



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:00 AM UTC

PDB ID : 9JOP / pdb_00009jop
Title : Caseinolytic protease P from bacteria
Authors : Lu, M.; Yin, J.; Xiao, Y.
Deposited on : 2024-09-25
Resolution : 2.17 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

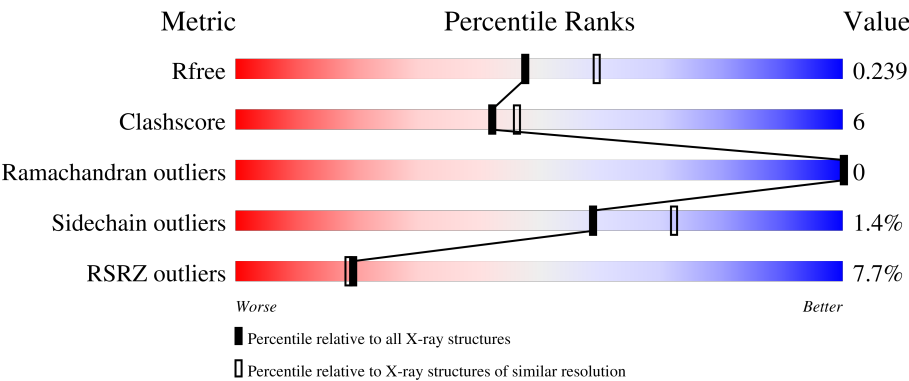
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	H	196	5% 81%15%..
1	I	196	8% 84%12%..
1	J	196	10% 87%11%.
1	K	196	8% 83%14%.
1	L	196	8% 87%11%.

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	196	
1	N	196	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	H	203	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10953 atoms, of which 256 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.

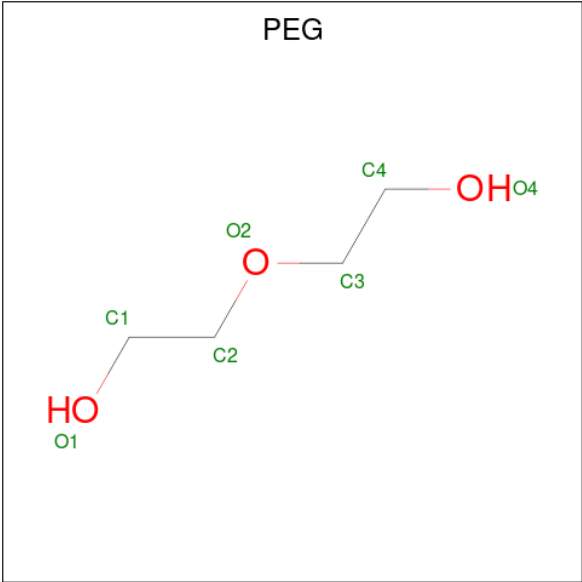
- Molecule 1 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	189	Total	C	N	O	S	0	1	0
			1427	897	243	280	7			
1	I	190	Total	C	N	O	S	0	3	0
			1454	914	248	284	8			
1	J	193	Total	C	N	O	S	0	2	0
			1469	919	253	291	6			
1	K	190	Total	C	N	O	S	0	1	0
			1445	908	244	286	7			
1	L	193	Total	C	N	O	S	0	0	0
			1448	911	250	281	6			
1	M	192	Total	C	N	O	S	0	0	0
			1471	923	252	290	6			
1	N	190	Total	C	N	O	S	0	2	0
			1436	904	244	281	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	0	SER	-	expression tag	UNP A0A0D1I3W4
I	0	SER	-	expression tag	UNP A0A0D1I3W4
J	0	SER	-	expression tag	UNP A0A0D1I3W4
K	0	SER	-	expression tag	UNP A0A0D1I3W4
L	0	SER	-	expression tag	UNP A0A0D1I3W4
M	0	SER	-	expression tag	UNP A0A0D1I3W4
N	0	SER	-	expression tag	UNP A0A0D1I3W4

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃) (labeled as "Ligand of Interest" by depositor).



