wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 05:24 pm BST

PDB ID	:	8OFR
Title	:	Human adenovirus type 25 fiber-knob protein complexed with sialic acid
Authors	:	Rizkallah, P.J.; Parker, A.L.; Mundy, R.M.; Baker, A.T.
Deposited on	:	2023-03-16
Resolution	:	2.51 Å(reported)

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

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

The 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:

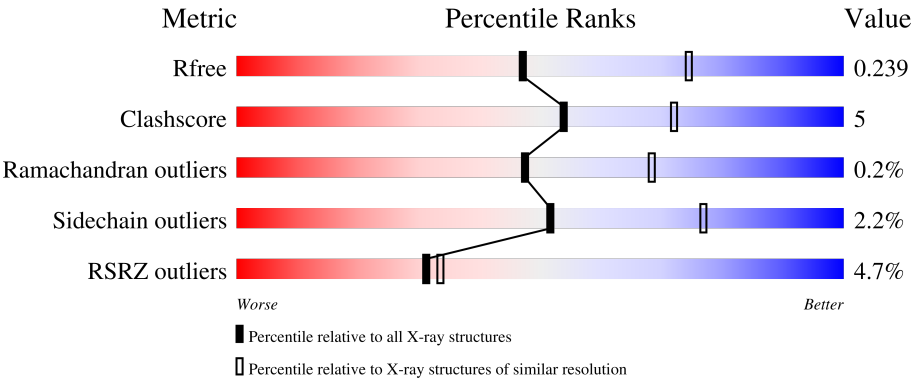
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	186	4% 86% 10%
1	B	186	7% 84% 15%
1	C	186	2% 84% 11% 5%
1	D	186	4% 87% 9%
1	E	186	6% 87% 9%

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Mol	Chain	Length	Quality of chain
1	F	186	4% 84% 10% 5%
1	G	186	6% 82% 11% 5%
1	H	186	3% 87% 10%
1	I	186	3% 82% 14%
1	J	186	3% 81% 13%
1	K	186	4% 83% 12% 5%
1	L	186	6% 82% 13%
1	M	186	8% 83% 10% 5%
1	N	186	4% 84% 11%
1	O	186	6% 83% 12%
1	P	186	4% 85% 9% 5%
1	Q	186	3% 87% 10%
1	R	186	5% 86% 10%
1	S	186	4% 87% 11%
1	T	186	3% 83% 11% 6%
1	U	186	2% 84% 10%
1	V	186	7% 85% 13%
1	W	186	5% 84% 11%
1	X	186	4% 83% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SLB	R	401	X	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35979 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 Fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	4	0
			1483	949	241	289	4			
1	B	186	Total	C	N	O	S	0	2	0
			1509	966	246	293	4			
1	C	177	Total	C	N	O	S	0	3	0
			1448	927	237	280	4			
1	D	180	Total	C	N	O	S	0	2	0
			1470	942	239	285	4			
1	E	179	Total	C	N	O	S	0	2	0
			1461	937	238	282	4			
1	F	176	Total	C	N	O	S	0	1	0
			1424	915	231	274	4			
1	G	177	Total	C	N	O	S	0	3	0
			1455	934	238	279	4			
1	H	181	Total	C	N	O	S	0	2	0
			1475	947	239	285	4			
1	I	179	Total	C	N	O	S	0	2	0
			1461	937	238	282	4			
1	J	178	Total	C	N	O	S	0	3	0
			1451	927	237	283	4			
1	K	177	Total	C	N	O	S	0	2	0
			1440	923	235	278	4			
1	L	179	Total	C	N	O	S	0	2	0
			1452	929	238	281	4			
1	M	176	Total	C	N	O	S	0	2	0
			1431	917	233	277	4			
1	N	178	Total	C	N	O	S	0	1	0
			1444	928	234	278	4			
1	O	178	Total	C	N	O	S	0	1	0
			1436	921	234	277	4			
1	P	177	Total	C	N	O	S	0	2	0
			1444	928	234	278	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	179	Total	C	N	O	S	0	2	0
			1461	937	238	282	4			
1	R	180	Total	C	N	O	S	0	2	0
			1465	939	239	283	4			
1	S	186	Total	C	N	O	S	0	2	0
			1509	966	246	293	4			
1	T	175	Total	C	N	O	S	0	2	0
			1423	913	231	275	4			
1	U	178	Total	C	N	O	S	0	2	0
			1452	932	236	280	4			
1	V	186	Total	C	N	O	S	0	1	0
			1501	962	244	291	4			
1	W	178	Total	C	N	O	S	0	2	0
			1453	933	236	280	4			
1	X	182	Total	C	N	O	S	0	2	0
			1482	948	242	288	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	LYS	-	expression tag	UNP M0QUM1
A	187	LEU	-	expression tag	UNP M0QUM1
B	186	LYS	-	expression tag	UNP M0QUM1
B	187	LEU	-	expression tag	UNP M0QUM1
C	186	LYS	-	expression tag	UNP M0QUM1
C	187	LEU	-	expression tag	UNP M0QUM1
D	186	LYS	-	expression tag	UNP M0QUM1
D	187	LEU	-	expression tag	UNP M0QUM1
E	186	LYS	-	expression tag	UNP M0QUM1
E	187	LEU	-	expression tag	UNP M0QUM1
F	186	LYS	-	expression tag	UNP M0QUM1
F	187	LEU	-	expression tag	UNP M0QUM1
G	186	LYS	-	expression tag	UNP M0QUM1
G	187	LEU	-	expression tag	UNP M0QUM1
H	186	LYS	-	expression tag	UNP M0QUM1
H	187	LEU	-	expression tag	UNP M0QUM1
I	186	LYS	-	expression tag	UNP M0QUM1
I	187	LEU	-	expression tag	UNP M0QUM1
J	186	LYS	-	expression tag	UNP M0QUM1
J	187	LEU	-	expression tag	UNP M0QUM1
K	186	LYS	-	expression tag	UNP M0QUM1
K	187	LEU	-	expression tag	UNP M0QUM1
L	186	LYS	-	expression tag	UNP M0QUM1

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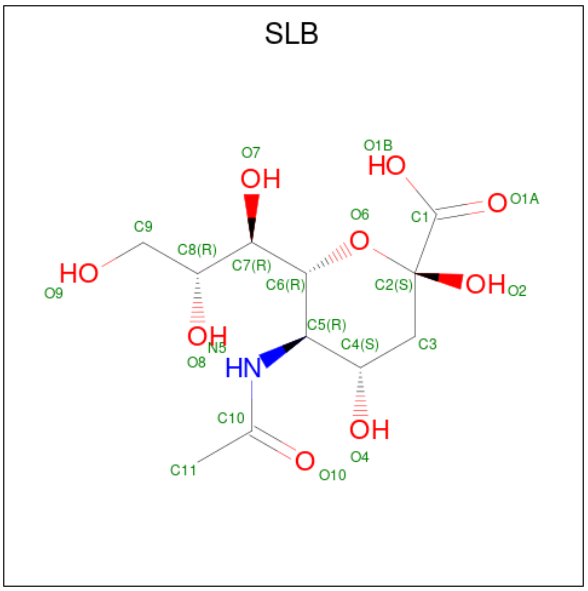
Chain	Residue	Modelled	Actual	Comment	Reference
L	187	LEU	-	expression tag	UNP M0QUM1
M	186	LYS	-	expression tag	UNP M0QUM1
M	187	LEU	-	expression tag	UNP M0QUM1
N	186	LYS	-	expression tag	UNP M0QUM1
N	187	LEU	-	expression tag	UNP M0QUM1
O	186	LYS	-	expression tag	UNP M0QUM1
O	187	LEU	-	expression tag	UNP M0QUM1
P	186	LYS	-	expression tag	UNP M0QUM1
P	187	LEU	-	expression tag	UNP M0QUM1
Q	186	LYS	-	expression tag	UNP M0QUM1
Q	187	LEU	-	expression tag	UNP M0QUM1
R	186	LYS	-	expression tag	UNP M0QUM1
R	187	LEU	-	expression tag	UNP M0QUM1
S	186	LYS	-	expression tag	UNP M0QUM1
S	187	LEU	-	expression tag	UNP M0QUM1
T	186	LYS	-	expression tag	UNP M0QUM1
T	187	LEU	-	expression tag	UNP M0QUM1
U	186	LYS	-	expression tag	UNP M0QUM1
U	187	LEU	-	expression tag	UNP M0QUM1
V	186	LYS	-	expression tag	UNP M0QUM1
V	187	LEU	-	expression tag	UNP M0QUM1
W	186	LYS	-	expression tag	UNP M0QUM1
W	187	LEU	-	expression tag	UNP M0QUM1
X	186	LYS	-	expression tag	UNP M0QUM1
X	187	LEU	-	expression tag	UNP M0QUM1

- Molecule 2 is N-acetyl-beta-neuraminic acid (three-letter code: SLB) (formula: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	11	1	9		
2	B	1	Total	C	N	O	0	0
			21	11	1	9		
2	C	1	Total	C	N	O	0	0
			21	11	1	9		
2	D	1	Total	C	N	O	0	0
			21	11	1	9		
2	E	1	Total	C	N	O	0	0
			21	11	1	9		
2	F	1	Total	C	N	O	0	0
			21	11	1	9		
2	G	1	Total	C	N	O	0	0
			21	11	1	9		
2	H	1	Total	C	N	O	0	0
			21	11	1	9		
2	I	1	Total	C	N	O	0	0
			21	11	1	9		
2	J	1	Total	C	N	O	0	0
			21	11	1	9		
2	K	1	Total	C	N	O	0	0
			21	11	1	9		
2	L	1	Total	C	N	O	0	0
			21	11	1	9		
2	M	1	Total	C	N	O	0	0
			21	11	1	9		
2	N	1	Total	C	N	O	0	0
			21	11	1	9		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			21	11	1	9		
2	P	1	Total	C	N	O	0	0
			21	11	1	9		
2	Q	1	Total	C	N	O	0	0
			21	11	1	9		
2	R	1	Total	C	N	O	0	0
			21	11	1	9		
2	S	1	Total	C	N	O	0	0
			21	11	1	9		
2	T	1	Total	C	N	O	0	0
			21	11	1	9		
2	U	1	Total	C	N	O	0	0
			21	11	1	9		
2	V	1	Total	C	N	O	0	0
			21	11	1	9		
2	W	1	Total	C	N	O	0	0
			21	11	1	9		
2	X	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	19	Total	O	0	0
			19	19		
3	C	13	Total	O	0	0
			13	13		
3	D	3	Total	O	0	0
			3	3		
3	E	3	Total	O	0	0
			3	3		
3	F	12	Total	O	0	0
			12	12		
3	G	24	Total	O	0	0
			24	24		
3	H	12	Total	O	0	0
			12	12		
3	I	32	Total	O	0	0
			32	32		

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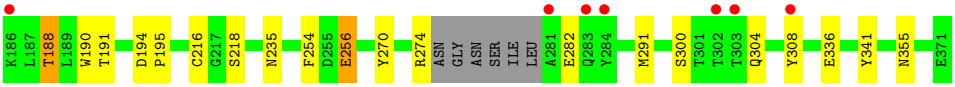
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	32	Total O 32 32	0	0
3	K	19	Total O 19 19	0	0
3	L	27	Total O 27 27	0	0
3	M	23	Total O 23 23	0	0
3	N	12	Total O 12 12	0	0
3	O	9	Total O 9 9	0	0
3	P	23	Total O 23 23	0	0
3	Q	7	Total O 7 7	0	0
3	R	12	Total O 12 12	0	0
3	S	40	Total O 40 40	0	0
3	T	28	Total O 28 28	0	0
3	U	15	Total O 15 15	0	0
3	V	20	Total O 20 20	0	0
3	W	23	Total O 23 23	0	0
3	X	21	Total O 21 21	0	0

3 Residue-property plots (i)

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

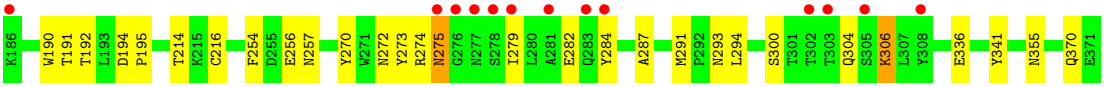
• Molecule 1: Fiber

Chain A:



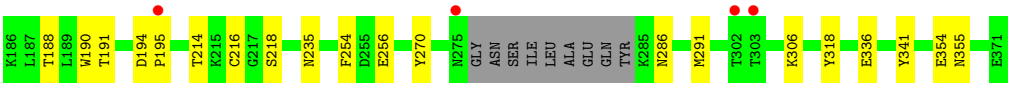
• Molecule 1: Fiber

Chain B:



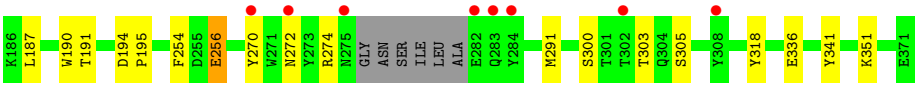
• Molecule 1: Fiber

Chain C:



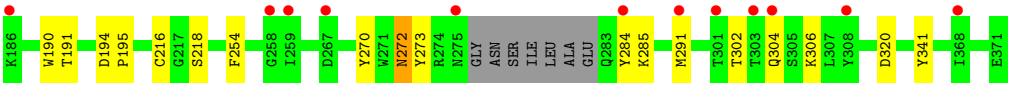
• Molecule 1: Fiber

Chain D:



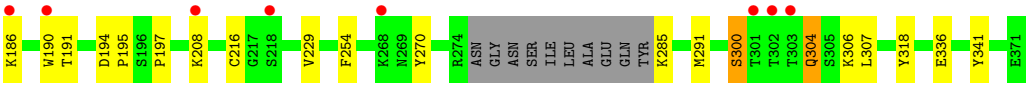
• Molecule 1: Fiber

Chain E:



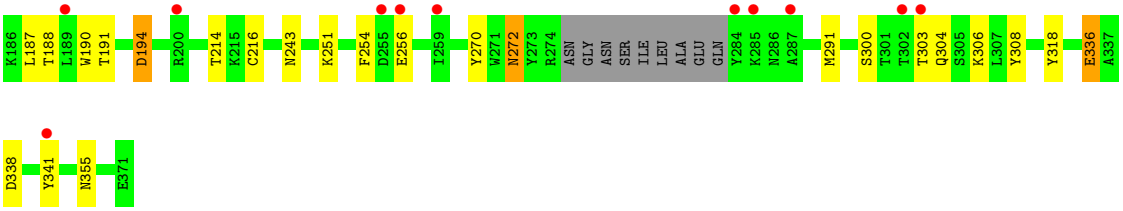
• Molecule 1: Fiber

Chain F:



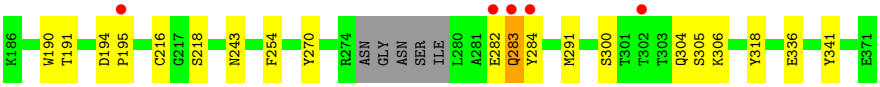
• Molecule 1: Fiber

Chain G:



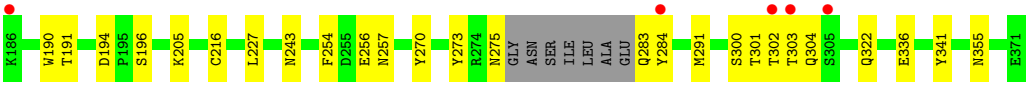
• Molecule 1: Fiber

Chain H:



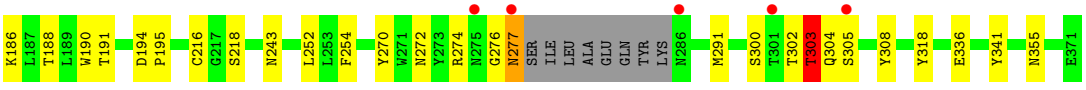
• Molecule 1: Fiber

Chain I:



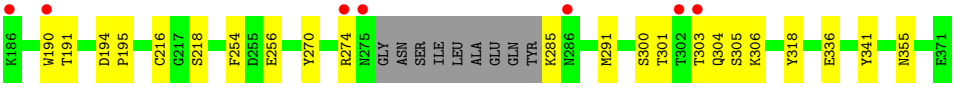
• Molecule 1: Fiber

Chain J:



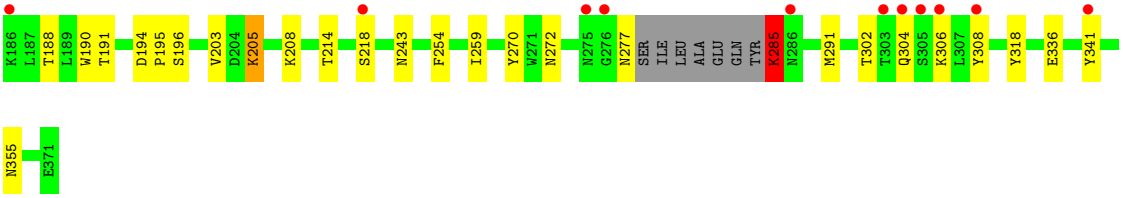
• Molecule 1: Fiber

Chain K:

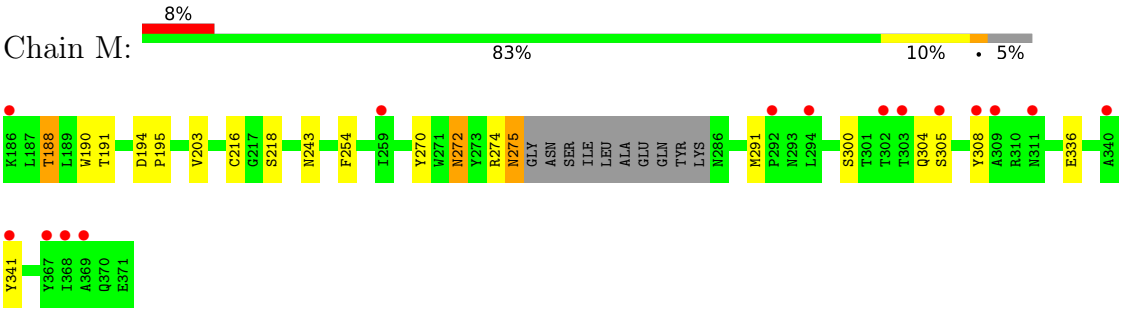


• Molecule 1: Fiber

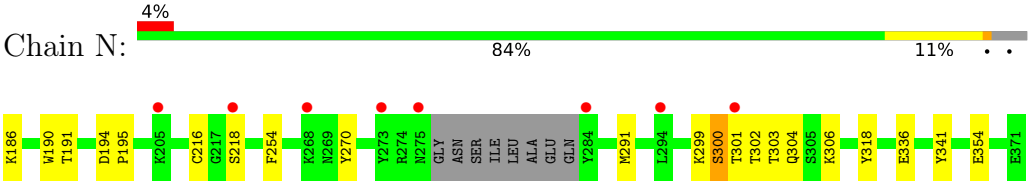
Chain L:



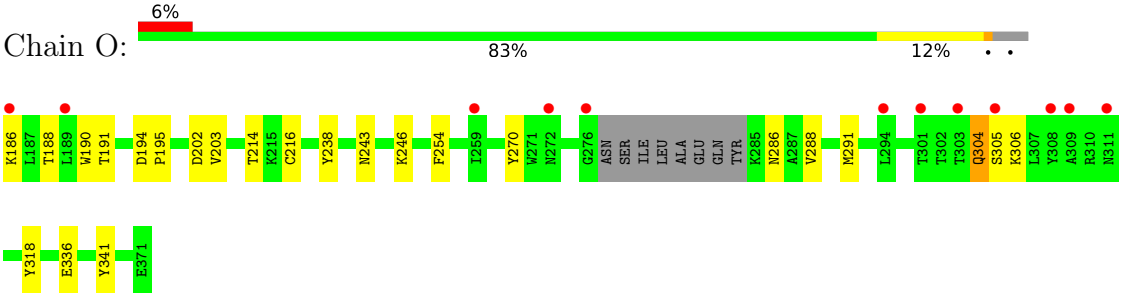
• Molecule 1: Fiber



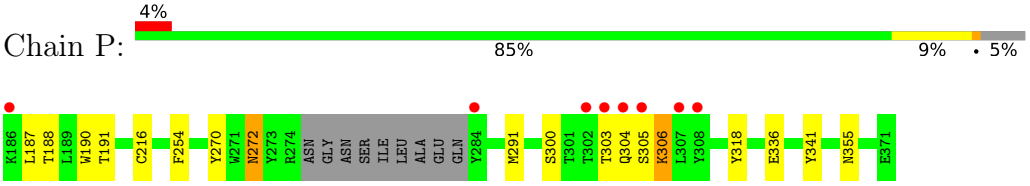
• Molecule 1: Fiber



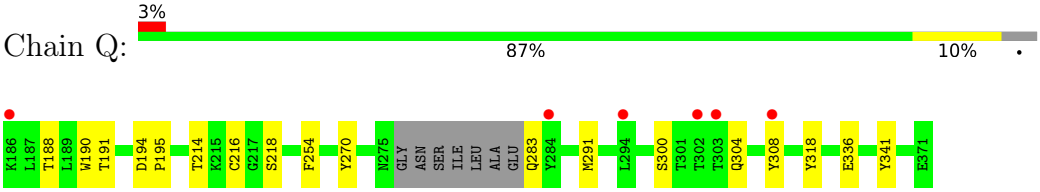
• Molecule 1: Fiber



• Molecule 1: Fiber

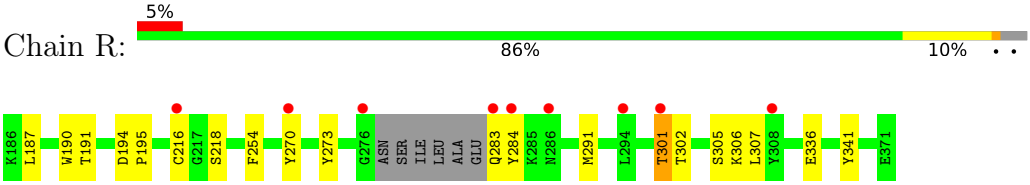


• Molecule 1: Fiber



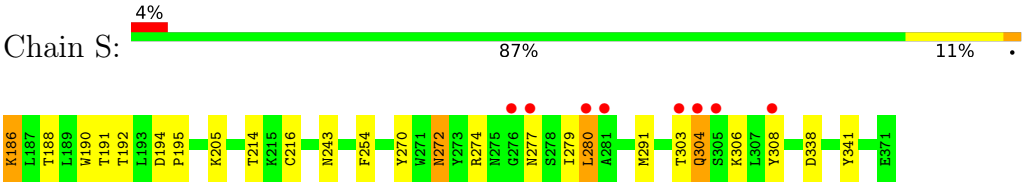
• Molecule 1: Fiber

Chain R:



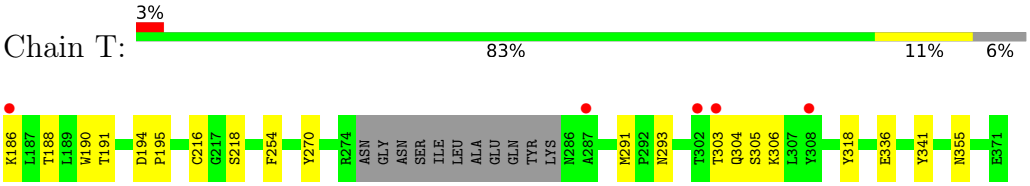
• Molecule 1: Fiber

Chain S:



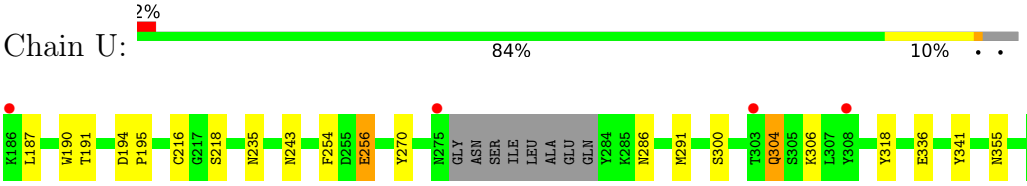
• Molecule 1: Fiber

Chain T:



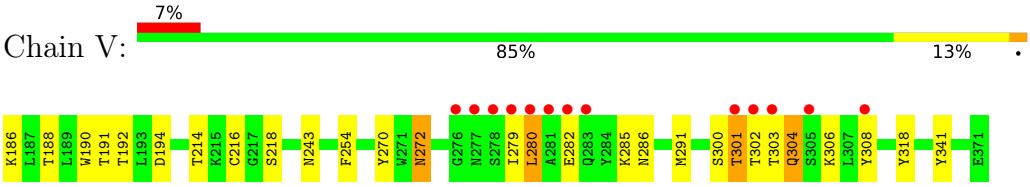
• Molecule 1: Fiber

Chain U:



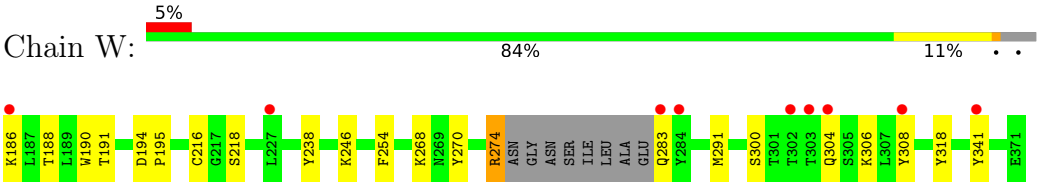
• Molecule 1: Fiber

Chain V:



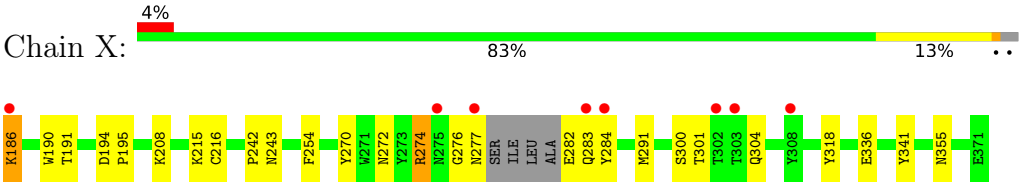
• Molecule 1: Fiber

Chain W:



• Molecule 1: Fiber

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.56Å 179.32Å 207.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.64 – 2.51 64.64 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.9 (64.64-2.51) 99.9 (64.64-2.51)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.239 0.222 , 0.239	Depositor DCC
R_{free} test set	7943 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	35979	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2584e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: SLB

