



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:10 PM UTC

PDB ID : 7DFU / pdb_00007dfu
Title : Crystal structure of Xanthomonas oryzae ClpP S68Y in complex with ADEP4.
Authors : Yang, C.-G.; Yang, T.
Deposited on : 2020-11-09
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

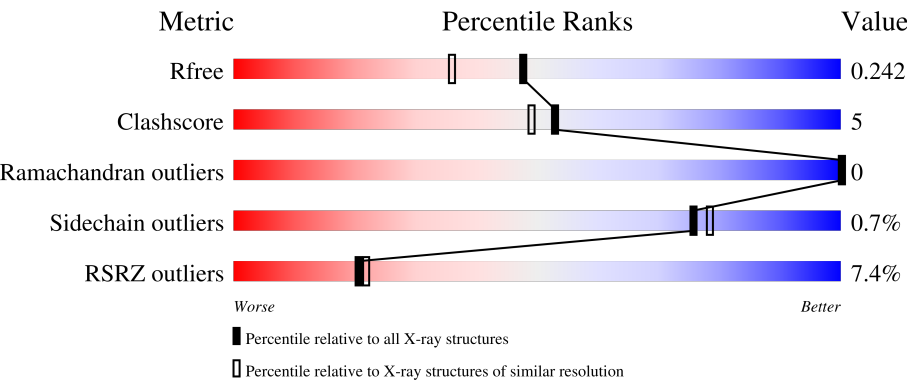
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	208	7% 81%10%8%
1	B	208	5% 81%6%12%
1	C	208	7% 77%11%11%
1	D	208	7% 79%11%9%
1	E	208	9% 76%10%13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	208	7% 80% 10% 10%
1	G	208	4% 75% 12% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10810 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.

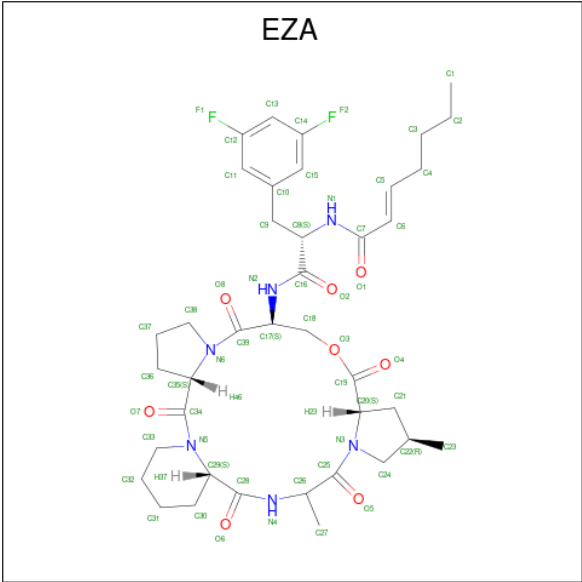
- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	1	0
			1462	923	254	278	7			
1	B	182	Total	C	N	O	S	0	0	0
			1381	875	237	262	7			
1	C	185	Total	C	N	O	S	0	0	0
			1422	899	247	269	7			
1	D	189	Total	C	N	O	S	0	0	0
			1440	909	249	275	7			
1	E	180	Total	C	N	O	S	0	0	0
			1374	867	239	262	6			
1	F	188	Total	C	N	O	S	0	0	0
			1435	906	250	272	7			
1	G	181	Total	C	N	O	S	0	0	0
			1386	879	237	263	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	TYR	SER	engineered mutation	UNP A0A0M1K022
B	68	TYR	SER	engineered mutation	UNP A0A0M1K022
C	68	TYR	SER	engineered mutation	UNP A0A0M1K022
D	68	TYR	SER	engineered mutation	UNP A0A0M1K022
E	68	TYR	SER	engineered mutation	UNP A0A0M1K022
F	68	TYR	SER	engineered mutation	UNP A0A0M1K022
G	68	TYR	SER	engineered mutation	UNP A0A0M1K022

- Molecule 2 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).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
2	B	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
2	C	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
2	D	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
2	E	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
2	F	1	Total	C	F	N	O	0	0
			55	39	2	6	8		
2	G	1	Total	C	F	N	O	0	0
			55	39	2	6	8		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

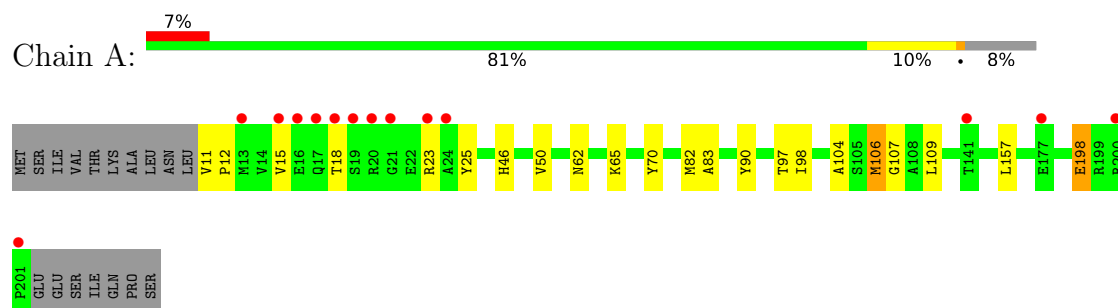
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	83	Total	O	0	0
			83	83		
5	B	73	Total	O	0	0
			73	73		
5	C	79	Total	O	0	0
			79	79		
5	D	67	Total	O	0	0
			67	67		
5	E	58	Total	O	0	0
			58	58		
5	F	78	Total	O	0	0
			78	78		
5	G	79	Total	O	0	0
			79	79		

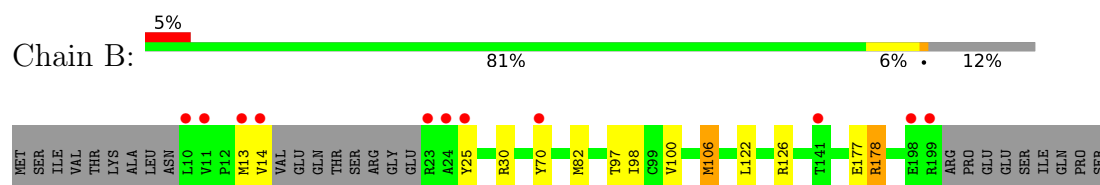
3 Residue-property plots [i](#)

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.

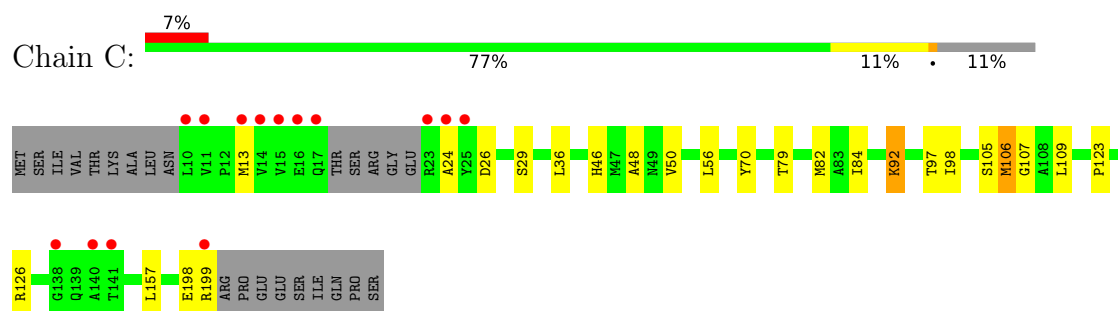
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



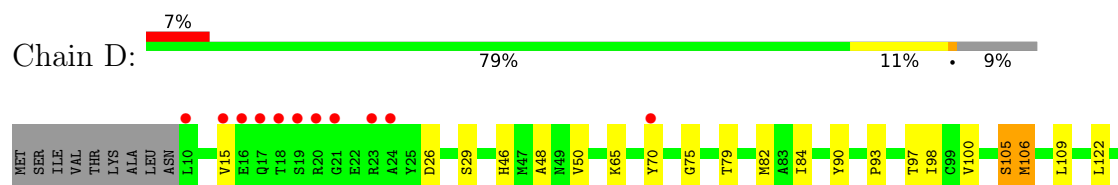
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

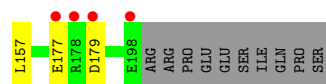


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

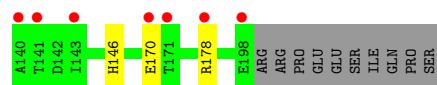
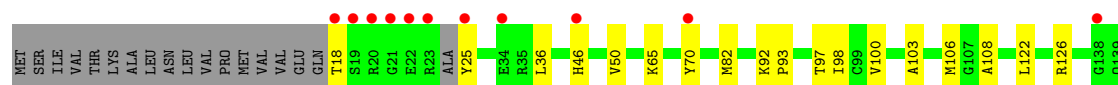
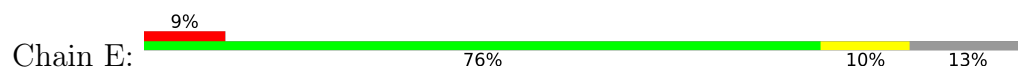


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

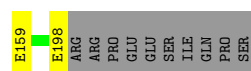
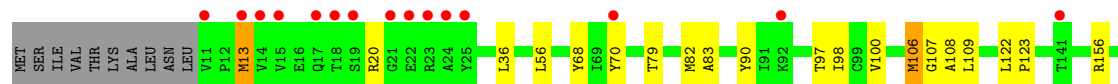
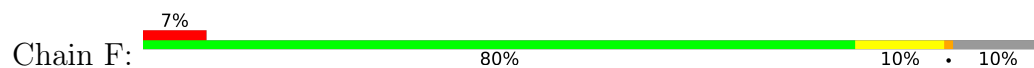




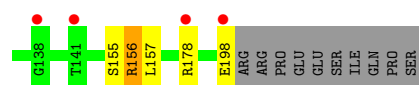
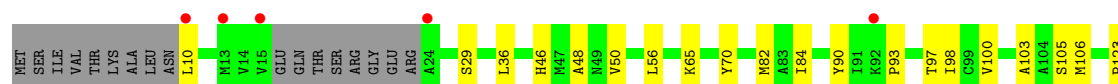
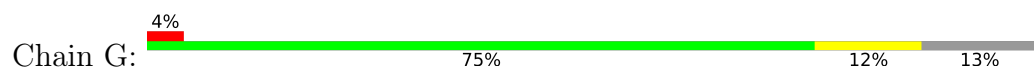
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- 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 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.50Å 132.50Å 187.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 1.90 29.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.3 (29.69-1.90) 90.2 (29.69-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 1.91Å)	Xtriage
Refinement program	PHENIX V1.0	Depositor
R, R_{free}	0.217 , 0.243 0.216 , 0.242	Depositor DCC
R_{free} test set	5807 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: CL, MG, 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	0.49	4/1488 (0.3%)	0.50	0/2019
1	B	0.46	3/1402 (0.2%)	0.43	0/1903
1	C	0.42	3/1443 (0.2%)	0.42	0/1955
1	D	0.35	2/1462 (0.1%)	0.44	0/1983
1	E	0.47	3/1394 (0.2%)	0.56	3/1888 (0.2%)
1	F	0.44	3/1457 (0.2%)	0.44	0/1976
1	G	0.51	5/1407 (0.4%)	0.51	2/1908 (0.1%)
All	All	0.45	23/10053 (0.2%)	0.47	5/13632 (0.0%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	105	SER	C-O	-7.33	1.14	1.24
1	A	106	MET	C-O	-7.30	1.15	1.24
1	B	106	MET	C-O	-6.59	1.16	1.24
1	C	106	MET	C-O	-6.49	1.16	1.24
1	C	105	SER	C-O	-6.24	1.16	1.24
1	G	157	LEU	C-O	-6.10	1.17	1.24
1	C	107	GLY	C-O	-6.04	1.16	1.23
1	B	177	GLU	C-O	-5.88	1.16	1.24
1	E	92	LYS	C-O	-5.79	1.19	1.24
1	D	106	MET	C-O	-5.77	1.17	1.24
1	F	108	ALA	C-O	-5.70	1.17	1.24
1	E	103	ALA	C-O	-5.68	1.17	1.23
1	B	178	ARG	C-O	-5.68	1.17	1.24
1	E	108	ALA	C-O	-5.68	1.17	1.24
1	F	107	GLY	C-O	-5.65	1.17	1.23
1	G	155	SER	C-O	-5.58	1.17	1.24
1	G	156	ARG	C-O	-5.50	1.17	1.24
1	G	103	ALA	C-O	-5.50	1.17	1.23
1	F	106	MET	C-O	-5.46	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLY	C-O	-5.37	1.17	1.23
1	A	198	GLU	CA-C	-5.21	1.45	1.52
1	D	105	SER	C-O	-5.09	1.17	1.24
1	A	104	ALA	C-O	-5.08	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	178	ARG	CA-CB-CG	6.21	126.51	114.10
1	E	170	GLU	CB-CA-C	-5.90	101.36	110.81
1	E	178	ARG	CB-CG-CD	5.77	124.58	111.30
1	G	178	ARG	CB-CG-CD	-5.69	98.22	111.30
1	G	178	ARG	CG-CD-NE	5.08	123.17	112.00