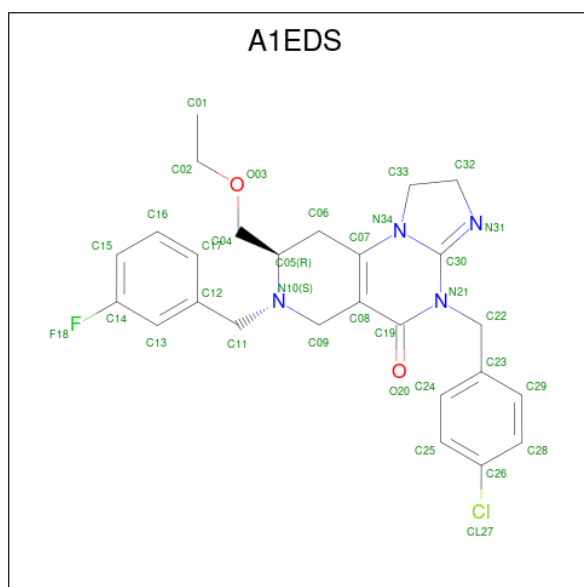
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	O		0	0
			7	4	3			
2	H	1	Total	C	O		0	0
			7	4	3			
2	H	1	Total	C	O		0	0
			7	4	3			
2	I	1	Total	C	O		0	0
			7	4	3			
2	I	1	Total	C	O		0	0
			7	4	3			
2	I	1	Total	C	H	O	0	0
			17	4	10	3		
2	I	1	Total	C	H	O	0	0
			17	4	10	3		
2	J	1	Total	C	O		0	0
			7	4	3			
2	J	1	Total	C	O		0	0
			7	4	3			
2	J	1	Total	C	O		0	0
			7	4	3			
2	K	1	Total	C	H	O	0	0
			17	4	10	3		
2	K	1	Total	C	H	O	0	0
			17	4	10	3		
2	K	1	Total	C	O		0	0
			7	4	3			
2	K	1	Total	C	O		0	0
			7	4	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total C O 7 4 3	0	0
2	L	1	Total C O 7 4 3	0	0
2	L	1	Total C O 7 4 3	0	0
2	L	1	Total C H O 17 4 10 3	0	0
2	M	1	Total C O 7 4 3	0	0
2	M	1	Total C O 7 4 3	0	0
2	N	1	Total C O 7 4 3	0	0
2	N	1	Total C O 7 4 3	0	0
2	N	1	Total C O 7 4 3	0	0
2	N	1	Total C H O 17 4 10 3	0	0

- Molecule 3 is (12 {R})-7-[(4-chlorophenyl)methyl]-12-(ethoxymethyl)-11-[(3-fluorophenyl)methyl]-2,5,7,11-tetrazatricyclo[7.4.0.0[^]{2,6}]trideca-1(9),5-dien-8-one (CCD ID: A1EDS) (formula: C₂₆H₂₈ClFN₄O₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	H	1	Total	C	Cl	F	H	N	O	0	0
			62	26	1	1	28	4	2		
3	I	1	Total	C	Cl	F	H	N	O	0	0
			62	26	1	1	28	4	2		
3	J	1	Total	C	Cl	F	H	N	O	0	0
			62	26	1	1	28	4	2		
3	K	1	Total	C	Cl	F	H	N	O	0	0
			62	26	1	1	28	4	2		
3	L	1	Total	C	Cl	F	H	N	O	0	0
			62	26	1	1	28	4	2		
3	M	1	Total	C	Cl	F	H	N	O	0	0
			62	26	1	1	28	4	2		
3	N	1	Total	C	Cl	F	H	N	O	0	0
			62	26	1	1	28	4	2		

