



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:19 PM UTC

PDB ID : 6CFD / pdb_00006cfd
Title : ADEP4 bound to E. faecium ClpP
Authors : Lee, R.E.; Griffith, E.C.
Deposited on : 2018-02-14
Resolution : 2.57 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

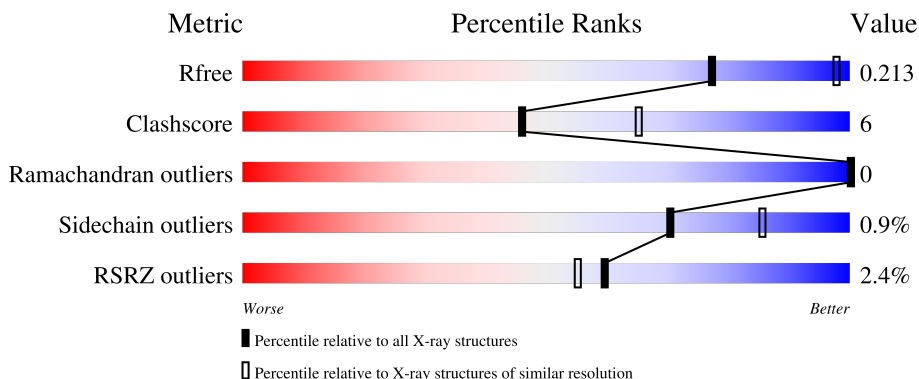
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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.



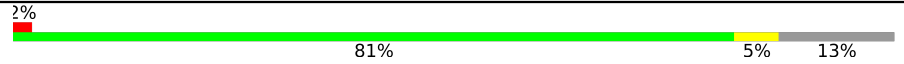

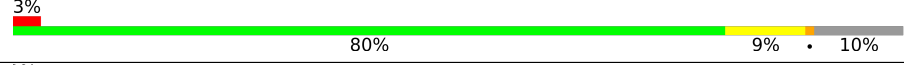



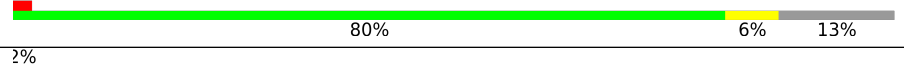


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	210	2% 80% 5% 14%
1	B	210	0% 80% 6% 13%
1	C	210	0% 78% 7% 14%
1	D	210	2% 80% 6% 14%
1	E	210	0% 80% 8% 12%

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Mol	Chain	Length	Quality of chain
1	F	210	
1	G	210	
1	I	210	
1	K	210	
1	L	210	
1	M	210	
1	N	210	
1	S	210	
1	T	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MPD	A	401	-	-	X	-
2	MPD	C	401	-	-	X	-
2	MPD	E	401	-	-	X	-
2	MPD	I	401	-	-	X	-
3	EZA	A	402	X	-	-	-
3	EZA	C	402	X	-	-	-
3	EZA	D	402	X	-	-	-
3	EZA	E	402	X	-	-	-
3	EZA	F	402	X	-	-	-
3	EZA	I	402	X	-	-	-
3	EZA	L	402	X	-	-	-
3	EZA	M	402	X	-	-	-
3	EZA	N	402	X	-	-	-
3	EZA	S	402	X	-	-	-
3	EZA	T	402	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20070 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	181	1370	862	231	268	9	0	0	0
1	B	182	1375	864	231	271	9	0	0	0
1	C	180	1361	856	229	267	9	0	0	0
1	D	181	1362	856	229	268	9	0	0	0
1	E	184	1385	871	234	271	9	0	0	0
1	F	183	1380	868	233	270	9	0	0	0
1	G	182	1367	859	230	269	9	0	0	0
1	I	188	1405	881	237	278	9	0	0	0
1	K	183	1380	868	233	270	9	0	0	0
1	L	180	1361	855	228	269	9	0	0	0
1	M	181	1370	862	231	268	9	0	0	0
1	N	182	1371	862	231	269	9	0	0	0
1	S	180	1357	853	228	267	9	0	0	0
1	T	181	1370	862	231	268	9	0	0	0

There are 196 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	LYS	-	expression tag	UNP A0A133CH35

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Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ILE	-	expression tag	UNP A0A133CH35
A	199	GLU	-	expression tag	UNP A0A133CH35
A	200	GLY	-	expression tag	UNP A0A133CH35
A	201	ARG	-	expression tag	UNP A0A133CH35
A	202	GLY	-	expression tag	UNP A0A133CH35
A	203	LEU	-	expression tag	UNP A0A133CH35
A	204	GLU	-	expression tag	UNP A0A133CH35
A	205	HIS	-	expression tag	UNP A0A133CH35
A	206	HIS	-	expression tag	UNP A0A133CH35
A	207	HIS	-	expression tag	UNP A0A133CH35
A	208	HIS	-	expression tag	UNP A0A133CH35
A	209	HIS	-	expression tag	UNP A0A133CH35
A	210	HIS	-	expression tag	UNP A0A133CH35
B	197	LYS	-	expression tag	UNP A0A133CH35
B	198	ILE	-	expression tag	UNP A0A133CH35
B	199	GLU	-	expression tag	UNP A0A133CH35
B	200	GLY	-	expression tag	UNP A0A133CH35
B	201	ARG	-	expression tag	UNP A0A133CH35
B	202	GLY	-	expression tag	UNP A0A133CH35
B	203	LEU	-	expression tag	UNP A0A133CH35
B	204	GLU	-	expression tag	UNP A0A133CH35
B	205	HIS	-	expression tag	UNP A0A133CH35
B	206	HIS	-	expression tag	UNP A0A133CH35
B	207	HIS	-	expression tag	UNP A0A133CH35
B	208	HIS	-	expression tag	UNP A0A133CH35
B	209	HIS	-	expression tag	UNP A0A133CH35
B	210	HIS	-	expression tag	UNP A0A133CH35
C	197	LYS	-	expression tag	UNP A0A133CH35
C	198	ILE	-	expression tag	UNP A0A133CH35
C	199	GLU	-	expression tag	UNP A0A133CH35
C	200	GLY	-	expression tag	UNP A0A133CH35
C	201	ARG	-	expression tag	UNP A0A133CH35
C	202	GLY	-	expression tag	UNP A0A133CH35
C	203	LEU	-	expression tag	UNP A0A133CH35
C	204	GLU	-	expression tag	UNP A0A133CH35
C	205	HIS	-	expression tag	UNP A0A133CH35
C	206	HIS	-	expression tag	UNP A0A133CH35
C	207	HIS	-	expression tag	UNP A0A133CH35
C	208	HIS	-	expression tag	UNP A0A133CH35
C	209	HIS	-	expression tag	UNP A0A133CH35
C	210	HIS	-	expression tag	UNP A0A133CH35
D	197	LYS	-	expression tag	UNP A0A133CH35

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Chain	Residue	Modelled	Actual	Comment	Reference
D	198	ILE	-	expression tag	UNP A0A133CH35
D	199	GLU	-	expression tag	UNP A0A133CH35
D	200	GLY	-	expression tag	UNP A0A133CH35
D	201	ARG	-	expression tag	UNP A0A133CH35
D	202	GLY	-	expression tag	UNP A0A133CH35
D	203	LEU	-	expression tag	UNP A0A133CH35
D	204	GLU	-	expression tag	UNP A0A133CH35
D	205	HIS	-	expression tag	UNP A0A133CH35
D	206	HIS	-	expression tag	UNP A0A133CH35
D	207	HIS	-	expression tag	UNP A0A133CH35
D	208	HIS	-	expression tag	UNP A0A133CH35
D	209	HIS	-	expression tag	UNP A0A133CH35
D	210	HIS	-	expression tag	UNP A0A133CH35
E	197	LYS	-	expression tag	UNP A0A133CH35
E	198	ILE	-	expression tag	UNP A0A133CH35
E	199	GLU	-	expression tag	UNP A0A133CH35
E	200	GLY	-	expression tag	UNP A0A133CH35
E	201	ARG	-	expression tag	UNP A0A133CH35
E	202	GLY	-	expression tag	UNP A0A133CH35
E	203	LEU	-	expression tag	UNP A0A133CH35
E	204	GLU	-	expression tag	UNP A0A133CH35
E	205	HIS	-	expression tag	UNP A0A133CH35
E	206	HIS	-	expression tag	UNP A0A133CH35
E	207	HIS	-	expression tag	UNP A0A133CH35
E	208	HIS	-	expression tag	UNP A0A133CH35
E	209	HIS	-	expression tag	UNP A0A133CH35
E	210	HIS	-	expression tag	UNP A0A133CH35
F	197	LYS	-	expression tag	UNP A0A133CH35
F	198	ILE	-	expression tag	UNP A0A133CH35
F	199	GLU	-	expression tag	UNP A0A133CH35
F	200	GLY	-	expression tag	UNP A0A133CH35
F	201	ARG	-	expression tag	UNP A0A133CH35
F	202	GLY	-	expression tag	UNP A0A133CH35
F	203	LEU	-	expression tag	UNP A0A133CH35
F	204	GLU	-	expression tag	UNP A0A133CH35
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F	207	HIS	-	expression tag	UNP A0A133CH35
F	208	HIS	-	expression tag	UNP A0A133CH35
F	209	HIS	-	expression tag	UNP A0A133CH35
F	210	HIS	-	expression tag	UNP A0A133CH35
G	197	LYS	-	expression tag	UNP A0A133CH35

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Chain	Residue	Modelled	Actual	Comment	Reference
G	198	ILE	-	expression tag	UNP A0A133CH35
G	199	GLU	-	expression tag	UNP A0A133CH35
G	200	GLY	-	expression tag	UNP A0A133CH35
G	201	ARG	-	expression tag	UNP A0A133CH35
G	202	GLY	-	expression tag	UNP A0A133CH35
G	203	LEU	-	expression tag	UNP A0A133CH35
G	204	GLU	-	expression tag	UNP A0A133CH35
G	205	HIS	-	expression tag	UNP A0A133CH35
G	206	HIS	-	expression tag	UNP A0A133CH35
G	207	HIS	-	expression tag	UNP A0A133CH35
G	208	HIS	-	expression tag	UNP A0A133CH35
G	209	HIS	-	expression tag	UNP A0A133CH35
G	210	HIS	-	expression tag	UNP A0A133CH35
I	197	LYS	-	expression tag	UNP A0A133CH35
I	198	ILE	-	expression tag	UNP A0A133CH35
I	199	GLU	-	expression tag	UNP A0A133CH35
I	200	GLY	-	expression tag	UNP A0A133CH35
I	201	ARG	-	expression tag	UNP A0A133CH35
I	202	GLY	-	expression tag	UNP A0A133CH35
I	203	LEU	-	expression tag	UNP A0A133CH35
I	204	GLU	-	expression tag	UNP A0A133CH35
I	205	HIS	-	expression tag	UNP A0A133CH35
I	206	HIS	-	expression tag	UNP A0A133CH35
I	207	HIS	-	expression tag	UNP A0A133CH35
I	208	HIS	-	expression tag	UNP A0A133CH35
I	209	HIS	-	expression tag	UNP A0A133CH35
I	210	HIS	-	expression tag	UNP A0A133CH35
K	197	LYS	-	expression tag	UNP A0A133CH35
K	198	ILE	-	expression tag	UNP A0A133CH35
K	199	GLU	-	expression tag	UNP A0A133CH35
K	200	GLY	-	expression tag	UNP A0A133CH35
K	201	ARG	-	expression tag	UNP A0A133CH35
K	202	GLY	-	expression tag	UNP A0A133CH35
K	203	LEU	-	expression tag	UNP A0A133CH35
K	204	GLU	-	expression tag	UNP A0A133CH35
K	205	HIS	-	expression tag	UNP A0A133CH35
K	206	HIS	-	expression tag	UNP A0A133CH35
K	207	HIS	-	expression tag	UNP A0A133CH35
K	208	HIS	-	expression tag	UNP A0A133CH35
K	209	HIS	-	expression tag	UNP A0A133CH35
K	210	HIS	-	expression tag	UNP A0A133CH35
L	197	LYS	-	expression tag	UNP A0A133CH35