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	0.70	1/1516 (0.1%)	0.72	0/2061
1	B	0.74	2/1543 (0.1%)	0.74	0/2099
1	C	0.70	2/1480 (0.1%)	0.73	0/2011
1	D	0.69	2/1503 (0.1%)	0.72	0/2043
1	E	0.67	0/1494	0.73	0/2031
1	F	0.72	3/1456 (0.2%)	0.74	0/1978
1	G	0.68	1/1488 (0.1%)	0.75	1/2022 (0.0%)
1	H	0.68	1/1508 (0.1%)	0.76	2/2050 (0.1%)
1	I	0.72	1/1494 (0.1%)	0.75	0/2031
1	J	0.75	2/1483 (0.1%)	0.74	0/2017
1	K	0.65	1/1472 (0.1%)	0.72	0/2001
1	L	0.70	2/1484 (0.1%)	0.74	0/2017
1	M	0.66	1/1463 (0.1%)	0.71	0/1990
1	N	0.68	3/1477 (0.2%)	0.73	0/2007
1	O	0.71	2/1468 (0.1%)	0.74	0/1994
1	P	0.67	1/1477 (0.1%)	0.72	0/2008
1	Q	0.65	1/1494 (0.1%)	0.71	0/2031
1	R	0.72	2/1498 (0.1%)	0.74	0/2036
1	S	0.75	0/1543	0.76	0/2099
1	T	0.69	1/1455 (0.1%)	0.73	0/1979
1	U	0.70	2/1485 (0.1%)	0.75	0/2019
1	V	0.69	0/1535	0.78	0/2087
1	W	0.67	1/1486 (0.1%)	0.73	0/2020
1	X	0.70	2/1515 (0.1%)	0.73	0/2059
All	All	0.70	34/35817 (0.1%)	0.74	3/48690 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	1
1	I	0	1
1	J	0	1
1	K	0	2
1	L	0	1
1	V	0	1
All	All	0	8

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	336	GLU	CD-OE1	8.47	1.34	1.25
1	D	256	GLU	CD-OE1	7.28	1.33	1.25
1	A	336	GLU	CD-OE1	7.22	1.33	1.25
1	G	336	GLU	CD-OE1	6.88	1.33	1.25
1	C	336	GLU	CD-OE2	6.78	1.33	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	284	TYR	CB-CG-CD2	-5.86	117.49	121.00
1	H	284	TYR	CB-CG-CD1	5.11	124.07	121.00
1	G	194	ASP	CB-CA-C	5.03	120.46	110.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	187	LEU	Mainchain
1	G	187	LEU	Mainchain
1	I	301	THR	Mainchain
1	J	303	THR	Peptide
1	K	285	LYS	Mainchain

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	1483	0	1452	17	1
1	B	1509	0	1486	25	0
1	C	1448	0	1425	18	0
1	D	1470	0	1444	11	1
1	E	1461	0	1438	10	0
1	F	1424	0	1410	19	0
1	G	1455	0	1436	23	0
1	H	1475	0	1454	15	0
1	I	1461	0	1437	21	0
1	J	1451	0	1420	28	0
1	K	1440	0	1422	17	0
1	L	1452	0	1429	27	1
1	M	1431	0	1409	19	0
1	N	1444	0	1425	15	1
1	O	1436	0	1419	18	0
1	P	1444	0	1424	16	1
1	Q	1461	0	1438	15	1
1	R	1465	0	1442	13	0
1	S	1509	0	1487	32	0
1	T	1423	0	1403	20	1
1	U	1452	0	1431	16	0
1	V	1501	0	1481	33	0
1	W	1453	0	1433	20	1
1	X	1482	0	1454	29	0
2	A	21	0	18	0	0
2	B	21	0	18	0	0
2	C	21	0	18	1	0
2	D	21	0	18	4	0
2	E	21	0	18	0	0
2	F	21	0	18	1	0
2	G	21	0	18	2	0
2	H	21	0	18	3	0
2	I	21	0	18	0	0
2	J	21	0	18	2	0
2	K	21	0	18	2	0
2	L	21	0	18	2	0
2	M	21	0	18	1	0
2	N	21	0	18	2	0
2	O	21	0	18	1	0
2	P	21	0	18	2	0
2	Q	21	0	18	4	0
2	R	21	0	18	0	0
2	S	21	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	21	0	18	2	0
2	U	21	0	18	2	0
2	V	21	0	18	1	0
2	W	21	0	18	1	0
2	X	21	0	18	2	0
3	A	16	0	0	0	0
3	B	19	0	0	1	0
3	C	13	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	12	0	0	1	0
3	G	24	0	0	1	0
3	H	12	0	0	0	0
3	I	32	0	0	1	0
3	J	32	0	0	2	0
3	K	19	0	0	1	0
3	L	27	0	0	2	0
3	M	23	0	0	0	0
3	N	12	0	0	0	0
3	O	9	0	0	0	0
3	P	23	0	0	1	0
3	Q	7	0	0	0	0
3	R	12	0	0	0	0
3	S	40	0	0	1	0
3	T	28	0	0	1	0
3	U	15	0	0	1	0
3	V	20	0	0	0	0
3	W	23	0	0	0	0
3	X	21	0	0	2	0
All	All	35979	0	34931	373	4

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

The worst 5 of 373 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:O:203:VAL:HG22	1:V:286:ASN:HB2	1.38	1.03
1:B:282:GLU:HA	1:X:194:ASP:OD2	1.60	1.02
1:L:355:ASN:HB3	3:L:527:HOH:O	1.67	0.95
1:F:197:PRO:HA	1:F:208:LYS:HG2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASN:HB3	1:B:279:ILE:HB	1.54	0.89

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:TYR:OH	1:T:303:THR:OG1[3_544]	1.39	0.81
1:N:303:THR:CB	1:Q:308:TYR:OH[2_554]	2.11	0.09
1:D:303:THR:O	1:W:308:TYR:OH[3_544]	2.15	0.05
1:L:308:TYR:OH	1:P:303:THR:O[1_455]	2.19	0.01

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	180/186 (97%)	173 (96%)	7 (4%)	0	100	100
1	B	186/186 (100%)	176 (95%)	10 (5%)	0	100	100
1	C	176/186 (95%)	168 (96%)	8 (4%)	0	100	100
1	D	178/186 (96%)	172 (97%)	6 (3%)	0	100	100
1	E	177/186 (95%)	168 (95%)	8 (4%)	1 (1%)	25	43
1	F	173/186 (93%)	166 (96%)	7 (4%)	0	100	100
1	G	176/186 (95%)	171 (97%)	5 (3%)	0	100	100
1	H	179/186 (96%)	169 (94%)	8 (4%)	2 (1%)	14	26
1	I	177/186 (95%)	170 (96%)	6 (3%)	1 (1%)	25	43
1	J	177/186 (95%)	167 (94%)	10 (6%)	0	100	100
1	K	175/186 (94%)	170 (97%)	5 (3%)	0	100	100
1	L	177/186 (95%)	166 (94%)	11 (6%)	0	100	100
1	M	174/186 (94%)	168 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	175/186 (94%)	167 (95%)	7 (4%)	1 (1%)	25 43
1	O	175/186 (94%)	168 (96%)	7 (4%)	0	100 100
1	P	175/186 (94%)	169 (97%)	6 (3%)	0	100 100
1	Q	177/186 (95%)	172 (97%)	5 (3%)	0	100 100
1	R	178/186 (96%)	166 (93%)	10 (6%)	2 (1%)	14 26
1	S	186/186 (100%)	179 (96%)	7 (4%)	0	100 100
1	T	173/186 (93%)	165 (95%)	8 (5%)	0	100 100
1	U	176/186 (95%)	168 (96%)	7 (4%)	1 (1%)	25 43
1	V	185/186 (100%)	175 (95%)	8 (4%)	2 (1%)	14 26
1	W	176/186 (95%)	170 (97%)	6 (3%)	0	100 100
1	X	180/186 (97%)	168 (93%)	12 (7%)	0	100 100
All	All	4261/4464 (96%)	4071 (96%)	180 (4%)	10 (0%)	47 68

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	302	THR
1	V	302	THR
1	H	283	GLN
1	R	302	THR
1	U	286	ASN

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	168/169 (99%)	165 (98%)	3 (2%)	59 81
1	B	171/169 (101%)	168 (98%)	3 (2%)	59 81
1	C	165/169 (98%)	160 (97%)	5 (3%)	41 68
1	D	167/169 (99%)	163 (98%)	4 (2%)	49 74
1	E	166/169 (98%)	161 (97%)	5 (3%)	41 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	162/169 (96%)	161 (99%)	1 (1%)	86 95
1	G	165/169 (98%)	161 (98%)	4 (2%)	49 74
1	H	167/169 (99%)	165 (99%)	2 (1%)	71 88
1	I	166/169 (98%)	162 (98%)	4 (2%)	49 74
1	J	165/169 (98%)	162 (98%)	3 (2%)	59 81
1	K	164/169 (97%)	160 (98%)	4 (2%)	49 74
1	L	165/169 (98%)	160 (97%)	5 (3%)	41 68
1	M	163/169 (96%)	158 (97%)	5 (3%)	40 67
1	N	164/169 (97%)	162 (99%)	2 (1%)	71 88
1	O	163/169 (96%)	160 (98%)	3 (2%)	59 81
1	P	164/169 (97%)	160 (98%)	4 (2%)	49 74
1	Q	166/169 (98%)	164 (99%)	2 (1%)	71 88
1	R	166/169 (98%)	161 (97%)	5 (3%)	41 68
1	S	171/169 (101%)	165 (96%)	6 (4%)	36 62
1	T	162/169 (96%)	158 (98%)	4 (2%)	47 73
1	U	165/169 (98%)	161 (98%)	4 (2%)	49 74
1	V	170/169 (101%)	163 (96%)	7 (4%)	30 55
1	W	165/169 (98%)	164 (99%)	1 (1%)	86 95
1	X	168/169 (99%)	166 (99%)	2 (1%)	71 88
All	All	3978/4056 (98%)	3890 (98%)	88 (2%)	52 77

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	190	TRP
1	T	190	TRP
1	R	190	TRP
1	S	190	TRP
1	U	190	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	311	ASN

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Mol	Chain	Res	Type
1	W	269	ASN
1	S	272	ASN
1	U	269	ASN
1	X	316	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	SLB	Q	401	-	21,21,21	1.18	3 (14%)	25,31,31	0.97	2 (8%)
2	SLB	T	401	-	21,21,21	1.39	3 (14%)	25,31,31	1.13	3 (12%)
2	SLB	C	401	-	21,21,21	1.00	2 (9%)	25,31,31	1.50	4 (16%)
2	SLB	L	401	-	21,21,21	0.85	1 (4%)	25,31,31	1.42	4 (16%)
2	SLB	H	401	-	21,21,21	1.24	3 (14%)	25,31,31	1.08	2 (8%)
2	SLB	V	401	-	21,21,21	1.78	5 (23%)	25,31,31	1.45	4 (16%)
2	SLB	M	401	-	21,21,21	0.79	1 (4%)	25,31,31	0.91	1 (4%)
2	SLB	D	401	-	21,21,21	1.58	6 (28%)	25,31,31	1.36	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SLB	R	401	-	21,21,21	1.12	2 (9%)	25,31,31	1.03	2 (8%)
2	SLB	G	401	-	21,21,21	0.99	2 (9%)	25,31,31	0.74	0
2	SLB	U	401	-	21,21,21	1.47	4 (19%)	25,31,31	1.14	3 (12%)
2	SLB	A	401	-	21,21,21	1.01	2 (9%)	25,31,31	0.95	3 (12%)
2	SLB	P	401	-	21,21,21	1.10	2 (9%)	25,31,31	0.93	1 (4%)
2	SLB	W	401	-	21,21,21	1.18	3 (14%)	25,31,31	1.17	3 (12%)
2	SLB	I	401	-	21,21,21	0.90	1 (4%)	25,31,31	1.05	3 (12%)
2	SLB	F	401	-	21,21,21	1.26	3 (14%)	25,31,31	1.34	4 (16%)
2	SLB	E	401	-	21,21,21	1.15	3 (14%)	25,31,31	0.85	1 (4%)
2	SLB	K	401	-	21,21,21	0.98	2 (9%)	25,31,31	1.03	3 (12%)
2	SLB	O	401	-	21,21,21	1.14	3 (14%)	25,31,31	0.86	1 (4%)
2	SLB	N	401	-	21,21,21	1.22	2 (9%)	25,31,31	1.26	3 (12%)
2	SLB	J	401	-	21,21,21	1.20	3 (14%)	25,31,31	0.98	2 (8%)
2	SLB	B	401	-	21,21,21	1.22	3 (14%)	25,31,31	1.07	3 (12%)
2	SLB	X	401	-	21,21,21	1.99	5 (23%)	25,31,31	1.45	4 (16%)
2	SLB	S	401	-	21,21,21	1.29	4 (19%)	25,31,31	1.11	1 (4%)

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	SLB	Q	401	-	-	5/20/38/38	0/1/1/1
2	SLB	T	401	-	-	9/20/38/38	0/1/1/1
2	SLB	C	401	-	-	7/20/38/38	0/1/1/1
2	SLB	L	401	-	-	9/20/38/38	0/1/1/1
2	SLB	H	401	-	-	10/20/38/38	0/1/1/1
2	SLB	V	401	-	-	8/20/38/38	0/1/1/1
2	SLB	M	401	-	-	6/20/38/38	0/1/1/1
2	SLB	D	401	-	-	1/20/38/38	0/1/1/1
2	SLB	R	401	-	1/1/8/9	4/20/38/38	0/1/1/1
2	SLB	G	401	-	-	10/20/38/38	0/1/1/1
2	SLB	U	401	-	-	8/20/38/38	0/1/1/1
2	SLB	A	401	-	-	8/20/38/38	0/1/1/1
2	SLB	P	401	-	-	8/20/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SLB	W	401	-	-	8/20/38/38	0/1/1/1
2	SLB	I	401	-	-	7/20/38/38	0/1/1/1
2	SLB	F	401	-	-	11/20/38/38	0/1/1/1
2	SLB	E	401	-	-	8/20/38/38	0/1/1/1
2	SLB	K	401	-	-	2/20/38/38	0/1/1/1
2	SLB	O	401	-	-	5/20/38/38	0/1/1/1
2	SLB	N	401	-	-	7/20/38/38	0/1/1/1
2	SLB	J	401	-	-	2/20/38/38	0/1/1/1
2	SLB	B	401	-	-	3/20/38/38	0/1/1/1
2	SLB	X	401	-	-	7/20/38/38	0/1/1/1
2	SLB	S	401	-	-	6/20/38/38	0/1/1/1

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	401	SLB	O6-C2	5.16	1.48	1.43
2	T	401	SLB	C8-C7	4.46	1.61	1.53
2	V	401	SLB	C11-C10	4.38	1.59	1.50
2	X	401	SLB	C8-C7	4.28	1.61	1.53
2	X	401	SLB	C2-C1	4.19	1.60	1.53

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	SLB	C8-C7-C6	4.82	122.18	113.03
2	V	401	SLB	C11-C10-N5	-4.47	108.53	116.10
2	X	401	SLB	O6-C6-C7	3.88	113.27	107.29
2	D	401	SLB	C11-C10-N5	-3.82	109.63	116.10
2	L	401	SLB	O1A-C1-C2	-3.63	118.09	123.59

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	R	401	SLB	C2

5 of 159 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SLB	O1A-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	401	SLB	O1B-C1-C2-O2
2	A	401	SLB	O1B-C1-C2-O6
2	A	401	SLB	O8-C8-C9-O9
2	B	401	SLB	O1B-C1-C2-O2

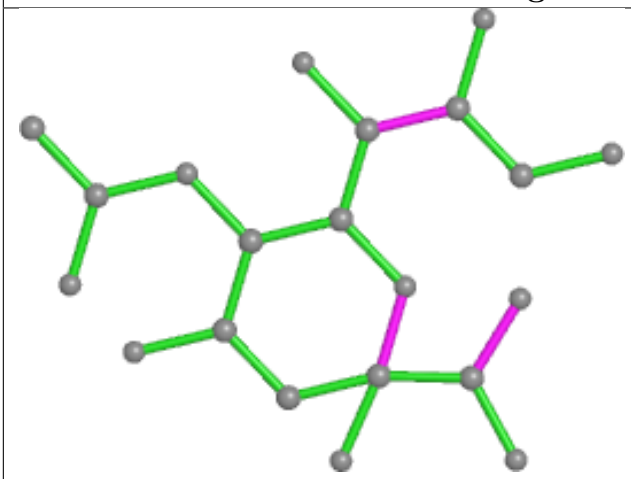
There are no ring outliers.

18 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	401	SLB	4	0
2	T	401	SLB	2	0
2	C	401	SLB	1	0
2	L	401	SLB	2	0
2	H	401	SLB	3	0
2	V	401	SLB	1	0
2	M	401	SLB	1	0
2	D	401	SLB	4	0
2	G	401	SLB	2	0
2	U	401	SLB	2	0
2	P	401	SLB	2	0
2	W	401	SLB	1	0
2	F	401	SLB	1	0
2	K	401	SLB	2	0
2	O	401	SLB	1	0
2	N	401	SLB	2	0
2	J	401	SLB	2	0
2	X	401	SLB	2	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 SLB Q 401



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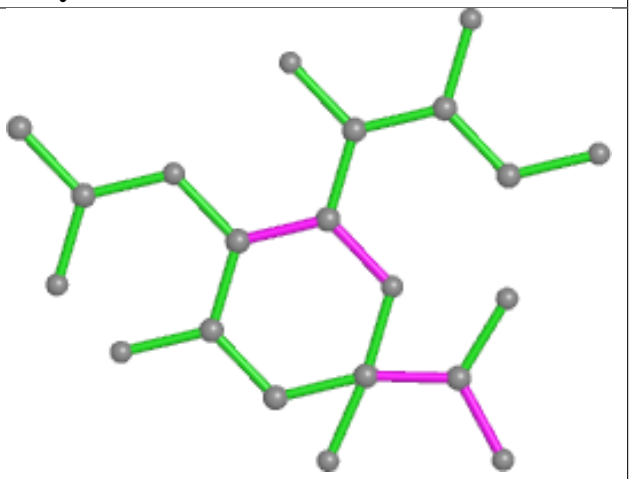
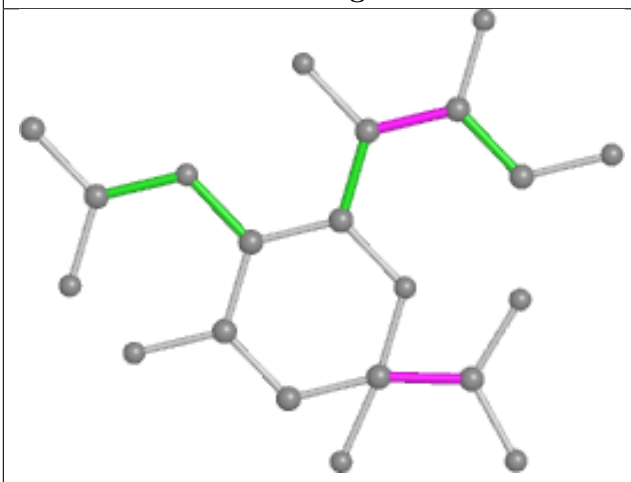


Bond angles



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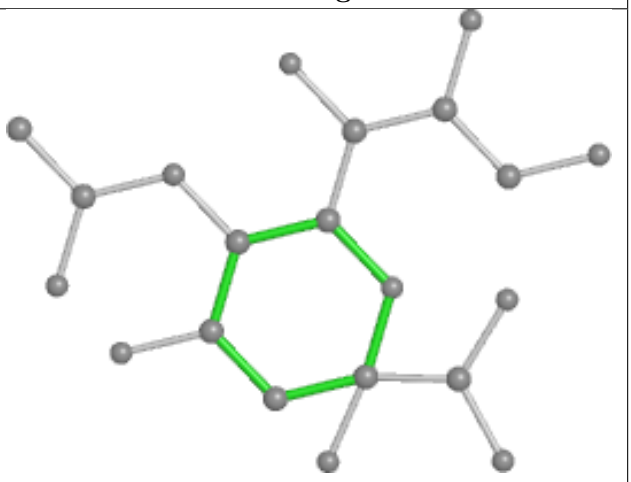
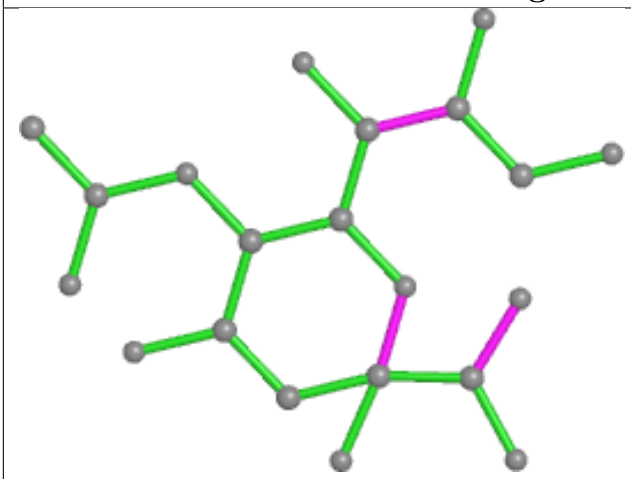


Rings

Ligand SLB T 401



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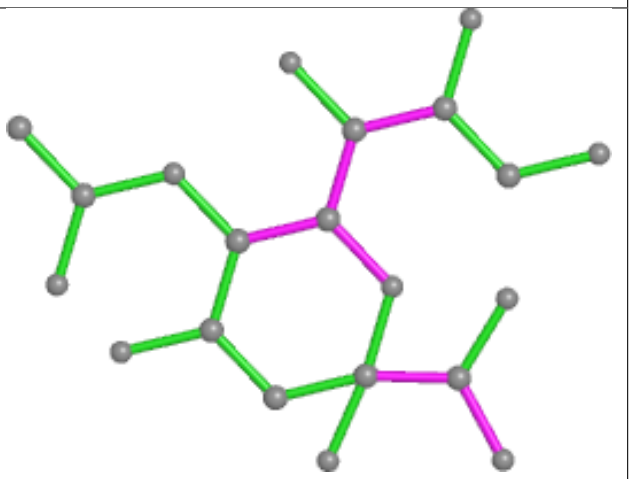

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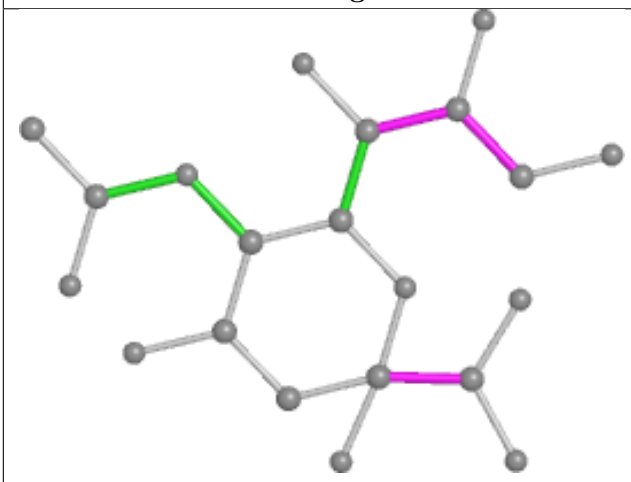

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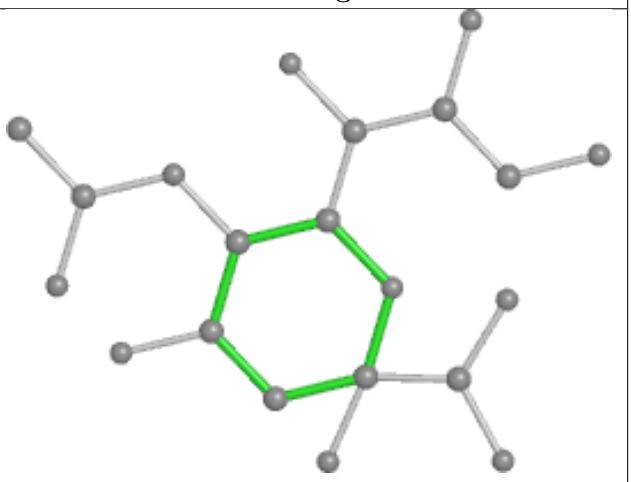
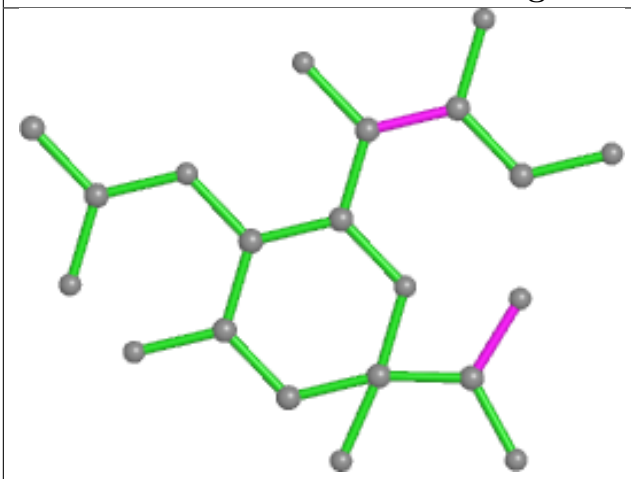


Rings

Ligand SLB C 401



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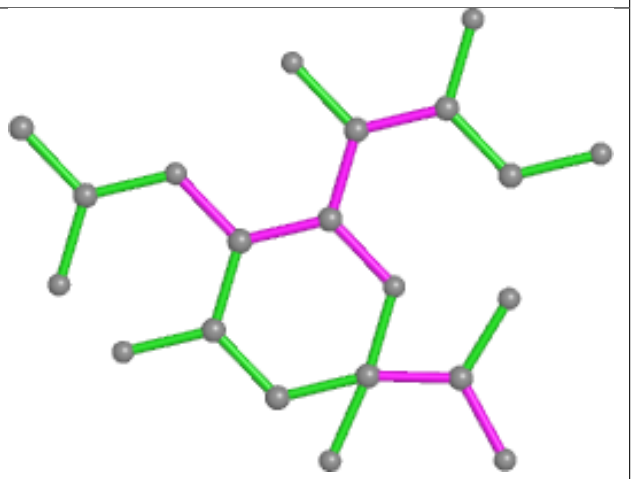

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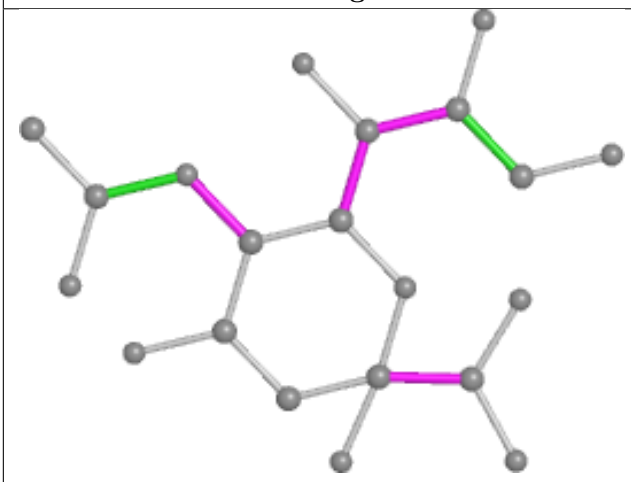

