



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:17 PM UTC

PDB ID : 8PI1 / pdb_00008pi1
Title : Bicyclic INCYPRO Pseudomonas fluorescens esterase
Authors : Kiehstaller, S.; Pearce, N.M.; Grossmann, T.N.; Hennig, S.
Deposited on : 2023-06-20
Resolution : 2.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

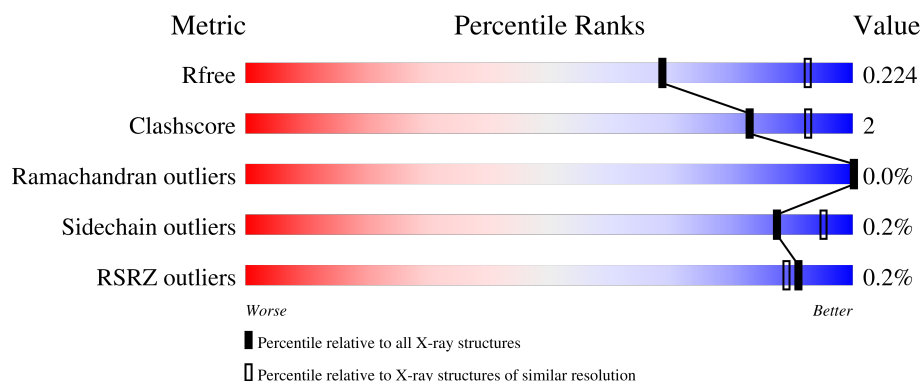
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

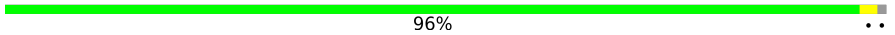
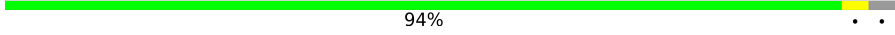
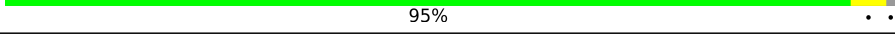
The reported resolution of this entry is 2.50 Å.

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



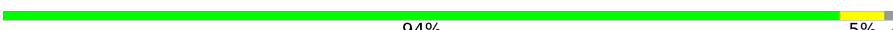
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	280	 91% 6% .
1	B	280	 96% ..
1	C	280	 94% . .
1	D	280	 95% . .
1	E	280	 90% 8% .

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Mol	Chain	Length	Quality of chain
1	F	280	 91% 6% .
1	G	280	 90% 6% .
1	H	280	 94% 5% .
1	I	280	 86% 11% .
1	J	280	 92% . .
1	K	280	 91% 5% .
1	L	280	 92% . .
1	M	280	 91% 5% .
1	N	280	 88% 9% .
1	O	280	 88% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	H	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32857 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 Arylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2119	1361	357	394	7			
1	B	276	Total	C	N	O	S	0	1	0
			2161	1385	368	401	7			
1	C	271	Total	C	N	O	S	0	0	0
			2115	1359	356	393	7			
1	D	276	Total	C	N	O	S	0	1	0
			2161	1385	368	401	7			
1	E	273	Total	C	N	O	S	0	0	0
			2125	1364	358	396	7			
1	F	272	Total	C	N	O	S	0	0	0
			2119	1361	357	394	7			
1	G	271	Total	C	N	O	S	0	0	0
			2115	1359	356	393	7			
1	H	275	Total	C	N	O	S	0	0	0
			2145	1376	364	398	7			
1	I	272	Total	C	N	O	S	0	0	0
			2119	1361	357	394	7			
1	J	271	Total	C	N	O	S	0	2	0
			2129	1366	358	398	7			
1	K	272	Total	C	N	O	S	0	1	0
			2128	1366	358	397	7			
1	L	271	Total	C	N	O	S	0	1	0
			2123	1365	357	394	7			
1	M	271	Total	C	N	O	S	0	0	0
			2115	1359	356	393	7			
1	N	271	Total	C	N	O	S	0	0	0
			2115	1359	356	393	7			
1	O	271	Total	C	N	O	S	0	0	0
			2115	1359	356	393	7			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	CYS	THR	engineered mutation	UNP P22862
A	174	CYS	GLN	engineered mutation	UNP P22862
A	273	GLY	-	expression tag	UNP P22862
A	274	SER	-	expression tag	UNP P22862
A	275	HIS	-	expression tag	UNP P22862
A	276	HIS	-	expression tag	UNP P22862
A	277	HIS	-	expression tag	UNP P22862
A	278	HIS	-	expression tag	UNP P22862
A	279	HIS	-	expression tag	UNP P22862
A	280	HIS	-	expression tag	UNP P22862
B	3	CYS	THR	engineered mutation	UNP P22862
B	174	CYS	GLN	engineered mutation	UNP P22862
B	273	GLY	-	expression tag	UNP P22862
B	274	SER	-	expression tag	UNP P22862
B	275	HIS	-	expression tag	UNP P22862
B	276	HIS	-	expression tag	UNP P22862
B	277	HIS	-	expression tag	UNP P22862
B	278	HIS	-	expression tag	UNP P22862
B	279	HIS	-	expression tag	UNP P22862
B	280	HIS	-	expression tag	UNP P22862
C	3	CYS	THR	engineered mutation	UNP P22862
C	174	CYS	GLN	engineered mutation	UNP P22862
C	273	GLY	-	expression tag	UNP P22862
C	274	SER	-	expression tag	UNP P22862
C	275	HIS	-	expression tag	UNP P22862
C	276	HIS	-	expression tag	UNP P22862
C	277	HIS	-	expression tag	UNP P22862
C	278	HIS	-	expression tag	UNP P22862
C	279	HIS	-	expression tag	UNP P22862
C	280	HIS	-	expression tag	UNP P22862
D	3	CYS	THR	engineered mutation	UNP P22862
D	174	CYS	GLN	engineered mutation	UNP P22862
D	273	GLY	-	expression tag	UNP P22862
D	274	SER	-	expression tag	UNP P22862
D	275	HIS	-	expression tag	UNP P22862
D	276	HIS	-	expression tag	UNP P22862
D	277	HIS	-	expression tag	UNP P22862
D	278	HIS	-	expression tag	UNP P22862
D	279	HIS	-	expression tag	UNP P22862
D	280	HIS	-	expression tag	UNP P22862
E	3	CYS	THR	engineered mutation	UNP P22862
E	174	CYS	GLN	engineered mutation	UNP P22862
E	273	GLY	-	expression tag	UNP P22862

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Chain	Residue	Modelled	Actual	Comment	Reference
E	274	SER	-	expression tag	UNP P22862
E	275	HIS	-	expression tag	UNP P22862
E	276	HIS	-	expression tag	UNP P22862
E	277	HIS	-	expression tag	UNP P22862
E	278	HIS	-	expression tag	UNP P22862
E	279	HIS	-	expression tag	UNP P22862
E	280	HIS	-	expression tag	UNP P22862
F	3	CYS	THR	engineered mutation	UNP P22862
F	174	CYS	GLN	engineered mutation	UNP P22862
F	273	GLY	-	expression tag	UNP P22862
F	274	SER	-	expression tag	UNP P22862
F	275	HIS	-	expression tag	UNP P22862
F	276	HIS	-	expression tag	UNP P22862
F	277	HIS	-	expression tag	UNP P22862
F	278	HIS	-	expression tag	UNP P22862
F	279	HIS	-	expression tag	UNP P22862
F	280	HIS	-	expression tag	UNP P22862
G	3	CYS	THR	engineered mutation	UNP P22862
G	174	CYS	GLN	engineered mutation	UNP P22862
G	273	GLY	-	expression tag	UNP P22862
G	274	SER	-	expression tag	UNP P22862
G	275	HIS	-	expression tag	UNP P22862
G	276	HIS	-	expression tag	UNP P22862
G	277	HIS	-	expression tag	UNP P22862
G	278	HIS	-	expression tag	UNP P22862
G	279	HIS	-	expression tag	UNP P22862
G	280	HIS	-	expression tag	UNP P22862
H	3	CYS	THR	engineered mutation	UNP P22862
H	174	CYS	GLN	engineered mutation	UNP P22862
H	273	GLY	-	expression tag	UNP P22862
H	274	SER	-	expression tag	UNP P22862
H	275	HIS	-	expression tag	UNP P22862
H	276	HIS	-	expression tag	UNP P22862
H	277	HIS	-	expression tag	UNP P22862
H	278	HIS	-	expression tag	UNP P22862
H	279	HIS	-	expression tag	UNP P22862
H	280	HIS	-	expression tag	UNP P22862
I	3	CYS	THR	engineered mutation	UNP P22862
I	174	CYS	GLN	engineered mutation	UNP P22862
I	273	GLY	-	expression tag	UNP P22862
I	274	SER	-	expression tag	UNP P22862
I	275	HIS	-	expression tag	UNP P22862

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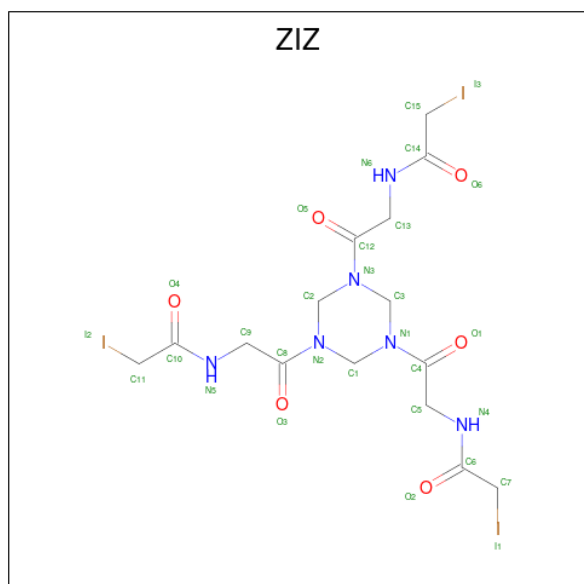
Chain	Residue	Modelled	Actual	Comment	Reference
I	276	HIS	-	expression tag	UNP P22862
I	277	HIS	-	expression tag	UNP P22862
I	278	HIS	-	expression tag	UNP P22862
I	279	HIS	-	expression tag	UNP P22862
I	280	HIS	-	expression tag	UNP P22862
J	3	CYS	THR	engineered mutation	UNP P22862
J	174	CYS	GLN	engineered mutation	UNP P22862
J	273	GLY	-	expression tag	UNP P22862
J	274	SER	-	expression tag	UNP P22862
J	275	HIS	-	expression tag	UNP P22862
J	276	HIS	-	expression tag	UNP P22862
J	277	HIS	-	expression tag	UNP P22862
J	278	HIS	-	expression tag	UNP P22862
J	279	HIS	-	expression tag	UNP P22862
J	280	HIS	-	expression tag	UNP P22862
K	3	CYS	THR	engineered mutation	UNP P22862
K	174	CYS	GLN	engineered mutation	UNP P22862
K	273	GLY	-	expression tag	UNP P22862
K	274	SER	-	expression tag	UNP P22862
K	275	HIS	-	expression tag	UNP P22862
K	276	HIS	-	expression tag	UNP P22862
K	277	HIS	-	expression tag	UNP P22862
K	278	HIS	-	expression tag	UNP P22862
K	279	HIS	-	expression tag	UNP P22862
K	280	HIS	-	expression tag	UNP P22862
L	3	CYS	THR	engineered mutation	UNP P22862
L	174	CYS	GLN	engineered mutation	UNP P22862
L	273	GLY	-	expression tag	UNP P22862
L	274	SER	-	expression tag	UNP P22862
L	275	HIS	-	expression tag	UNP P22862
L	276	HIS	-	expression tag	UNP P22862
L	277	HIS	-	expression tag	UNP P22862
L	278	HIS	-	expression tag	UNP P22862
L	279	HIS	-	expression tag	UNP P22862
L	280	HIS	-	expression tag	UNP P22862
M	3	CYS	THR	engineered mutation	UNP P22862
M	174	CYS	GLN	engineered mutation	UNP P22862
M	273	GLY	-	expression tag	UNP P22862
M	274	SER	-	expression tag	UNP P22862
M	275	HIS	-	expression tag	UNP P22862
M	276	HIS	-	expression tag	UNP P22862
M	277	HIS	-	expression tag	UNP P22862

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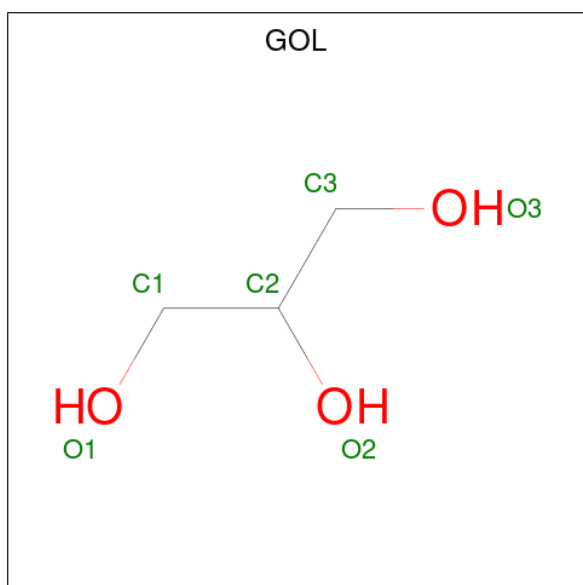
Chain	Residue	Modelled	Actual	Comment	Reference
M	278	HIS	-	expression tag	UNP P22862
M	279	HIS	-	expression tag	UNP P22862
M	280	HIS	-	expression tag	UNP P22862
N	3	CYS	THR	engineered mutation	UNP P22862
N	174	CYS	GLN	engineered mutation	UNP P22862
N	273	GLY	-	expression tag	UNP P22862
N	274	SER	-	expression tag	UNP P22862
N	275	HIS	-	expression tag	UNP P22862
N	276	HIS	-	expression tag	UNP P22862
N	277	HIS	-	expression tag	UNP P22862
N	278	HIS	-	expression tag	UNP P22862
N	279	HIS	-	expression tag	UNP P22862
N	280	HIS	-	expression tag	UNP P22862
O	3	CYS	THR	engineered mutation	UNP P22862
O	174	CYS	GLN	engineered mutation	UNP P22862
O	273	GLY	-	expression tag	UNP P22862
O	274	SER	-	expression tag	UNP P22862
O	275	HIS	-	expression tag	UNP P22862
O	276	HIS	-	expression tag	UNP P22862
O	277	HIS	-	expression tag	UNP P22862
O	278	HIS	-	expression tag	UNP P22862
O	279	HIS	-	expression tag	UNP P22862
O	280	HIS	-	expression tag	UNP P22862

- Molecule 2 is N-[2-[3,5-bis[2-(2-iodanylethanoylamino)ethanoyl]-1,3,5-triazinan-1-yl]-2-oxidanylidene-ethyl]-2-iodanyl-ethanamide (CCD ID: ZIZ) (formula: $C_{15}H_{21}I_3N_6O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	6	6		
2	A	1	Total	C	N	O	0	0
			27	15	6	6		
2	D	1	Total	C	N	O	0	0
			27	15	6	6		
2	D	1	Total	C	N	O	0	0
			27	15	6	6		
2	G	1	Total	C	N	O	0	0
			27	15	6	6		
2	G	1	Total	C	N	O	0	0
			27	15	6	6		
2	J	1	Total	C	N	O	0	0
			27	15	6	6		
2	J	1	Total	C	N	O	0	0
			27	15	6	6		
2	M	1	Total	C	N	O	0	0
			27	15	6	6		
2	M	1	Total	C	N	O	0	0
			27	15	6	6		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	46	Total	O	0	0
			46	46		
4	C	25	Total	O	0	0
			25	25		
4	D	55	Total	O	0	0
			55	55		
4	E	39	Total	O	0	0
			39	39		
4	F	43	Total	O	0	0
			43	43		
4	G	14	Total	O	0	0
			14	14		
4	H	58	Total	O	0	0
			58	58		
4	I	6	Total	O	0	0
			6	6		
4	J	62	Total	O	0	0
			62	62		
4	K	60	Total	O	0	0
			60	60		
4	L	63	Total	O	0	0
			63	63		
4	M	22	Total	O	0	0
			22	22		
4	N	7	Total	O	0	0
			7	7		
4	O	10	Total	O	0	0
			10	10		

3 Residue-property plots [i](#)

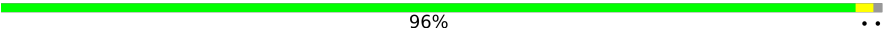
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Arylesterase

Chain A:  91% 6% .



