



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:00 am BST

PDB ID : 2FZS  
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](mailto: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.

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

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

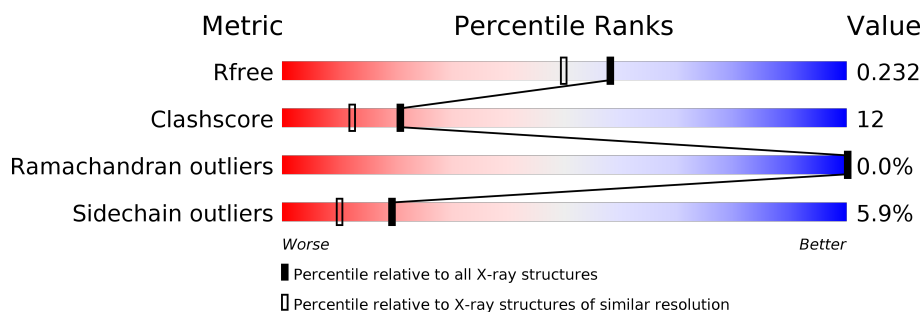
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	193	77% 13% 6% . .
1	B	193	79% 17% . .
1	C	193	75% 15% 5% 5%
1	D	193	75% 17% . . .
1	E	193	80% 16% . .
1	F	193	79% 15% . . .
1	G	193	74% 18% . 5%

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Mol	Chain	Length	Quality of chain
1	H	193	 78%13%5%
1	I	193	 72%21%5%
1	J	193	 76%18%5%
1	K	193	 76%18%5%
1	L	193	 75%17%5%
1	M	193	 76%18%5%
1	N	193	 83%10%5%

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 [i](#)

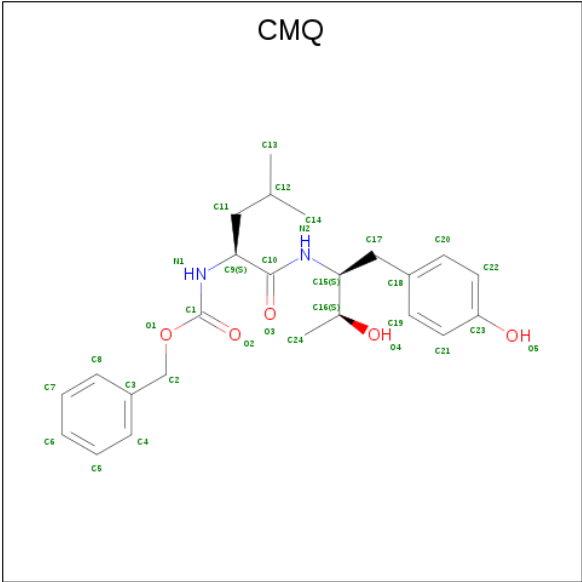
There are 5 unique types of molecules in this entry. The entry contains 24125 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

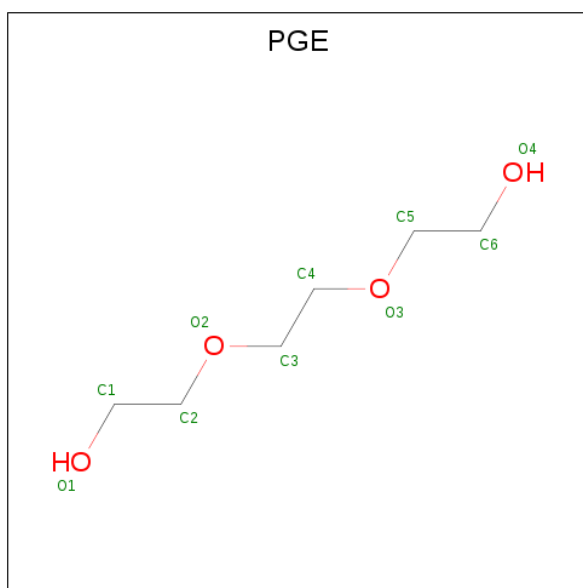
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	7	0
			1487	946	252	274	15			
1	B	192	Total	C	N	O	S	0	10	0
			1554	981	268	290	15			
1	C	183	Total	C	N	O	S	0	7	0
			1467	931	254	270	12			
1	D	185	Total	C	N	O	S	0	3	0
			1462	926	249	275	12			
1	E	188	Total	C	N	O	S	0	2	0
			1479	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<sup>2</sup> -[(BENZYLOXY)CARBONYL]-N-[(1S,2S)-2-HYDROXY-1-(4-HYDROXYBENZYL)PROPYL]-L-LEUCINAMIDE (three-letter code: CMQ) (formula: C<sub>24</sub>H<sub>32</sub>N<sub>2</sub>O<sub>5</sub>).



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 (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



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 (three-letter code: 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.

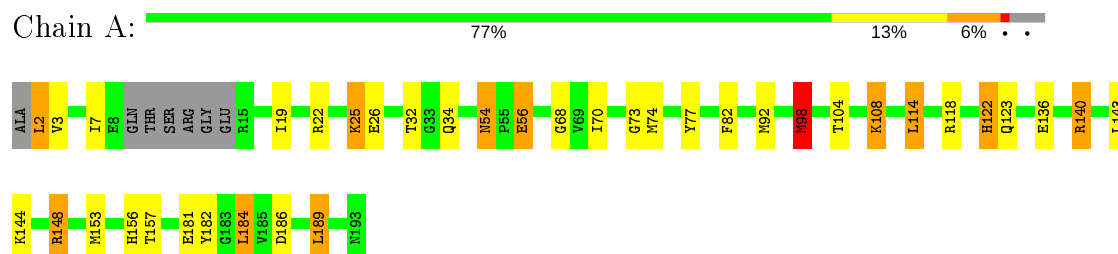
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	234	Total	O		0	0
			234	234			
5	B	188	Total	O		0	0
			188	188			
5	C	189	Total	O		0	0
			189	189			
5	D	165	Total	O		0	0
			165	165			
5	E	199	Total	O		0	0
			199	199			
5	F	218	Total	O		0	0
			218	218			
5	G	232	Total	O		0	0
			232	232			
5	H	176	Total	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			



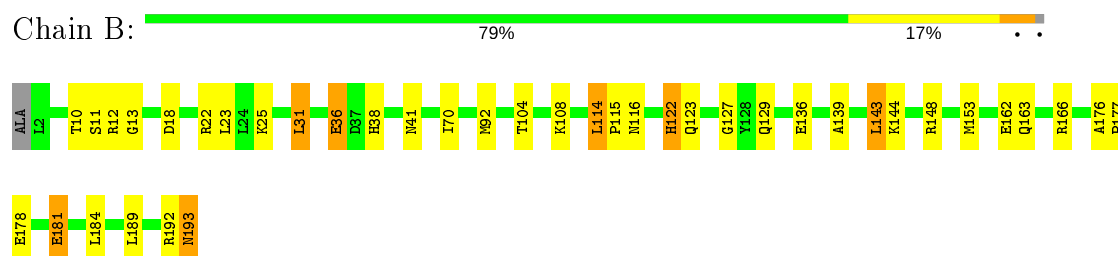
### 3 Residue-property plots [i](#)

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

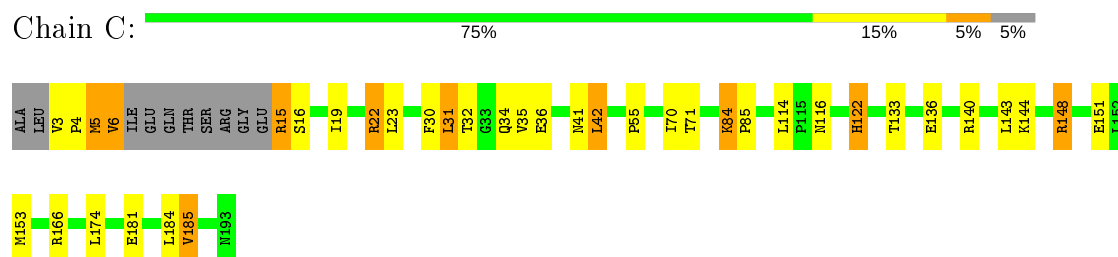
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



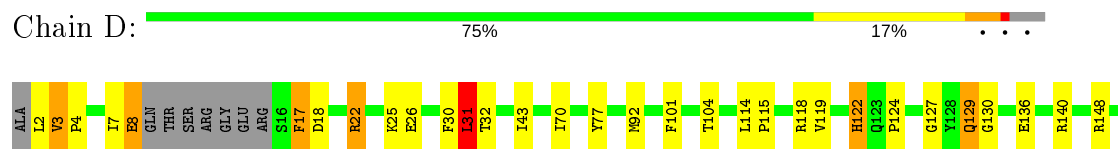
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- Molecule 1: ATP-dependent Clp protease proteolytic subunit



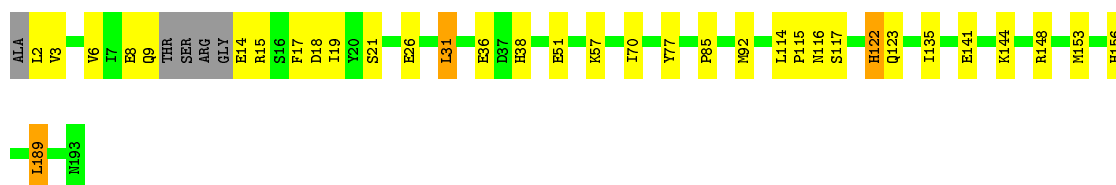
- Molecule 1: ATP-dependent Clp protease proteolytic subunit





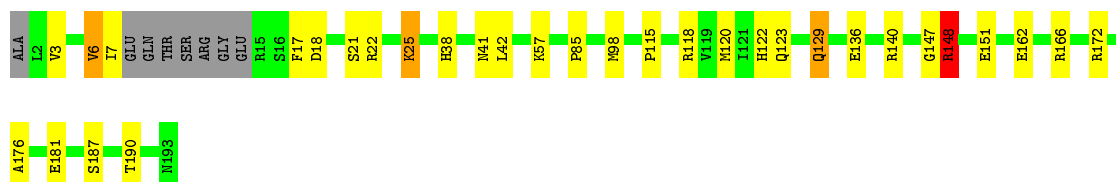
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E: 80% 16%



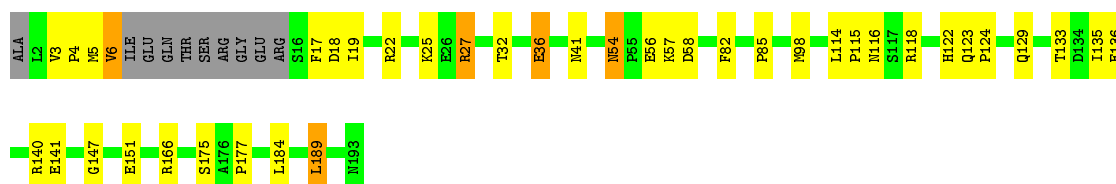
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F: 79% 15%



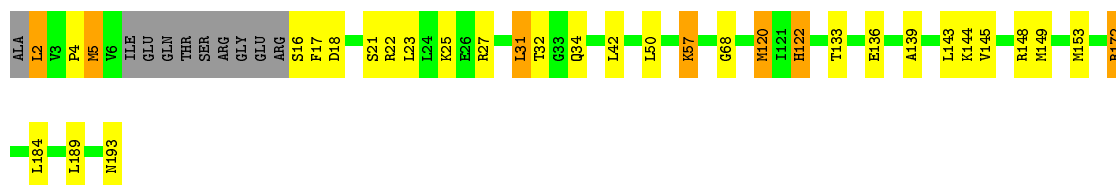
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G: 74% 18% 5%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H: 78% 13% 5%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I: 72% 21% 5%





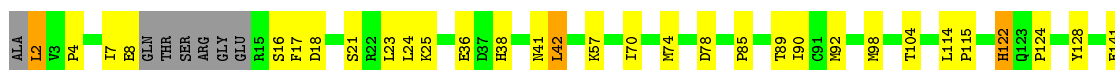
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J: 76% 18%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K: 76% 18%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L: 75% 17% 5%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M: 76% 18%



- Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N: 83% 10% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.70 Å   101.00 Å   155.40 Å 90.00°   99.00°   90.00°	Depositor
Resolution (Å)	15.00 – 1.90 29.85 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.8 (15.00-1.90) 93.4 (29.85-1.90)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.173   ,   0.233 0.173   ,   0.232	Depositor DCC
$R_{free}$ test set	10777 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.90	0/1538	0.85	2/2069 (0.1%)
1	B	0.81	1/1618 (0.1%)	0.87	4/2175 (0.2%)
1	C	0.83	1/1518 (0.1%)	0.88	4/2043 (0.2%)
1	D	0.79	0/1497	0.85	2/2016 (0.1%)
1	E	0.88	0/1510	0.84	2/2032 (0.1%)
1	F	1.03	2/1484 (0.1%)	0.97	5/1999 (0.3%)
1	G	0.99	1/1487 (0.1%)	1.26	10/2001 (0.5%)
1	H	0.83	2/1470 (0.1%)	0.84	3/1980 (0.2%)
1	I	0.74	0/1512	0.85	3/2034 (0.1%)
1	J	0.75	0/1487	0.80	3/2002 (0.1%)
1	K	0.84	0/1489	0.86	3/2006 (0.1%)
1	L	1.00	6/1545 (0.4%)	0.91	4/2079 (0.2%)
1	M	0.96	0/1572	0.94	2/2113 (0.1%)
1	N	0.86	0/1532	0.89	4/2063 (0.2%)
All	All	0.88	13/21259 (0.1%)	0.91	51/28612 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	136	GLU	CD-OE1	8.13	1.34	1.25
1	C	181	GLU	CG-CD	6.54	1.61	1.51
1	L	181[A]	GLU	CD-OE1	6.41	1.32	1.25
1	L	181[B]	GLU	CD-OE1	6.41	1.32	1.25
1	H	136	GLU	CG-CD	6.24	1.61	1.51

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	27	ARG	NE-CZ-NH2	-28.69	105.95	120.30
1	G	27	ARG	NE-CZ-NH1	20.06	130.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	27	ARG	CD-NE-CZ	10.11	137.75	123.60
1	I	27	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	K	98	MET	CG-SD-CE	-9.80	84.52	100.20

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	61	0
1	B	1554	0	1567	53	0
1	C	1467	0	1487	44	0
1	D	1462	0	1471	49	0
1	E	1479	0	1486	39	0
1	F	1453	0	1456	20	0
1	G	1448	0	1455	39	0
1	H	1439	0	1448	37	0
1	I	1461	0	1477	47	0
1	J	1456	0	1463	36	0
1	K	1462	0	1476	42	0
1	L	1478	0	1483	43	0
1	M	1505	0	1533	37	0
1	N	1469	0	1492	23	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	12	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	4	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	514	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 12.