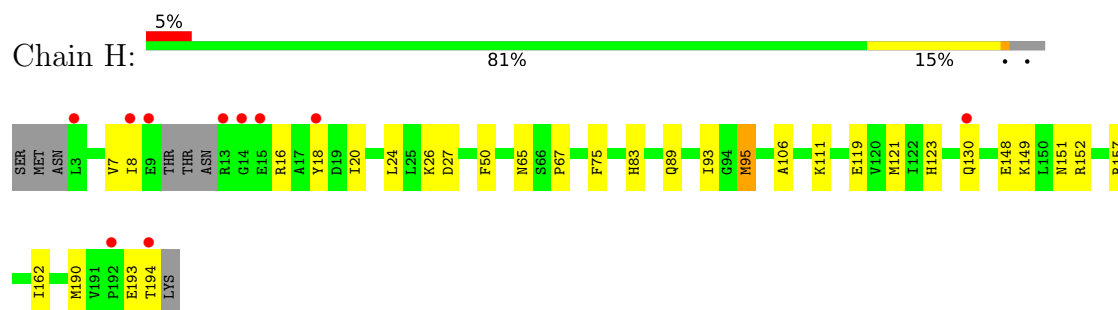
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	29	Total	O	0	0
			29	29		
4	I	26	Total	O	0	0
			26	26		
4	J	21	Total	O	0	0
			21	21		
4	K	15	Total	O	0	0
			15	15		
4	L	9	Total	O	0	0
			9	9		
4	M	9	Total	O	0	0
			9	9		
4	N	32	Total	O	0	0
			32	32		

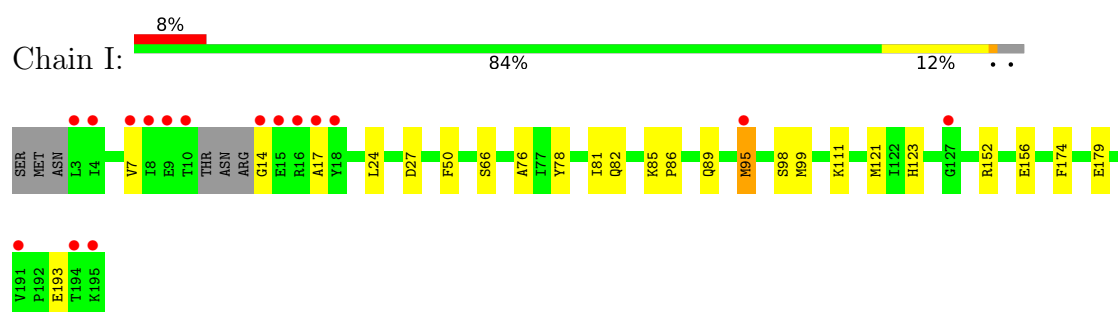
3 Residue-property plots [i](#)

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.

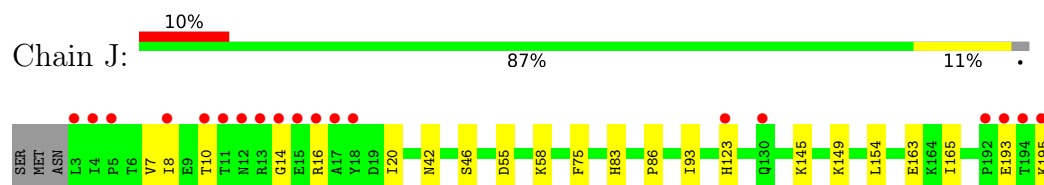
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



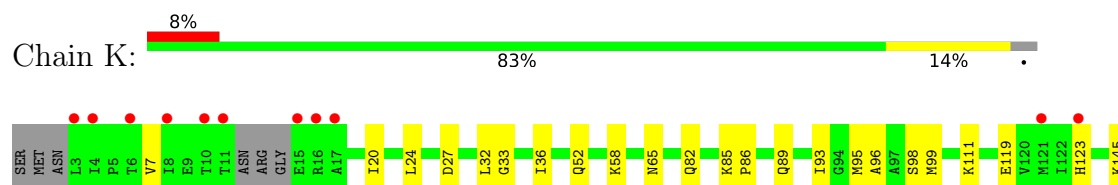
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

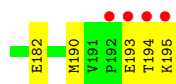


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

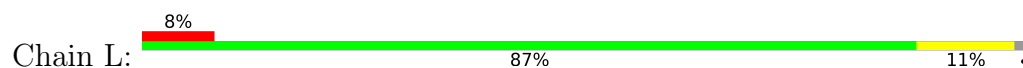


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

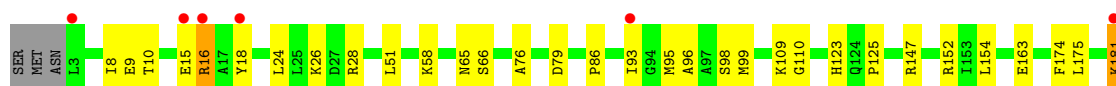
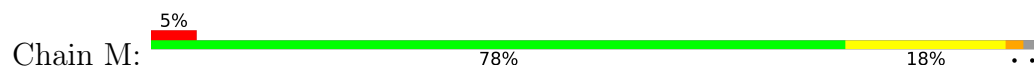




