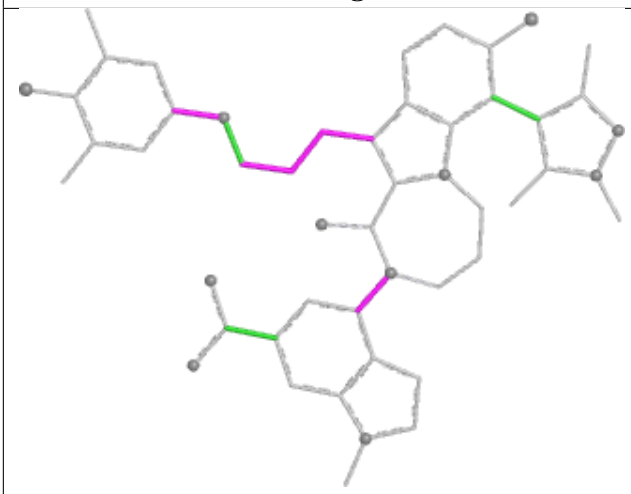

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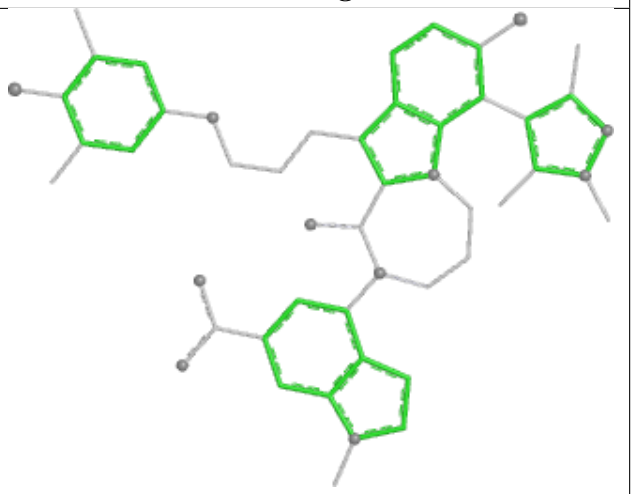
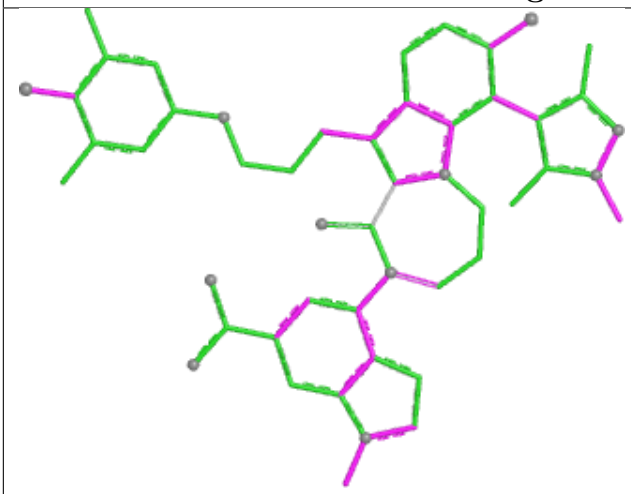


Rings

Ligand 6AK F 405



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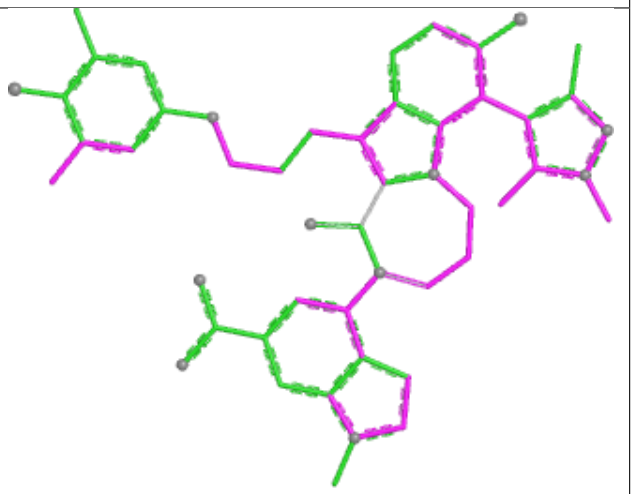

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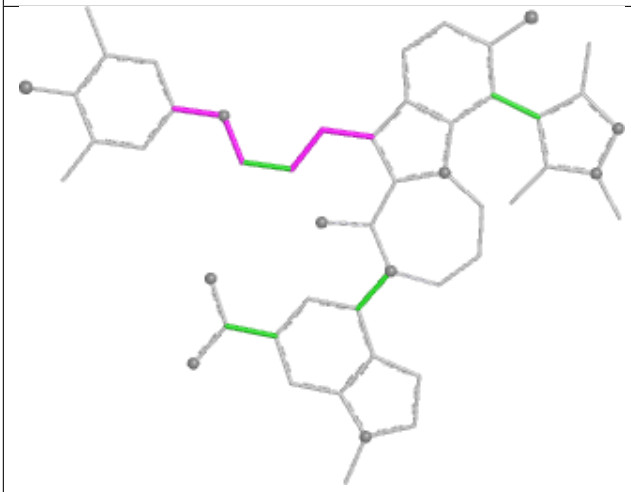

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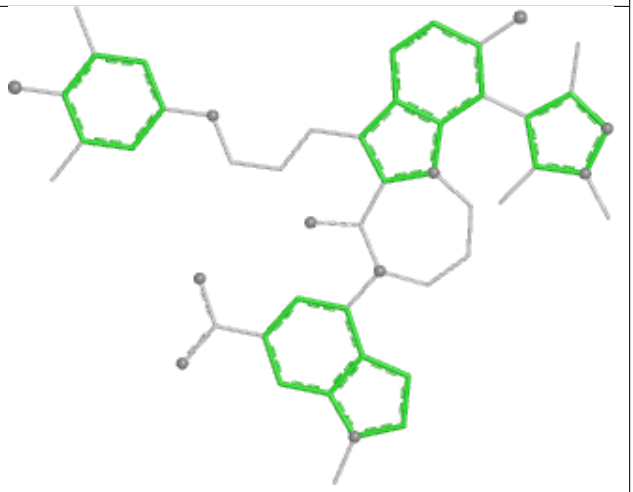

Rings

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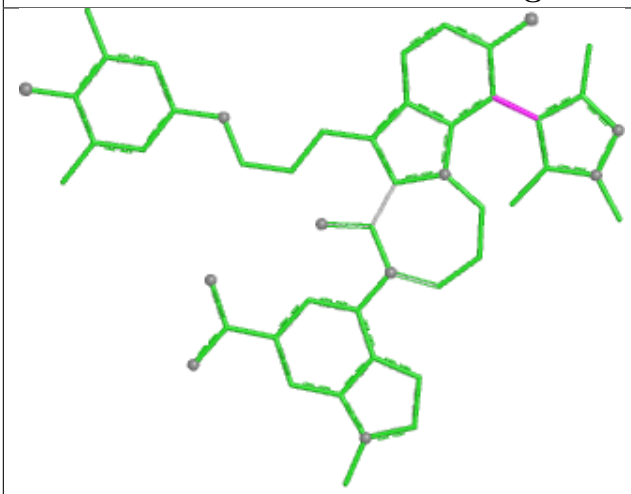

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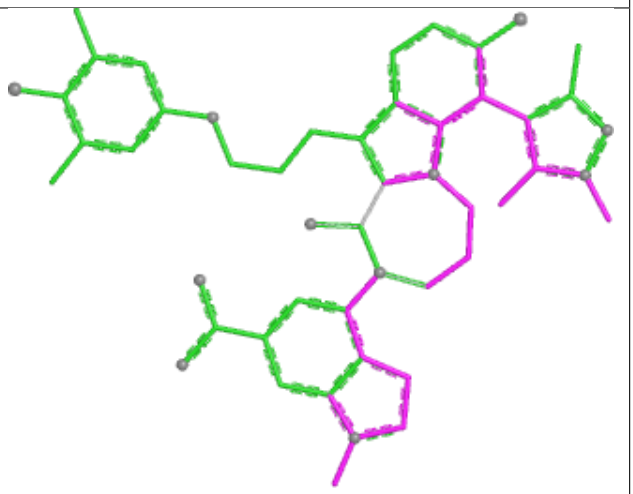

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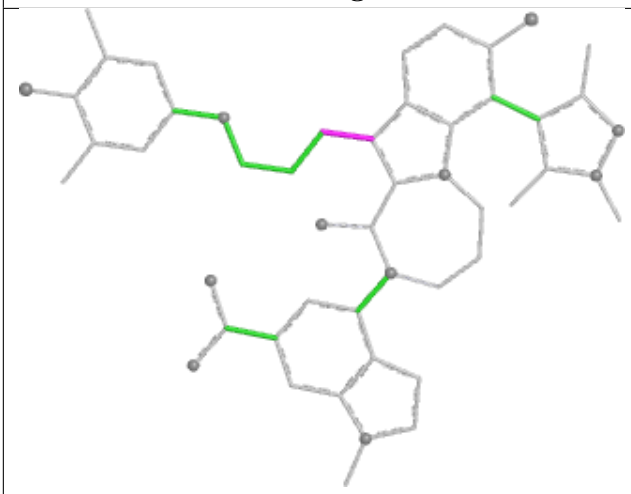

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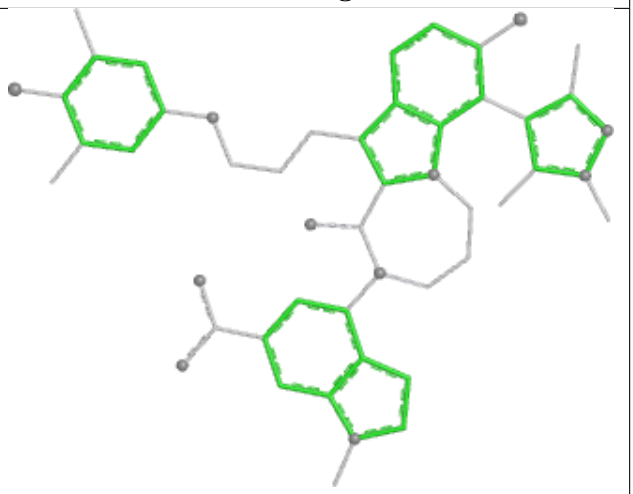

Rings

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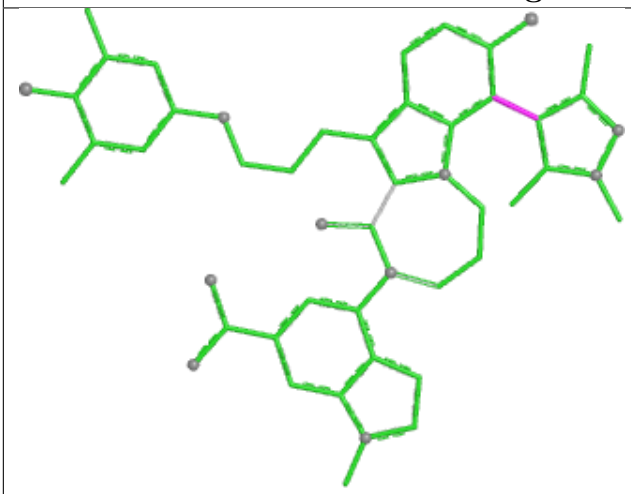

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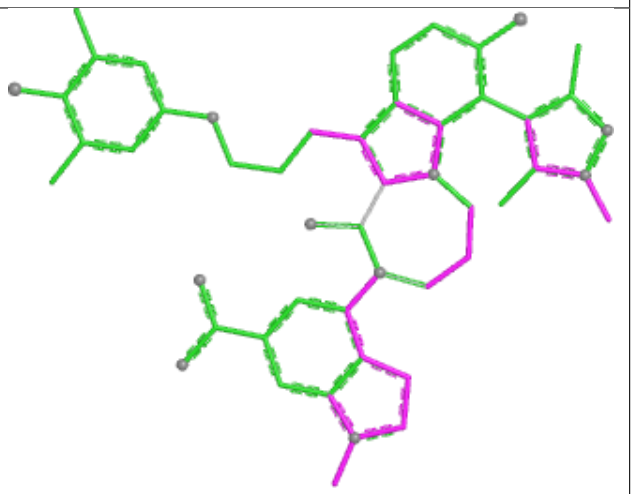

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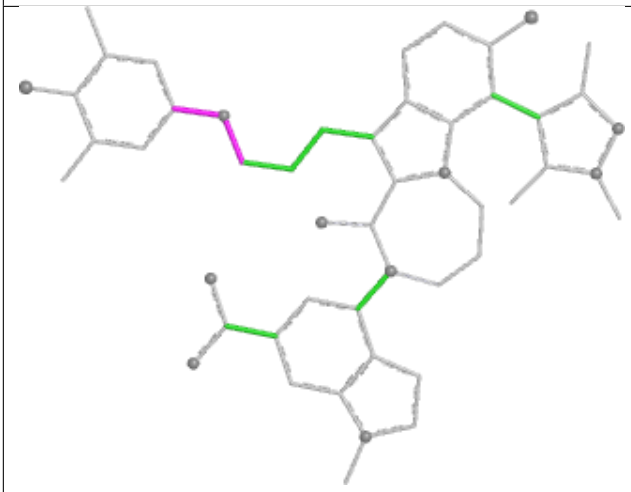

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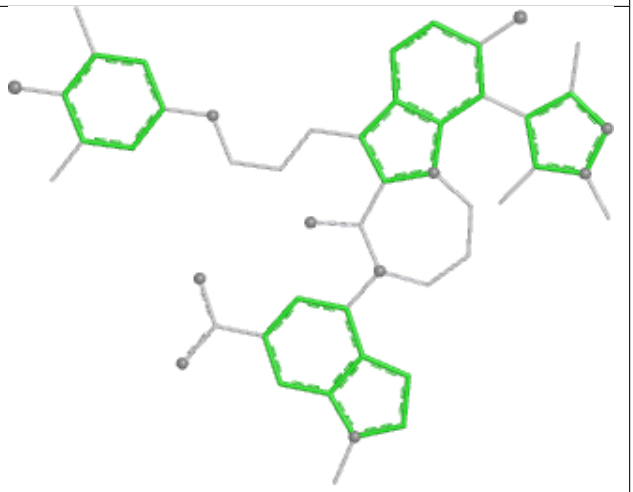

Rings

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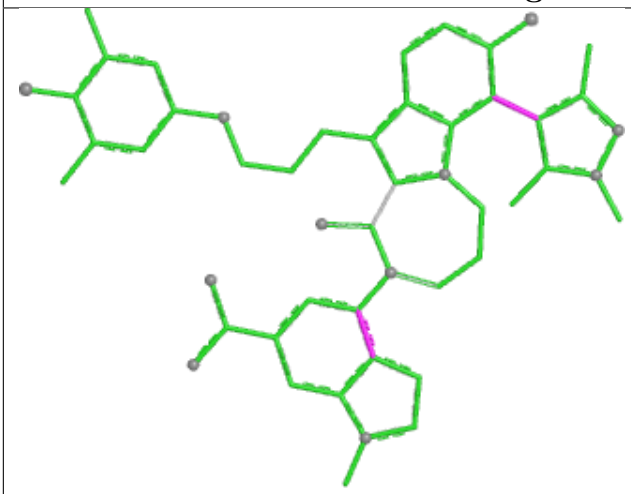

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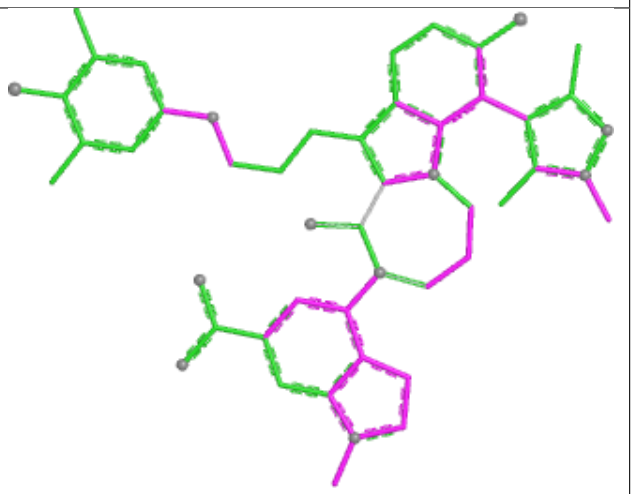

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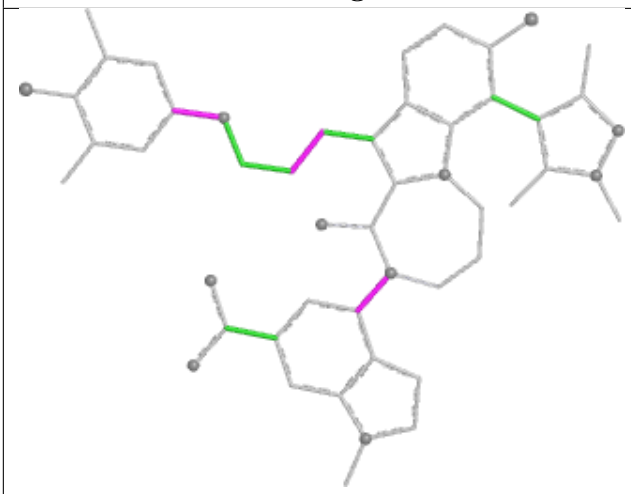

