



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:15 AM BST

PDB ID : 4MZU  
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 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

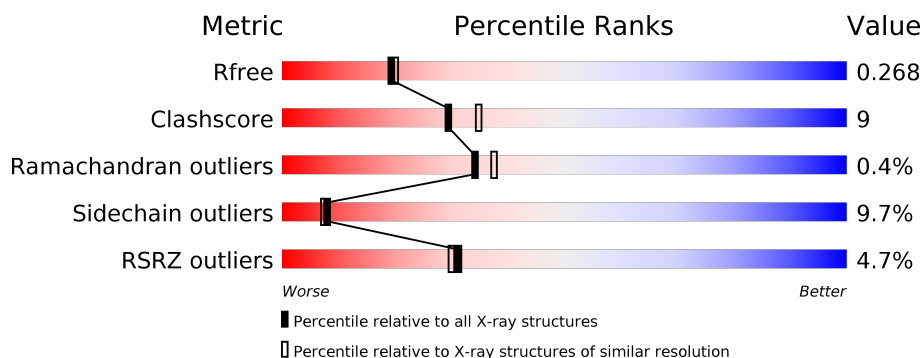
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	312	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>• • 9%</div> </div> </div>
1	B	312	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	C	312	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>• • 9%</div> </div> </div>
1	D	312	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div>• 9%</div> </div> </div>
1	E	312	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>• 8%</div> </div> </div>
1	F	312	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	312	<div><div></div><div>2%70%19%9%</div></div>
1	H	312	<div><div></div><div>9%58%28%11%</div></div>
1	I	312	<div><div></div><div>4%66%22%9%</div></div>
1	J	312	<div><div></div><div>7%65%18%12%</div></div>
1	K	312	<div><div></div><div>5%71%17%9%</div></div>
1	L	312	<div><div></div><div>3%66%22%8%</div></div>

## 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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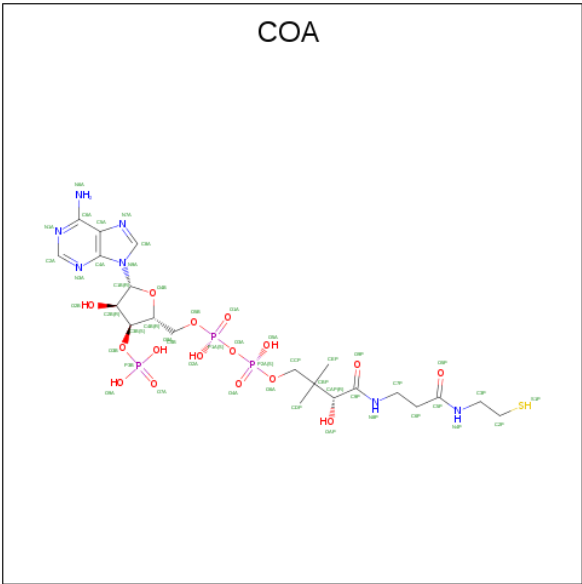
Chain	Residue	Modelled	Actual	Comment	Reference
F	312	HIS	-	EXPRESSION TAG	UNP Q12KT8
G	305	LEU	-	EXPRESSION TAG	UNP Q12KT8
G	306	GLU	-	EXPRESSION TAG	UNP Q12KT8
G	307	HIS	-	EXPRESSION TAG	UNP Q12KT8
G	308	HIS	-	EXPRESSION TAG	UNP Q12KT8
G	309	HIS	-	EXPRESSION TAG	UNP Q12KT8
G	310	HIS	-	EXPRESSION TAG	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 (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



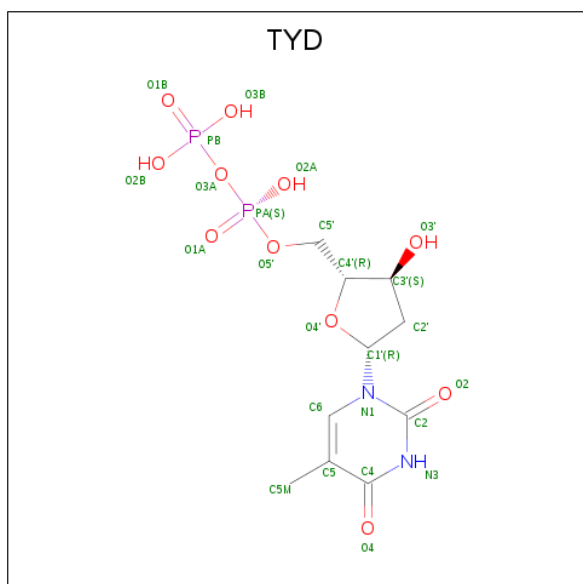
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			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 (three-letter code: TYD) (formula:  $C_{10}H_{16}N_2O_{11}P_2$ ).



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

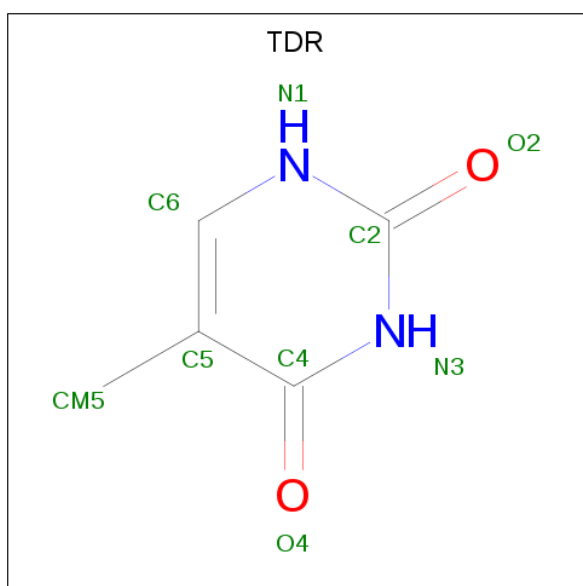
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	I	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	J	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	K	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
3	L	1	Total	C	N	O	P	0	0
			25	10	2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

- Molecule 4 is THYMINE (three-letter code: TDR) (formula: C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>).



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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	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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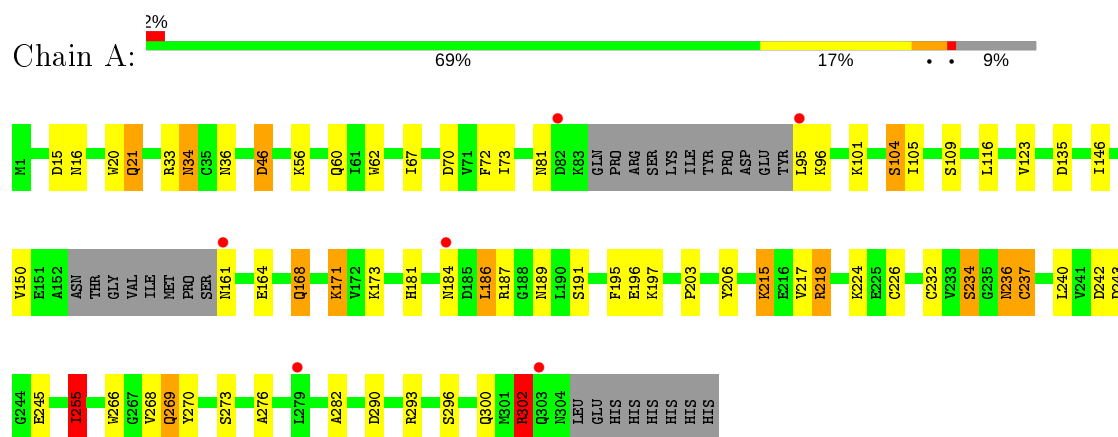
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	54	Total 54	O 54	0	0
6	K	82	Total 82	O 82	0	0
6	L	62	Total 62	O 62	0	0

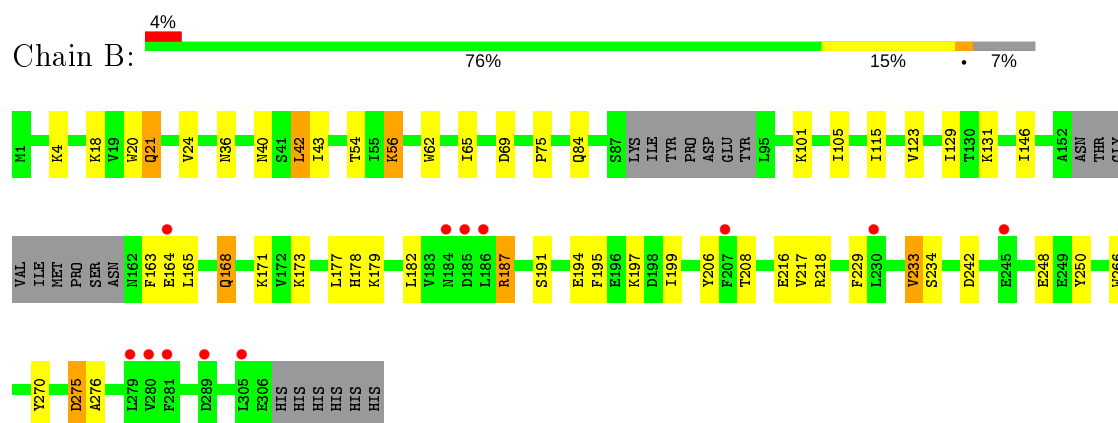
### 3 Residue-property plots [i](#)

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.

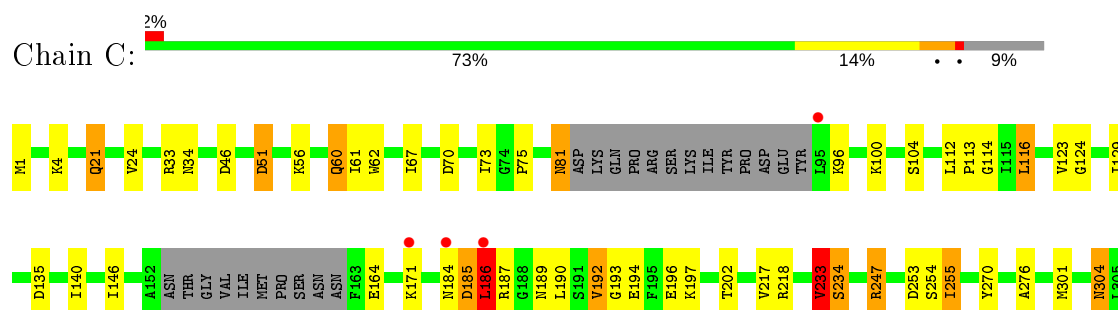
#### • Molecule 1: WxcM-like protein

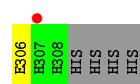


#### • Molecule 1: WxcM-like protein

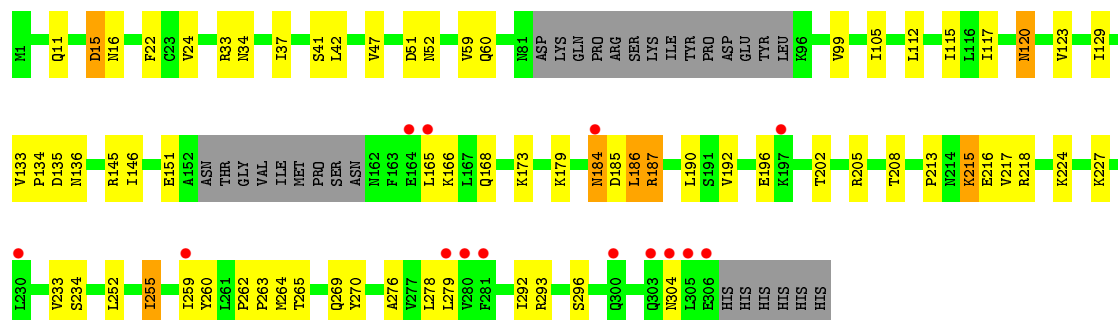


#### • Molecule 1: WxcM-like protein

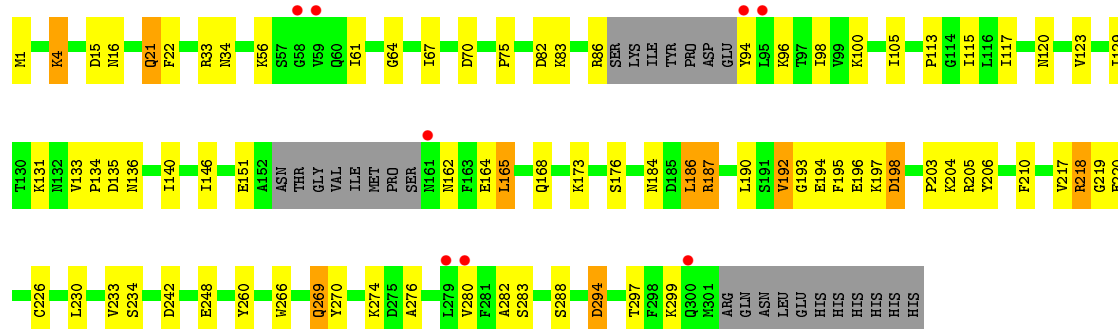




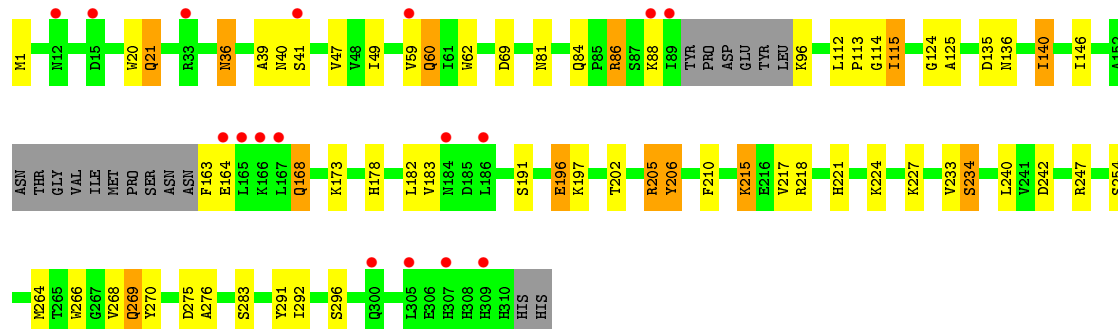
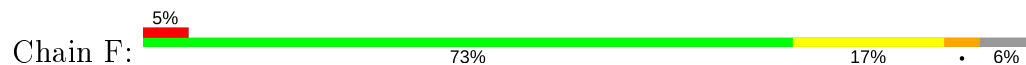
• Molecule 1: WxcM-like protein



• Molecule 1: WxcM-like protein

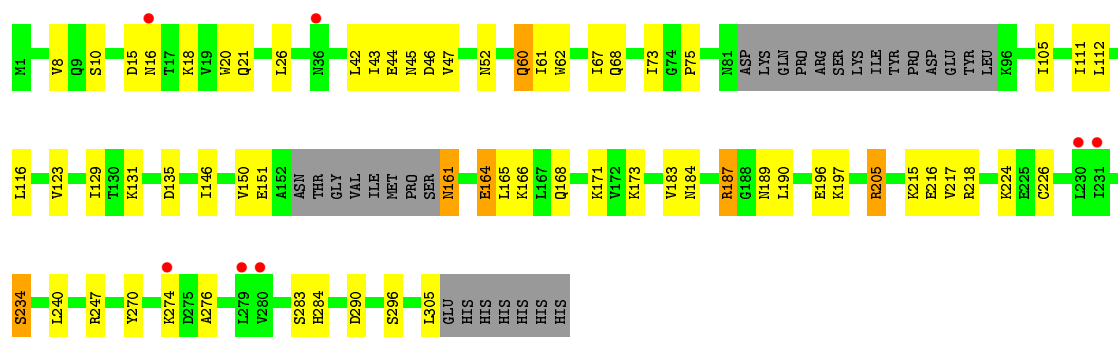


• Molecule 1: WxcM-like protein

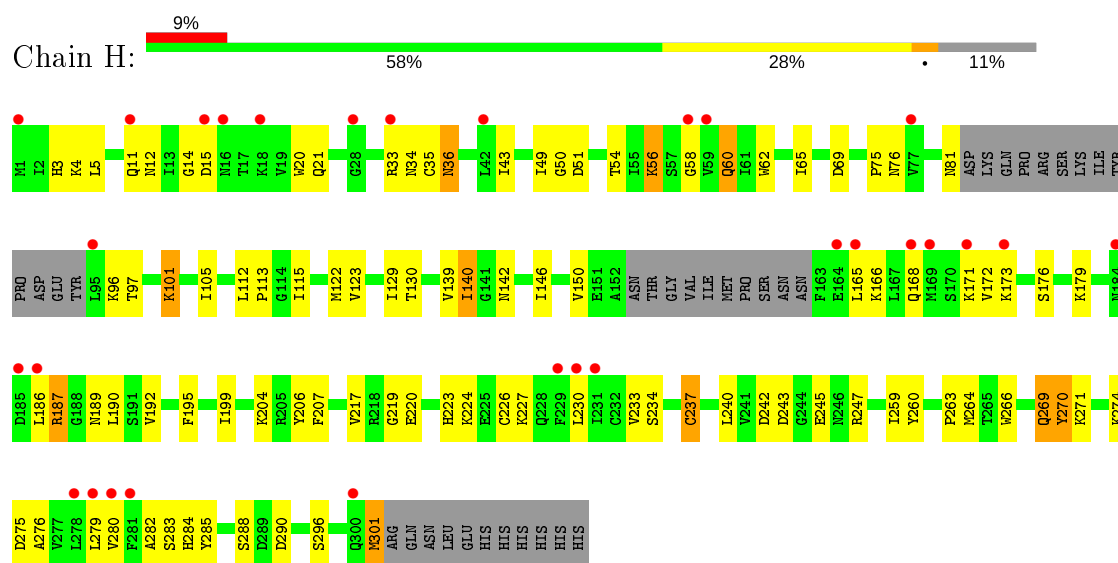


• Molecule 1: WxcM-like protein

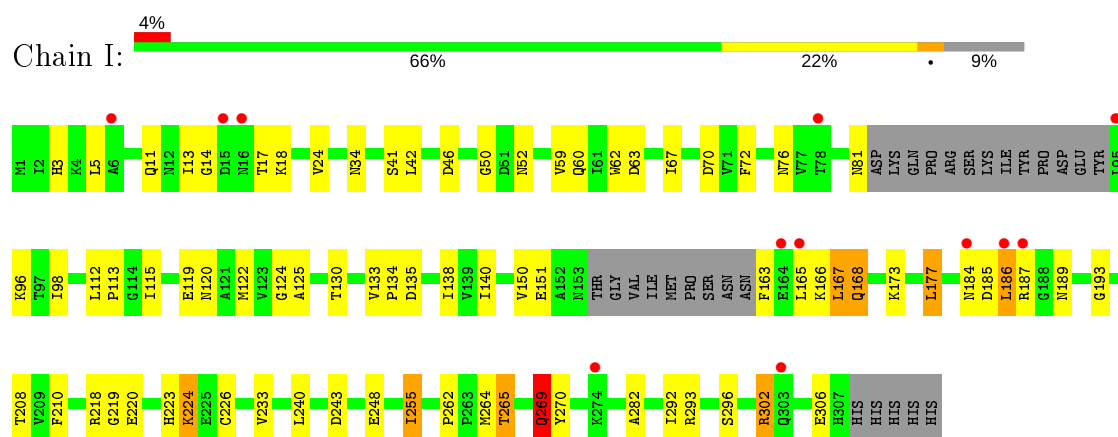




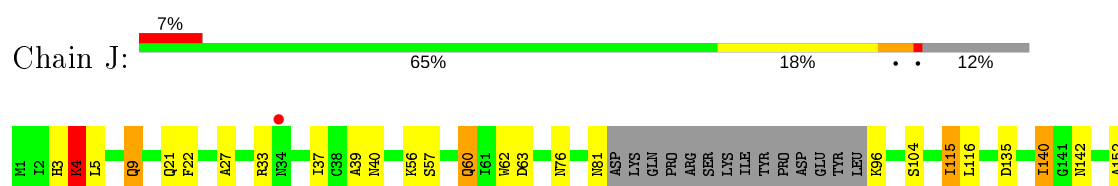
• Molecule 1: WxcM-like protein

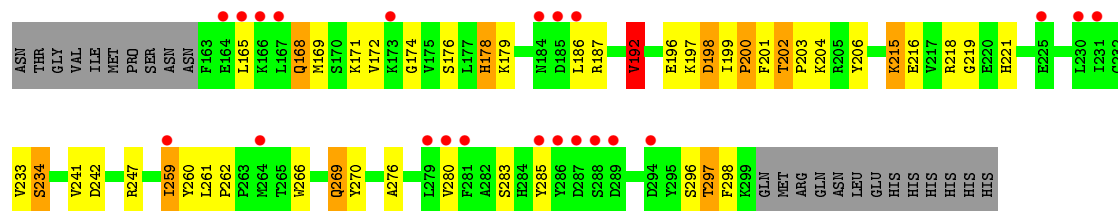


• Molecule 1: WxcM-like protein

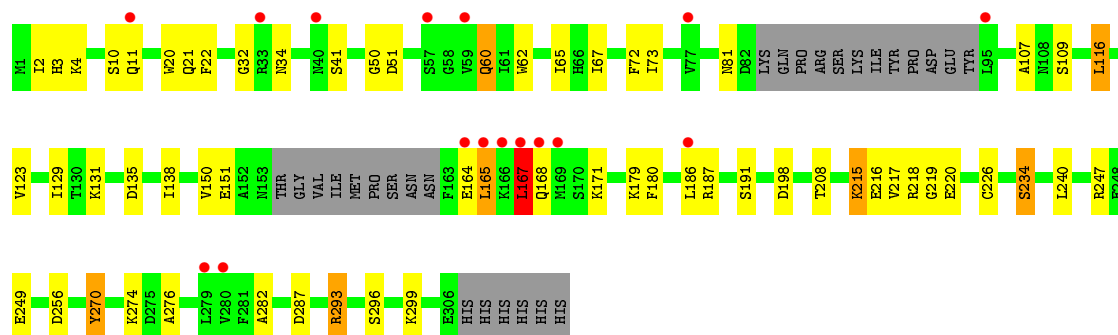
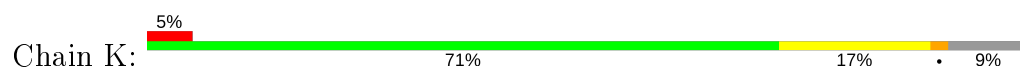


• Molecule 1: WxcM-like protein

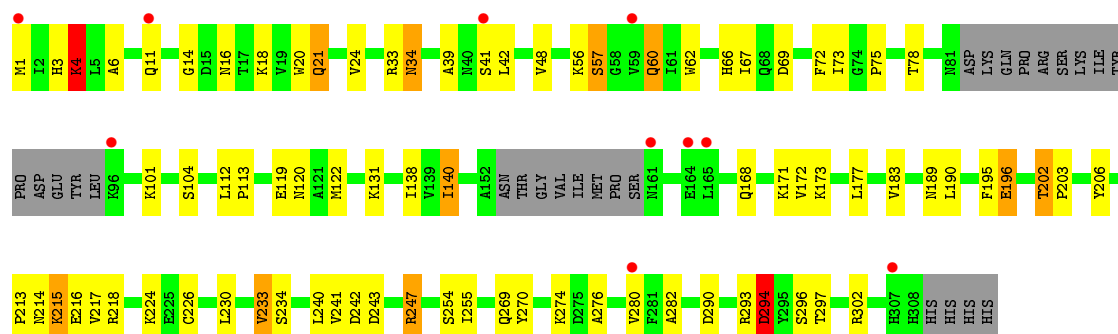




• Molecule 1: WxcM-like protein



• Molecule 1: WxcM-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.31Å 109.44Å 127.85Å 79.23° 79.98° 84.89°	Depositor
Resolution (Å)	30.00 – 2.20 28.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.9 (30.00-2.20) 90.9 (28.75-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.70	1/2261 (0.0%)	1.11	9/3059 (0.3%)
1	B	0.66	0/2304	1.06	4/3117 (0.1%)
1	C	0.68	0/2266	1.13	11/3066 (0.4%)
1	D	0.60	0/2245	1.06	6/3038 (0.2%)
1	E	0.61	0/2274	1.06	7/3078 (0.2%)
1	F	0.64	0/2331	1.09	6/3153 (0.2%)
1	G	0.63	0/2250	1.04	4/3045 (0.1%)
1	H	0.52	1/2200 (0.0%)	0.95	5/2978 (0.2%)
1	I	0.60	0/2258	1.04	4/3056 (0.1%)
1	J	0.56	0/2184	0.98	5/2956 (0.2%)
1	K	0.65	0/2270	1.08	10/3071 (0.3%)
1	L	0.61	0/2272	1.05	3/3074 (0.1%)
All	All	0.62	2/27115 (0.0%)	1.05	74/36691 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	CYS	CB-SG	-6.57	1.71	1.82
1	H	237	CYS	CB-SG	-5.43	1.73	1.81

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	ARG	NE-CZ-NH2	-14.92	112.84	120.30
1	C	247	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	56	LYS	CD-CE-NZ	7.64	129.28	111.70
1	A	237	CYS	N-CA-CB	-7.60	96.93	110.60
1	K	135	ASP	CB-CG-OD1	7.56	125.10	118.30
1	E	218	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	I	218	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	G	135	ASP	CB-CG-OD1	7.10	124.69	118.30
1	E	56	LYS	CD-CE-NZ	7.07	127.95	111.70
1	F	115	ILE	CG1-CB-CG2	-7.03	95.92	111.40
1	F	275	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	302	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	C	218	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	B	69	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	135	ASP	CB-CG-OD1	6.70	124.33	118.30
1	G	187	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	K	293	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	K	293	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	L	294	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	F	69	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	247	ARG	CG-CD-NE	-6.20	98.78	111.80
1	K	116	LEU	CB-CG-CD1	6.12	121.41	111.00
1	B	101	LYS	CD-CE-NZ	-5.98	97.94	111.70
1	J	63	ASP	CB-CG-OD1	5.97	123.68	118.30
1	C	135	ASP	CB-CG-OD1	5.97	123.67	118.30
1	E	33	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	46	ASP	N-CA-CB	5.92	121.25	110.60
1	D	112	LEU	CA-CB-CG	-5.90	101.73	115.30
1	K	109	SER	CB-CA-C	-5.87	98.94	110.10
1	B	69	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	185	ASP	CB-CG-OD1	5.81	123.53	118.30
1	K	256	ASP	CB-CG-OD1	5.81	123.53	118.30
1	I	135	ASP	CB-CG-OD1	5.75	123.48	118.30
1	J	115	ILE	CG1-CB-CG2	-5.75	98.76	111.40
1	H	237	CYS	CB-CA-C	-5.73	98.95	110.40
1	D	145	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	K	167	LEU	CA-CB-CG	5.65	128.29	115.30
1	H	269	GLN	CA-CB-CG	5.64	125.82	113.40
1	F	86	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	H	187	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	131	LYS	CB-CA-C	-5.61	99.19	110.40
1	G	218	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	I	269	GLN	CA-CB-CG	5.58	125.69	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	142	ASN	C-N-CD	-5.55	108.40	120.60
1	J	192	VAL	CB-CA-C	-5.50	100.95	111.40
1	D	145	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	218	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	51	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	46	ASP	CB-CA-C	5.40	121.20	110.40
1	K	218	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	E	133	VAL	C-N-CD	5.34	139.62	128.40
1	F	86	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	E	192	VAL	CB-CA-C	-5.33	101.28	111.40
1	C	186	LEU	CA-CB-CG	5.32	127.54	115.30
1	L	247	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	H	301	MET	CG-SD-CE	5.30	108.68	100.20
1	L	294	ASP	N-CA-CB	-5.28	101.09	110.60
1	D	255	ILE	CG1-CB-CG2	-5.28	99.79	111.40
1	C	192	VAL	CB-CA-C	-5.27	101.39	111.40
1	C	21	GLN	CA-CB-CG	5.26	124.97	113.40
1	K	287	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	E	187	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	G	46	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	D	192	VAL	CB-CA-C	-5.13	101.65	111.40
1	A	109	SER	CB-CA-C	-5.13	100.36	110.10
1	D	47	VAL	N-CA-C	-5.12	97.18	111.00
1	I	177	LEU	CA-CB-CG	-5.10	103.58	115.30
1	A	56	LYS	CB-CA-C	5.09	120.58	110.40
1	A	302	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	F	206	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	K	81	ASN	N-CA-C	5.04	124.60	111.00
1	J	135	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	255	ILE	CB-CA-C	-5.01	101.59	111.60
1	J	186	LEU	CA-CB-CG	5.00	126.81	115.30

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 ⓘ

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	57	0
1	B	2262	0	2258	38	0
1	C	2222	0	2219	48	0
1	D	2204	0	2197	37	0
1	E	2231	0	2224	45	0
1	F	2288	0	2278	51	0
1	G	2206	0	2202	48	0
1	H	2159	0	2158	61	0
1	I	2217	0	2210	57	0
1	J	2140	0	2143	45	0
1	K	2226	0	2225	37	0
1	L	2228	0	2220	49	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	1	0
2	I	48	0	32	2	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	517	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 9.