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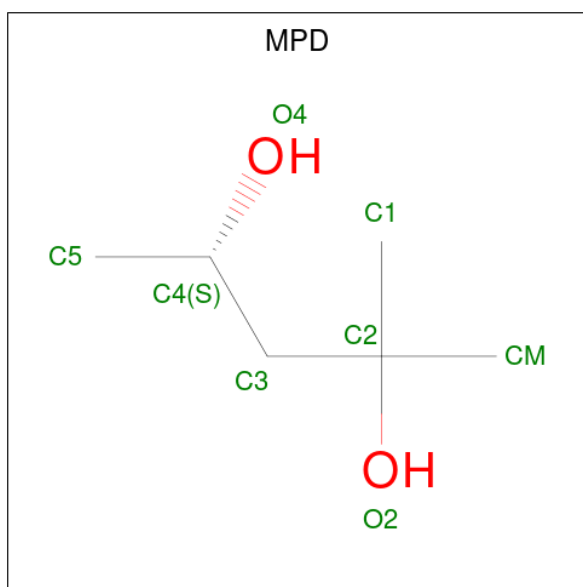
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L	199	GLU	-	expression tag	UNP A0A133CH35
L	200	GLY	-	expression tag	UNP A0A133CH35
L	201	ARG	-	expression tag	UNP A0A133CH35
L	202	GLY	-	expression tag	UNP A0A133CH35
L	203	LEU	-	expression tag	UNP A0A133CH35
L	204	GLU	-	expression tag	UNP A0A133CH35
L	205	HIS	-	expression tag	UNP A0A133CH35
L	206	HIS	-	expression tag	UNP A0A133CH35
L	207	HIS	-	expression tag	UNP A0A133CH35
L	208	HIS	-	expression tag	UNP A0A133CH35
L	209	HIS	-	expression tag	UNP A0A133CH35
L	210	HIS	-	expression tag	UNP A0A133CH35
M	197	LYS	-	expression tag	UNP A0A133CH35
M	198	ILE	-	expression tag	UNP A0A133CH35
M	199	GLU	-	expression tag	UNP A0A133CH35
M	200	GLY	-	expression tag	UNP A0A133CH35
M	201	ARG	-	expression tag	UNP A0A133CH35
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M	204	GLU	-	expression tag	UNP A0A133CH35
M	205	HIS	-	expression tag	UNP A0A133CH35
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M	207	HIS	-	expression tag	UNP A0A133CH35
M	208	HIS	-	expression tag	UNP A0A133CH35
M	209	HIS	-	expression tag	UNP A0A133CH35
M	210	HIS	-	expression tag	UNP A0A133CH35
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N	198	ILE	-	expression tag	UNP A0A133CH35
N	199	GLU	-	expression tag	UNP A0A133CH35
N	200	GLY	-	expression tag	UNP A0A133CH35
N	201	ARG	-	expression tag	UNP A0A133CH35
N	202	GLY	-	expression tag	UNP A0A133CH35
N	203	LEU	-	expression tag	UNP A0A133CH35
N	204	GLU	-	expression tag	UNP A0A133CH35
N	205	HIS	-	expression tag	UNP A0A133CH35
N	206	HIS	-	expression tag	UNP A0A133CH35
N	207	HIS	-	expression tag	UNP A0A133CH35
N	208	HIS	-	expression tag	UNP A0A133CH35
N	209	HIS	-	expression tag	UNP A0A133CH35
N	210	HIS	-	expression tag	UNP A0A133CH35
S	197	LYS	-	expression tag	UNP A0A133CH35

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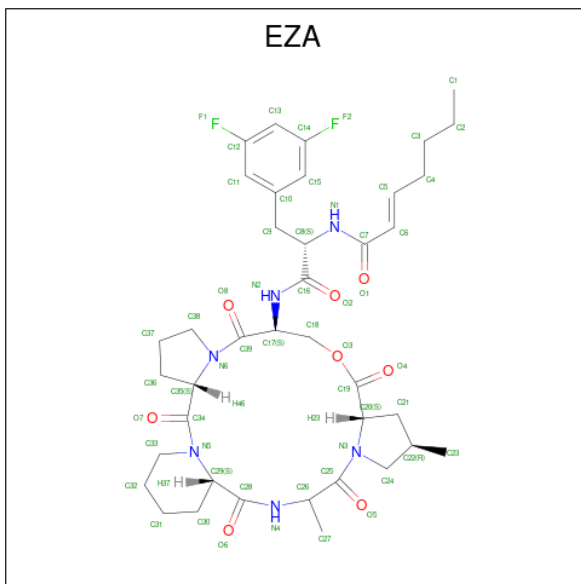
Chain	Residue	Modelled	Actual	Comment	Reference
S	198	ILE	-	expression tag	UNP A0A133CH35
S	199	GLU	-	expression tag	UNP A0A133CH35
S	200	GLY	-	expression tag	UNP A0A133CH35
S	201	ARG	-	expression tag	UNP A0A133CH35
S	202	GLY	-	expression tag	UNP A0A133CH35
S	203	LEU	-	expression tag	UNP A0A133CH35
S	204	GLU	-	expression tag	UNP A0A133CH35
S	205	HIS	-	expression tag	UNP A0A133CH35
S	206	HIS	-	expression tag	UNP A0A133CH35
S	207	HIS	-	expression tag	UNP A0A133CH35
S	208	HIS	-	expression tag	UNP A0A133CH35
S	209	HIS	-	expression tag	UNP A0A133CH35
S	210	HIS	-	expression tag	UNP A0A133CH35
T	197	LYS	-	expression tag	UNP A0A133CH35
T	198	ILE	-	expression tag	UNP A0A133CH35
T	199	GLU	-	expression tag	UNP A0A133CH35
T	200	GLY	-	expression tag	UNP A0A133CH35
T	201	ARG	-	expression tag	UNP A0A133CH35
T	202	GLY	-	expression tag	UNP A0A133CH35
T	203	LEU	-	expression tag	UNP A0A133CH35
T	204	GLU	-	expression tag	UNP A0A133CH35
T	205	HIS	-	expression tag	UNP A0A133CH35
T	206	HIS	-	expression tag	UNP A0A133CH35
T	207	HIS	-	expression tag	UNP A0A133CH35
T	208	HIS	-	expression tag	UNP A0A133CH35
T	209	HIS	-	expression tag	UNP A0A133CH35
T	210	HIS	-	expression tag	UNP A0A133CH35

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 8 6 2	0	0
2	B	1	Total C O 8 6 2	0	0
2	C	1	Total C O 8 6 2	0	0
2	D	1	Total C O 8 6 2	0	0
2	E	1	Total C O 8 6 2	0	0
2	F	1	Total C O 8 6 2	0	0
2	G	1	Total C O 8 6 2	0	0
2	I	1	Total C O 8 6 2	0	0
2	K	1	Total C O 8 6 2	0	0
2	L	1	Total C O 8 6 2	0	0
2	M	1	Total C O 8 6 2	0	0
2	N	1	Total C O 8 6 2	0	0
2	S	1	Total C O 8 6 2	0	0
2	T	1	Total C O 8 6 2	0	0

- Molecule 3 is N-[(6aS,12S,15aS,17R,21R,23aS)-17,21-dimethyl-6,11,15,20,23-pentaoxooctadecahydro-2H,6H,11H,15H-pyrido[2,1-i]dipyrrolo[2,1-c:2',1'-l][1,4,7,10,13]oxatetraazacyclohexadecin-12-yl]-3,5-difluoro-Nalpha-[(2E)-hept-2-enoyl]-L-phenylalaninamide (CCD ID: EZA) (formula: C₃₉H₅₂F₂N₆O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
3	A	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	C	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	D	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	E	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	F	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	I	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	L	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	M	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	N	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	S	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
3	T	1	Total	C	F	N	O	0	0
			55	39	2	6	8		

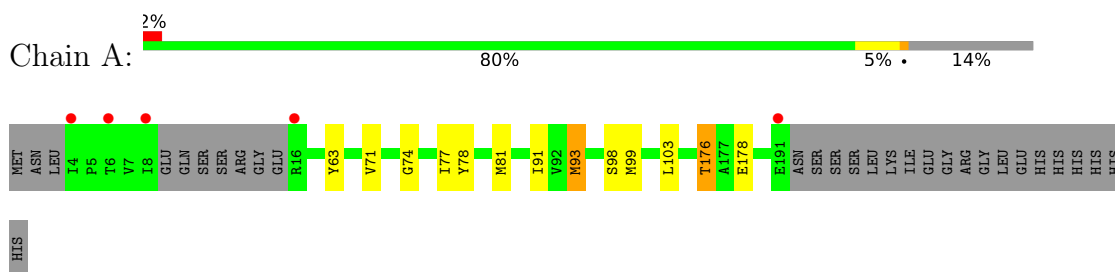
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	11	Total O 11 11	0	0
4	C	8	Total O 8 8	0	0
4	D	8	Total O 8 8	0	0
4	E	6	Total O 6 6	0	0
4	F	11	Total O 11 11	0	0
4	G	15	Total O 15 15	0	0
4	I	9	Total O 9 9	0	0
4	K	14	Total O 14 14	0	0
4	L	10	Total O 10 10	0	0
4	M	7	Total O 7 7	0	0
4	N	12	Total O 12 12	0	0
4	S	13	Total O 13 13	0	0
4	T	6	Total O 6 6	0	0

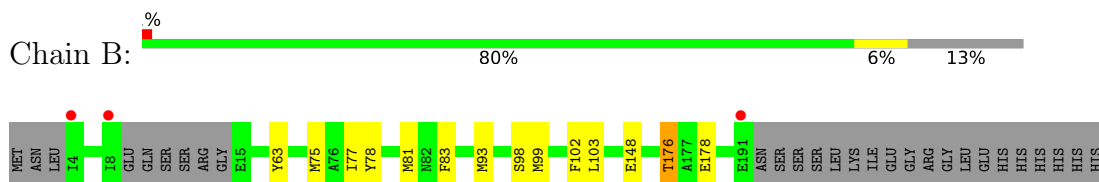
3 Residue-property plots [i](#)

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.

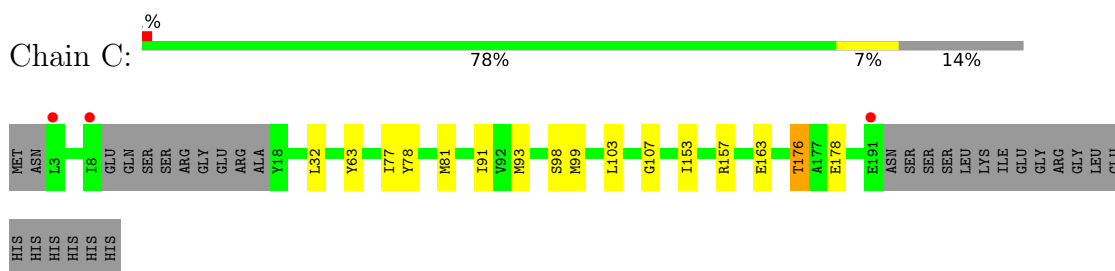
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



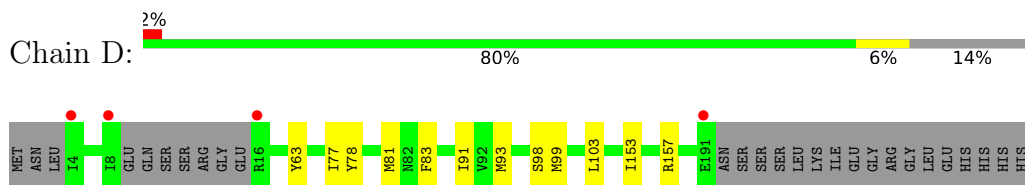
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



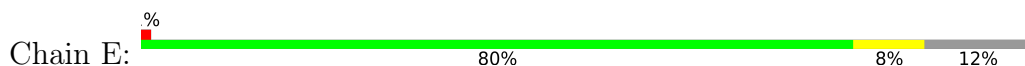
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



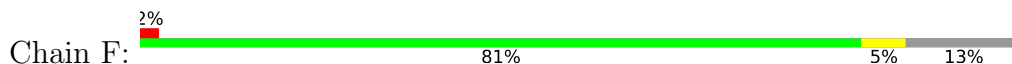
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



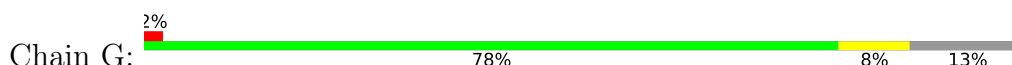


HIS

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

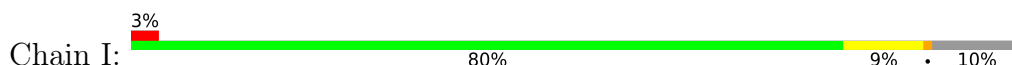


• Molecule 1: ATP-dependent Clp protease proteolytic subunit



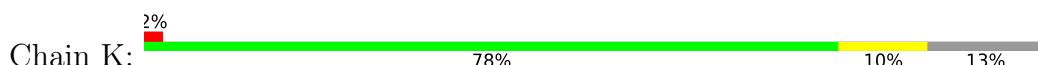
LEU
GLU
HIS
HIS
HIS
HIS
HIS

• Molecule 1: ATP-dependent Clp protease proteolytic subunit



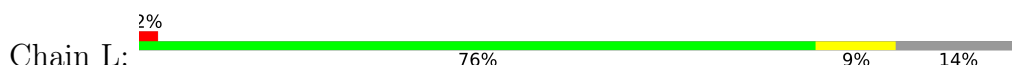
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: ATP-dependent Clp protease proteolytic subunit



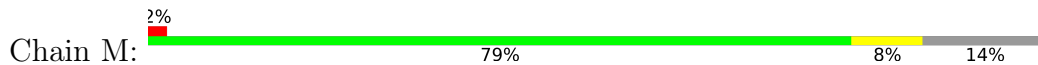
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS

• Molecule 1: ATP-dependent Clp protease proteolytic subunit



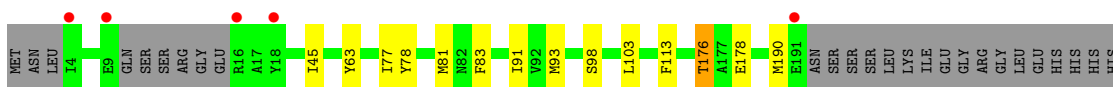
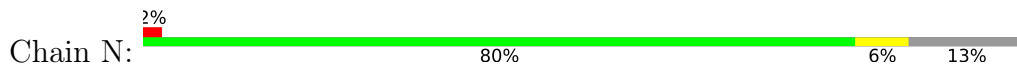
LYS
ILE
GLU
GLY
ARG
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS

● Molecule 1: ATP-dependent Clp protease proteolytic subunit



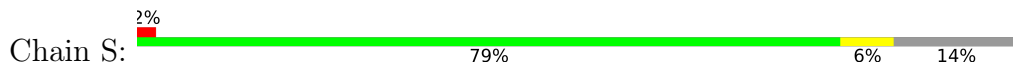
HIS
HIS
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HIS

