



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:47 PM UTC

PDB ID : 4MZU / pdb_00004mzu
Title : Crystal structure of FdtD, a bifunctional ketoisomerase/N-acetyltransferase from *Shewanella denitrificans*
Authors : Chantigian, D.P.; Thoden, J.B.; Holden, H.M.
Deposited on : 2013-09-30
Resolution : 2.20 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 types of validation reports are described at

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

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

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

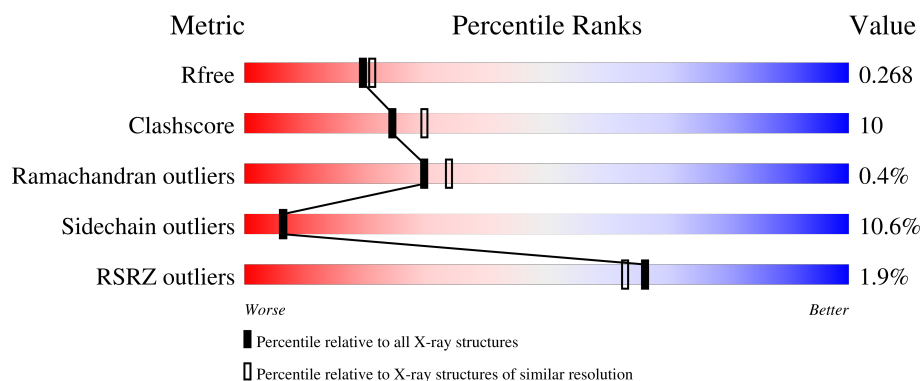
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	312	2% 68% 19% 9%
1	B	312	2% 72% 18% 7%
1	C	312	2% 72% 16% 9%
1	D	312	2% 65% 22% 9%
1	E	312	2% 64% 23% 8%

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Mol	Chain	Length	Quality of chain
1	F	312	
1	G	312	
1	H	312	
1	I	312	
1	J	312	
1	K	312	
1	L	312	

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
4	TDR	A	403	-	X	-	-
4	TDR	B	403	-	X	-	-
4	TDR	C	403	-	X	-	-
4	TDR	D	403	-	X	-	-
4	TDR	E	403	-	X	-	-
4	TDR	J	403	-	X	-	-
4	TDR	L	403	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28412 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 WxcM-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2220	1412	379	418	11			
1	B	290	Total	C	N	O	S	0	0	0
			2262	1438	387	426	11			
1	C	285	Total	C	N	O	S	0	1	0
			2222	1416	379	416	11			
1	D	283	Total	C	N	O	S	0	0	0
			2204	1403	375	415	11			
1	E	286	Total	C	N	O	S	0	0	0
			2231	1422	379	419	11			
1	F	294	Total	C	N	O	S	0	0	0
			2288	1455	393	429	11			
1	G	283	Total	C	N	O	S	0	1	0
			2206	1404	376	415	11			
1	H	278	Total	C	N	O	S	0	0	0
			2159	1379	364	405	11			
1	I	285	Total	C	N	O	S	0	0	0
			2217	1412	377	417	11			
1	J	275	Total	C	N	O	S	0	1	0
			2140	1368	361	401	10			
1	K	285	Total	C	N	O	S	0	1	0
			2226	1418	378	419	11			
1	L	286	Total	C	N	O	S	0	1	0
			2228	1418	380	419	11			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	LEU	-	expression tag	UNP Q12KT8
A	306	GLU	-	expression tag	UNP Q12KT8
A	307	HIS	-	expression tag	UNP Q12KT8
A	308	HIS	-	expression tag	UNP Q12KT8
A	309	HIS	-	expression tag	UNP Q12KT8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	310	HIS	-	expression tag	UNP Q12KT8
A	311	HIS	-	expression tag	UNP Q12KT8
A	312	HIS	-	expression tag	UNP Q12KT8
B	305	LEU	-	expression tag	UNP Q12KT8
B	306	GLU	-	expression tag	UNP Q12KT8
B	307	HIS	-	expression tag	UNP Q12KT8
B	308	HIS	-	expression tag	UNP Q12KT8
B	309	HIS	-	expression tag	UNP Q12KT8
B	310	HIS	-	expression tag	UNP Q12KT8
B	311	HIS	-	expression tag	UNP Q12KT8
B	312	HIS	-	expression tag	UNP Q12KT8
C	305	LEU	-	expression tag	UNP Q12KT8
C	306	GLU	-	expression tag	UNP Q12KT8
C	307	HIS	-	expression tag	UNP Q12KT8
C	308	HIS	-	expression tag	UNP Q12KT8
C	309	HIS	-	expression tag	UNP Q12KT8
C	310	HIS	-	expression tag	UNP Q12KT8
C	311	HIS	-	expression tag	UNP Q12KT8
C	312	HIS	-	expression tag	UNP Q12KT8
D	305	LEU	-	expression tag	UNP Q12KT8
D	306	GLU	-	expression tag	UNP Q12KT8
D	307	HIS	-	expression tag	UNP Q12KT8
D	308	HIS	-	expression tag	UNP Q12KT8
D	309	HIS	-	expression tag	UNP Q12KT8
D	310	HIS	-	expression tag	UNP Q12KT8
D	311	HIS	-	expression tag	UNP Q12KT8
D	312	HIS	-	expression tag	UNP Q12KT8
E	305	LEU	-	expression tag	UNP Q12KT8
E	306	GLU	-	expression tag	UNP Q12KT8
E	307	HIS	-	expression tag	UNP Q12KT8
E	308	HIS	-	expression tag	UNP Q12KT8
E	309	HIS	-	expression tag	UNP Q12KT8
E	310	HIS	-	expression tag	UNP Q12KT8
E	311	HIS	-	expression tag	UNP Q12KT8
E	312	HIS	-	expression tag	UNP Q12KT8
F	305	LEU	-	expression tag	UNP Q12KT8
F	306	GLU	-	expression tag	UNP Q12KT8
F	307	HIS	-	expression tag	UNP Q12KT8
F	308	HIS	-	expression tag	UNP Q12KT8
F	309	HIS	-	expression tag	UNP Q12KT8
F	310	HIS	-	expression tag	UNP Q12KT8
F	311	HIS	-	expression tag	UNP Q12KT8

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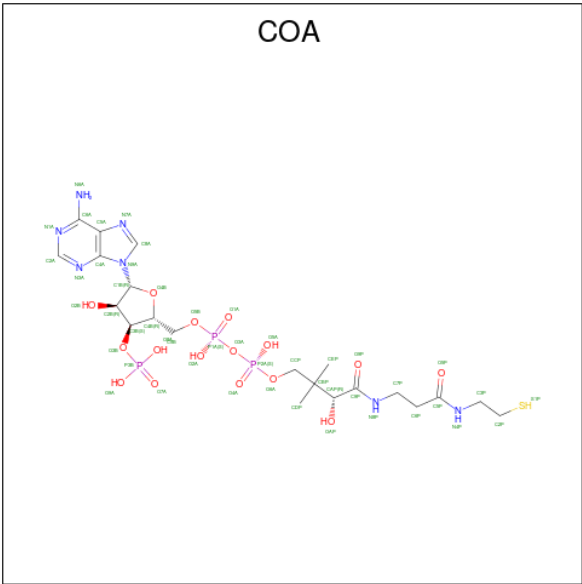
Chain	Residue	Modelled	Actual	Comment	Reference
F	312	HIS	-	expression tag	UNP Q12KT8
G	305	LEU	-	expression tag	UNP Q12KT8
G	306	GLU	-	expression tag	UNP Q12KT8
G	307	HIS	-	expression tag	UNP Q12KT8
G	308	HIS	-	expression tag	UNP Q12KT8
G	309	HIS	-	expression tag	UNP Q12KT8
G	310	HIS	-	expression tag	UNP Q12KT8
G	311	HIS	-	expression tag	UNP Q12KT8
G	312	HIS	-	expression tag	UNP Q12KT8
H	305	LEU	-	expression tag	UNP Q12KT8
H	306	GLU	-	expression tag	UNP Q12KT8
H	307	HIS	-	expression tag	UNP Q12KT8
H	308	HIS	-	expression tag	UNP Q12KT8
H	309	HIS	-	expression tag	UNP Q12KT8
H	310	HIS	-	expression tag	UNP Q12KT8
H	311	HIS	-	expression tag	UNP Q12KT8
H	312	HIS	-	expression tag	UNP Q12KT8
I	305	LEU	-	expression tag	UNP Q12KT8
I	306	GLU	-	expression tag	UNP Q12KT8
I	307	HIS	-	expression tag	UNP Q12KT8
I	308	HIS	-	expression tag	UNP Q12KT8
I	309	HIS	-	expression tag	UNP Q12KT8
I	310	HIS	-	expression tag	UNP Q12KT8
I	311	HIS	-	expression tag	UNP Q12KT8
I	312	HIS	-	expression tag	UNP Q12KT8
J	305	LEU	-	expression tag	UNP Q12KT8
J	306	GLU	-	expression tag	UNP Q12KT8
J	307	HIS	-	expression tag	UNP Q12KT8
J	308	HIS	-	expression tag	UNP Q12KT8
J	309	HIS	-	expression tag	UNP Q12KT8
J	310	HIS	-	expression tag	UNP Q12KT8
J	311	HIS	-	expression tag	UNP Q12KT8
J	312	HIS	-	expression tag	UNP Q12KT8
K	305	LEU	-	expression tag	UNP Q12KT8
K	306	GLU	-	expression tag	UNP Q12KT8
K	307	HIS	-	expression tag	UNP Q12KT8
K	308	HIS	-	expression tag	UNP Q12KT8
K	309	HIS	-	expression tag	UNP Q12KT8
K	310	HIS	-	expression tag	UNP Q12KT8
K	311	HIS	-	expression tag	UNP Q12KT8
K	312	HIS	-	expression tag	UNP Q12KT8
L	305	LEU	-	expression tag	UNP Q12KT8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	306	GLU	-	expression tag	UNP Q12KT8
L	307	HIS	-	expression tag	UNP Q12KT8
L	308	HIS	-	expression tag	UNP Q12KT8
L	309	HIS	-	expression tag	UNP Q12KT8
L	310	HIS	-	expression tag	UNP Q12KT8
L	311	HIS	-	expression tag	UNP Q12KT8
L	312	HIS	-	expression tag	UNP Q12KT8

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



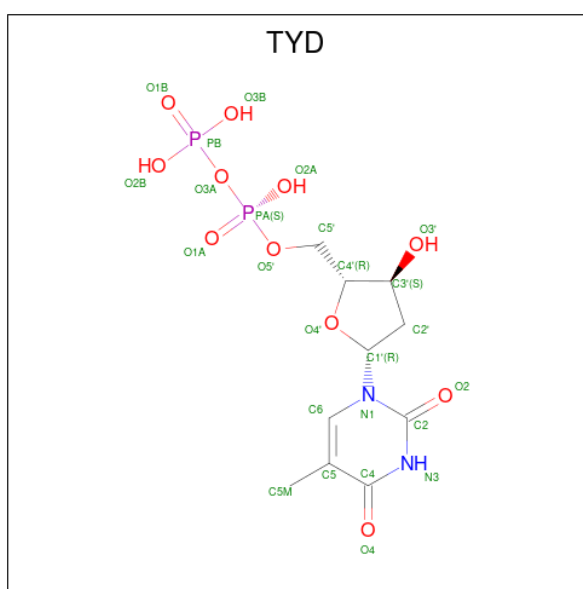
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	I	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	J	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	K	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	L	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 3 is THYMIDINE-5'-DIPHOSPHATE (CCD ID: TYD) (formula: $C_{10}H_{16}N_2O_{11}P_2$).



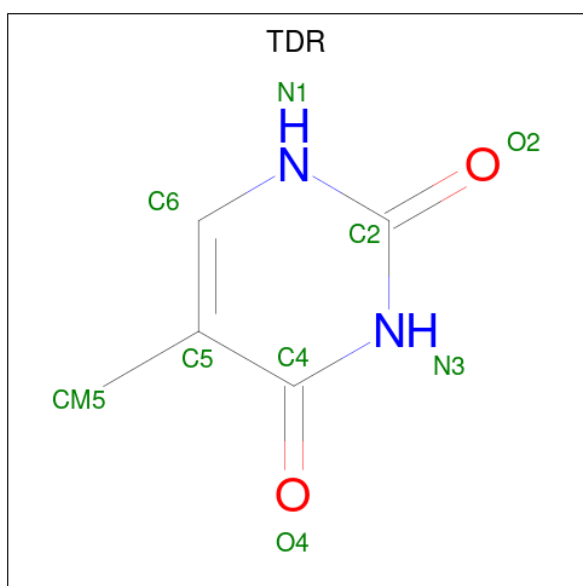
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P		
			25	10	2	11	2	0	0
3	B	1	Total	C	N	O	P		
			25	10	2	11	2	0	0
3	C	1	Total	C	N	O	P		
			25	10	2	11	2	0	0
3	D	1	Total	C	N	O	P		
			25	10	2	11	2	0	0
3	E	1	Total	C	N	O	P		
			25	10	2	11	2	0	0
3	F	1	Total	C	N	O	P		
			25	10	2	11	2	0	0
3	G	1	Total	C	N	O	P		
			25	10	2	11	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	I	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	J	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	K	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	L	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 4 is THYMINE (CCD ID: TDR) (formula: $C_5H_6N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	5	2	2		
4	B	1	Total	C	N	O	0	0
			9	5	2	2		
4	C	1	Total	C	N	O	0	0
			9	5	2	2		
4	D	1	Total	C	N	O	0	0
			9	5	2	2		
4	E	1	Total	C	N	O	0	0
			9	5	2	2		
4	F	1	Total	C	N	O	0	0
			9	5	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	J	1	Total	C	N	O	0	0
			9	5	2	2		
4	K	1	Total	C	N	O	0	0
			9	5	2	2		
4	L	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		

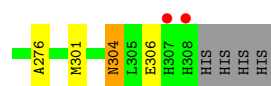
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	93	Total	O	0	0
			93	93		
6	B	100	Total	O	0	0
			100	100		
6	C	87	Total	O	0	0
			87	87		
6	D	53	Total	O	0	0
			53	53		
6	E	66	Total	O	0	0
			66	66		
6	F	61	Total	O	0	0
			61	61		
6	G	80	Total	O	0	0
			80	80		
6	H	42	Total	O	0	0
			42	42		
6	I	67	Total	O	0	0
			67	67		

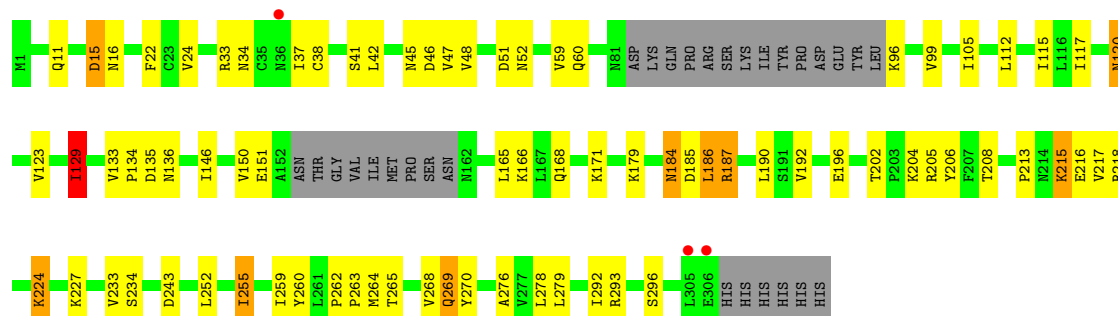
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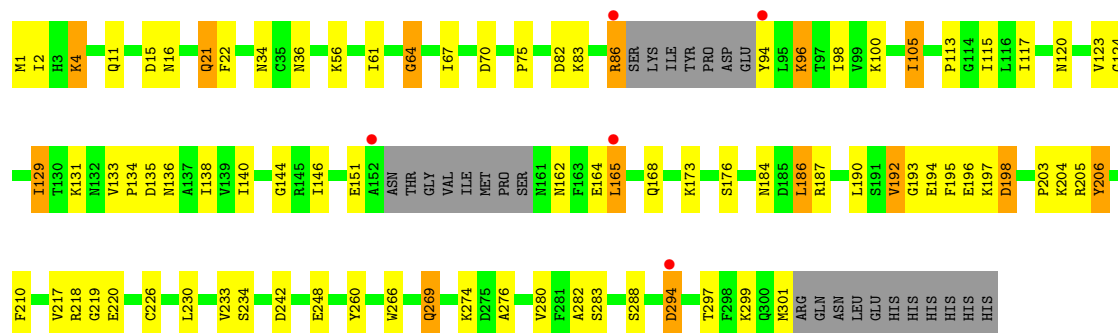
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	54	Total 54	O 54	0	0
6	K	82	Total 82	O 82	0	0
6	L	62	Total 62	O 62	0	0



