



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 05:43 PM BST

PDB ID : 6S5U
Title : Strictosidine Synthase from *Ophiorrhiza pumila* in complex with N-[2-(1H-Indol-3-yl)ethyl]-3-methyl-1-butanamine
Authors : Eger, E.; Sharma, M.; Kroutil, W.; Grogan, G.
Deposited on : 2019-07-02
Resolution : 2.03 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

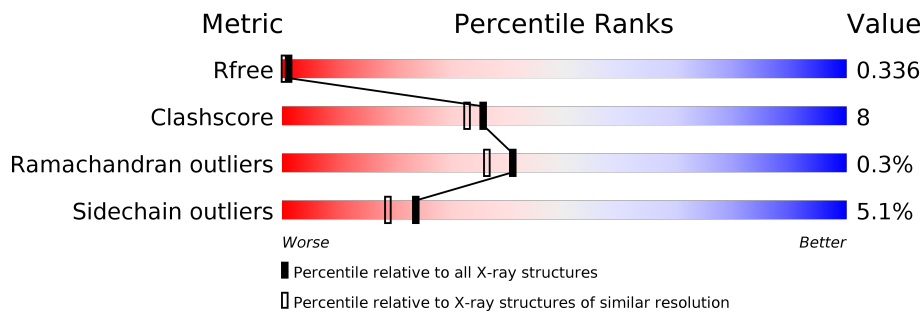
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	331	74% 15% 9%
1	B	331	76% 12% 9%
1	C	331	73% 14% 9%
1	D	331	77% 12% 9%
1	E	331	77% 12% 9%
1	F	331	77% 13% 9%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14917 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 Strictosidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	302	Total 2340	C 1508	N 386	O 442	S 4	0	0	0
1	C	301	Total 2336	C 1505	N 382	O 445	S 4	0	2	0
1	B	300	Total 2312	C 1493	N 379	O 436	S 4	0	0	0
1	D	301	Total 2344	C 1510	N 386	O 444	S 4	0	1	0
1	E	300	Total 2319	C 1495	N 380	O 440	S 4	0	0	0
1	F	301	Total 2334	C 1505	N 380	O 445	S 4	0	2	0

There are 24 discrepancies between the modelled and reference sequences:

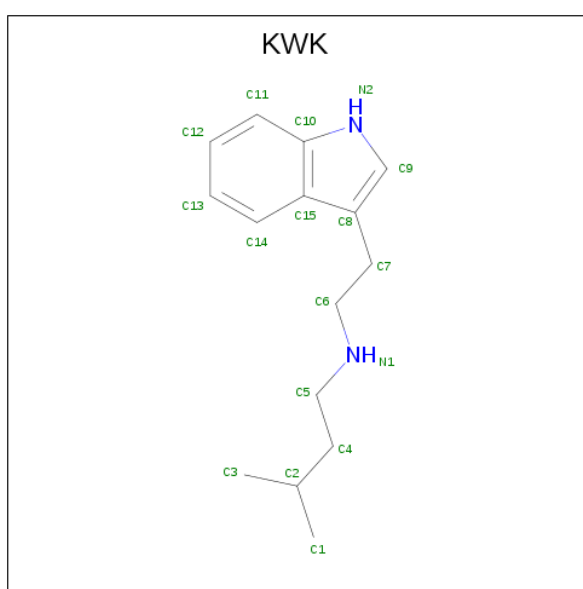
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q94LW9
A	2	ALA	-	expression tag	UNP Q94LW9
A	330	GLY	-	expression tag	UNP Q94LW9
A	331	SER	-	expression tag	UNP Q94LW9
C	1	MET	-	initiating methionine	UNP Q94LW9
C	2	ALA	-	expression tag	UNP Q94LW9
C	330	GLY	-	expression tag	UNP Q94LW9
C	331	SER	-	expression tag	UNP Q94LW9
B	1	MET	-	initiating methionine	UNP Q94LW9
B	2	ALA	-	expression tag	UNP Q94LW9
B	330	GLY	-	expression tag	UNP Q94LW9
B	331	SER	-	expression tag	UNP Q94LW9
D	1	MET	-	initiating methionine	UNP Q94LW9
D	2	ALA	-	expression tag	UNP Q94LW9
D	330	GLY	-	expression tag	UNP Q94LW9
D	331	SER	-	expression tag	UNP Q94LW9
E	1	MET	-	initiating methionine	UNP Q94LW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ALA	-	expression tag	UNP Q94LW9
E	330	GLY	-	expression tag	UNP Q94LW9
E	331	SER	-	expression tag	UNP Q94LW9
F	1	MET	-	initiating methionine	UNP Q94LW9
F	2	ALA	-	expression tag	UNP Q94LW9
F	330	GLY	-	expression tag	UNP Q94LW9
F	331	SER	-	expression tag	UNP Q94LW9

- Molecule 2 is {N}-[2-(1 {H}-indol-3-yl)ethyl]-3-methyl-butan-1-amine (three-letter code: KWK) (formula: C₁₅H₂₂N₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			17	15	2		
2	A	1	Total	C	N	0	1
			17	15	2		
2	C	1	Total	C	N	0	0
			17	15	2		
2	C	1	Total	C	N	0	0
			17	15	2		
2	B	1	Total	C	N	0	0
			17	15	2		
2	B	1	Total	C	N	0	0
			17	15	2		
2	B	1	Total	C	N	0	1
			17	15	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	N	0	0
			17	15	2		
2	D	1	Total	C	N	0	0
			17	15	2		
2	E	1	Total	C	N	0	0
			17	15	2		
2	E	1	Total	C	N	0	0
			17	15	2		
2	F	1	Total	C	N	0	0
			17	15	2		
2	F	1	Total	C	N	0	0
			17	15	2		

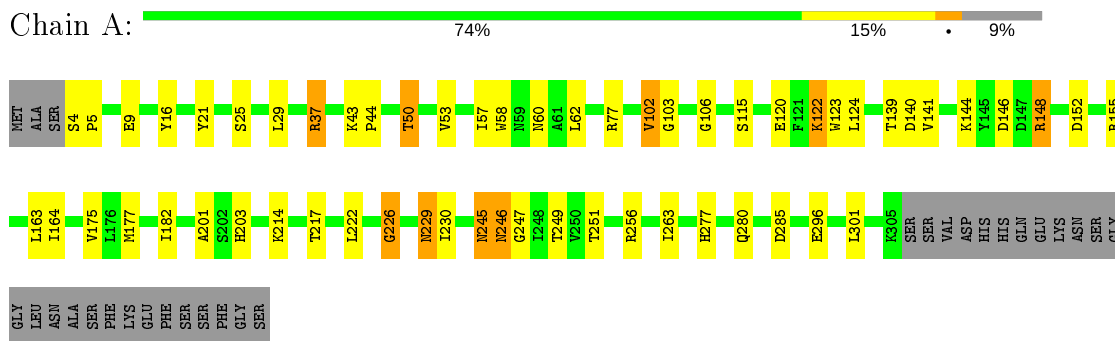
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		
3	C	123	Total	O	0	0
			123	123		
3	B	107	Total	O	0	0
			107	107		
3	D	134	Total	O	0	0
			134	134		
3	E	111	Total	O	0	0
			111	111		
3	F	130	Total	O	0	0
			130	130		

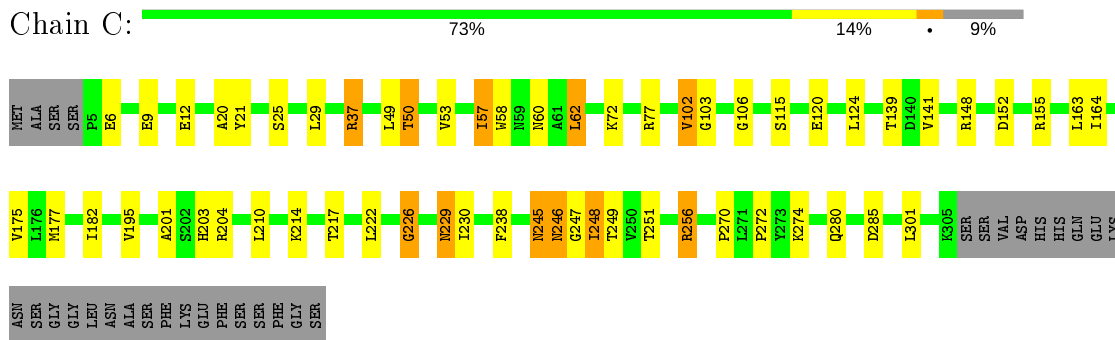
3 Residue-property plots [i](#)

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. 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. 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.