The worst 5 of 514 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:I:122:HIS:NE2	2:I:509:CMQ:H242	1.24	1.45
1:D:122:HIS:NE2	2:D:504:CMQ:H242	1.14	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%)	29	18
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%)	150 (91%)	15 (9%)	9	3
1	B	173/163 (106%)	163 (94%)	10 (6%)	20	10
1	C	162/163 (99%)	145 (90%)	17 (10%)	7	2
1	D	160/163 (98%)	146 (91%)	14 (9%)	10	4
1	E	161/163 (99%)	154 (96%)	7 (4%)	29	19
1	F	158/163 (97%)	148 (94%)	10 (6%)	18	8
1	G	159/163 (98%)	151 (95%)	8 (5%)	24	15
1	H	157/163 (96%)	146 (93%)	11 (7%)	15	7
1	I	162/163 (99%)	156 (96%)	6 (4%)	34	25
1	J	159/163 (98%)	151 (95%)	8 (5%)	24	15
1	K	159/163 (98%)	152 (96%)	7 (4%)	28	19
1	L	166/163 (102%)	156 (94%)	10 (6%)	19	9
1	M	168/163 (103%)	156 (93%)	12 (7%)	14	6
1	N	165/163 (101%)	154 (93%)	11 (7%)	16	7
All	All	2274/2282 (100%)	2128 (94%)	146 (6%)	19	8

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	21	SER

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Mol	Chain	Res	Type
1	H	2	LEU
1	M	192	ARG
1	F	25	LYS
1	G	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	34	GLN
1	G	54	ASN
1	M	123	GLN
1	F	41	ASN
1	G	191	HIS

### 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 carbohydrates 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
3	PGE	H	4008	-	9,9,9	0.42	0	8,8,8	0.54	0
2	CMQ	E	505	1	31,32,32	1.32	1 (3%)	39,42,42	1.59	11 (28%)
4	GOL	B	3003	-	5,5,5	0.43	0	5,5,5	0.34	0
4	GOL	L	3011	-	5,5,5	0.46	0	5,5,5	0.66	0
3	PGE	K	4015	-	9,9,9	0.22	0	8,8,8	0.90	0
3	PGE	F	4006	-	9,9,9	0.38	0	8,8,8	0.51	0
2	CMQ	I	509	1	31,32,32	1.21	1 (3%)	39,42,42	1.59	5 (12%)
3	PGE	K	4011	-	9,9,9	0.52	0	8,8,8	0.45	0
2	CMQ	D	504	1	31,32,32	1.22	1 (3%)	39,42,42	1.53	6 (15%)
3	PGE	D	4004	-	9,9,9	0.47	0	8,8,8	0.35	0
3	PGE	N	4014	-	9,9,9	0.43	0	8,8,8	0.45	0
2	CMQ	K	511	1	31,32,32	1.15	1 (3%)	39,42,42	1.20	5 (12%)
4	GOL	K	3010	-	5,5,5	0.32	0	5,5,5	0.79	0
3	PGE	I	4009	-	9,9,9	0.45	0	8,8,8	0.45	0
2	CMQ	B	502	1	31,32,32	1.11	1 (3%)	39,42,42	1.27	3 (7%)
3	PGE	B	4002	-	9,9,9	0.51	0	8,8,8	0.18	0
2	CMQ	M	513	1	31,32,32	1.18	2 (6%)	39,42,42	1.29	5 (12%)
2	CMQ	H	508	1	31,32,32	1.21	1 (3%)	39,42,42	1.52	8 (20%)
3	PGE	J	4010	-	9,9,9	0.60	0	8,8,8	0.49	0
3	PGE	M	4013	-	9,9,9	0.43	0	8,8,8	0.51	0
3	PGE	G	4007	-	9,9,9	0.50	0	8,8,8	0.48	0
4	GOL	H	3008	-	5,5,5	0.37	0	5,5,5	0.88	0
2	CMQ	F	506	1	31,32,32	1.15	1 (3%)	39,42,42	1.32	6 (15%)
2	CMQ	L	512	1	31,32,32	1.23	2 (6%)	39,42,42	1.31	5 (12%)
4	GOL	G	3009	-	5,5,5	0.49	0	5,5,5	0.37	0
2	CMQ	C	503	1	31,32,32	1.26	2 (6%)	39,42,42	1.35	5 (12%)
3	PGE	E	4005	-	9,9,9	0.49	0	8,8,8	0.37	0
4	GOL	C	3005	-	5,5,5	0.27	0	5,5,5	0.63	0
4	GOL	B	3002	-	5,5,5	0.23	0	5,5,5	0.62	0
2	CMQ	J	510	1	31,32,32	1.23	1 (3%)	39,42,42	1.44	6 (15%)
4	GOL	F	3004	-	5,5,5	0.60	0	5,5,5	0.70	0
2	CMQ	A	501	1	31,32,32	1.26	1 (3%)	39,42,42	1.45	8 (20%)
3	PGE	C	4003	-	9,9,9	0.51	0	8,8,8	0.32	0
3	PGE	L	4012	-	9,9,9	0.59	0	8,8,8	0.31	0
4	GOL	N	3007	-	5,5,5	0.31	0	5,5,5	0.74	0
4	GOL	C	3006	-	5,5,5	0.35	0	5,5,5	0.54	0
4	GOL	A	3001	-	5,5,5	0.30	0	5,5,5	0.48	0
2	CMQ	G	507	1	31,32,32	1.43	1 (3%)	39,42,42	1.26	6 (15%)
3	PGE	A	4001	-	9,9,9	0.50	0	8,8,8	0.29	0
2	CMQ	N	514	1	31,32,32	1.23	1 (3%)	39,42,42	1.12	4 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	H	4008	-	-	3/7/7/7	-
2	CMQ	E	505	1	-	10/29/29/29	0/2/2/2
4	GOL	B	3003	-	-	2/4/4/4	-
4	GOL	L	3011	-	-	2/4/4/4	-
3	PGE	K	4015	-	-	6/7/7/7	-
3	PGE	F	4006	-	-	6/7/7/7	-
2	CMQ	I	509	1	-	6/29/29/29	0/2/2/2
3	PGE	K	4011	-	-	5/7/7/7	-
2	CMQ	D	504	1	-	8/29/29/29	0/2/2/2
3	PGE	D	4004	-	-	6/7/7/7	-
3	PGE	N	4014	-	-	3/7/7/7	-
2	CMQ	K	511	1	-	7/29/29/29	0/2/2/2
4	GOL	K	3010	-	-	3/4/4/4	-
3	PGE	I	4009	-	-	3/7/7/7	-
2	CMQ	B	502	1	-	6/29/29/29	0/2/2/2
3	PGE	B	4002	-	-	3/7/7/7	-
2	CMQ	M	513	1	-	7/29/29/29	0/2/2/2
2	CMQ	H	508	1	-	10/29/29/29	0/2/2/2
3	PGE	J	4010	-	-	0/7/7/7	-
3	PGE	M	4013	-	-	3/7/7/7	-
3	PGE	G	4007	-	-	5/7/7/7	-
4	GOL	H	3008	-	-	0/4/4/4	-
2	CMQ	F	506	1	-	4/29/29/29	0/2/2/2
2	CMQ	L	512	1	-	7/29/29/29	0/2/2/2
4	GOL	G	3009	-	-	2/4/4/4	-
2	CMQ	C	503	1	-	6/29/29/29	0/2/2/2
3	PGE	E	4005	-	-	4/7/7/7	-
4	GOL	C	3005	-	-	4/4/4/4	-
4	GOL	B	3002	-	-	2/4/4/4	-
2	CMQ	J	510	1	-	9/29/29/29	0/2/2/2
4	GOL	F	3004	-	-	2/4/4/4	-
2	CMQ	A	501	1	-	4/29/29/29	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	C	4003	-	-	6/7/7/7	-
3	PGE	L	4012	-	-	4/7/7/7	-
4	GOL	N	3007	-	-	4/4/4/4	-
4	GOL	C	3006	-	-	2/4/4/4	-
4	GOL	A	3001	-	-	2/4/4/4	-
2	CMQ	G	507	1	-	4/29/29/29	0/2/2/2
3	PGE	A	4001	-	-	3/7/7/7	-
2	CMQ	N	514	1	-	9/29/29/29	0/2/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	507	CMQ	O1-C1	6.19	1.47	1.35
2	C	503	CMQ	O1-C1	5.93	1.46	1.35
2	D	504	CMQ	O1-C1	5.80	1.46	1.35
2	J	510	CMQ	O1-C1	5.56	1.45	1.35
2	H	508	CMQ	O1-C1	5.39	1.45	1.35

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	509	CMQ	O1-C1-O2	-5.42	113.85	124.25
2	D	504	CMQ	O1-C1-N1	4.48	119.62	110.50
2	B	502	CMQ	O1-C1-N1	4.48	119.60	110.50
2	E	505	CMQ	O1-C1-O2	-4.33	115.95	124.25
2	B	502	CMQ	O1-C1-O2	-4.08	116.42	124.25

There are no chirality outliers.

5 of 182 torsion outliers are listed below:

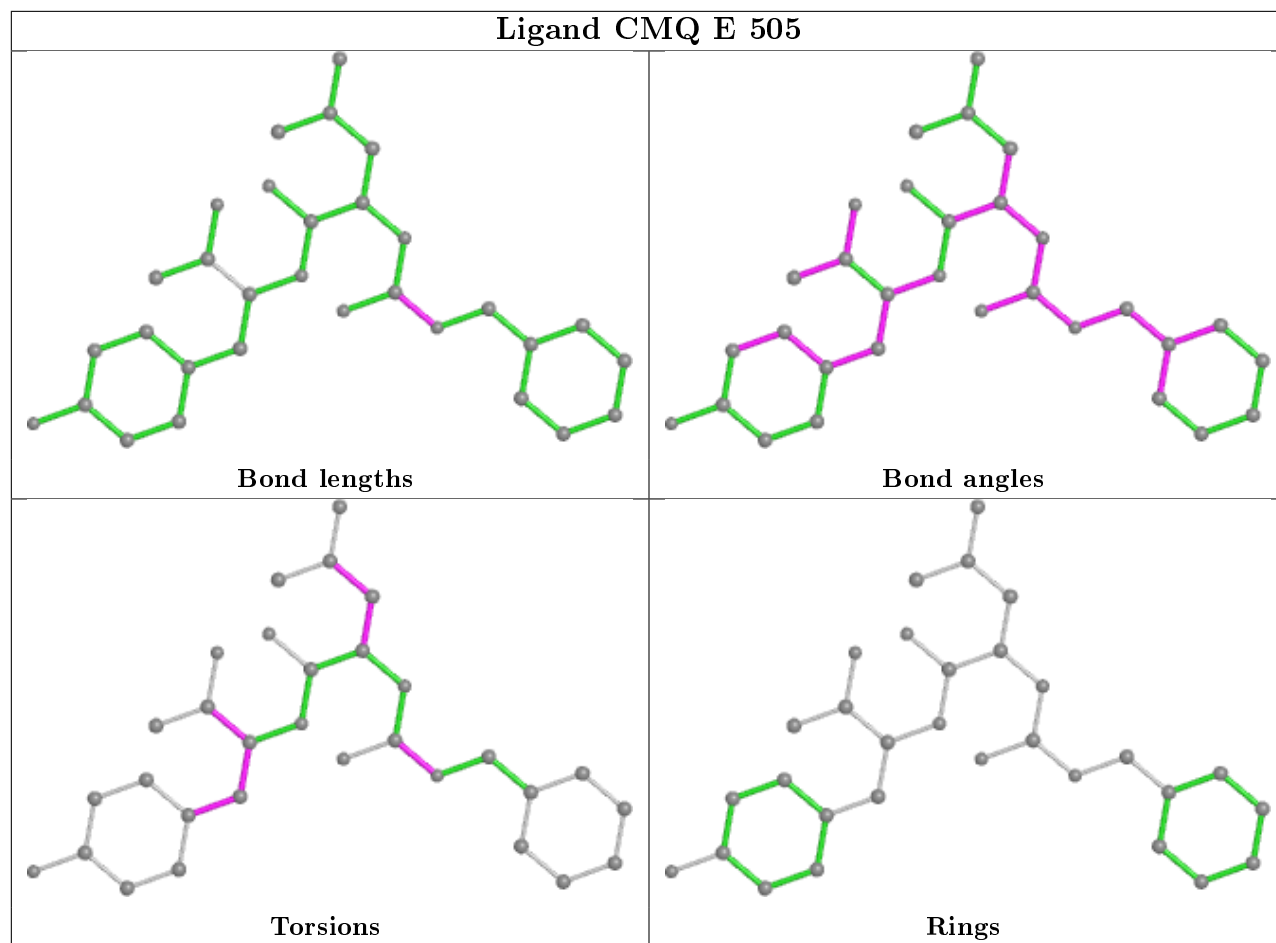
Mol	Chain	Res	Type	Atoms
2	E	505	CMQ	O2-C1-O1-C2
2	E	505	CMQ	N1-C1-O1-C2
2	E	505	CMQ	N2-C15-C17-C18
2	E	505	CMQ	C16-C15-C17-C18
4	B	3003	GOL	C1-C2-C3-O3