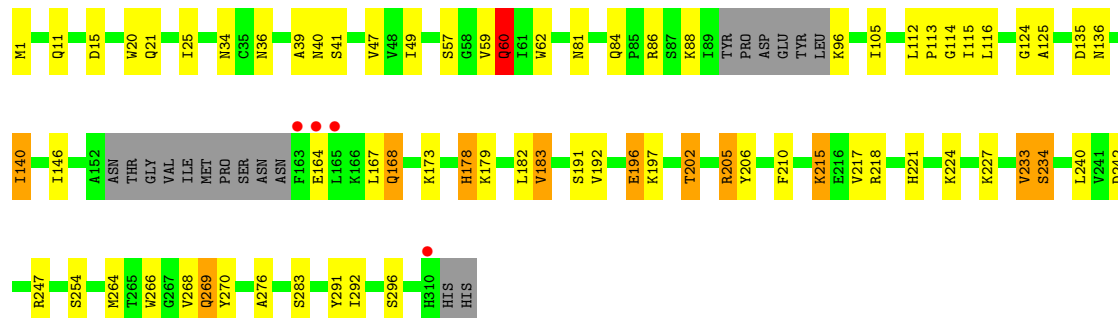
• Molecule 1: WxcM-like protein



• Molecule 1: WxcM-like protein

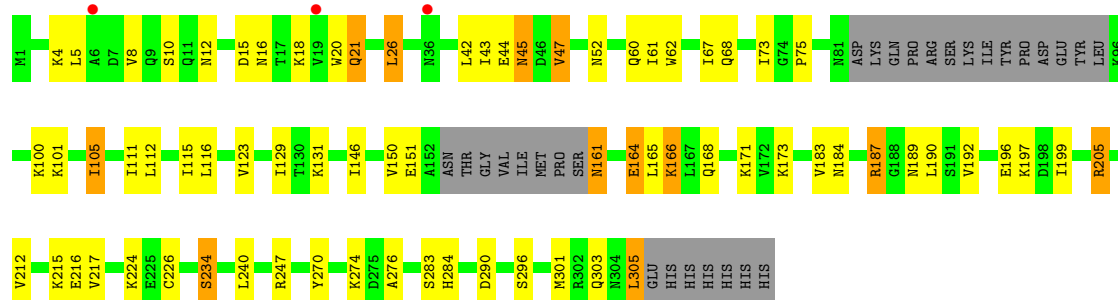


• Molecule 1: WxcM-like protein

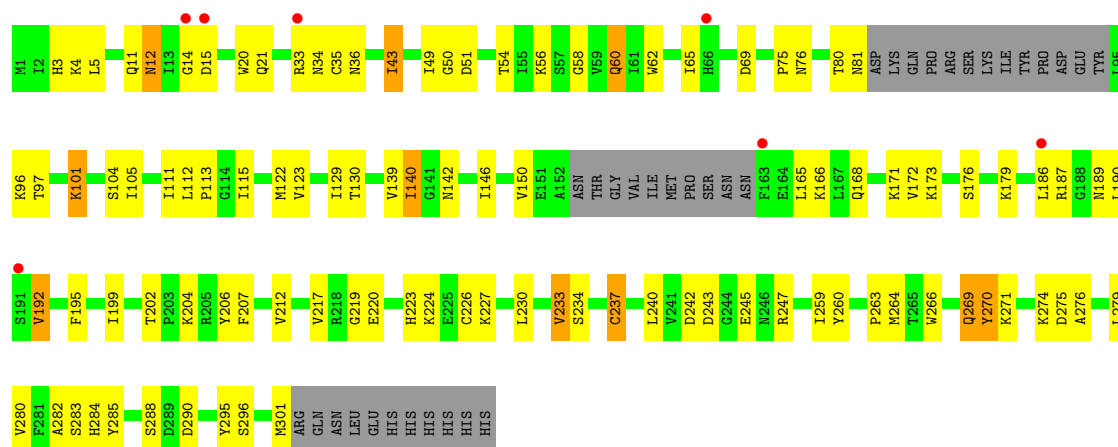


• Molecule 1: WxcM-like protein

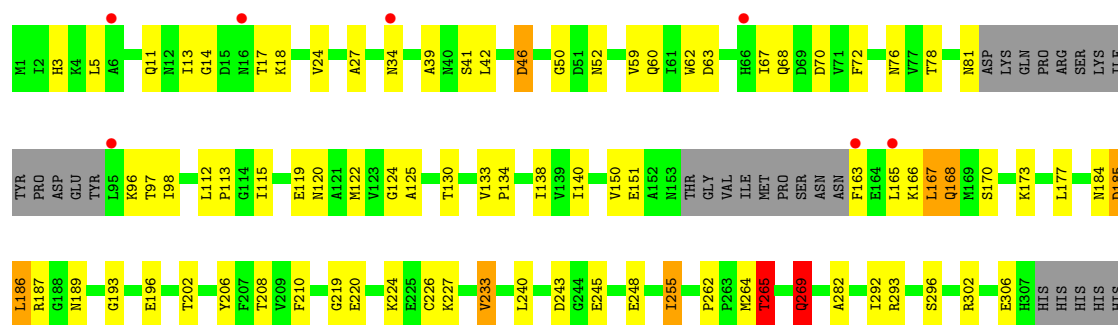




• Molecule 1: WxcM-like protein

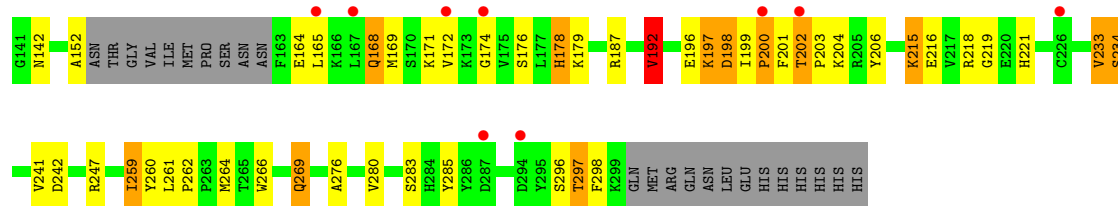


• Molecule 1: WxcM-like protein

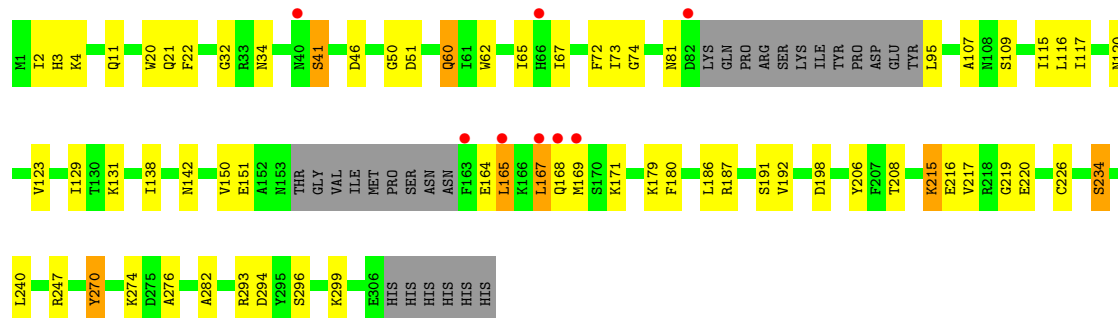


• Molecule 1: WxcM-like protein

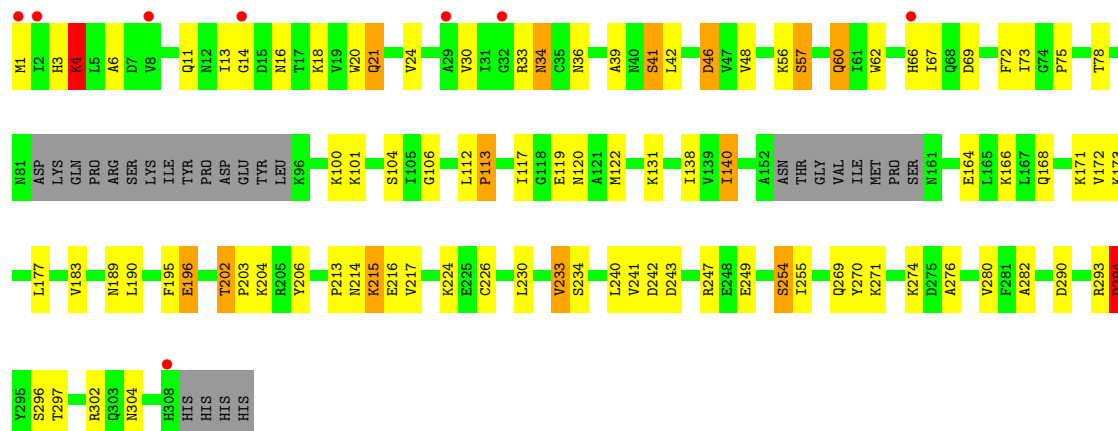




• Molecule 1: WxcM-like protein



• Molecule 1: WxcM-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.31Å 109.44Å 127.85Å 79.23° 79.98° 84.89°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.9 (30.00-2.20) 90.9 (30.00-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.270 0.204 , 0.268	Depositor DCC
R_{free} test set	10284 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28412	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TDR, TYD, COA

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	0.83	0/2261	1.40	16/3059 (0.5%)
1	B	0.83	0/2304	1.29	6/3117 (0.2%)
1	C	0.82	0/2266	1.37	12/3066 (0.4%)
1	D	0.72	0/2245	1.35	12/3038 (0.4%)
1	E	0.73	0/2274	1.34	13/3078 (0.4%)
1	F	0.77	0/2331	1.38	9/3153 (0.3%)
1	G	0.74	0/2250	1.30	12/3045 (0.4%)
1	H	0.61	0/2200	1.25	13/2978 (0.4%)
1	I	0.72	0/2258	1.31	13/3056 (0.4%)
1	J	0.67	0/2184	1.26	9/2956 (0.3%)
1	K	0.77	0/2270	1.33	9/3071 (0.3%)
1	L	0.73	0/2272	1.31	10/3074 (0.3%)
All	All	0.75	0/27115	1.33	134/36691 (0.4%)

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	C	0	1

There are no bond length outliers.

The worst 5 of 134 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	133	VAL	CA-C-N	-12.82	107.83	120.52
1	E	133	VAL	C-N-CA	-12.82	107.83	120.52
1	D	45	ASN	N-CA-C	8.74	120.74	111.03
1	K	81	ASN	N-CA-C	8.72	124.60	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	47	VAL	N-CA-C	-8.46	97.18	108.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	233	VAL	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	2220	0	2214	59	0
1	B	2262	0	2258	42	0
1	C	2222	0	2219	50	0
1	D	2204	0	2197	39	0
1	E	2231	0	2224	46	0
1	F	2288	0	2278	52	0
1	G	2206	0	2202	50	0
1	H	2159	0	2158	63	0
1	I	2217	0	2210	56	0
1	J	2140	0	2143	46	0
1	K	2226	0	2225	39	0
1	L	2228	0	2220	53	0
2	A	48	0	32	0	0
2	B	48	0	32	1	0
2	C	48	0	32	0	0
2	D	48	0	32	1	0
2	E	48	0	32	0	0
2	F	48	0	32	0	0
2	G	96	0	64	2	0
2	I	48	0	32	3	0
2	J	48	0	32	4	0
2	K	48	0	32	3	0
2	L	48	0	32	3	0
3	A	25	0	13	0	0
3	B	25	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	25	0	13	0	0
3	D	25	0	13	2	0
3	E	25	0	13	4	0
3	F	25	0	13	1	0
3	G	25	0	13	1	0
3	H	25	0	13	1	0
3	I	25	0	13	0	0
3	J	25	0	13	0	0
3	K	25	0	13	0	0
3	L	25	0	13	1	0
4	A	9	0	6	1	0
4	B	9	0	6	0	0
4	C	9	0	6	0	0
4	D	9	0	6	0	0
4	E	9	0	6	0	0
4	F	9	0	6	0	0
4	J	9	0	6	0	0
4	K	9	0	6	0	0
4	L	9	0	6	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
6	A	93	0	0	1	0
6	B	100	0	0	2	0
6	C	87	0	0	1	0
6	D	53	0	0	0	0
6	E	66	0	0	1	0
6	F	61	0	0	3	0
6	G	80	0	0	1	1
6	H	42	0	0	1	0
6	I	67	0	0	1	0
6	J	54	0	0	1	1
6	K	82	0	0	2	0
6	L	62	0	0	2	0
All	All	28412	0	27142	539	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 10.

The worst 5 of 539 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:I:264:MET:HE1	1:I:292:ILE:CD1	1.76	1.15
1:A:236:ASN:HD21	1:A:273:SER:HB3	1.05	1.12
1:A:236:ASN:ND2	1:A:273:SER:HB3	1.64	1.11
1:I:264:MET:HE1	1:I:292:ILE:HD12	1.27	1.10
1:F:224:LYS:HA	1:F:264:MET:HE2	1.28	1.07

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)
6:G:566:HOH:O	6:J:526:HOH:O[1_545]	1.99	0.21

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	279/312 (89%)	269 (96%)	9 (3%)	1 (0%)	30	34
1	B	284/312 (91%)	270 (95%)	14 (5%)	0	100	100
1	C	280/312 (90%)	270 (96%)	10 (4%)	0	100	100
1	D	277/312 (89%)	263 (95%)	13 (5%)	1 (0%)	30	34
1	E	280/312 (90%)	266 (95%)	13 (5%)	1 (0%)	30	34
1	F	288/312 (92%)	268 (93%)	20 (7%)	0	100	100
1	G	278/312 (89%)	267 (96%)	10 (4%)	1 (0%)	30	34
1	H	272/312 (87%)	252 (93%)	19 (7%)	1 (0%)	30	34
1	I	279/312 (89%)	261 (94%)	16 (6%)	2 (1%)	18	19
1	J	270/312 (86%)	258 (96%)	9 (3%)	3 (1%)	11	10
1	K	280/312 (90%)	261 (93%)	16 (6%)	3 (1%)	11	10
1	L	281/312 (90%)	260 (92%)	19 (7%)	2 (1%)	18	19
All	All	3348/3744 (89%)	3165 (94%)	168 (5%)	15 (0%)	30	34

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	H	14	GLY
1	K	3	HIS
1	J	297	THR
1	E	197	LYS

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	246/272 (90%)	222 (90%)	24 (10%)	7	8
1	B	251/272 (92%)	225 (90%)	26 (10%)	7	7
1	C	245/272 (90%)	224 (91%)	21 (9%)	10	10
1	D	244/272 (90%)	213 (87%)	31 (13%)	4	4
1	E	247/272 (91%)	217 (88%)	30 (12%)	5	4
1	F	252/272 (93%)	227 (90%)	25 (10%)	7	8
1	G	245/272 (90%)	221 (90%)	24 (10%)	7	8
1	H	239/272 (88%)	212 (89%)	27 (11%)	5	5
1	I	245/272 (90%)	228 (93%)	17 (7%)	14	16
1	J	237/272 (87%)	206 (87%)	31 (13%)	4	3
1	K	247/272 (91%)	222 (90%)	25 (10%)	7	7
1	L	246/272 (90%)	212 (86%)	34 (14%)	3	3
All	All	2944/3264 (90%)	2629 (89%)	315 (11%)	6	6

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	56	LYS
1	L	30	VAL
1	J	140	ILE
1	K	60	GLN

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Mol	Chain	Res	Type
1	L	166	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	168	GLN
1	J	60	GLN
1	H	221	HIS
1	I	136	ASN
1	J	221	HIS

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 38 ligands modelled in this entry, 5 are monoatomic - leaving 33 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
2	COA	I	401	-	47,50,50	0.92	1 (2%)	69,75,75	1.84	17 (24%)
3	TYD	E	402	-	25,26,26	1.47	6 (24%)	38,40,40	2.40	15 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	G	403	-	47,50,50	0.98	3 (6%)	69,75,75	1.78	16 (23%)
2	COA	K	401	-	47,50,50	0.88	3 (6%)	69,75,75	1.85	17 (24%)
3	TYD	G	402	-	25,26,26	1.45	4 (16%)	38,40,40	2.58	16 (42%)
2	COA	L	401	-	47,50,50	1.02	3 (6%)	69,75,75	1.82	20 (28%)
4	TDR	D	403	-	9,9,9	2.28	3 (33%)	12,12,12	3.76	8 (66%)
2	COA	B	401	-	47,50,50	0.95	3 (6%)	69,75,75	1.94	21 (30%)
3	TYD	K	402	-	25,26,26	1.41	5 (20%)	38,40,40	2.05	14 (36%)
2	COA	E	401	-	47,50,50	0.93	4 (8%)	69,75,75	1.68	14 (20%)
3	TYD	I	402	-	25,26,26	1.38	3 (12%)	38,40,40	2.67	11 (28%)
3	TYD	J	402	-	25,26,26	1.49	4 (16%)	38,40,40	2.35	10 (26%)
2	COA	F	401	-	47,50,50	1.07	4 (8%)	69,75,75	1.98	18 (26%)
3	TYD	A	402	-	25,26,26	1.45	4 (16%)	38,40,40	2.09	10 (26%)
3	TYD	H	401	-	25,26,26	1.48	5 (20%)	38,40,40	1.81	8 (21%)
3	TYD	D	402	-	25,26,26	1.45	5 (20%)	38,40,40	2.47	13 (34%)
4	TDR	E	403	-	9,9,9	2.21	3 (33%)	12,12,12	3.11	7 (58%)
4	TDR	J	403	-	9,9,9	2.24	2 (22%)	12,12,12	3.44	7 (58%)
3	TYD	F	402	-	25,26,26	1.45	5 (20%)	38,40,40	2.31	14 (36%)
4	TDR	L	403	-	9,9,9	2.13	3 (33%)	12,12,12	3.83	8 (66%)
3	TYD	C	402	-	25,26,26	1.37	4 (16%)	38,40,40	2.80	12 (31%)
4	TDR	K	403	-	9,9,9	2.10	2 (22%)	12,12,12	2.66	5 (41%)
2	COA	A	401	-	47,50,50	1.07	4 (8%)	69,75,75	2.00	21 (30%)
2	COA	J	401	-	47,50,50	0.86	2 (4%)	69,75,75	1.95	18 (26%)
3	TYD	B	402	-	25,26,26	1.45	5 (20%)	38,40,40	2.33	9 (23%)
4	TDR	A	403	-	9,9,9	2.17	2 (22%)	12,12,12	4.86	8 (66%)
4	TDR	B	403	-	9,9,9	2.48	2 (22%)	12,12,12	2.87	7 (58%)
4	TDR	F	403	-	9,9,9	2.21	2 (22%)	12,12,12	3.13	6 (50%)
2	COA	G	401	-	47,50,50	1.03	4 (8%)	69,75,75	1.85	18 (26%)
2	COA	D	401	-	47,50,50	0.98	3 (6%)	69,75,75	1.86	19 (27%)
4	TDR	C	403	-	9,9,9	2.28	3 (33%)	12,12,12	3.70	7 (58%)
3	TYD	L	402	-	25,26,26	1.38	4 (16%)	38,40,40	2.18	13 (34%)
2	COA	C	401	-	47,50,50	0.87	2 (4%)	69,75,75	2.06	15 (21%)

