



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:41 AM EDT

PDB ID : 7LTL  
Title : STRUCTURE OF HUMAN HDAC2 IN COMPLEX WITH AN INHIBITOR  
LACKING A ZINC BINDING GROUP (COMPOUND 19)  
Authors : Klein, D.J.; Beshore, D.C.  
Deposited on : 2021-02-19  
Resolution : 1.49 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

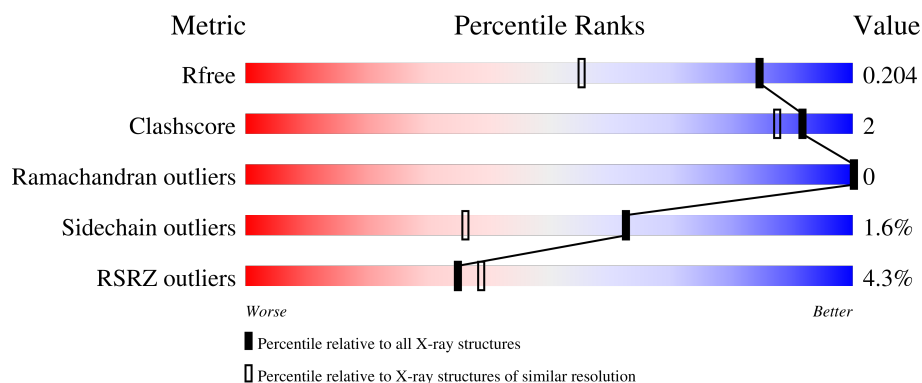
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.49 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\geq 3$ , 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	376	<div> <div>3%</div> <div>93%</div> <div>6%</div> <div>• •</div> </div>
1	B	376	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	C	376	<div> <div>9%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>

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
3	SO4	B	404	-	-	-	X
3	SO4	C	406	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10339 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 Histone deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	12	0
			2989	1910	505	547	27			
1	B	365	Total	C	N	O	S	0	14	0
			3006	1924	503	550	29			
1	C	367	Total	C	N	O	S	0	7	0
			2978	1901	504	547	26			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

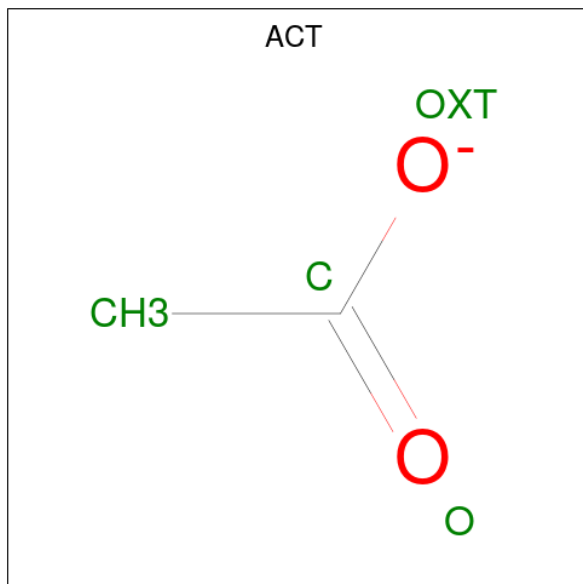


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



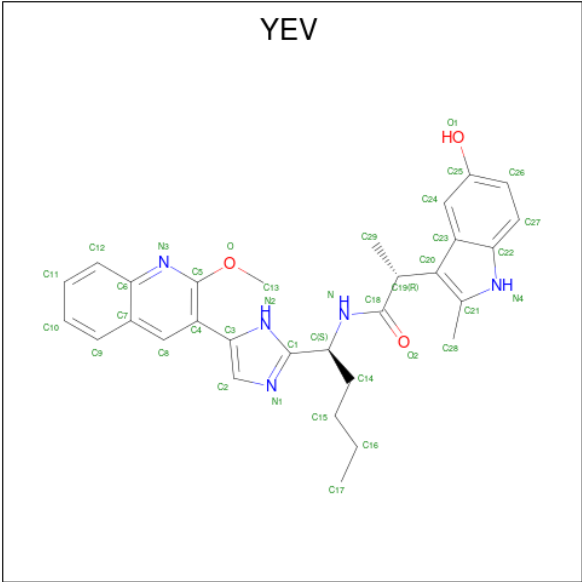
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is (2R)-2-(5-hydroxy-2-methyl-1H-indol-3-yl)-N-{(1S)-1-[5-(2-methoxyquinolin-3-yl)-1H-imidazol-2-yl]pentyl}propanamide (three-letter code: YEV) (formula: C<sub>30</sub>H<sub>33</sub>N<sub>5</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			38	30	5	3		
7	B	1	Total	C	N	O	0	0
			38	30	5	3		
7	C	1	Total	C	N	O	0	0
			38	30	5	3		

- Molecule 8 is water.