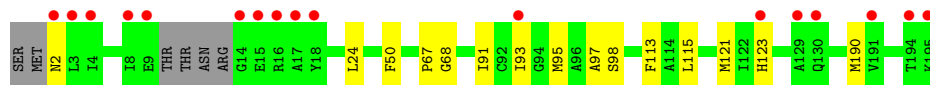
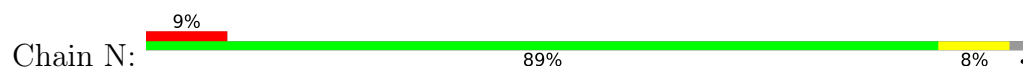
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



- 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	Depositor
Cell constants a, b, c, α , β , γ	123.64Å 123.64Å 107.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.21 – 2.17 41.21 – 2.17	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.21-2.17) 100.0 (41.21-2.17)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.201 , 0.238 0.203 , 0.239	Depositor DCC
R_{free} test set	4292 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: PEG, A1EDS

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	H	0.35	0/1445	0.45	0/1954
1	I	0.31	1/1472 (0.1%)	0.40	0/1990
1	J	0.35	0/1488	0.47	0/2015
1	K	0.35	0/1463	0.44	0/1979
1	L	0.33	0/1467	0.38	0/1987
1	M	0.34	0/1490	0.42	0/2014
1	N	0.23	0/1456	0.35	0/1970
All	All	0.32	1/10281 (0.0%)	0.42	0/13909

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	66	SER	C-N	6.82	1.39	1.33

There are no bond angle outliers.