● Molecule 1: ATP-dependent Clp protease proteolytic subunit



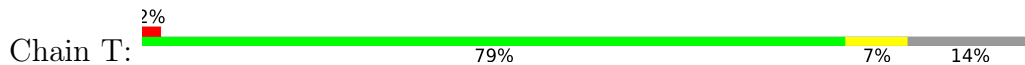
HIS
HIS

● Molecule 1: ATP-dependent Clp protease proteolytic subunit



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● Molecule 1: ATP-dependent Clp protease proteolytic subunit



HIS
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4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.39Å 202.17Å 97.39Å 90.00° 102.69° 90.00°	Depositor
Resolution (Å)	101.08 – 2.57 101.08 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.9 (101.08-2.57) 98.9 (101.08-2.58)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.58Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.209 0.179 , 0.213	Depositor DCC
R_{free} test set	5708 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtrriage
Anisotropy	0.569	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.176 for l,-k,h	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20070	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.92	0/1386	0.93	1/1875 (0.1%)
1	B	1.06	0/1391	0.96	0/1883
1	C	1.05	0/1377	1.00	1/1864 (0.1%)
1	D	1.03	0/1378	0.97	0/1867
1	E	1.04	0/1401	0.98	1/1896 (0.1%)
1	F	1.00	0/1396	0.96	0/1889
1	G	1.03	2/1383 (0.1%)	0.97	0/1874
1	I	1.07	2/1421 (0.1%)	1.00	0/1924
1	K	1.06	1/1396 (0.1%)	0.97	1/1889 (0.1%)
1	L	1.00	0/1377	0.98	0/1865
1	M	1.00	1/1386 (0.1%)	0.97	0/1875
1	N	0.96	0/1387	0.94	0/1878
1	S	1.04	1/1373 (0.1%)	1.00	0/1860
1	T	1.05	0/1386	1.00	1/1875 (0.1%)
All	All	1.02	7/19438 (0.0%)	0.97	5/26314 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	4	ILE	N-CA	6.42	1.51	1.46
1	M	174	TYR	C-O	-5.53	1.17	1.24
1	K	4	ILE	N-CA	5.34	1.50	1.46
1	G	69	GLY	C-O	-5.23	1.20	1.23
1	S	69	GLY	C-O	-5.23	1.20	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	GLY	N-CA-C	-6.61	105.06	112.33
1	E	4	ILE	N-CA-C	6.19	114.22	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	4	ILE	N-CA-C	6.15	114.18	107.60
1	A	93	MET	CG-SD-CE	-6.09	87.50	100.90
1	T	4	ILE	N-CA-C	5.83	113.83	107.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1370	0	1363	18	0
1	B	1375	0	1358	18	0
1	C	1361	0	1347	16	0
1	D	1362	0	1341	12	0
1	E	1385	0	1369	18	0
1	F	1380	0	1367	13	0
1	G	1367	0	1343	13	0
1	I	1405	0	1374	21	0
1	K	1380	0	1367	19	0
1	L	1361	0	1343	18	0
1	M	1370	0	1363	15	0
1	N	1371	0	1354	12	0
1	S	1357	0	1339	15	0
1	T	1370	0	1363	13	0
2	A	8	0	14	6	0
2	B	8	0	14	5	0
2	C	8	0	14	7	0
2	D	8	0	14	4	0
2	E	8	0	14	7	0
2	F	8	0	14	4	0
2	G	8	0	14	5	0
2	I	8	0	14	7	0
2	K	8	0	14	5	0
2	L	8	0	14	4	0
2	M	8	0	14	4	0
2	N	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	8	0	14	5	0
2	T	8	0	14	4	0
3	A	55	0	0	2	0
3	C	55	0	0	1	0
3	D	55	0	0	1	0
3	E	55	0	0	0	0
3	F	55	0	0	1	0
3	I	55	0	0	0	0
3	L	55	0	0	1	0
3	M	55	0	0	2	0
3	N	55	0	0	1	0
3	S	55	0	0	2	0
3	T	55	0	0	0	0
4	A	9	0	0	1	0
4	B	11	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	0	0
4	E	6	0	0	0	0
4	F	11	0	0	0	0
4	G	15	0	0	0	0
4	I	9	0	0	0	0
4	K	14	0	0	1	0
4	L	10	0	0	0	0
4	M	7	0	0	0	0
4	N	12	0	0	0	0
4	S	13	0	0	0	0
4	T	6	0	0	0	0
All	All	20070	0	19187	226	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 6.

The worst 5 of 226 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:93:MET:HE1	3:A:402:EZA:F2	1.71	0.81
1:K:147:ARG:HD2	4:K:513:HOH:O	1.80	0.80
1:I:77:ILE:HG22	1:I:81:MET:HE2	1.66	0.76
1:T:77:ILE:HG22	1:T:81:MET:HE2	1.69	0.75
1:A:77:ILE:HG22	1:A:81:MET:HE2	1.71	0.72

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	177/210 (84%)	174 (98%)	3 (2%)	0	100	100
1	B	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	C	176/210 (84%)	173 (98%)	3 (2%)	0	100	100
1	D	177/210 (84%)	173 (98%)	4 (2%)	0	100	100
1	E	180/210 (86%)	177 (98%)	3 (2%)	0	100	100
1	F	179/210 (85%)	177 (99%)	2 (1%)	0	100	100
1	G	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	I	184/210 (88%)	181 (98%)	3 (2%)	0	100	100
1	K	179/210 (85%)	175 (98%)	4 (2%)	0	100	100
1	L	176/210 (84%)	173 (98%)	3 (2%)	0	100	100
1	M	177/210 (84%)	174 (98%)	3 (2%)	0	100	100
1	N	178/210 (85%)	175 (98%)	3 (2%)	0	100	100
1	S	176/210 (84%)	174 (99%)	2 (1%)	0	100	100
1	T	177/210 (84%)	175 (99%)	2 (1%)	0	100	100
All	All	2492/2940 (85%)	2451 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/174 (82%)	141 (99%)	1 (1%)	76	88
1	B	142/174 (82%)	140 (99%)	2 (1%)	59	79
1	C	141/174 (81%)	139 (99%)	2 (1%)	59	79
1	D	140/174 (80%)	140 (100%)	0	100	100
1	E	142/174 (82%)	141 (99%)	1 (1%)	76	88
1	F	142/174 (82%)	141 (99%)	1 (1%)	76	88
1	G	140/174 (80%)	138 (99%)	2 (1%)	59	79
1	I	143/174 (82%)	141 (99%)	2 (1%)	59	79
1	K	142/174 (82%)	141 (99%)	1 (1%)	76	88
1	L	141/174 (81%)	140 (99%)	1 (1%)	76	88
1	M	142/174 (82%)	141 (99%)	1 (1%)	76	88
1	N	141/174 (81%)	140 (99%)	1 (1%)	76	88
1	S	140/174 (80%)	139 (99%)	1 (1%)	76	88
1	T	142/174 (82%)	141 (99%)	1 (1%)	76	88
All	All	1980/2436 (81%)	1963 (99%)	17 (1%)	70	85

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	176	THR
1	T	176	THR
1	G	148	GLU
1	G	176	THR
1	I	11	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	142	HIS
1	I	54	GLN
1	S	160	GLN
1	N	65	ASN
1	G	42	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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	MPD	E	401	-	7,7,7	0.65	0	9,10,10	0.70	0
2	MPD	K	401	-	7,7,7	0.68	0	9,10,10	0.92	1 (11%)
3	EZA	C	402	-	58,59,59	2.85	16 (27%)	79,83,83	2.38	24 (30%)
3	EZA	L	402	-	58,59,59	2.86	14 (24%)	79,83,83	2.18	20 (25%)
2	MPD	T	401	-	7,7,7	0.84	0	9,10,10	0.95	0
2	MPD	B	401	-	7,7,7	0.51	0	9,10,10	0.80	0
3	EZA	F	402	-	58,59,59	2.94	14 (24%)	79,83,83	2.17	17 (21%)
3	EZA	D	402	-	58,59,59	2.85	15 (25%)	79,83,83	2.22	17 (21%)
3	EZA	A	402	-	58,59,59	2.85	15 (25%)	79,83,83	1.92	14 (17%)
2	MPD	F	401	-	7,7,7	0.49	0	9,10,10	0.77	0
2	MPD	A	401	-	7,7,7	0.51	0	9,10,10	0.25	0
3	EZA	M	402	-	58,59,59	2.89	16 (27%)	79,83,83	2.41	21 (26%)
3	EZA	N	402	-	58,59,59	2.92	16 (27%)	79,83,83	2.27	23 (29%)
2	MPD	M	401	-	7,7,7	0.41	0	9,10,10	0.95	1 (11%)
2	MPD	I	401	-	7,7,7	0.48	0	9,10,10	0.55	0
2	MPD	S	401	-	7,7,7	0.75	0	9,10,10	0.82	0
3	EZA	T	402	-	58,59,59	2.87	15 (25%)	79,83,83	2.31	17 (21%)
2	MPD	N	401	-	7,7,7	0.76	0	9,10,10	0.99	1 (11%)
3	EZA	S	402	-	58,59,59	2.78	18 (31%)	79,83,83	2.27	28 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EZA	E	402	-	58,59,59	2.79	13 (22%)	79,83,83	2.42	22 (27%)
2	MPD	D	401	-	7,7,7	0.47	0	9,10,10	0.47	0
2	MPD	C	401	-	7,7,7	0.83	0	9,10,10	1.10	1 (11%)
2	MPD	L	401	-	7,7,7	0.55	0	9,10,10	0.79	0
2	MPD	G	401	-	7,7,7	0.68	0	9,10,10	1.33	0
3	EZA	I	402	-	58,59,59	2.72	13 (22%)	79,83,83	2.43	24 (30%)

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	MPD	E	401	-	-	4/5/5/5	-
2	MPD	K	401	-	-	3/5/5/5	-
3	EZA	C	402	-	2/2/17/22	16/63/96/96	0/4/5/5
3	EZA	L	402	-	1/1/17/22	11/63/96/96	0/4/5/5
2	MPD	T	401	-	-	1/5/5/5	-
2	MPD	B	401	-	-	2/5/5/5	-
3	EZA	F	402	-	1/1/17/22	13/63/96/96	0/4/5/5
3	EZA	D	402	-	1/1/17/22	13/63/96/96	0/4/5/5
3	EZA	A	402	-	1/1/17/22	9/63/96/96	0/4/5/5
2	MPD	F	401	-	-	2/5/5/5	-
2	MPD	A	401	-	-	3/5/5/5	-
3	EZA	M	402	-	2/2/17/22	12/63/96/96	0/4/5/5
3	EZA	N	402	-	1/1/17/22	11/63/96/96	0/4/5/5
2	MPD	M	401	-	-	4/5/5/5	-
2	MPD	I	401	-	-	2/5/5/5	-
3	EZA	T	402	-	1/1/17/22	13/63/96/96	0/4/5/5
2	MPD	S	401	-	-	0/5/5/5	-
2	MPD	N	401	-	-	3/5/5/5	-
3	EZA	S	402	-	2/2/17/22	14/63/96/96	0/4/5/5
3	EZA	E	402	-	2/2/17/22	13/63/96/96	0/4/5/5
2	MPD	D	401	-	-	2/5/5/5	-
2	MPD	C	401	-	-	1/5/5/5	-
2	MPD	L	401	-	-	2/5/5/5	-
2	MPD	G	401	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EZA	I	402	-	2/2/17/22	14/63/96/96	0/4/5/5

The worst 5 of 165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	EZA	C20-C19	-8.40	1.37	1.52
3	I	402	EZA	C34-N5	8.38	1.53	1.34
3	S	402	EZA	C34-N5	8.11	1.52	1.34
3	F	402	EZA	C20-C19	-8.04	1.37	1.52
3	L	402	EZA	C20-C19	-7.99	1.37	1.52

The worst 5 of 231 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	402	EZA	C19-C20-N3	10.30	132.38	112.08
3	E	402	EZA	C19-C20-N3	10.09	131.97	112.08
3	I	402	EZA	C19-C20-N3	9.73	131.26	112.08
3	C	402	EZA	C19-C20-N3	9.53	130.88	112.08
3	D	402	EZA	C19-C20-N3	9.31	130.44	112.08

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	402	EZA	C26
3	C	402	EZA	C20
3	C	402	EZA	C26
3	D	402	EZA	C26
3	E	402	EZA	C20

5 of 172 torsion outliers are listed below:

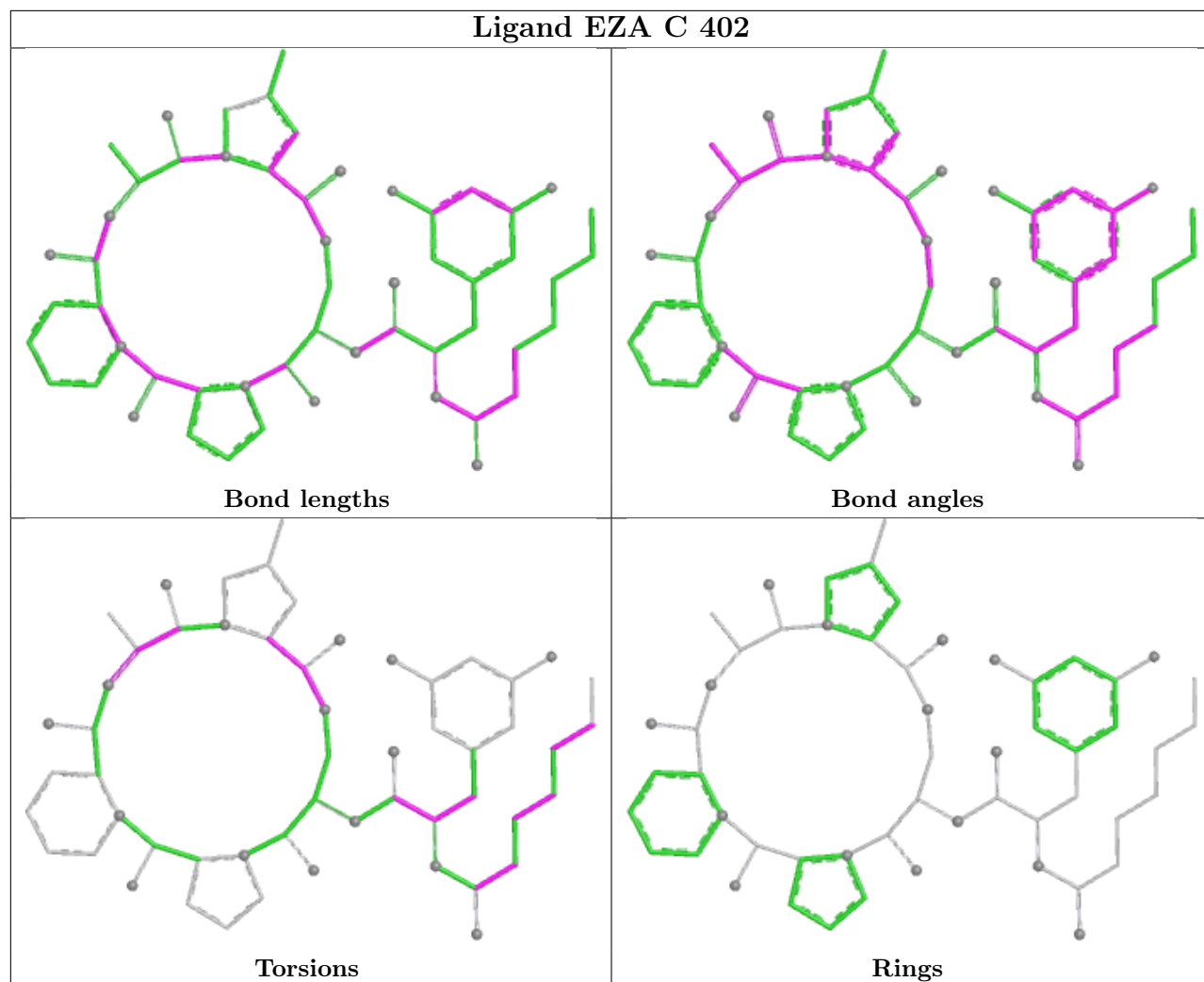
Mol	Chain	Res	Type	Atoms
2	A	401	MPD	C2-C3-C4-C5
2	E	401	MPD	C2-C3-C4-O4
2	E	401	MPD	C2-C3-C4-C5
2	F	401	MPD	C2-C3-C4-O4
2	F	401	MPD	C2-C3-C4-C5

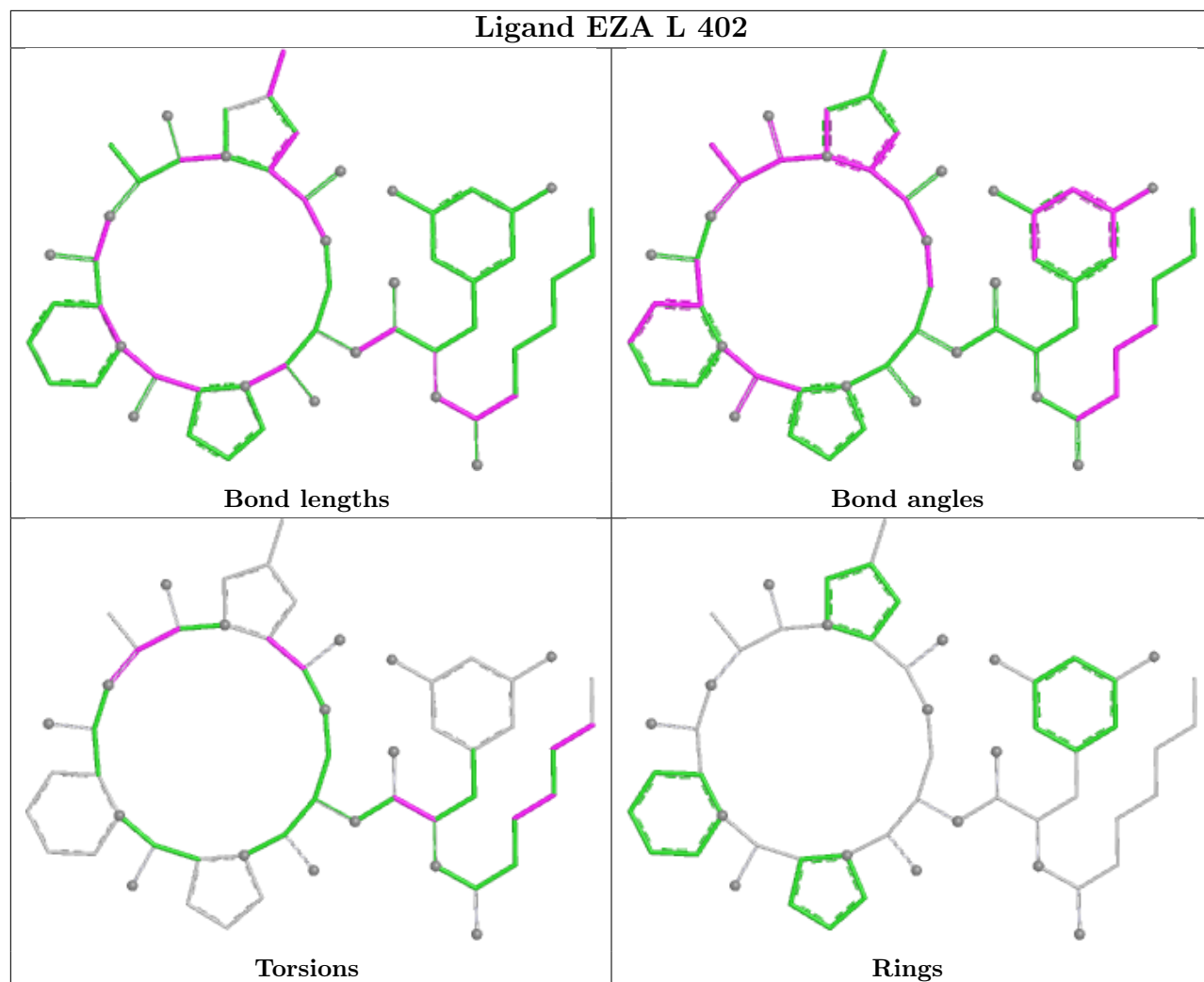
There are no ring outliers.

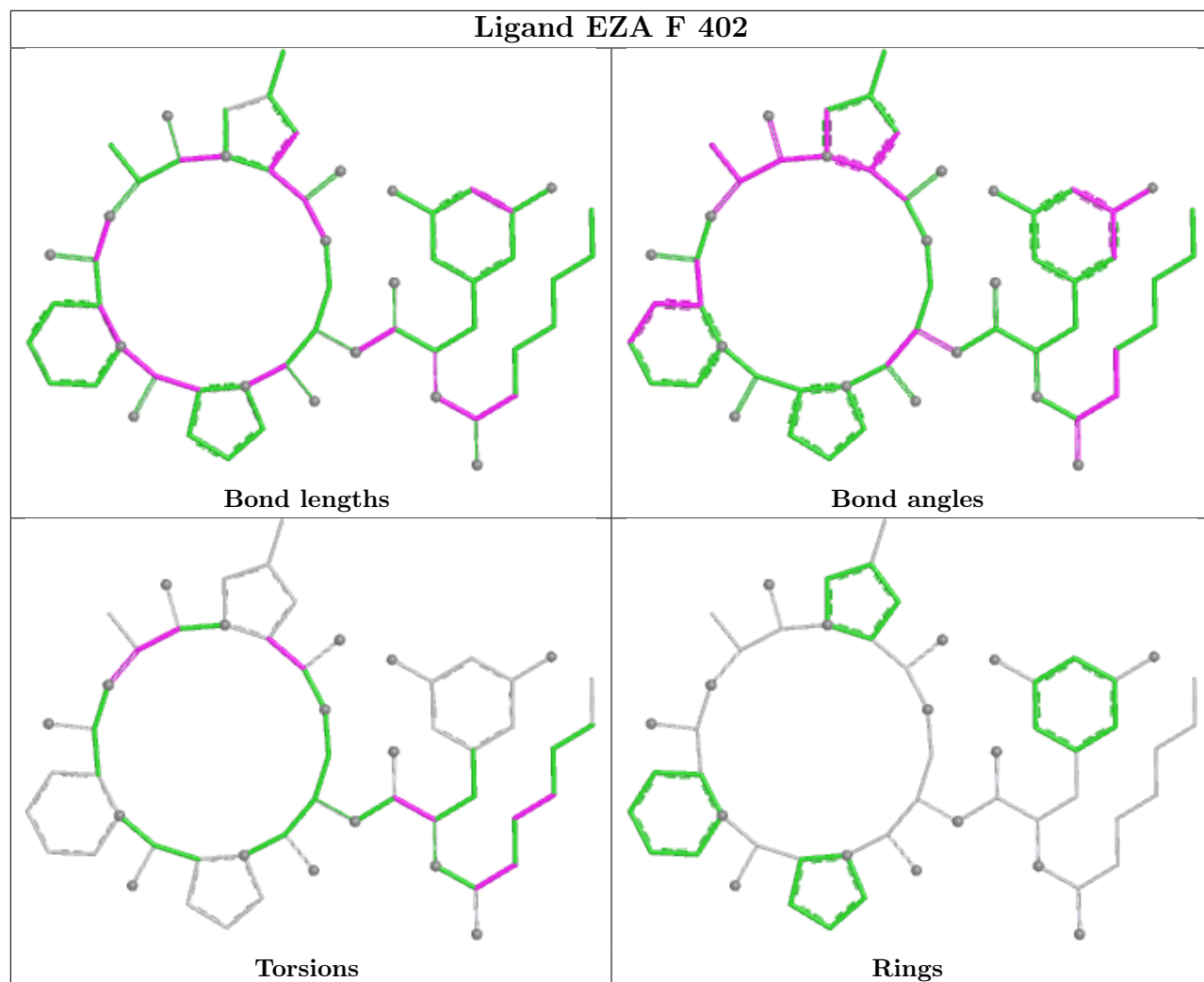
22 monomers are involved in 80 short contacts:

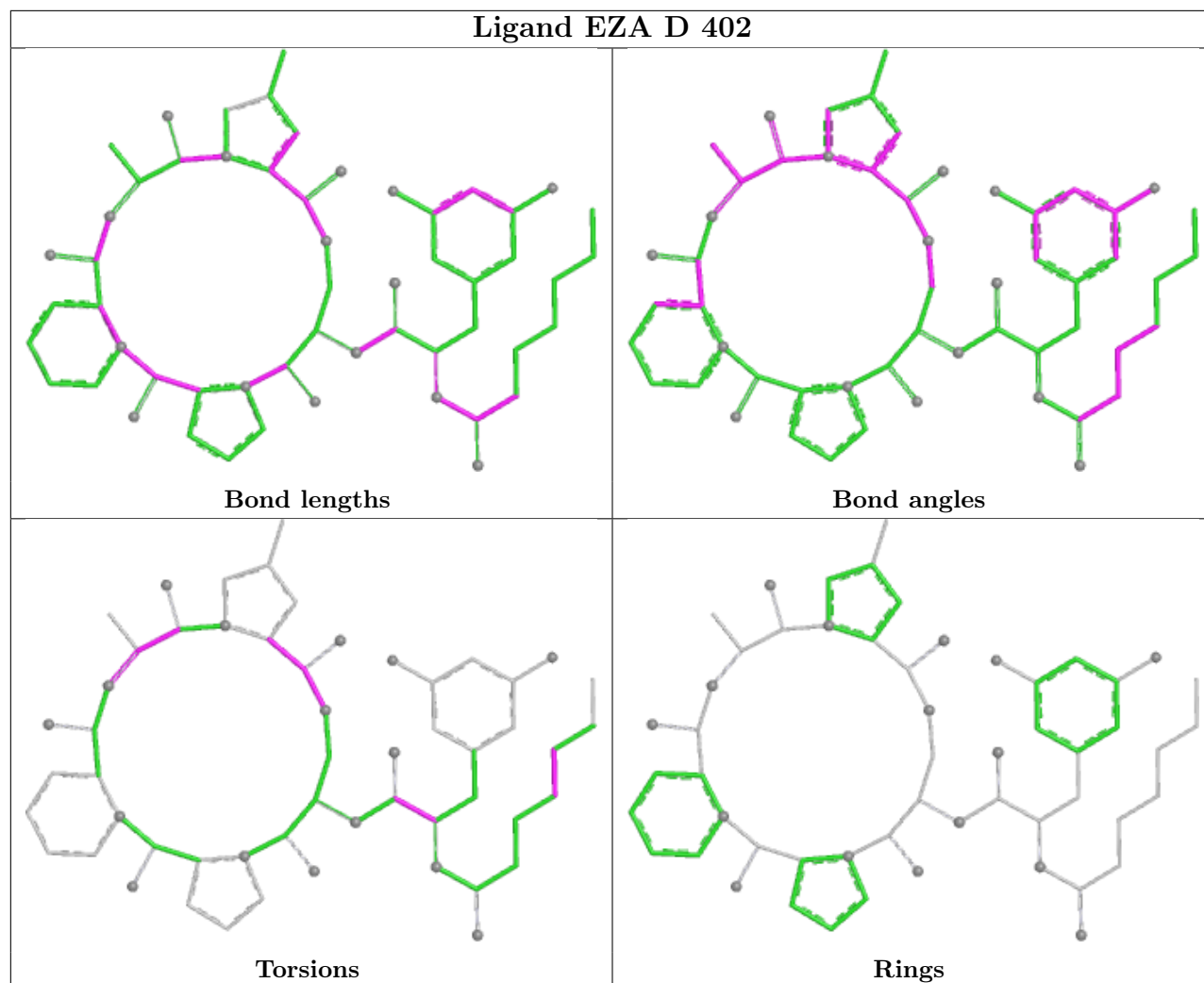
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	MPD	7	0
2	K	401	MPD	5	0
3	C	402	EZA	1	0
3	L	402	EZA	1	0
2	T	401	MPD	4	0
2	B	401	MPD	5	0
3	F	402	EZA	1	0
3	D	402	EZA	1	0
3	A	402	EZA	2	0
2	F	401	MPD	4	0
2	A	401	MPD	6	0
3	M	402	EZA	2	0
3	N	402	EZA	1	0
2	M	401	MPD	4	0
2	I	401	MPD	7	0
2	S	401	MPD	5	0
2	N	401	MPD	2	0
3	S	402	EZA	2	0
2	D	401	MPD	4	0
2	C	401	MPD	7	0
2	L	401	MPD	4	0
2	G	401	MPD	5	0