All (517) 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: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:A:60:GLN:HG3	1:A:62:TRP:CZ2	1.91	1.05
1:A:184:ASN:HB3	1:A:189:ASN:HD22	1.23	1.04
1:K:215[A]:LYS:H	1:K:215[A]:LYS:HE3	1.22	1.03
1:I:264:MET:HE1	1:I:292:ILE:HD12	1.39	1.00
1:B:123:VAL:HG13	1:B:129:ILE:HD11	1.48	0.95
1:C:100:LYS:HD2	1:C:116:LEU:HD21	1.46	0.94
1:A:236:ASN:HD21	1:A:273:SER:CB	1.80	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:GLN:HE21	1:E:21:GLN:H	1.14	0.92
1:A:168:GLN:HE22	1:G:168:GLN:HE22	1.10	0.92
3:G:402:TYD:O1B	1:K:187:ARG:NH1	2.02	0.92
1:D:187:ARG:HH11	1:D:187:ARG:HG2	1.34	0.91
1:F:215:LYS:HE3	1:F:215:LYS:H	1.33	0.91
1:H:207:PHE:HB3	1:J:192:VAL:HG13	1.53	0.90
2:J:401:COA:H143	1:L:140:ILE:HD11	1.52	0.90
1:A:236:ASN:ND2	1:A:273:SER:CB	2.35	0.89
1:I:60:GLN:HG3	1:I:62:TRP:CZ2	2.08	0.89
1:F:215:LYS:HE3	1:F:215:LYS:N	1.88	0.87
1:I:150:VAL:HG12	1:I:151:GLU:HG2	1.57	0.86
1:A:168:GLN:HE22	1:G:168:GLN:NE2	1.73	0.86
1:A:184:ASN:HB3	1:A:189:ASN:ND2	1.92	0.85
1:H:242:ASP:HB3	1:H:266:TRP:HB3	1.60	0.84
1:A:21:GLN:NE2	1:A:21:GLN:H	1.75	0.84
1:E:21:GLN:NE2	1:E:21:GLN:H	1.75	0.83
1:C:123:VAL:HG13	1:C:129:ILE:CD1	2.07	0.83
1:B:242:ASP:HB3	1:B:266:TRP:HB3	1.60	0.83
1:I:186:LEU:CD2	1:I:186:LEU:H	1.92	0.81
1:D:185:ASP:HB2	1:D:186:LEU:HD23	1.62	0.81
1:F:224:LYS:HA	1:F:264:MET:CE	2.10	0.81
1:E:269:GLN:HG3	6:E:526:HOH:O	1.81	0.81
1:A:21:GLN:HE21	1:A:21:GLN:H	1.28	0.80
1:I:186:LEU:HD23	1:I:186:LEU:H	1.45	0.80
1:G:216:GLU:OE1	1:K:187:ARG:HD2	1.82	0.80
1:C:56:LYS:NZ	6:C:547:HOH:O	2.15	0.79
1:B:187:ARG:HH11	1:B:187:ARG:HG2	1.48	0.78
1:C:100:LYS:HD2	1:C:116:LEU:CD2	2.14	0.78
1:H:123:VAL:HG13	1:H:129:ILE:HD11	1.65	0.78
1:I:264:MET:CE	1:I:292:ILE:HD12	2.14	0.78
1:A:168:GLN:NE2	1:G:168:GLN:HE22	1.81	0.78
1:I:173:LYS:HG3	1:I:243:ASP:OD1	1.83	0.78
1:D:227:LYS:HG2	1:D:260:TYR:OH	1.84	0.77
1:C:60:GLN:HG3	1:C:62:TRP:CZ2	2.18	0.77
1:F:224:LYS:HA	1:F:264:MET:HE2	1.65	0.77
1:A:21:GLN:NE2	4:A:403:TDR:O4	2.17	0.76
1:J:60:GLN:HE21	1:L:75:PRO:HB2	1.50	0.76
1:H:140:ILE:HD11	2:I:401:COA:CEP	2.16	0.76
1:A:302:ARG:HH11	1:A:302:ARG:HG3	1.51	0.75
1:F:60:GLN:HG3	1:F:62:TRP:CZ2	2.22	0.75
1:J:269:GLN:HG3	6:J:521:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ARG:N	1:H:51:ASP:OD1	2.17	0.74
1:I:185:ASP:HB2	1:I:186:LEU:HD23	1.69	0.73
1:C:123:VAL:HG13	1:C:129:ILE:HD11	1.68	0.73
1:C:123:VAL:CG1	1:C:129:ILE:CD1	2.66	0.73
1:B:123:VAL:HG13	1:B:129:ILE:CD1	2.18	0.73
1:C:190:LEU:HD21	1:C:192:VAL:HG22	1.70	0.73
1:B:187:ARG:HG2	1:D:216:GLU:OE1	1.89	0.73
1:A:184:ASN:CB	1:A:189:ASN:HD22	2.01	0.72
1:H:69:ASP:HB2	1:H:101:LYS:HD3	1.70	0.72
1:K:72:PHE:CZ	2:L:401:COA:H22	2.24	0.72
1:G:60:GLN:NE2	1:I:76:ASN:HD21	1.87	0.71
1:A:302:ARG:CG	1:A:302:ARG:HH11	2.02	0.71
1:I:269:GLN:HG2	6:I:553:HOH:O	1.90	0.71
1:C:100:LYS:CD	1:C:116:LEU:HD21	2.21	0.70
1:A:184:ASN:CB	1:A:189:ASN:ND2	2.52	0.70
1:A:171:LYS:HG3	1:G:165:LEU:HD21	1.71	0.70
1:H:65:ILE:HG13	1:H:97:THR:HB	1.73	0.70
1:B:21:GLN:HG3	1:C:24:VAL:CG2	2.21	0.70
1:F:20:TRP:HB3	1:F:21:GLN:OE1	1.92	0.70
1:H:176:SER:OG	1:H:260:TYR:HB3	1.92	0.70
1:E:204:LYS:HG3	1:E:283:SER:O	1.92	0.69
1:I:3:HIS:HE1	1:I:5:LEU:HD12	1.56	0.69
1:F:146:ILE:HD12	1:F:217:VAL:HG21	1.73	0.69
1:H:140:ILE:HD11	2:I:401:COA:H143	1.75	0.69
1:H:283:SER:OG	1:H:284:HIS:HD2	1.75	0.69
2:J:401:COA:CEP	1:L:140:ILE:HD11	2.22	0.69
1:C:185:ASP:HB2	1:C:186:LEU:HD23	1.73	0.69
1:F:264:MET:HE3	1:F:292:ILE:HD11	1.75	0.68
1:A:67:ILE:HD13	1:A:73:ILE:HD11	1.76	0.68
1:I:184:ASN:HD22	1:I:189:ASN:HD21	1.42	0.68
1:I:264:MET:CE	1:I:292:ILE:CD1	2.72	0.68
1:A:70:ASP:OD2	1:A:101:LYS:NZ	2.27	0.68
2:K:401:COA:S1P	6:K:515:HOH:O	2.52	0.67
1:K:216:GLU:OE1	6:K:566:HOH:O	2.10	0.67
1:E:186:LEU:HD23	1:E:186:LEU:H	1.60	0.67
1:J:242:ASP:OD2	1:J:247:ARG:HB3	1.95	0.66
1:C:184:ASN:ND2	1:C:189:ASN:OD1	2.28	0.66
3:F:402:TYD:H5'1	3:F:402:TYD:H6	1.76	0.66
1:J:76:ASN:OD1	1:K:60:GLN:NE2	2.28	0.66
1:L:242:ASP:OD2	1:L:247:ARG:NH1	2.28	0.66
1:B:234:SER:O	1:B:276:ALA:HA	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:LEU:HG	1:I:168:GLN:N	2.08	0.65
1:B:21:GLN:HG3	1:C:24:VAL:HG22	1.77	0.65
1:K:60:GLN:HG3	1:K:62:TRP:CZ2	2.32	0.65
1:K:62:TRP:N	1:K:65:ILE:HD12	2.11	0.65
1:H:233:VAL:HG11	1:J:233:VAL:HG11	1.76	0.65
1:C:61:ILE:HD12	1:C:67:ILE:HD11	1.78	0.64
1:G:42:LEU:HD23	1:G:43:ILE:N	2.13	0.64
1:H:20:TRP:HB3	1:H:21:GLN:OE1	1.97	0.64
1:C:186:LEU:H	1:C:186:LEU:HD23	1.63	0.64
1:G:26:LEU:HD22	1:G:44:GLU:HA	1.80	0.64
1:H:20:TRP:HE1	1:H:36:ASN:HD21	1.45	0.63
1:E:21:GLN:N	1:E:21:GLN:HE21	1.91	0.63
1:E:123:VAL:HG13	1:E:129:ILE:HD11	1.81	0.63
1:A:224:LYS:HB2	1:A:290:ASP:OD1	1.98	0.62
1:H:15:ASP:O	1:H:33:ARG:HB2	2.00	0.62
1:I:224:LYS:HA	1:I:264:MET:HE2	1.81	0.62
1:C:194:GLU:HG2	1:F:205:ARG:HB2	1.79	0.62
1:C:96:LYS:O	1:C:114:GLY:HA2	2.00	0.62
1:F:96:LYS:O	1:F:114:GLY:HA2	2.00	0.62
1:G:60:GLN:HG3	1:G:62:TRP:CZ2	2.35	0.62
1:G:60:GLN:NE2	1:I:76:ASN:ND2	2.47	0.61
1:A:60:GLN:HE21	1:C:75:PRO:HB2	1.64	0.61
1:J:204:LYS:HD3	1:J:285:TYR:CE1	2.35	0.61
1:B:233:VAL:HG11	1:D:233:VAL:HG21	1.81	0.61
1:J:152:ALA:HB2	1:J:247:ARG:HG3	1.82	0.61
1:H:58:GLY:HA3	1:H:76:ASN:ND2	2.16	0.61
1:H:58:GLY:HA3	1:H:76:ASN:HD22	1.64	0.61
1:L:39:ALA:O	1:L:57:SER:HB3	2.01	0.61
1:B:216:GLU:OE1	1:D:187:ARG:NH1	2.33	0.60
1:F:224:LYS:HA	1:F:264:MET:HE1	1.82	0.60
1:G:67:ILE:HD13	1:G:73:ILE:HD11	1.84	0.60
1:K:240:LEU:HD11	1:K:247:ARG:HG2	1.84	0.60
1:F:264:MET:CE	1:F:292:ILE:HD11	2.31	0.60
1:E:164:GLU:H	1:E:168:GLN:HE22	1.49	0.60
1:D:146:ILE:HD12	1:D:217:VAL:HG21	1.84	0.60
1:J:199:ILE:O	1:J:201:PHE:N	2.31	0.60
3:L:402:TYD:O3B	6:L:512:HOH:O	2.16	0.60
1:I:264:MET:HE1	1:I:292:ILE:CD1	2.21	0.59
1:K:123:VAL:HG13	1:K:129:ILE:HD11	1.82	0.59
1:J:241:VAL:O	1:J:247:ARG:HA	2.03	0.59
1:L:20:TRP:HB3	1:L:21:GLN:OE1	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:ARG:O	1:L:34:ASN:CB	2.51	0.59
1:H:242:ASP:OD2	1:H:247:ARG:NH1	2.36	0.59
1:A:146:ILE:HD12	1:A:217:VAL:HG21	1.84	0.58
1:G:10:SER:HB2	1:G:26:LEU:O	2.02	0.58
1:D:135:ASP:O	1:D:136:ASN:HB2	2.03	0.58
1:A:60:GLN:HG3	1:A:62:TRP:HZ2	1.57	0.58
1:C:112:LEU:HB3	1:C:113:PRO:CD	2.34	0.58
1:H:165:LEU:HD22	6:H:526:HOH:O	2.04	0.58
1:D:184:ASN:HD22	1:D:184:ASN:C	2.07	0.58
2:G:403:COA:H21	1:H:81:ASN:H	1.68	0.58
1:I:122:MET:HB3	1:I:138:ILE:CD1	2.34	0.58
1:H:240:LEU:HD11	1:H:247:ARG:HG2	1.86	0.58
1:H:33:ARG:HG3	1:H:34:ASN:HD22	1.68	0.58
1:J:234:SER:O	1:J:276:ALA:HA	2.03	0.58
1:E:234:SER:O	1:E:276:ALA:HA	2.04	0.58
1:G:26:LEU:HD23	1:G:45:ASN:ND2	2.18	0.58
1:H:224:LYS:HB2	1:H:290:ASP:OD1	2.03	0.58
1:L:33:ARG:O	1:L:34:ASN:HB2	2.03	0.58
1:D:205:ARG:NH2	3:D:402:TYD:O4	2.36	0.57
1:G:123:VAL:HG13	1:G:129:ILE:HD11	1.86	0.57
1:L:122:MET:HB3	1:L:138:ILE:HD13	1.85	0.57
1:A:195:PHE:CE1	1:A:203:PRO:HG3	2.40	0.57
1:G:283:SER:OG	1:G:284:HIS:HD2	1.88	0.57
1:B:21:GLN:CG	1:C:24:VAL:HG21	2.34	0.57
1:I:3:HIS:CE1	1:I:5:LEU:HD12	2.39	0.57
1:G:123:VAL:CG1	1:G:129:ILE:HD11	2.33	0.57
1:G:161:ASN:HA	1:G:164:GLU:OE1	2.05	0.57
1:H:204:LYS:HB3	1:H:285:TYR:CE2	2.39	0.57
1:K:226:CYS:SG	1:K:282:ALA:HB1	2.45	0.57
1:A:187:ARG:HH22	3:E:402:TYD:PB	2.28	0.57
1:F:60:GLN:HG2	6:F:557:HOH:O	2.04	0.57
1:D:252:LEU:HD21	1:D:259:ILE:HG13	1.87	0.56
1:K:107:ALA:HB1	1:L:78:THR:HG21	1.87	0.56
1:B:168:GLN:HB2	6:B:542:HOH:O	2.05	0.56
1:B:123:VAL:CG1	1:B:129:ILE:CD1	2.84	0.56
1:F:234:SER:O	1:F:276:ALA:HA	2.06	0.56
1:I:46:ASP:OD1	1:I:63:ASP:HB3	2.06	0.56
1:J:297:THR:O	1:J:298:PHE:C	2.44	0.56
1:H:172:VAL:HG13	1:H:243:ASP:HB3	1.88	0.55
1:A:293:ARG:HG3	1:A:293:ARG:HH11	1.72	0.55
1:E:15:ASP:O	1:E:16:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LEU:HD23	1:D:186:LEU:H	1.71	0.55
1:D:22:PHE:CZ	1:E:22:PHE:HA	2.41	0.55
1:E:230:LEU:HD21	1:E:269:GLN:HE22	1.71	0.55
1:E:218:ARG:HD2	3:E:402:TYD:O1B	2.07	0.55
1:F:60:GLN:HG3	1:F:62:TRP:HZ2	1.69	0.55
1:F:41:SER:HB2	1:F:59:VAL:O	2.06	0.55
1:J:178:HIS:N	1:J:178:HIS:CD2	2.74	0.55
1:A:242:ASP:HB3	1:A:266:TRP:HB3	1.87	0.55
1:J:174:GLY:HA3	1:J:262:PRO:HG2	1.87	0.55
1:F:242:ASP:OD2	1:F:247:ARG:NH1	2.40	0.54
1:J:215[A]:LYS:H	1:J:215[A]:LYS:HD2	1.72	0.54
1:C:233:VAL:HA	1:C:255:ILE:HG23	1.90	0.54
1:G:161:ASN:N	1:G:161:ASN:OD1	2.41	0.54
1:B:163:PHE:O	1:B:179:LYS:HD2	2.08	0.54
1:K:167:LEU:HD12	1:K:168:GLN:N	2.22	0.54
1:J:204:LYS:HG3	1:J:283:SER:O	2.08	0.54
1:K:62:TRP:H	1:K:65:ILE:HD12	1.71	0.54
1:A:168:GLN:NE2	1:G:168:GLN:NE2	2.48	0.54
1:C:190:LEU:CD2	1:C:192:VAL:HG22	2.38	0.53
1:I:34:ASN:ND2	1:I:52:ASN:OD1	2.40	0.53
1:E:96:LYS:HE3	1:E:98:ILE:HD11	1.90	0.53
1:I:41:SER:HB2	1:I:59:VAL:O	2.09	0.53
1:G:240:LEU:HD11	1:G:247:ARG:HG2	1.90	0.53
1:J:140:ILE:HD11	2:K:401:COA:H143	1.89	0.53
1:D:184:ASN:HD22	1:D:185:ASP:N	2.06	0.53
1:I:122:MET:HB3	1:I:138:ILE:HD13	1.90	0.53
1:E:242:ASP:HB3	1:E:266:TRP:HB3	1.91	0.53
1:A:60:GLN:NE2	1:C:75:PRO:HB2	2.24	0.53
1:E:195:PHE:CD1	1:E:203:PRO:HD3	2.44	0.53
1:H:146:ILE:HD12	1:H:217:VAL:HG21	1.91	0.52
1:K:20:TRP:HB3	1:K:21:GLN:OE1	2.09	0.52
1:B:187:ARG:NH2	3:D:402:TYD:O2B	2.42	0.52
1:I:186:LEU:HD23	1:I:186:LEU:N	2.21	0.52
1:A:255:ILE:HD11	1:E:210:PHE:CZ	2.45	0.52
1:C:190:LEU:HD23	1:C:190:LEU:C	2.30	0.52
1:H:54:THR:HG22	1:H:56:LYS:HD3	1.91	0.52
1:H:166:LYS:HD3	1:H:179:LYS:O	2.10	0.52
1:J:198:ASP:O	1:J:200:PRO:HD3	2.10	0.52
1:A:217:VAL:O	1:E:187:ARG:NH2	2.43	0.52
1:F:112:LEU:HB3	1:F:113:PRO:CD	2.40	0.51
1:D:123:VAL:HG13	1:D:129:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:LEU:H	1:E:168:GLN:NE2	2.08	0.51
1:L:234:SER:O	1:L:276:ALA:HA	2.10	0.51
1:F:47:VAL:CG1	1:F:49:ILE:HD12	2.40	0.51
1:B:177:LEU:HD11	1:B:250:TYR:CE1	2.45	0.51
1:A:20:TRP:HB3	1:A:21:GLN:NE2	2.26	0.51
1:G:111:ILE:HD12	1:G:129:ILE:HD13	1.92	0.51
1:I:210:PHE:CE2	1:L:255:ILE:HG21	2.45	0.51
1:K:219:GLY:O	1:K:220:GLU:HB2	2.09	0.51
1:J:22:PHE:CZ	1:K:22:PHE:HA	2.45	0.51
1:C:33:ARG:HG2	1:C:51:ASP:OD1	2.09	0.51
1:H:139:VAL:O	1:H:140:ILE:HD12	2.10	0.51
2:D:401:COA:H143	1:F:140:ILE:HD11	1.92	0.51
1:I:302:ARG:O	1:I:306:GLU:HG2	2.11	0.51
1:A:72:PHE:CZ	2:B:401:COA:H22	2.45	0.51
1:B:146:ILE:HD12	1:B:217:VAL:HG21	1.92	0.51
1:C:234:SER:O	1:C:276:ALA:HA	2.11	0.51
1:H:112:LEU:HB3	1:H:113:PRO:HD2	1.91	0.51
1:J:176:SER:OG	1:J:260:TYR:HB3	2.11	0.51
1:L:196:GLU:OE2	1:L:202:THR:HG23	2.11	0.50
1:A:72:PHE:HB3	1:A:104:SER:HB2	1.93	0.50
1:J:172:VAL:HG21	1:J:241:VAL:HG23	1.92	0.50
1:L:21:GLN:N	1:L:21:GLN:OE1	2.26	0.50
1:C:146:ILE:HD12	1:C:217:VAL:HG21	1.92	0.50
1:H:60:GLN:HB2	1:H:62:TRP:CE2	2.47	0.50
1:C:60:GLN:HG3	1:C:62:TRP:HZ2	1.74	0.50
1:H:263:PRO:O	1:H:264:MET:HB2	2.11	0.50
1:E:186:LEU:H	1:E:186:LEU:CD2	2.25	0.50
1:J:259:ILE:HG22	1:J:261:LEU:HD12	1.93	0.50
2:J:401:COA:S1P	1:L:56:LYS:NZ	2.84	0.50
1:K:138:ILE:HD11	1:K:150:VAL:CG2	2.42	0.50
1:D:41:SER:HB2	1:D:59:VAL:O	2.12	0.49
1:L:20:TRP:CE3	4:L:403:TDR:C2	2.95	0.49
1:H:230:LEU:HG	1:H:280:VAL:HG22	1.93	0.49
1:H:187:ARG:O	1:J:218:ARG:NH2	2.45	0.49
1:H:123:VAL:CG1	1:H:129:ILE:HD11	2.38	0.49
1:H:227:LYS:HB2	1:H:283:SER:HB3	1.95	0.49
1:H:234:SER:O	1:H:276:ALA:HA	2.13	0.49
1:L:48:VAL:HB	1:L:66:HIS:ND1	2.27	0.49
1:C:1:MET:C	1:C:1:MET:SD	2.90	0.49
1:F:221:HIS:CE1	1:F:291:TYR:HE2	2.30	0.49
1:G:15:ASP:HB3	1:G:16:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:VAL:HG12	1:K:151:GLU:HG3	1.93	0.49
1:D:99:VAL:HG22	1:D:117:ILE:HD12	1.94	0.49
1:I:124:GLY:HA3	1:I:140:ILE:HG22	1.93	0.49
1:J:168:GLN:HE21	1:J:169:MET:N	2.11	0.49
1:E:64:GLY:O	1:E:96:LYS:HG3	2.13	0.49
1:I:224:LYS:HA	1:I:264:MET:CE	2.42	0.49
1:G:283:SER:OG	1:G:284:HIS:CD2	2.65	0.49
1:G:60:GLN:HE21	1:I:76:ASN:HD21	1.61	0.49
1:B:187:ARG:O	1:D:218:ARG:NH2	2.46	0.49
1:E:206:TYR:HA	1:E:280:VAL:O	2.12	0.49
1:J:9:GLN:O	1:J:27:ALA:HA	2.12	0.49
1:K:234:SER:O	1:K:276:ALA:HA	2.13	0.49
1:H:195:PHE:CE1	1:H:199:ILE:HD12	2.48	0.49
1:H:223:HIS:O	1:H:264:MET:N	2.42	0.49
1:I:223:HIS:O	1:I:264:MET:HE2	2.13	0.49
1:A:15:ASP:O	1:A:16:ASN:HB2	2.13	0.48
1:E:146:ILE:HD12	1:E:217:VAL:HG21	1.95	0.48
1:L:1:MET:C	1:L:1:MET:SD	2.92	0.48
1:C:184:ASN:CG	1:C:189:ASN:OD1	2.52	0.48
1:G:224:LYS:HB2	1:G:290:ASP:OD1	2.13	0.48
1:L:215[A]:LYS:HE2	2:L:401:COA:O8A	2.13	0.48
1:F:1:MET:C	1:F:1:MET:SD	2.92	0.48
1:L:243:ASP:O	1:L:302:ARG:HG2	2.13	0.48
1:E:294:ASP:HB2	1:E:297:THR:HB	1.95	0.48
1:I:72:PHE:CD2	1:I:72:PHE:C	2.86	0.48
1:K:67:ILE:HG12	1:K:73:ILE:HD11	1.96	0.48
1:E:134:PRO:CD	1:E:146:ILE:HD11	2.43	0.48
1:J:242:ASP:OD2	1:J:247:ARG:NE	2.45	0.48
1:A:236:ASN:ND2	1:A:273:SER:OG	2.45	0.48
1:B:177:LEU:N	1:B:177:LEU:HD23	2.29	0.48
1:L:240:LEU:HD11	1:L:247:ARG:HG2	1.95	0.48
1:L:67:ILE:HD13	1:L:73:ILE:CD1	2.44	0.48
1:L:67:ILE:HD13	1:L:73:ILE:HD11	1.94	0.48
1:B:168:GLN:HB3	1:B:168:GLN:HE21	1.47	0.48
1:H:35:CYS:SG	1:H:50:GLY:O	2.71	0.48
1:K:2:ILE:O	1:K:2:ILE:HG22	2.14	0.48
1:B:18:LYS:HE3	1:B:36:ASN:OD1	2.14	0.48
1:I:208:THR:O	1:L:190:LEU:HA	2.14	0.48
1:B:195:PHE:CE1	1:B:199:ILE:HD12	2.48	0.48
1:C:306:GLU:OE1	1:C:306:GLU:HA	2.14	0.48
1:I:138:ILE:HD11	1:I:150:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3:HIS:HE1	1:J:5:LEU:HD12	1.78	0.48
1:D:263:PRO:O	1:D:264:MET:HB2	2.14	0.47
1:I:262:PRO:O	1:I:265:THR:OG1	2.32	0.47
1:A:240:LEU:HB3	1:A:268:VAL:HB	1.96	0.47
1:D:262:PRO:HG2	1:D:265:THR:CG2	2.44	0.47
1:H:226:CYS:SG	1:H:282:ALA:HB1	2.54	0.47
1:H:43:ILE:HD13	1:H:49:ILE:CD1	2.44	0.47
1:L:224:LYS:HB2	1:L:290:ASP:OD1	2.13	0.47
1:A:269:GLN:HG2	6:A:528:HOH:O	2.14	0.47
1:G:105:ILE:HA	1:G:123:VAL:HB	1.97	0.47
1:G:61:ILE:HD12	1:G:67:ILE:HD11	1.96	0.47
1:G:112:LEU:HD11	1:I:125:ALA:HB3	1.97	0.47
1:A:302:ARG:NH1	1:A:302:ARG:HG3	2.17	0.47
1:K:60:GLN:HG3	1:K:62:TRP:HZ2	1.77	0.47
1:H:43:ILE:HD13	1:H:49:ILE:HD11	1.97	0.47
1:D:51:ASP:O	1:D:52:ASN:HB2	2.15	0.47
1:G:42:LEU:HD23	1:G:42:LEU:C	2.35	0.47
1:C:187[A]:ARG:NH2	1:F:217:VAL:O	2.48	0.47
1:D:187:ARG:NH1	1:D:187:ARG:HG2	2.13	0.47
1:E:219:GLY:O	1:E:220:GLU:HB2	2.15	0.47
1:J:142:ASN:OD1	2:J:401:COA:H2A	2.15	0.47
1:D:234:SER:O	1:D:276:ALA:HA	2.15	0.47
1:F:240:LEU:HB3	1:F:268:VAL:HB	1.97	0.47
1:G:234:SER:O	1:G:276:ALA:HA	2.14	0.47
1:C:100:LYS:CE	1:C:116:LEU:HD21	2.45	0.46
1:C:193:GLY:HA3	1:F:206:TYR:CE2	2.49	0.46
1:L:168:GLN:HG3	1:L:177:LEU:HD12	1.96	0.46
1:A:215:LYS:HB3	1:A:215:LYS:HE3	1.67	0.46
1:E:194:GLU:N	1:E:198:ASP:OD2	2.39	0.46
1:I:264:MET:HE3	1:I:292:ILE:HD11	1.96	0.46
1:A:105:ILE:HA	1:A:123:VAL:HB	1.96	0.46
1:C:123:VAL:HG11	1:C:129:ILE:CD1	2.44	0.46
1:E:135:ASP:O	1:E:136:ASN:HB2	2.15	0.46
1:F:196:GLU:OE2	1:F:202:THR:OG1	2.34	0.46
1:A:195:PHE:CD1	1:A:203:PRO:HD3	2.50	0.46
1:B:75:PRO:HB3	1:C:62:TRP:HZ2	1.79	0.46
1:H:105:ILE:HA	1:H:123:VAL:HB	1.98	0.46
1:E:205:ARG:NH2	3:E:402:TYD:O4	2.47	0.46
1:F:39:ALA:HB1	1:F:40:ASN:ND2	2.31	0.46
1:L:195:PHE:CD1	1:L:203:PRO:HD3	2.50	0.46
1:E:4:LYS:HB3	1:E:4:LYS:HE2	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:GLN:CG	1:F:62:TRP:CZ2	2.98	0.46
1:K:249:GLU:OE1	1:K:270:TYR:OH	2.32	0.46
1:K:65:ILE:HG22	1:K:67:ILE:CD1	2.46	0.46
1:B:206:TYR:C	1:B:206:TYR:CD1	2.89	0.46
1:K:150:VAL:HG12	1:K:151:GLU:CG	2.46	0.46
1:D:105:ILE:HA	1:D:123:VAL:HB	1.97	0.45
1:D:255:ILE:HD13	1:D:255:ILE:HG21	1.48	0.45
1:J:22:PHE:CE2	1:K:22:PHE:HA	2.51	0.45
1:I:112:LEU:HD22	1:I:130:THR:HA	1.99	0.45
1:F:240:LEU:HD11	1:F:247:ARG:HG2	1.97	0.45
1:F:227:LYS:HB2	1:F:283:SER:HB3	1.99	0.45
1:F:47:VAL:HG12	1:F:49:ILE:HD12	1.99	0.45
1:G:60:GLN:HE21	1:I:76:ASN:ND2	2.14	0.45
1:A:234:SER:O	1:A:276:ALA:HA	2.17	0.45
1:E:206:TYR:C	1:E:206:TYR:CD1	2.90	0.45
1:L:213:PRO:HG2	1:L:216:GLU:HG2	1.98	0.45
1:C:123:VAL:CG1	1:C:129:ILE:HD12	2.47	0.45
1:C:233:VAL:HG11	1:F:233:VAL:HG21	1.99	0.45
1:F:36:ASN:OD1	1:F:36:ASN:N	2.50	0.45
1:J:140:ILE:HD11	2:K:401:COA:CEP	2.47	0.45
1:K:165:LEU:HD13	1:K:167:LEU:O	2.17	0.45
1:K:138:ILE:HD11	1:K:150:VAL:HG22	1.99	0.45
1:A:181:HIS:O	1:A:191:SER:HA	2.17	0.45
1:A:67:ILE:HD13	1:A:73:ILE:CD1	2.45	0.45
1:B:21:GLN:CG	1:C:24:VAL:CG2	2.90	0.45
1:I:193:GLY:HA3	1:L:206:TYR:CE2	2.52	0.45
1:L:24:VAL:HB	1:L:42:LEU:HD12	1.99	0.45
1:L:60:GLN:HB2	1:L:62:TRP:CZ2	2.51	0.45
1:H:33:ARG:NH1	1:H:33:ARG:HB3	2.31	0.45
1:D:123:VAL:HG13	1:D:129:ILE:CD1	2.47	0.45
1:H:101:LYS:HE3	1:H:101:LYS:HB2	1.60	0.45
1:H:21:GLN:N	1:H:21:GLN:OE1	2.34	0.45
1:H:275:ASP:N	1:H:275:ASP:OD2	2.44	0.45
1:G:205:ARG:NH2	1:G:284:HIS:O	2.39	0.44
1:F:227:LYS:HD2	1:F:283:SER:CB	2.47	0.44
1:F:269:GLN:HG2	6:F:516:HOH:O	2.17	0.44
1:J:201:PHE:CD1	1:J:283:SER:HB3	2.52	0.44
1:A:95:LEU:HB3	1:A:96:LYS:H	1.67	0.44
1:L:6:ALA:HB2	1:L:20:TRP:O	2.18	0.44
1:G:43:ILE:HG23	1:G:47:VAL:HG11	2.00	0.44
1:G:60:GLN:HE22	1:I:76:ASN:HD21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:215[B]:LYS:H	1:L:215[B]:LYS:HG2	1.58	0.44
1:L:247:ARG:HG3	1:L:247:ARG:HH11	1.81	0.44
1:D:224:LYS:HG3	1:D:292:ILE:HD11	1.99	0.44
1:E:105:ILE:HA	1:E:123:VAL:HB	1.99	0.44
1:E:226:CYS:SG	1:E:282:ALA:HB1	2.58	0.44
1:B:20:TRP:HB3	1:B:21:GLN:OE1	2.17	0.44
1:I:240:LEU:HD12	1:I:248:GLU:O	2.18	0.44
1:F:124:GLY:O	1:F:125:ALA:C	2.55	0.44
1:F:182:LEU:HD13	1:F:191:SER:HB3	1.99	0.44
1:H:75:PRO:HB2	1:I:60:GLN:NE2	2.33	0.44
1:J:39:ALA:O	1:J:57:SER:HB3	2.18	0.44
1:C:124:GLY:HA3	1:C:140:ILE:HG22	1.98	0.43
1:D:187:ARG:CG	1:D:187:ARG:HH11	2.15	0.43
1:H:112:LEU:HD22	1:H:130:THR:HA	2.00	0.43
1:I:119:GLU:O	1:I:120:ASN:HB2	2.18	0.43
1:L:3:HIS:O	1:L:4:LYS:C	2.57	0.43
1:E:100:LYS:HB2	1:E:117:ILE:O	2.18	0.43
1:A:187:ARG:NH2	3:E:402:TYD:O1B	2.50	0.43
1:I:11:GLN:HA	1:I:11:GLN:OE1	2.18	0.43
1:I:226:CYS:SG	1:I:282:ALA:HB1	2.58	0.43
1:E:83:LYS:HA	1:E:113:PRO:HG2	2.00	0.43
1:J:3:HIS:O	1:J:4:LYS:C	2.56	0.43
1:J:62:TRP:CH2	1:L:56:LYS:HD3	2.53	0.43
1:L:230:LEU:HG	1:L:280:VAL:HG22	2.01	0.43
1:G:75:PRO:HB3	1:H:62:TRP:HZ2	1.84	0.43
1:B:54:THR:HG22	1:B:56:LYS:HD3	2.00	0.43
1:I:52:ASN:O	1:I:70:ASP:HA	2.19	0.43
1:F:218:ARG:NH2	6:F:554:HOH:O	2.50	0.43
1:L:69:ASP:O	1:L:101:LYS:HG3	2.18	0.43
1:A:226:CYS:SG	1:A:282:ALA:HB1	2.59	0.43
1:B:42:LEU:HG	1:B:43:ILE:N	2.33	0.43
1:C:81:ASN:HA	1:C:81:ASN:HD22	1.40	0.43
1:E:75:PRO:HB3	1:F:62:TRP:HZ2	1.84	0.43
1:J:3:HIS:CE1	1:J:5:LEU:HD12	2.52	0.43
1:B:21:GLN:HG2	1:C:24:VAL:HG21	2.01	0.43
1:B:208:THR:O	1:D:190:LEU:HA	2.19	0.43
1:B:275:ASP:N	1:B:275:ASP:OD2	2.39	0.43
1:B:62:TRP:H	1:B:65:ILE:HD12	1.84	0.43
1:C:253:ASP:OD1	1:C:253:ASP:N	2.51	0.43
1:H:219:GLY:O	1:H:220:GLU:HB2	2.19	0.43
1:H:21:GLN:CD	1:H:21:GLN:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:180:PHE:HE2	1:K:198:ASP:HB3	1.84	0.43
1:H:217:VAL:O	1:J:187:ARG:NH2	2.52	0.42
1:I:112:LEU:HB3	1:I:113:PRO:CD	2.48	0.42
3:H:401:TYD:O1B	1:J:187:ARG:NH1	2.52	0.42
1:K:32:GLY:HA3	1:K:51:ASP:OD1	2.19	0.42
1:L:72:PHE:CD2	1:L:72:PHE:C	2.91	0.42
1:A:218:ARG:HB3	1:A:218:ARG:HE	1.44	0.42
1:J:219:GLY:HA2	1:J:221:HIS:CE1	2.54	0.42
1:E:269:GLN:HE21	1:E:269:GLN:HB3	1.72	0.42
1:F:197:LYS:HB2	1:F:197:LYS:HE3	1.68	0.42
1:C:301:MET:O	1:C:304:ASN:HB2	2.20	0.42
1:F:182:LEU:CD1	1:F:191:SER:HB3	2.49	0.42
1:H:3:HIS:CE1	1:H:5:LEU:HG	2.53	0.42
1:F:135:ASP:O	1:F:136:ASN:HB2	2.19	0.42
1:F:168:GLN:HB3	1:F:168:GLN:HE21	1.64	0.42
1:H:270:TYR:CE1	1:H:271:LYS:HE3	2.55	0.42
1:I:115:ILE:HD13	1:I:115:ILE:HA	1.85	0.42
1:I:233:VAL:HG11	1:L:233:VAL:HG11	2.02	0.42
1:K:72:PHE:HZ	2:L:401:COA:H22	1.79	0.42
1:H:187:ARG:HG2	1:J:216:GLU:OE1	2.19	0.42
1:A:206:TYR:CE2	1:E:193:GLY:HA3	2.54	0.42
1:B:199:ILE:HG23	1:B:229:PHE:CD2	2.54	0.42
1:G:15:ASP:HB3	1:G:16:ASN:HD22	1.85	0.42
1:G:150:VAL:O	1:G:151:GLU:HB2	2.19	0.42
1:H:227:LYS:HG2	1:H:260:TYR:OH	2.19	0.42
1:H:230:LEU:HB2	1:H:259:ILE:CG2	2.49	0.42
1:J:215[A]:LYS:HB3	1:J:215[A]:LYS:HE3	1.73	0.42
1:A:243:ASP:OD2	1:A:243:ASP:C	2.58	0.42
1:F:81:ASN:HA	1:F:113:PRO:HB3	2.01	0.42
1:G:68:GLN:HB3	6:G:572:HOH:O	2.19	0.42
1:I:96:LYS:NZ	1:I:98:ILE:HD11	2.33	0.42
1:F:242:ASP:HB3	1:F:266:TRP:HB3	2.01	0.42
1:F:264:MET:CE	1:F:292:ILE:CD1	2.96	0.42
1:G:8:VAL:HG12	1:G:10:SER:H	1.85	0.42
1:J:242:ASP:HB3	1:J:266:TRP:HB3	2.00	0.42
1:I:187:ARG:NH2	1:L:217:VAL:O	2.53	0.42
1:L:294:ASP:HB3	1:L:297:THR:HB	2.02	0.42
1:D:15:ASP:OD2	1:D:33:ARG:NE	2.37	0.41
1:B:24:VAL:HB	1:B:42:LEU:HD12	2.02	0.41
1:C:73:ILE:HG21	1:C:73:ILE:HD13	1.84	0.41
1:D:187:ARG:CG	1:D:187:ARG:NH1	2.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LEU:HD21	1:E:192:VAL:HG22	2.01	0.41
1:A:33:ARG:O	1:A:34:ASN:CB	2.67	0.41
1:G:226:CYS:HA	1:G:284:HIS:CD2	2.56	0.41
1:D:213:PRO:CB	1:D:215:LYS:HE2	2.51	0.41
1:D:22:PHE:CE2	1:E:22:PHE:HA	2.56	0.41
1:C:255:ILE:HD11	1:F:210:PHE:CZ	2.55	0.41
1:H:206:TYR:HA	1:H:280:VAL:O	2.20	0.41
1:H:60:GLN:HB2	1:H:62:TRP:NE1	2.36	0.41
1:A:232:CYS:SG	1:A:237:CYS:HB2	2.61	0.41
1:E:294:ASP:HB2	1:E:297:THR:CB	2.51	0.41
1:F:60:GLN:HB2	1:F:62:TRP:CZ2	2.55	0.41
1:L:247:ARG:HG3	1:L:247:ARG:NH1	2.35	0.41
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.94	0.41
1:A:21:GLN:N	1:A:21:GLN:HE21	2.07	0.41
1:B:105:ILE:HA	1:B:123:VAL:HB	2.02	0.41
1:G:146:ILE:HD12	1:G:217:VAL:HG21	2.03	0.41
1:G:183:VAL:O	1:G:189:ASN:HA	2.21	0.41
1:I:133:VAL:HA	1:I:134:PRO:HD3	1.91	0.41
1:I:219:GLY:O	1:I:220:GLU:HB2	2.21	0.41
1:J:206:TYR:HA	1:J:280:VAL:O	2.21	0.41
1:K:138:ILE:CD1	1:K:150:VAL:HG23	2.50	0.41
1:C:60:GLN:CG	1:C:62:TRP:CZ2	2.98	0.41
1:F:215:LYS:CE	1:F:215:LYS:H	2.17	0.41
1:G:123:VAL:HG11	1:G:129:ILE:HD11	2.02	0.41
1:G:247:ARG:HH21	1:G:247:ARG:HD2	1.76	0.41
1:K:138:ILE:CD1	1:K:150:VAL:CG2	2.98	0.41
1:B:36:ASN:ND2	6:B:508:HOH:O	2.54	0.41
1:J:206:TYR:C	1:J:206:TYR:CD1	2.93	0.41
1:J:215[A]:LYS:H	1:J:215[A]:LYS:CD	2.32	0.41
1:L:214:ASN:HB3	6:L:547:HOH:O	2.20	0.41
1:B:218:ARG:HB3	1:B:218:ARG:HE	1.76	0.41
1:D:133:VAL:HA	1:D:134:PRO:HD3	1.93	0.41
1:G:190:LEU:HA	1:K:208:THR:O	2.20	0.41
1:D:120:ASN:O	1:E:86:ARG:NH2	2.54	0.41
1:G:18:LYS:N	1:G:18:LYS:HD3	2.36	0.41
1:H:56:LYS:HD2	1:H:56:LYS:HA	1.88	0.41
1:J:202:THR:HA	1:J:203:PRO:HD3	1.77	0.41
1:F:178:HIS:N	1:F:178:HIS:CD2	2.89	0.40
1:D:24:VAL:HG22	1:F:21:GLN:HG3	2.02	0.40
1:I:13:ILE:HG23	1:I:17:THR:HG21	2.02	0.40
1:I:255:ILE:N	1:I:255:ILE:HD12	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:112:LEU:HB3	1:L:113:PRO:HD2	2.01	0.40
1:E:176:SER:OG	1:E:260:TYR:HB3	2.21	0.40
1:I:67:ILE:HG22	1:I:67:ILE:O	2.20	0.40
1:L:226:CYS:SG	1:L:282:ALA:HB1	2.61	0.40
1:C:255:ILE:HD12	1:C:255:ILE:N	2.36	0.40
1:G:44:GLU:HB3	1:G:45:ASN:H	1.77	0.40
1:L:42:LEU:O	1:L:60:GLN:HA	2.22	0.40
1:D:208:THR:HA	1:D:278:LEU:O	2.21	0.40
1:A:255:ILE:CD1	1:E:210:PHE:CZ	3.05	0.40
1:L:172:VAL:HG21	1:L:241:VAL:HG23	2.03	0.40
1:L:183:VAL:O	1:L:189:ASN:HA	2.21	0.40
1:B:178:HIS:N	1:B:178:HIS:CD2	2.90	0.40
1:E:61:ILE:HD12	1:E:67:ILE:HD11	2.04	0.40
1:I:24:VAL:O	1:I:42:LEU:HA	2.22	0.40
1:G:187:ARG:NH2	1:K:217:VAL:O	2.50	0.40