• Molecule 1: Arylesterase

Chain B:  96% ..

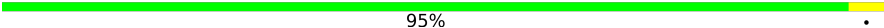


• Molecule 1: Arylesterase

Chain C:  94% ..



• Molecule 1: Arylesterase

Chain D:  95% ..



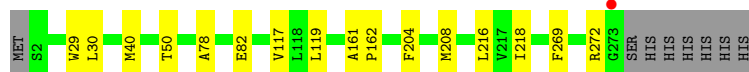
• Molecule 1: Arylesterase

Chain E:  90% 8% .



• Molecule 1: Arylesterase

Chain F:  91% 6% .



• Molecule 1: Arylesterase

Chain G:  90% 6% .



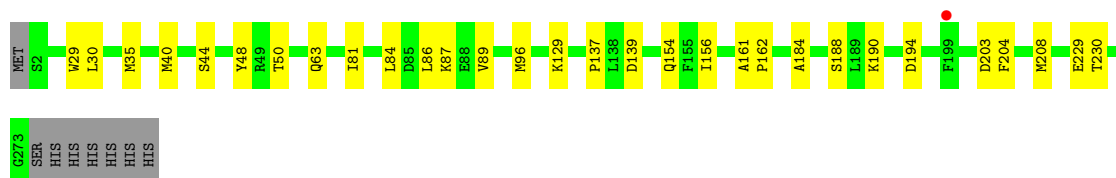
• Molecule 1: Arylesterase

Chain H:  94% 5% .



• Molecule 1: Arylesterase

Chain I:  86% 11% .



• Molecule 1: Arylesterase

Chain J:  92% . .



• Molecule 1: Arylesterase

Chain K:  91% 5% .



• Molecule 1: Arylesterase

Chain L:  92% . .



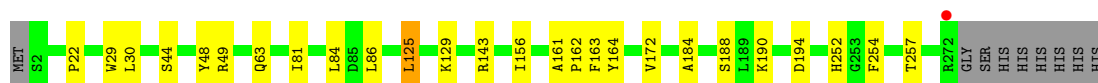
● Molecule 1: Arylesterase

Chain M:  91% 5% .

● Molecule 1: Arylesterase

Chain N:  88% 9% .

● Molecule 1: Arylesterase

Chain O:  88% 9% .

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.80Å 146.25Å 154.59Å 90.00° 122.63° 90.00°	Depositor
Resolution (Å)	77.72 – 2.50 77.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.72-2.50) 100.0 (77.72-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0411, PDB-REDO	Depositor
R, R_{free}	0.182 , 0.223 0.182 , 0.224	Depositor DCC
R_{free} test set	8234 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.088 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.115 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32857	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.43	0/2170	0.91	0/2942
1	B	0.44	0/2215	0.90	0/3003
1	C	0.43	0/2166	0.90	0/2937
1	D	0.44	0/2215	0.90	0/3003
1	E	0.44	0/2176	0.92	0/2950
1	F	0.44	0/2170	0.92	0/2942
1	G	0.42	0/2166	0.91	0/2937
1	H	0.44	0/2198	0.91	0/2980
1	I	0.42	0/2170	0.92	0/2942
1	J	0.43	0/2180	0.90	0/2956
1	K	0.43	0/2179	0.89	1/2954 (0.0%)
1	L	0.44	0/2174	0.92	0/2948
1	M	0.44	0/2166	0.93	0/2937
1	N	0.43	0/2166	0.93	0/2937
1	O	0.43	0/2166	0.93	0/2937
All	All	0.43	0/32677	0.91	1/44305 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	199	PHE	CA-CB-CG	5.32	119.12	113.80

There are no chirality outliers.

There are no planarity outliers.

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	2119	0	2075	13	0
1	B	2161	0	2105	5	0
1	C	2115	0	2072	8	0
1	D	2161	0	2105	6	0
1	E	2125	0	2080	13	0
1	F	2119	0	2075	8	0
1	G	2115	0	2072	15	0
1	H	2145	0	2094	7	0
1	I	2119	0	2075	23	0
1	J	2129	0	2079	6	0
1	K	2128	0	2080	9	0
1	L	2123	0	2082	9	0
1	M	2115	0	2072	8	0
1	N	2115	0	2072	14	0
1	O	2115	0	2072	16	0
2	A	54	0	0	0	0
2	D	54	0	0	0	0
2	G	54	0	0	0	0
2	J	54	0	0	0	0
2	M	54	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	3	0
3	D	18	0	24	1	0
3	E	6	0	8	0	0
3	F	12	0	16	1	0
3	G	6	0	8	2	0
3	H	6	0	8	4	0
3	I	6	0	8	0	0
3	J	12	0	16	1	0
3	K	24	0	32	0	0
3	L	18	0	24	3	0
3	M	18	0	24	1	0
3	O	6	0	8	0	0
4	A	23	0	0	0	0
4	B	46	0	0	0	0
4	C	25	0	0	0	0
4	D	55	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	39	0	0	0	0
4	F	43	0	0	0	0
4	G	14	0	0	0	0
4	H	58	0	0	0	0
4	I	6	0	0	0	0
4	J	62	0	0	0	0
4	K	60	0	0	0	0
4	L	63	0	0	0	0
4	M	22	0	0	0	0
4	N	7	0	0	0	0
4	O	10	0	0	0	0
All	All	32857	0	31410	155	0

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

All (155) 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:63:GLN:H	3:B:301:GOL:H32	1.18	1.03
1:G:63:GLN:H	3:H:301:GOL:H11	1.25	1.02
1:G:244:LEU:HD21	1:G:246:VAL:HG23	1.71	0.73
1:C:21:LYS:HG2	1:I:87:LYS:HZ1	1.59	0.67
1:A:63:GLN:N	3:B:301:GOL:H32	2.02	0.66
1:G:63:GLN:N	3:H:301:GOL:H11	2.06	0.66
1:I:81:ILE:HG23	1:I:86:LEU:HB2	1.78	0.65
1:L:2:SER:OG	3:L:301:GOL:H31	1.98	0.64
1:M:164:TYR:HB3	1:M:172:VAL:HG21	1.80	0.63
3:G:302:GOL:H11	1:I:63:GLN:H	1.63	0.62
1:K:269:PHE:O	1:K:272:ARG:HG3	2.00	0.61
1:G:44:SER:HA	1:G:48:TYR:O	2.01	0.61
1:K:125:LEU:HD13	1:K:203:ASP:HA	1.83	0.59
1:J:142:ALA:HA	3:J:302:GOL:H32	1.87	0.57
1:A:125:LEU:HD11	1:A:205:ARG:NE	2.19	0.57
1:J:7:LYS:HG2	1:J:79:GLN:OE1	2.06	0.56
1:N:270:LEU:O	1:N:271:LYS:HG2	2.04	0.56
1:G:63:GLN:H	3:H:301:GOL:C1	2.10	0.56
1:L:15:LYS:HA	3:L:301:GOL:H32	1.89	0.55
1:L:2:SER:N	3:L:301:GOL:H2	2.22	0.55
1:E:81:ILE:HG23	1:E:86:LEU:HB2	1.88	0.54
1:I:204:PHE:O	1:I:208:MET:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:29:TRP:O	1:J:30:LEU:HB2	2.06	0.54
1:J:164:TYR:HB3	1:J:172:VAL:HG21	1.90	0.53
1:M:81:ILE:HG23	1:M:86:LEU:HB2	1.91	0.53
1:C:81:ILE:HG23	1:C:86:LEU:HB2	1.91	0.53
1:I:229:GLU:HG2	1:I:230:THR:HG23	1.92	0.52
1:N:81:ILE:HG23	1:N:86:LEU:HB2	1.91	0.52
1:N:63:GLN:HB3	1:N:188:SER:HB2	1.90	0.52
1:A:81:ILE:HG23	1:A:86:LEU:HB2	1.92	0.52
1:C:21:LYS:HG2	1:I:87:LYS:NZ	2.23	0.52
1:I:129:LYS:HE3	1:I:203:ASP:HB2	1.92	0.51
1:A:63:GLN:H	3:B:301:GOL:C3	2.07	0.51
3:M:303:GOL:HO2	1:N:2:SER:N	2.08	0.51
1:C:21:LYS:NZ	1:I:87:LYS:HE3	2.26	0.51
1:A:29:TRP:O	1:A:30:LEU:HB2	2.09	0.51
1:I:161:ALA:HB3	1:I:162:PRO:HD3	1.93	0.51
1:E:44:SER:HA	1:E:48:TYR:O	2.11	0.50
1:E:125:LEU:HD13	1:E:203:ASP:HA	1.94	0.50
1:F:269:PHE:O	1:F:272:ARG:HG3	2.12	0.50
1:I:63:GLN:HB3	1:I:188:SER:HB2	1.94	0.50
1:D:29:TRP:O	1:D:30:LEU:HB2	2.12	0.50
1:G:29:TRP:O	1:G:30:LEU:HB2	2.12	0.50
1:L:125[B]:LEU:N	1:L:125[B]:LEU:HD23	2.27	0.49
1:G:244:LEU:C	1:G:244:LEU:HD23	2.37	0.49
1:G:2:SER:N	3:G:302:GOL:H12	2.28	0.49
1:O:81:ILE:HG23	1:O:86:LEU:HB2	1.95	0.49
1:N:161:ALA:HB3	1:N:162:PRO:HD3	1.95	0.49
1:D:2:SER:OG	3:F:301:GOL:H11	2.13	0.48
1:M:29:TRP:O	1:M:30:LEU:HB2	2.14	0.48
1:A:156:ILE:HD13	1:A:184:ALA:HB1	1.96	0.47
1:D:125:LEU:HD13	1:D:203:ASP:HA	1.97	0.47
1:F:29:TRP:O	1:F:30:LEU:HB2	2.15	0.47
1:N:78:ALA:O	1:N:82:GLU:HG2	2.14	0.47
1:O:44:SER:HA	1:O:48:TYR:O	2.15	0.47
1:M:44:SER:HA	1:M:48:TYR:O	2.14	0.47
1:E:161:ALA:HB3	1:E:162:PRO:CD	2.45	0.47
1:K:7:LYS:HG2	1:K:79:GLN:OE1	2.15	0.47
1:I:190:LYS:HE3	1:I:194:ASP:OD2	2.15	0.47
1:H:40:MET:HG2	1:H:50:THR:HB	1.97	0.47
1:J:125:LEU:HD13	1:J:132:TYR:CD2	2.50	0.46
1:D:190:LYS:HE3	1:D:194:ASP:OD2	2.15	0.46
1:O:29:TRP:O	1:O:30:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:MET:HG2	1:I:50:THR:HB	1.98	0.46
1:O:254:PHE:HA	1:O:257:THR:OG1	2.16	0.46
1:K:120:GLY:HA2	1:K:219:HIS:CE1	2.51	0.46
1:G:244:LEU:CD2	1:G:246:VAL:HG23	2.44	0.45
1:M:25:PHE:HB3	1:M:36:TRP:CD1	2.51	0.45
1:E:120:GLY:HA2	1:E:219:HIS:ND1	2.31	0.45
1:N:40:MET:HG2	1:N:50:THR:HB	1.97	0.45
1:O:63:GLN:HB3	1:O:188:SER:HB2	1.98	0.45
1:F:161:ALA:HB3	1:F:162:PRO:HD3	1.98	0.45
1:G:35:MET:HE3	1:G:35:MET:HB2	1.87	0.45
1:L:44:SER:HA	1:L:48:TYR:O	2.15	0.45
1:N:216:LEU:HD21	1:N:218:ILE:HD11	1.98	0.45
1:E:161:ALA:HB3	1:E:162:PRO:HD3	1.98	0.45
1:N:124:PRO:O	1:N:204:PHE:HB2	2.17	0.45
1:B:161:ALA:HB3	1:B:162:PRO:HD3	1.99	0.45
1:D:204:PHE:O	1:D:207:ASP:HB2	2.16	0.45
1:I:161:ALA:HB3	1:I:162:PRO:CD	2.46	0.45
1:E:120:GLY:HA2	1:E:219:HIS:CE1	2.52	0.45
1:E:96:MET:HE3	1:E:96:MET:HB2	1.91	0.45
1:B:164:TYR:HB3	1:B:172:VAL:HG21	1.99	0.44
1:K:164:TYR:HB3	1:K:172:VAL:HG21	1.98	0.44
1:N:127:GLY:HA3	1:N:200:ALA:O	2.16	0.44
1:J:96:MET:HE3	1:J:96:MET:HB2	1.89	0.44
1:I:44:SER:HA	1:I:48:TYR:O	2.18	0.44
1:C:116:LEU:O	1:C:215:THR:HA	2.18	0.44
1:M:40:MET:HG2	1:M:50:THR:HB	1.98	0.44
1:O:22:PRO:HA	1:O:49:ARG:O	2.17	0.44
1:I:84:LEU:HB2	1:I:86:LEU:HG	1.99	0.44
1:O:163:PHE:CE1	1:O:252:HIS:HD2	2.36	0.44
1:E:40:MET:HG2	1:E:50:THR:HB	2.00	0.44
1:A:120:GLY:HA2	1:A:219:HIS:CE1	2.52	0.43
1:G:110:SER:HB2	1:G:113:VAL:HG13	2.00	0.43
1:N:161:ALA:HB3	1:N:162:PRO:CD	2.48	0.43
1:H:3:CYS:HA	1:H:12:ILE:O	2.18	0.43
1:O:161:ALA:HB3	1:O:162:PRO:HD3	1.99	0.43
1:A:152:ARG:O	1:A:156:ILE:HG13	2.18	0.43
1:N:50:THR:C	1:N:51:ILE:HG13	2.43	0.43
1:C:21:LYS:HZ3	1:I:87:LYS:HE3	1.82	0.43
1:I:96:MET:HE3	1:I:96:MET:HB2	1.82	0.43
1:K:125:LEU:HD21	1:K:129:LYS:HG3	2.01	0.43
1:L:50:THR:C	1:L:51:ILE:HG13	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LYS:O	1:B:51:ILE:HA	2.19	0.43
1:I:86:LEU:HB3	1:I:89:VAL:CG2	2.48	0.43
1:A:164:TYR:HB3	1:A:172:VAL:HG21	2.00	0.43
1:H:29:TRP:O	1:H:30:LEU:HB2	2.19	0.43
1:I:156:ILE:HD13	1:I:184:ALA:HB1	2.01	0.43
1:C:161:ALA:HB3	1:C:162:PRO:HD3	2.01	0.43
1:H:2:SER:N	3:H:301:GOL:H2	2.33	0.43
1:O:164:TYR:HB3	1:O:172:VAL:HG21	2.00	0.43
1:G:120:GLY:HA2	1:G:219:HIS:CE1	2.54	0.42
1:H:44:SER:HA	1:H:48:TYR:O	2.20	0.42
1:K:3:CYS:HB2	1:K:12:ILE:O	2.19	0.42
1:B:96:MET:HE3	1:B:96:MET:HB2	1.98	0.42
1:A:181:LEU:O	1:A:185:LEU:HG	2.18	0.42
1:G:173:SER:HB2	1:I:154:GLN:OE1	2.19	0.42
1:I:137:PRO:C	1:I:139:ASP:H	2.26	0.42
1:L:125[A]:LEU:HD21	1:L:129:LYS:HG3	2.00	0.42
1:E:3:CYS:HA	1:E:12:ILE:O	2.20	0.42
1:C:96:MET:HE3	1:C:96:MET:HB2	1.85	0.42
1:M:24:LEU:C	1:M:24:LEU:HD23	2.45	0.42
1:A:51:ILE:HD13	1:A:86:LEU:HD11	2.01	0.41
1:F:40:MET:HG2	1:F:50:THR:HB	2.01	0.41
1:D:152:ARG:O	1:D:156:ILE:HG13	2.20	0.41
1:E:29:TRP:O	1:E:30:LEU:HB2	2.20	0.41
1:G:161:ALA:HB3	1:G:162:PRO:HD3	2.02	0.41
1:K:29:TRP:O	1:K:30:LEU:HB2	2.21	0.41
1:L:116:LEU:O	1:L:215:THR:HA	2.20	0.41
1:O:156:ILE:HD13	1:O:184:ALA:HB1	2.02	0.41
1:H:267:LEU:O	1:H:271:LYS:HG2	2.21	0.41
1:M:78:ALA:O	1:M:82:GLU:HG2	2.21	0.41
1:N:269:PHE:HA	1:N:272:ARG:HD3	2.01	0.41
1:B:161:ALA:HB3	1:B:162:PRO:CD	2.51	0.41
1:E:25:PHE:HB3	1:E:36:TRP:CE2	2.56	0.41
1:F:117:VAL:HA	1:F:216:LEU:O	2.21	0.41
1:K:120:GLY:HA2	1:K:219:HIS:ND1	2.36	0.41
1:O:156:ILE:HG21	1:O:184:ALA:HB3	2.03	0.41
1:O:190:LYS:HE3	1:O:194:ASP:OD2	2.21	0.41
1:F:119:LEU:HD23	1:F:218:ILE:HB	2.02	0.41
1:I:29:TRP:O	1:I:30:LEU:HB2	2.21	0.41
1:I:35:MET:HE3	1:I:35:MET:HB2	1.97	0.41
1:N:125:LEU:HD23	1:N:132:TYR:CG	2.55	0.41
3:D:404:GOL:H31	1:E:2:SER:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:MET:HE3	1:H:96:MET:HB2	2.01	0.40
1:O:125:LEU:HD11	1:O:129:LYS:HG3	2.03	0.40
1:A:125:LEU:HD11	1:A:205:ARG:CD	2.51	0.40
1:F:204:PHE:O	1:F:208:MET:HG2	2.22	0.40
1:L:120:GLY:HA2	1:L:219:HIS:CE1	2.57	0.40
1:F:78:ALA:O	1:F:82:GLU:HG2	2.21	0.40
1:O:84:LEU:HB2	1:O:86:LEU:HG	2.03	0.40
1:O:143:ARG:HA	1:O:143:ARG:HD2	1.96	0.40
1:O:156:ILE:HG21	1:O:184:ALA:CB	2.52	0.40
1:G:22:PRO:HG2	1:G:89:VAL:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/280 (96%)	261 (97%)	9 (3%)	0	100	100
1	B	275/280 (98%)	267 (97%)	8 (3%)	0	100	100
1	C	269/280 (96%)	260 (97%)	9 (3%)	0	100	100
1	D	275/280 (98%)	267 (97%)	8 (3%)	0	100	100
1	E	271/280 (97%)	262 (97%)	8 (3%)	1 (0%)	30	49
1	F	270/280 (96%)	259 (96%)	11 (4%)	0	100	100
1	G	269/280 (96%)	259 (96%)	10 (4%)	0	100	100
1	H	273/280 (98%)	265 (97%)	8 (3%)	0	100	100
1	I	270/280 (96%)	256 (95%)	14 (5%)	0	100	100
1	J	271/280 (97%)	261 (96%)	10 (4%)	0	100	100
1	K	271/280 (97%)	263 (97%)	8 (3%)	0	100	100
1	L	270/280 (96%)	264 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	269/280 (96%)	259 (96%)	10 (4%)	0	100	100
1	N	269/280 (96%)	261 (97%)	8 (3%)	0	100	100
1	O	269/280 (96%)	262 (97%)	7 (3%)	0	100	100
All	All	4061/4200 (97%)	3926 (97%)	134 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	273	GLY