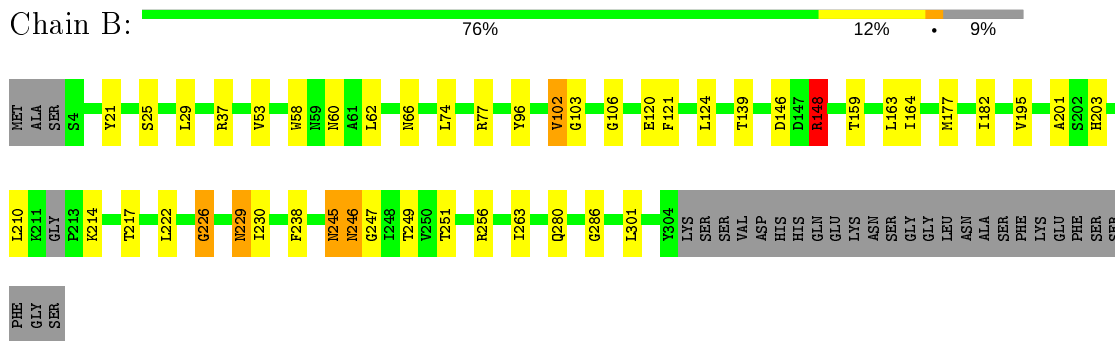
- Molecule 1: Strictosidine synthase



- Molecule 1: Strictosidine synthase



- Molecule 1: Strictosidine synthase



- Molecule 1: Strictosidine synthase

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	125.75Å 125.75Å 117.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.90 – 2.03 39.87 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.90-2.03) 99.7 (39.87-2.03)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.312 , 0.334 0.315 , 0.336	Depositor DCC
R_{free} test set	6605 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	1.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 19.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l 0.049 for h,-h-k,-l 0.407 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14917	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KWK

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	0.75	0/2404	0.85	4/3273 (0.1%)
1	B	0.75	0/2375	0.83	1/3235 (0.0%)
1	C	0.76	0/2406	0.85	3/3277 (0.1%)
1	D	0.77	0/2411	0.84	2/3280 (0.1%)
1	E	0.75	0/2383	0.84	2/3246 (0.1%)
1	F	0.75	0/2404	0.83	2/3274 (0.1%)
All	All	0.75	0/14383	0.84	14/19585 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	NE-CZ-NH1	-9.63	115.48	120.30
1	C	256	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	148	ARG	CG-CD-NE	-7.19	96.70	111.80
1	F	148	ARG	NE-CZ-NH2	-7.14	116.73	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	148	ARG	NE-CZ-NH1	-6.88	116.86	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37	ARG	Peptide
1	B	37	ARG	Peptide
1	C	37	ARG	Peptide
1	D	37	ARG	Peptide
1	E	37	ARG	Peptide

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	2340	0	2195	40	0
1	B	2312	0	2155	38	0
1	C	2336	0	2181	47	0
1	D	2344	0	2210	40	0
1	E	2319	0	2164	32	0
1	F	2334	0	2181	37	0
2	A	34	0	0	1	0
2	B	51	0	0	0	0
2	C	34	0	0	1	0
2	D	34	0	0	0	0
2	E	34	0	0	0	0
2	F	34	0	0	0	0
3	A	106	0	0	7	0
3	B	107	0	0	5	0
3	C	123	0	0	13	1
3	D	134	0	0	12	1
3	E	111	0	0	4	0
3	F	130	0	0	7	0
All	All	14917	0	13086	220	1

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 8.

The worst 5 of 220 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:159:THR:HB	3:B:523:HOH:O	1.56	1.04
1:B:214:LYS:O	1:B:217:THR:HG22	1.66	0.96
1:A:214:LYS:O	1:A:217:THR:HG22	1.66	0.95
1:E:214:LYS:O	1:E:217:THR:HG22	1.67	0.94
1:C:214:LYS:O	1:C:217:THR:HG22	1.67	0.92

All (1) 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)
3:C:605:HOH:O	3:D:597:HOH:O 3_664	2.05	0.15

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	300/331 (91%)	291 (97%)	8 (3%)	1 (0%)	41 36
1	B	296/331 (89%)	289 (98%)	6 (2%)	1 (0%)	41 36
1	C	301/331 (91%)	293 (97%)	7 (2%)	1 (0%)	41 36
1	D	300/331 (91%)	292 (97%)	7 (2%)	1 (0%)	41 36
1	E	298/331 (90%)	290 (97%)	7 (2%)	1 (0%)	41 36
1	F	301/331 (91%)	292 (97%)	8 (3%)	1 (0%)	41 36
All	All	1796/1986 (90%)	1747 (97%)	43 (2%)	6 (0%)	41 36

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLY
1	B	226	GLY
1	D	226	GLY
1	F	226	GLY
1	C	226	GLY

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	239/277 (86%)	224 (94%)	15 (6%)	18	12
1	B	234/277 (84%)	224 (96%)	10 (4%)	29	25
1	C	239/277 (86%)	221 (92%)	18 (8%)	13	8
1	D	242/277 (87%)	232 (96%)	10 (4%)	30	27
1	E	236/277 (85%)	226 (96%)	10 (4%)	30	26
1	F	239/277 (86%)	229 (96%)	10 (4%)	30	26
All	All	1429/1662 (86%)	1356 (95%)	73 (5%)	24	19

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	SER
1	B	245	ASN
1	F	148	ARG
1	B	102	VAL
1	B	301	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	245	ASN
1	D	69	GLN
1	F	245	ASN
1	B	246	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	280	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	KWK	F	401	-	17,18,18	0.56	0	16,23,23	0.73	1 (6%)
2	KWK	B	402	-	17,18,18	0.56	0	16,23,23	0.76	0
2	KWK	D	402	-	17,18,18	0.54	0	16,23,23	0.78	1 (6%)
2	KWK	F	402	-	17,18,18	0.50	0	16,23,23	0.78	1 (6%)
2	KWK	C	401	-	17,18,18	0.54	0	16,23,23	0.80	1 (6%)
2	KWK	E	402	-	17,18,18	0.59	0	16,23,23	0.89	1 (6%)
2	KWK	A	401	-	17,18,18	0.50	0	16,23,23	0.82	1 (6%)
2	KWK	B	403[B]	-	17,18,18	0.55	0	16,23,23	0.85	1 (6%)
2	KWK	B	401	-	17,18,18	0.58	0	16,23,23	0.82	0
2	KWK	E	401	-	17,18,18	0.54	0	16,23,23	0.91	1 (6%)
2	KWK	C	402	-	17,18,18	0.52	0	16,23,23	0.93	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KWK	A	402[A]	-	17,18,18	0.54	0	16,23,23	0.80	0
2	KWK	D	401	-	17,18,18	0.45	0	16,23,23	1.38	2 (12%)

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	KWK	F	401	-	-	1/8/8/8	0/2/2/2
2	KWK	B	402	-	-	2/8/8/8	0/2/2/2
2	KWK	D	402	-	-	1/8/8/8	0/2/2/2
2	KWK	F	402	-	-	3/8/8/8	0/2/2/2
2	KWK	C	401	-	-	4/8/8/8	0/2/2/2
2	KWK	E	402	-	-	1/8/8/8	0/2/2/2
2	KWK	A	401	-	-	5/8/8/8	0/2/2/2
2	KWK	B	403[B]	-	-	0/8/8/8	0/2/2/2
2	KWK	B	401	-	-	2/8/8/8	0/2/2/2
2	KWK	E	401	-	-	4/8/8/8	0/2/2/2
2	KWK	C	402	-	-	2/8/8/8	0/2/2/2
2	KWK	A	402[A]	-	-	7/8/8/8	0/2/2/2
2	KWK	D	401	-	-	5/8/8/8	0/2/2/2

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	KWK	C6-C7-C8	4.04	119.08	111.28
2	D	401	KWK	C12-C11-C10	-2.27	116.81	120.08
2	B	403[B]	KWK	C12-C11-C10	-2.20	116.92	120.08
2	E	401	KWK	C12-C11-C10	-2.18	116.95	120.08
2	D	402	KWK	C12-C11-C10	-2.13	117.02	120.08

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401	KWK	N1-C6-C7-C8
2	B	402	KWK	C2-C4-C5-N1

Continued on next page...

Continued from previous page...