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%)	34	37
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%)	34	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	280/312 (90%)	266 (95%)	13 (5%)	1 (0%)	34	37
1	F	288/312 (92%)	268 (93%)	20 (7%)	0	100	100
1	G	278/312 (89%)	267 (96%)	10 (4%)	1 (0%)	34	37
1	H	272/312 (87%)	252 (93%)	19 (7%)	1 (0%)	34	37
1	I	279/312 (89%)	261 (94%)	16 (6%)	2 (1%)	22	22
1	J	270/312 (86%)	258 (96%)	9 (3%)	3 (1%)	14	12
1	K	280/312 (90%)	261 (93%)	16 (6%)	3 (1%)	14	12
1	L	281/312 (90%)	260 (92%)	19 (7%)	2 (1%)	22	22
All	All	3348/3744 (89%)	3165 (94%)	168 (5%)	15 (0%)	34	37

All (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
1	G	20	TRP
1	I	14	GLY
1	J	4	LYS
1	L	14	GLY
1	I	50	GLY
1	K	50	GLY
1	K	164	GLU
1	L	4	LYS
1	D	151	GLU
1	J	200	PRO

### 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%)	220 (89%)	26 (11%)	6	6
1	B	251/272 (92%)	230 (92%)	21 (8%)	11	11
1	C	245/272 (90%)	224 (91%)	21 (9%)	10	10
1	D	244/272 (90%)	218 (89%)	26 (11%)	6	6
1	E	247/272 (91%)	220 (89%)	27 (11%)	6	5
1	F	252/272 (93%)	231 (92%)	21 (8%)	11	11
1	G	245/272 (90%)	225 (92%)	20 (8%)	11	11
1	H	239/272 (88%)	211 (88%)	28 (12%)	5	4
1	I	245/272 (90%)	228 (93%)	17 (7%)	15	16
1	J	237/272 (87%)	206 (87%)	31 (13%)	4	3
1	K	247/272 (91%)	225 (91%)	22 (9%)	9	9
1	L	246/272 (90%)	217 (88%)	29 (12%)	5	4
All	All	2944/3264 (90%)	2655 (90%)	289 (10%)	8	7

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	34	ASN
1	A	36	ASN
1	A	46	ASP
1	A	81	ASN
1	A	104	SER
1	A	116	LEU
1	A	150	VAL
1	A	161	ASN
1	A	164	GLU
1	A	168	GLN
1	A	171	LYS
1	A	173	LYS
1	A	186	LEU
1	A	196	GLU
1	A	215	LYS
1	A	218	ARG
1	A	234	SER
1	A	236	ASN
1	A	245	GLU
1	A	255	ILE
1	A	269	GLN

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Mol	Chain	Res	Type
1	A	270	TYR
1	A	296	SER
1	A	300	GLN
1	A	302	ARG
1	B	4	LYS
1	B	21	GLN
1	B	40	ASN
1	B	42	LEU
1	B	56	LYS
1	B	84	GLN
1	B	115	ILE
1	B	164	GLU
1	B	165	LEU
1	B	168	GLN
1	B	171	LYS
1	B	173	LYS
1	B	182	LEU
1	B	187	ARG
1	B	191	SER
1	B	194	GLU
1	B	197	LYS
1	B	233	VAL
1	B	248	GLU
1	B	270	TYR
1	B	275	ASP
1	C	4	LYS
1	C	21	GLN
1	C	34	ASN
1	C	60	GLN
1	C	70	ASP
1	C	81	ASN
1	C	104	SER
1	C	116	LEU
1	C	164	GLU
1	C	171	LYS
1	C	186	LEU
1	C	196	GLU
1	C	197	LYS
1	C	202	THR
1	C	233	VAL
1	C	234	SER
1	C	247	ARG

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Mol	Chain	Res	Type
1	C	254	SER
1	C	255	ILE
1	C	270	TYR
1	C	304	ASN
1	D	11	GLN
1	D	15	ASP
1	D	16	ASN
1	D	34	ASN
1	D	37	ILE
1	D	42	LEU
1	D	60	GLN
1	D	115	ILE
1	D	120	ASN
1	D	165	LEU
1	D	166	LYS
1	D	168	GLN
1	D	173	LYS
1	D	179	LYS
1	D	184	ASN
1	D	186	LEU
1	D	187	ARG
1	D	196	GLU
1	D	202	THR
1	D	215	LYS
1	D	269	GLN
1	D	270	TYR
1	D	279	LEU
1	D	293	ARG
1	D	296	SER
1	D	304	ASN
1	E	1	MET
1	E	4	LYS
1	E	21	GLN
1	E	34	ASN
1	E	70	ASP
1	E	82	ASP
1	E	94	TYR
1	E	115	ILE
1	E	120	ASN
1	E	131	LYS
1	E	140	ILE
1	E	151	GLU

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Mol	Chain	Res	Type
1	E	162	ASN
1	E	165	LEU
1	E	173	LYS
1	E	184	ASN
1	E	186	LEU
1	E	196	GLU
1	E	198	ASP
1	E	233	VAL
1	E	248	GLU
1	E	269	GLN
1	E	270	TYR
1	E	274	LYS
1	E	288	SER
1	E	294	ASP
1	E	299	LYS
1	F	21	GLN
1	F	36	ASN
1	F	60	GLN
1	F	84	GLN
1	F	86	ARG
1	F	88	LYS
1	F	115	ILE
1	F	140	ILE
1	F	163	PHE
1	F	164	GLU
1	F	168	GLN
1	F	173	LYS
1	F	183	VAL
1	F	196	GLU
1	F	205	ARG
1	F	215	LYS
1	F	234	SER
1	F	254	SER
1	F	269	GLN
1	F	270	TYR
1	F	296	SER
1	G	21	GLN
1	G	52	ASN
1	G	60	GLN
1	G	116	LEU
1	G	131	LYS
1	G	161	ASN

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Mol	Chain	Res	Type
1	G	164	GLU
1	G	166	LYS
1	G	171	LYS
1	G	173	LYS
1	G	184	ASN
1	G	196	GLU
1	G	197	LYS
1	G	205	ARG
1	G	215	LYS
1	G	234	SER
1	G	270	TYR
1	G	274	LYS
1	G	296	SER
1	G	305	LEU
1	H	4	LYS
1	H	11	GLN
1	H	12	ASN
1	H	36	ASN
1	H	56	LYS
1	H	60	GLN
1	H	96	LYS
1	H	101	LYS
1	H	115	ILE
1	H	122	MET
1	H	140	ILE
1	H	150	VAL
1	H	168	GLN
1	H	171	LYS
1	H	173	LYS
1	H	186	LEU
1	H	189	ASN
1	H	190	LEU
1	H	192	VAL
1	H	237	CYS
1	H	245	GLU
1	H	269	GLN
1	H	270	TYR
1	H	274	LYS
1	H	279	LEU
1	H	288	SER
1	H	296	SER
1	H	301	MET

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Mol	Chain	Res	Type
1	I	18	LYS
1	I	81	ASN
1	I	163	PHE
1	I	165	LEU
1	I	166	LYS
1	I	167	LEU
1	I	168	GLN
1	I	177	LEU
1	I	186	LEU
1	I	224	LYS
1	I	255	ILE
1	I	265	THR
1	I	269	GLN
1	I	270	TYR
1	I	293	ARG
1	I	296	SER
1	I	302	ARG
1	J	4	LYS
1	J	9	GLN
1	J	21	GLN
1	J	33	ARG
1	J	37	ILE
1	J	40	ASN
1	J	56	LYS
1	J	60	GLN
1	J	81	ASN
1	J	96	LYS
1	J	104	SER
1	J	115	ILE
1	J	116	LEU
1	J	140	ILE
1	J	165	LEU
1	J	168	GLN
1	J	171	LYS
1	J	178	HIS
1	J	179	LYS
1	J	192	VAL
1	J	196	GLU
1	J	197	LYS
1	J	198	ASP
1	J	202	THR
1	J	215[A]	LYS

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Mol	Chain	Res	Type
1	J	215[B]	LYS
1	J	234	SER
1	J	259	ILE
1	J	269	GLN
1	J	270	TYR
1	J	296	SER
1	K	4	LYS
1	K	10	SER
1	K	11	GLN
1	K	34	ASN
1	K	41	SER
1	K	60	GLN
1	K	116	LEU
1	K	131	LYS
1	K	165	LEU
1	K	167	LEU
1	K	171	LYS
1	K	179	LYS
1	K	186	LEU
1	K	191	SER
1	K	215[A]	LYS
1	K	215[B]	LYS
1	K	234	SER
1	K	270	TYR
1	K	274	LYS
1	K	293	ARG
1	K	296	SER
1	K	299	LYS
1	L	4	LYS
1	L	11	GLN
1	L	16	ASN
1	L	18	LYS
1	L	21	GLN
1	L	34	ASN
1	L	41	SER
1	L	57	SER
1	L	60	GLN
1	L	104	SER
1	L	119	GLU
1	L	120	ASN
1	L	131	LYS
1	L	140	ILE

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Mol	Chain	Res	Type
1	L	171	LYS
1	L	173	LYS
1	L	196	GLU
1	L	202	THR
1	L	215[A]	LYS
1	L	215[B]	LYS
1	L	218	ARG
1	L	233	VAL
1	L	254	SER
1	L	269	GLN
1	L	270	TYR
1	L	274	LYS
1	L	293	ARG
1	L	294	ASP
1	L	296	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	60	GLN
1	A	81	ASN
1	A	189	ASN
1	A	236	ASN
1	A	300	GLN
1	B	168	GLN
1	B	189	ASN
1	B	221	HIS
1	C	66	HIS
1	C	81	ASN
1	C	184	ASN
1	C	221	HIS
1	D	184	ASN
1	D	189	ASN
1	D	221	HIS
1	D	236	ASN
1	D	304	ASN
1	E	21	GLN
1	E	162	ASN
1	E	168	GLN
1	E	184	ASN
1	E	189	ASN

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Mol	Chain	Res	Type
1	E	269	GLN
1	F	40	ASN
1	F	168	GLN
1	F	189	ASN
1	F	221	HIS
1	F	246	ASN
1	G	16	ASN
1	G	60	GLN
1	G	161	ASN
1	G	168	GLN
1	G	221	HIS
1	G	284	HIS
1	H	16	ASN
1	H	34	ASN
1	H	36	ASN
1	H	66	HIS
1	H	76	ASN
1	H	81	ASN
1	H	168	GLN
1	H	221	HIS
1	H	236	ASN
1	H	284	HIS
1	I	81	ASN
1	I	168	GLN
1	I	189	ASN
1	I	221	HIS
1	I	300	GLN
1	I	304	ASN
1	J	40	ASN
1	J	60	GLN
1	J	81	ASN
1	J	168	GLN
1	J	184	ASN
1	J	221	HIS
1	J	269	GLN
1	K	60	GLN
1	K	136	ASN
1	K	184	ASN
1	K	189	ASN
1	K	236	ASN
1	L	52	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 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	K	401	-	41,50,50	0.72	1 (2%)	52,75,75	1.62	9 (17%)
4	TDR	A	403	-	8,9,9	1.84	1 (12%)	6,12,12	6.69	4 (66%)
4	TDR	J	403	-	8,9,9	1.89	1 (12%)	6,12,12	5.10	4 (66%)
2	COA	F	401	-	41,50,50	0.78	2 (4%)	52,75,75	1.76	10 (19%)
4	TDR	E	403	-	8,9,9	1.79	1 (12%)	6,12,12	5.22	4 (66%)
3	TYD	B	402	-	23,26,26	2.15	3 (13%)	33,40,40	2.58	11 (33%)
3	TYD	L	402	-	23,26,26	2.32	2 (8%)	33,40,40	2.50	9 (27%)
4	TDR	K	403	-	8,9,9	1.70	1 (12%)	6,12,12	5.69	4 (66%)
4	TDR	F	403	-	8,9,9	1.79	1 (12%)	6,12,12	5.27	4 (66%)
2	COA	E	401	-	41,50,50	0.72	1 (2%)	52,75,75	1.67	12 (23%)
2	COA	J	401	-	41,50,50	0.75	1 (2%)	52,75,75	1.99	11 (21%)
2	COA	D	401	-	41,50,50	0.75	1 (2%)	52,75,75	1.58	12 (23%)
2	COA	G	403	-	41,50,50	0.73	0	52,75,75	1.54	9 (17%)
2	COA	B	401	-	41,50,50	0.83	2 (4%)	52,75,75	1.70	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TYD	E	402	-	23,26,26	2.37	2 (8%)	33,40,40	2.65	10 (30%)
4	TDR	B	403	-	8,9,9	1.94	1 (12%)	6,12,12	5.65	4 (66%)
2	COA	A	401	-	41,50,50	0.91	2 (4%)	52,75,75	1.84	15 (28%)
4	TDR	L	403	-	8,9,9	1.89	1 (12%)	6,12,12	5.69	5 (83%)
3	TYD	I	402	-	23,26,26	2.22	3 (13%)	33,40,40	2.41	10 (30%)
3	TYD	J	402	-	23,26,26	2.34	2 (8%)	33,40,40	2.37	9 (27%)
2	COA	I	401	-	41,50,50	0.83	2 (4%)	52,75,75	1.58	8 (15%)
3	TYD	G	402	-	23,26,26	2.19	3 (13%)	33,40,40	2.72	13 (39%)
4	TDR	D	403	-	8,9,9	1.98	1 (12%)	6,12,12	4.86	4 (66%)
2	COA	G	401	-	41,50,50	0.82	1 (2%)	52,75,75	1.76	14 (26%)
3	TYD	C	402	-	23,26,26	2.24	2 (8%)	33,40,40	2.66	10 (30%)
3	TYD	A	402	-	23,26,26	2.23	3 (13%)	33,40,40	2.23	9 (27%)
2	COA	C	401	-	41,50,50	0.86	2 (4%)	52,75,75	1.98	11 (21%)
2	COA	L	401	-	41,50,50	0.76	1 (2%)	52,75,75	1.66	13 (25%)
3	TYD	K	402	-	23,26,26	2.31	2 (8%)	33,40,40	2.46	10 (30%)
3	TYD	F	402	-	23,26,26	2.25	3 (13%)	33,40,40	2.16	11 (33%)
3	TYD	D	402	-	23,26,26	2.46	2 (8%)	33,40,40	2.23	10 (30%)
3	TYD	H	401	-	23,26,26	2.22	4 (17%)	33,40,40	1.88	7 (21%)
4	TDR	C	403	-	8,9,9	2.00	1 (12%)	6,12,12	4.58	4 (66%)