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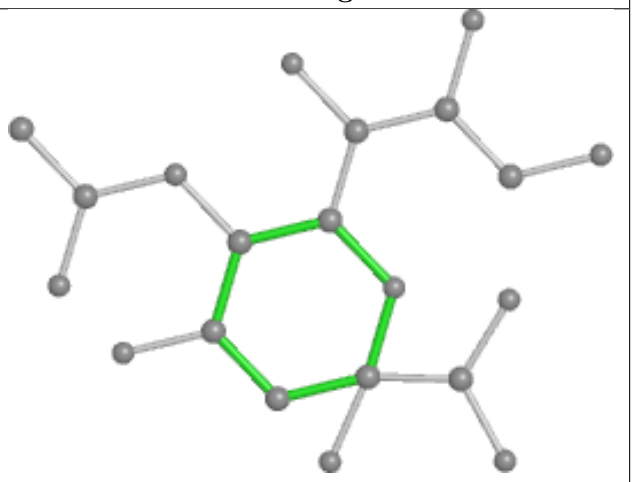
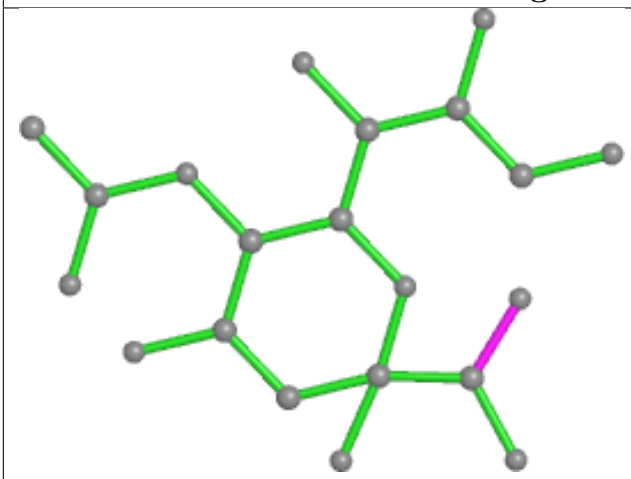


Rings

Ligand SLB L 401



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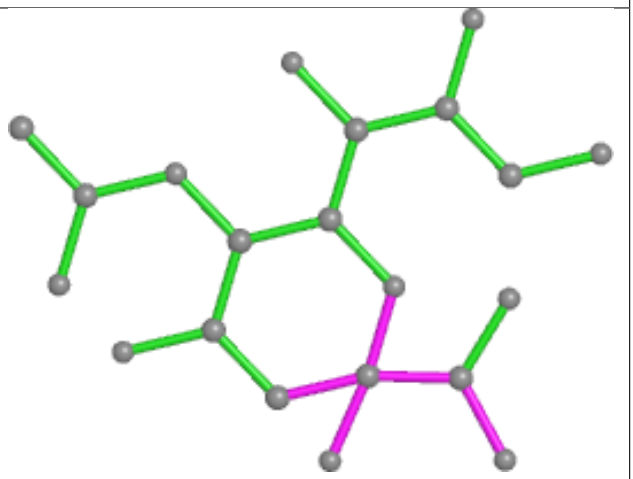

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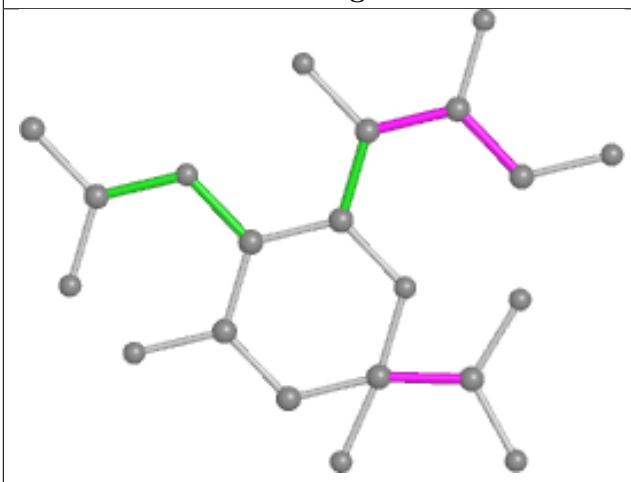

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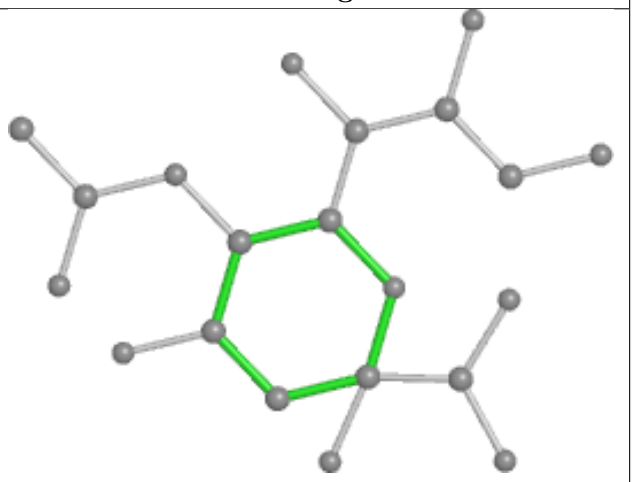
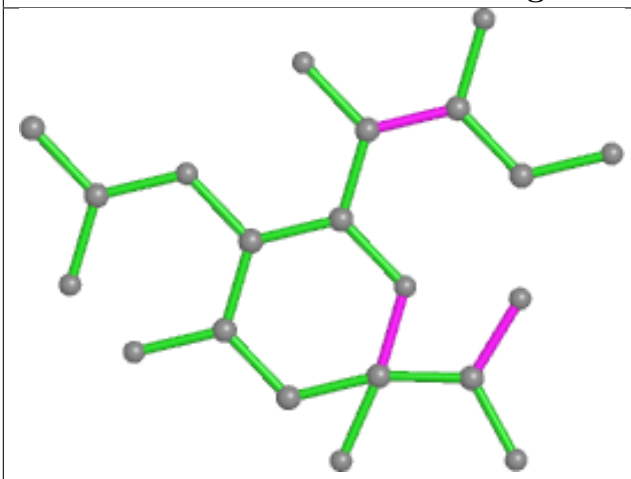


Rings

Ligand SLB H 401



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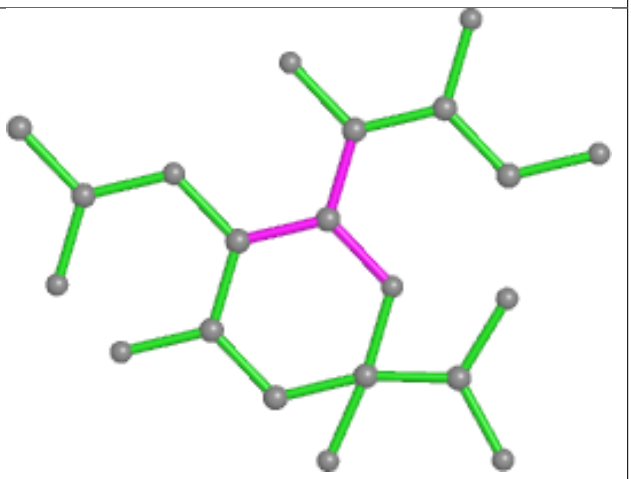

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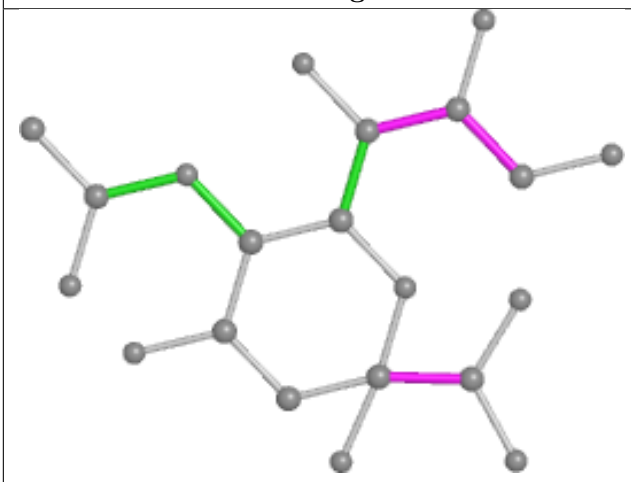

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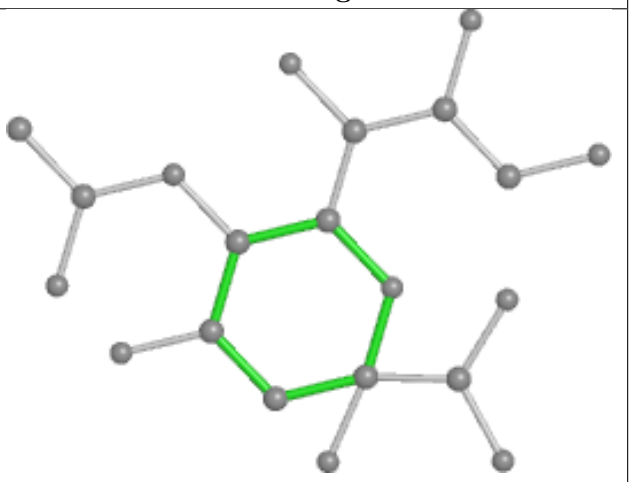

Rings

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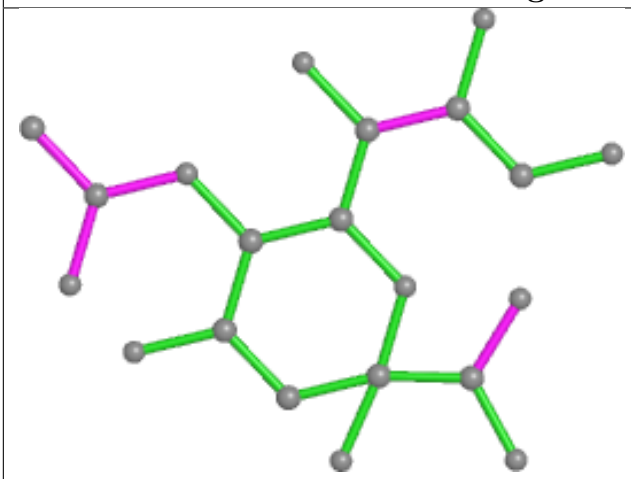

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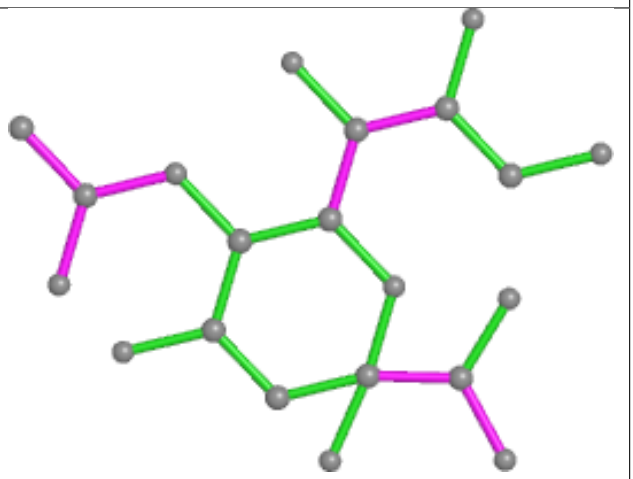

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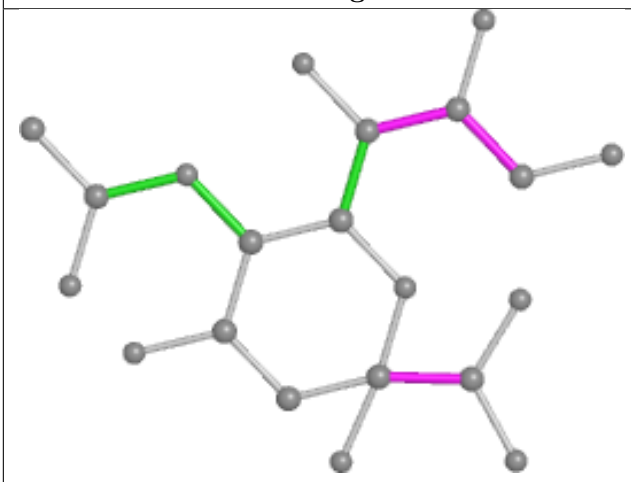

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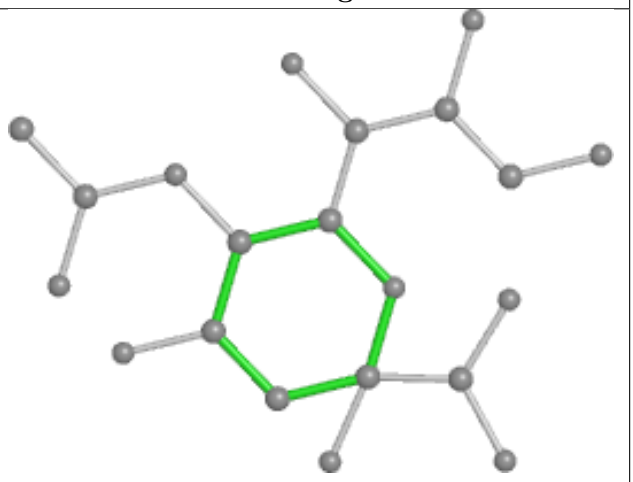
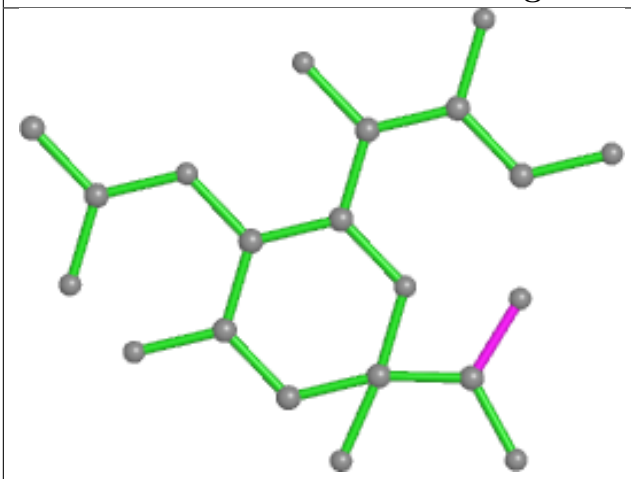


Rings

Ligand SLB M 401



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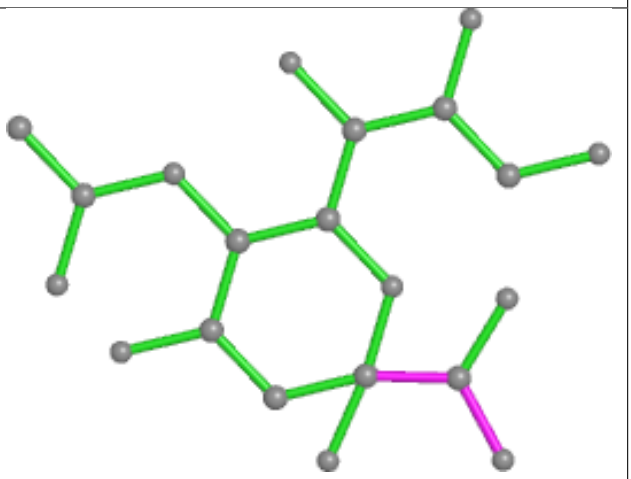

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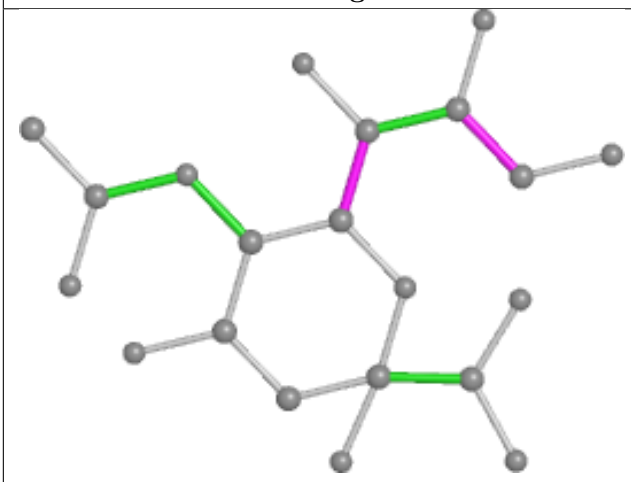

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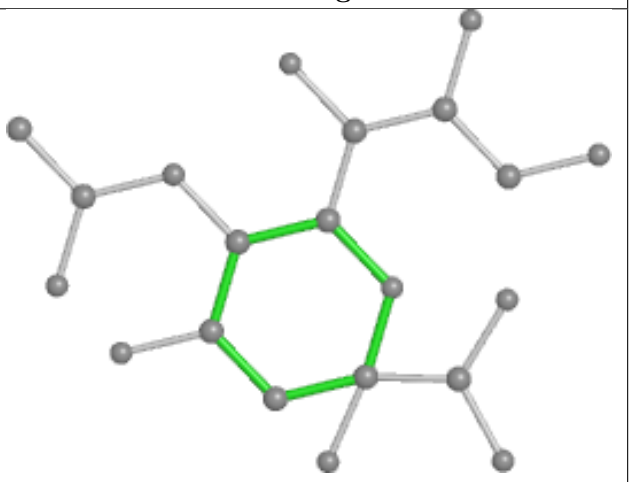

Rings

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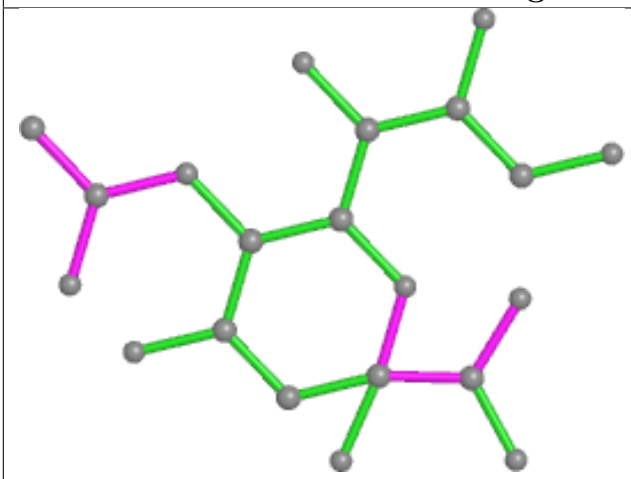

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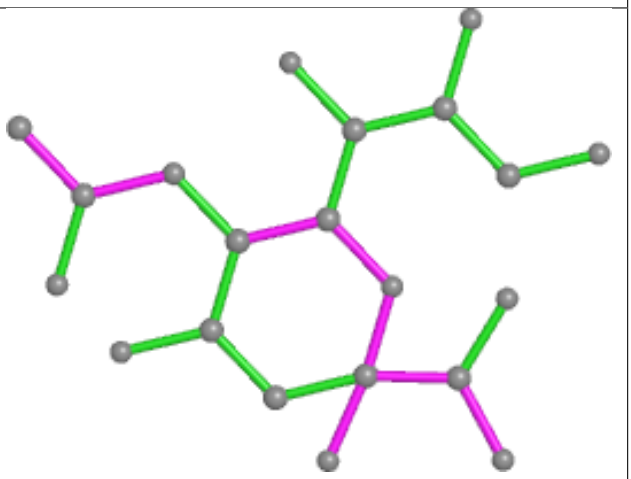

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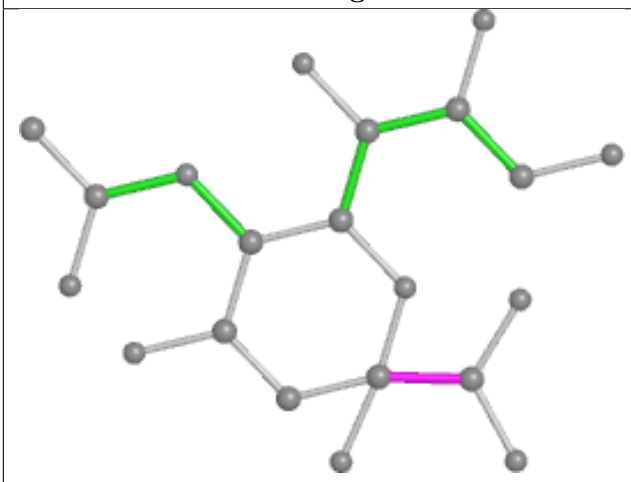

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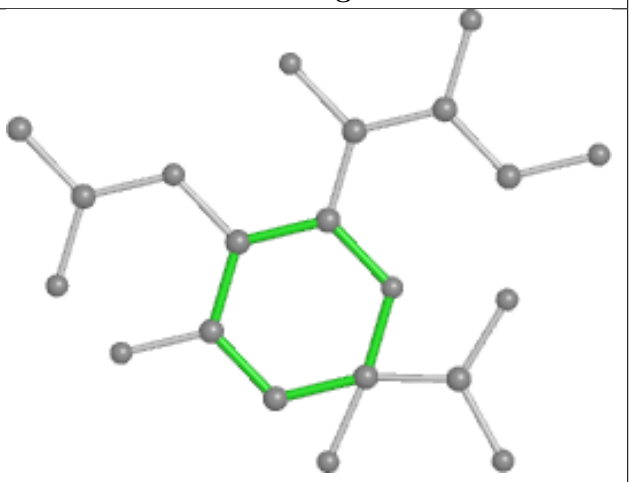

Rings

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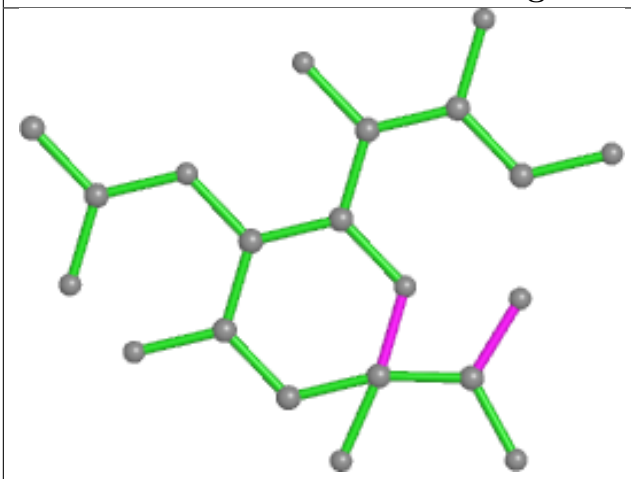

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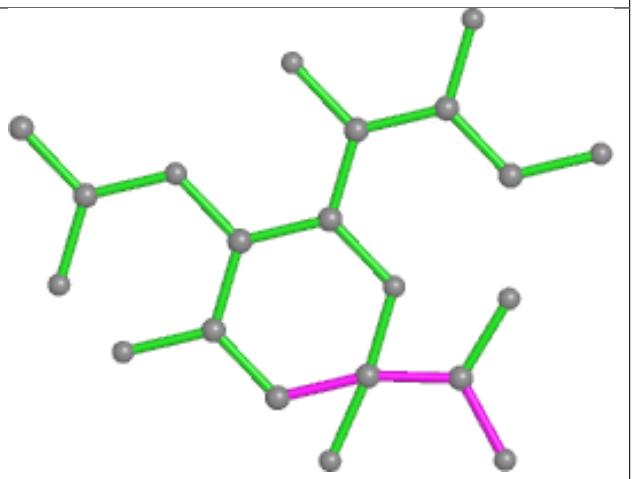

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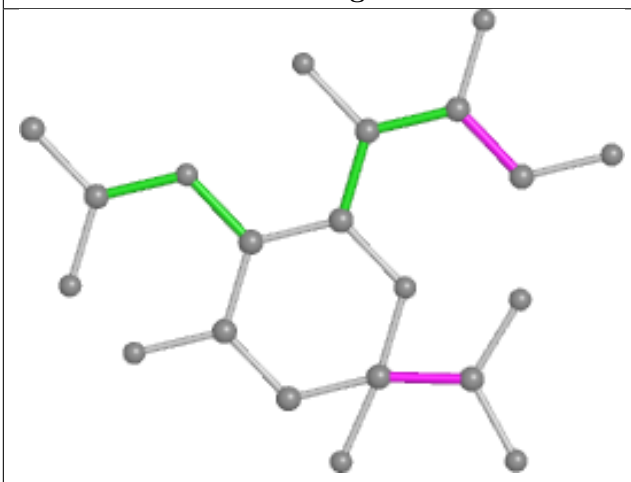

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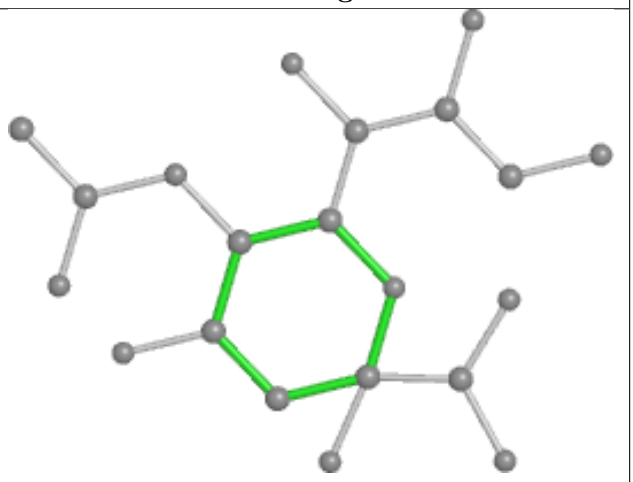
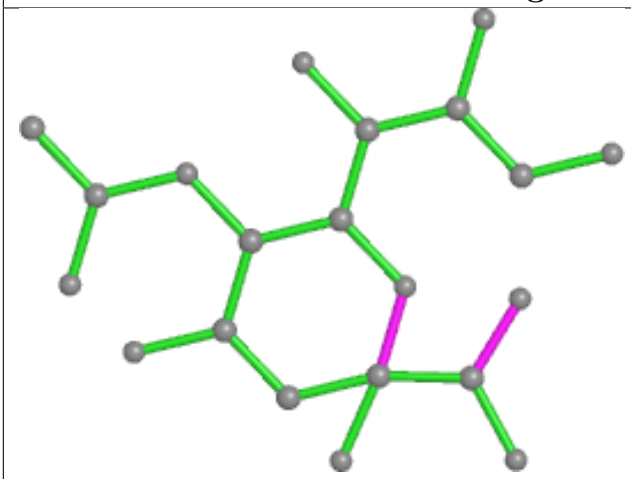