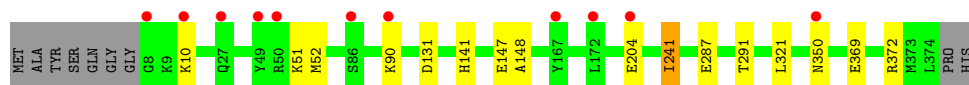
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	368	Total	O	0	0
			368	368		
8	B	432	Total	O	0	3
			435	435		
8	C	324	Total	O	0	3
			326	326		



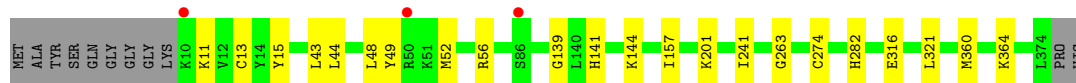
### 3 Residue-property plots

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.

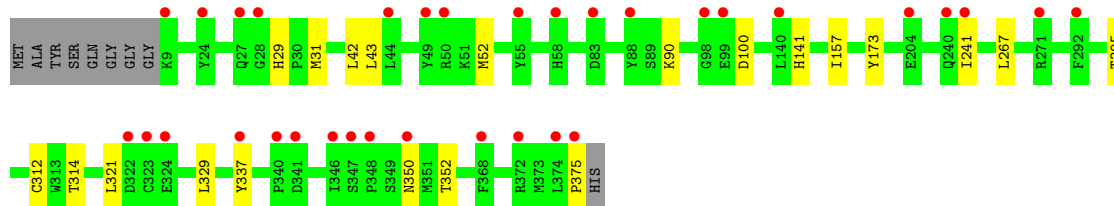
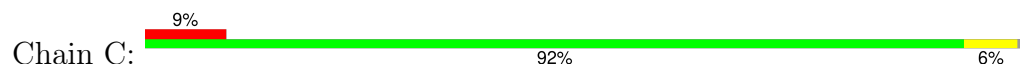
- Molecule 1: Histone deacetylase 2



- Molecule 1: Histone deacetylase 2



- Molecule 1: Histone deacetylase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.35Å 98.76Å 139.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.77 – 1.49 21.77 – 1.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (21.77-1.49) 98.7 (21.77-1.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.49Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.170 , 0.195 0.178 , 0.204	Depositor DCC
$R_{free}$ test set	10293 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: YEV, ACT, ZN, SO4, PEG, CA

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	0.53	0/3079	0.66	1/4154 (0.0%)
1	B	0.55	0/3104	0.67	0/4189
1	C	0.49	0/3063	0.63	2/4134 (0.0%)
All	All	0.52	0/9246	0.65	3/12477 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	PRO	N-CA-CB	5.59	110.01	103.30
1	C	305	THR	N-CA-C	-5.33	96.61	111.00
1	A	241	ILE	N-CA-CB	-5.02	99.25	110.80

