



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2024 – 12:35 pm GMT

PDB ID : 8RBB  
Title : p53-Y220C Core Domain Covalently Bound to 2,5,6-trifluoropyridine-3-carbonitrile Soaked at 40 mM  
Authors : Stahlecker, J.; Klett, T.; Stehle, T.; Boeckler, F.M.  
Deposited on : 2023-12-04  
Resolution : 1.69 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

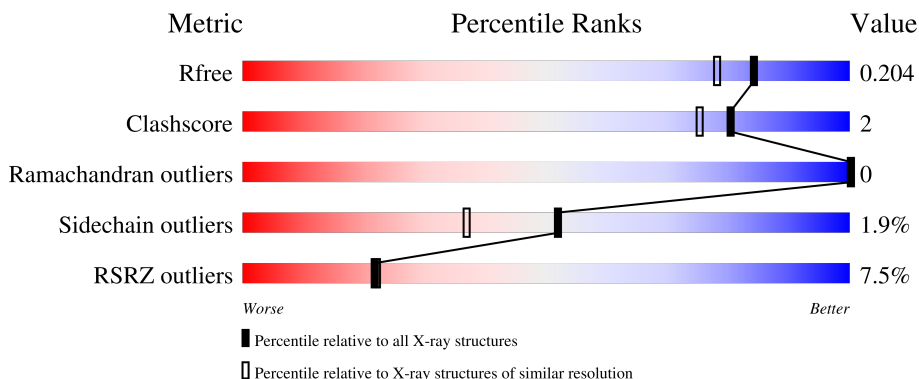
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	219	 6% 82% 5% 13%
1	B	219	 7% 84% 5% 10%

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	YLW	A	401	-	-	X	-
5	EPE	A	409	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3429 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.

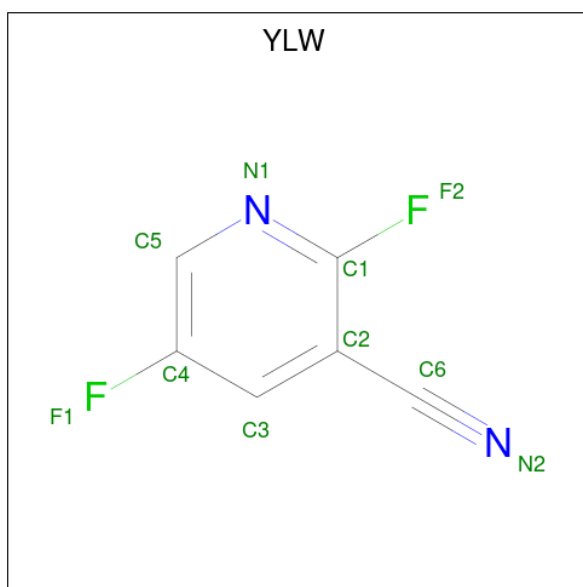
- Molecule 1 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	191	1476	916	268	276	16	0	2	0
1	B	197	1542	953	283	290	16	0	6	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	LEU	MET	engineered mutation	UNP P04637
A	203	ALA	VAL	engineered mutation	UNP P04637
A	220	CYS	TYR	engineered mutation	UNP P04637
A	239	TYR	ASN	engineered mutation	UNP P04637
A	268	ASP	ASN	engineered mutation	UNP P04637
B	133	LEU	MET	engineered mutation	UNP P04637
B	203	ALA	VAL	engineered mutation	UNP P04637
B	220	CYS	TYR	engineered mutation	UNP P04637
B	239	TYR	ASN	engineered mutation	UNP P04637
B	268	ASP	ASN	engineered mutation	UNP P04637

- Molecule 2 is 2,5-bis(fluoranyl)pyridine-3-carbonitrile (three-letter code: YLW) (formula: C<sub>6</sub>H<sub>2</sub>F<sub>2</sub>N<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			10	6	2	2		
2	A	1	Total	C	F	N	0	0
			10	6	2	2		
2	A	1	Total	C	F	N	0	0
			10	6	2	2		
2	A	1	Total	C	F	N	0	0
			9	6	2	1		
2	A	1	Total	C	F	N	0	0
			10	6	2	2		
2	B	1	Total	C	F	N	0	0
			8	5	2	1		
2	B	1	Total	C	F	N	0	0
			10	6	2	2		
2	B	1	Total	C	F	N	0	0
			10	6	2	2		
2	B	1	Total	C	F	N	0	0
			9	6	2	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



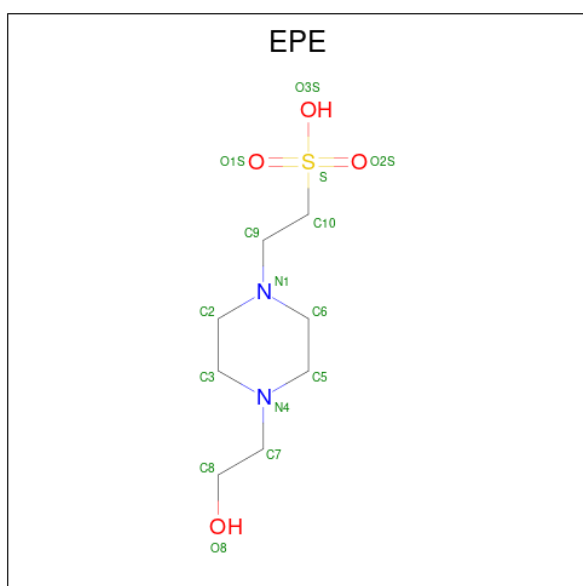
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 7 2 1 3 1	0	0
5	A	1	Total C O S 6 2 3 1	0	0
5	B	1	Total C N O S 13 7 2 3 1	0	0
5	B	1	Total C N O S 7 2 1 3 1	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	128	Total	O	0	0
			128	128		
7	B	128	Total	O	0	0
			128	128		

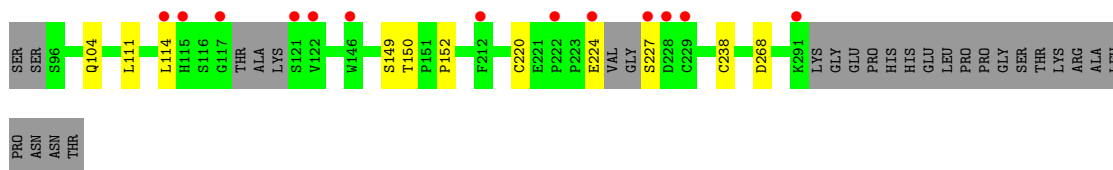


### 3 Residue-property plots [i](#)


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.

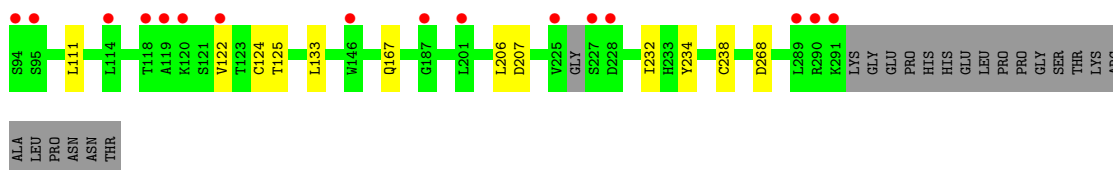
- Molecule 1: Cellular tumor antigen p53

Chain A: 



- Molecule 1: Cellular tumor antigen p53

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.08Å 70.99Å 105.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.97 – 1.69 47.97 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.97-1.69) 99.5 (47.97-1.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 1.69Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.164 , 0.207 0.165 , 0.204	Depositor DCC
$R_{free}$ test set	1507 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.0	Xtrriage
Anisotropy	0.237	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.41$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.97 % 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 6.9143e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, ZN, YLW, EDO, EPE

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	0.49	0/1509	0.68	0/2050
1	B	0.49	0/1577	0.66	0/2145
All	All	0.49	0/3086	0.67	0/4195

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1476	0	1393	10	0
1	B	1542	0	1442	5	0
2	A	49	0	0	5	0
2	B	37	0	0	0	0
3	A	6	0	8	2	0
4	A	16	0	24	0	0
4	B	12	0	18	1	0
5	A	13	0	6	0	0
5	B	20	0	16	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	128	0	0	1	0
7	B	128	0	0	0	0
All	All	3429	0	2907	15	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (15) 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:A:114:LEU:N	2:A:401:YLW:N2	2.37	0.72
1:A:114:LEU:O	2:A:401:YLW:N2	2.23	0.71
1:A:114:LEU:CA	2:A:401:YLW:N2	2.59	0.65
1:A:114:LEU:C	2:A:401:YLW:N2	2.50	0.64
1:B:111[B]:LEU:HG	1:B:268:ASP:HB3	1.82	0.62
1:A:111:LEU:HG	1:A:268:ASP:HB3	1.89	0.55
1:A:104:GLN:NE2	7:A:502:HOH:O	2.29	0.51
1:B:122:VAL:HG11	1:B:125:THR:HB	1.93	0.48
1:A:152:PRO:HG3	3:A:406:GOL:H2	1.97	0.46
1:A:150:THR:O	3:A:406:GOL:O2	2.28	0.45
1:B:206:LEU:HD21	4:B:409:EDO:H22	1.99	0.44
1:A:114:LEU:CB	2:A:401:YLW:N2	2.81	0.43
1:B:232[B]:ILE:HD12	1:B:234:TYR:CZ	2.54	0.42
1:A:224:GLU:O	1:A:227:SER:N	2.52	0.42
1:B:124:CYS:SG	1:B:133:LEU:HD11	2.59	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/219 (85%)	186 (100%)	1 (0%)	0	100	100
1	B	199/219 (91%)	199 (100%)	0	0	100	100
All	All	386/438 (88%)	385 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	162/195 (83%)	159 (98%)	3 (2%)	52	37
1	B	168/195 (86%)	165 (98%)	3 (2%)	54	39
All	All	330/390 (85%)	324 (98%)	6 (2%)	52	39

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	220	CYS
1	A	238	CYS
1	B	167	GLN
1	B	207	ASP
1	B	238	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 for Mogul analysis.