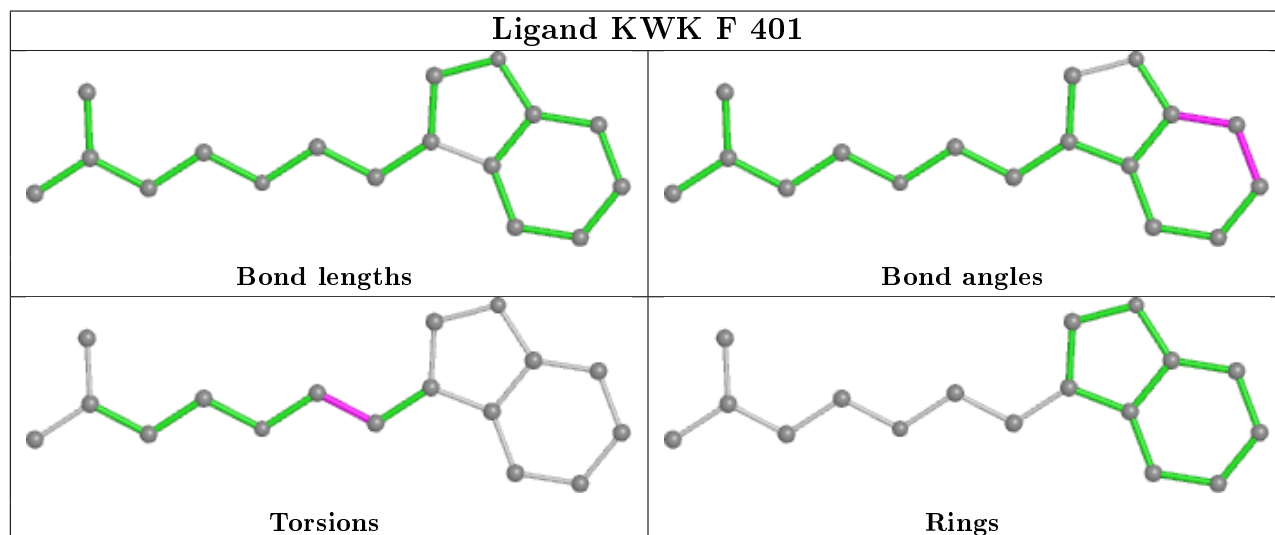
Mol	Chain	Res	Type	Atoms
2	F	402	KWK	N1-C6-C7-C8
2	C	401	KWK	C2-C4-C5-N1
2	C	401	KWK	C6-C7-C8-C15

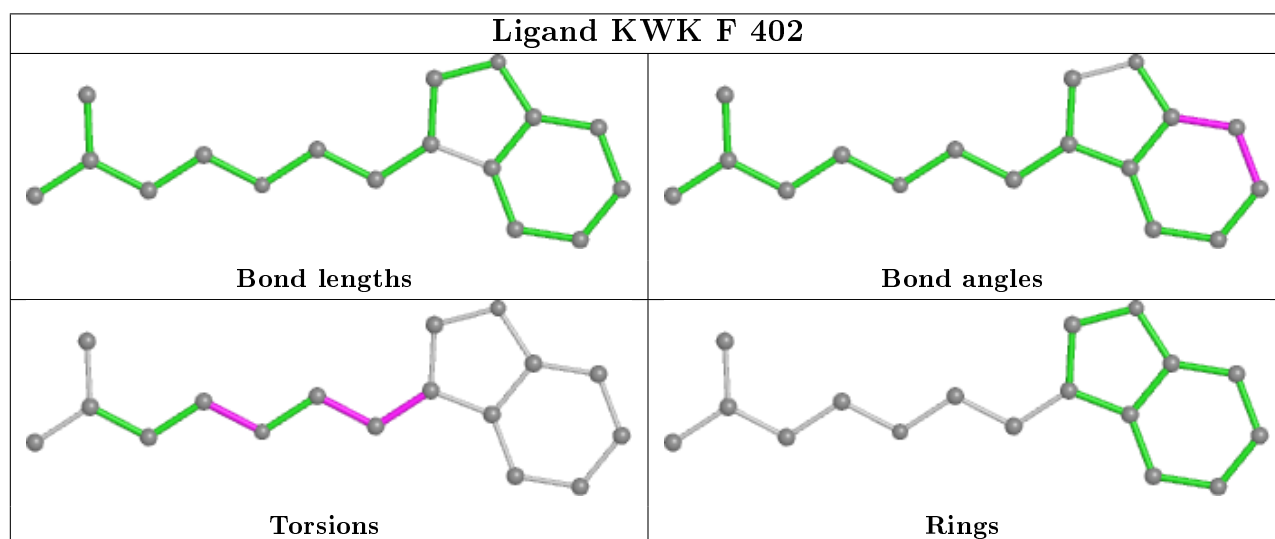
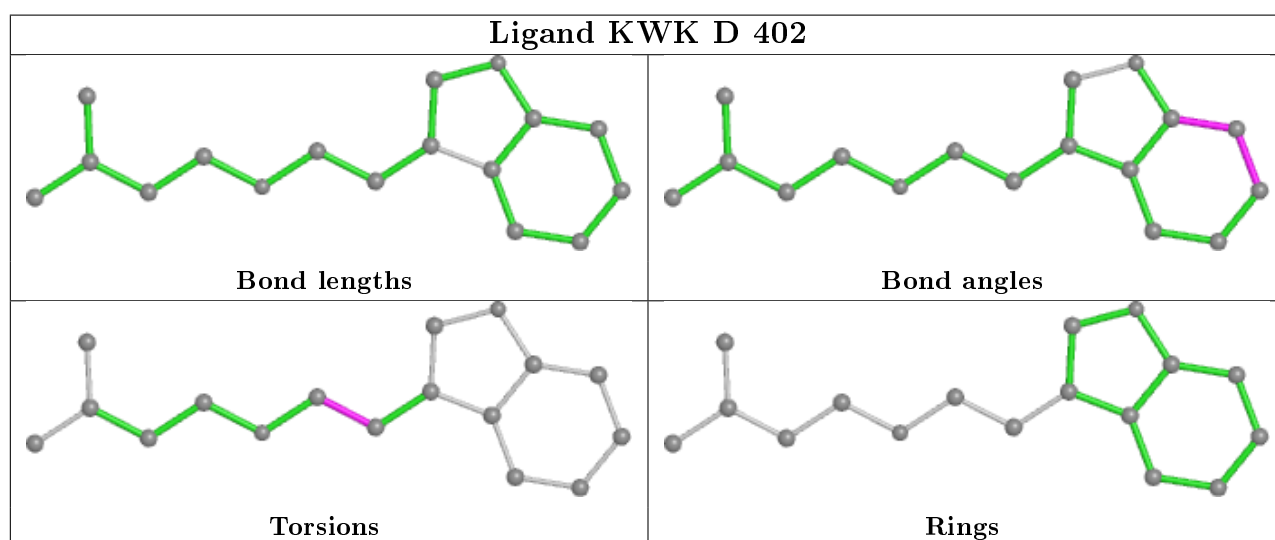
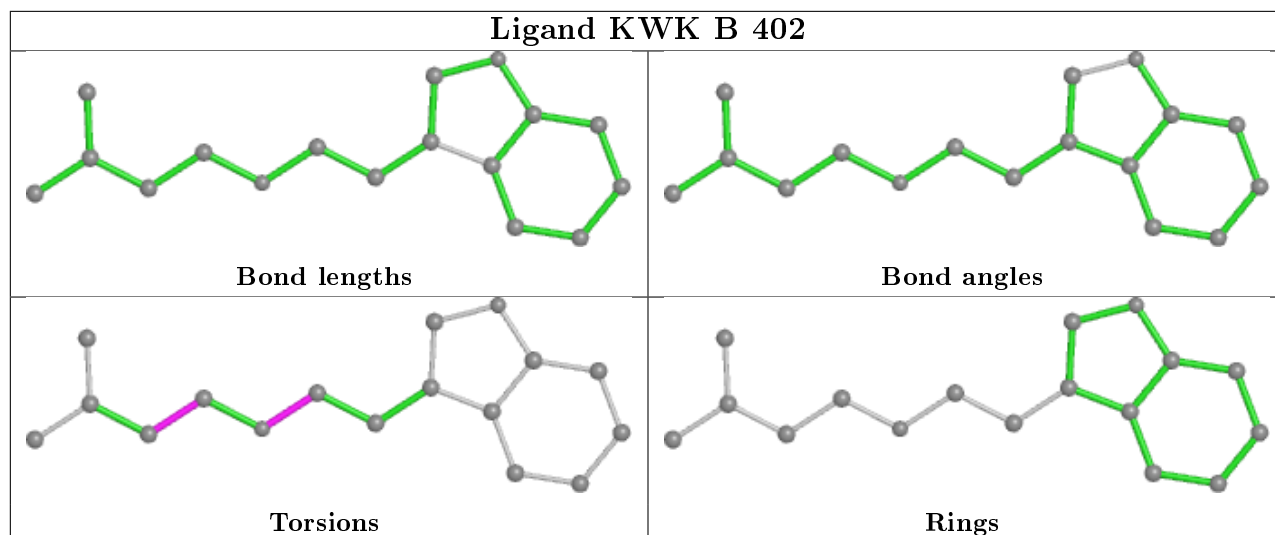
There are no ring outliers.