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	2989	0	2888	5	0
1	B	3006	0	2905	15	0
1	C	2978	0	2873	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	20	0	0	0	0
3	B	15	0	0	0	0
3	C	25	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
6	A	21	0	30	0	0
6	B	14	0	20	0	0
6	C	7	0	10	0	0
7	A	38	0	0	0	0
7	B	38	0	0	0	0
7	C	38	0	0	0	0
8	A	368	0	0	0	0
8	B	435	0	0	1	0
8	C	326	0	0	0	0
All	All	10339	0	8735	28	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 (28) 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:201:LYS:HD2	1:B:274[B]:CYS:SG	2.13	0.89
1:B:282:HIS:HD2	1:B:316:GLU:OE2	1.60	0.84
1:C:29:HIS:HD2	1:C:31:MET:H	1.32	0.77
1:B:43[A]:LEU:HD12	1:B:49:TYR:HE1	1.54	0.71
1:A:287:GLU:O	1:A:291:THR:HG23	1.95	0.67
1:B:144:LYS:HE3	8:B:536:HOH:O	1.95	0.67
1:C:29:HIS:CD2	1:C:31:MET:H	2.16	0.62
1:B:43[A]:LEU:HD12	1:B:49:TYR:CE1	2.34	0.61
1:B:201:LYS:HD2	1:B:274[B]:CYS:HG	1.66	0.60
1:B:201:LYS:CD	1:B:274[B]:CYS:SG	2.89	0.60
1:A:52:MET:HG2	1:A:321:LEU:HD21	1.83	0.59
1:B:44:LEU:HB2	1:B:49:TYR:CZ	2.41	0.56
1:B:52:MET:HB3	1:B:321:LEU:HD21	1.93	0.49
1:B:241:ILE:HG12	1:B:360:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:HIS:HE1	1:C:100:ASP:O	1.95	0.49
1:A:369:GLU:HG2	1:A:372[A]:ARG:NH2	2.28	0.48
1:C:43:LEU:HD21	1:C:314:THR:HA	1.97	0.47
1:B:263:GLY:O	1:B:282:HIS:HE1	1.98	0.46
1:B:43[B]:LEU:HD23	1:B:48:LEU:HD12	1.98	0.45
1:A:147:GLU:HG2	1:A:148:ALA:O	2.17	0.45
1:B:241:ILE:HG22	1:B:364:LYS:HD3	1.98	0.45
1:C:42:LEU:HD11	1:C:329:LEU:HD22	2.00	0.43
1:A:10:LYS:HB3	1:A:131:ASP:HB2	2.00	0.43
1:C:267:LEU:HD11	1:C:312:CYS:HB2	2.01	0.43
1:B:139:GLY:HA2	1:B:157:ILE:HD11	2.01	0.42
1:C:52:MET:HG2	1:C:321:LEU:HD21	2.01	0.41
1:C:157:ILE:HG21	1:C:173:TYR:CE1	2.56	0.41
1:B:13[B]:CYS:HG	1:B:15:TYR:HE1	1.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/376 (99%)	365 (98%)	6 (2%)	0	100	100
1	B	374/376 (100%)	369 (99%)	5 (1%)	0	100	100
1	C	369/376 (98%)	363 (98%)	6 (2%)	0	100	100
All	All	1114/1128 (99%)	1097 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	322/322 (100%)	316 (98%)	6 (2%)	57	27
1	B	326/322 (101%)	323 (99%)	3 (1%)	78	61
1	C	319/322 (99%)	313 (98%)	6 (2%)	57	27
All	All	967/966 (100%)	952 (98%)	15 (2%)	62	36

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	90	LYS
1	A	141	HIS
1	A	204	GLU
1	A	241	ILE
1	A	350	ASN
1	B	11	LYS
1	B	56	ARG
1	B	141	HIS
1	C	90	LYS
1	C	141	HIS
1	C	241	ILE
1	C	337	TYR
1	C	350	ASN
1	C	352	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	350	ASN
1	B	91	GLN
1	B	282	HIS
1	B	354	GLN
1	C	29	HIS
1	C	240	GLN

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Mol	Chain	Res	Type
1	C	350	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 9 are monoatomic - leaving 24 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	$\# Z  > 2$
3	SO4	B	404	-	4,4,4	0.23	0	6,6,6	0.09	0
6	PEG	A	409	-	6,6,6	0.15	0	5,5,5	0.11	0
3	SO4	C	403	-	4,4,4	0.50	0	6,6,6	0.18	0
7	YEV	A	412	-	35,42,42	0.62	0	39,60,60	0.72	1 (2%)
3	SO4	C	404	-	4,4,4	0.27	0	6,6,6	0.16	0
3	SO4	A	405	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	B	403	-	4,4,4	0.26	0	6,6,6	0.12	0
6	PEG	A	411	-	6,6,6	0.17	0	5,5,5	0.11	0
5	ACT	A	408	2	3,3,3	1.40	1 (33%)	3,3,3	0.74	0
3	SO4	A	403	-	4,4,4	0.39	0	6,6,6	0.71	0
6	PEG	C	410	-	6,6,6	0.06	0	5,5,5	0.06	0
5	ACT	B	407	2	3,3,3	1.57	0	3,3,3	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	YEV	C	411	-	35,42,42	0.65	0	39,60,60	0.77	1 (2%)
6	PEG	B	409	-	6,6,6	0.11	0	5,5,5	0.08	0
5	ACT	C	409	2	3,3,3	1.57	1 (33%)	3,3,3	0.94	0
3	SO4	C	406	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	404	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	B	402	-	4,4,4	0.50	0	6,6,6	0.15	0
6	PEG	A	410	-	6,6,6	0.13	0	5,5,5	0.12	0
6	PEG	B	408	-	6,6,6	0.06	0	5,5,5	0.06	0
3	SO4	C	402	-	4,4,4	0.29	0	6,6,6	0.05	0
3	SO4	C	405	-	4,4,4	0.25	0	6,6,6	0.08	0
7	YEV	B	410	-	35,42,42	0.67	1 (2%)	39,60,60	0.79	1 (2%)
3	SO4	A	402	-	4,4,4	0.22	0	6,6,6	0.16	0