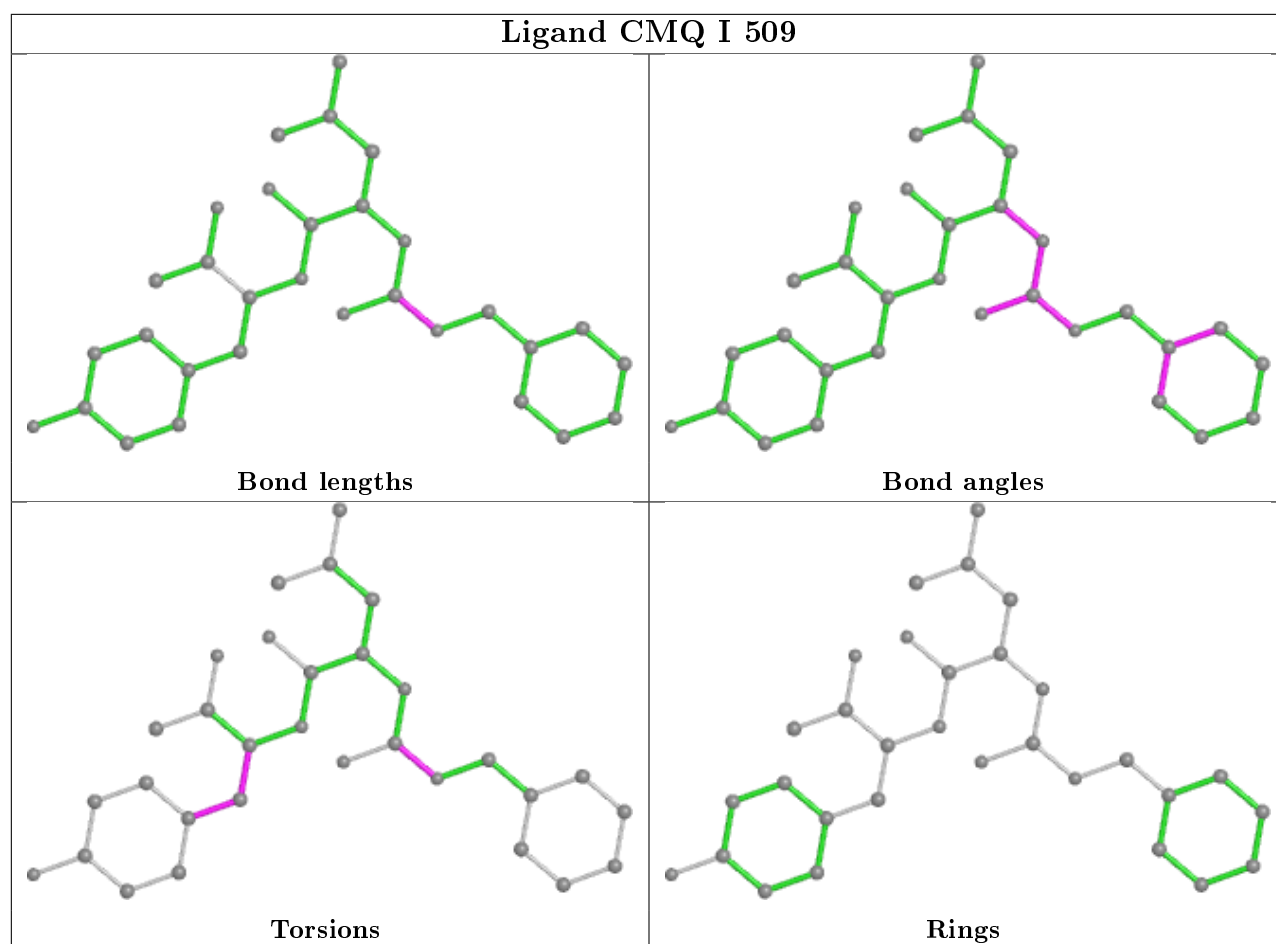
There are no ring outliers.

28 monomers are involved in 107 short contacts:

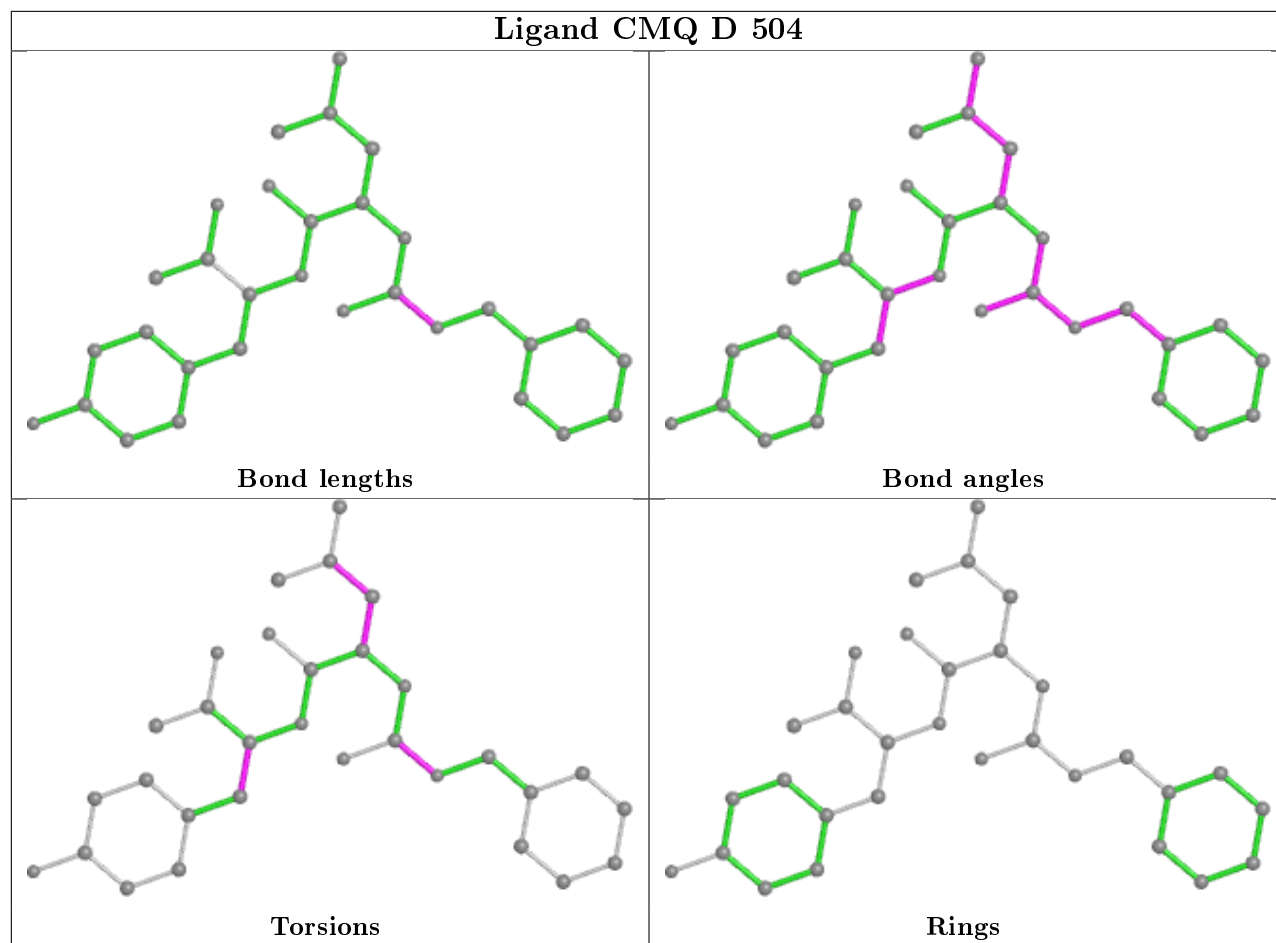
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	505	CMQ	8	0
3	K	4015	PGE	2	0
3	F	4006	PGE	1	0
2	I	509	CMQ	7	0
2	D	504	CMQ	8	0
3	N	4014	PGE	2	0
2	K	511	CMQ	9	0
4	K	3010	GOL	1	0
2	B	502	CMQ	7	0
3	B	4002	PGE	2	0
2	M	513	CMQ	1	0
2	H	508	CMQ	6	0
3	J	4010	PGE	1	0
3	M	4013	PGE	1	0
4	H	3008	GOL	2	0
2	F	506	CMQ	1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

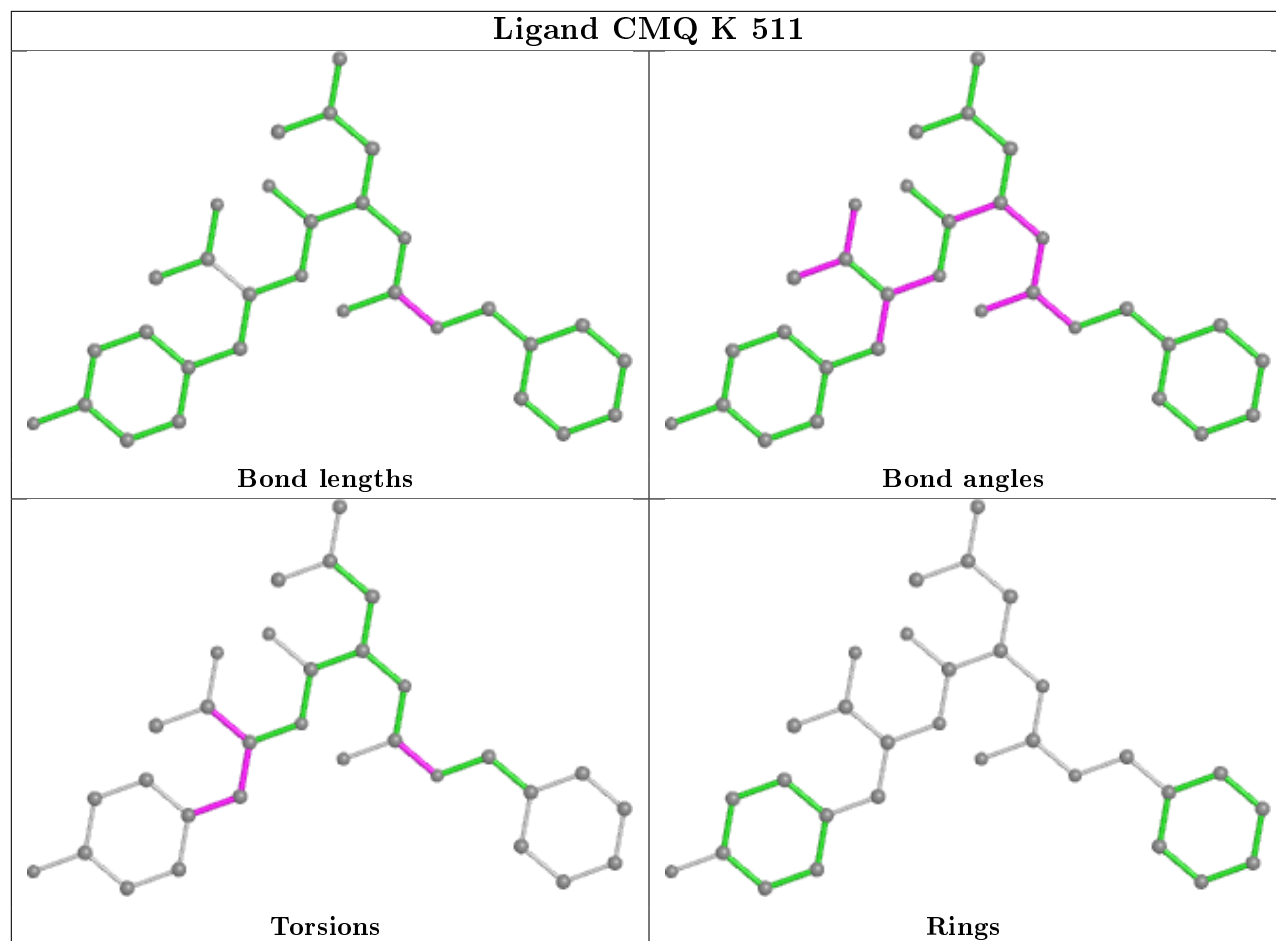
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