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	K	401	-	-	12/44/64/64	0/3/3/3
4	TDR	A	403	-	-	-	0/1/1/1
4	TDR	J	403	-	-	-	0/1/1/1
2	COA	F	401	-	-	6/44/64/64	0/3/3/3
4	TDR	E	403	-	-	-	0/1/1/1
3	TYD	B	402	-	-	8/16/28/28	0/2/2/2
3	TYD	L	402	-	-	3/16/28/28	0/2/2/2
4	TDR	K	403	-	-	-	0/1/1/1
4	TDR	F	403	-	-	-	0/1/1/1
2	COA	E	401	-	-	9/44/64/64	0/3/3/3
2	COA	J	401	-	-	10/44/64/64	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	D	401	-	-	9/44/64/64	0/3/3/3
2	COA	G	403	-	-	6/44/64/64	0/3/3/3
2	COA	B	401	-	-	5/44/64/64	0/3/3/3
3	TYD	E	402	-	-	4/16/28/28	0/2/2/2
4	TDR	B	403	-	-	-	0/1/1/1
2	COA	A	401	-	-	9/44/64/64	0/3/3/3
4	TDR	L	403	-	-	-	0/1/1/1
3	TYD	I	402	-	-	7/16/28/28	0/2/2/2
3	TYD	J	402	-	-	9/16/28/28	0/2/2/2
2	COA	I	401	-	-	4/44/64/64	0/3/3/3
3	TYD	G	402	-	-	2/16/28/28	0/2/2/2
4	TDR	D	403	-	-	-	0/1/1/1
2	COA	G	401	-	-	5/44/64/64	0/3/3/3
3	TYD	C	402	-	-	3/16/28/28	0/2/2/2
3	TYD	A	402	-	-	4/16/28/28	0/2/2/2
2	COA	C	401	-	-	6/44/64/64	0/3/3/3
2	COA	L	401	-	-	10/44/64/64	0/3/3/3
3	TYD	K	402	-	-	3/16/28/28	0/2/2/2
3	TYD	F	402	-	-	8/16/28/28	0/2/2/2
3	TYD	D	402	-	-	0/16/28/28	0/2/2/2
3	TYD	H	401	-	-	2/16/28/28	0/2/2/2
4	TDR	C	403	-	-	-	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	TYD	C6-N1	-10.46	1.33	1.46
3	E	402	TYD	C6-N1	-9.89	1.34	1.46
3	L	402	TYD	C6-N1	-9.82	1.34	1.46
3	J	402	TYD	C6-N1	-9.75	1.34	1.46
3	K	402	TYD	C6-N1	-9.68	1.34	1.46
3	C	402	TYD	C6-N1	-9.30	1.35	1.46
3	I	402	TYD	C6-N1	-9.29	1.35	1.46
3	F	402	TYD	C6-N1	-9.29	1.35	1.46
3	A	402	TYD	C6-N1	-9.20	1.35	1.46
3	G	402	TYD	C6-N1	-9.12	1.35	1.46
3	H	401	TYD	C6-N1	-9.08	1.35	1.46
3	B	402	TYD	C6-N1	-8.75	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	403	TDR	C4-C5	4.70	1.51	1.41
4	C	403	TDR	C4-C5	4.68	1.51	1.41
4	B	403	TDR	C4-C5	4.59	1.51	1.41
4	L	403	TDR	C4-C5	4.51	1.51	1.41
4	J	403	TDR	C4-C5	4.34	1.50	1.41
3	D	402	TYD	C6-C5	-4.20	1.38	1.51
4	E	403	TDR	C4-C5	4.17	1.50	1.41
4	F	403	TDR	C4-C5	4.17	1.50	1.41
4	A	403	TDR	C4-C5	4.13	1.50	1.41
3	F	402	TYD	C6-C5	-4.12	1.38	1.51
3	J	402	TYD	C6-C5	-4.11	1.39	1.51
3	K	402	TYD	C6-C5	-4.04	1.39	1.51
4	K	403	TDR	C4-C5	4.01	1.50	1.41
3	G	402	TYD	C6-C5	-3.97	1.39	1.51
3	C	402	TYD	C6-C5	-3.92	1.39	1.51
3	I	402	TYD	C6-C5	-3.91	1.39	1.51
3	E	402	TYD	C6-C5	-3.85	1.39	1.51
3	B	402	TYD	C6-C5	-3.85	1.39	1.51
3	A	402	TYD	C6-C5	-3.77	1.40	1.51
3	H	401	TYD	C6-C5	-3.75	1.40	1.51
3	L	402	TYD	C6-C5	-3.69	1.40	1.51
2	A	401	COA	C2A-N3A	3.31	1.37	1.32
2	C	401	COA	O4B-C1B	3.23	1.45	1.41
2	L	401	COA	O4B-C1B	2.63	1.44	1.41
2	B	401	COA	P3B-O3B	2.47	1.64	1.59
2	C	401	COA	C2A-N3A	2.47	1.36	1.32
3	B	402	TYD	C1'-N1	2.44	1.48	1.45
2	J	401	COA	P3B-O3B	2.43	1.63	1.59
3	G	402	TYD	C1'-N1	2.41	1.48	1.45
2	I	401	COA	O4B-C1B	2.32	1.44	1.41
2	K	401	COA	O4B-C1B	2.30	1.44	1.41
2	F	401	COA	O4B-C1B	2.29	1.44	1.41
2	A	401	COA	O4B-C1B	2.24	1.44	1.41
2	B	401	COA	O4B-C1B	2.24	1.44	1.41
2	E	401	COA	O4B-C1B	2.22	1.44	1.41
3	I	402	TYD	C1'-N1	2.21	1.48	1.45
3	A	402	TYD	C1'-N1	2.20	1.48	1.45
2	I	401	COA	C2A-N3A	2.18	1.35	1.32
3	H	401	TYD	O2-C2	2.13	1.26	1.23
2	F	401	COA	P3B-O3B	2.10	1.63	1.59
2	G	401	COA	O4B-C1B	2.04	1.43	1.41
3	F	402	TYD	C1'-N1	2.03	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	401	TYD	C1'-N1	2.03	1.48	1.45
2	D	401	COA	O4B-C1B	2.03	1.43	1.41

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	TDR	N1-C2-N3	-12.63	118.39	128.43
4	F	403	TDR	C4-N3-C2	9.69	123.32	115.14
4	K	403	TDR	N1-C2-N3	-9.60	120.80	128.43
4	L	403	TDR	N1-C2-N3	-9.44	120.92	128.43
4	E	403	TDR	N1-C2-N3	-8.91	121.34	128.43
4	B	403	TDR	N1-C2-N3	-8.89	121.36	128.43
4	J	403	TDR	N1-C2-N3	-8.66	121.55	128.43
4	E	403	TDR	C4-N3-C2	8.08	121.96	115.14
4	K	403	TDR	C4-N3-C2	7.94	121.85	115.14
4	F	403	TDR	N1-C2-N3	-7.80	122.23	128.43
4	D	403	TDR	C4-N3-C2	7.76	121.69	115.14
4	D	403	TDR	N1-C2-N3	-7.72	122.29	128.43
4	J	403	TDR	C4-N3-C2	7.42	121.41	115.14
3	K	402	TYD	C2'-C1'-N1	-7.39	106.58	115.61
3	J	402	TYD	O4'-C1'-N1	7.34	117.76	108.41
3	C	402	TYD	O4'-C1'-N1	7.33	117.75	108.41
4	A	403	TDR	C6-N1-C2	7.10	127.07	115.36
3	I	402	TYD	C4-N3-C2	-7.08	118.20	126.86
4	B	403	TDR	C4-N3-C2	7.02	121.07	115.14
3	C	402	TYD	C4-N3-C2	-6.97	118.33	126.86
4	C	403	TDR	N1-C2-N3	-6.82	123.01	128.43
2	F	401	COA	C7P-N8P-C9P	6.69	134.52	122.59
3	G	402	TYD	C4-N3-C2	-6.57	118.82	126.86
4	L	403	TDR	C4-N3-C2	6.55	120.68	115.14
3	B	402	TYD	O4'-C1'-N1	6.52	116.72	108.41
3	G	402	TYD	N3-C2-N1	6.49	123.51	116.65
3	E	402	TYD	O4'-C1'-N1	6.46	116.65	108.41
2	C	401	COA	C3P-N4P-C5P	6.44	134.79	122.84
2	I	401	COA	C3P-N4P-C5P	6.39	134.69	122.84
3	I	402	TYD	N3-C2-N1	6.34	123.36	116.65
3	D	402	TYD	C4-N3-C2	-6.33	119.11	126.86
4	B	403	TDR	C5-C6-N1	-6.32	118.72	125.16
4	C	403	TDR	C4-N3-C2	6.28	120.44	115.14
4	A	403	TDR	C5-C6-N1	-6.26	118.78	125.16
3	E	402	TYD	C2'-C1'-N1	-6.17	108.07	115.61
3	G	402	TYD	C2'-C1'-N1	-6.11	108.14	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	COA	N3A-C2A-N1A	-6.09	119.16	128.68
3	E	402	TYD	C4-N3-C2	-6.08	119.42	126.86
3	A	402	TYD	C5-C6-N1	5.92	122.77	111.11
3	L	402	TYD	C2'-C1'-N1	-5.90	108.40	115.61
3	C	402	TYD	N3-C2-N1	5.80	122.79	116.65
3	F	402	TYD	C4-N3-C2	-5.78	119.80	126.86
3	E	402	TYD	N3-C2-N1	5.75	122.73	116.65
3	B	402	TYD	C4-N3-C2	-5.69	119.90	126.86
2	J	401	COA	C7P-N8P-C9P	5.60	132.57	122.59
2	J	401	COA	N3A-C2A-N1A	-5.60	119.93	128.68
3	A	402	TYD	N3-C2-N1	5.56	122.54	116.65
3	L	402	TYD	C4-N3-C2	-5.52	120.11	126.86
3	G	402	TYD	C5-C6-N1	5.49	121.92	111.11
3	B	402	TYD	N3-C2-N1	5.47	122.44	116.65
3	L	402	TYD	N3-C2-N1	5.47	122.43	116.65
3	L	402	TYD	O4'-C1'-N1	5.45	115.36	108.41
3	B	402	TYD	C5-C6-N1	5.41	121.77	111.11
2	J	401	COA	O4B-C1B-C2B	-5.40	99.03	106.93
4	L	403	TDR	C5-C6-N1	-5.24	119.82	125.16
3	J	402	TYD	C4-N3-C2	-5.24	120.45	126.86
3	F	402	TYD	N3-C2-N1	5.19	122.14	116.65
3	J	402	TYD	C5-C6-N1	5.16	121.28	111.11
2	K	401	COA	C7P-C6P-C5P	-5.08	103.90	112.36
3	F	402	TYD	C5-C6-N1	5.01	120.98	111.11
3	L	402	TYD	C5-C6-N1	4.91	120.79	111.11
3	K	402	TYD	O4'-C1'-N1	4.91	114.67	108.41
4	L	403	TDR	C6-N1-C2	4.90	123.44	115.36
3	H	401	TYD	C5-C6-N1	4.86	120.69	111.11
3	K	402	TYD	C5-C6-N1	4.86	120.68	111.11
3	D	402	TYD	N3-C2-N1	4.82	121.75	116.65
3	I	402	TYD	C5-C6-N1	4.82	120.60	111.11
4	C	403	TDR	C5-C6-N1	-4.79	120.28	125.16
3	B	402	TYD	C5M-C5-C6	4.78	122.55	112.34
2	E	401	COA	N3A-C2A-N1A	-4.75	121.26	128.68
4	B	403	TDR	C6-N1-C2	4.73	123.16	115.36
3	D	402	TYD	C5-C6-N1	4.62	120.21	111.11
3	K	402	TYD	C4-N3-C2	-4.60	121.23	126.86
3	K	402	TYD	N3-C2-N1	4.55	121.47	116.65
4	K	403	TDR	C5-C6-N1	-4.54	120.54	125.16
2	D	401	COA	C7P-N8P-C9P	4.54	130.68	122.59
2	G	401	COA	N3A-C2A-N1A	-4.45	121.72	128.68
3	A	402	TYD	C4-N3-C2	-4.41	121.46	126.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	TYD	C5M-C5-C6	4.39	121.73	112.34
3	H	401	TYD	C4-N3-C2	-4.38	121.50	126.86
2	L	401	COA	N3A-C2A-N1A	-4.38	121.83	128.68
2	G	403	COA	C7P-N8P-C9P	4.37	130.39	122.59
2	G	401	COA	CEP-CBP-CCP	-4.36	101.11	108.23
3	J	402	TYD	C1'-N1-C2	4.34	124.26	118.50
2	L	401	COA	C2P-C3P-N4P	-4.34	102.39	112.31
2	G	403	COA	N3A-C2A-N1A	-4.18	122.14	128.68
4	K	403	TDR	C6-N1-C2	4.15	122.20	115.36
2	A	401	COA	N3A-C2A-N1A	-4.14	122.20	128.68
2	F	401	COA	C6P-C5P-N4P	4.11	123.34	116.42
2	B	401	COA	C2P-C3P-N4P	-4.07	103.00	112.31
2	J	401	COA	O5P-C5P-N4P	-4.07	115.33	123.01
3	E	402	TYD	C5-C6-N1	4.04	119.06	111.11
2	F	401	COA	N3A-C2A-N1A	-4.01	122.42	128.68
3	C	402	TYD	O2-C2-N3	-4.00	114.06	121.50
2	C	401	COA	OAP-CAP-CBP	-3.96	100.92	110.25
3	G	402	TYD	O4'-C1'-N1	3.90	113.38	108.41
2	A	401	COA	C2P-C3P-N4P	-3.90	103.40	112.31
2	D	401	COA	N3A-C2A-N1A	-3.89	122.60	128.68
3	I	402	TYD	O2-C2-N1	-3.81	118.33	123.11
2	E	401	COA	O9A-P3B-O7A	3.79	125.52	110.68
2	C	401	COA	C7P-N8P-C9P	3.75	129.28	122.59
3	B	402	TYD	C2'-C1'-N1	-3.75	111.02	115.61
2	A	401	COA	C3P-N4P-C5P	3.75	129.79	122.84
2	G	401	COA	C6P-C5P-N4P	3.73	122.71	116.42
3	D	402	TYD	C1'-N1-C2	3.67	123.36	118.50
4	C	403	TDR	C6-N1-C2	3.66	121.40	115.36
4	A	403	TDR	C4-N3-C2	3.66	118.23	115.14
2	G	401	COA	O5P-C5P-N4P	-3.64	116.14	123.01
3	A	402	TYD	C1'-N1-C2	3.63	123.32	118.50
2	E	401	COA	C7P-N8P-C9P	3.62	129.05	122.59
4	J	403	TDR	C6-N1-C2	3.62	121.33	115.36
3	C	402	TYD	C3'-C2'-C1'	-3.60	93.52	102.54
2	J	401	COA	O6A-CCP-CBP	-3.59	104.78	110.55
3	C	402	TYD	C5-C6-N1	3.54	118.09	111.11
3	A	402	TYD	O4'-C1'-N1	3.53	112.91	108.41
3	H	401	TYD	N3-C2-N1	3.50	120.36	116.65
2	B	401	COA	CDP-CBP-CCP	3.42	113.82	108.23
3	K	402	TYD	C5M-C5-C6	3.39	119.57	112.34
2	J	401	COA	P2A-O3A-P1A	-3.37	121.25	132.83
2	K	401	COA	N3A-C2A-N1A	-3.34	123.46	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	401	COA	C4A-C5A-N7A	-3.32	105.94	109.40
2	G	403	COA	O9A-P3B-O7A	3.32	123.67	110.68
2	K	401	COA	C7P-N8P-C9P	3.31	128.49	122.59
3	D	402	TYD	C2'-C1'-N1	-3.30	111.58	115.61
2	L	401	COA	O9A-P3B-O7A	3.28	123.50	110.68
2	E	401	COA	O3B-P3B-O7A	-3.27	96.78	109.39
2	I	401	COA	O3B-P3B-O7A	-3.25	96.84	109.39
2	A	401	COA	C4A-C5A-N7A	-3.24	106.02	109.40
2	A	401	COA	C7P-N8P-C9P	3.24	128.37	122.59
3	J	402	TYD	N3-C2-N1	3.23	120.07	116.65
2	B	401	COA	C7P-C6P-C5P	-3.23	106.98	112.36
4	J	403	TDR	C5-C6-N1	-3.20	121.91	125.16
2	F	401	COA	O5P-C5P-N4P	-3.19	116.99	123.01
2	B	401	COA	N3A-C2A-N1A	-3.18	123.70	128.68
2	D	401	COA	CEP-CBP-CAP	3.17	114.33	108.82
3	E	402	TYD	C5M-C5-C6	3.17	119.12	112.34
3	G	402	TYD	O2-C2-N1	-3.17	119.12	123.11
3	F	402	TYD	C2'-C1'-N1	-3.17	111.74	115.61
3	C	402	TYD	C1'-N1-C2	3.16	122.70	118.50
2	I	401	COA	N3A-C2A-N1A	-3.16	123.75	128.68
4	E	403	TDR	C6-N1-C2	3.09	120.46	115.36
2	K	401	COA	O5A-P2A-O4A	3.09	127.51	112.24
2	D	401	COA	C3P-N4P-C5P	3.08	128.56	122.84
3	L	402	TYD	C5M-C5-C6	3.07	118.90	112.34
2	A	401	COA	O5P-C5P-N4P	-3.07	117.22	123.01
3	A	402	TYD	C2'-C1'-N1	-3.07	111.86	115.61
2	C	401	COA	O3B-P3B-O7A	-3.05	97.61	109.39
3	J	402	TYD	C5M-C5-C6	3.03	118.81	112.34
2	L	401	COA	O5P-C5P-N4P	-3.02	117.32	123.01
2	G	403	COA	O2A-P1A-O1A	2.99	127.02	112.24
4	D	403	TDR	C6-N1-C2	2.98	120.28	115.36
3	L	402	TYD	O2-C2-N3	-2.96	115.99	121.50
4	L	403	TDR	CM5-C5-C4	2.95	126.66	121.37
3	K	402	TYD	C6-C5-C4	2.94	119.96	111.53
4	D	403	TDR	C5-C6-N1	-2.93	122.18	125.16
2	C	401	COA	O4B-C1B-C2B	-2.93	102.65	106.93
3	E	402	TYD	C6-C5-C4	2.93	119.93	111.53
3	E	402	TYD	O2-C2-N1	-2.92	119.44	123.11
2	G	401	COA	C7P-N8P-C9P	2.92	127.79	122.59
3	G	402	TYD	O4'-C4'-C5'	2.89	118.87	109.37
2	E	401	COA	P2A-O3A-P1A	-2.88	122.94	132.83
2	J	401	COA	C2B-C3B-C4B	-2.87	98.14	103.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	402	TYD	C6-N1-C1'	-2.85	115.33	120.94
2	L	401	COA	C7P-N8P-C9P	2.85	127.67	122.59
3	K	402	TYD	O3A-PB-O1B	-2.85	95.41	111.19
2	F	401	COA	C7P-C6P-C5P	-2.84	107.63	112.36
3	F	402	TYD	O4-C4-N3	-2.84	115.95	121.01
3	A	402	TYD	C5M-C5-C6	2.83	118.39	112.34
3	C	402	TYD	C6-C5-C4	2.82	119.63	111.53
2	C	401	COA	C2P-C3P-N4P	-2.81	105.88	112.31
3	A	402	TYD	O2-C2-N3	-2.78	116.33	121.50
2	B	401	COA	C7P-N8P-C9P	2.77	127.53	122.59
2	G	401	COA	P2A-O3A-P1A	-2.76	123.34	132.83
2	G	401	COA	O4B-C1B-C2B	-2.76	102.90	106.93
2	E	401	COA	C3P-N4P-C5P	2.75	127.94	122.84
3	I	402	TYD	C1'-N1-C2	2.72	122.11	118.50
3	K	402	TYD	O2-C2-N3	-2.70	116.46	121.50
2	G	403	COA	CEP-CBP-CAP	2.69	113.49	108.82
3	G	402	TYD	C1'-N1-C2	2.69	122.07	118.50
2	F	401	COA	C4A-C5A-N7A	-2.68	106.60	109.40
2	B	401	COA	C4A-C5A-N7A	-2.68	106.60	109.40
2	F	401	COA	C1B-N9A-C4A	-2.68	121.94	126.64
3	I	402	TYD	C2'-C1'-N1	-2.66	112.36	115.61
2	E	401	COA	C2P-C3P-N4P	-2.66	106.23	112.31
3	L	402	TYD	C6-C5-C4	2.65	119.14	111.53
2	A	401	COA	O8A-P3B-O7A	2.65	121.05	110.68
3	G	402	TYD	C5M-C5-C6	2.65	117.99	112.34
2	A	401	COA	O3B-C3B-C4B	-2.65	100.52	110.08
2	I	401	COA	C2P-C3P-N4P	-2.64	106.27	112.31
2	A	401	COA	O3B-P3B-O7A	-2.63	99.24	109.39
3	H	401	TYD	O2-C2-N1	-2.62	119.81	123.11
2	A	401	COA	C1B-N9A-C4A	-2.62	122.04	126.64
2	F	401	COA	C2P-C3P-N4P	-2.62	106.32	112.31
3	E	402	TYD	O3A-PB-O1B	-2.62	96.67	111.19
2	K	401	COA	C2P-C3P-N4P	-2.61	106.34	112.31
2	L	401	COA	O3B-C3B-C4B	-2.59	100.70	110.08
3	I	402	TYD	C6-C5-C4	2.59	118.97	111.53
2	D	401	COA	CDP-CBP-CCP	2.59	112.45	108.23
2	B	401	COA	CDP-CBP-CAP	-2.58	104.34	108.82
2	D	401	COA	CDP-CBP-CAP	-2.58	104.34	108.82
3	F	402	TYD	O2-C2-N3	-2.58	116.69	121.50
3	C	402	TYD	O4-C4-N3	-2.58	116.42	121.01
3	L	402	TYD	C1'-N1-C2	2.57	121.91	118.50
2	A	401	COA	C6P-C5P-N4P	2.56	120.73	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	COA	O9A-P3B-O7A	2.55	120.67	110.68
2	G	403	COA	C3P-N4P-C5P	2.54	127.56	122.84
3	D	402	TYD	O4'-C1'-N1	2.54	111.65	108.41
2	B	401	COA	O5A-P2A-O4A	2.54	124.80	112.24
2	K	401	COA	O9A-P3B-O7A	2.54	120.61	110.68
2	D	401	COA	CAP-C9P-N8P	-2.53	111.54	116.58
2	L	401	COA	CDP-CBP-CCP	2.52	112.35	108.23
2	L	401	COA	O3B-P3B-O7A	-2.52	99.65	109.39
2	B	401	COA	C6P-C7P-N8P	-2.52	106.80	111.90
2	A	401	COA	O4B-C4B-C5B	2.51	117.64	109.37
4	E	403	TDR	C5-C6-N1	-2.49	122.62	125.16
3	D	402	TYD	O2-C2-N1	-2.47	120.01	123.11
2	B	401	COA	O9A-P3B-O3B	-2.46	94.95	105.99
2	L	401	COA	O2B-C2B-C1B	-2.46	101.76	110.85
3	C	402	TYD	C6-N1-C1'	-2.46	116.10	120.94
2	E	401	COA	C2A-N1A-C6A	2.45	122.95	118.75
2	G	401	COA	C5A-C6A-N6A	2.45	124.07	120.35
3	F	402	TYD	O4'-C1'-N1	2.45	111.53	108.41
3	F	402	TYD	C6-C5-C4	2.44	118.55	111.53
3	H	401	TYD	C6-C5-C4	2.44	118.54	111.53
2	K	401	COA	O3B-C3B-C4B	-2.44	101.28	110.08
2	B	401	COA	C3P-N4P-C5P	2.44	127.36	122.84
3	D	402	TYD	C6-C5-C4	2.42	118.48	111.53
3	D	402	TYD	C6-N1-C1'	-2.42	116.19	120.94
2	G	401	COA	C4A-C5A-N7A	-2.41	106.88	109.40
3	B	402	TYD	O2-C2-N3	-2.41	117.02	121.50
3	A	402	TYD	C6-C5-C4	2.40	118.43	111.53
3	K	402	TYD	O3B-PB-O1B	2.37	119.95	110.68
3	I	402	TYD	C2'-C3'-C4'	2.37	107.69	102.76
3	D	402	TYD	O3'-C3'-C2'	-2.36	102.44	110.90
2	A	401	COA	CEP-CBP-CAP	2.35	112.90	108.82
2	D	401	COA	C2P-C3P-N4P	-2.35	106.94	112.31
4	F	403	TDR	C5-C6-N1	-2.34	122.78	125.16
3	F	402	TYD	C1'-N1-C2	2.34	121.61	118.50
2	I	401	COA	C7P-N8P-C9P	2.33	126.74	122.59
2	C	401	COA	CAP-C9P-N8P	2.32	121.20	116.58
2	L	401	COA	P2A-O3A-P1A	-2.32	124.87	132.83
2	J	401	COA	C7P-C6P-C5P	-2.31	108.50	112.36
2	I	401	COA	O5A-P2A-O4A	2.30	123.62	112.24
2	D	401	COA	C4A-C5A-N7A	-2.29	107.01	109.40
2	G	403	COA	C4A-C5A-N7A	-2.29	107.01	109.40
3	I	402	TYD	O4-C4-N3	-2.29	116.94	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	COA	C3P-N4P-C5P	2.29	127.08	122.84
2	D	401	COA	N6A-C6A-N1A	2.28	123.31	118.57
2	I	401	COA	O3B-C3B-C2B	-2.28	103.42	111.68
2	A	401	COA	O4B-C1B-C2B	-2.28	103.59	106.93
2	B	401	COA	O9A-P3B-O7A	2.27	119.58	110.68
3	H	401	TYD	O3A-PB-O1B	-2.27	98.61	111.19
2	J	401	COA	O9A-P3B-O7A	2.26	119.52	110.68
3	G	402	TYD	O3'-C3'-C2'	2.26	118.97	110.90
3	G	402	TYD	C6-C5-C4	2.24	117.96	111.53
3	B	402	TYD	C3'-C2'-C1'	2.24	108.15	102.54
2	F	401	COA	CDP-CBP-CAP	2.23	112.70	108.82
2	E	401	COA	CEP-CBP-CDP	2.23	113.72	109.17
4	F	403	TDR	C6-N1-C2	2.23	119.04	115.36
3	G	402	TYD	O2-C2-N3	-2.23	117.34	121.50
2	J	401	COA	C2P-C3P-N4P	-2.23	107.21	112.31
2	C	401	COA	P2A-O3A-P1A	-2.23	125.19	132.83
2	J	401	COA	O9A-P3B-O3B	-2.23	96.02	105.99
3	J	402	TYD	O2-C2-N3	-2.22	117.37	121.50
2	K	401	COA	O3B-P3B-O7A	-2.21	100.84	109.39
2	D	401	COA	O3B-P3B-O7A	-2.21	100.85	109.39
3	G	402	TYD	O3B-PB-O2B	2.21	116.07	107.64
2	E	401	COA	CDP-CBP-CCP	-2.20	104.64	108.23
2	E	401	COA	O2A-P1A-O1A	2.17	122.97	112.24
2	C	401	COA	O2B-C2B-C3B	2.17	117.33	111.17
3	I	402	TYD	O3'-C3'-C2'	-2.17	103.14	110.90
3	B	402	TYD	C6-C5-C4	2.16	117.74	111.53
2	B	401	COA	O3B-C3B-C4B	-2.16	102.26	110.08
2	I	401	COA	CEP-CBP-CCP	-2.16	104.70	108.23
2	E	401	COA	O3B-C3B-C4B	-2.16	102.27	110.08
2	D	401	COA	O5A-P2A-O4A	2.16	122.92	112.24
2	G	401	COA	O5A-P2A-O4A	2.16	122.90	112.24
2	G	401	COA	O3B-C3B-C4B	-2.15	102.32	110.08
3	F	402	TYD	O5'-PA-O1A	-2.14	100.70	109.07
3	J	402	TYD	C6-C5-C4	2.14	117.67	111.53
2	A	401	COA	O5A-P2A-O4A	2.14	122.81	112.24
3	B	402	TYD	O5'-PA-O1A	-2.12	100.78	109.07
2	L	401	COA	O2A-P1A-O1A	2.12	122.73	112.24
2	G	401	COA	C2P-C3P-N4P	-2.12	107.47	112.31
2	G	403	COA	C6P-C7P-N8P	-2.09	107.67	111.90
2	L	401	COA	O3B-C3B-C2B	-2.05	104.24	111.68
2	G	403	COA	O6A-CCP-CBP	2.05	113.85	110.55
3	B	402	TYD	O2-C2-N1	-2.05	120.54	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	COA	C2A-N1A-C6A	2.04	122.25	118.75
3	E	402	TYD	O2A-PA-O1A	2.02	122.24	112.24
2	G	401	COA	O6A-CCP-CBP	2.02	113.80	110.55
3	F	402	TYD	O2A-PA-O1A	2.00	122.15	112.24
2	L	401	COA	C3P-N4P-C5P	2.00	126.55	122.84

There are no chirality outliers.