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	220/228 (96%)	220 (100%)	0	100	100
1	B	225/228 (99%)	225 (100%)	0	100	100
1	C	220/228 (96%)	220 (100%)	0	100	100
1	D	225/228 (99%)	225 (100%)	0	100	100
1	E	221/228 (97%)	220 (100%)	1 (0%)	81	92
1	F	220/228 (96%)	220 (100%)	0	100	100
1	G	220/228 (96%)	220 (100%)	0	100	100
1	H	223/228 (98%)	222 (100%)	1 (0%)	84	93
1	I	220/228 (96%)	220 (100%)	0	100	100
1	J	222/228 (97%)	219 (99%)	3 (1%)	59	81
1	K	221/228 (97%)	220 (100%)	1 (0%)	81	92
1	L	221/228 (97%)	221 (100%)	0	100	100
1	M	220/228 (96%)	220 (100%)	0	100	100
1	N	220/228 (96%)	220 (100%)	0	100	100
1	O	220/228 (96%)	219 (100%)	1 (0%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3318/3420 (97%)	3311 (100%)	7 (0%)	87 95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	157	SER
1	H	199	PHE
1	J	3	CYS
1	J	125	LEU
1	J	272	ARG
1	K	3	CYS
1	O	125	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	B	39	GLN
1	B	68	ASN
1	C	39	GLN
1	C	108	HIS
1	G	108	HIS
1	G	128	GLN
1	H	39	GLN
1	H	79	GLN
1	H	275	HIS
1	J	39	GLN
1	K	39	GLN
1	L	39	GLN
1	L	108	HIS
1	M	108	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

35 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ZIZ	A	402	1	27,27,30	0.83	0	36,36,39	1.11	2 (5%)
2	ZIZ	D	402	1	27,27,30	0.82	0	36,36,39	1.06	3 (8%)
2	ZIZ	D	401	1	27,27,30	0.85	0	36,36,39	1.35	5 (13%)
3	GOL	M	303	-	5,5,5	0.10	0	5,5,5	0.35	0
2	ZIZ	G	301	1	27,27,30	0.81	0	36,36,39	0.88	1 (2%)
3	GOL	F	302	-	5,5,5	0.09	0	5,5,5	0.34	0
3	GOL	D	403	-	5,5,5	0.09	0	5,5,5	0.37	0
3	GOL	H	301	-	5,5,5	0.07	0	5,5,5	0.37	0
3	GOL	B	301	-	5,5,5	0.08	0	5,5,5	0.40	0
2	ZIZ	A	401	1	27,27,30	0.85	0	36,36,39	1.12	2 (5%)
3	GOL	M	301	-	5,5,5	0.12	0	5,5,5	0.44	0
3	GOL	O	301	-	5,5,5	0.09	0	5,5,5	0.34	0
3	GOL	E	301	-	5,5,5	0.11	0	5,5,5	0.43	0
2	ZIZ	J	304	1	27,27,30	0.87	0	36,36,39	1.12	2 (5%)
3	GOL	K	301	-	5,5,5	0.09	0	5,5,5	0.43	0
3	GOL	D	405	-	5,5,5	0.09	0	5,5,5	0.37	0
3	GOL	J	302	-	5,5,5	0.09	0	5,5,5	0.33	0
2	ZIZ	J	303	1	27,27,30	0.88	0	36,36,39	1.92	4 (11%)
3	GOL	L	301	-	5,5,5	0.08	0	5,5,5	0.43	0
3	GOL	B	302	-	5,5,5	0.09	0	5,5,5	0.29	0
2	ZIZ	M	304	1	27,27,30	0.84	0	36,36,39	0.82	1 (2%)
2	ZIZ	G	303	1	27,27,30	0.84	0	36,36,39	1.19	2 (5%)
3	GOL	M	302	-	5,5,5	0.10	0	5,5,5	0.38	0
3	GOL	K	304	-	5,5,5	0.10	0	5,5,5	0.35	0
3	GOL	K	302	-	5,5,5	0.06	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	404	-	5,5,5	0.10	0	5,5,5	0.33	0
3	GOL	J	301	-	5,5,5	0.09	0	5,5,5	0.36	0
3	GOL	L	302	-	5,5,5	0.09	0	5,5,5	0.34	0
2	ZIZ	M	305	1	27,27,30	0.83	0	36,36,39	1.14	3 (8%)
3	GOL	K	303	-	5,5,5	0.10	0	5,5,5	0.39	0
3	GOL	F	301	-	5,5,5	0.12	0	5,5,5	0.46	0
3	GOL	A	403	-	5,5,5	0.08	0	5,5,5	0.34	0
3	GOL	L	303	-	5,5,5	0.08	0	5,5,5	0.30	0
3	GOL	I	301	-	5,5,5	0.09	0	5,5,5	0.36	0
3	GOL	G	302	-	5,5,5	0.10	0	5,5,5	0.39	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZIZ	A	402	1	-	5/27/39/45	0/0/1/1
2	ZIZ	D	402	1	-	4/27/39/45	0/0/1/1
2	ZIZ	D	401	1	-	8/27/39/45	0/0/1/1
3	GOL	M	303	-	-	1/4/4/4	-
2	ZIZ	G	301	1	-	5/27/39/45	0/0/1/1
3	GOL	F	302	-	-	0/4/4/4	-
3	GOL	D	403	-	-	2/4/4/4	-
3	GOL	H	301	-	-	2/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-
2	ZIZ	A	401	1	-	0/27/39/45	0/0/1/1
3	GOL	M	301	-	-	4/4/4/4	-
3	GOL	O	301	-	-	2/4/4/4	-
3	GOL	E	301	-	-	0/4/4/4	-
2	ZIZ	J	304	1	-	1/27/39/45	0/0/1/1
3	GOL	K	301	-	-	0/4/4/4	-
3	GOL	D	405	-	-	0/4/4/4	-
3	GOL	J	302	-	-	2/4/4/4	-
2	ZIZ	J	303	1	-	6/27/39/45	0/0/1/1
3	GOL	L	301	-	-	0/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-
2	ZIZ	M	304	1	-	2/27/39/45	0/0/1/1
2	ZIZ	G	303	1	-	0/27/39/45	0/0/1/1
3	GOL	M	302	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	K	304	-	-	2/4/4/4	-
3	GOL	K	302	-	-	2/4/4/4	-
3	GOL	D	404	-	-	3/4/4/4	-
3	GOL	J	301	-	-	0/4/4/4	-
3	GOL	L	302	-	-	1/4/4/4	-
2	ZIZ	M	305	1	-	10/27/39/45	0/0/1/1
3	GOL	K	303	-	-	0/4/4/4	-
3	GOL	F	301	-	-	3/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	L	303	-	-	2/4/4/4	-
3	GOL	I	301	-	-	2/4/4/4	-
3	GOL	G	302	-	-	4/4/4/4	-

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	303	ZIZ	N1-C3-N3	-7.80	98.65	110.77
2	J	303	ZIZ	N1-C1-N2	-5.35	102.46	110.77
2	D	401	ZIZ	N1-C1-N2	-4.75	103.39	110.77
2	G	303	ZIZ	N2-C2-N3	-4.45	103.86	110.77
2	J	303	ZIZ	N2-C2-N3	-4.39	103.96	110.77
2	G	303	ZIZ	N1-C3-N3	-4.02	104.52	110.77
2	D	402	ZIZ	N1-C3-N3	-3.75	104.95	110.77
2	A	401	ZIZ	N1-C3-N3	-3.65	105.10	110.77
2	A	402	ZIZ	N1-C1-N2	-3.65	105.11	110.77
2	A	401	ZIZ	N2-C2-N3	-3.51	105.32	110.77
2	M	304	ZIZ	N2-C2-N3	-2.97	106.16	110.77
2	M	305	ZIZ	N2-C2-N3	-2.96	106.17	110.77
2	A	402	ZIZ	N1-C3-N3	-2.92	106.24	110.77
2	M	305	ZIZ	C4-C5-N4	-2.81	103.97	110.90
2	M	305	ZIZ	N1-C1-N2	-2.77	106.46	110.77
2	D	401	ZIZ	C8-C9-N5	-2.65	104.37	110.90
2	G	301	ZIZ	N1-C3-N3	-2.59	106.75	110.77
2	D	401	ZIZ	N2-C2-N3	-2.57	106.77	110.77
2	J	304	ZIZ	N1-C1-N2	-2.55	106.81	110.77
2	D	402	ZIZ	N2-C2-N3	-2.55	106.81	110.77
2	J	304	ZIZ	N1-C3-N3	2.36	114.44	110.77
2	J	303	ZIZ	C8-C9-N5	-2.32	105.18	110.90
2	D	401	ZIZ	N1-C3-N3	-2.26	107.26	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	402	ZIZ	C4-C5-N4	-2.05	105.84	110.90
2	D	401	ZIZ	C9-N5-C10	2.03	127.70	121.65