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	1462	0	1467	13	0
1	B	1381	0	1378	13	1
1	C	1422	0	1432	20	0
1	D	1440	0	1440	17	1
1	E	1374	0	1376	15	0
1	F	1435	0	1444	16	0
1	G	1386	0	1398	16	0
2	A	55	0	0	1	0
2	B	55	0	0	1	0
2	C	55	0	0	1	0
2	D	55	0	0	1	0
2	E	55	0	0	2	0
2	F	55	0	0	2	0
2	G	55	0	0	2	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	B	1	0	0	0	0
5	A	83	0	0	0	0
5	B	73	0	0	0	0
5	C	79	0	0	0	0
5	D	67	0	0	0	0
5	E	58	0	0	0	0
5	F	78	0	0	1	0
5	G	79	0	0	1	0
All	All	10810	0	9935	101	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (101) 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:D:15:VAL:HG22	1:E:25:TYR:CZ	2.25	0.71
1:C:82:MET:HE3	1:C:106:MET:HE1	1.79	0.64
1:A:82:MET:HE3	1:A:106:MET:HE1	1.80	0.63
1:B:82:MET:HE3	1:B:106:MET:HE1	1.79	0.63
1:F:82:MET:HE3	1:F:106:MET:HE1	1.81	0.63
1:E:82:MET:HE3	1:E:106:MET:HE1	1.81	0.62
1:C:13:MET:HE2	1:C:24:ALA:HB1	1.81	0.61
1:C:92:LYS:HD3	1:C:92:LYS:O	1.98	0.61
1:D:82:MET:HE3	1:D:106:MET:HE1	1.85	0.58
1:C:123:PRO:HG3	1:C:198:GLU:HG2	1.87	0.57
1:A:18:THR:HG22	1:A:23:ARG:HH21	1.72	0.55
1:A:62:ASN:ND2	1:A:65:LYS:HE2	2.22	0.55
1:A:23:ARG:HH11	1:A:25:TYR:HE1	1.52	0.55
1:D:46:HIS:O	1:D:50:VAL:HG23	2.07	0.55
1:G:82:MET:HE3	1:G:106:MET:HE1	1.89	0.55
1:F:123:PRO:HG3	1:F:198:GLU:HG2	1.90	0.54
1:D:179:ASP:OD2	1:E:146:HIS:NE2	2.29	0.53
1:C:82:MET:HE2	1:C:82:MET:HA	1.91	0.53
1:A:46:HIS:O	1:A:50:VAL:HG23	2.08	0.53
1:G:82:MET:HE2	1:G:82:MET:HA	1.91	0.53
1:E:82:MET:HA	1:E:82:MET:HE2	1.92	0.52
1:B:82:MET:HA	1:B:82:MET:HE2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:MET:HA	1:A:82:MET:HE2	1.92	0.52
1:D:100:VAL:HG13	1:D:122:LEU:HD12	1.92	0.52
1:F:82:MET:HA	1:F:82:MET:HE2	1.91	0.52
1:A:15:VAL:HB	1:B:25:TYR:OH	2.11	0.51
1:G:36:LEU:HD21	1:G:70:TYR:CZ	2.46	0.51
1:D:82:MET:HA	1:D:82:MET:HE2	1.92	0.51
1:F:100:VAL:HG13	1:F:122:LEU:HD12	1.94	0.50
2:F:401:EZA:O7	1:G:90:TYR:OH	2.29	0.49
1:F:36:LEU:HD23	1:F:68:TYR:HB2	1.94	0.48
1:F:70:TYR:HE2	1:G:56:LEU:HD13	1.77	0.48
1:F:156:ARG:NH1	1:F:159:GLU:OE1	2.45	0.48
2:D:401:EZA:C19	2:D:401:EZA:N4	2.76	0.48
1:E:65:LYS:O	1:E:93:PRO:HB3	2.14	0.48
1:C:97:THR:C	1:C:98:ILE:HD12	2.40	0.47
1:E:100:VAL:HG13	1:E:122:LEU:HD12	1.95	0.47
1:B:100:VAL:HG13	1:B:122:LEU:HD12	1.96	0.47
1:G:97:THR:C	1:G:98:ILE:HD12	2.40	0.47
1:B:70:TYR:CE1	1:B:98:ILE:HD13	2.49	0.46
1:C:70:TYR:CE1	1:C:98:ILE:HD13	2.50	0.46
1:E:70:TYR:CE1	1:E:98:ILE:HD13	2.49	0.46
1:D:70:TYR:CE1	1:D:98:ILE:HD13	2.51	0.46
1:A:109:LEU:HD13	1:A:157:LEU:HD22	1.98	0.46
1:G:70:TYR:CE1	1:G:98:ILE:HD13	2.51	0.46
1:D:15:VAL:HG22	1:E:25:TYR:CE2	2.51	0.45
1:G:46:HIS:O	1:G:50:VAL:HG23	2.16	0.45
1:C:70:TYR:HE1	1:C:98:ILE:HD13	1.82	0.45
1:E:36:LEU:HD21	1:E:70:TYR:CD2	2.52	0.45
1:D:97:THR:C	1:D:98:ILE:HD12	2.41	0.45
1:C:199:ARG:HG3	1:D:90:TYR:CE1	2.52	0.45
1:E:97:THR:C	1:E:98:ILE:HD12	2.42	0.45
1:A:97:THR:C	1:A:98:ILE:HD12	2.41	0.45
1:G:36:LEU:HD21	1:G:70:TYR:CE1	2.52	0.45
1:C:46:HIS:O	1:C:50:VAL:HG23	2.17	0.44
1:G:10:LEU:N	5:G:505:HOH:O	2.50	0.44
2:B:401:EZA:N4	2:B:401:EZA:C19	2.80	0.44
1:C:26:ASP:OD1	1:C:29:SER:OG	2.26	0.44
1:B:14:VAL:HG11	1:B:30:ARG:HH21	1.82	0.44
1:B:70:TYR:HE1	1:B:98:ILE:HD13	1.82	0.44
1:F:156:ARG:NH2	5:F:501:HOH:O	2.39	0.44
1:B:97:THR:C	1:B:98:ILE:HD12	2.41	0.44
1:E:46:HIS:O	1:E:50:VAL:HG23	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:TYR:HE1	1:D:98:ILE:HD13	1.82	0.44
1:D:75:GLY:HA3	1:D:105:SER:OG	2.18	0.44
1:B:13:MET:HG2	1:C:26:ASP:OD1	2.17	0.44
1:C:36:LEU:HD21	1:C:70:TYR:CE2	2.53	0.44
2:F:401:EZA:N4	2:F:401:EZA:C19	2.81	0.44
2:G:401:EZA:N4	2:G:401:EZA:C19	2.81	0.44
1:E:70:TYR:HE2	1:F:56:LEU:HD13	1.82	0.44
2:E:401:EZA:O7	1:F:90:TYR:OH	2.32	0.44
1:D:65:LYS:O	1:D:93:PRO:HB3	2.18	0.43
1:D:109:LEU:HD13	1:D:157:LEU:HD22	2.00	0.43
1:F:70:TYR:CE1	1:F:98:ILE:HD13	2.53	0.43
1:F:156:ARG:HA	1:F:156:ARG:HD2	1.84	0.43
1:C:48:ALA:HA	1:C:84:ILE:HD11	2.00	0.43
1:C:109:LEU:HD13	1:C:157:LEU:HD22	2.01	0.43
1:A:90:TYR:OH	2:G:401:EZA:O7	2.33	0.43
1:B:70:TYR:HE2	1:C:56:LEU:HD13	1.83	0.43
1:E:126:ARG:CZ	1:F:79:THR:HG21	2.49	0.43
1:A:70:TYR:CE1	1:A:98:ILE:HD13	2.54	0.43
1:F:97:THR:C	1:F:98:ILE:HD12	2.44	0.43
2:A:401:EZA:C19	2:A:401:EZA:N4	2.82	0.42
1:G:48:ALA:HA	1:G:84:ILE:HD11	2.00	0.42
1:G:123:PRO:HG3	1:G:198:GLU:HG2	2.02	0.42
1:B:126:ARG:CZ	1:C:79:THR:HG21	2.50	0.42
1:E:100:VAL:HG12	1:F:83:ALA:HB1	2.01	0.42
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.89	0.42
2:E:401:EZA:C19	2:E:401:EZA:N4	2.83	0.42
1:G:70:TYR:HE1	1:G:98:ILE:HD13	1.83	0.42
1:B:13:MET:N	1:C:29:SER:OG	2.33	0.41
1:C:92:LYS:HD3	1:C:92:LYS:C	2.45	0.41
1:A:83:ALA:HB1	1:G:100:VAL:HG12	2.03	0.41
1:D:48:ALA:HA	1:D:84:ILE:HD11	2.01	0.41
1:B:13:MET:HA	1:B:25:TYR:O	2.20	0.41
2:C:401:EZA:C19	2:C:401:EZA:N4	2.84	0.41
1:D:26:ASP:OD1	1:D:29:SER:OG	2.39	0.41
1:E:70:TYR:HE1	1:E:98:ILE:HD13	1.86	0.40
1:G:65:LYS:O	1:G:93:PRO:HB3	2.20	0.40
1:C:126:ARG:CZ	1:D:79:THR:HG21	2.51	0.40
1:F:13:MET:HG3	1:G:29:SER:OG	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:NH2	1:D:177:GLU:CG[2_675]	2.12	0.08

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	190/208 (91%)	186 (98%)	4 (2%)	0	100	100
1	B	178/208 (86%)	175 (98%)	3 (2%)	0	100	100
1	C	181/208 (87%)	177 (98%)	4 (2%)	0	100	100
1	D	187/208 (90%)	183 (98%)	4 (2%)	0	100	100
1	E	176/208 (85%)	173 (98%)	3 (2%)	0	100	100
1	F	186/208 (89%)	182 (98%)	4 (2%)	0	100	100
1	G	177/208 (85%)	174 (98%)	3 (2%)	0	100	100
All	All	1275/1456 (88%)	1250 (98%)	25 (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	154/173 (89%)	153 (99%)	1 (1%)	78	81
1	B	144/173 (83%)	144 (100%)	0	100	100
1	C	150/173 (87%)	149 (99%)	1 (1%)	76	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	151/173 (87%)	151 (100%)	0	100	100
1	E	144/173 (83%)	143 (99%)	1 (1%)	76	78
1	F	151/173 (87%)	148 (98%)	3 (2%)	48	46
1	G	147/173 (85%)	146 (99%)	1 (1%)	76	78
All	All	1041/1211 (86%)	1034 (99%)	7 (1%)	76	78

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

Mol	Chain	Res	Type
1	A	198	GLU
1	C	92	LYS
1	E	18	THR
1	F	13	MET
1	F	20	ARG
1	F	109	LEU
1	G	156	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	49	ASN
1	A	72	ASN
1	A	180	ASN
1	B	49	ASN
1	B	72	ASN
1	B	180	ASN
1	C	49	ASN
1	C	72	ASN
1	C	180	ASN
1	D	49	ASN
1	D	72	ASN
1	E	49	ASN
1	F	72	ASN
1	F	180	ASN
1	G	49	ASN
1	G	72	ASN
1	G	180	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	EZA	D	401	-	58,59,59	1.93	3 (5%)	79,83,83	1.75	19 (24%)
2	EZA	C	401	-	58,59,59	1.93	3 (5%)	79,83,83	1.57	16 (20%)
2	EZA	F	401	-	58,59,59	1.93	3 (5%)	79,83,83	1.60	15 (18%)
2	EZA	B	401	-	58,59,59	1.93	3 (5%)	79,83,83	1.61	17 (21%)
2	EZA	G	401	-	58,59,59	1.93	3 (5%)	79,83,83	1.55	15 (18%)
2	EZA	A	401	-	58,59,59	1.92	3 (5%)	79,83,83	1.59	17 (21%)
2	EZA	E	401	-	58,59,59	1.92	3 (5%)	79,83,83	1.62	15 (18%)

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	EZA	D	401	-	-	19/63/96/96	0/4/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EZA	C	401	-	-	16/63/96/96	0/4/5/5
2	EZA	F	401	-	-	15/63/96/96	0/4/5/5
2	EZA	B	401	-	-	12/63/96/96	0/4/5/5
2	EZA	G	401	-	-	14/63/96/96	0/4/5/5
2	EZA	A	401	-	-	9/63/96/96	0/4/5/5
2	EZA	E	401	-	-	14/63/96/96	0/4/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	EZA	C21-C20	-11.15	1.34	1.53
2	C	401	EZA	C21-C20	-11.14	1.34	1.53
2	A	401	EZA	C21-C20	-11.13	1.34	1.53
2	G	401	EZA	C21-C20	-11.13	1.34	1.53
2	E	401	EZA	C21-C20	-11.10	1.34	1.53
2	B	401	EZA	C21-C20	-11.07	1.34	1.53
2	F	401	EZA	C21-C20	-11.06	1.34	1.53
2	G	401	EZA	C20-N3	-6.39	1.34	1.47
2	F	401	EZA	C20-N3	-6.38	1.34	1.47
2	B	401	EZA	C20-N3	-6.37	1.34	1.47
2	C	401	EZA	C20-N3	-6.31	1.34	1.47
2	A	401	EZA	C20-N3	-6.31	1.34	1.47
2	D	401	EZA	C20-N3	-6.26	1.34	1.47
2	E	401	EZA	C20-N3	-6.26	1.34	1.47
2	C	401	EZA	O3-C19	5.87	1.45	1.33
2	B	401	EZA	O3-C19	5.87	1.45	1.33
2	E	401	EZA	O3-C19	5.85	1.45	1.33
2	F	401	EZA	O3-C19	5.82	1.45	1.33
2	D	401	EZA	O3-C19	5.80	1.45	1.33
2	A	401	EZA	O3-C19	5.80	1.45	1.33
2	G	401	EZA	O3-C19	5.78	1.45	1.33