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	H	1427	0	1399	25	0
1	I	1454	0	1428	20	0
1	J	1469	0	1431	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1445	0	1420	20	0
1	L	1448	0	1430	16	0
1	M	1471	0	1469	39	0
1	N	1436	0	1418	11	0
2	H	21	0	30	5	0
2	I	28	20	40	1	0
2	J	21	0	30	0	0
2	K	28	20	40	3	0
2	L	28	10	40	3	0
2	M	14	0	20	1	0
2	N	28	10	40	1	0
3	H	34	28	0	1	0
3	I	34	28	0	1	0
3	J	34	28	0	0	0
3	K	34	28	0	0	0
3	L	34	28	0	1	0
3	M	34	28	0	1	0
3	N	34	28	0	1	0
4	H	29	0	0	0	0
4	I	26	0	0	0	0
4	J	21	0	0	0	0
4	K	15	0	0	0	0
4	L	9	0	0	0	0
4	M	9	0	0	0	0
4	N	32	0	0	0	0
All	All	10697	256	10235	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (132) 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:H:18:TYR:HH	1:I:14:GLY:N	1.88	0.71
1:H:83:HIS:NE2	2:H:203:PEG:H42	2.06	0.70
1:H:83:HIS:HE2	2:H:203:PEG:H42	1.56	0.70
1:H:24:LEU:HD12	3:H:204:A1EDS:CL27	2.29	0.69
1:L:16:ARG:HH21	1:M:10:THR:HG23	1.58	0.68
1:L:125:PRO:HD2	1:L:147:ARG:HG3	1.75	0.67
1:L:24:LEU:HD23	3:L:205:A1EDS:CL27	2.32	0.66
1:L:83:HIS:O	1:M:193:GLU:HB3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:TYR:CE1	1:M:8:ILE:HD12	2.31	0.66
1:M:152:ARG:NH1	1:M:152:ARG:HB3	2.12	0.64
1:M:65:ASN:HB2	1:M:93:ILE:HG13	1.79	0.63
1:H:83:HIS:CD2	2:H:203:PEG:H42	2.33	0.62
1:M:181:LYS:HD3	1:M:188:GLU:HA	1.81	0.62
1:N:24:LEU:HD23	3:N:205:A1EDS:CL27	2.37	0.62
1:H:50:PHE:CZ	1:I:7:VAL:HG13	2.34	0.61
1:K:194:THR:O	1:K:195:LYS:C	2.43	0.61
1:J:83:HIS:O	1:K:193:GLU:HB2	2.00	0.61
1:M:16:ARG:CG	1:M:16:ARG:HH11	2.14	0.61
1:M:24:LEU:HD12	3:M:203:A1EDS:CL27	2.38	0.61
1:H:151:ASN:HB3	1:H:162:ILE:HD11	1.83	0.60
1:I:24:LEU:HD12	3:I:205:A1EDS:CL27	2.39	0.60
1:I:121[B]:MET:HG3	1:I:174:PHE:CD1	2.36	0.59
1:K:95[A]:MET:HE3	1:K:119:GLU:O	2.02	0.59
1:H:93:ILE:HG13	1:H:93:ILE:O	2.00	0.59
1:L:4:ILE:HG23	1:L:20:ILE:HG22	1.86	0.57
1:K:123:HIS:HE2	2:K:204:PEG:HO4	1.51	0.57
1:I:81:ILE:O	1:J:195:LYS:HE3	2.05	0.56
1:L:174:PHE:H	2:L:204:PEG:C1	2.17	0.56
1:L:123:HIS:HE2	2:L:202:PEG:HO1	1.53	0.56
1:M:16:ARG:HH11	1:M:16:ARG:HG2	1.70	0.55
1:M:95:MET:HG2	1:M:96:ALA:N	2.23	0.54
1:H:151:ASN:HB3	1:H:162:ILE:CD1	2.39	0.53
1:I:89:GLN:HG2	1:I:111:LYS:HB3	1.92	0.52
1:K:82:GLN:O	1:L:192:PRO:HB3	2.09	0.52
1:M:79:ASP:HB3	1:N:115:LEU:HD13	1.92	0.52
1:M:16:ARG:HG2	1:M:16:ARG:NH1	2.25	0.52
1:K:93:ILE:O	1:K:93:ILE:HG13	2.11	0.51
1:H:95[B]:MET:HG2	1:H:119:GLU:HB2	1.91	0.51
1:M:98:SER:OG	1:M:99:MET:N	2.37	0.51
1:M:9:GLU:HB2	1:M:16:ARG:HH12	1.75	0.51
1:H:18:TYR:OH	1:H:26:LYS:NZ	2.45	0.50
1:M:174:PHE:C	1:M:175:LEU:HD12	2.37	0.50
1:I:82:GLN:HA	1:J:195:LYS:HG2	1.93	0.50
1:J:7:VAL:HG11	1:J:20:ILE:HD12	1.94	0.49
1:J:55:ASP:CG	1:J:58:LYS:HG3	2.37	0.49