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	ZIZ	C9-C8-N2-C1
2	D	401	ZIZ	O3-C8-C9-N5
2	M	305	ZIZ	C5-C4-N1-C1
2	M	305	ZIZ	C5-C4-N1-C3
3	A	403	GOL	C1-C2-C3-O3
3	A	403	GOL	O2-C2-C3-O3
3	B	301	GOL	O1-C1-C2-C3
3	G	302	GOL	O1-C1-C2-C3
3	G	302	GOL	C1-C2-C3-O3
3	H	301	GOL	C1-C2-C3-O3
3	I	301	GOL	C1-C2-C3-O3
3	I	301	GOL	O2-C2-C3-O3
3	K	302	GOL	C1-C2-C3-O3
3	L	303	GOL	C1-C2-C3-O3
3	M	301	GOL	C1-C2-C3-O3
2	D	401	ZIZ	C11-C10-N5-C9
2	D	401	ZIZ	O4-C10-N5-C9
2	G	301	ZIZ	C15-C14-N6-C13
2	G	301	ZIZ	O6-C14-N6-C13
2	J	303	ZIZ	C11-C10-N5-C9
2	J	303	ZIZ	O4-C10-N5-C9
2	M	305	ZIZ	C7-C6-N4-C5
2	M	305	ZIZ	O2-C6-N4-C5
2	A	402	ZIZ	C12-C13-N6-C14
3	K	302	GOL	O2-C2-C3-O3
3	L	303	GOL	O2-C2-C3-O3
3	M	301	GOL	O1-C1-C2-O2
3	M	301	GOL	O2-C2-C3-O3
3	D	403	GOL	O1-C1-C2-C3
3	D	404	GOL	O1-C1-C2-C3
3	F	301	GOL	O1-C1-C2-C3
3	J	302	GOL	O1-C1-C2-C3
3	M	301	GOL	O1-C1-C2-C3
3	O	301	GOL	C1-C2-C3-O3
3	B	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	F	301	GOL	O1-C1-C2-O2
3	G	302	GOL	O1-C1-C2-O2
3	G	302	GOL	O2-C2-C3-O3
3	H	301	GOL	O2-C2-C3-O3
3	O	301	GOL	O2-C2-C3-O3
2	J	303	ZIZ	N2-C8-C9-N5
3	D	403	GOL	O1-C1-C2-O2
3	D	404	GOL	O1-C1-C2-O2
2	J	303	ZIZ	C9-C8-N2-C1
2	D	401	ZIZ	O3-C8-N2-C1
2	G	301	ZIZ	O5-C12-C13-N6
2	J	303	ZIZ	O3-C8-C9-N5
2	D	401	ZIZ	N2-C8-C9-N5
2	G	301	ZIZ	N3-C12-C13-N6
2	M	305	ZIZ	O1-C4-N1-C3
2	D	401	ZIZ	C9-C8-N2-C2
3	D	404	GOL	O2-C2-C3-O3
3	L	302	GOL	O2-C2-C3-O3
3	J	302	GOL	O1-C1-C2-O2
2	M	305	ZIZ	N2-C8-C9-N5
3	K	304	GOL	C1-C2-C3-O3
2	D	402	ZIZ	O3-C8-C9-N5
2	D	402	ZIZ	N3-C12-C13-N6
2	D	402	ZIZ	O5-C12-C13-N6
2	M	304	ZIZ	O1-C4-C5-N4
2	M	305	ZIZ	O3-C8-C9-N5
3	M	303	GOL	C1-C2-C3-O3
3	K	304	GOL	O2-C2-C3-O3
2	D	402	ZIZ	N2-C8-C9-N5
2	M	304	ZIZ	N1-C4-C5-N4
2	M	305	ZIZ	N1-C4-C5-N4
2	M	305	ZIZ	O1-C4-N1-C1
2	A	402	ZIZ	N3-C12-C13-N6
2	M	305	ZIZ	O1-C4-C5-N4
2	J	303	ZIZ	C8-C9-N5-C10
2	D	401	ZIZ	O3-C8-N2-C2
2	A	402	ZIZ	C8-C9-N5-C10
2	A	402	ZIZ	O5-C12-C13-N6
2	A	402	ZIZ	O1-C4-C5-N4
2	J	304	ZIZ	O1-C4-C5-N4
2	G	301	ZIZ	C12-C13-N6-C14
3	F	301	GOL	O2-C2-C3-O3

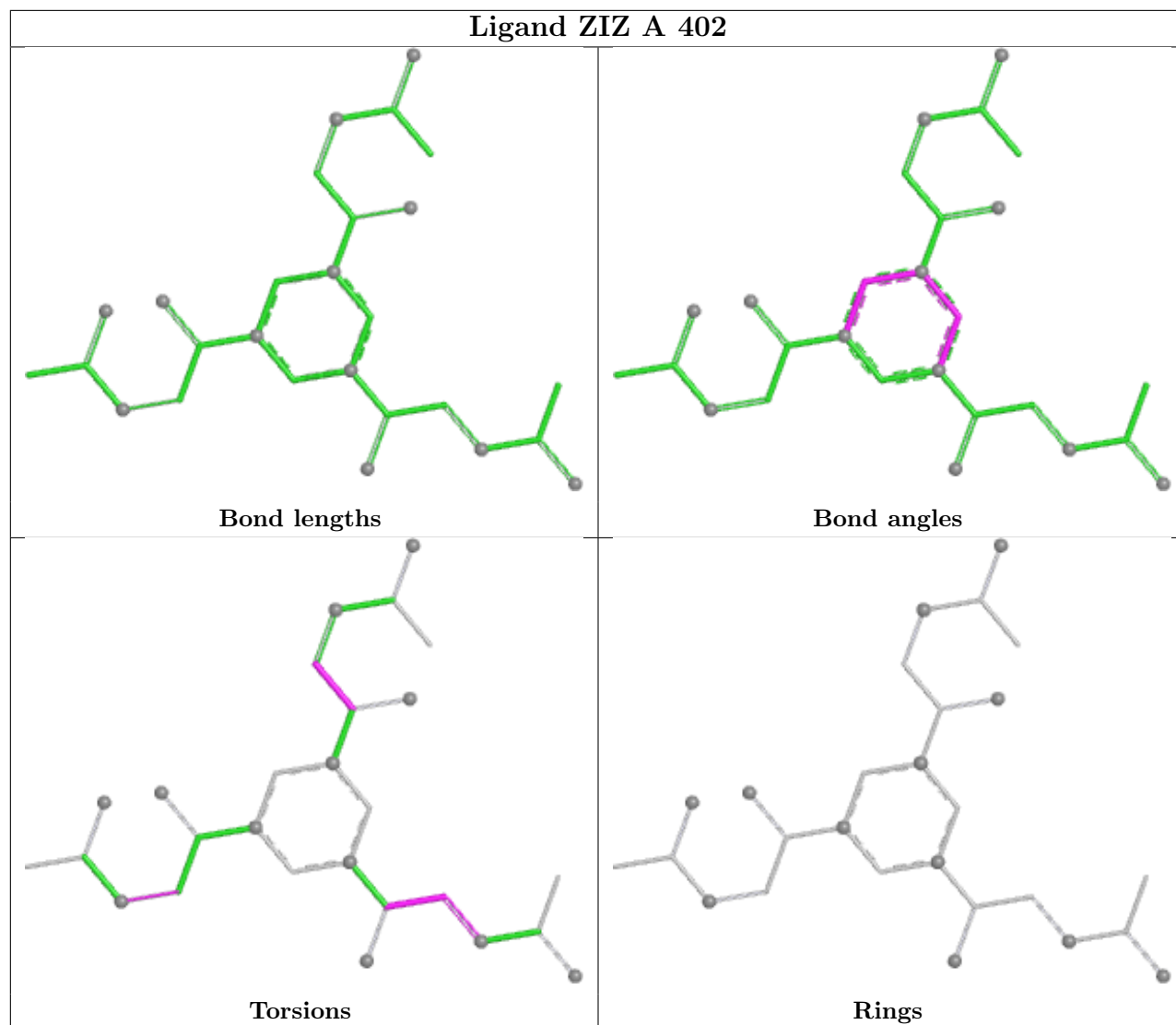
There are no ring outliers.

8 monomers are involved in 16 short contacts:

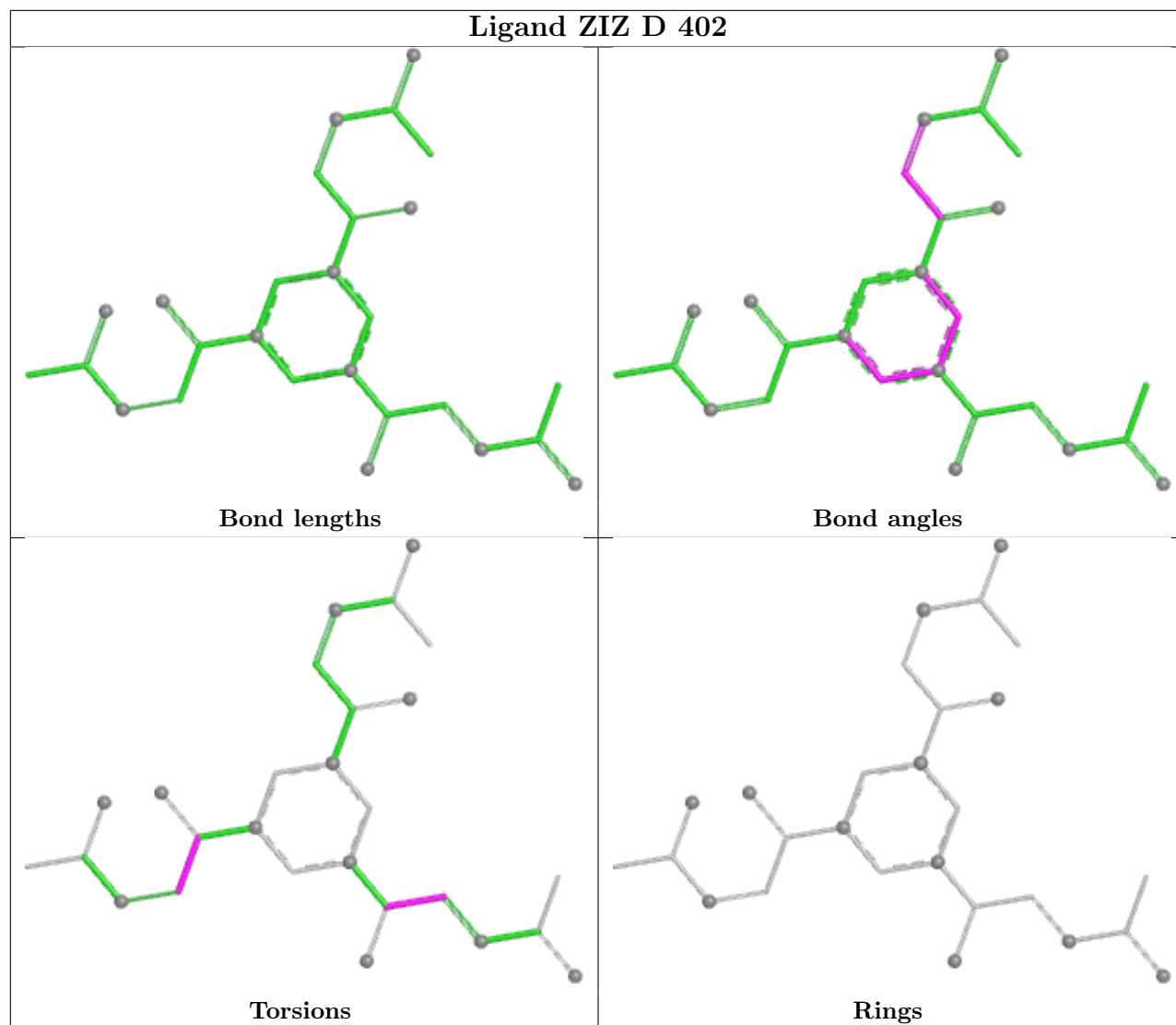
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	303	GOL	1	0
3	H	301	GOL	4	0
3	B	301	GOL	3	0
3	J	302	GOL	1	0
3	L	301	GOL	3	0
3	D	404	GOL	1	0
3	F	301	GOL	1	0
3	G	302	GOL	2	0

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.