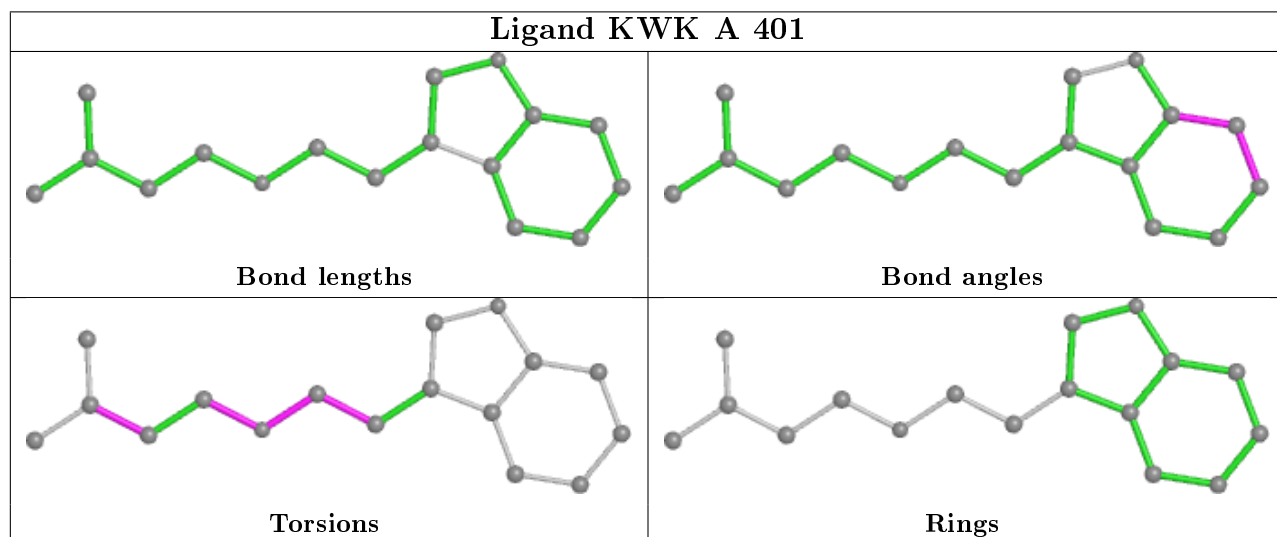
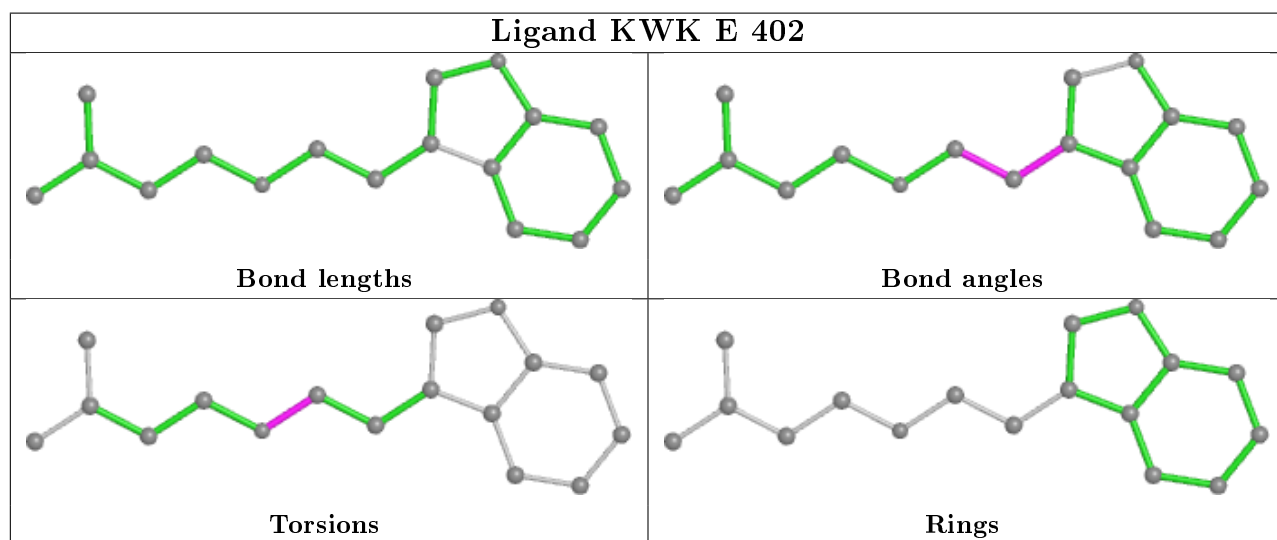
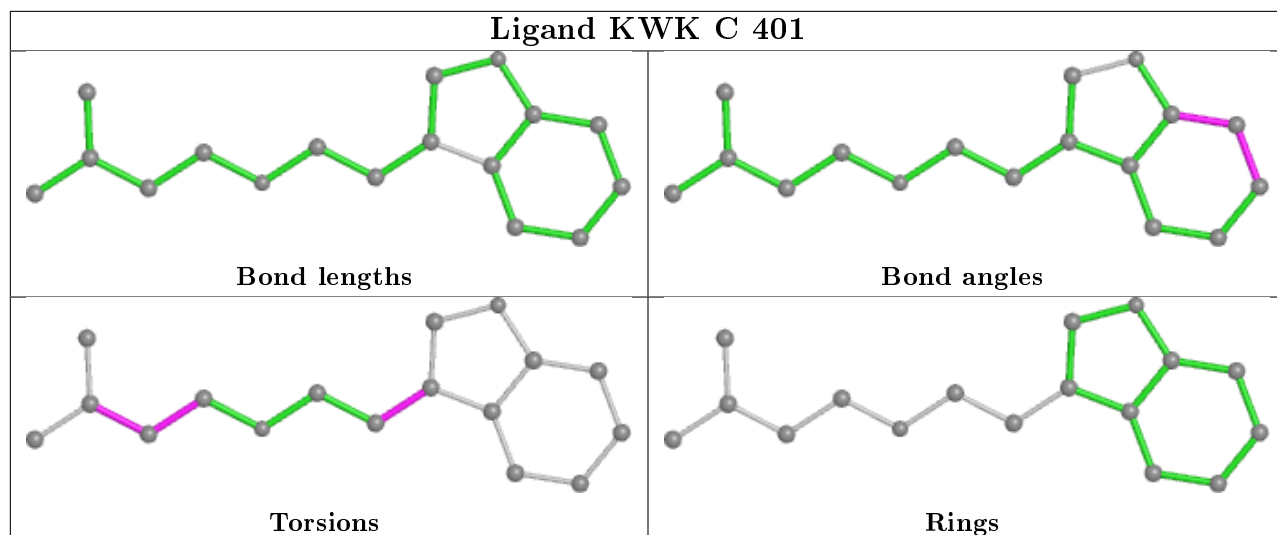
2 monomers are involved in 2 short contacts:

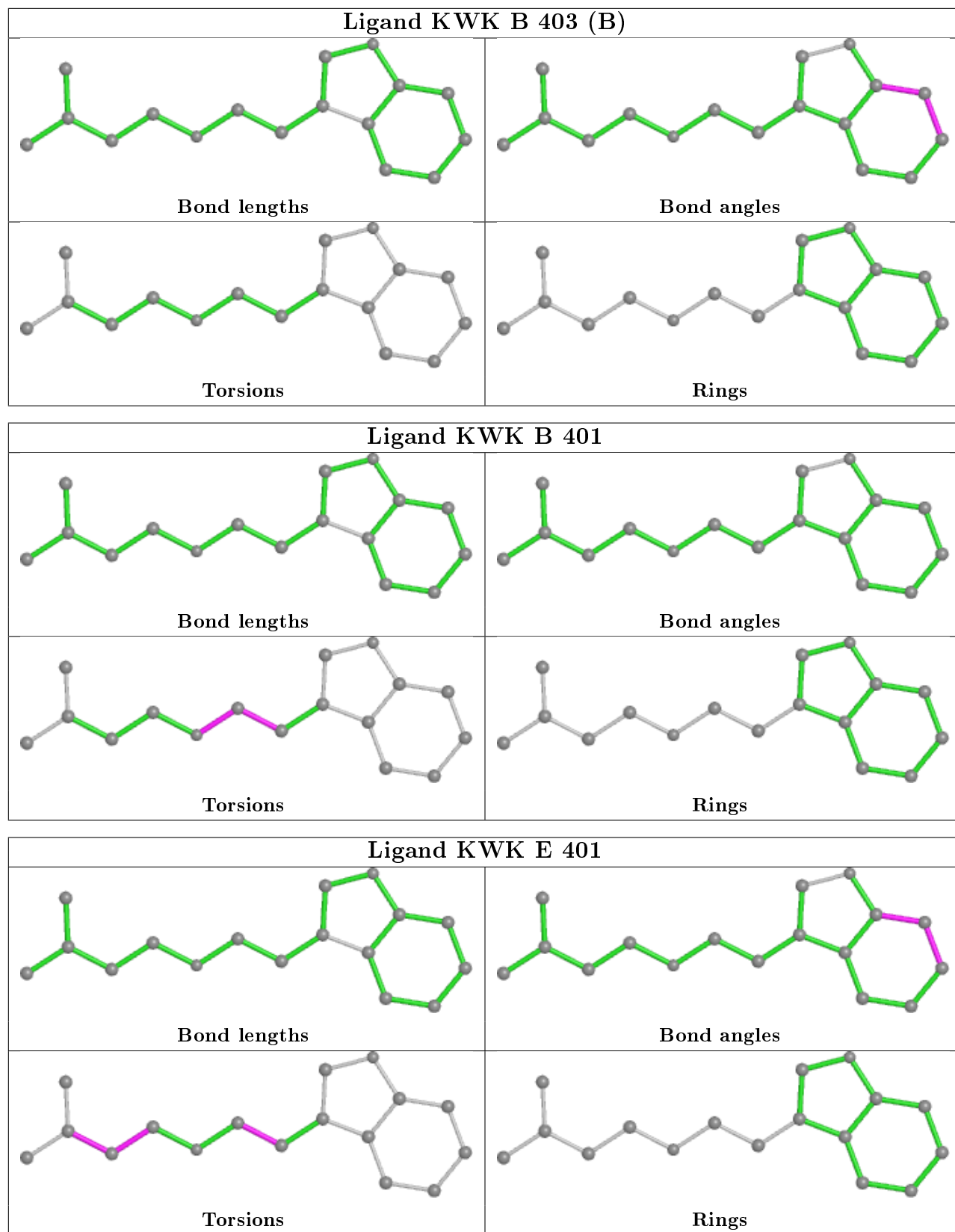
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	KWK	1	0
2	A	402[A]	KWK	1	0

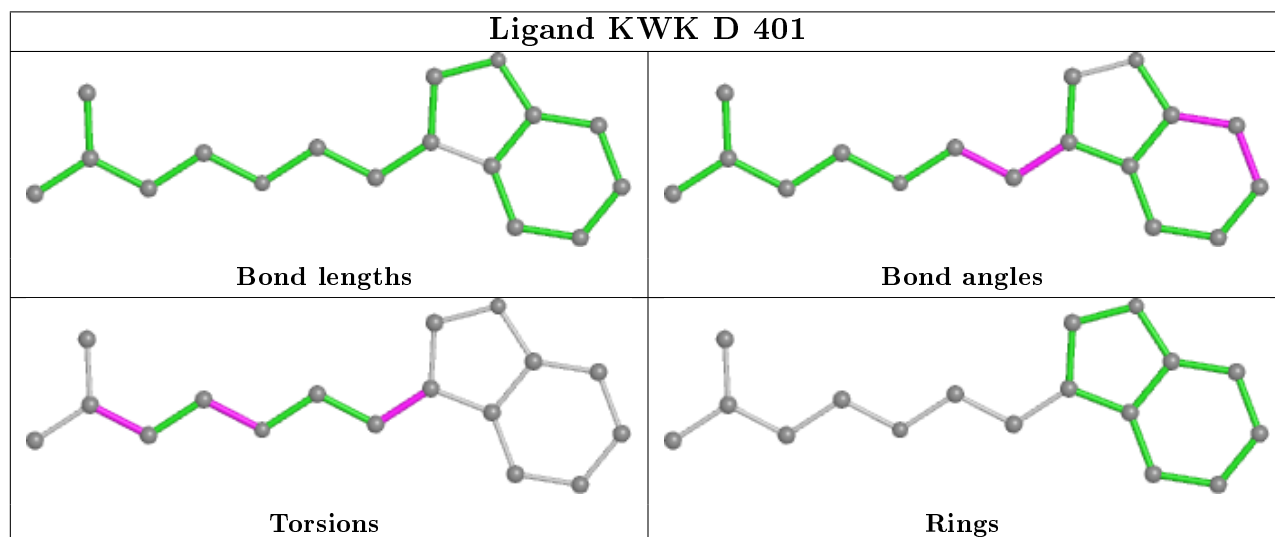
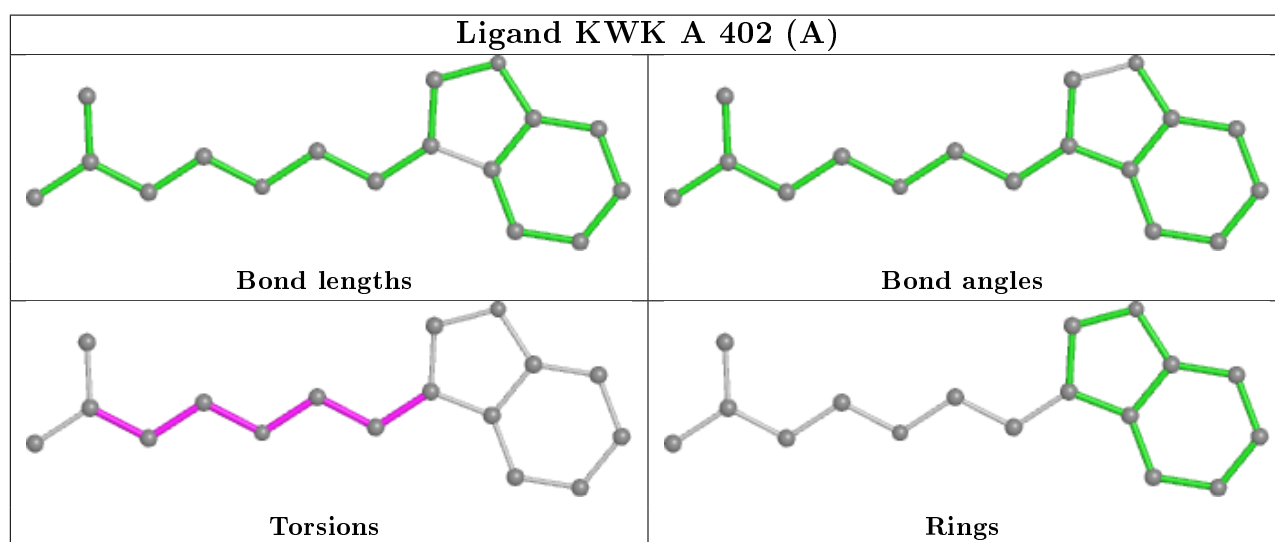
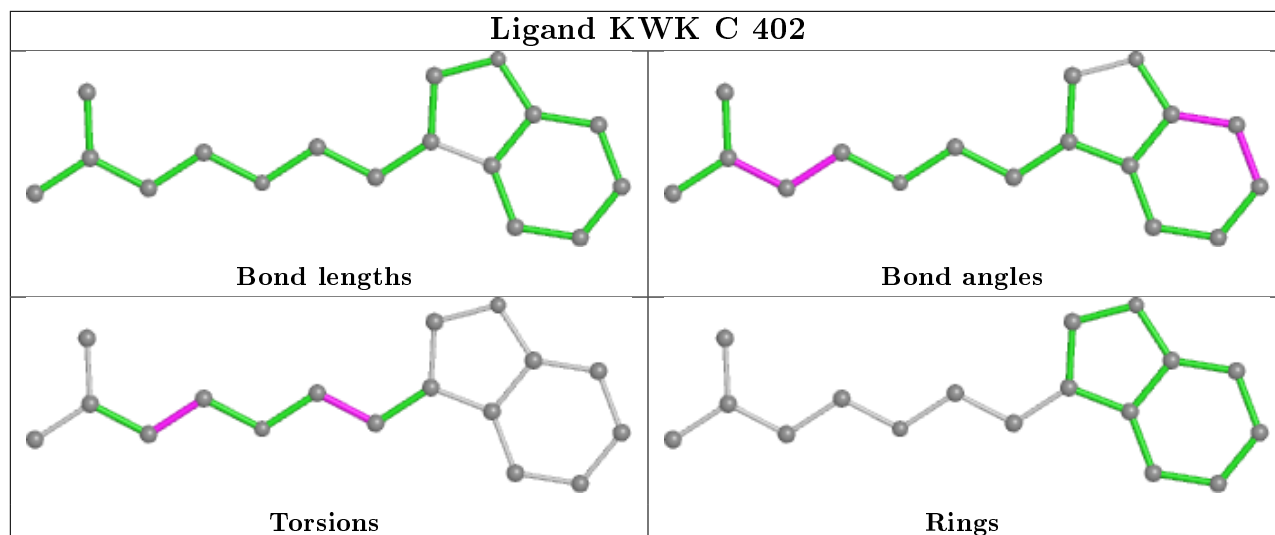
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

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

Unable to reproduce the depositor's R factor - this section is therefore empty.