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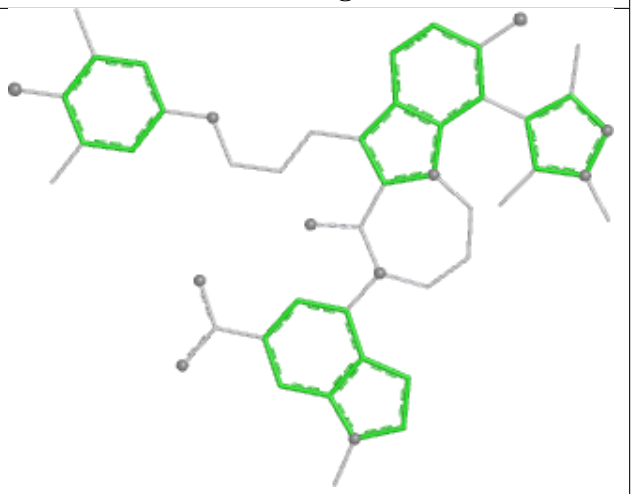

Rings

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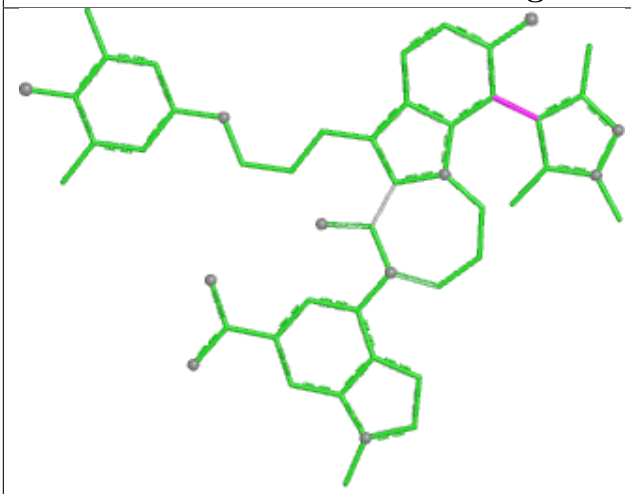

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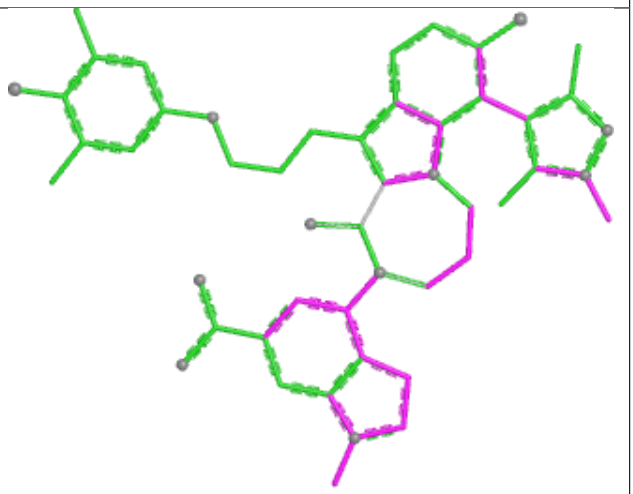

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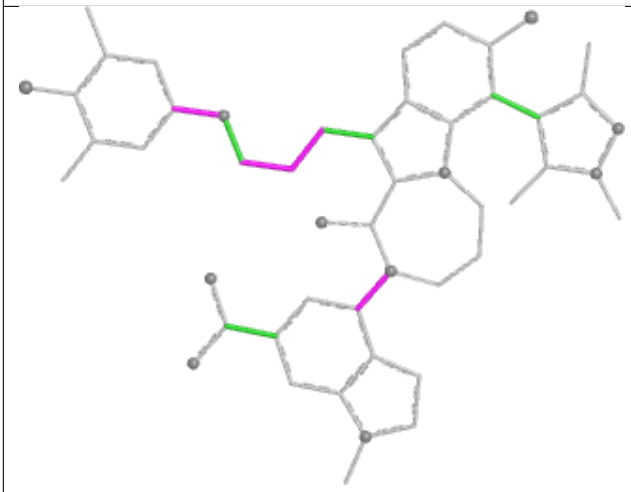

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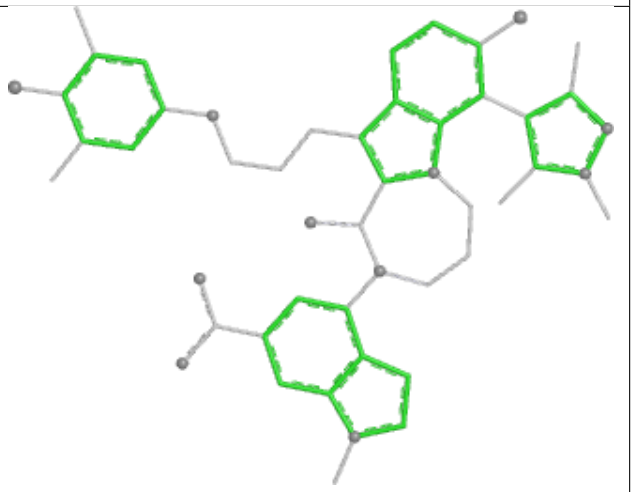
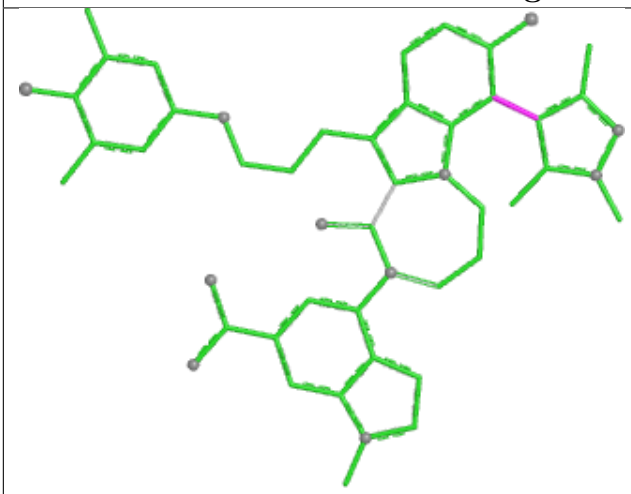


Rings

Ligand 6AK H 301



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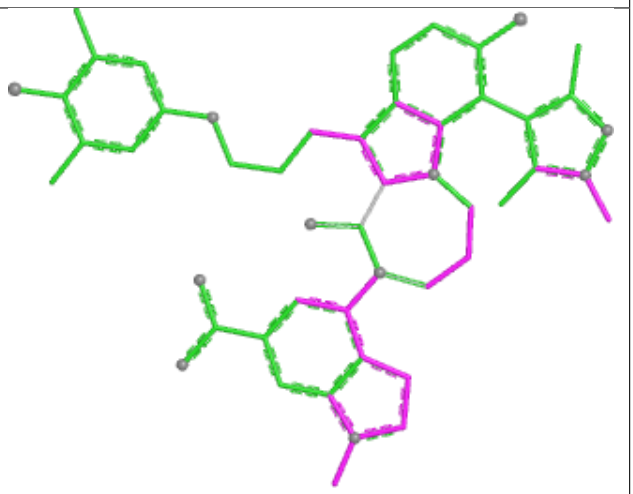

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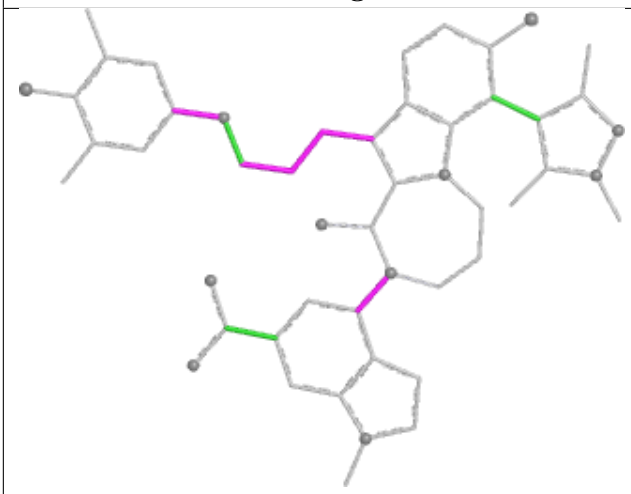

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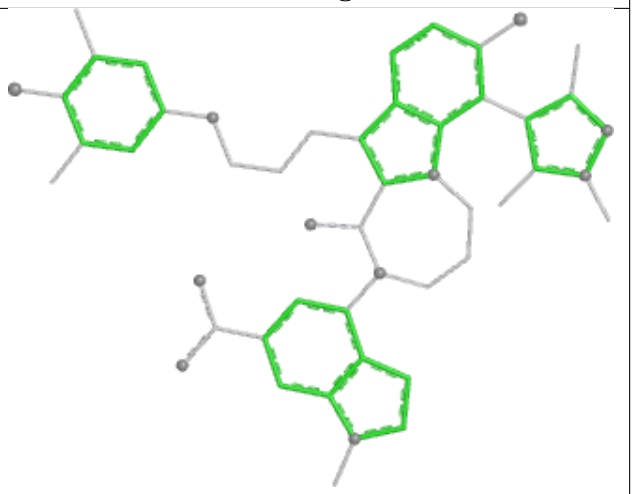
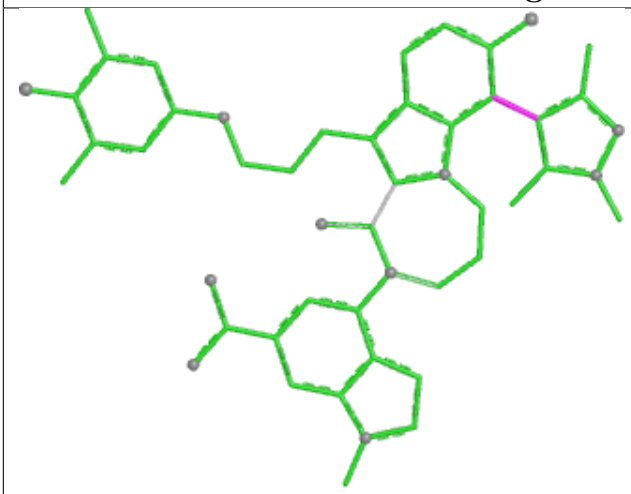


Rings

Ligand 6AK B 402



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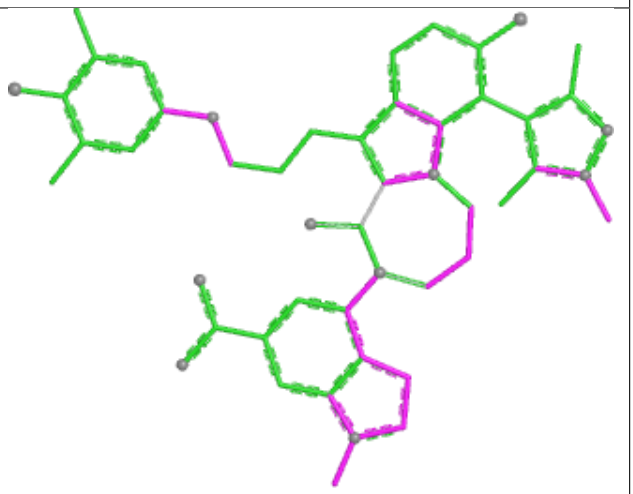

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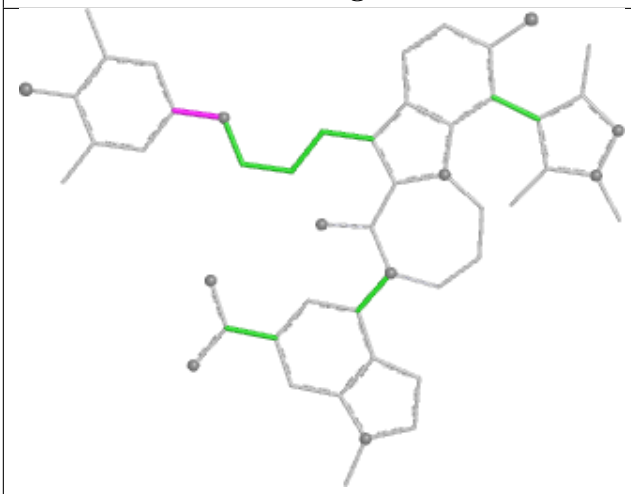

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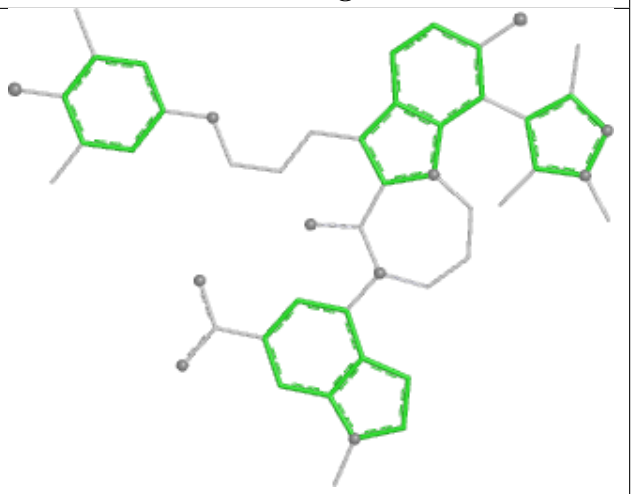
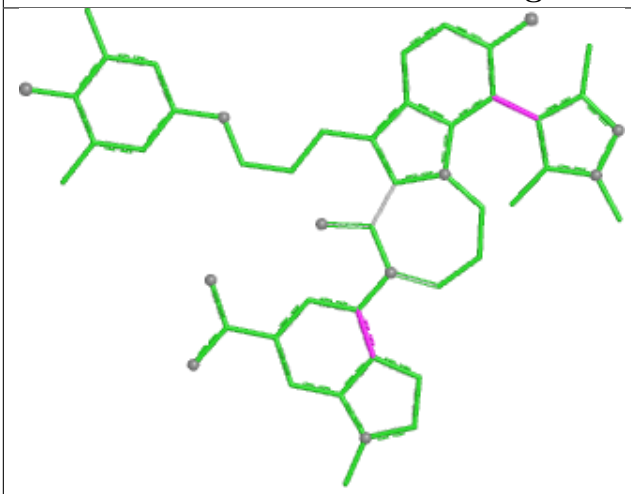


Rings

Ligand 6AK C 404



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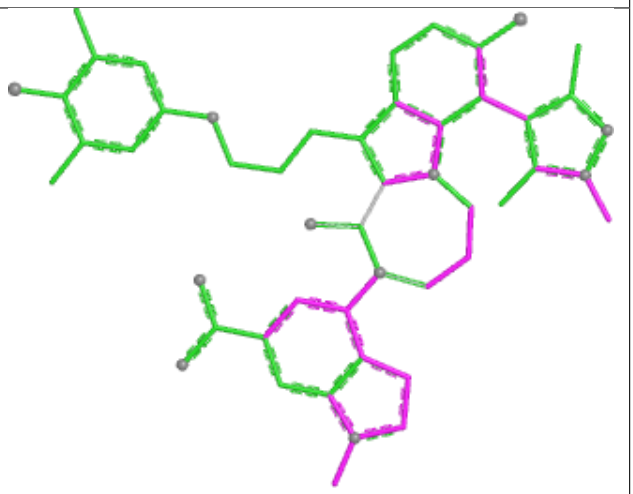

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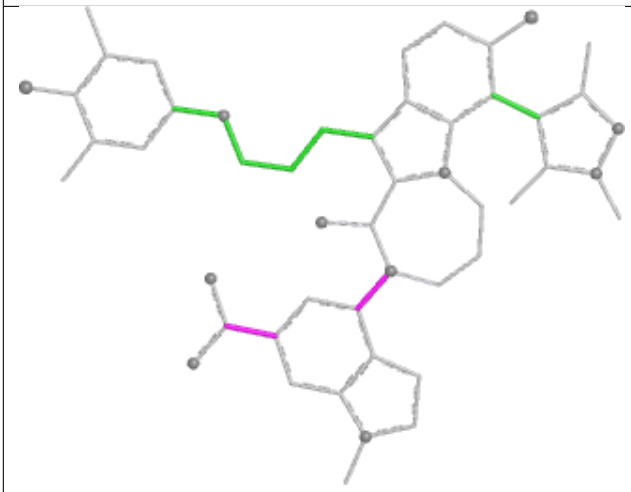