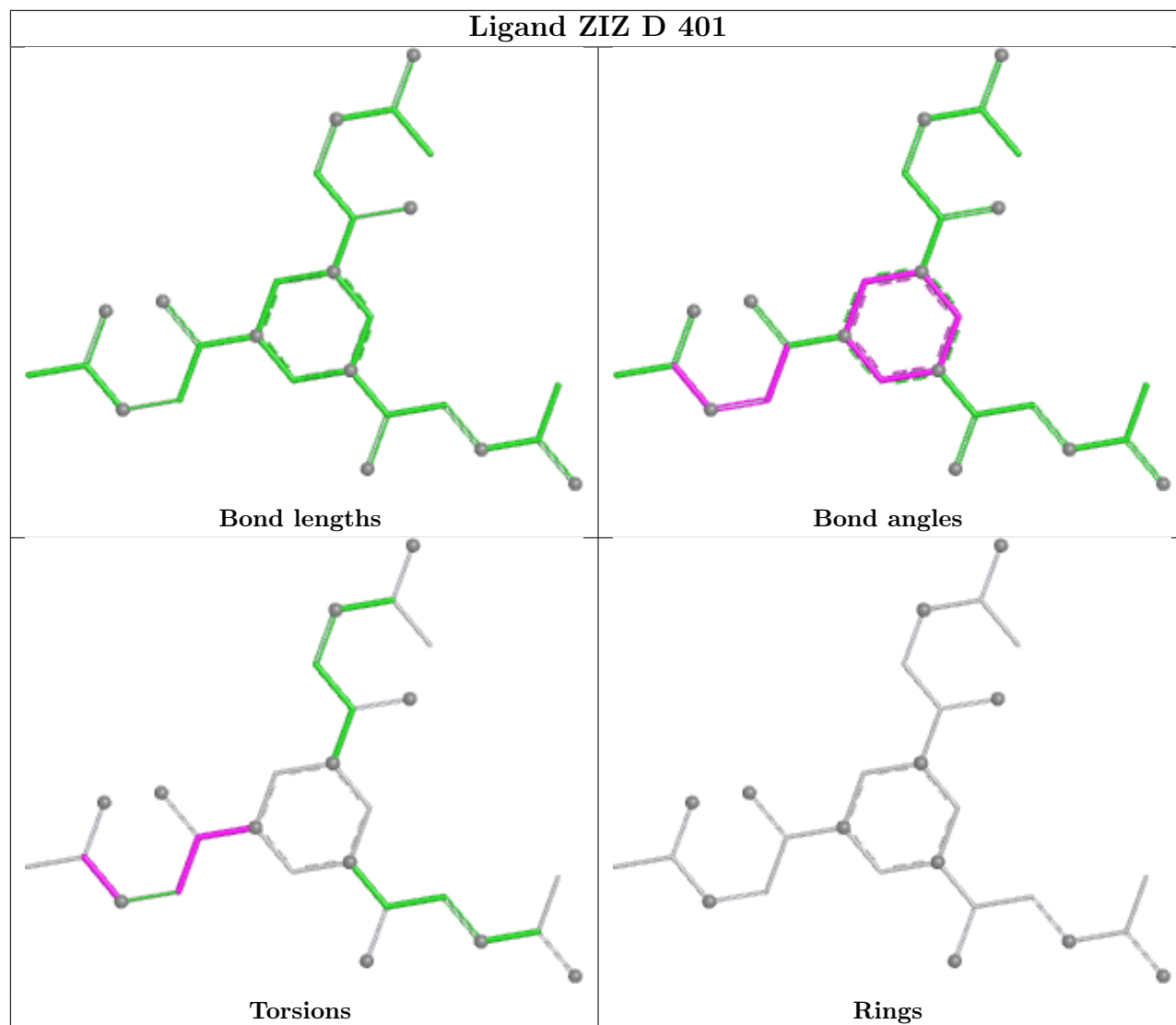
Ligand ZIZ A 402



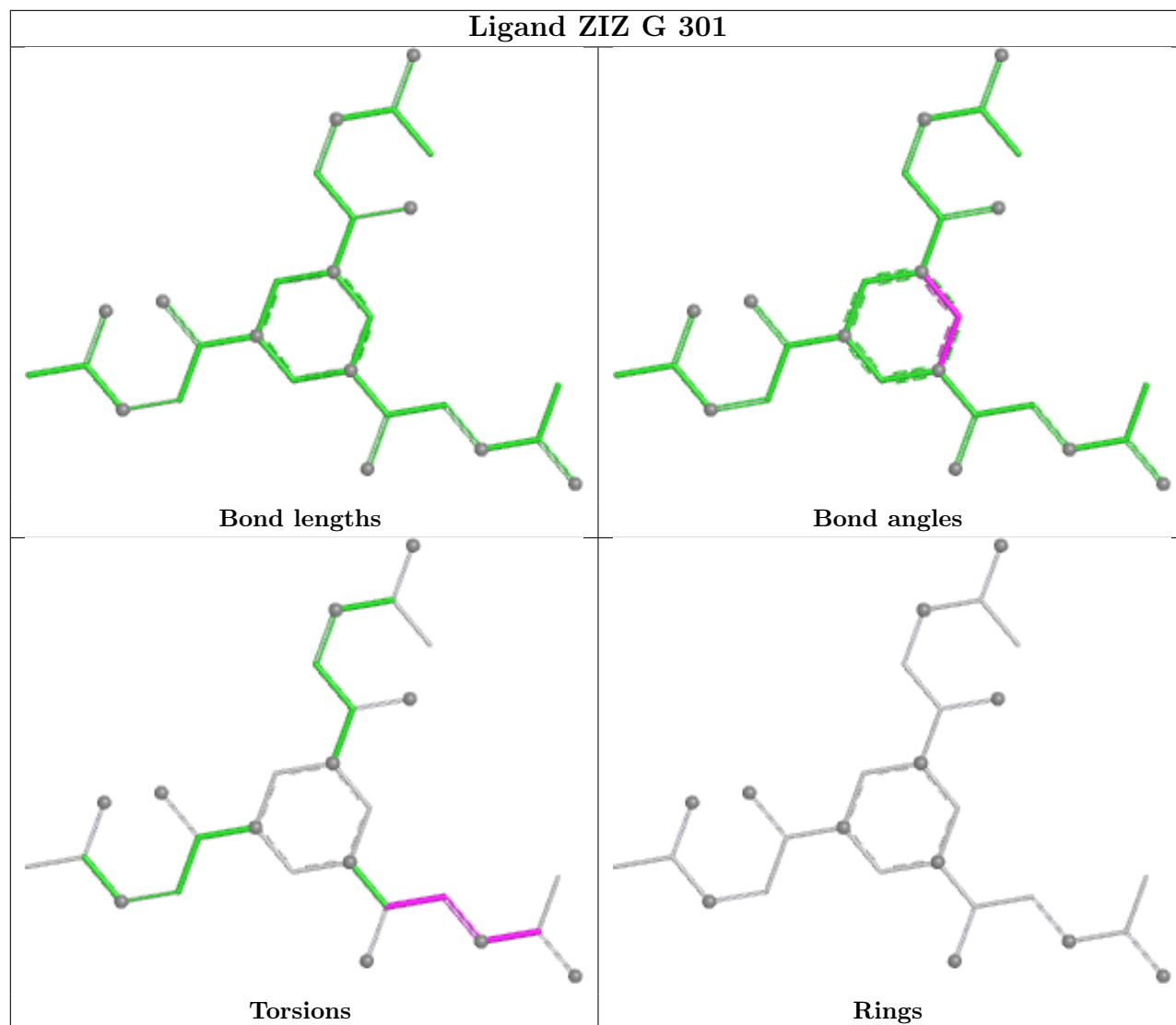
Ligand ZIZ D 402



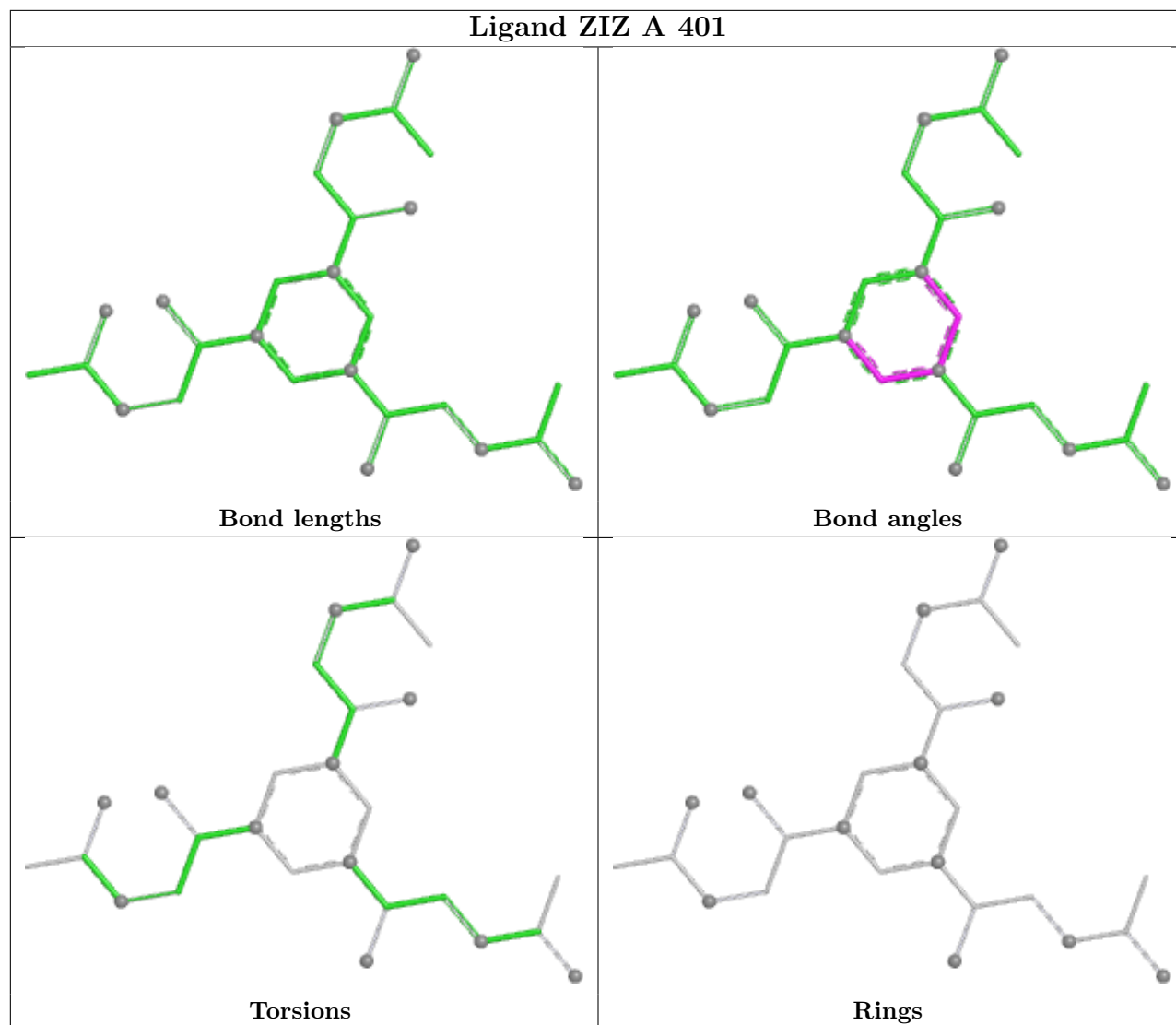
Ligand ZIZ D 401



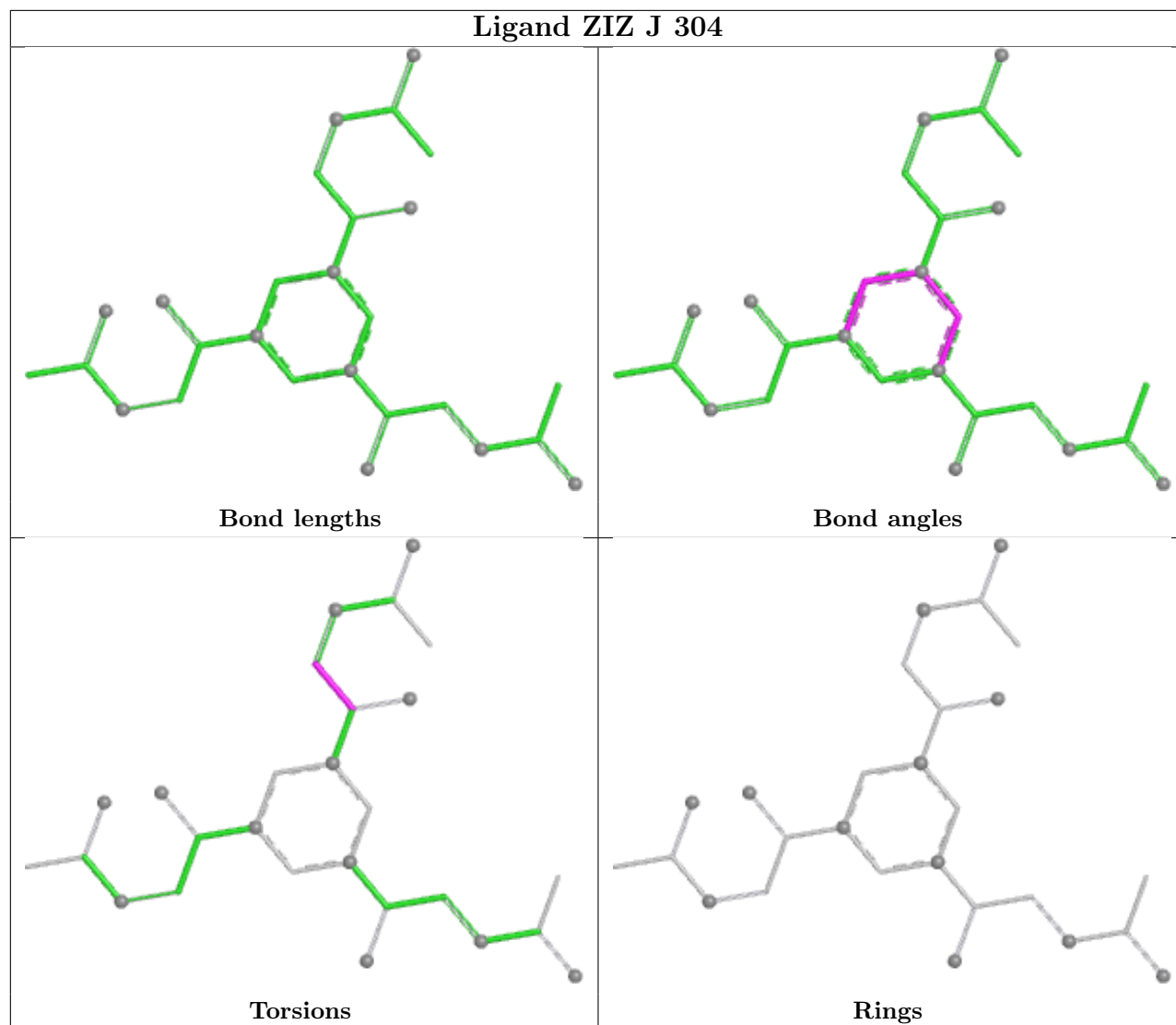
Ligand ZIZ G 301



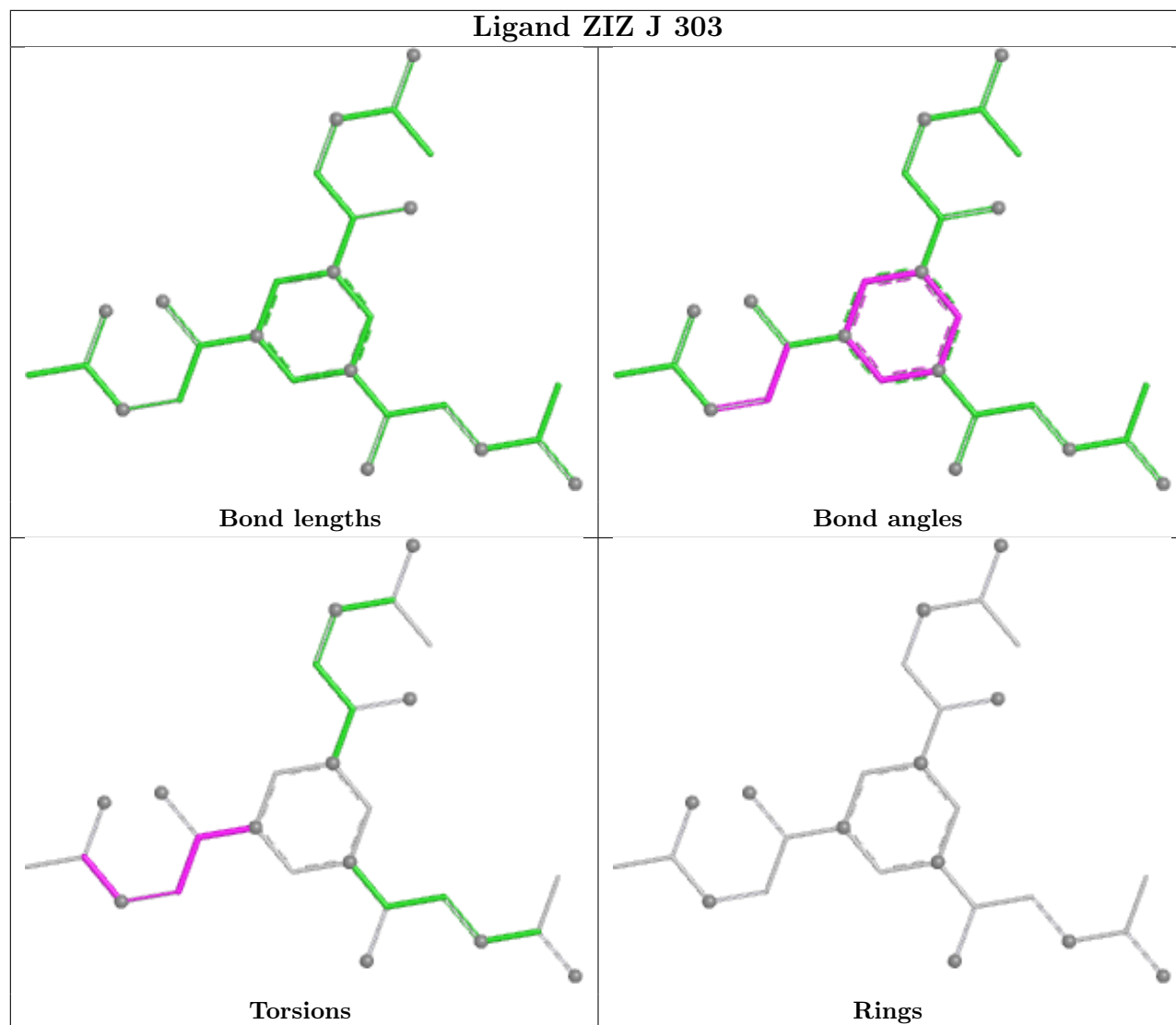
Ligand ZIZ A 401



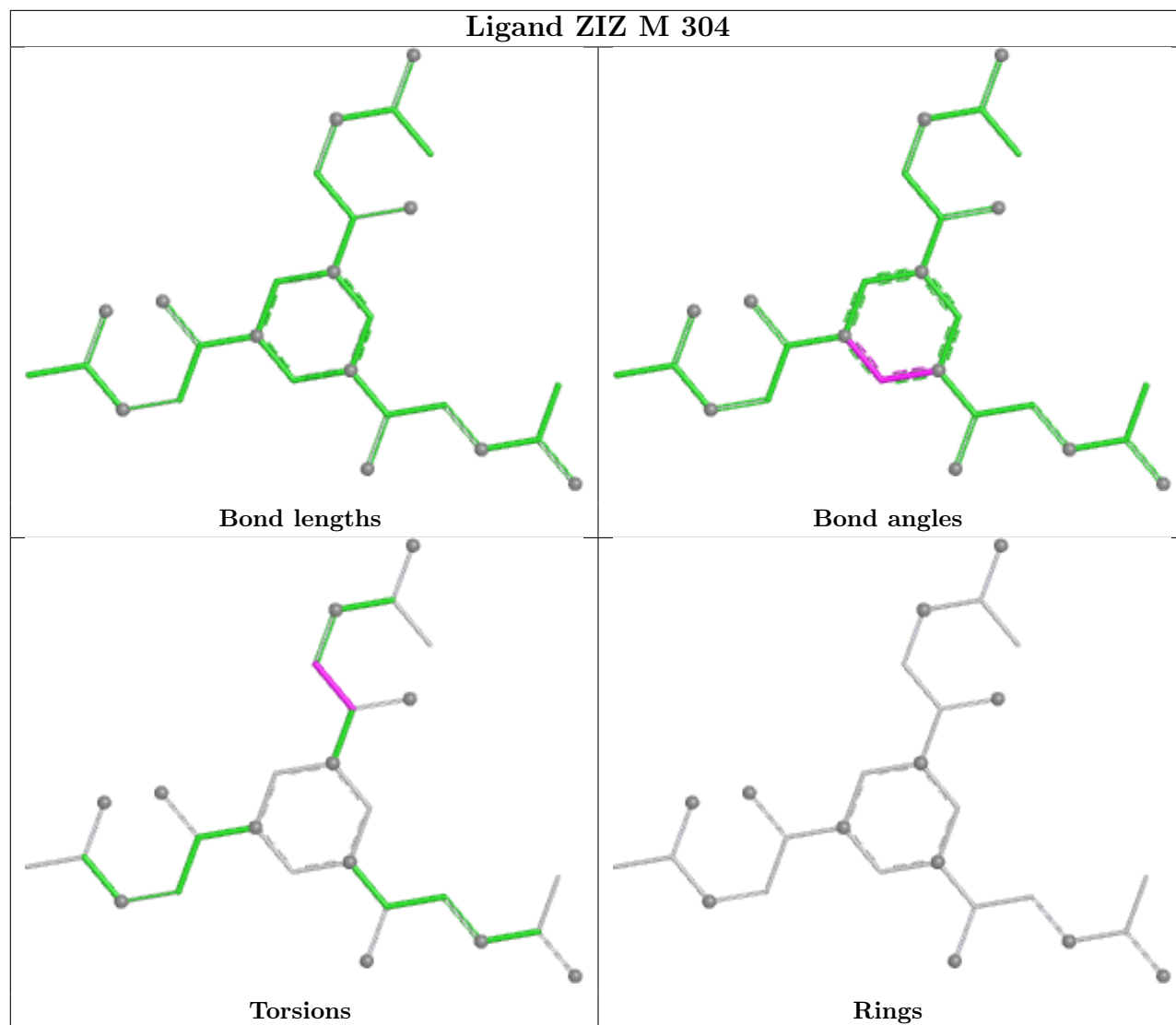
Ligand ZIZ J 304



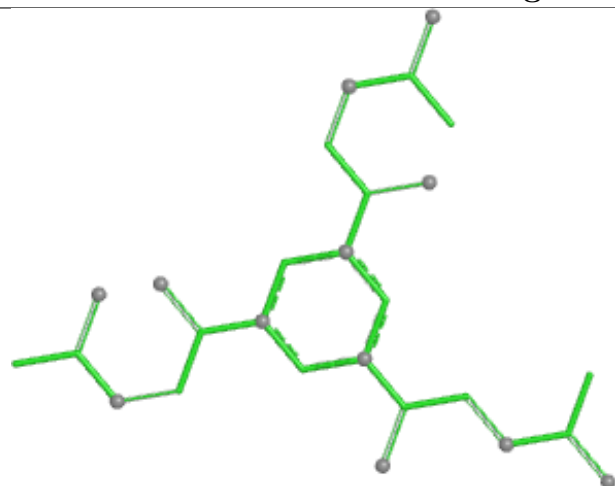
Ligand ZIZ J 303



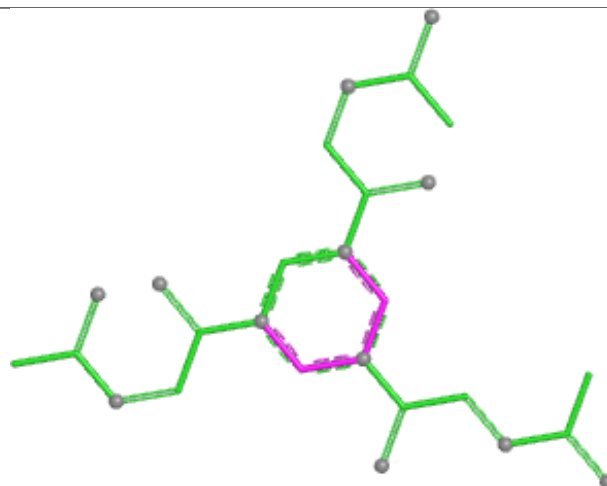
Ligand ZIZ M 304



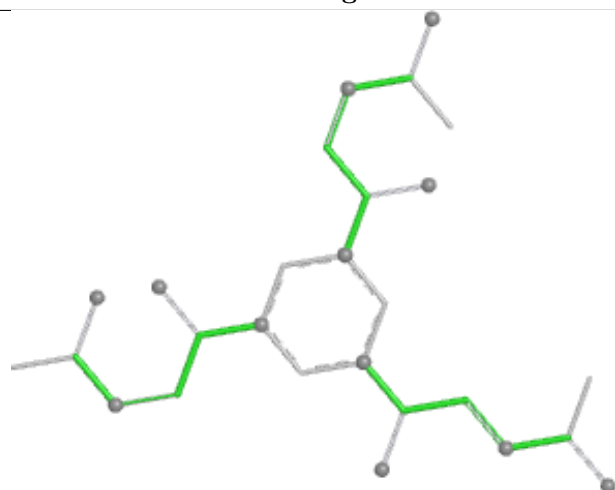
Ligand ZIZ G 303



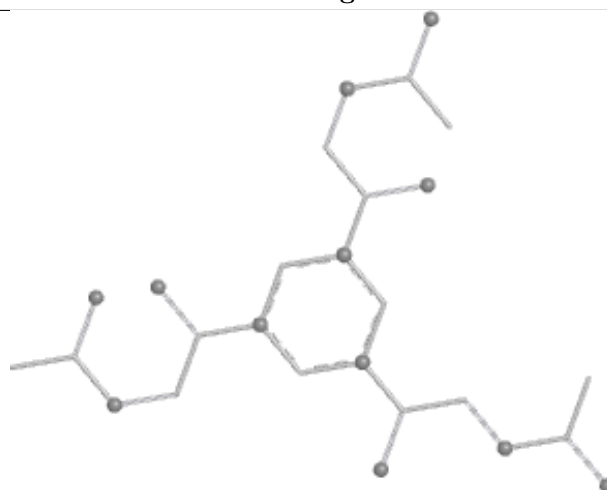
Bond lengths



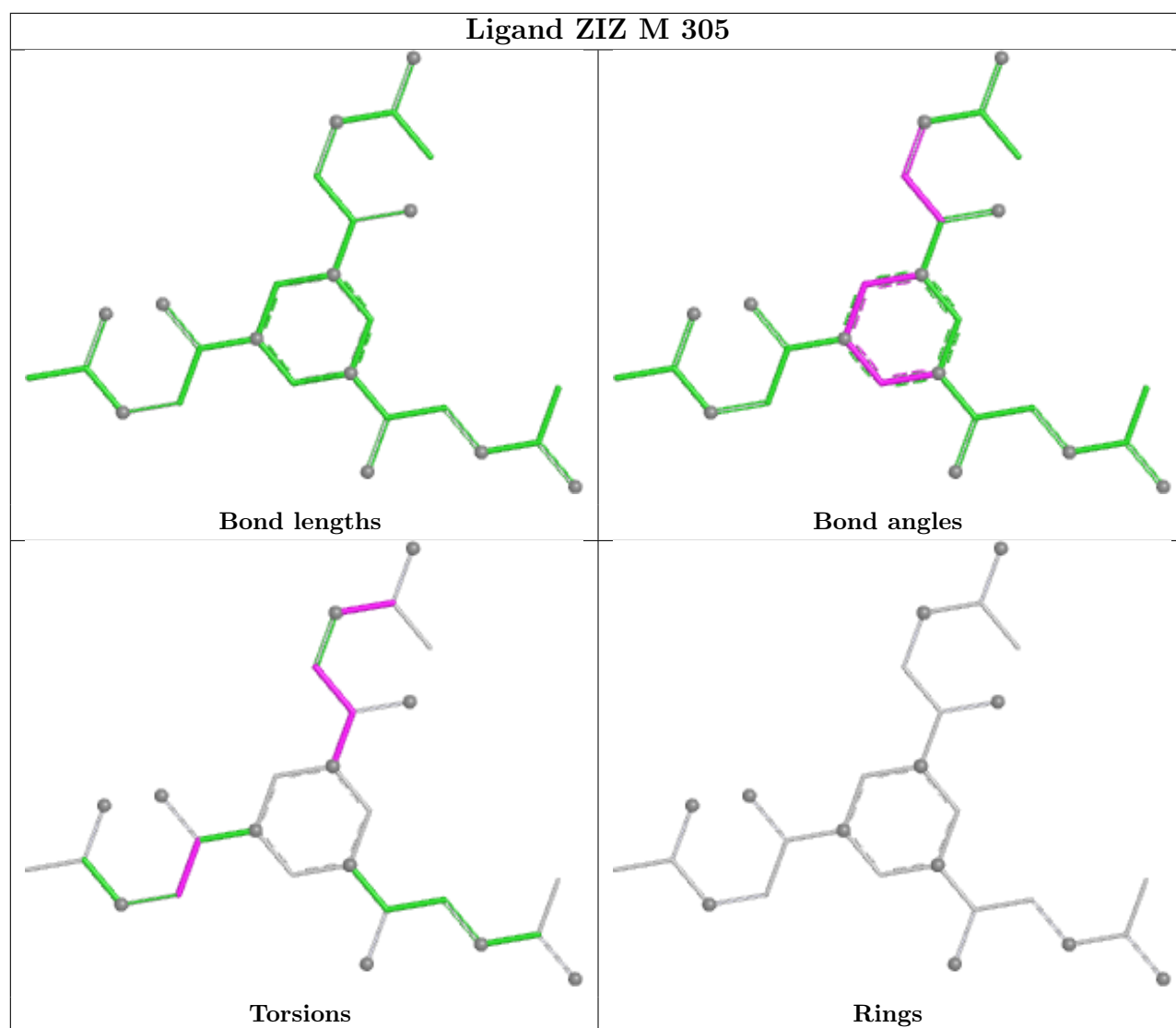
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	272/280 (97%)	-0.42	1 (0%) 88 86	51, 70, 93, 111	0
1	B	276/280 (98%)	-0.61	1 (0%) 88 86	26, 56, 73, 104	1 (0%)
1	C	271/280 (96%)	-0.41	0 100 100	53, 66, 86, 99	0