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	EZA	C26-C25-N3	5.16	128.31	118.09
2	B	401	EZA	C26-C25-N3	5.06	128.12	118.09
2	F	401	EZA	C26-C25-N3	4.94	127.88	118.09
2	D	401	EZA	C26-C25-N3	4.89	127.78	118.09
2	C	401	EZA	C26-C25-N3	4.81	127.61	118.09
2	A	401	EZA	C26-C25-N3	4.79	127.58	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	EZA	C26-C25-N3	4.74	127.47	118.09
2	D	401	EZA	C26-N4-C28	4.55	130.90	121.32
2	F	401	EZA	C25-C26-N4	4.23	119.57	109.03
2	D	401	EZA	C30-C29-N5	-4.22	104.90	110.55
2	E	401	EZA	C4-C5-C6	-4.19	117.19	125.92
2	E	401	EZA	C25-C26-N4	4.05	119.11	109.03
2	D	401	EZA	C32-C33-N5	-4.01	104.45	110.65
2	E	401	EZA	O3-C19-C20	4.01	118.86	110.58
2	G	401	EZA	C25-C26-N4	3.98	118.94	109.03
2	B	401	EZA	C25-C26-N4	3.98	118.93	109.03
2	C	401	EZA	C25-C26-N4	3.95	118.88	109.03
2	B	401	EZA	O3-C19-C20	3.94	118.72	110.58
2	D	401	EZA	O3-C19-C20	3.92	118.67	110.58
2	A	401	EZA	O3-C19-C20	3.92	118.67	110.58
2	D	401	EZA	C25-C26-N4	3.86	118.64	109.03
2	G	401	EZA	O3-C19-C20	3.86	118.55	110.58
2	A	401	EZA	C25-C26-N4	3.79	118.46	109.03
2	C	401	EZA	O3-C19-C20	3.76	118.35	110.58
2	F	401	EZA	O3-C19-C20	3.69	118.21	110.58
2	B	401	EZA	C26-N4-C28	3.69	129.09	121.32
2	A	401	EZA	C26-N4-C28	3.66	129.02	121.32
2	C	401	EZA	C22-C24-N3	-3.54	100.01	103.54
2	F	401	EZA	C26-N4-C28	3.47	128.61	121.32
2	A	401	EZA	C22-C24-N3	-3.45	100.10	103.54
2	G	401	EZA	C26-N4-C28	3.39	128.44	121.32
2	E	401	EZA	C22-C24-N3	-3.38	100.17	103.54
2	C	401	EZA	C26-N4-C28	3.36	128.39	121.32
2	E	401	EZA	C26-N4-C28	3.35	128.36	121.32
2	G	401	EZA	C22-C24-N3	-3.34	100.22	103.54
2	F	401	EZA	C22-C24-N3	-3.23	100.33	103.54
2	D	401	EZA	C22-C24-N3	-3.21	100.35	103.54
2	B	401	EZA	C4-C5-C6	-3.17	119.31	125.92
2	B	401	EZA	C22-C24-N3	-3.16	100.39	103.54
2	F	401	EZA	C4-C5-C6	-3.08	119.51	125.92
2	C	401	EZA	C4-C5-C6	-3.05	119.56	125.92
2	A	401	EZA	C4-C5-C6	-2.98	119.71	125.92
2	D	401	EZA	C4-C5-C6	-2.96	119.76	125.92
2	E	401	EZA	C13-C12-C11	-2.93	119.94	123.50
2	G	401	EZA	C4-C5-C6	-2.92	119.84	125.92
2	F	401	EZA	C6-C7-N1	2.86	119.50	114.61
2	D	401	EZA	C13-C12-C11	-2.86	120.03	123.50
2	A	401	EZA	C15-C14-C13	-2.82	120.07	123.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	EZA	C15-C14-C13	-2.82	120.07	123.50
2	D	401	EZA	C15-C14-C13	-2.81	120.08	123.50
2	F	401	EZA	C13-C12-C11	-2.80	120.09	123.50
2	C	401	EZA	C13-C12-C11	-2.80	120.10	123.50
2	B	401	EZA	C15-C14-C13	-2.79	120.11	123.50
2	C	401	EZA	C15-C14-C13	-2.77	120.14	123.50
2	F	401	EZA	C15-C14-C13	-2.75	120.16	123.50
2	E	401	EZA	O5-C25-C26	-2.75	114.49	120.15
2	D	401	EZA	C6-C7-N1	2.73	119.28	114.61
2	B	401	EZA	C13-C12-C11	-2.73	120.19	123.50
2	G	401	EZA	C13-C12-C11	-2.72	120.20	123.50
2	A	401	EZA	C13-C12-C11	-2.68	120.24	123.50
2	D	401	EZA	C14-C13-C12	2.67	119.97	116.08
2	E	401	EZA	C15-C14-C13	-2.65	120.28	123.50
2	B	401	EZA	O5-C25-C26	-2.65	114.70	120.15
2	E	401	EZA	C14-C13-C12	2.64	119.92	116.08
2	G	401	EZA	O5-C25-C26	-2.63	114.73	120.15
2	C	401	EZA	C6-C7-N1	2.62	119.10	114.61
2	F	401	EZA	O5-C25-C26	-2.61	114.78	120.15
2	D	401	EZA	O5-C25-C26	-2.61	114.79	120.15
2	A	401	EZA	C30-C29-N5	-2.57	107.11	110.55
2	F	401	EZA	C14-C13-C12	2.57	119.82	116.08
2	B	401	EZA	C14-C13-C12	2.55	119.80	116.08
2	A	401	EZA	O5-C25-C26	-2.55	114.91	120.15
2	C	401	EZA	C14-C13-C12	2.54	119.79	116.08
2	G	401	EZA	C14-C13-C12	2.54	119.78	116.08
2	A	401	EZA	C14-C13-C12	2.54	119.78	116.08
2	C	401	EZA	O5-C25-C26	-2.54	114.93	120.15
2	G	401	EZA	O3-C19-O4	-2.46	119.64	124.14
2	A	401	EZA	O3-C19-O4	-2.45	119.66	124.14
2	E	401	EZA	O3-C19-O4	-2.44	119.68	124.14
2	G	401	EZA	C6-C7-N1	2.43	118.77	114.61
2	B	401	EZA	O3-C19-O4	-2.40	119.75	124.14
2	C	401	EZA	C24-N3-C20	2.39	115.00	111.83
2	C	401	EZA	O3-C19-O4	-2.38	119.79	124.14
2	B	401	EZA	C24-N3-C20	2.37	114.98	111.83
2	E	401	EZA	C24-N3-C20	2.35	114.95	111.83
2	B	401	EZA	O5-C25-N3	-2.34	117.17	121.38
2	E	401	EZA	C24-N3-C25	-2.33	119.03	126.93
2	A	401	EZA	C24-N3-C20	2.33	114.93	111.83
2	F	401	EZA	C24-N3-C20	2.33	114.92	111.83
2	E	401	EZA	O5-C25-N3	-2.33	117.19	121.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	EZA	C27-C26-N4	2.30	114.60	110.38
2	B	401	EZA	C24-N3-C25	-2.28	119.23	126.93
2	D	401	EZA	O3-C19-O4	-2.27	119.98	124.14
2	F	401	EZA	O3-C19-O4	-2.26	120.01	124.14
2	F	401	EZA	O5-C25-N3	-2.25	117.34	121.38
2	D	401	EZA	C34-C35-N6	2.25	116.08	110.83
2	D	401	EZA	C33-N5-C29	-2.24	111.16	115.81
2	D	401	EZA	C24-N3-C20	2.24	114.80	111.83
2	A	401	EZA	C24-N3-C25	-2.23	119.37	126.93
2	B	401	EZA	C34-C35-N6	2.23	116.04	110.83
2	G	401	EZA	C24-N3-C20	2.22	114.78	111.83
2	A	401	EZA	C6-C7-N1	2.22	118.40	114.61
2	C	401	EZA	C24-N3-C25	-2.21	119.47	126.93
2	D	401	EZA	O5-C25-N3	-2.20	117.42	121.38
2	B	401	EZA	C6-C7-N1	2.19	118.35	114.61
2	C	401	EZA	O5-C25-N3	-2.19	117.46	121.38
2	F	401	EZA	C24-N3-C25	-2.16	119.61	126.93
2	A	401	EZA	O5-C25-N3	-2.15	117.51	121.38
2	E	401	EZA	C27-C26-N4	2.14	114.31	110.38
2	D	401	EZA	C24-N3-C25	-2.14	119.69	126.93
2	G	401	EZA	C24-N3-C25	-2.11	119.80	126.93
2	B	401	EZA	C27-C26-N4	2.08	114.19	110.38
2	C	401	EZA	C28-C29-N5	2.01	116.09	111.21
2	G	401	EZA	O5-C25-N3	-2.00	117.79	121.38

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	EZA	N3-C25-C26-N4
2	A	401	EZA	C27-C26-N4-C28
2	B	401	EZA	C17-C39-N6-C35
2	B	401	EZA	O8-C39-N6-C35
2	B	401	EZA	C17-C39-N6-C38
2	B	401	EZA	O8-C39-N6-C38
2	B	401	EZA	N3-C25-C26-N4
2	B	401	EZA	O5-C25-C26-N4
2	B	401	EZA	C27-C26-N4-C28
2	C	401	EZA	N3-C25-C26-N4
2	C	401	EZA	O5-C25-C26-N4
2	D	401	EZA	C17-C39-N6-C35
2	D	401	EZA	O8-C39-N6-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	401	EZA	C17-C39-N6-C38
2	D	401	EZA	O8-C39-N6-C38
2	D	401	EZA	N3-C25-C26-N4
2	D	401	EZA	O5-C25-C26-N4
2	D	401	EZA	C27-C26-N4-C28
2	E	401	EZA	C27-C26-N4-C28
2	F	401	EZA	N3-C25-C26-N4
2	F	401	EZA	O5-C25-C26-N4
2	F	401	EZA	C27-C26-N4-C28
2	G	401	EZA	N3-C25-C26-N4
2	G	401	EZA	O5-C25-C26-N4
2	G	401	EZA	C27-C26-N4-C28
2	D	401	EZA	O6-C28-N4-C26
2	D	401	EZA	C29-C28-N4-C26
2	C	401	EZA	C27-C26-N4-C28
2	G	401	EZA	O6-C28-N4-C26
2	B	401	EZA	O6-C28-N4-C26
2	F	401	EZA	O6-C28-N4-C26
2	E	401	EZA	O6-C28-N4-C26
2	A	401	EZA	O5-C25-C26-N4
2	E	401	EZA	O5-C25-C26-N4
2	E	401	EZA	N3-C25-C26-N4
2	G	401	EZA	C29-C28-N4-C26
2	F	401	EZA	O5-C25-N3-C24
2	A	401	EZA	O6-C28-N4-C26
2	G	401	EZA	O5-C25-N3-C24
2	D	401	EZA	O5-C25-N3-C24
2	E	401	EZA	C2-C3-C4-C5
2	C	401	EZA	O6-C28-N4-C26
2	B	401	EZA	C29-C28-N4-C26
2	D	401	EZA	O5-C25-C26-C27
2	D	401	EZA	N3-C25-C26-C27
2	F	401	EZA	C29-C28-N4-C26
2	F	401	EZA	O5-C25-N3-C20
2	F	401	EZA	C26-C25-N3-C24
2	C	401	EZA	C1-C2-C3-C4
2	G	401	EZA	O5-C25-N3-C20
2	C	401	EZA	O5-C25-N3-C24
2	D	401	EZA	C26-C25-N3-C24
2	G	401	EZA	C26-C25-N3-C24
2	E	401	EZA	C29-C28-N4-C26
2	D	401	EZA	O5-C25-N3-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	401	EZA	O2-C16-C8-C9
2	A	401	EZA	O2-C16-C8-N1
2	D	401	EZA	O2-C16-C8-C9
2	F	401	EZA	O2-C16-C8-C9
2	C	401	EZA	O5-C25-N3-C20
2	F	401	EZA	C26-C25-N3-C20
2	E	401	EZA	O8-C39-N6-C38
2	D	401	EZA	C1-C2-C3-C4
2	C	401	EZA	O2-C16-C8-C9
2	E	401	EZA	O2-C16-C8-C9
2	G	401	EZA	O2-C16-C8-C9
2	A	401	EZA	C29-C28-N4-C26
2	B	401	EZA	N2-C16-C8-C9
2	D	401	EZA	C26-C25-N3-C20
2	G	401	EZA	C26-C25-N3-C20
2	D	401	EZA	N2-C16-C8-C9
2	A	401	EZA	N2-C16-C8-N1
2	F	401	EZA	N2-C16-C8-C9
2	F	401	EZA	N3-C25-C26-C27
2	C	401	EZA	C26-C25-N3-C24
2	C	401	EZA	N2-C16-C8-C9
2	E	401	EZA	N2-C16-C8-C9
2	G	401	EZA	N2-C16-C8-C9
2	A	401	EZA	O2-C16-C8-C9
2	C	401	EZA	C25-C26-N4-C28
2	E	401	EZA	O2-C16-C8-N1
2	C	401	EZA	C26-C25-N3-C20
2	G	401	EZA	O2-C16-C8-N1
2	F	401	EZA	C25-C26-N4-C28
2	E	401	EZA	C17-C39-N6-C38
2	C	401	EZA	O2-C16-C8-N1
2	E	401	EZA	C1-C2-C3-C4
2	A	401	EZA	N2-C16-C8-C9
2	G	401	EZA	C25-C26-N4-C28
2	E	401	EZA	N2-C16-C8-N1
2	B	401	EZA	O2-C16-C8-N1
2	F	401	EZA	O2-C16-C8-N1
2	C	401	EZA	C29-C28-N4-C26
2	G	401	EZA	N2-C16-C8-N1
2	D	401	EZA	O2-C16-C8-N1
2	C	401	EZA	O8-C39-N6-C38
2	E	401	EZA	C25-C26-N4-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	401	EZA	N2-C16-C8-N1
2	F	401	EZA	N2-C16-C8-N1

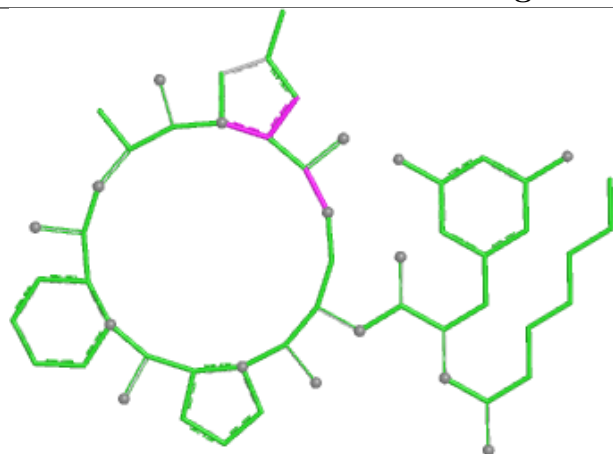
There are no ring outliers.

7 monomers are involved in 10 short contacts:

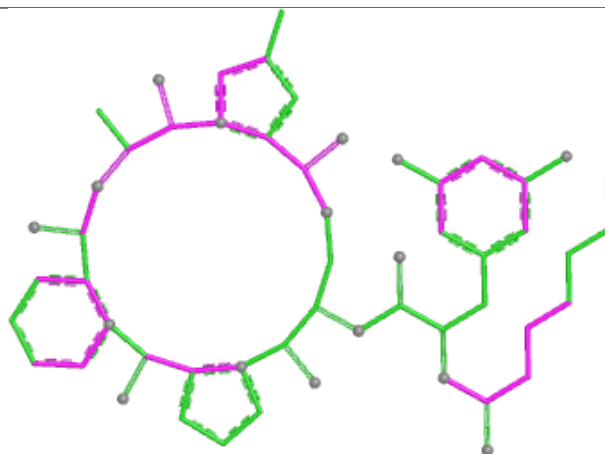
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	EZA	1	0
2	C	401	EZA	1	0
2	F	401	EZA	2	0
2	B	401	EZA	1	0
2	G	401	EZA	2	0
2	A	401	EZA	1	0
2	E	401	EZA	2	0