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	COA	I	401	-	-	5/48/64/64	0/3/3/3
3	TYD	E	402	-	-	3/16/28/28	0/2/2/2
2	COA	G	403	-	-	8/48/64/64	0/3/3/3
2	COA	K	401	-	-	13/48/64/64	0/3/3/3
3	TYD	G	402	-	-	1/16/28/28	0/2/2/2
2	COA	L	401	-	-	11/48/64/64	0/3/3/3
4	TDR	D	403	-	-	-	0/1/1/1
2	COA	B	401	-	-	7/48/64/64	0/3/3/3
3	TYD	K	402	-	-	3/16/28/28	0/2/2/2
2	COA	E	401	-	-	10/48/64/64	0/3/3/3
3	TYD	I	402	-	-	7/16/28/28	0/2/2/2
3	TYD	J	402	-	-	8/16/28/28	0/2/2/2
2	COA	F	401	-	-	7/48/64/64	0/3/3/3
3	TYD	A	402	-	-	2/16/28/28	0/2/2/2
3	TYD	H	401	-	-	2/16/28/28	0/2/2/2
3	TYD	D	402	-	-	0/16/28/28	0/2/2/2
4	TDR	E	403	-	-	-	0/1/1/1
4	TDR	J	403	-	-	-	0/1/1/1
3	TYD	F	402	-	-	7/16/28/28	0/2/2/2
4	TDR	L	403	-	-	-	0/1/1/1
3	TYD	C	402	-	-	3/16/28/28	0/2/2/2
4	TDR	K	403	-	-	-	0/1/1/1
2	COA	A	401	-	-	10/48/64/64	0/3/3/3
2	COA	J	401	-	-	11/48/64/64	0/3/3/3
3	TYD	B	402	-	-	8/16/28/28	0/2/2/2
4	TDR	A	403	-	-	-	0/1/1/1
4	TDR	B	403	-	-	-	0/1/1/1
4	TDR	F	403	-	-	-	0/1/1/1
2	COA	G	401	-	-	6/48/64/64	0/3/3/3
2	COA	D	401	-	-	10/48/64/64	0/3/3/3
4	TDR	C	403	-	-	-	0/1/1/1
3	TYD	L	402	-	-	4/16/28/28	0/2/2/2
2	COA	C	401	-	-	7/48/64/64	0/3/3/3

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	TDR	C6-C5	5.07	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	TDR	C6-C5	4.71	1.40	1.34
4	J	403	TDR	C6-C5	4.62	1.40	1.34
4	E	403	TDR	C6-C5	4.52	1.40	1.34
4	F	403	TDR	C6-C5	4.47	1.40	1.34

The worst 5 of 422 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	TDR	C5-C4-N3	10.97	124.86	115.32
4	C	403	TDR	N1-C2-N3	7.43	123.01	115.17
4	L	403	TDR	CM5-C5-C4	7.38	126.66	118.78
3	I	402	TYD	C4-N3-C2	-6.97	118.20	127.34
3	C	402	TYD	C4-N3-C2	-6.87	118.33	127.34

There are no chirality outliers.

5 of 153 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	COA	OAP-CAP-CBP-CCP
2	A	401	COA	C9P-CAP-CBP-CCP
2	A	401	COA	OAP-CAP-CBP-CDP
2	A	401	COA	C9P-CAP-CBP-CDP
2	A	401	COA	OAP-CAP-CBP-CEP

There are no ring outliers.

16 monomers are involved in 29 short contacts:

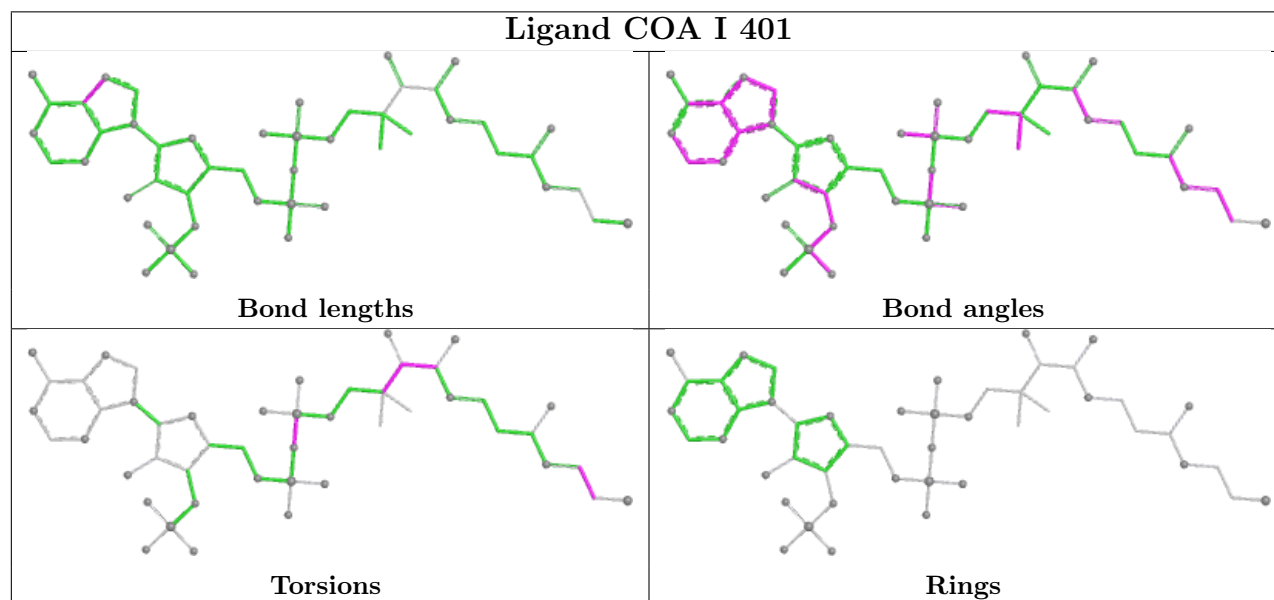
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	COA	3	0
3	E	402	TYD	4	0
2	G	403	COA	1	0
2	K	401	COA	3	0
3	G	402	TYD	1	0
2	L	401	COA	3	0
2	B	401	COA	1	0
3	H	401	TYD	1	0
3	D	402	TYD	2	0
3	F	402	TYD	1	0
4	L	403	TDR	1	0
2	J	401	COA	4	0
4	A	403	TDR	1	0

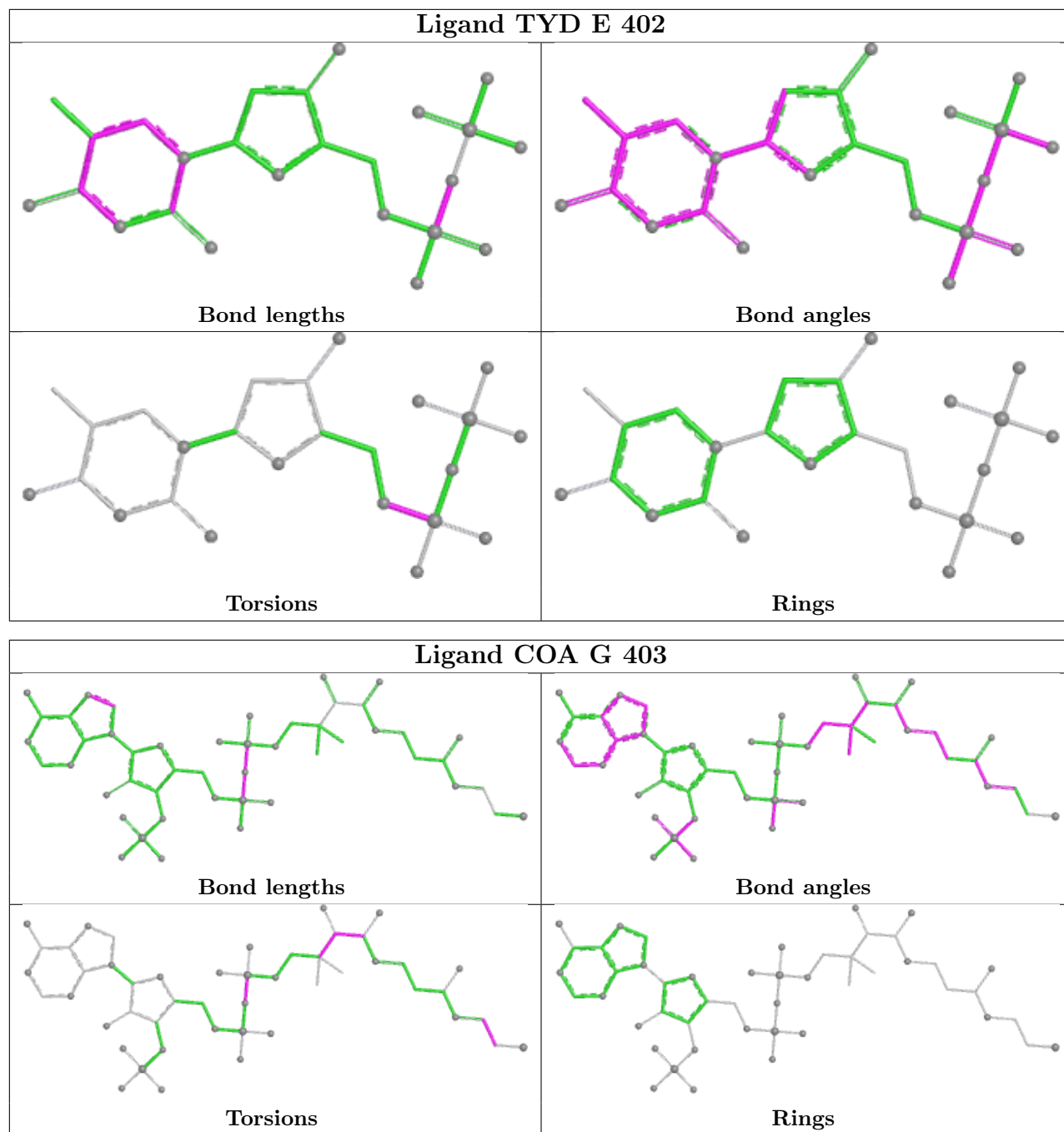
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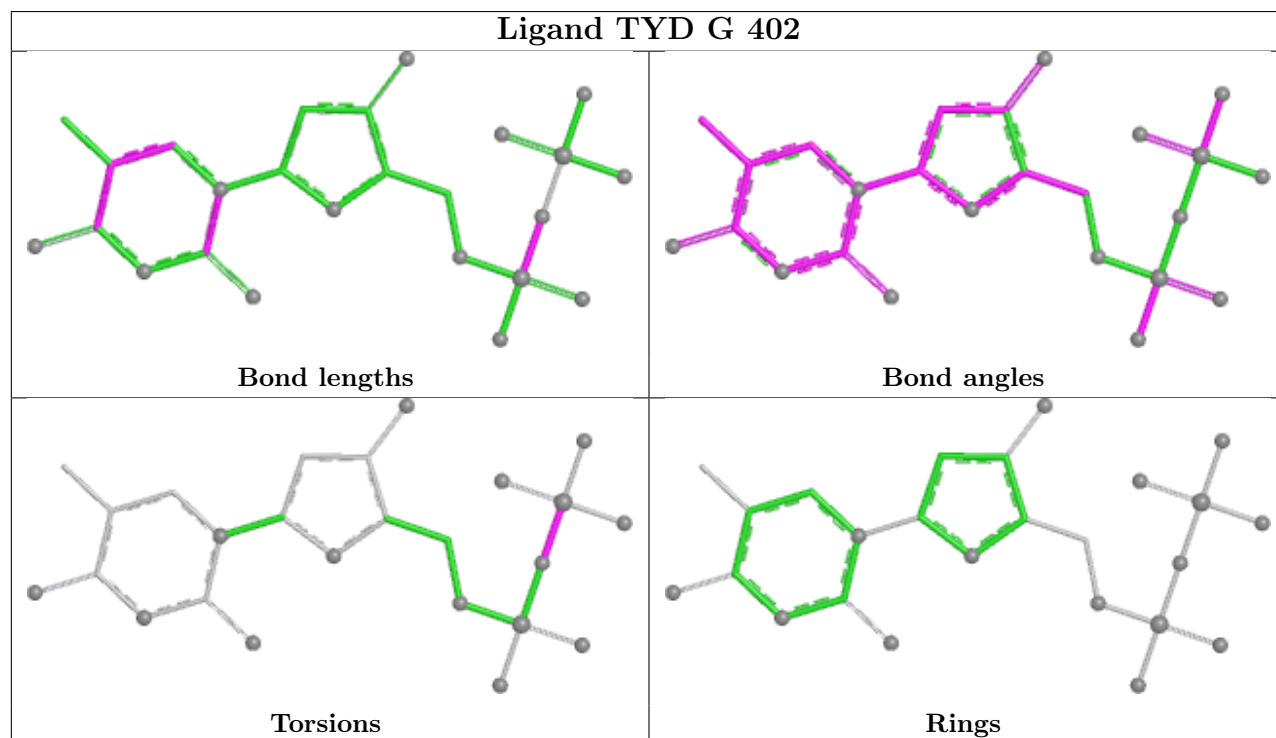
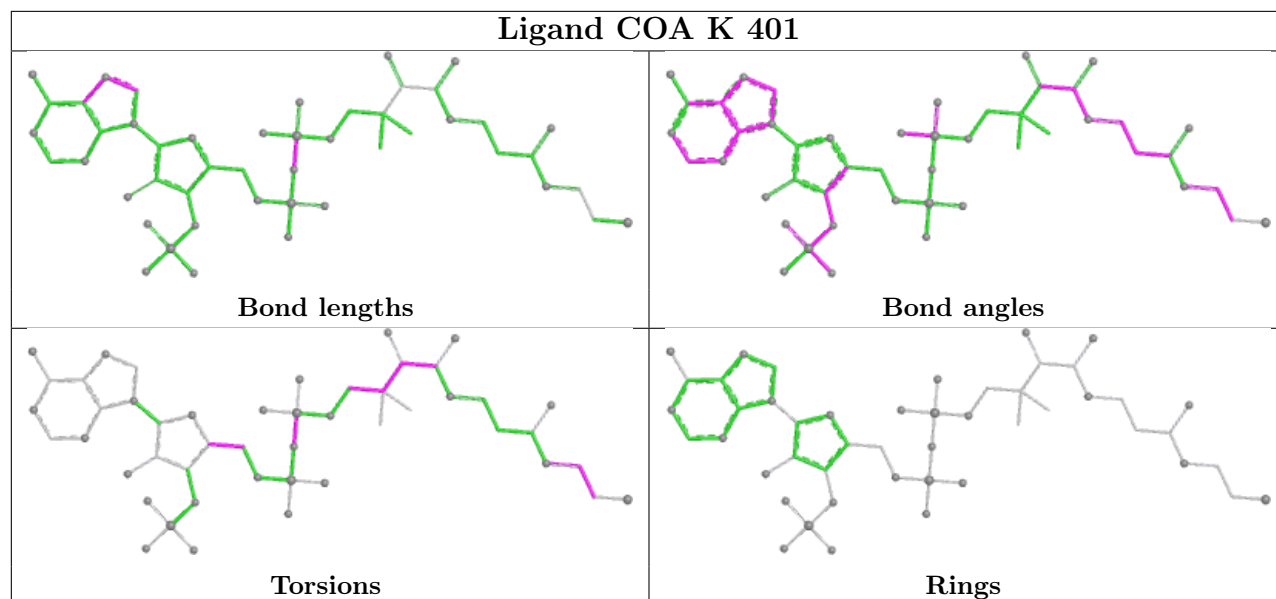
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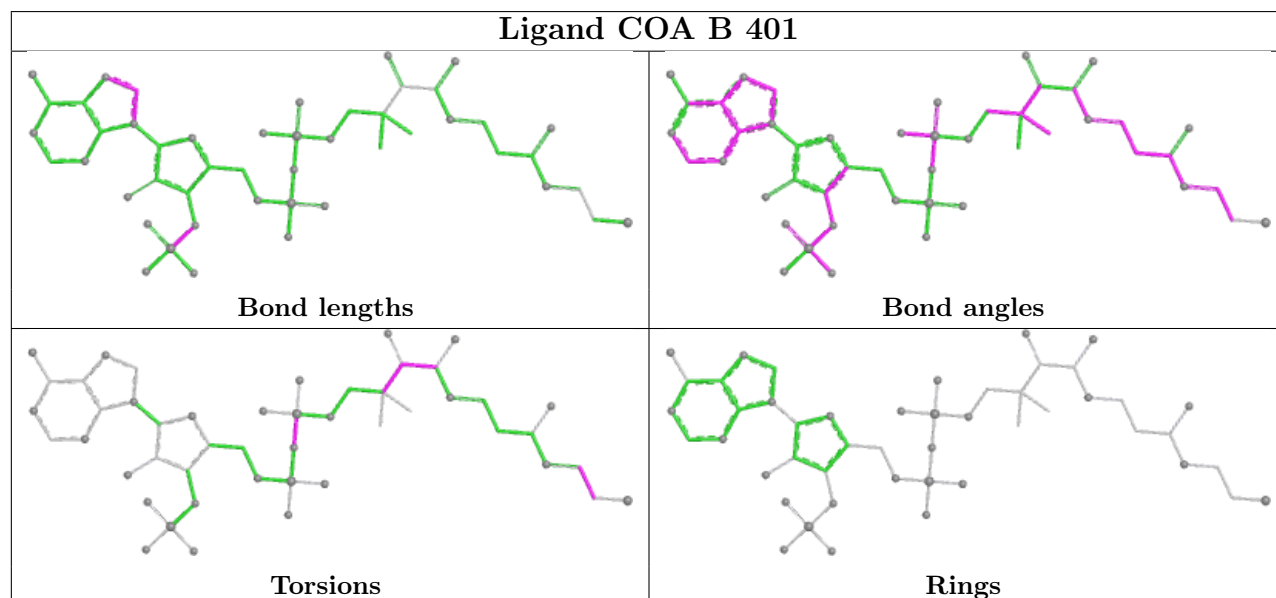
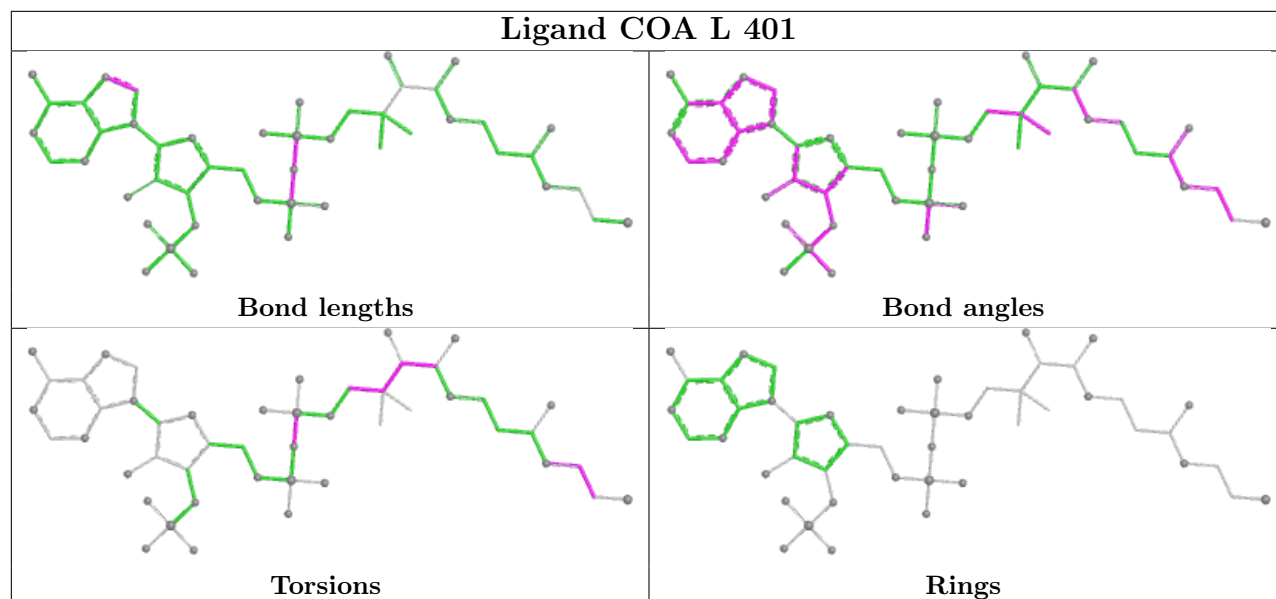
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	COA	1	0
2	D	401	COA	1	0
3	L	402	TYD	1	0