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	401	COA	CAP-CBP-CCP-O6A
2	K	401	COA	OAP-CAP-CBP-CCP
2	K	401	COA	OAP-CAP-CBP-CEP
2	K	401	COA	S1P-C2P-C3P-N4P
3	B	402	TYD	C5'-O5'-PA-O3A
3	B	402	TYD	PA-O3A-PB-O2B
2	E	401	COA	OAP-CAP-CBP-CCP
2	E	401	COA	C9P-CAP-CBP-CCP
2	E	401	COA	OAP-CAP-CBP-CDP
2	E	401	COA	C9P-CAP-CBP-CDP
2	E	401	COA	OAP-CAP-CBP-CEP
2	E	401	COA	C9P-CAP-CBP-CEP
2	E	401	COA	S1P-C2P-C3P-N4P
2	J	401	COA	OAP-CAP-CBP-CCP
2	J	401	COA	C9P-CAP-CBP-CCP
2	J	401	COA	C9P-CAP-CBP-CDP
2	J	401	COA	OAP-CAP-CBP-CEP
2	J	401	COA	C9P-CAP-CBP-CEP
2	J	401	COA	S1P-C2P-C3P-N4P
2	D	401	COA	OAP-CAP-CBP-CCP
2	D	401	COA	C9P-CAP-CBP-CCP
2	D	401	COA	OAP-CAP-CBP-CDP
2	D	401	COA	C9P-CAP-CBP-CDP
2	D	401	COA	OAP-CAP-CBP-CEP
2	D	401	COA	C9P-CAP-CBP-CEP
2	D	401	COA	S1P-C2P-C3P-N4P
2	G	403	COA	OAP-CAP-CBP-CCP
2	G	403	COA	OAP-CAP-CBP-CEP
2	G	403	COA	S1P-C2P-C3P-N4P
2	B	401	COA	OAP-CAP-CBP-CCP
2	B	401	COA	OAP-CAP-CBP-CEP
3	E	402	TYD	C5'-O5'-PA-O2A

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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
2	A	401	COA	C9P-CAP-CBP-CEP
2	A	401	COA	S1P-C2P-C3P-N4P
3	I	402	TYD	C5'-O5'-PA-O1A
3	I	402	TYD	C5'-O5'-PA-O2A
3	J	402	TYD	C5'-O5'-PA-O1A
3	J	402	TYD	PA-O3A-PB-O2B
3	J	402	TYD	C3'-C4'-C5'-O5'
2	G	401	COA	OAP-CAP-CBP-CCP
3	C	402	TYD	C5'-O5'-PA-O2A
3	C	402	TYD	C5'-O5'-PA-O3A
3	A	402	TYD	O4'-C4'-C5'-O5'
2	C	401	COA	OAP-CAP-CBP-CCP
2	C	401	COA	S1P-C2P-C3P-N4P
2	L	401	COA	S1P-C2P-C3P-N4P
3	F	402	TYD	C5'-O5'-PA-O3A
3	F	402	TYD	PA-O3A-PB-O2B
3	H	401	TYD	O4'-C4'-C5'-O5'
3	B	402	TYD	O4'-C4'-C5'-O5'
3	B	402	TYD	C3'-C4'-C5'-O5'
3	L	402	TYD	O4'-C4'-C5'-O5'
3	L	402	TYD	C3'-C4'-C5'-O5'
3	A	402	TYD	C3'-C4'-C5'-O5'
3	H	401	TYD	C3'-C4'-C5'-O5'
3	J	402	TYD	C2'-C1'-N1-C2
3	I	402	TYD	C3'-C4'-C5'-O5'
3	J	402	TYD	C2'-C1'-N1-C6
3	J	402	TYD	O4'-C4'-C5'-O5'
3	K	402	TYD	O4'-C4'-C5'-O5'
3	I	402	TYD	O4'-C4'-C5'-O5'
3	K	402	TYD	C3'-C4'-C5'-O5'
2	K	401	COA	CEP-CBP-CCP-O6A
3	G	402	TYD	PA-O3A-PB-O1B
2	K	401	COA	OAP-CAP-CBP-CDP
2	J	401	COA	OAP-CAP-CBP-CDP
2	G	403	COA	OAP-CAP-CBP-CDP
2	G	401	COA	OAP-CAP-CBP-CDP
2	C	401	COA	OAP-CAP-CBP-CDP

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Mol	Chain	Res	Type	Atoms
3	F	402	TYD	PB-O3A-PA-O1A
2	I	401	COA	S1P-C2P-C3P-N4P
3	B	402	TYD	C4'-C5'-O5'-PA
3	J	402	TYD	C4'-C5'-O5'-PA
2	K	401	COA	CDP-CBP-CCP-O6A
2	B	401	COA	C9P-CAP-CBP-CEP
2	L	401	COA	C9P-CAP-CBP-CEP
2	F	401	COA	C3B-O3B-P3B-O9A
3	E	402	TYD	C5'-O5'-PA-O3A
3	A	402	TYD	C5'-O5'-PA-O3A
2	F	401	COA	P1A-O3A-P2A-O5A
2	D	401	COA	P1A-O3A-P2A-O4A
2	G	403	COA	P1A-O3A-P2A-O5A
3	I	402	TYD	PB-O3A-PA-O2A
2	G	401	COA	P1A-O3A-P2A-O5A
2	L	401	COA	P1A-O3A-P2A-O5A
3	B	402	TYD	C5'-O5'-PA-O1A
3	E	402	TYD	C5'-O5'-PA-O1A
3	F	402	TYD	C5'-O5'-PA-O1A
2	K	401	COA	C3B-C4B-C5B-O5B
2	C	401	COA	C9P-CAP-CBP-CCP
2	L	401	COA	C9P-CAP-CBP-CCP
2	F	401	COA	CAP-CBP-CCP-O6A
2	I	401	COA	OAP-CAP-CBP-CCP
2	L	401	COA	CAP-CBP-CCP-O6A
2	L	401	COA	OAP-CAP-CBP-CCP
3	F	402	TYD	C4'-C5'-O5'-PA
2	A	401	COA	O9P-C9P-CAP-OAP
2	I	401	COA	O9P-C9P-CAP-OAP
2	E	401	COA	P1A-O3A-P2A-O4A
2	E	401	COA	P1A-O3A-P2A-O5A
2	J	401	COA	P1A-O3A-P2A-O5A
2	D	401	COA	P1A-O3A-P2A-O5A
2	B	401	COA	P1A-O3A-P2A-O5A
3	I	402	TYD	PB-O3A-PA-O1A
2	C	401	COA	P1A-O3A-P2A-O5A
3	K	402	TYD	PB-O3A-PA-O2A
3	F	402	TYD	PB-O3A-PA-O2A
2	K	401	COA	C2P-C3P-N4P-C5P
2	J	401	COA	C2P-C3P-N4P-C5P
2	G	401	COA	C2P-C3P-N4P-C5P
2	L	401	COA	C2P-C3P-N4P-C5P

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Mol	Chain	Res	Type	Atoms
2	F	401	COA	CDP-CBP-CCP-O6A
2	F	401	COA	CEP-CBP-CCP-O6A
3	B	402	TYD	PA-O3A-PB-O1B
2	L	401	COA	CDP-CBP-CCP-O6A
2	L	401	COA	CEP-CBP-CCP-O6A
3	F	402	TYD	PA-O3A-PB-O1B
2	K	401	COA	P1A-O3A-P2A-O5A
3	B	402	TYD	PB-O3A-PA-O2A
2	G	403	COA	P1A-O3A-P2A-O4A
2	K	401	COA	O4B-C4B-C5B-O5B
3	C	402	TYD	C3'-C4'-C5'-O5'
3	J	402	TYD	PA-O3A-PB-O1B
2	C	401	COA	C9P-CAP-CBP-CDP
3	I	402	TYD	C5'-O5'-PA-O3A
3	J	402	TYD	C5'-O5'-PA-O3A
3	F	402	TYD	O4'-C4'-C5'-O5'
2	K	401	COA	P1A-O3A-P2A-O4A
2	F	401	COA	P1A-O3A-P2A-O4A
3	L	402	TYD	PB-O3A-PA-O1A
2	J	401	COA	P1A-O3A-P2A-O4A
2	A	401	COA	P1A-O3A-P2A-O5A
2	I	401	COA	P1A-O3A-P2A-O4A
2	G	401	COA	P1A-O3A-P2A-O4A
2	L	401	COA	P1A-O3A-P2A-O4A
3	A	402	TYD	C5'-O5'-PA-O1A
3	E	402	TYD	O4'-C4'-C5'-O5'
3	G	402	TYD	O4'-C4'-C5'-O5'
2	B	401	COA	C9P-CAP-CBP-CCP

There are no ring outliers.

15 monomers are involved in 27 short contacts:

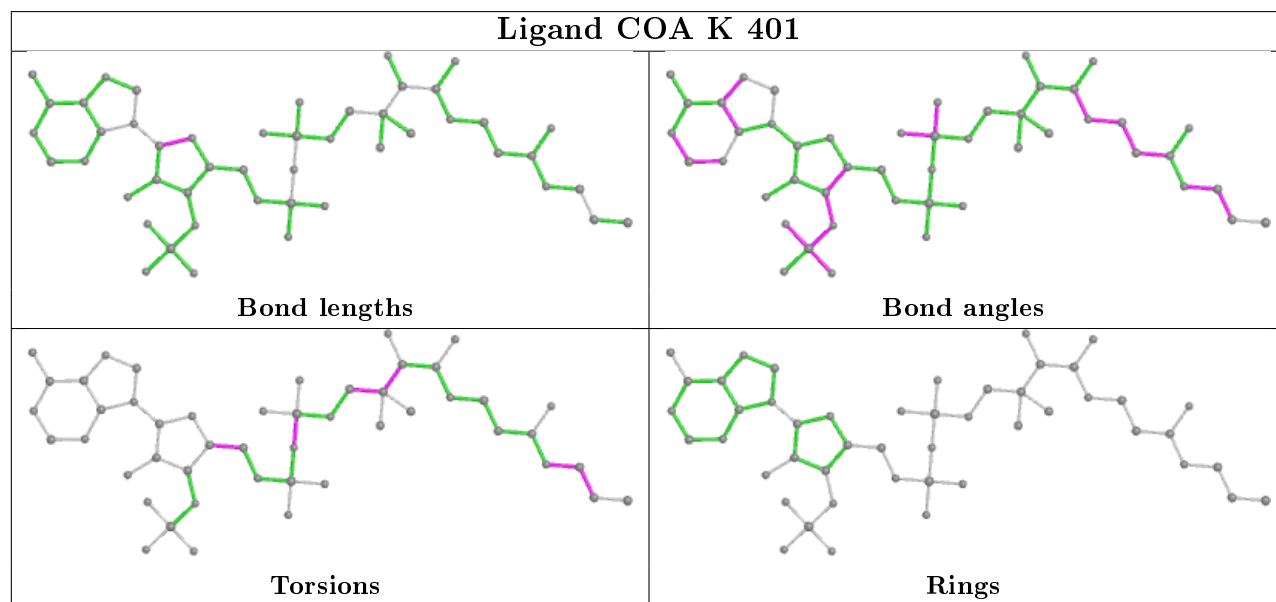
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	401	COA	3	0
4	A	403	TDR	1	0
3	L	402	TYD	1	0
2	J	401	COA	4	0
2	D	401	COA	1	0
2	G	403	COA	1	0
2	B	401	COA	1	0
3	E	402	TYD	4	0
4	L	403	TDR	1	0

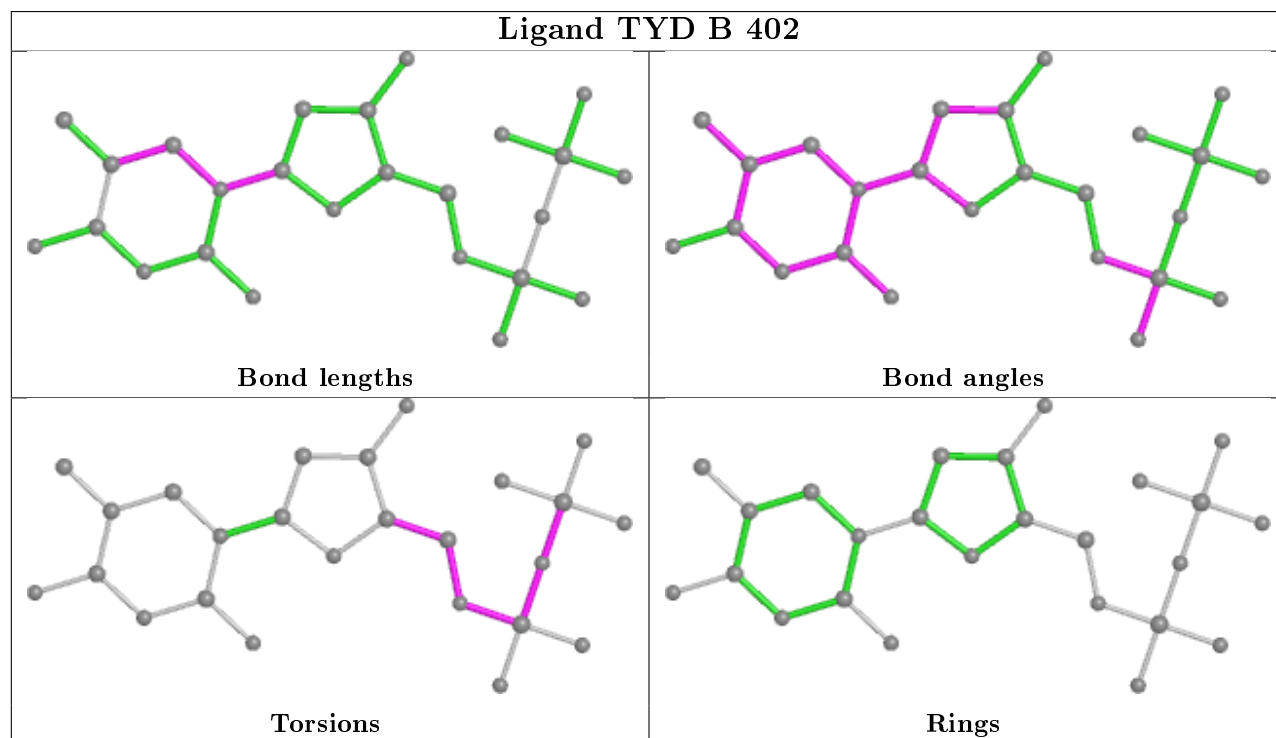
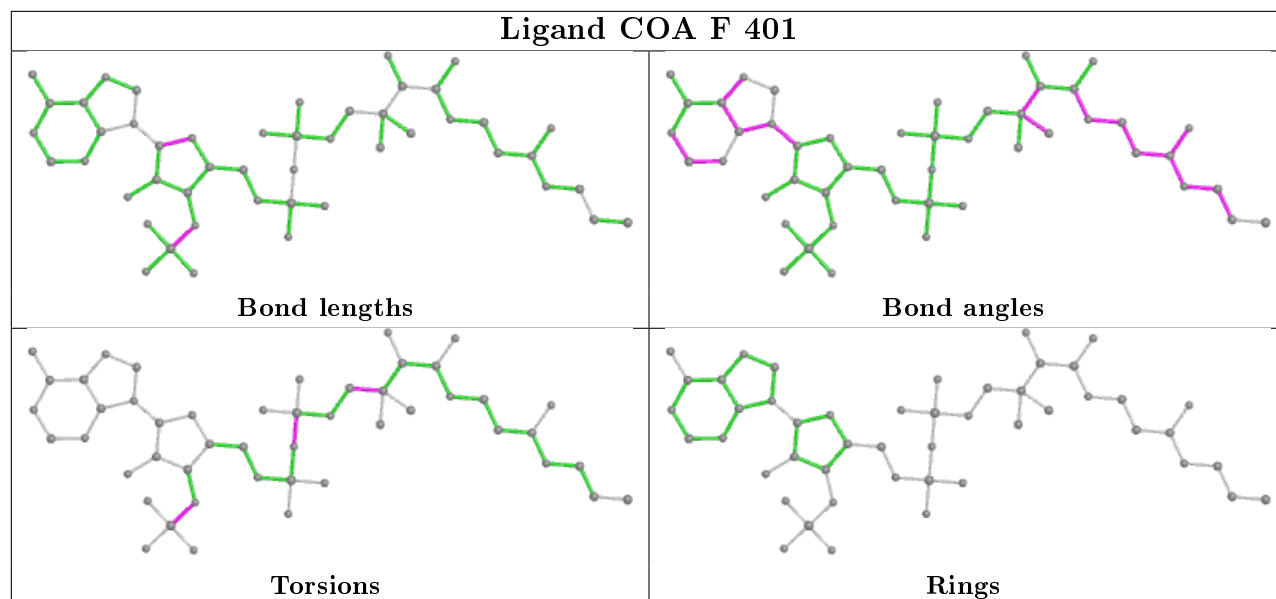
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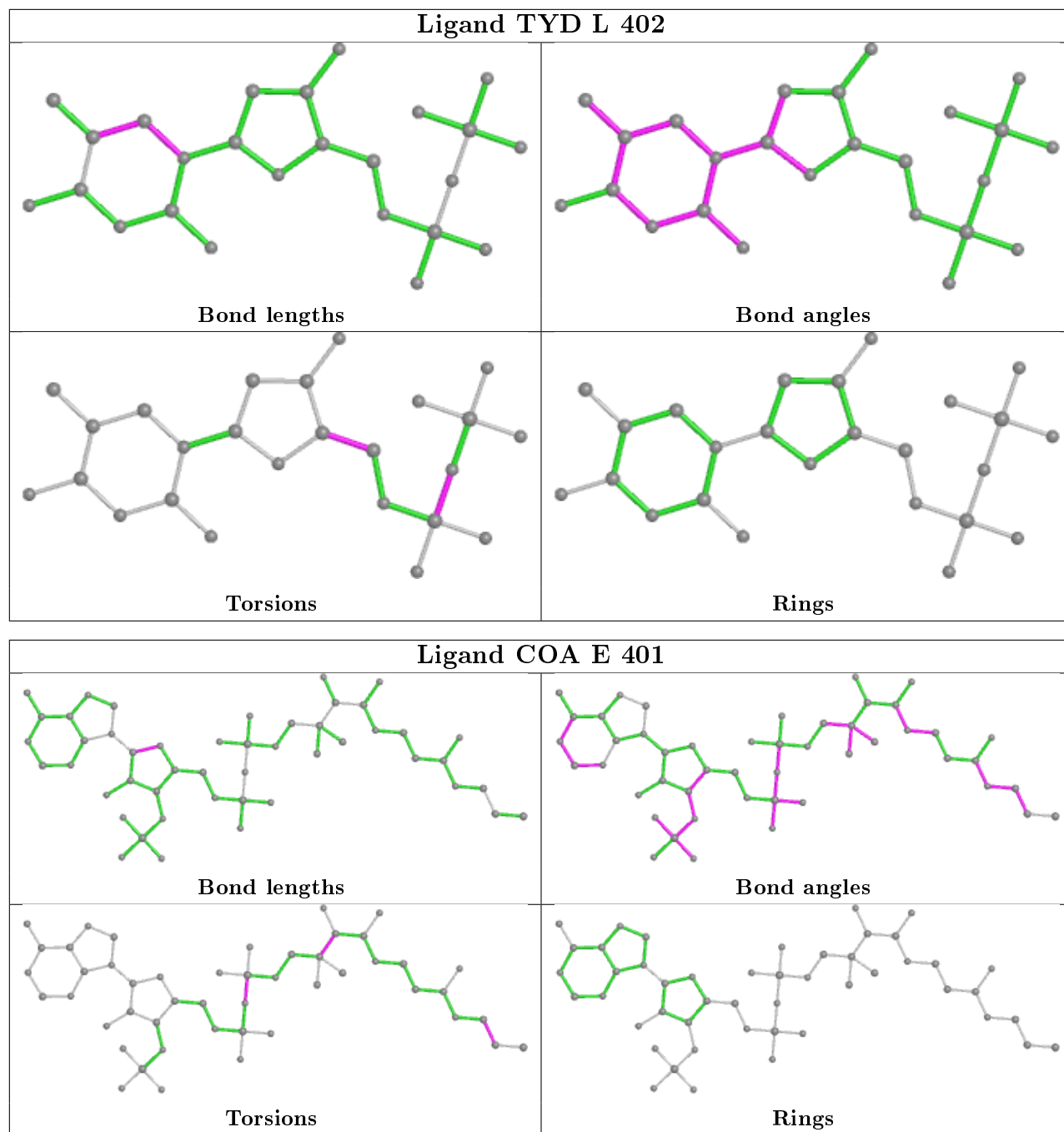
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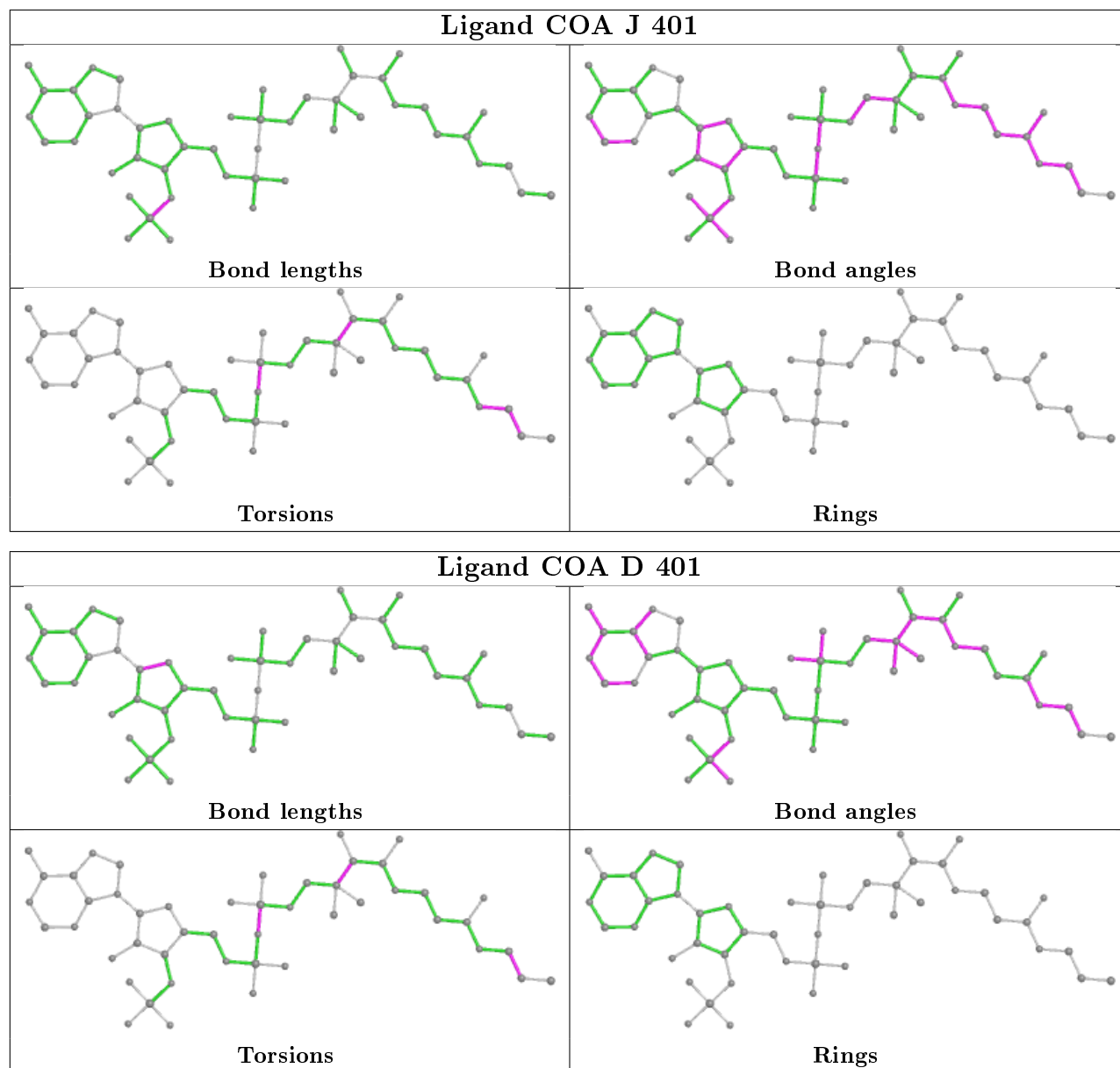
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	COA	2	0
3	G	402	TYD	1	0
2	L	401	COA	3	0
3	F	402	TYD	1	0
3	D	402	TYD	2	0
3	H	401	TYD	1	0

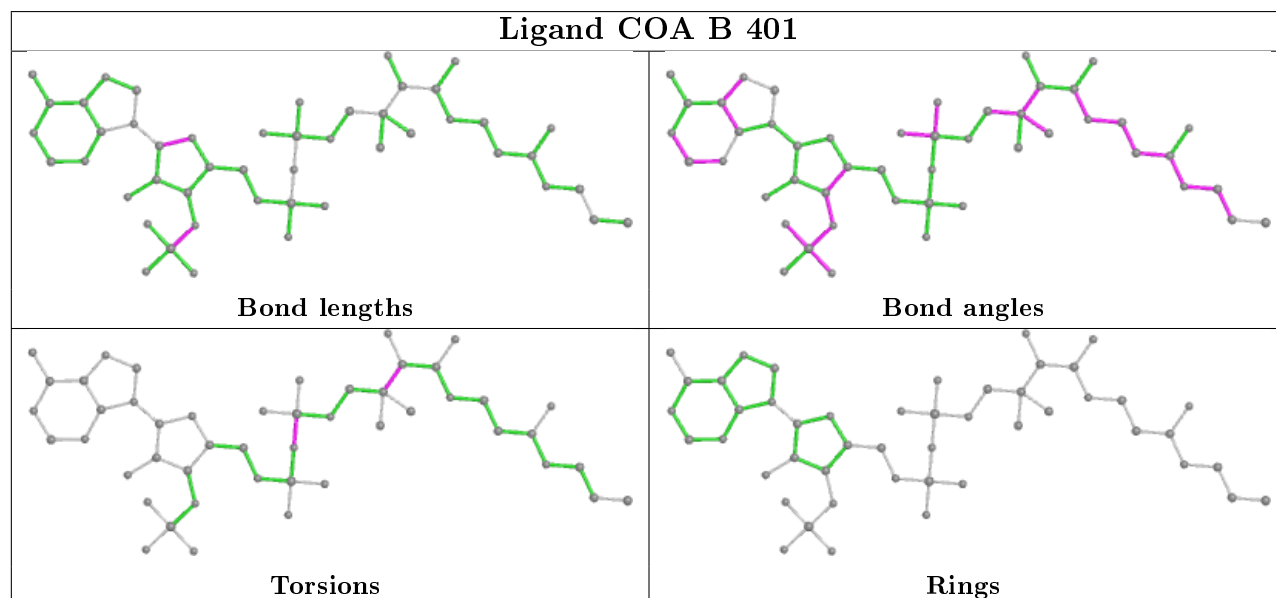
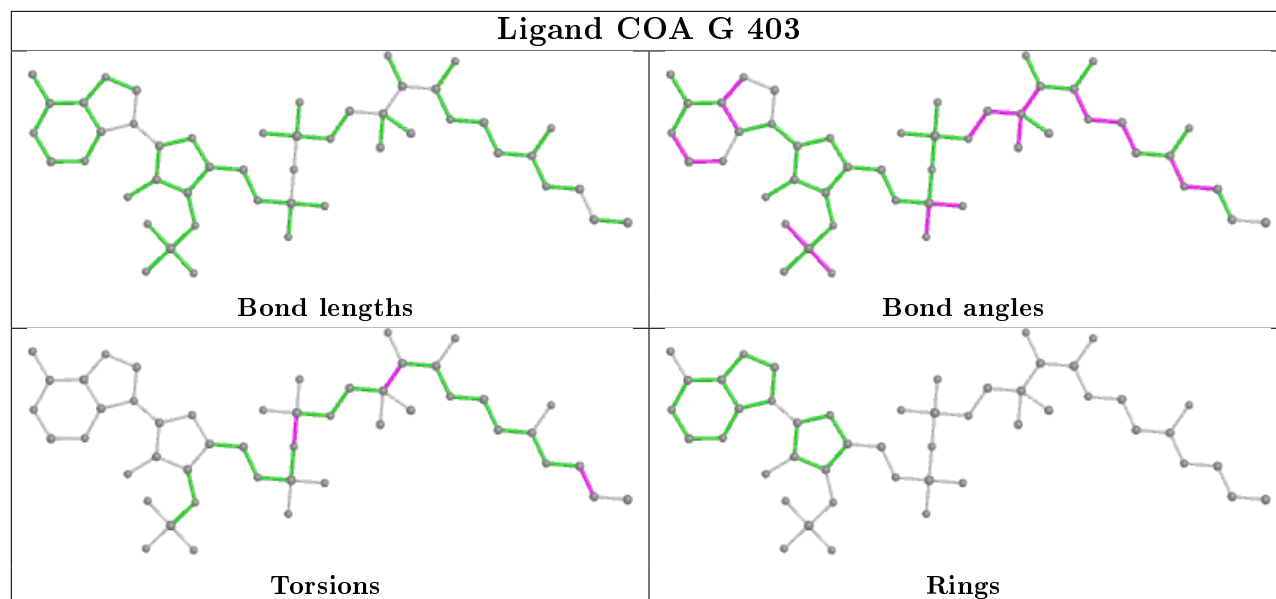
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



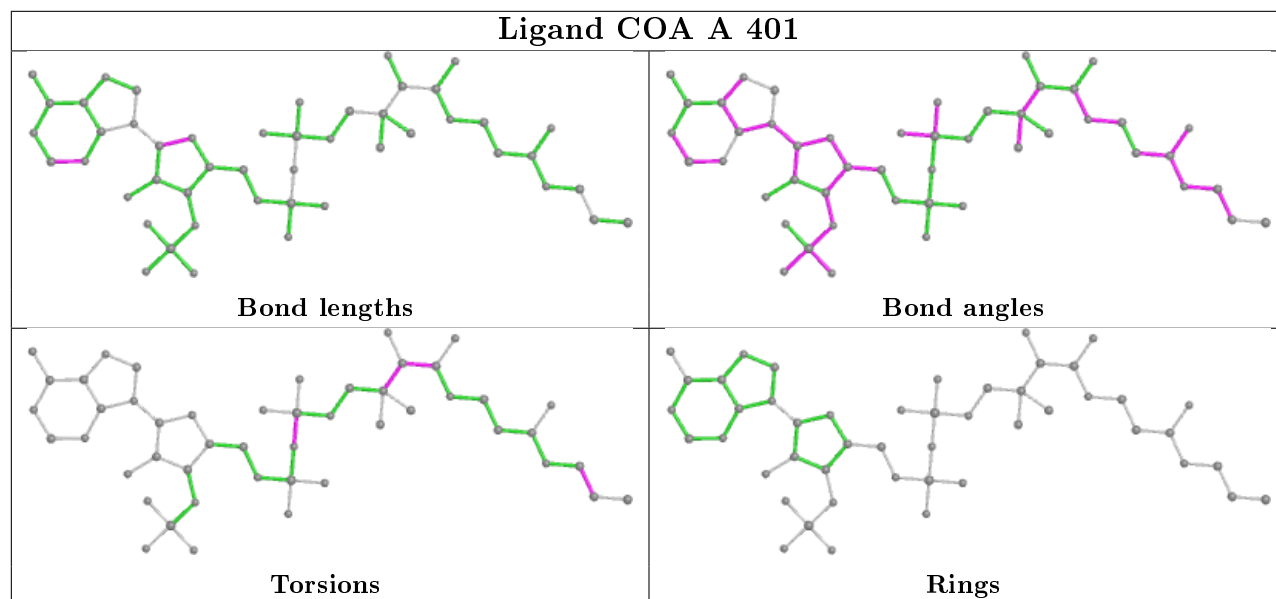
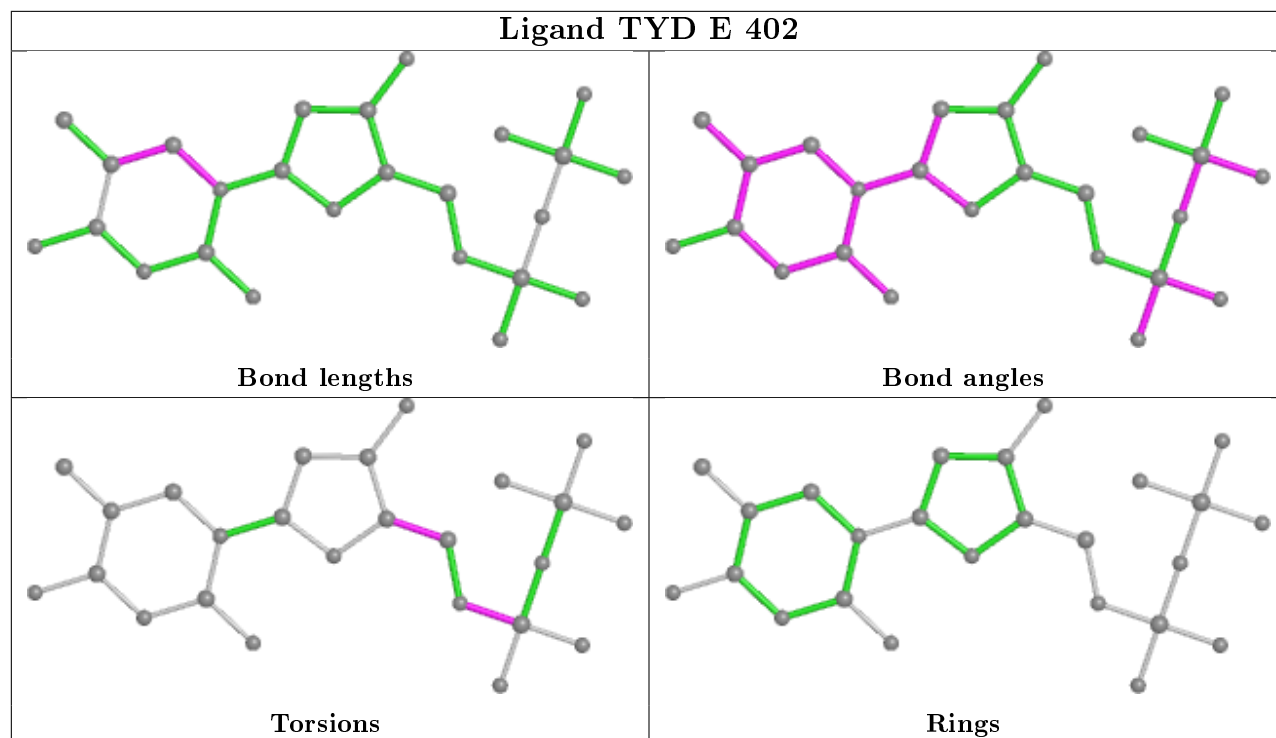