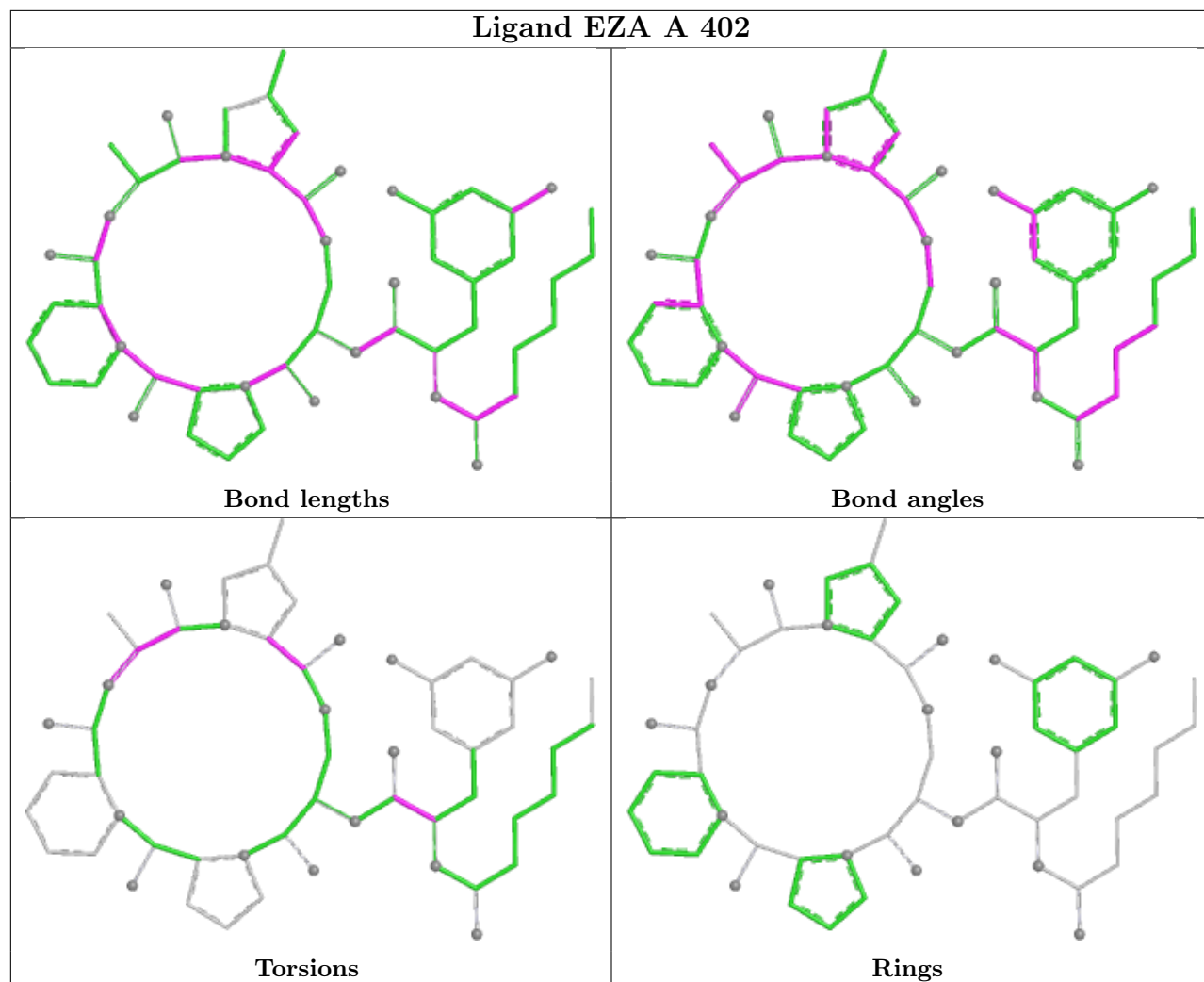
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

