



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 10:00 AM EDT

PDB ID : 2FZS / pdb_00002fzs
Title : Crystal structure of E. coli ClpP with a Peptide Chloromethyl Ketone Covalently Bound at the Active Site
Authors : Szyk, A.; Maurizi, M.R.
Deposited on : 2006-02-10
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

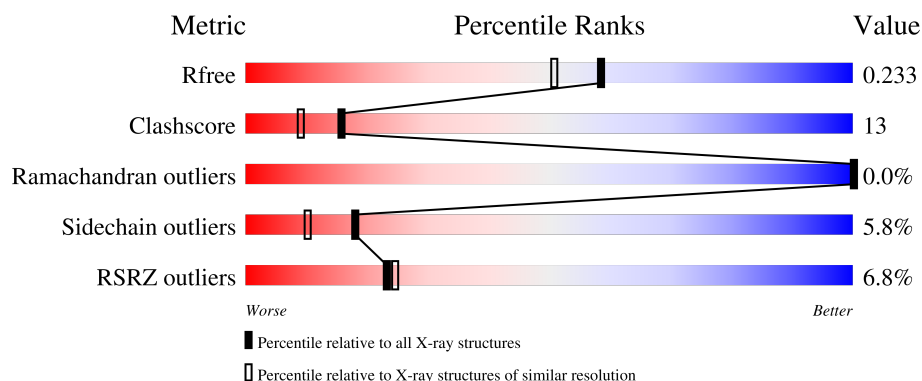
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	193	5% 74% 17% 6% •
1	B	193	14% 77% 19% •
1	C	193	7% 76% 13% 5% •
1	D	193	8% 74% 18% •
1	E	193	12% 76% 20% •

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Mol	Chain	Length	Quality of chain
1	F	193	
1	G	193	
1	H	193	
1	I	193	
1	J	193	
1	K	193	
1	L	193	
1	M	193	
1	N	193	

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
4	GOL	C	3006	-	-	X	-

2 Entry composition

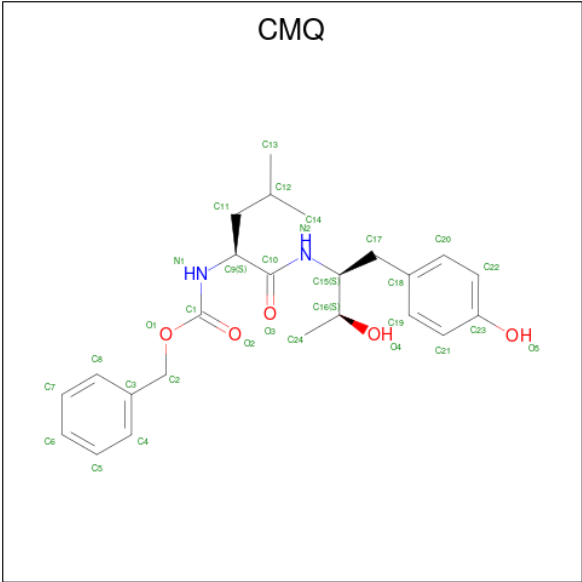
There are 5 unique types of molecules in this entry. The entry contains 24125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

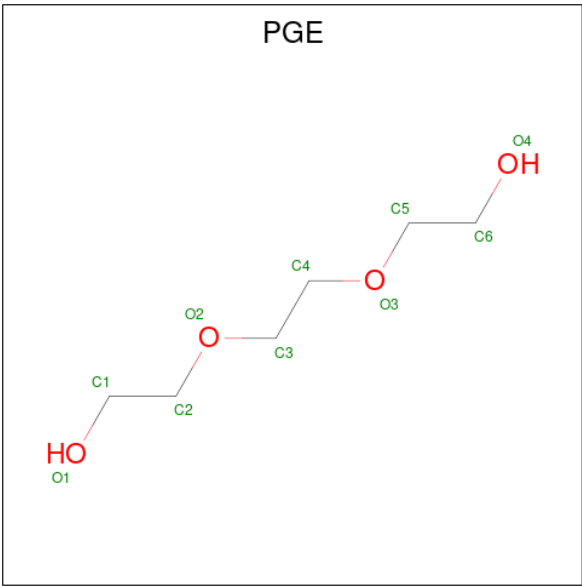
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	7	0
			1487	946	252	274	15			
1	B	192	Total	C	N	O	S	0	10	0
			1554	981	268	290	15			
1	C	183	Total	C	N	O	S	0	7	0
			1467	931	254	270	12			
1	D	185	Total	C	N	O	S	0	3	0
			1462	926	249	275	12			
1	E	188	Total	C	N	O	S	0	2	0
			1479	936	252	278	13			
1	F	185	Total	C	N	O	S	0	2	0
			1453	920	247	274	12			
1	G	183	Total	C	N	O	S	0	4	0
			1448	917	246	271	14			
1	H	183	Total	C	N	O	S	0	2	0
			1439	912	245	270	12			
1	I	183	Total	C	N	O	S	0	7	0
			1461	928	248	270	15			
1	J	185	Total	C	N	O	S	0	2	0
			1456	922	247	274	13			
1	K	186	Total	C	N	O	S	0	1	0
			1462	926	251	273	12			
1	L	183	Total	C	N	O	S	0	11	0
			1478	939	246	278	15			
1	M	186	Total	C	N	O	S	0	11	0
			1505	958	256	276	15			
1	N	183	Total	C	N	O	S	0	10	0
			1469	938	245	271	15			

- Molecule 2 is N 2 -[(BENZYLOXY)CARBONYL]-N-[(1S,2S)-2-HYDROXY-1-(4-HYDROXYBENZYL)PROPYL]-L-LEUCINAMIDE (CCD ID: CMQ) (formula: C₂₄H₃₂N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	24	2	5		
2	B	1	Total	C	N	O	0	0
			31	24	2	5		
2	C	1	Total	C	N	O	0	0
			31	24	2	5		
2	D	1	Total	C	N	O	0	0
			31	24	2	5		
2	E	1	Total	C	N	O	0	0
			31	24	2	5		
2	F	1	Total	C	N	O	0	0
			31	24	2	5		
2	G	1	Total	C	N	O	0	0
			31	24	2	5		
2	H	1	Total	C	N	O	0	0
			31	24	2	5		
2	I	1	Total	C	N	O	0	0
			31	24	2	5		
2	J	1	Total	C	N	O	0	0
			31	24	2	5		
2	K	1	Total	C	N	O	0	0
			31	24	2	5		
2	L	1	Total	C	N	O	0	0
			31	24	2	5		
2	M	1	Total	C	N	O	0	0
			31	24	2	5		
2	N	1	Total	C	N	O	0	0
			31	24	2	5		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	E	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		
3	G	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			10	6	4		
3	I	1	Total	C	O	0	0
			10	6	4		
3	J	1	Total	C	O	0	0
			10	6	4		
3	K	1	Total	C	O	0	0
			10	6	4		
3	K	1	Total	C	O	0	0
			10	6	4		
3	L	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	0
			10	6	4		
3	N	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	K	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			6	3	3		
4	N	1	Total	C	O	0	0
			6	3	3		

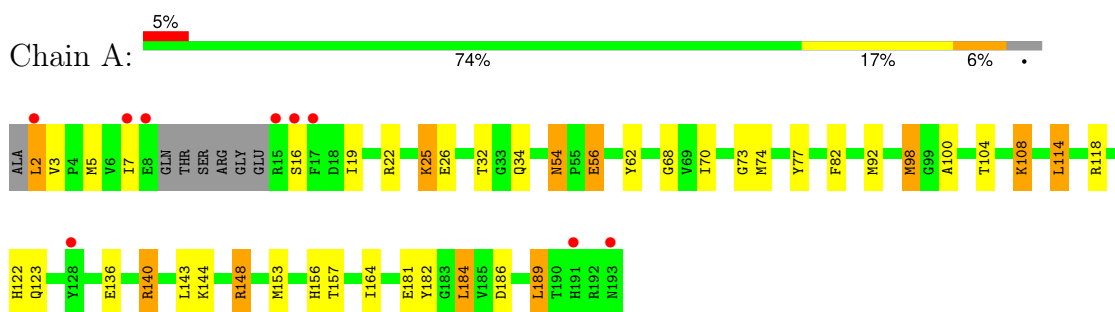
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	234	Total	O		0	0
			234	234			
5	B	188	Total	O		0	0
			188	188			
5	C	189	Total	O		0	0
			189	189			
5	D	165	Total	O		0	0
			165	165			
5	E	199	Total	O		0	0
			199	199			
5	F	218	Total	O		0	0
			218	218			
5	G	232	Total	O		0	0
			232	232			
5	H	176	Total	O		0	0
			176	176			
5	I	171	Total	O		0	0
			171	171			
5	J	176	Total	O		0	0
			176	176			
5	K	192	Total	O		0	0
			192	192			
5	L	247	Total	O		0	0
			247	247			
5	M	251	Total	O		0	0
			251	251			
5	N	217	Total	O		0	0
			217	217			

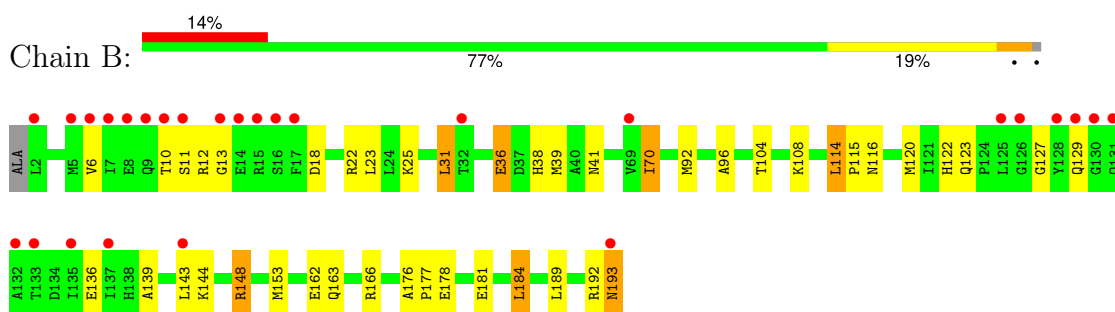
3 Residue-property plots [i](#)

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.

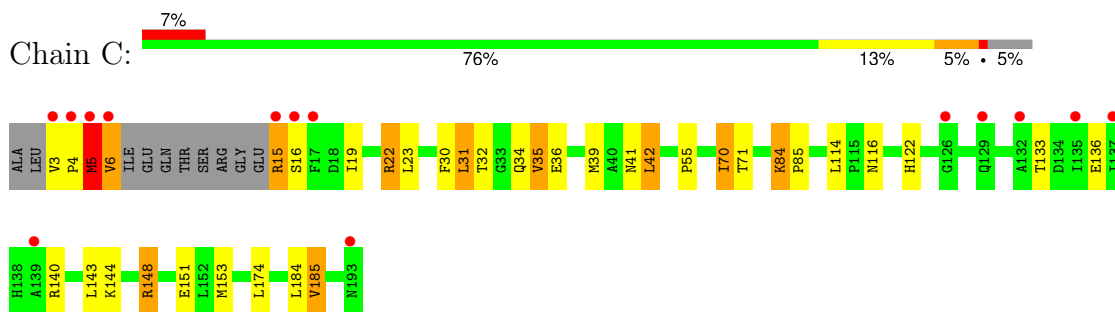
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



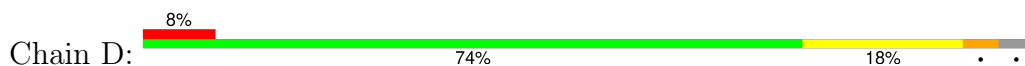
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

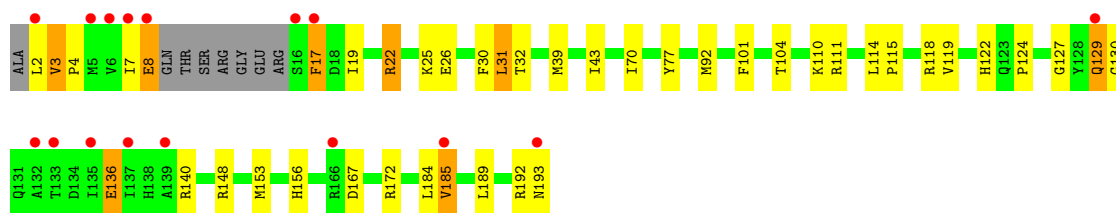


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

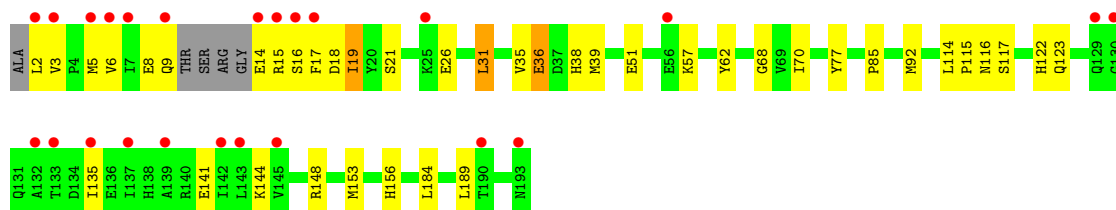
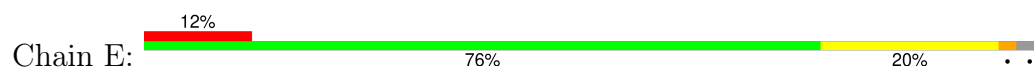


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

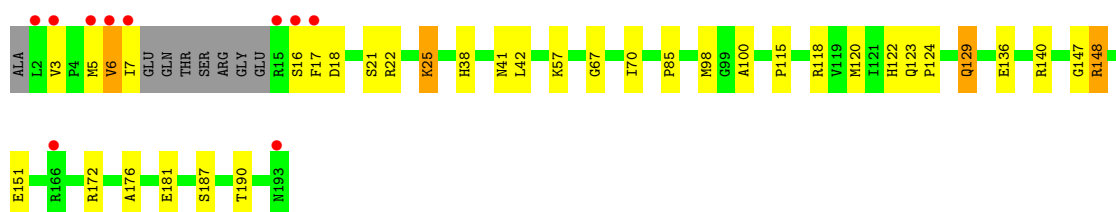
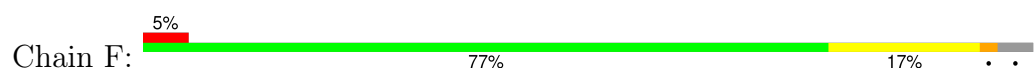




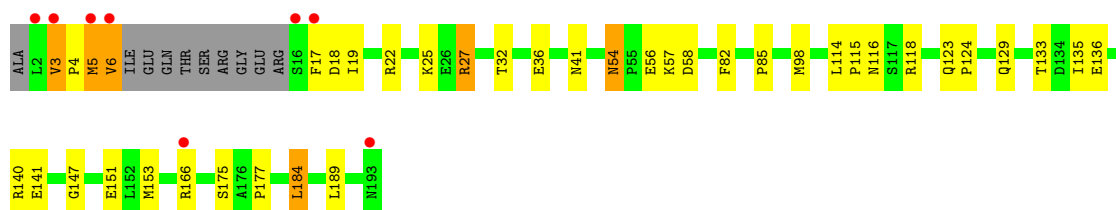
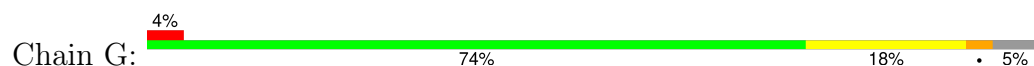
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



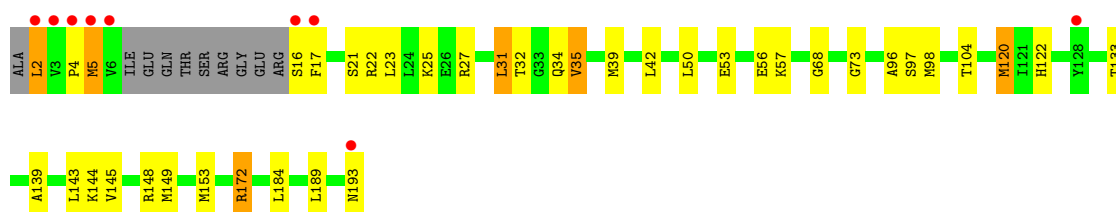
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