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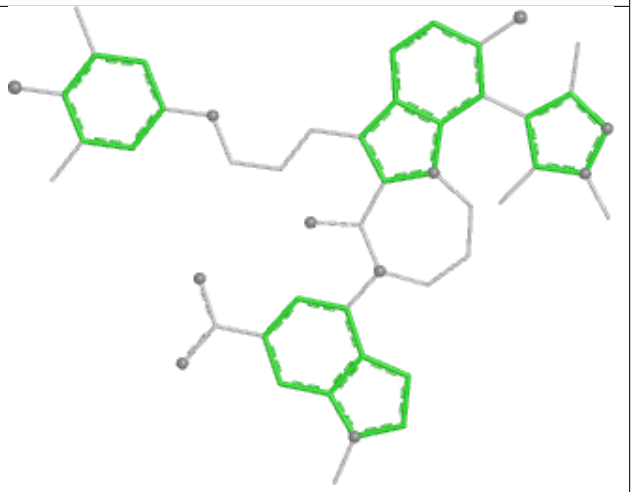
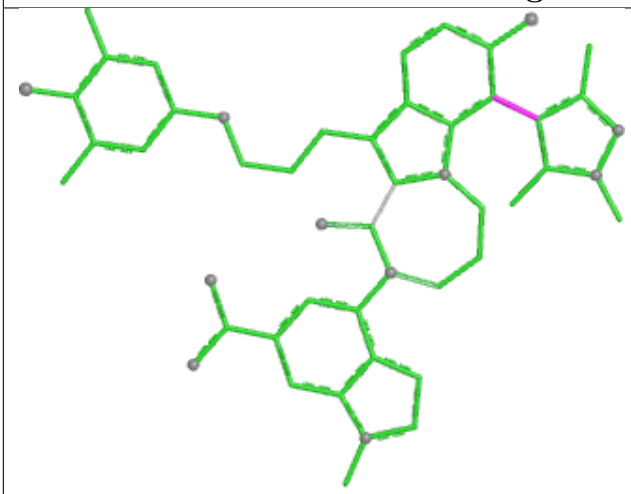


Rings

Ligand 6AK E 403



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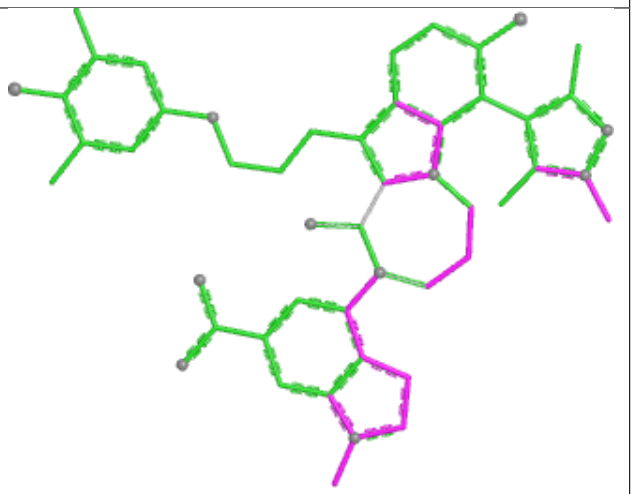

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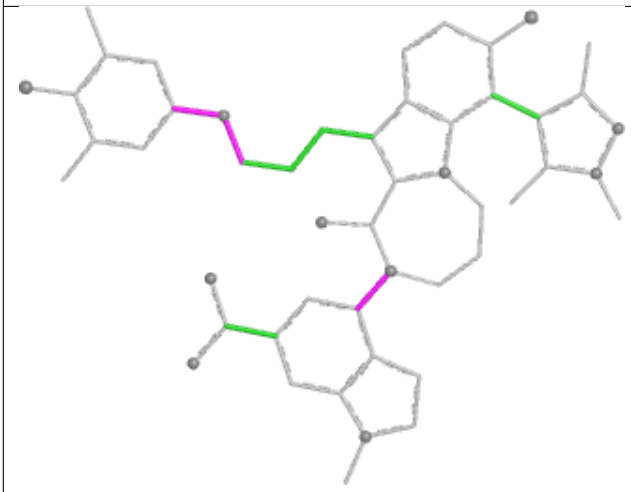

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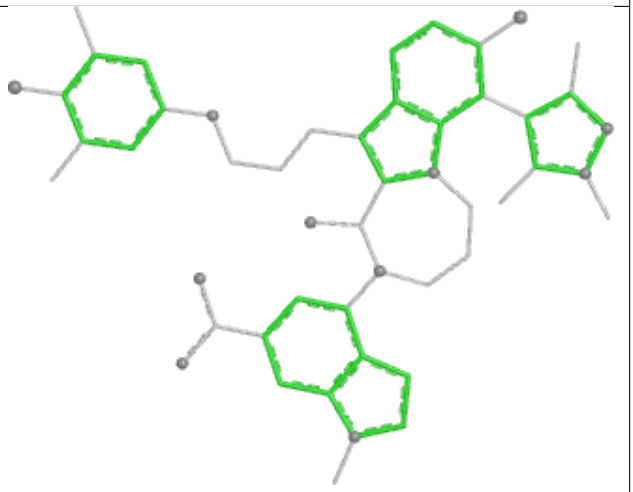
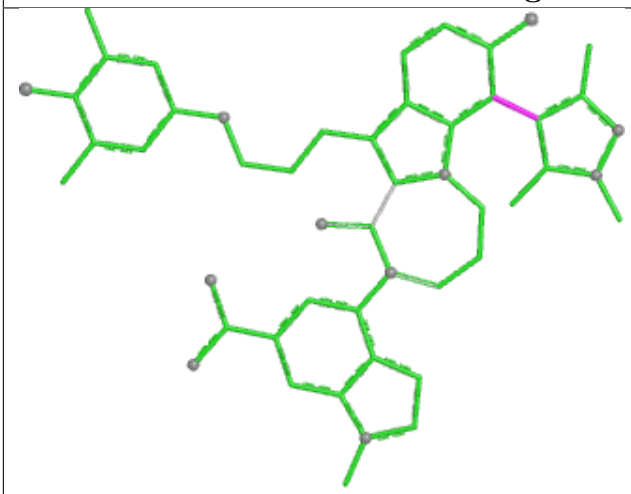


Rings

Ligand 6AK A 401



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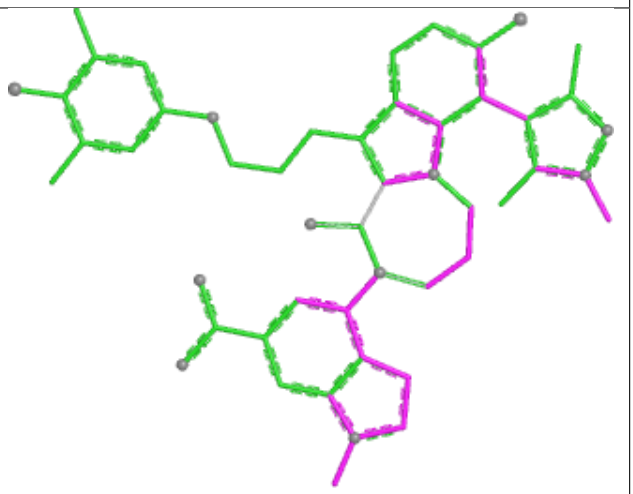
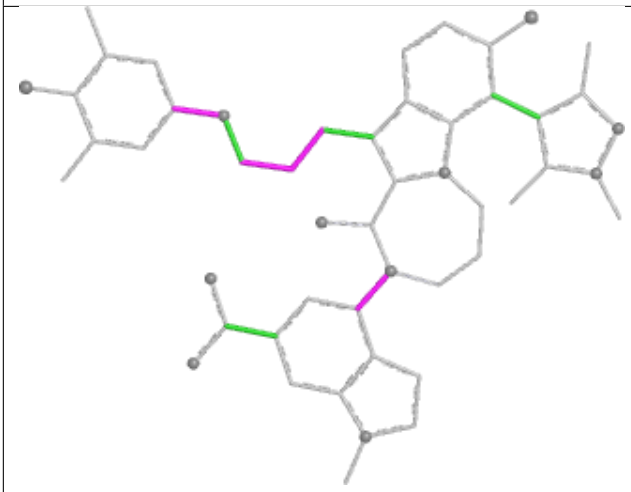


Bond angles



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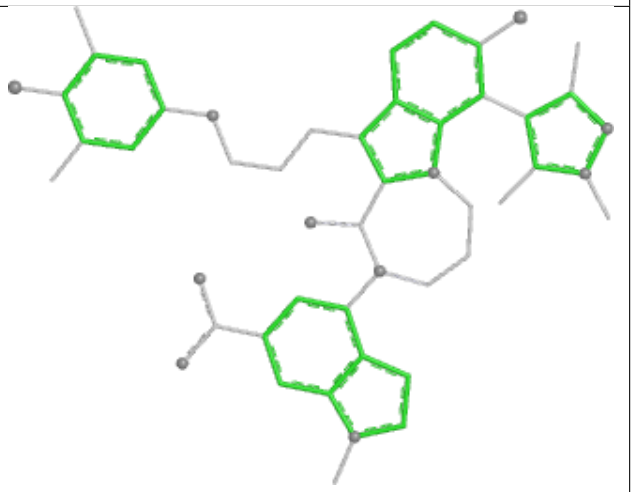
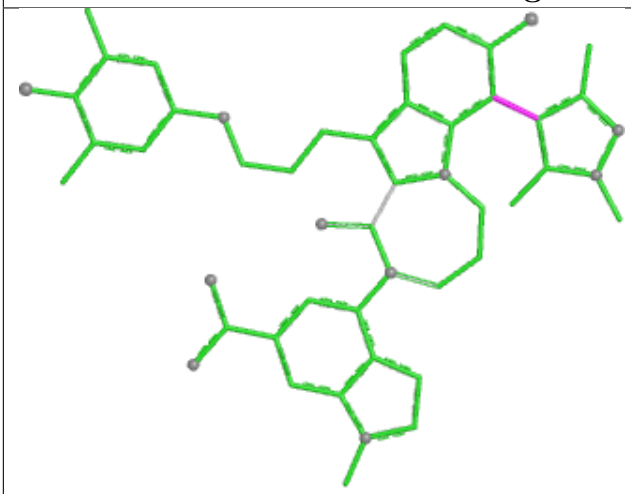


Rings

Ligand 6AK H 305



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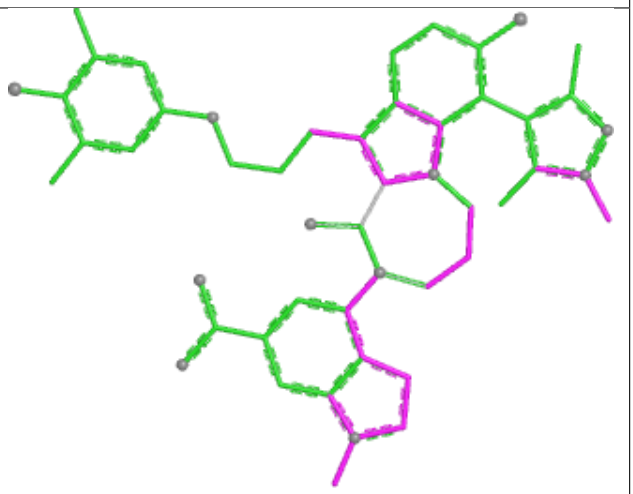
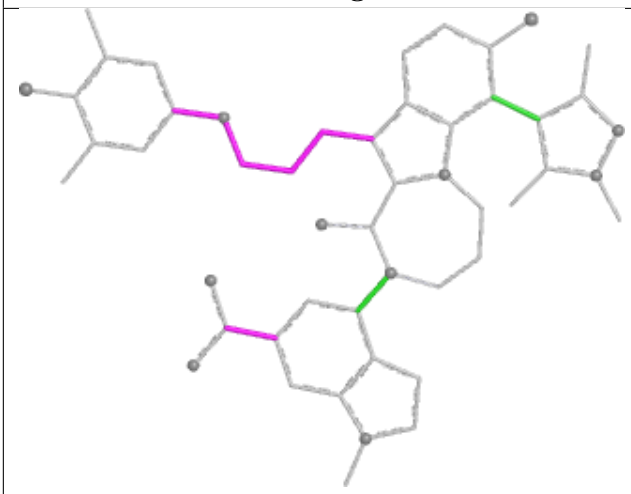
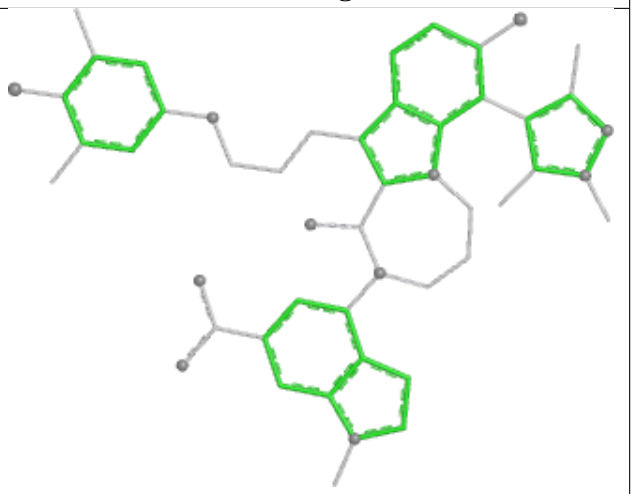


Bond angles

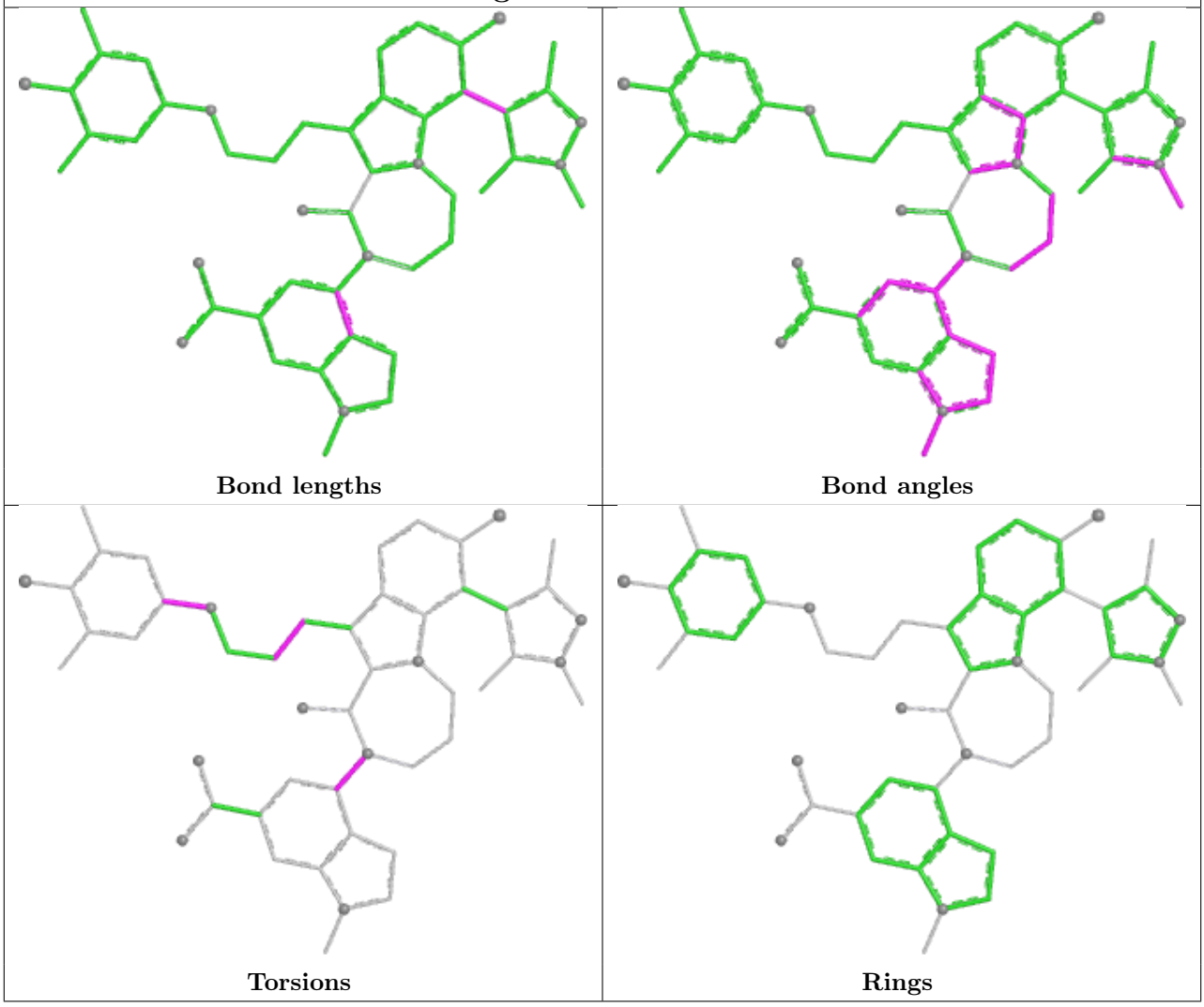


Torsions



Rings

Ligand 6AK C 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	513/518 (99%)	-1.55	0	100	100	29, 45, 64, 81	1 (0%)
1	B	507/518 (97%)	-1.57	0	100	100	29, 45, 69, 92	1 (0%)
1	C	508/518 (98%)	-1.56	0	100	100	25, 45, 70, 83	1 (0%)
1	D	504/518 (97%)	-1.53	0	100	100	29, 51, 75, 91	1 (0%)
1	E	507/518 (97%)	-1.58	0	100	100	31, 45, 62, 77	0
1	F	504/518 (97%)	-1.52	0	100	100	29, 51, 75, 92	0
1	G	506/518 (97%)	-1.52	0	100	100	27, 49, 77, 88	1 (0%)
1	H	501/518 (96%)	-1.50	0	100	100	29, 48, 82, 107	2 (0%)
All	All	4050/4144 (97%)	-1.54	0	100	100	25, 47, 73, 107	7 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