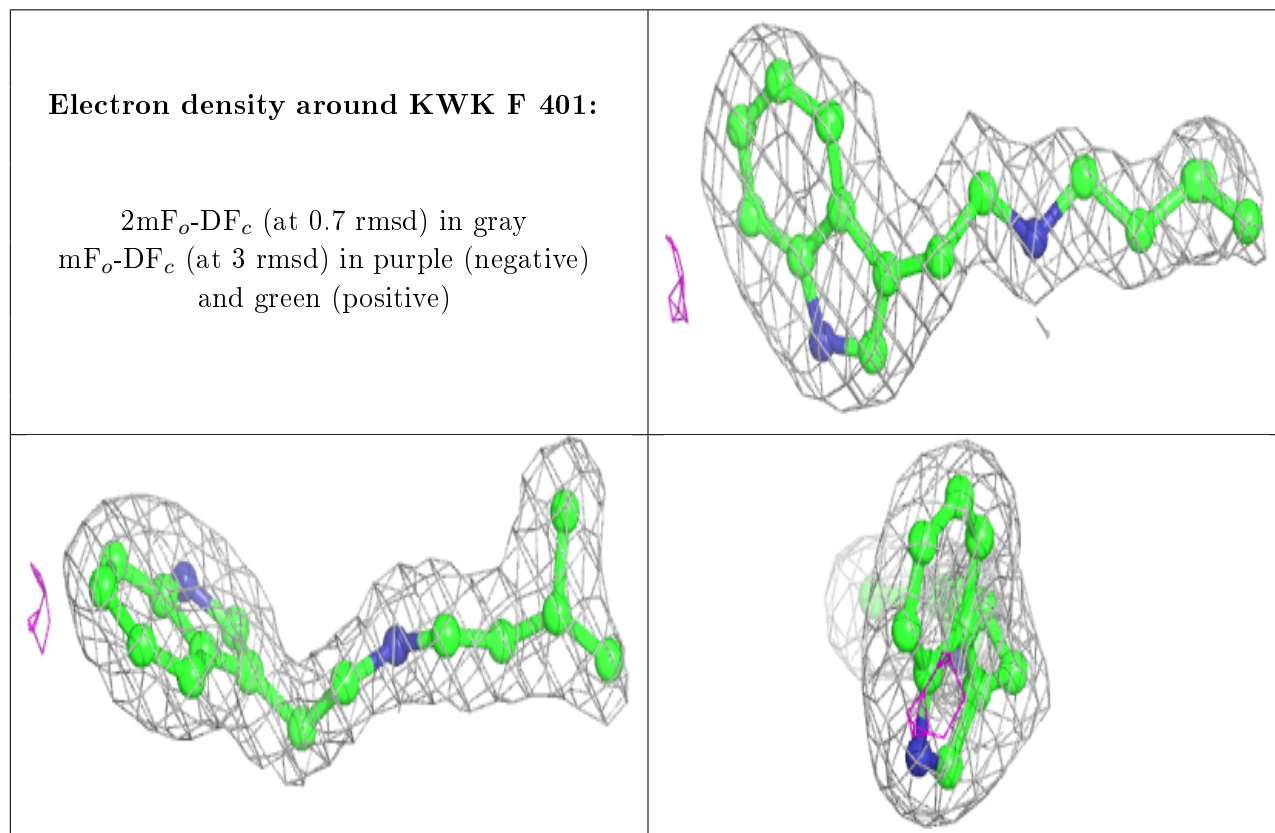
6.3 Carbohydrates [i](#)

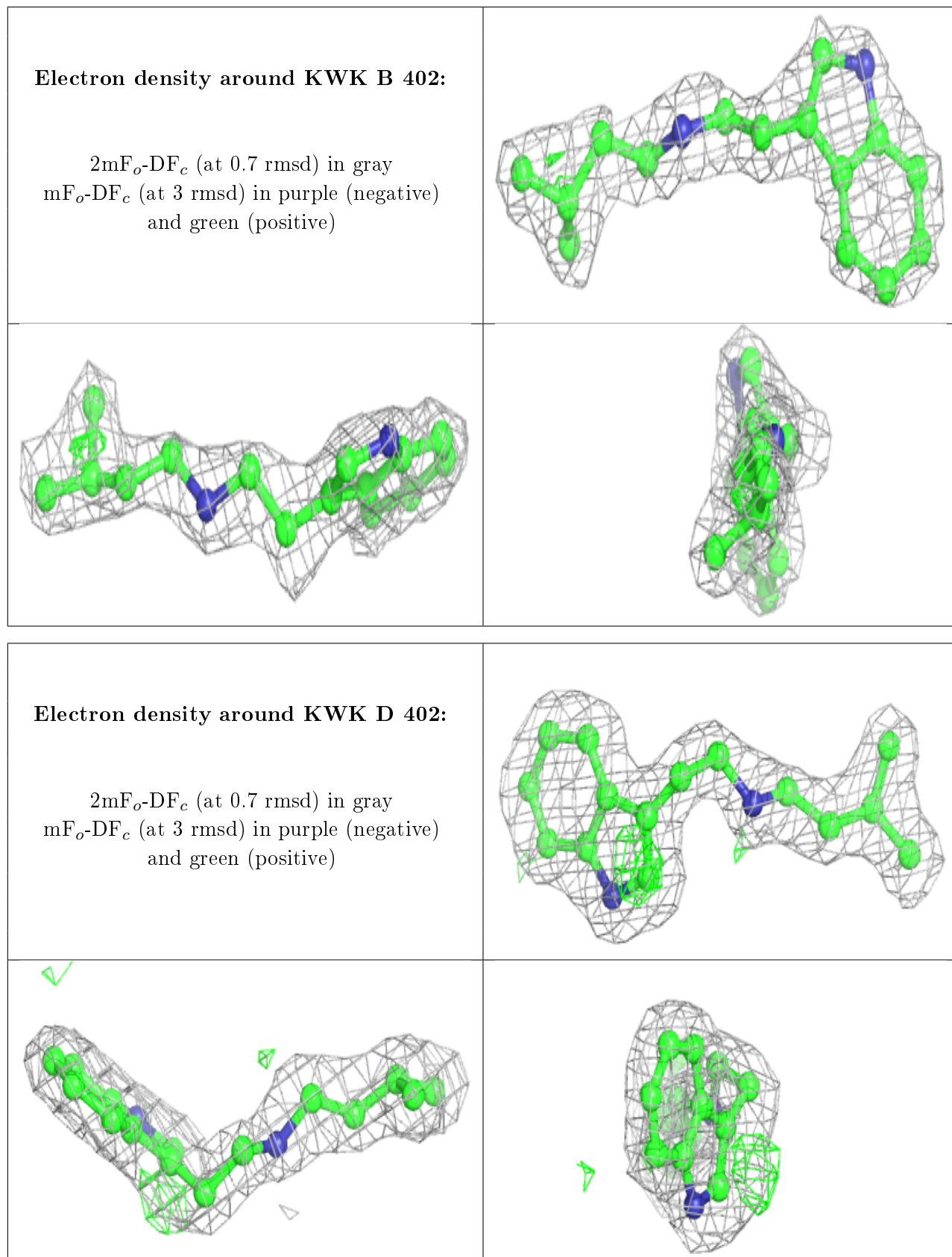
Unable to reproduce the depositor's R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

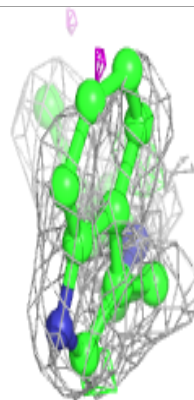
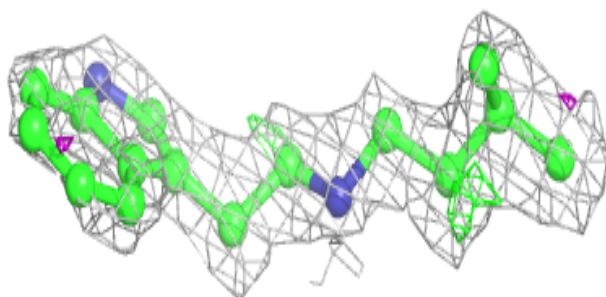
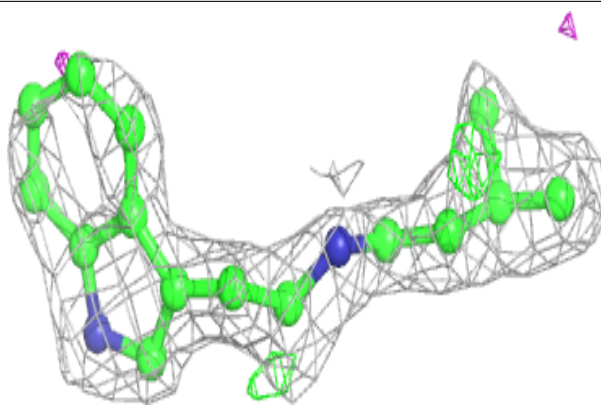
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