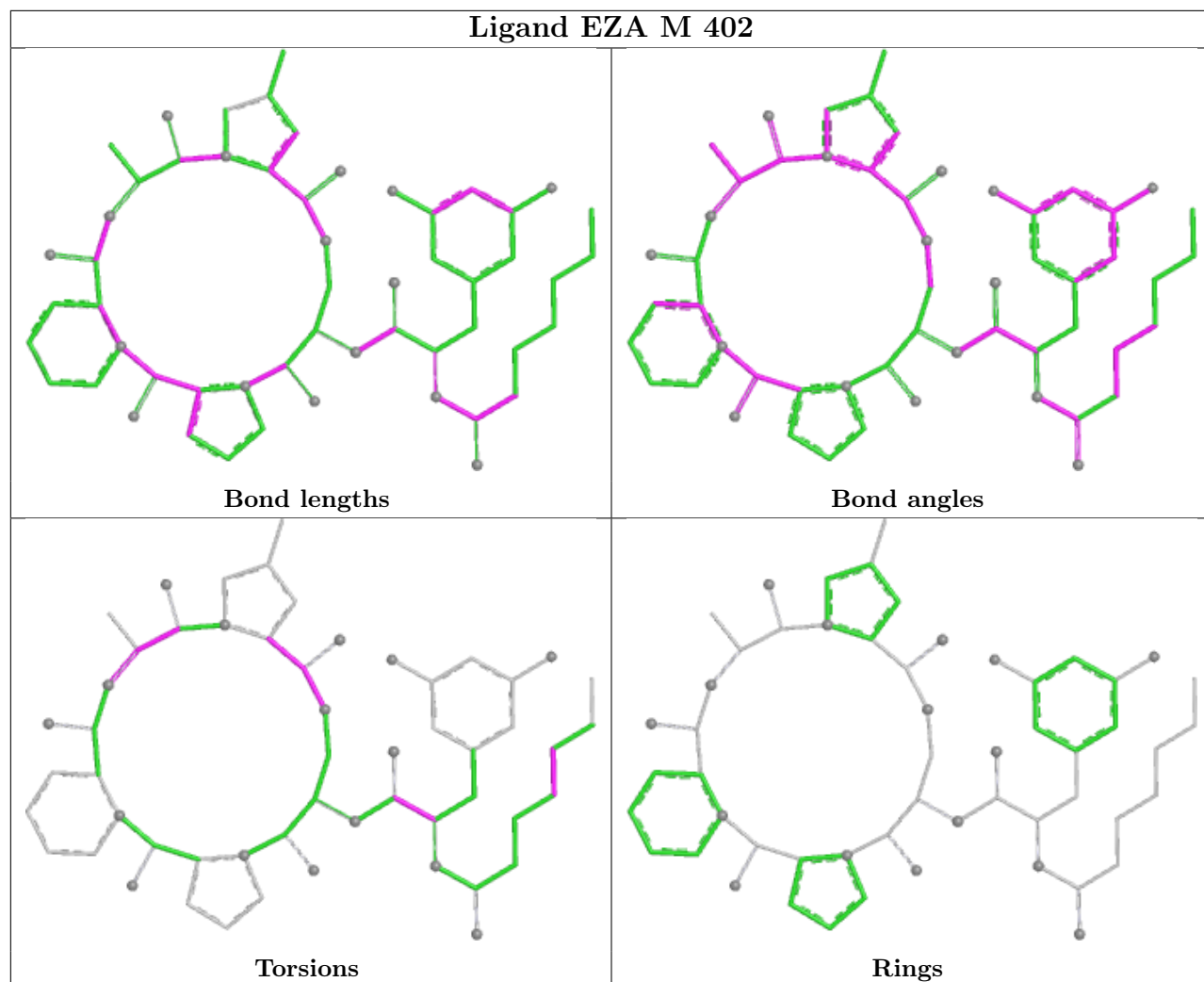


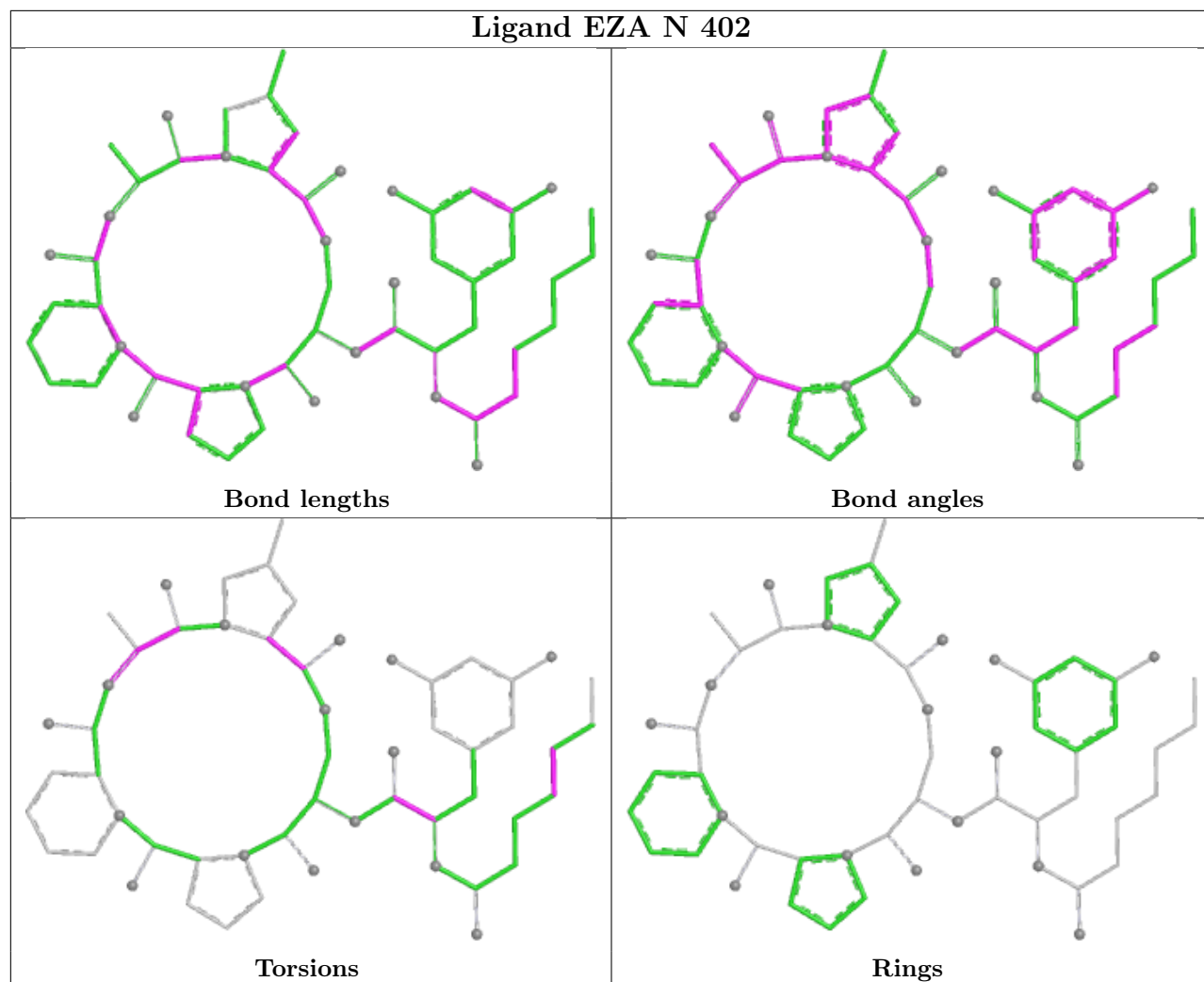


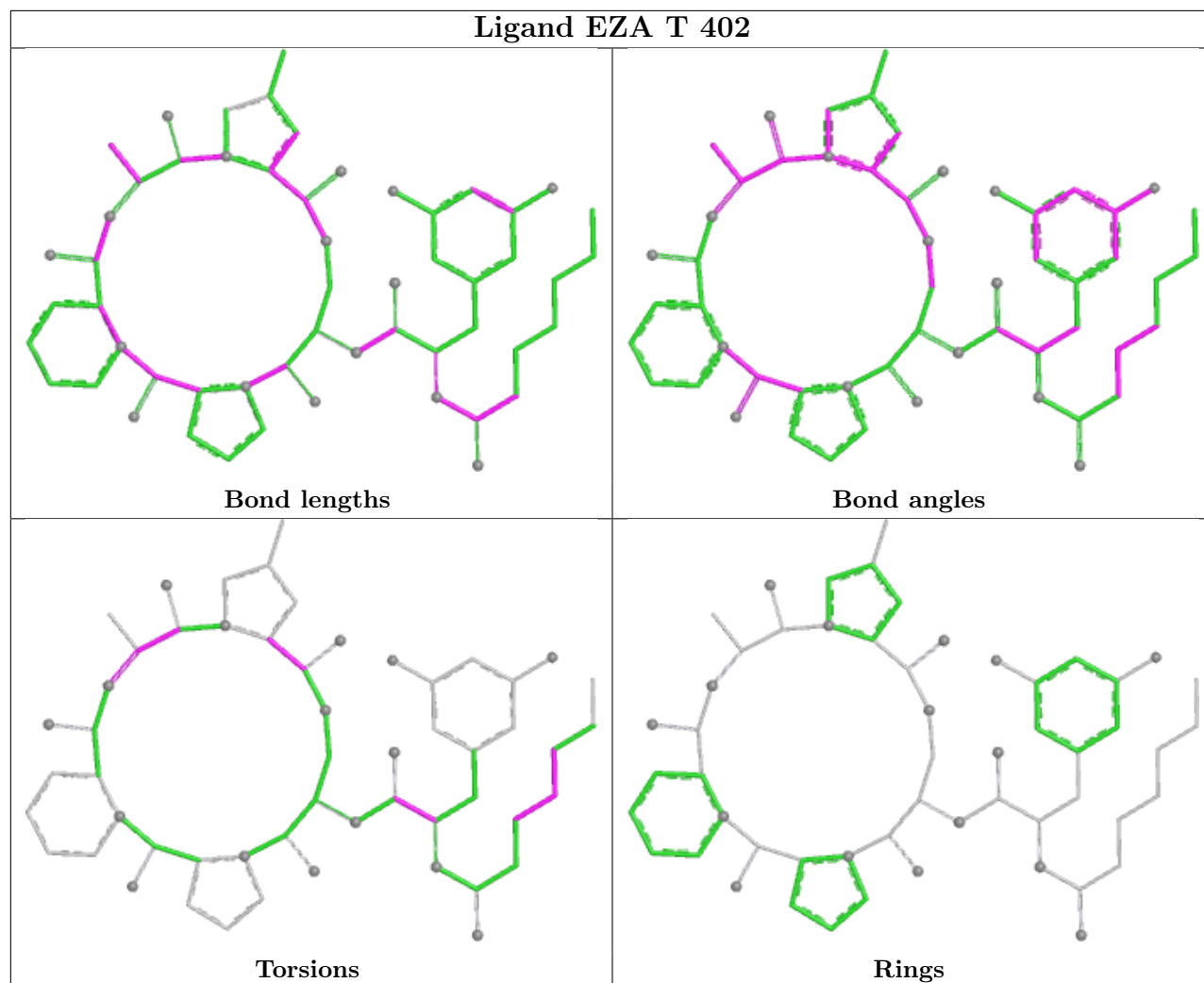


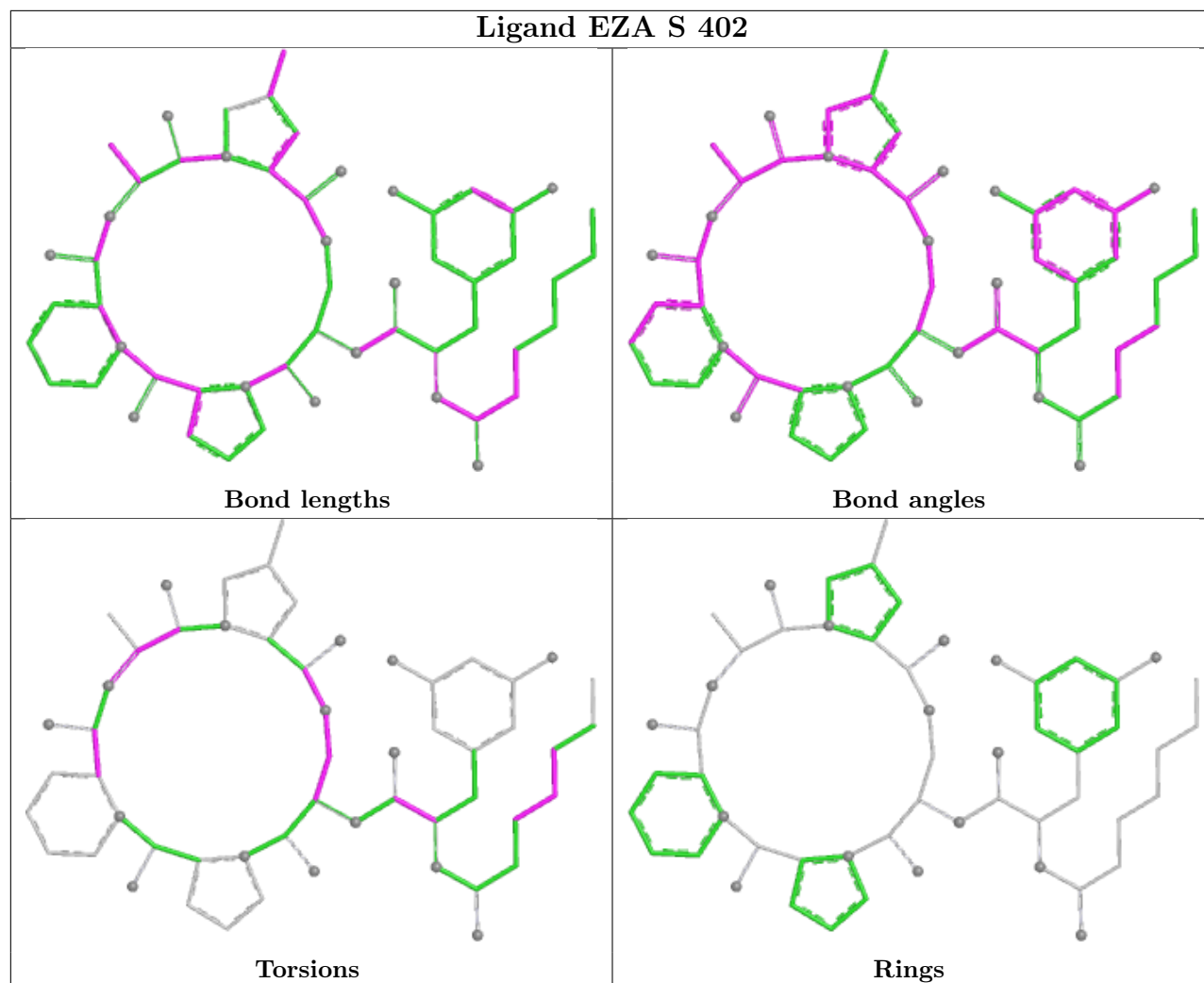


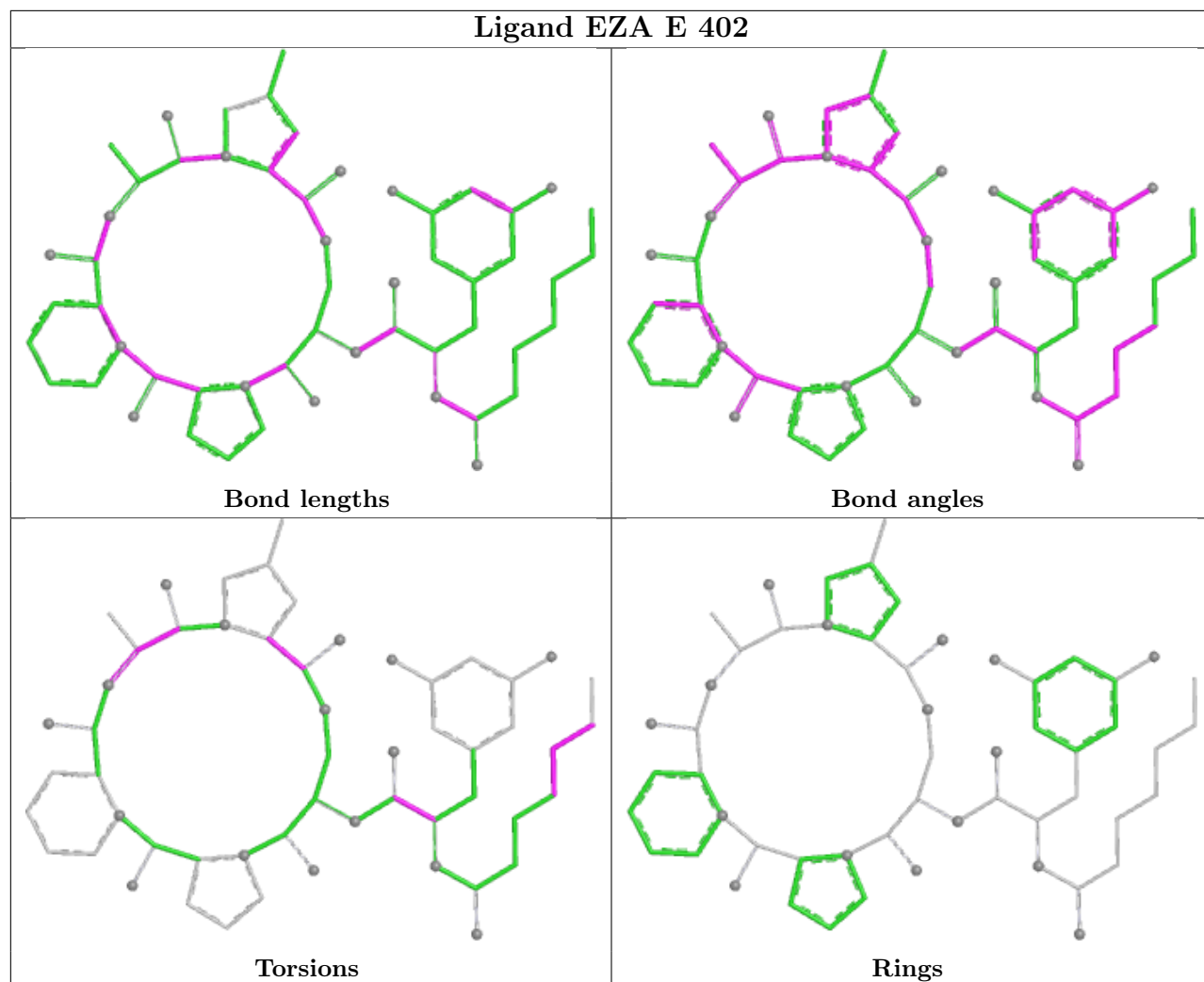


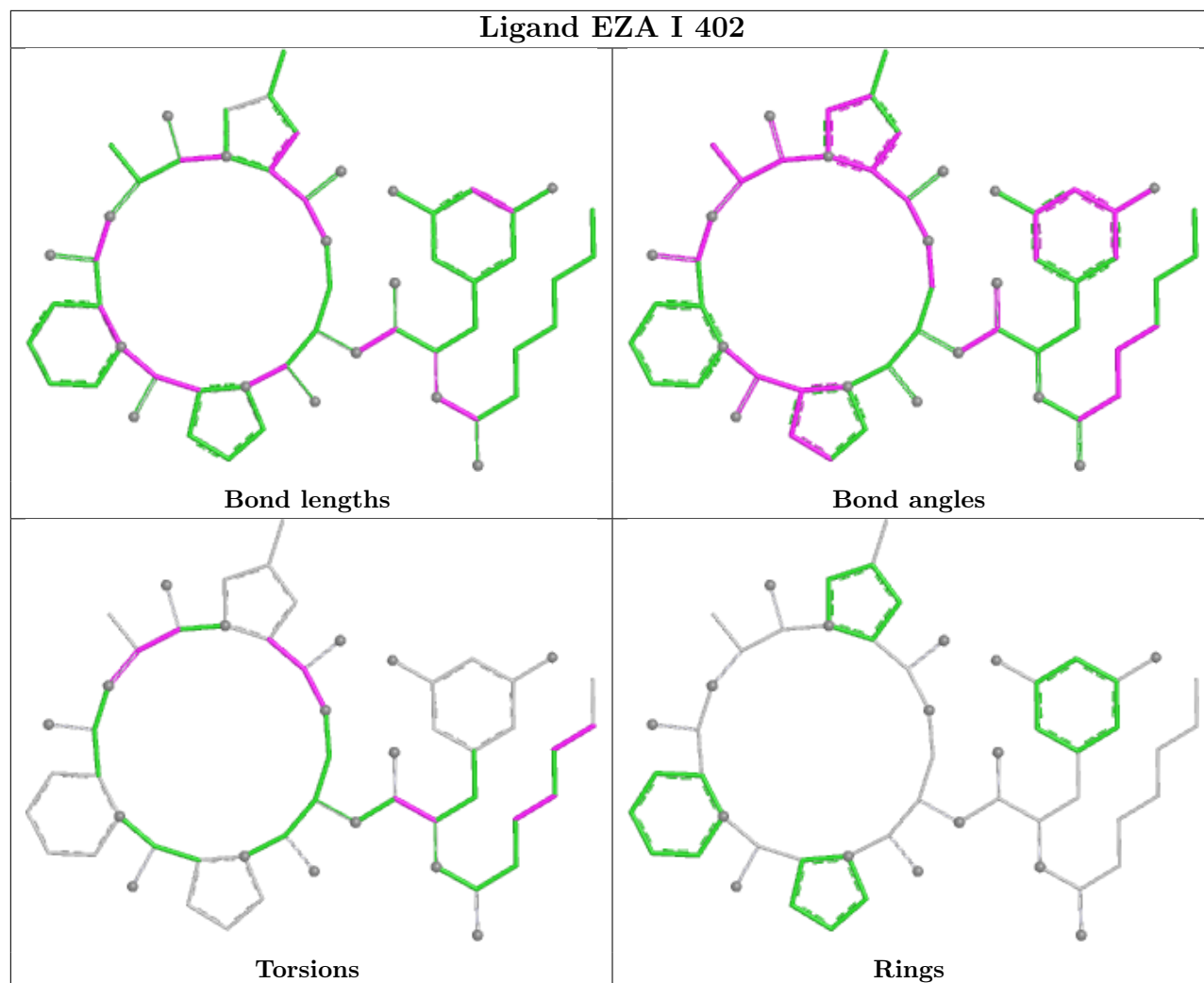












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	181/210 (86%)	-0.13	5 (2%) 55 50	40, 53, 83, 104	0
1	B	182/210 (86%)	-0.20	3 (1%) 70 67	37, 50, 84, 106	0
1	C	180/210 (85%)	-0.16	3 (1%) 69 65	36, 49, 83, 108	0
1	D	181/210 (86%)	-0.09	4 (2%) 62 58	38, 53, 84, 101	0
1	E	184/210 (87%)	-0.14	3 (1%) 70 67	37, 50, 87, 114	0
1	F	183/210 (87%)	-0.23	4 (2%) 62 58	35, 49, 82, 110	0
1	G	182/210 (86%)	-0.21	5 (2%) 56 52	36, 49, 81, 106	0
1	I	188/210 (89%)	-0.06	7 (3%) 45 40	36, 53, 90, 121	0
1	K	183/210 (87%)	-0.20	5 (2%) 56 52	36, 48, 87, 115	0
1	L	180/210 (85%)	-0.20	4 (2%) 62 58	36, 50, 82, 108	0
1	M	181/210 (86%)	-0.20	5 (2%) 55 50	36, 50, 83, 105	0
1	N	182/210 (86%)	-0.19	5 (2%) 56 52	41, 53, 87, 109	0
1	S	180/210 (85%)	-0.11	5 (2%) 55 50	37, 51, 80, 96	0
1	T	181/210 (86%)	-0.17	4 (2%) 62 58	35, 50, 81, 101	0
All	All	2548/2940 (86%)	-0.16	62 (2%) 59 55	35, 51, 85, 121	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	GLU	7.3
1	E	191	GLU	6.5
1	I	191	GLU	6.1
1	B	191	GLU	6.0
1	F	191	GLU	5.9

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.

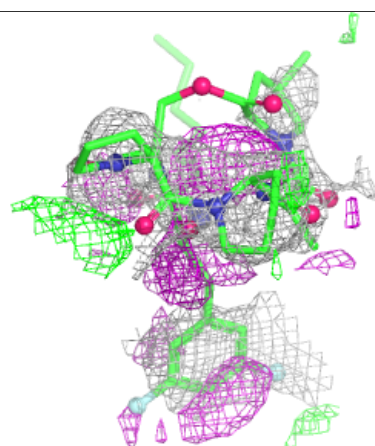
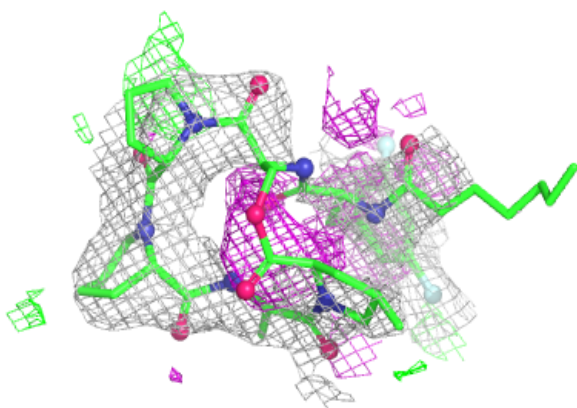
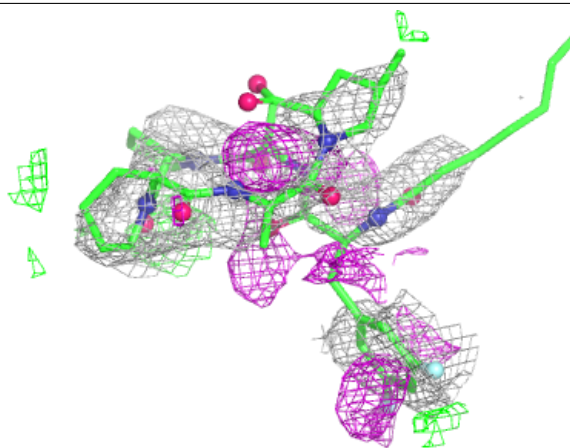
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EZA	S	402	55/55	0.76	0.24	96,135,177,184	0
3	EZA	I	402	55/55	0.80	0.23	93,132,159,187	0
3	EZA	M	402	55/55	0.82	0.20	96,129,159,162	0
3	EZA	N	402	55/55	0.83	0.20	98,127,147,158	0
3	EZA	T	402	55/55	0.83	0.17	84,111,135,138	0