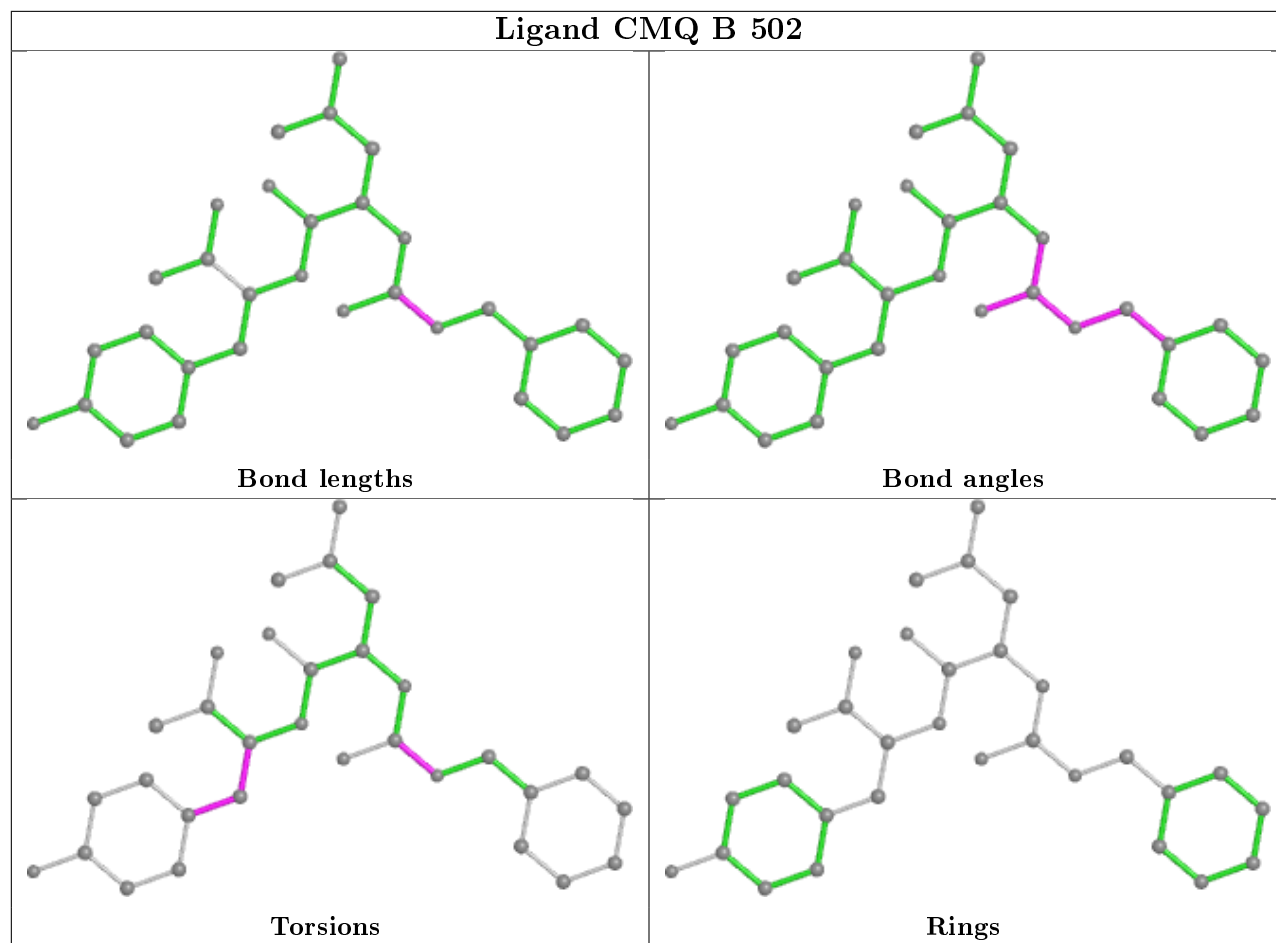




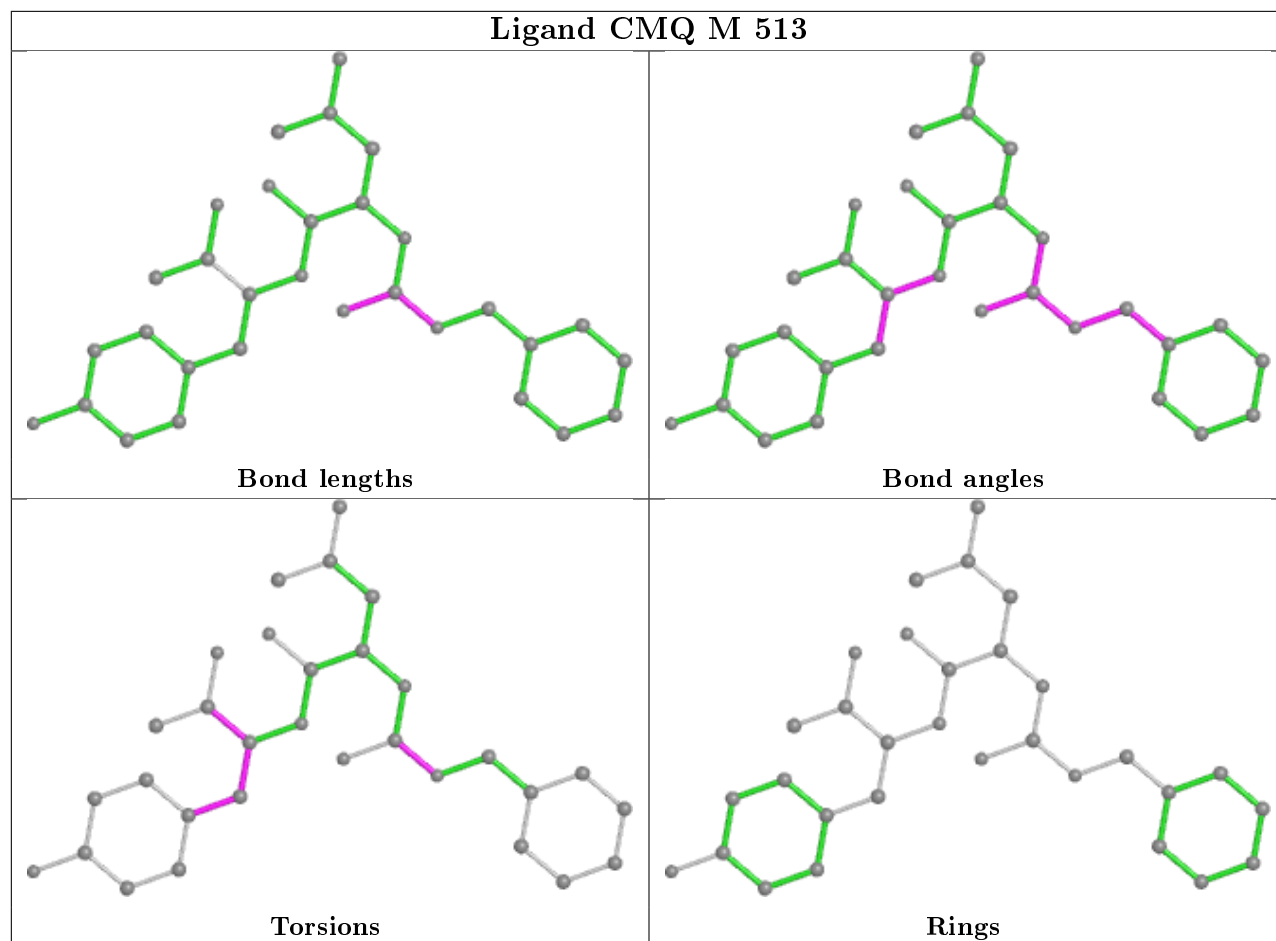


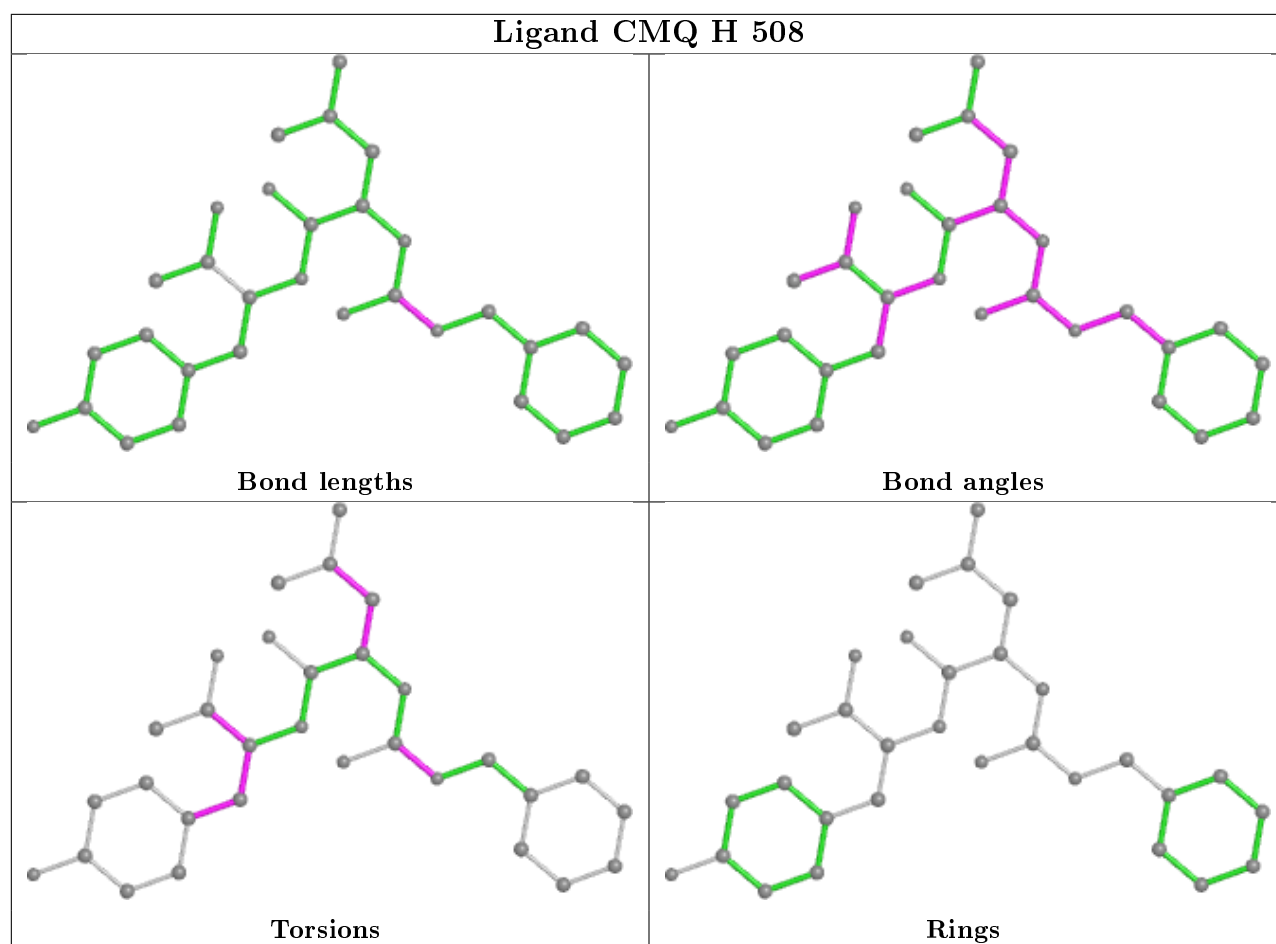


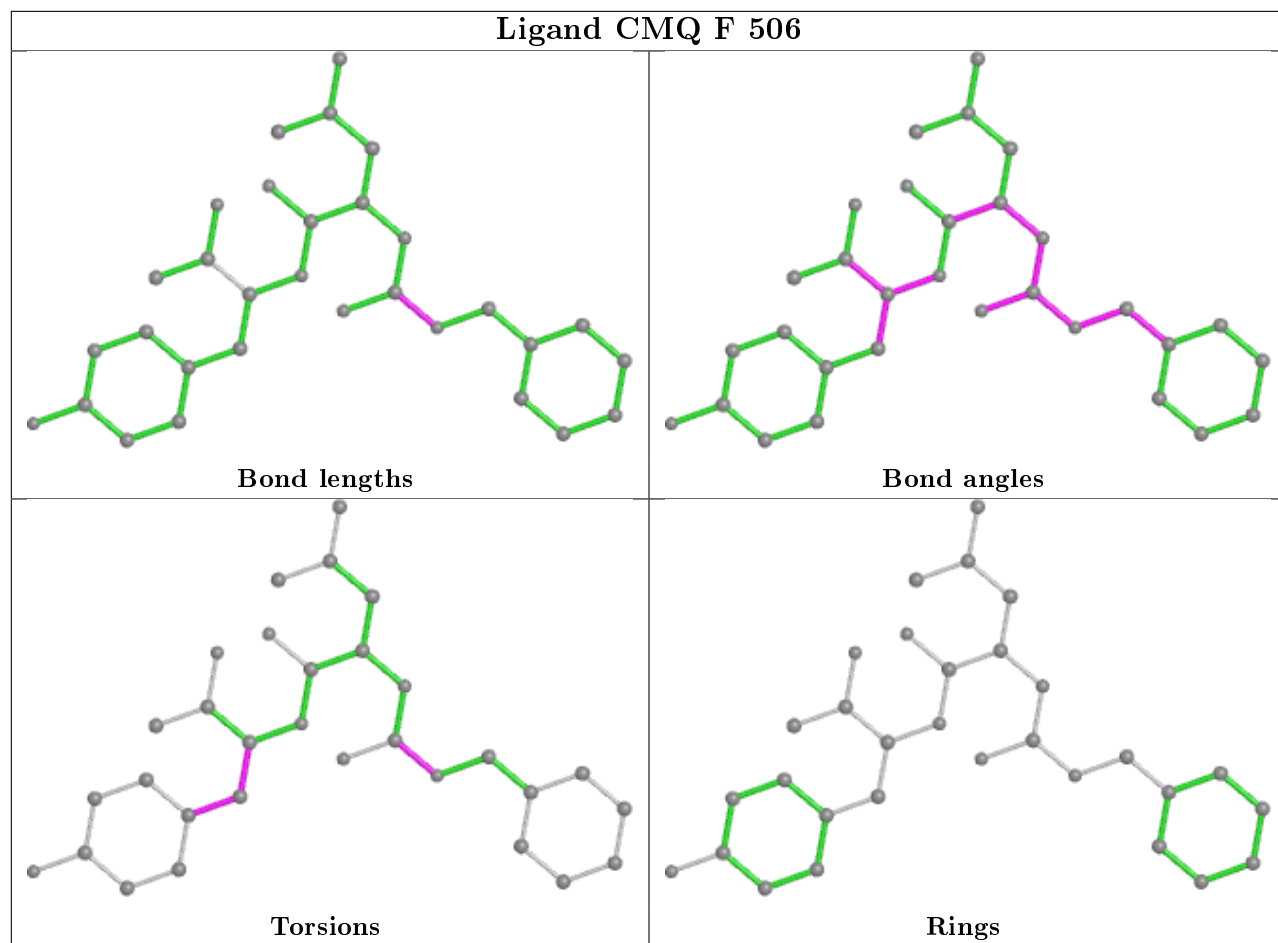


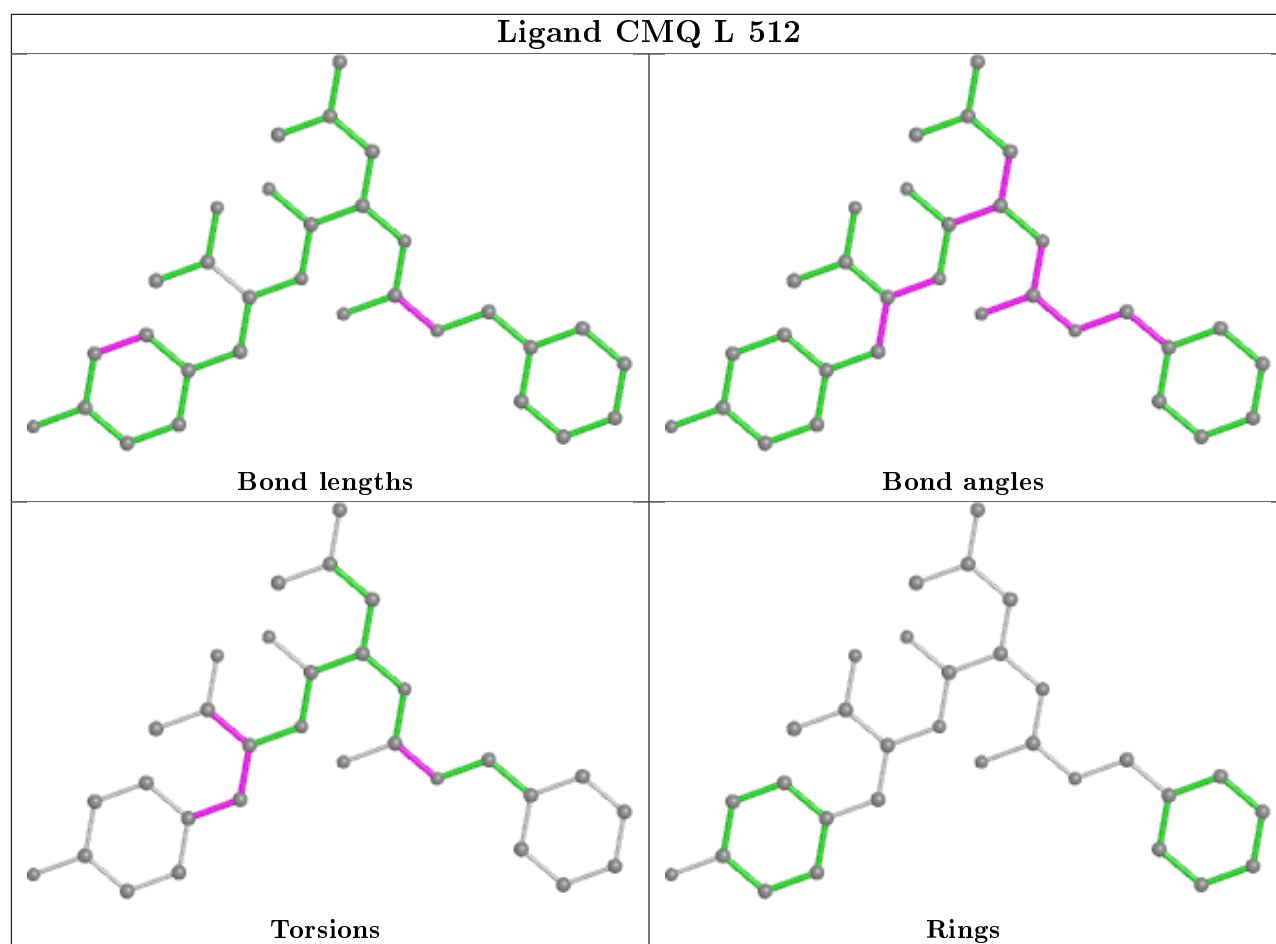


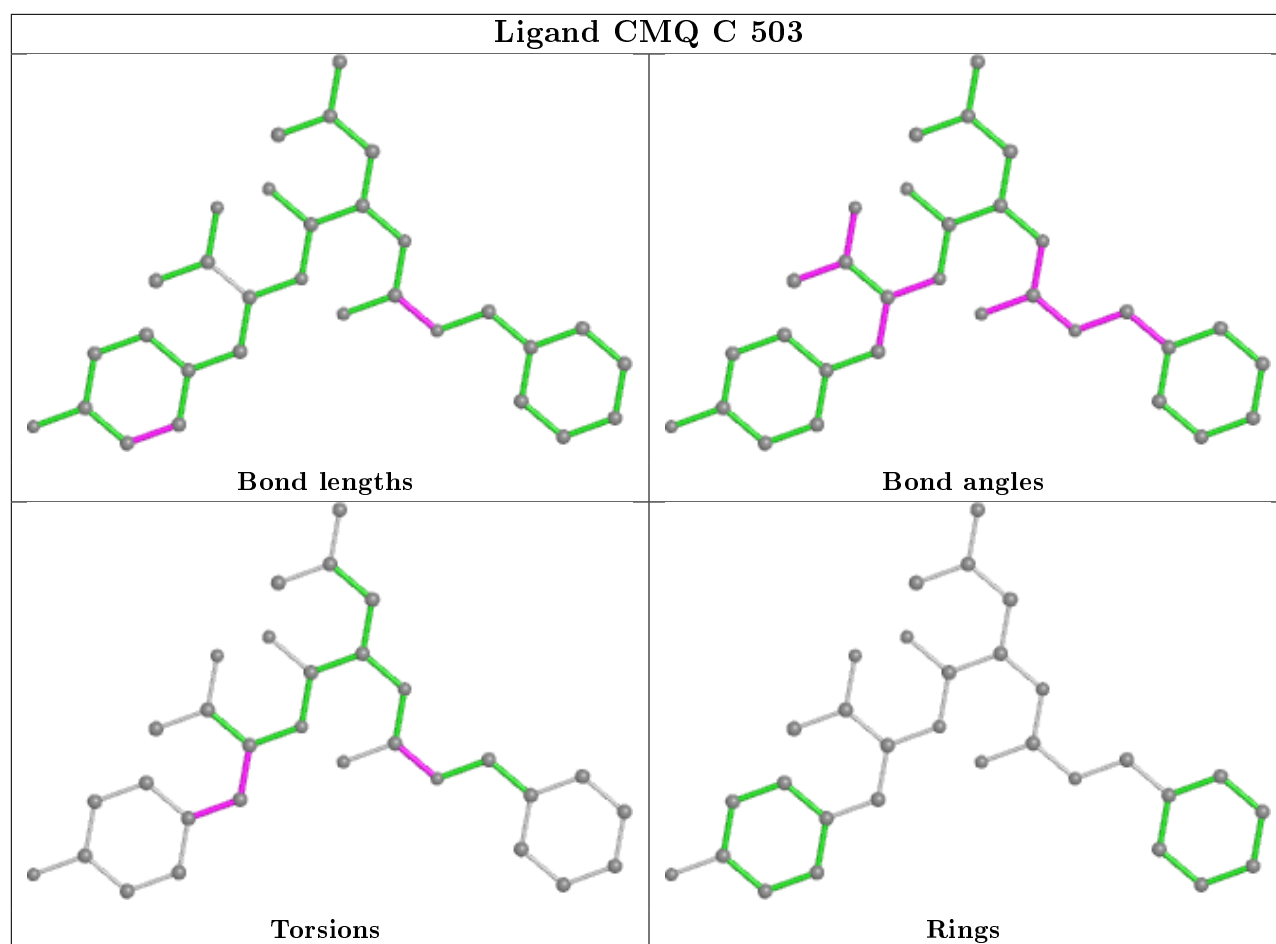