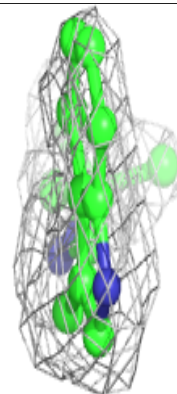
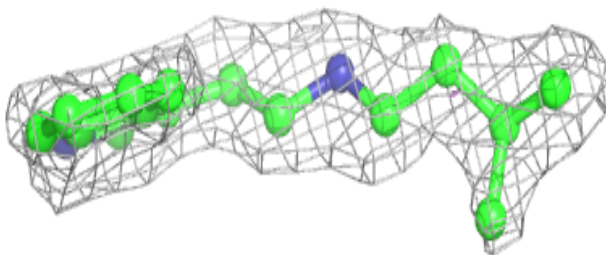
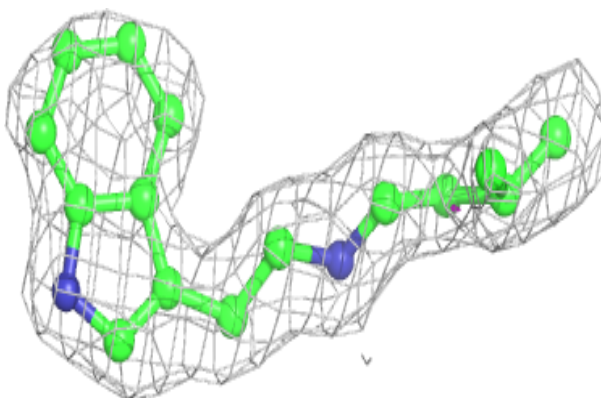


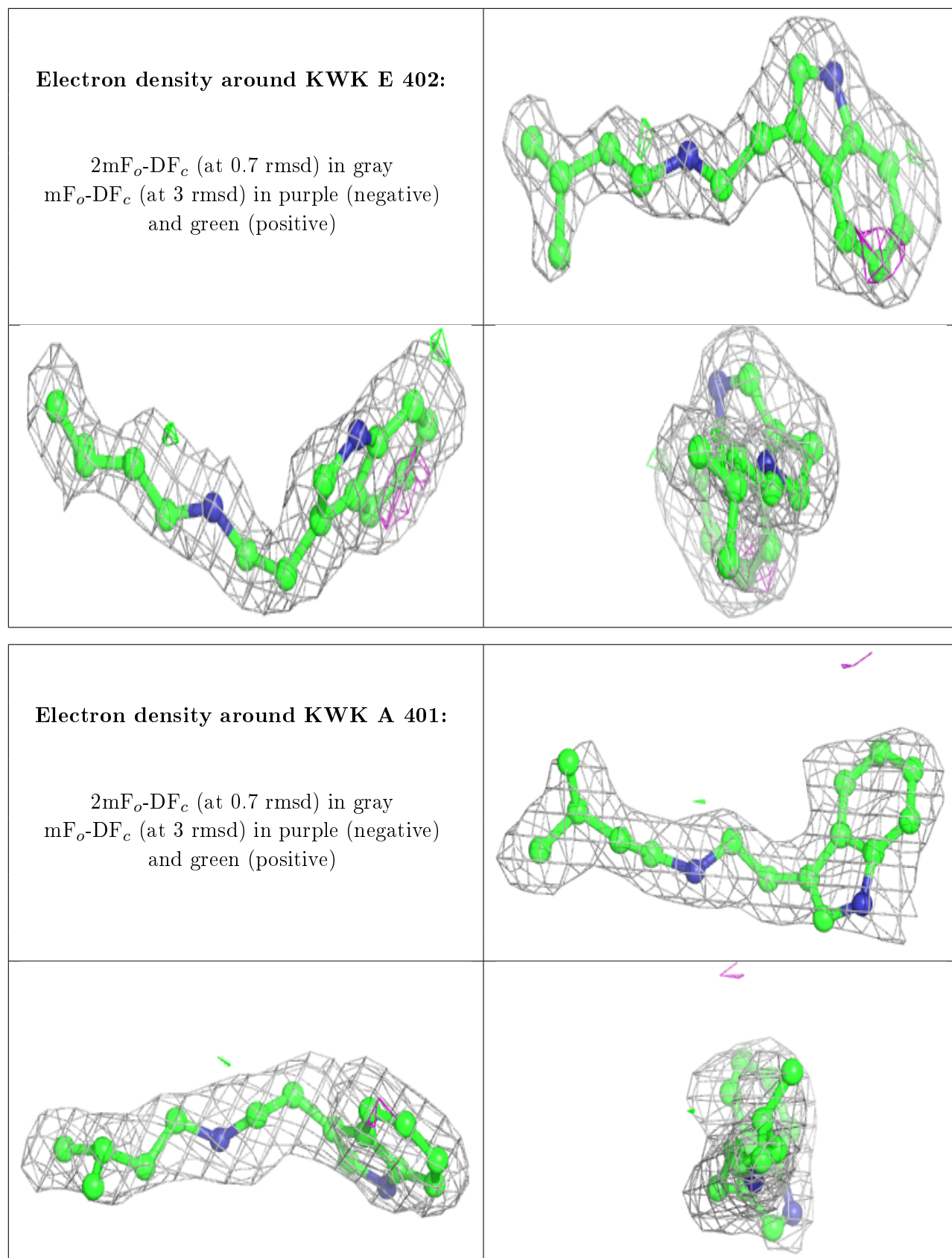
Electron density around KWK F 402:

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

**Electron density around KWK C 401:**

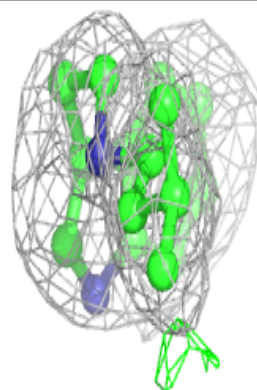
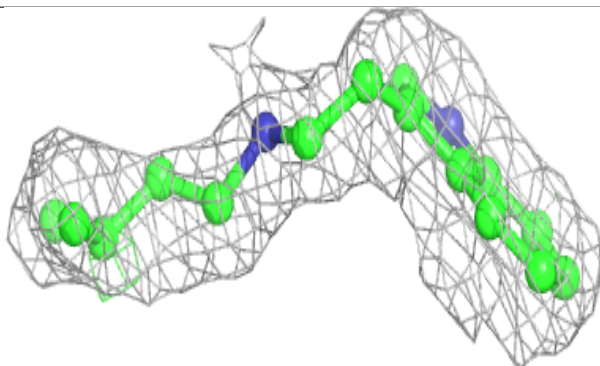
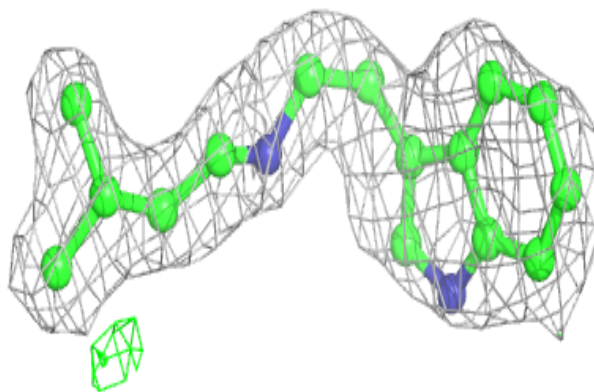
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