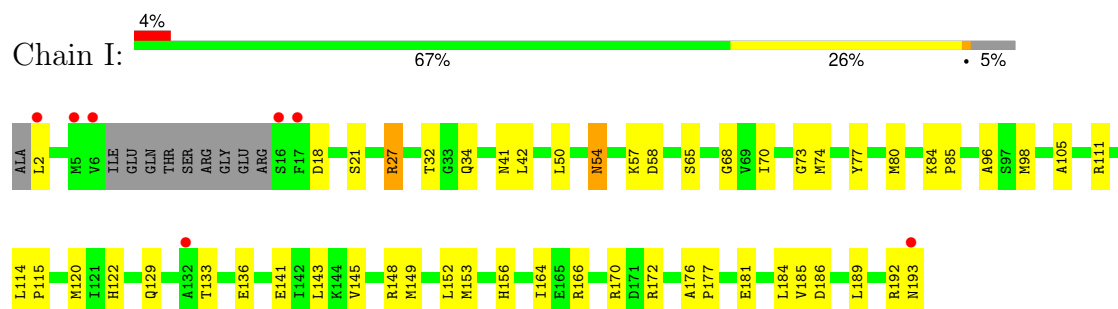
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



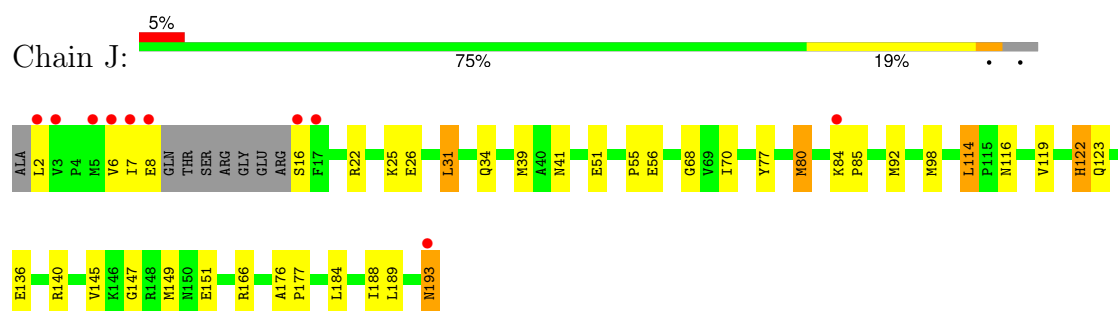
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



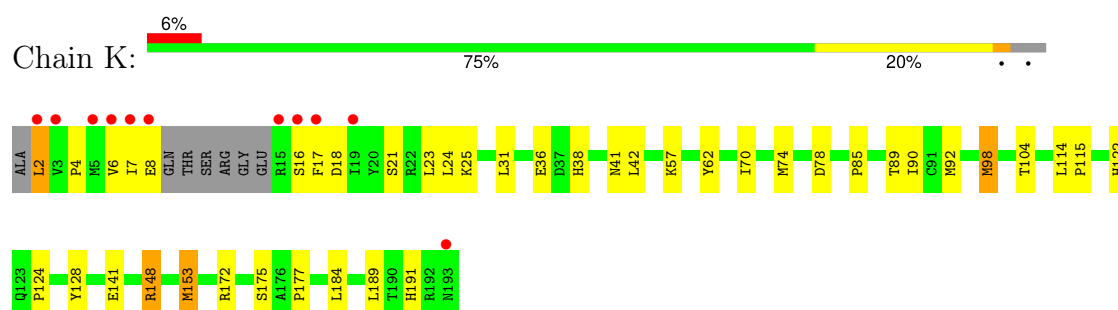
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



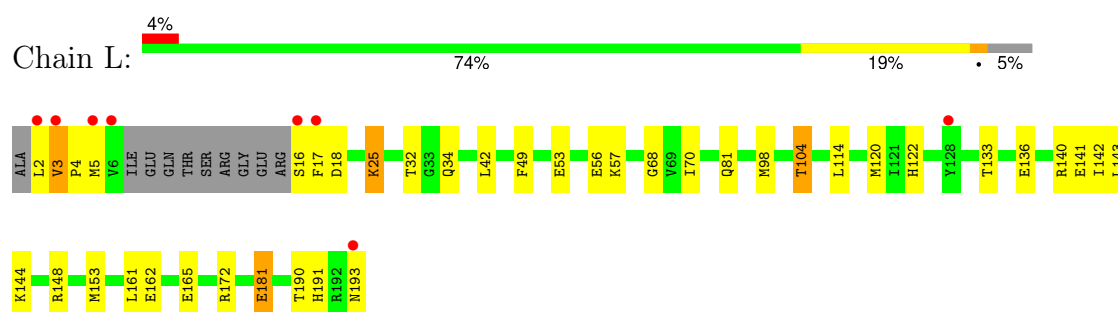
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



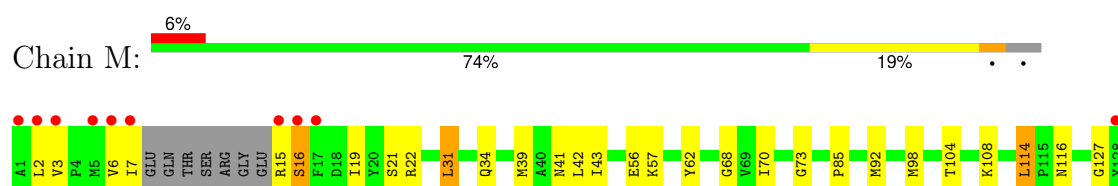
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

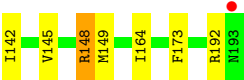
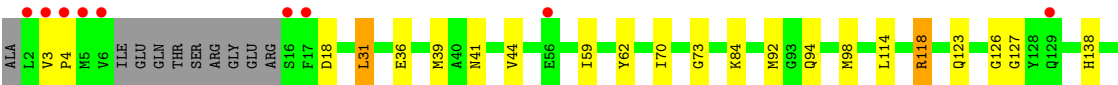
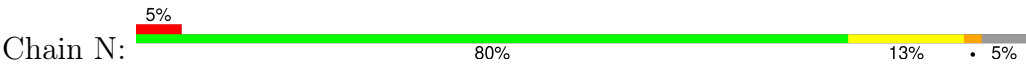


- Molecule 1: ATP-dependent Clp protease proteolytic subunit





● Molecule 1: ATP-dependent Clp protease proteolytic subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	190.70Å 101.00Å 155.40Å 90.00° 99.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90 15.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (15.00-1.90) 93.6 (15.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.173 , 0.233 0.174 , 0.233	Depositor DCC
R_{free} test set	10777 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24125	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: PGE, CMQ, GOL

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	1.09	2/1538 (0.1%)	1.02	0/2069
1	B	0.99	0/1618	1.04	2/2175 (0.1%)
1	C	1.01	0/1518	1.09	4/2043 (0.2%)
1	D	0.98	3/1497 (0.2%)	1.04	1/2016 (0.0%)
1	E	1.09	0/1510	1.03	1/2032 (0.0%)
1	F	1.28	3/1484 (0.2%)	1.15	4/1999 (0.2%)
1	G	1.21	2/1487 (0.1%)	1.22	7/2001 (0.3%)
1	H	1.01	0/1470	1.06	2/1980 (0.1%)
1	I	0.91	0/1512	1.04	5/2034 (0.2%)
1	J	0.92	0/1487	1.02	0/2002
1	K	1.03	0/1489	1.06	1/2006 (0.0%)
1	L	1.13	0/1545	1.02	0/2079
1	M	1.17	1/1572 (0.1%)	1.08	1/2113 (0.0%)
1	N	1.06	2/1532 (0.1%)	1.02	2/2063 (0.1%)
All	All	1.07	13/21259 (0.1%)	1.06	30/28612 (0.1%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	176	ALA	CA-CB	7.75	1.63	1.53
1	G	27	ARG	CD-NE	-6.74	1.36	1.46
1	D	19	ILE	CA-CB	5.88	1.60	1.54
1	F	67	GLY	C-O	-5.63	1.20	1.24
1	A	100	ALA	C-O	5.60	1.30	1.24

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	27	ARG	NE-CZ-NH2	-14.72	105.95	119.20
1	G	27	ARG	CD-NE-CZ	9.54	137.75	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	27	ARG	NE-CZ-NH1	8.83	130.33	121.50
1	G	27	ARG	CG-CD-NE	-8.38	93.56	112.00
1	G	3	VAL	CA-C-N	8.22	128.73	119.93

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	1487	0	1509	65	0
1	B	1554	0	1567	57	0
1	C	1467	0	1487	45	0
1	D	1462	0	1471	51	0
1	E	1479	0	1486	43	0
1	F	1453	0	1456	21	0
1	G	1448	0	1455	40	0
1	H	1439	0	1448	43	0
1	I	1461	0	1477	51	0
1	J	1456	0	1463	39	0
1	K	1462	0	1476	47	0
1	L	1478	0	1483	47	0
1	M	1505	0	1533	44	0
1	N	1469	0	1492	26	0
2	A	31	0	31	9	0
2	B	31	0	30	7	0
2	C	31	0	30	6	0
2	D	31	0	31	8	0
2	E	31	0	31	8	0
2	F	31	0	28	1	0
2	G	31	0	29	1	0
2	H	31	0	31	6	0
2	I	31	0	31	7	0
2	J	31	0	31	8	0
2	K	31	0	31	9	0
2	L	31	0	29	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	31	0	29	1	0
2	N	31	0	29	2	0
3	A	10	0	14	1	0
3	B	10	0	14	2	0
3	C	10	0	14	0	0
3	D	10	0	14	0	0
3	E	10	0	14	0	0
3	F	10	0	14	1	0
3	G	10	0	14	0	0
3	H	10	0	14	0	0
3	I	10	0	14	0	0
3	J	10	0	14	1	0
3	K	20	0	28	2	0
3	L	10	0	14	0	0
3	M	10	0	14	1	0
3	N	10	0	14	2	0
4	A	6	0	8	2	0
4	B	12	0	16	0	0
4	C	12	0	16	6	0
4	F	6	0	8	2	0
4	G	6	0	8	1	0
4	H	6	0	8	2	0
4	K	6	0	8	1	0
4	L	6	0	8	0	0
4	N	6	0	8	3	0
5	A	234	0	0	13	0
5	B	188	0	0	6	0
5	C	189	0	0	8	0
5	D	165	0	0	5	0
5	E	199	0	0	10	0
5	F	218	0	0	7	0
5	G	232	0	0	8	0
5	H	176	0	0	5	0
5	I	171	0	0	5	0
5	J	176	0	0	6	0
5	K	192	0	0	8	0
5	L	247	0	0	12	0
5	M	251	0	0	5	0
5	N	217	0	0	6	0
All	All	24125	0	21522	563	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 13.

The worst 5 of 563 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:122:HIS:NE2	2:D:504:CMQ:H242	1.14	1.45
1:I:122:HIS:NE2	2:I:509:CMQ:H242	1.24	1.45
1:B:122:HIS:NE2	2:B:502:CMQ:H242	1.20	1.43
1:H:122:HIS:NE2	2:H:508:CMQ:H242	1.14	1.43
1:A:122:HIS:NE2	2:A:501:CMQ:H242	1.20	1.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	189/193 (98%)	184 (97%)	5 (3%)	0	100	100
1	B	200/193 (104%)	195 (98%)	5 (2%)	0	100	100
1	C	186/193 (96%)	182 (98%)	4 (2%)	0	100	100
1	D	184/193 (95%)	180 (98%)	3 (2%)	1 (0%)	24	16
1	E	186/193 (96%)	180 (97%)	6 (3%)	0	100	100
1	F	183/193 (95%)	180 (98%)	3 (2%)	0	100	100
1	G	183/193 (95%)	179 (98%)	4 (2%)	0	100	100
1	H	181/193 (94%)	178 (98%)	3 (2%)	0	100	100
1	I	186/193 (96%)	183 (98%)	3 (2%)	0	100	100
1	J	183/193 (95%)	179 (98%)	4 (2%)	0	100	100
1	K	183/193 (95%)	178 (97%)	5 (3%)	0	100	100
1	L	190/193 (98%)	187 (98%)	3 (2%)	0	100	100
1	M	193/193 (100%)	188 (97%)	5 (3%)	0	100	100
1	N	189/193 (98%)	186 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2616/2702 (97%)	2559 (98%)	56 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	17	PHE

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	165/163 (101%)	151 (92%)	14 (8%)	10	4
1	B	173/163 (106%)	160 (92%)	13 (8%)	12	6
1	C	162/163 (99%)	147 (91%)	15 (9%)	8	3
1	D	160/163 (98%)	149 (93%)	11 (7%)	14	7
1	E	161/163 (99%)	153 (95%)	8 (5%)	22	14
1	F	158/163 (97%)	148 (94%)	10 (6%)	16	8
1	G	159/163 (98%)	151 (95%)	8 (5%)	22	14
1	H	157/163 (96%)	146 (93%)	11 (7%)	14	7
1	I	162/163 (99%)	155 (96%)	7 (4%)	26	18
1	J	159/163 (98%)	149 (94%)	10 (6%)	16	8
1	K	159/163 (98%)	151 (95%)	8 (5%)	22	14
1	L	166/163 (102%)	156 (94%)	10 (6%)	17	9
1	M	168/163 (103%)	157 (94%)	11 (6%)	15	8
1	N	165/163 (101%)	156 (94%)	9 (6%)	19	11
All	All	2274/2282 (100%)	2129 (94%)	145 (6%)	18	8

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL

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Mol	Chain	Res	Type
1	N	114[B]	LEU
1	L	104[B]	THR
1	M	108[A]	LYS
1	D	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	163	GLN
1	N	41	ASN
1	H	159	GLN
1	N	34	GLN
1	L	193	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

40 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CMQ	H	508	1	31,32,32	1.21	1 (3%)	40,42,42	1.71	9 (22%)
3	PGE	D	4004	-	9,9,9	0.48	0	8,8,8	0.34	0
3	PGE	K	4011	-	9,9,9	0.52	0	8,8,8	0.45	0
3	PGE	B	4002	-	9,9,9	0.51	0	8,8,8	0.18	0
3	PGE	A	4001	-	9,9,9	0.51	0	8,8,8	0.29	0
4	GOL	G	3009	-	5,5,5	0.51	0	5,5,5	0.38	0
2	CMQ	G	507	1	31,32,32	1.43	3 (9%)	40,42,42	1.40	7 (17%)
4	GOL	N	3007	-	5,5,5	0.31	0	5,5,5	0.79	0
4	GOL	A	3001	-	5,5,5	0.30	0	5,5,5	0.52	0
4	GOL	H	3008	-	5,5,5	0.38	0	5,5,5	0.95	0
3	PGE	F	4006	-	9,9,9	0.38	0	8,8,8	0.51	0
2	CMQ	J	510	1	31,32,32	1.22	1 (3%)	40,42,42	1.59	7 (17%)
2	CMQ	B	502	1	31,32,32	1.12	1 (3%)	40,42,42	1.51	4 (10%)
2	CMQ	C	503	1	31,32,32	1.25	2 (6%)	40,42,42	1.48	6 (15%)
3	PGE	G	4007	-	9,9,9	0.50	0	8,8,8	0.48	0
2	CMQ	A	501	1	31,32,32	1.26	2 (6%)	40,42,42	1.69	9 (22%)
3	PGE	L	4012	-	9,9,9	0.59	0	8,8,8	0.31	0
4	GOL	B	3003	-	5,5,5	0.44	0	5,5,5	0.37	0
2	CMQ	E	505	1	31,32,32	1.34	2 (6%)	40,42,42	1.82	12 (30%)
2	CMQ	N	514	1	31,32,32	1.24	1 (3%)	40,42,42	1.19	4 (10%)
2	CMQ	M	513	1	31,32,32	1.20	2 (6%)	40,42,42	1.33	3 (7%)
2	CMQ	D	504	1	31,32,32	1.21	1 (3%)	40,42,42	1.57	7 (17%)
2	CMQ	L	512	1	31,32,32	1.24	2 (6%)	40,42,42	1.43	6 (15%)
4	GOL	K	3010	-	5,5,5	0.34	0	5,5,5	0.86	0
4	GOL	C	3006	-	5,5,5	0.35	0	5,5,5	0.59	0
3	PGE	J	4010	-	9,9,9	0.61	0	8,8,8	0.48	0
4	GOL	F	3004	-	5,5,5	0.61	0	5,5,5	0.76	0
4	GOL	B	3002	-	5,5,5	0.23	0	5,5,5	0.67	0
3	PGE	I	4009	-	9,9,9	0.45	0	8,8,8	0.45	0
3	PGE	E	4005	-	9,9,9	0.49	0	8,8,8	0.36	0
2	CMQ	F	506	1	31,32,32	1.16	1 (3%)	40,42,42	1.43	7 (17%)
3	PGE	C	4003	-	9,9,9	0.51	0	8,8,8	0.31	0
3	PGE	N	4014	-	9,9,9	0.44	0	8,8,8	0.45	0
4	GOL	C	3005	-	5,5,5	0.28	0	5,5,5	0.67	0
3	PGE	H	4008	-	9,9,9	0.43	0	8,8,8	0.53	0
2	CMQ	K	511	1	31,32,32	1.15	1 (3%)	40,42,42	1.34	6 (15%)
3	PGE	K	4015	-	9,9,9	0.23	0	8,8,8	0.89	0
4	GOL	L	3011	-	5,5,5	0.46	0	5,5,5	0.69	0
3	PGE	M	4013	-	9,9,9	0.43	0	8,8,8	0.50	0
2	CMQ	I	509	1	31,32,32	1.21	1 (3%)	40,42,42	1.79	9 (22%)