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
5	EPE	A	408	-	6,6,15	1.26	1 (16%)	6,8,20	1.80	2 (33%)
2	YLW	B	404	1	9,10,10	0.30	0	12,13,13	2.37	4 (33%)
2	YLW	B	405	1	8,9,10	1.20	1 (12%)	11,12,13	3.01	4 (36%)
4	EDO	B	406	-	3,3,3	0.39	0	2,2,2	0.54	0
2	YLW	A	405	1	9,10,10	0.41	0	12,13,13	2.22	2 (16%)
4	EDO	A	412	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	B	401	-	3,3,3	0.48	0	2,2,2	0.31	0
2	YLW	B	402	1	8,8,10	1.69	2 (25%)	10,10,13	3.07	4 (40%)
4	EDO	B	409	-	3,3,3	0.56	0	2,2,2	0.14	0
2	YLW	A	404	1	8,9,10	1.22	1 (12%)	11,12,13	2.99	4 (36%)
5	EPE	B	408	-	6,6,15	1.31	1 (16%)	6,8,20	1.94	3 (50%)
4	EDO	A	407	-	3,3,3	0.52	0	2,2,2	0.27	0
4	EDO	A	411	-	3,3,3	0.44	0	2,2,2	0.33	0
4	EDO	A	410	-	3,3,3	0.47	0	2,2,2	0.34	0
3	GOL	A	406	-	5,5,5	0.96	0	5,5,5	0.98	0
2	YLW	A	401	1	9,10,10	0.26	0	12,13,13	2.30	3 (25%)
2	YLW	B	403	1	9,10,10	0.27	0	12,13,13	2.07	3 (25%)
2	YLW	A	403	1	9,10,10	0.29	0	12,13,13	2.33	3 (25%)
5	EPE	A	409	-	5,5,15	0.72	0	7,7,20	1.62	3 (42%)
5	EPE	B	407	-	13,13,15	0.84	1 (7%)	16,18,20	2.92	6 (37%)
2	YLW	A	402	1	9,10,10	0.33	0	12,13,13	1.87	2 (16%)

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
5	EPE	A	408	-	-	1/4/4/19	-
2	YLW	B	404	1	-	0/1/2/2	0/1/1/1
2	YLW	B	405	1	-	-	0/1/1/1
4	EDO	B	406	-	-	1/1/1/1	-
2	YLW	A	405	1	-	0/1/2/2	0/1/1/1
4	EDO	A	412	-	-	1/1/1/1	-
4	EDO	B	401	-	-	0/1/1/1	-
4	EDO	B	409	-	-	0/1/1/1	-
2	YLW	B	402	1	-	-	0/1/1/1
2	YLW	A	404	1	-	-	0/1/1/1
5	EPE	B	408	-	-	0/4/4/19	-
4	EDO	A	407	-	-	1/1/1/1	-
4	EDO	A	411	-	-	1/1/1/1	-
4	EDO	A	410	-	-	0/1/1/1	-
3	GOL	A	406	-	-	2/4/4/4	-
2	YLW	A	401	1	-	0/1/2/2	0/1/1/1
2	YLW	B	403	1	-	0/1/2/2	0/1/1/1
2	YLW	A	403	1	-	0/1/2/2	0/1/1/1
5	EPE	A	409	-	-	3/3/3/19	-
5	EPE	B	407	-	-	4/6/16/19	0/1/1/1
2	YLW	A	402	1	-	0/1/2/2	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	YLW	C1-N1	3.59	1.34	1.30
2	B	405	YLW	C6-C2	-3.26	1.44	1.51
2	A	404	YLW	C6-C2	-3.22	1.44	1.51
5	B	408	EPE	C10-S	3.08	1.81	1.77
5	A	408	EPE	C10-S	2.98	1.81	1.77
2	B	402	YLW	C2-C1	2.95	1.40	1.37
5	B	407	EPE	C10-S	2.50	1.81	1.77

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	404	YLW	C5-N1-C1	7.81	118.57	115.79
2	B	405	YLW	C5-N1-C1	7.45	118.44	115.79
5	B	407	EPE	C5-N4-C3	7.02	119.33	109.52
2	A	405	YLW	C5-N1-C1	6.82	118.22	115.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	YLW	C2-C1-N1	-6.55	123.23	126.83
2	B	404	YLW	C5-N1-C1	6.42	118.07	115.79
2	A	401	YLW	C5-N1-C1	6.38	118.06	115.79
2	A	403	YLW	C5-N1-C1	6.27	118.02	115.79
2	B	402	YLW	C5-N1-C1	5.64	117.59	115.75
2	B	403	YLW	C5-N1-C1	5.48	117.74	115.79
5	B	407	EPE	C7-N4-C3	5.02	118.17	110.66
2	A	402	YLW	C5-N1-C1	4.99	117.57	115.79
5	B	407	EPE	C7-N4-C5	4.38	117.22	110.66
2	B	405	YLW	C3-C2-C1	4.27	118.31	114.46
2	A	404	YLW	C3-C2-C1	4.11	118.17	114.46
5	B	407	EPE	C6-N1-C2	3.56	116.83	108.83
2	A	403	YLW	C2-C3-C4	-3.39	117.17	119.35
5	B	407	EPE	O3S-S-C10	3.35	111.19	105.77
2	B	405	YLW	F2-C1-C2	3.21	120.38	117.46
5	B	408	EPE	O2S-S-C10	3.17	110.73	106.92
2	B	402	YLW	F2-C1-N1	2.98	116.89	114.95
5	A	408	EPE	O1S-S-C10	2.94	110.46	106.92
2	A	404	YLW	F2-C1-C2	2.81	120.02	117.46
5	A	408	EPE	O3S-S-C10	2.73	110.19	105.77
2	A	401	YLW	C2-C3-C4	-2.63	117.66	119.35
2	B	404	YLW	C3-C2-C6	2.60	123.66	119.74
2	B	404	YLW	C2-C3-C4	-2.59	117.69	119.35
2	B	402	YLW	C3-C2-C1	2.56	118.26	116.35
2	B	403	YLW	C4-C5-N1	2.49	122.96	121.46
5	B	407	EPE	C2-C3-N4	2.48	113.60	110.80
2	A	404	YLW	C2-C1-N1	-2.38	122.64	127.43
2	B	405	YLW	C2-C1-N1	-2.38	122.65	127.43
2	A	403	YLW	C3-C2-C6	2.37	123.31	119.74
5	A	409	EPE	O3S-S-C10	2.36	109.58	105.77
5	A	409	EPE	O2S-S-C10	2.28	109.66	106.92
2	A	401	YLW	C4-C5-N1	2.28	122.83	121.46
2	A	402	YLW	C4-C5-N1	2.23	122.80	121.46
5	A	409	EPE	O1S-S-C10	2.16	109.51	106.92
5	B	408	EPE	O1S-S-C10	2.12	109.47	106.92
2	B	404	YLW	C1-C2-C6	-2.07	117.98	120.98
5	B	408	EPE	O3S-S-C10	2.06	109.11	105.77
2	A	405	YLW	C2-C3-C4	-2.03	118.05	119.35
2	B	403	YLW	C2-C3-C4	-2.02	118.05	119.35

There are no chirality outliers.