1	D	276/280 (98%)	-0.65	1 (0%) 88 86	26, 52, 70, 103	1 (0%)
1	E	273/280 (97%)	-0.42	0 100 100	50, 64, 87, 109	0
1	F	272/280 (97%)	-0.48	1 (0%) 88 86	47, 62, 82, 93	0
1	G	271/280 (96%)	-0.11	0 100 100	56, 87, 111, 136	0
1	H	275/280 (98%)	-0.55	0 100 100	43, 58, 77, 88	0
1	I	272/280 (97%)	0.11	1 (0%) 88 86	71, 95, 128, 148	0
1	J	271/280 (96%)	-0.61	0 100 100	26, 53, 69, 91	2 (0%)
1	K	272/280 (97%)	-0.61	0 100 100	28, 54, 72, 100	1 (0%)
1	L	271/280 (96%)	-0.67	0 100 100	27, 51, 67, 87	1 (0%)
1	M	271/280 (96%)	-0.34	1 (0%) 88 86	57, 75, 98, 113	0
1	N	271/280 (96%)	0.09	0 100 100	66, 94, 129, 150	0
1	O	271/280 (96%)	-0.00	1 (0%) 88 86	60, 89, 121, 139	0
All	All	4085/4200 (97%)	-0.38	7 (0%) 91 89	26, 66, 108, 150	6 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	GLY	3.5
1	B	277	HIS	2.4
1	O	272	ARG	2.4
1	D	277	HIS	2.3
1	F	273	GLY	2.3
1	I	199	PHE	2.2
1	M	111	ALA	2.1