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	CMQ	H	508	1	-	9/29/29/29	0/2/2/2
3	PGE	D	4004	-	-	5/7/7/7	-
3	PGE	K	4011	-	-	5/7/7/7	-
3	PGE	B	4002	-	-	3/7/7/7	-
3	PGE	A	4001	-	-	3/7/7/7	-
4	GOL	G	3009	-	-	2/4/4/4	-
2	CMQ	G	507	1	-	5/29/29/29	0/2/2/2
4	GOL	N	3007	-	-	4/4/4/4	-
4	GOL	A	3001	-	-	2/4/4/4	-
4	GOL	H	3008	-	-	0/4/4/4	-
3	PGE	F	4006	-	-	6/7/7/7	-
2	CMQ	J	510	1	-	9/29/29/29	0/2/2/2
2	CMQ	B	502	1	-	6/29/29/29	0/2/2/2
2	CMQ	C	503	1	-	6/29/29/29	0/2/2/2
3	PGE	G	4007	-	-	5/7/7/7	-
2	CMQ	A	501	1	-	4/29/29/29	0/2/2/2
3	PGE	L	4012	-	-	4/7/7/7	-
4	GOL	B	3003	-	-	2/4/4/4	-
2	CMQ	E	505	1	-	10/29/29/29	0/2/2/2
2	CMQ	N	514	1	-	9/29/29/29	0/2/2/2
2	CMQ	M	513	1	-	7/29/29/29	0/2/2/2
2	CMQ	D	504	1	-	8/29/29/29	0/2/2/2
2	CMQ	L	512	1	-	8/29/29/29	0/2/2/2
4	GOL	K	3010	-	-	3/4/4/4	-
4	GOL	C	3006	-	-	2/4/4/4	-
3	PGE	J	4010	-	-	0/7/7/7	-
4	GOL	F	3004	-	-	2/4/4/4	-
4	GOL	B	3002	-	-	1/4/4/4	-
3	PGE	I	4009	-	-	3/7/7/7	-
3	PGE	E	4005	-	-	4/7/7/7	-
2	CMQ	F	506	1	-	4/29/29/29	0/2/2/2
3	PGE	C	4003	-	-	6/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	N	4014	-	-	3/7/7/7	-
4	GOL	C	3005	-	-	4/4/4/4	-
3	PGE	H	4008	-	-	3/7/7/7	-
2	CMQ	K	511	1	-	7/29/29/29	0/2/2/2
3	PGE	K	4015	-	-	6/7/7/7	-
4	GOL	L	3011	-	-	2/4/4/4	-
3	PGE	M	4013	-	-	3/7/7/7	-
2	CMQ	I	509	1	-	5/29/29/29	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	507	CMQ	O1-C1	5.95	1.47	1.35
2	C	503	CMQ	O1-C1	5.70	1.46	1.35
2	D	504	CMQ	O1-C1	5.57	1.46	1.35
2	J	510	CMQ	O1-C1	5.34	1.45	1.35
2	H	508	CMQ	O1-C1	5.18	1.45	1.35

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	505	CMQ	C16-C15-N2	-5.67	100.61	110.90
2	I	509	CMQ	O1-C1-O2	-5.43	113.85	124.26
2	A	501	CMQ	C16-C15-N2	-5.39	101.12	110.90
2	B	502	CMQ	C16-C15-N2	-5.36	101.17	110.90
2	I	509	CMQ	C16-C15-N2	-5.34	101.20	110.90

There are no chirality outliers.

5 of 180 torsion outliers are listed below:

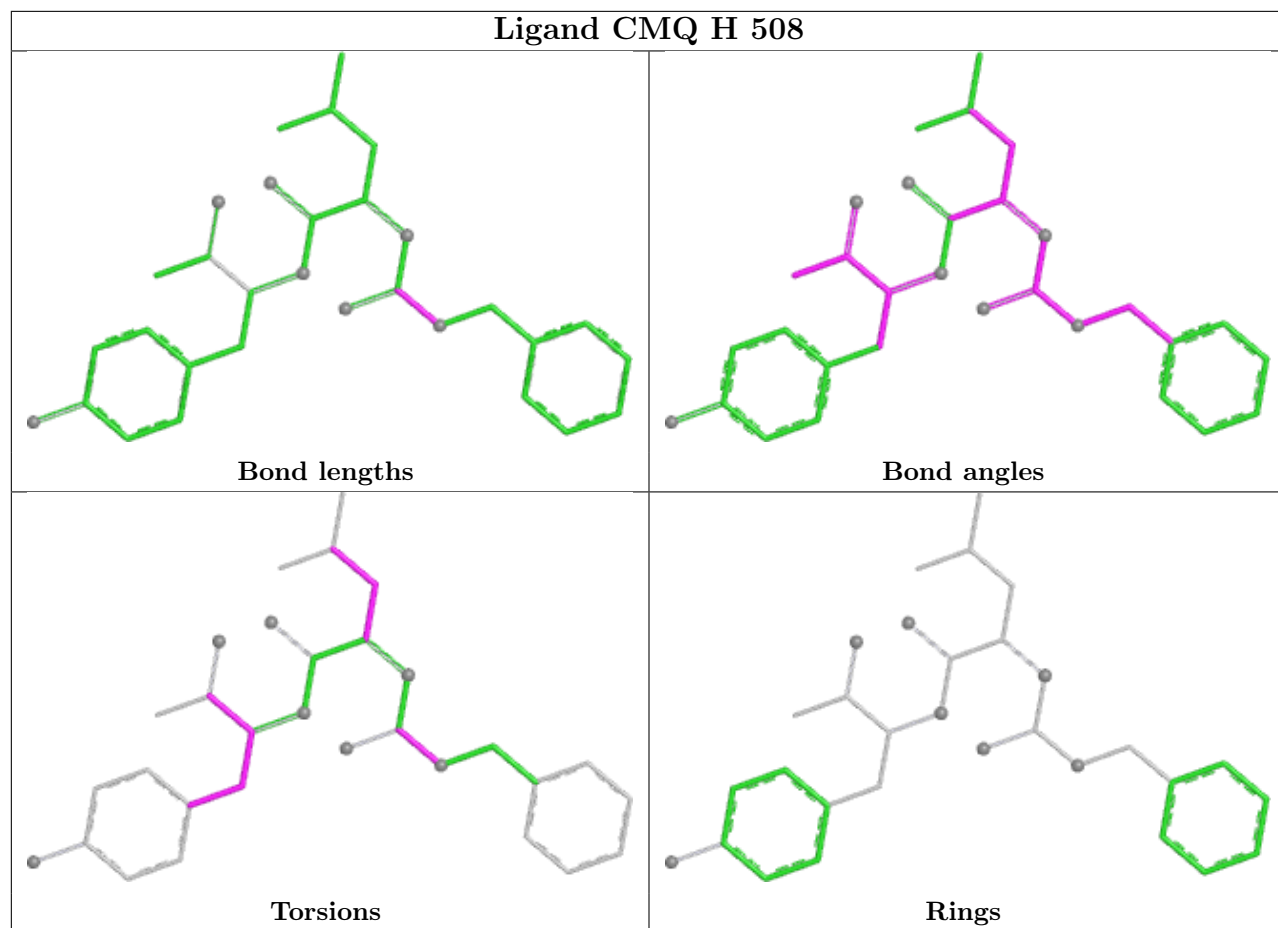
Mol	Chain	Res	Type	Atoms
2	A	501	CMQ	N2-C15-C17-C18
2	A	501	CMQ	C16-C15-C17-C18
2	B	502	CMQ	N2-C15-C17-C18
2	B	502	CMQ	C16-C15-C17-C18
2	C	503	CMQ	N2-C15-C17-C18

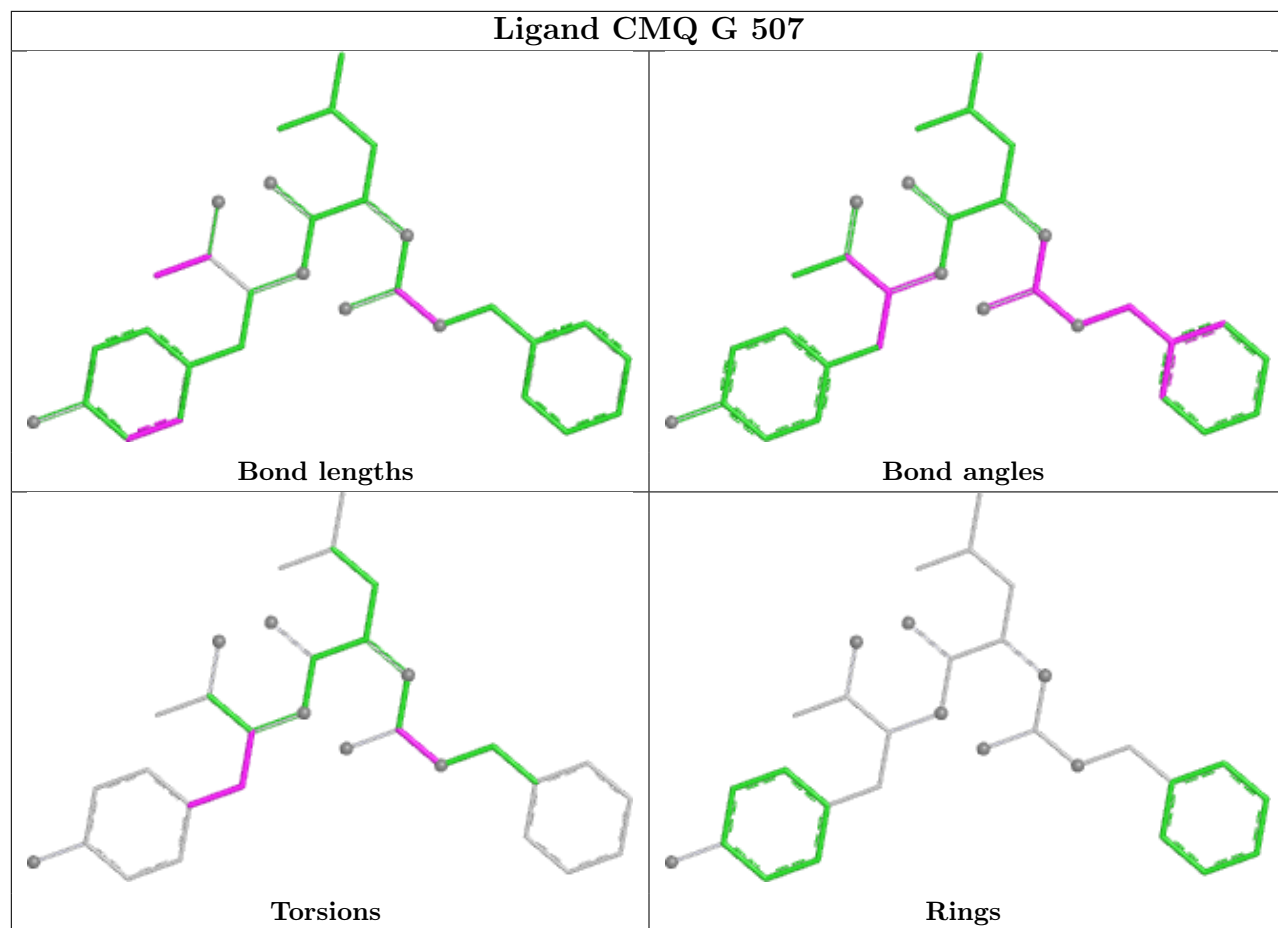
There are no ring outliers.

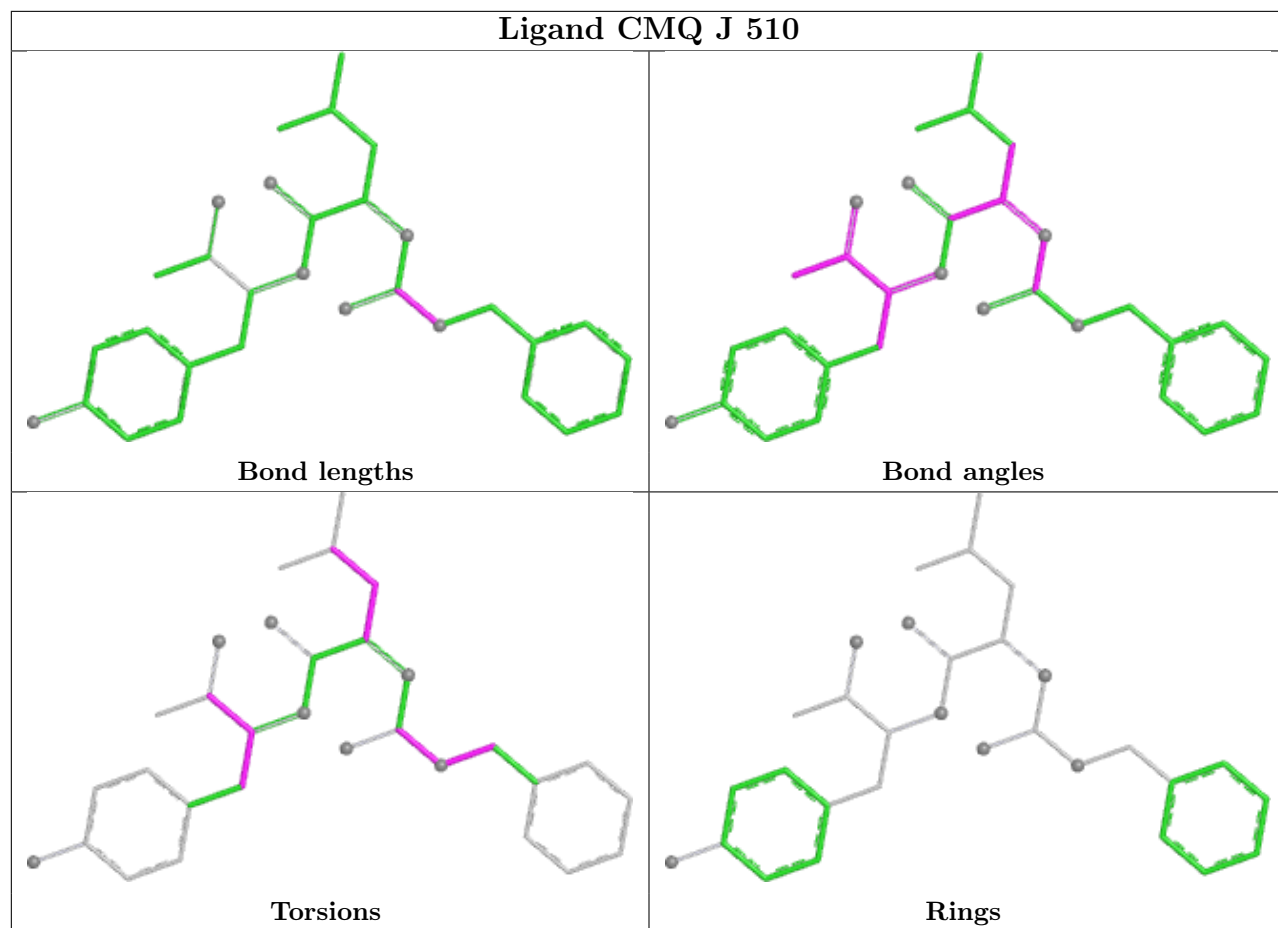
28 monomers are involved in 107 short contacts:

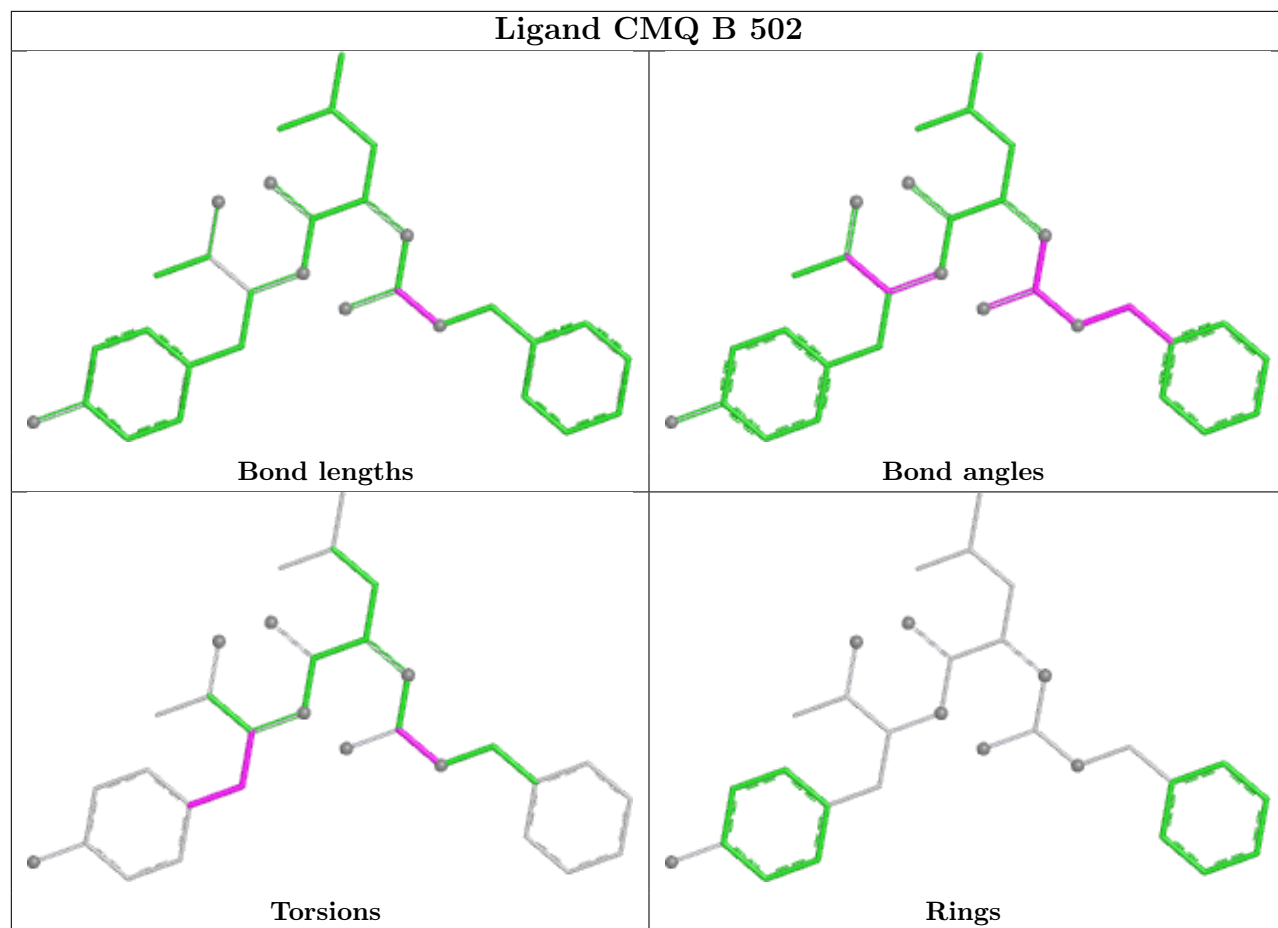
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	508	CMQ	6	0
3	B	4002	PGE	2	0
3	A	4001	PGE	1	0
4	G	3009	GOL	1	0
2	G	507	CMQ	1	0
4	N	3007	GOL	3	0
4	A	3001	GOL	2	0
4	H	3008	GOL	2	0
3	F	4006	PGE	1	0
2	J	510	CMQ	8	0
2	B	502	CMQ	7	0
2	C	503	CMQ	6	0
2	A	501	CMQ	9	0
2	E	505	CMQ	8	0
2	N	514	CMQ	2	0
2	M	513	CMQ	1	0
2	D	504	CMQ	8	0
2	L	512	CMQ	7	0
4	K	3010	GOL	1	0
4	C	3006	GOL	6	0
3	J	4010	PGE	1	0
4	F	3004	GOL	2	0
2	F	506	CMQ	1	0
3	N	4014	PGE	2	0
2	K	511	CMQ	9	0
3	K	4015	PGE	2	0
3	M	4013	PGE	1	0
2	I	509	CMQ	7	0

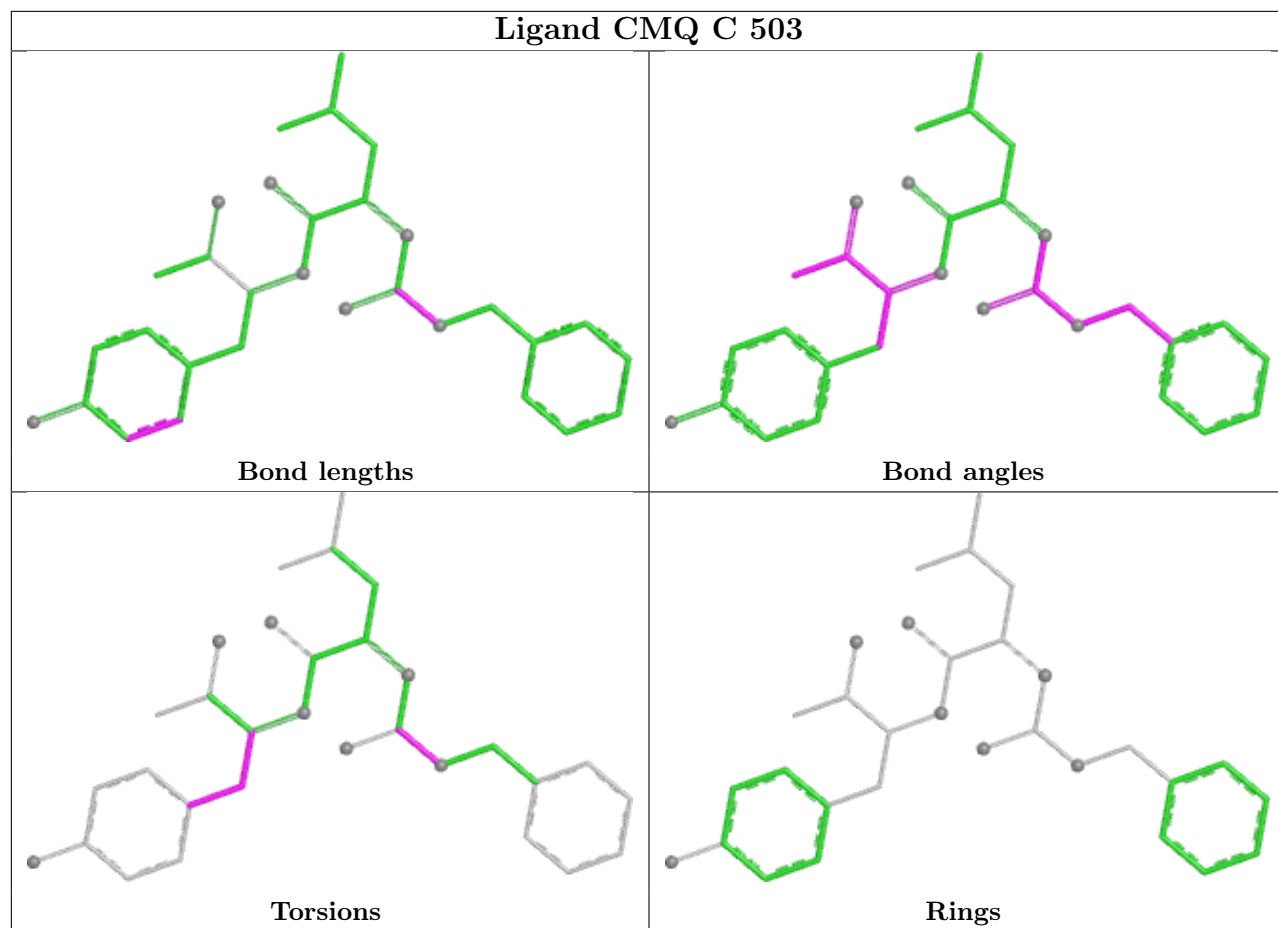
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

