



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:11 am BST

PDB ID : 6CFD
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 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

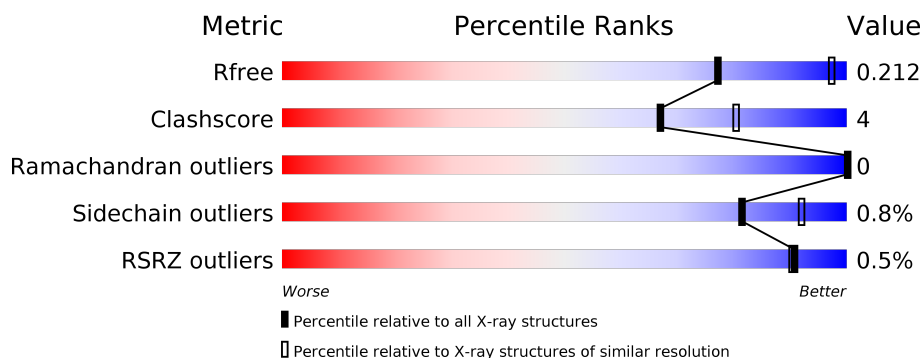
1 Overall quality at a glance

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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (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 on 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	<div> <div>80%</div> <div>6%</div> <div>14%</div> </div>
1	B	210	<div> <div>83%</div> <div>•</div> <div>13%</div> </div>
1	C	210	<div> <div>%</div> <div>80%</div> <div>5%</div> <div>14%</div> </div>
1	D	210	<div> <div>81%</div> <div>•</div> <div>14%</div> </div>
1	E	210	<div> <div>81%</div> <div>6%</div> <div>12%</div> </div>
1	F	210	<div> <div>83%</div> <div>•</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
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	-
2	MPD	K	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	-	-	X
3	EZA	L	402	X	-	-	-
3	EZA	M	402	X	-	-	-
3	EZA	N	402	X	-	-	-
3	EZA	S	402	X	-	-	X
3	EZA	T	402	X	-	-	-

2 Entry composition

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

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
F	205	HIS	-	expression tag	UNP A0A133CH35
F	206	HIS	-	expression tag	UNP A0A133CH35
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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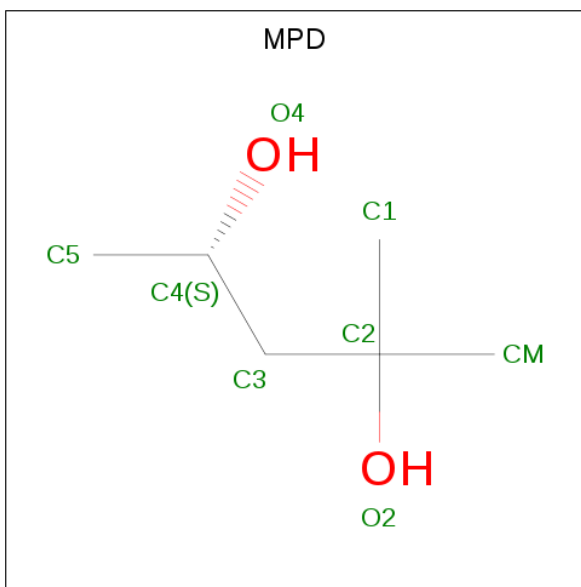
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L	199	GLU	-	expression tag	UNP A0A133CH35
L	200	GLY	-	expression tag	UNP A0A133CH35
L	201	ARG	-	expression tag	UNP A0A133CH35
L	202	GLY	-	expression tag	UNP A0A133CH35
L	203	LEU	-	expression tag	UNP A0A133CH35
L	204	GLU	-	expression tag	UNP A0A133CH35
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
M	202	GLY	-	expression tag	UNP A0A133CH35
M	203	LEU	-	expression tag	UNP A0A133CH35
M	204	GLU	-	expression tag	UNP A0A133CH35
M	205	HIS	-	expression tag	UNP A0A133CH35
M	206	HIS	-	expression tag	UNP A0A133CH35
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
N	197	LYS	-	expression tag	UNP A0A133CH35
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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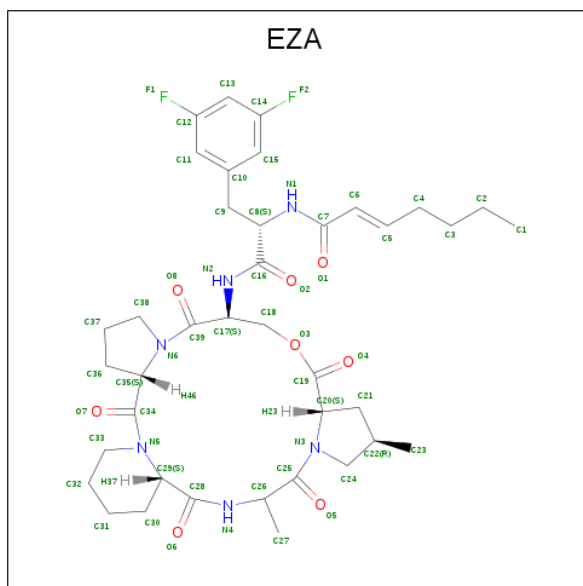
Chain	Residue	Modelled	Actual	Comment	Reference
S	198	ILE	-	expression tag	UNP A0A133CH35
S	199	GLU	-	expression tag	UNP A0A133CH35
S	200	GLY	-	expression tag	UNP A0A133CH35
S	201	ARG	-	expression tag	UNP A0A133CH35
S	202	GLY	-	expression tag	UNP A0A133CH35
S	203	LEU	-	expression tag	UNP A0A133CH35
S	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 (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- 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 (three-letter code: EZA) (formula: C₃₉H₅₂F₂N₆O₈) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 and DNA 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

Chain A: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D: 




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E: 




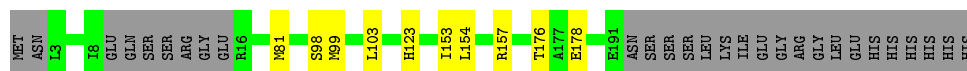
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:  83% 13%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:  82% 5% 13%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I:  82% 7% 10%




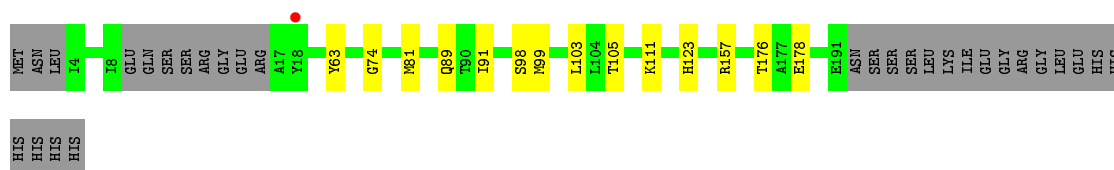
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:  82% 5% 13%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:  79% 7% 14%




- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:  81% 5% 14%

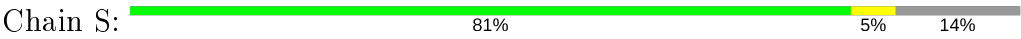


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

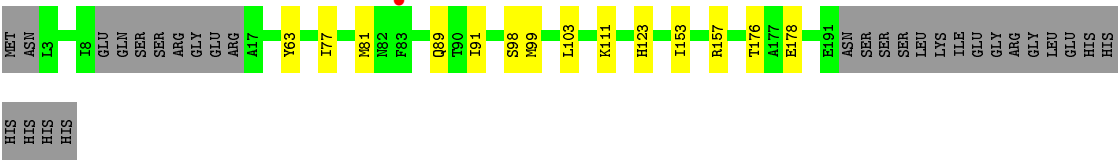
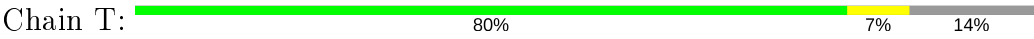
Chain N:  82% 5% 13%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

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 47.50 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.9 (101.08-2.57) 99.0 (47.50-2.57)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.209 0.179 , 0.212	Depositor DCC
R_{free} test set	5708 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.176 for l,-k,h	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	0.67	0/1386	0.80	1/1875 (0.1%)
1	B	0.75	0/1391	0.79	0/1883
1	C	0.74	0/1377	0.82	0/1864
1	D	0.73	0/1378	0.80	0/1867
1	E	0.71	0/1401	0.77	1/1896 (0.1%)
1	F	0.71	0/1396	0.81	0/1889
1	G	0.73	0/1383	0.78	0/1874
1	I	0.74	0/1421	0.81	0/1924
1	K	0.74	0/1396	0.80	0/1889
1	L	0.72	0/1377	0.80	0/1865
1	M	0.71	0/1386	0.80	0/1875
1	N	0.68	0/1387	0.78	0/1878
1	S	0.74	0/1373	0.80	0/1860
1	T	0.74	0/1386	0.81	0/1875
All	All	0.72	0/19438	0.80	2/26314 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	MET	CG-SD-CE	-7.94	87.50	100.20
1	E	79	ASP	CB-CG-OD1	5.03	122.82	118.30

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	1370	0	1363	15	0
1	B	1375	0	1358	8	0
1	C	1361	0	1347	12	0
1	D	1362	0	1341	10	0
1	E	1385	0	1369	13	0
1	F	1380	0	1367	7	0
1	G	1367	0	1343	8	0
1	I	1405	0	1374	13	0
1	K	1380	0	1367	10	0
1	L	1361	0	1343	10	0
1	M	1370	0	1363	8	0
1	N	1371	0	1354	5	0
1	S	1357	0	1339	10	0
1	T	1370	0	1363	11	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	6	0
2	K	8	0	14	6	0
2	L	8	0	14	4	0
2	M	8	0	14	4	0
2	N	8	0	14	2	0
2	S	8	0	14	5	0
2	T	8	0	14	4	0
3	A	55	0	0	3	0
3	C	55	0	0	0	0
3	D	55	0	0	1	0
3	E	55	0	0	0	0
3	F	55	0	0	0	0
3	I	55	0	0	0	0
3	L	55	0	0	0	0
3	M	55	0	0	1	0
3	N	55	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	154	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 4.

All (154) 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:K:147:ARG:HD2	4:K:513:HOH:O	1.80	0.80
1:B:99:MET:HE2	2:B:401:MPD:C1	2.19	0.73
1:S:99:MET:HE2	2:S:401:MPD:H12	1.72	0.71
2:B:401:MPD:HM2	2:B:401:MPD:H52	1.73	0.69
1:S:98:SER:HA	2:S:401:MPD:H32	1.75	0.68
1:I:99:MET:HE2	2:I:401:MPD:C1	2.25	0.66
1:A:176:THR:HG21	4:A:509:HOH:O	1.95	0.66
1:G:99:MET:HE2	2:G:401:MPD:C1	2.26	0.65
1:M:98:SER:HA	2:M:401:MPD:H32	1.79	0.64
2:A:401:MPD:HM2	2:A:401:MPD:H52	1.79	0.64
1:A:99:MET:HE2	2:A:401:MPD:C1	2.28	0.62
1:E:99:MET:HE2	2:E:401:MPD:C1	2.28	0.62
1:A:99:MET:HE2	2:A:401:MPD:H13	1.81	0.62
1:C:99:MET:HE2	2:C:401:MPD:C1	2.30	0.62
1:B:99:MET:HE2	2:B:401:MPD:H12	1.80	0.62
2:T:401:MPD:HM2	2:T:401:MPD:H52	1.82	0.62
1:T:99:MET:HE2	2:T:401:MPD:H12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:98:SER:HA	2:T:401:MPD:H32	1.82	0.62
1:C:98:SER:HA	2:C:401:MPD:H32	1.82	0.61
1:F:98:SER:HA	2:F:401:MPD:H32	1.83	0.60
1:F:99:MET:HE2	2:F:401:MPD:C1	2.32	0.60
2:L:401:MPD:HM2	2:L:401:MPD:H52	1.83	0.60
2:D:401:MPD:H52	2:D:401:MPD:HM2	1.84	0.59
1:C:99:MET:HE2	2:C:401:MPD:H12	1.85	0.59
1:A:99:MET:CE	2:A:401:MPD:H13	2.33	0.59
1:B:98:SER:HA	2:B:401:MPD:H32	1.84	0.59
1:G:98:SER:HA	2:G:401:MPD:H32	1.83	0.58
1:A:93:MET:CE	3:A:402:EZA:F2	2.41	0.58
1:S:61:TYR:CD1	3:S:402:EZA:O5	2.56	0.58
1:E:98:SER:HA	2:E:401:MPD:H32	1.85	0.58
1:S:99:MET:HE2	2:S:401:MPD:C1	2.33	0.58
1:B:81:MET:CE	1:B:103:LEU:HD22	2.33	0.58
1:I:81:MET:CE	1:I:103:LEU:HD22	2.34	0.58
1:N:98:SER:HA	2:N:401:MPD:H32	1.87	0.57
1:S:81:MET:CE	1:S:103:LEU:HD22	2.35	0.57
2:I:401:MPD:HM2	2:I:401:MPD:H52	1.87	0.56
1:D:81:MET:CE	1:D:103:LEU:HD22	2.36	0.56
1:M:99:MET:HE2	2:M:401:MPD:H12	1.86	0.56
1:A:98:SER:HA	2:A:401:MPD:H32	1.88	0.56
1:K:99:MET:HE2	2:K:401:MPD:C1	2.35	0.56
1:T:81:MET:CE	1:T:103:LEU:HD22	2.36	0.56
1:A:93:MET:HE1	3:A:402:EZA:F2	1.95	0.56
1:I:98:SER:HA	2:I:401:MPD:H32	1.88	0.56
1:K:98:SER:HA	2:K:401:MPD:H32	1.88	0.56
2:C:401:MPD:HM2	2:C:401:MPD:H52	1.88	0.55
1:C:81:MET:CE	1:C:103:LEU:HD22	2.36	0.55
1:T:99:MET:HE2	2:T:401:MPD:C1	2.35	0.55
1:G:81:MET:CE	1:G:103:LEU:HD22	2.35	0.55
1:D:99:MET:HE2	2:D:401:MPD:C1	2.37	0.55
1:G:99:MET:HE2	2:G:401:MPD:H12	1.89	0.54
1:M:99:MET:HE2	2:M:401:MPD:C1	2.36	0.54
1:A:81:MET:CE	1:A:103:LEU:HD22	2.38	0.54
1:L:98:SER:HA	2:L:401:MPD:H32	1.89	0.53
1:D:98:SER:HA	2:D:401:MPD:H32	1.89	0.53
2:F:401:MPD:HM2	2:F:401:MPD:H52	1.89	0.53
1:D:99:MET:HE2	2:D:401:MPD:H12	1.90	0.53
1:L:99:MET:HE2	2:L:401:MPD:H12	1.91	0.53
1:B:75:MET:CE	1:B:99:MET:SD	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:MET:HE2	2:I:401:MPD:H13	1.90	0.52
1:M:63:TYR:CZ	3:M:402:EZA:C15	2.93	0.51
1:I:99:MET:CE	2:I:401:MPD:H13	2.41	0.51
1:N:81:MET:CE	1:N:103:LEU:HD22	2.40	0.51
1:E:81:MET:CE	1:E:103:LEU:HD22	2.41	0.51
2:M:401:MPD:H52	2:M:401:MPD:HM2	1.93	0.50
1:K:81:MET:CE	1:K:103:LEU:HD22	2.41	0.50
1:F:99:MET:HE2	2:F:401:MPD:H12	1.92	0.50
1:M:81:MET:CE	1:M:103:LEU:HD22	2.42	0.50
1:E:99:MET:HE2	2:E:401:MPD:H12	1.94	0.50
1:I:99:MET:HE2	2:I:401:MPD:H12	1.95	0.49
1:K:99:MET:CE	2:K:401:MPD:H13	2.43	0.49
1:C:99:MET:CE	2:C:401:MPD:H13	2.43	0.48
1:B:99:MET:CE	2:B:401:MPD:C1	2.90	0.48
1:E:99:MET:CE	2:E:401:MPD:H13	2.43	0.48
1:E:99:MET:HE2	2:E:401:MPD:H13	1.95	0.48
2:K:401:MPD:HM2	2:K:401:MPD:H52	1.95	0.48
1:G:153:ILE:O	1:G:157:ARG:HG2	2.13	0.48
2:G:401:MPD:HM2	2:G:401:MPD:H52	1.95	0.48
1:T:91:ILE:HD12	1:T:91:ILE:N	2.29	0.48
1:L:105:THR:O	1:L:157:ARG:HD3	2.14	0.47
1:L:99:MET:HE2	2:L:401:MPD:C1	2.44	0.47
1:L:63:TYR:CE1	1:L:91:ILE:HD13	2.49	0.47
1:S:63:TYR:CE1	1:S:91:ILE:HD13	2.49	0.47
1:E:153:ILE:O	1:E:157:ARG:HG2	2.14	0.47
1:L:81:MET:CE	1:L:103:LEU:HD22	2.44	0.47
1:A:176:THR:HG22	1:A:178:GLU:N	2.29	0.47
1:B:75:MET:HE3	1:B:99:MET:SD	2.54	0.47
1:C:91:ILE:HD12	1:C:91:ILE:N	2.30	0.47
1:E:91:ILE:N	1:E:91:ILE:HD12	2.30	0.46
1:C:63:TYR:CE1	1:C:91:ILE:HD13	2.50	0.46
1:F:81:MET:CE	1:F:103:LEU:HD22	2.45	0.46
1:M:63:TYR:CE1	1:M:91:ILE:HD13	2.50	0.46
1:I:63:TYR:CE1	1:I:91:ILE:HD13	2.50	0.46
1:K:99:MET:HE2	2:K:401:MPD:H12	1.97	0.46
1:N:176:THR:HG22	1:N:178:GLU:N	2.31	0.46
1:N:113:PHE:CD1	1:N:190:MET:HE3	2.51	0.46
1:S:176:THR:HG22	1:S:178:GLU:N	2.31	0.45
1:F:63:TYR:CE1	1:F:91:ILE:HD13	2.52	0.45
1:K:153:ILE:O	1:K:157:ARG:HG2	2.16	0.45
1:L:91:ILE:HD12	1:L:91:ILE:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:401:MPD:H52	2:S:401:MPD:HM2	1.99	0.44
1:C:176:THR:HG22	1:C:178:GLU:N	2.33	0.44
1:E:113:PHE:CD1	1:E:190:MET:HE3	2.52	0.44
1:L:176:THR:HG22	1:L:178:GLU:N	2.33	0.44
3:D:402:EZA:N4	3:D:402:EZA:O2	2.51	0.44
1:B:176:THR:HG22	1:B:178:GLU:N	2.33	0.44
1:D:63:TYR:CE1	1:D:91:ILE:HD13	2.53	0.44
1:G:176:THR:HG22	1:G:178:GLU:N	2.33	0.43
1:F:91:ILE:N	1:F:91:ILE:HD12	2.34	0.43
1:M:105:THR:O	1:M:157:ARG:HD3	2.18	0.43
1:S:91:ILE:N	1:S:91:ILE:HD12	2.34	0.43
1:A:99:MET:HE2	2:A:401:MPD:H12	1.99	0.43
1:D:153:ILE:O	1:D:157:ARG:HG2	2.19	0.43
1:I:81:MET:HE1	1:I:103:LEU:HD22	2.00	0.43
1:I:176:THR:HG22	1:I:178:GLU:N	2.34	0.43
1:N:63:TYR:CE1	1:N:91:ILE:HD13	2.54	0.43
1:A:93:MET:HE2	3:A:402:EZA:F2	2.08	0.42
1:E:123:HIS:O	2:E:401:MPD:H31	2.19	0.42
1:F:176:THR:HG22	1:F:178:GLU:N	2.35	0.42
1:T:63:TYR:CE1	1:T:91:ILE:HD13	2.53	0.42
1:E:99:MET:CE	2:E:401:MPD:C1	2.98	0.42
1:I:91:ILE:N	1:I:91:ILE:HD12	2.35	0.42
1:C:81:MET:HE1	1:C:103:LEU:HD22	2.00	0.42
1:D:98:SER:HG	1:D:123:HIS:CE1	2.33	0.42
1:K:99:MET:HE2	2:K:401:MPD:H13	2.01	0.42
1:G:81:MET:HE1	1:G:103:LEU:HD22	2.02	0.42
1:K:107:GLY:O	1:K:157:ARG:NH2	2.53	0.42
1:L:74:GLY:HA3	1:L:99:MET:HG2	2.02	0.42
1:D:91:ILE:HD12	1:D:91:ILE:N	2.35	0.42
1:E:83:PHE:CD1	1:E:83:PHE:C	2.92	0.42
2:N:401:MPD:HM2	2:N:401:MPD:H52	2.02	0.41
1:C:99:MET:HE2	2:C:401:MPD:H13	2.00	0.41
1:T:77:ILE:HG22	1:T:81:MET:HE3	2.01	0.41
1:D:81:MET:HE1	1:D:103:LEU:HD22	2.02	0.41
1:A:63:TYR:CE1	1:A:91:ILE:HD13	2.55	0.41
1:D:83:PHE:CD1	1:D:83:PHE:C	2.94	0.41
1:I:153:ILE:O	1:I:157:ARG:HG2	2.20	0.41
1:I:83:PHE:CD1	1:I:83:PHE:C	2.94	0.41
1:C:99:MET:CE	2:C:401:MPD:C1	2.98	0.41
1:G:154:LEU:HD11	2:G:401:MPD:H51	2.03	0.41
1:K:74:GLY:HA3	1:K:99:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:81:MET:HE2	1:T:103:LEU:HD22	2.02	0.41
1:S:99:MET:CE	2:S:401:MPD:C1	2.98	0.41
1:I:93:MET:HB3	1:I:115:LEU:HD12	2.03	0.41
1:M:74:GLY:HA3	1:M:99:MET:HG2	2.03	0.41
1:T:153:ILE:O	1:T:157:ARG:HG2	2.21	0.41
1:A:113:PHE:CD1	1:A:190:MET:HE3	2.56	0.41
1:E:74:GLY:HA3	1:E:99:MET:HG2	2.03	0.40
1:C:153:ILE:O	1:C:157:ARG:HG2	2.21	0.40
1:A:74:GLY:HA3	1:A:99:MET:HG2	2.03	0.40
1:T:176:THR:HG22	1:T:178:GLU:N	2.37	0.40
1:A:63:TYR:HB3	1:A:93:MET:CE	2.51	0.40
1:T:89:GLN:HG2	1:T:111:LYS:HB3	2.04	0.40
1:L:89:GLN:HG2	1:L:111:LYS:HB3	2.02	0.40
1:S:63:TYR:CD2	3:S:402:EZA:F2	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	84	93
1	B	142/174 (82%)	141 (99%)	1 (1%)	84	93
1	C	141/174 (81%)	140 (99%)	1 (1%)	84	93
1	D	140/174 (80%)	139 (99%)	1 (1%)	84	93
1	E	142/174 (82%)	141 (99%)	1 (1%)	84	93
1	F	142/174 (82%)	141 (99%)	1 (1%)	84	93
1	G	140/174 (80%)	139 (99%)	1 (1%)	84	93
1	I	143/174 (82%)	141 (99%)	2 (1%)	67	84
1	K	142/174 (82%)	141 (99%)	1 (1%)	84	93
1	L	141/174 (81%)	140 (99%)	1 (1%)	84	93
1	M	142/174 (82%)	141 (99%)	1 (1%)	84	93
1	N	141/174 (81%)	140 (99%)	1 (1%)	84	93
1	S	140/174 (80%)	139 (99%)	1 (1%)	84	93
1	T	142/174 (82%)	141 (99%)	1 (1%)	84	93
All	All	1980/2436 (81%)	1965 (99%)	15 (1%)	81	92