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

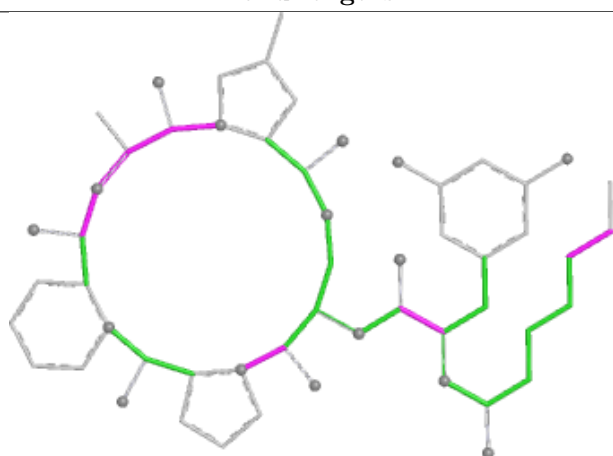
Ligand EZA D 401



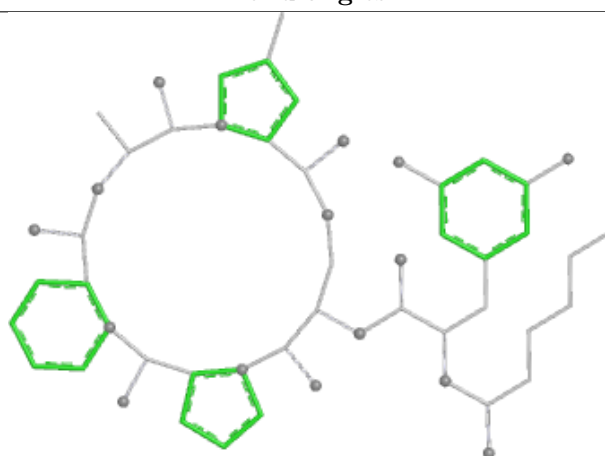
Bond lengths



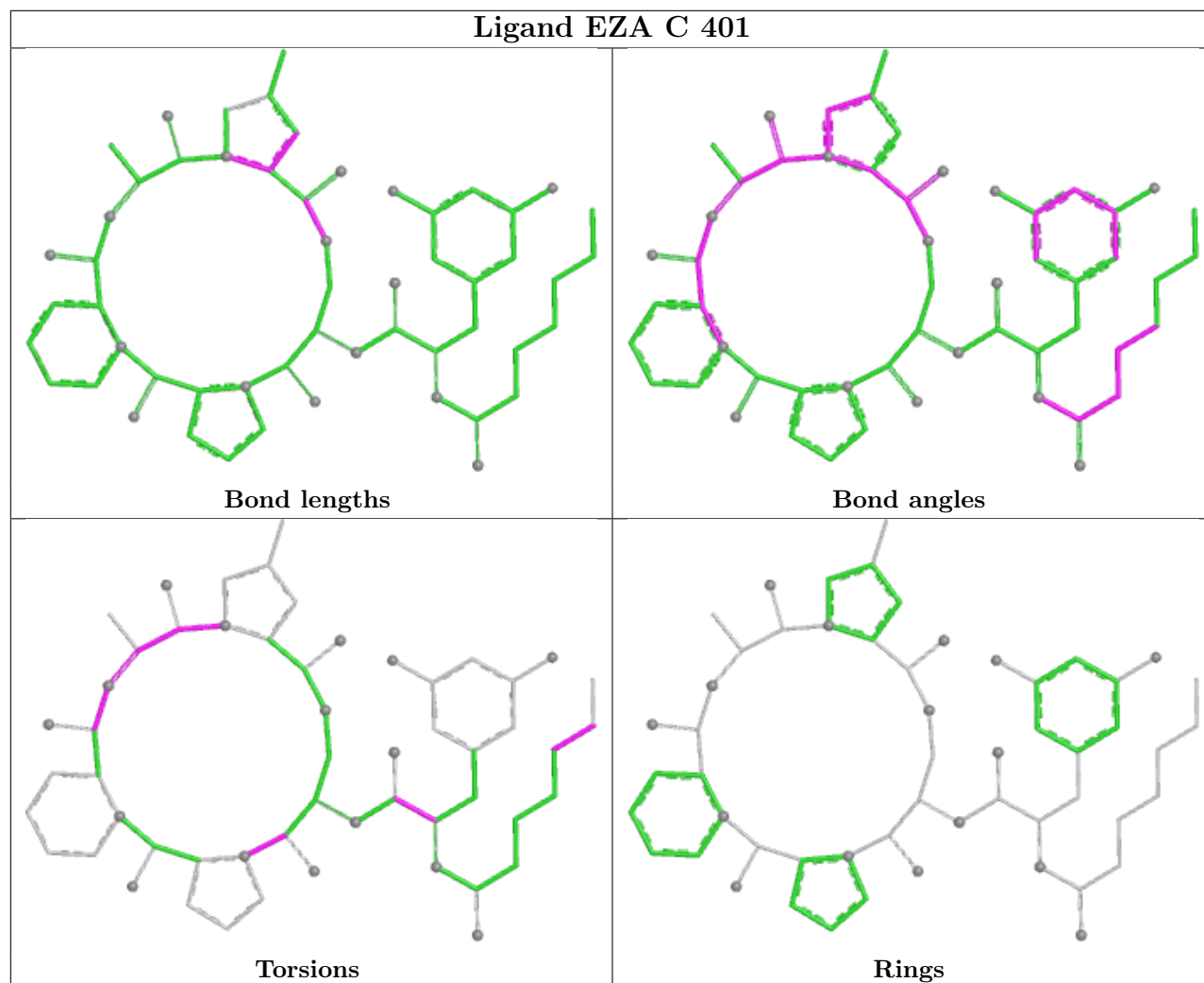
Bond angles



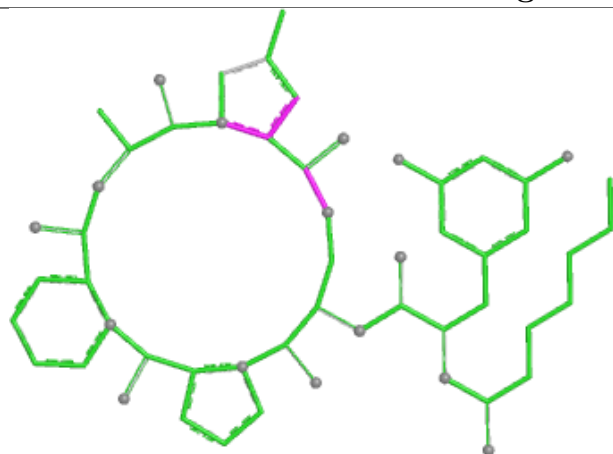
Torsions



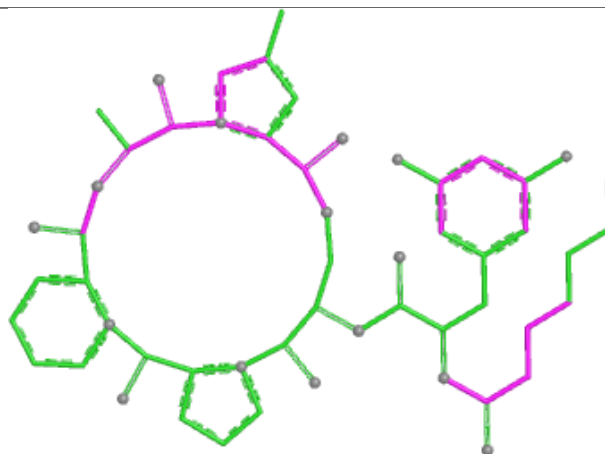
Rings



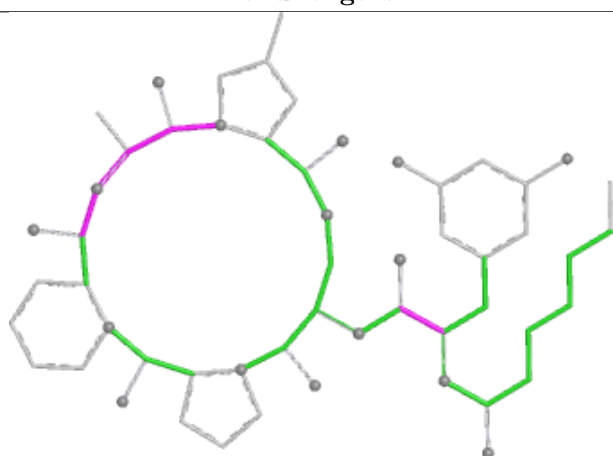
Ligand EZA F 401



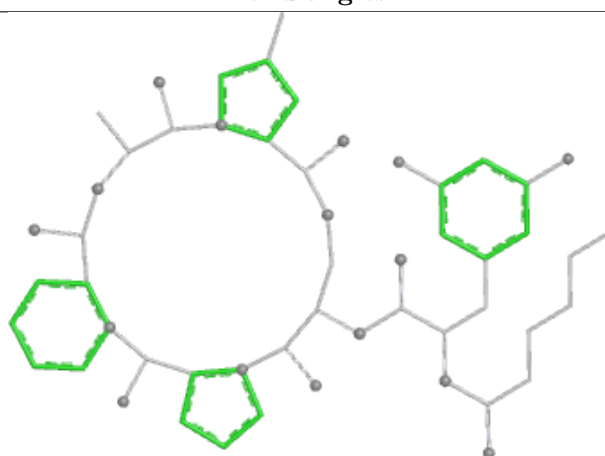
Bond lengths



Bond angles

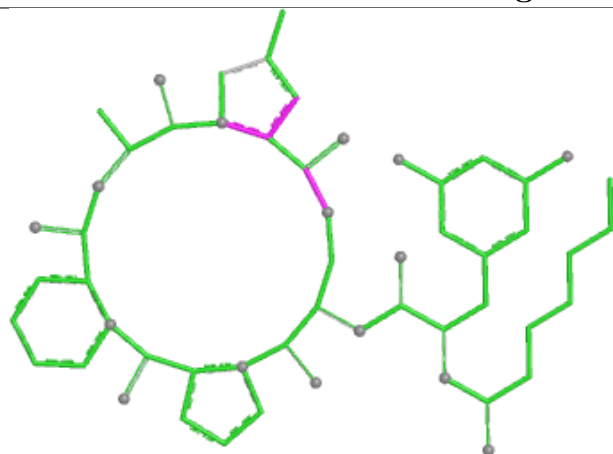


Torsions

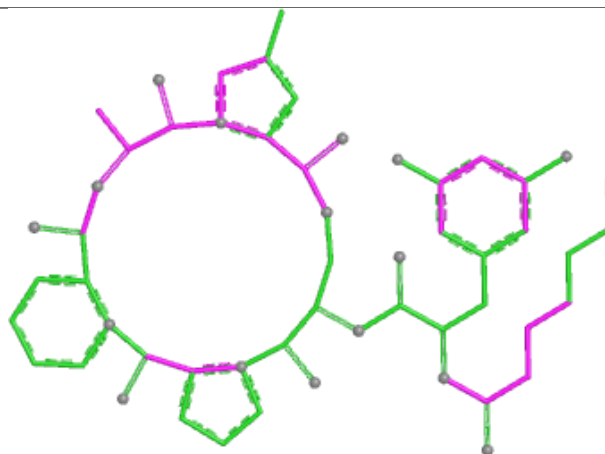


Rings

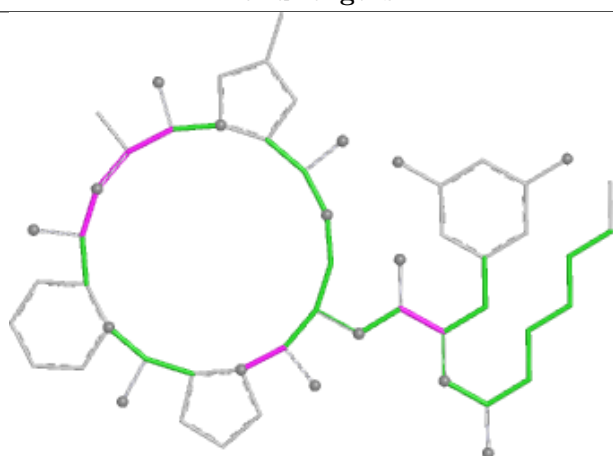
Ligand EZA B 401



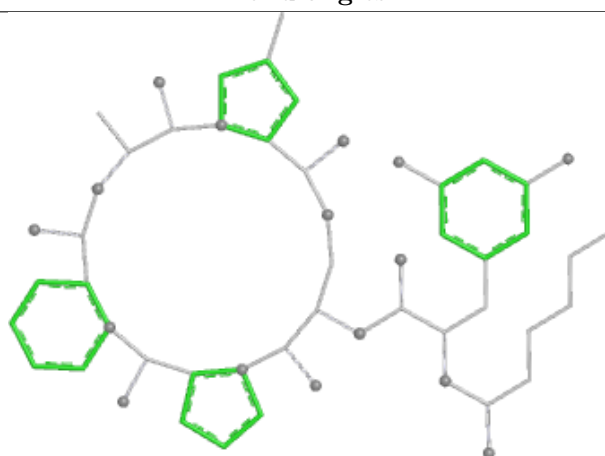
Bond lengths



Bond angles

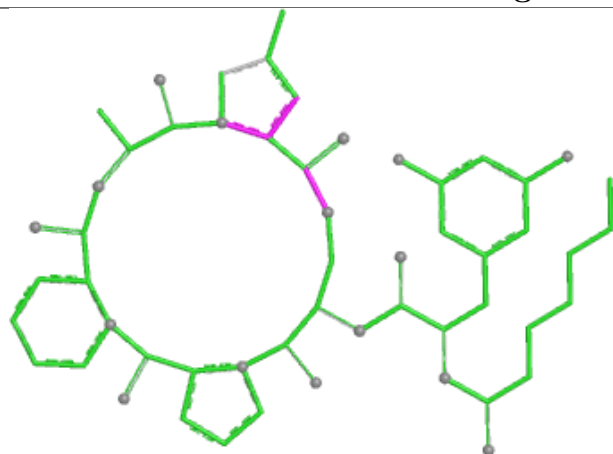


Torsions

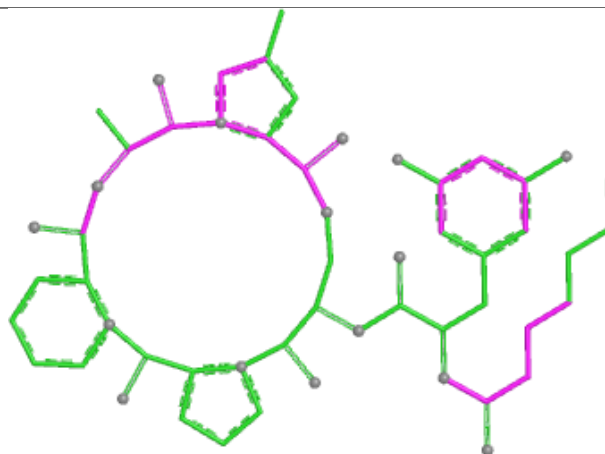


Rings

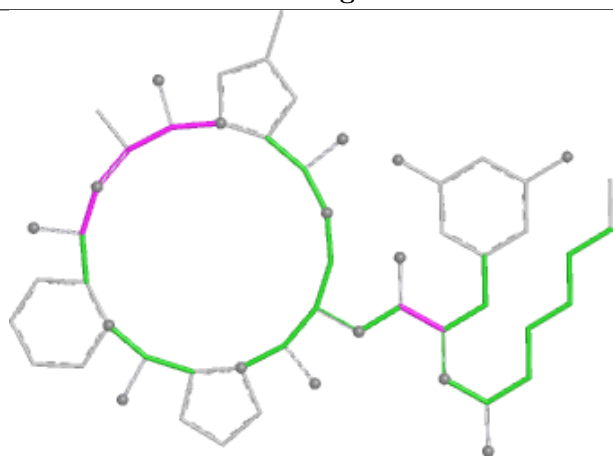
Ligand EZA G 401



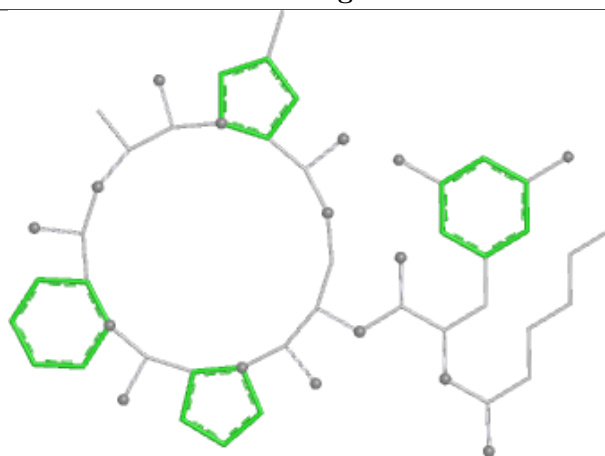
Bond lengths



Bond angles

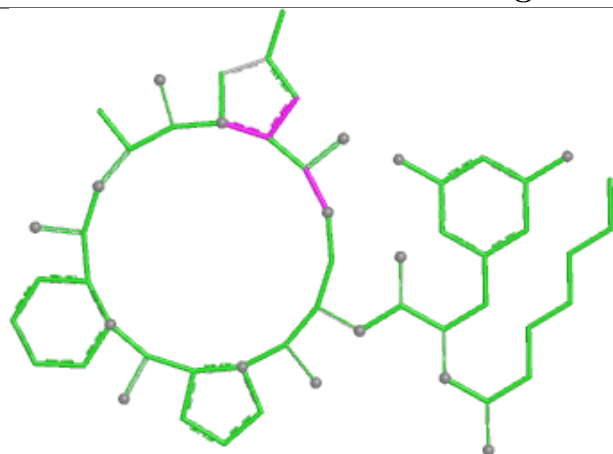


Torsions

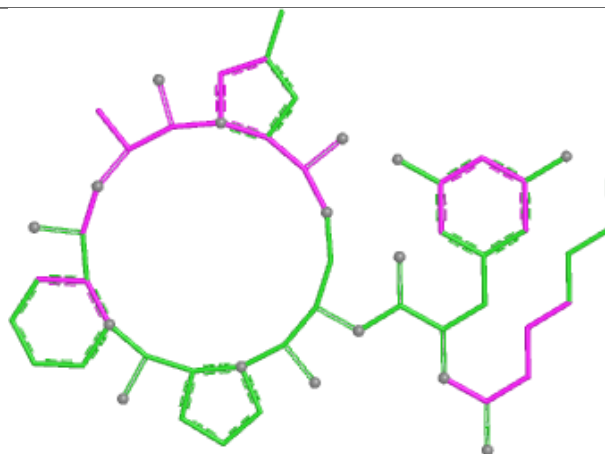


Rings

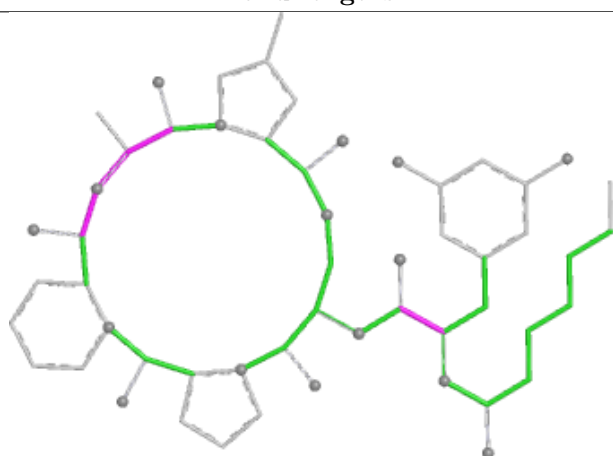
Ligand EZA A 401



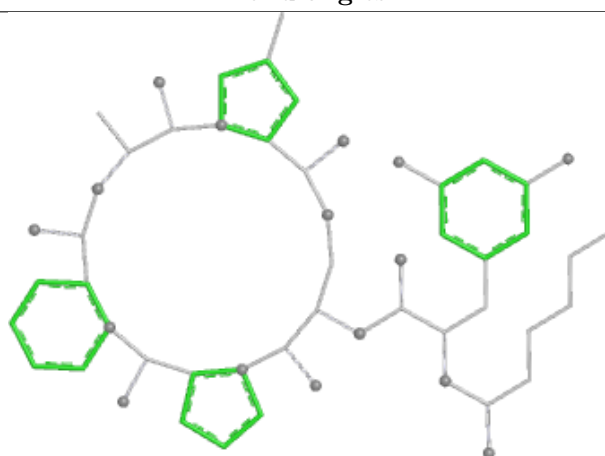
Bond lengths



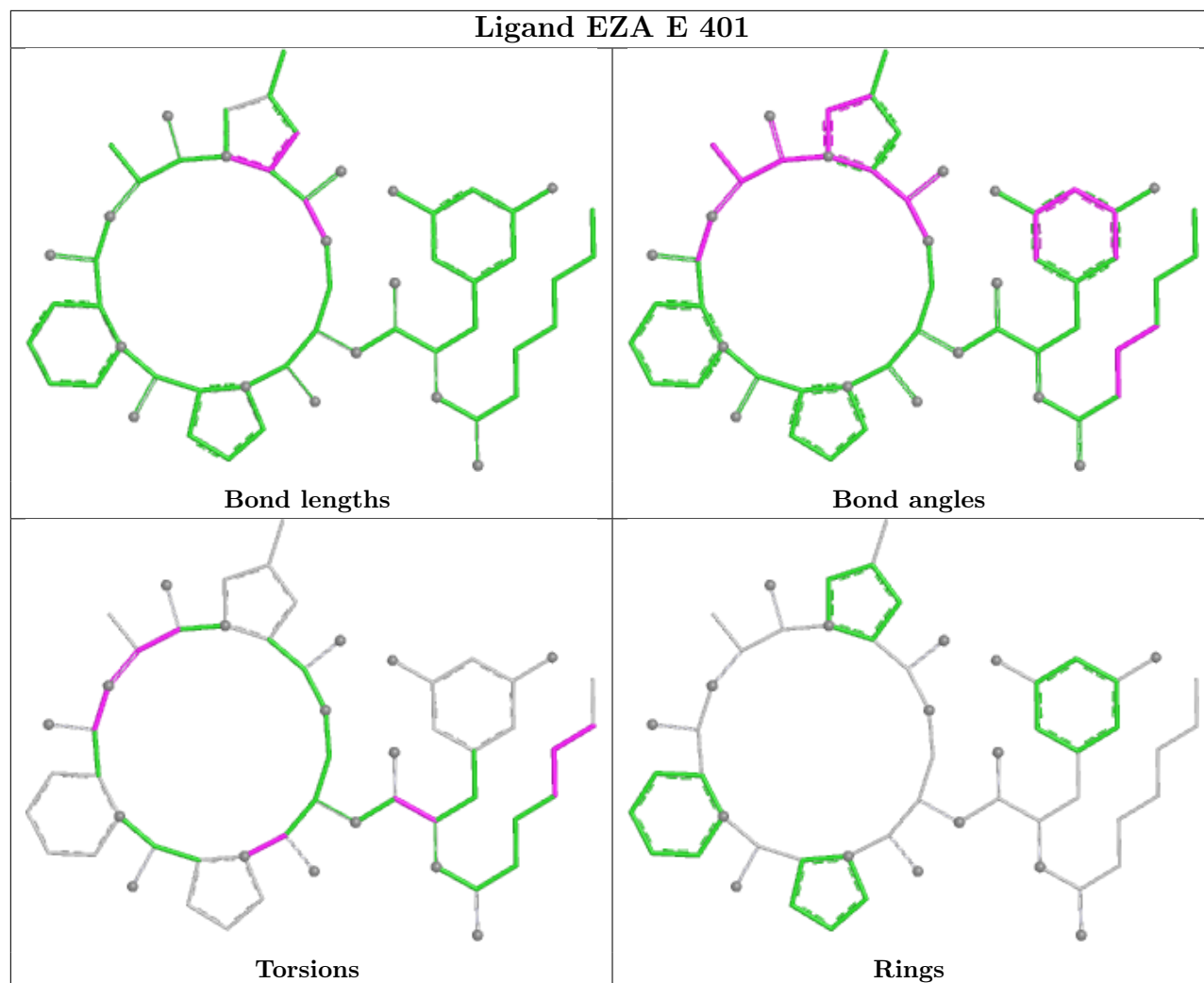
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	191/208 (91%)	-0.01	14 (7%)	21	22	7, 16, 48, 77	1 (0%)
1	B	182/208 (87%)	-0.00	11 (6%)	27	29	10, 17, 39, 55	0
1	C	185/208 (88%)	0.08	14 (7%)	20	21	6, 15, 42, 54	0
1	D	189/208 (90%)	0.06	15 (7%)	18	20	8, 17, 45, 74	0
1	E	180/208 (86%)	0.15	18 (10%)	12	13	9, 18, 40, 50	0
1	F	188/208 (90%)	0.10	15 (7%)	18	19	9, 17, 40, 52	0
1	G	181/208 (87%)	-0.22	9 (4%)	34	36	8, 14, 32, 51	0
All	All	1296/1456 (89%)	0.02	96 (7%)	20	22	6, 16, 42, 77	1 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	24	ALA	9.6
1	B	24	ALA	6.9
1	B	25	TYR	6.1
1	A	19	SER	6.0
1	E	21	GLY	6.0
1	A	24	ALA	5.9
1	C	11	VAL	5.7
1	D	23	ARG	5.7
1	A	23	ARG	5.4
1	B	10	LEU	5.1
1	F	11	VAL	5.1
1	C	10	LEU	4.8
1	C	15	VAL	4.5
1	F	13	MET	4.5
1	A	20	ARG	4.4
1	C	13	MET	4.3
1	D	15	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	201	PRO	4.3
1	E	18	THR	4.1
1	A	21	GLY	4.1
1	F	22	GLU	4.0