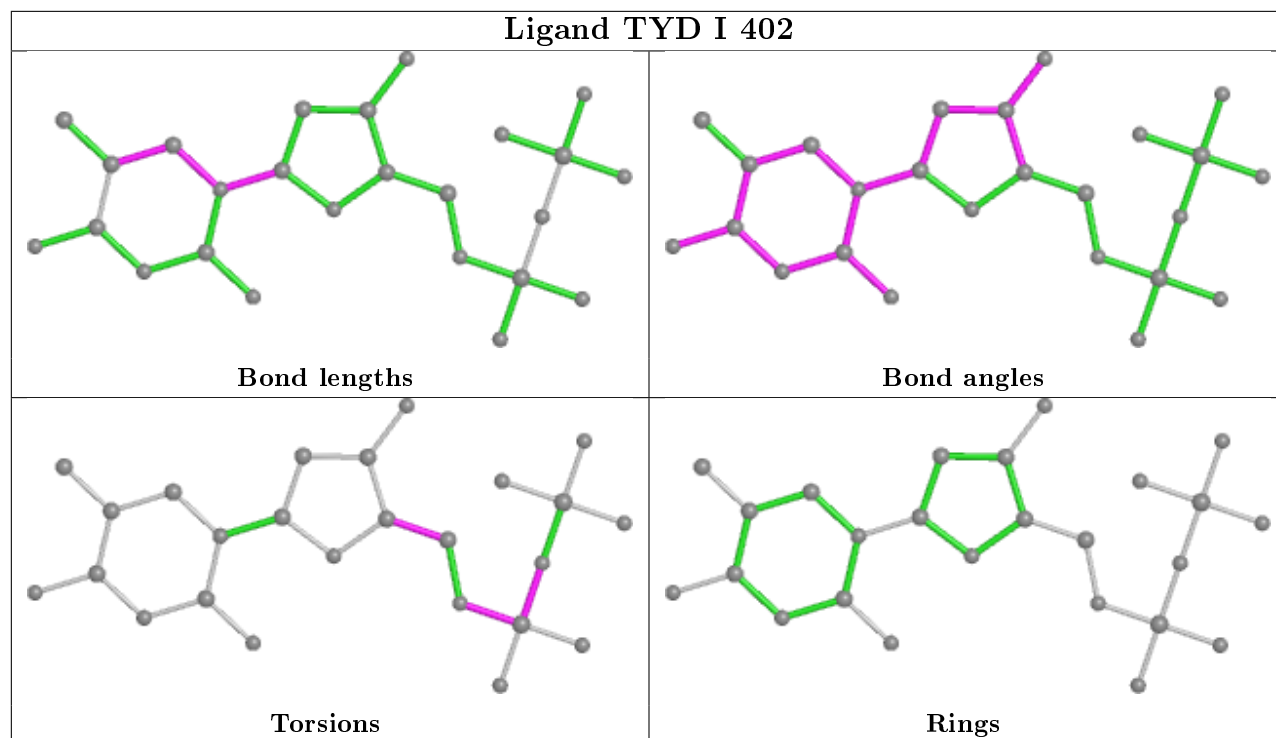




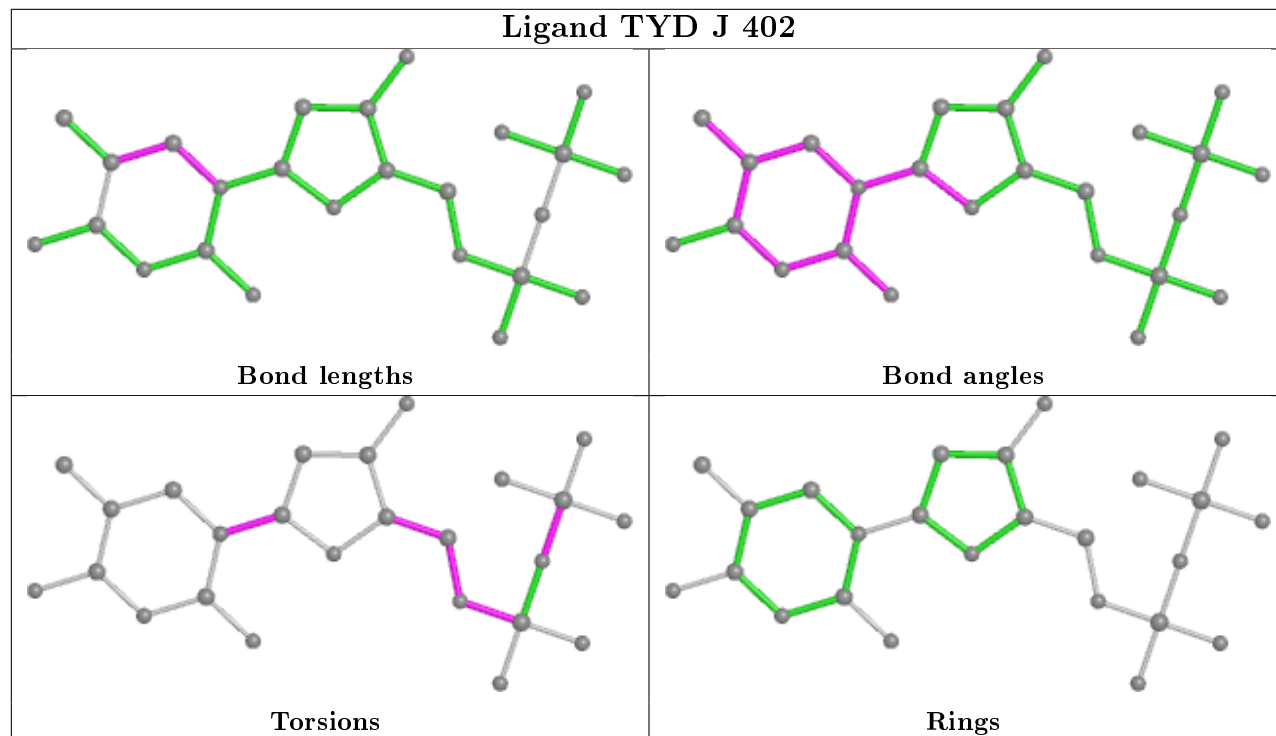




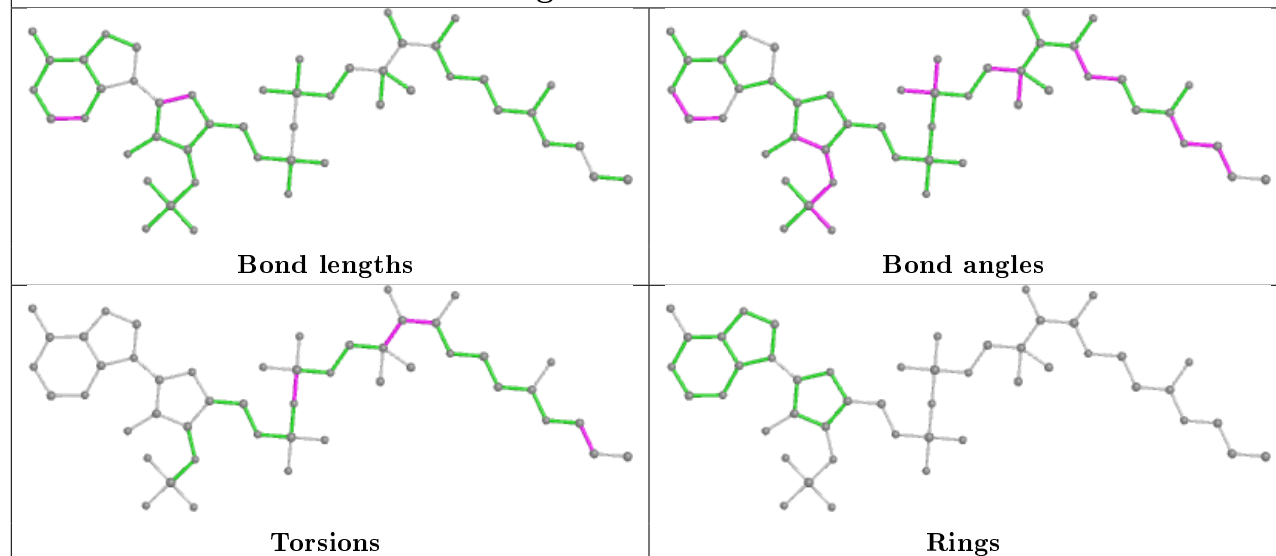
## Ligand TYD I 402



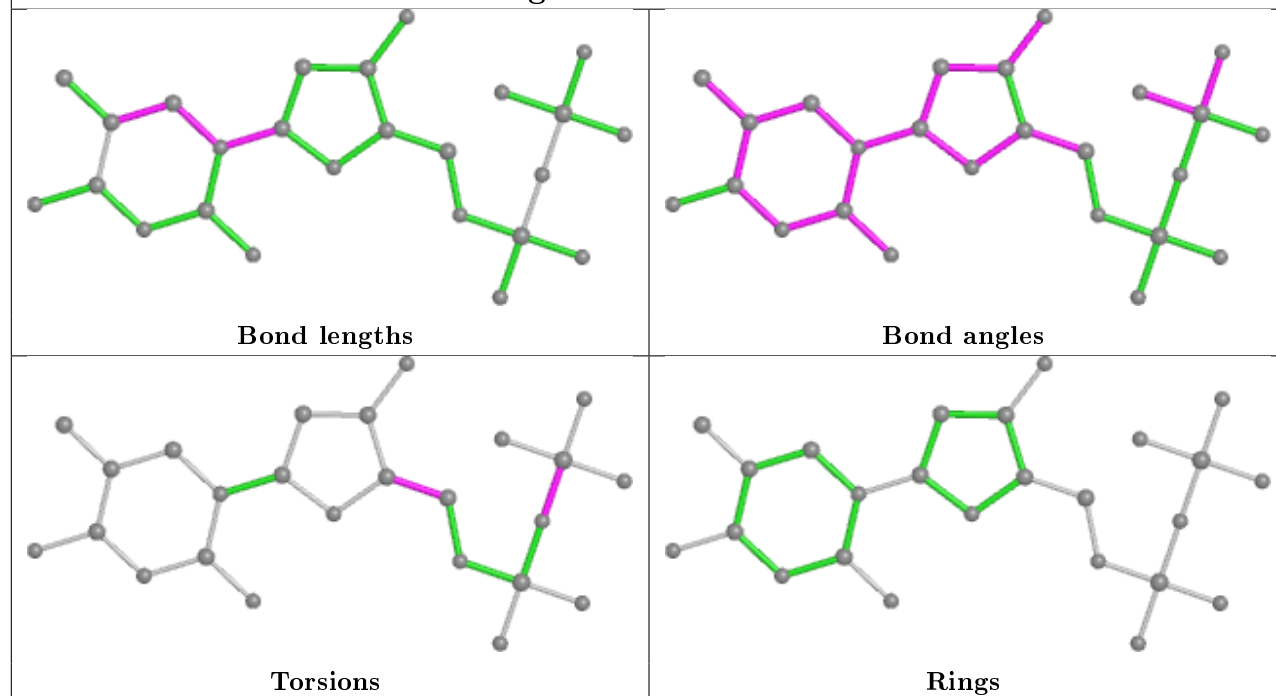
## Ligand TYD J 402

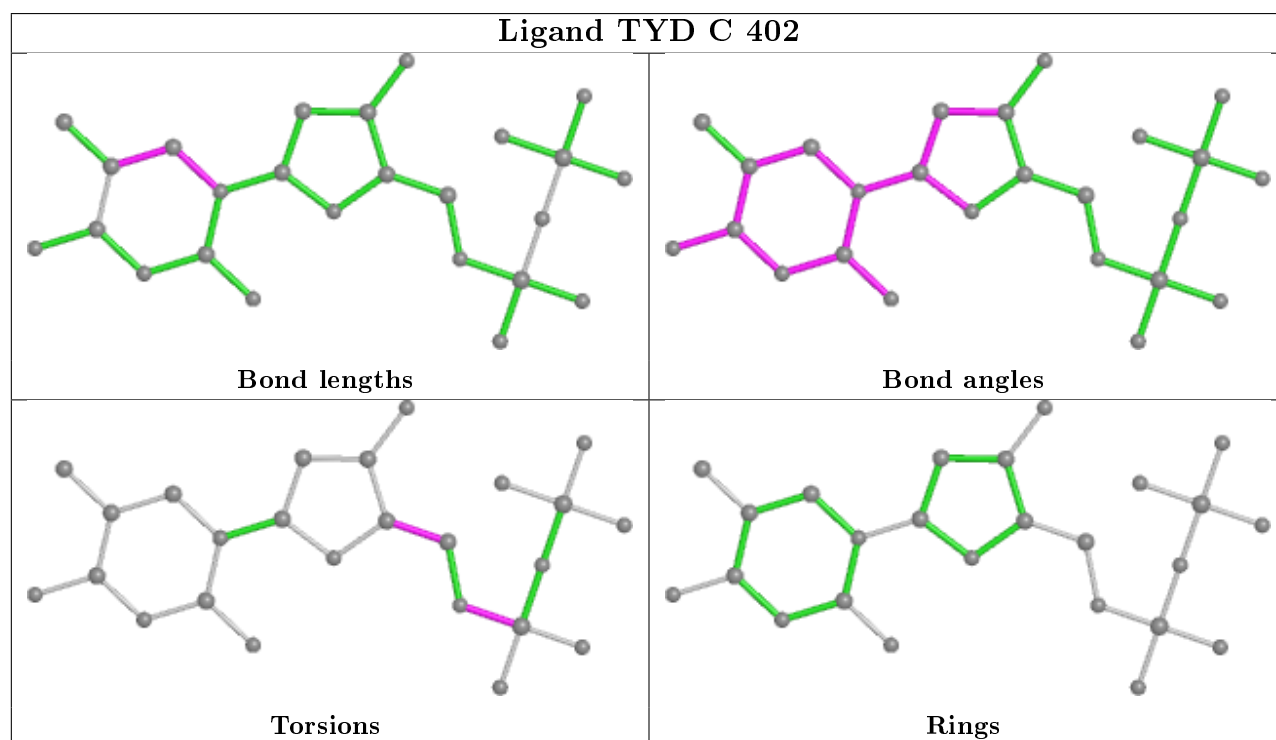
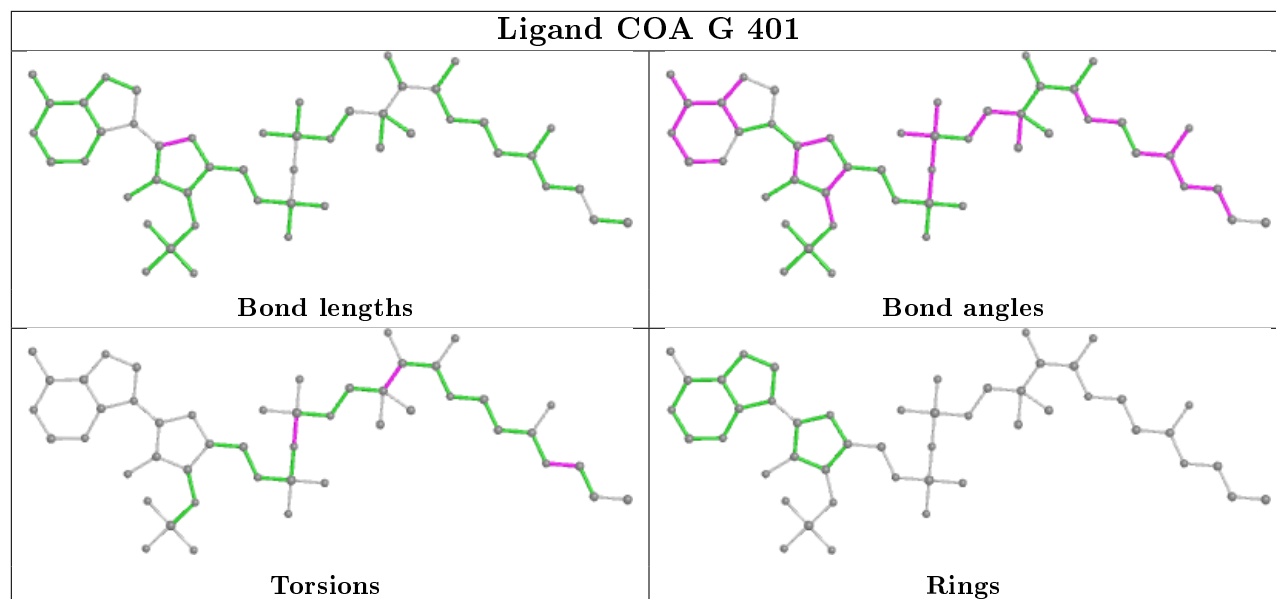


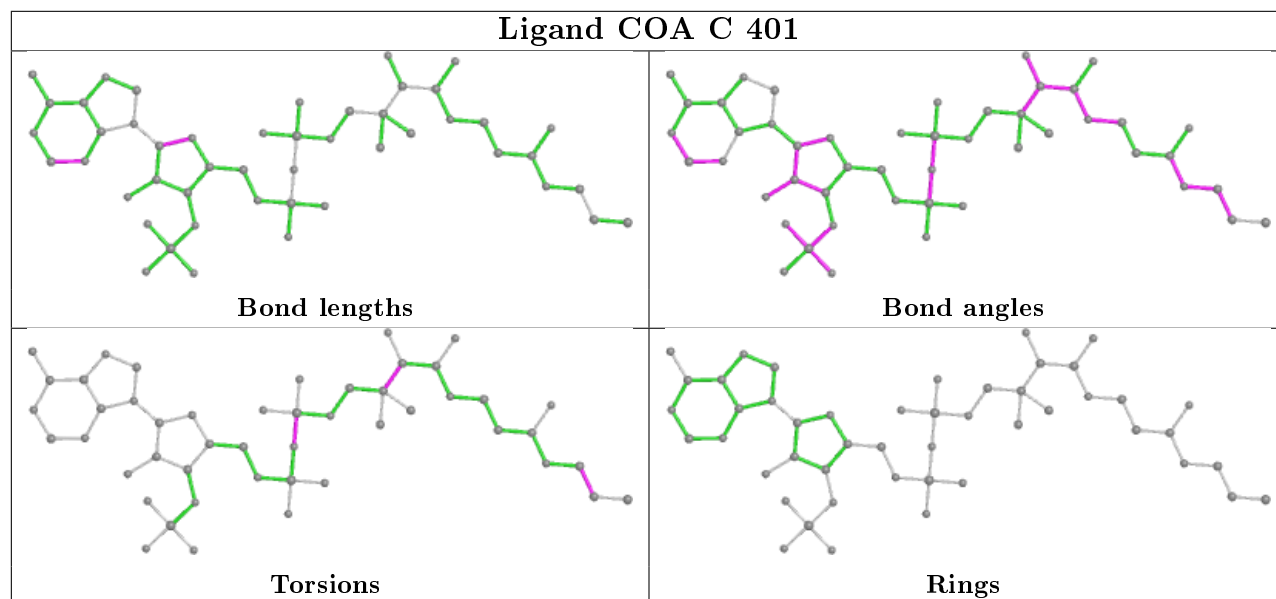
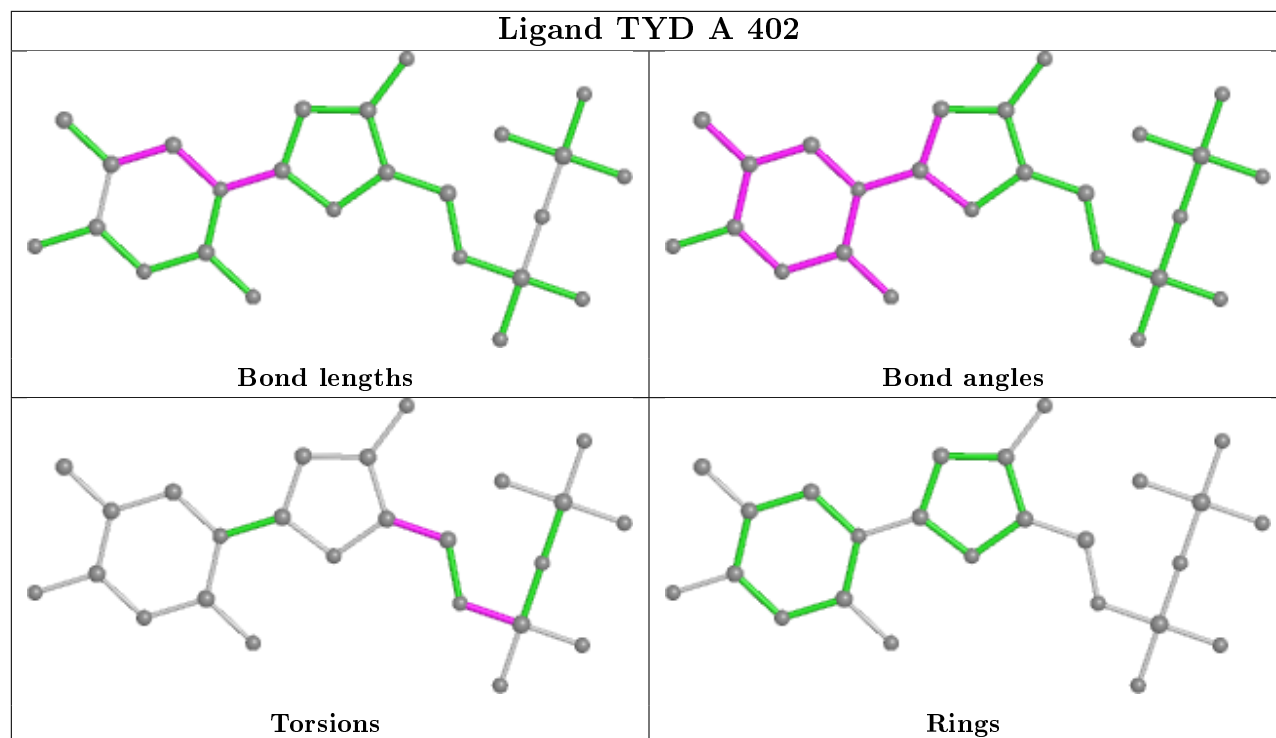
## Ligand COA I 401