All (14) torsion outliers are listed below:



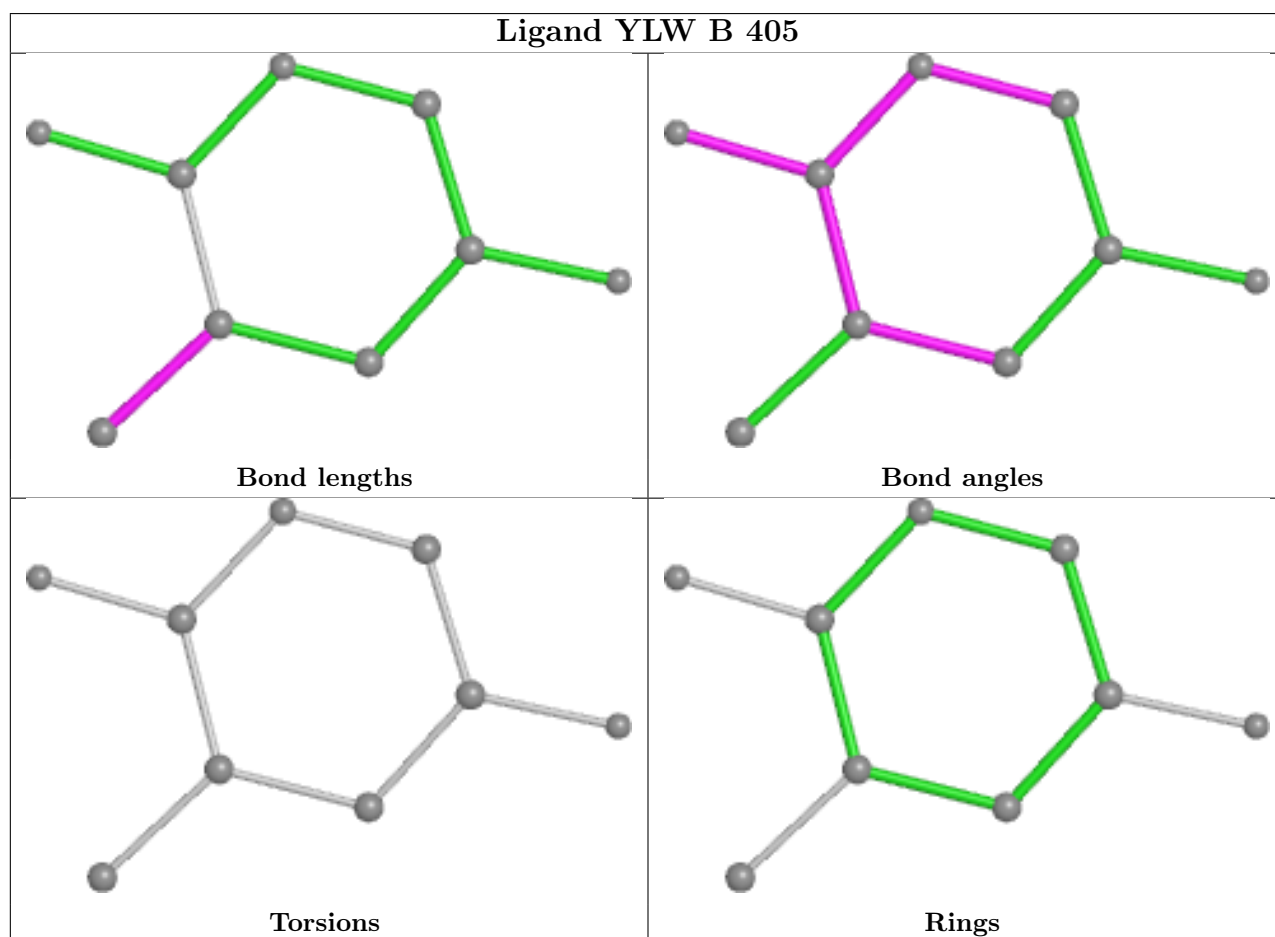
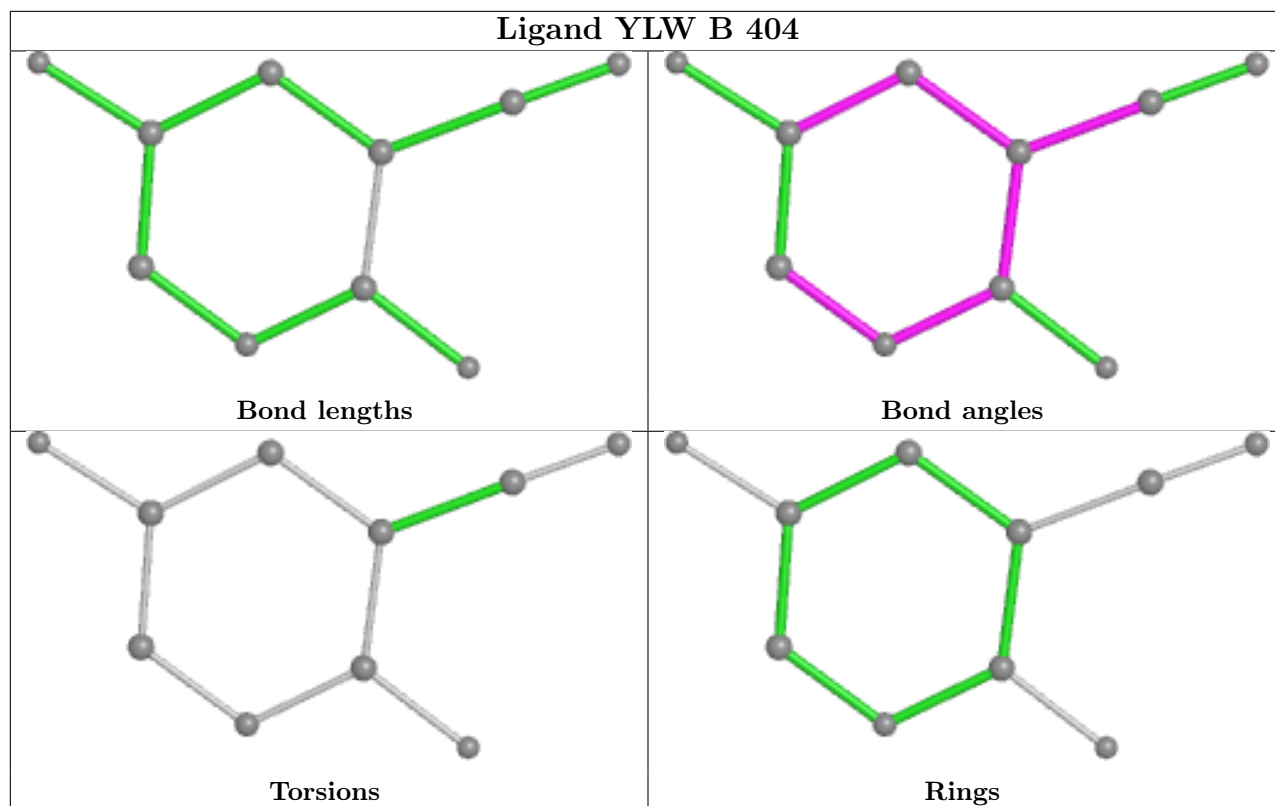
Mol	Chain	Res	Type	Atoms
5	A	408	EPE	S-C10-C9-N1
5	A	409	EPE	C9-C10-S-O1S
5	A	409	EPE	C9-C10-S-O2S
5	A	409	EPE	C9-C10-S-O3S
5	B	407	EPE	C9-C10-S-O2S
5	B	407	EPE	C9-C10-S-O3S
3	A	406	GOL	O1-C1-C2-C3
4	A	407	EDO	O1-C1-C2-O2
4	A	411	EDO	O1-C1-C2-O2
3	A	406	GOL	O1-C1-C2-O2
5	B	407	EPE	S-C10-C9-N1
4	A	412	EDO	O1-C1-C2-O2
5	B	407	EPE	C9-C10-S-O1S
4	B	406	EDO	O1-C1-C2-O2