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
7	YEV	C	411	-	-	1/17/26/26	0/5/5/5
6	PEG	A	409	-	-	1/4/4/4	-
6	PEG	A	410	-	-	2/4/4/4	-
6	PEG	B	408	-	-	0/4/4/4	-
7	YEV	A	412	-	-	1/17/26/26	0/5/5/5
6	PEG	A	411	-	-	2/4/4/4	-
6	PEG	B	409	-	-	3/4/4/4	-
6	PEG	C	410	-	-	2/4/4/4	-
7	YEV	B	410	-	-	1/17/26/26	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	410	YEV	C19-C18	2.30	1.56	1.53
5	C	409	ACT	CH3-C	2.08	1.57	1.49
5	A	408	ACT	CH3-C	2.03	1.57	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	410	YEV	O-C5-C4	-2.30	115.03	117.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	411	YEV	O-C5-C4	-2.26	115.08	117.74
7	A	412	YEV	O-C5-C4	-2.18	115.17	117.74

There are no chirality outliers.

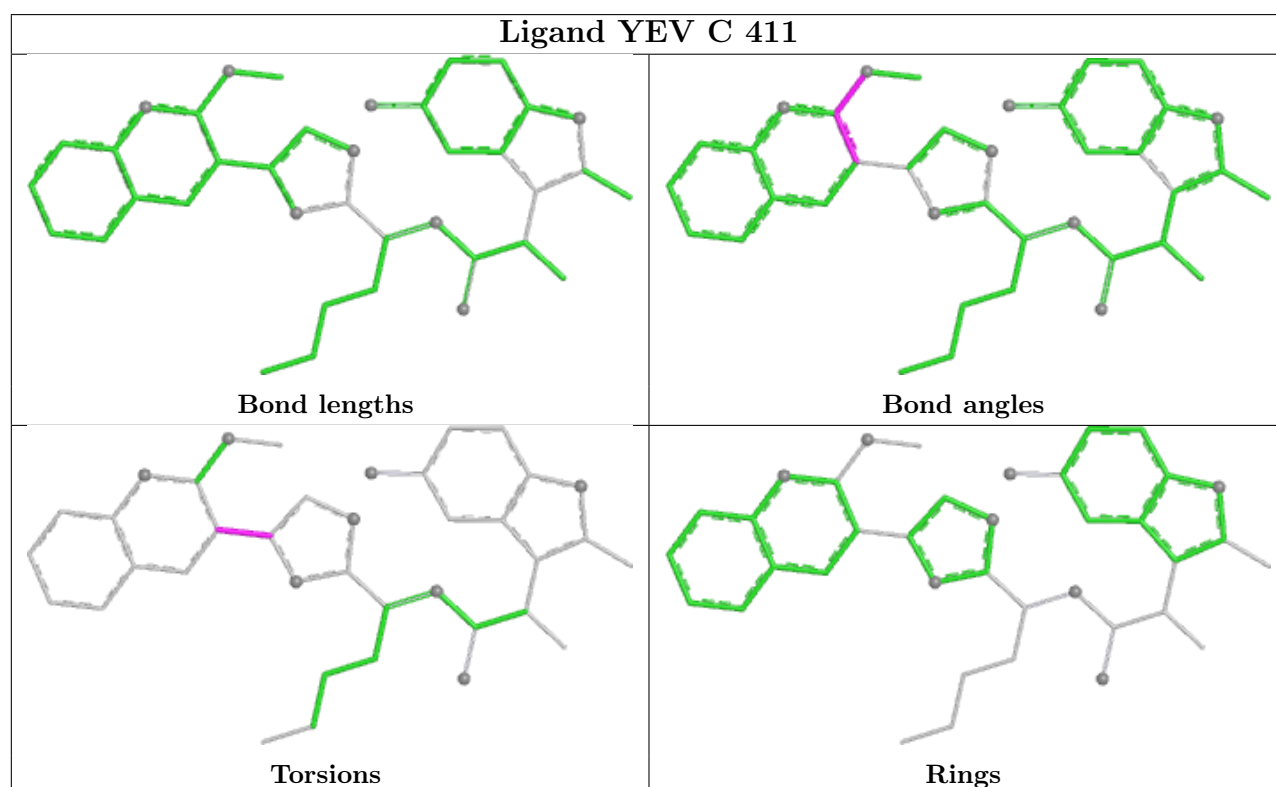
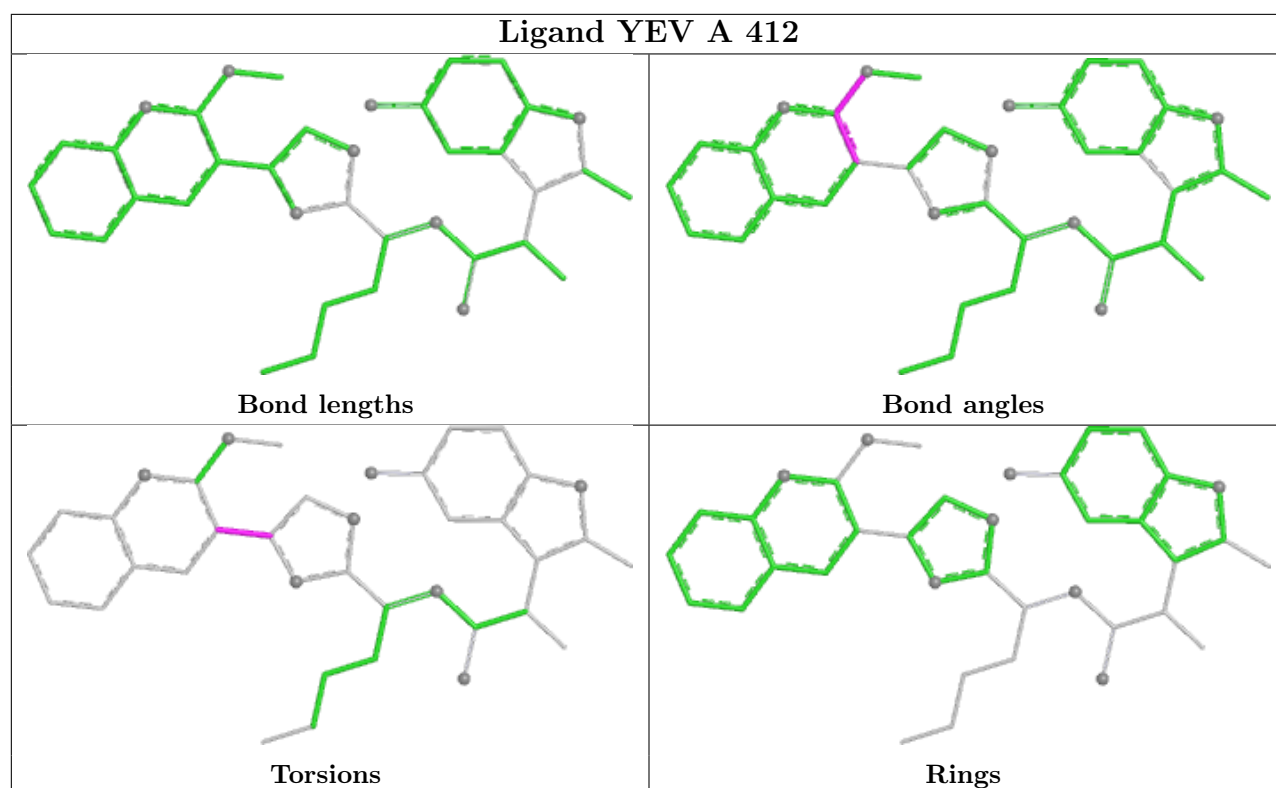
All (13) torsion outliers are listed below:

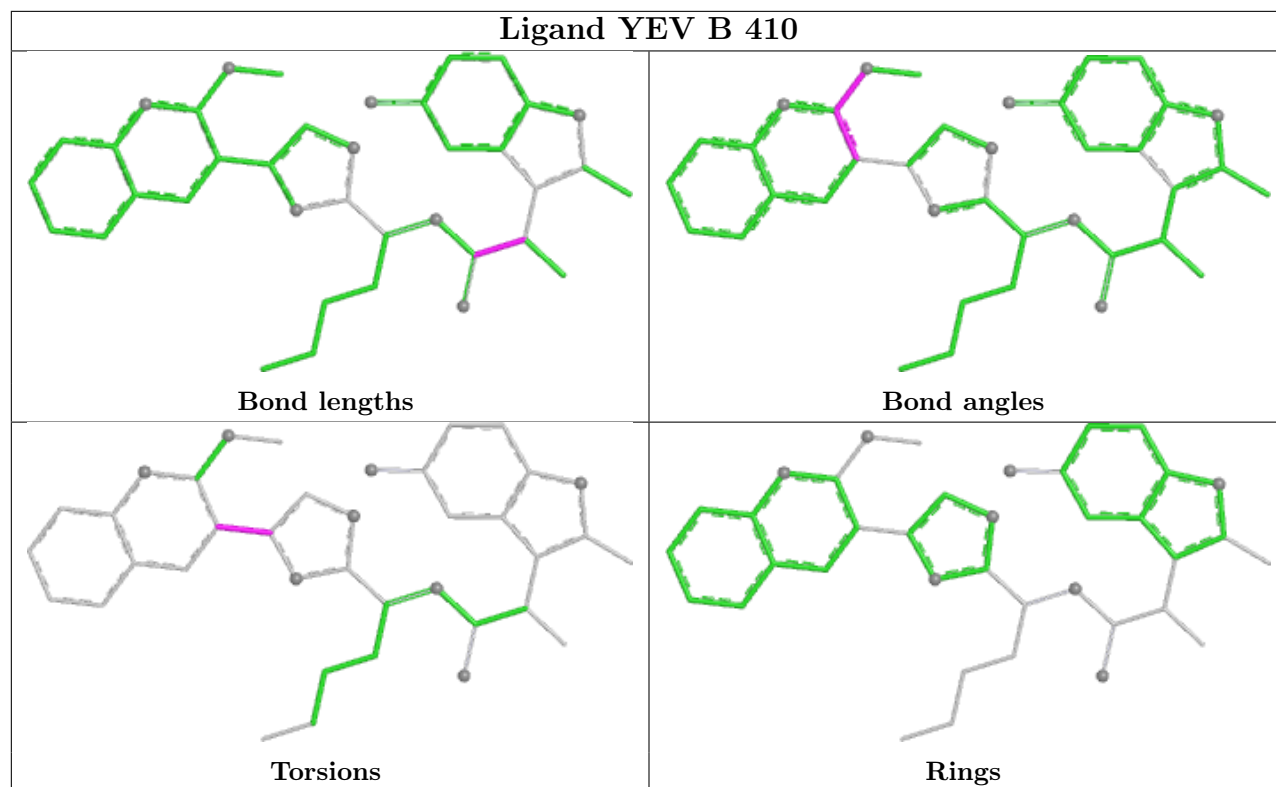
Mol	Chain	Res	Type	Atoms
7	A	412	YEV	C2-C3-C4-C5
7	B	410	YEV	C2-C3-C4-C5
7	C	411	YEV	C2-C3-C4-C5
6	A	409	PEG	O2-C3-C4-O4
6	A	410	PEG	C1-C2-O2-C3
6	A	411	PEG	C1-C2-O2-C3
6	B	409	PEG	C4-C3-O2-C2
6	A	410	PEG	C4-C3-O2-C2
6	C	410	PEG	C1-C2-O2-C3
6	C	410	PEG	C4-C3-O2-C2
6	B	409	PEG	O1-C1-C2-O2
6	B	409	PEG	O2-C3-C4-O4
6	A	411	PEG	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	367/376 (97%)	0.06	11 (2%) 50 55	15, 22, 41, 61	5 (1%)
1	B	365/376 (97%)	-0.00	3 (0%) 86 89	13, 19, 38, 56	3 (0%)
1	C	367/376 (97%)	0.41	33 (8%) 9 10	17, 27, 45, 85	3 (0%)
All	All	1099/1128 (97%)	0.16	47 (4%) 35 39	13, 22, 43, 85	11 (1%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	375	PRO	8.8
1	C	9	LYS	6.4
1	C	337	TYR	6.0
1	A	49	TYR	5.6
1	C	350	ASN	4.8
1	C	50	ARG	4.6
1	C	98	GLY	4.6
1	C	49	TYR	4.4
1	C	340	PRO	4.1
1	C	58	HIS	4.1
1	C	346	ILE	4.0
1	C	24	TYR	3.8
1	C	27	GLN	3.6
1	A	350	ASN	3.6
1	A	50[A]	ARG	3.5
1	A	204	GLU	3.4
1	C	44	LEU	3.3
1	C	348	PRO	3.2
1	A	27	GLN	3.1
1	C	347	SER	3.0
1	A	8	GLY	2.8
1	C	374	LEU	2.8
1	C	140[A]	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	28	GLY	2.8
1	A	10	LYS	2.7
1	A	167	TYR	2.7
1	C	324	GLU	2.7
1	B	10	LYS	2.6
1	A	90	LYS	2.6
1	C	204	GLU	2.6
1	A	86	SER	2.5
1	C	88	TYR	2.4
1	C	241	ILE	2.4
1	C	323	CYS	2.3
1	C	292	PHE	2.3
1	C	240	GLN	2.3
1	B	86	SER	2.2
1	C	368	PHE	2.1
1	C	271	ARG	2.1
1	C	372[A]	ARG	2.1
1	B	50	ARG	2.1
1	A	172	LEU	2.1
1	C	83	ASP	2.1
1	C	322	ASP	2.0
1	C	99	GLU	2.0
1	C	55	TYR	2.0
1	C	341	ASP	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](#)