## Ligand CMQ M 513



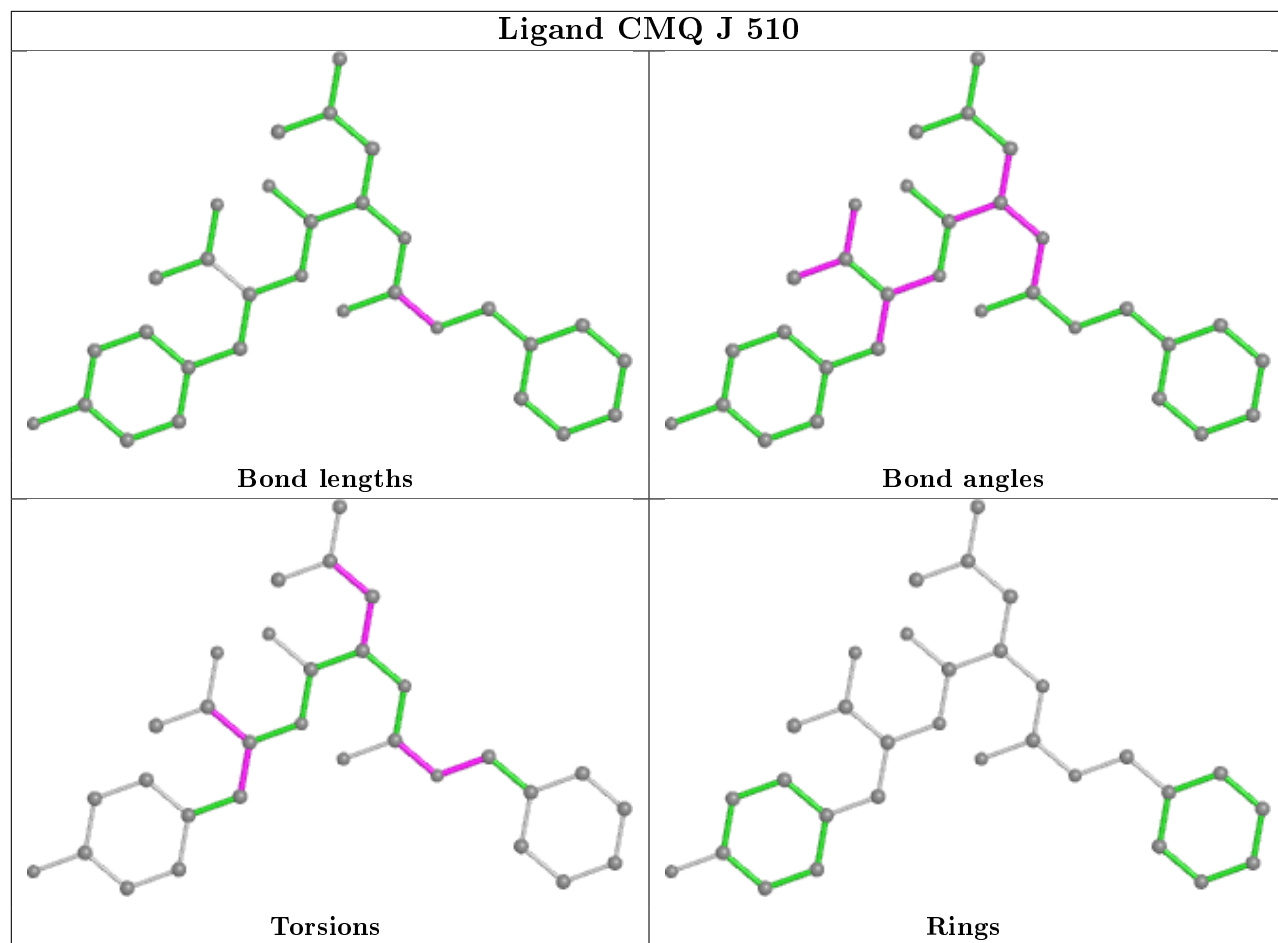


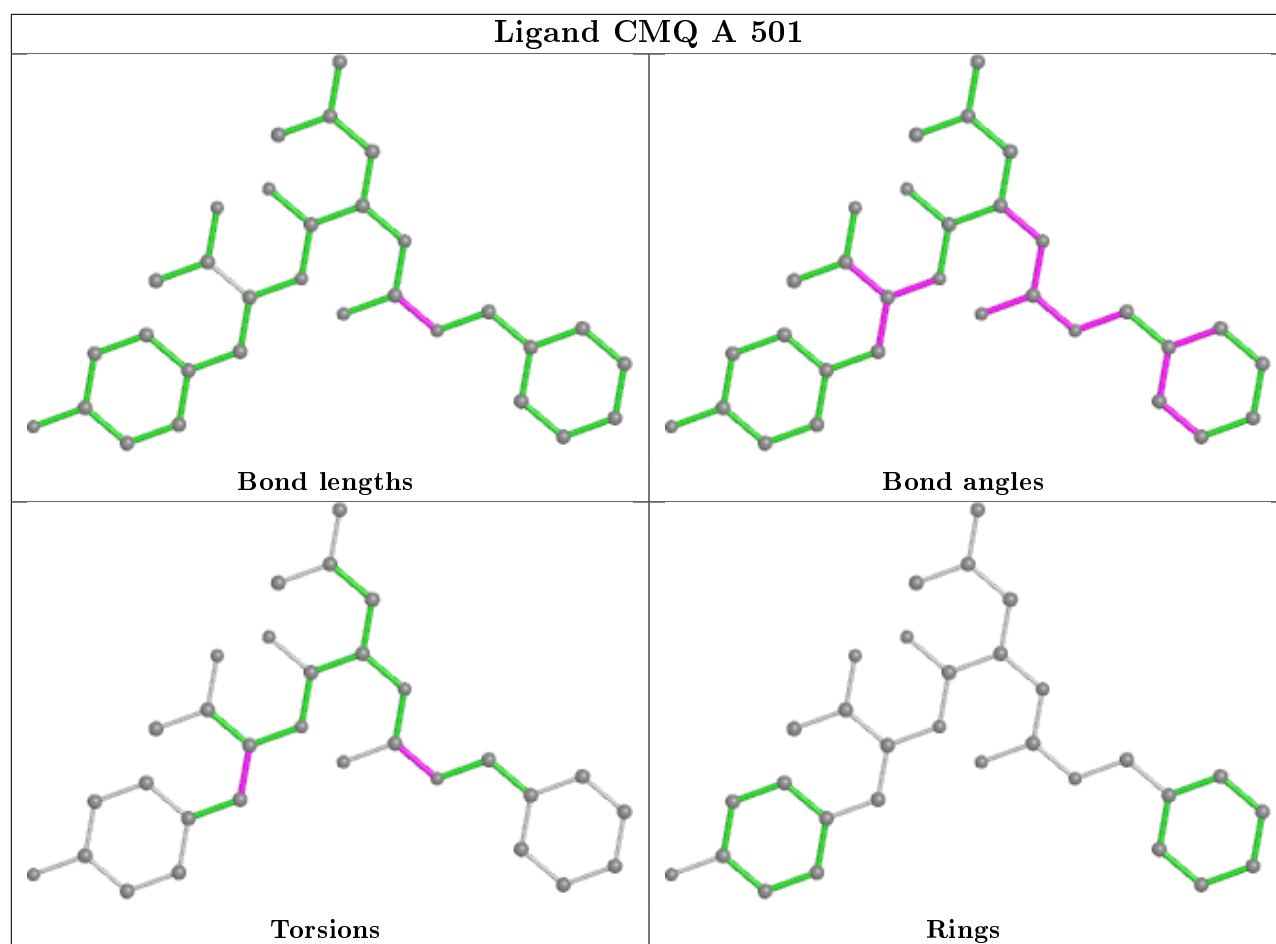


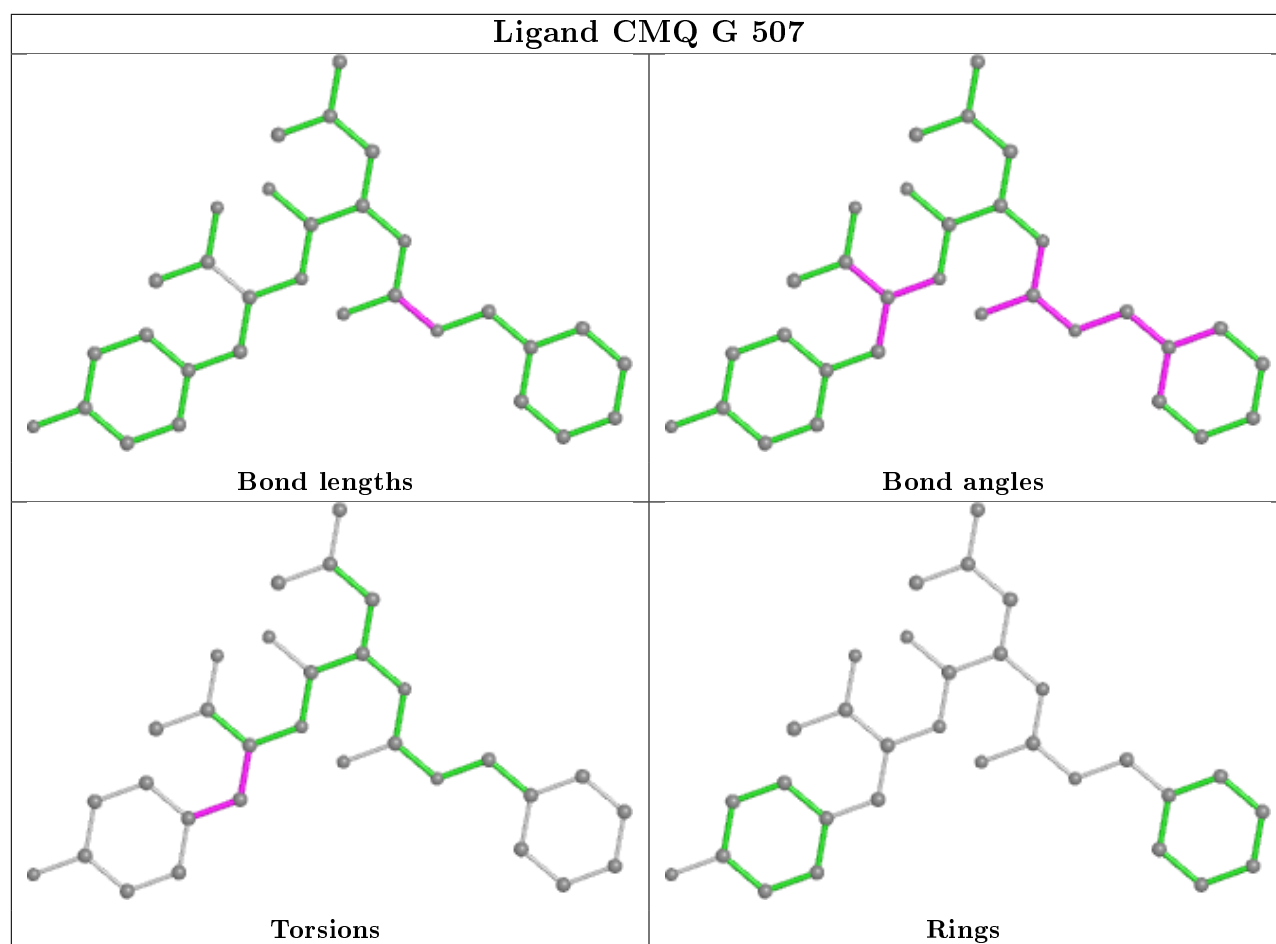


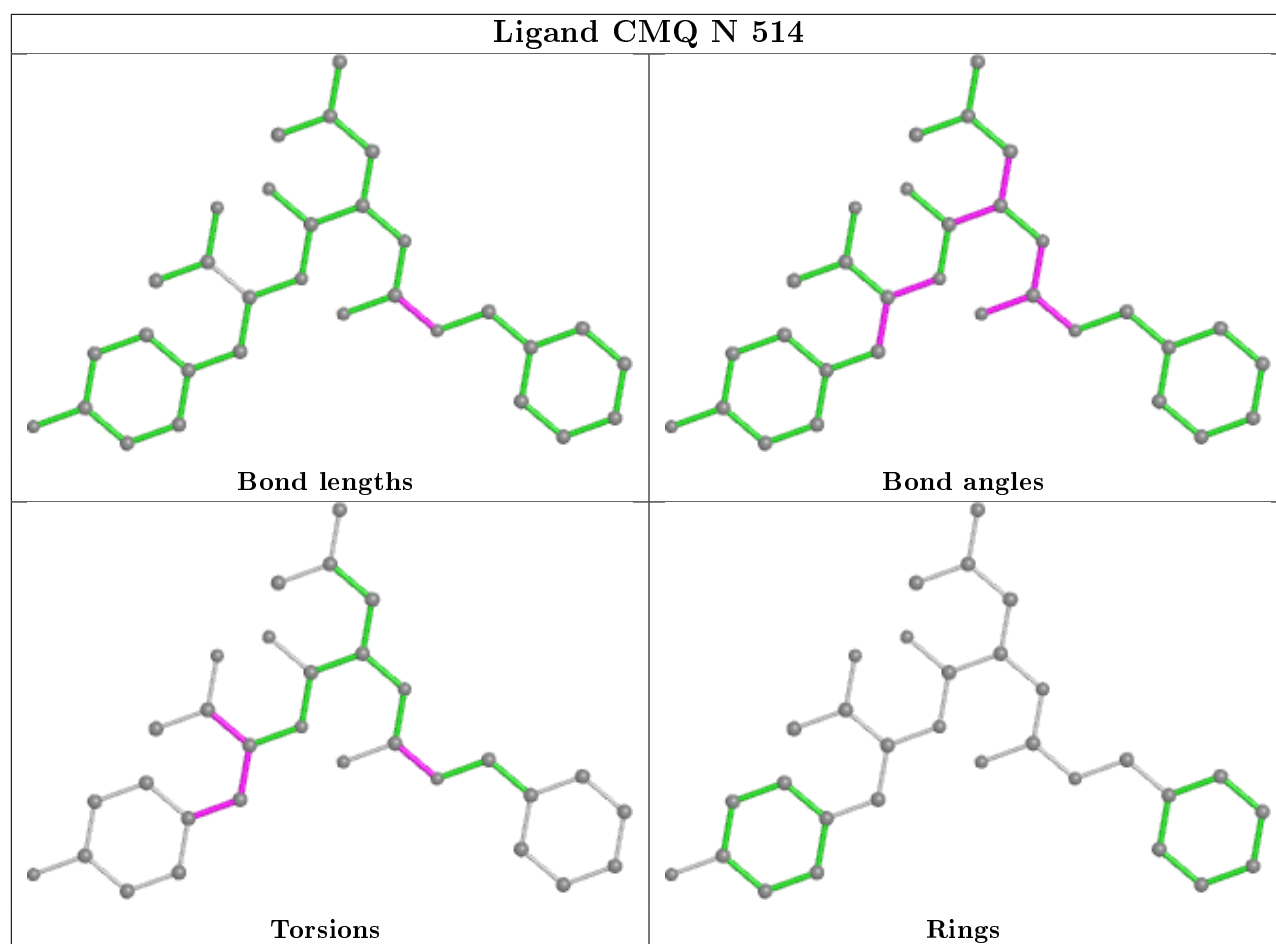