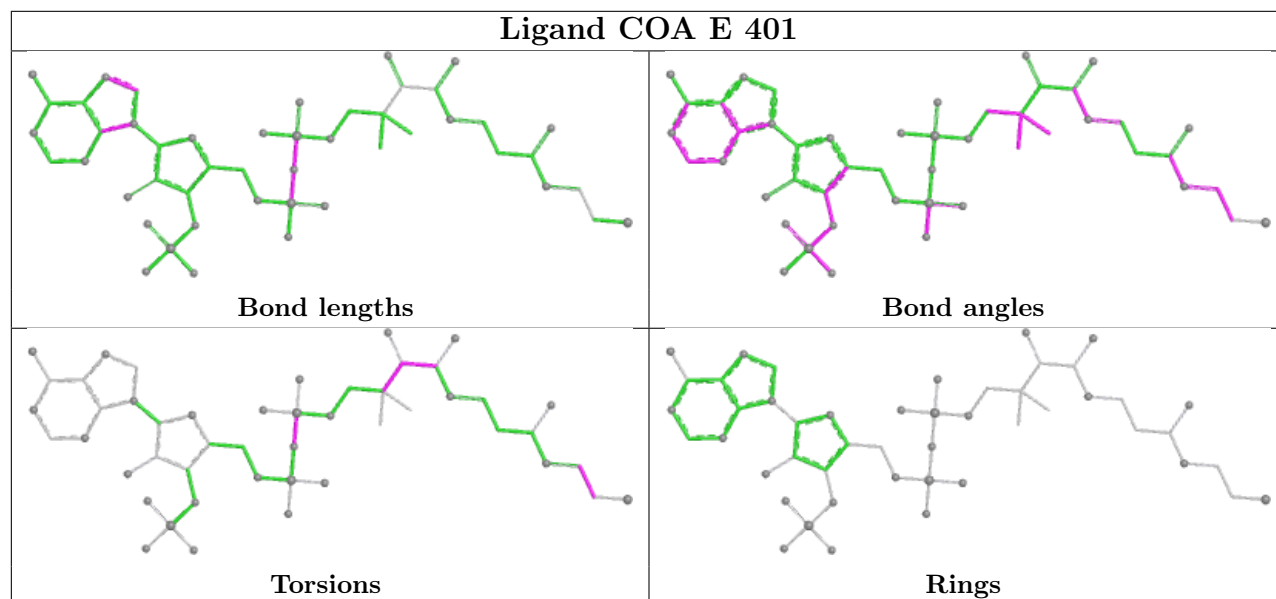
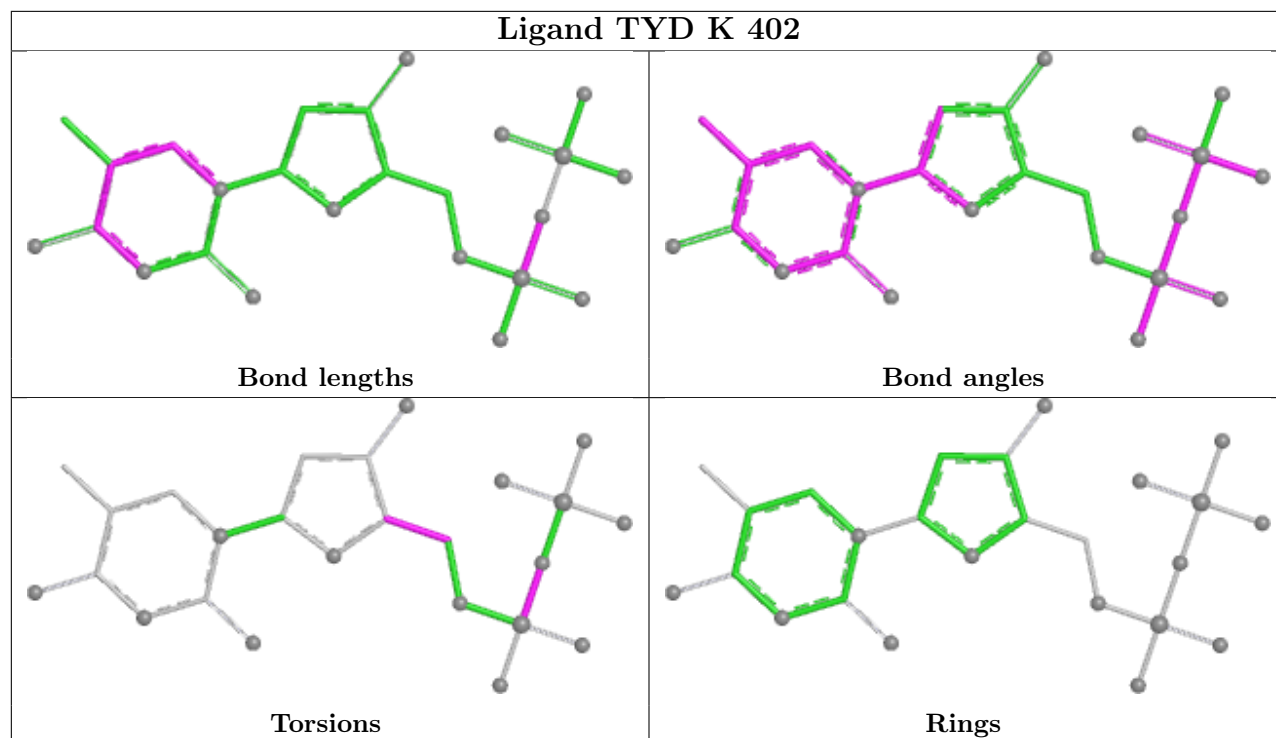
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



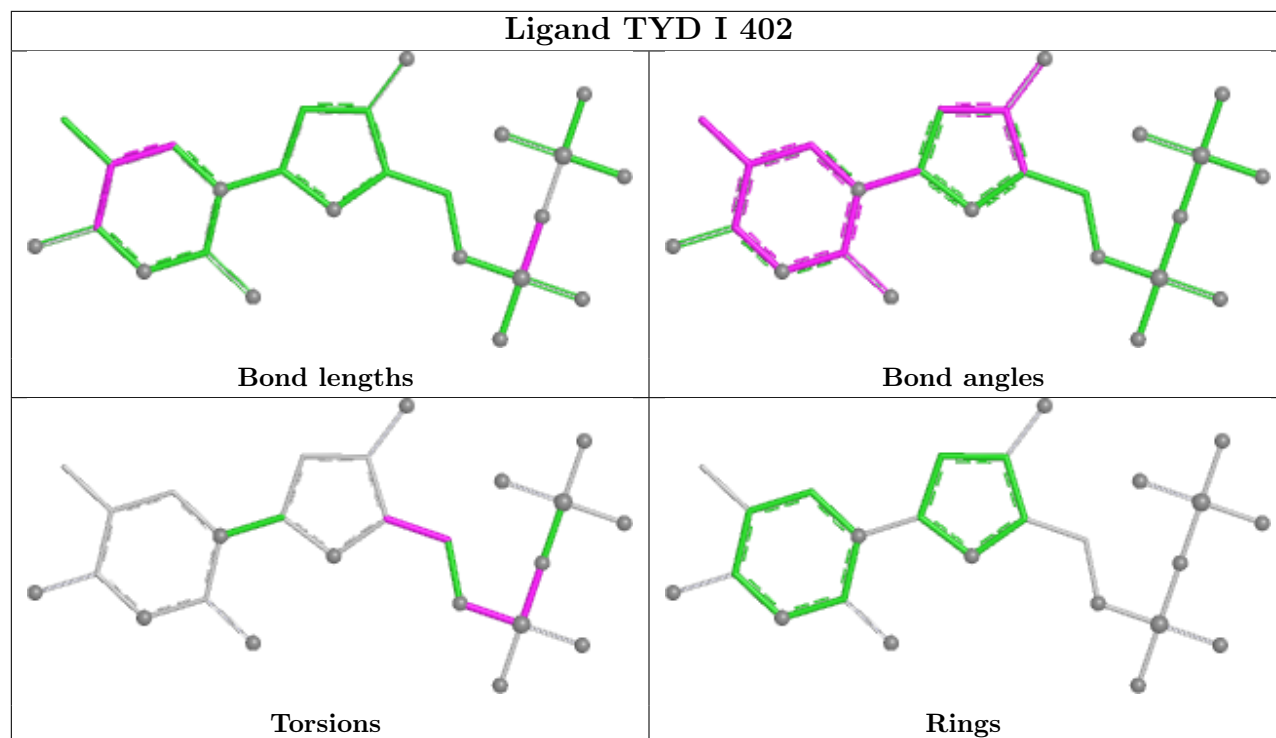




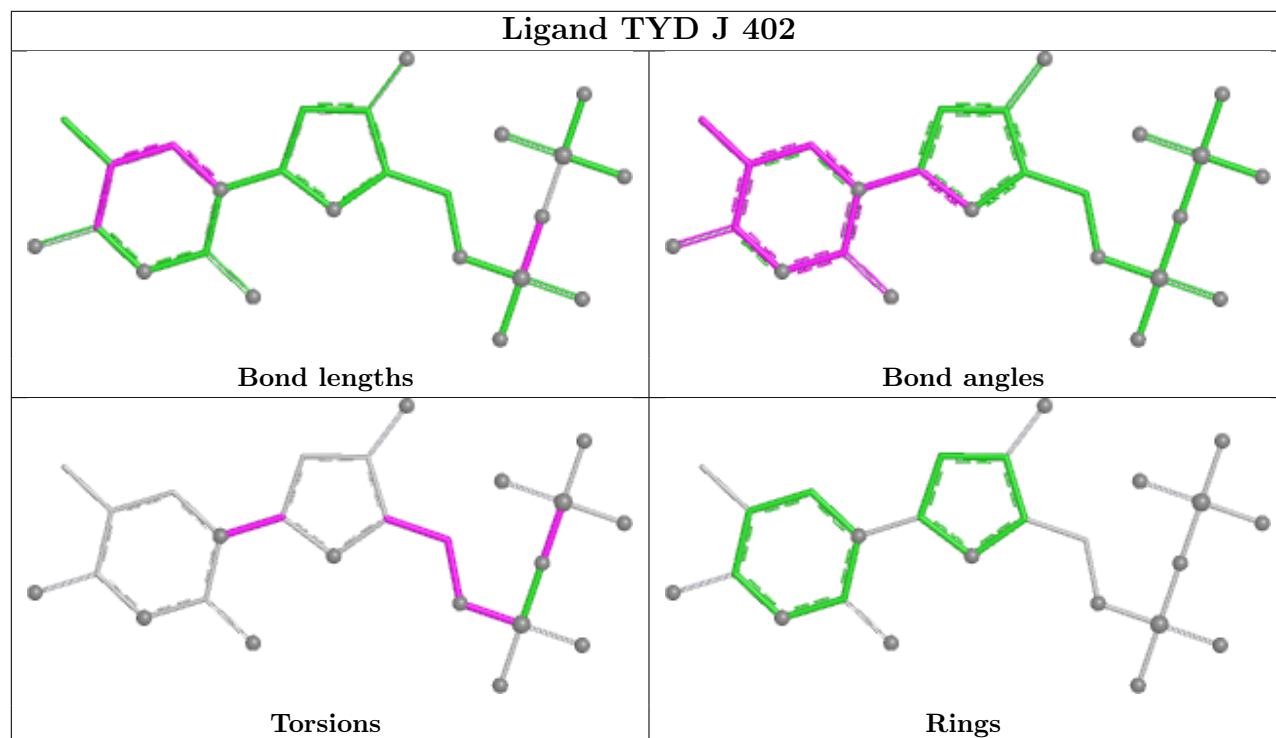


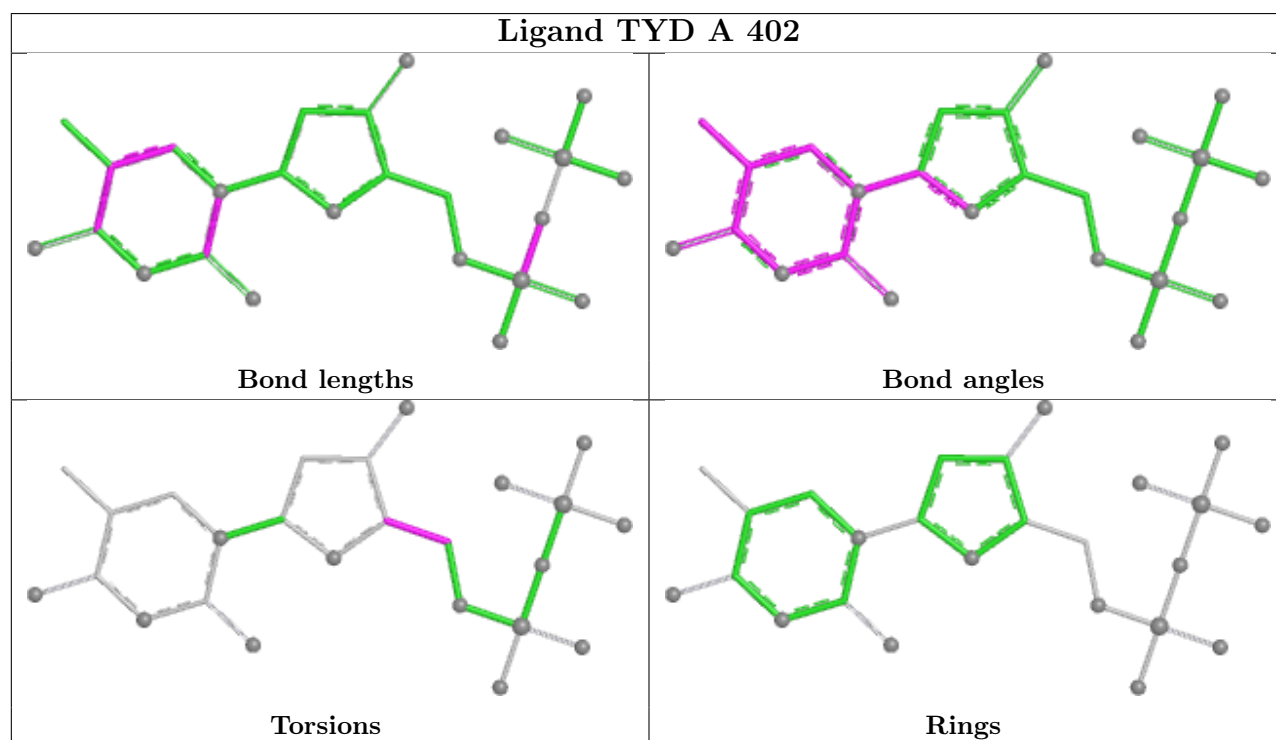
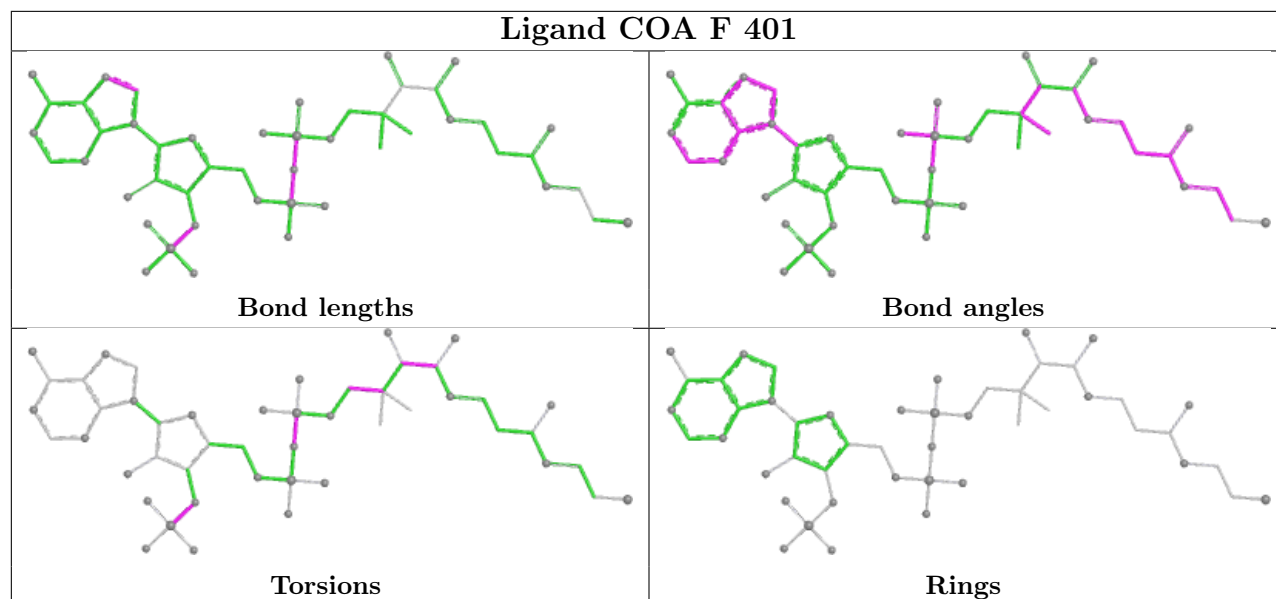