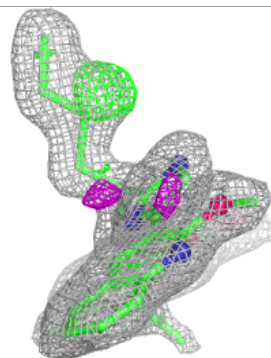
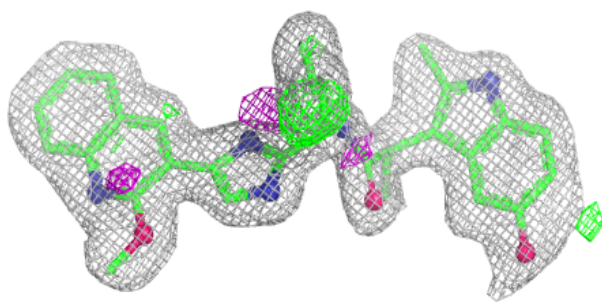
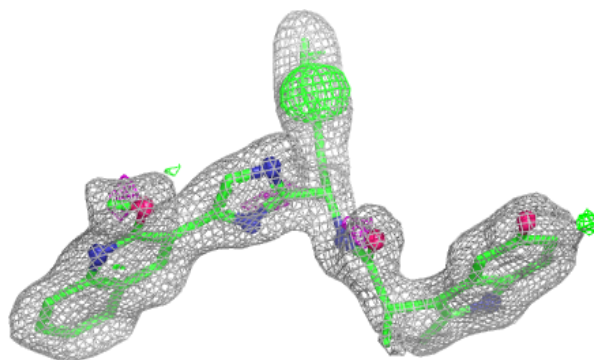
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	404	5/5	0.38	0.42	134,135,135,135	0
3	SO4	A	404	5/5	0.56	0.36	118,119,119,120	0
6	PEG	A	411	7/7	0.61	0.16	59,61,63,64	0
3	SO4	C	406	5/5	0.68	0.69	165,165,165,165	0
3	SO4	C	404	5/5	0.68	0.25	87,87,88,89	0
3	SO4	A	405	5/5	0.72	0.30	102,103,103,103	0
7	YEV	B	410	38/38	0.74	0.21	25,35,40,42	0
7	YEV	A	412	38/38	0.75	0.20	24,36,41,44	0
6	PEG	A	410	7/7	0.75	0.23	60,61,63,64	0
7	YEV	C	411	38/38	0.78	0.23	30,42,46,50	0
6	PEG	A	409	7/7	0.80	0.21	46,48,56,59	0
6	PEG	B	408	7/7	0.81	0.15	67,67,68,69	0
6	PEG	B	409	7/7	0.82	0.13	51,52,55,57	0
3	SO4	C	402	5/5	0.82	0.20	104,104,104,104	0
3	SO4	B	403	5/5	0.83	0.31	82,83,84,85	0
3	SO4	A	403	5/5	0.84	0.25	25,27,39,40	0
5	ACT	C	409	4/4	0.84	0.13	22,22,22,24	0
3	SO4	C	403	5/5	0.87	0.23	41,45,48,51	0
6	PEG	C	410	7/7	0.89	0.12	50,51,56,58	0
3	SO4	C	405	5/5	0.91	0.33	83,84,85,85	0
3	SO4	B	402	5/5	0.94	0.24	38,41,43,47	0
3	SO4	A	402	5/5	0.94	0.13	76,76,77,77	0
5	ACT	A	408	4/4	0.96	0.09	18,19,20,21	0
5	ACT	B	407	4/4	0.97	0.08	16,18,19,20	0
4	CA	C	408	1/1	0.98	0.13	40,40,40,40	0
4	CA	A	406	1/1	0.99	0.14	33,33,33,33	0
4	CA	A	407	1/1	0.99	0.11	39,39,39,39	0
4	CA	B	405	1/1	0.99	0.11	31,31,31,31	0
4	CA	B	406	1/1	0.99	0.13	39,39,39,39	0
4	CA	C	407	1/1	0.99	0.20	40,40,40,40	0
2	ZN	C	401	1/1	0.99	0.05	20,20,20,20	0
2	ZN	B	401	1/1	1.00	0.07	15,15,15,15	0
2	ZN	A	401	1/1	1.00	0.06	16,16,16,16	0