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

Mol	Chain	Res	Type
1	A	123	HIS
1	B	123	HIS
1	C	123	HIS
1	D	123	HIS
1	E	123	HIS
1	F	123	HIS
1	G	123	HIS
1	I	11	SER
1	I	123	HIS
1	K	123	HIS
1	L	123	HIS
1	M	123	HIS
1	N	123	HIS
1	S	123	HIS
1	T	123	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
3	EZA	N	402	-	59,59,59	2.85	17 (28%)	78,83,83	2.22	22 (28%)
3	EZA	C	402	-	59,59,59	2.80	16 (27%)	78,83,83	2.33	24 (30%)
3	EZA	F	402	-	59,59,59	2.88	16 (27%)	78,83,83	2.09	17 (21%)
3	EZA	D	402	-	59,59,59	2.79	16 (27%)	78,83,83	2.17	15 (19%)
2	MPD	S	401	-	7,7,7	0.71	0	9,10,10	0.81	0
2	MPD	L	401	-	7,7,7	0.54	0	9,10,10	0.77	0
3	EZA	S	402	-	59,59,59	2.76	19 (32%)	78,83,83	2.26	30 (38%)
3	EZA	T	402	-	59,59,59	2.80	16 (27%)	78,83,83	2.27	17 (21%)
2	MPD	T	401	-	7,7,7	0.80	0	9,10,10	0.95	0
3	EZA	L	402	-	59,59,59	2.79	15 (25%)	78,83,83	2.14	19 (24%)
2	MPD	K	401	-	7,7,7	0.65	0	9,10,10	0.92	1 (11%)
2	MPD	I	401	-	7,7,7	0.45	0	9,10,10	0.56	0
2	MPD	F	401	-	7,7,7	0.51	0	9,10,10	0.78	0
2	MPD	M	401	-	7,7,7	0.39	0	9,10,10	0.99	1 (11%)
2	MPD	B	401	-	7,7,7	0.48	0	9,10,10	0.81	0
2	MPD	E	401	-	7,7,7	0.61	0	9,10,10	0.70	0
2	MPD	A	401	-	7,7,7	0.47	0	9,10,10	0.27	0
3	EZA	E	402	-	59,59,59	2.74	14 (23%)	78,83,83	2.35	21 (26%)
3	EZA	A	402	-	59,59,59	2.79	16 (27%)	78,83,83	1.87	13 (16%)
2	MPD	N	401	-	7,7,7	0.74	0	9,10,10	1.01	1 (11%)
3	EZA	M	402	-	59,59,59	2.84	17 (28%)	78,83,83	2.36	21 (26%)
2	MPD	C	401	-	7,7,7	0.79	0	9,10,10	1.10	1 (11%)
2	MPD	D	401	-	7,7,7	0.43	0	9,10,10	0.48	0
3	EZA	I	402	-	59,59,59	2.66	16 (27%)	78,83,83	2.37	20 (25%)
2	MPD	G	401	-	7,7,7	0.65	0	9,10,10	1.34	1 (11%)

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
3	EZA	N	402	-	1/1/17/22	11/63/96/96	0/4/5/5
3	EZA	C	402	-	2/2/17/22	17/63/96/96	0/4/5/5
3	EZA	F	402	-	1/1/17/22	14/63/96/96	0/4/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EZA	D	402	-	1/1/17/22	12/63/96/96	0/4/5/5
2	MPD	S	401	-	-	1/5/5/5	-
2	MPD	L	401	-	-	3/5/5/5	-
3	EZA	S	402	-	2/2/17/22	14/63/96/96	0/4/5/5
3	EZA	T	402	-	1/1/17/22	13/63/96/96	0/4/5/5
2	MPD	T	401	-	-	1/5/5/5	-
3	EZA	L	402	-	1/1/17/22	11/63/96/96	0/4/5/5
2	MPD	K	401	-	-	2/5/5/5	-
2	MPD	I	401	-	-	0/5/5/5	-
2	MPD	F	401	-	-	1/5/5/5	-
2	MPD	M	401	-	-	1/5/5/5	-
2	MPD	B	401	-	-	1/5/5/5	-
2	MPD	E	401	-	-	3/5/5/5	-
2	MPD	A	401	-	-	2/5/5/5	-
3	EZA	E	402	-	2/2/17/22	13/63/96/96	0/4/5/5
2	MPD	C	401	-	-	1/5/5/5	-
2	MPD	N	401	-	-	2/5/5/5	-
3	EZA	M	402	-	2/2/17/22	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	D	401	-	-	1/5/5/5	-
3	EZA	I	402	-	2/2/17/22	15/63/96/96	0/4/5/5
2	MPD	G	401	-	-	1/5/5/5	-