Rings

Ligand SLB G 401



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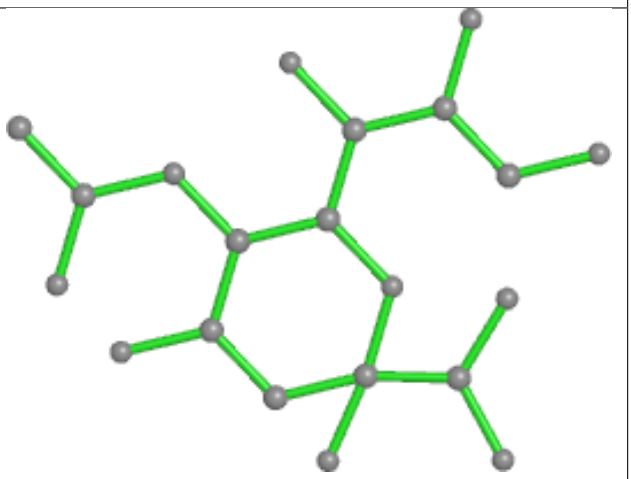

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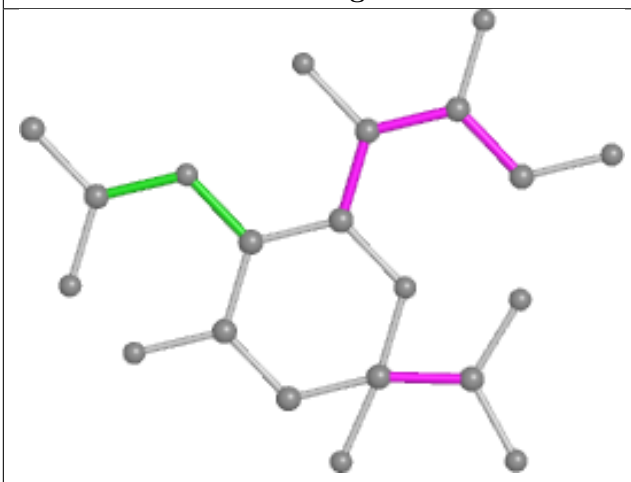

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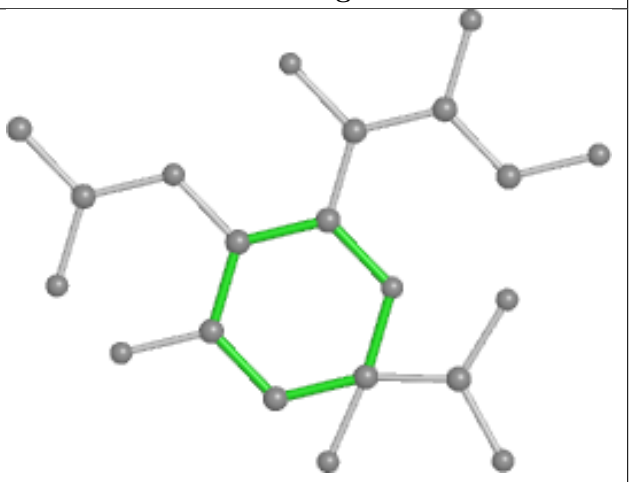
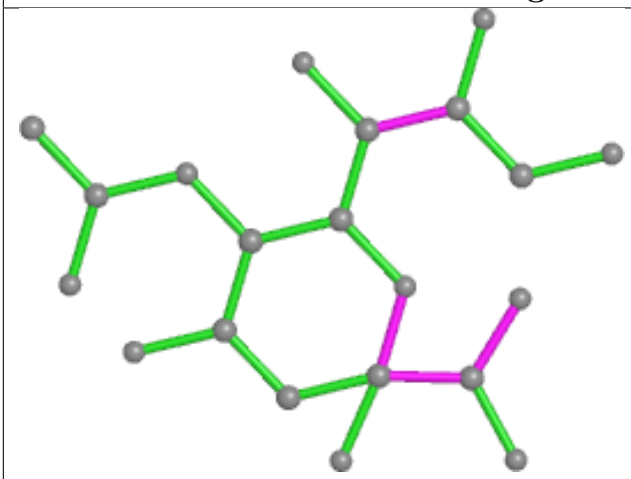


Rings

Ligand SLB U 401



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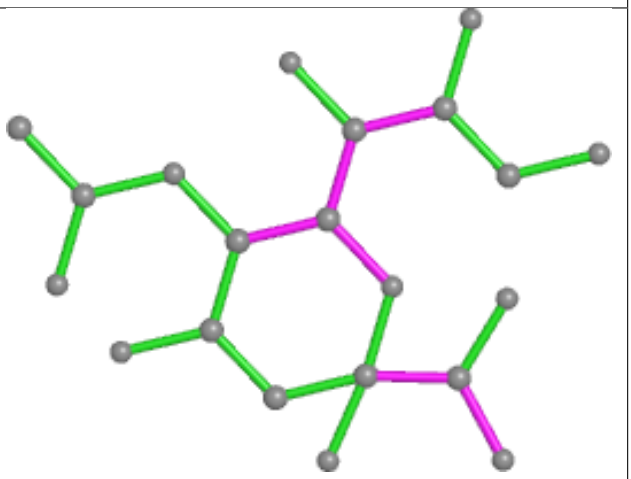

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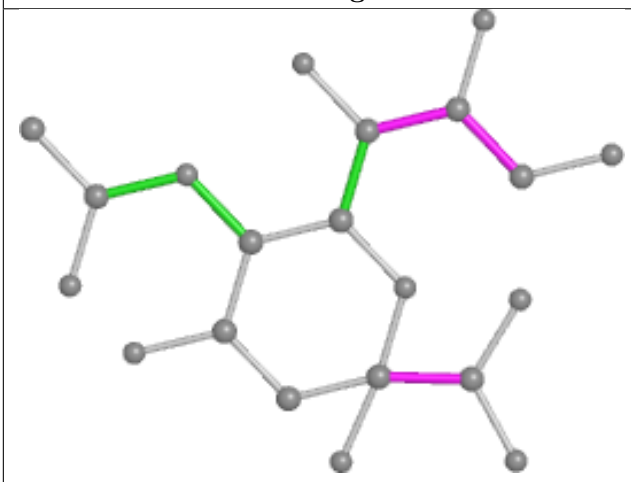

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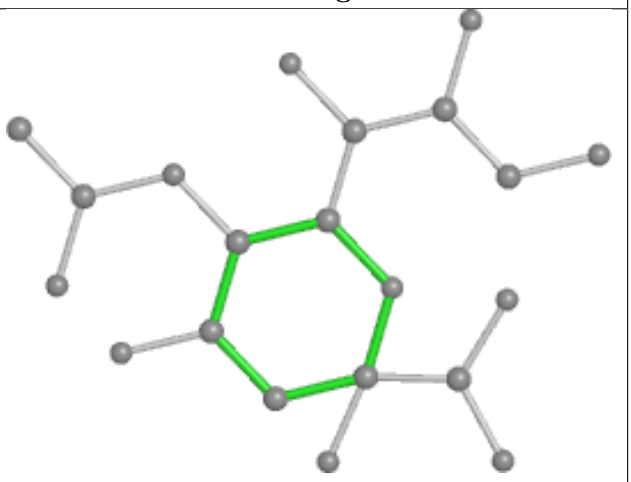
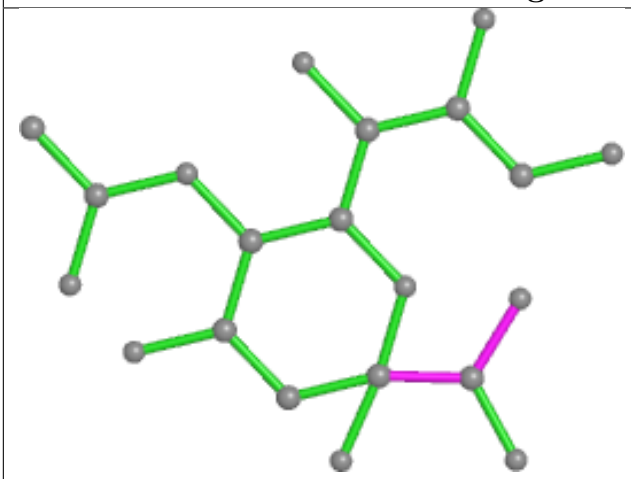


Rings

Ligand SLB A 401



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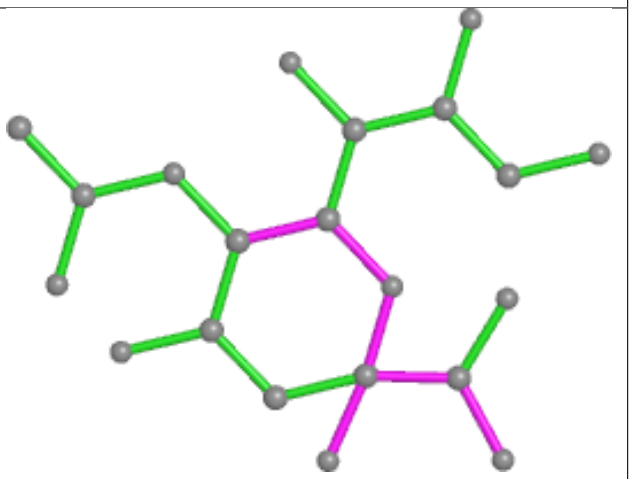

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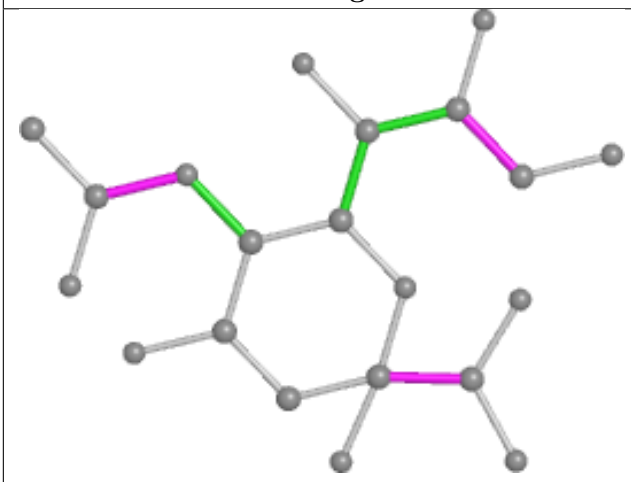

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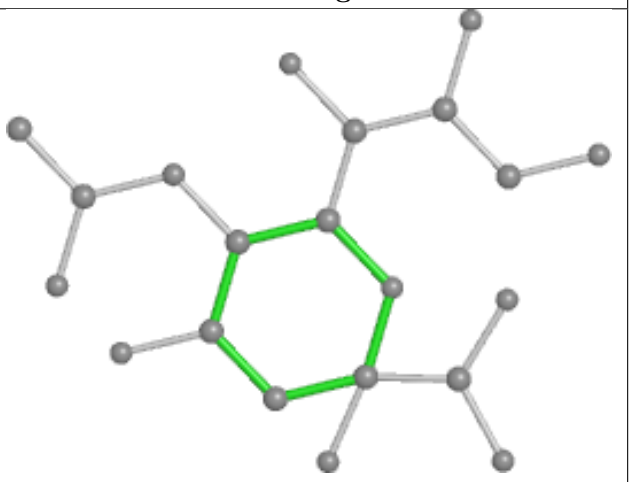
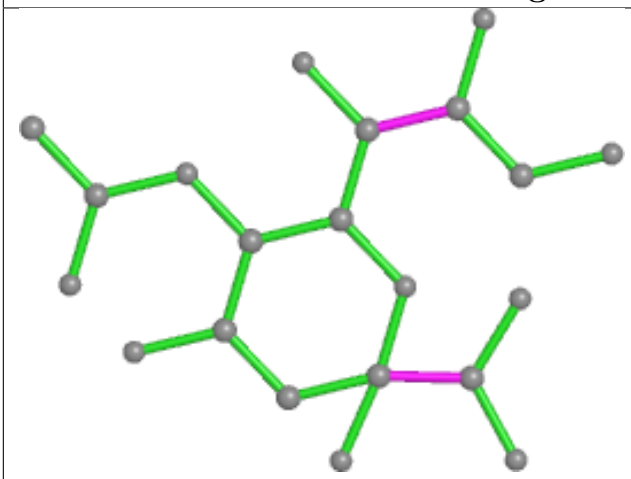
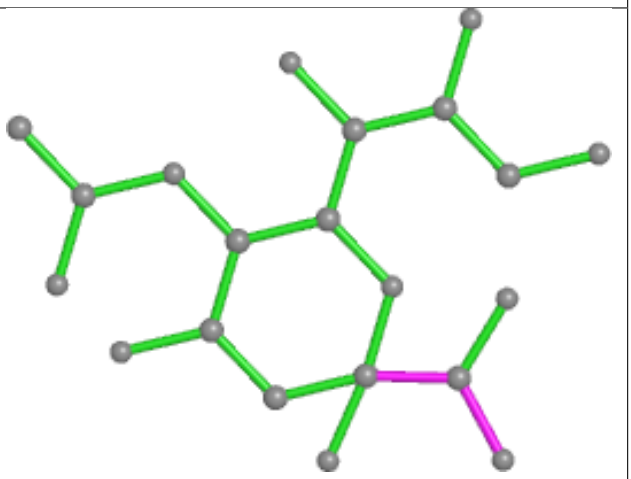


Rings

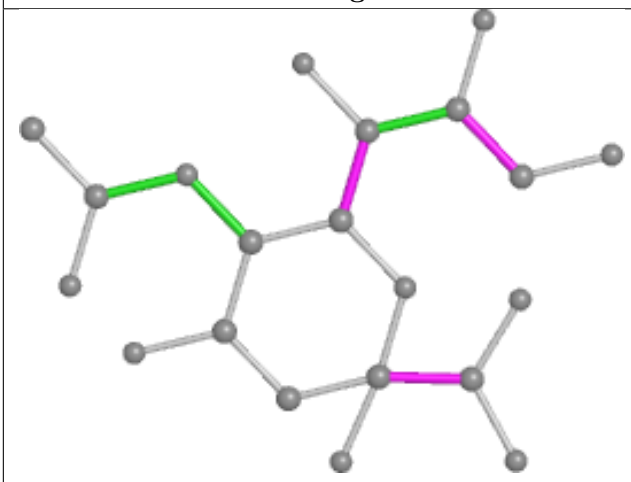
Ligand SLB P 401



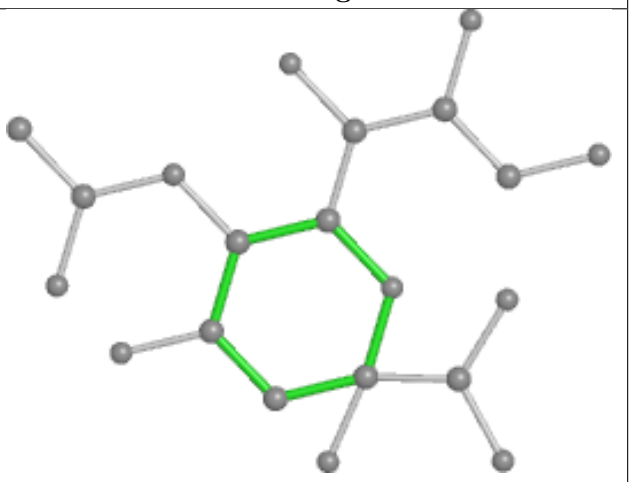
Bond lengths



Bond angles

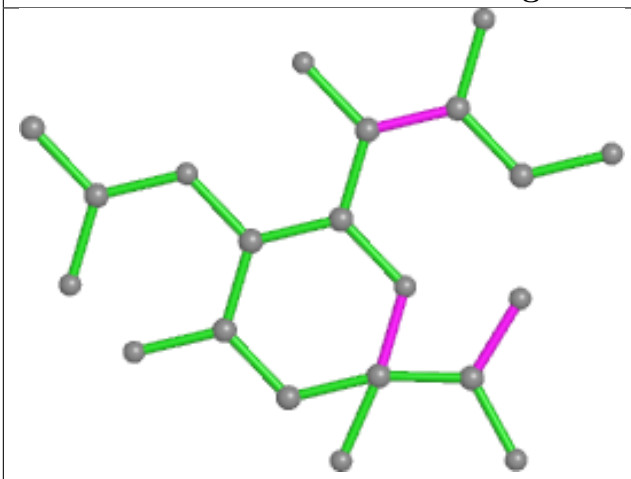


Torsions

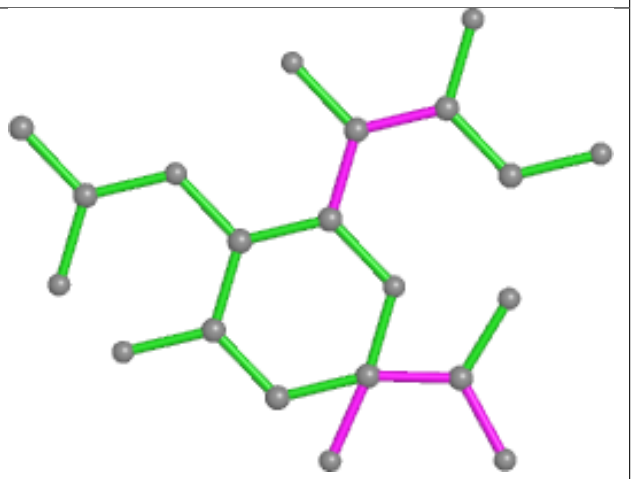


Rings

Ligand SLB W 401



Bond lengths



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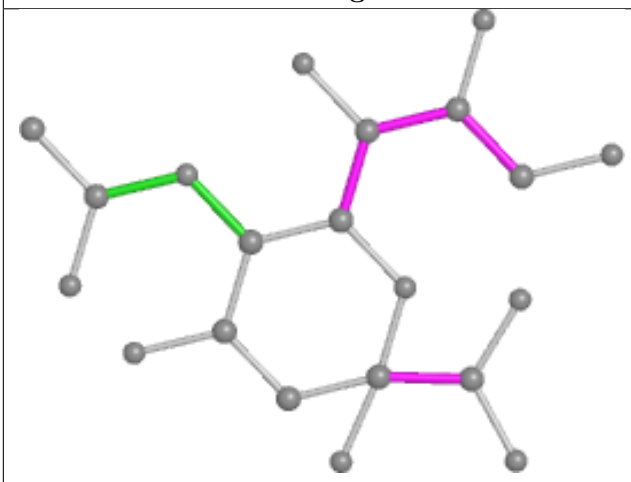

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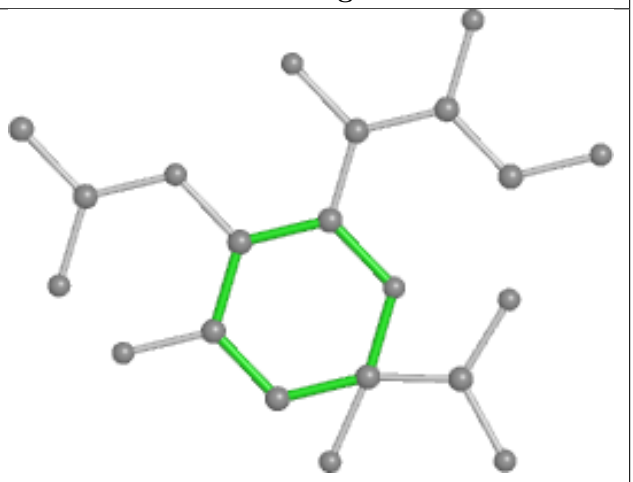
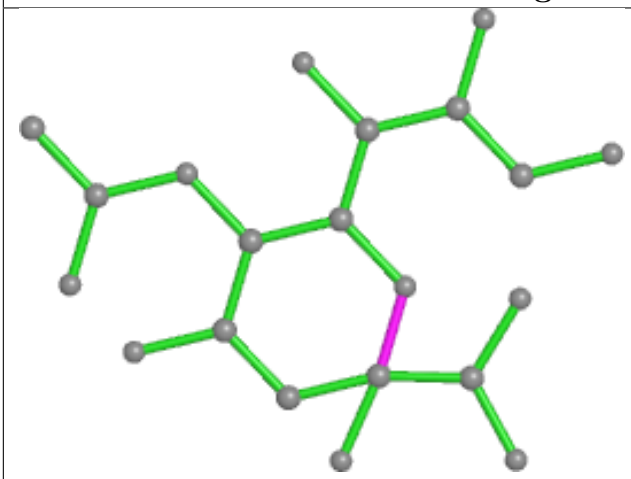


Rings

Ligand SLB I 401



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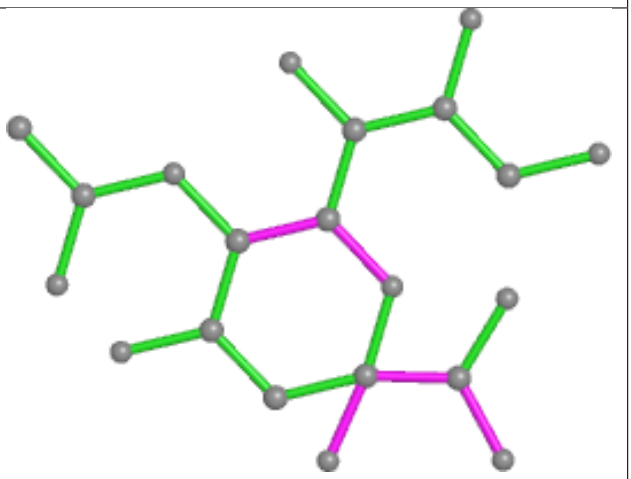
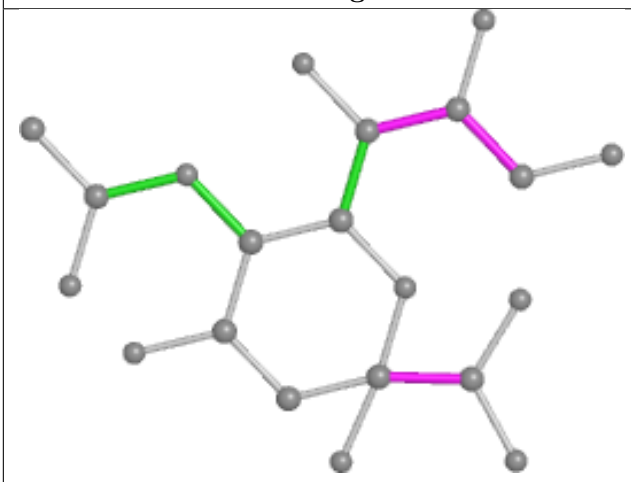
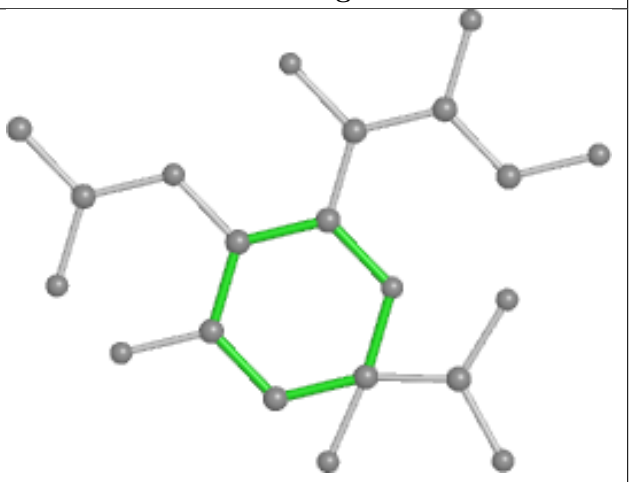