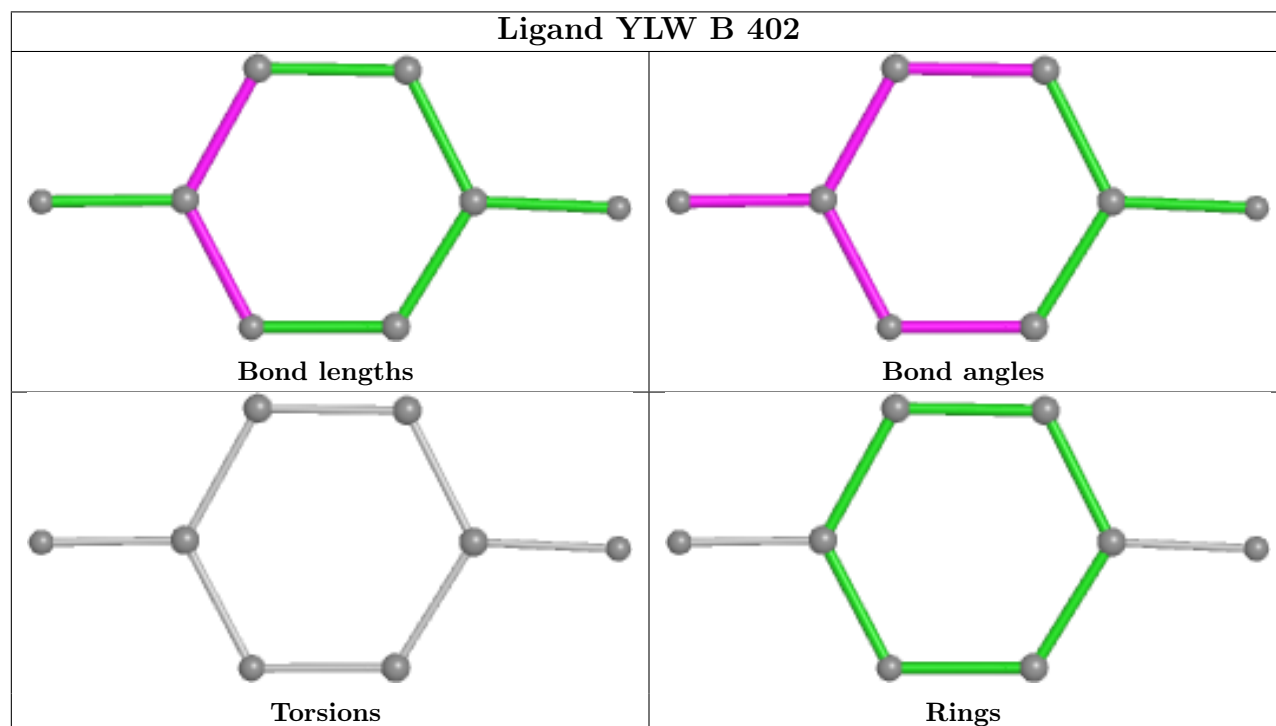
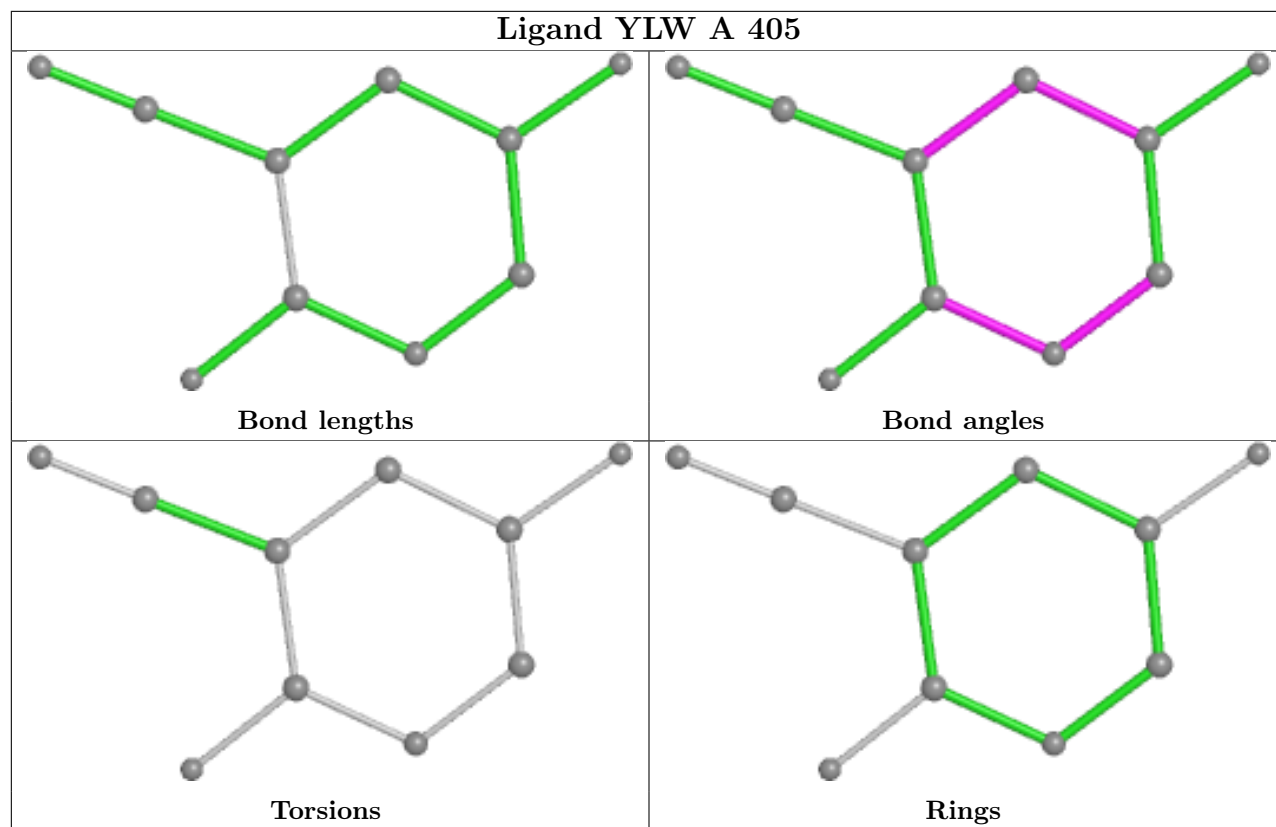
There are no ring outliers.

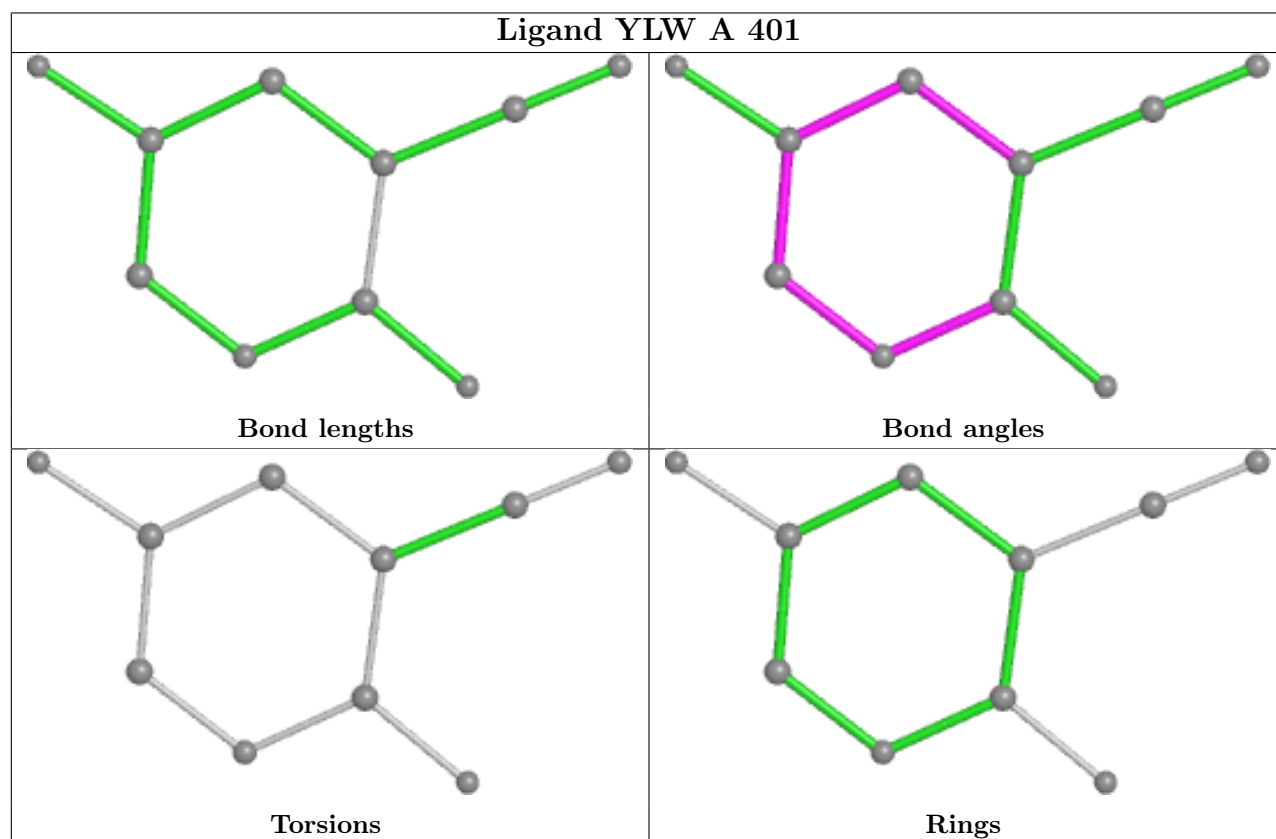
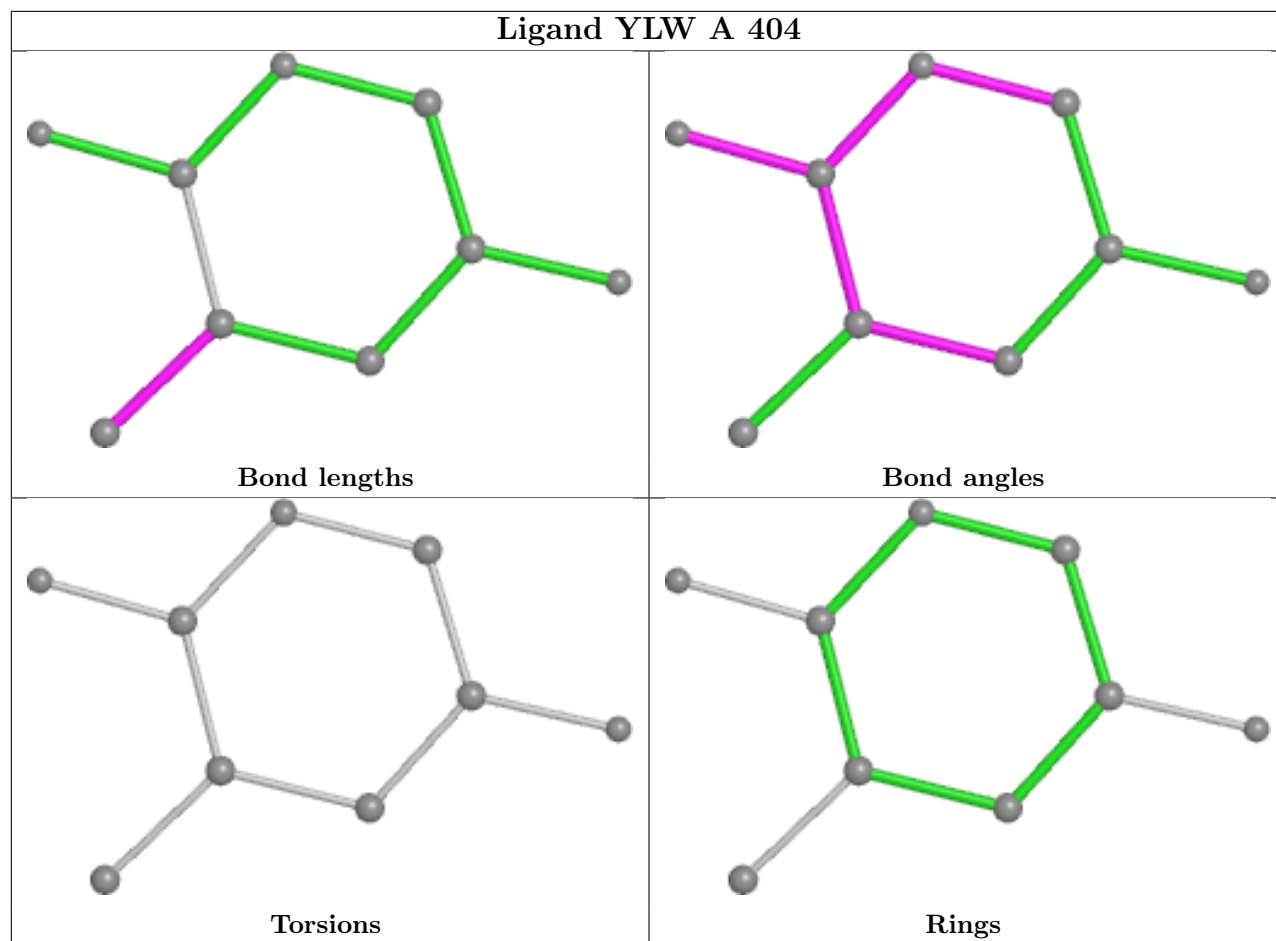
3 monomers are involved in 8 short contacts:

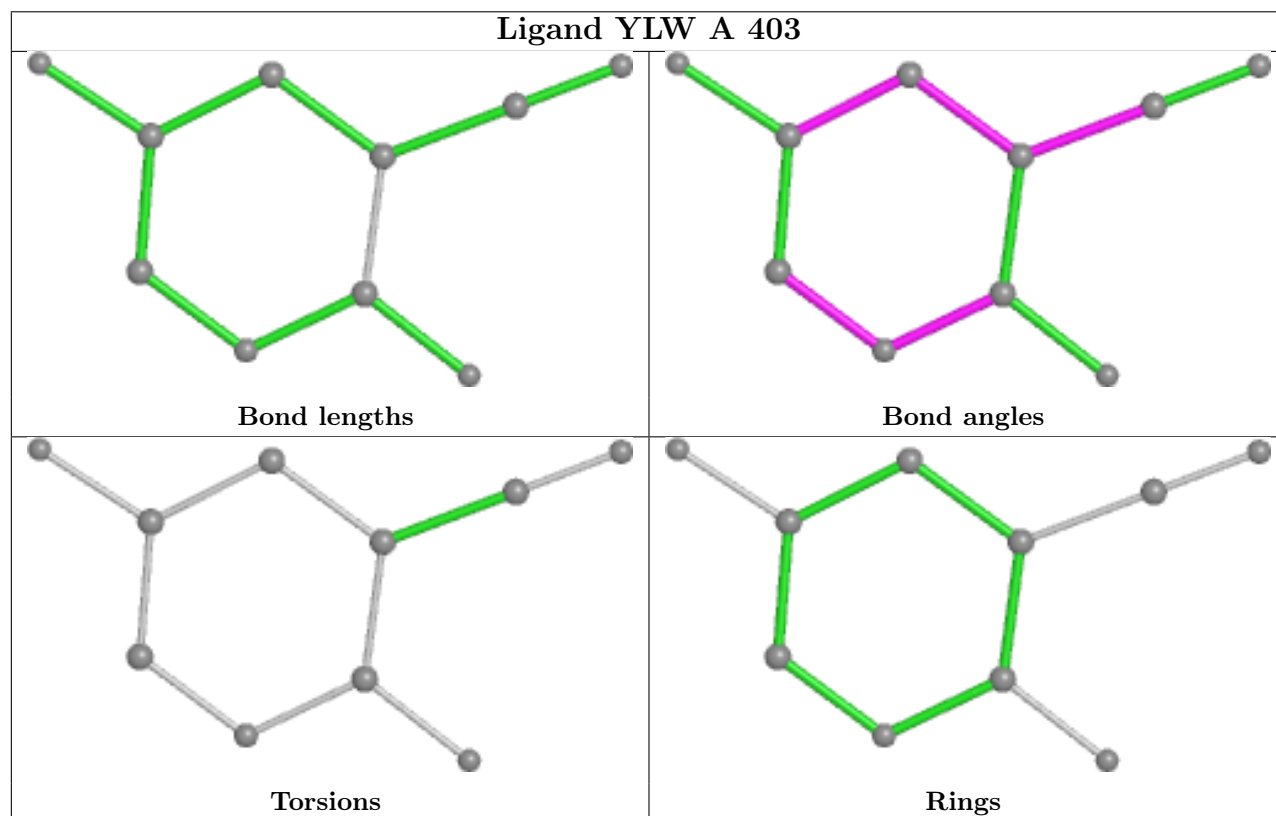
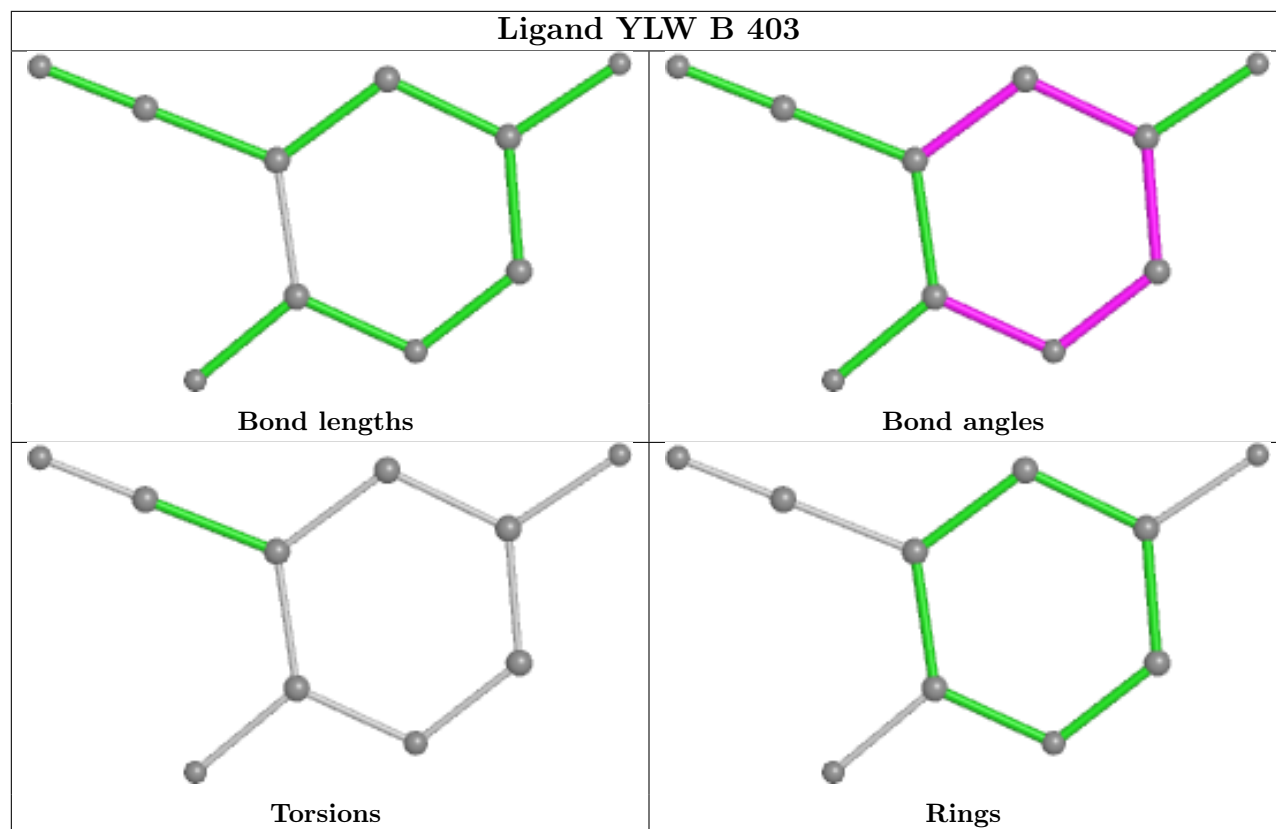
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	409	EDO	1	0
3	A	406	GOL	2	0
2	A	401	YLW	5	0