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	402	EZA	C34-N5	8.20	1.53	1.34
3	A	402	EZA	C20-C19	-8.09	1.37	1.52
3	S	402	EZA	C34-N5	7.93	1.52	1.34
3	E	402	EZA	C34-N5	7.82	1.52	1.34
3	D	402	EZA	C34-N5	7.75	1.52	1.34
3	F	402	EZA	C20-C19	-7.75	1.37	1.52
3	L	402	EZA	C20-C19	-7.70	1.37	1.52
3	T	402	EZA	C34-N5	7.64	1.52	1.34
3	N	402	EZA	C34-N5	7.61	1.52	1.34
3	F	402	EZA	C34-N5	7.61	1.52	1.34
3	C	402	EZA	C34-N5	7.57	1.52	1.34
3	S	402	EZA	O3-C19	7.41	1.48	1.33
3	M	402	EZA	C34-N5	7.39	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	402	EZA	C34-N5	7.28	1.51	1.34
3	M	402	EZA	O3-C19	7.27	1.48	1.33
3	A	402	EZA	C34-N5	7.12	1.51	1.34
3	N	402	EZA	C20-C19	-7.08	1.39	1.52
3	I	402	EZA	O3-C19	7.02	1.47	1.33
3	T	402	EZA	C28-N4	6.98	1.49	1.34
3	D	402	EZA	C28-N4	6.91	1.49	1.34
3	T	402	EZA	C20-C19	-6.86	1.39	1.52
3	F	402	EZA	C16-N2	6.85	1.49	1.34
3	N	402	EZA	C16-N2	6.84	1.49	1.34
3	E	402	EZA	O3-C19	6.81	1.47	1.33
3	C	402	EZA	O3-C19	6.80	1.47	1.33
3	F	402	EZA	C28-N4	6.80	1.49	1.34
3	I	402	EZA	C16-N2	6.74	1.48	1.34
3	E	402	EZA	C20-C19	-6.71	1.39	1.52
3	N	402	EZA	C28-N4	6.69	1.48	1.34
3	L	402	EZA	O3-C19	6.69	1.47	1.33
3	T	402	EZA	O3-C19	6.69	1.47	1.33
3	C	402	EZA	C28-N4	6.67	1.48	1.34
3	D	402	EZA	O3-C19	6.65	1.47	1.33
3	T	402	EZA	C16-N2	6.65	1.48	1.34
3	D	402	EZA	C16-N2	6.64	1.48	1.34
3	D	402	EZA	C20-C19	-6.62	1.39	1.52
3	L	402	EZA	C28-N4	6.61	1.48	1.34
3	N	402	EZA	O3-C19	6.60	1.46	1.33
3	L	402	EZA	C16-N2	6.60	1.48	1.34
3	F	402	EZA	O3-C19	6.59	1.46	1.33
3	E	402	EZA	C16-N2	6.59	1.48	1.34
3	M	402	EZA	C16-N2	6.57	1.48	1.34
3	A	402	EZA	C16-N2	6.56	1.48	1.34
3	C	402	EZA	C16-N2	6.55	1.48	1.34
3	A	402	EZA	C28-N4	6.51	1.48	1.34
3	A	402	EZA	O3-C19	6.49	1.46	1.33
3	M	402	EZA	C29-N5	-6.42	1.39	1.47
3	C	402	EZA	C20-C19	-6.38	1.40	1.52
3	C	402	EZA	C7-N1	6.38	1.49	1.34
3	S	402	EZA	C16-N2	6.31	1.47	1.34
3	E	402	EZA	C39-N6	6.31	1.49	1.34
3	M	402	EZA	C28-N4	6.28	1.47	1.34
3	M	402	EZA	C39-N6	6.27	1.49	1.34
3	N	402	EZA	C39-N6	6.21	1.48	1.34
3	F	402	EZA	C39-N6	6.17	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	402	EZA	C25-N3	6.16	1.48	1.34
3	T	402	EZA	C7-N1	6.16	1.49	1.34
3	I	402	EZA	C28-N4	6.14	1.47	1.34
3	A	402	EZA	C7-N1	6.12	1.49	1.34
3	E	402	EZA	C28-N4	6.10	1.47	1.34
3	S	402	EZA	C7-N1	6.05	1.48	1.34
3	M	402	EZA	C7-N1	6.03	1.48	1.34
3	M	402	EZA	C25-N3	6.01	1.48	1.34
3	N	402	EZA	C7-N1	6.00	1.48	1.34
3	S	402	EZA	C28-N4	5.99	1.47	1.34
3	N	402	EZA	C25-N3	5.99	1.48	1.34
3	F	402	EZA	C7-N1	5.98	1.48	1.34
3	M	402	EZA	C20-C19	-5.89	1.41	1.52
3	F	402	EZA	C21-C20	-5.87	1.42	1.53
3	L	402	EZA	C21-C20	-5.86	1.42	1.53
3	D	402	EZA	C7-N1	5.86	1.48	1.34
3	I	402	EZA	C20-C19	-5.83	1.41	1.52
3	L	402	EZA	C25-N3	5.77	1.47	1.34
3	T	402	EZA	C39-N6	5.76	1.47	1.34
3	L	402	EZA	C39-N6	5.75	1.47	1.34
3	D	402	EZA	C39-N6	5.75	1.47	1.34
3	S	402	EZA	C39-N6	5.72	1.47	1.34
3	I	402	EZA	C7-N1	5.69	1.48	1.34
3	T	402	EZA	C25-N3	5.67	1.47	1.34
3	C	402	EZA	C25-N3	5.66	1.47	1.34
3	I	402	EZA	C25-N3	5.62	1.47	1.34
3	I	402	EZA	C39-N6	5.61	1.47	1.34
3	C	402	EZA	C39-N6	5.60	1.47	1.34
3	D	402	EZA	C25-N3	5.56	1.47	1.34
3	L	402	EZA	C7-N1	5.56	1.47	1.34
3	E	402	EZA	C25-N3	5.55	1.47	1.34
3	A	402	EZA	C39-N6	5.55	1.47	1.34
3	D	402	EZA	C21-C20	-5.55	1.43	1.53
3	F	402	EZA	C25-N3	5.41	1.47	1.34
3	N	402	EZA	C29-N5	-5.28	1.41	1.47
3	C	402	EZA	C29-N5	-5.26	1.41	1.47
3	S	402	EZA	C29-N5	-5.26	1.41	1.47
3	C	402	EZA	C21-C20	-5.20	1.43	1.53
3	A	402	EZA	C21-C20	-5.19	1.43	1.53
3	E	402	EZA	C29-N5	-5.16	1.41	1.47
3	F	402	EZA	C29-N5	-5.13	1.41	1.47
3	E	402	EZA	C7-N1	5.13	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	402	EZA	C21-C20	-5.11	1.44	1.53
3	A	402	EZA	C29-N5	-4.94	1.41	1.47
3	M	402	EZA	C21-C20	-4.89	1.44	1.53
3	T	402	EZA	C29-N5	-4.86	1.41	1.47
3	A	402	EZA	C25-N3	4.82	1.45	1.34
3	S	402	EZA	C20-C19	-4.82	1.43	1.52
3	E	402	EZA	C21-C20	-4.63	1.45	1.53
3	L	402	EZA	C29-N5	-4.53	1.42	1.47
3	S	402	EZA	C24-C22	-4.34	1.45	1.52
3	D	402	EZA	C29-N5	-4.31	1.42	1.47
3	T	402	EZA	C21-C20	-4.18	1.45	1.53
3	I	402	EZA	C29-N5	-3.94	1.42	1.47
3	I	402	EZA	C21-C20	-3.93	1.46	1.53
3	C	402	EZA	C24-C22	-3.39	1.47	1.52
3	F	402	EZA	C24-C22	-3.37	1.47	1.52
3	A	402	EZA	C24-C22	-3.23	1.47	1.52
3	M	402	EZA	C24-C22	-3.19	1.47	1.52
3	S	402	EZA	C21-C20	-3.17	1.47	1.53
3	L	402	EZA	C24-C22	-3.15	1.47	1.52
3	D	402	EZA	C24-C22	-3.08	1.47	1.52
3	T	402	EZA	C8-N1	-3.05	1.39	1.45
3	E	402	EZA	C8-N1	-3.04	1.39	1.45
3	E	402	EZA	C24-C22	-3.03	1.47	1.52
3	T	402	EZA	C13-C14	2.90	1.42	1.37
3	N	402	EZA	C24-C22	-2.86	1.48	1.52
3	M	402	EZA	C13-C14	2.85	1.42	1.37
3	M	402	EZA	C35-C34	-2.85	1.46	1.53
3	I	402	EZA	C24-C22	-2.83	1.48	1.52
3	T	402	EZA	C24-C22	-2.81	1.48	1.52
3	N	402	EZA	C6-C7	2.78	1.54	1.48
3	S	402	EZA	C35-C34	-2.77	1.46	1.53
3	L	402	EZA	C8-N1	-2.76	1.40	1.45
3	E	402	EZA	C13-C14	2.76	1.42	1.37
3	T	402	EZA	C6-C7	2.75	1.54	1.48
3	N	402	EZA	C35-C34	-2.74	1.46	1.53
3	C	402	EZA	C13-C14	2.72	1.42	1.37
3	N	402	EZA	C13-C14	2.71	1.42	1.37
3	M	402	EZA	C8-N1	-2.68	1.40	1.45
3	S	402	EZA	C13-C14	2.67	1.42	1.37
3	D	402	EZA	C13-C14	2.66	1.42	1.37
3	E	402	EZA	C35-C34	-2.63	1.47	1.53
3	A	402	EZA	C20-N3	-2.62	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	EZA	C35-C34	-2.60	1.47	1.53
3	F	402	EZA	C6-C7	2.57	1.53	1.48
3	S	402	EZA	C27-C26	-2.55	1.45	1.52
3	A	402	EZA	F2-C14	-2.55	1.30	1.36
3	C	402	EZA	C35-C34	-2.54	1.47	1.53
3	C	402	EZA	C8-N1	-2.54	1.40	1.45
3	I	402	EZA	C13-C14	2.51	1.41	1.37
3	M	402	EZA	C13-C12	2.51	1.41	1.37
3	M	402	EZA	C6-C7	2.49	1.53	1.48
3	L	402	EZA	C35-C34	-2.47	1.47	1.53
3	D	402	EZA	C8-N1	-2.46	1.40	1.45
3	T	402	EZA	C35-C34	-2.46	1.47	1.53
3	A	402	EZA	C6-C7	2.44	1.53	1.48
3	A	402	EZA	C8-N1	-2.38	1.40	1.45
3	N	402	EZA	C8-N1	-2.37	1.40	1.45
3	C	402	EZA	C6-C7	2.34	1.53	1.48
3	F	402	EZA	C8-N1	-2.34	1.40	1.45
3	S	402	EZA	C6-C7	2.30	1.53	1.48
3	C	402	EZA	C6-C5	2.30	1.38	1.32
3	N	402	EZA	C6-C5	2.30	1.38	1.32
3	I	402	EZA	C8-N1	-2.29	1.41	1.45
3	F	402	EZA	C35-C34	-2.29	1.48	1.53
3	L	402	EZA	C6-C7	2.29	1.53	1.48
3	S	402	EZA	C6-C5	2.27	1.37	1.32
3	F	402	EZA	C13-C14	2.21	1.41	1.37
3	A	402	EZA	C35-C34	-2.19	1.48	1.53
3	T	402	EZA	C27-C26	-2.17	1.46	1.52
3	S	402	EZA	C8-N1	-2.10	1.41	1.45
3	D	402	EZA	C13-C12	2.09	1.41	1.37
3	M	402	EZA	C36-C35	-2.08	1.48	1.53
3	I	402	EZA	C35-C34	-2.07	1.48	1.53
3	S	402	EZA	C36-C35	-2.07	1.48	1.53
3	D	402	EZA	C6-C7	2.04	1.52	1.48
3	S	402	EZA	C23-C22	2.04	1.59	1.52
3	N	402	EZA	C36-C35	-2.04	1.49	1.53
3	L	402	EZA	C23-C22	2.04	1.59	1.52
3	F	402	EZA	C6-C5	2.03	1.37	1.32
3	I	402	EZA	C6-C5	2.02	1.37	1.32
3	I	402	EZA	C6-C7	2.00	1.52	1.48

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	402	EZA	C19-C20-N3	10.05	132.38	112.07
3	E	402	EZA	C19-C20-N3	9.85	131.97	112.07
3	I	402	EZA	C19-C20-N3	9.50	131.26	112.07
3	C	402	EZA	C19-C20-N3	9.31	130.88	112.07
3	D	402	EZA	C19-C20-N3	9.09	130.44	112.07
3	T	402	EZA	C19-C20-N3	9.04	130.34	112.07
3	I	402	EZA	C25-C26-N4	7.97	129.10	109.14
3	N	402	EZA	C19-C20-N3	7.76	127.75	112.07
3	D	402	EZA	C25-C26-N4	7.59	128.17	109.14
3	L	402	EZA	C19-C20-N3	7.56	127.34	112.07
3	C	402	EZA	C25-C26-N4	7.47	127.86	109.14
3	T	402	EZA	C25-C26-N4	7.29	127.41	109.14
3	F	402	EZA	C19-C20-N3	7.27	126.75	112.07
3	S	402	EZA	C26-C25-N3	7.14	131.90	118.10
3	A	402	EZA	C25-C26-N4	7.07	126.86	109.14
3	M	402	EZA	C25-C26-N4	7.04	126.78	109.14
3	M	402	EZA	C24-N3-C20	-6.81	101.87	111.70
3	E	402	EZA	C24-N3-C20	-6.78	101.91	111.70
3	F	402	EZA	C25-C26-N4	6.77	126.11	109.14
3	I	402	EZA	C24-N3-C20	-6.74	101.96	111.70
3	T	402	EZA	C24-N3-C20	-6.62	102.14	111.70
3	N	402	EZA	C24-N3-C20	-6.58	102.19	111.70
3	N	402	EZA	C25-C26-N4	6.54	125.53	109.14
3	L	402	EZA	C24-N3-C20	-6.44	102.40	111.70
3	I	402	EZA	C21-C20-N3	6.43	111.59	103.10
3	S	402	EZA	C25-C26-N4	6.38	125.13	109.14
3	L	402	EZA	C25-C26-N4	6.31	124.96	109.14
3	E	402	EZA	C25-C26-N4	6.25	124.80	109.14
3	T	402	EZA	C21-C20-N3	6.23	111.33	103.10
3	E	402	EZA	C21-C20-N3	6.03	111.07	103.10
3	F	402	EZA	C24-N3-C20	-6.00	103.04	111.70
3	D	402	EZA	C24-N3-C20	-5.99	103.04	111.70
3	C	402	EZA	C24-N3-C20	-5.76	103.38	111.70
3	A	402	EZA	C21-C20-N3	5.68	110.60	103.10
3	A	402	EZA	C27-C26-N4	5.13	120.02	110.38
3	N	402	EZA	C27-C26-N4	5.13	120.01	110.38
3	E	402	EZA	C27-C26-N4	5.11	119.97	110.38
3	N	402	EZA	C21-C20-N3	4.93	109.62	103.10
3	L	402	EZA	C21-C20-C19	4.92	120.27	111.37
3	A	402	EZA	C19-C20-N3	4.85	121.86	112.07
3	M	402	EZA	C21-C20-N3	4.83	109.48	103.10
3	A	402	EZA	C24-N3-C20	-4.83	104.73	111.70
3	T	402	EZA	C4-C5-C6	-4.74	115.68	125.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	EZA	C21-C20-N3	4.65	109.24	103.10
3	M	402	EZA	C27-C26-N4	4.59	119.00	110.38
3	S	402	EZA	C27-C26-N4	4.58	118.99	110.38
3	N	402	EZA	C21-C20-C19	4.45	119.41	111.37
3	S	402	EZA	O5-C25-N3	-4.39	113.55	121.38
3	S	402	EZA	O3-C19-C20	4.21	119.42	110.54
3	C	402	EZA	C20-N3-C25	4.17	135.81	121.41
3	T	402	EZA	C27-C26-C25	4.17	117.30	109.73
3	C	402	EZA	F2-C14-C13	4.16	124.19	118.25
3	L	402	EZA	C27-C26-N4	4.14	118.16	110.38
3	M	402	EZA	C20-N3-C25	4.14	135.71	121.41
3	C	402	EZA	C21-C20-N3	4.10	108.51	103.10
3	E	402	EZA	C20-N3-C25	4.09	135.53	121.41
3	M	402	EZA	C4-C5-C6	-4.07	117.13	125.85
3	S	402	EZA	C20-N3-C25	3.99	135.17	121.41
3	C	402	EZA	C26-C25-N3	3.96	125.77	118.10
3	F	402	EZA	C27-C26-N4	3.96	117.82	110.38
3	D	402	EZA	C21-C20-N3	3.89	108.24	103.10
3	L	402	EZA	C27-C26-C25	3.88	116.78	109.73
3	I	402	EZA	C20-N3-C25	3.82	134.60	121.41
3	E	402	EZA	C26-C25-N3	3.82	125.48	118.10
3	C	402	EZA	O5-C25-N3	-3.80	114.60	121.38
3	L	402	EZA	C21-C20-N3	3.76	108.07	103.10
3	N	402	EZA	C20-N3-C25	3.75	134.35	121.41
3	D	402	EZA	C20-N3-C25	3.75	134.35	121.41
3	I	402	EZA	C26-C25-N3	3.74	125.33	118.10
3	T	402	EZA	C20-N3-C25	3.73	134.28	121.41
3	D	402	EZA	C21-C20-C19	3.72	118.11	111.37
3	C	402	EZA	C21-C20-C19	3.71	118.09	111.37
3	F	402	EZA	C21-C20-C19	3.70	118.07	111.37
3	S	402	EZA	C24-N3-C20	-3.62	106.47	111.70
3	N	402	EZA	F2-C14-C13	3.56	123.34	118.25
3	F	402	EZA	O5-C25-N3	-3.55	115.04	121.38
3	F	402	EZA	C20-N3-C25	3.54	133.64	121.41
3	S	402	EZA	C4-C5-C6	-3.51	118.32	125.85
3	T	402	EZA	F2-C14-C13	3.50	123.25	118.25
3	L	402	EZA	C20-N3-C25	3.49	133.44	121.41
3	E	402	EZA	C4-C5-C6	-3.46	118.43	125.85
3	E	402	EZA	F2-C14-C13	3.45	123.18	118.25
3	M	402	EZA	F2-C14-C13	3.43	123.15	118.25
3	C	402	EZA	O1-C7-N1	3.42	126.88	122.35
3	F	402	EZA	C27-C26-C25	3.41	115.92	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	EZA	C4-C5-C6	-3.36	118.65	125.85
3	D	402	EZA	F2-C14-C13	3.35	123.05	118.25
3	D	402	EZA	C27-C26-N4	3.33	116.63	110.38
3	N	402	EZA	C26-C25-N3	3.32	124.52	118.10
3	T	402	EZA	C26-C25-N3	3.31	124.50	118.10
3	I	402	EZA	O5-C25-N3	-3.30	115.49	121.38
3	C	402	EZA	C27-C26-N4	3.28	116.55	110.38
3	M	402	EZA	C15-C14-C13	-3.28	119.38	123.52
3	I	402	EZA	C27-C26-C25	3.24	115.62	109.73
3	S	402	EZA	C22-C24-N3	3.24	106.87	103.53
3	E	402	EZA	O5-C25-N3	-3.18	115.70	121.38
3	I	402	EZA	F2-C14-C13	3.16	122.77	118.25
3	M	402	EZA	O5-C25-N3	-3.16	115.75	121.38
3	D	402	EZA	O5-C25-N3	-3.15	115.77	121.38
3	M	402	EZA	C18-O3-C19	3.14	123.04	116.84
3	T	402	EZA	O5-C25-N3	-3.13	115.80	121.38
3	C	402	EZA	C15-C14-C13	-3.12	119.58	123.52
3	I	402	EZA	C18-O3-C19	3.12	122.99	116.84
3	N	402	EZA	C15-C14-C13	-3.11	119.59	123.52
3	N	402	EZA	C18-O3-C19	3.10	122.95	116.84
3	F	402	EZA	C39-C17-N2	3.07	115.99	108.81
3	A	402	EZA	C18-O3-C19	3.07	122.89	116.84
3	C	402	EZA	C27-C26-C25	3.06	115.29	109.73
3	S	402	EZA	C19-C20-N3	3.06	118.24	112.07
3	C	402	EZA	C18-O3-C19	3.05	122.86	116.84
3	E	402	EZA	C27-C26-C25	3.02	115.22	109.73
3	S	402	EZA	O2-C16-N2	-3.02	117.33	122.93
3	S	402	EZA	C13-C12-C11	-3.02	119.70	123.52
3	M	402	EZA	C26-C25-N3	3.00	123.91	118.10
3	E	402	EZA	C18-O3-C19	3.00	122.74	116.84
3	D	402	EZA	C27-C26-C25	2.99	115.16	109.73
3	S	402	EZA	C10-C11-C12	2.98	121.52	118.81
3	S	402	EZA	C15-C14-C13	-2.97	119.76	123.52
3	L	402	EZA	C18-O3-C19	2.97	122.69	116.84
3	F	402	EZA	C26-C25-N3	2.92	123.75	118.10
3	A	402	EZA	F1-C12-C11	2.87	122.36	118.25
3	L	402	EZA	F2-C14-C13	2.86	122.34	118.25
3	S	402	EZA	C21-C20-C19	-2.85	106.21	111.37
3	L	402	EZA	C4-C5-C6	-2.83	119.78	125.85
3	A	402	EZA	O7-C34-N5	-2.79	116.40	121.38
3	S	402	EZA	O5-C25-C26	-2.78	114.44	120.19
3	S	402	EZA	O3-C19-O4	-2.77	118.88	124.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	402	EZA	O5-C25-N3	-2.77	116.45	121.38
3	D	402	EZA	C13-C12-C11	-2.74	120.05	123.52
3	S	402	EZA	C35-C34-N5	2.73	124.45	117.72
3	S	402	EZA	C27-C26-C25	2.72	114.67	109.73
3	F	402	EZA	C31-C30-C29	2.71	116.28	111.23
3	M	402	EZA	F1-C12-C13	2.69	122.09	118.25
3	M	402	EZA	C21-C20-C19	2.68	116.22	111.37
3	M	402	EZA	C35-C34-N5	2.67	124.30	117.72
3	D	402	EZA	C18-O3-C19	2.67	122.09	116.84
3	N	402	EZA	O5-C25-N3	-2.66	116.63	121.38
3	I	402	EZA	C4-C5-C6	-2.66	120.15	125.85
3	E	402	EZA	C35-C34-N5	2.66	124.26	117.72
3	I	402	EZA	C13-C12-C11	-2.66	120.16	123.52
3	T	402	EZA	C18-O3-C19	2.65	122.07	116.84
3	C	402	EZA	C9-C8-C16	-2.64	103.41	110.25
3	D	402	EZA	C26-C25-N3	2.62	123.17	118.10
3	I	402	EZA	C21-C20-C19	2.62	116.11	111.37
3	I	402	EZA	C27-C26-N4	2.60	115.25	110.38
3	L	402	EZA	C26-C25-N3	2.59	123.11	118.10
3	E	402	EZA	C30-C29-N5	-2.58	106.94	110.53
3	T	402	EZA	C15-C14-C13	-2.58	120.26	123.52
3	N	402	EZA	C4-C5-C6	-2.56	120.36	125.85
3	L	402	EZA	C15-C14-C13	-2.55	120.30	123.52
3	S	402	EZA	C31-C30-C29	2.53	115.94	111.23
3	N	402	EZA	C27-C26-C25	2.52	114.31	109.73
3	T	402	EZA	C27-C26-N4	2.51	115.09	110.38
3	L	402	EZA	C35-C34-N5	2.51	123.89	117.72
3	S	402	EZA	O7-C34-N5	-2.49	116.94	121.38
2	C	401	MPD	O4-C4-C3	-2.48	101.36	111.36
3	C	402	EZA	C13-C12-C11	-2.47	120.39	123.52
3	M	402	EZA	O1-C7-N1	2.47	125.62	122.35
3	N	402	EZA	C35-C34-N5	2.47	123.79	117.72
2	K	401	MPD	O4-C4-C3	-2.45	101.48	111.36
3	S	402	EZA	C8-C16-N2	2.44	122.05	116.70
3	M	402	EZA	C10-C15-C14	2.43	121.02	118.81
3	S	402	EZA	F2-C14-C13	2.43	121.72	118.25
3	L	402	EZA	C31-C30-C29	2.42	115.75	111.23
3	A	402	EZA	C16-C8-N1	-2.42	104.58	111.16
2	N	401	MPD	O4-C4-C3	-2.41	101.64	111.36
3	C	402	EZA	C35-C34-N5	2.40	123.63	117.72
3	A	402	EZA	C4-C5-C6	-2.39	120.72	125.85
3	N	402	EZA	C8-C16-N2	2.39	121.94	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	402	EZA	C13-C12-C11	-2.38	120.51	123.52
3	E	402	EZA	C21-C20-C19	2.38	115.67	111.37
3	N	402	EZA	C9-C8-C16	-2.37	104.09	110.25
3	T	402	EZA	C13-C12-C11	-2.37	120.52	123.52
3	M	402	EZA	C27-C26-C25	2.36	114.01	109.73
3	C	402	EZA	C9-C10-C15	-2.35	116.40	120.44
3	S	402	EZA	C24-N3-C25	-2.35	118.12	126.64
3	A	402	EZA	C30-C29-C28	-2.35	107.86	112.12
3	L	402	EZA	O7-C34-N5	-2.33	117.22	121.38
3	I	402	EZA	C22-C24-N3	2.33	105.93	103.53
3	C	402	EZA	C31-C30-C29	2.32	115.55	111.23
2	M	401	MPD	CM-C2-C1	-2.31	105.75	110.57
3	A	402	EZA	C20-N3-C25	2.31	129.38	121.41
3	F	402	EZA	F2-C14-C13	2.29	121.53	118.25
3	S	402	EZA	C18-O3-C19	2.29	121.35	116.84
3	L	402	EZA	C39-C17-N2	2.28	114.14	108.81
3	E	402	EZA	O1-C7-N1	2.28	125.37	122.35
3	N	402	EZA	C22-C24-N3	2.27	105.87	103.53
3	C	402	EZA	C4-C5-C6	-2.27	120.98	125.85
3	E	402	EZA	C22-C24-N3	2.26	105.86	103.53
3	S	402	EZA	C30-C29-C28	-2.25	108.03	112.12
3	F	402	EZA	C15-C14-C13	-2.24	120.68	123.52
3	S	402	EZA	C14-C13-C12	2.24	119.62	116.13
3	C	402	EZA	C10-C15-C14	2.23	120.84	118.81
3	I	402	EZA	C37-C36-C35	2.23	108.84	104.18
3	C	402	EZA	O7-C34-N5	-2.22	117.43	121.38
3	A	402	EZA	C35-C34-N5	2.21	123.16	117.72
3	M	402	EZA	O7-C34-N5	-2.21	117.44	121.38
3	N	402	EZA	C30-C29-C28	-2.20	108.12	112.12
3	S	402	EZA	O6-C28-N4	-2.17	118.91	122.93
3	E	402	EZA	C15-C14-C13	-2.17	120.78	123.52
3	M	402	EZA	C30-C29-N5	-2.17	107.52	110.53
3	F	402	EZA	C30-C29-C28	-2.15	108.21	112.12
3	D	402	EZA	C30-C29-C28	-2.15	108.22	112.12
3	I	402	EZA	C15-C14-C13	-2.14	120.81	123.52
3	M	402	EZA	C8-C16-N2	2.14	121.39	116.70
3	I	402	EZA	C35-C34-N5	2.14	122.98	117.72
3	F	402	EZA	O1-C7-C6	-2.13	118.17	123.03
2	G	401	MPD	O2-C2-C3	-2.11	101.87	109.80
3	C	402	EZA	O1-C7-C6	-2.10	118.25	123.03
3	S	402	EZA	C33-N5-C34	-2.10	114.97	122.59
3	E	402	EZA	O7-C34-N5	-2.09	117.66	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	402	EZA	C31-C30-C29	2.09	115.12	111.23
3	L	402	EZA	C30-C29-C28	-2.08	108.34	112.12
3	E	402	EZA	C13-C12-C11	-2.07	120.90	123.52
3	N	402	EZA	C14-C13-C12	2.06	119.34	116.13
3	I	402	EZA	O7-C34-N5	-2.06	117.70	121.38
3	S	402	EZA	O3-C18-C17	2.06	114.38	108.43
3	F	402	EZA	C18-O3-C19	2.05	120.89	116.84
3	T	402	EZA	O7-C34-N5	-2.05	117.73	121.38
3	N	402	EZA	O7-C34-N5	-2.04	117.74	121.38
3	C	402	EZA	C14-C13-C12	2.03	119.29	116.13
3	I	402	EZA	O6-C28-N4	-2.03	119.17	122.93
3	T	402	EZA	C35-C34-N5	2.03	122.70	117.72
3	E	402	EZA	C8-C16-N2	2.01	121.11	116.70