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
2	GLC	I	1	12/12	0.99	0.03	24,30,37,37	0
2	GLC	I	2	11/12	0.99	0.03	24,35,42,48	0
2	GLC	J	1	12/12	0.99	0.04	27,33,42,43	0

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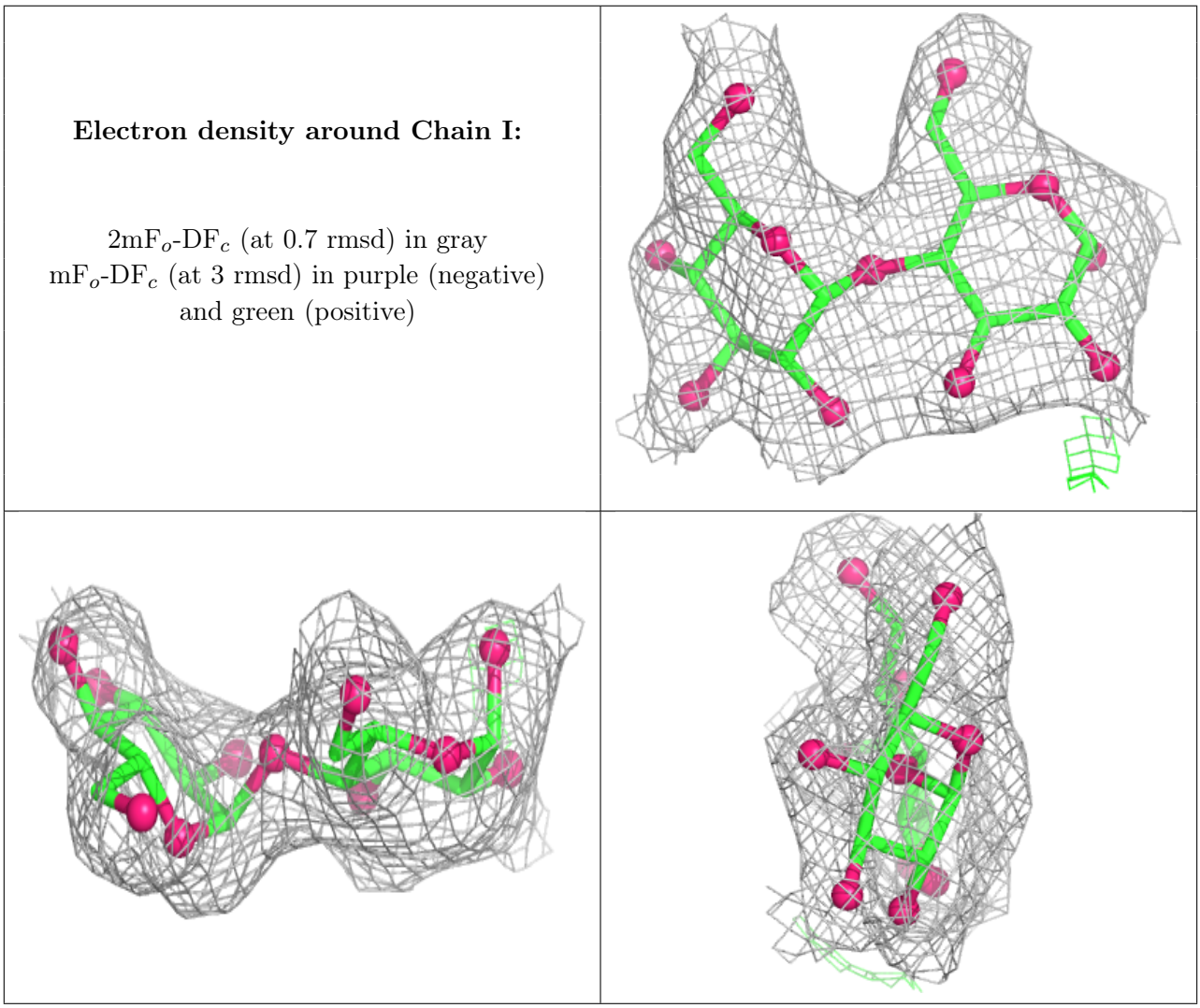
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	J	2	11/12	0.99	0.03	23,26,38,38	0
2	GLC	K	1	12/12	0.99	0.03	19,36,42,48	0
2	GLC	K	2	11/12	0.99	0.03	23,27,36,39	0
2	GLC	L	2	11/12	0.99	0.03	37,43,49,52	0
2	GLC	M	1	12/12	0.99	0.03	36,43,52,57	0
2	GLC	M	2	11/12	0.99	0.03	25,30,38,43	0
2	GLC	N	1	12/12	0.99	0.03	31,37,45,45	0
2	GLC	N	2	11/12	0.99	0.03	24,29,49,49	0
2	GLC	O	2	11/12	0.99	0.03	19,30,38,39	0
2	GLC	P	1	12/12	0.99	0.03	19,25,32,33	0
2	GLC	P	2	11/12	0.99	0.03	19,28,35,36	0
2	GLC	O	1	12/12	1.00	0.02	19,30,34,35	0
2	GLC	L	1	12/12	1.00	0.02	25,33,38,42	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

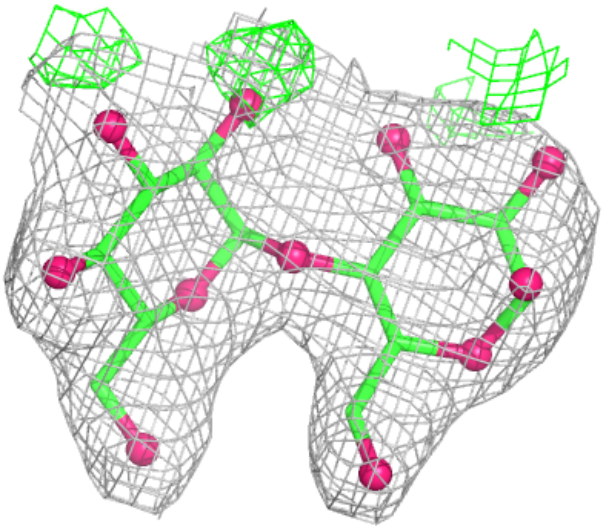
Electron density around Chain I:

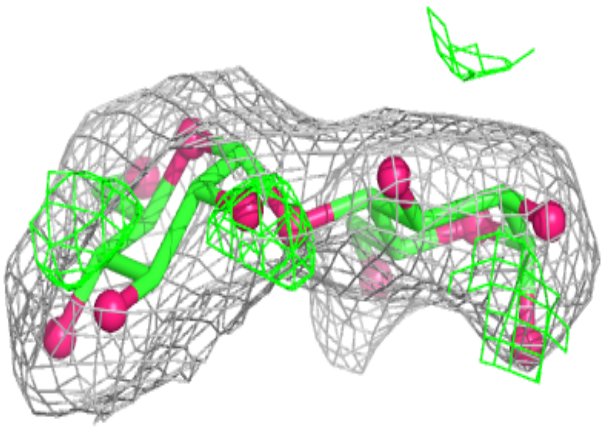
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

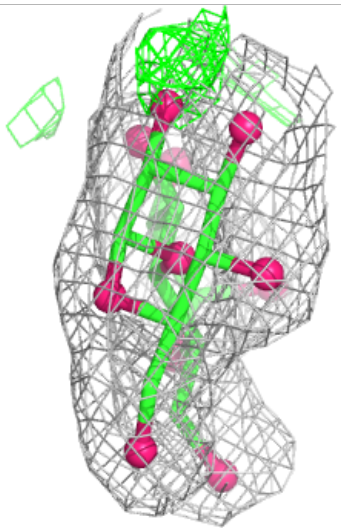


Electron density around Chain J:

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

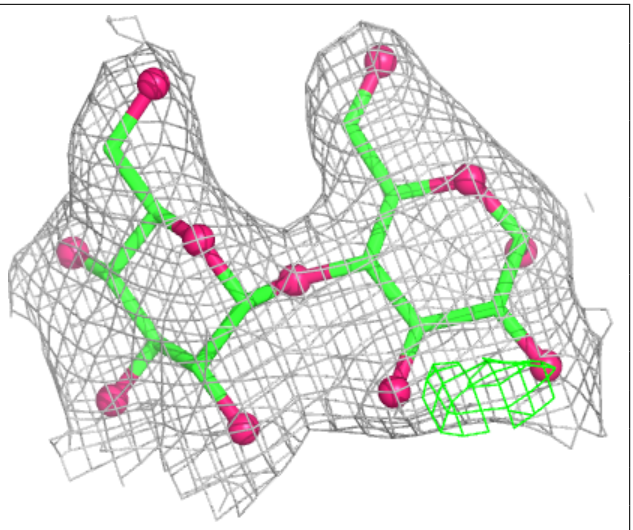


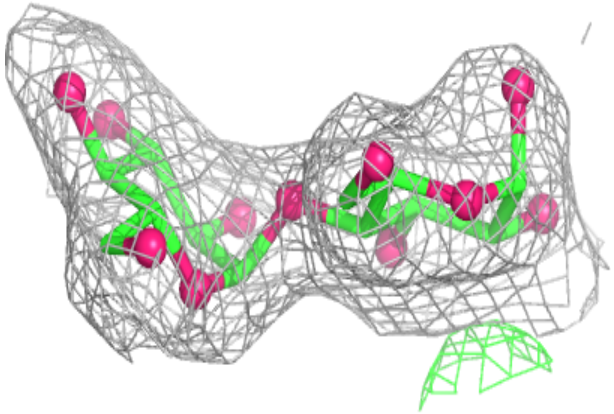


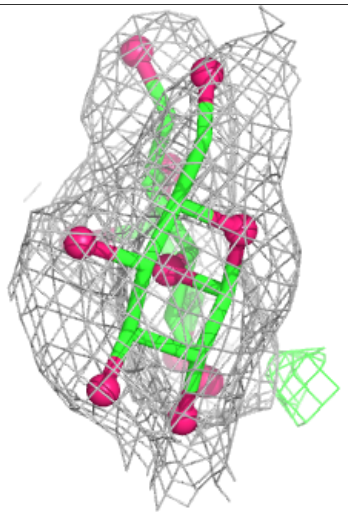


Electron density around Chain K:

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

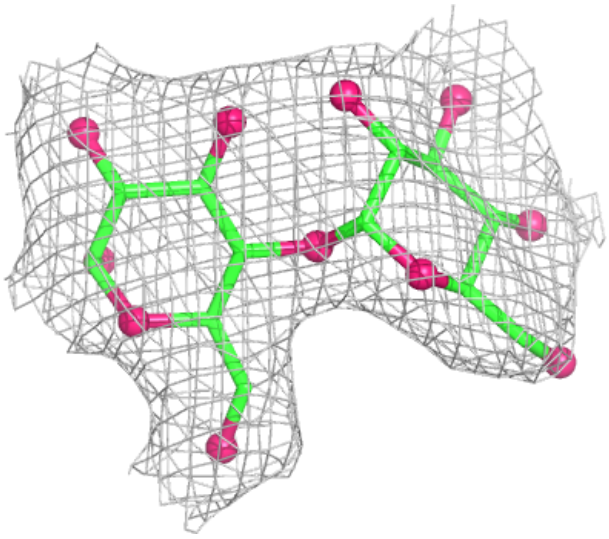


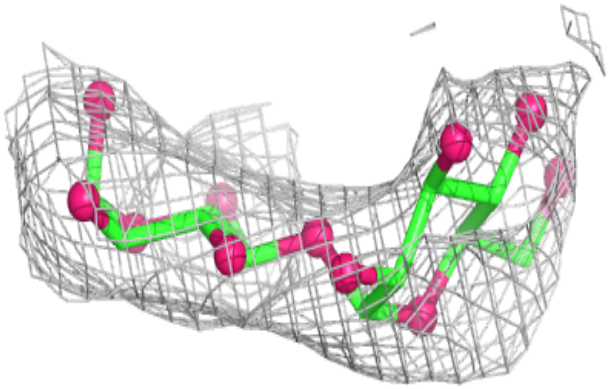




Electron density around Chain L:

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

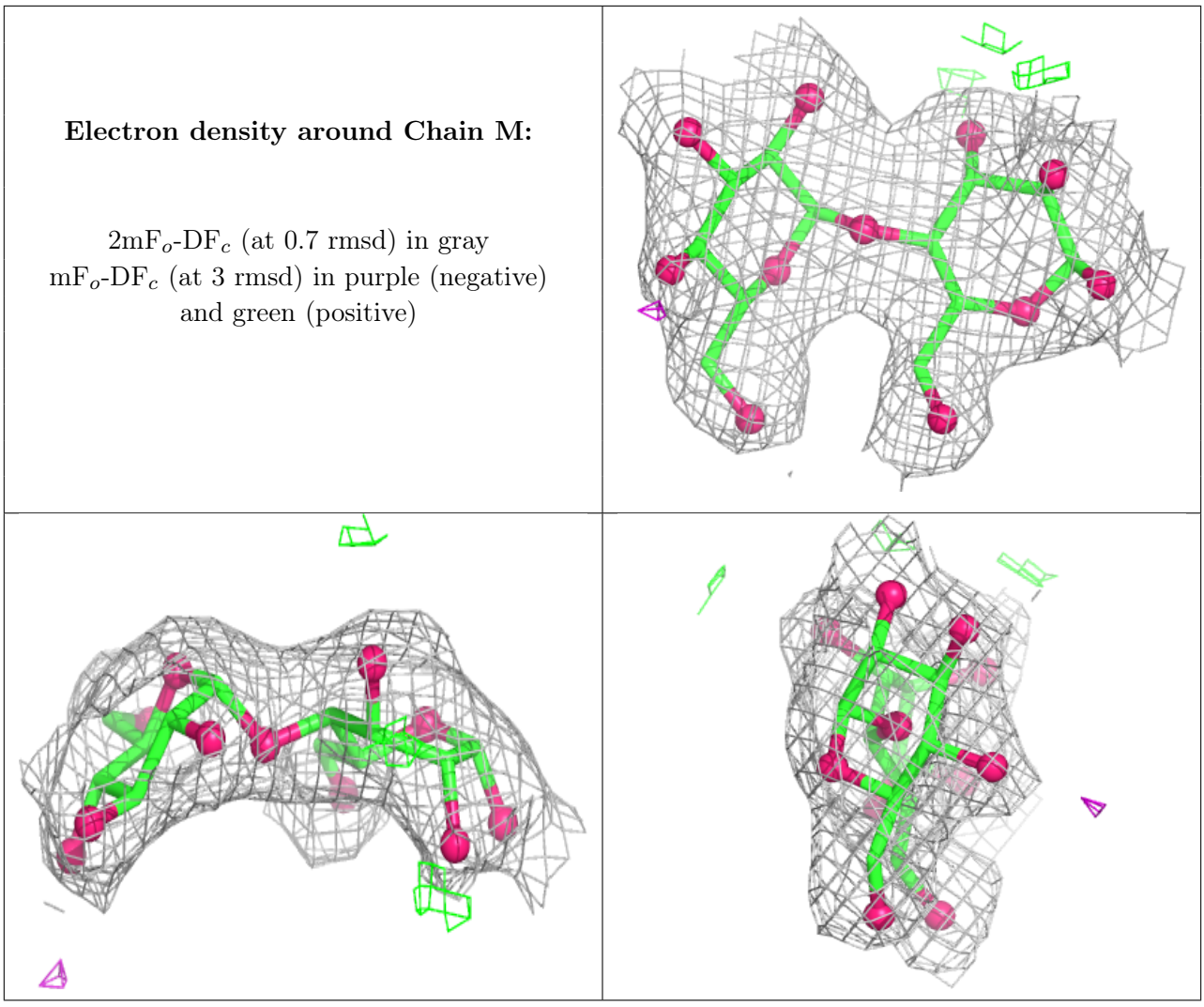






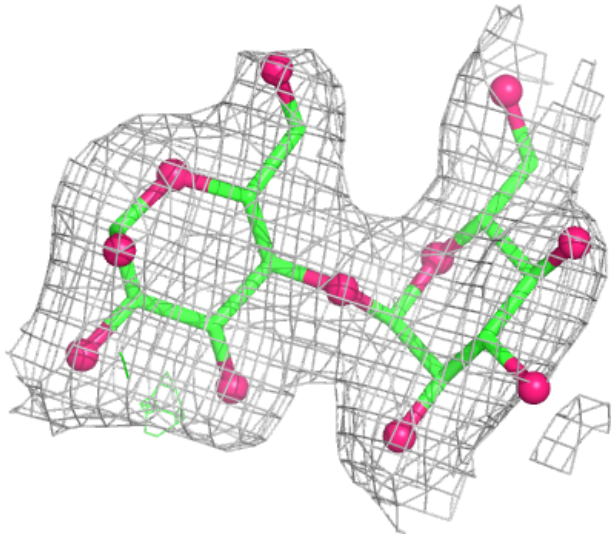
Electron density around Chain M:

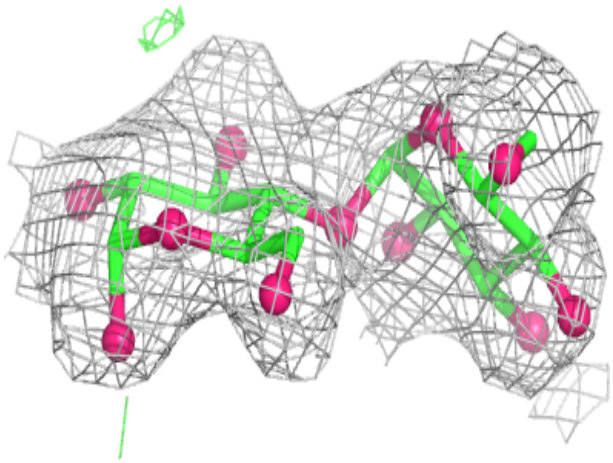
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

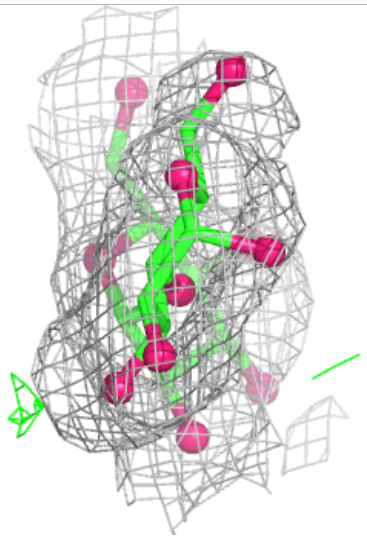


Electron density around Chain N:

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

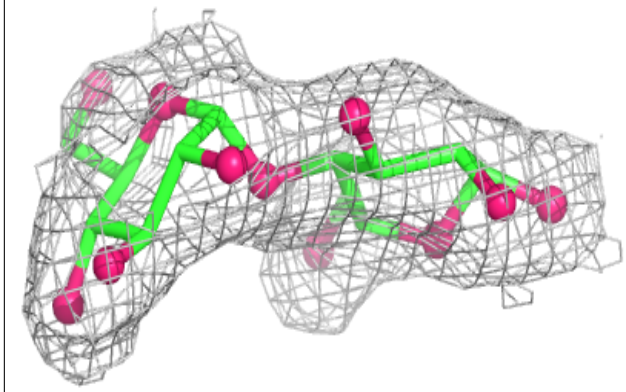


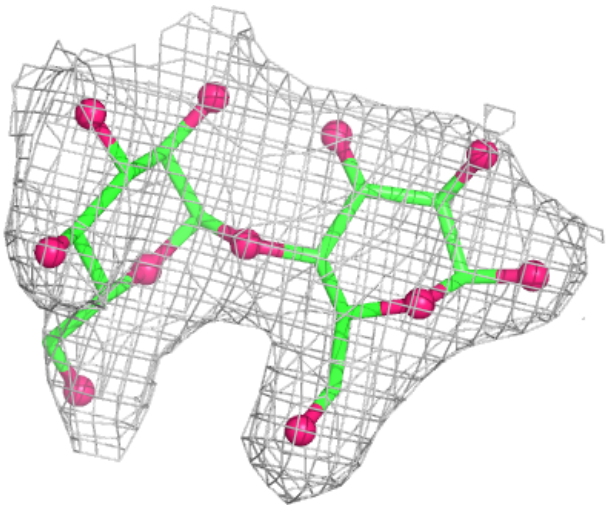


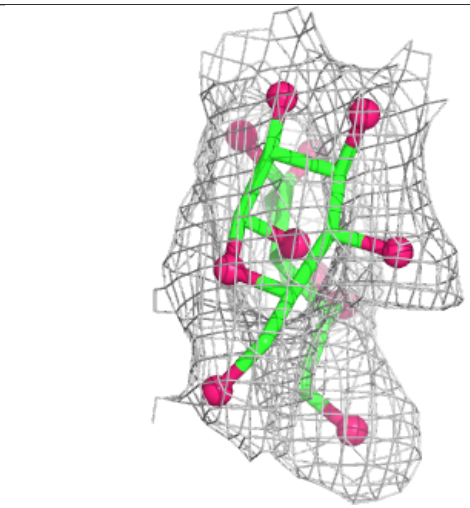


Electron density around Chain O:

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

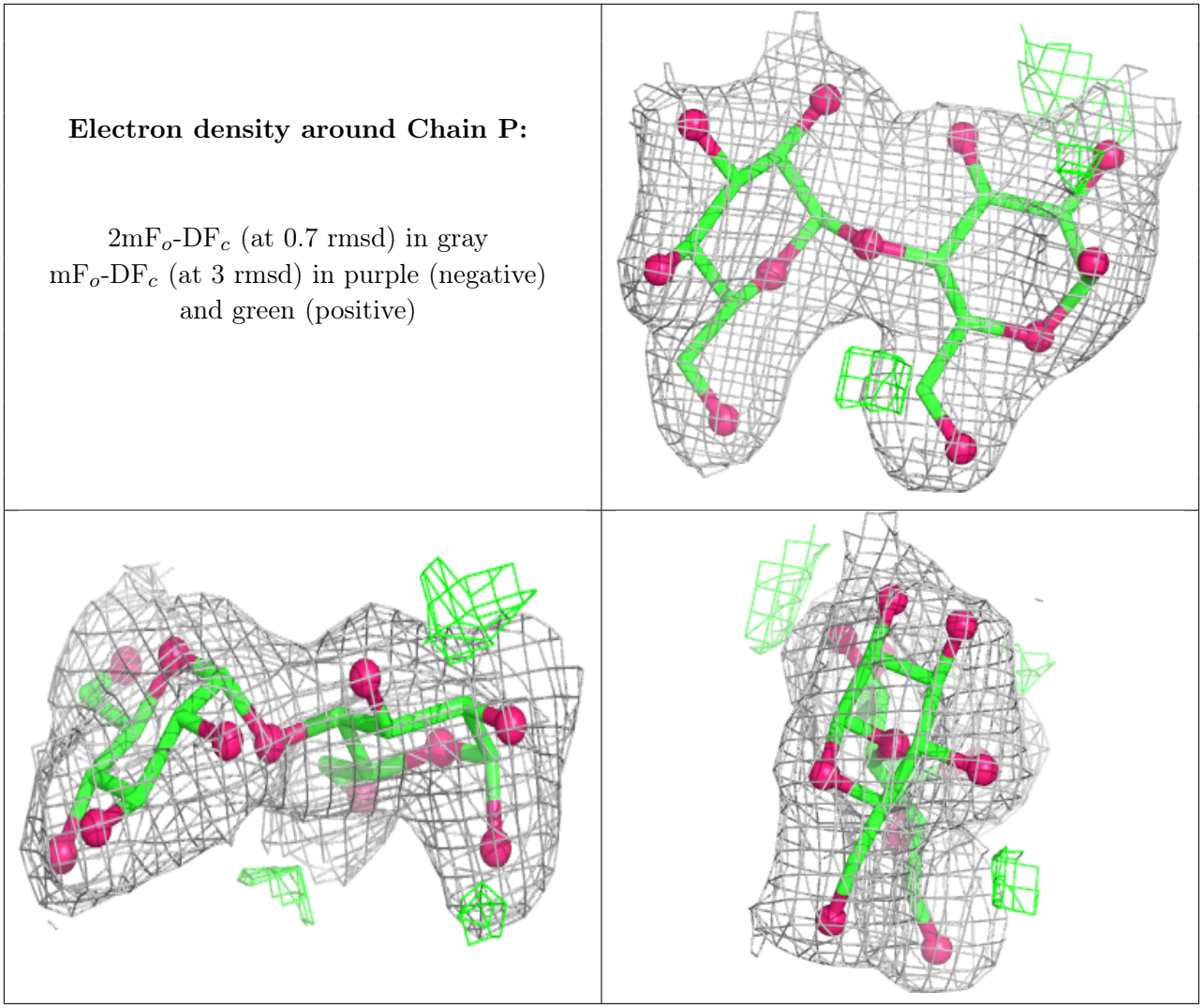






Electron density around Chain P:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	6AK	A	401	50/50	0.99	0.03	23,41,53,59	0
3	6AK	A	403	50/50	0.99	0.03	32,46,66,79	0
3	6AK	A	404	50/50	0.99	0.03	34,46,62,66	0
3	6AK	B	402	50/50	0.99	0.03	26,47,56,59	0
3	6AK	B	403	50/50	0.99	0.03	22,36,50,51	0
3	6AK	C	401	50/50	0.99	0.03	22,40,61,69	0
3	6AK	C	403	50/50	0.99	0.04	24,47,55,57	0
3	6AK	C	404	50/50	0.99	0.03	24,50,56,66	0

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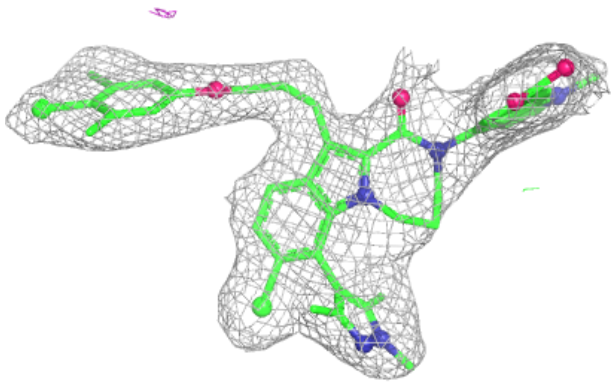
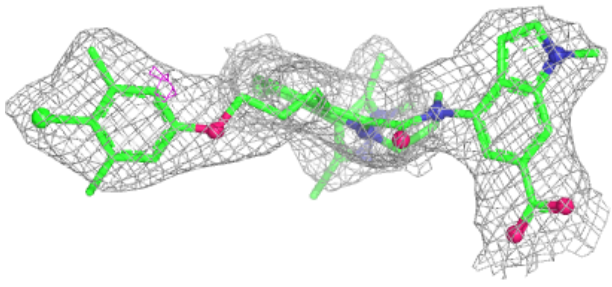
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	6AK	C	405	50/50	0.99	0.03	38,50,71,76	0
3	6AK	D	401	50/50	0.99	0.04	23,38,47,55	0
3	6AK	D	403	50/50	0.99	0.03	30,45,58,61	0
3	6AK	E	401	50/50	0.99	0.04	21,36,44,46	0
3	6AK	E	403	50/50	0.99	0.03	29,46,55,65	0
3	6AK	F	401	50/50	0.99	0.03	27,41,51,63	0
3	6AK	F	403	50/50	0.99	0.04	27,43,52,55	0
3	6AK	F	404	50/50	0.99	0.04	31,48,54,61	0
3	6AK	F	405	50/50	0.99	0.04	36,51,80,86	0
3	6AK	G	401	50/50	0.99	0.04	25,47,62,76	0
3	6AK	G	403	50/50	0.99	0.03	21,39,50,56	0
3	6AK	G	404	50/50	0.99	0.04	20,45,63,76	0
3	6AK	H	301	50/50	0.99	0.03	27,41,53,65	0
3	6AK	H	303	50/50	0.99	0.03	28,53,84,93	0
3	6AK	H	304	50/50	0.99	0.03	30,44,53,56	0
3	6AK	H	305	50/50	0.99	0.03	21,40,52,53	0

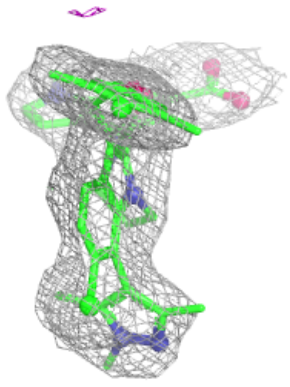
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6AK A 401:

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

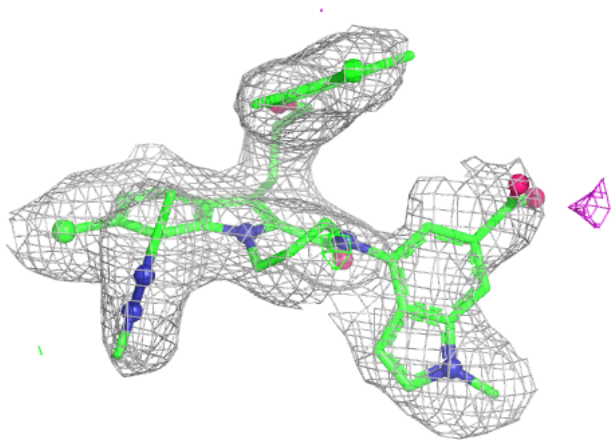


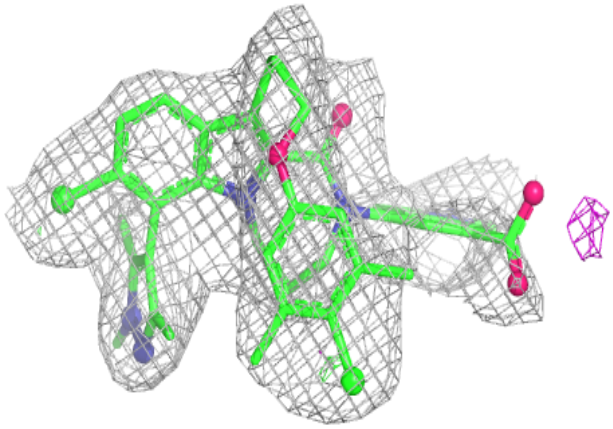


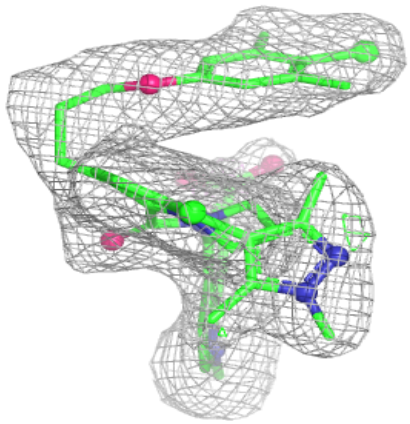


Electron density around 6AK A 403:

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

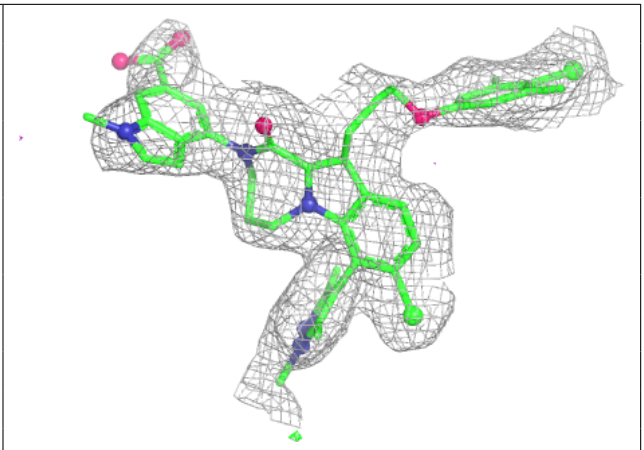


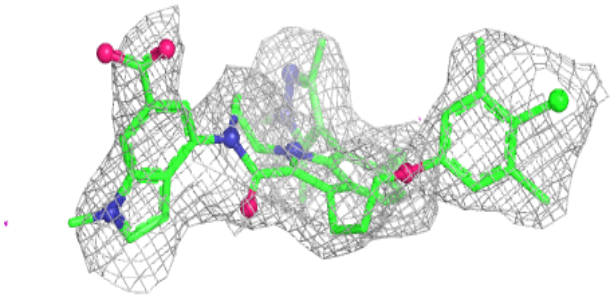


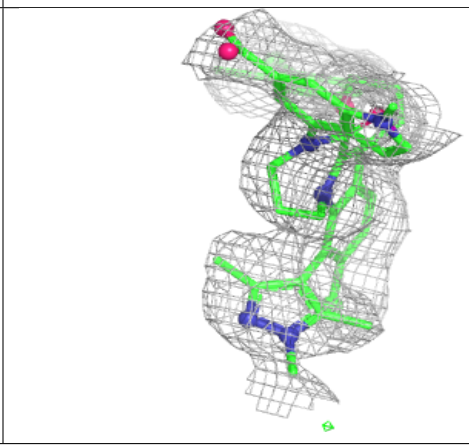


Electron density around 6AK A 404:

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

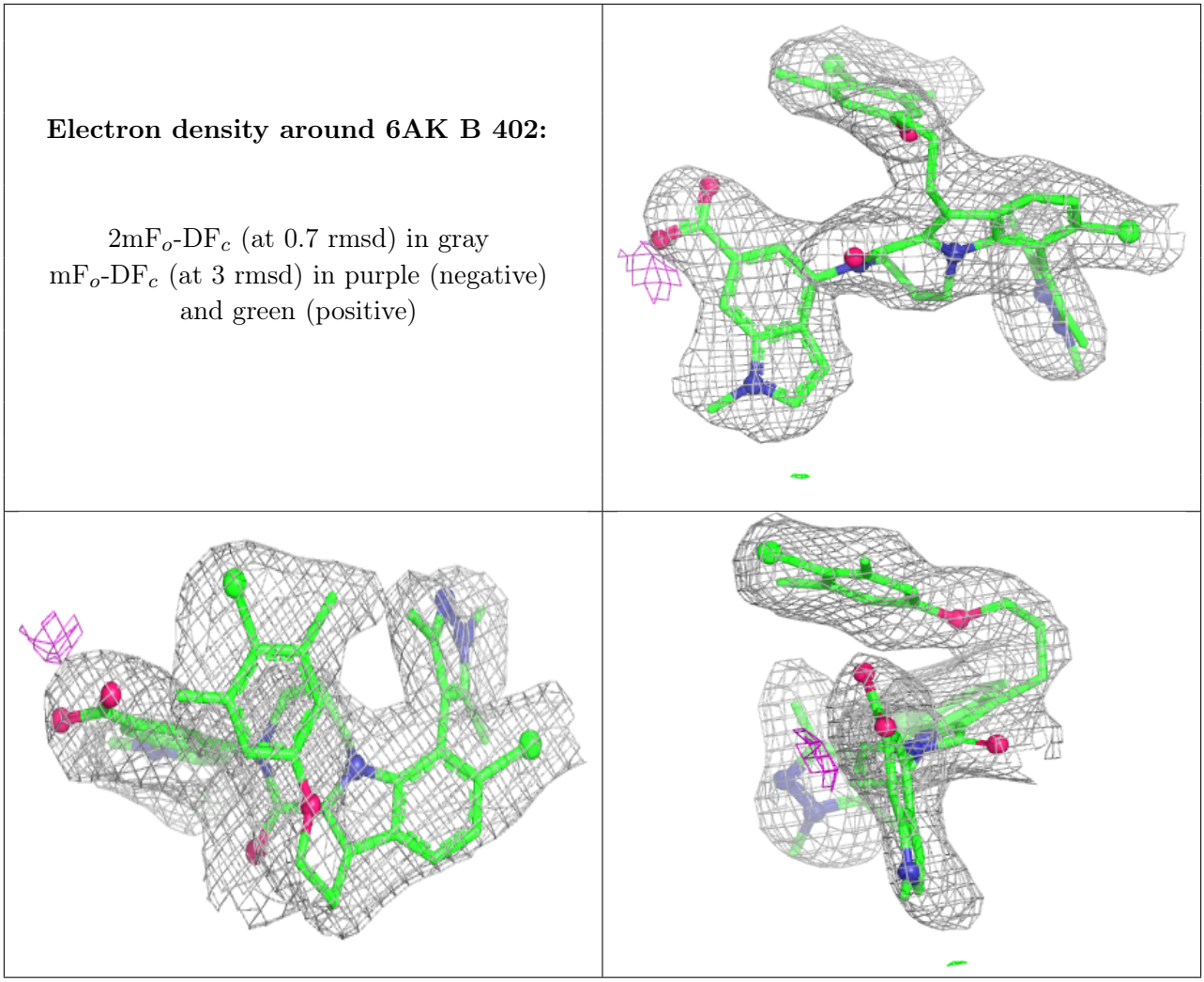






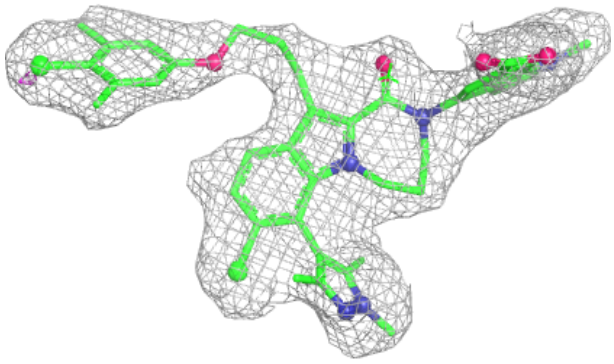
Electron density around 6AK B 402:

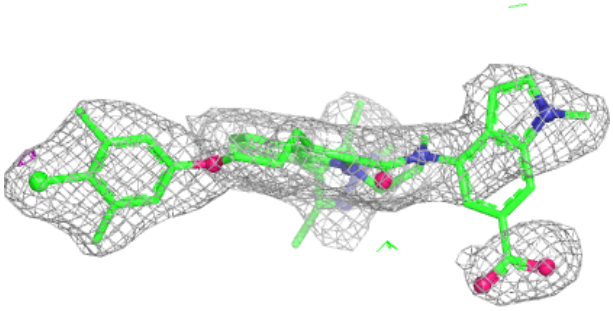
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

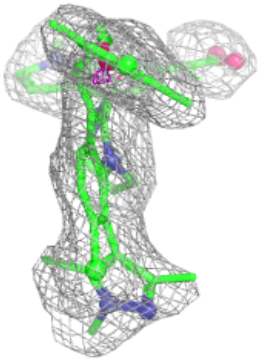


Electron density around 6AK B 403:

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

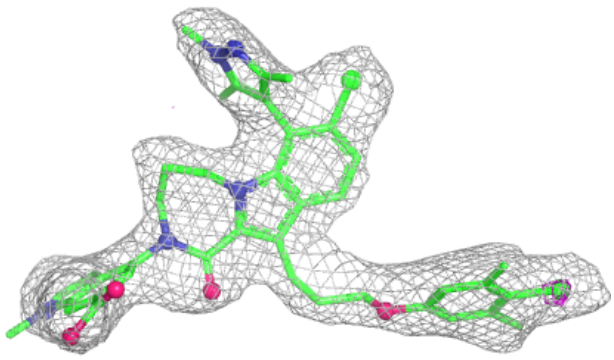


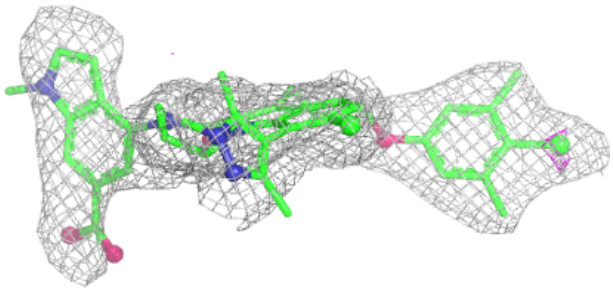


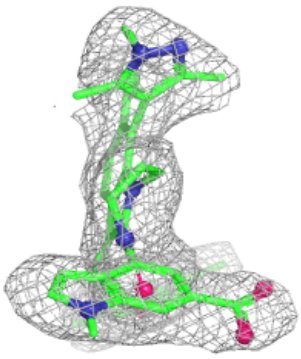


Electron density around 6AK C 401:

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

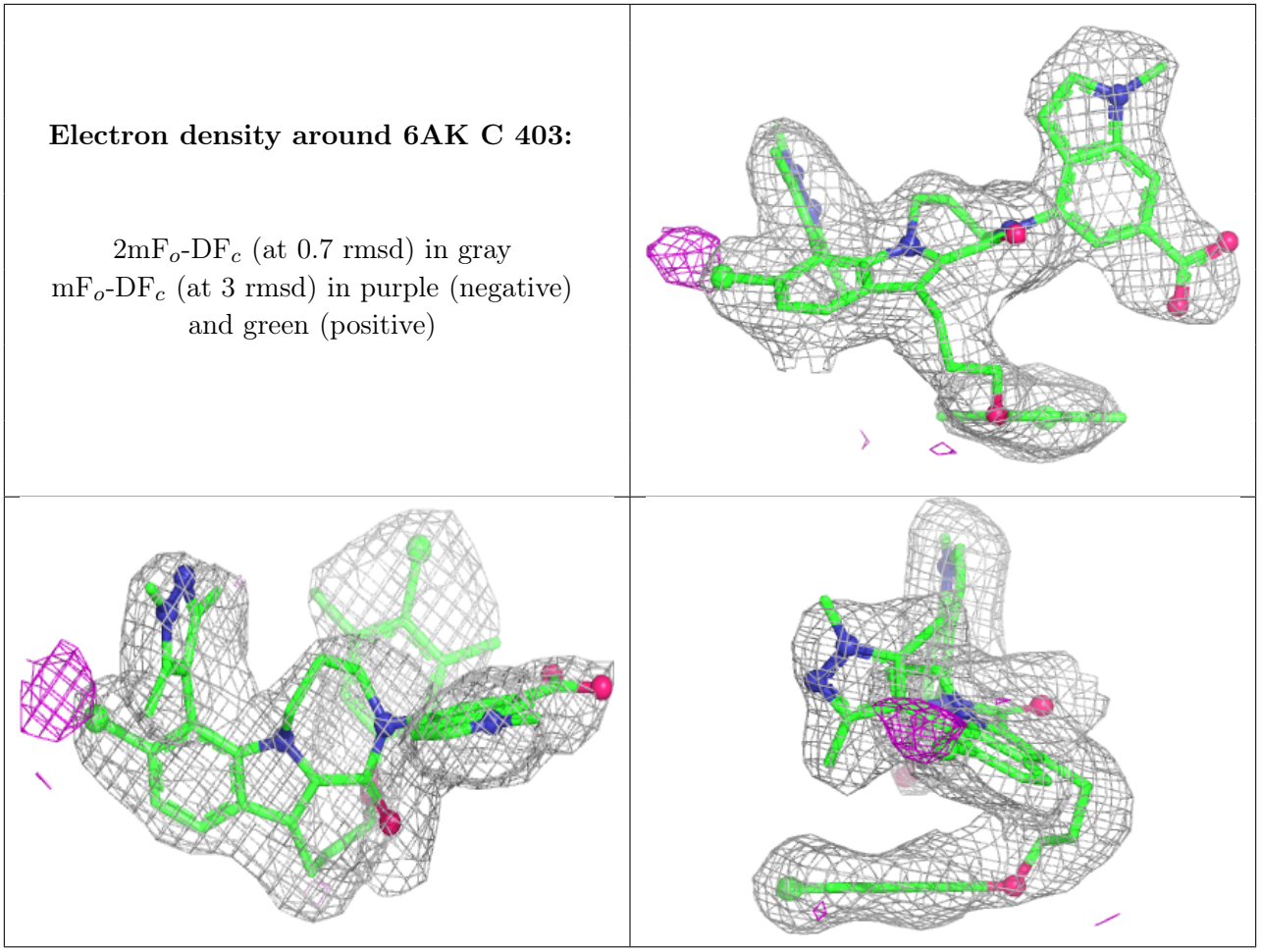






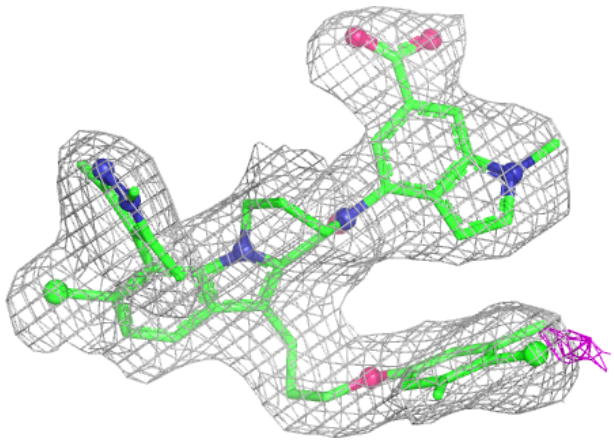
Electron density around 6AK C 403:

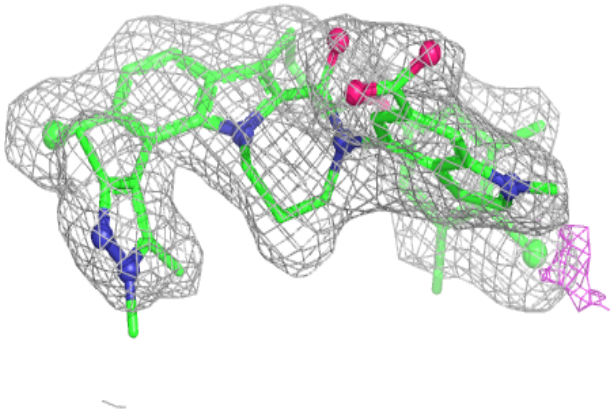
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

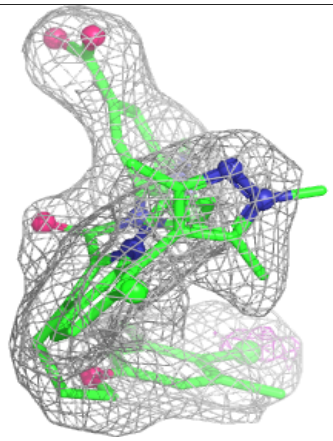


Electron density around 6AK C 404:

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

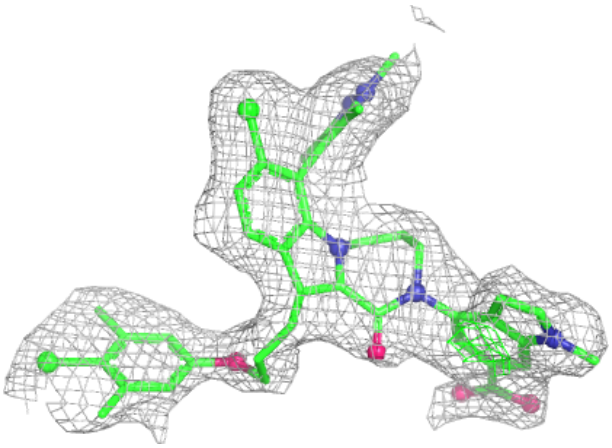


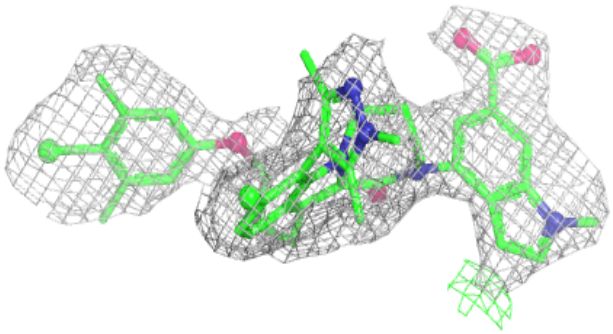


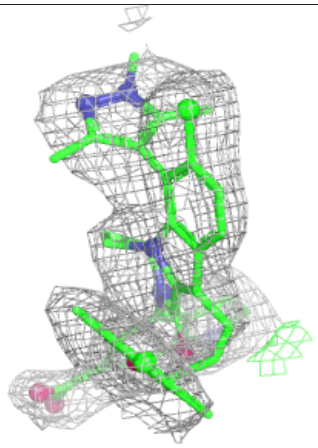


Electron density around 6AK C 405:

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

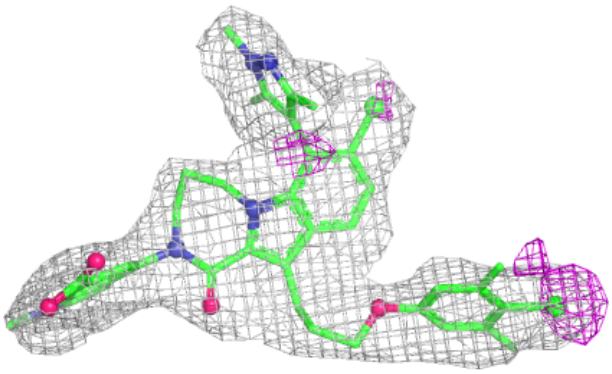


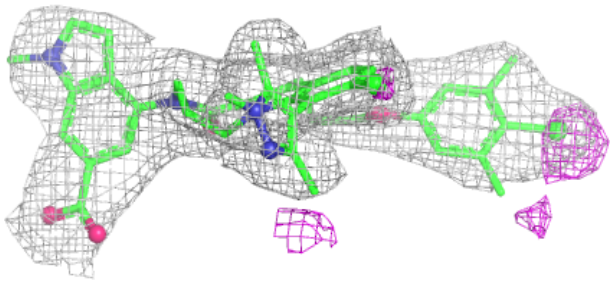


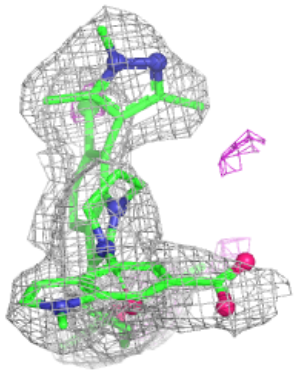


Electron density around 6AK D 401:

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

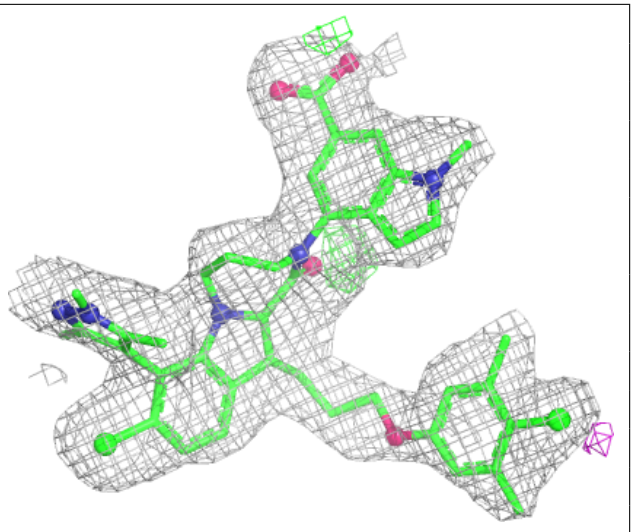


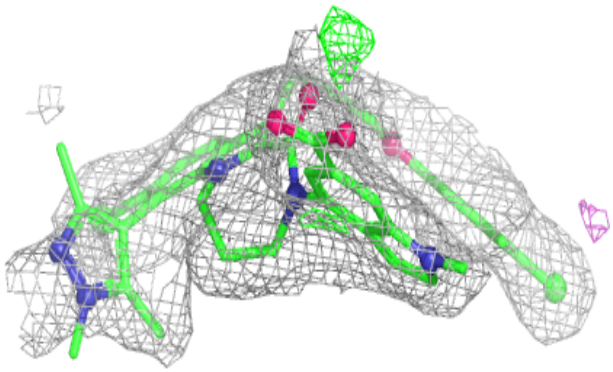


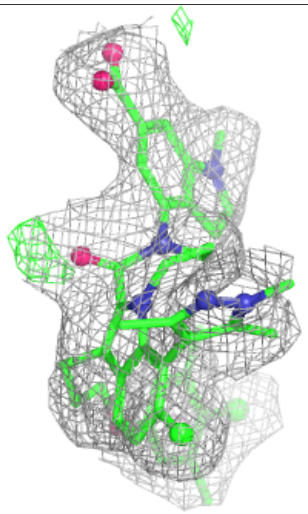


Electron density around 6AK D 403:

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

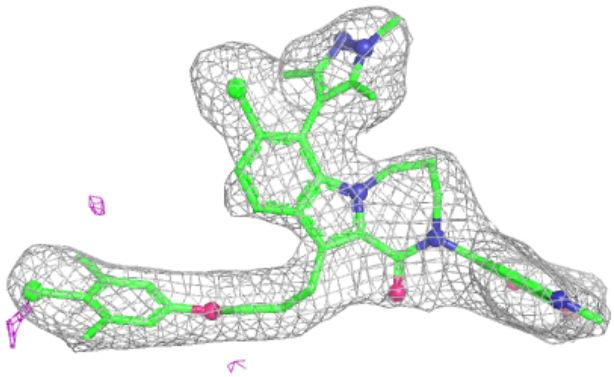


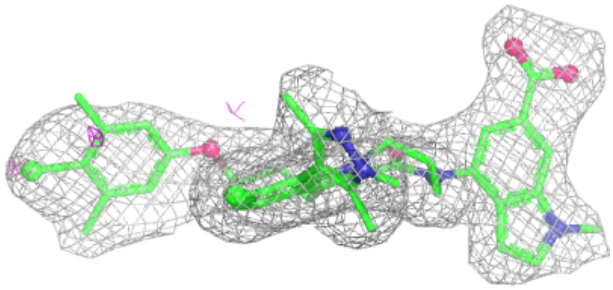


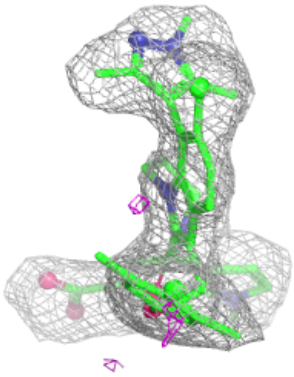


Electron density around 6AK E 401:

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

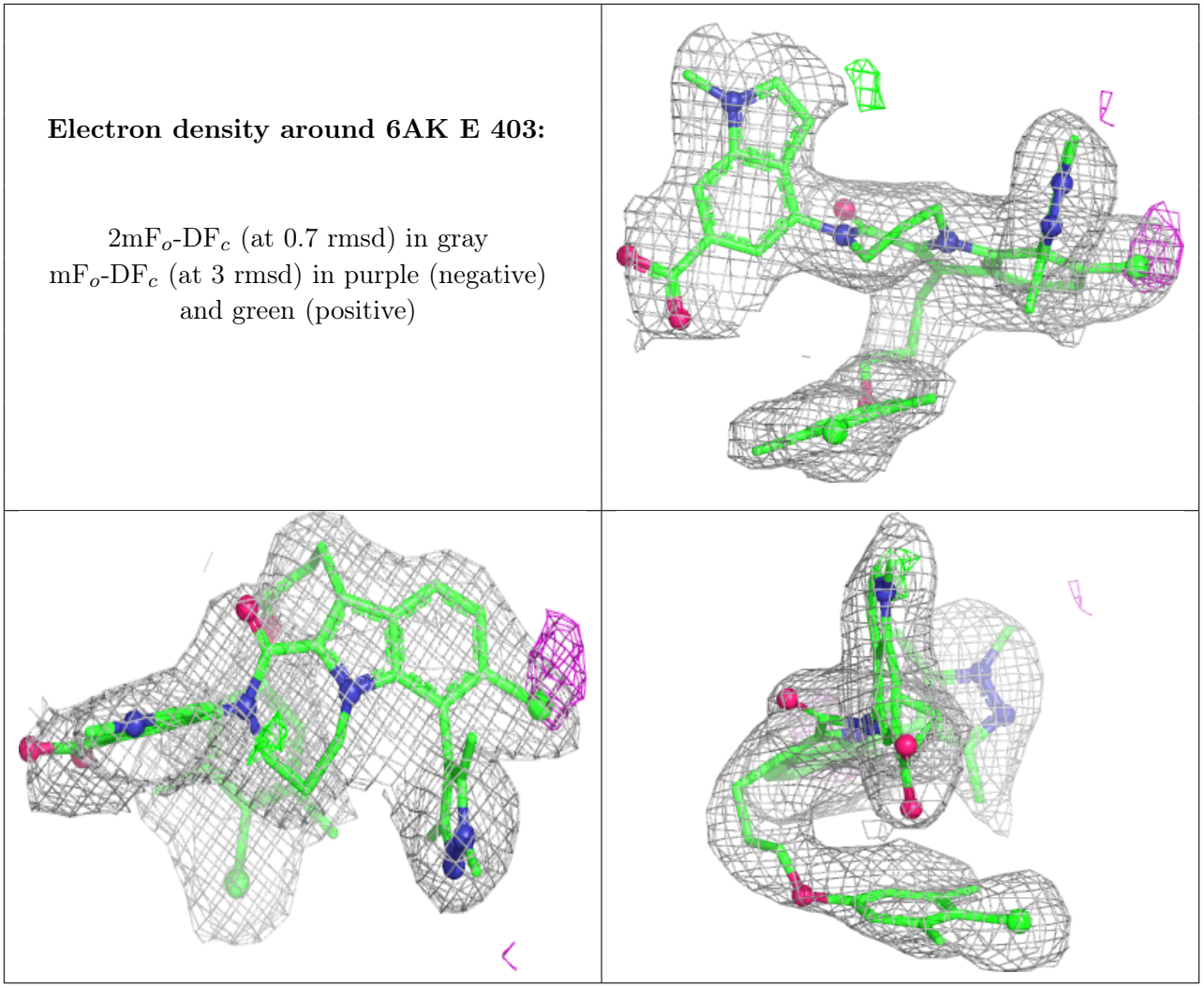






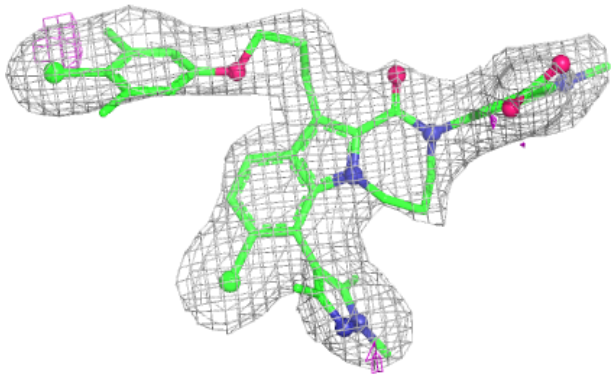
Electron density around 6AK E 403:

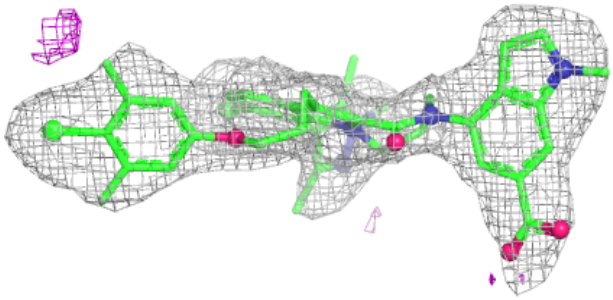
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

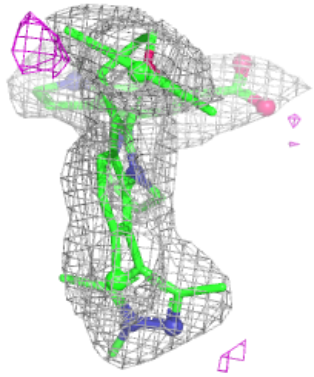


Electron density around 6AK F 401:

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

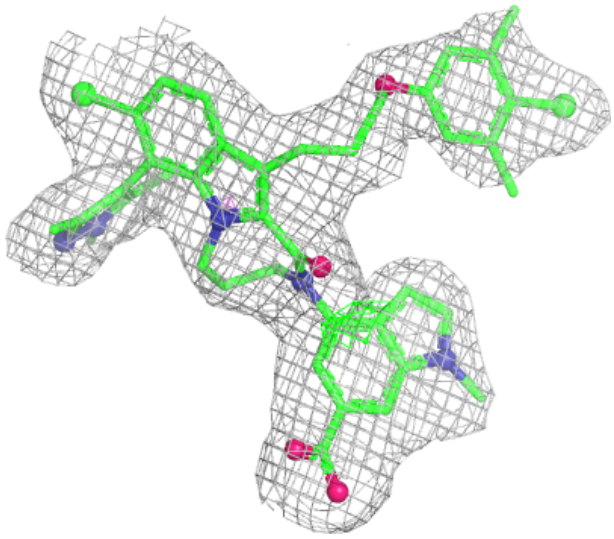


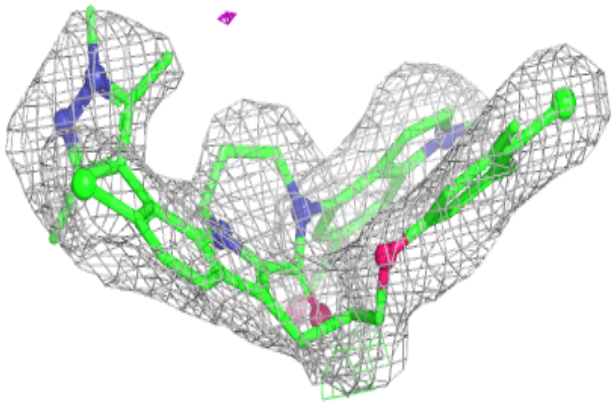


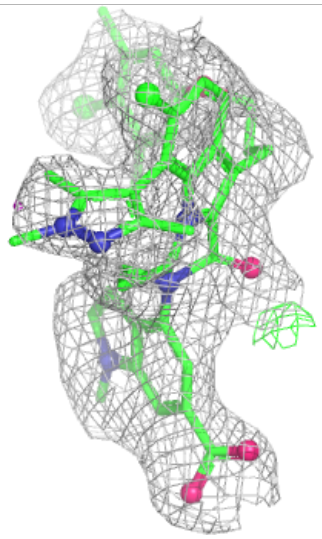


Electron density around 6AK F 403:

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

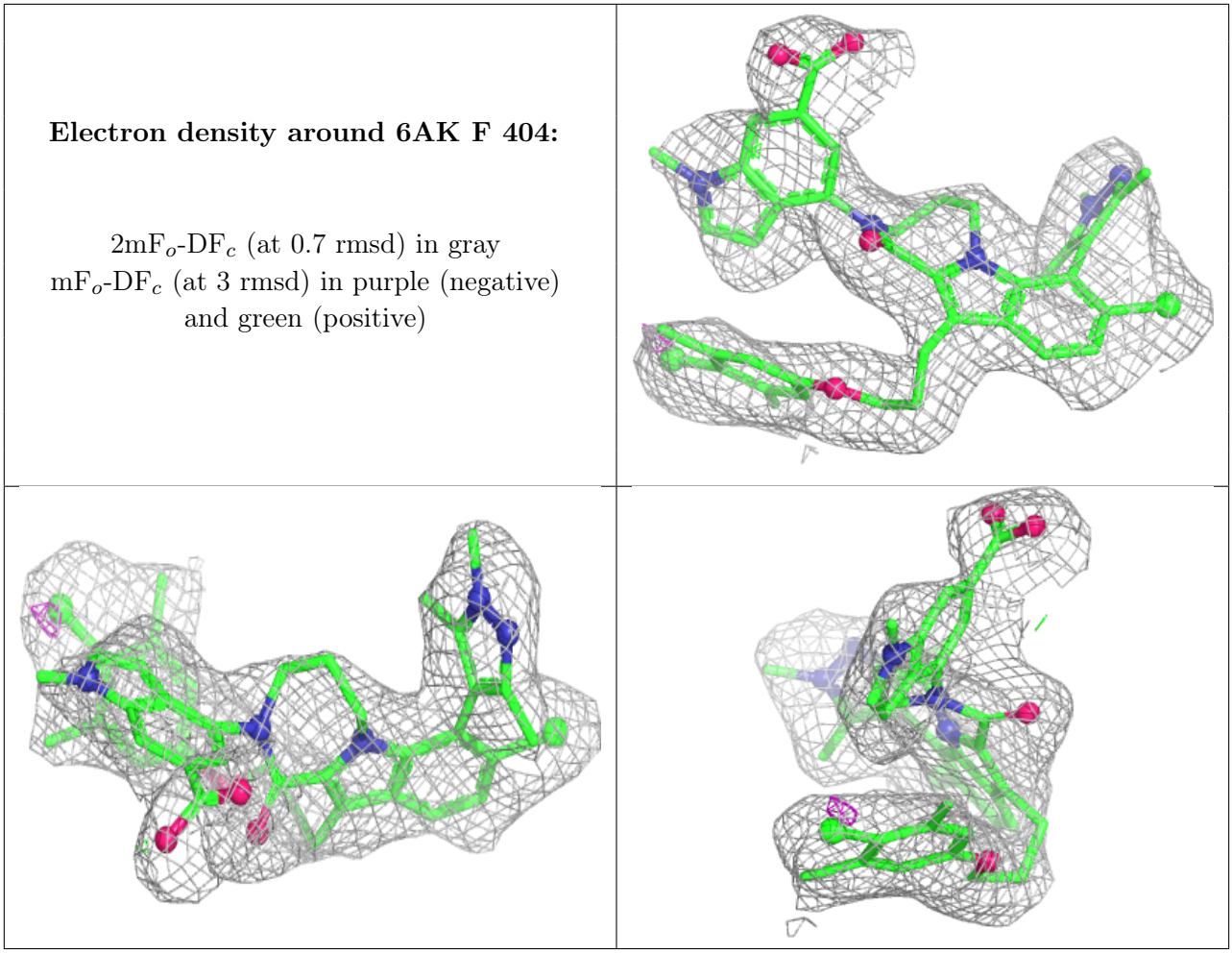






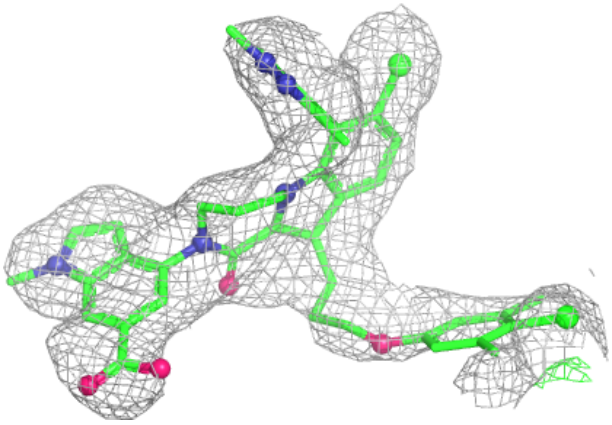
Electron density around 6AK F 404:

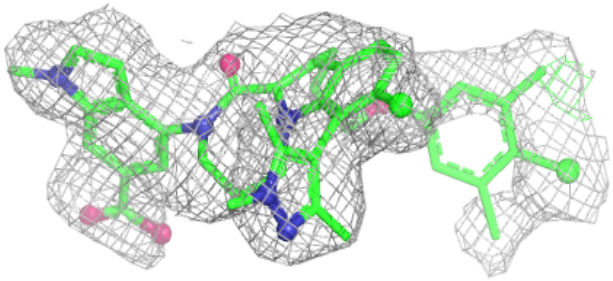
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