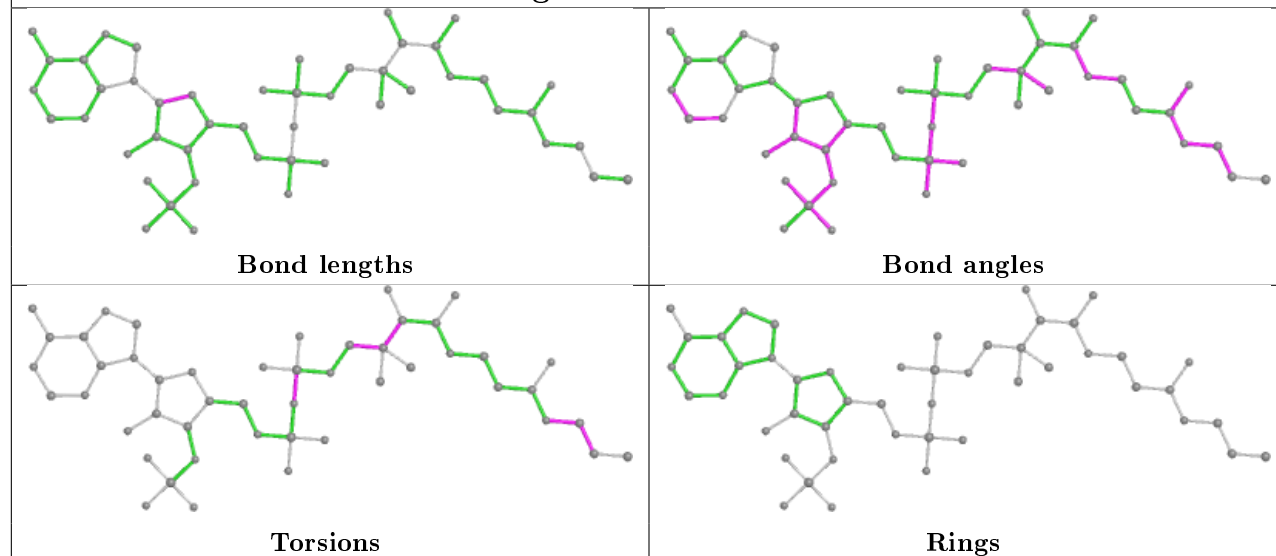
## Ligand TYD G 402



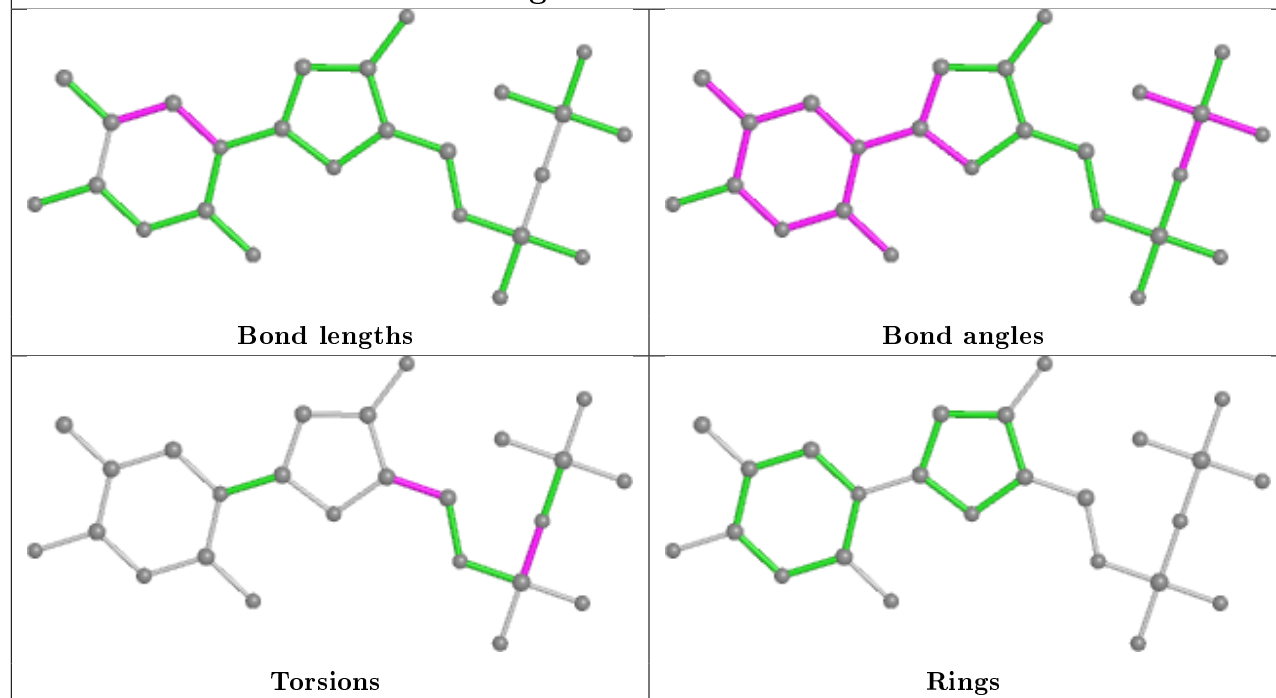


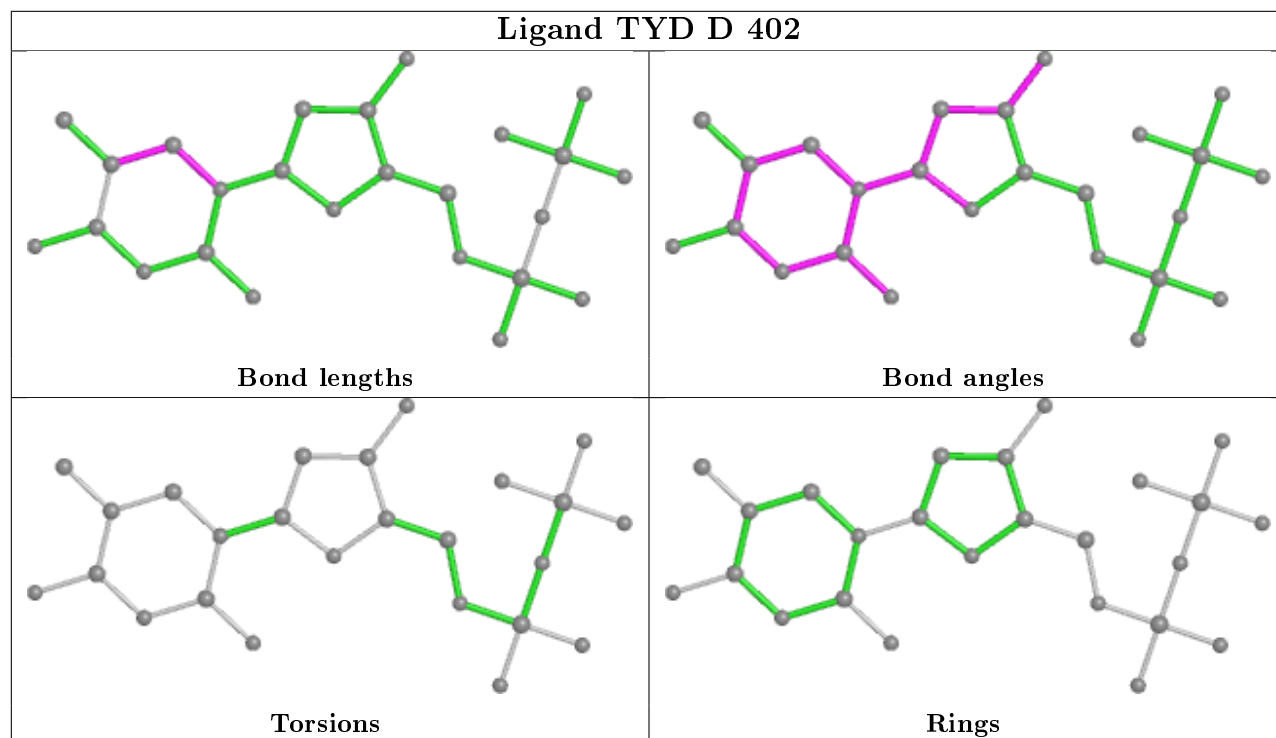
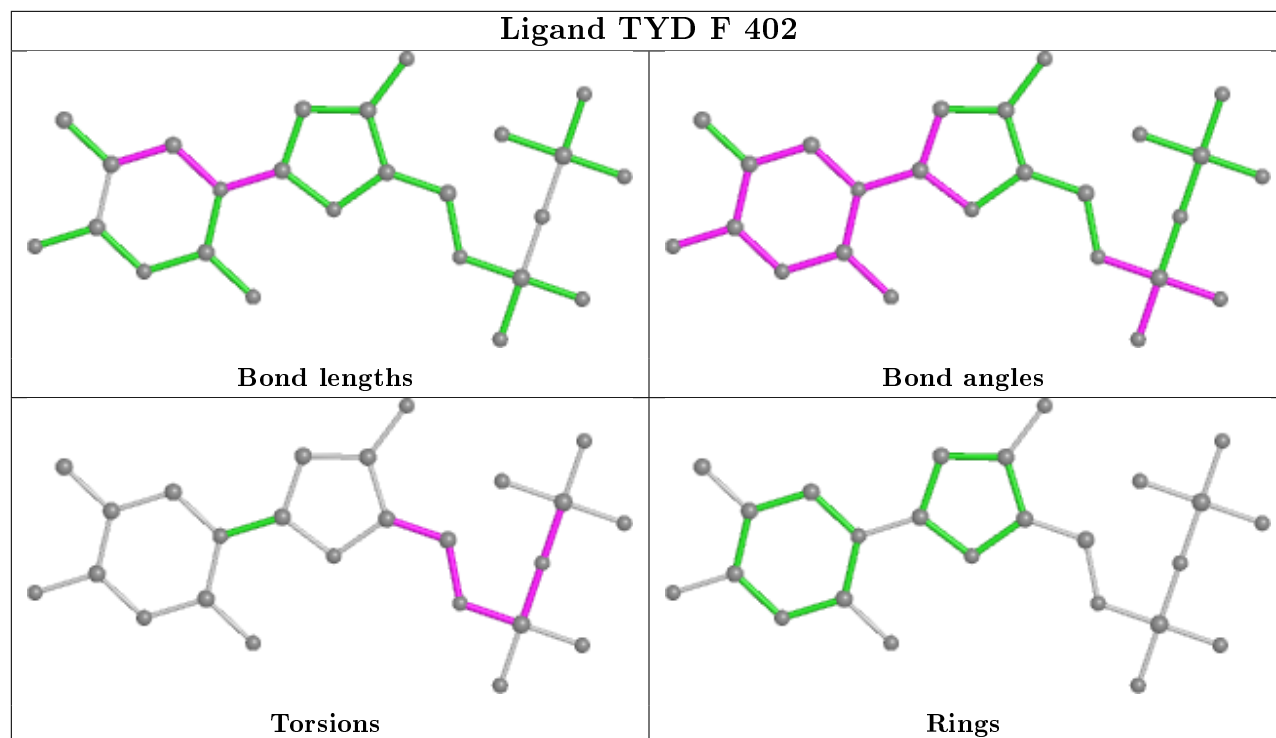


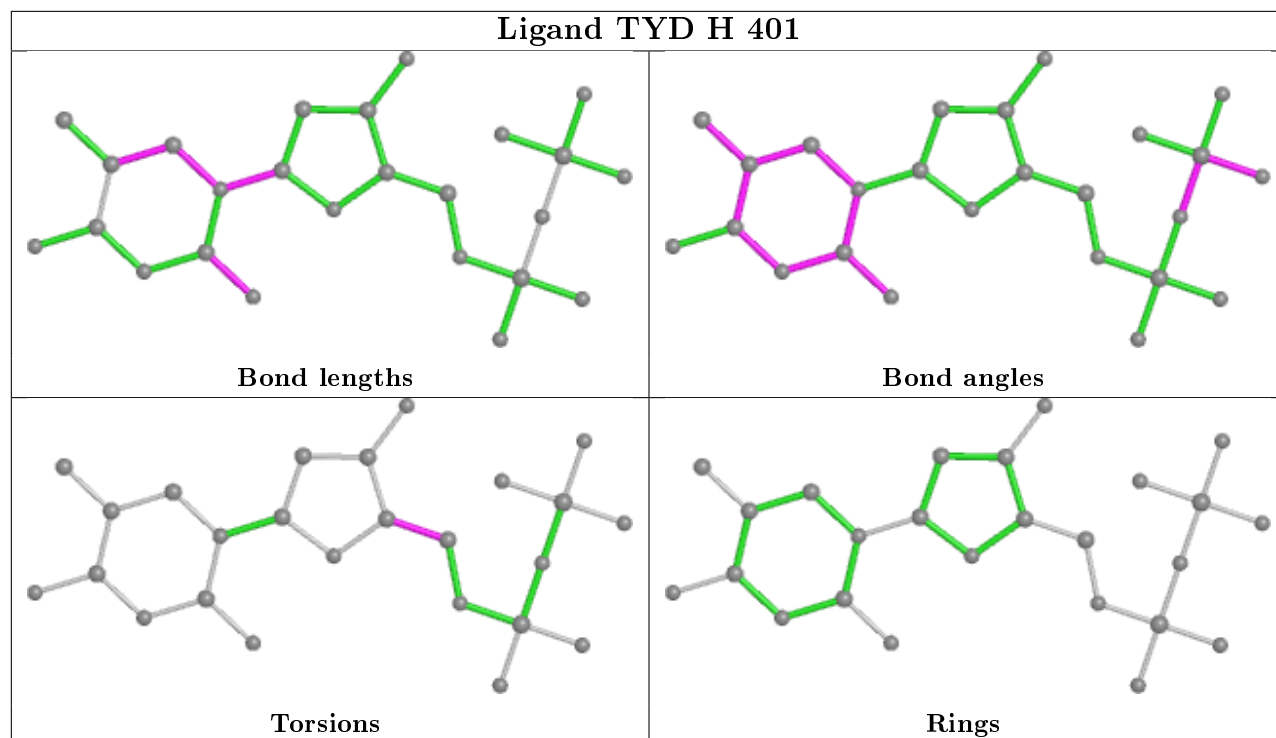
## Ligand COA L 401



## Ligand TYD K 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, 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	285/312 (91%)	-0.03	6 (2%) 63 61	12, 27, 46, 67	0
1	B	290/312 (92%)	0.09	12 (4%) 37 35	12, 28, 51, 65	0
1	C	285/312 (91%)	-0.01	5 (1%) 68 66	14, 28, 47, 66	0
1	D	283/312 (90%)	0.16	14 (4%) 29 28	18, 33, 53, 75	0
1	E	286/312 (91%)	0.12	8 (2%) 53 51	17, 32, 53, 67	0
1	F	294/312 (94%)	0.26	17 (5%) 23 22	20, 33, 54, 67	0
1	G	283/312 (90%)	0.01	7 (2%) 57 55	17, 31, 56, 63	0
1	H	278/312 (89%)	0.53	29 (10%) 6 5	27, 47, 65, 74	0
1	I	285/312 (91%)	0.20	12 (4%) 36 34	18, 34, 58, 65	0
1	J	275/312 (88%)	0.41	23 (8%) 11 9	18, 40, 63, 70	0
1	K	285/312 (91%)	0.16	16 (5%) 24 23	16, 29, 55, 81	0
1	L	286/312 (91%)	0.15	10 (3%) 44 42	20, 32, 58, 65	0
All	All	3415/3744 (91%)	0.17	159 (4%) 31 30	12, 33, 58, 81	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	165	LEU	8.7
1	E	94	TYR	6.6
1	F	165	LEU	6.0
1	K	167	LEU	5.5
1	E	161	ASN	5.2
1	C	95	LEU	5.1
1	I	95	LEU	5.0
1	K	165	LEU	5.0
1	H	186	LEU	4.7
1	H	11	GLN	4.5
1	K	168	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	J	279	LEU	4.4
1	D	305	LEU	4.3
1	H	33	ARG	4.3
1	K	186	LEU	4.2
1	K	169	MET	4.1
1	D	165	LEU	3.9
1	J	164	GLU	3.8
1	J	184	ASN	3.8
1	I	16	ASN	3.8
1	K	166	LYS	3.8
1	L	161	ASN	3.8
1	J	186	LEU	3.7
1	A	161	ASN	3.7
1	K	164	GLU	3.7
1	J	230	LEU	3.7
1	C	186	LEU	3.6
1	B	280	VAL	3.5
1	H	169	MET	3.5
1	G	16	ASN	3.4
1	L	1	MET	3.4
1	B	305	LEU	3.4
1	F	166	LYS	3.4
1	B	186	LEU	3.3
1	H	95	LEU	3.3
1	B	164	GLU	3.3
1	J	280	VAL	3.2
1	F	89	ILE	3.2
1	B	289	ASP	3.2
1	B	279	LEU	3.2
1	F	33	ARG	3.2
1	H	15	ASP	3.2
1	K	95	LEU	3.0
1	J	287	ASP	3.0
1	L	307	HIS	3.0
1	D	306	GLU	3.0
1	H	164	GLU	3.0
1	H	300	GLN	3.0
1	J	286	TYR	3.0
1	E	280	VAL	3.0
1	E	279	LEU	3.0
1	H	165	LEU	3.0
1	J	165	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	225	GLU	2.9
1	H	280	VAL	2.9
1	E	300	GLN	2.9
1	B	184	ASN	2.9
1	D	279	LEU	2.9
1	I	186	LEU	2.9
1	F	307	HIS	2.9
1	K	280	VAL	2.9
1	I	303	GLN	2.8
1	L	280	VAL	2.8
1	K	59	VAL	2.8
1	A	279	LEU	2.8
1	D	230	LEU	2.8
1	C	171	LYS	2.8
1	H	230	LEU	2.7
1	H	279	LEU	2.7
1	F	88	LYS	2.7
1	H	173	LYS	2.7
1	F	186	LEU	2.7
1	H	16	ASN	2.7
1	F	164	GLU	2.7
1	D	280	VAL	2.7
1	J	167	LEU	2.7
1	J	264	MET	2.7
1	D	164	GLU	2.6
1	G	279	LEU	2.6
1	K	57	SER	2.6
1	C	307	HIS	2.6
1	G	231	ILE	2.6
1	G	230	LEU	2.6
1	J	285	TYR	2.6
1	F	167	LEU	2.6
1	A	303	GLN	2.6
1	G	36	ASN	2.6
1	F	59	VAL	2.6
1	J	281	PHE	2.6
1	D	197	LYS	2.6
1	H	184	ASN	2.6
1	A	95	LEU	2.5
1	H	1	MET	2.5
1	D	300	GLN	2.5
1	J	185	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	184	ASN	2.5
1	I	15	ASP	2.5
1	H	58	GLY	2.5
1	K	279	LEU	2.5
1	L	11	GLN	2.5
1	J	289	ASP	2.5
1	L	59	VAL	2.5
1	F	309	HIS	2.5
1	J	231	ILE	2.5
1	F	12	ASN	2.4
1	B	281	PHE	2.4
1	K	77	VAL	2.4
1	B	230	LEU	2.4
1	L	165	LEU	2.4
1	E	59	VAL	2.3
1	H	18	LYS	2.3
1	J	173	LYS	2.3
1	D	281	PHE	2.3
1	E	58	GLY	2.3
1	D	259	ILE	2.3
1	H	278	LEU	2.3
1	E	95	LEU	2.3
1	I	184	ASN	2.3
1	A	82	ASP	2.3
1	F	15	ASP	2.3
1	D	303	GLN	2.3
1	I	164	GLU	2.3
1	I	274	LYS	2.3
1	C	184	ASN	2.2
1	H	59	VAL	2.2
1	K	33	ARG	2.2
1	H	28	GLY	2.2
1	K	11	GLN	2.2
1	J	166	LYS	2.2
1	F	305	LEU	2.2
1	L	96	LYS	2.2
1	J	34	ASN	2.2
1	K	40	ASN	2.2
1	F	300	GLN	2.2
1	B	185	ASP	2.2
1	A	184	ASN	2.2
1	B	207	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	274	LYS	2.2
1	L	164	GLU	2.2
1	H	77	VAL	2.1
1	B	245	GLU	2.1
1	J	288	SER	2.1
1	D	304	ASN	2.1
1	H	281	PHE	2.1
1	I	6	ALA	2.1
1	H	231	ILE	2.1
1	J	259	ILE	2.1
1	J	294	ASP	2.1
1	H	42	LEU	2.1
1	D	184	ASN	2.1
1	I	78	THR	2.1
1	L	41	SER	2.1
1	H	171	LYS	2.0
1	G	280	VAL	2.0
1	H	168	GLN	2.0
1	H	229	PHE	2.0
1	F	41	SER	2.0
1	H	185	ASP	2.0
1	I	187	ARG	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
4	TDR	L	403	9/9	0.71	0.20	71,72,73,74	0

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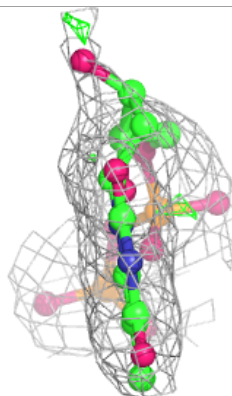
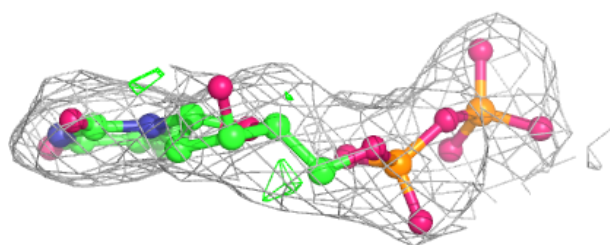
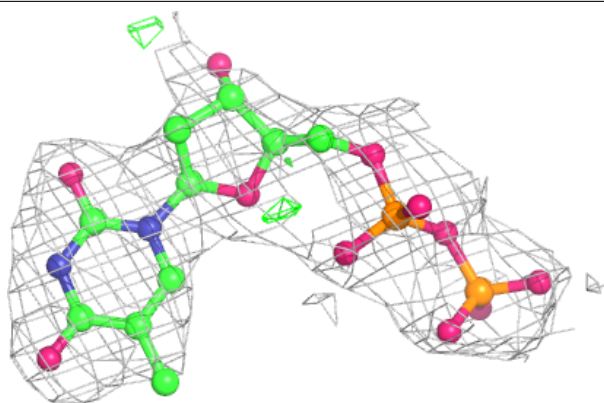
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TDR	D	403	9/9	0.74	0.20	43,47,49,50	0
4	TDR	C	403	9/9	0.75	0.18	51,55,57,59	0
4	TDR	K	403	9/9	0.76	0.20	69,72,74,74	0
4	TDR	J	403	9/9	0.77	0.25	58,62,64,65	0
3	TYD	J	402	25/25	0.82	0.19	69,81,92,93	0
4	TDR	A	403	9/9	0.83	0.17	31,41,43,44	0
4	TDR	B	403	9/9	0.84	0.17	41,43,47,47	0
4	TDR	F	403	9/9	0.85	0.14	52,54,56,56	0
4	TDR	E	403	9/9	0.85	0.13	41,46,48,49	0
3	TYD	G	402	25/25	0.86	0.17	40,58,72,72	0
3	TYD	F	402	25/25	0.88	0.13	35,56,79,79	0
3	TYD	D	402	25/25	0.88	0.17	47,71,75,77	0
3	TYD	H	401	25/25	0.88	0.14	44,61,73,74	0
3	TYD	A	402	25/25	0.88	0.16	39,63,74,75	0
3	TYD	C	402	25/25	0.90	0.14	31,56,66,68	0
3	TYD	L	402	25/25	0.90	0.14	46,63,71,72	0
3	TYD	B	402	25/25	0.91	0.12	34,57,71,73	0
3	TYD	E	402	25/25	0.92	0.13	31,49,61,63	0
3	TYD	K	402	25/25	0.92	0.12	22,39,55,57	0
3	TYD	I	402	25/25	0.92	0.11	22,40,66,68	0
2	COA	I	401	48/48	0.94	0.14	27,43,62,71	0
2	COA	D	401	48/48	0.95	0.13	20,41,56,64	0
2	COA	G	403	48/48	0.95	0.12	35,42,57,70	0
2	COA	G	401	48/48	0.95	0.11	26,36,41,53	0
2	COA	E	401	48/48	0.95	0.12	20,37,49,59	0
2	COA	J	401	48/48	0.95	0.12	21,36,48,60	0
2	COA	F	401	48/48	0.96	0.10	21,35,43,49	0
2	COA	C	401	48/48	0.96	0.10	14,32,42,45	0
2	COA	L	401	48/48	0.96	0.11	15,33,45,53	0
2	COA	A	401	48/48	0.96	0.12	17,29,42,55	0
2	COA	K	401	48/48	0.97	0.12	21,37,64,70	0
5	MG	C	404	1/1	0.97	0.19	20,20,20,20	0
5	MG	J	404	1/1	0.98	0.19	26,26,26,26	0
2	COA	B	401	48/48	0.98	0.09	9,24,33,42	0
5	MG	G	404	1/1	0.98	0.14	27,27,27,27	0
5	MG	D	404	1/1	0.99	0.20	21,21,21,21	0
5	MG	B	404	1/1	0.99	0.20	26,26,26,26	0

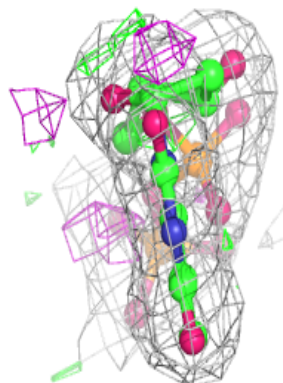
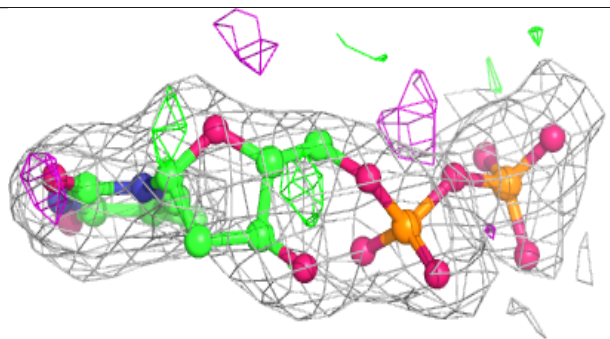
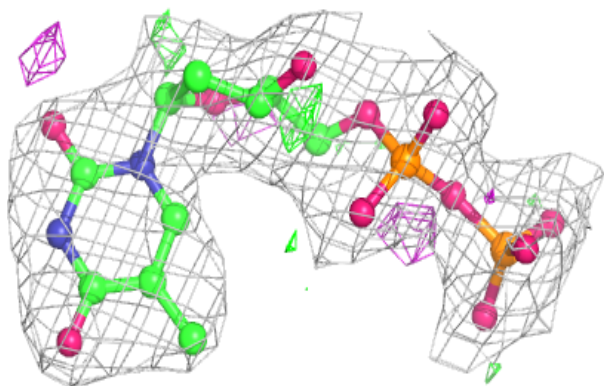
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TYD J 402:**

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

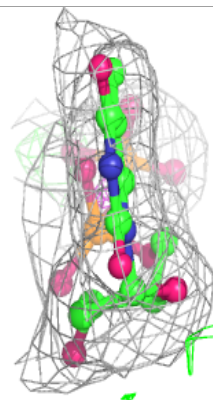
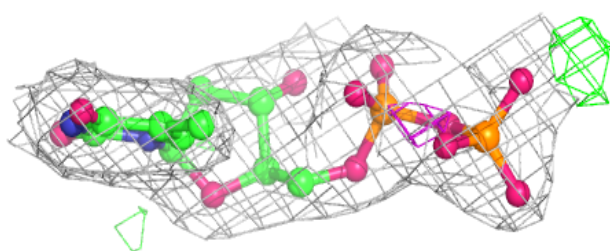
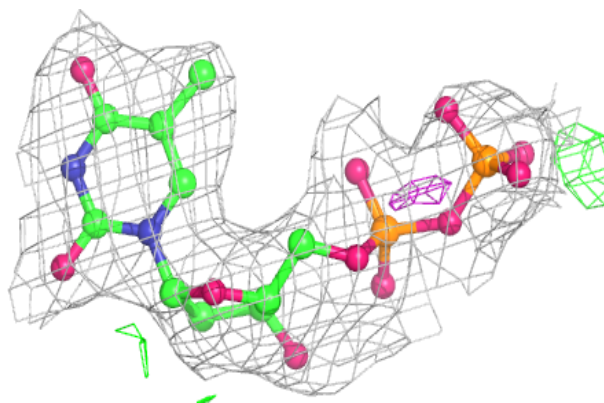
**Electron density around TYD G 402:**

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

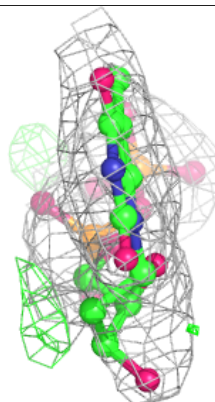
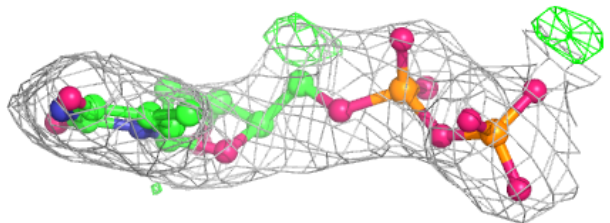
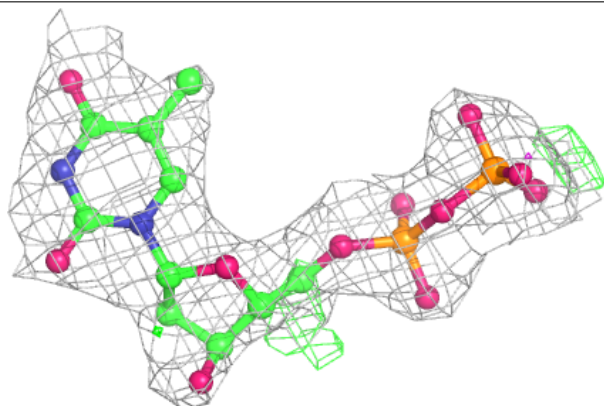


**Electron density around TYD F 402:**

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

**Electron density around TYD D 402:**

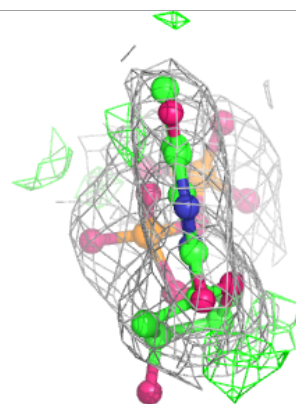
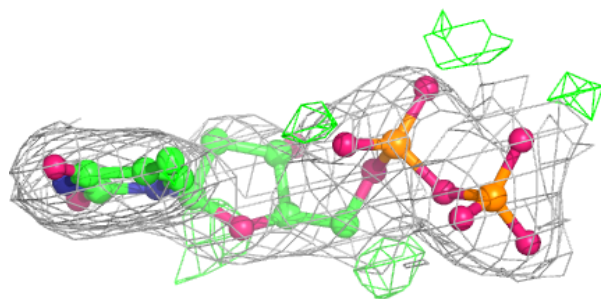
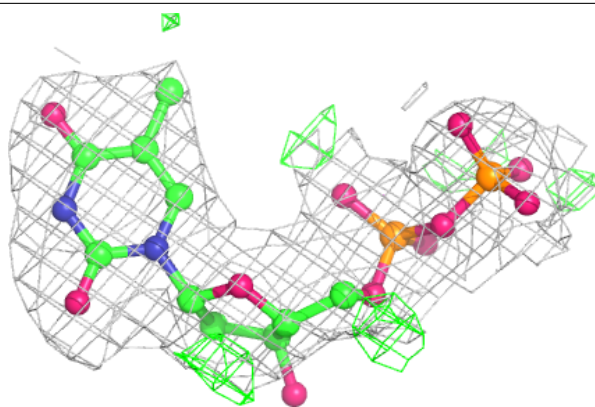
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



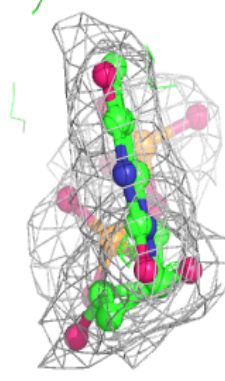
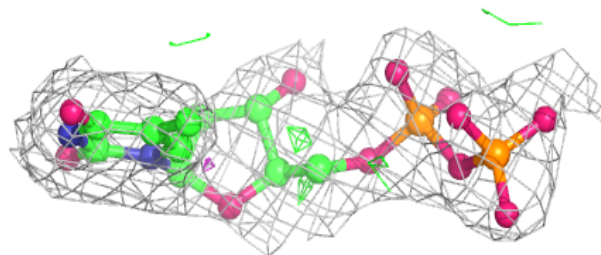
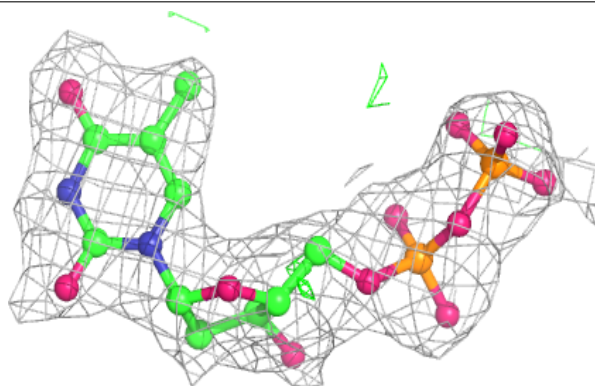


**Electron density around TYD H 401:**

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

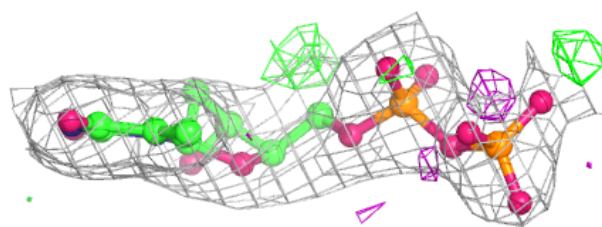
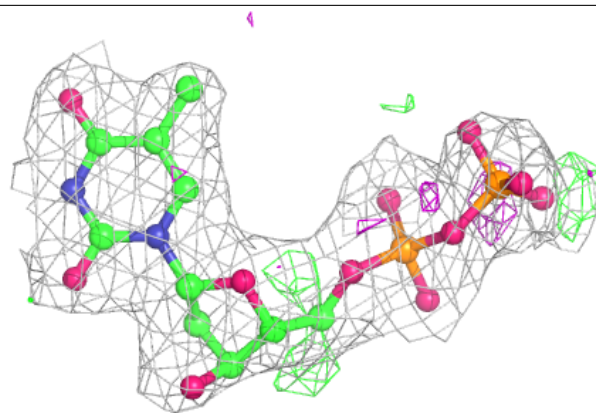
**Electron density around TYD A 402:**