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	N	402	EZA	C26
3	C	402	EZA	C26
3	C	402	EZA	C20
3	F	402	EZA	C26
3	D	402	EZA	C26
3	S	402	EZA	C20
3	S	402	EZA	C26
3	T	402	EZA	C26
3	L	402	EZA	C26
3	E	402	EZA	C26
3	E	402	EZA	C20
3	A	402	EZA	C26
3	M	402	EZA	C26
3	M	402	EZA	C20
3	I	402	EZA	C26
3	I	402	EZA	C20

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	401	MPD	C2-C3-C4-O4
3	S	402	EZA	N2-C17-C18-O3
3	S	402	EZA	C39-C17-C18-O3
3	S	402	EZA	C17-C18-O3-C19
3	S	402	EZA	O4-C19-O3-C18

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Mol	Chain	Res	Type	Atoms
3	S	402	EZA	C20-C19-O3-C18
3	S	402	EZA	N3-C25-C26-N4
3	S	402	EZA	O5-C25-C26-N4
2	F	401	MPD	C2-C3-C4-O4
2	M	401	MPD	C2-C3-C4-O4
2	E	401	MPD	C2-C3-C4-O4
2	G	401	MPD	C2-C3-C4-O4
3	N	402	EZA	C27-C26-N4-C28
3	E	402	EZA	C27-C26-N4-C28
3	A	402	EZA	C27-C26-N4-C28
3	S	402	EZA	C27-C26-N4-C28
3	L	402	EZA	C27-C26-N4-C28
3	M	402	EZA	C27-C26-N4-C28
3	F	402	EZA	C5-C6-C7-N1
3	C	402	EZA	C5-C6-C7-O1
3	F	402	EZA	C5-C6-C7-O1
3	C	402	EZA	C5-C6-C7-N1
3	C	402	EZA	C27-C26-N4-C28
3	F	402	EZA	C27-C26-N4-C28
3	D	402	EZA	C27-C26-N4-C28
3	I	402	EZA	C27-C26-N4-C28
3	T	402	EZA	C2-C3-C4-C5
3	E	402	EZA	C2-C3-C4-C5
3	D	402	EZA	O5-C25-C26-C27
3	N	402	EZA	N3-C25-C26-C27
3	M	402	EZA	N3-C25-C26-C27
3	E	402	EZA	O4-C19-C20-N3
3	N	402	EZA	O3-C19-C20-N3
3	D	402	EZA	O3-C19-C20-N3
3	M	402	EZA	O3-C19-C20-N3
3	I	402	EZA	O3-C19-C20-N3
3	N	402	EZA	C2-C3-C4-C5
3	M	402	EZA	C2-C3-C4-C5
3	N	402	EZA	O4-C19-C20-N3
3	C	402	EZA	O4-C19-C20-N3
3	D	402	EZA	O4-C19-C20-N3
3	D	402	EZA	C2-C3-C4-C5
3	T	402	EZA	O3-C19-C20-N3
3	A	402	EZA	O3-C19-C20-N3
3	F	402	EZA	O4-C19-C20-N3
3	T	402	EZA	O4-C19-C20-N3
3	M	402	EZA	O4-C19-C20-N3

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Mol	Chain	Res	Type	Atoms
3	I	402	EZA	O4-C19-C20-N3
3	C	402	EZA	O3-C19-C20-N3
3	F	402	EZA	O3-C19-C20-N3
3	E	402	EZA	O3-C19-C20-N3
3	N	402	EZA	O5-C25-C26-C27
3	C	402	EZA	O5-C25-C26-C27
3	F	402	EZA	O5-C25-C26-C27
3	T	402	EZA	O5-C25-C26-C27
3	L	402	EZA	O5-C25-C26-C27
3	M	402	EZA	O5-C25-C26-C27
3	I	402	EZA	O5-C25-C26-N4
3	E	402	EZA	N3-C25-C26-C27
3	E	402	EZA	N3-C25-C26-N4
3	I	402	EZA	N3-C25-C26-N4
3	L	402	EZA	O3-C19-C20-N3
3	I	402	EZA	C1-C2-C3-C4
3	S	402	EZA	C2-C3-C4-C5
3	A	402	EZA	O4-C19-C20-N3
3	N	402	EZA	O2-C16-C8-N1
3	C	402	EZA	O4-C19-O3-C18
3	C	402	EZA	C1-C2-C3-C4
3	E	402	EZA	N2-C16-C8-N1
3	A	402	EZA	N2-C16-C8-N1
3	L	402	EZA	C1-C2-C3-C4
3	E	402	EZA	C1-C2-C3-C4
3	T	402	EZA	C27-C26-N4-C28
3	N	402	EZA	N2-C16-C8-N1
3	E	402	EZA	O2-C16-C8-N1
3	A	402	EZA	O2-C16-C8-N1
3	E	402	EZA	O5-C25-C26-N4
3	F	402	EZA	O2-C16-C8-N1
3	C	402	EZA	N3-C25-C26-C27
3	F	402	EZA	N3-C25-C26-C27
3	T	402	EZA	N3-C25-C26-C27
3	L	402	EZA	N3-C25-C26-C27
3	I	402	EZA	N3-C25-C26-C27
3	C	402	EZA	C3-C4-C5-C6
3	T	402	EZA	O2-C16-C8-N1
3	T	402	EZA	N2-C16-C8-N1
3	L	402	EZA	O4-C19-C20-N3
3	F	402	EZA	N2-C16-C8-N1
3	D	402	EZA	N2-C16-C8-N1

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Mol	Chain	Res	Type	Atoms
3	M	402	EZA	N2-C16-C8-N1
3	N	402	EZA	O5-C25-C26-N4
3	D	402	EZA	O2-C16-C8-N1
3	L	402	EZA	O2-C16-C8-N1
3	M	402	EZA	O2-C16-C8-N1
3	C	402	EZA	N1-C8-C9-C10
2	T	401	MPD	C2-C3-C4-C5
2	B	401	MPD	C2-C3-C4-C5
3	C	402	EZA	O2-C16-C8-C9
3	I	402	EZA	N2-C16-C8-N1
3	D	402	EZA	N3-C25-C26-C27
3	L	402	EZA	N2-C16-C8-N1
2	E	401	MPD	C1-C2-C3-C4
3	I	402	EZA	O2-C16-C8-N1
3	C	402	EZA	O5-C25-C26-N4
3	T	402	EZA	O5-C25-C26-N4
3	M	402	EZA	O5-C25-C26-N4
3	C	402	EZA	C20-C19-O3-C18
3	N	402	EZA	N3-C25-C26-N4
3	C	402	EZA	N2-C16-C8-C9
3	T	402	EZA	C25-C26-N4-C28
3	F	402	EZA	O5-C25-C26-N4
3	A	402	EZA	O5-C25-C26-N4
3	M	402	EZA	N3-C25-C26-N4
3	L	402	EZA	C3-C4-C5-C6
3	N	402	EZA	O6-C28-C29-N5
3	S	402	EZA	O6-C28-C29-N5
3	I	402	EZA	O6-C28-C29-N5
3	I	402	EZA	O4-C19-O3-C18
3	D	402	EZA	O4-C19-O3-C18
3	M	402	EZA	O4-C19-O3-C18
3	E	402	EZA	O5-C25-C26-C27
3	I	402	EZA	O2-C16-C8-C9
3	T	402	EZA	N3-C25-C26-N4
2	L	401	MPD	O2-C2-C3-C4
2	K	401	MPD	O2-C2-C3-C4
2	E	401	MPD	O2-C2-C3-C4
2	A	401	MPD	O2-C2-C3-C4
2	N	401	MPD	O2-C2-C3-C4
3	C	402	EZA	N3-C25-C26-N4
3	F	402	EZA	C3-C4-C5-C6
3	S	402	EZA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	402	EZA	O5-C25-C26-C27
3	I	402	EZA	O5-C25-C26-C27
3	D	402	EZA	O5-C25-C26-N4
3	L	402	EZA	O5-C25-C26-N4
3	S	402	EZA	O2-C16-C8-C9
3	T	402	EZA	O2-C16-C8-C9
3	M	402	EZA	O2-C16-C8-C9
3	S	402	EZA	N4-C28-C29-N5
3	M	402	EZA	O6-C28-C29-N5
3	S	402	EZA	N3-C25-C26-C27
3	F	402	EZA	O2-C16-C8-C9
3	F	402	EZA	N3-C25-C26-N4
3	D	402	EZA	N3-C25-C26-N4
3	L	402	EZA	N3-C25-C26-N4
3	A	402	EZA	N3-C25-C26-N4
3	E	402	EZA	O2-C16-C8-C9
3	A	402	EZA	O2-C16-C8-C9
3	D	402	EZA	O2-C16-C8-C9
2	S	401	MPD	C2-C3-C4-C5
2	L	401	MPD	C2-C3-C4-C5
2	K	401	MPD	C2-C3-C4-C5
2	A	401	MPD	C2-C3-C4-C5
2	N	401	MPD	C2-C3-C4-C5
2	C	401	MPD	C2-C3-C4-C5
2	D	401	MPD	C2-C3-C4-C5
3	C	402	EZA	C25-C26-N4-C28
3	F	402	EZA	C25-C26-N4-C28
3	I	402	EZA	C25-C26-N4-C28
3	T	402	EZA	C3-C4-C5-C6
3	I	402	EZA	C3-C4-C5-C6
3	E	402	EZA	N2-C16-C8-C9

There are no ring outliers.

18 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	EZA	1	0
2	S	401	MPD	5	0
2	L	401	MPD	4	0
3	S	402	EZA	2	0
2	T	401	MPD	4	0
2	K	401	MPD	6	0

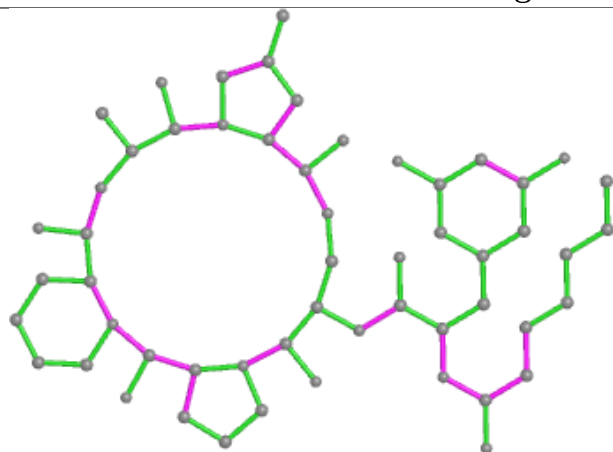
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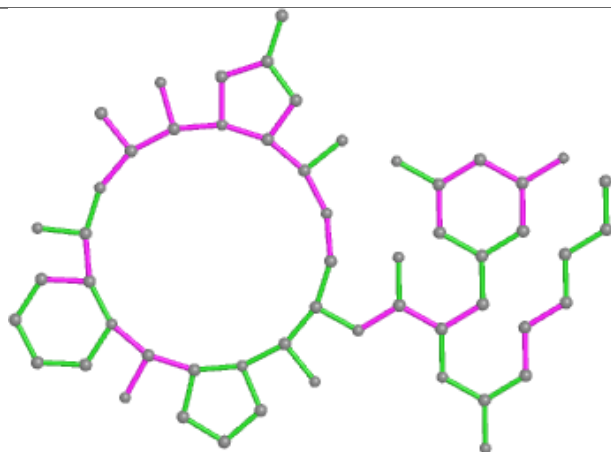
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	MPD	6	0
2	F	401	MPD	4	0
2	M	401	MPD	4	0
2	B	401	MPD	5	0
2	E	401	MPD	7	0
2	A	401	MPD	6	0
3	A	402	EZA	3	0
2	N	401	MPD	2	0
3	M	402	EZA	1	0
2	C	401	MPD	7	0
2	D	401	MPD	4	0
2	G	401	MPD	5	0

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.