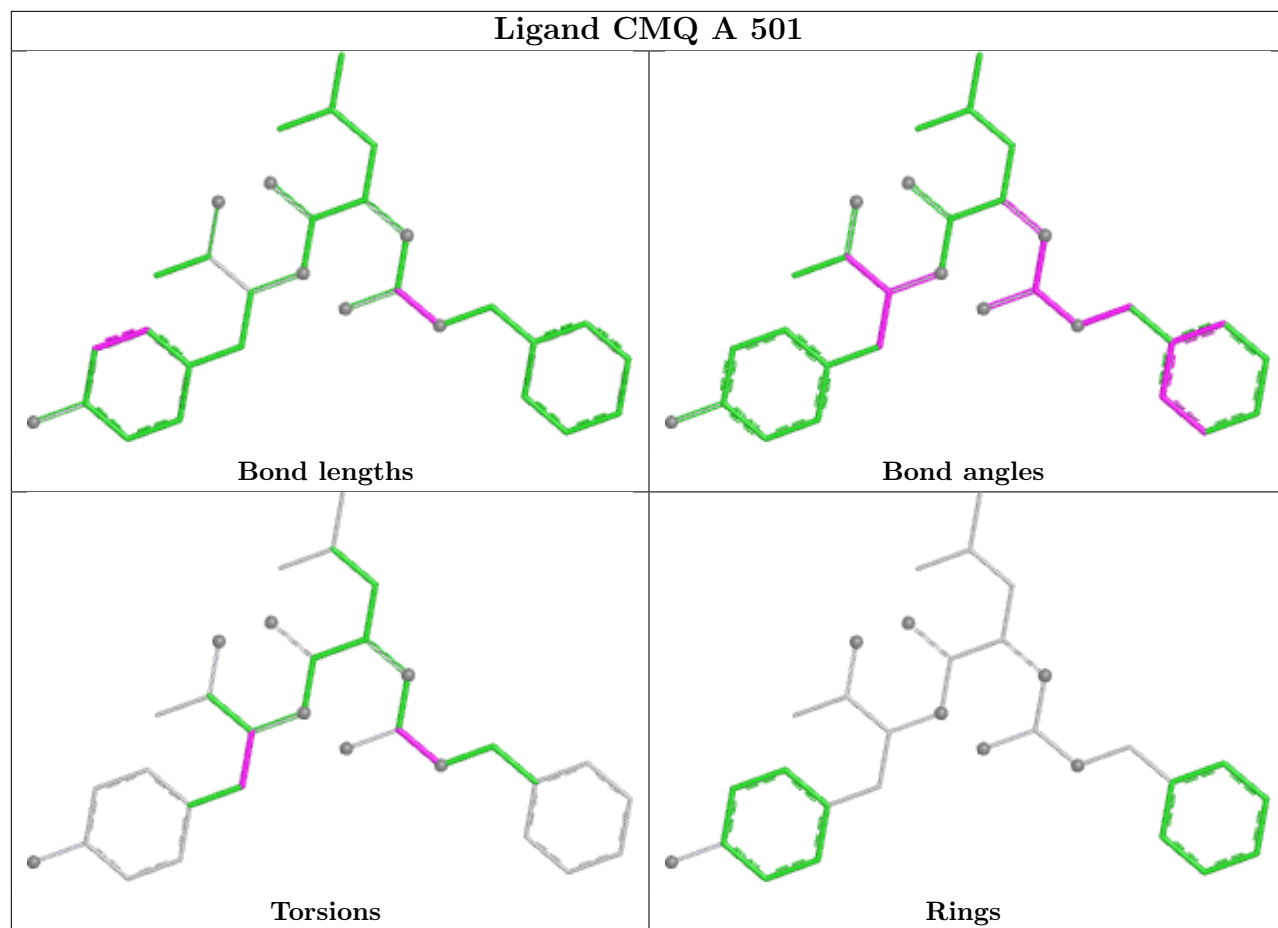


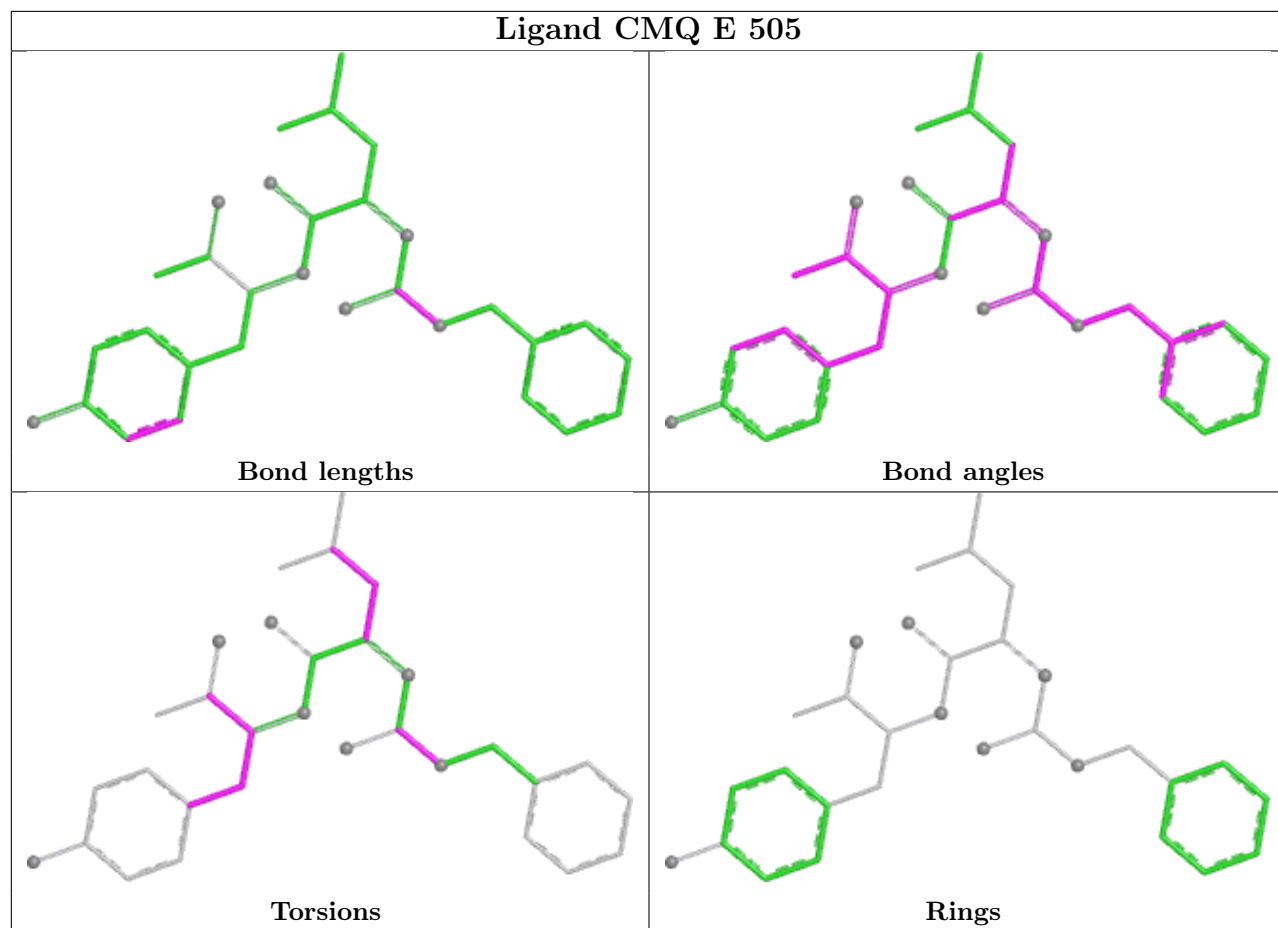


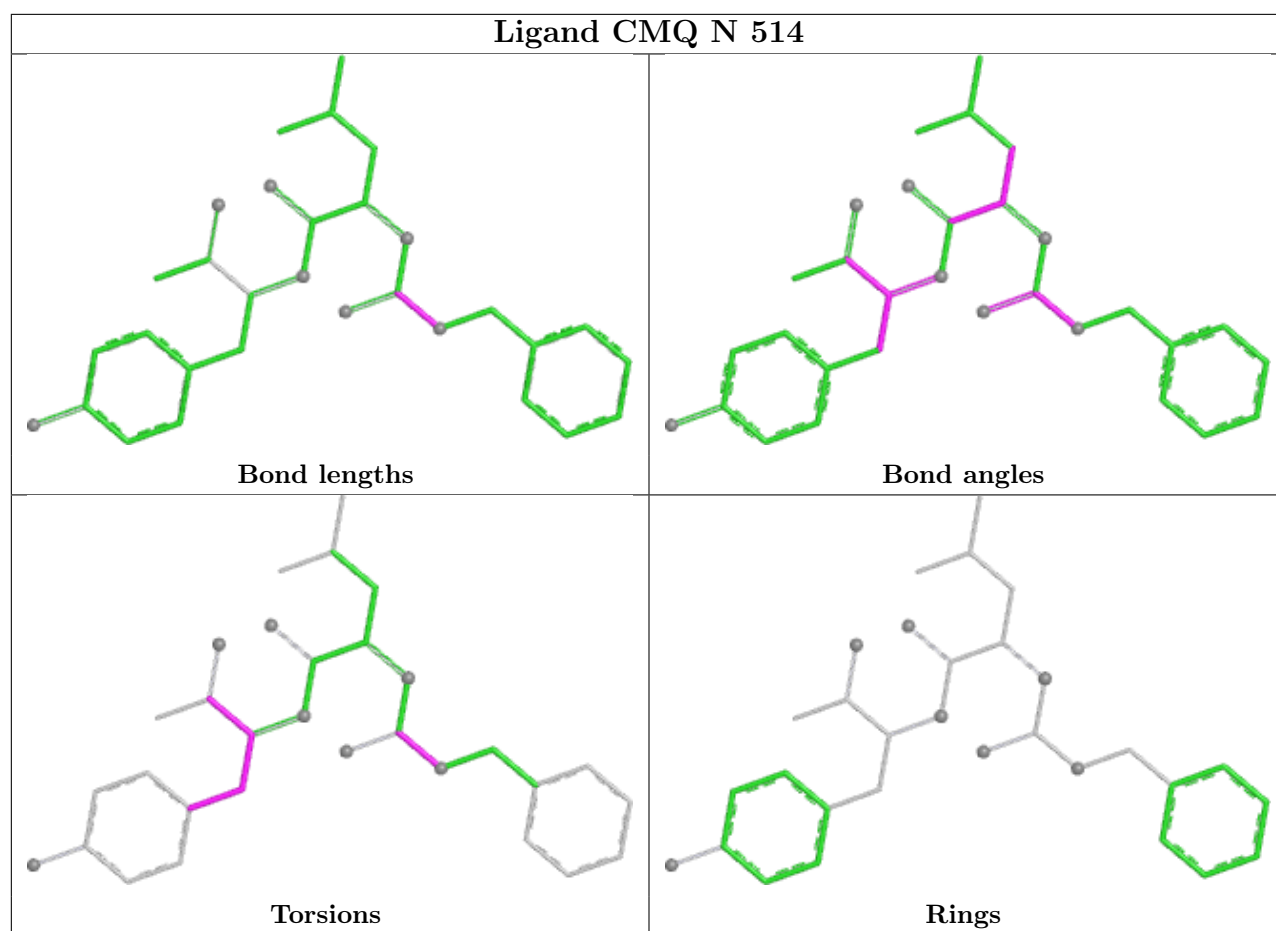


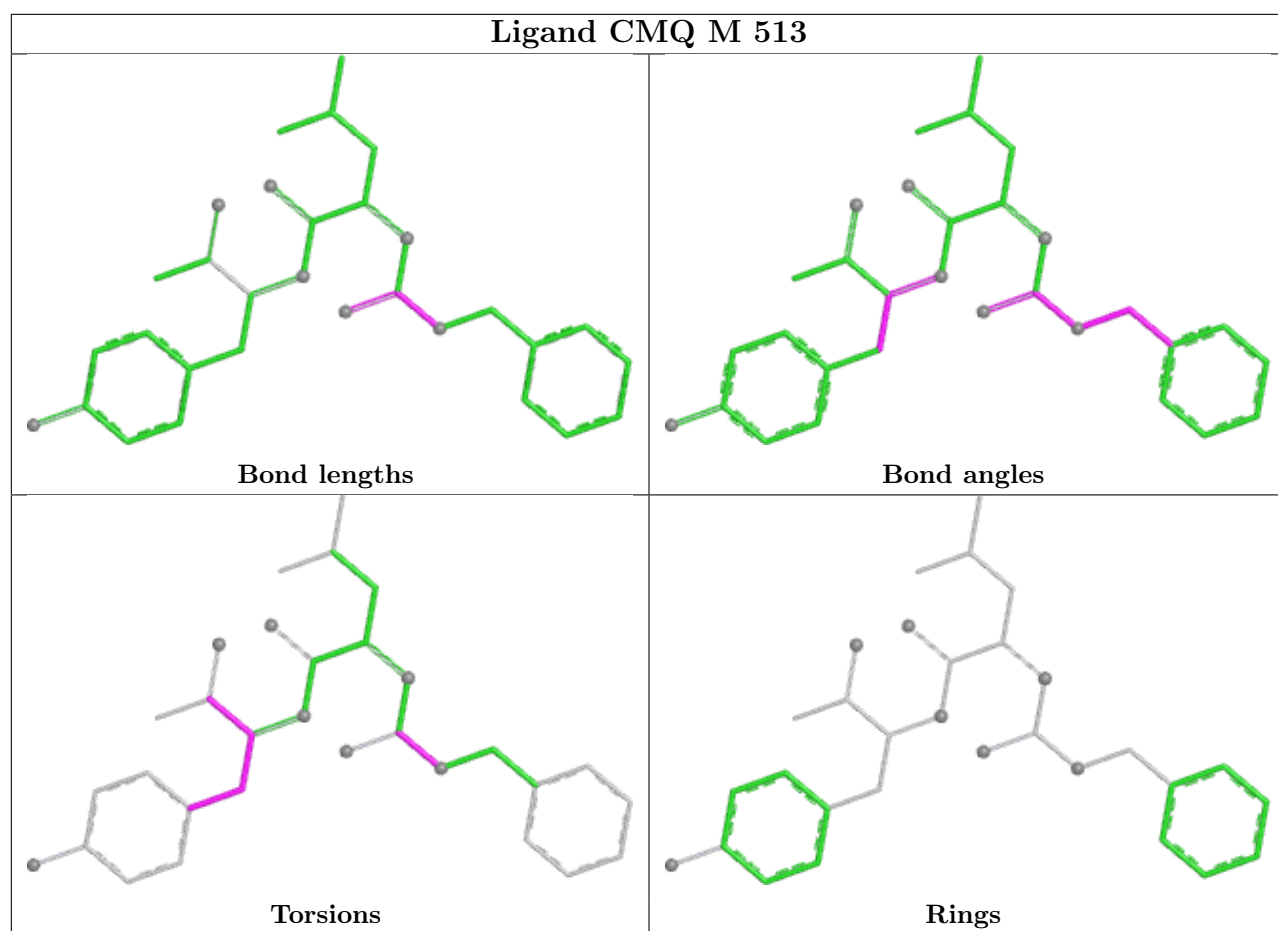


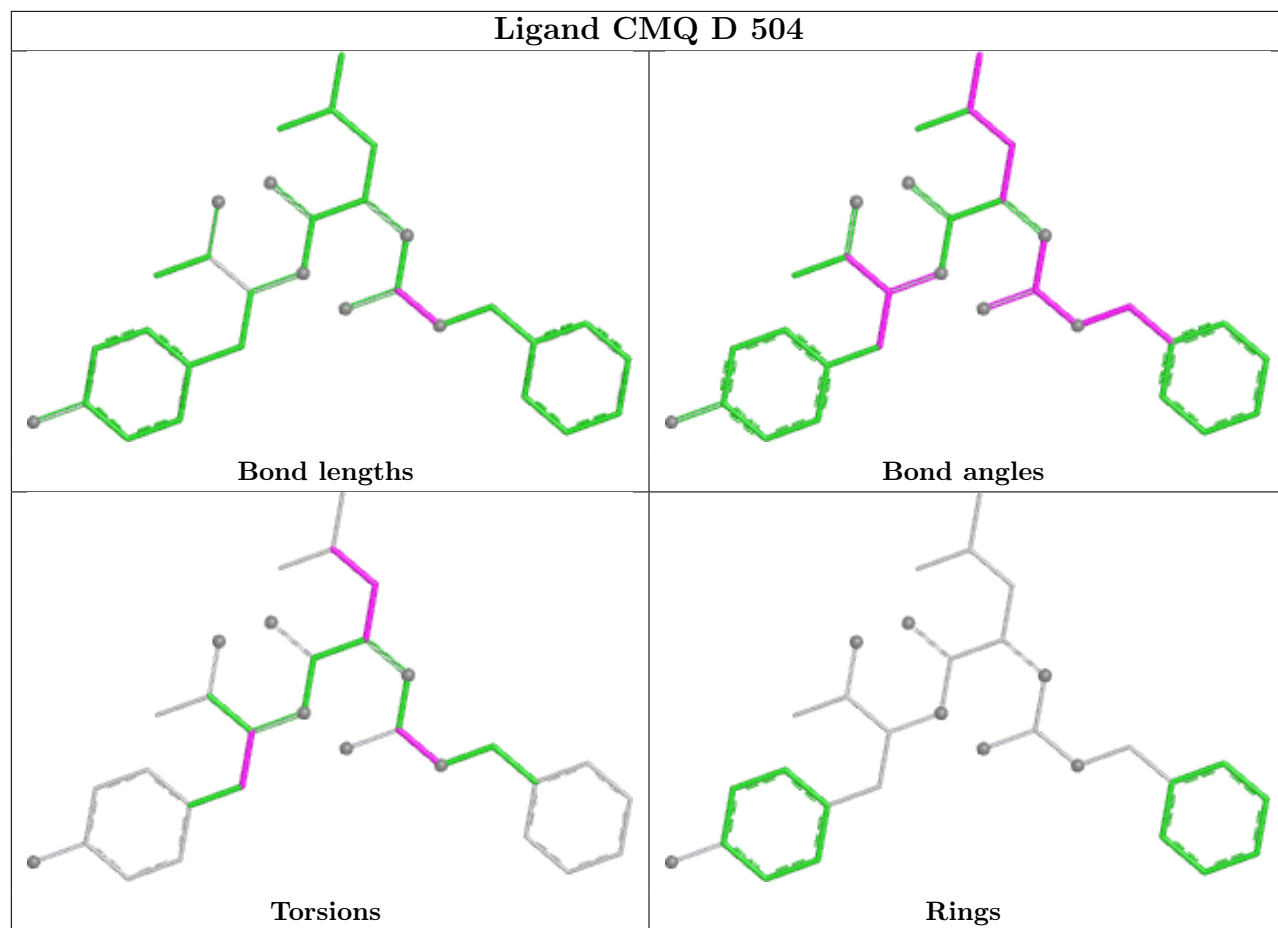


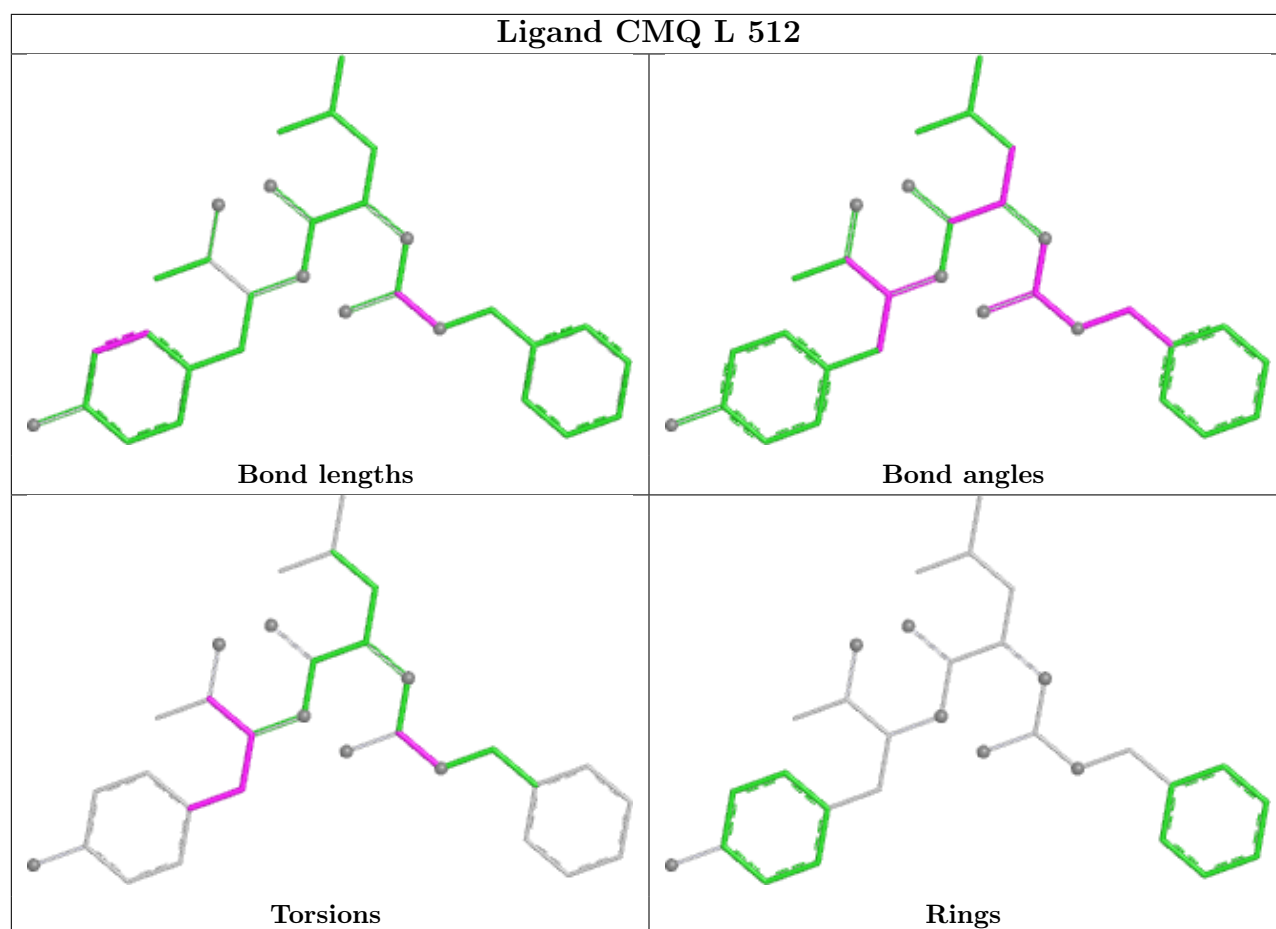


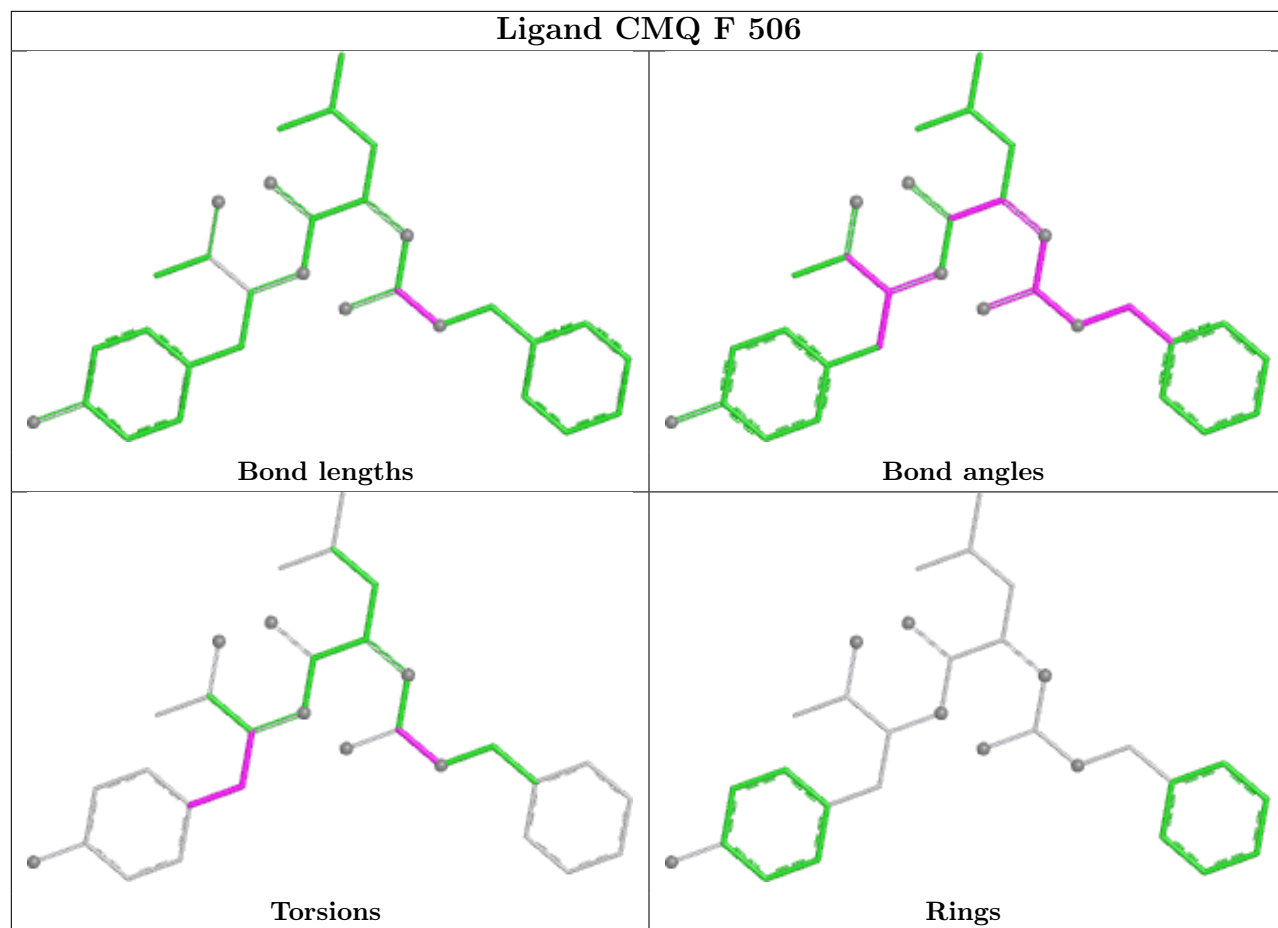


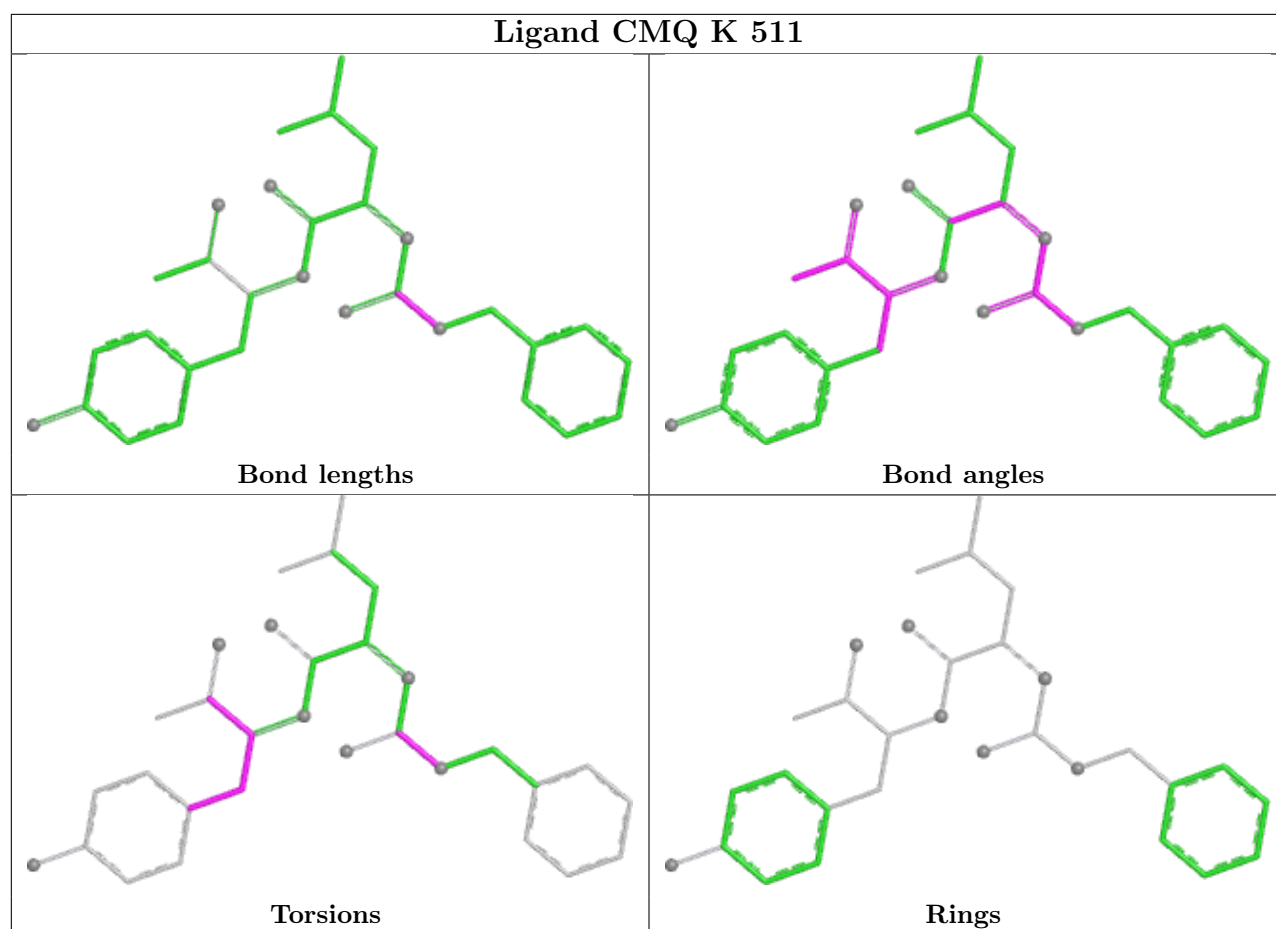


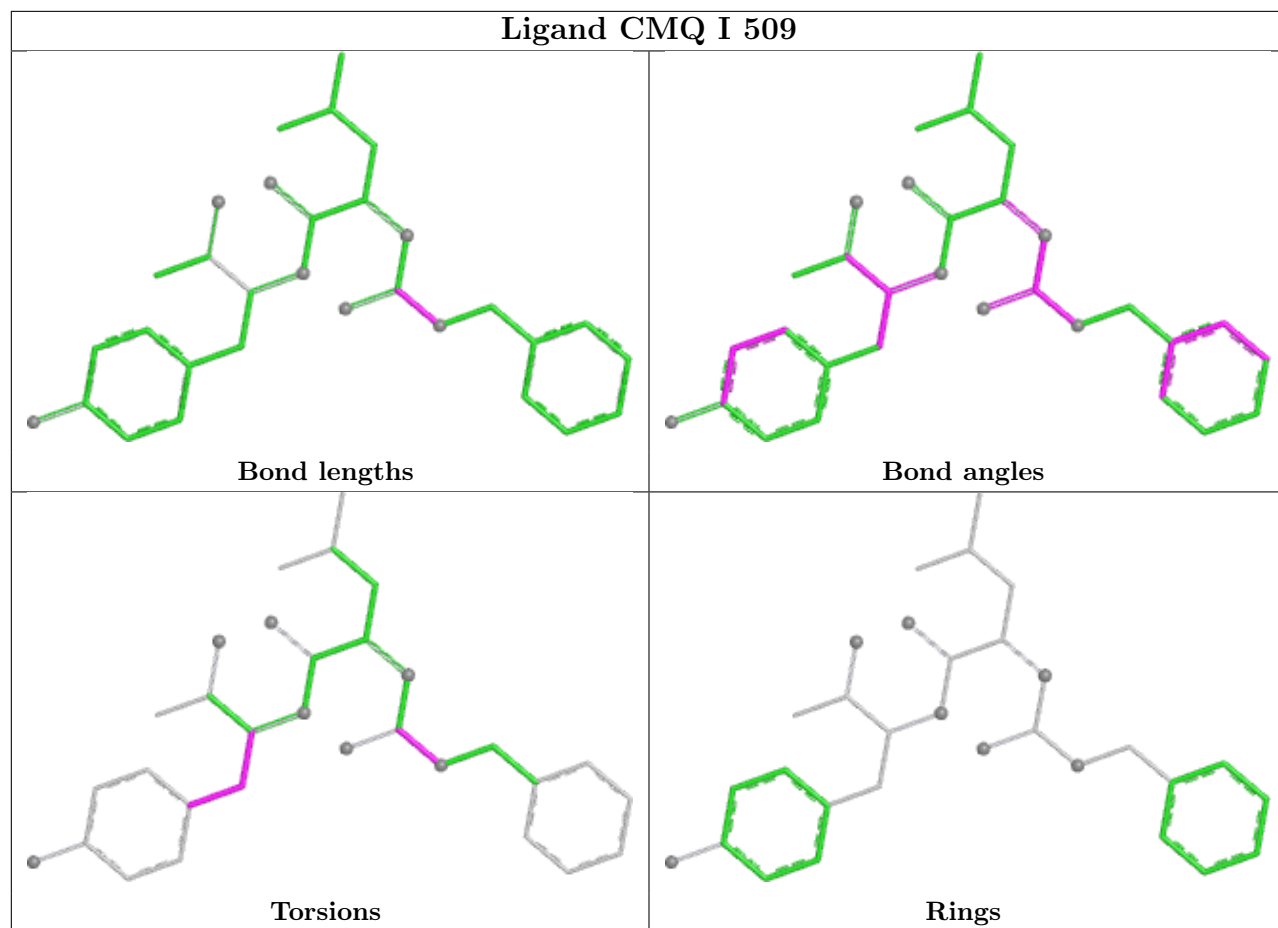












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	186/193 (96%)	0.55	9 (4%) 35 38	20, 32, 50, 69	7 (3%)
1	B	192/193 (99%)	0.89	27 (14%) 6 6	21, 33, 53, 69	10 (5%)
1	C	183/193 (94%)	0.76	14 (7%) 19 21	20, 33, 43, 66	7 (3%)
1	D	185/193 (95%)	0.72	16 (8%) 16 17	20, 33, 52, 72	3 (1%)
1	E	188/193 (97%)	0.98	24 (12%) 7 8	22, 32, 50, 66	2 (1%)
1	F	185/193 (95%)	0.51	10 (5%) 31 33	21, 32, 46, 59	2 (1%)
1	G	183/193 (94%)	0.53	8 (4%) 39 41	20, 32, 46, 68	4 (2%)
1	H	183/193 (94%)	0.49	9 (4%) 35 37	21, 32, 46, 78	2 (1%)
1	I	183/193 (94%)	0.54	7 (3%) 44 47	17, 32, 43, 64	7 (3%)
1	J	185/193 (95%)	0.56	10 (5%) 31 33	21, 32, 48, 79	2 (1%)
1	K	186/193 (96%)	0.55	11 (5%) 28 30	20, 33, 53, 70	1 (0%)
1	L	183/193 (94%)	0.55	8 (4%) 39 41	20, 32, 45, 68	11 (6%)
1	M	186/193 (96%)	0.62	12 (6%) 25 26	20, 32, 52, 70	11 (5%)
1	N	183/193 (94%)	0.50	10 (5%) 30 32	20, 32, 44, 73	10 (5%)
All	All	2591/2702 (95%)	0.63	175 (6%) 23 24	17, 33, 51, 79	79 (3%)

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	1	ALA	7.7