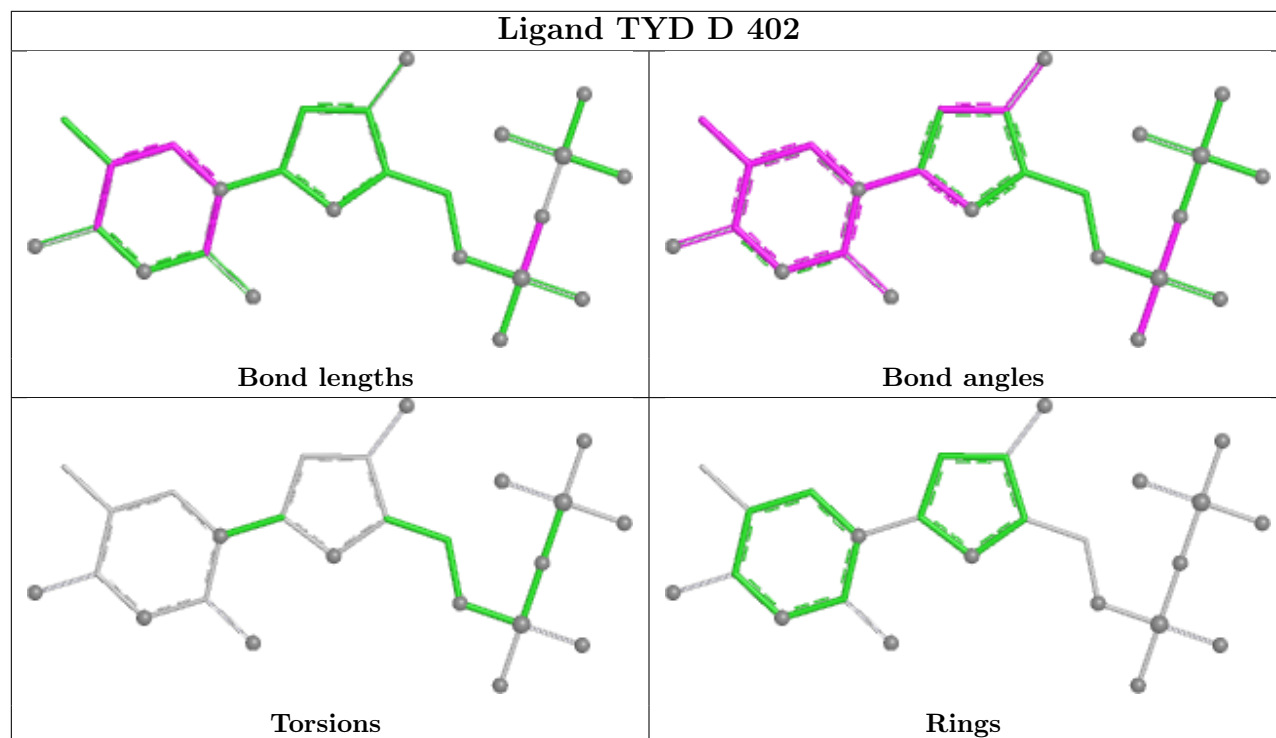
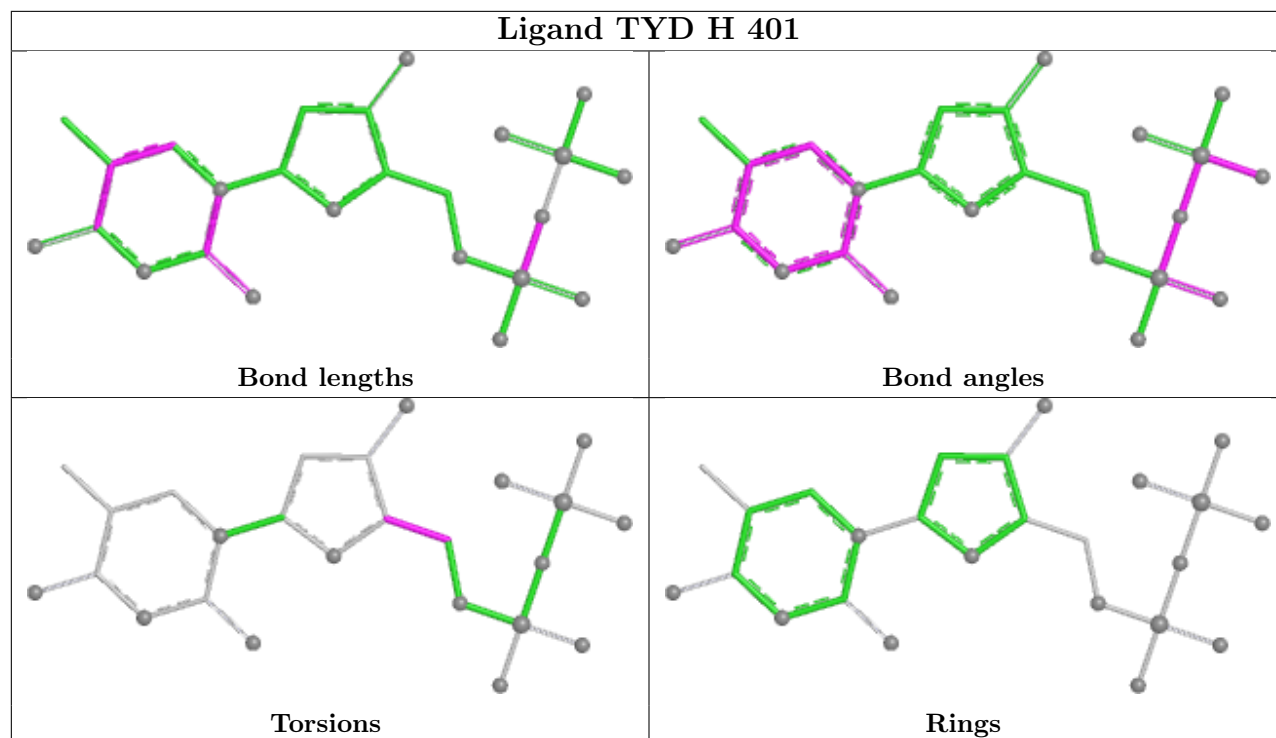
Ligand TYD I 402

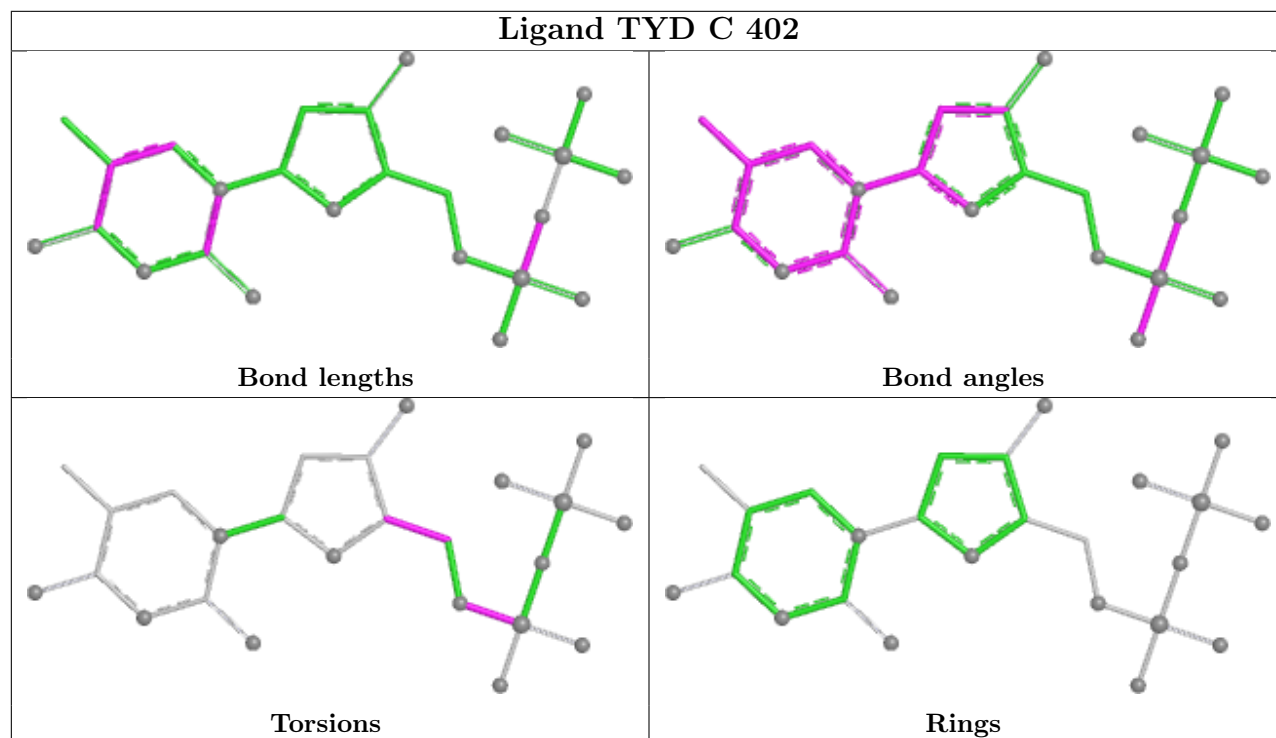
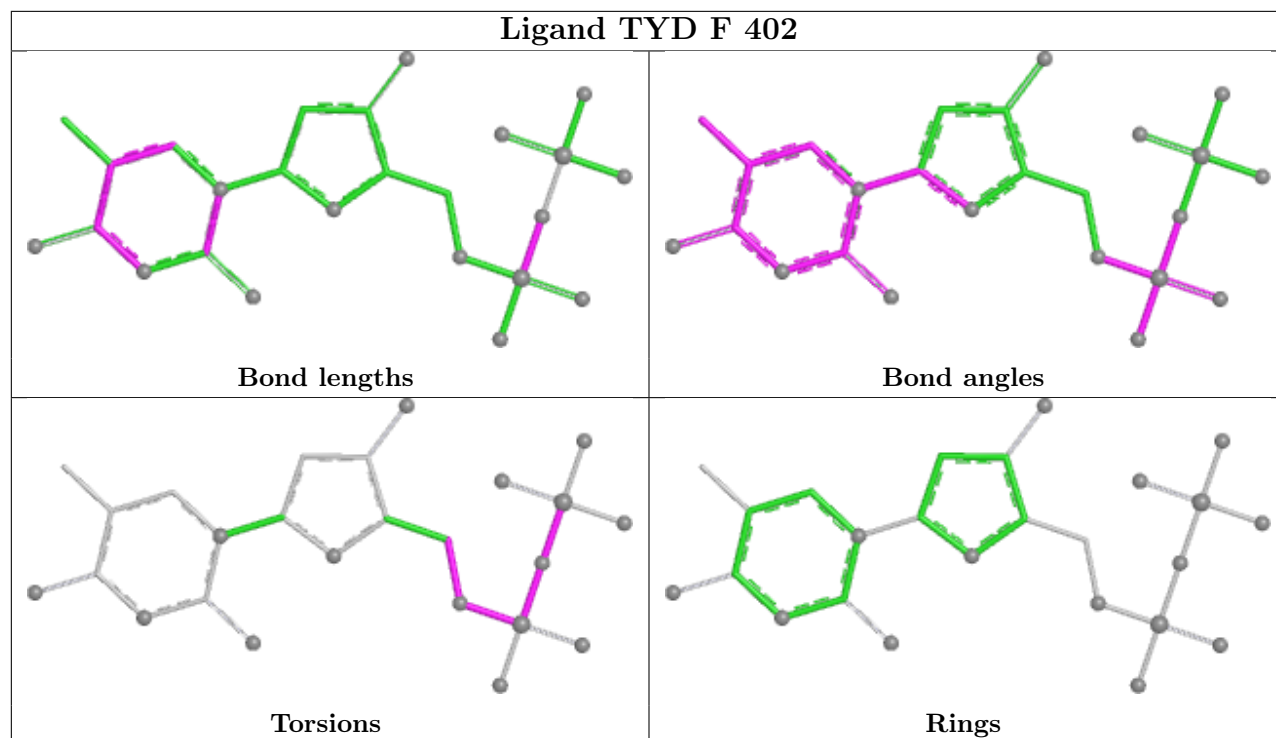