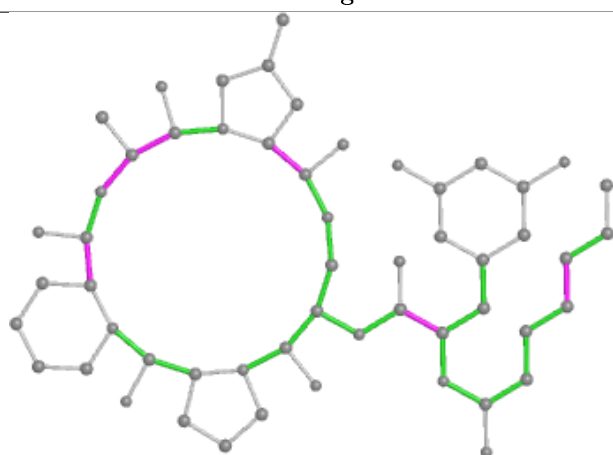
Ligand EZA N 402



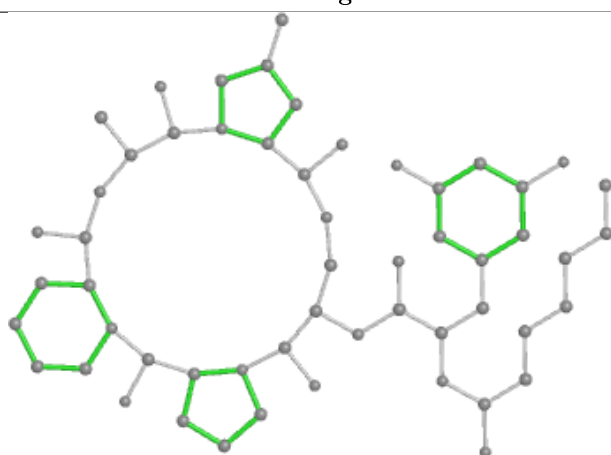
Bond lengths



Bond angles

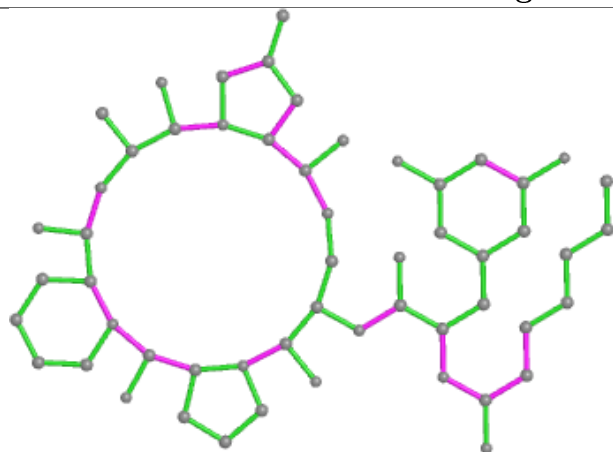


Torsions

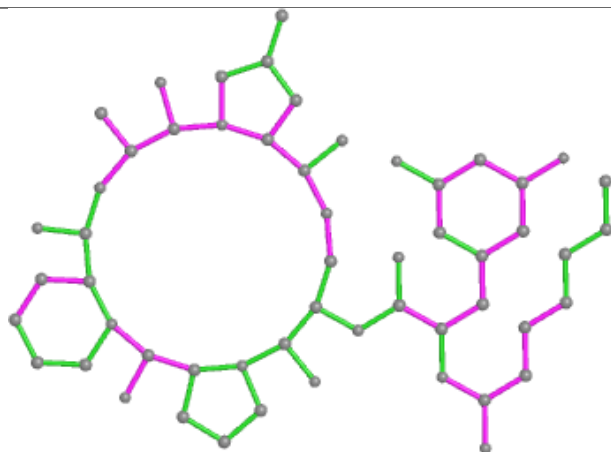


Rings

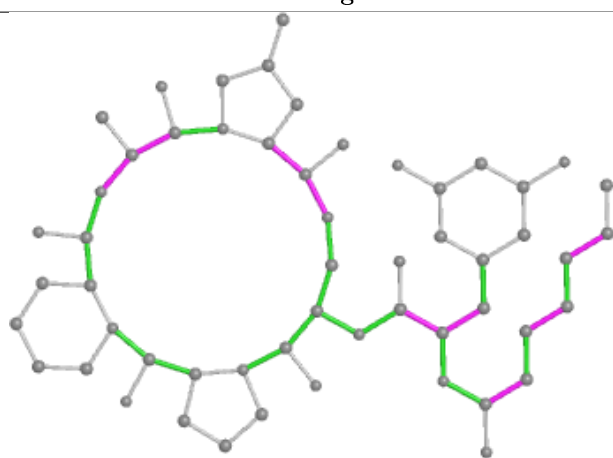
Ligand EZA C 402



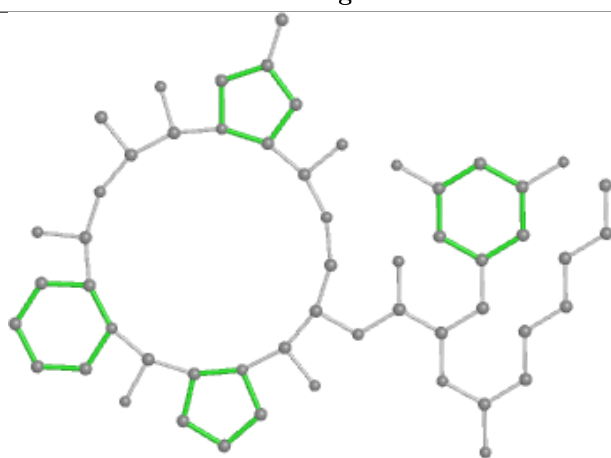
Bond lengths



Bond angles

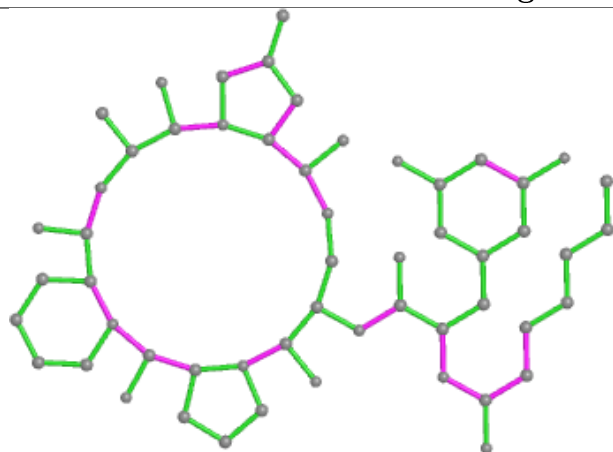


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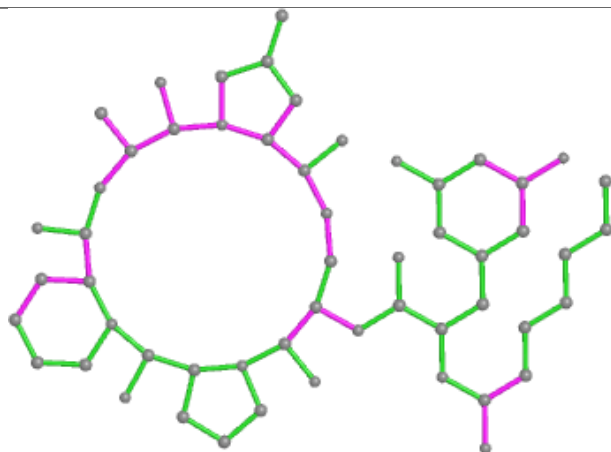


Rings

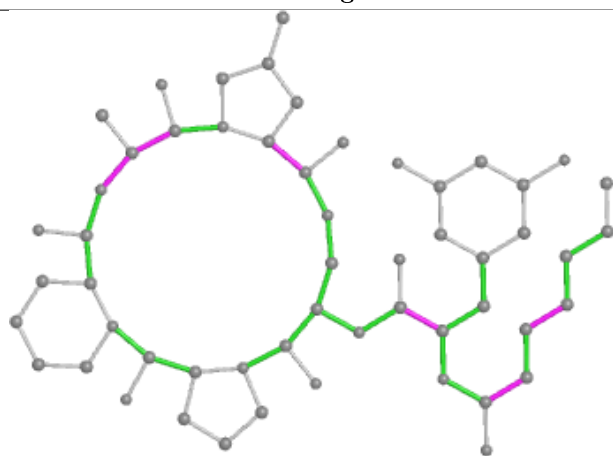
Ligand EZA F 402



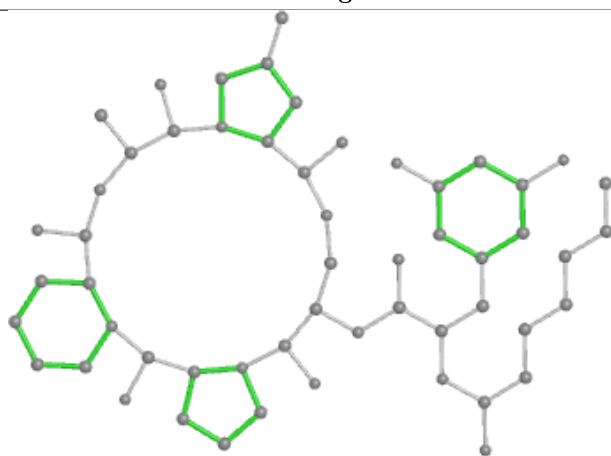
Bond lengths



Bond angles

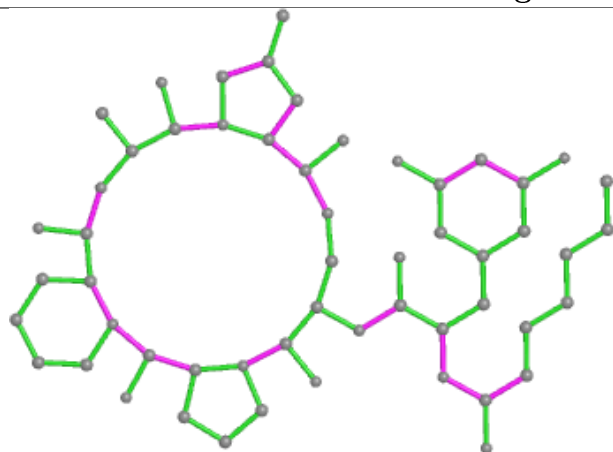


Torsions

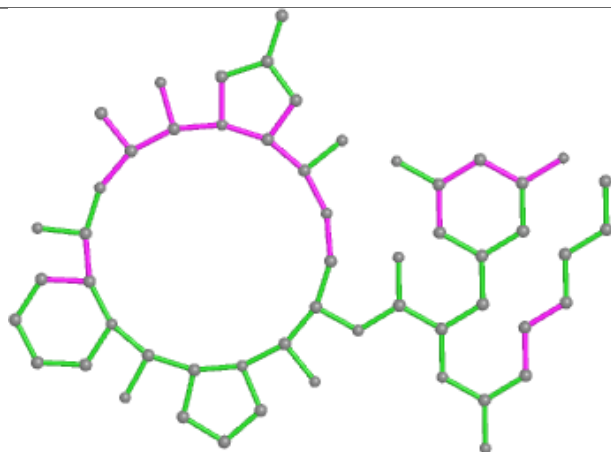


Rings

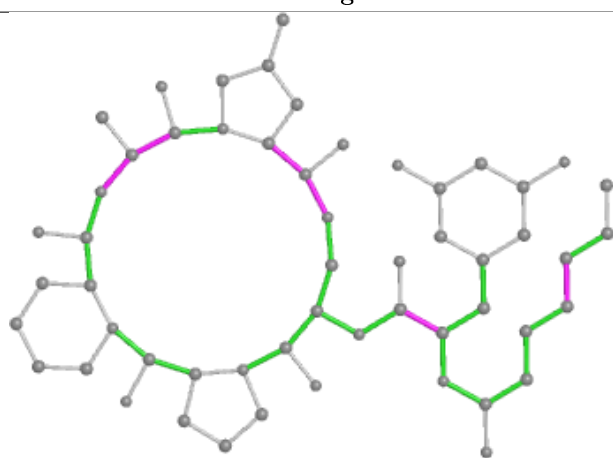
Ligand EZA D 402



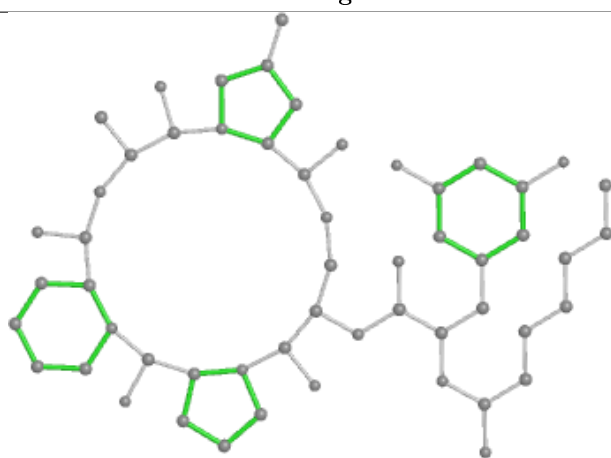
Bond lengths



Bond angles

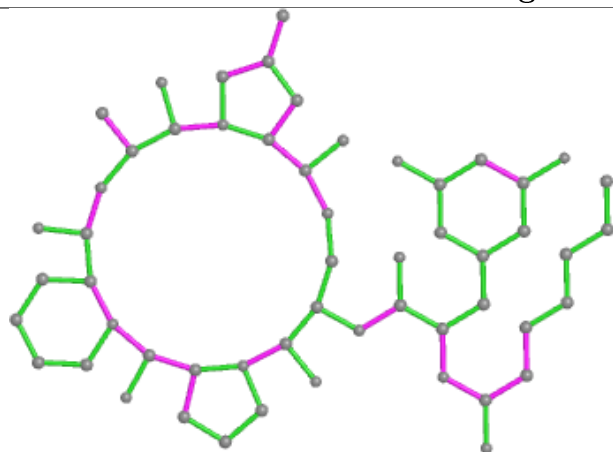


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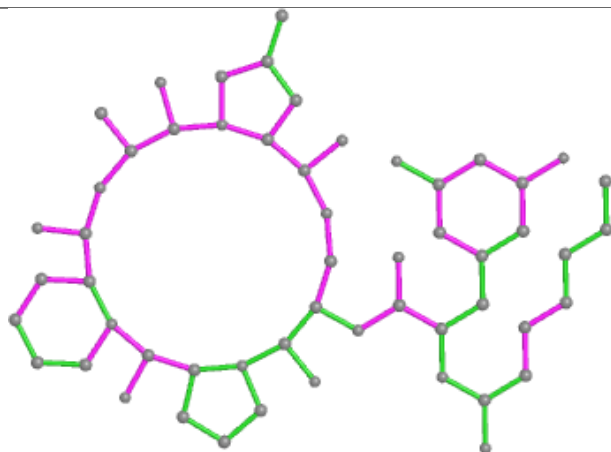