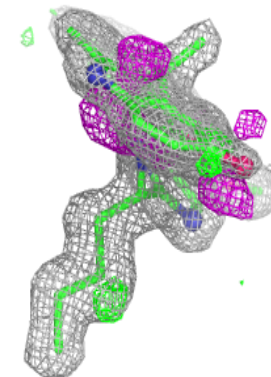
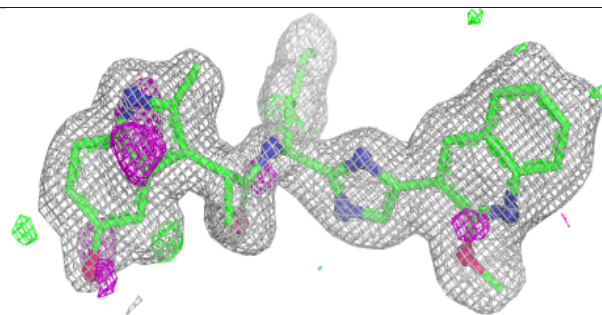
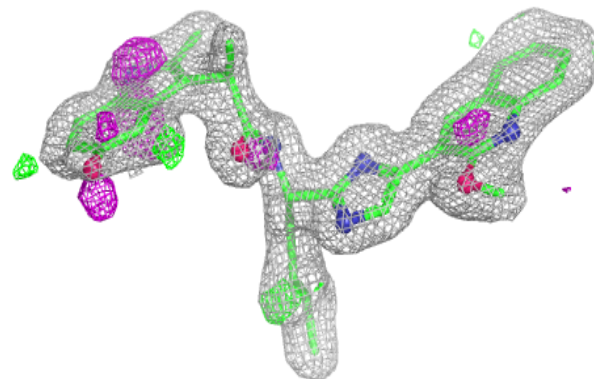
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