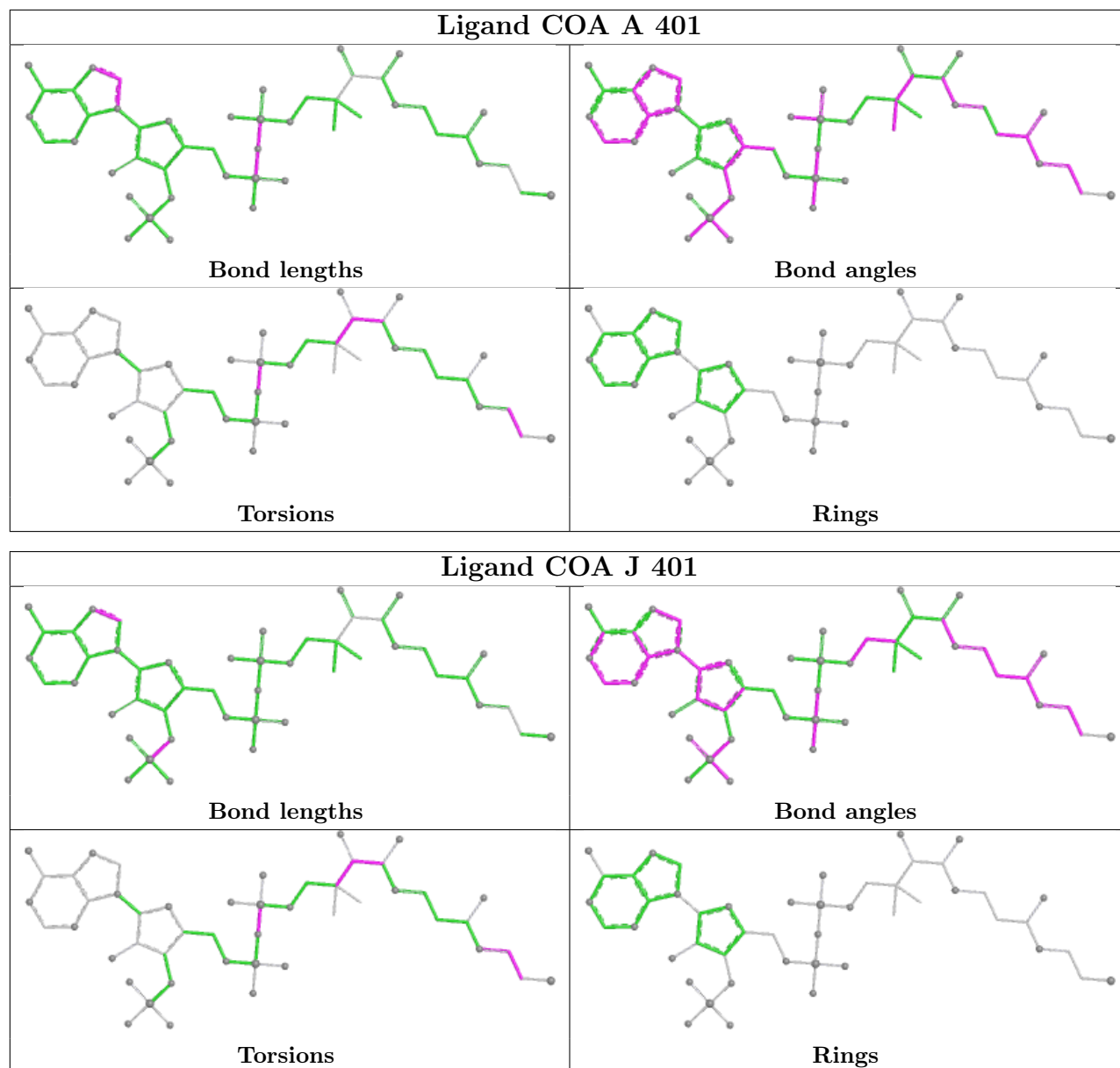
Ligand TYD J 402

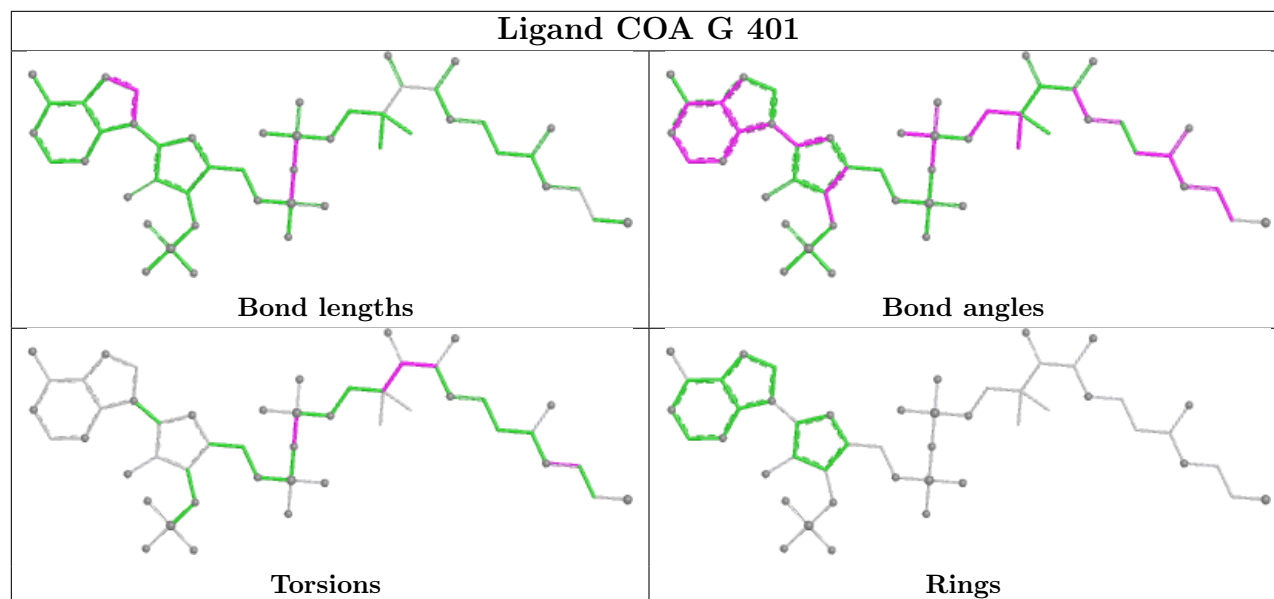
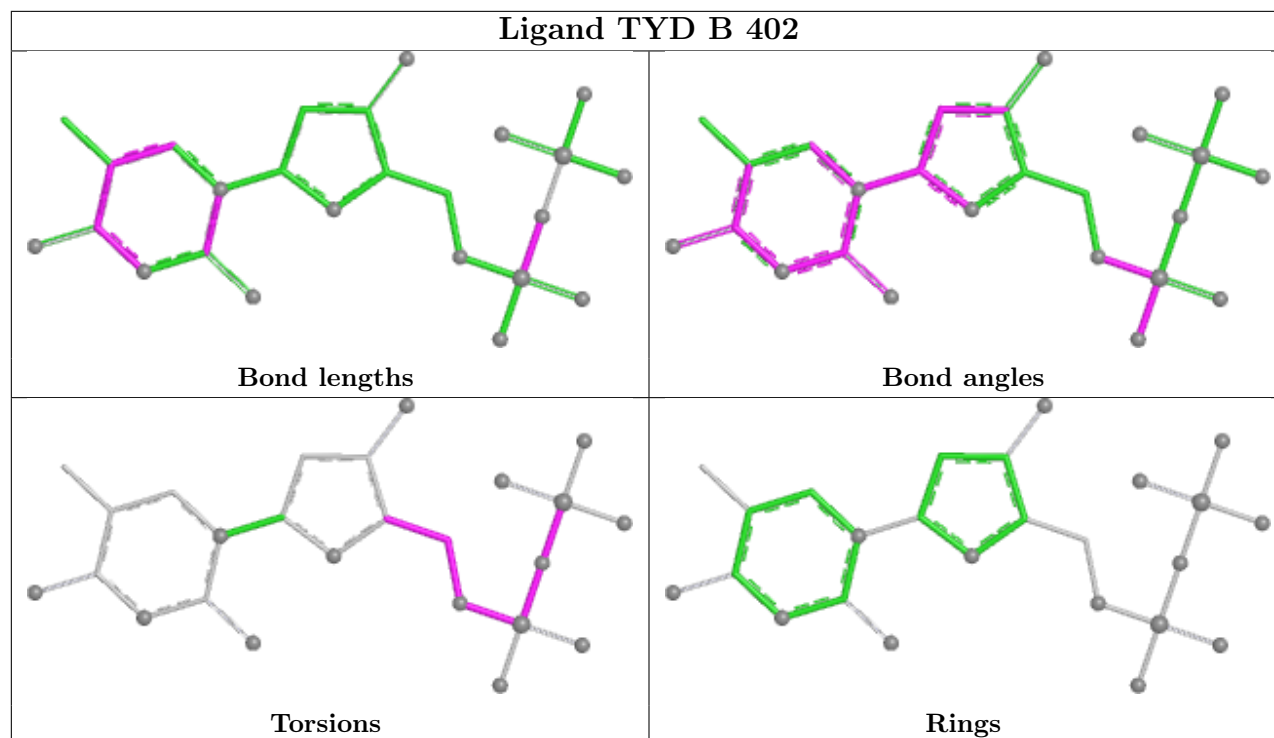


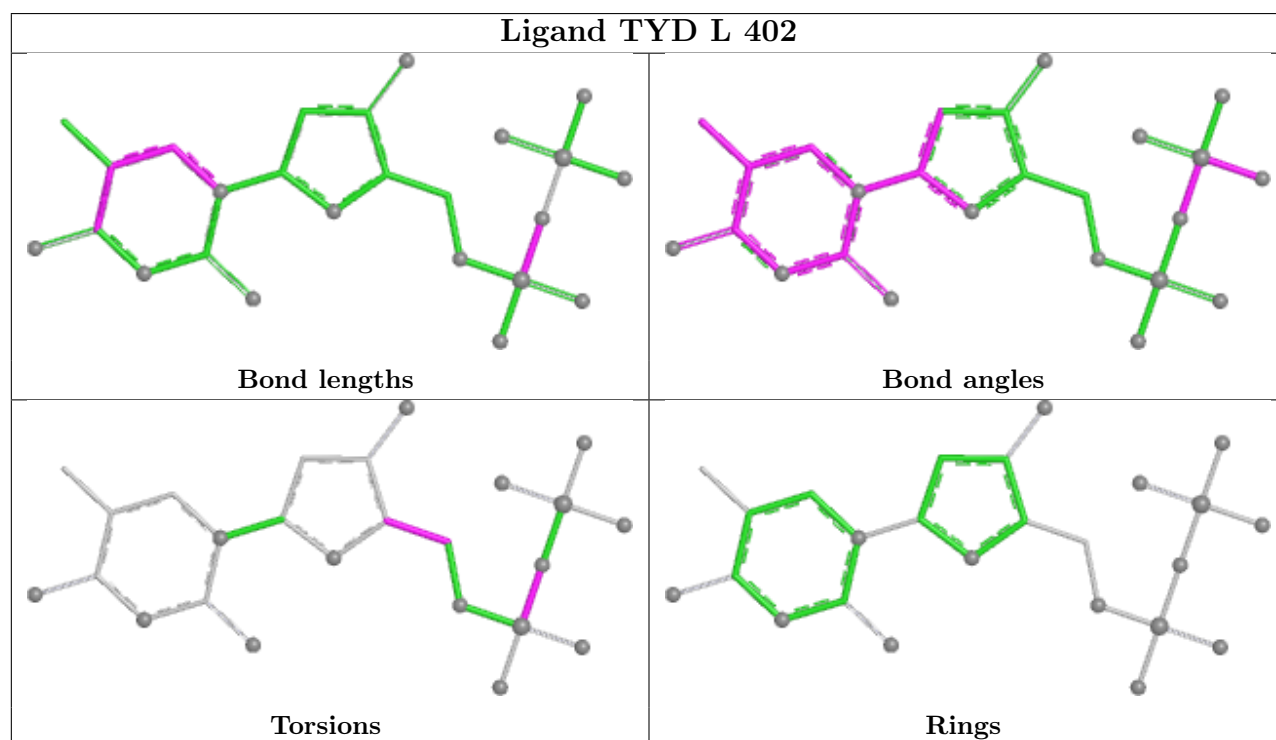
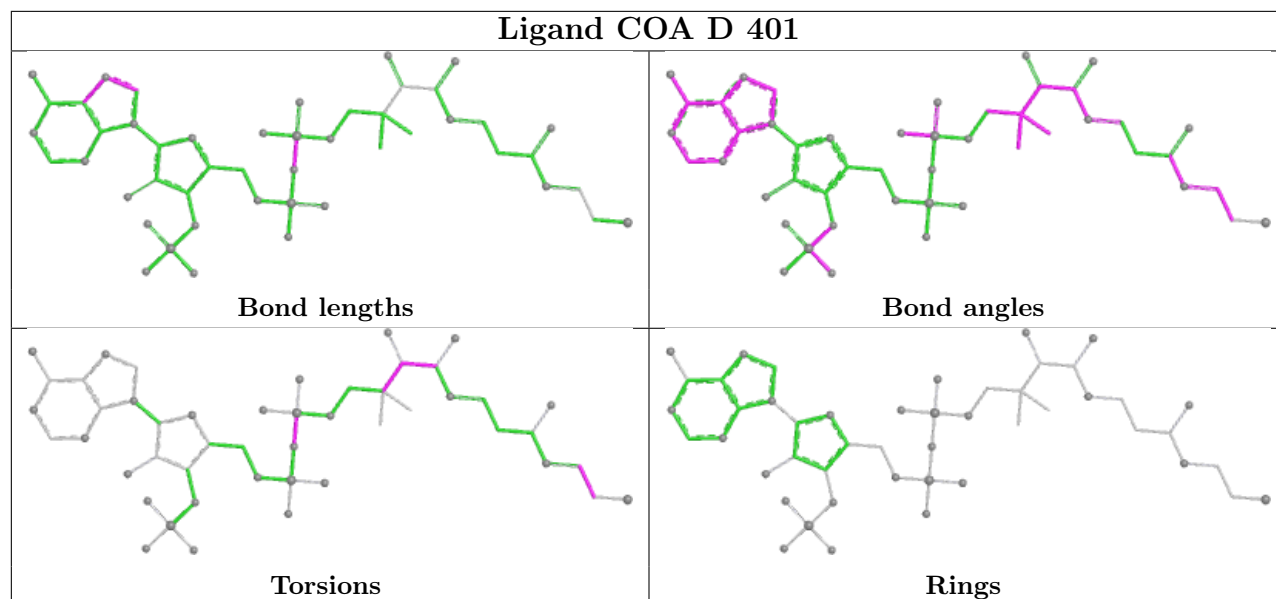


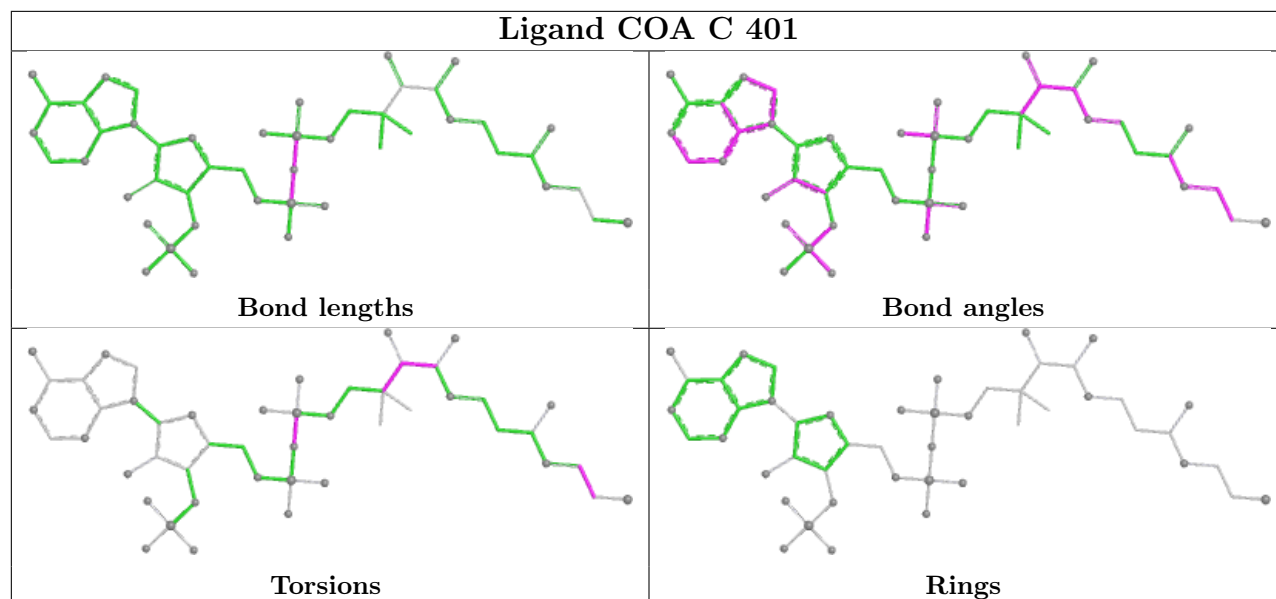












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/312 (91%)	-0.23	2 (0%) 84 82	12, 27, 46, 67	0
1	B	290/312 (92%)	-0.19	4 (1%) 73 71	12, 28, 51, 65	0
1	C	285/312 (91%)	-0.18	3 (1%) 78 76	14, 28, 47, 66	1 (0%)
1	D	283/312 (90%)	-0.00	3 (1%) 78 76	18, 33, 53, 75	0
1	E	286/312 (91%)	-0.00	5 (1%) 69 66	17, 32, 53, 67	0
1	F	294/312 (94%)	0.12	4 (1%) 73 71	20, 33, 54, 67	0
1	G	283/312 (90%)	-0.07	3 (1%) 78 76	17, 31, 56, 63	1 (0%)
1	H	278/312 (89%)	0.53	7 (2%) 58 55	27, 47, 65, 74	0
1	I	285/312 (91%)	0.16	7 (2%) 58 55	18, 34, 58, 65	0
1	J	275/312 (88%)	0.41	12 (4%) 39 36	18, 40, 63, 70	1 (0%)
1	K	285/312 (91%)	-0.06	8 (2%) 55 52	14, 29, 55, 81	1 (0%)
1	L	286/312 (91%)	0.10	8 (2%) 55 52	18, 32, 58, 65	1 (0%)
All	All	3415/3744 (91%)	0.05	66 (1%) 66 63	12, 33, 58, 81	5 (0%)

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	165	LEU	6.6
1	K	165	LEU	4.9
1	C	308	HIS	4.7
1	G	36	ASN	4.3
1	K	168	GLN	4.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TDR	J	403	9/9	0.62	0.19	58,62,64,65	0
4	TDR	D	403	9/9	0.65	0.17	43,47,49,50	0
4	TDR	L	403	9/9	0.67	0.20	71,72,73,74	0
4	TDR	C	403	9/9	0.72	0.18	51,55,57,59	0
4	TDR	B	403	9/9	0.74	0.13	41,43,47,47	0
4	TDR	E	403	9/9	0.74	0.15	41,46,48,49	0
4	TDR	K	403	9/9	0.75	0.20	69,72,74,74	0
4	TDR	F	403	9/9	0.75	0.15	52,54,56,56	0
3	TYD	J	402	25/25	0.78	0.15	69,81,92,93	0
4	TDR	A	403	9/9	0.78	0.13	31,41,43,44	0
3	TYD	G	402	25/25	0.80	0.14	40,58,72,72	0
3	TYD	L	402	25/25	0.84	0.12	46,63,71,72	0
3	TYD	C	402	25/25	0.84	0.13	31,56,66,68	0
3	TYD	H	401	25/25	0.85	0.14	44,61,73,74	0
3	TYD	D	402	25/25	0.85	0.12	47,71,75,77	0
3	TYD	F	402	25/25	0.87	0.12	35,56,79,79	0
3	TYD	I	402	25/25	0.88	0.10	22,40,66,68	0
3	TYD	A	402	25/25	0.88	0.10	39,63,74,75	0
3	TYD	B	402	25/25	0.90	0.10	34,57,71,73	0
3	TYD	E	402	25/25	0.91	0.09	31,49,61,63	0
3	TYD	K	402	25/25	0.91	0.09	22,39,55,57	0
2	COA	G	403	48/48	0.94	0.08	35,42,57,70	0
2	COA	I	401	48/48	0.94	0.09	27,43,62,71	0
2	COA	J	401	48/48	0.94	0.08	21,36,48,60	0
2	COA	D	401	48/48	0.94	0.08	20,41,56,64	0
5	MG	C	404	1/1	0.94	0.05	20,20,20,20	0
2	COA	G	401	48/48	0.95	0.07	26,36,41,53	0
2	COA	L	401	48/48	0.95	0.07	15,33,45,53	0
2	COA	A	401	48/48	0.95	0.07	17,29,42,55	0
2	COA	E	401	48/48	0.95	0.08	20,37,49,59	0
2	COA	K	401	48/48	0.96	0.07	21,37,64,70	0
2	COA	F	401	48/48	0.96	0.06	21,35,43,49	0

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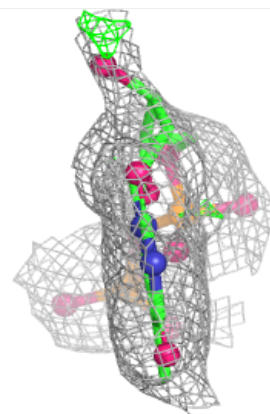
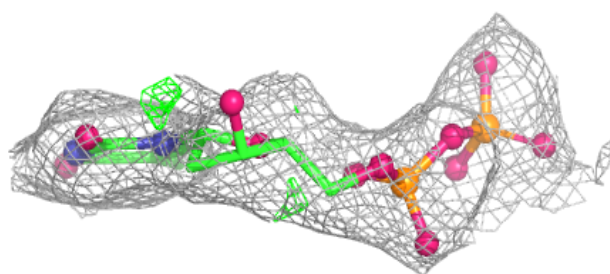
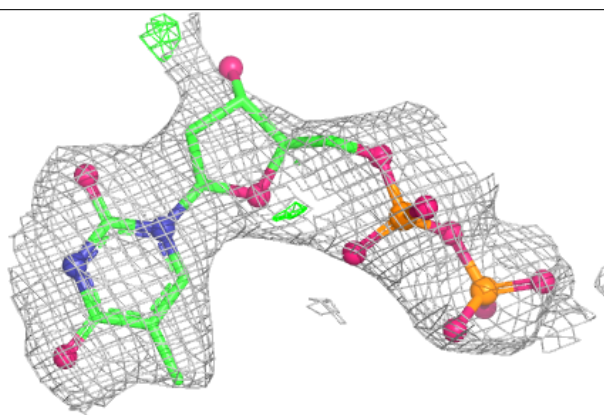
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	COA	C	401	48/48	0.97	0.06	14,32,42,45	0
2	COA	B	401	48/48	0.97	0.06	9,24,33,42	0
5	MG	B	404	1/1	0.98	0.05	26,26,26,26	0
5	MG	J	404	1/1	0.98	0.02	26,26,26,26	0
5	MG	G	404	1/1	0.99	0.02	27,27,27,27	0
5	MG	D	404	1/1	0.99	0.03	21,21,21,21	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.