1	F	24	ALA	3.9
1	E	170	GLU	3.8
1	F	14	VAL	3.8
1	E	19	SER	3.8
1	F	141	THR	3.8
1	B	199	ARG	3.8
1	D	24	ALA	3.7
1	D	177	GLU	3.7
1	F	15	VAL	3.7
1	F	21	GLY	3.7
1	E	141	THR	3.7
1	D	19	SER	3.6
1	C	23	ARG	3.6
1	G	24	ALA	3.5
1	A	18	THR	3.5
1	G	15	VAL	3.5
1	C	17	GLN	3.5
1	E	25	TYR	3.4
1	B	13	MET	3.4
1	C	141	THR	3.4
1	D	18	THR	3.4
1	C	25	TYR	3.3
1	D	10	LEU	3.3
1	E	20	ARG	3.3
1	F	25	TYR	3.2
1	D	16	GLU	3.2
1	A	13	MET	3.2
1	A	16	GLU	3.2
1	C	138	GLY	3.2
1	C	199	ARG	3.2
1	F	17	GLN	3.1
1	F	18	THR	3.0
1	D	20	ARG	3.0
1	B	141	THR	2.9
1	B	23	ARG	2.9
1	D	70	TYR	2.8
1	B	14	VAL	2.8
1	G	178	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	70	TYR	2.8
1	F	23	ARG	2.8
1	E	70	TYR	2.8
1	D	17	GLN	2.7
1	E	138	GLY	2.7
1	D	178	ARG	2.7
1	D	198	GLU	2.7
1	D	21	GLY	2.7
1	G	141	THR	2.7
1	E	23	ARG	2.6
1	E	22	GLU	2.6
1	E	198	GLU	2.6
1	A	200	ARG	2.5
1	B	11	VAL	2.5
1	C	16	GLU	2.5
1	G	13	MET	2.5
1	B	70	TYR	2.4
1	B	198	GLU	2.4
1	A	177	GLU	2.4
1	C	14	VAL	2.3
1	A	141	THR	2.3
1	E	46	HIS	2.2
1	D	179	ASP	2.2
1	E	143	ILE	2.2
1	G	198	GLU	2.2
1	E	178	ARG	2.2
1	A	15	VAL	2.2
1	F	19	SER	2.2
1	C	140	ALA	2.2
1	G	10	LEU	2.1
1	F	92	LYS	2.1
1	E	140	ALA	2.1
1	G	138	GLY	2.0
1	A	17	GLN	2.0
1	E	34	GLU	2.0
1	G	92	LYS	2.0
1	E	171	THR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

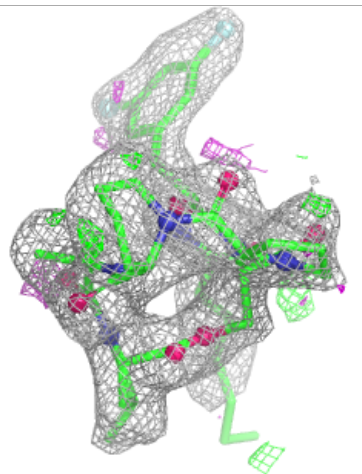
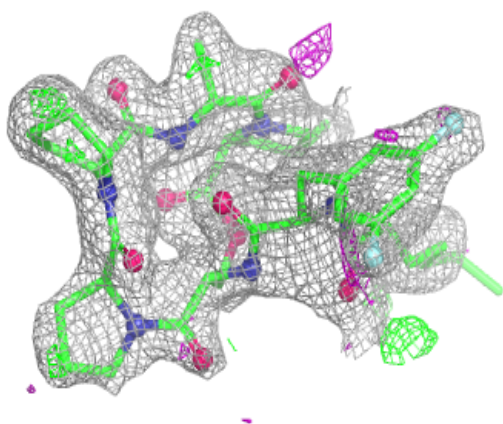
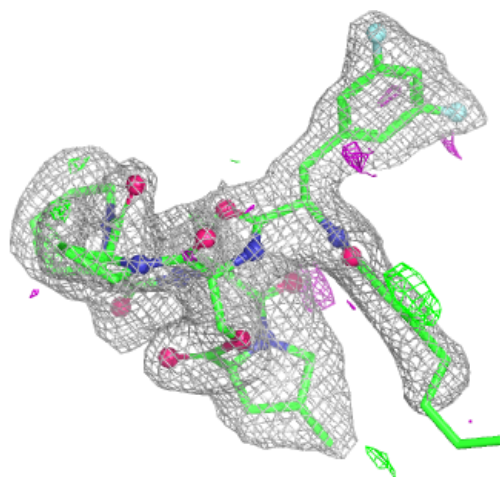
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EZA	B	401	55/55	0.81	0.14	29,41,44,49	0
2	EZA	F	401	55/55	0.81	0.14	23,40,44,48	0
2	EZA	E	401	55/55	0.84	0.14	30,41,50,60	0
2	EZA	D	401	55/55	0.85	0.12	28,38,43,49	0
2	EZA	C	401	55/55	0.86	0.12	25,36,45,46	0
2	EZA	A	401	55/55	0.91	0.10	21,27,34,39	0
2	EZA	G	401	55/55	0.91	0.10	19,29,42,46	0
4	MG	B	402	1/1	0.96	0.09	32,32,32,32	0
3	CL	A	404	1/1	0.98	0.06	28,28,28,28	0
3	CL	A	402	1/1	0.99	0.03	18,18,18,18	0
3	CL	B	403	1/1	0.99	0.03	19,19,19,19	0
3	CL	C	402	1/1	0.99	0.03	17,17,17,17	0
3	CL	D	402	1/1	0.99	0.03	14,14,14,14	0
3	CL	E	402	1/1	0.99	0.03	20,20,20,20	0
3	CL	A	403	1/1	0.99	0.04	18,18,18,18	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.