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

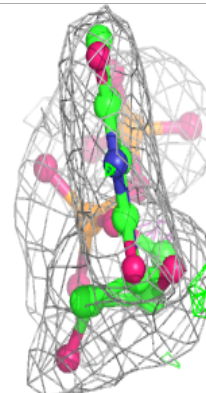
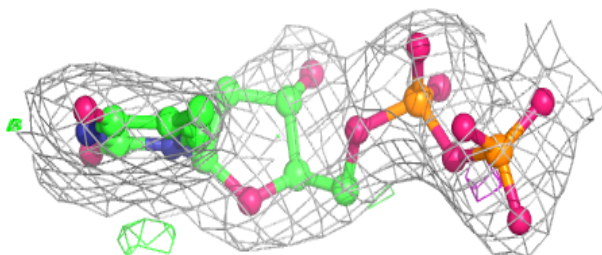
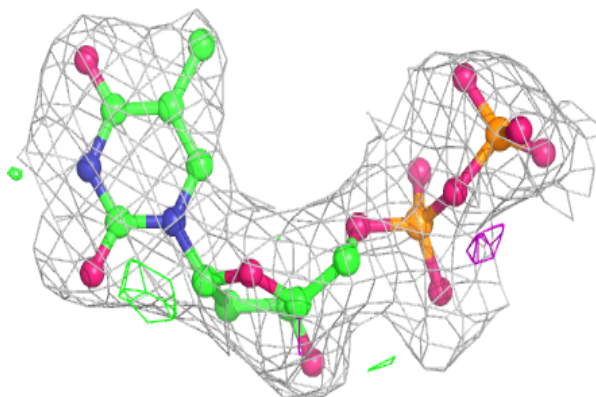


**Electron density around TYD C 402:**

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

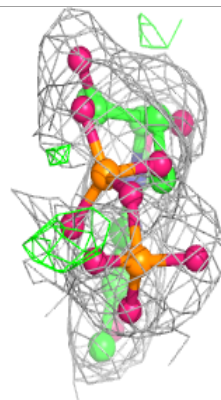
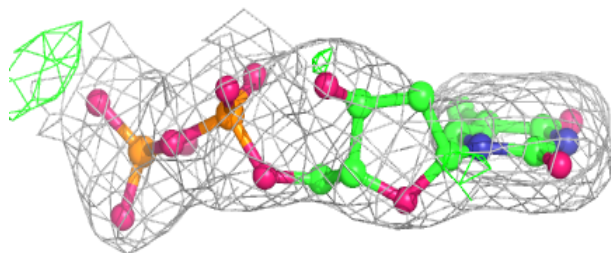
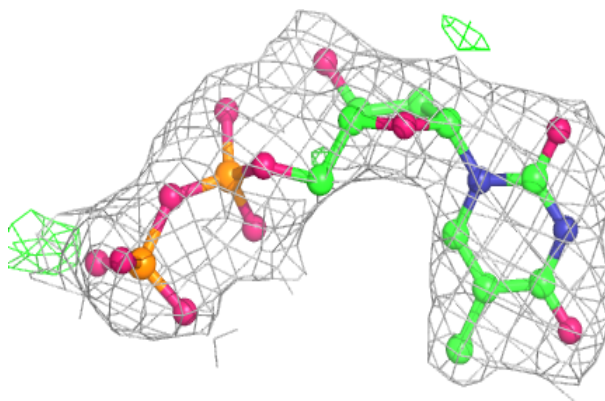
**Electron density around TYD L 402:**

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

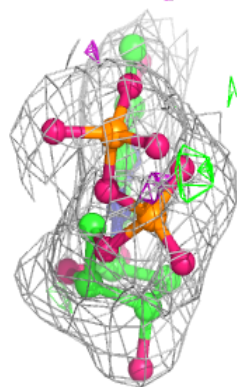
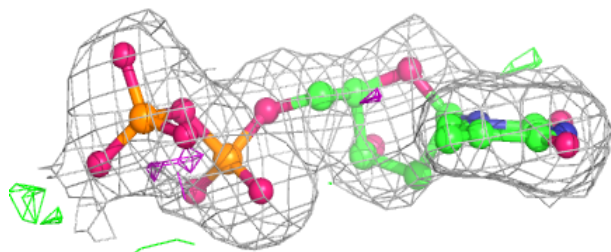
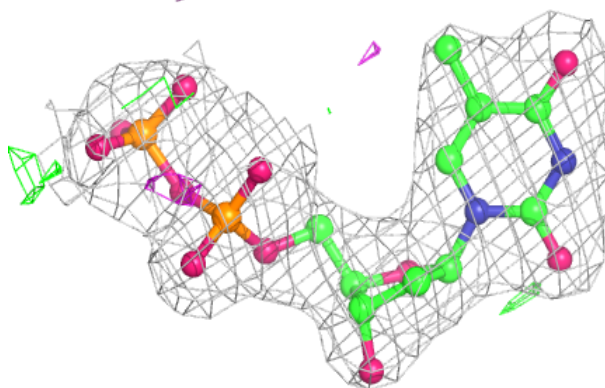


**Electron density around TYD B 402:**

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

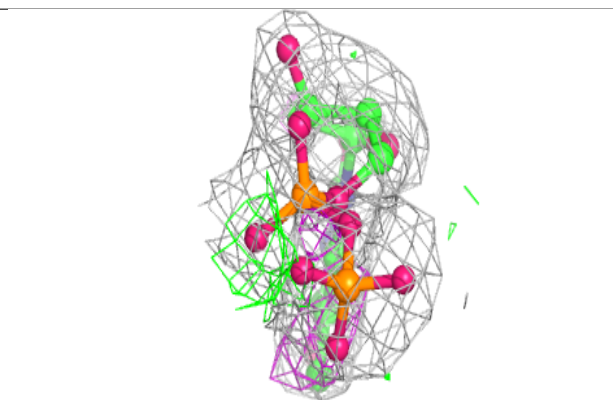
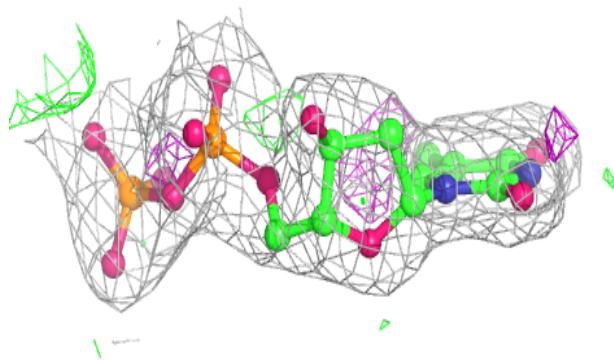
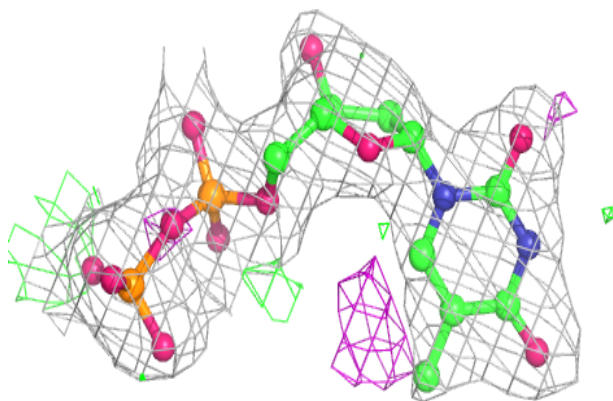
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and green (positive)

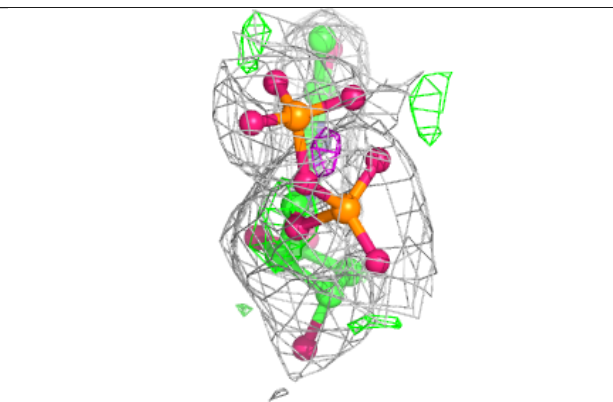
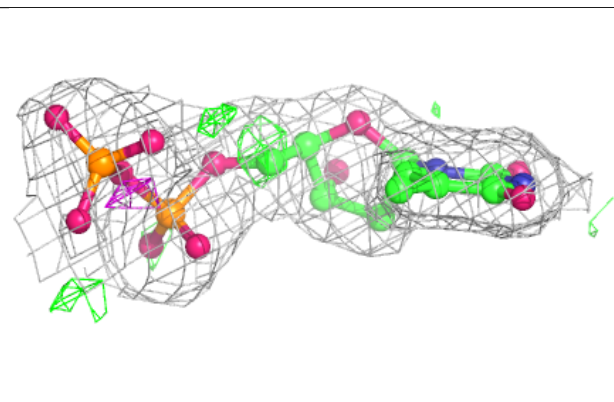
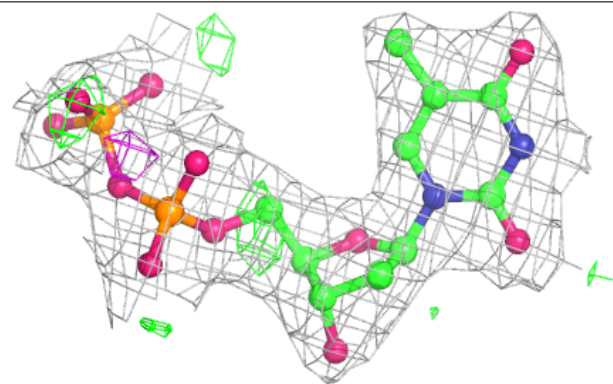


**Electron density around TYD K 402:**

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

**Electron density around TYD I 402:**

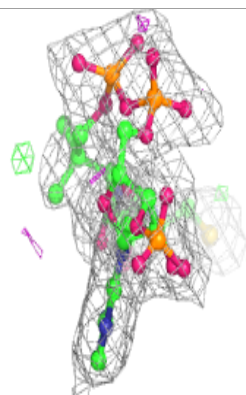
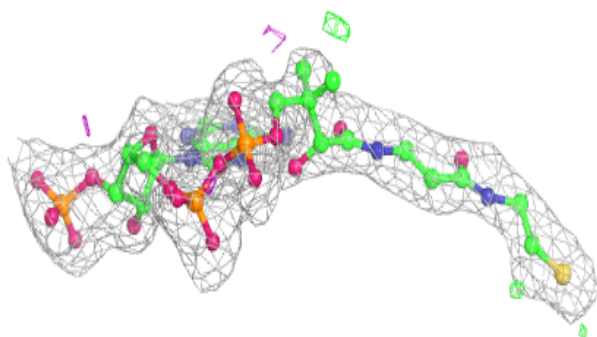
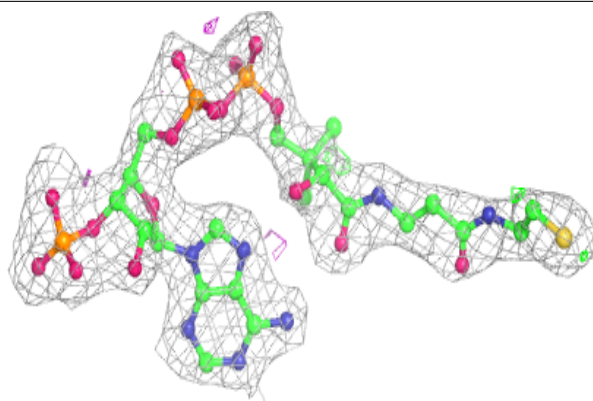
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



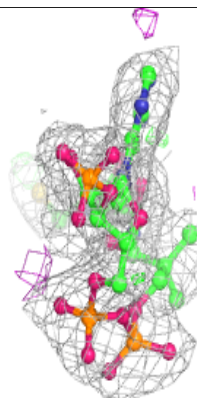
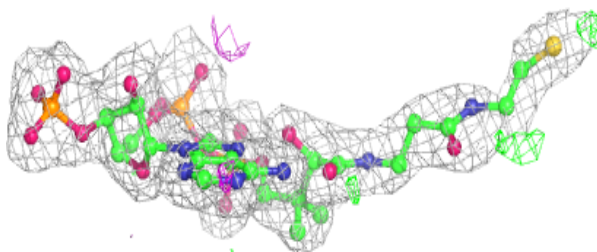
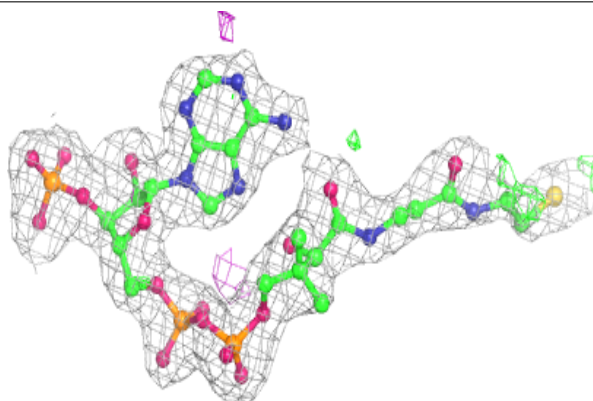


**Electron density around COA I 401:**

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

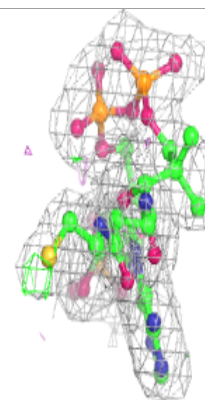
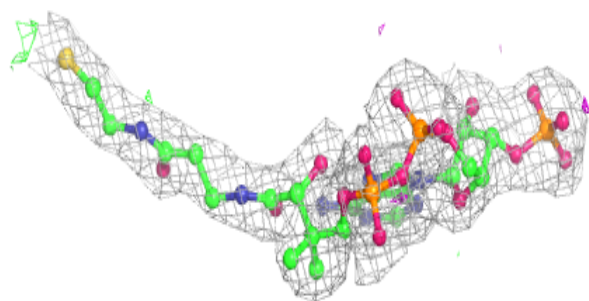
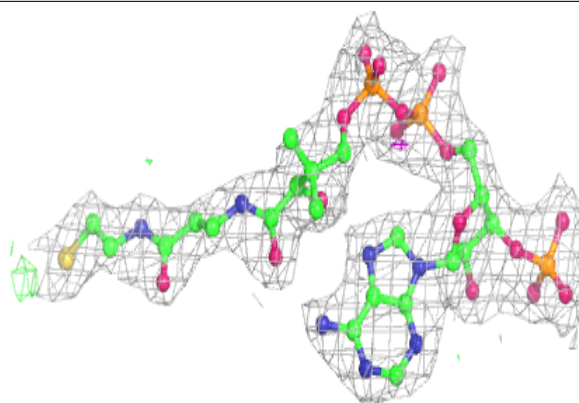
**Electron density around COA D 401:**

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and green (positive)

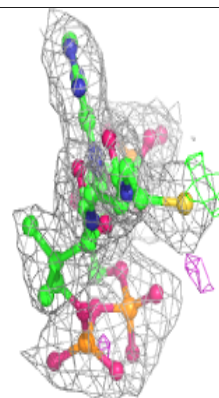
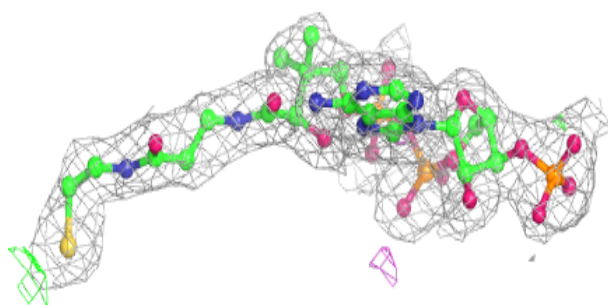
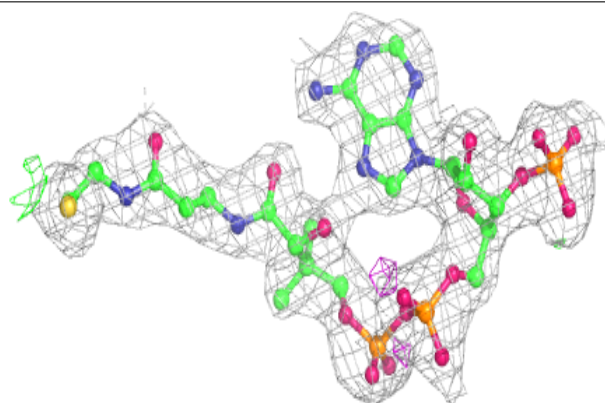


**Electron density around COA G 403:**

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

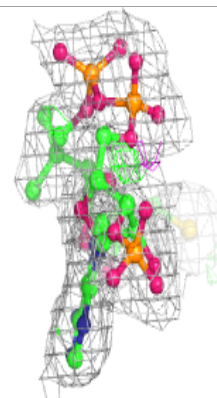
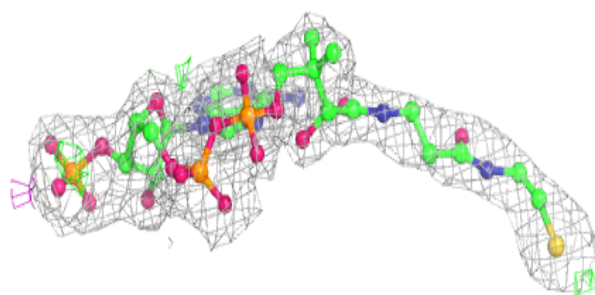
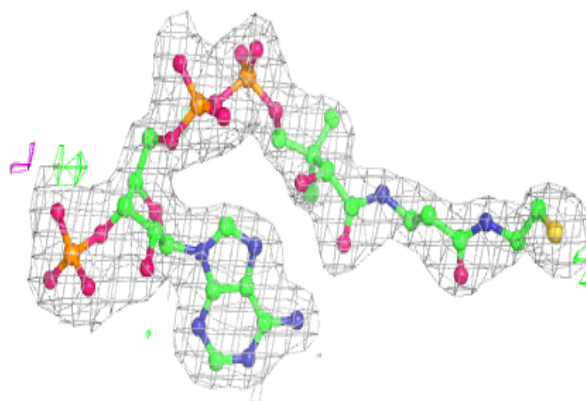
**Electron density around COA G 401:**

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

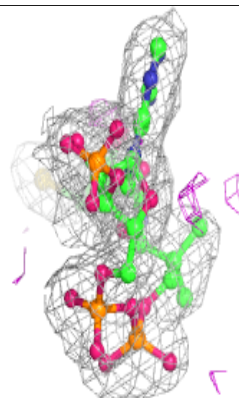
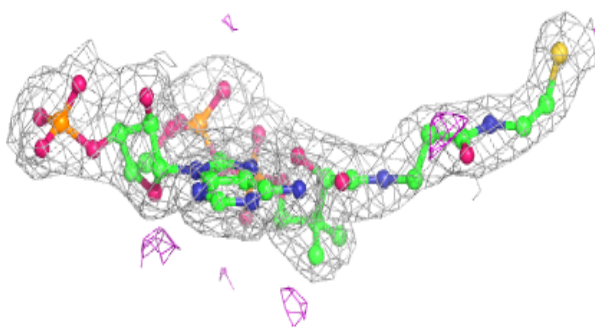
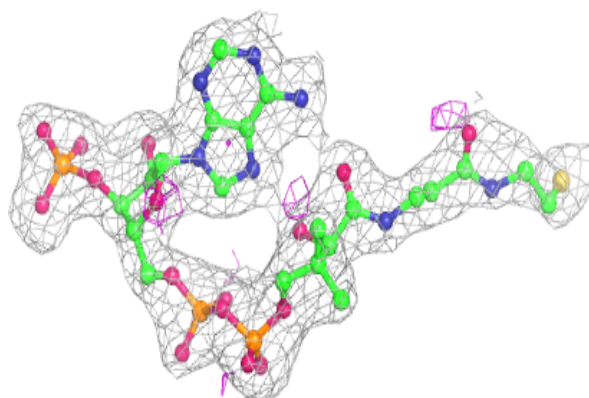


**Electron density around COA E 401:**

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

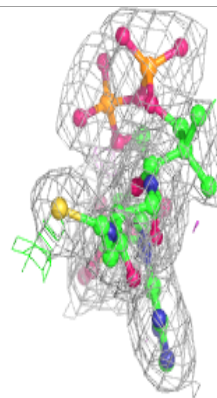
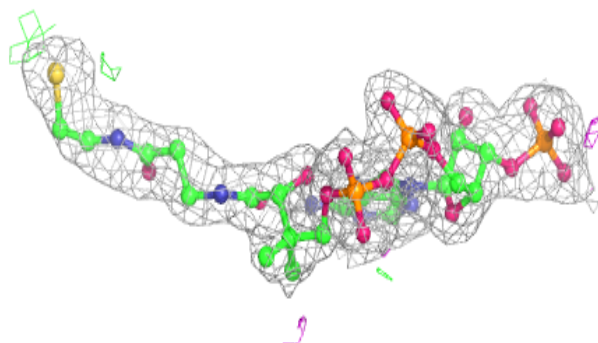
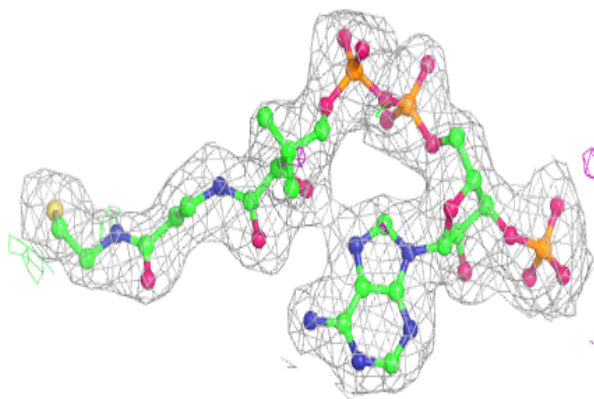
**Electron density around COA J 401:**

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

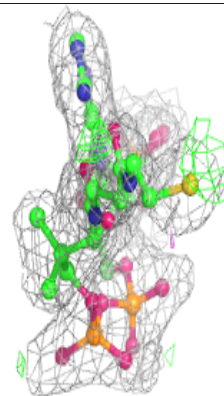
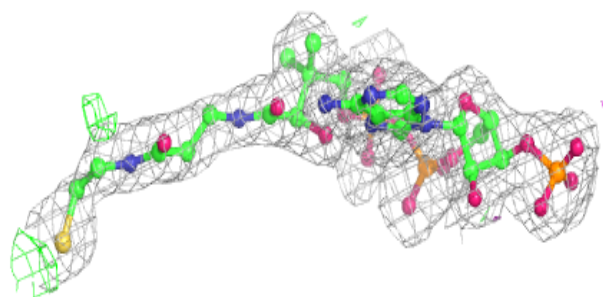
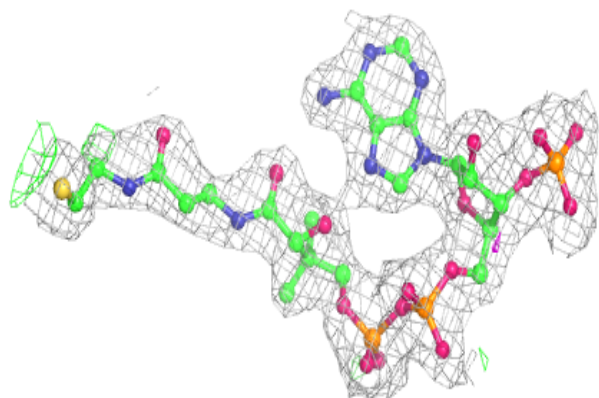


**Electron density around COA F 401:**

$2mF_o-DF_c$  (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:**

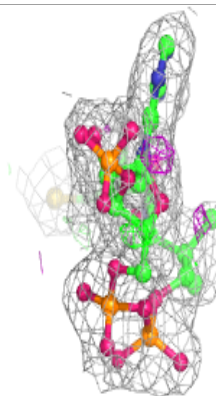
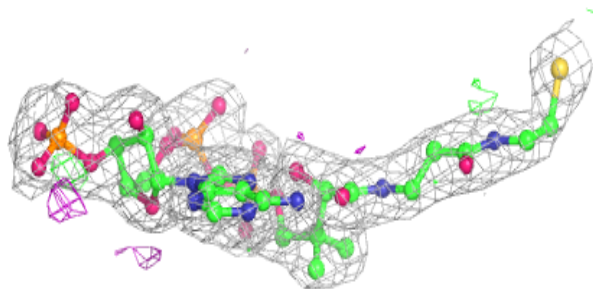
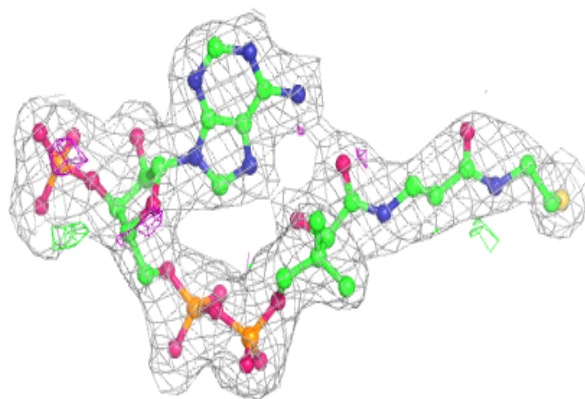
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



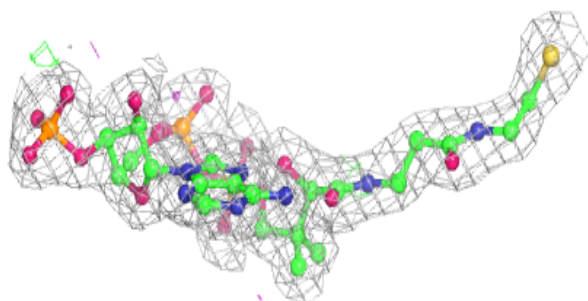
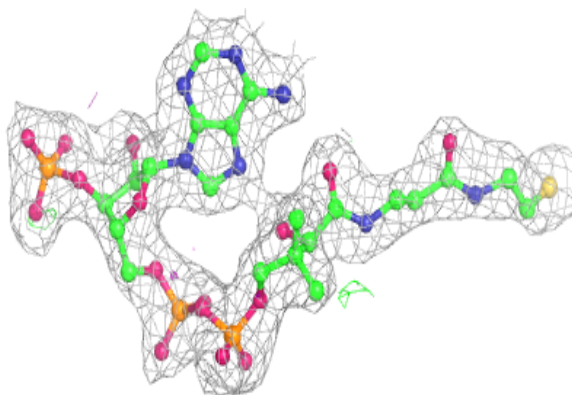


**Electron density around COA L 401:**

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

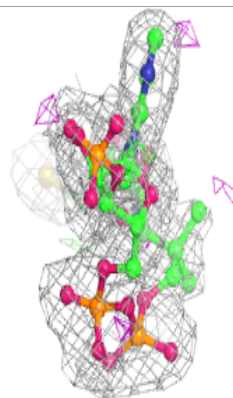
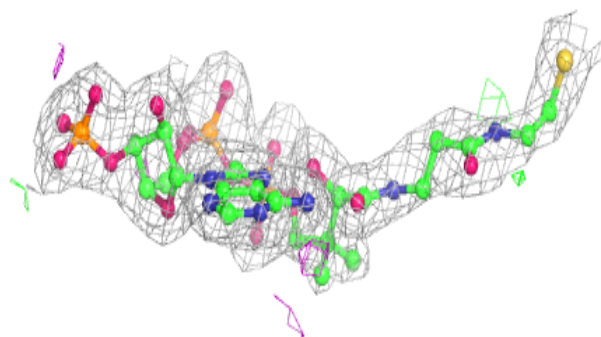
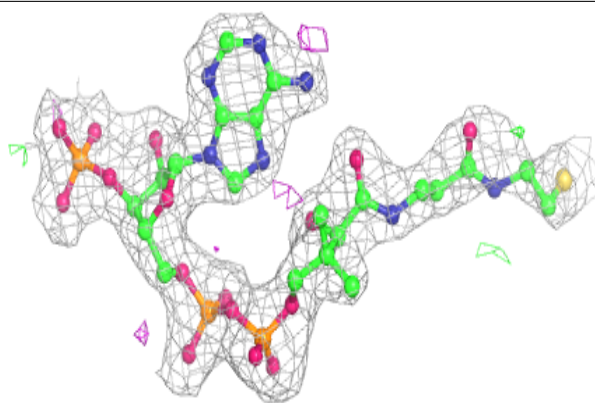
**Electron density around COA A 401:**

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

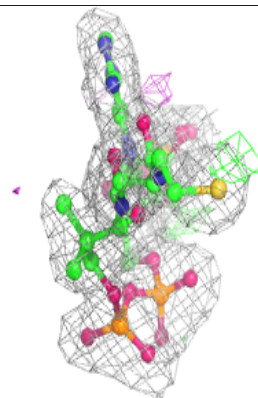
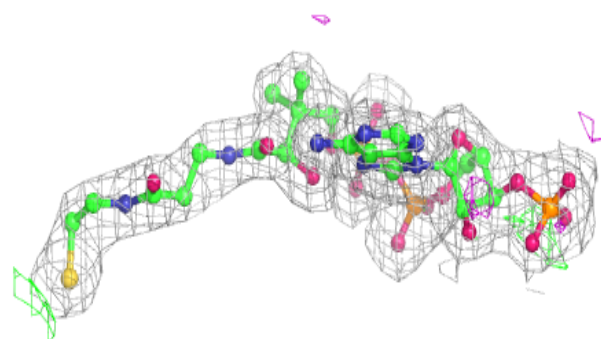
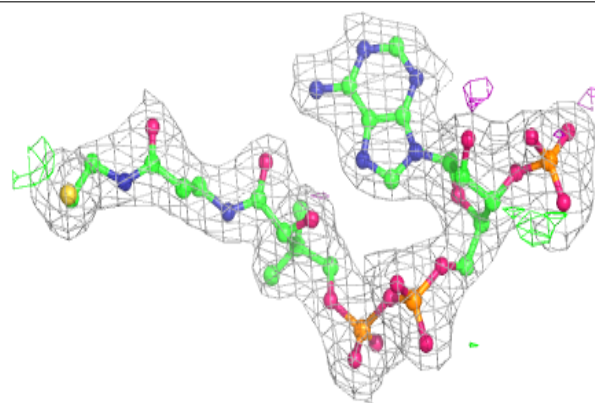


**Electron density around COA K 401:**

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

**Electron density around COA 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

There are no such residues in this entry.