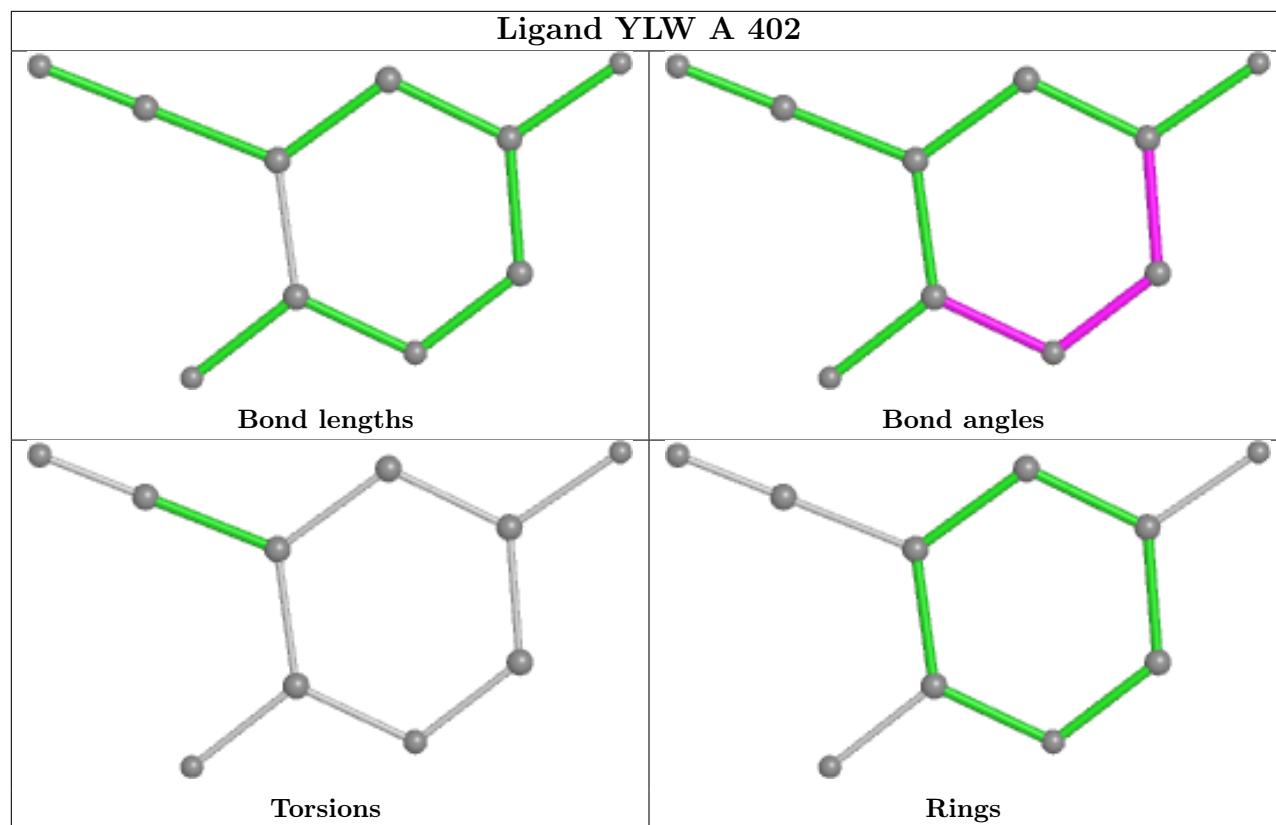
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	191/219 (87%)	0.18	13 (6%) 25 25	14, 37, 65, 75	2 (1%)
1	B	197/219 (89%)	0.19	16 (8%) 19 20	14, 37, 66, 81	6 (3%)
All	All	388/438 (88%)	0.18	29 (7%) 22 22	14, 37, 66, 81	8 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	118	THR	5.4
1	A	227	SER	4.2
1	A	114	LEU	4.1
1	B	119	ALA	3.8
1	B	225	VAL	3.7
1	A	228	ASP	3.7
1	A	146	TRP	3.6
1	A	117	GLY	3.5
1	A	115	HIS	3.3
1	A	224	GLU	3.3
1	B	94	SER	3.3
1	A	121	SER	3.2
1	B	289	LEU	3.1
1	A	122	VAL	2.9
1	B	146	TRP	2.9
1	B	228	ASP	2.7
1	B	95	SER	2.6
1	A	229	CYS	2.6
1	B	291	LYS	2.6
1	B	120	LYS	2.4
1	B	114	LEU	2.4
1	A	291	LYS	2.4
1	B	290	ARG	2.4
1	A	222	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	122	VAL	2.3
1	B	201	LEU	2.2
1	B	187	GLY	2.1
1	B	227	SER	2.1
1	A	212	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	YLW	B	405	9/10	0.71	0.15	74,77,78,80	0
2	YLW	A	404	9/10	0.73	0.14	69,76,78,79	0
5	EPE	B	407	13/15	0.73	0.18	73,76,99,100	0
4	EDO	B	406	4/4	0.78	0.19	73,74,75,76	0
2	YLW	A	405	10/10	0.80	0.13	66,75,81,84	0
5	EPE	A	409	6/15	0.81	0.21	96,100,101,102	0
4	EDO	A	410	4/4	0.83	0.17	75,75,76,77	0
2	YLW	B	402	8/10	0.83	0.13	58,61,65,69	0
4	EDO	A	411	4/4	0.84	0.17	56,60,62,64	0
3	GOL	A	406	6/6	0.85	0.13	69,70,70,71	0
5	EPE	A	408	7/15	0.86	0.14	88,93,96,97	0
2	YLW	A	401	10/10	0.86	0.11	61,64,68,70	0
4	EDO	B	409	4/4	0.86	0.14	58,61,63,66	0
5	EPE	B	408	7/15	0.87	0.13	85,87,90,91	0
4	EDO	A	407	4/4	0.88	0.15	72,74,75,76	0
4	EDO	A	412	4/4	0.89	0.17	69,70,70,71	0
4	EDO	B	401	4/4	0.89	0.17	65,66,67,68	0
2	YLW	A	402	10/10	0.92	0.11	59,61,64,66	0