## 5.7 Other polymers [i](#)

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

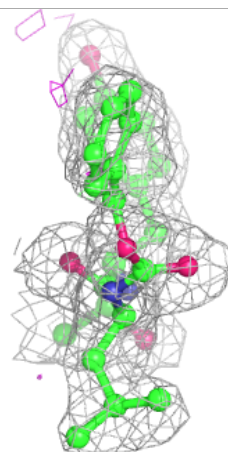
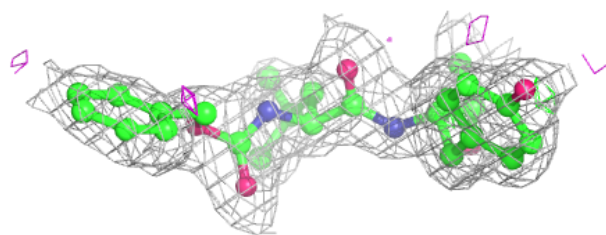
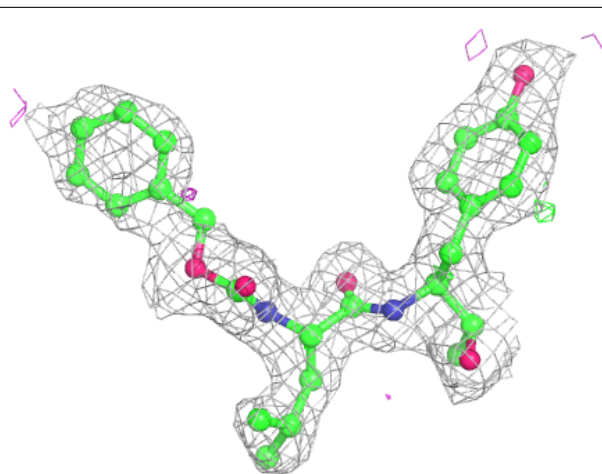
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