1	G	16	SER	7.2
1	G	5	MET	7.1
1	F	16	SER	6.7
1	G	6	VAL	6.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

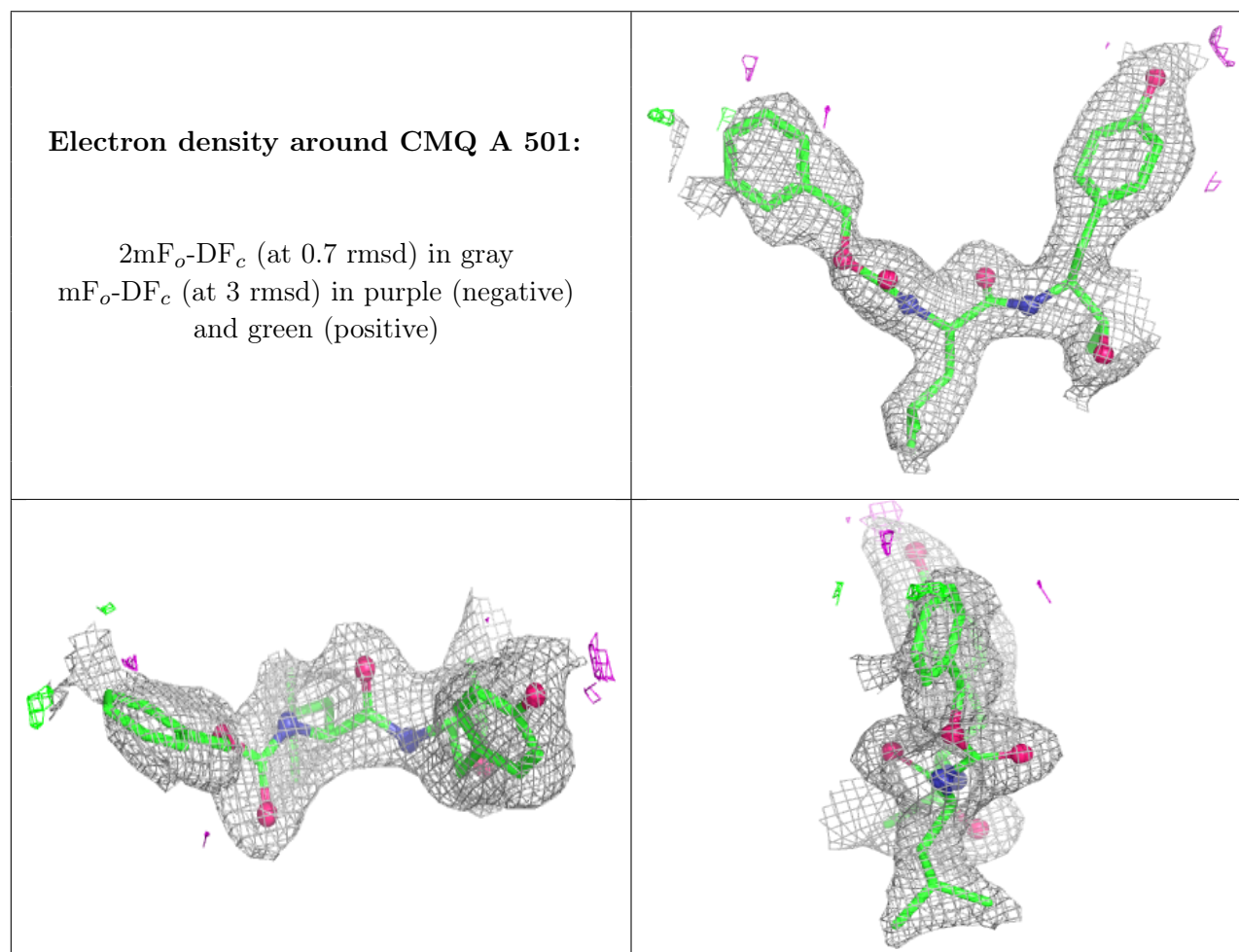
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PGE	C	4003	10/10	0.70	0.12	63,64,66,66	0
3	PGE	N	4014	10/10	0.71	0.12	59,65,69,70	0
3	PGE	B	4002	10/10	0.72	0.12	61,62,63,64	0
4	GOL	B	3002	6/6	0.72	0.12	52,54,56,56	0
3	PGE	K	4011	10/10	0.73	0.11	48,51,57,59	0
4	GOL	H	3008	6/6	0.73	0.12	53,55,57,58	0
3	PGE	E	4005	10/10	0.75	0.11	59,60,63,63	0
3	PGE	H	4008	10/10	0.75	0.12	52,55,58,59	0
4	GOL	C	3006	6/6	0.76	0.12	60,62,63,64	0
3	PGE	J	4010	10/10	0.76	0.12	41,46,51,52	0
4	GOL	K	3010	6/6	0.77	0.20	43,46,46,46	0
4	GOL	C	3005	6/6	0.78	0.11	53,55,56,56	0
3	PGE	D	4004	10/10	0.79	0.10	55,57,58,60	0
3	PGE	K	4015	10/10	0.80	0.12	37,40,42,45	0
3	PGE	A	4001	10/10	0.82	0.10	43,46,50,50	0
3	PGE	I	4009	10/10	0.84	0.10	48,52,60,60	0
4	GOL	N	3007	6/6	0.84	0.14	44,48,50,50	0
4	GOL	F	3004	6/6	0.85	0.16	30,33,34,40	0
4	GOL	B	3003	6/6	0.85	0.10	56,58,58,60	0
3	PGE	G	4007	10/10	0.85	0.10	36,39,44,44	0
3	PGE	L	4012	10/10	0.85	0.09	45,46,49,50	0
4	GOL	G	3009	6/6	0.86	0.15	42,46,48,49	0
3	PGE	F	4006	10/10	0.86	0.09	41,43,49,50	0
2	CMQ	A	501	31/31	0.87	0.11	36,41,56,58	0
3	PGE	M	4013	10/10	0.87	0.09	43,45,49,54	0
2	CMQ	I	509	31/31	0.87	0.11	35,41,55,58	0
4	GOL	L	3011	6/6	0.87	0.14	30,36,38,42	0