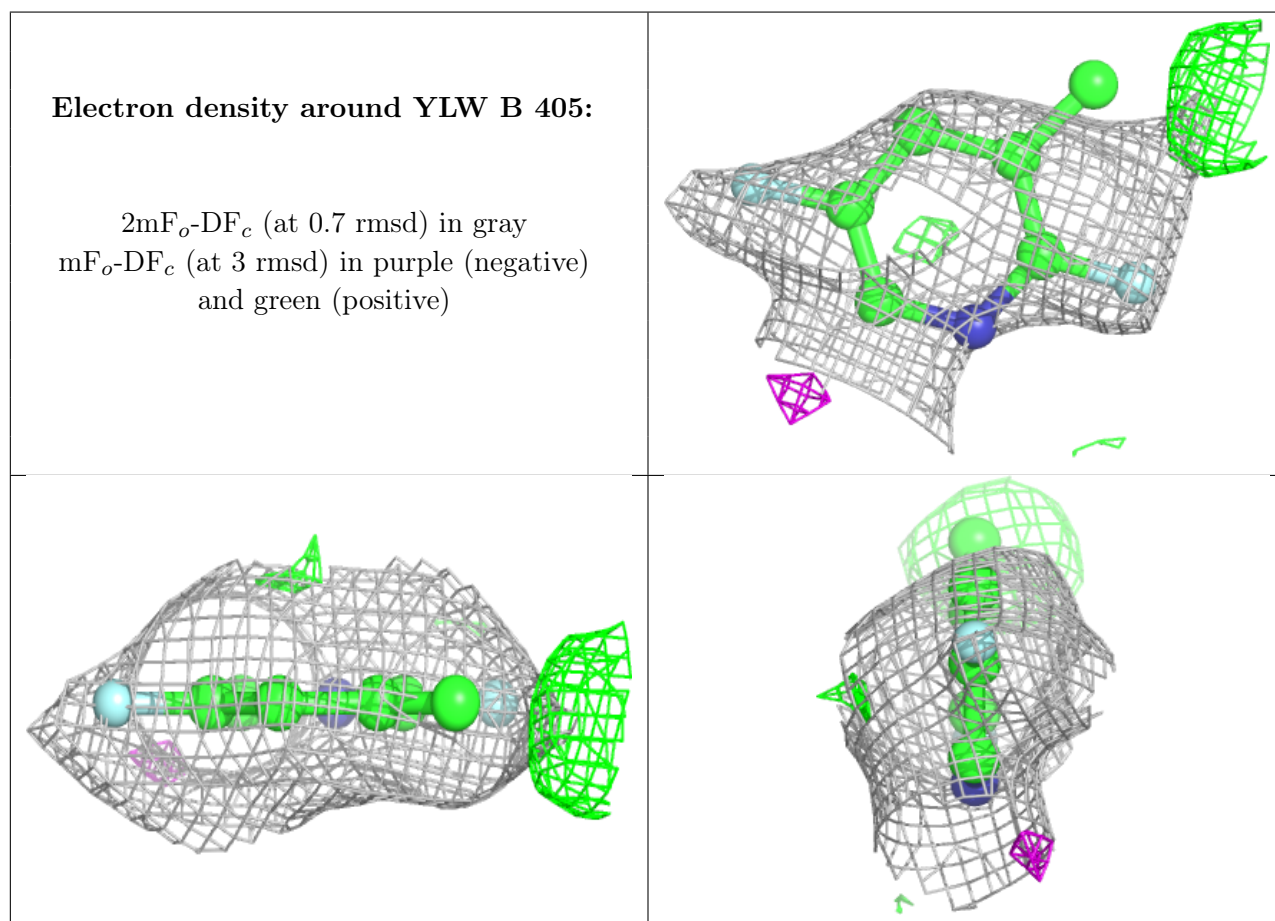
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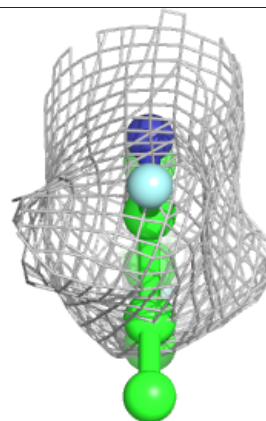
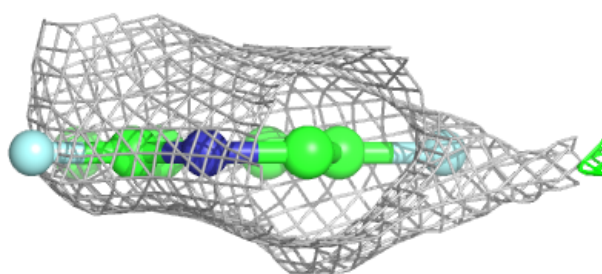
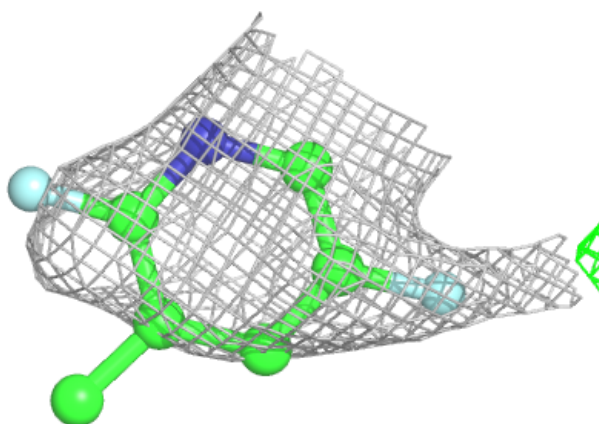
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	YLW	A	403	10/10	0.92	0.14	52,55,58,59	0
2	YLW	B	403	10/10	0.93	0.08	45,49,52,56	0
2	YLW	B	404	10/10	0.94	0.09	49,51,53,54	0
6	ZN	A	413	1/1	1.00	0.02	35,35,35,35	0
6	ZN	B	410	1/1	1.00	0.03	37,37,37,37	0

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.

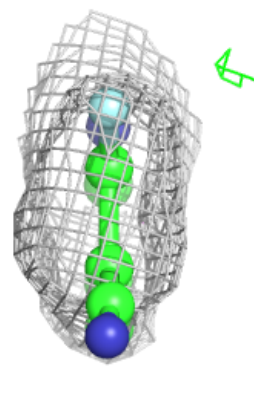
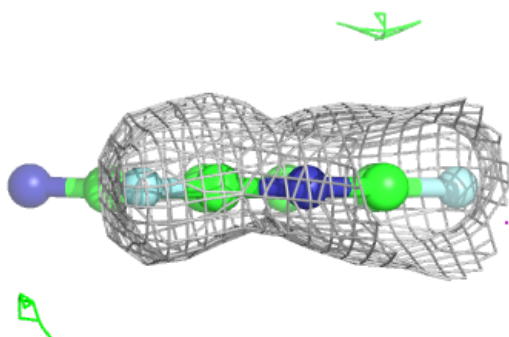
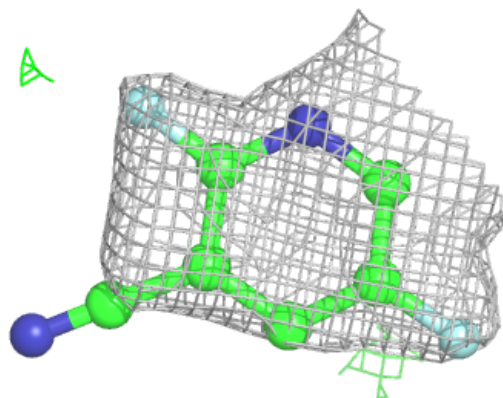


**Electron density around YLW A 404:**

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

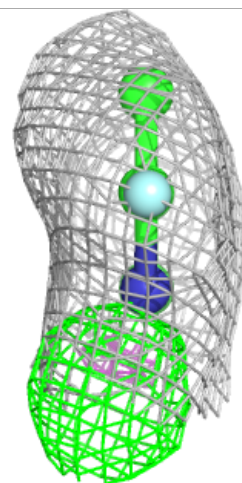
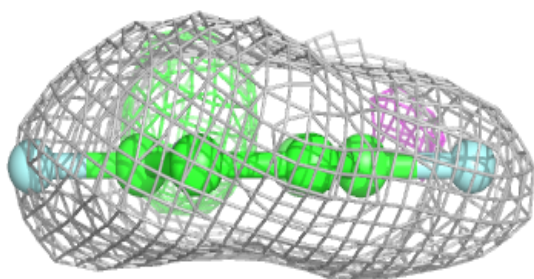
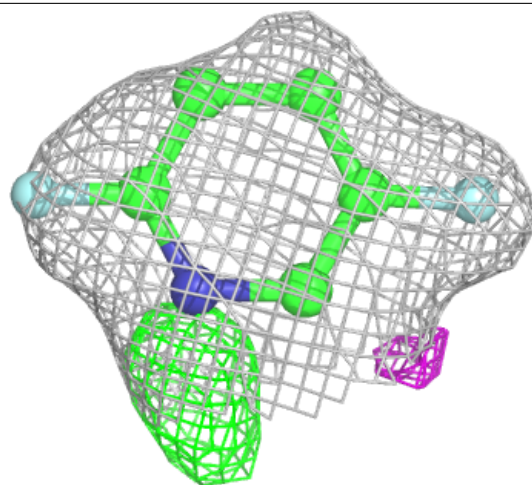
**Electron density around YLW A 405:**

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



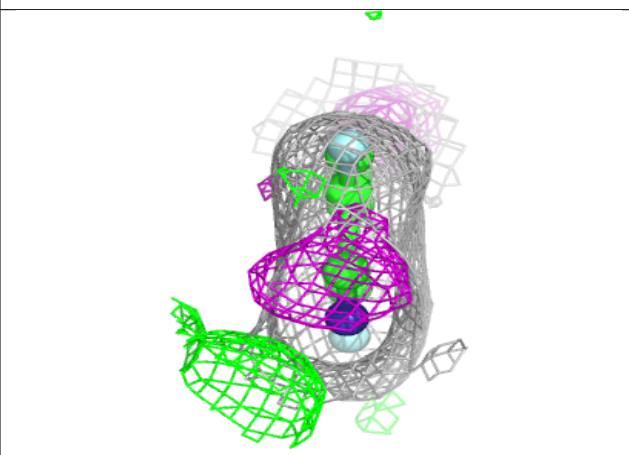
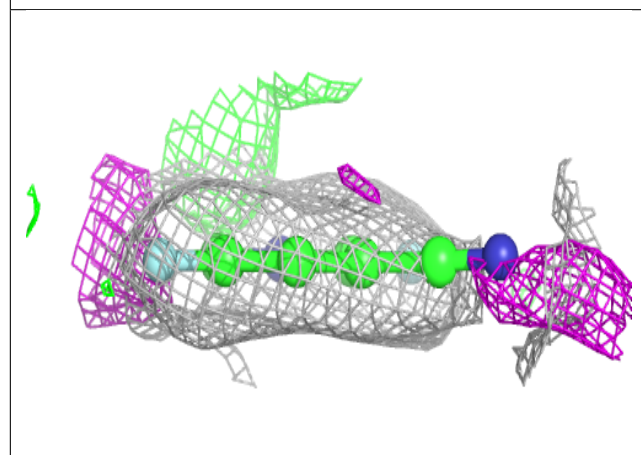
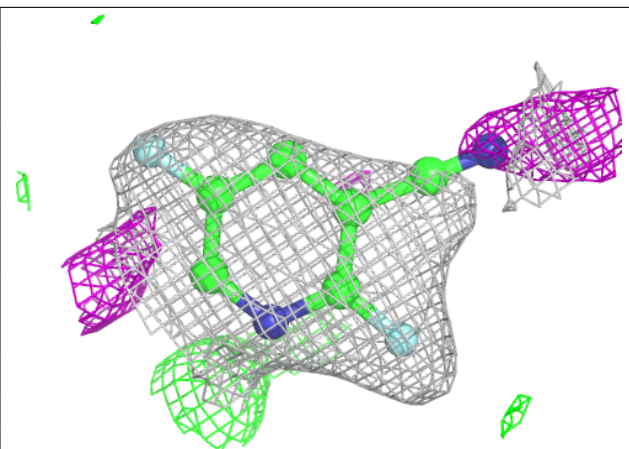
**Electron density around YLW B 402:**