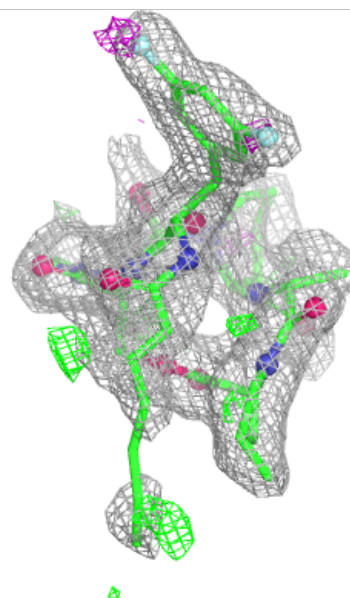
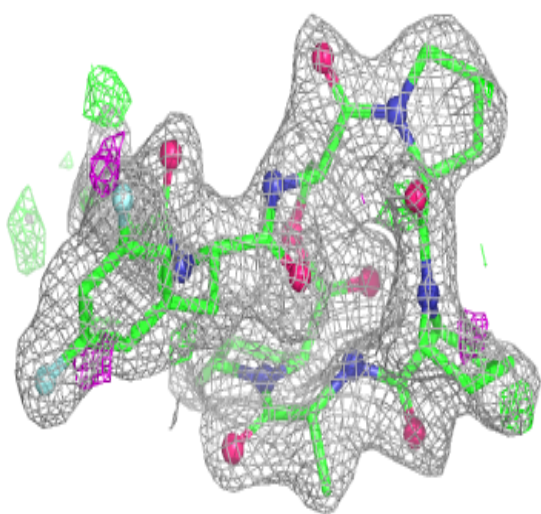
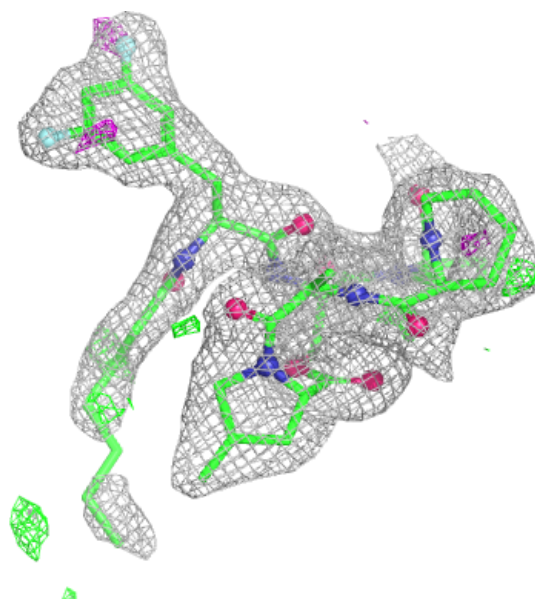
Electron density around EZA B 401:

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



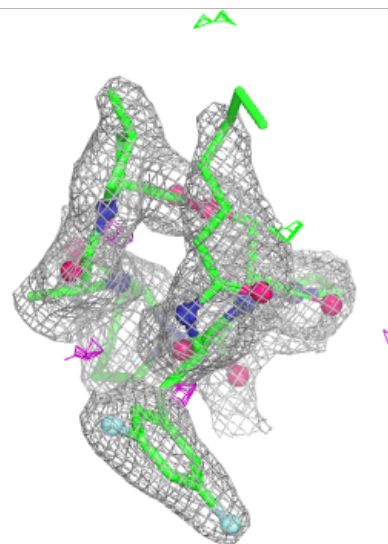
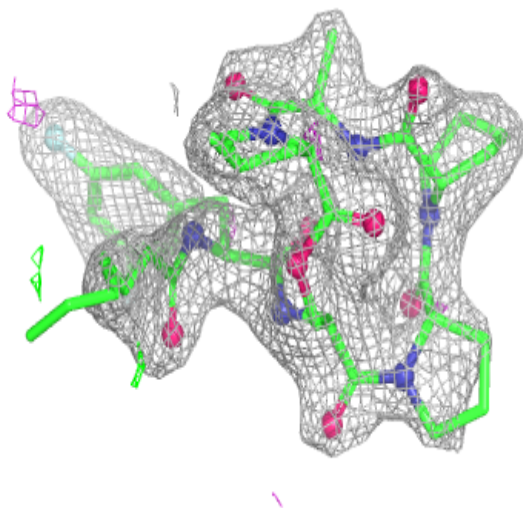
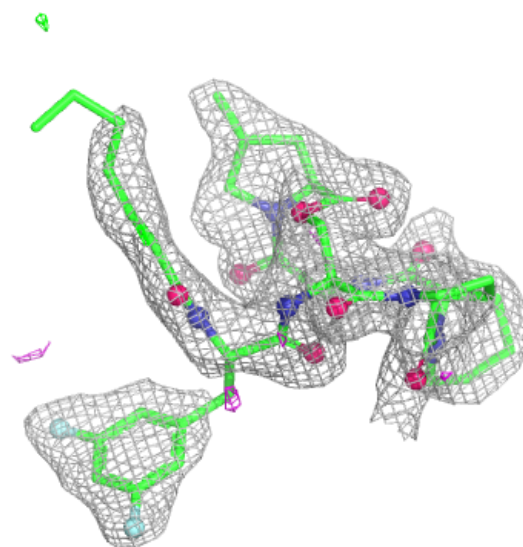
Electron density around EZA F 401:

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



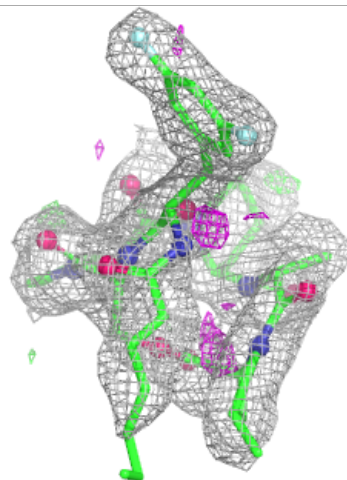
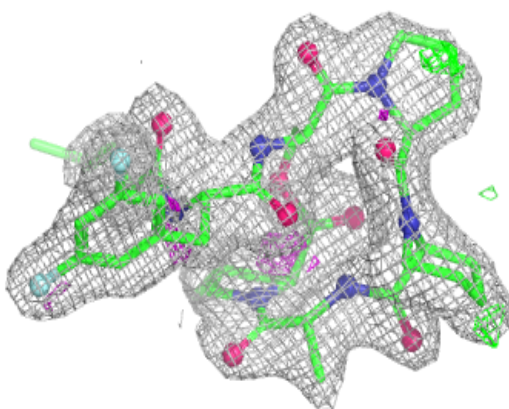
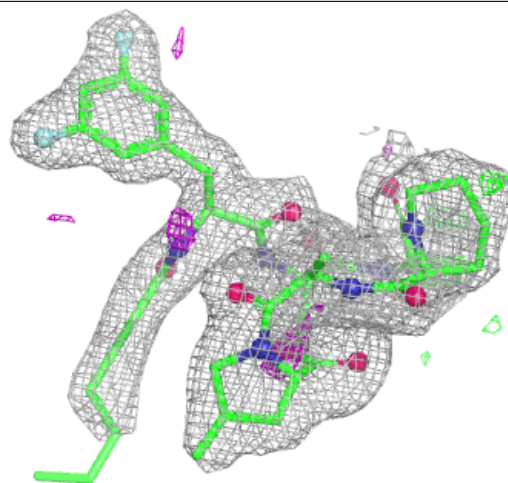
Electron density around EZA E 401:

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



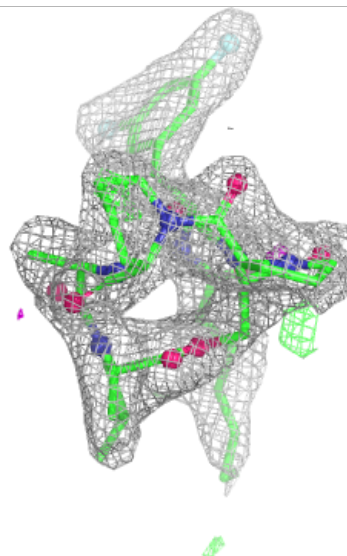
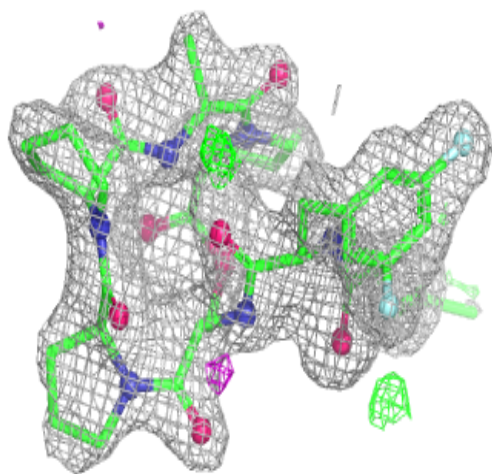
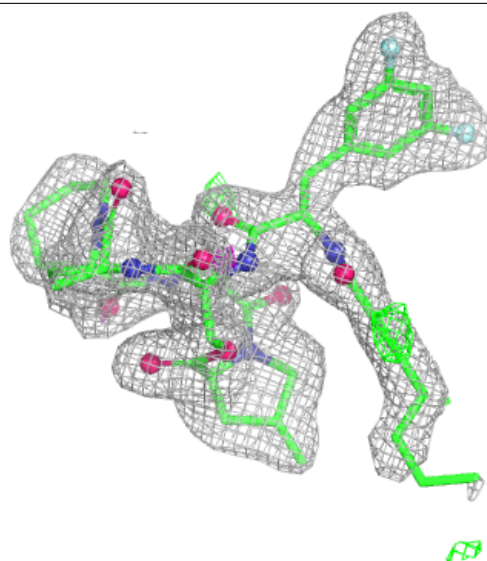
Electron density around EZA D 401:

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



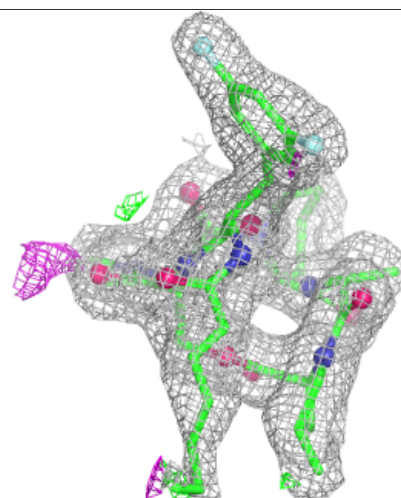
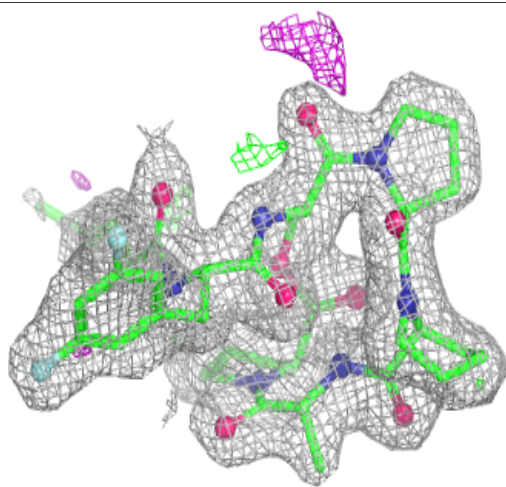
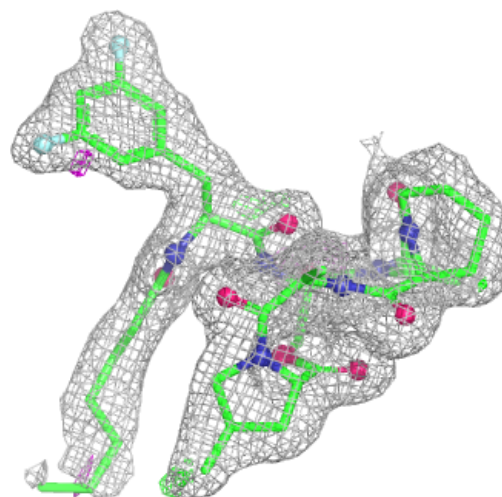
Electron density around EZA C 401:

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



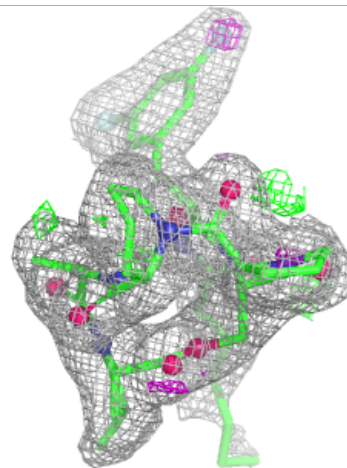
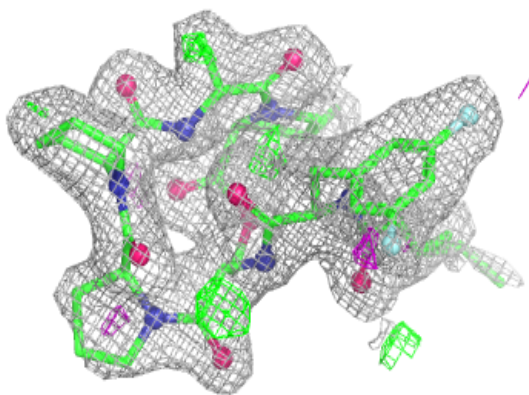
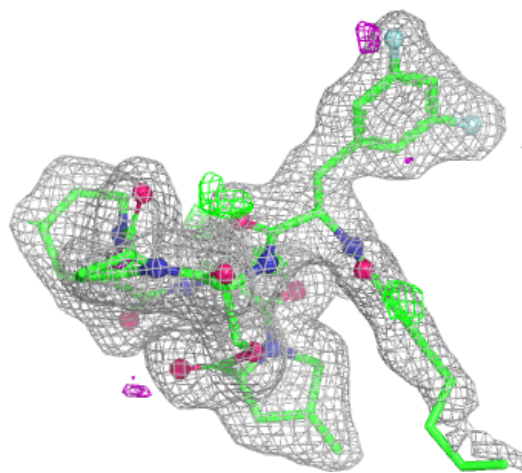
Electron density around EZA A 401:

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



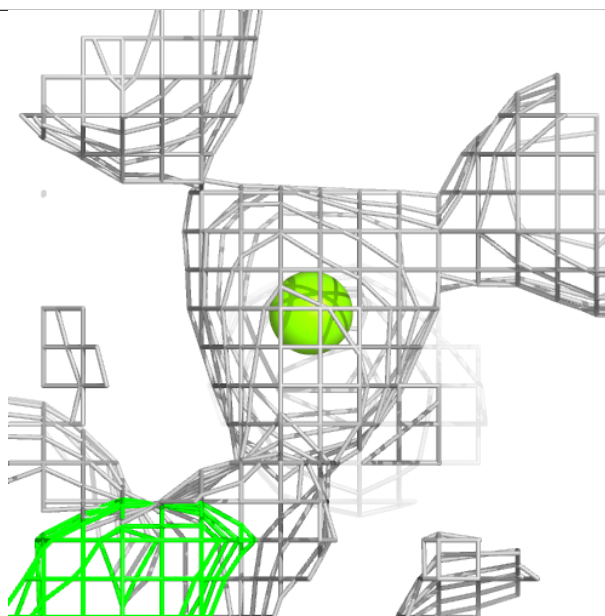
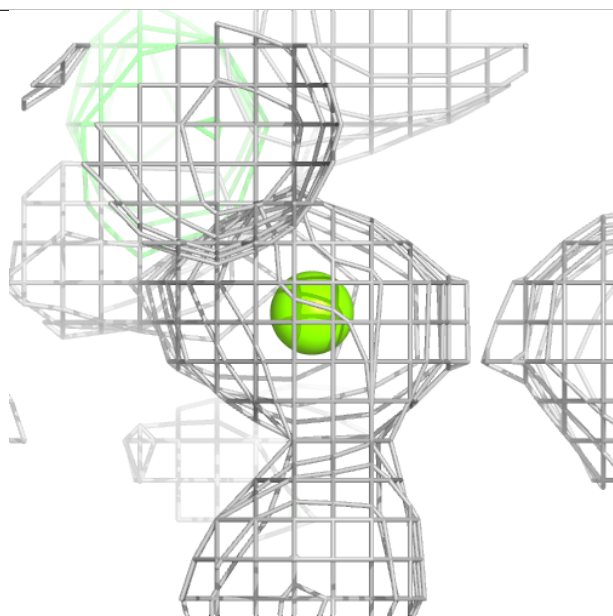
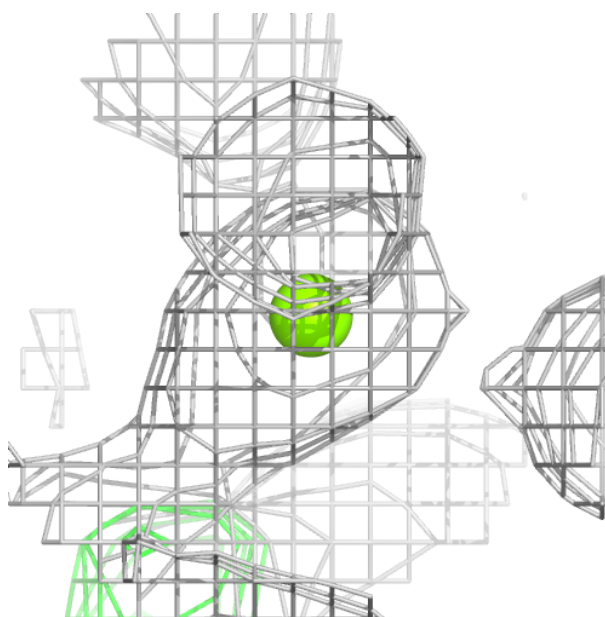
Electron density around EZA G 401:

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



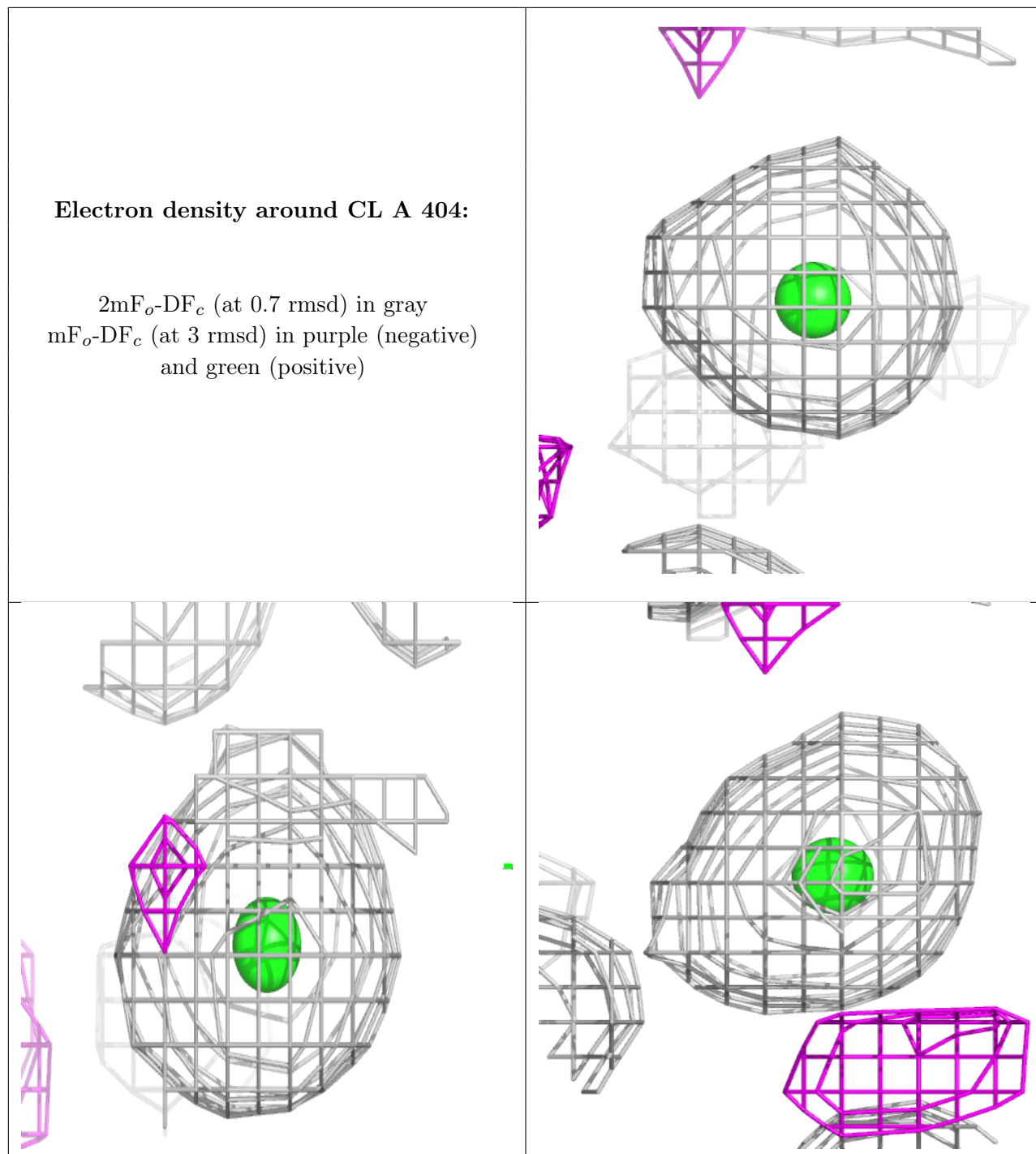
Electron density around MG B 402:

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



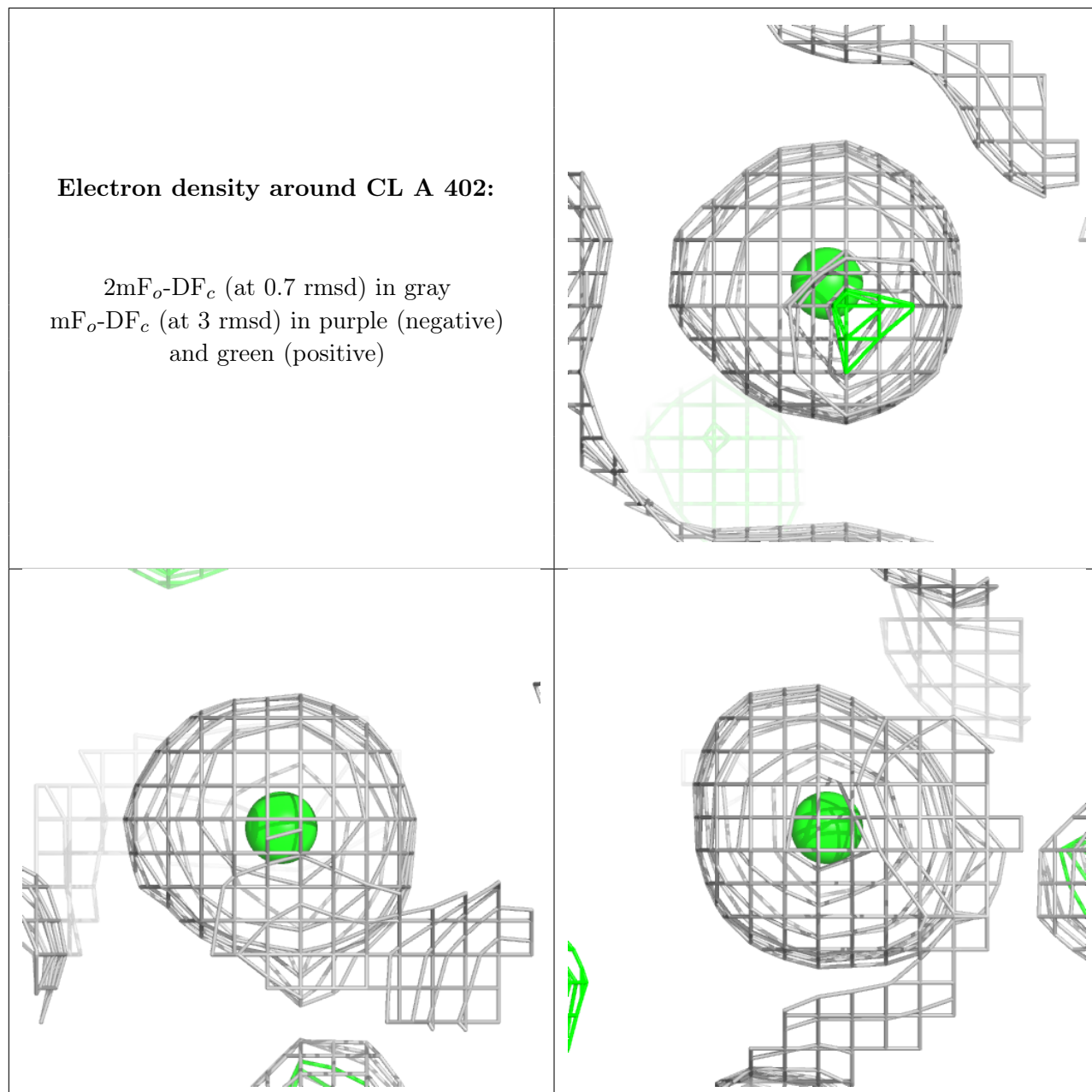
Electron density around CL A 404:

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



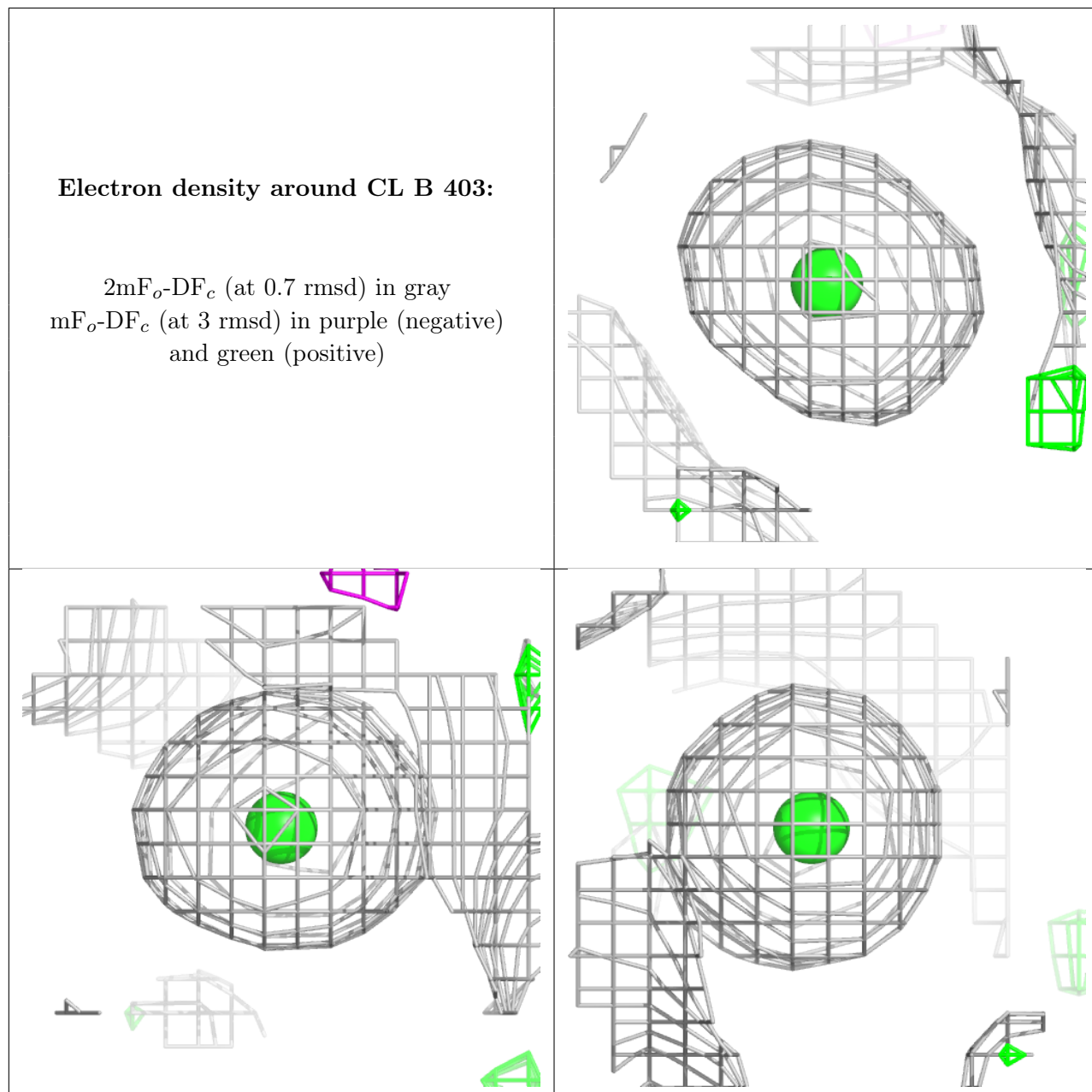
Electron density around CL A 402:

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



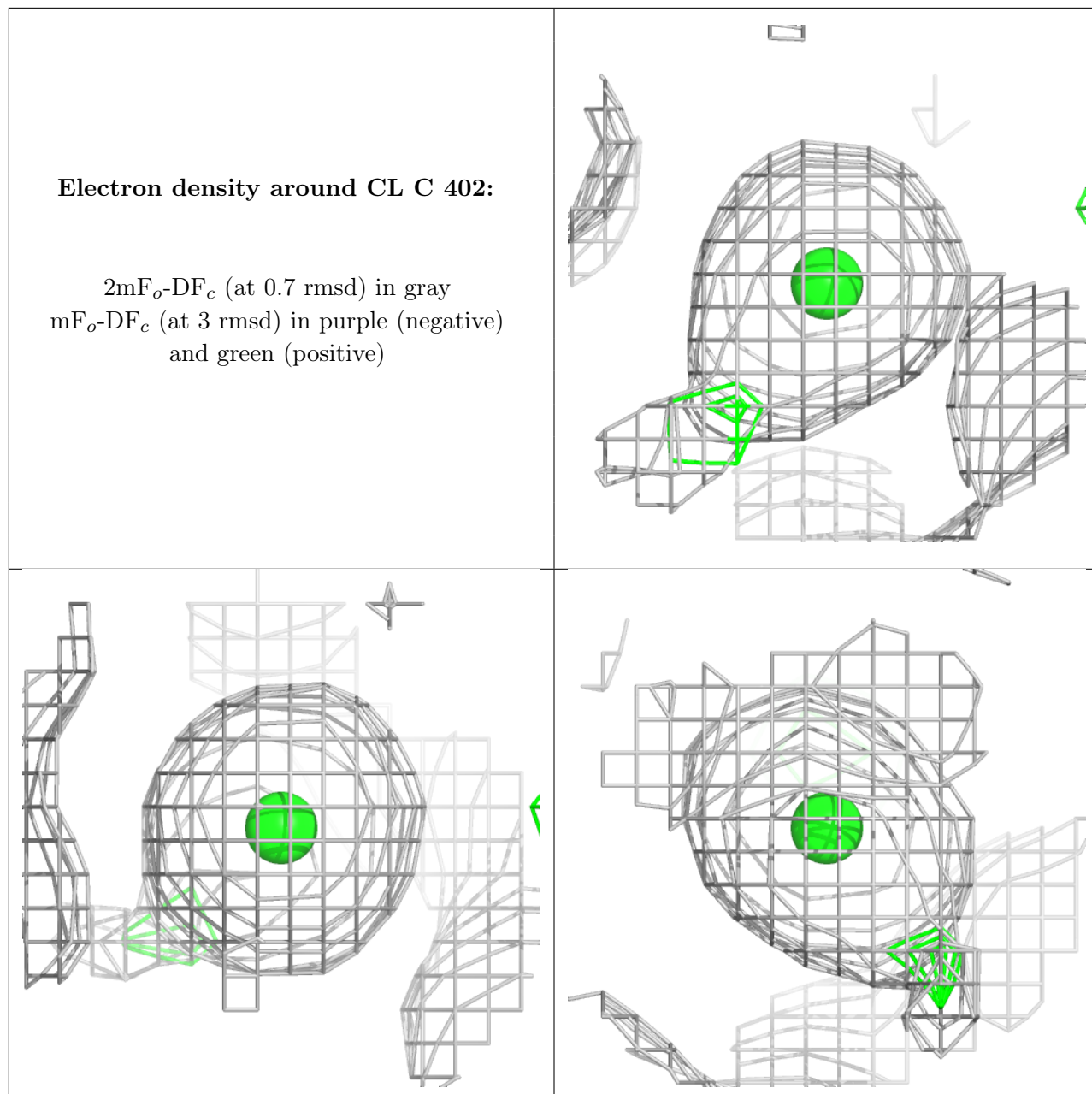
Electron density around CL B 403:

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



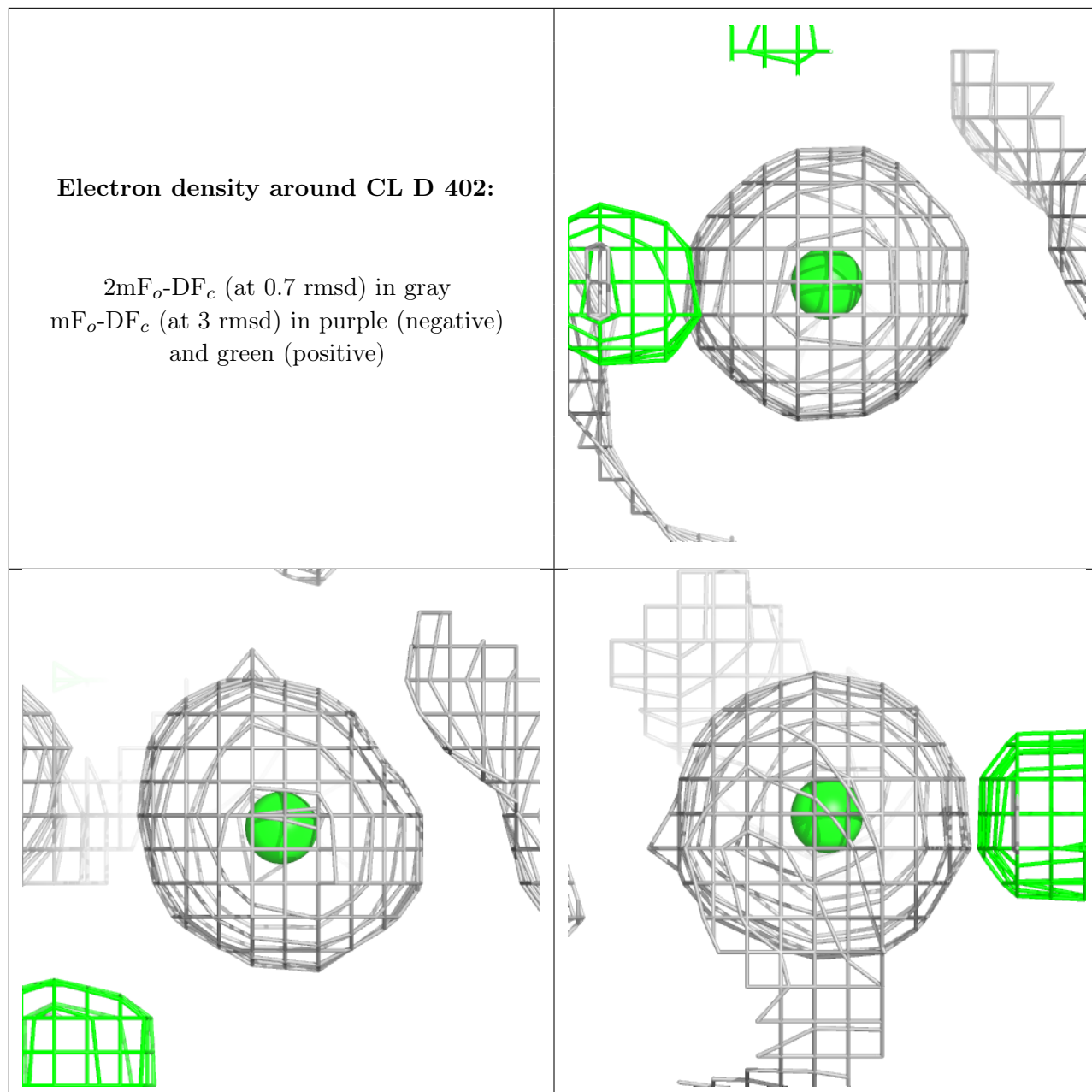
Electron density around CL C 402:

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



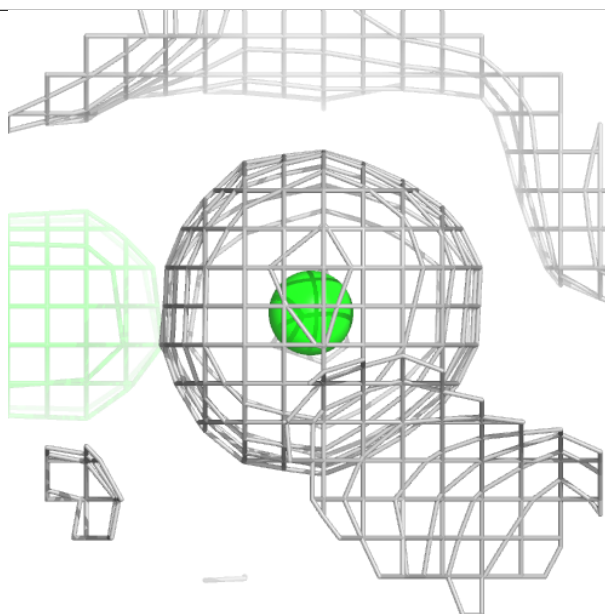
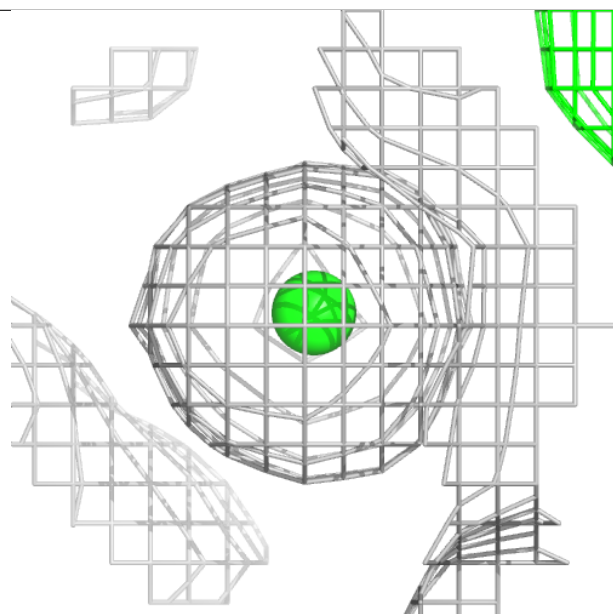
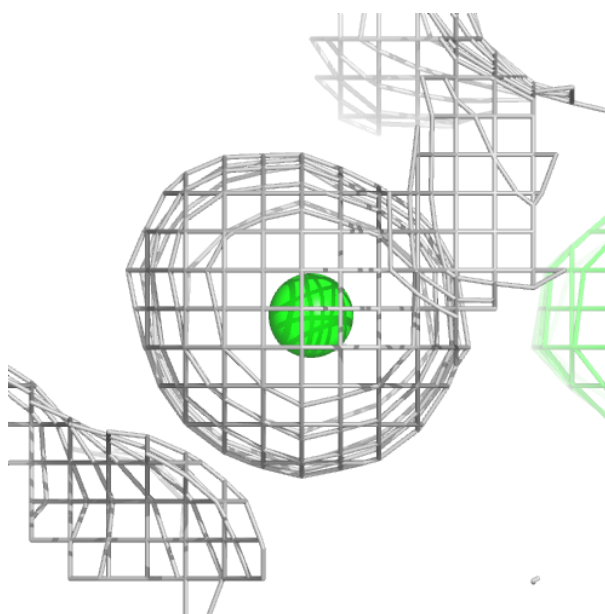
Electron density around CL D 402:

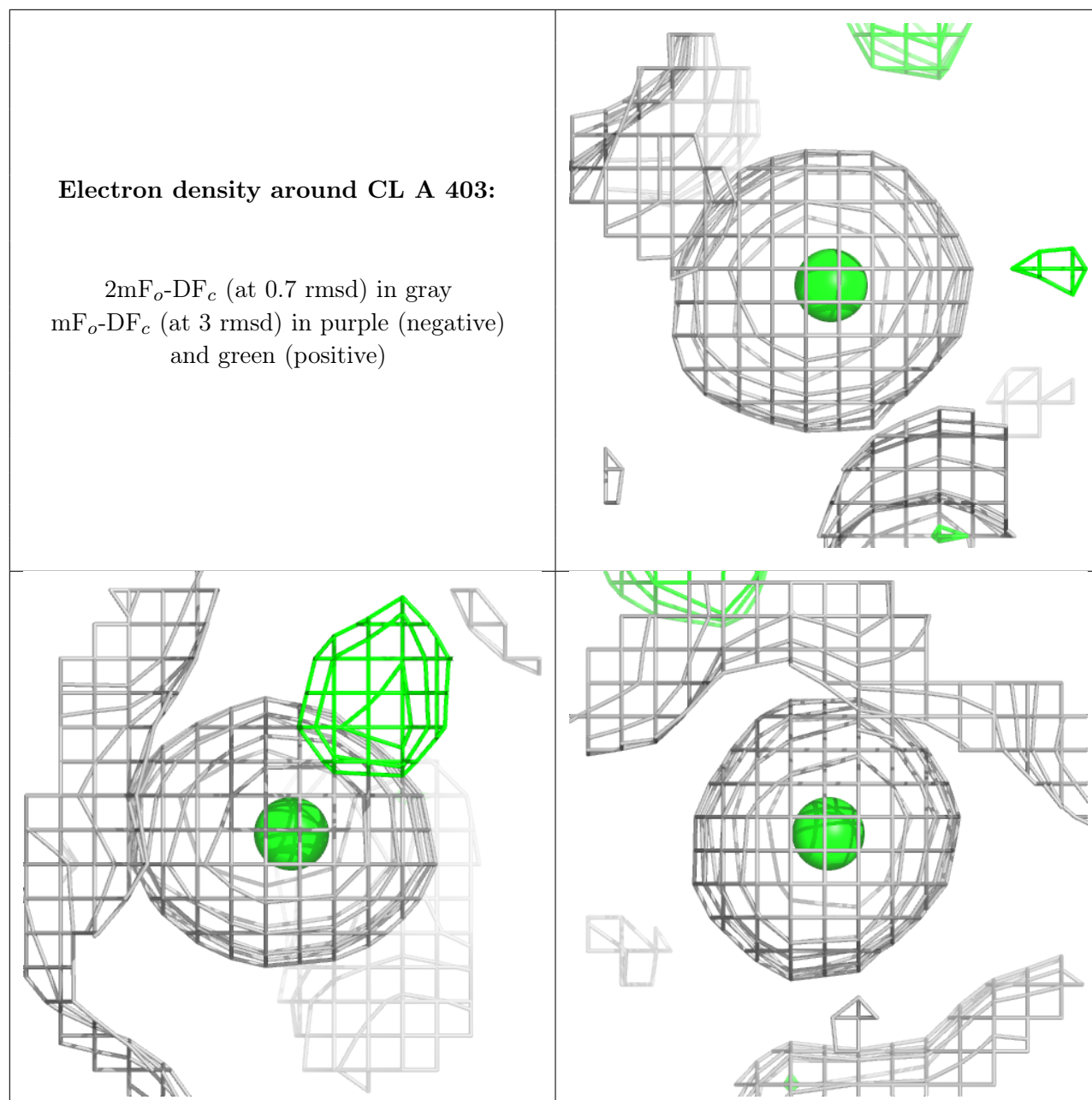
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CL E 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.