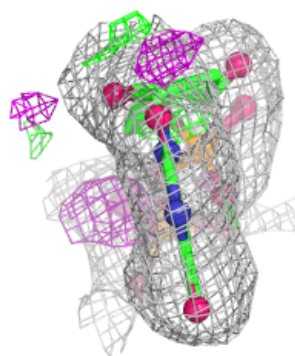
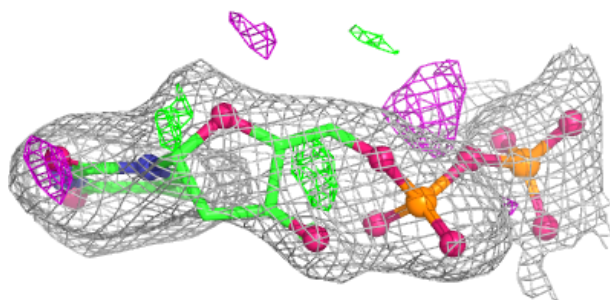
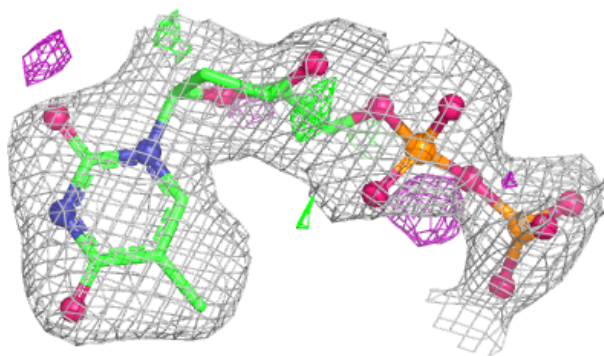
Electron density around TYD J 402:

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

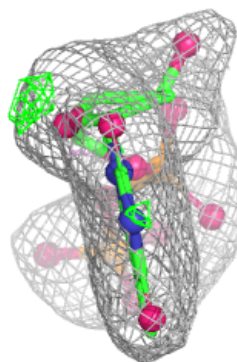
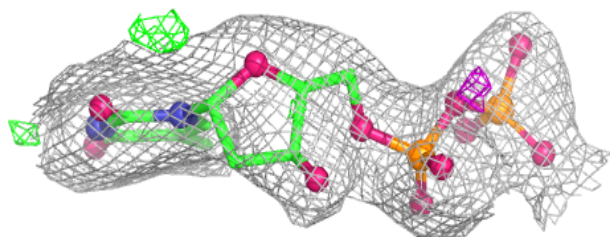
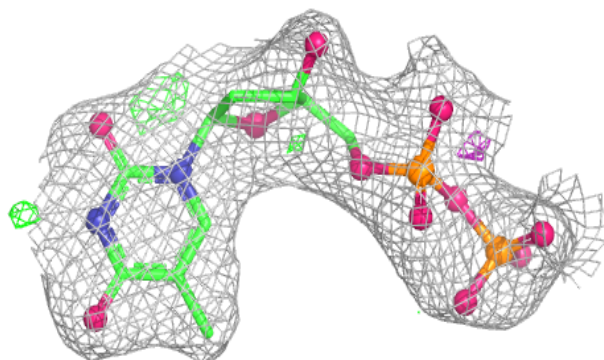


Electron density around TYD G 402:

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

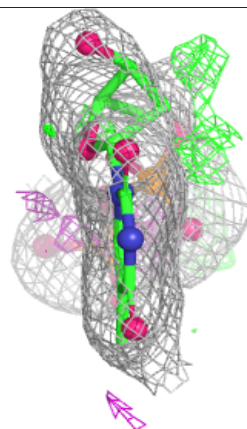
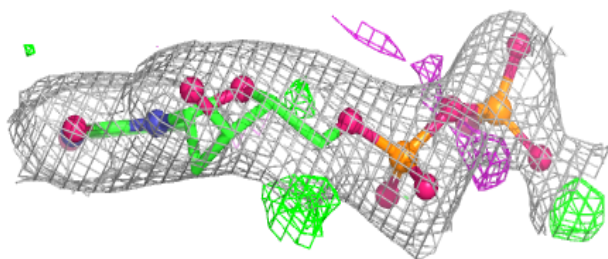
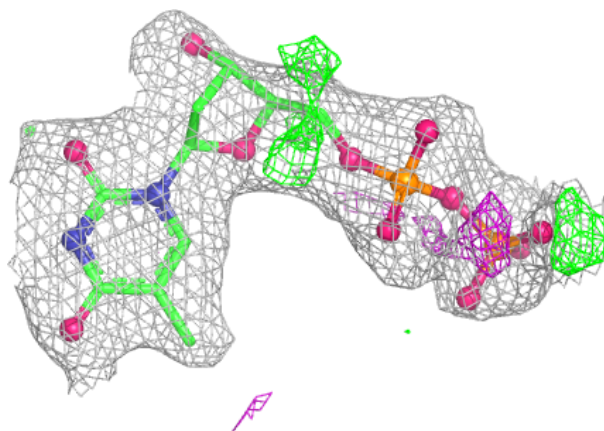
**Electron density around TYD L 402:**

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and green (positive)



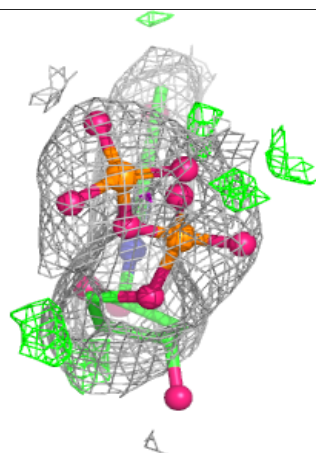
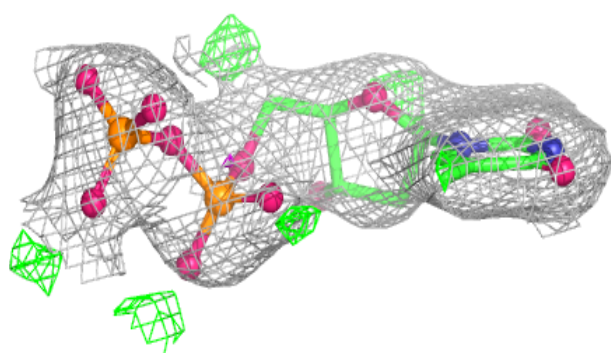
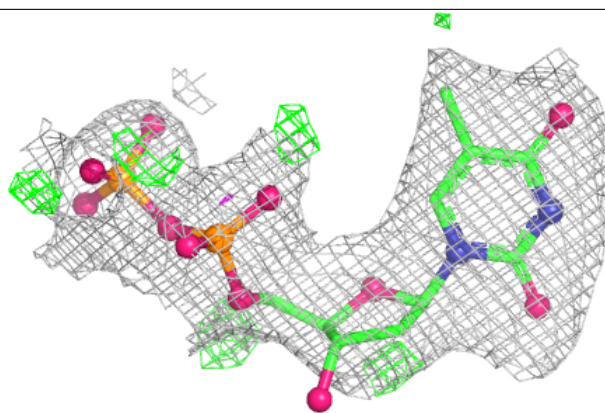
Electron density around TYD C 402:

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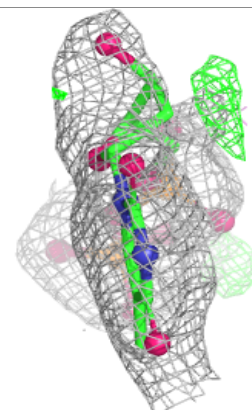
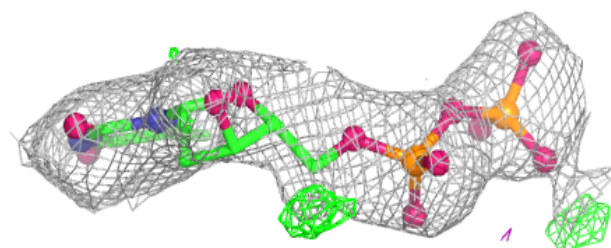
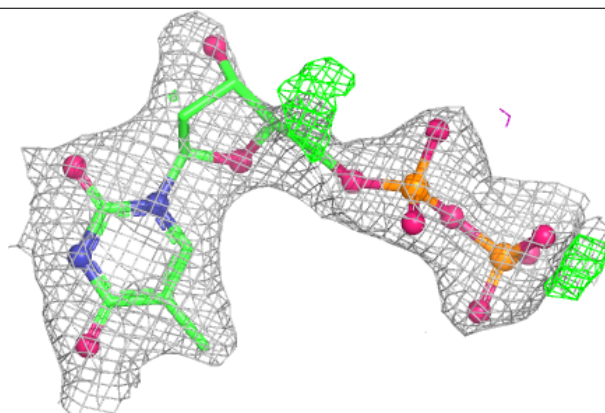


Electron density around TYD H 401:

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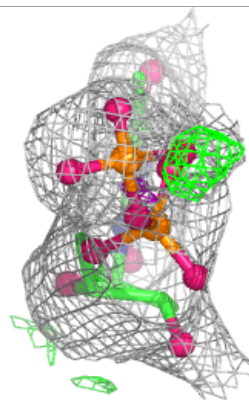
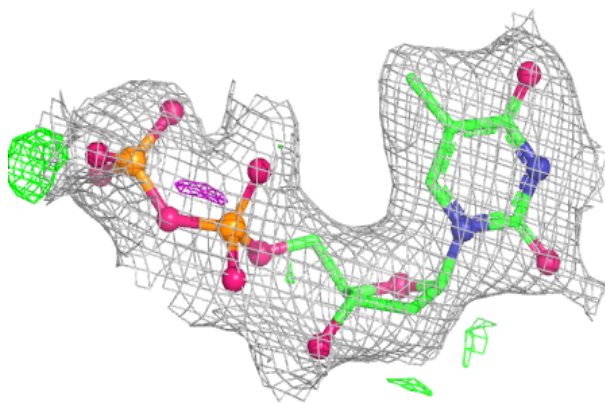
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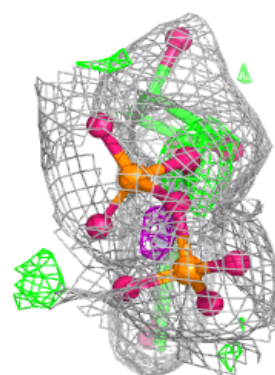
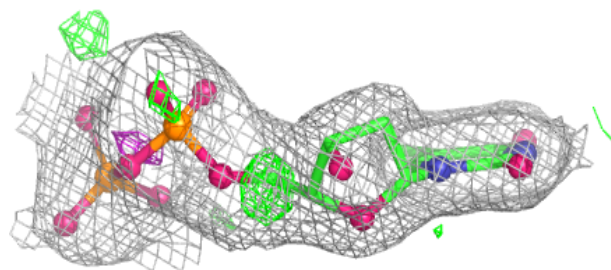
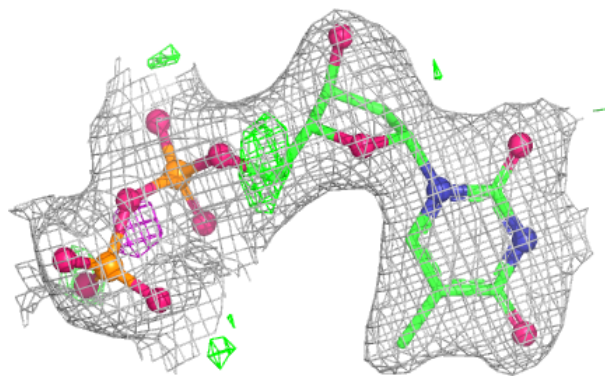


Electron density around TYD F 402:

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and green (positive)

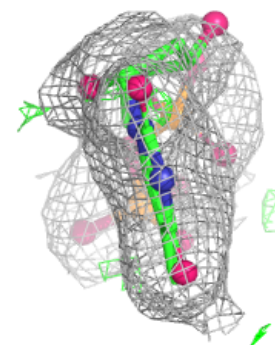
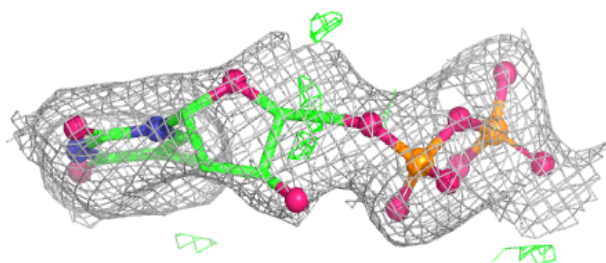
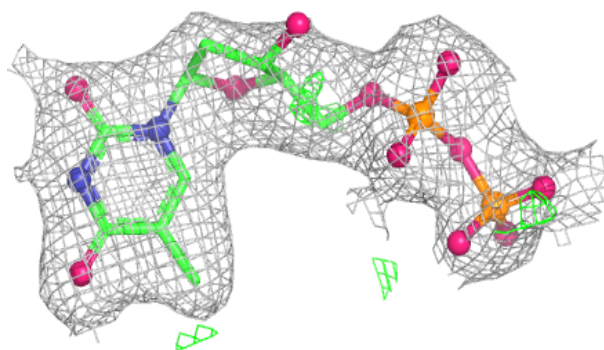
**Electron density around TYD I 402:**

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and green (positive)

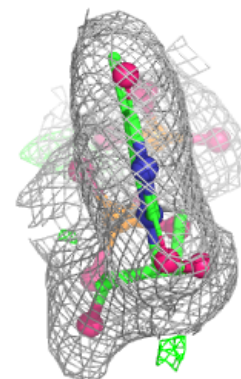
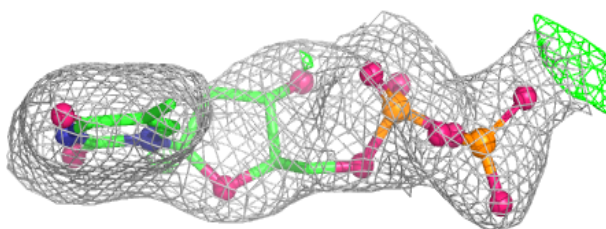
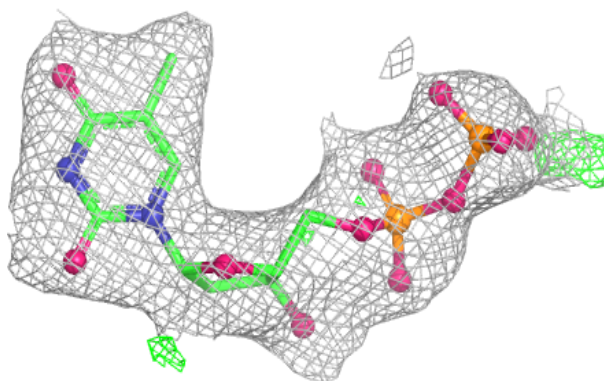


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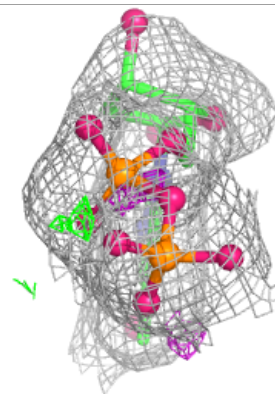
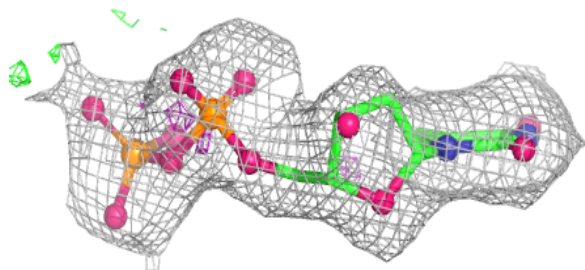
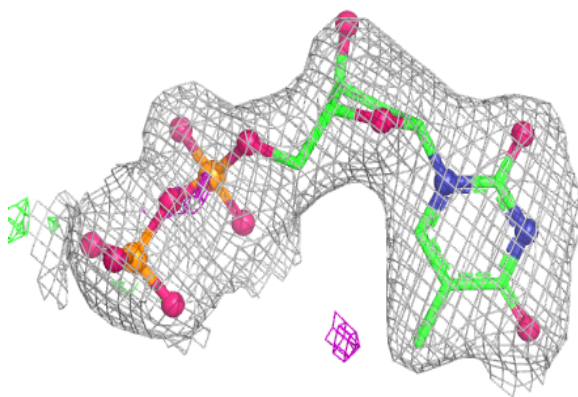
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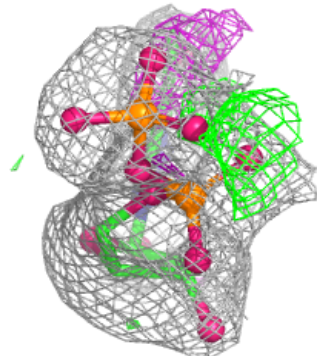
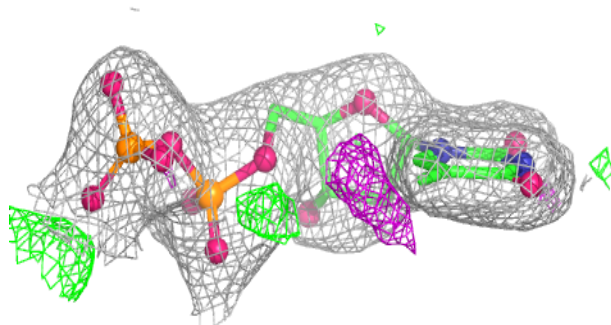
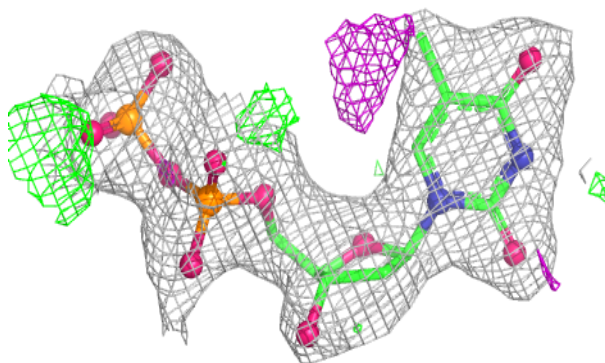