Bond angles

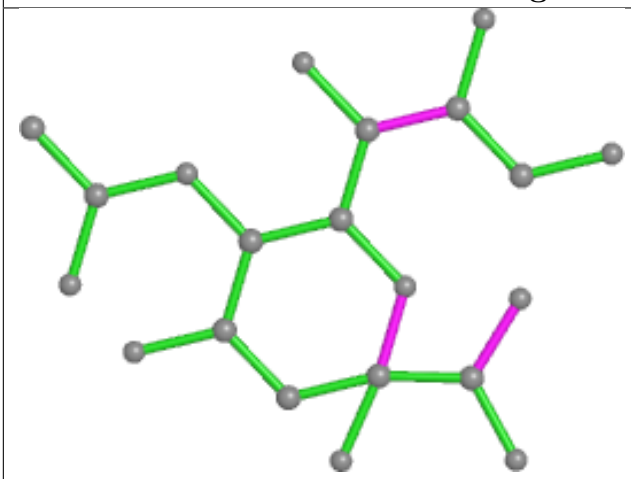


Torsions

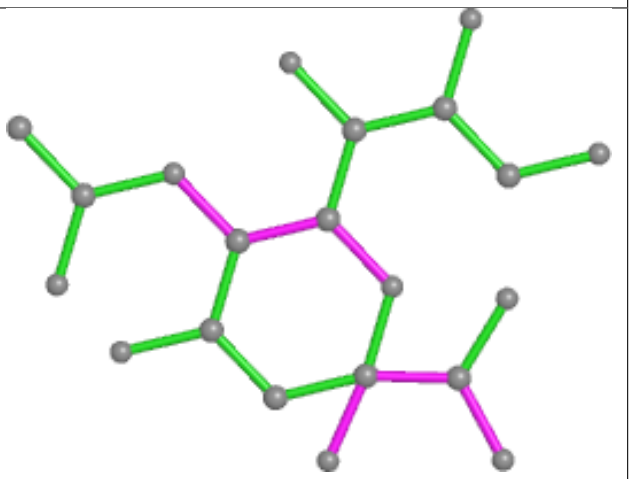


Rings

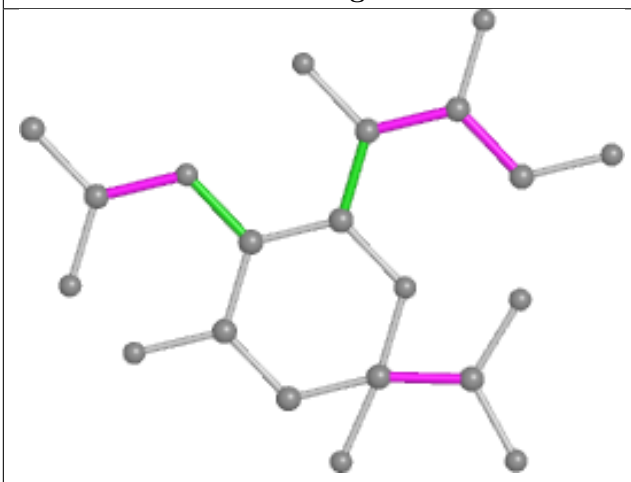
Ligand SLB F 401



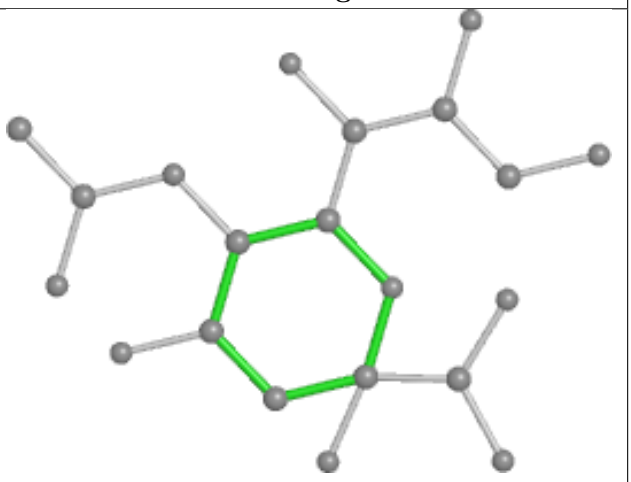
Bond lengths



Bond angles

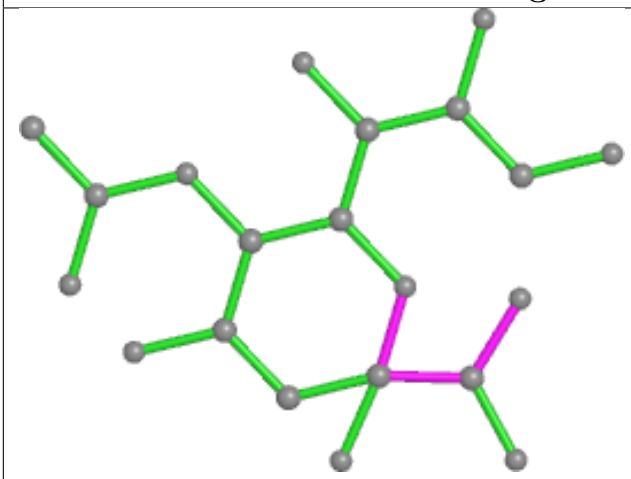


Torsions

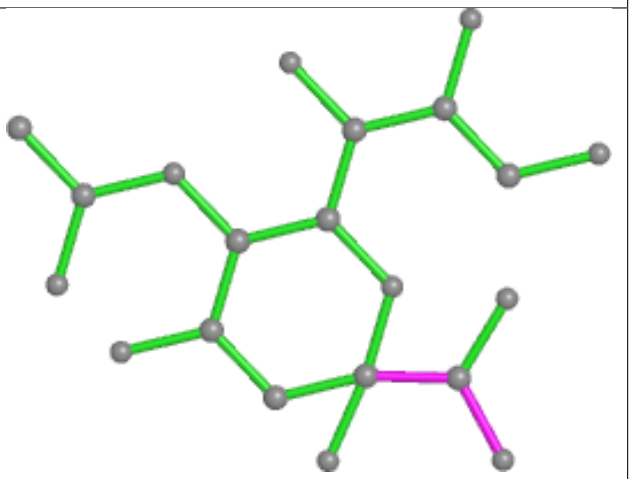


Rings

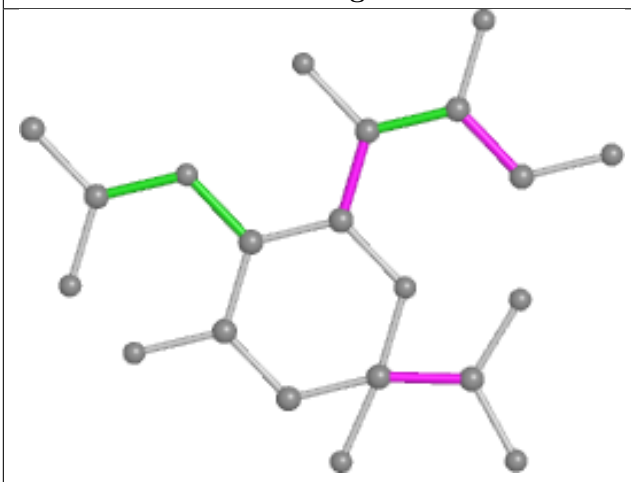
Ligand SLB E 401



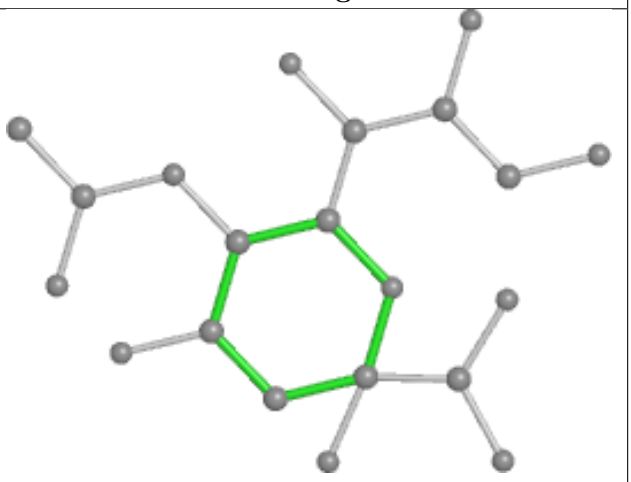
Bond lengths



Bond angles

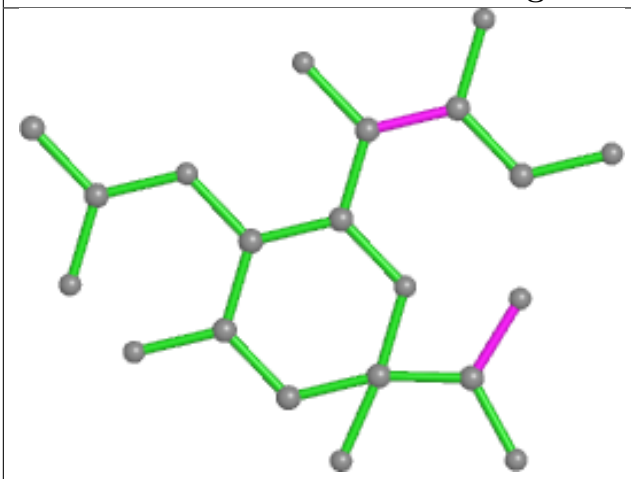


Torsions

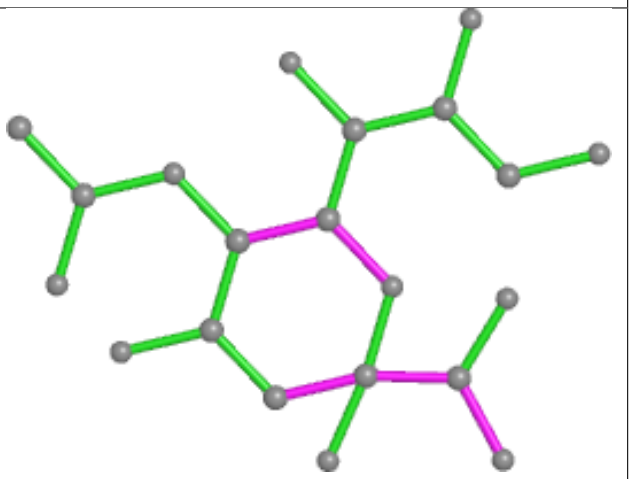


Rings

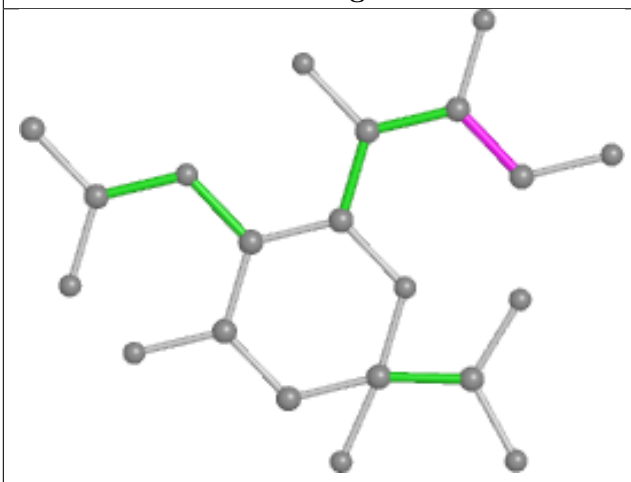
Ligand SLB K 401



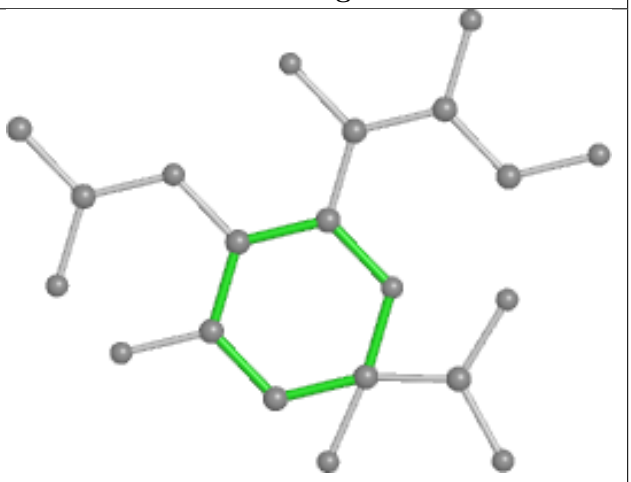
Bond lengths



Bond angles

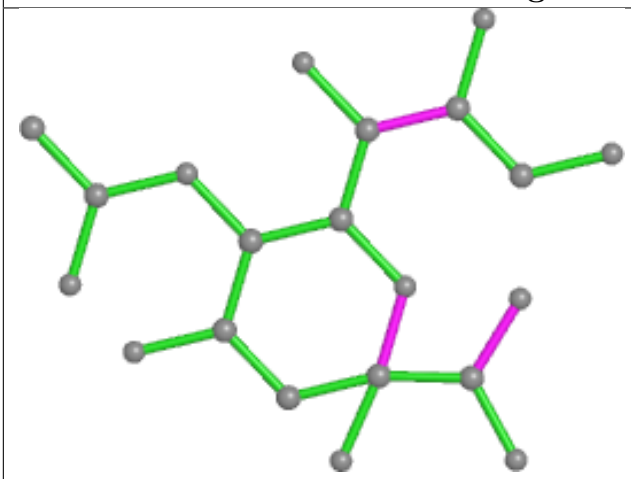


Torsions

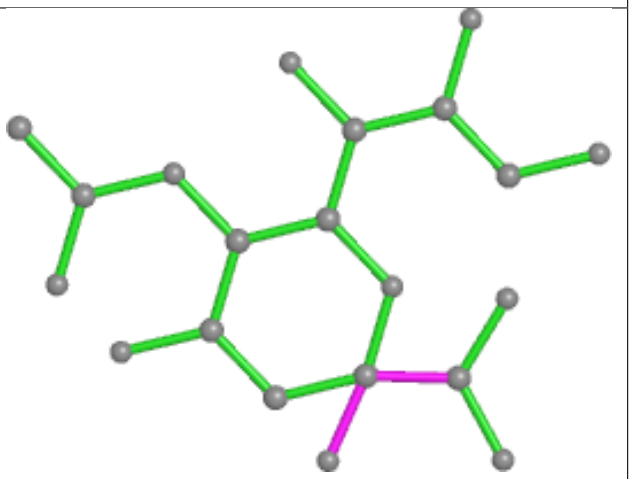


Rings

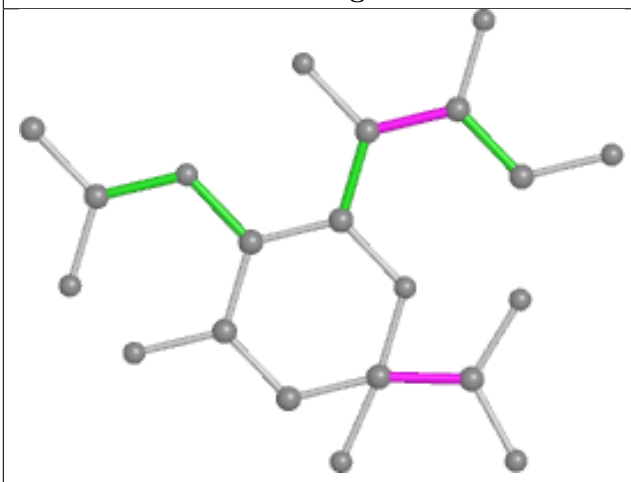
Ligand SLB O 401



Bond lengths



Bond angles



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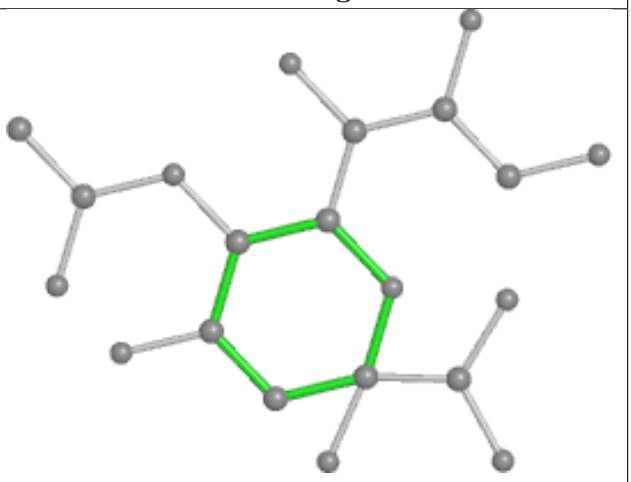
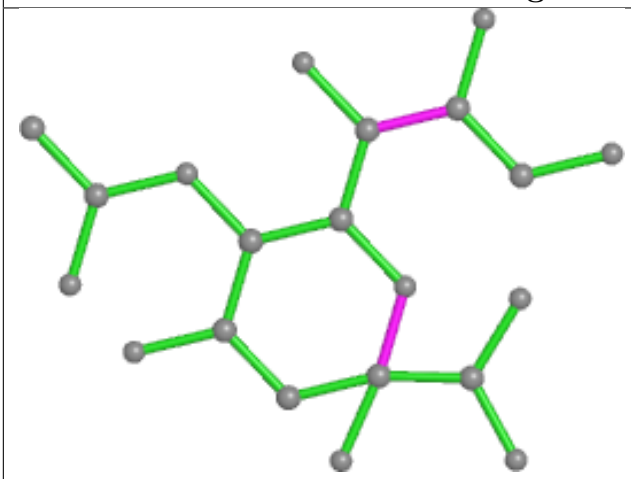
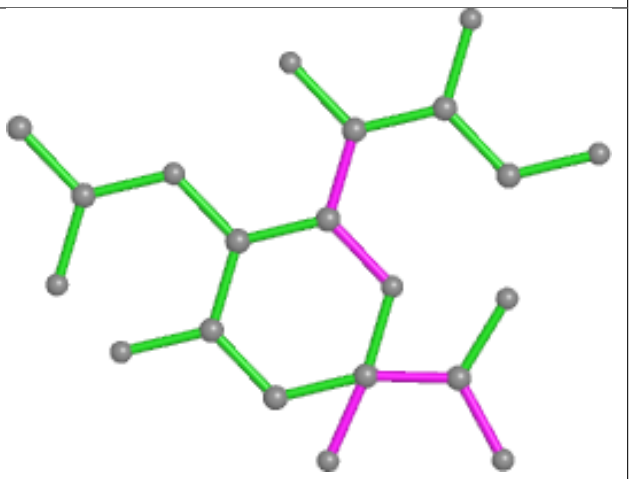