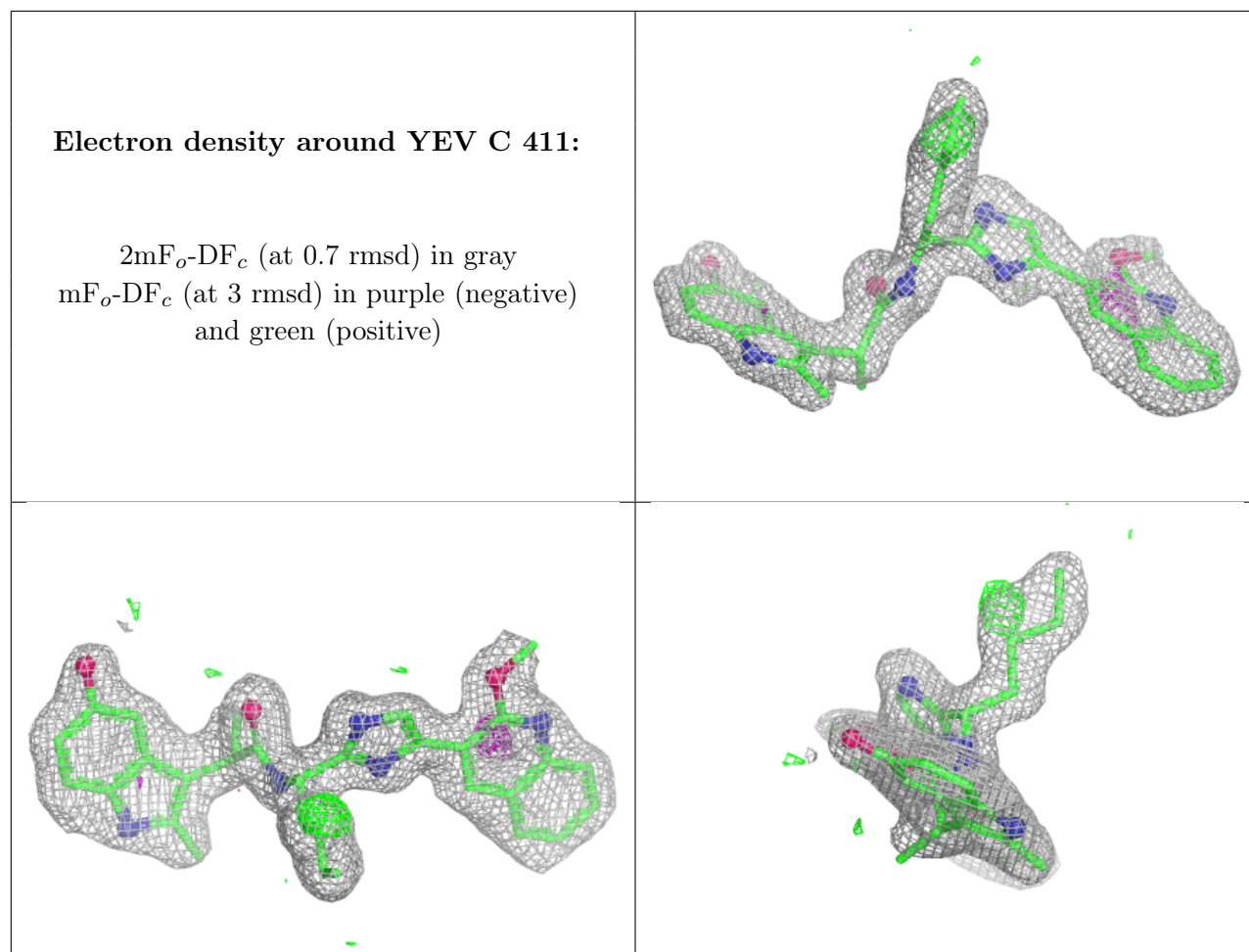
**Electron density around YEVS B 410:**

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

**Electron density around YEVS A 412:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.