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



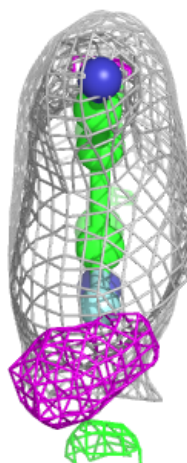
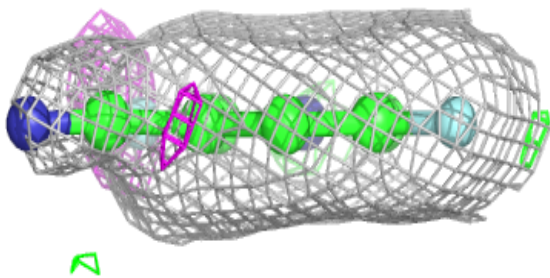
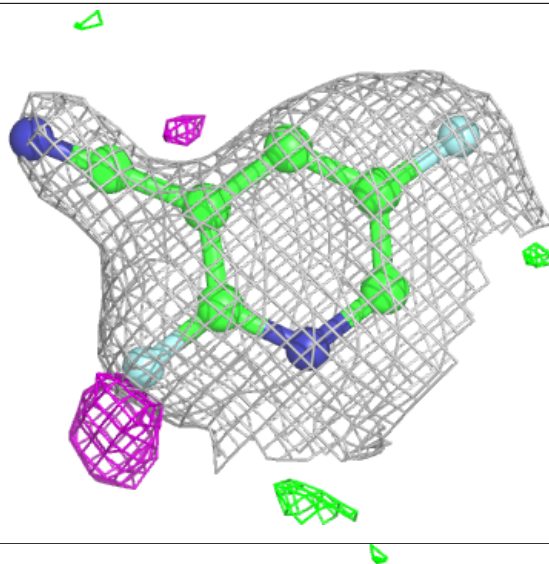
**Electron density around YLW A 401:**

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



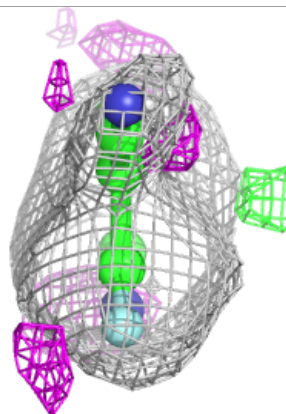
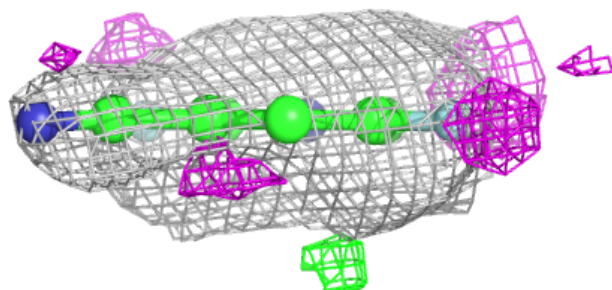
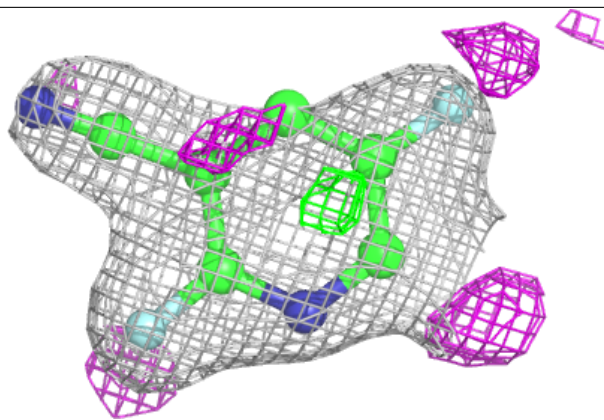
**Electron density around YLW A 402:**

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

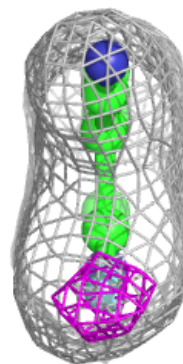
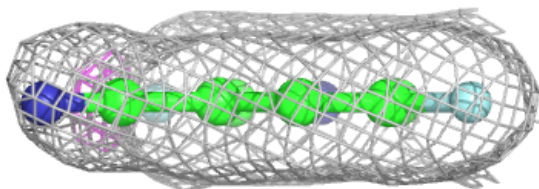
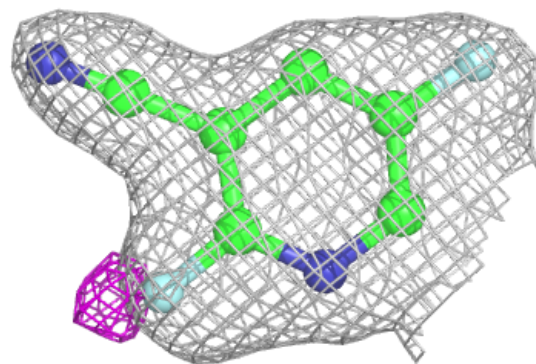


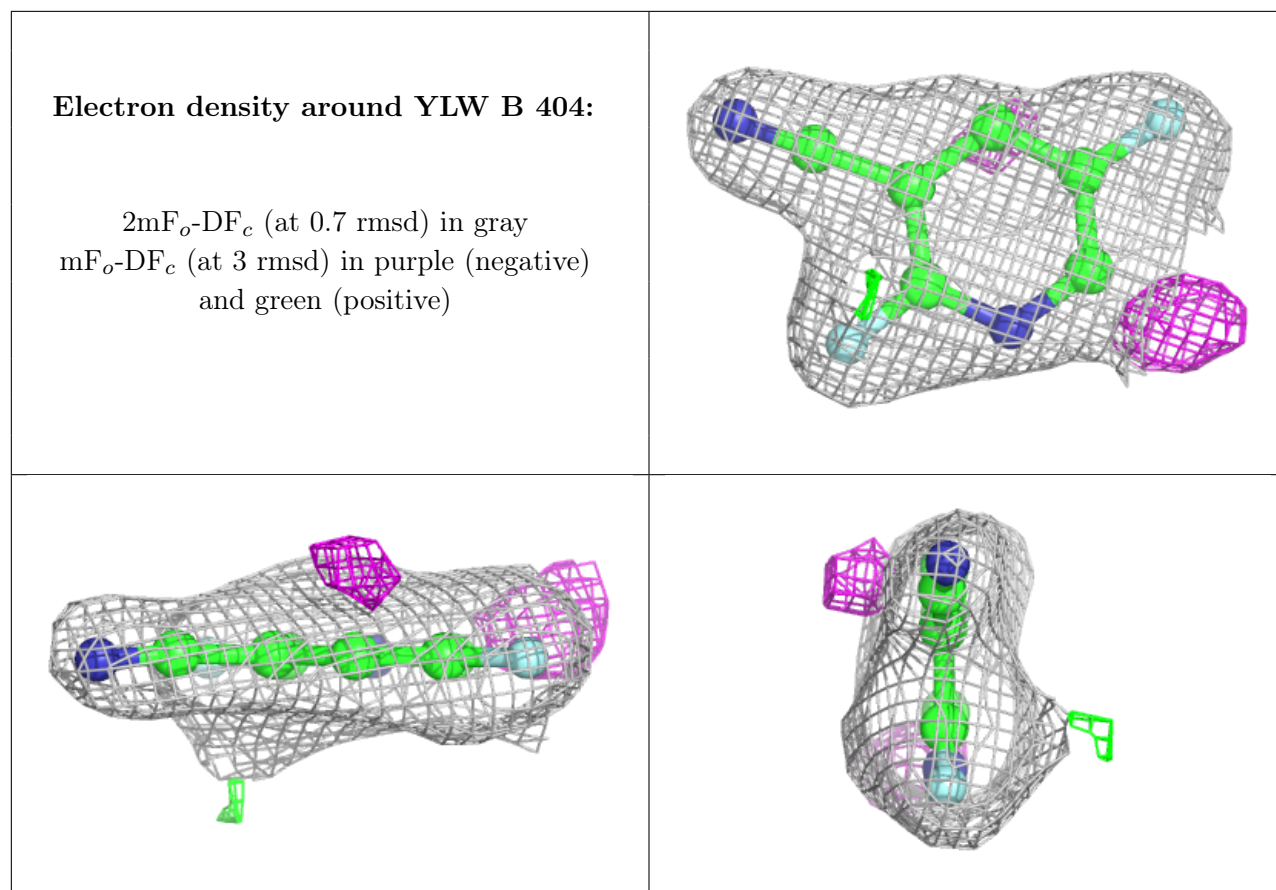
**Electron density around YLW A 403:**

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

**Electron density around YLW B 403:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.