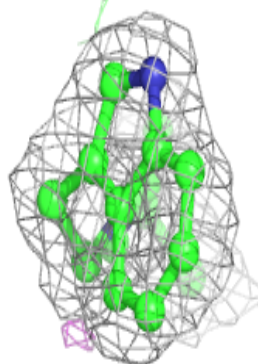
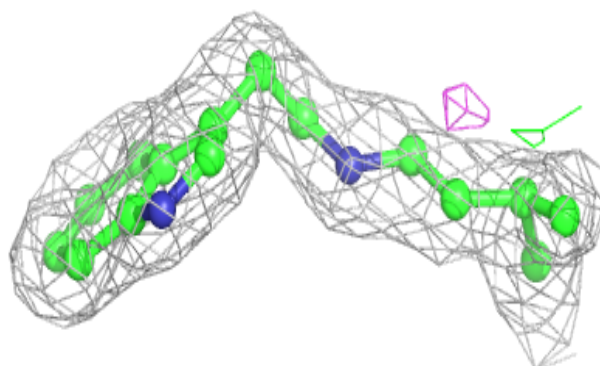
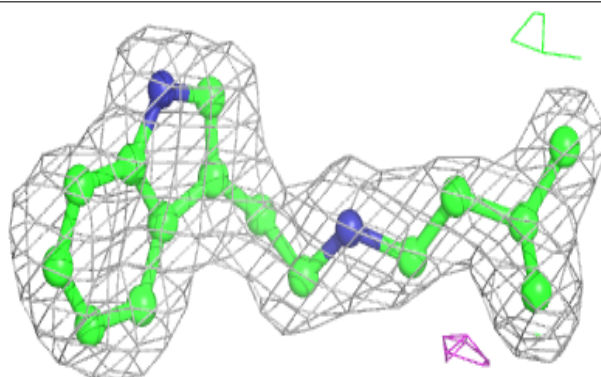


Electron density around KWK B 403 (B):

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

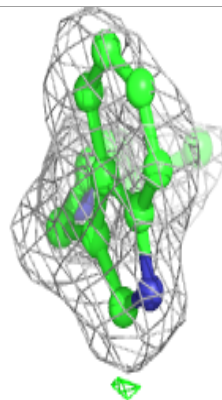
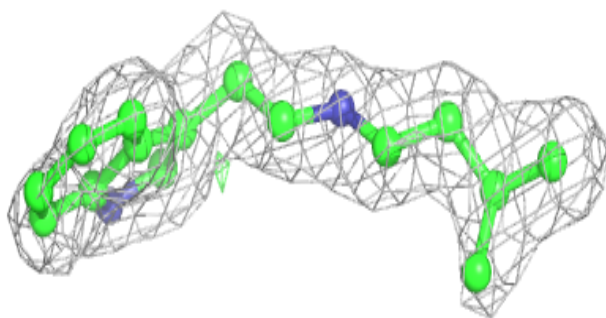
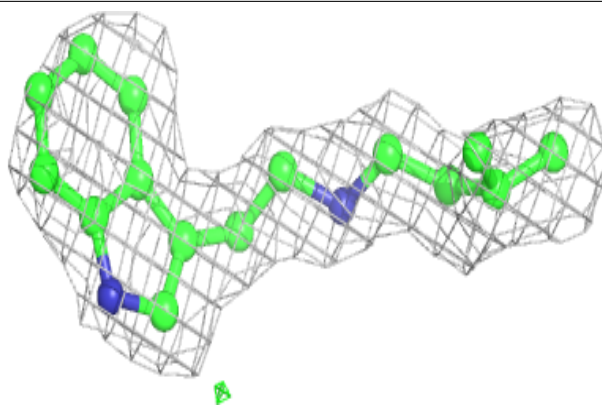
**Electron density around KWK B 401:**

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

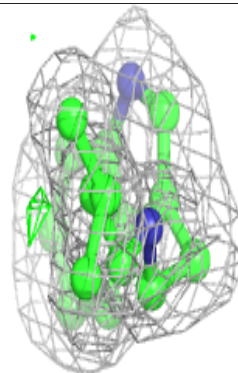
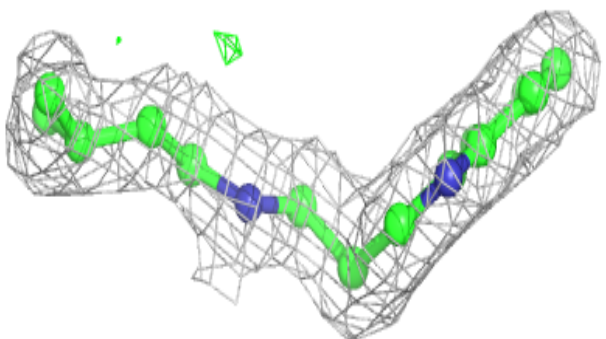
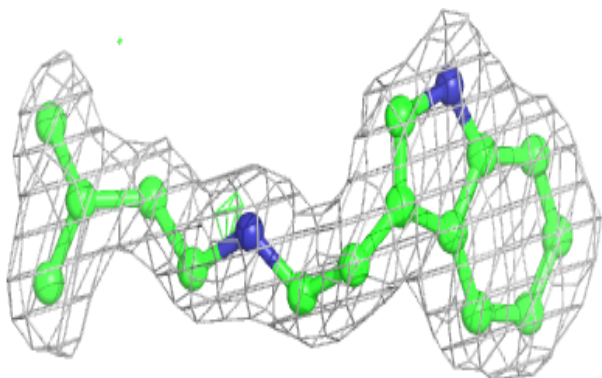


Electron density around KWK E 401:

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

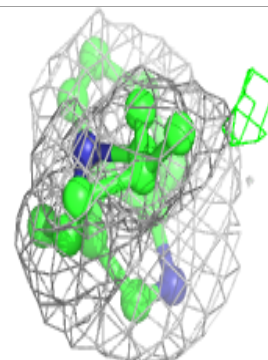
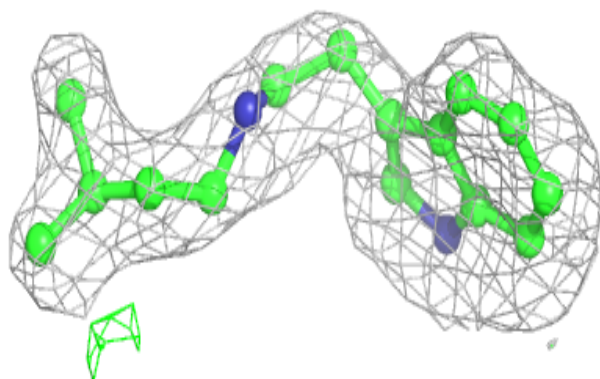
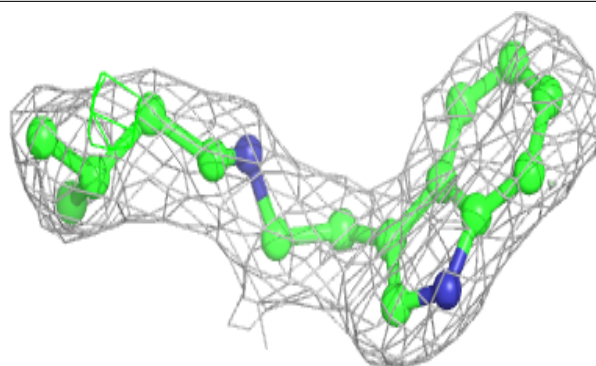
**Electron density around KWK C 402:**

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

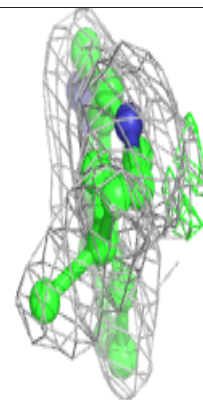
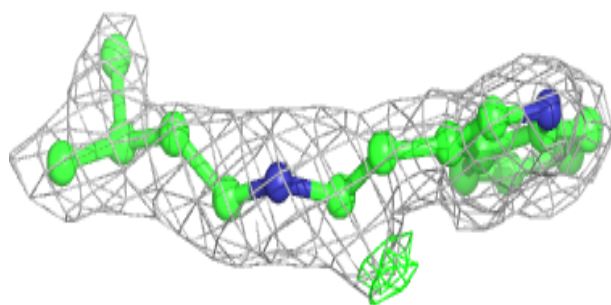
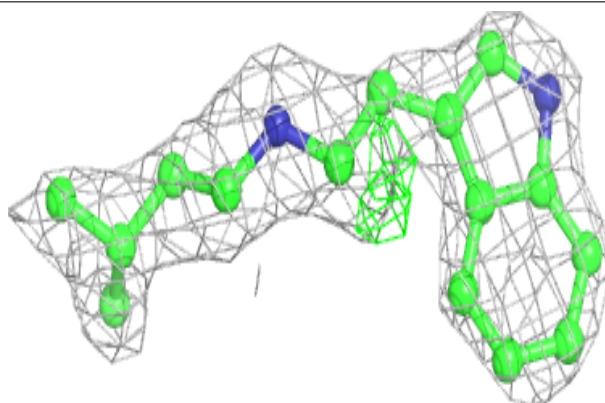


Electron density around KWK A 402 (A):

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

**Electron density around KWK 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)



6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.