Rings

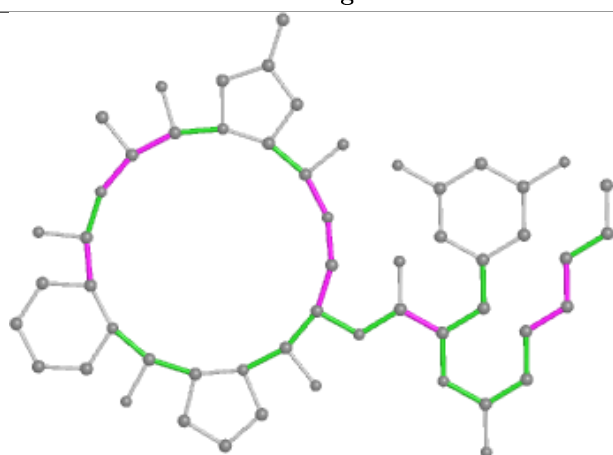
Ligand EZA S 402



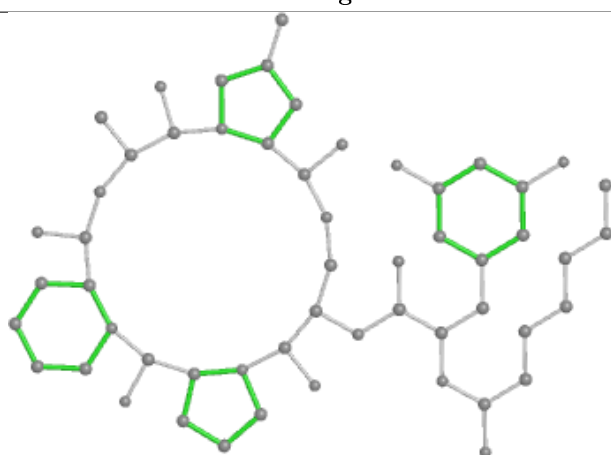
Bond lengths



Bond angles

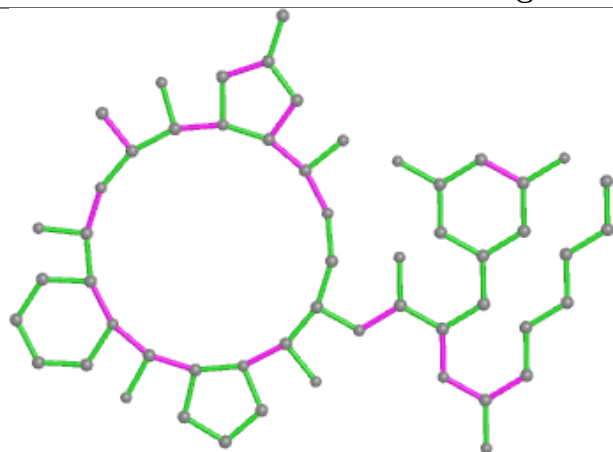


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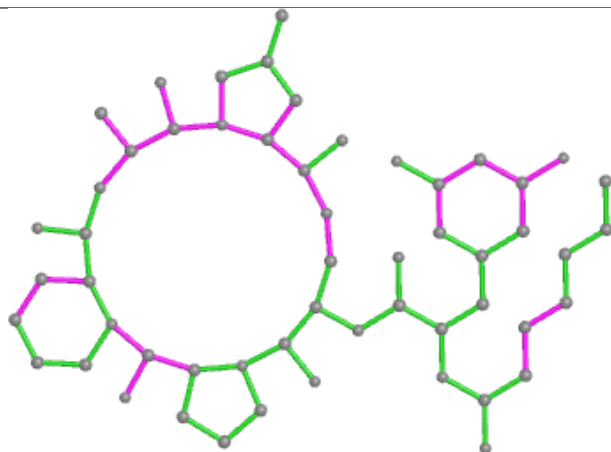


Rings

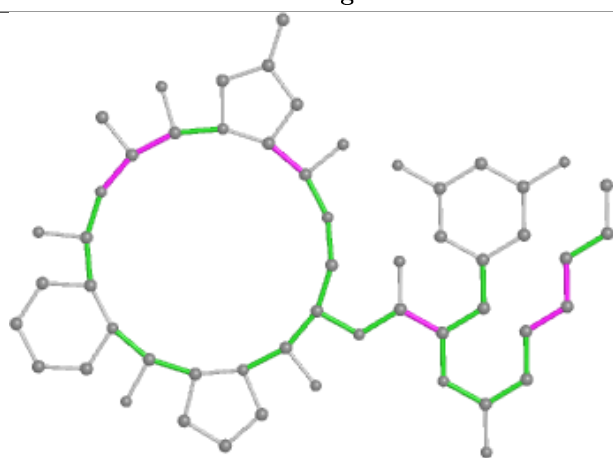
Ligand EZA T 402



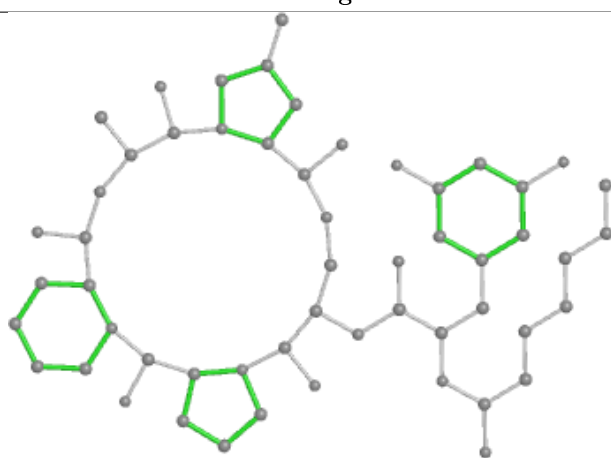
Bond lengths



Bond angles

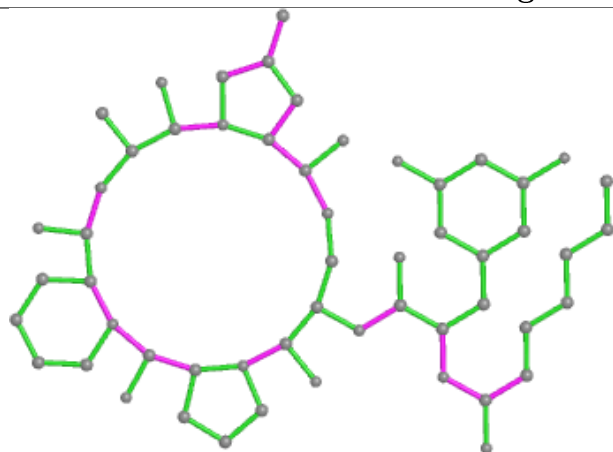


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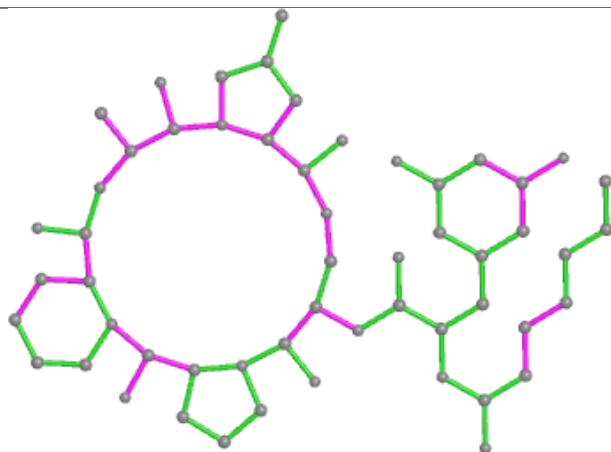


Rings

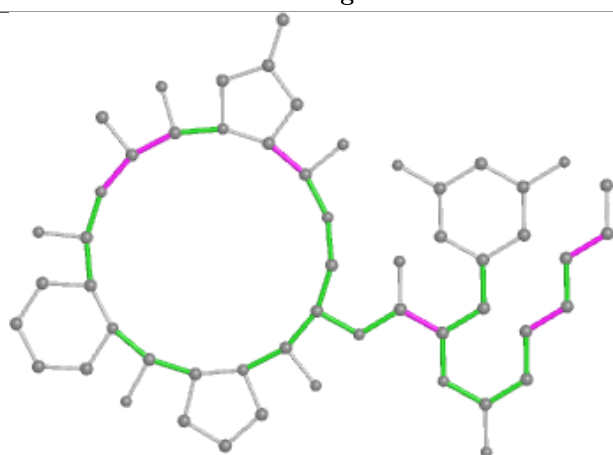
Ligand EZA L 402



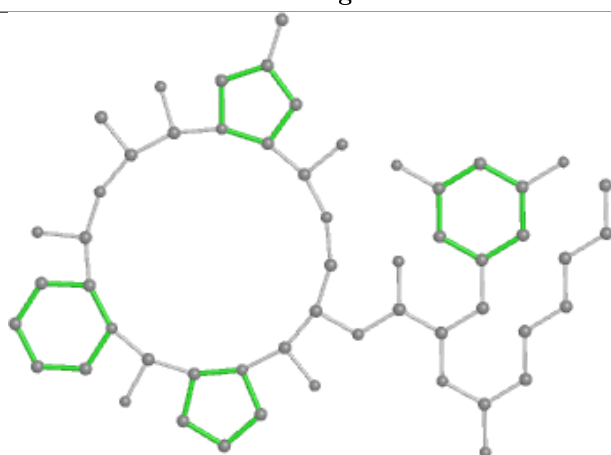
Bond lengths



Bond angles

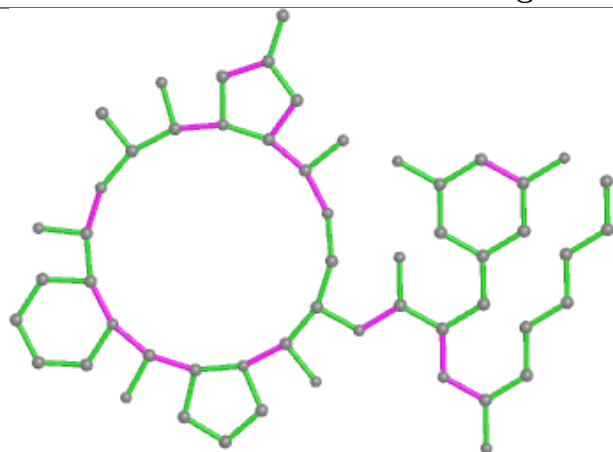


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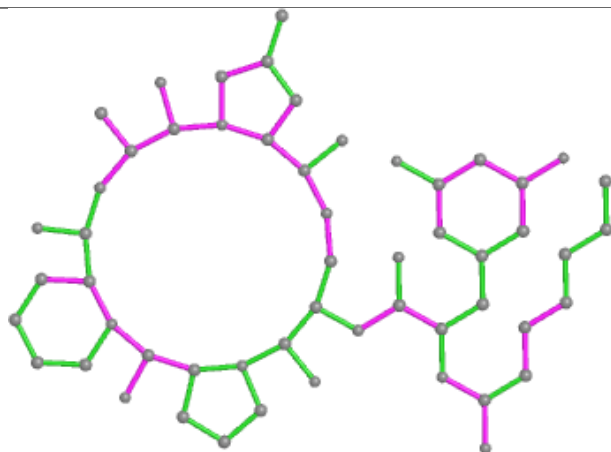