Electron density around TYD E 402:

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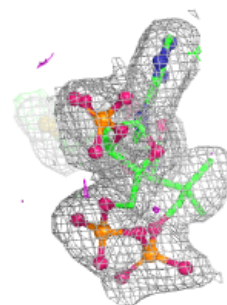
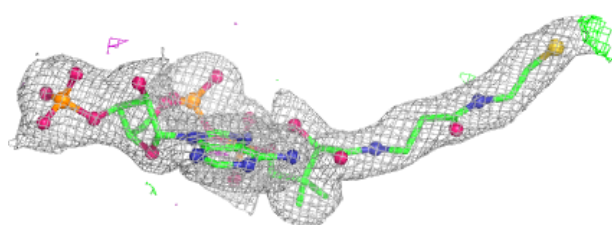
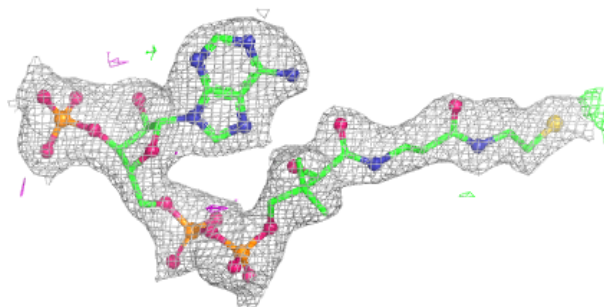
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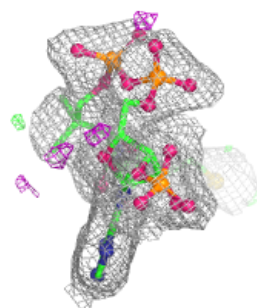
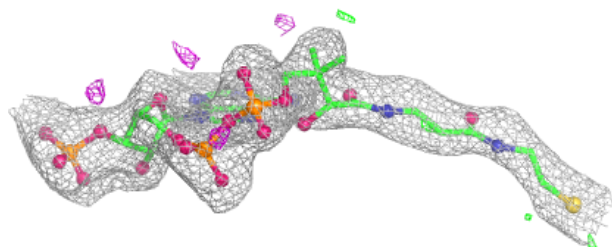
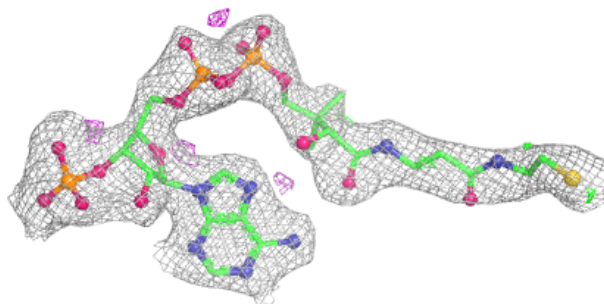


Electron density around COA G 403:

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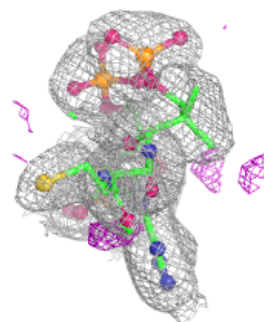
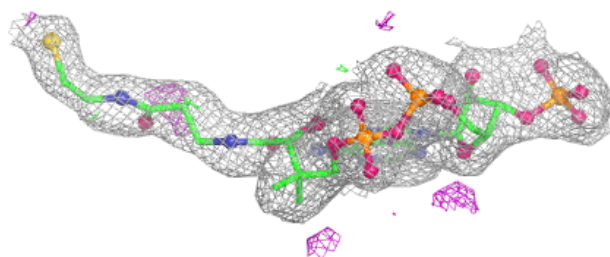
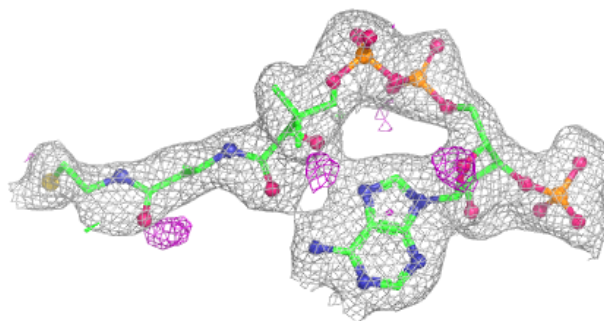
**Electron density around COA I 401:**

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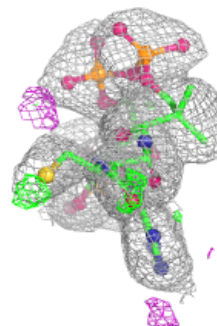
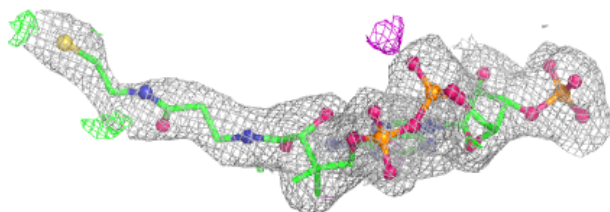
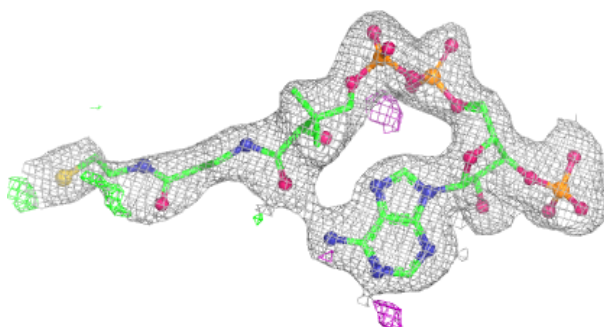


Electron density around COA J 401:

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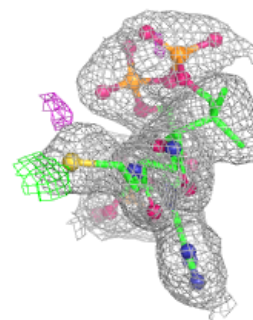
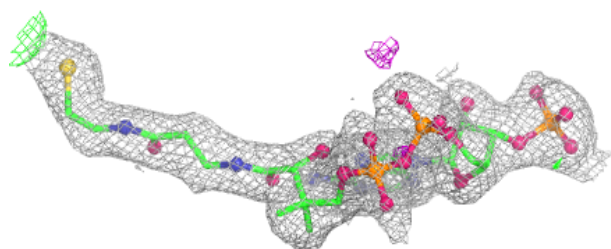
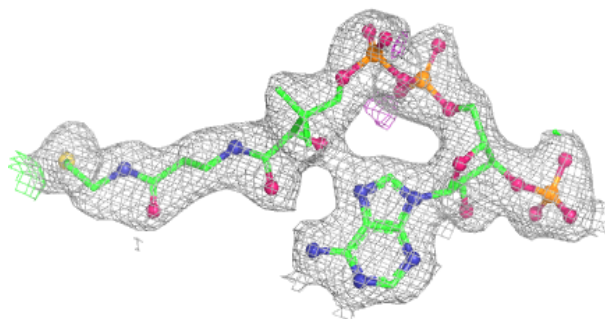
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

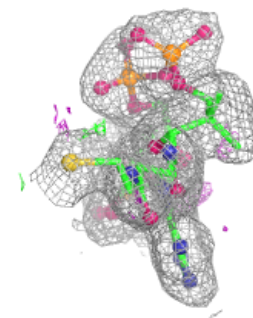
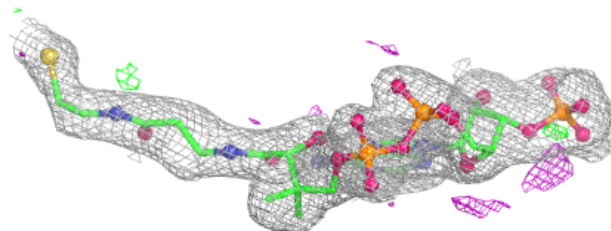
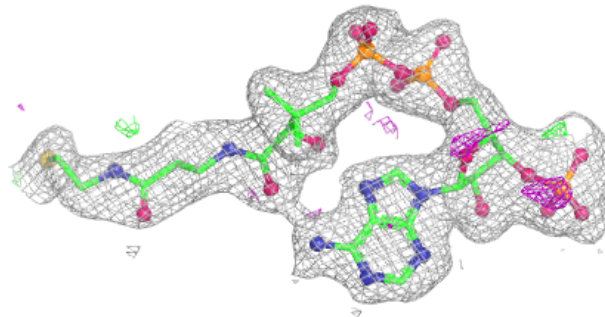


Electron density around COA G 401:

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

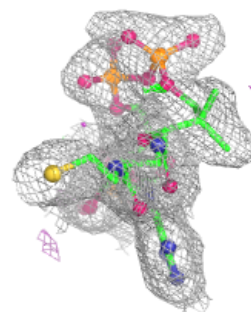
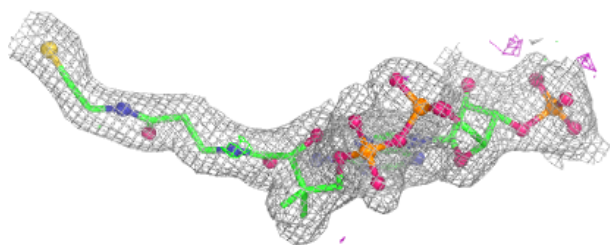
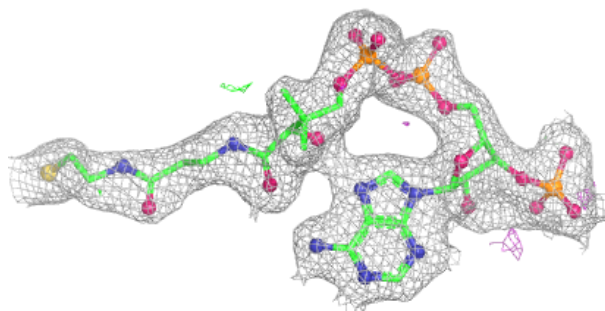
**Electron density around COA L 401:**

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

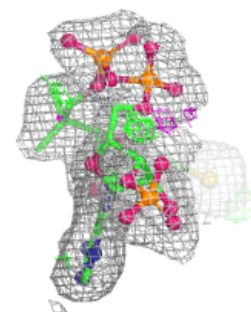
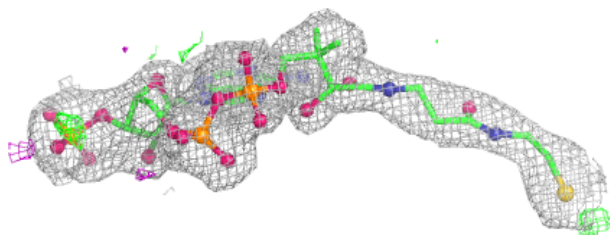
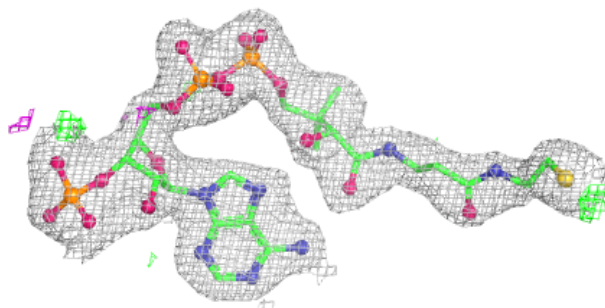


Electron density around COA A 401:

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

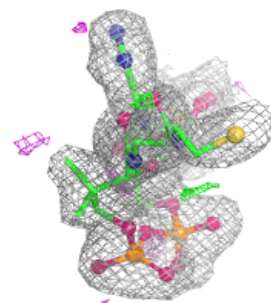
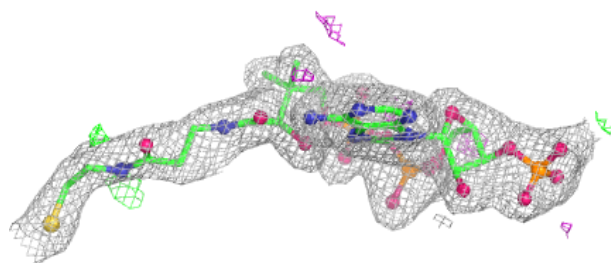
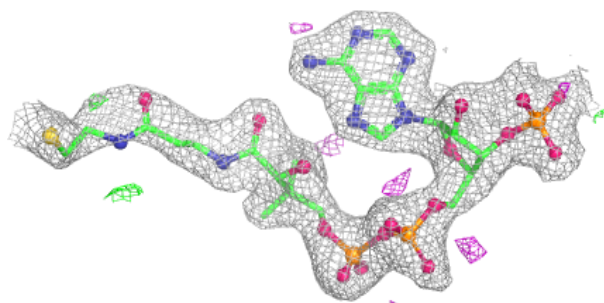
**Electron density around COA E 401:**

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

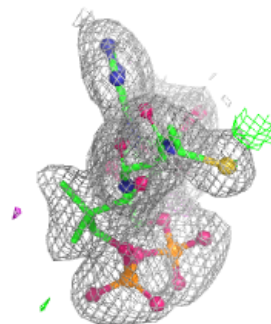
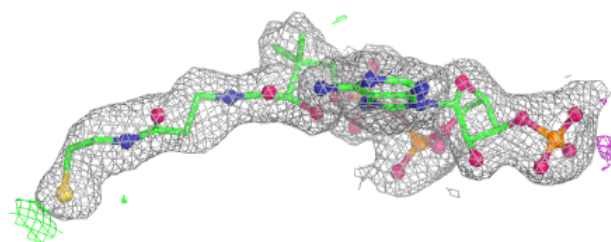
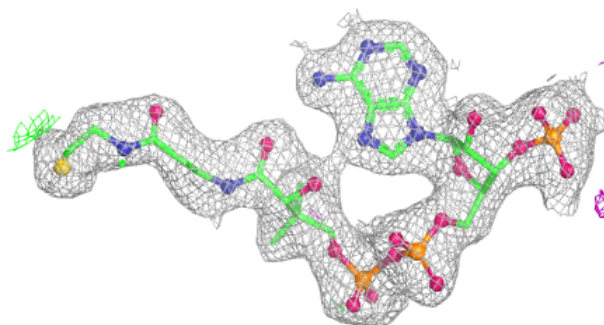


Electron density around COA K 401:

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

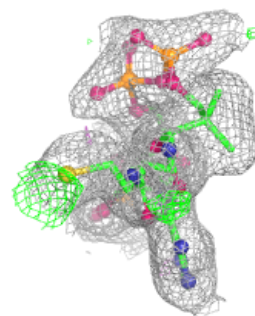
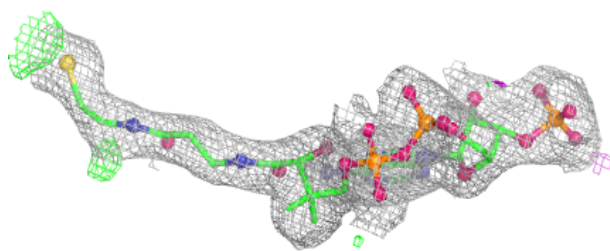
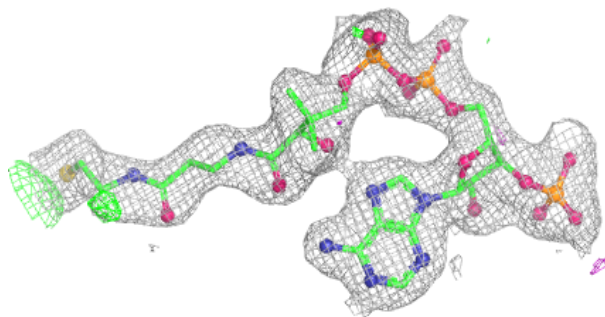
**Electron density around COA F 401:**

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

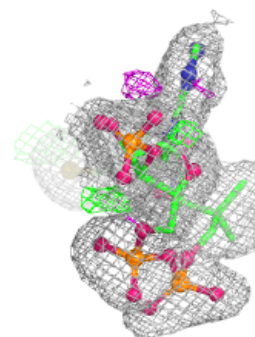
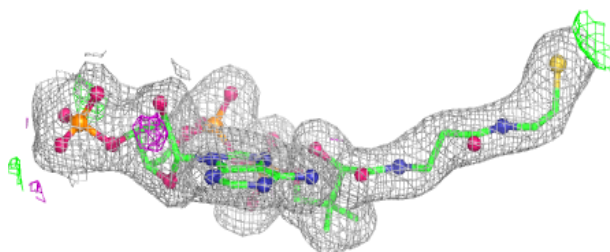
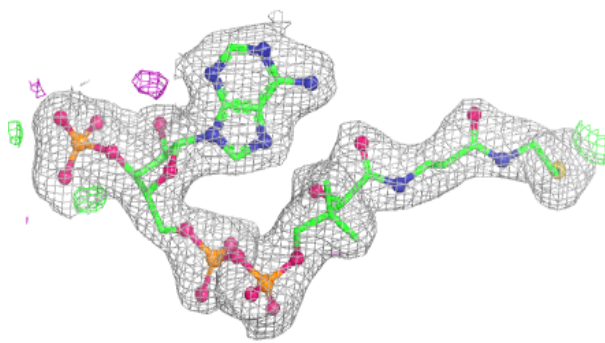


Electron density around COA C 401:

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

**Electron density around COA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.