Rings

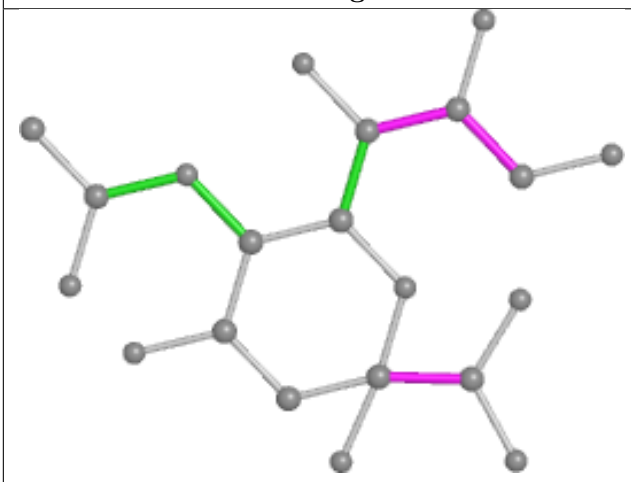
Ligand SLB N 401



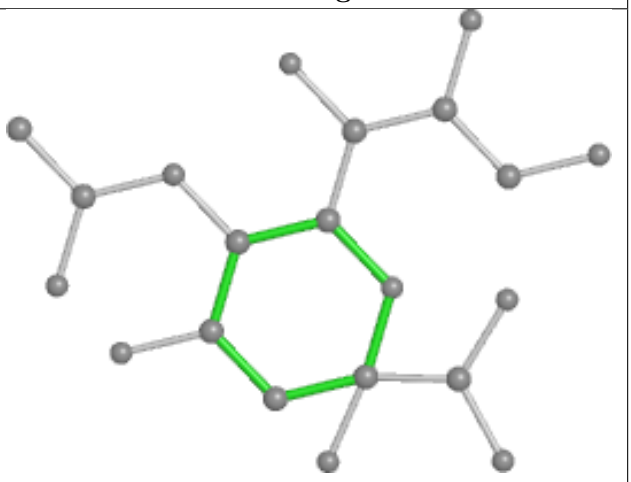
Bond lengths



Bond angles

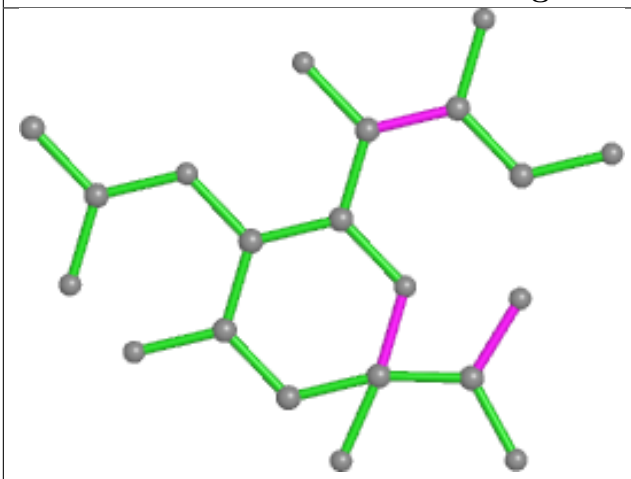


Torsions

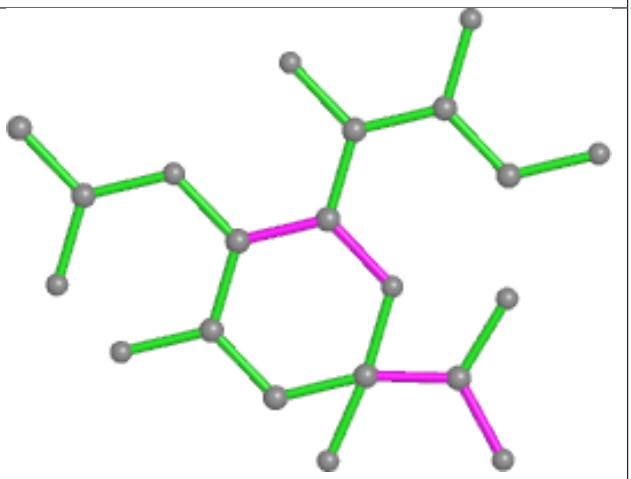


Rings

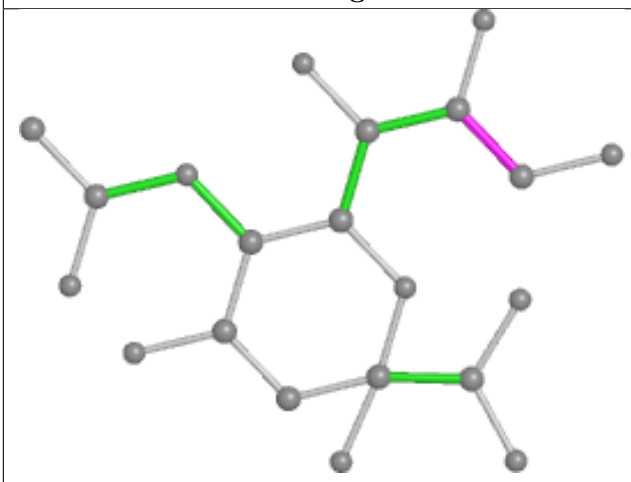
Ligand SLB J 401



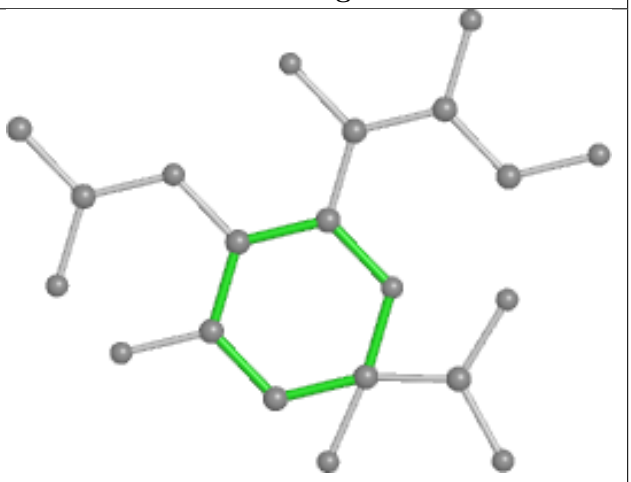
Bond lengths



Bond angles

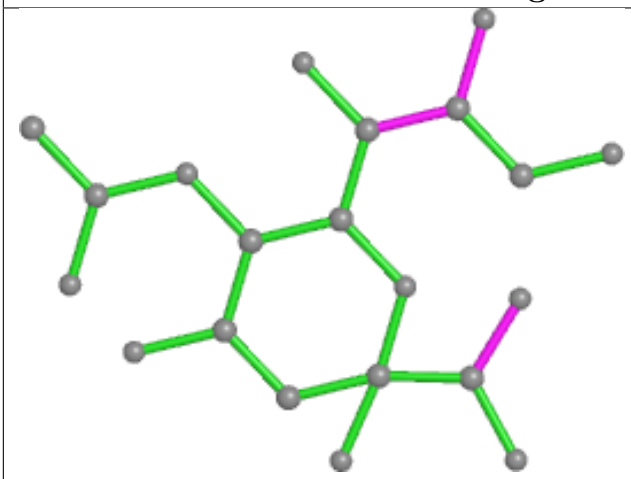


Torsions

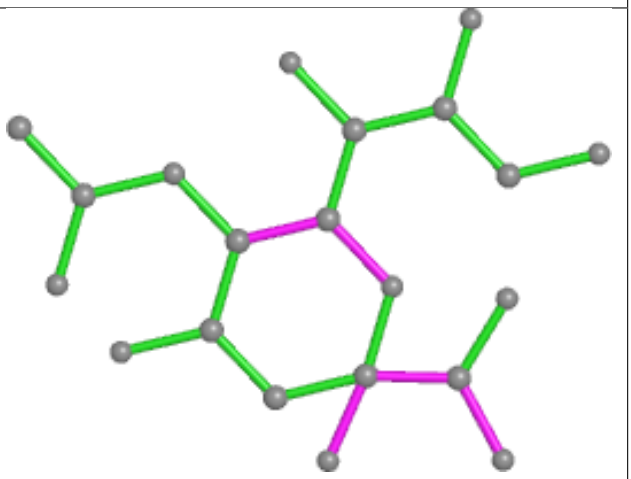


Rings

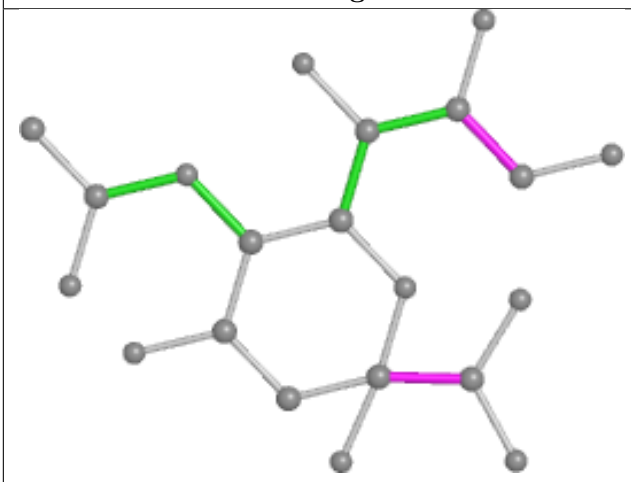
Ligand SLB B 401



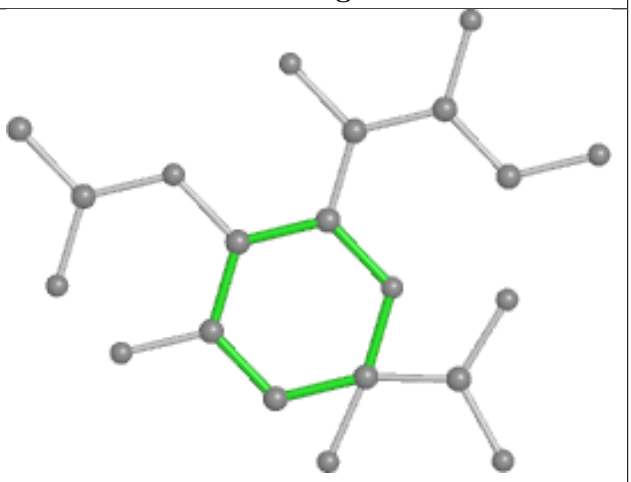
Bond lengths



Bond angles

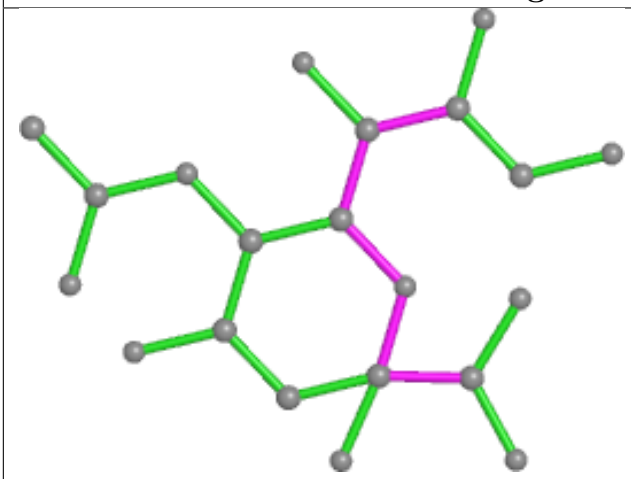


Torsions

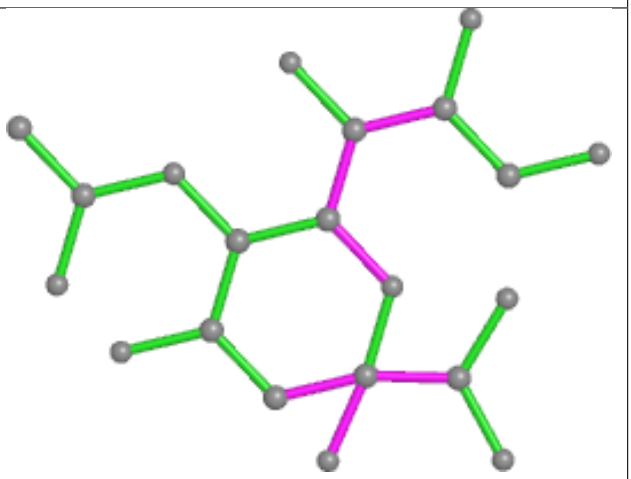


Rings

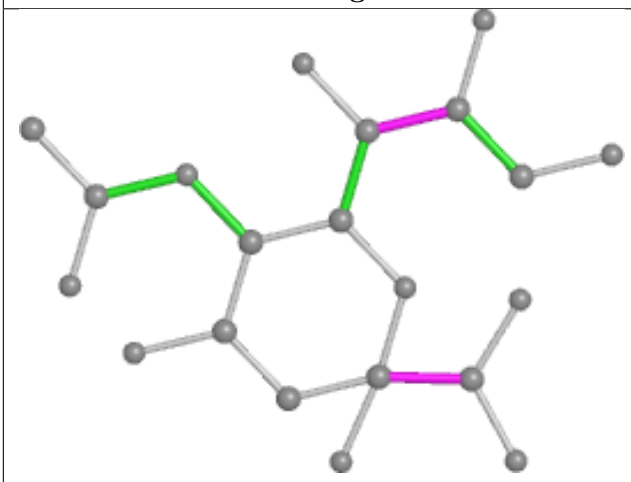
Ligand SLB X 401



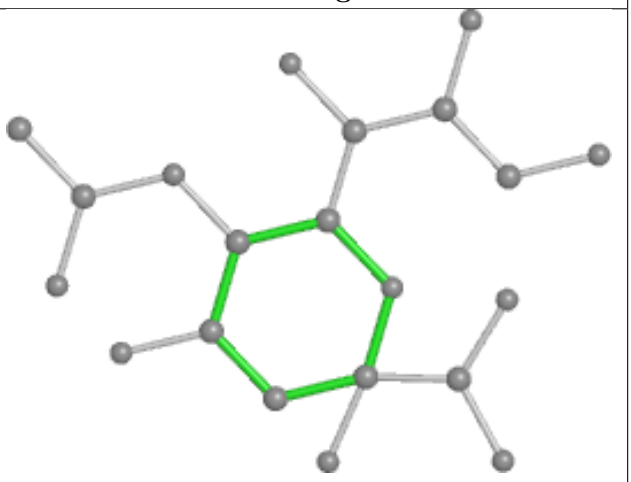
Bond lengths



Bond angles

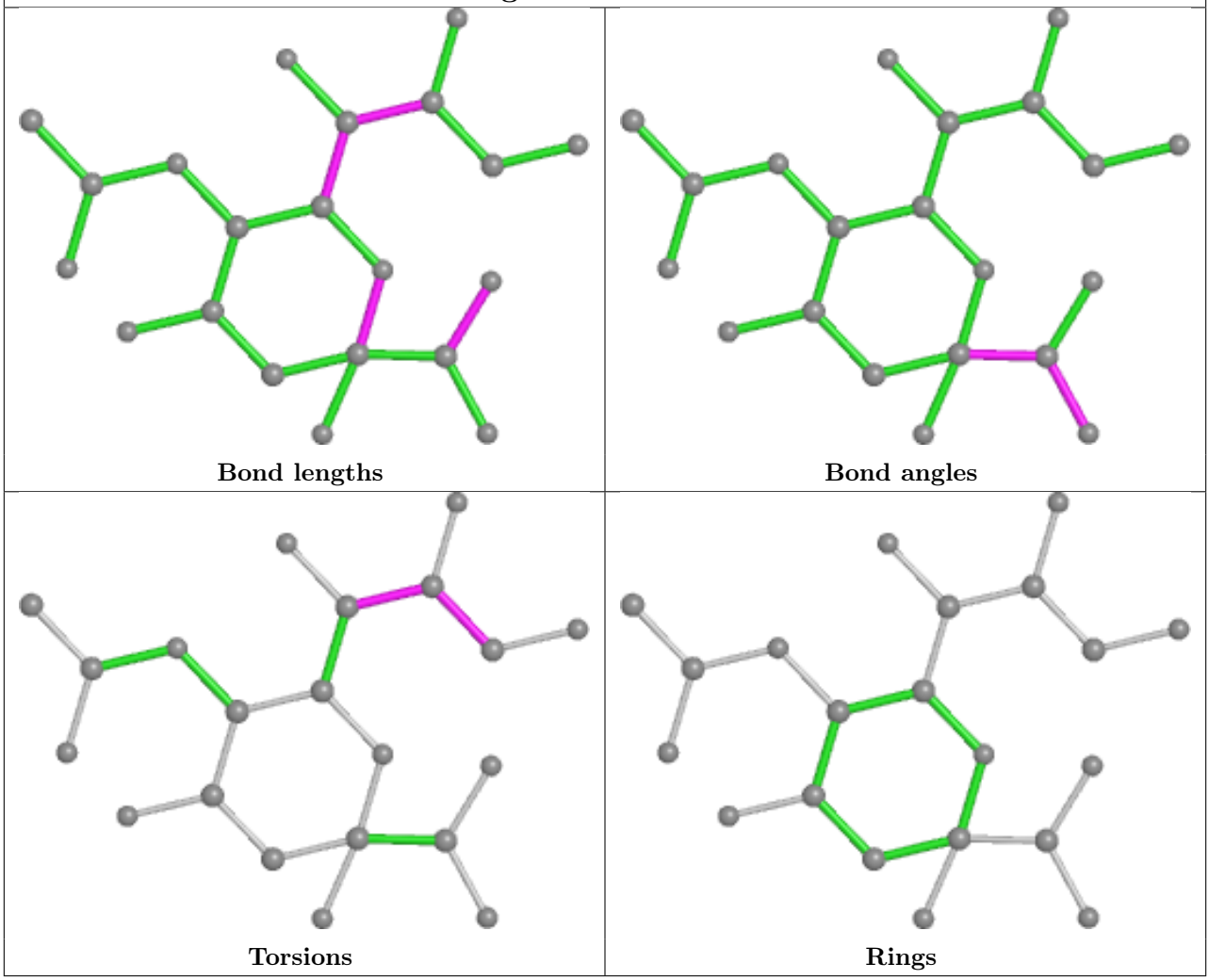


Torsions



Rings

Ligand SLB S 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	180/186 (96%)	0.09	7 (3%)	39	42	30, 45, 98, 158	0
1	B	186/186 (100%)	0.19	13 (6%)	16	16	33, 47, 116, 182	0
1	C	177/186 (95%)	-0.00	4 (2%)	60	63	31, 49, 89, 164	0
1	D	180/186 (96%)	0.22	8 (4%)	34	37	42, 61, 114, 164	0
1	E	179/186 (96%)	0.29	12 (6%)	17	18	48, 67, 116, 149	0
1	F	176/186 (94%)	0.33	8 (4%)	33	36	42, 67, 109, 178	0
1	G	177/186 (95%)	0.24	11 (6%)	20	21	41, 58, 105, 173	0
1	H	181/186 (97%)	0.11	5 (2%)	53	56	41, 62, 114, 167	0
1	I	179/186 (96%)	0.18	5 (2%)	53	56	33, 47, 107, 159	0
1	J	178/186 (95%)	0.11	5 (2%)	53	56	36, 57, 108, 140	0
1	K	177/186 (95%)	0.20	7 (3%)	38	41	36, 63, 108, 168	0
1	L	179/186 (96%)	0.33	11 (6%)	21	22	35, 54, 111, 139	0
1	M	176/186 (94%)	0.47	15 (8%)	10	10	43, 63, 104, 167	0
1	N	178/186 (95%)	0.18	8 (4%)	33	36	38, 63, 109, 169	0
1	O	178/186 (95%)	0.39	12 (6%)	17	18	37, 57, 112, 151	0
1	P	177/186 (95%)	0.16	8 (4%)	33	36	41, 56, 103, 169	0
1	Q	179/186 (96%)	0.20	6 (3%)	45	48	42, 65, 121, 176	0
1	R	180/186 (96%)	0.21	9 (5%)	28	30	39, 58, 117, 159	0
1	S	186/186 (100%)	0.33	8 (4%)	35	38	31, 46, 105, 126	0
1	T	175/186 (94%)	0.15	5 (2%)	51	55	33, 54, 96, 177	0
1	U	178/186 (95%)	0.03	4 (2%)	62	65	36, 60, 109, 188	0
1	V	186/186 (100%)	0.38	13 (6%)	16	16	37, 53, 118, 147	0
1	W	178/186 (95%)	0.19	9 (5%)	28	29	41, 59, 117, 174	0
1	X	182/186 (97%)	0.25	8 (4%)	34	37	35, 59, 127, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	4302/4464 (96%)	0.22	201 (4%)	31	33	30, 57, 112, 206	0

The worst 5 of 201 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	186	LYS	10.7
1	W	302	THR	10.4
1	X	303	THR	10.1
1	V	280	LEU	9.3
1	T	302	THR	9.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SLB	M	401	21/21	0.76	0.32	80,93,108,109	0
2	SLB	D	401	21/21	0.77	0.29	74,90,98,101	0
2	SLB	H	401	21/21	0.78	0.24	70,88,101,108	0
2	SLB	R	401	21/21	0.78	0.42	84,100,104,106	0
2	SLB	C	401	21/21	0.81	0.26	77,82,92,95	0
2	SLB	F	401	21/21	0.82	0.30	83,95,97,100	0
2	SLB	E	401	21/21	0.82	0.25	79,84,91,96	0
2	SLB	O	401	21/21	0.83	0.32	72,88,94,96	0
2	SLB	B	401	21/21	0.83	0.24	69,81,87,90	0
2	SLB	W	401	21/21	0.84	0.33	69,78,83,83	0
2	SLB	A	401	21/21	0.85	0.22	74,88,96,104	0
2	SLB	G	401	21/21	0.85	0.35	81,92,101,103	0
2	SLB	N	401	21/21	0.85	0.23	72,84,96,103	0

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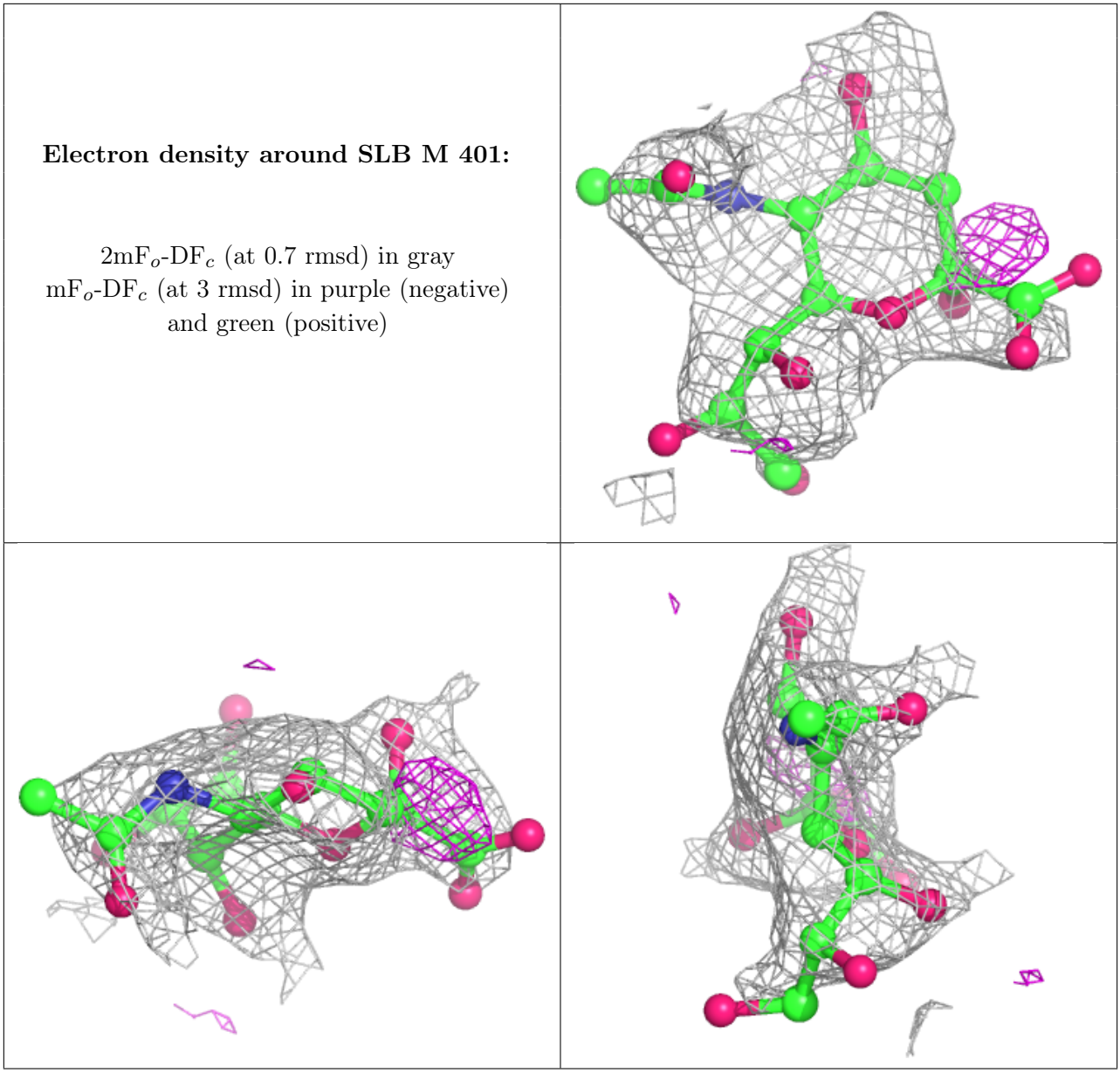
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SLB	U	401	21/21	0.86	0.27	74,80,84,88	0
2	SLB	P	401	21/21	0.86	0.32	74,88,99,104	0
2	SLB	T	401	21/21	0.87	0.28	71,81,86,87	0
2	SLB	J	401	21/21	0.87	0.23	69,79,84,88	0
2	SLB	I	401	21/21	0.87	0.18	73,81,88,90	0
2	SLB	Q	401	21/21	0.88	0.19	67,77,83,86	0
2	SLB	L	401	21/21	0.88	0.19	62,75,81,86	0
2	SLB	V	401	21/21	0.88	0.21	69,77,82,87	0
2	SLB	S	401	21/21	0.88	0.16	55,65,73,77	0
2	SLB	X	401	21/21	0.88	0.34	68,75,86,91	0
2	SLB	K	401	21/21	0.89	0.21	70,77,81,84	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.

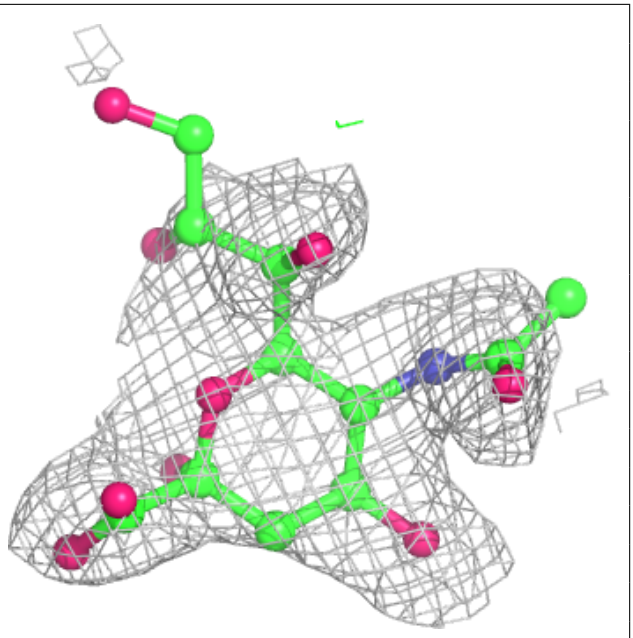
Electron density around SLB M 401:

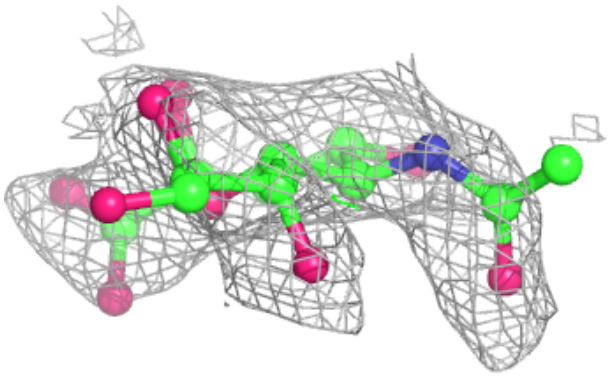
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

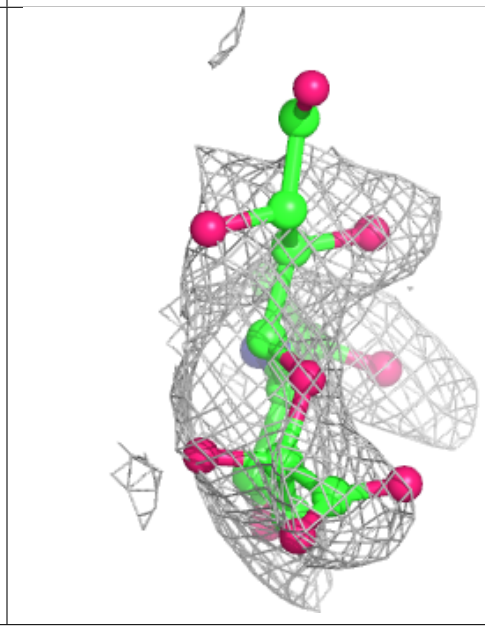


Electron density around SLB D 401:

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

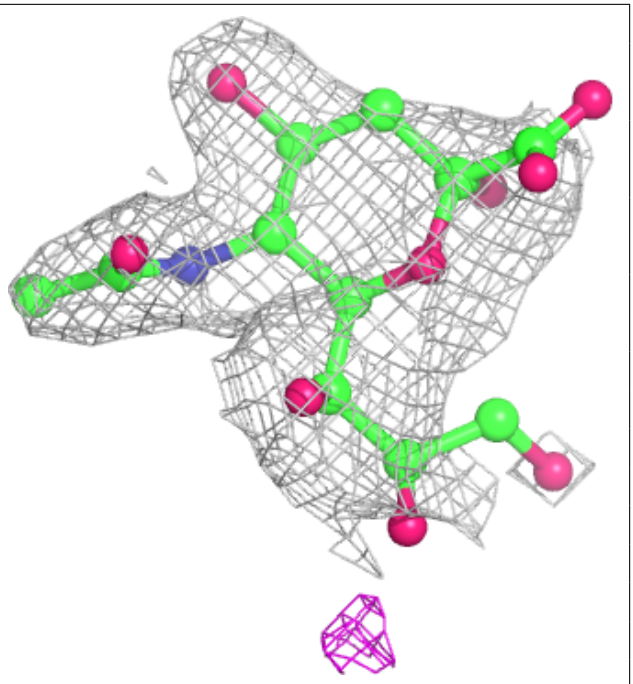


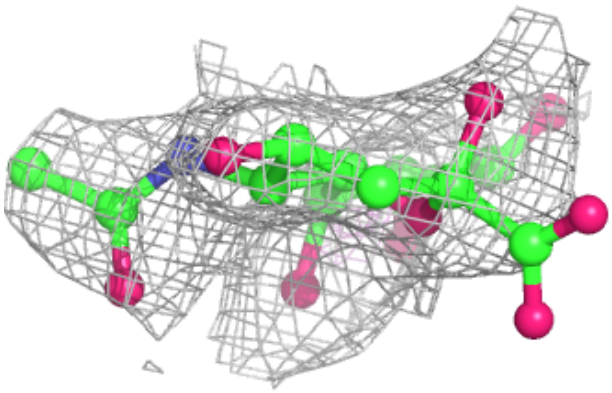


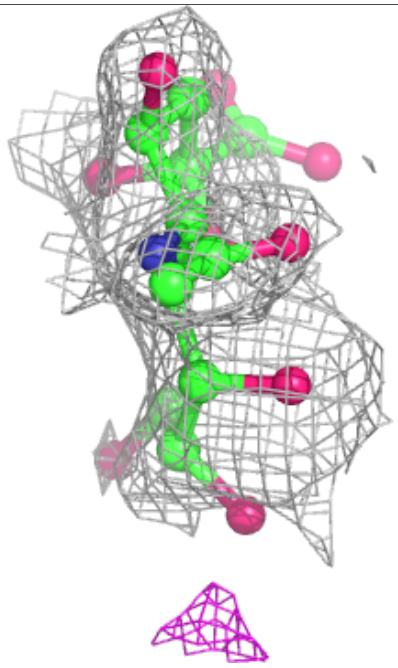


Electron density around SLB H 401:

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

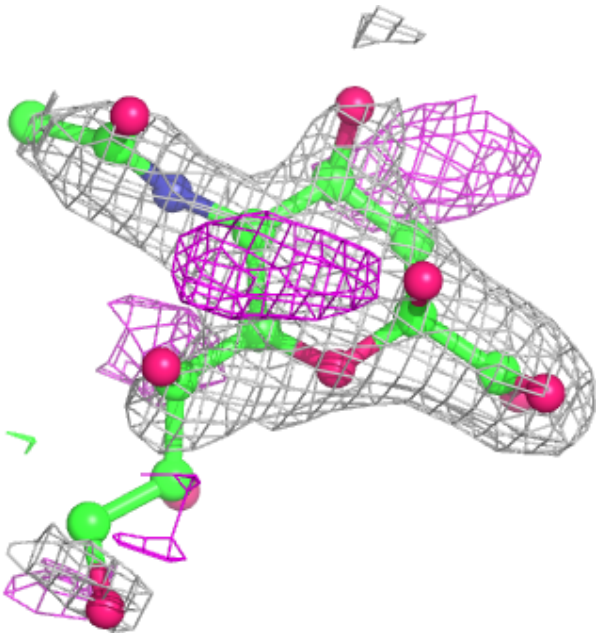


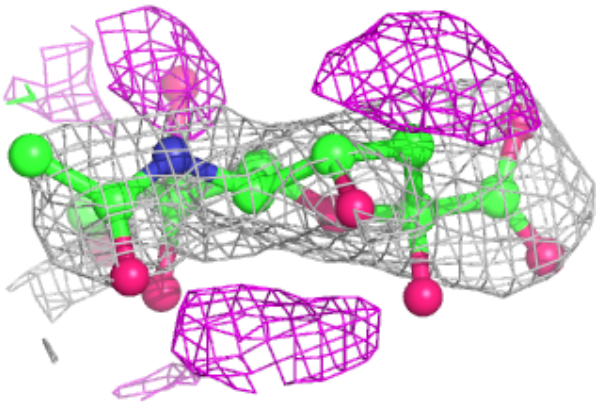


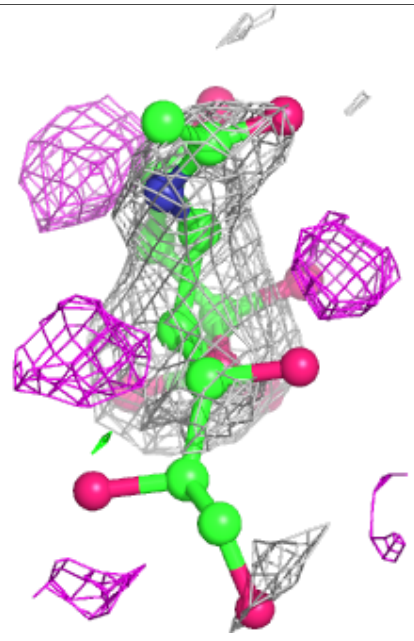


Electron density around SLB R 401:

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

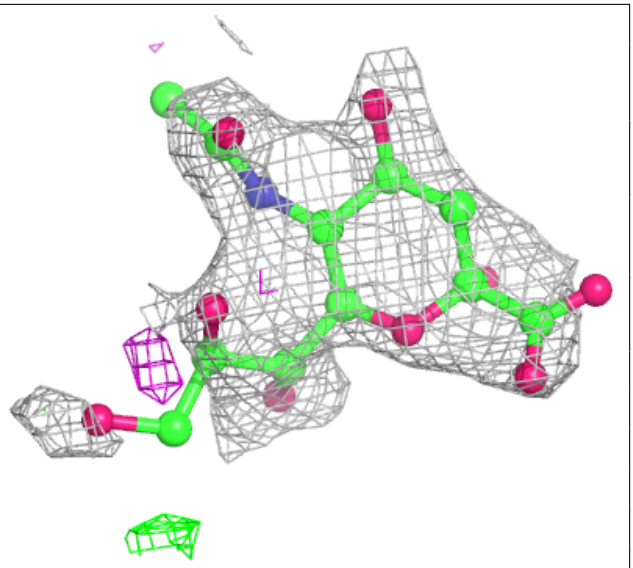


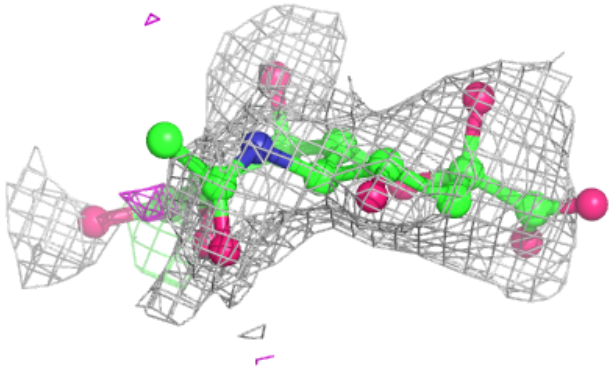


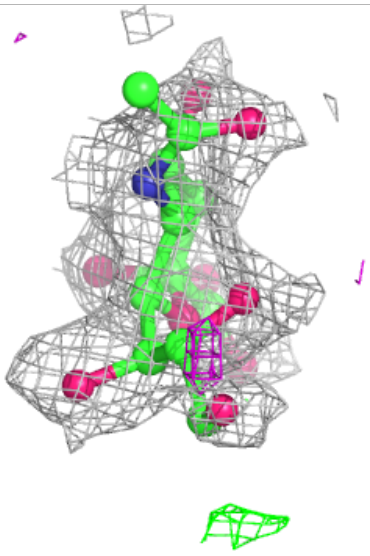


Electron density around SLB C 401:

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

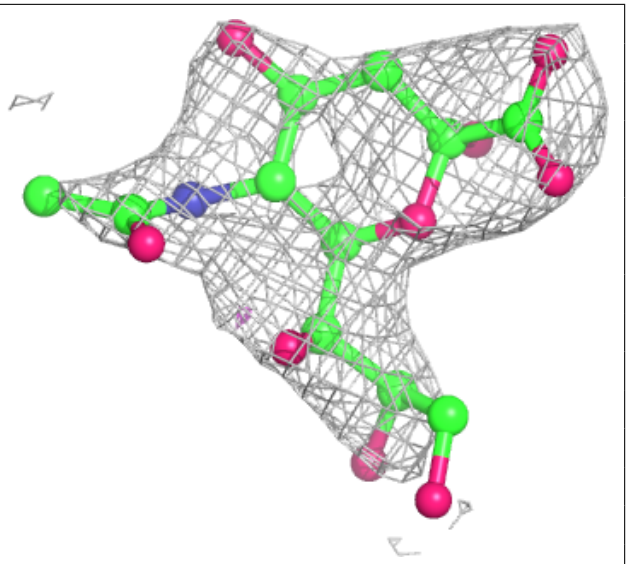


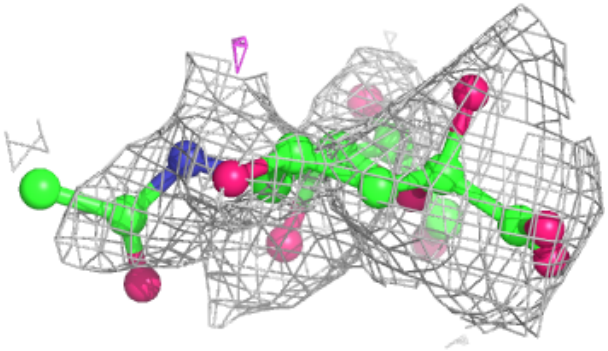


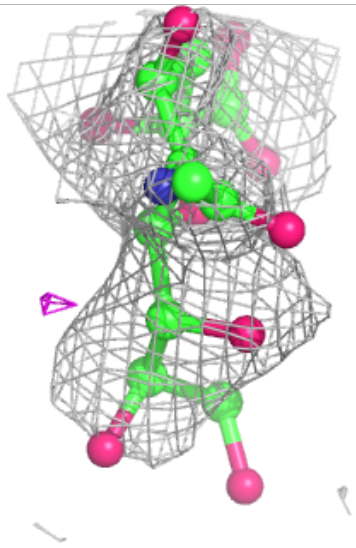


Electron density around SLB F 401:

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

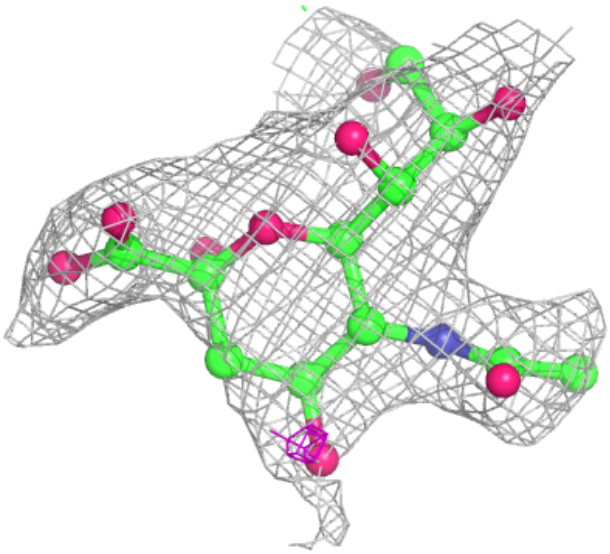


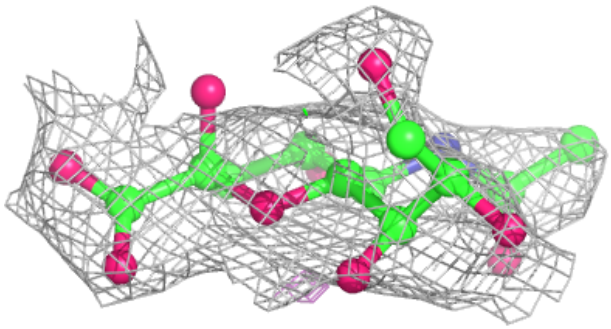


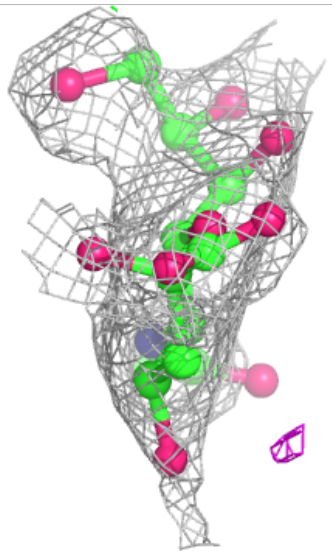


Electron density around SLB E 401:

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

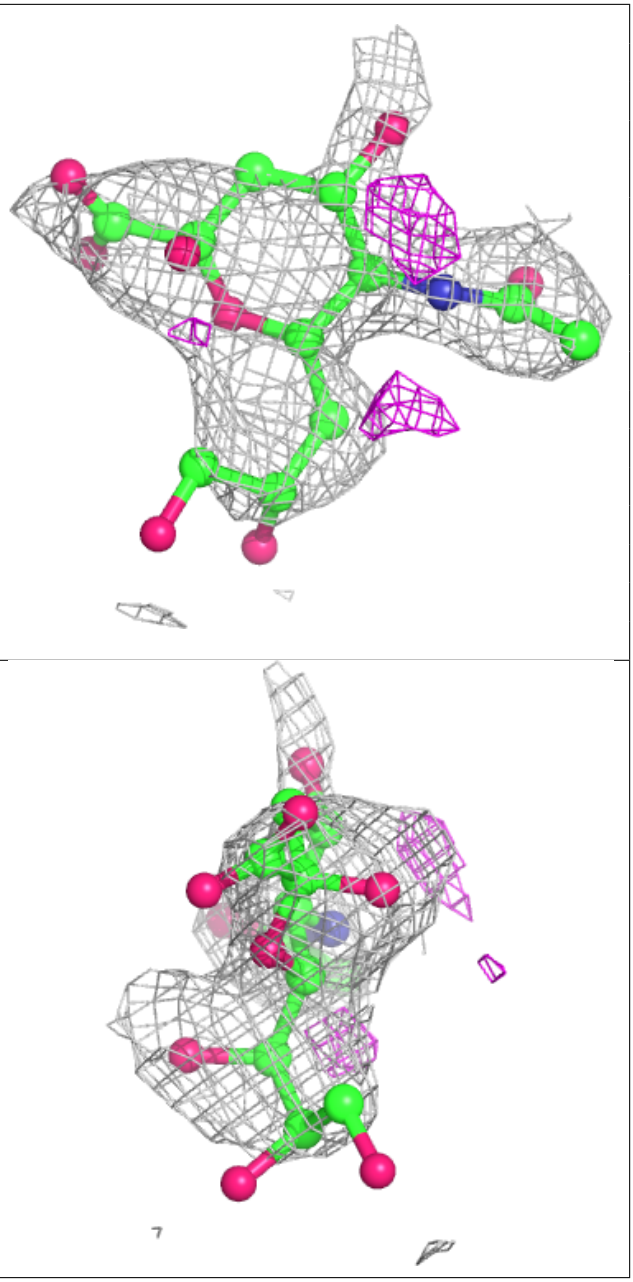






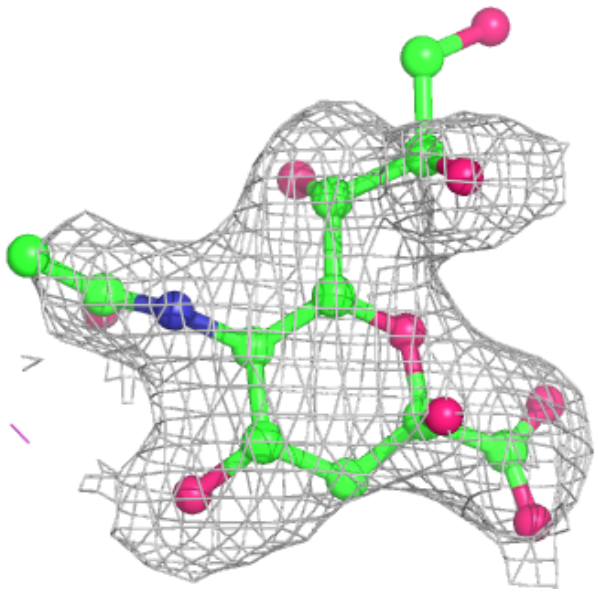
Electron density around SLB O 401:

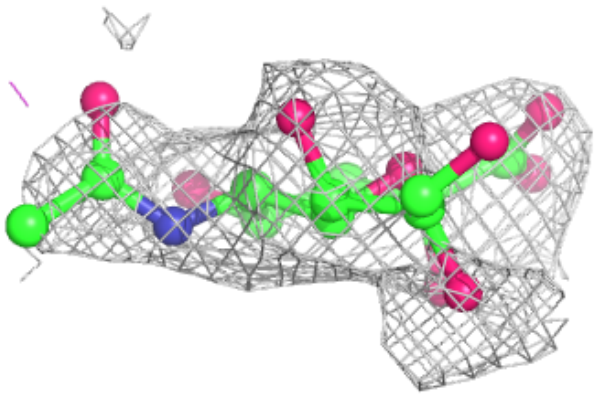
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

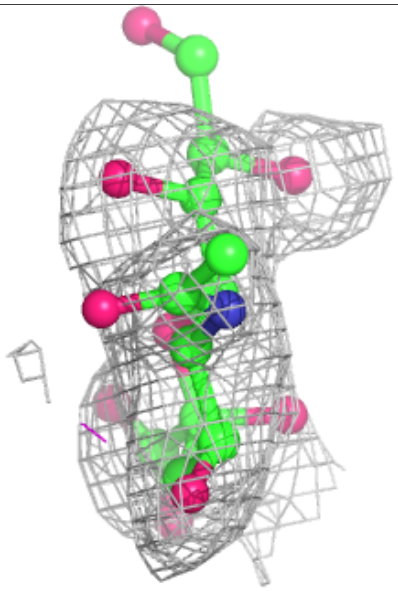


Electron density around SLB B 401:

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

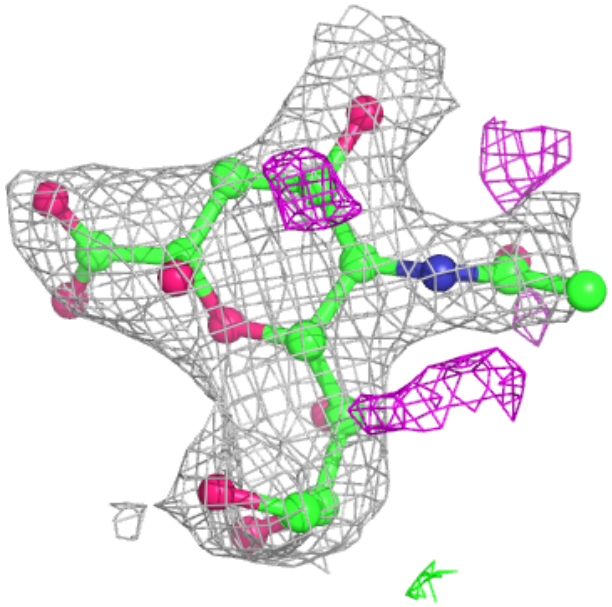


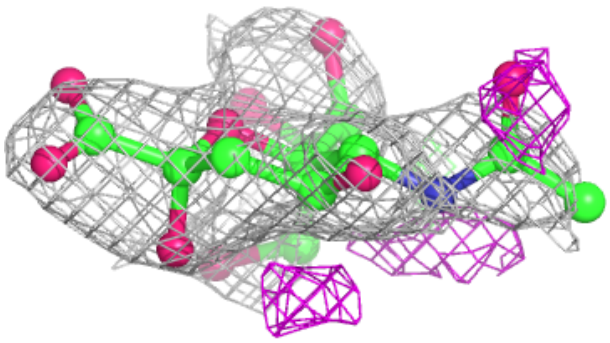


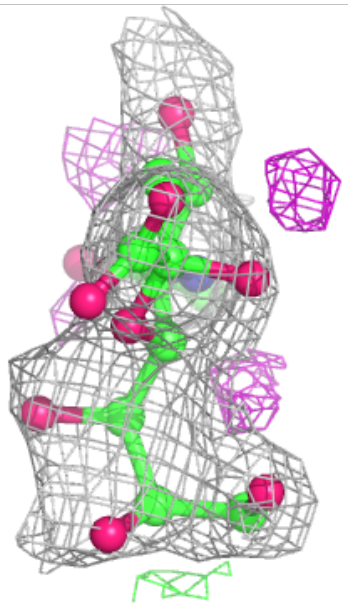


Electron density around SLB W 401:

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

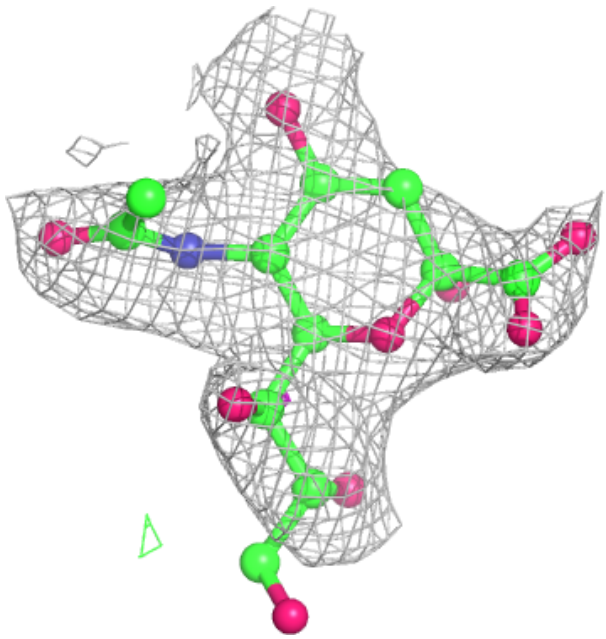


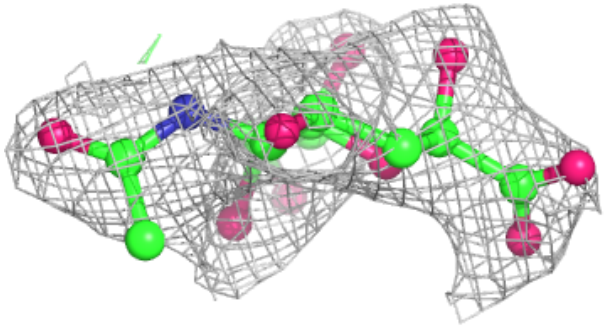


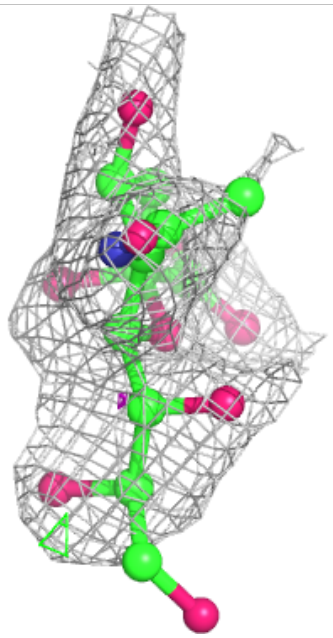


Electron density around SLB A 401:

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

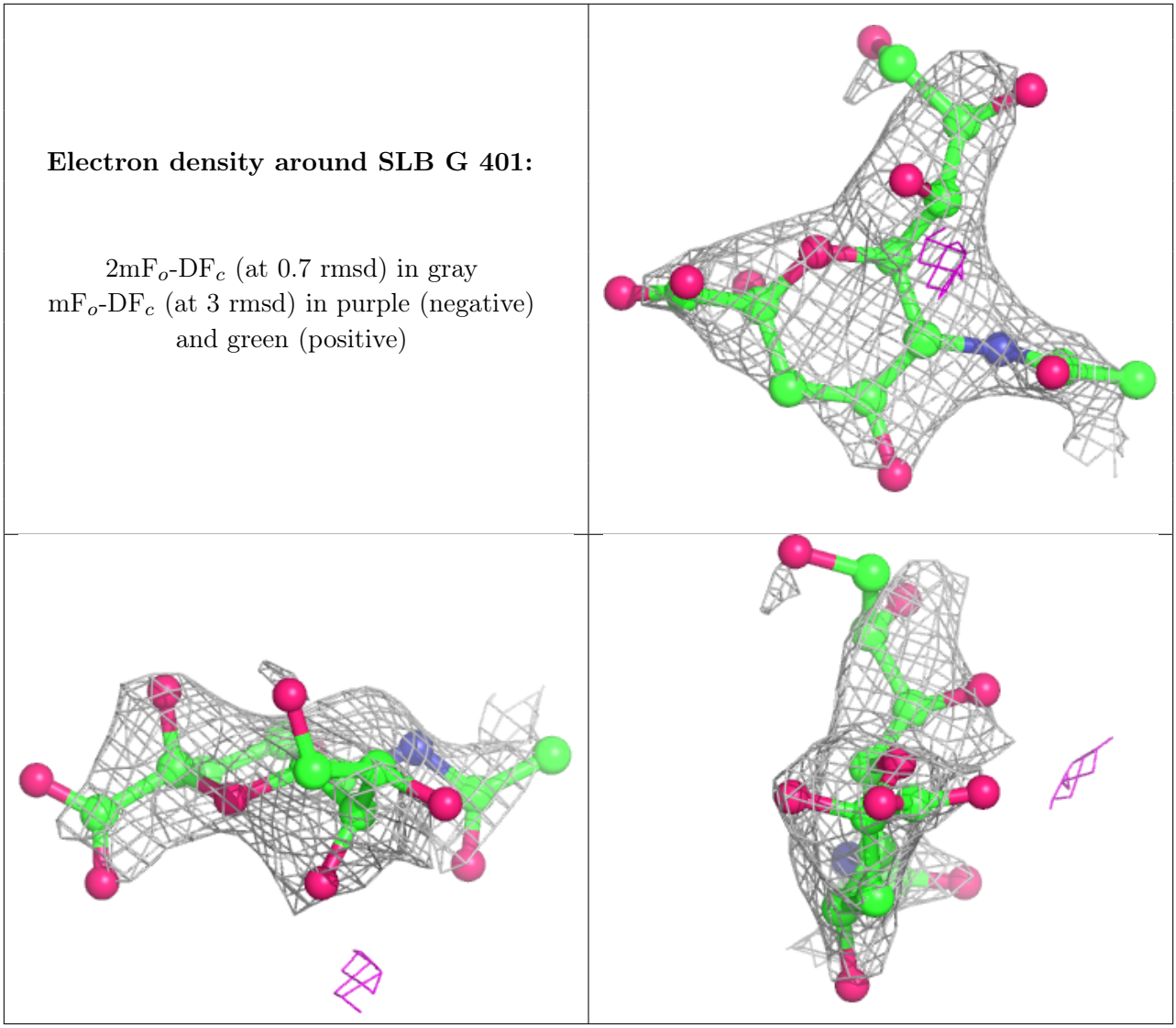






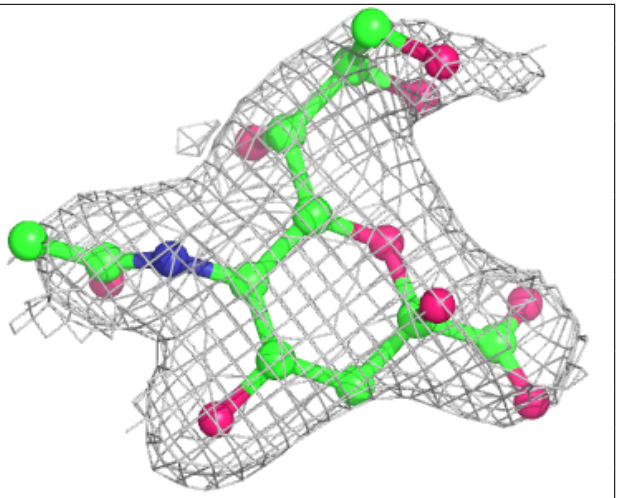
Electron density around SLB G 401:

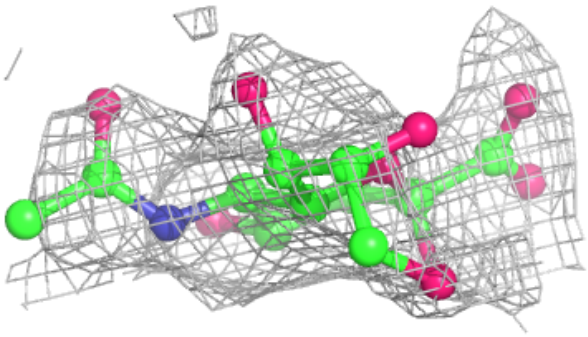
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

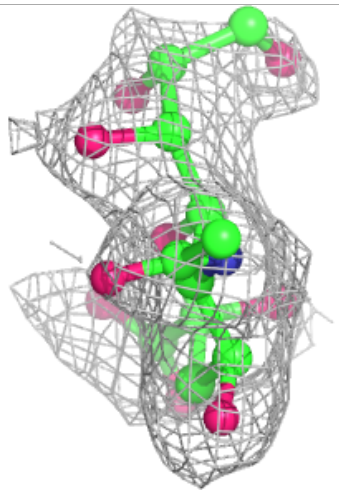


Electron density around SLB N 401:

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

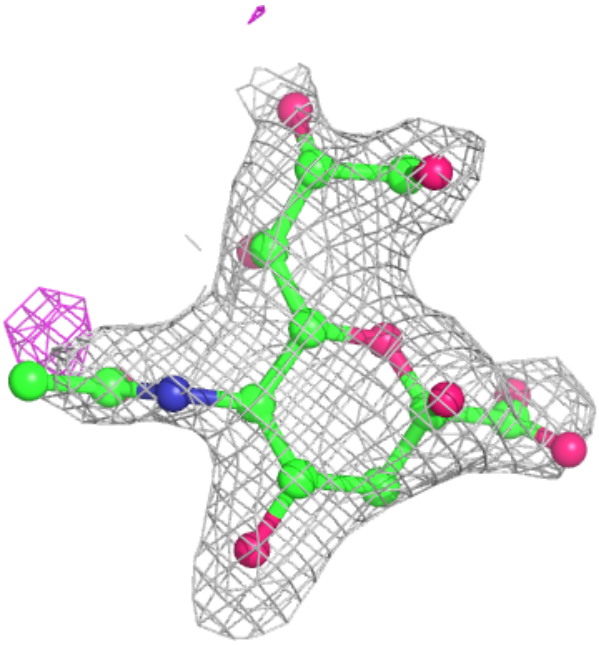


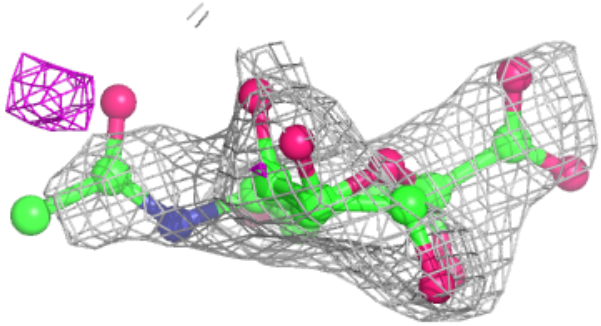


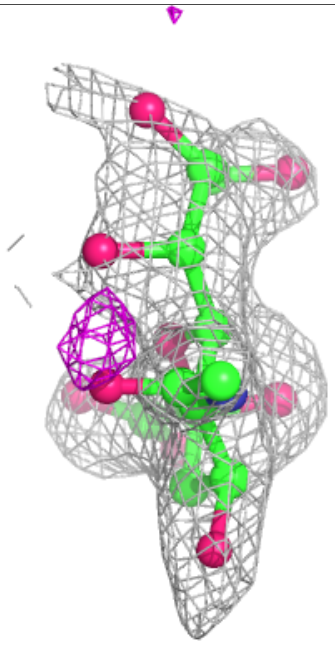


Electron density around SLB U 401:

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

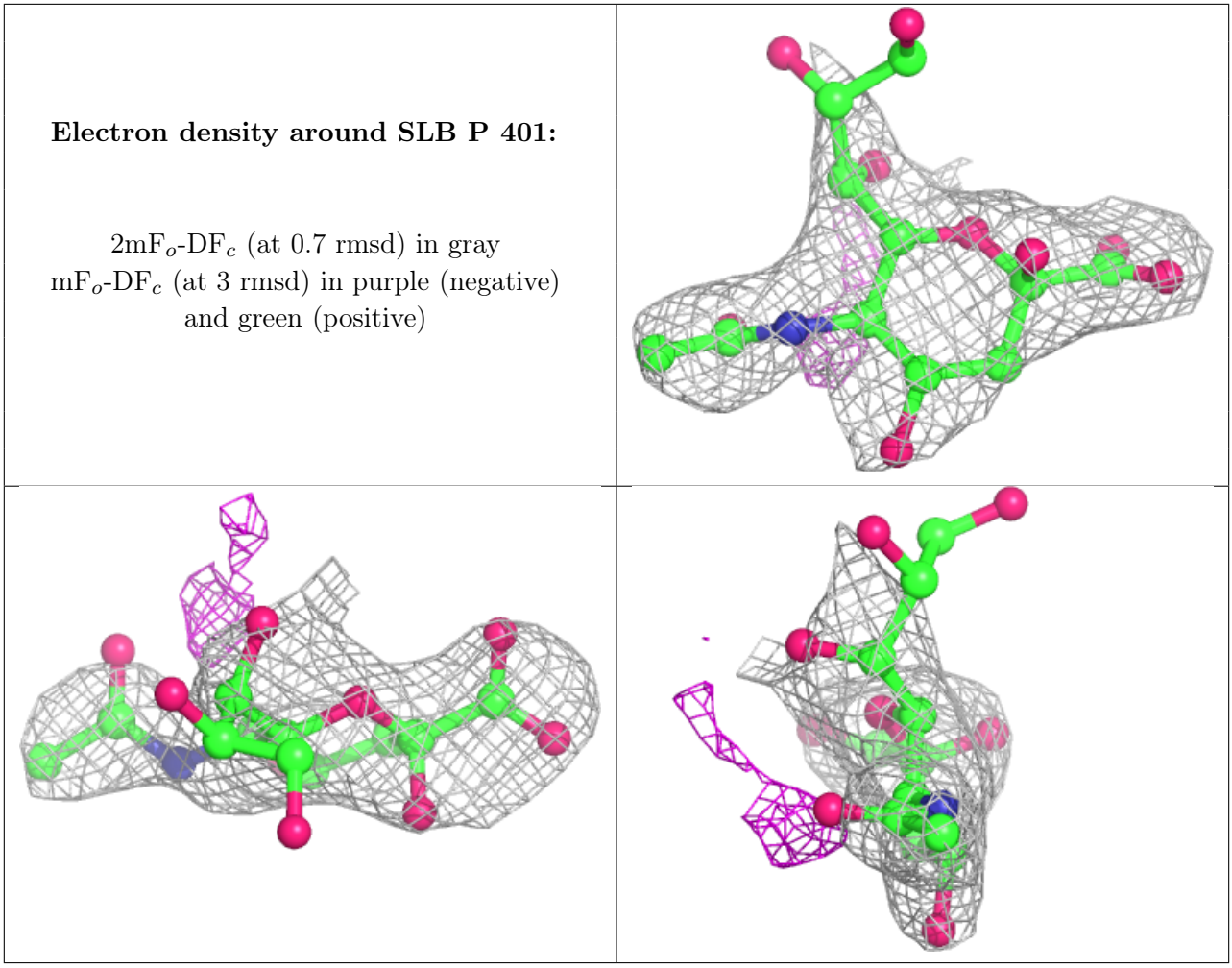






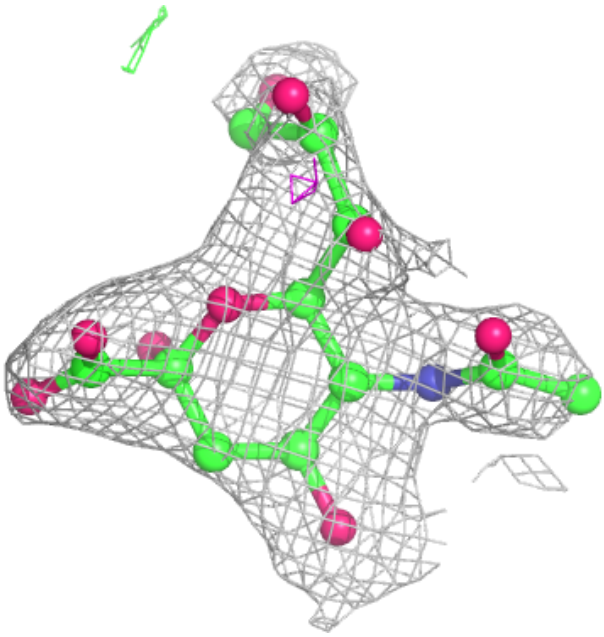
Electron density around SLB P 401:

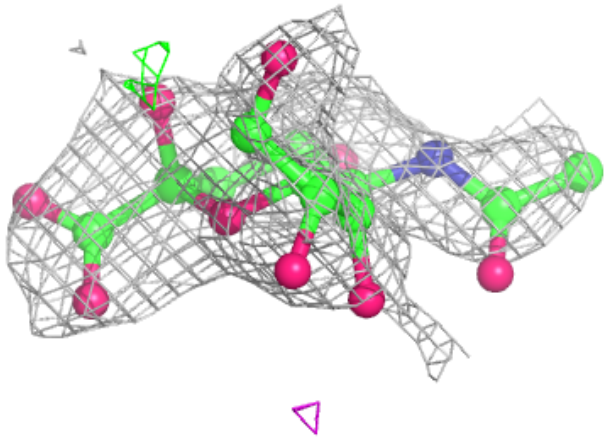
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

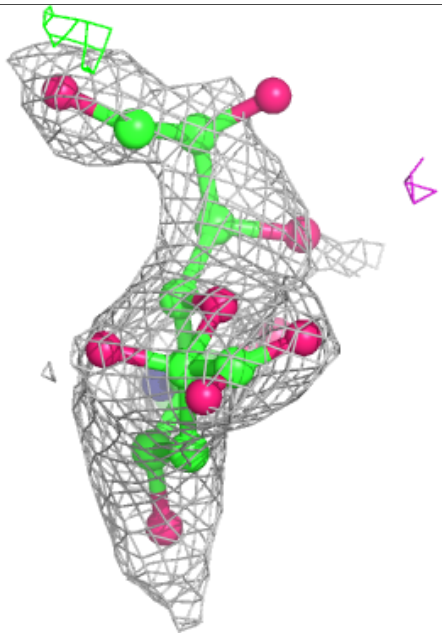


Electron density around SLB T 401:

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

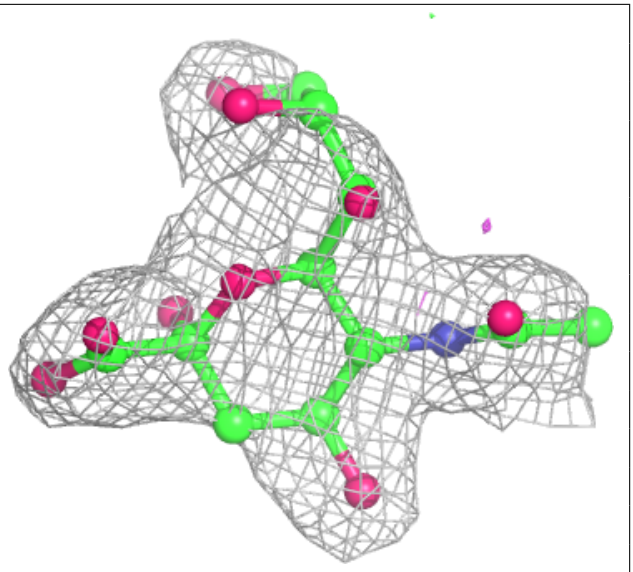


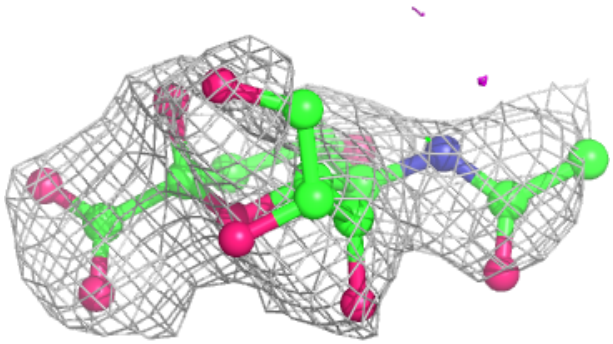


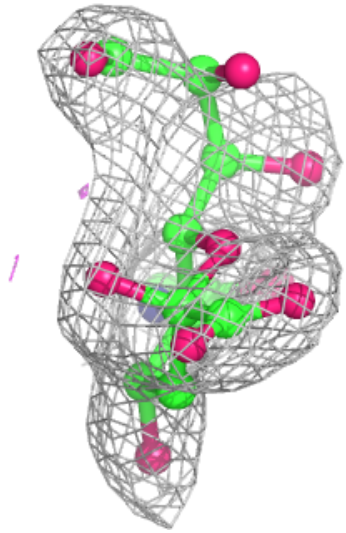


Electron density around SLB J 401:

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

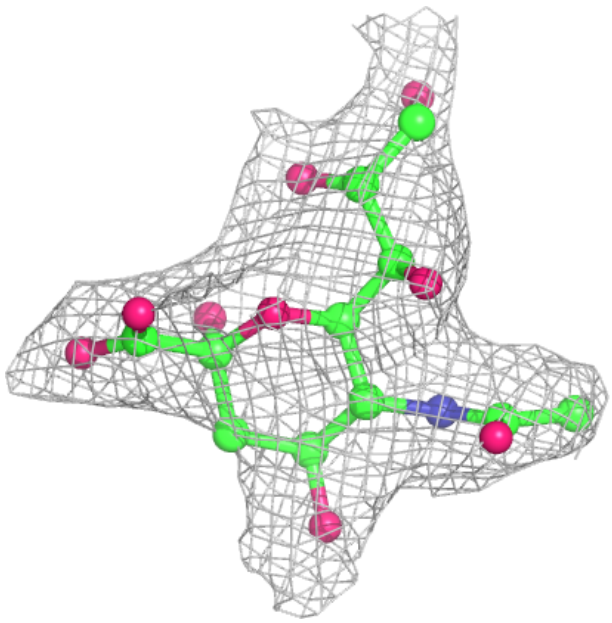


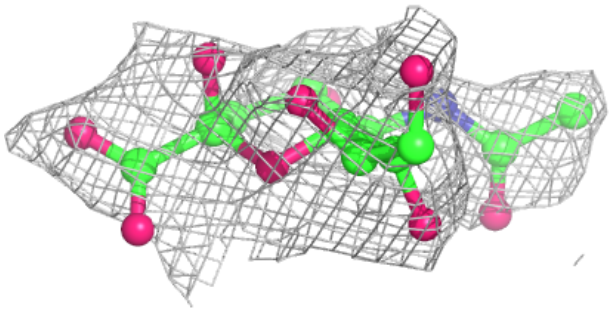


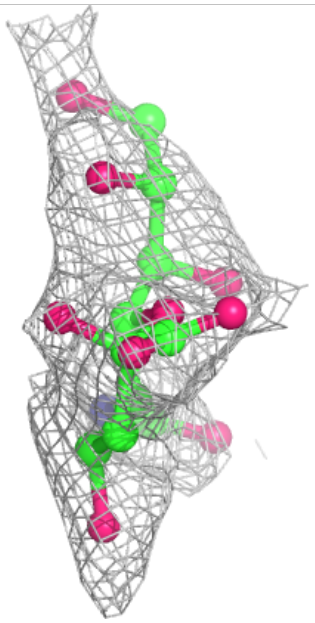


Electron density around SLB I 401:

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

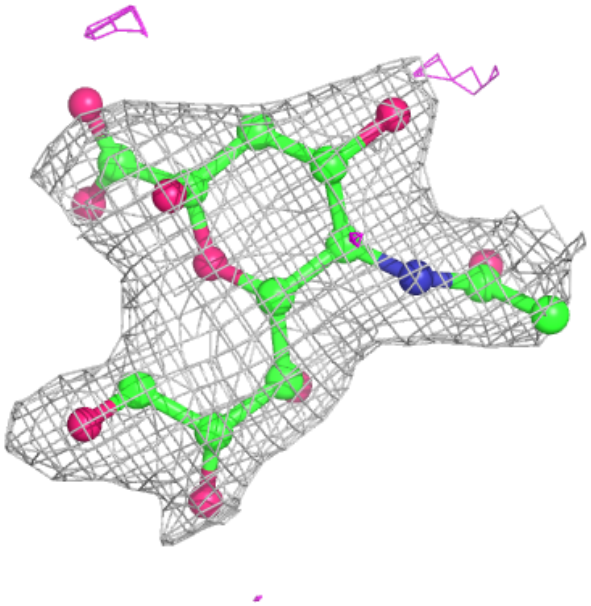


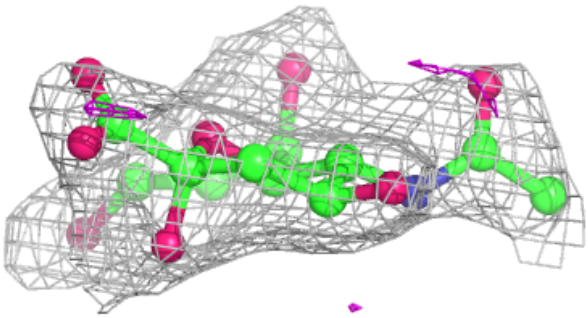


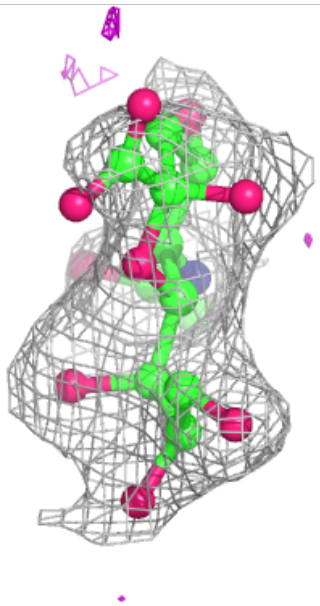


Electron density around SLB Q 401:

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

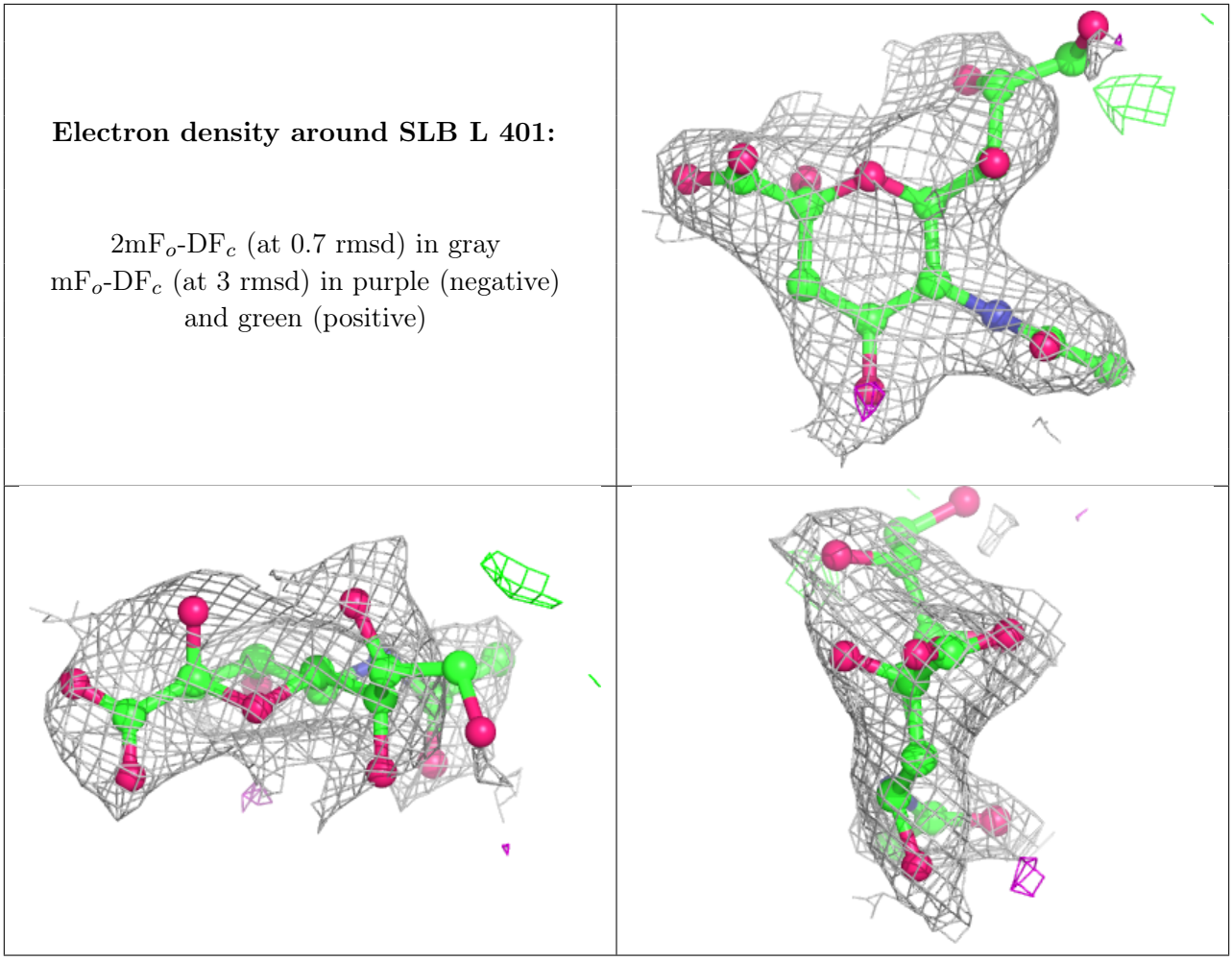






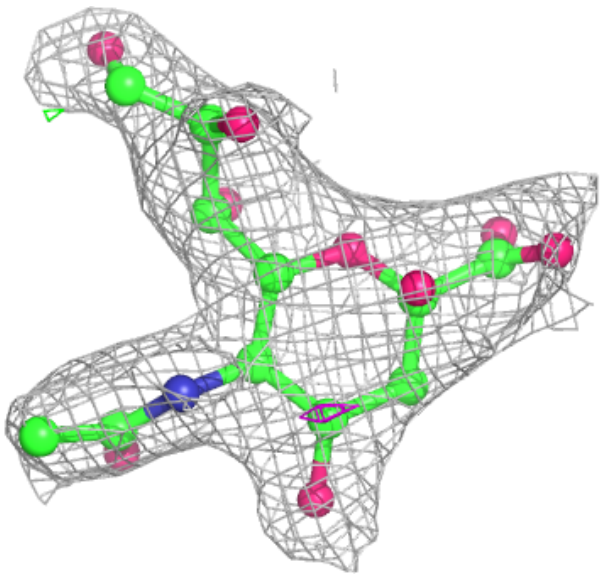
Electron density around SLB L 401:

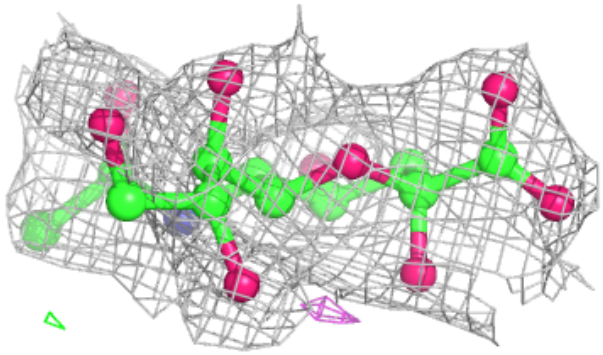
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

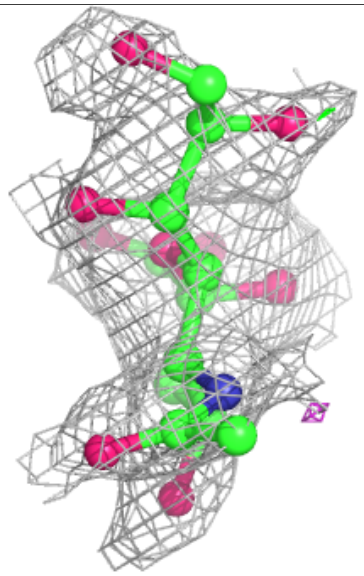


Electron density around SLB V 401:

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

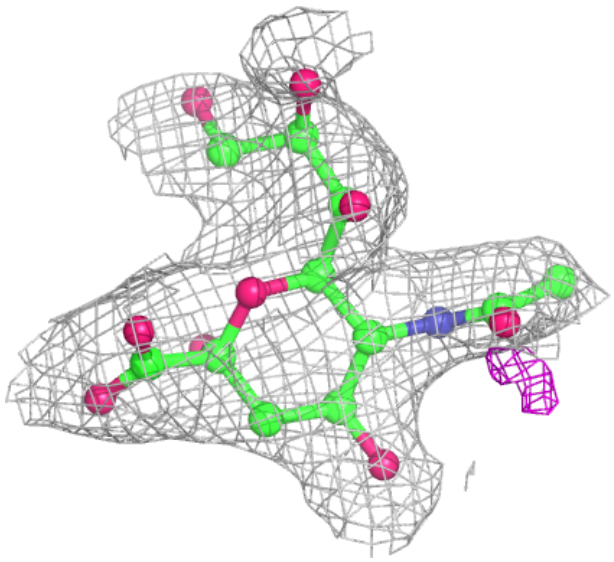


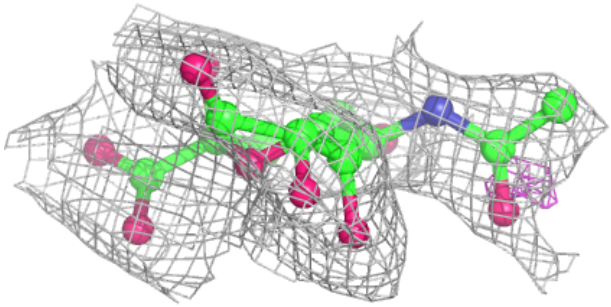


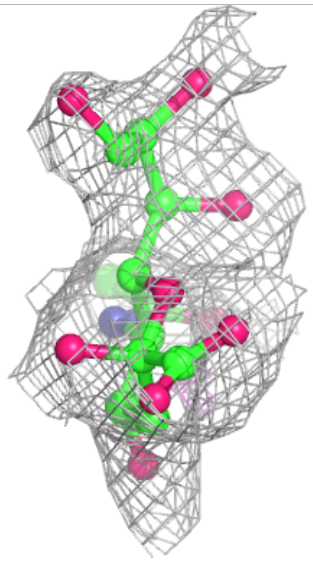


Electron density around SLB S 401:

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

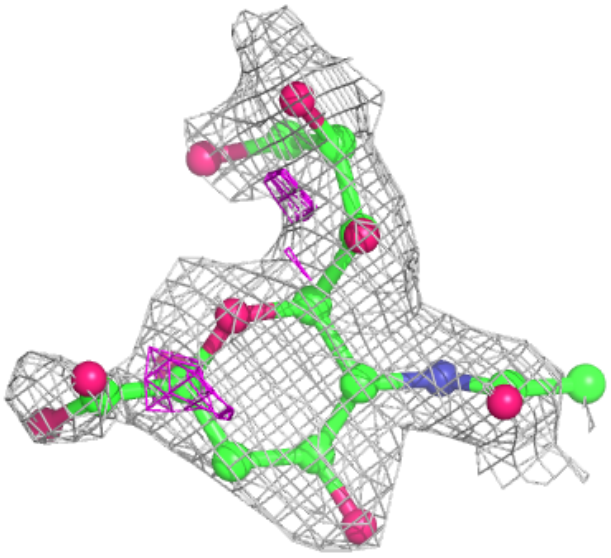


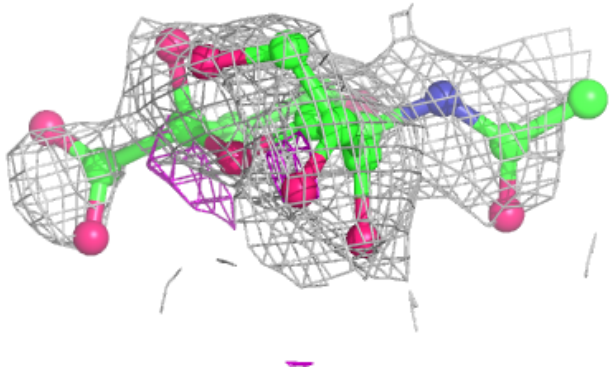


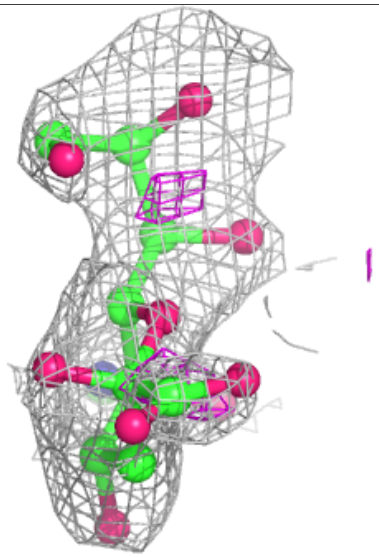


Electron density around SLB X 401:

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

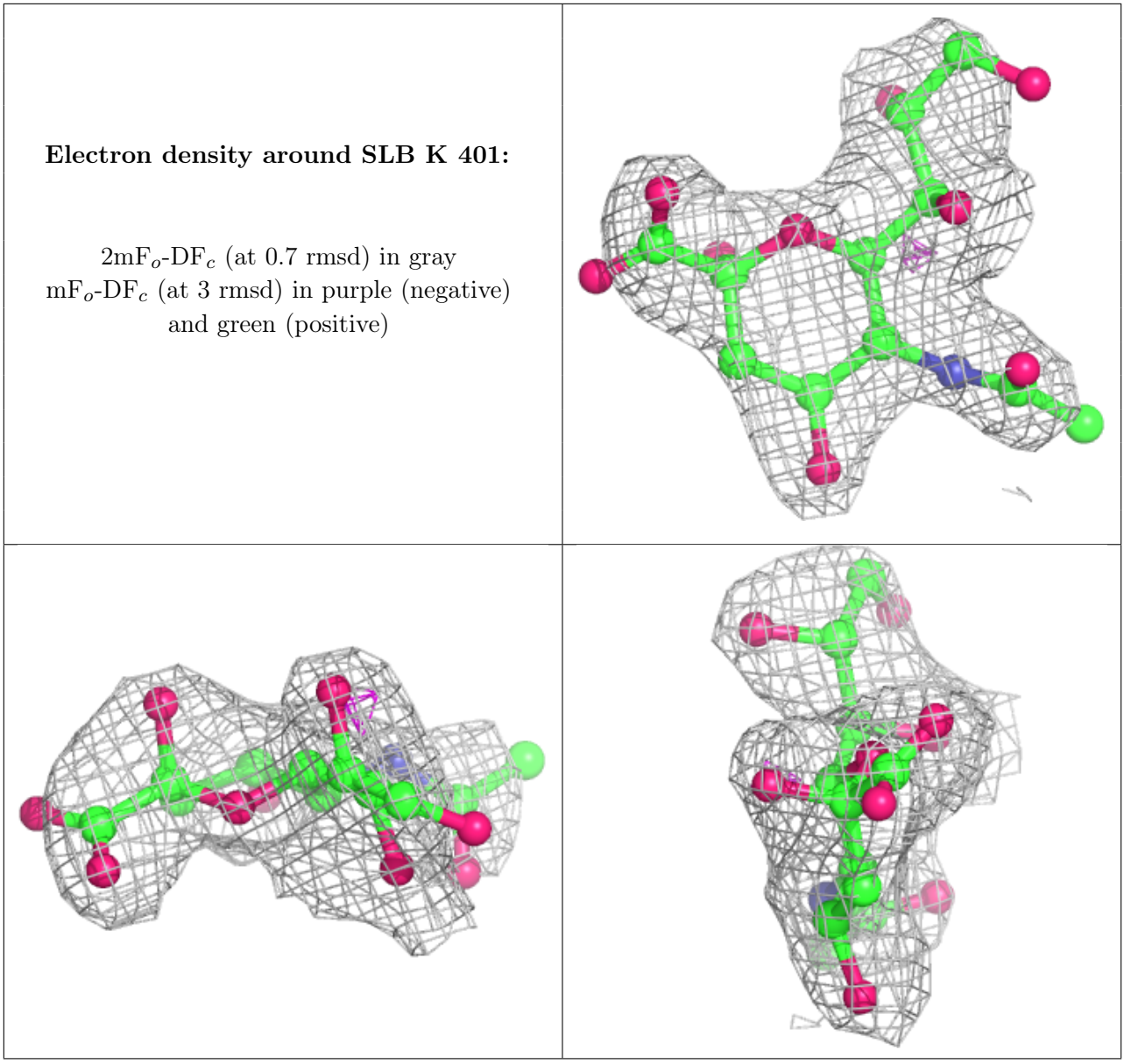






Electron density around SLB K 401:

$2mF_o$-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.