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZIZ	G	301	27/30	0.71	0.11	110,125,135,139	0
2	ZIZ	M	304	27/30	0.73	0.12	115,131,138,143	0
2	ZIZ	M	305	27/30	0.73	0.12	100,123,126,129	0
3	GOL	K	303	6/6	0.73	0.14	83,90,94,99	0
2	ZIZ	D	401	27/30	0.78	0.12	81,99,107,110	0
2	ZIZ	D	402	27/30	0.78	0.12	96,111,121,127	0
2	ZIZ	J	304	27/30	0.80	0.12	78,94,99,102	0
2	ZIZ	A	402	27/30	0.81	0.11	88,104,112,112	0
2	ZIZ	G	303	27/30	0.81	0.12	105,117,124,125	0
2	ZIZ	J	303	27/30	0.83	0.12	91,96,105,107	0
3	GOL	F	302	6/6	0.85	0.10	87,92,95,97	0
2	ZIZ	A	401	27/30	0.85	0.10	84,96,104,107	0
3	GOL	F	301	6/6	0.88	0.10	49,51,52,57	0
3	GOL	M	301	6/6	0.88	0.14	74,80,83,84	0
3	GOL	D	403	6/6	0.91	0.10	81,87,91,91	0
3	GOL	D	404	6/6	0.92	0.13	62,73,76,79	0
3	GOL	L	301	6/6	0.92	0.09	49,49,51,51	0
3	GOL	K	302	6/6	0.92	0.11	70,75,78,79	0
3	GOL	B	301	6/6	0.93	0.09	50,55,55,58	0
3	GOL	G	302	6/6	0.93	0.08	72,78,81,81	0
3	GOL	K	304	6/6	0.93	0.13	71,80,83,85	0
3	GOL	H	301	6/6	0.93	0.08	57,59,61,62	0
3	GOL	L	302	6/6	0.93	0.12	79,81,84,84	0
3	GOL	I	301	6/6	0.93	0.10	68,79,80,80	0
3	GOL	M	303	6/6	0.93	0.10	64,69,72,76	0
3	GOL	O	301	6/6	0.93	0.09	75,78,78,80	0
3	GOL	J	302	6/6	0.94	0.10	66,74,82,87	0

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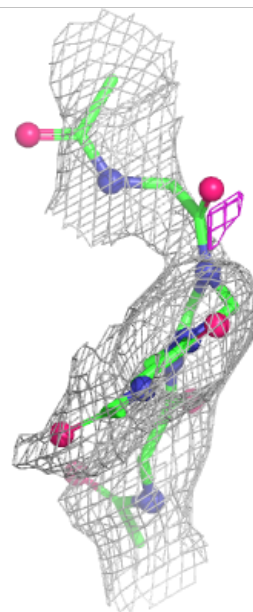
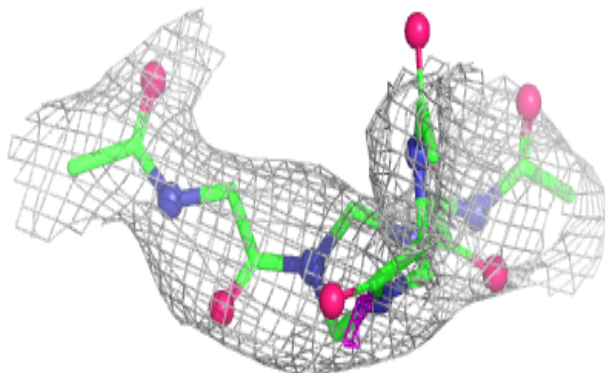
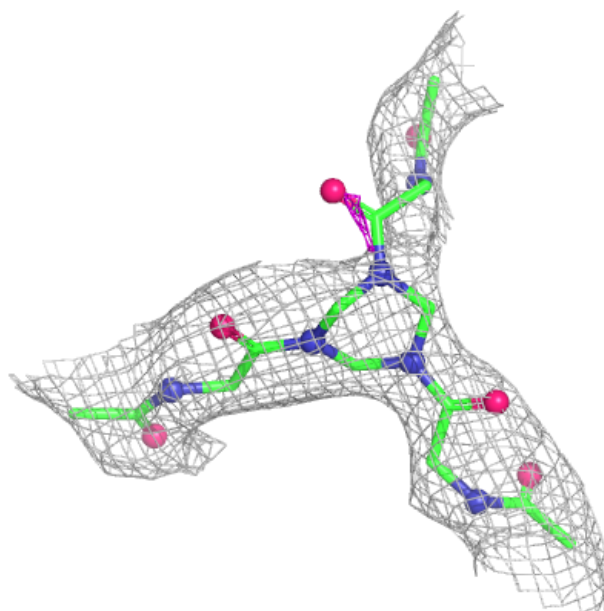
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	405	6/6	0.95	0.07	71,76,77,78	0
3	GOL	M	302	6/6	0.95	0.07	67,70,72,73	0
3	GOL	A	403	6/6	0.95	0.12	64,67,68,72	0
3	GOL	B	302	6/6	0.95	0.07	62,65,70,70	0
3	GOL	L	303	6/6	0.96	0.08	68,73,74,78	0
3	GOL	E	301	6/6	0.98	0.06	57,59,60,61	0
3	GOL	K	301	6/6	0.98	0.05	45,50,52,53	0
3	GOL	J	301	6/6	0.98	0.05	44,52,54,54	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.

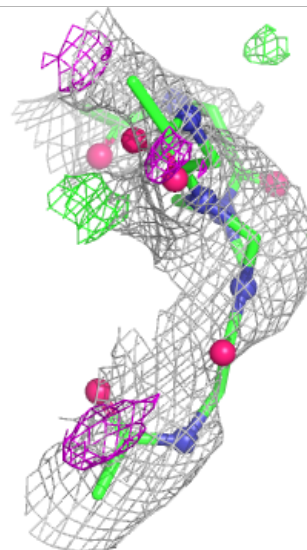
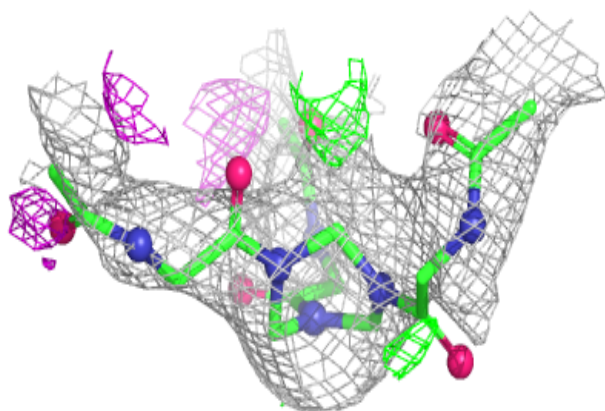
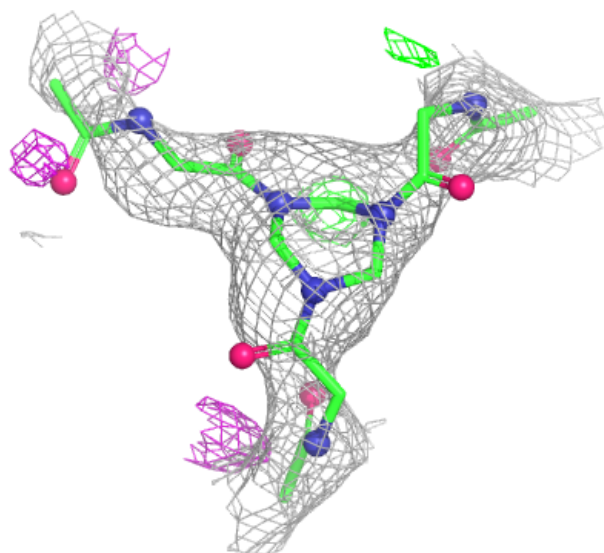
Electron density around ZIZ G 301:

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



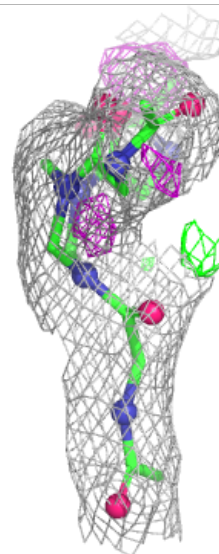
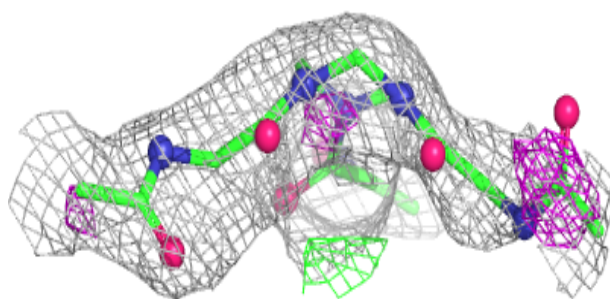
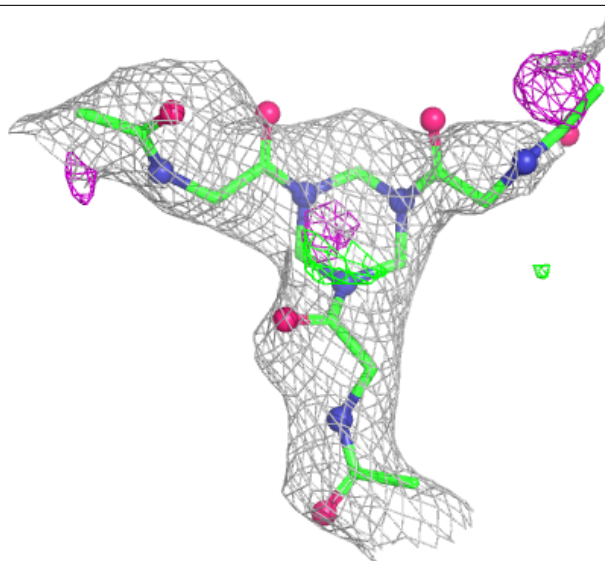
Electron density around ZIZ M 304:

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



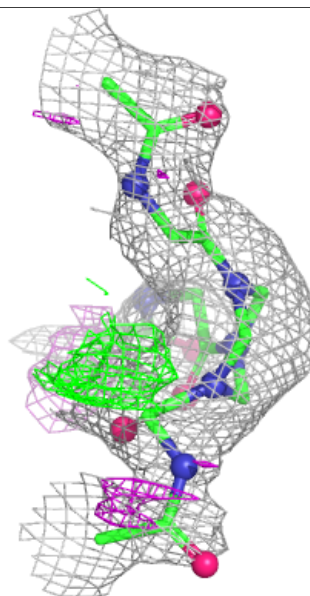
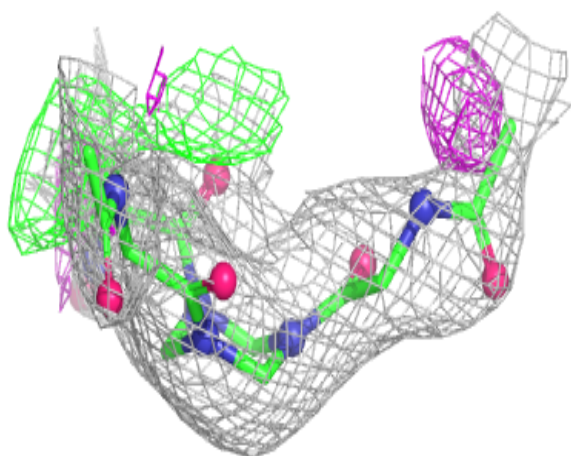
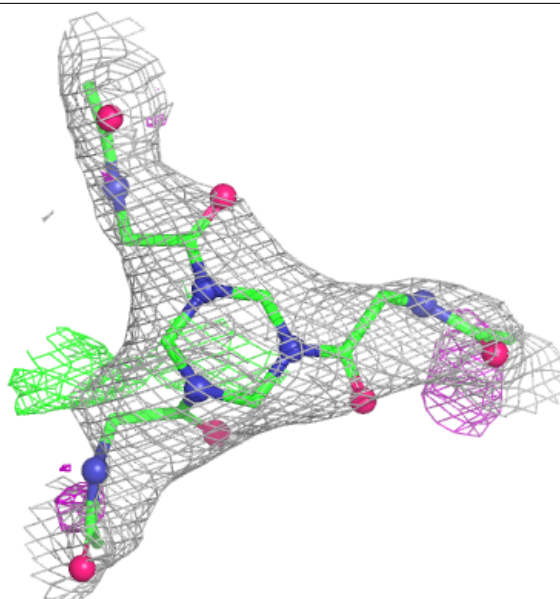
Electron density around ZIZ M 305:

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and green (positive)