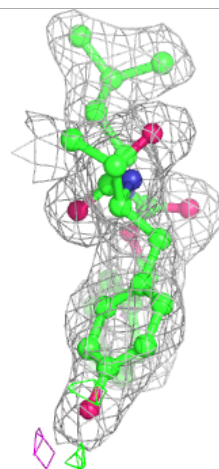
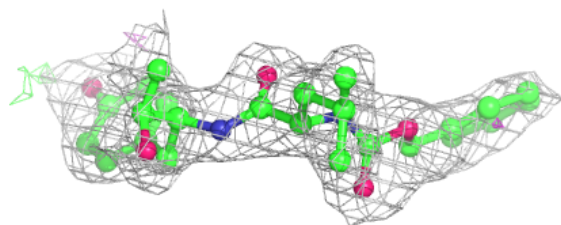
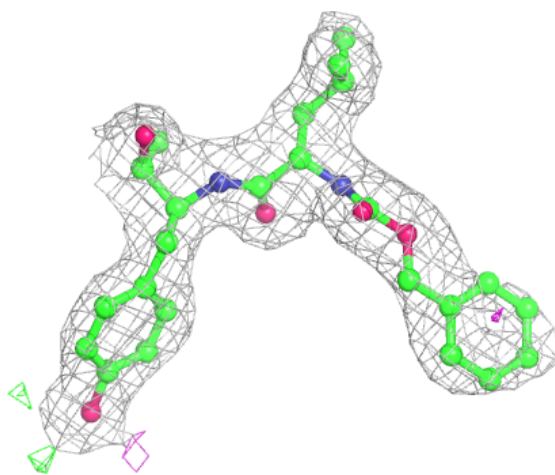
**Electron density around CMQ E 505:**

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



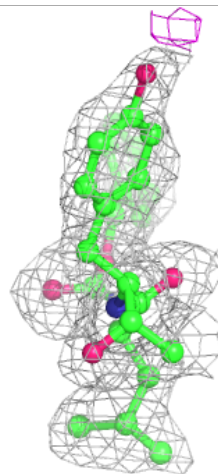
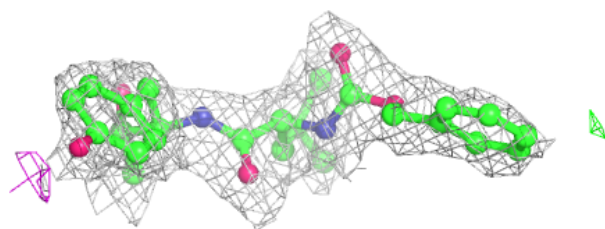
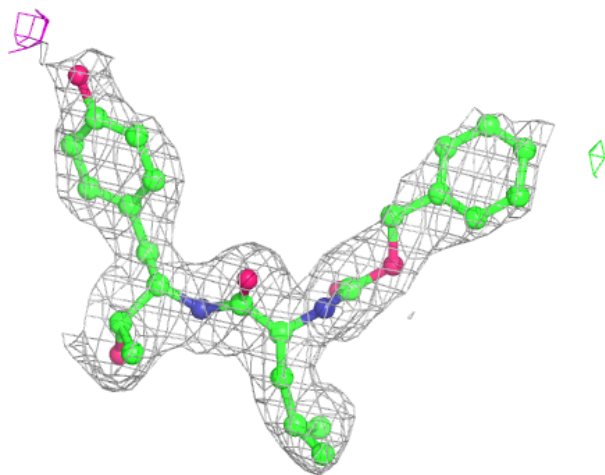
**Electron density around CMQ I 509:**

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



**Electron density around CMQ D 504:**

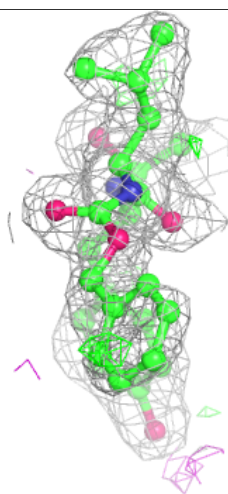
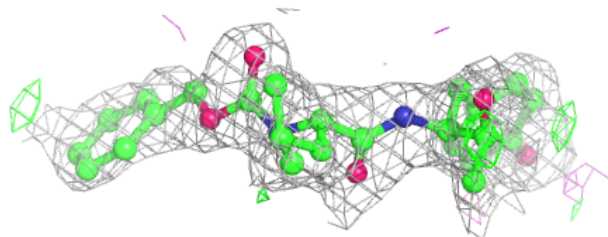
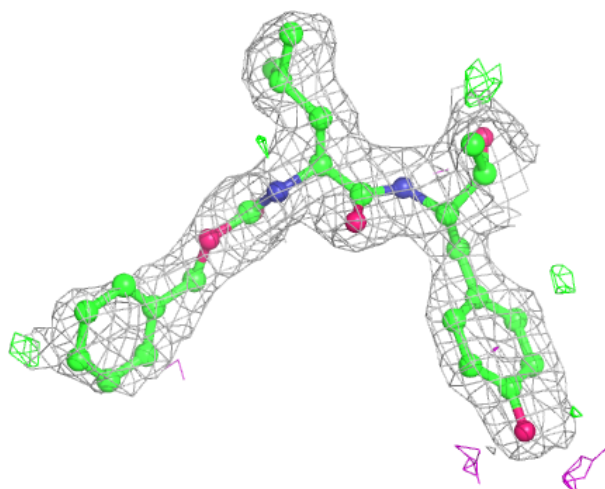
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





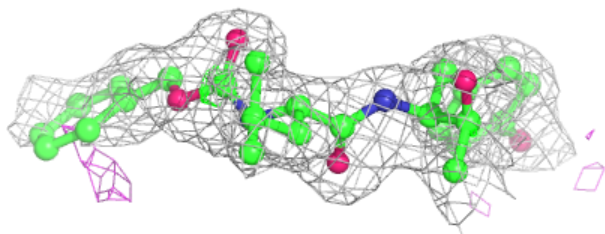
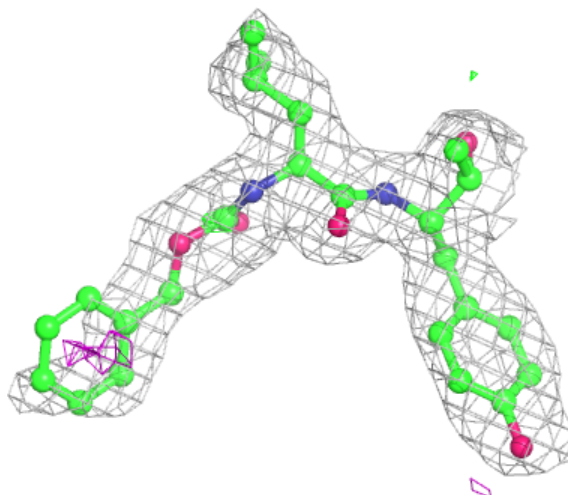
**Electron density around CMQ K 511:**

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



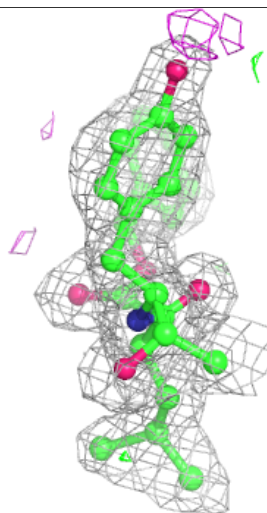
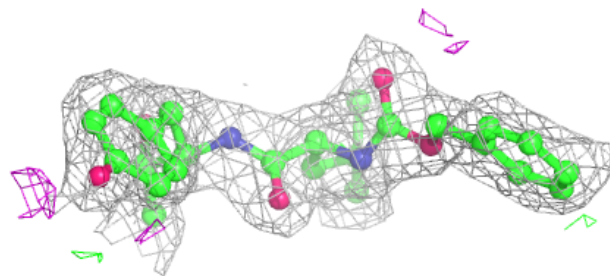
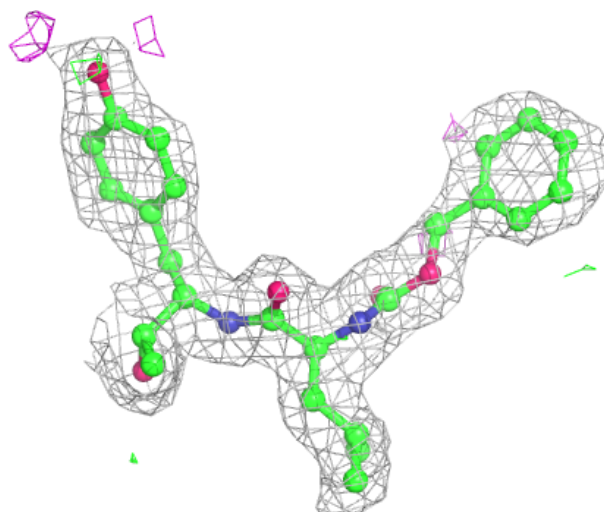
**Electron density around CMQ B 502:**

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



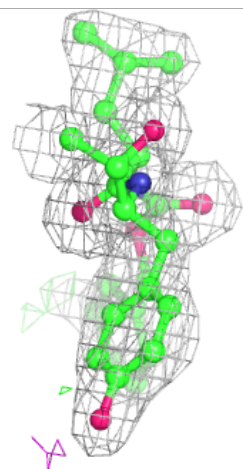
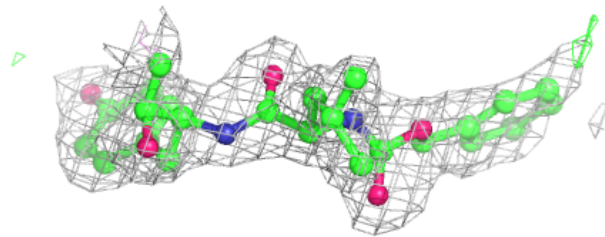
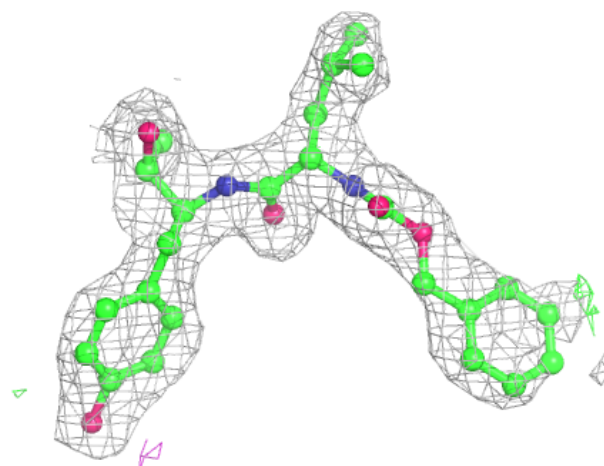
**Electron density around CMQ M 513:**

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



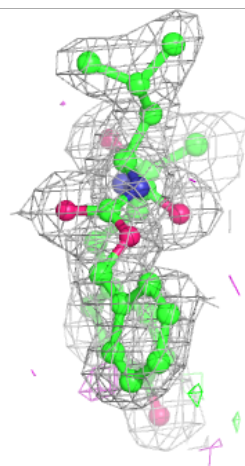
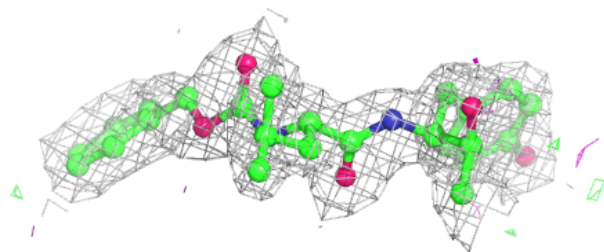
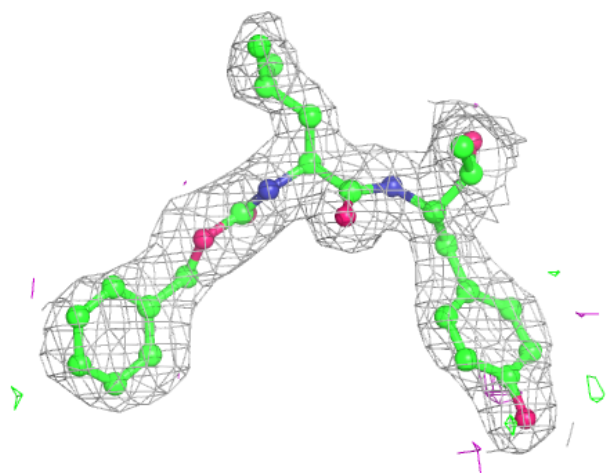
**Electron density around CMQ H 508:**