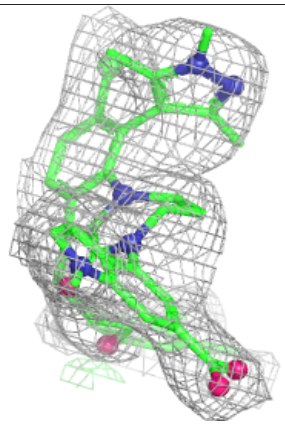


Electron density around 6AK F 405:

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

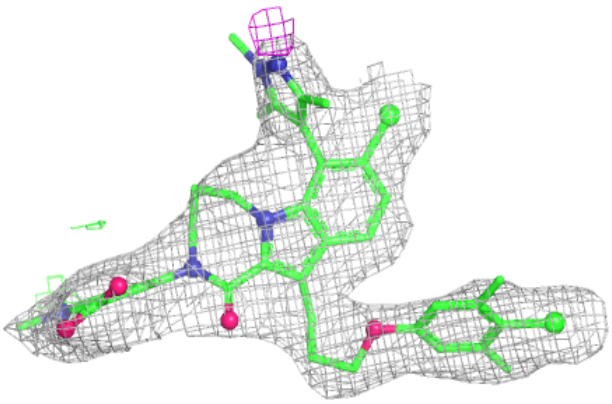


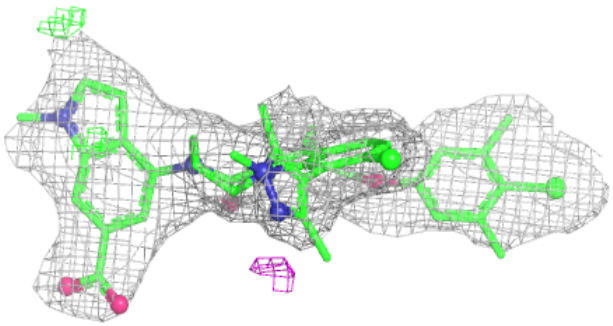


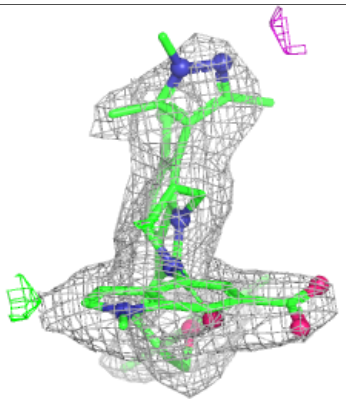


Electron density around 6AK G 401:

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

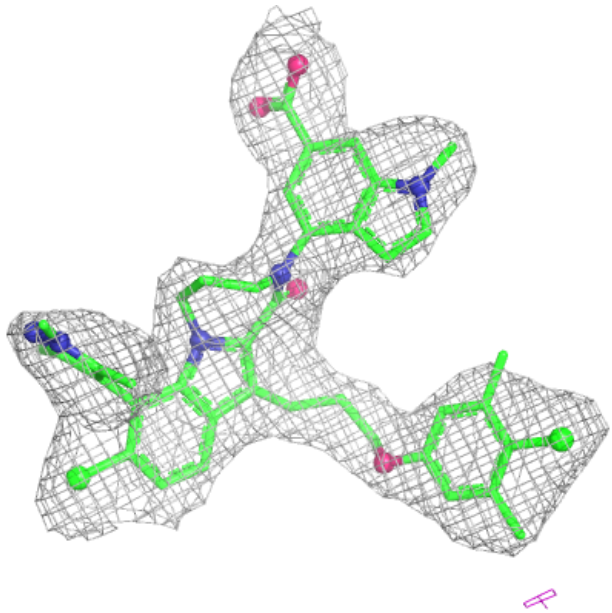


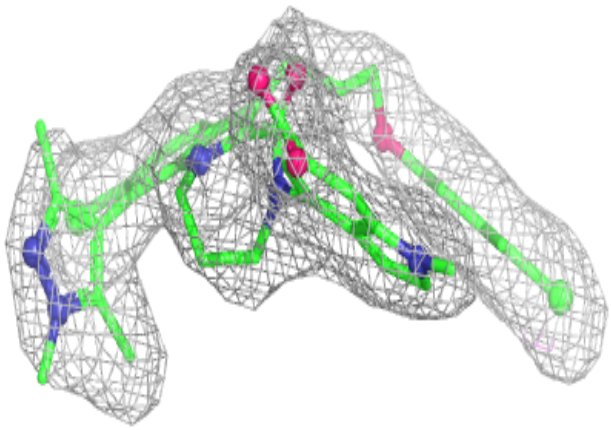


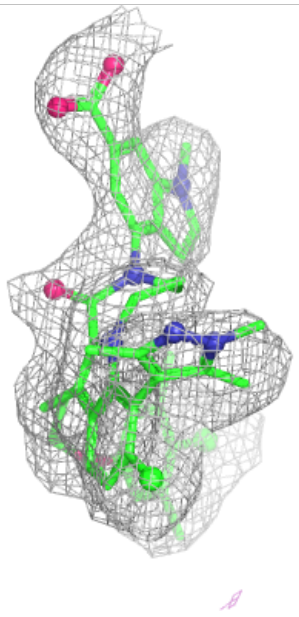


Electron density around 6AK G 403:

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

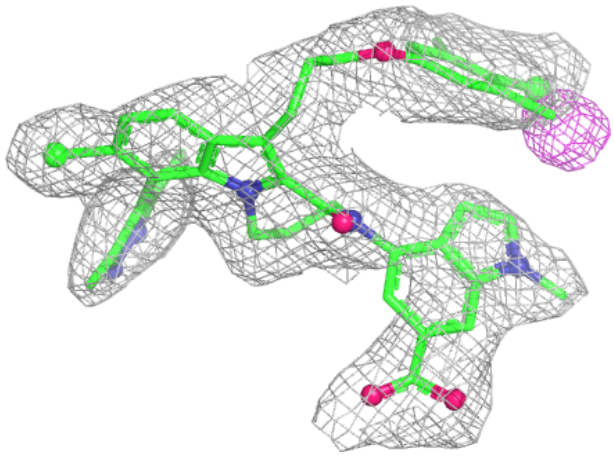


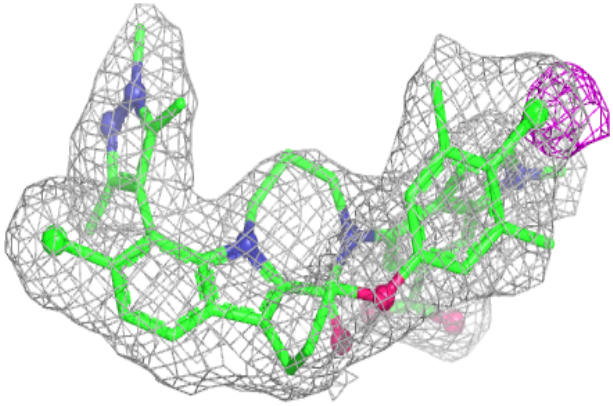


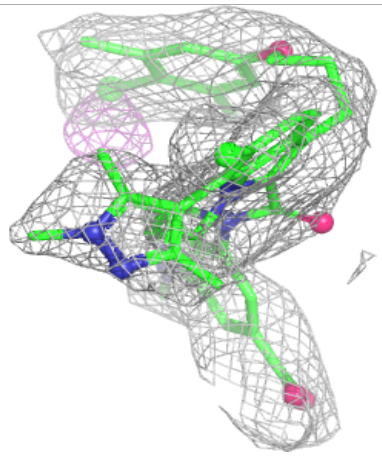


Electron density around 6AK G 404:

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

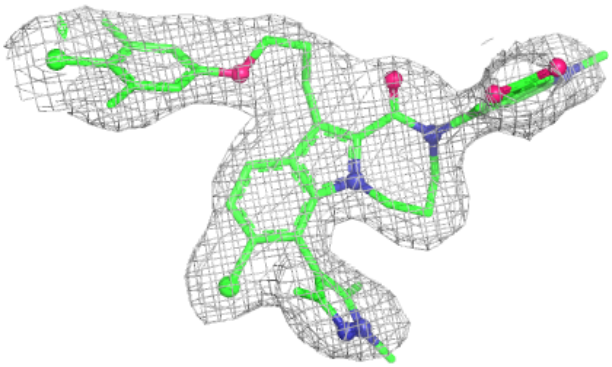


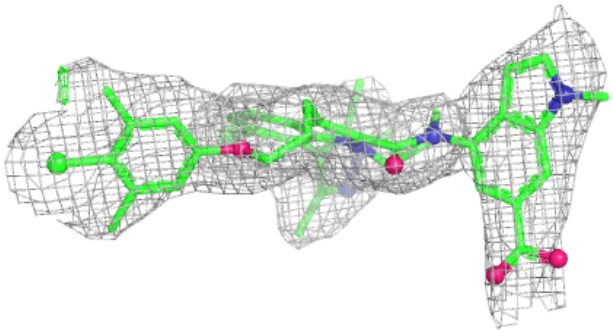


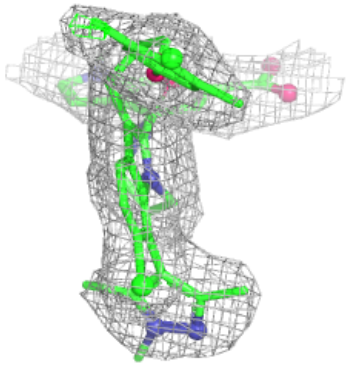


Electron density around 6AK H 301:

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

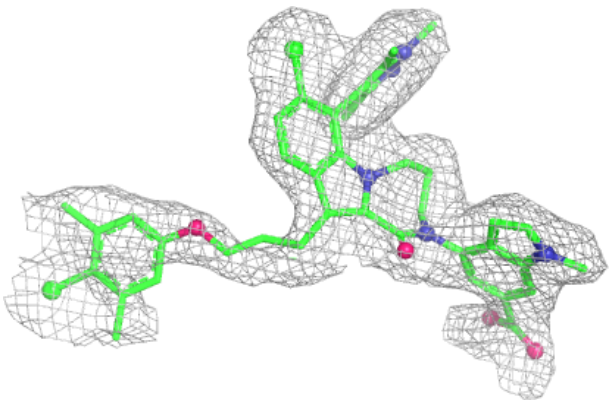


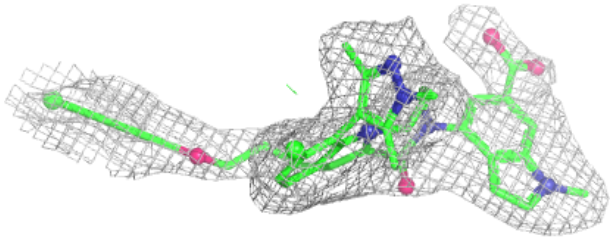


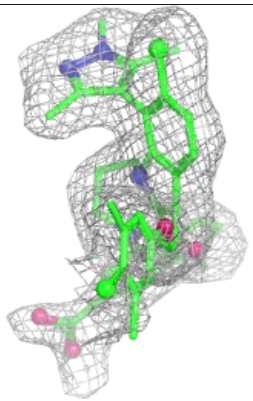


Electron density around 6AK H 303:

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

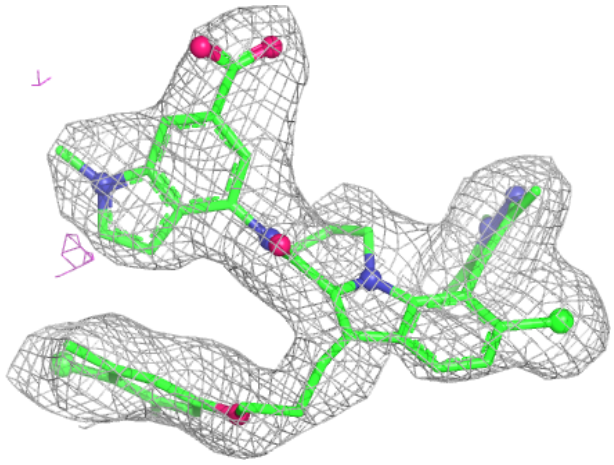


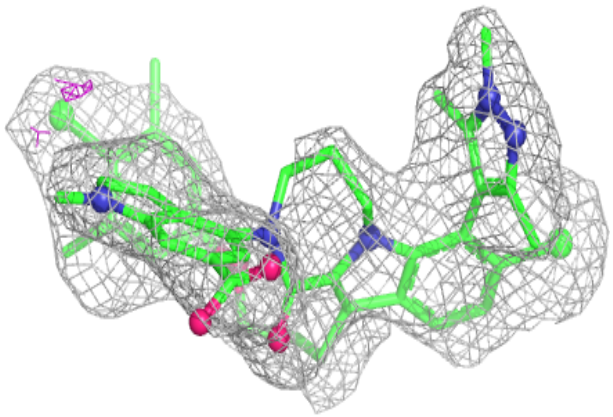


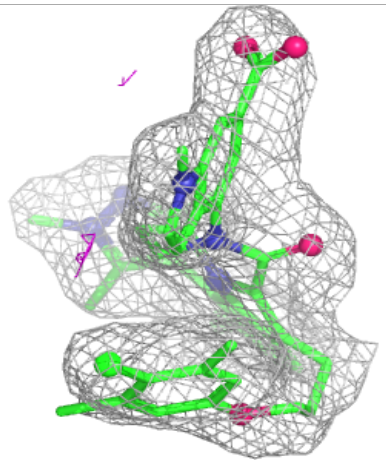


Electron density around 6AK H 304:

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

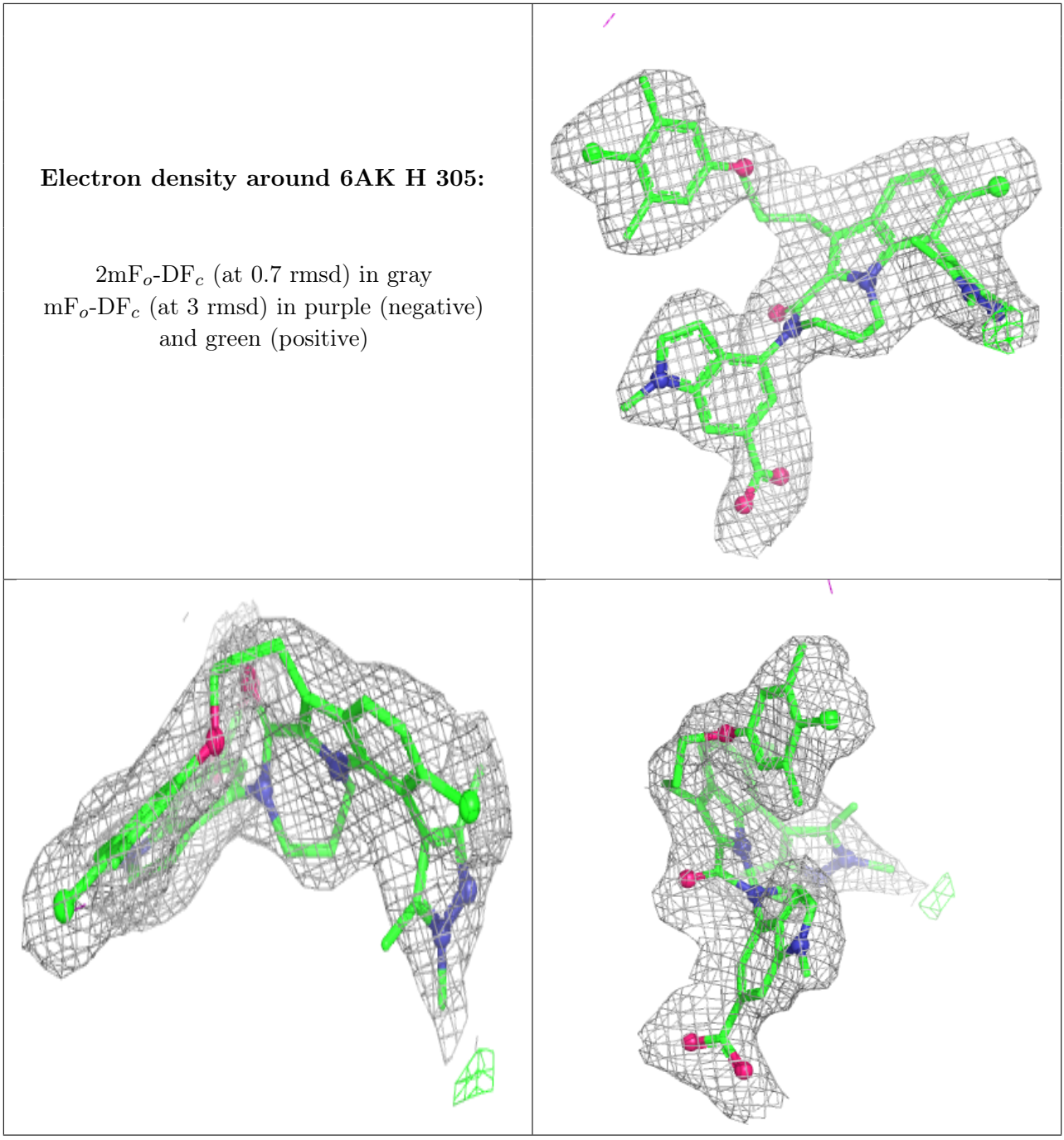






Electron density around 6AK H 305:

$2mF_o$-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.