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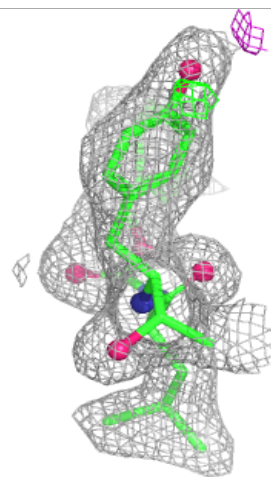
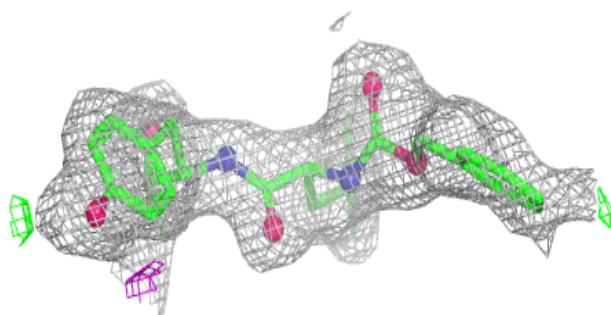
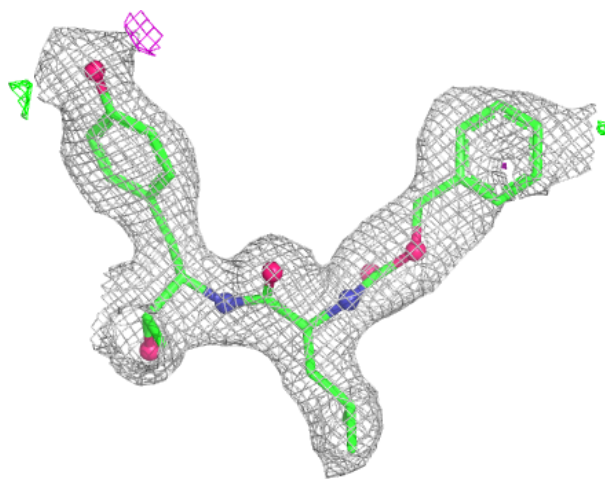
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CMQ	K	511	31/31	0.87	0.11	36,40,56,57	0
2	CMQ	N	514	31/31	0.88	0.11	34,41,59,60	0
2	CMQ	E	505	31/31	0.88	0.12	33,39,59,60	0
2	CMQ	H	508	31/31	0.89	0.10	33,39,62,63	0
2	CMQ	C	503	31/31	0.89	0.10	34,40,56,58	0
2	CMQ	J	510	31/31	0.89	0.09	36,41,53,54	0
2	CMQ	B	502	31/31	0.89	0.12	33,42,58,59	0
2	CMQ	F	506	31/31	0.89	0.10	34,40,58,59	0
2	CMQ	M	513	31/31	0.90	0.10	33,39,54,55	0
2	CMQ	D	504	31/31	0.91	0.10	34,38,55,56	0
4	GOL	A	3001	6/6	0.91	0.14	32,35,37,42	0
2	CMQ	L	512	31/31	0.91	0.12	35,40,62,64	0
2	CMQ	G	507	31/31	0.92	0.09	32,41,56,57	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.



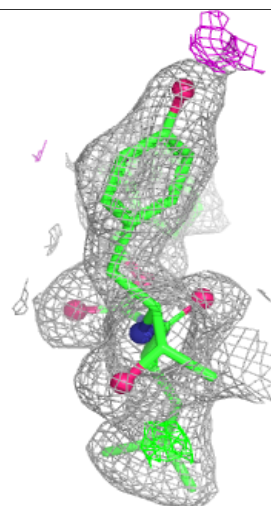
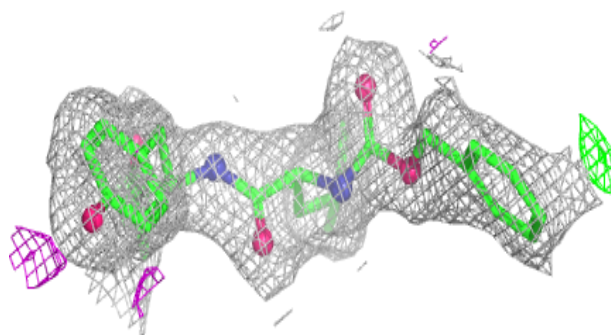
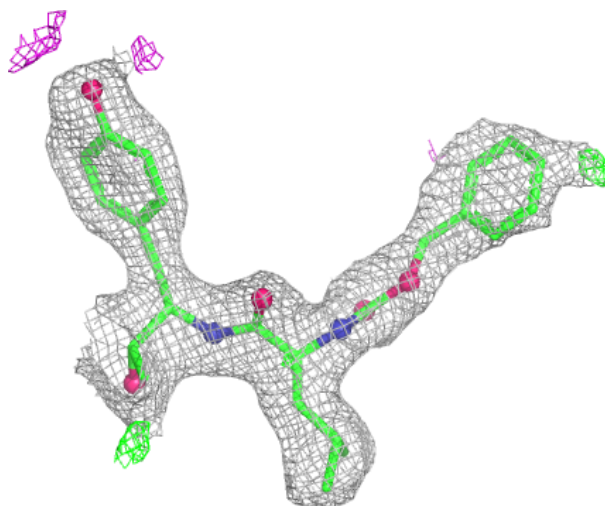
Electron density around CMQ I 509:

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



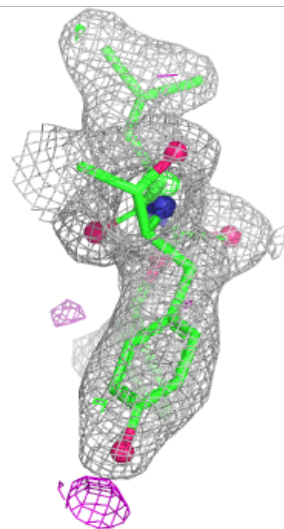
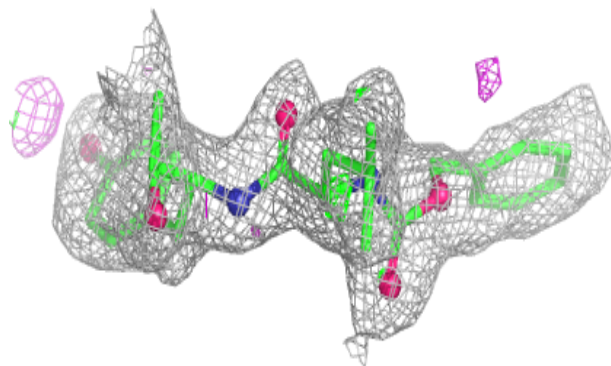
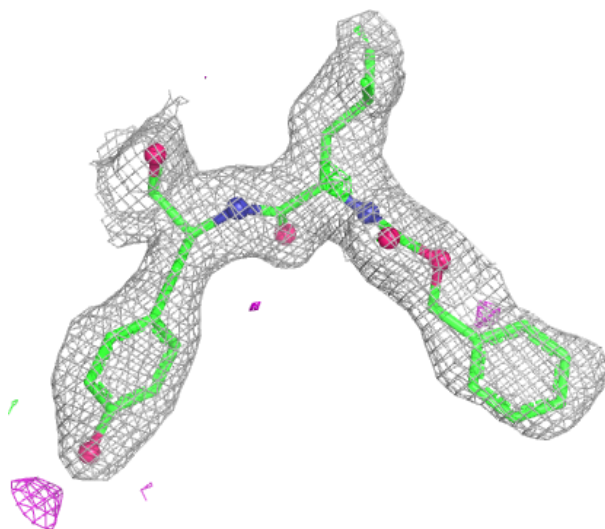
Electron density around CMQ K 511:

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



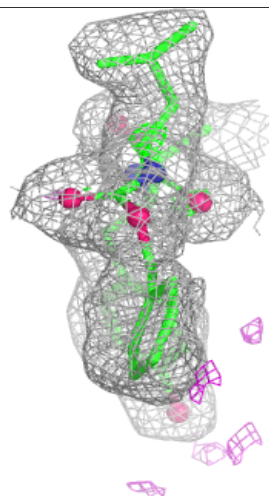
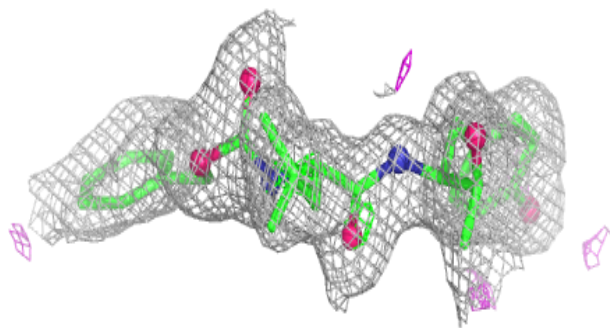
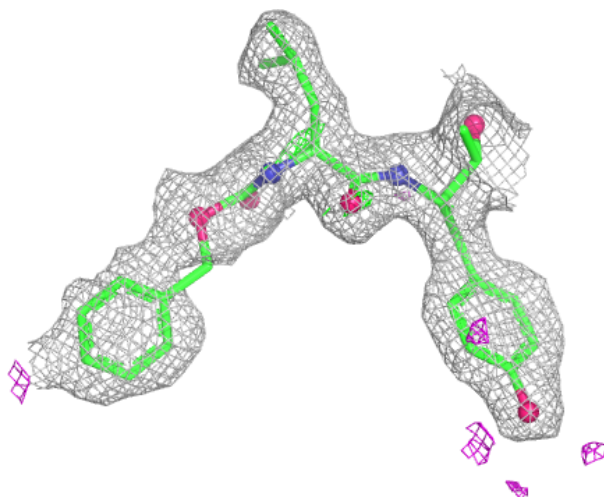
Electron density around CMQ N 514:

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



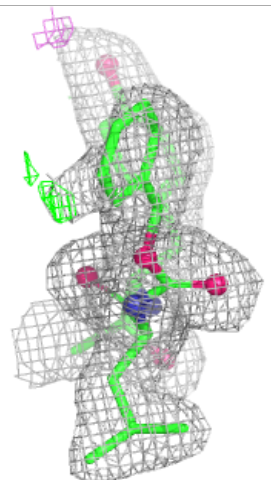
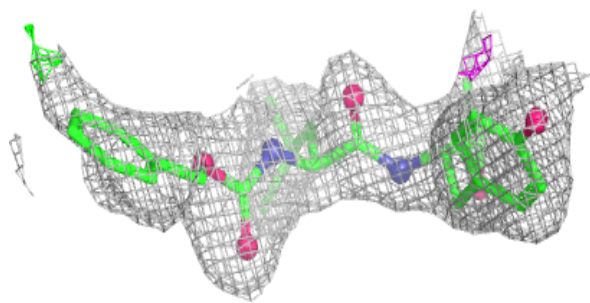
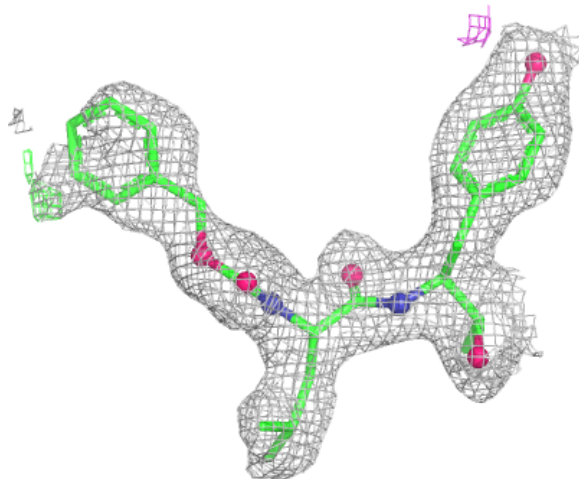
Electron density around CMQ E 505:

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



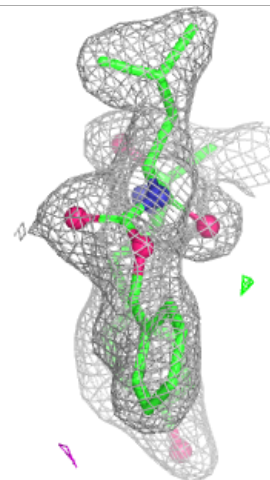
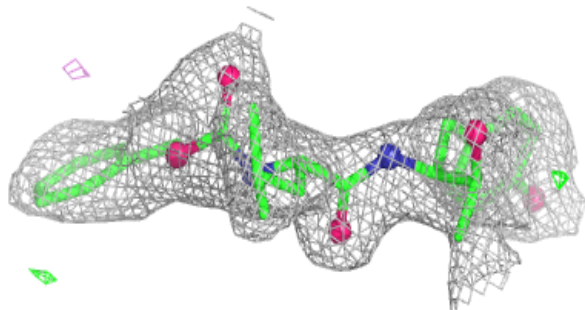
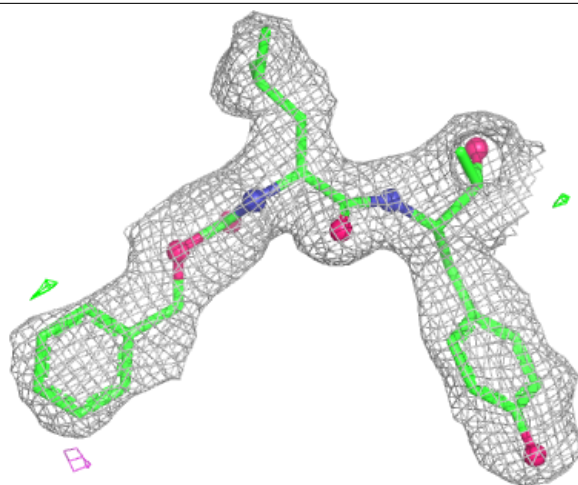
Electron density around CMQ H 508:

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



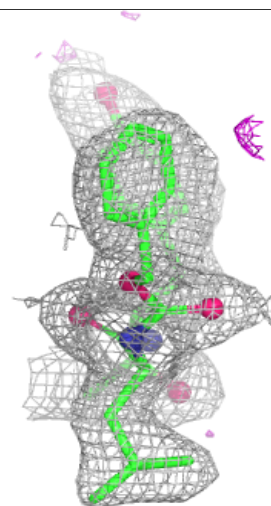
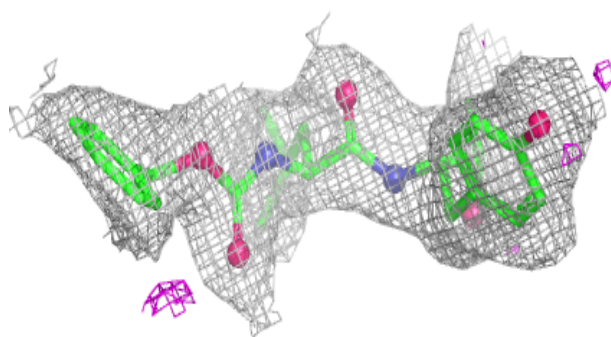
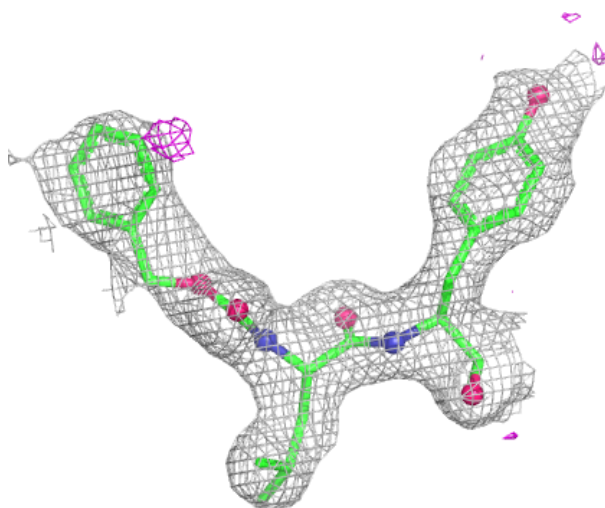
Electron density around CMQ C 503:

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



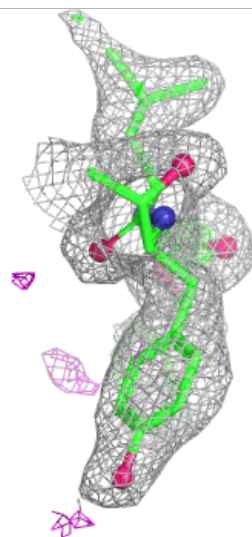
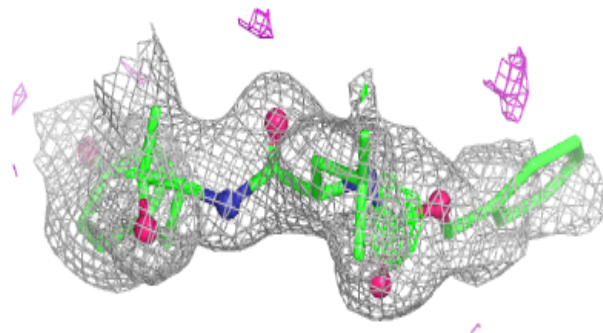
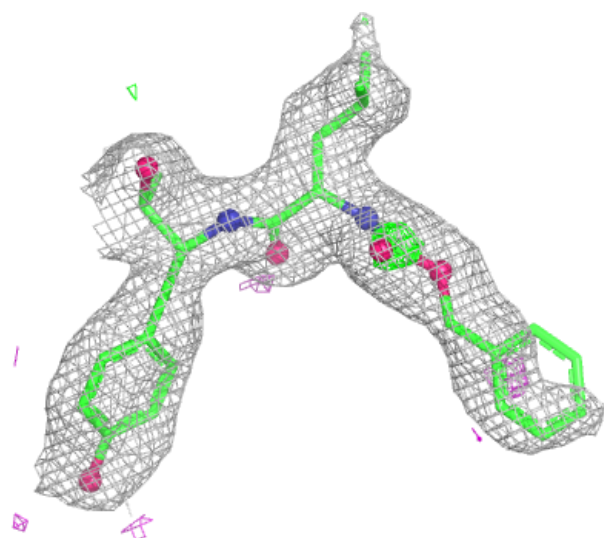
Electron density around CMQ J 510:

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



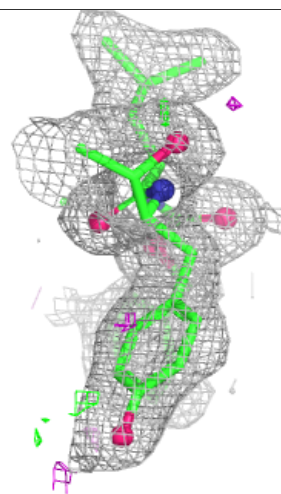
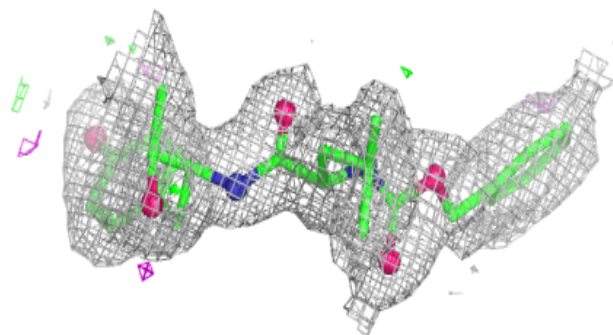
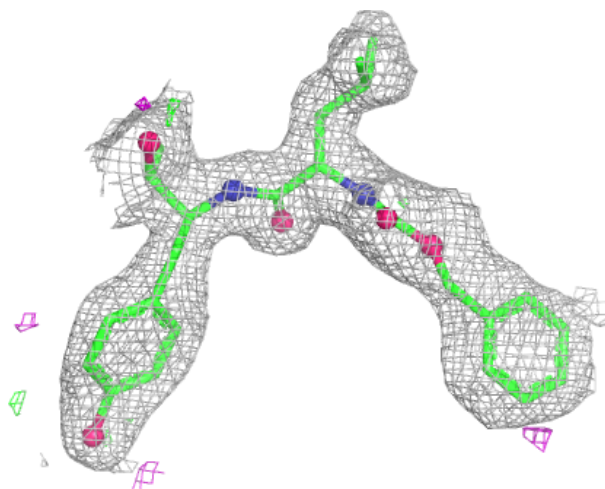
Electron density around CMQ B 502:

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



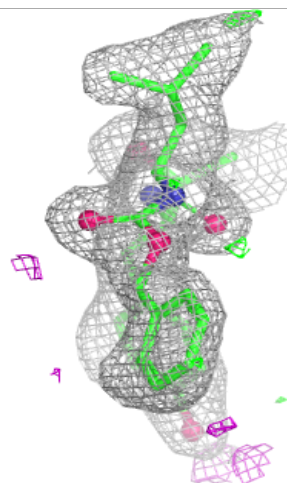
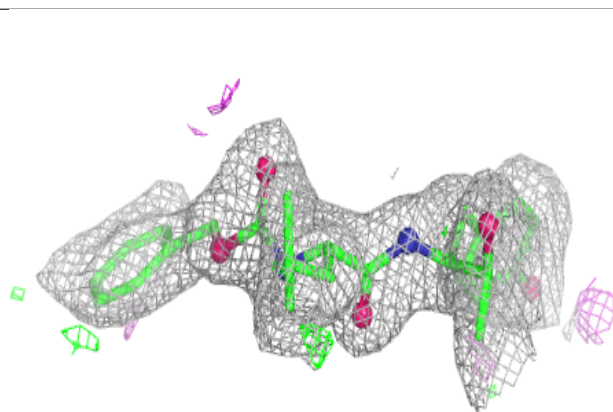
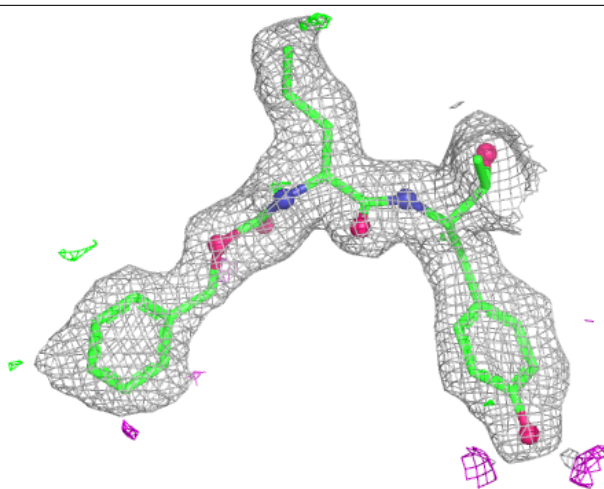
Electron density around CMQ F 506:

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



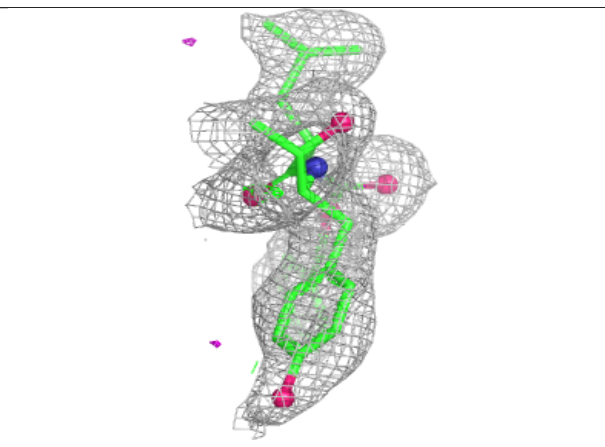
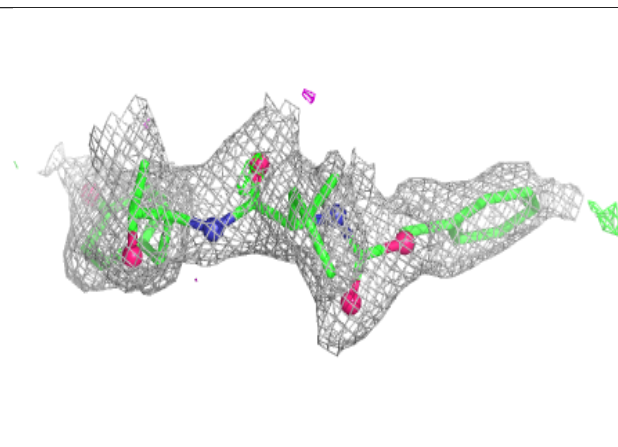
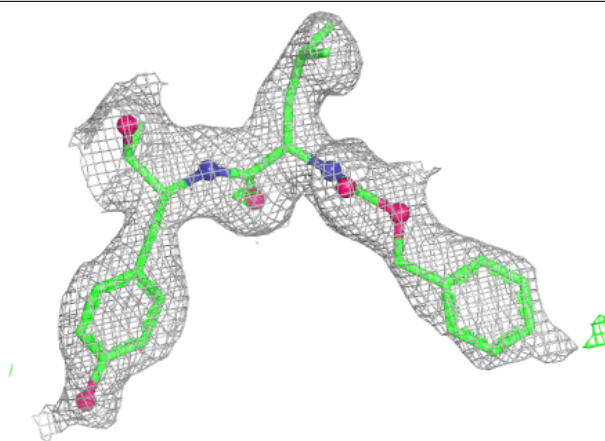
Electron density around CMQ M 513:

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



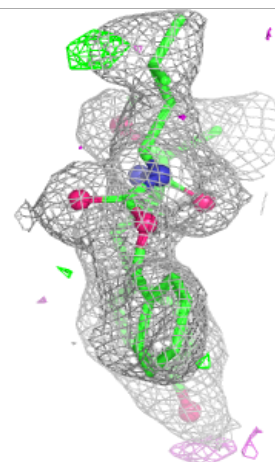
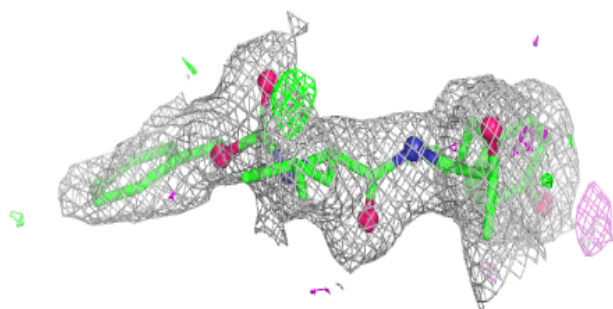
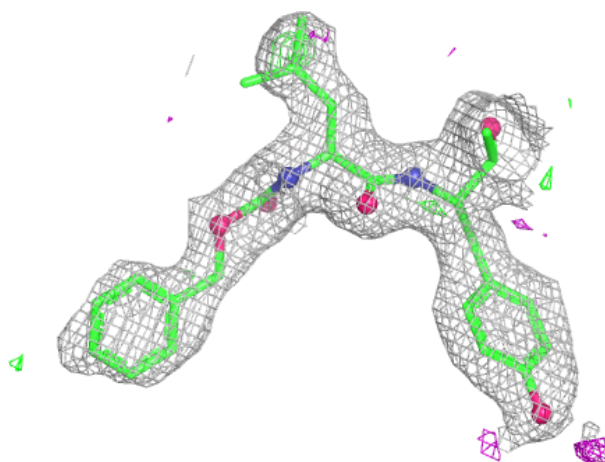
Electron density around CMQ D 504:

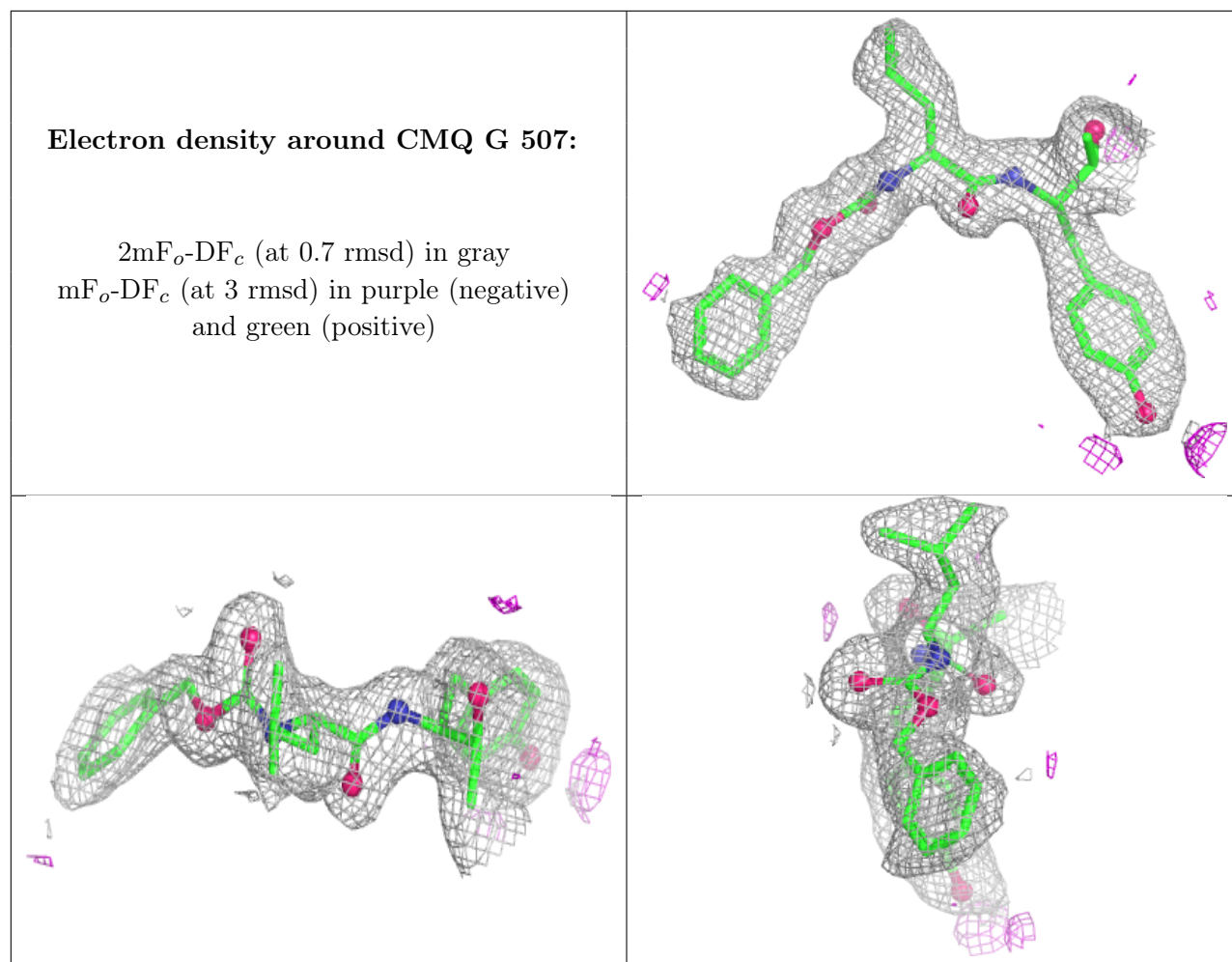
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and green (positive)



Electron density around CMQ L 512:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.