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



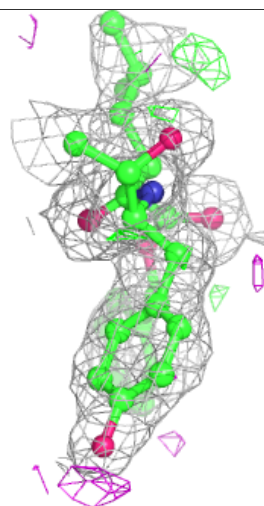
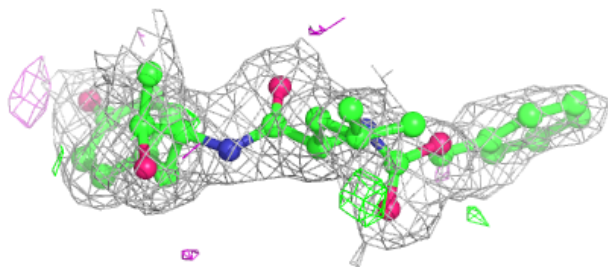
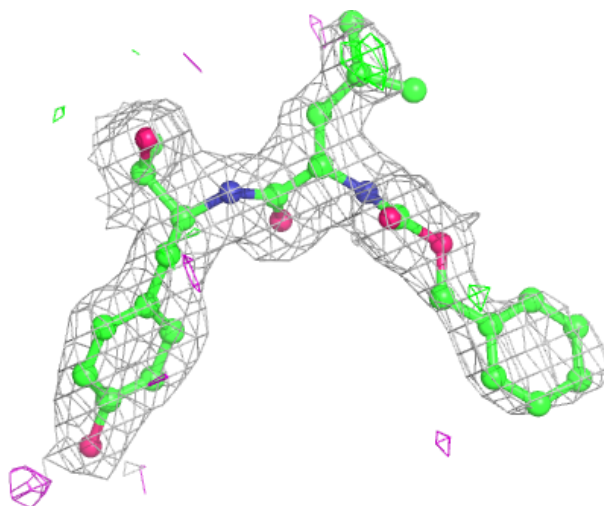
**Electron density around CMQ F 506:**

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



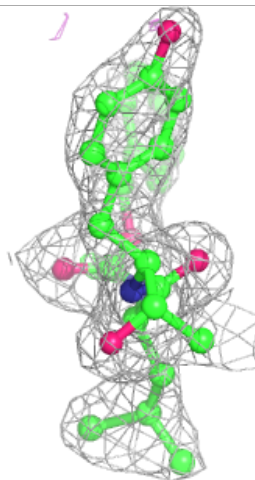
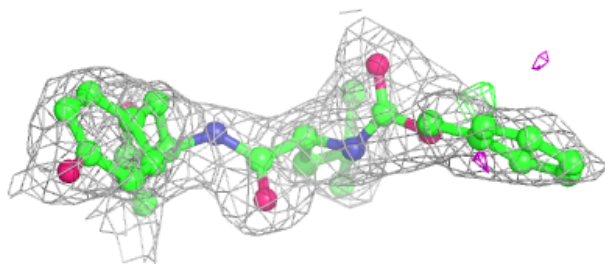
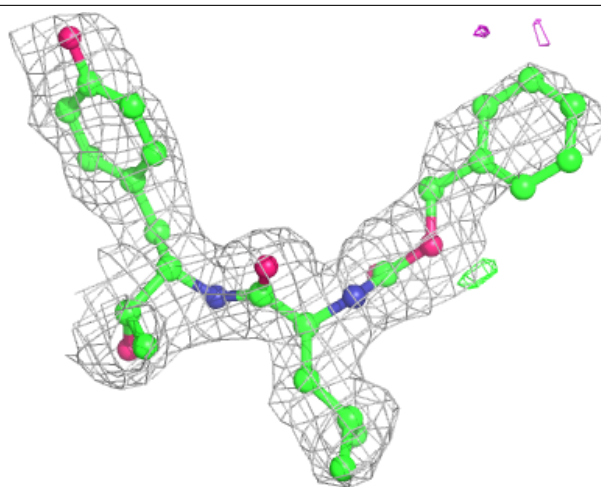
**Electron density around CMQ L 512:**

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



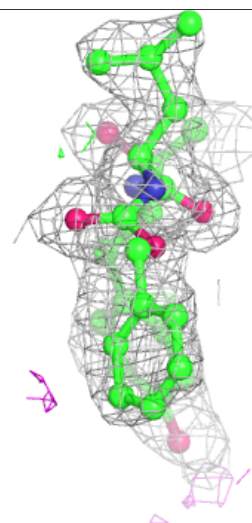
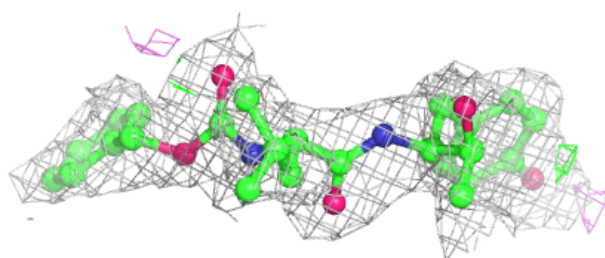
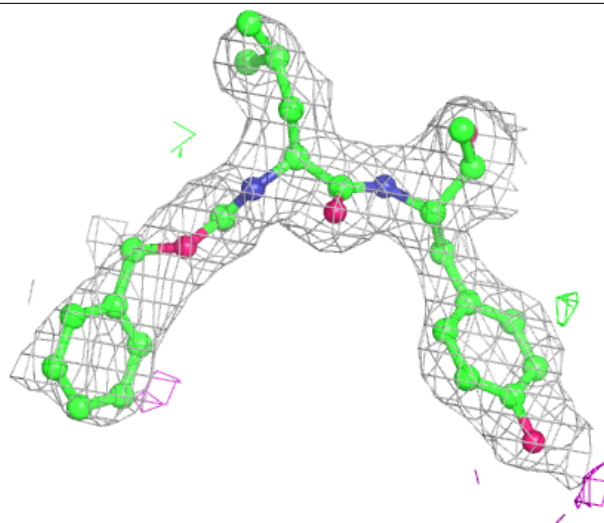
**Electron density around CMQ C 503:**

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



**Electron density around CMQ J 510:**

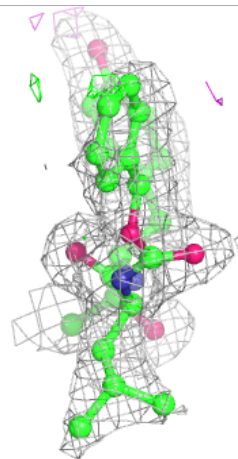
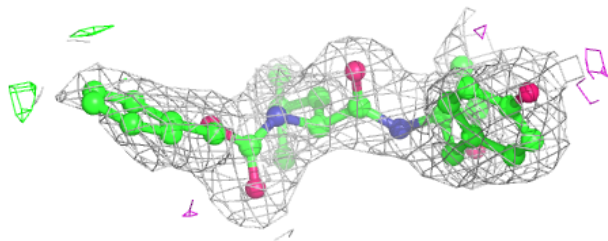
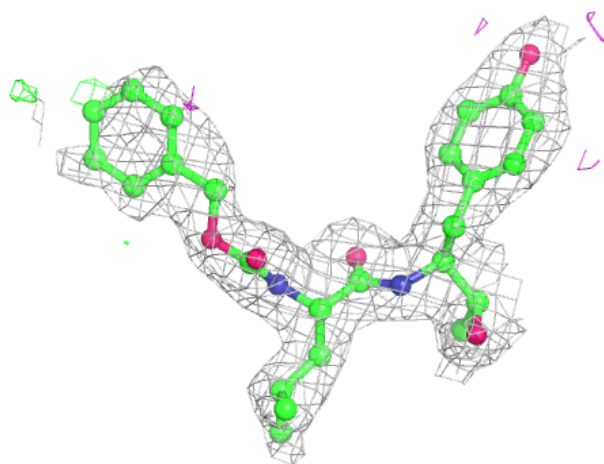
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





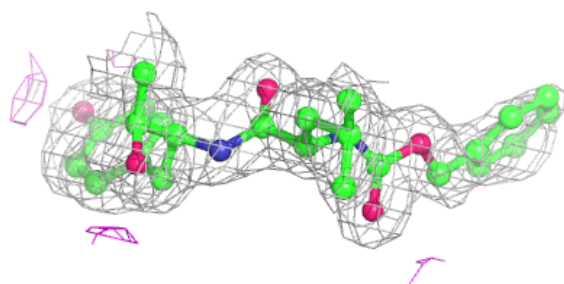
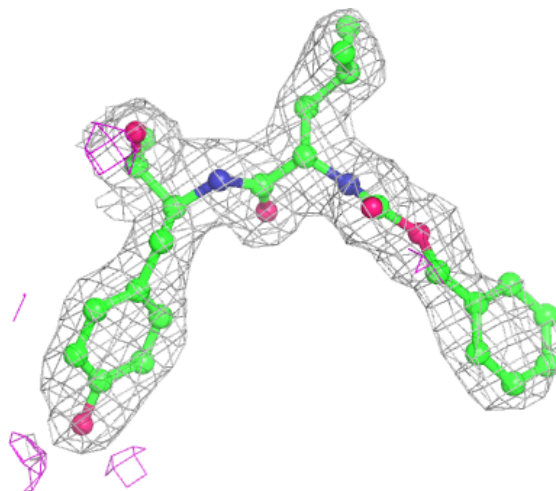
**Electron density around CMQ A 501:**

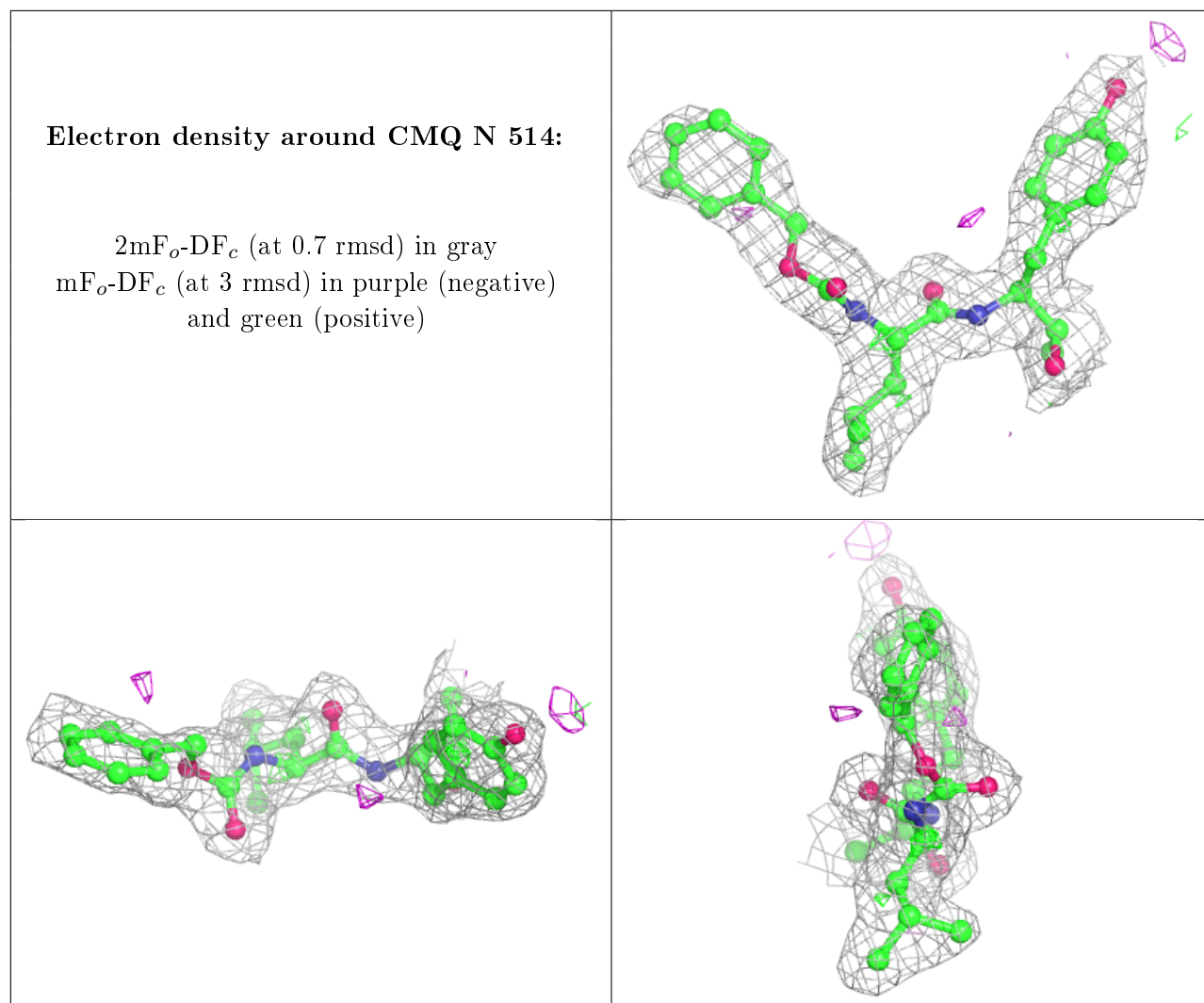
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CMQ G 507:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.