Rings

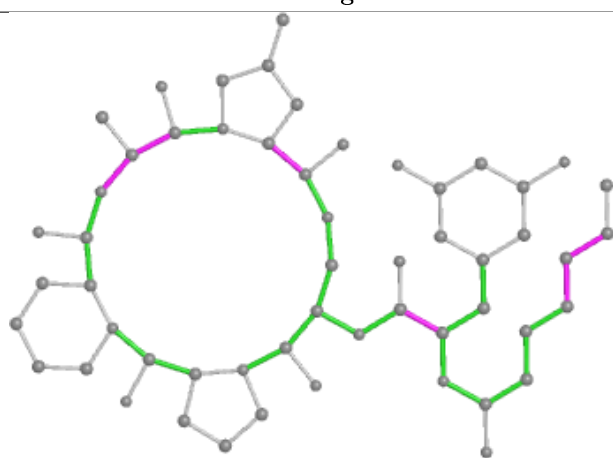
Ligand EZA E 402



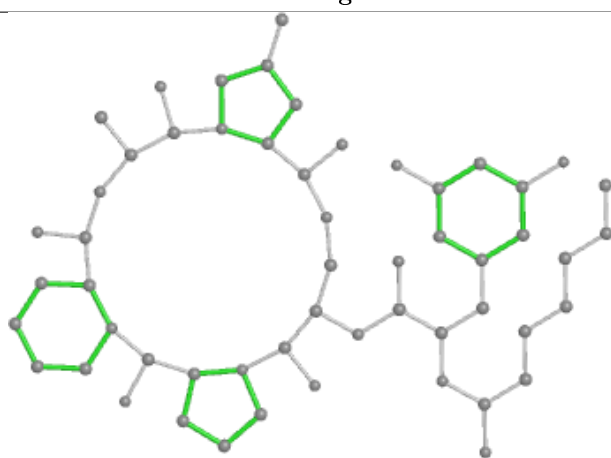
Bond lengths



Bond angles

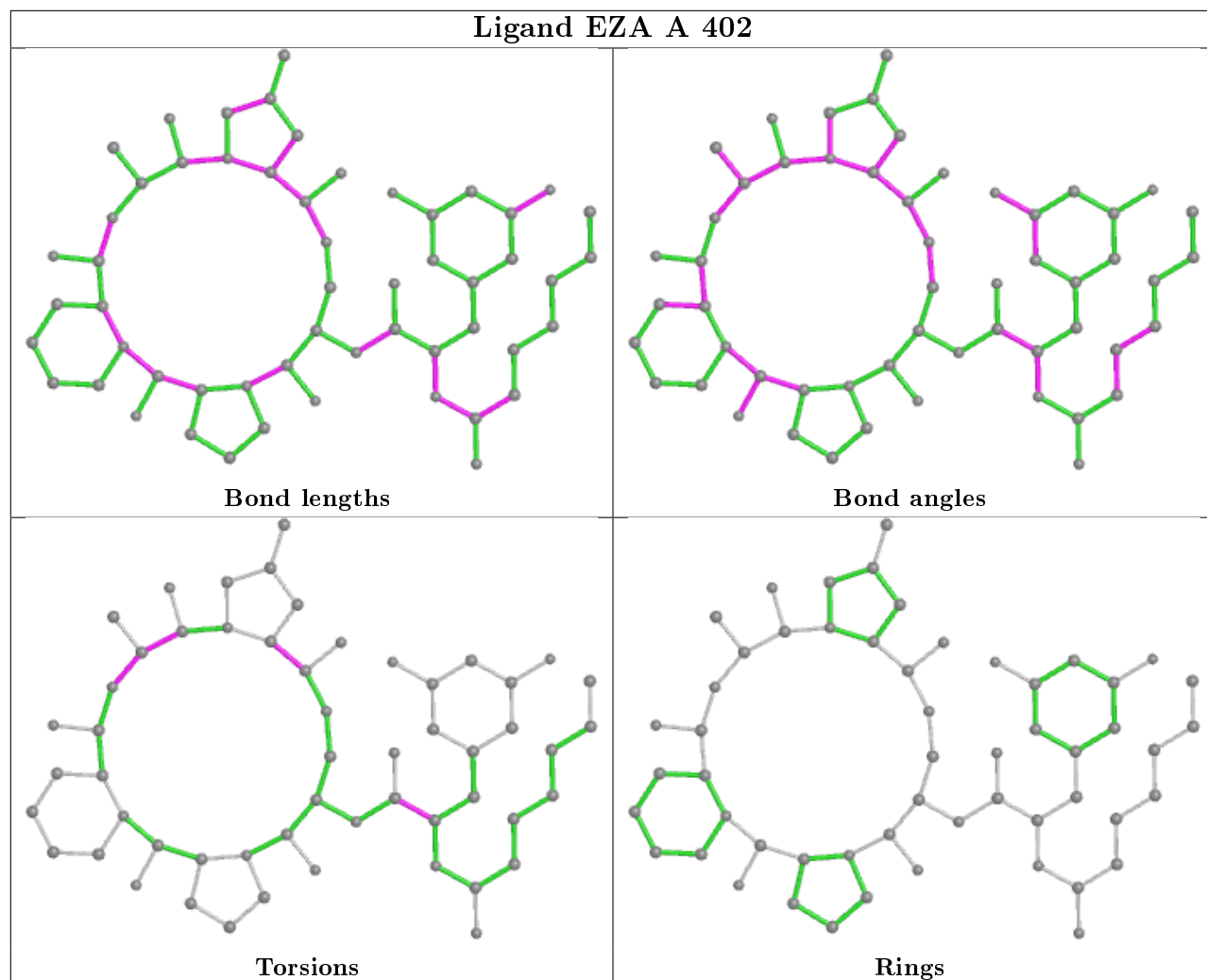


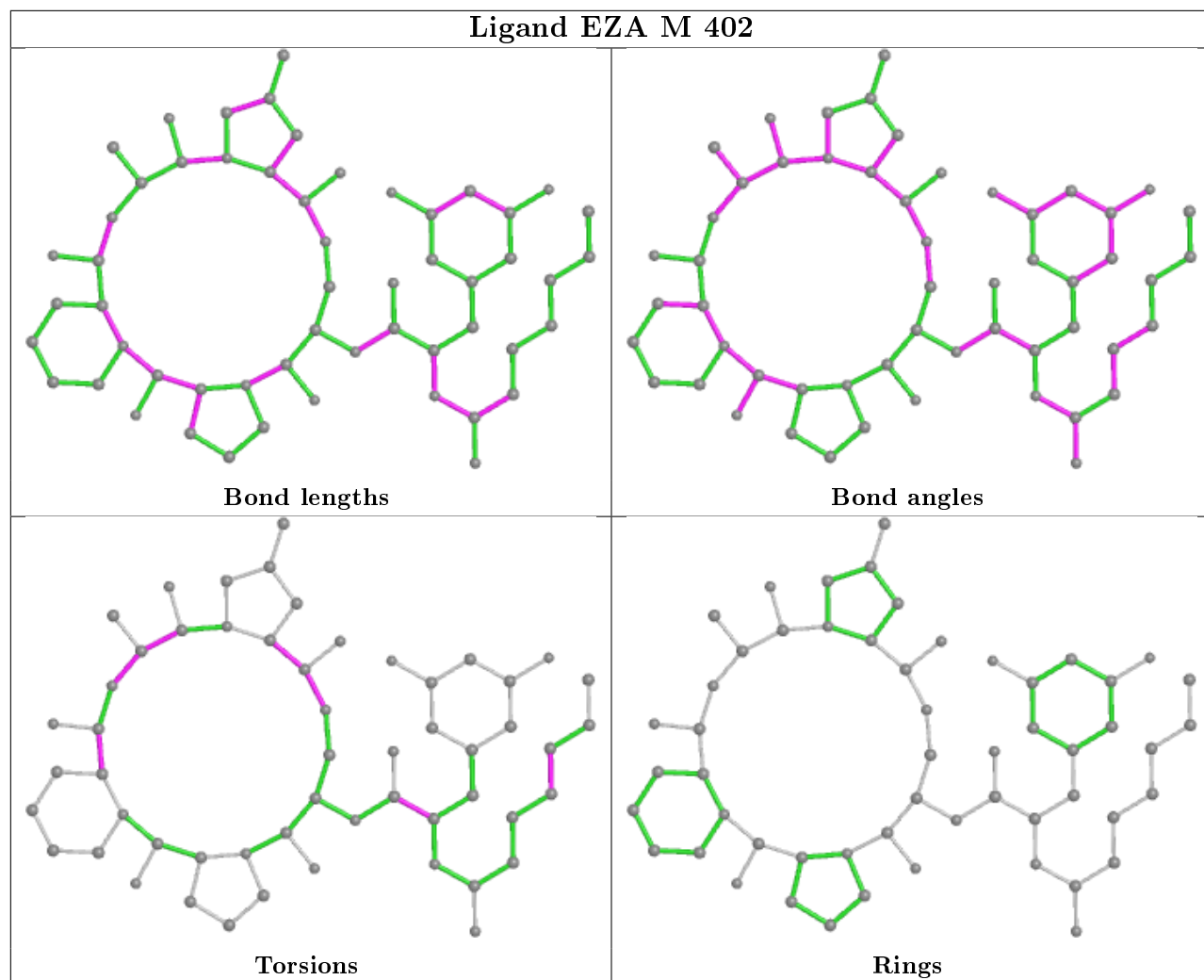
Torsions

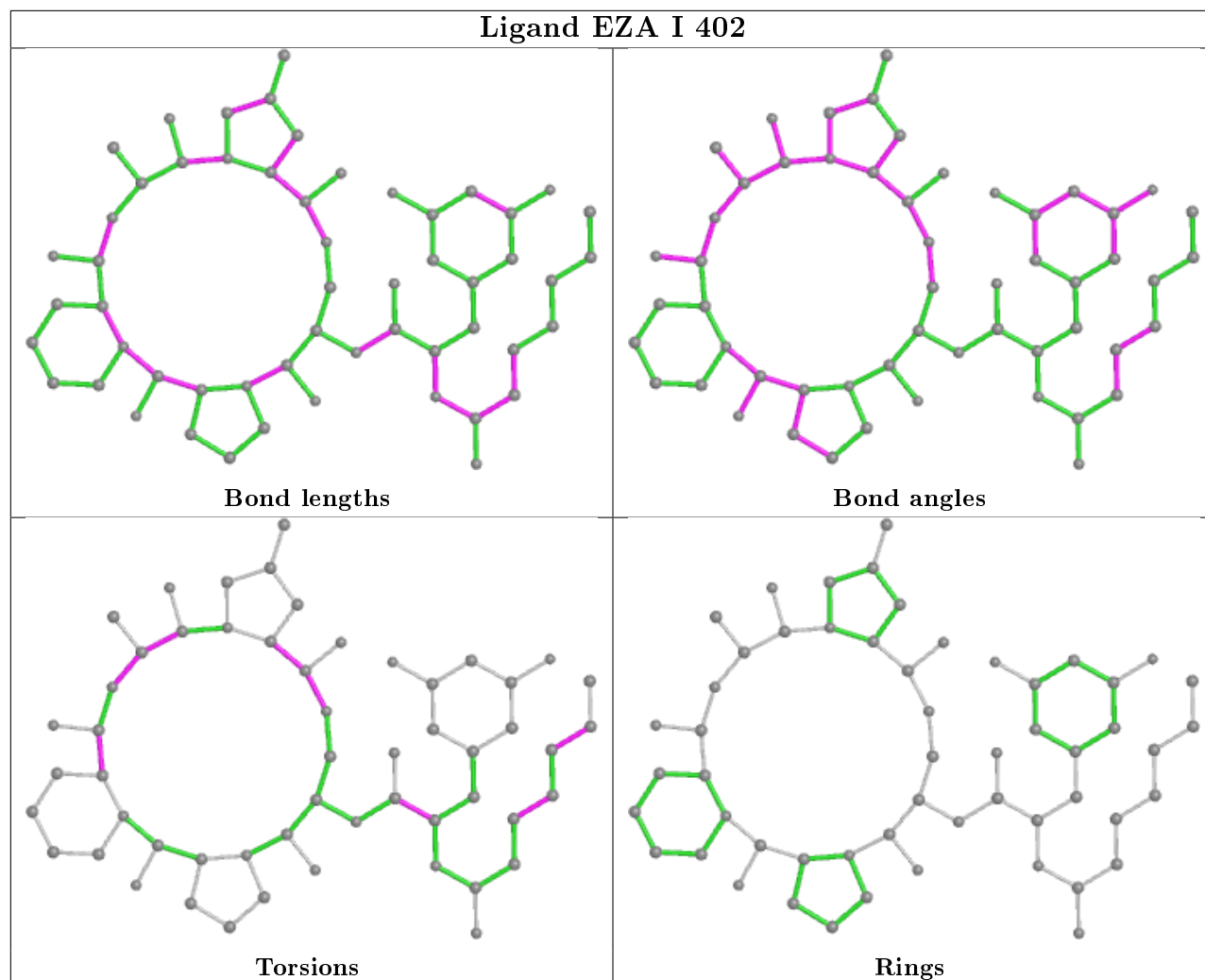


Rings

Ligand EZA A 402







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	181/210 (86%)	-0.18	0 100 100	40, 53, 83, 104	0
1	B	182/210 (86%)	-0.17	1 (0%) 91 90	37, 50, 84, 106	0
1	C	180/210 (85%)	-0.08	2 (1%) 80 79	36, 49, 83, 108	0
1	D	181/210 (86%)	-0.19	0 100 100	38, 53, 84, 101	0
1	E	184/210 (87%)	-0.16	1 (0%) 91 90	37, 50, 87, 114	0
1	F	183/210 (87%)	-0.19	0 100 100	35, 49, 82, 110	0
1	G	182/210 (86%)	-0.18	0 100 100	36, 49, 81, 106	0
1	I	188/210 (89%)	-0.17	4 (2%) 63 60	36, 53, 90, 121	0
1	K	183/210 (87%)	-0.17	1 (0%) 91 90	36, 48, 87, 115	0
1	L	180/210 (85%)	-0.16	1 (0%) 89 89	36, 50, 82, 108	0
1	M	181/210 (86%)	-0.15	1 (0%) 89 89	36, 50, 83, 105	0
1	N	182/210 (86%)	-0.15	0 100 100	41, 53, 87, 109	0
1	S	180/210 (85%)	-0.15	0 100 100	37, 51, 80, 96	0
1	T	181/210 (86%)	-0.14	1 (0%) 89 89	35, 50, 81, 101	0
All	All	2548/2940 (86%)	-0.16	12 (0%) 91 90	35, 51, 85, 121	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	18	TYR	2.6
1	I	63	TYR	2.6
1	E	18	TYR	2.5
1	L	18	TYR	2.3
1	M	4	ILE	2.3
1	T	83	PHE	2.3
1	C	23	ARG	2.2
1	I	3	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	3	LEU	2.2
1	I	18	TYR	2.1
1	I	12	SER	2.1
1	B	50	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EZA	I	402	55/55	0.75	0.49	93,132,159,187	0
3	EZA	S	402	55/55	0.79	0.55	96,135,177,184	0
3	EZA	N	402	55/55	0.80	0.39	98,127,147,158	0
3	EZA	M	402	55/55	0.82	0.42	96,129,159,162	0
3	EZA	D	402	55/55	0.83	0.43	85,118,141,147	0
3	EZA	C	402	55/55	0.83	0.33	84,111,147,153	0
3	EZA	T	402	55/55	0.85	0.36	84,111,135,138	0
3	EZA	E	402	55/55	0.86	0.36	92,116,138,177	0
2	MPD	B	401	8/8	0.90	0.22	65,68,73,79	0
3	EZA	F	402	55/55	0.91	0.43	77,102,123,130	0
3	EZA	L	402	55/55	0.91	0.49	80,101,122,130	0
2	MPD	D	401	8/8	0.92	0.30	72,77,80,82	0
2	MPD	C	401	8/8	0.92	0.27	51,68,74,80	0
2	MPD	I	401	8/8	0.93	0.31	65,71,76,78	0
3	EZA	A	402	55/55	0.94	0.28	64,78,93,98	0
2	MPD	F	401	8/8	0.94	0.38	58,68,74,76	0
2	MPD	M	401	8/8	0.94	0.28	55,68,69,73	0
2	MPD	L	401	8/8	0.94	0.26	57,64,66,73	0
2	MPD	T	401	8/8	0.94	0.30	66,76,83,85	0

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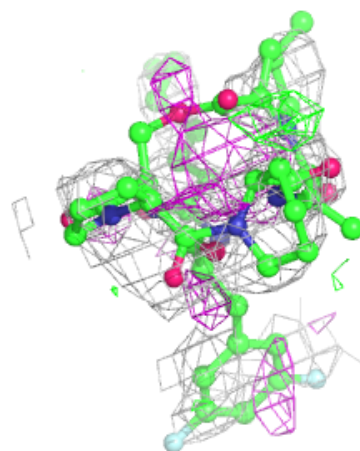
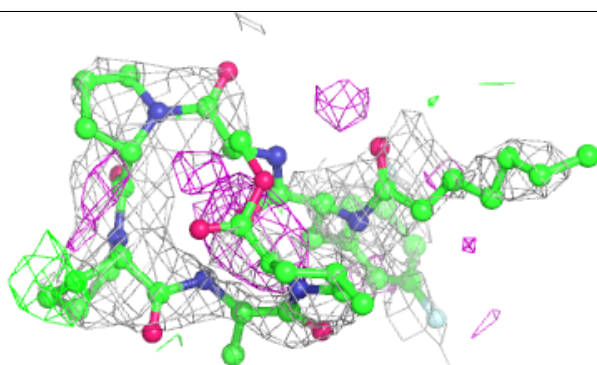
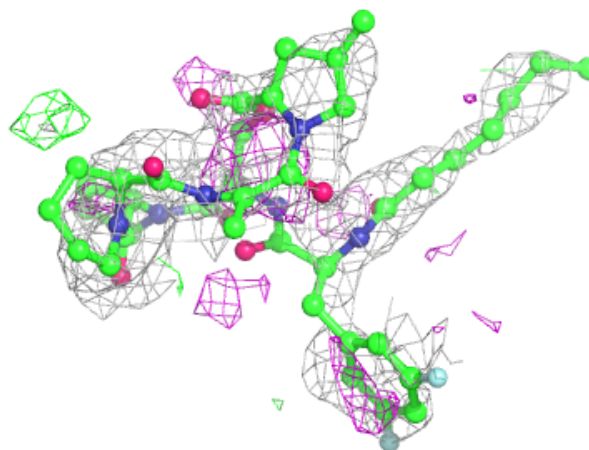
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MPD	E	401	8/8	0.95	0.24	68,74,82,84	0
2	MPD	S	401	8/8	0.95	0.30	63,65,78,79	0
2	MPD	K	401	8/8	0.95	0.23	67,69,72,74	0
2	MPD	N	401	8/8	0.95	0.26	62,67,70,75	0
2	MPD	G	401	8/8	0.95	0.24	58,60,66,67	0
2	MPD	A	401	8/8	0.96	0.37	65,68,71,71	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.

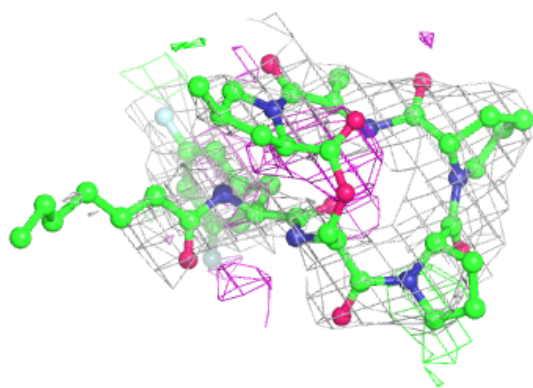
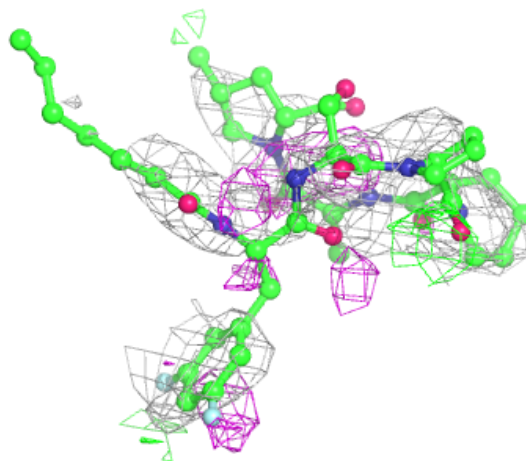
Electron density around EZA I 402:

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



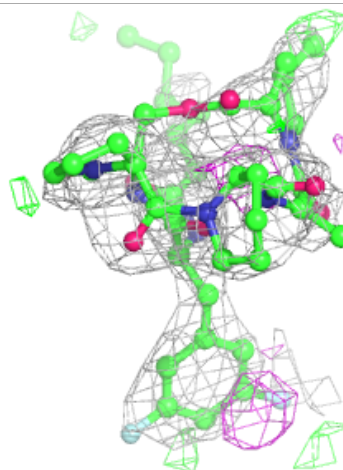
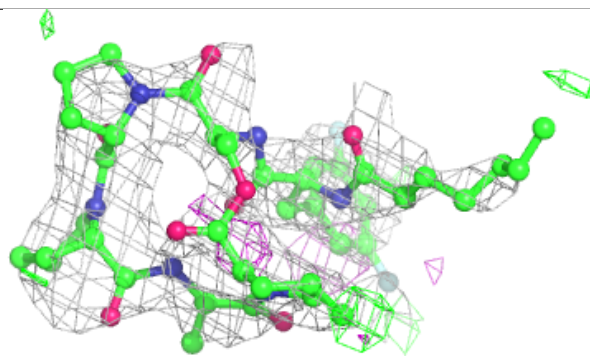
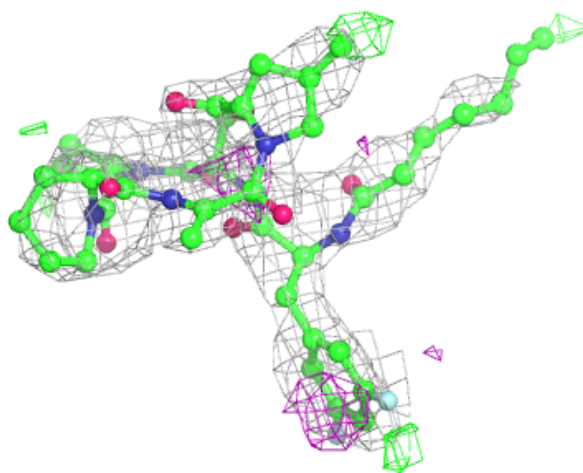
Electron density around EZA S 402:

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



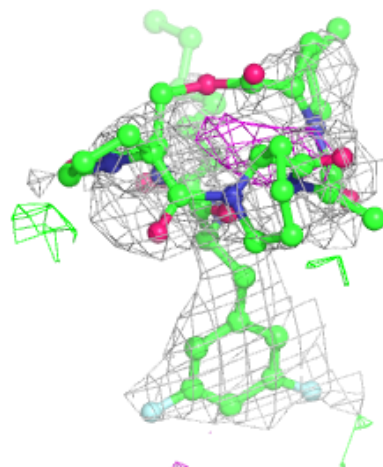
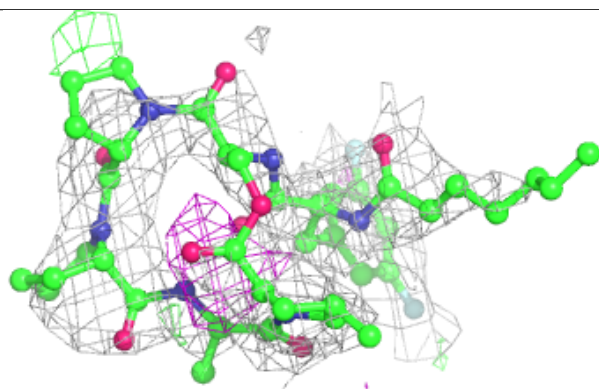
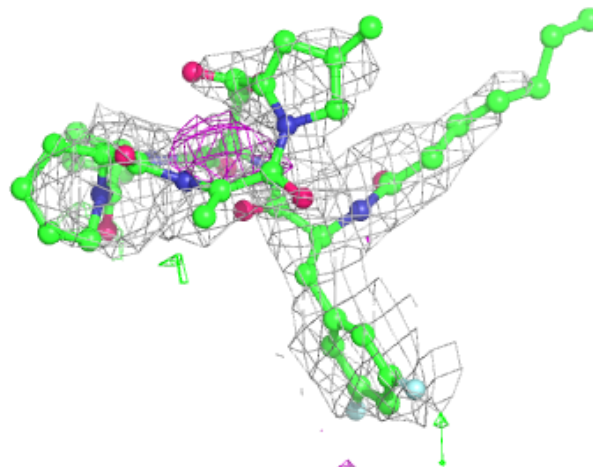
Electron density around EZA N 402:

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and green (positive)



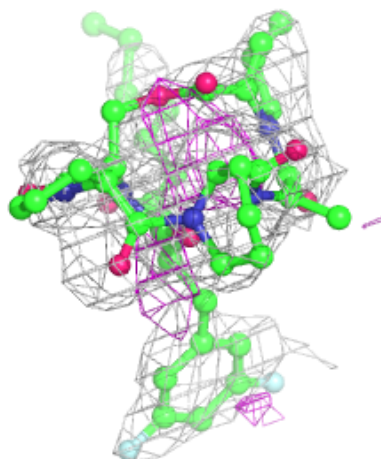
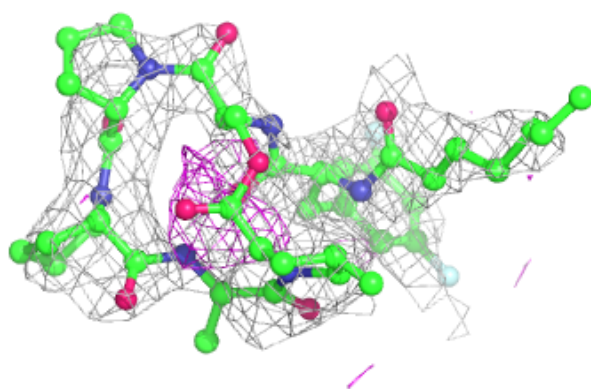
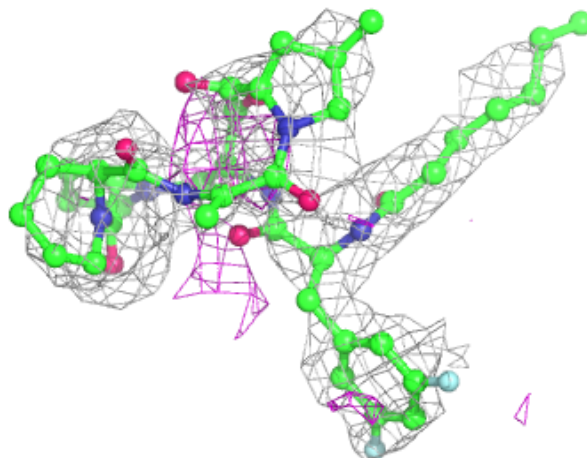
Electron density around EZA M 402:

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



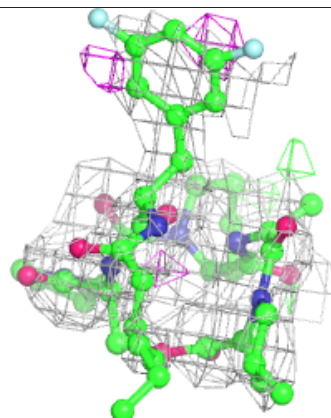
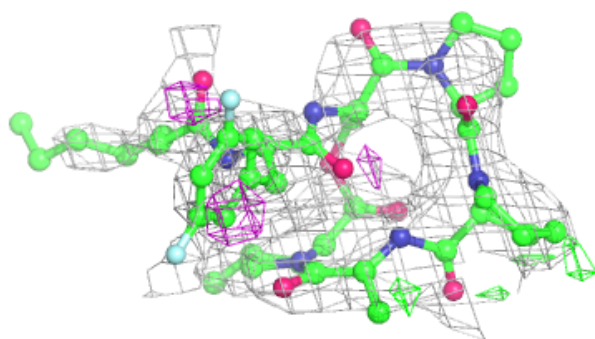
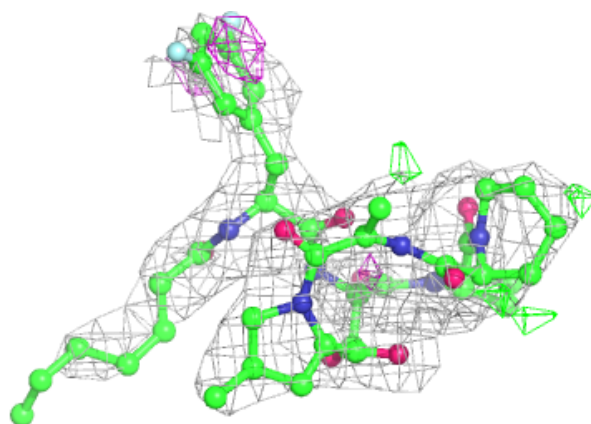
Electron density around EZA D 402:

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



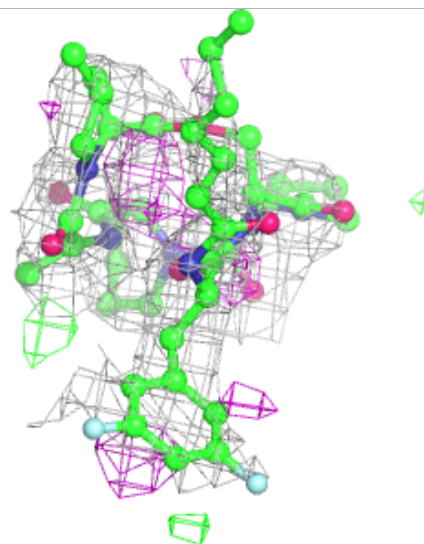
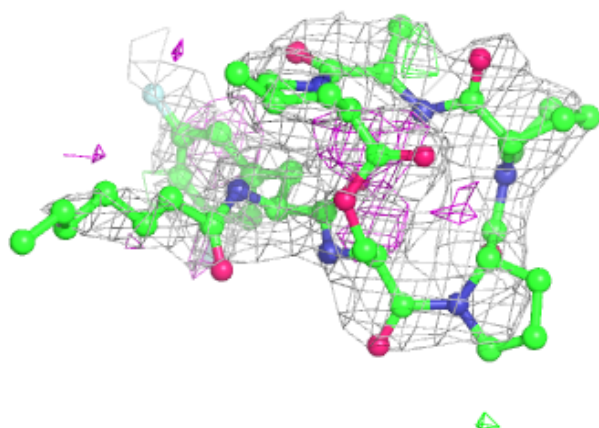
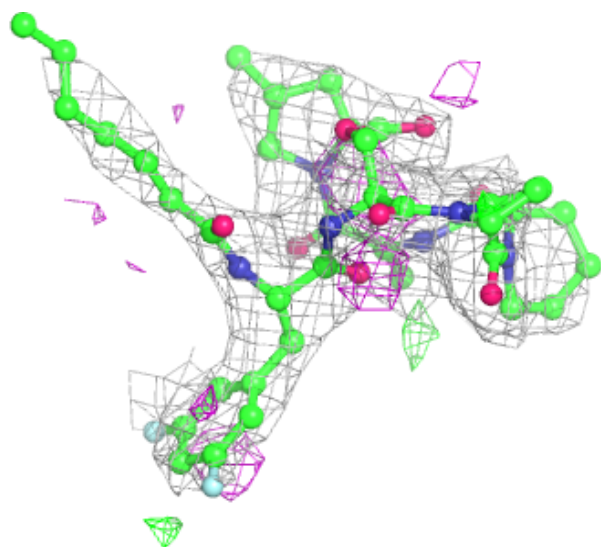
Electron density around EZA C 402:

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



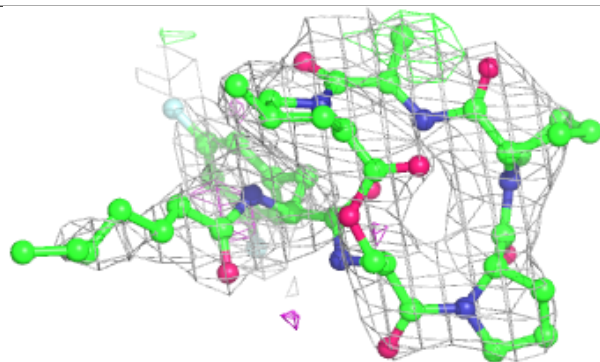
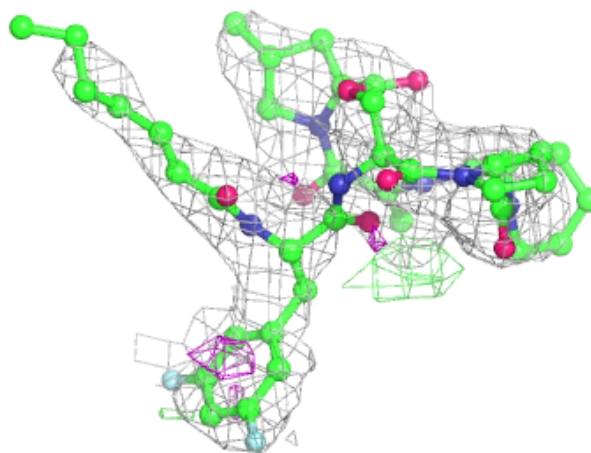
Electron density around EZA T 402:

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and green (positive)



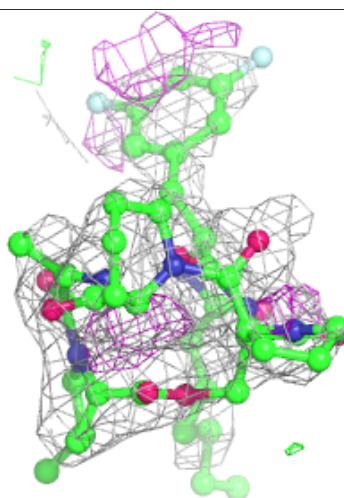
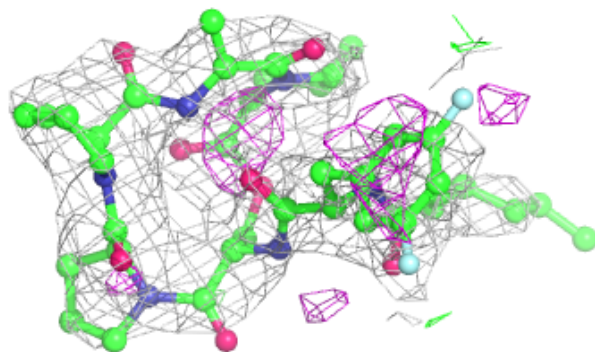
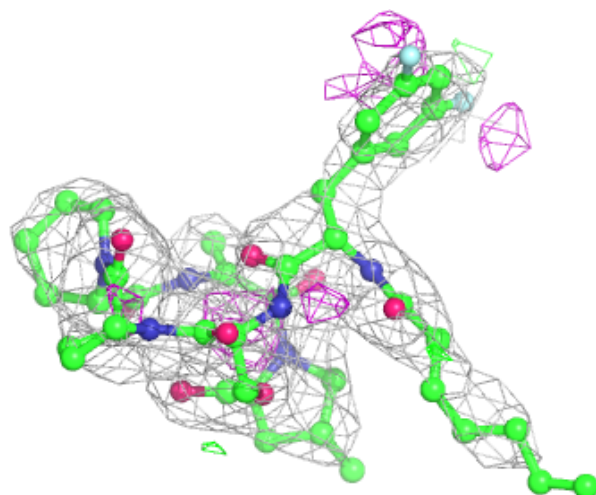
Electron density around EZA E 402:

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



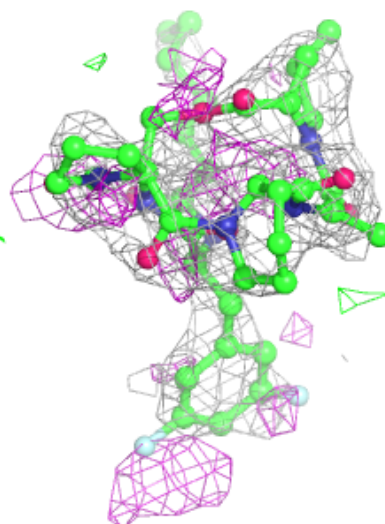
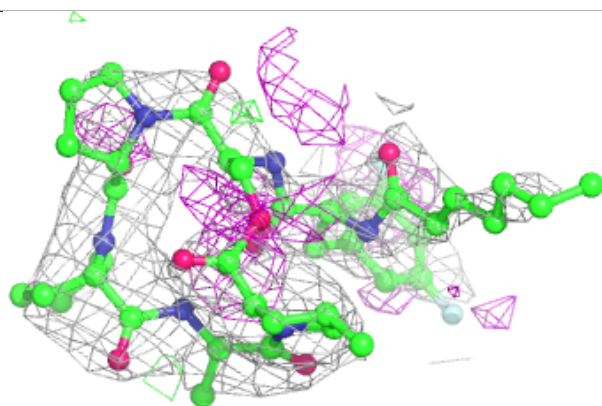
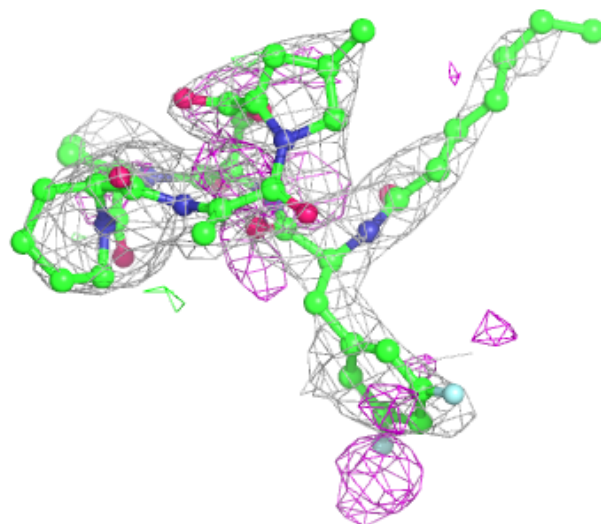
Electron density around EZA F 402:

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and green (positive)



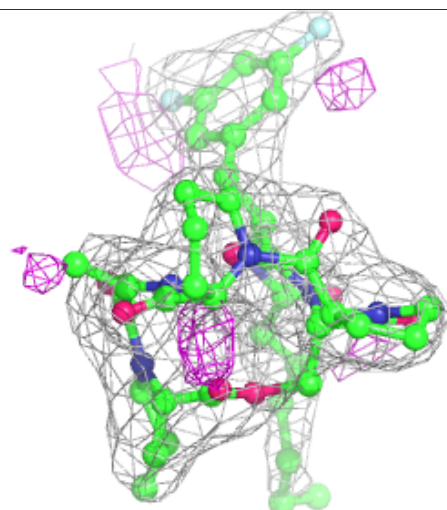
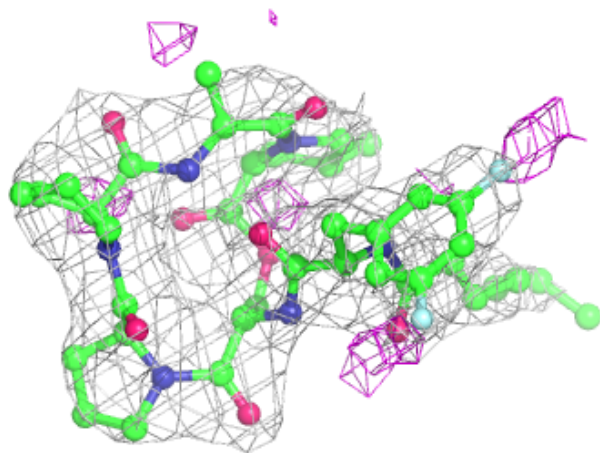
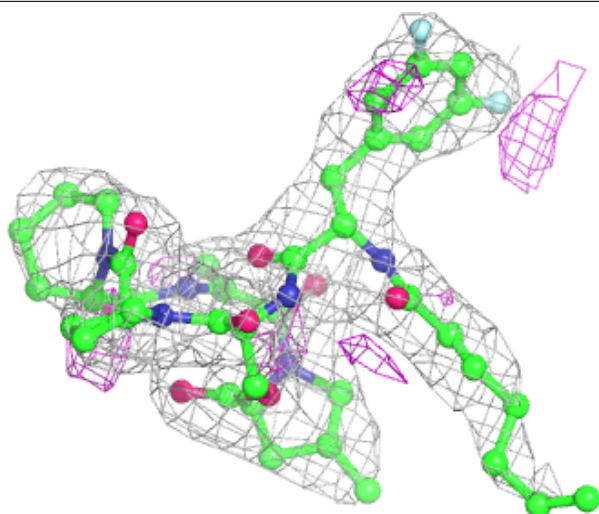
Electron density around EZA L 402:

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



Electron density around EZA A 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.