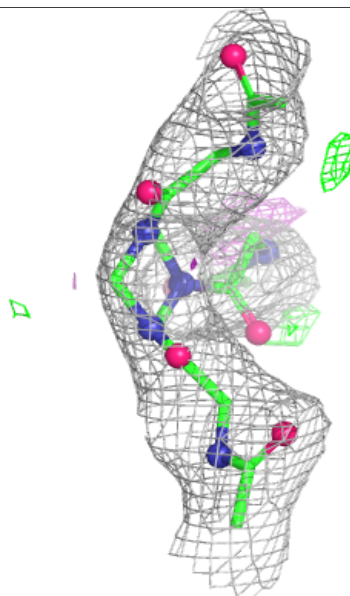
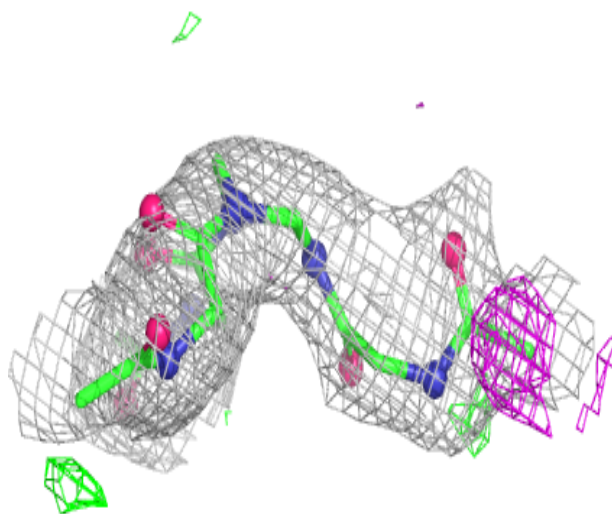
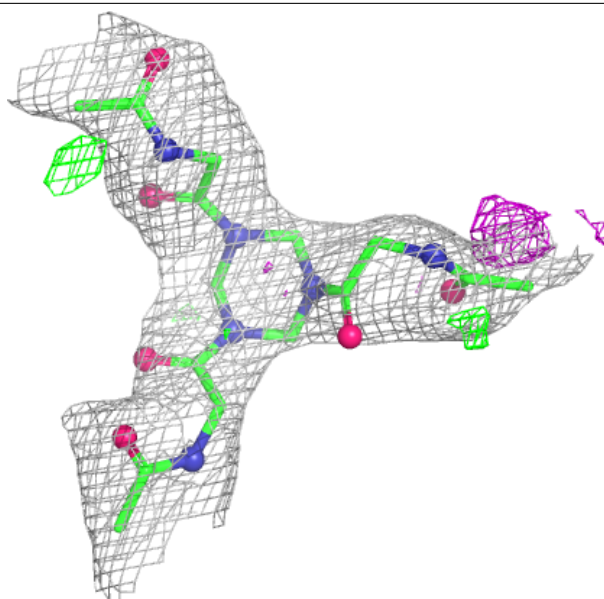
Electron density around ZIZ D 401:

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and green (positive)



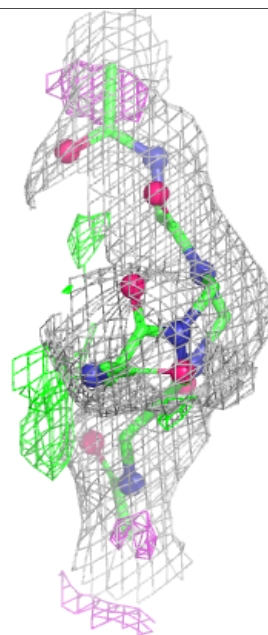
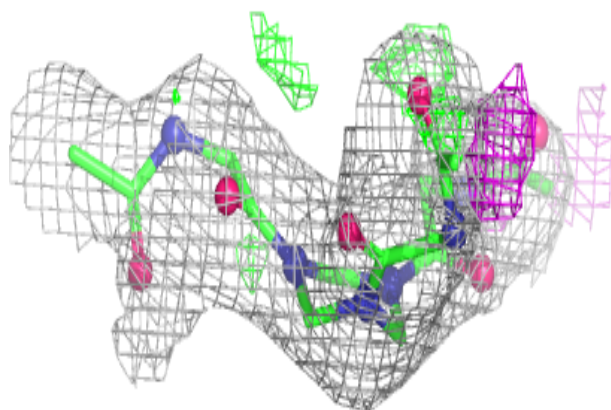
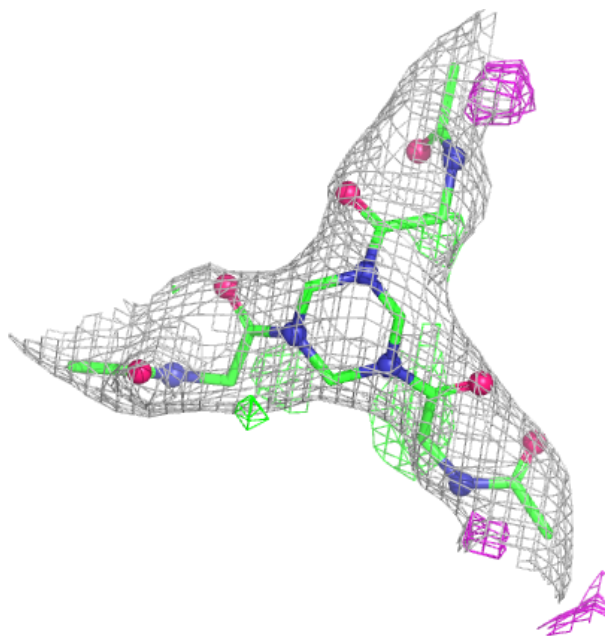
Electron density around ZIZ D 402:

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



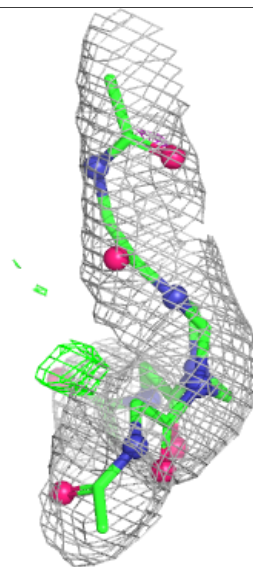
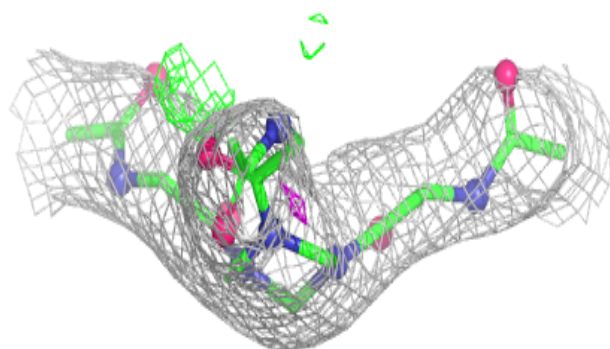
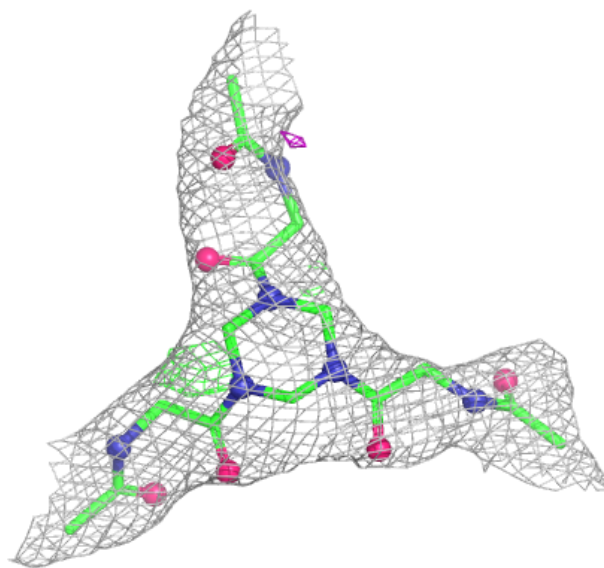
Electron density around ZIZ J 304:

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and green (positive)



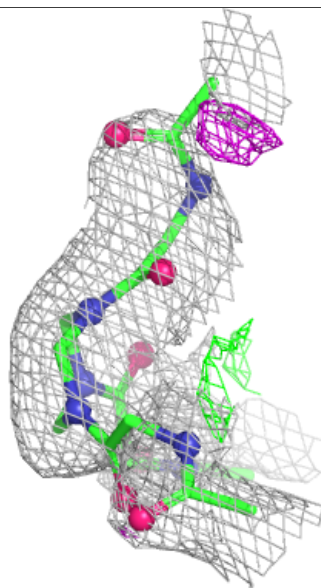
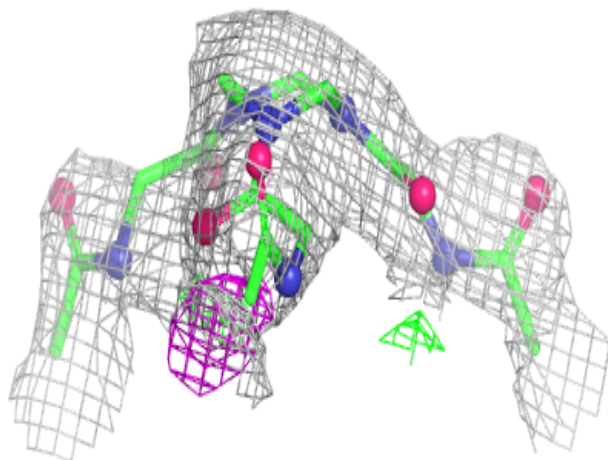
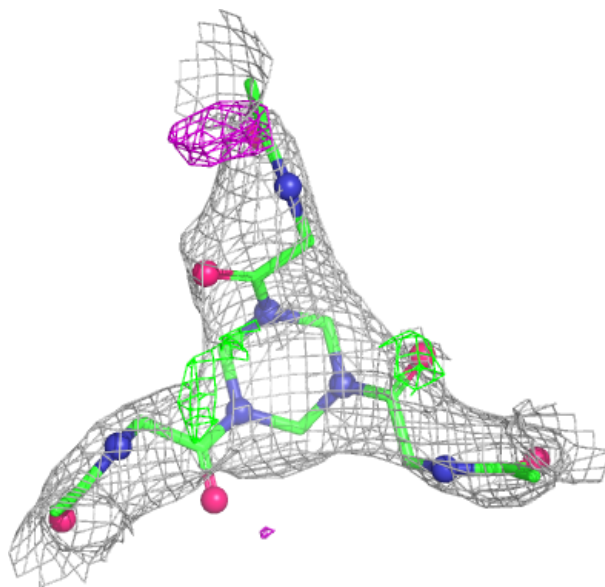
Electron density around ZIZ A 402:

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



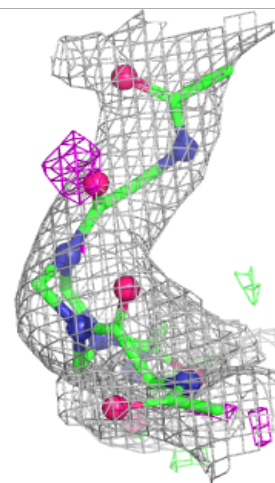
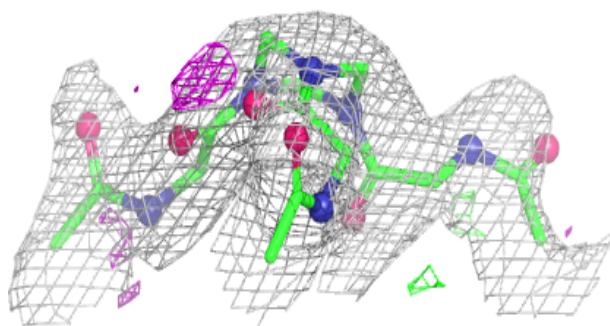
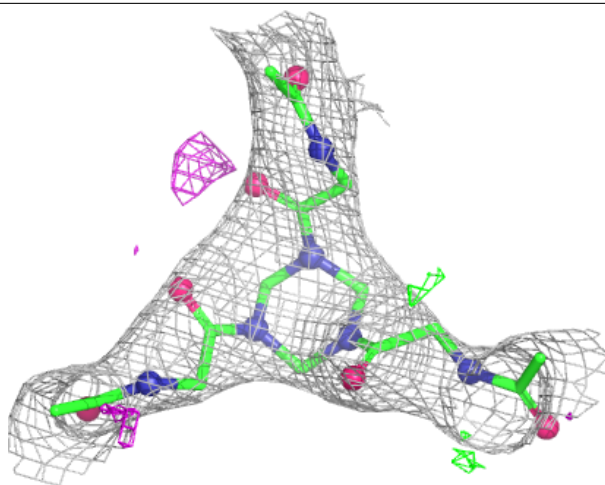
Electron density around ZIZ G 303:

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



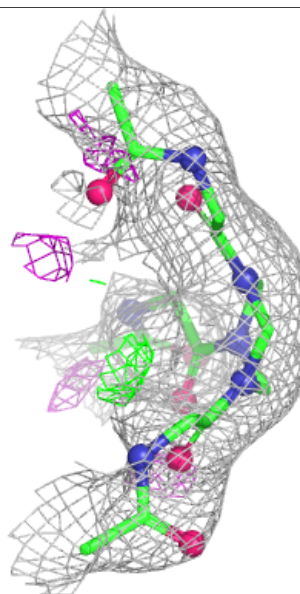
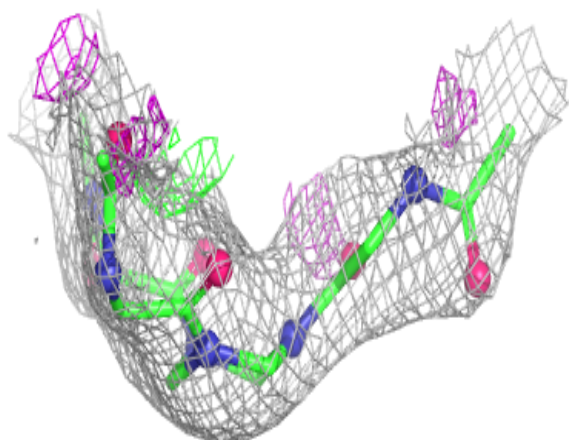
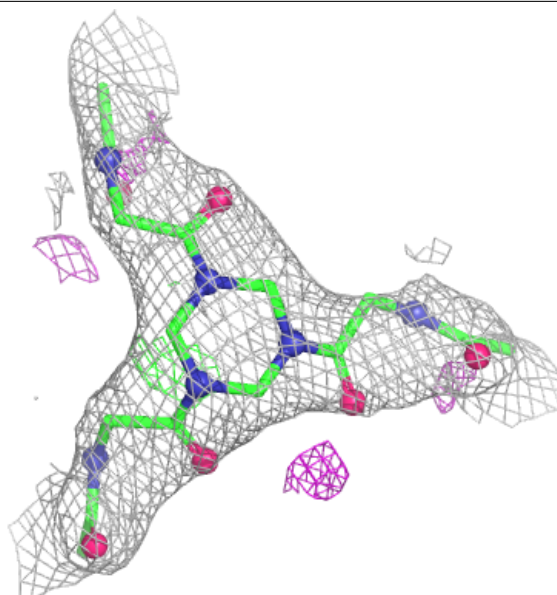
Electron density around ZIZ J 303:

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



Electron density around ZIZ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.