3	EZA	D	402	55/55	0.84	0.19	85,118,141,147	0
3	EZA	E	402	55/55	0.84	0.17	92,116,138,177	0
3	EZA	C	402	55/55	0.84	0.19	84,111,147,153	0
3	EZA	L	402	55/55	0.84	0.17	80,101,122,130	0
3	EZA	F	402	55/55	0.87	0.17	77,102,123,130	0
3	EZA	A	402	55/55	0.92	0.12	64,78,93,98	0
2	MPD	G	401	8/8	0.93	0.16	58,60,66,67	0
2	MPD	A	401	8/8	0.93	0.15	65,68,71,71	0
2	MPD	B	401	8/8	0.93	0.18	65,68,73,79	0
2	MPD	D	401	8/8	0.93	0.20	72,77,80,82	0
2	MPD	L	401	8/8	0.94	0.15	57,64,66,73	0
2	MPD	M	401	8/8	0.94	0.16	55,68,69,73	0
2	MPD	N	401	8/8	0.94	0.15	62,67,70,75	0
2	MPD	T	401	8/8	0.94	0.18	66,76,83,85	0
2	MPD	I	401	8/8	0.94	0.19	65,71,76,78	0
2	MPD	C	401	8/8	0.95	0.15	51,68,74,80	0
2	MPD	E	401	8/8	0.95	0.15	68,74,82,84	0
2	MPD	K	401	8/8	0.95	0.15	67,69,72,74	0
2	MPD	S	401	8/8	0.95	0.15	63,65,78,79	0
2	MPD	F	401	8/8	0.96	0.14	58,68,74,76	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.

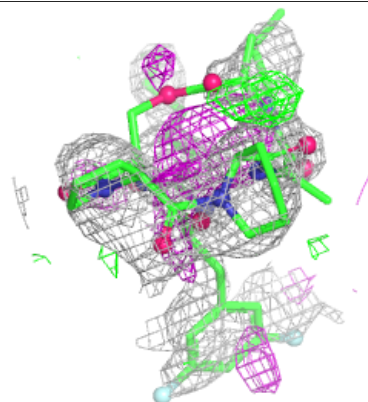
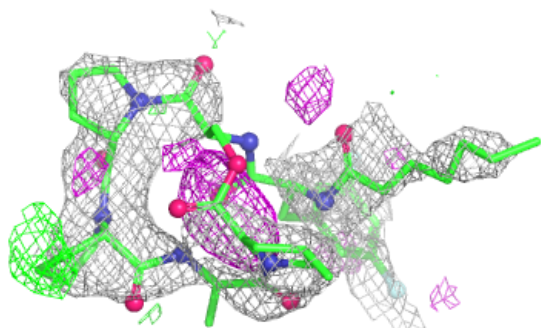
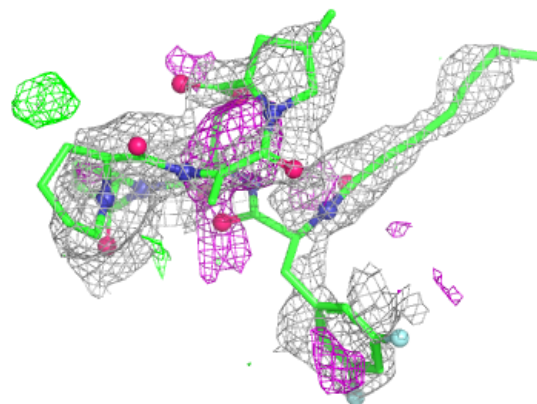
Electron density around EZA S 402:

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

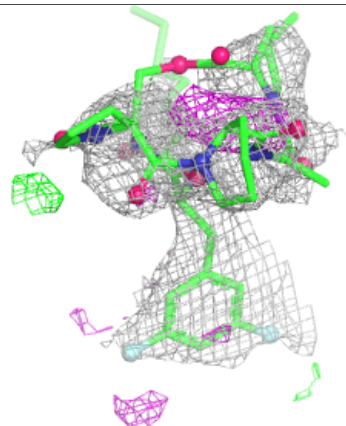
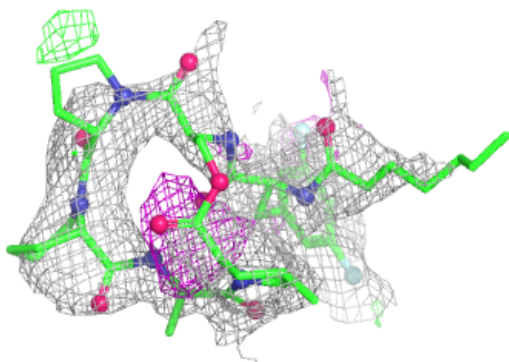
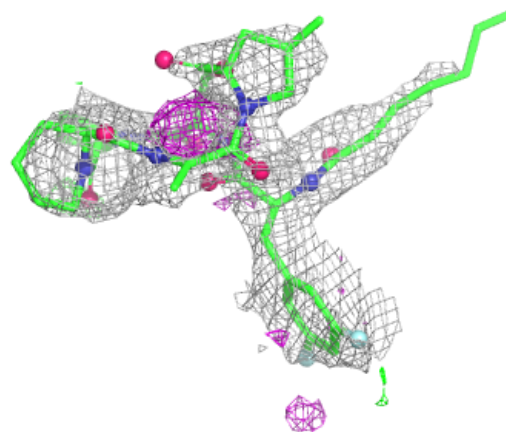


Electron density around EZA I 402:

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

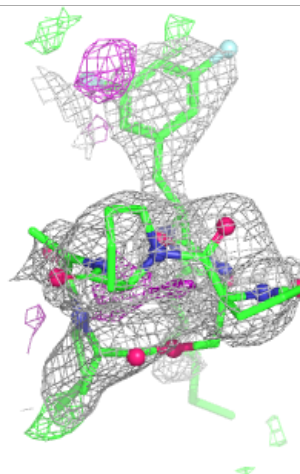
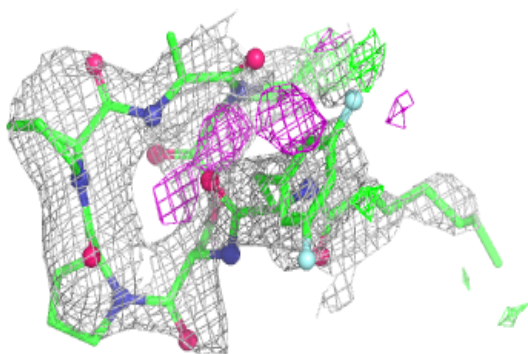
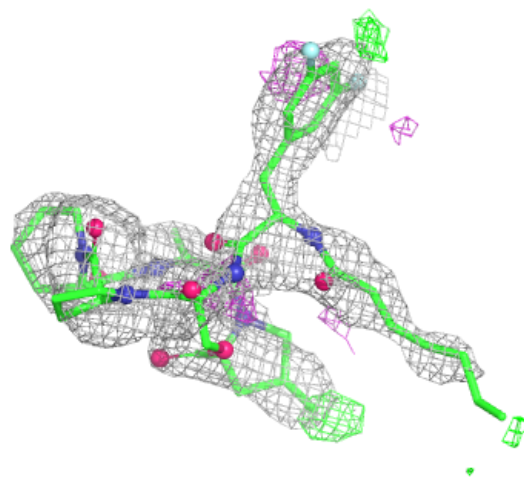
**Electron density around EZA M 402:**

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



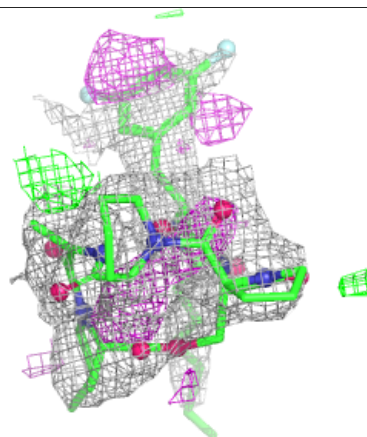
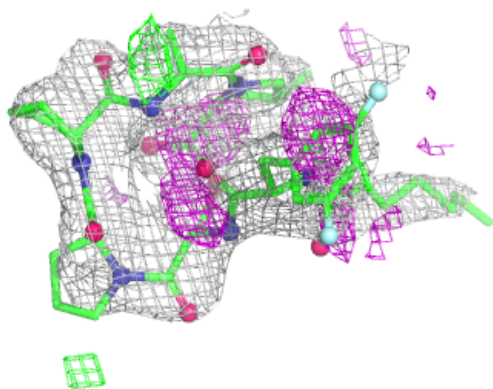
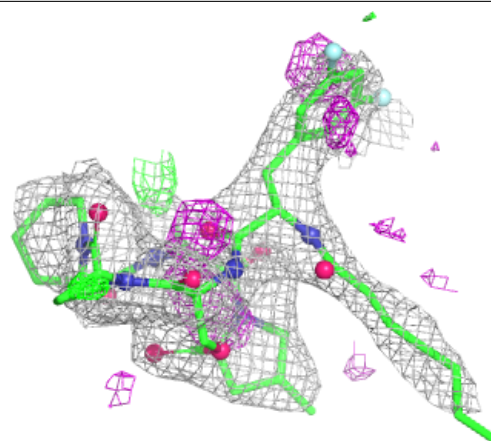
Electron density around EZA N 402:

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



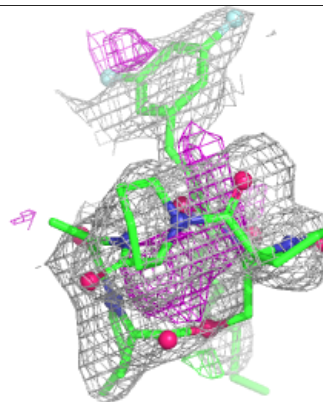
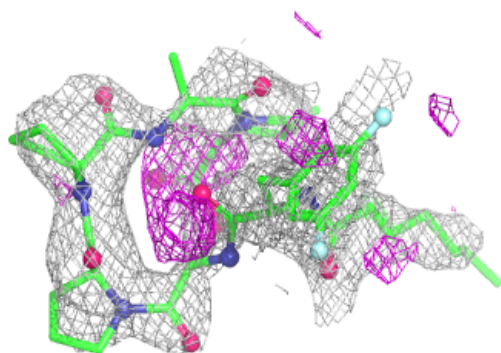
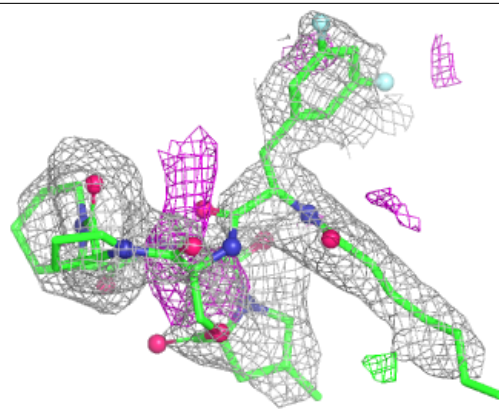
Electron density around EZA T 402:

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



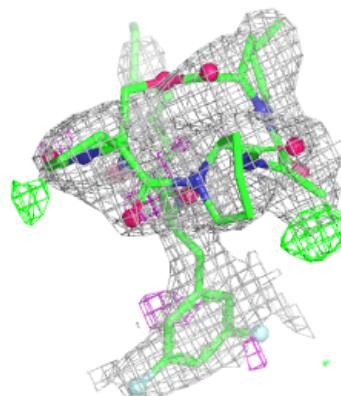
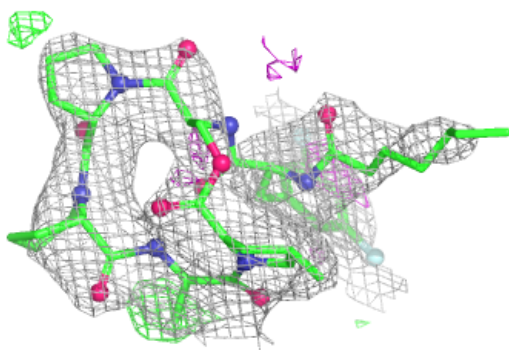
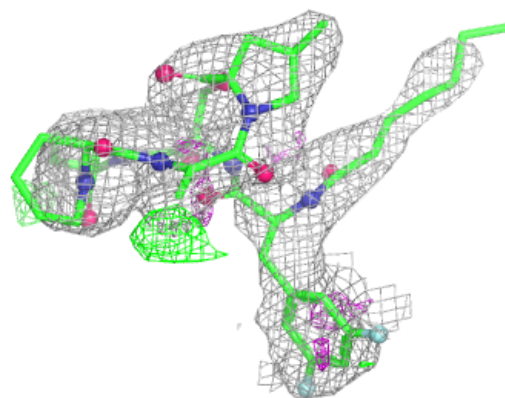
Electron density around EZA D 402:

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

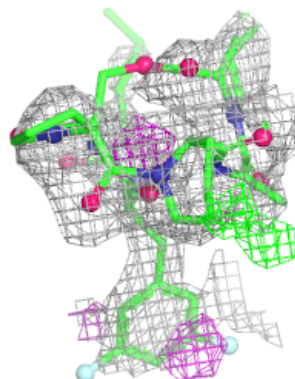
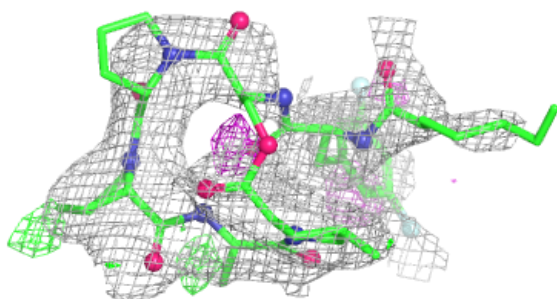
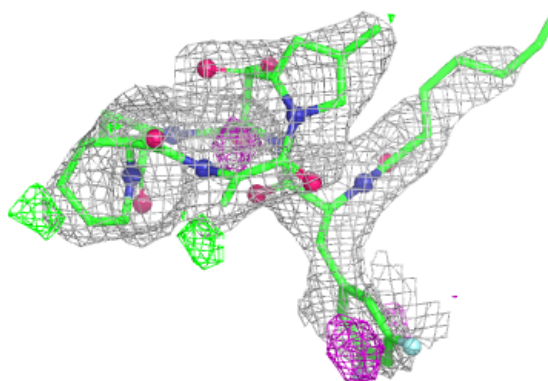


Electron density around EZA E 402:

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

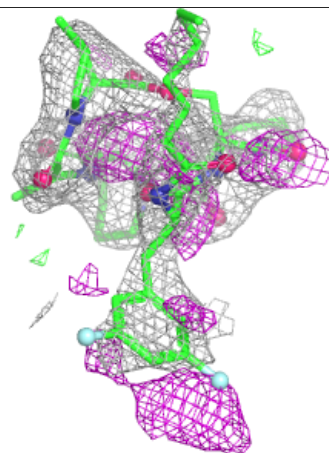
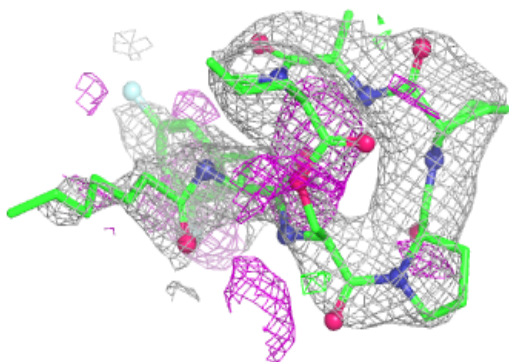
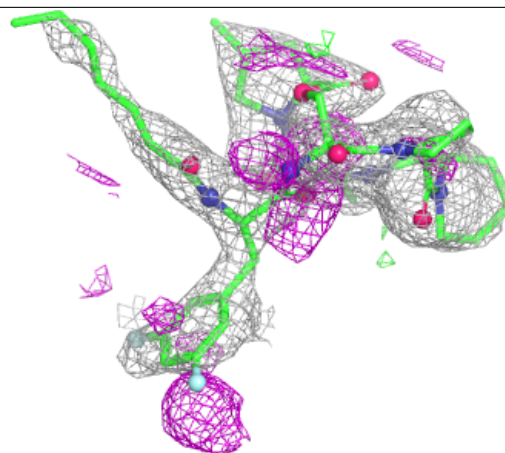
**Electron density around EZA C 402:**

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



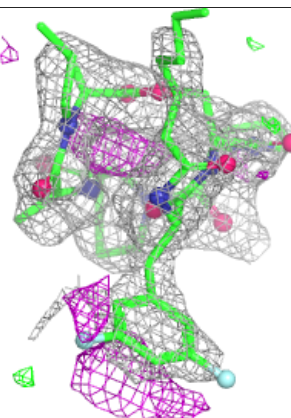
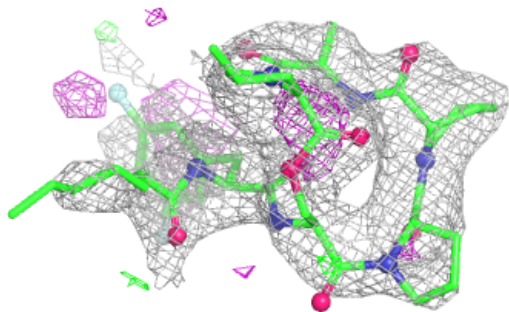
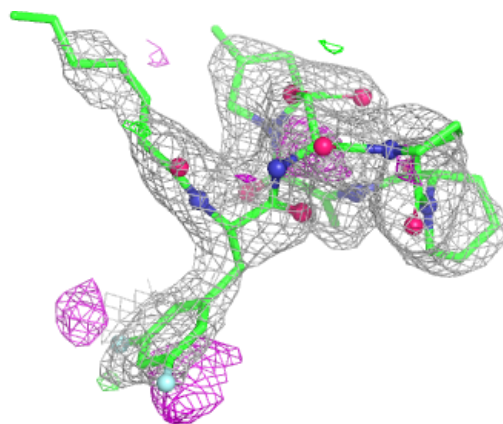
Electron density around EZA L 402:

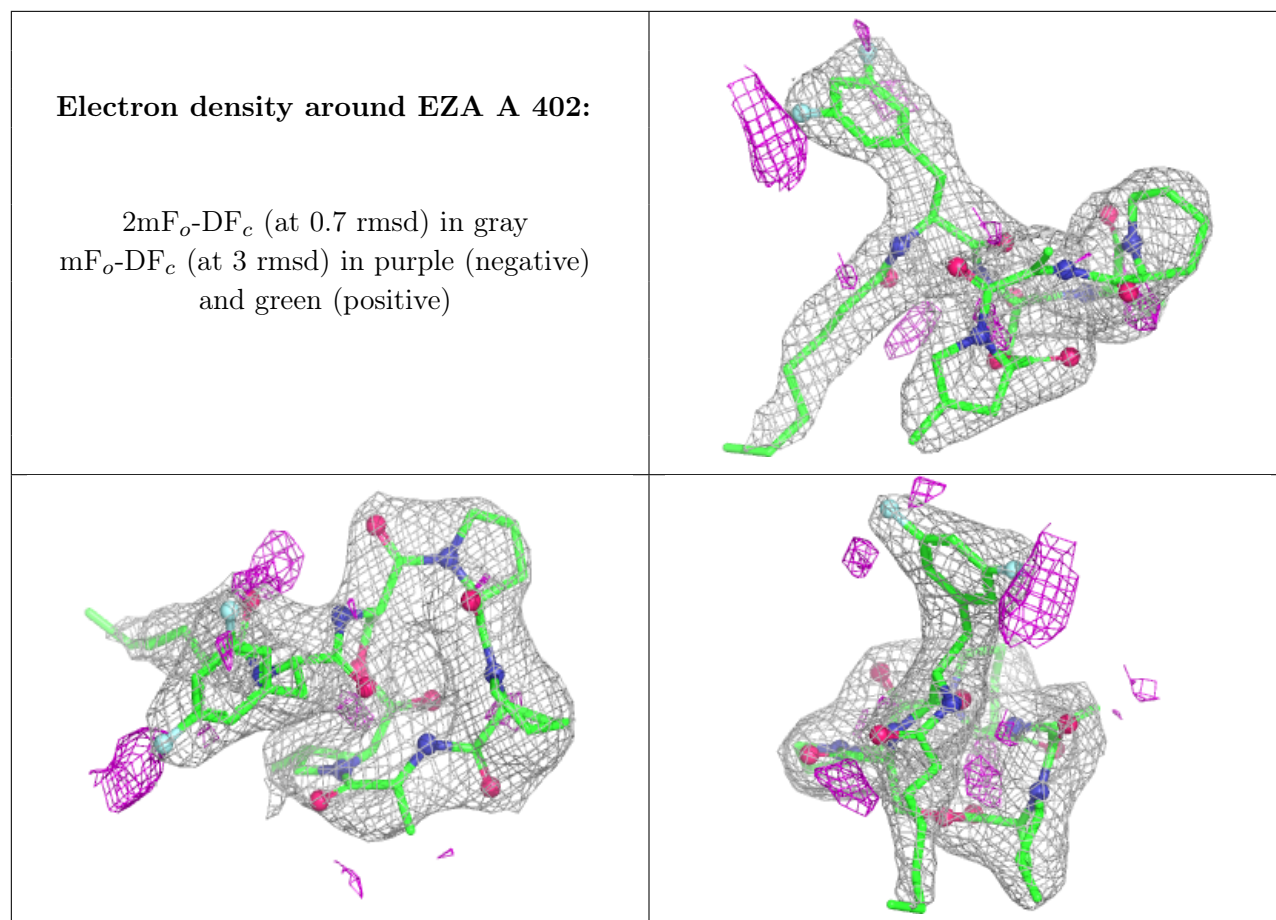
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EZA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.