1:K:123:HIS:NE2	2:K:204:PEG:O4	2.43	0.49
1:M:125:PRO:HD2	1:M:147:ARG:HG3	1.94	0.49
1:J:123:HIS:C	1:J:123:HIS:CD2	2.89	0.49
1:I:121[A]:MET:HE2	1:I:174:PHE:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:154:LEU:HB3	1:J:165:ILE:HD13	1.95	0.48
1:I:123:HIS:C	1:I:123:HIS:CD2	2.92	0.48
1:N:91:ILE:HG23	1:N:93:ILE:HD13	1.95	0.48
1:H:193:GLU:O	1:H:194:THR:C	2.56	0.48
1:H:8:ILE:HA	1:H:16:ARG:O	2.13	0.48
1:H:123:HIS:CD2	1:H:123:HIS:C	2.92	0.48
1:K:89:GLN:HG2	1:K:111:LYS:HB3	1.93	0.48
1:L:89:GLN:HG2	1:L:111:LYS:HB3	1.96	0.48
1:N:91:ILE:HA	1:N:113:PHE:O	2.13	0.48
1:H:148:GLU:HG2	1:H:152:ARG:HH21	1.78	0.48
1:J:46:SER:OG	1:K:24:LEU:HD11	2.14	0.48
1:L:82:GLN:HA	1:L:82:GLN:OE1	2.13	0.48
1:M:28:ARG:HG2	1:M:51:LEU:HD22	1.96	0.47
1:M:123:HIS:CD2	1:M:123:HIS:C	2.92	0.47
1:H:95[B]:MET:HE1	1:H:121:MET:HB2	1.97	0.47
1:H:106:ALA:HA	1:H:157:ARG:HD2	1.96	0.47
1:M:16:ARG:CZ	1:M:18:TYR:HE2	2.26	0.47
1:N:68:GLY:HA3	1:N:98:SER:HB3	1.96	0.47
1:N:190:MET:HE3	1:N:190:MET:HB2	1.68	0.47
1:I:50:PHE:CZ	1:J:7:VAL:HB	2.50	0.47
2:H:203:PEG:H41	1:I:193:GLU:CD	2.39	0.47
1:H:67:PRO:HB3	1:H:95[A]:MET:HE1	1.97	0.47
1:M:175:LEU:HD12	1:M:175:LEU:N	2.30	0.46
1:I:95[A]:MET:HE3	1:I:95[A]:MET:HB3	1.71	0.46
1:H:89:GLN:HG2	1:H:111:LYS:HB3	1.98	0.46
1:M:16:ARG:HH11	1:M:16:ARG:CB	2.28	0.46
1:M:154:LEU:HD12	1:M:154:LEU:HA	1.78	0.46
1:J:75:PHE:CE2	1:J:149:LYS:HE3	2.52	0.45
1:M:16:ARG:HH11	1:M:16:ARG:HB3	1.80	0.45
1:K:98:SER:OG	1:K:99:MET:N	2.48	0.45
1:N:97:ALA:CB	1:N:121:MET:HE3	2.46	0.45
1:M:10:THR:HG22	1:M:15:GLU:OE1	2.17	0.45
1:M:16:ARG:HH21	1:M:26:LYS:HE3	1.81	0.45
1:M:8:ILE:CG2	1:M:15:GLU:HG3	2.47	0.45
1:M:152:ARG:CB	1:M:152:ARG:CZ	2.95	0.45
1:H:65:ASN:HB2	1:H:93:ILE:HG13	2.00	0.44
1:K:95[A]:MET:HG3	1:K:96:ALA:N	2.33	0.44
1:H:75:PHE:CE2	1:H:149:LYS:HE3	2.52	0.44
1:K:190:MET:HE3	1:K:190:MET:HB2	1.85	0.44
1:L:98:SER:OG	1:L:99:MET:N	2.50	0.44
1:L:190:MET:HE3	1:L:190:MET:HB2	1.79	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:7:VAL:O	1:I:17:ALA:HA	2.18	0.44
1:M:93:ILE:HG13	1:M:93:ILE:O	2.18	0.43
1:M:193:GLU:O	1:M:194:THR:C	2.61	0.43
1:M:163:GLU:CD	1:M:163:GLU:N	2.77	0.43
1:M:182:GLU:O	2:M:201:PEG:H41	2.18	0.43
1:L:174:PHE:H	2:L:204:PEG:H12	1.82	0.43
1:M:26:LYS:O	1:M:26:LYS:HG2	2.18	0.43
1:M:191:VAL:O	1:M:192:PRO:C	2.61	0.43
1:M:109:LYS:HE3	1:M:109:LYS:HB2	1.87	0.43
1:I:98:SER:OG	1:I:99:MET:N	2.43	0.43
1:H:123:HIS:NE2	2:H:201:PEG:O1	2.52	0.43
1:K:52:GLN:HE22	2:K:202:PEG:C1	2.32	0.43
1:I:78:TYR:O	1:I:82:GLN:HG2	2.20	0.42
1:N:98:SER:HB2	1:N:123:HIS:HE1	1.84	0.42
1:M:110:GLY:H	1:M:187:ASP:CG	2.27	0.42
1:N:67:PRO:HB3	1:N:95[B]:MET:HE1	2.00	0.42
1:J:10:THR:HA	1:J:14:GLY:O	2.20	0.42
1:K:95[B]:MET:HE2	1:K:95[B]:MET:HB3	1.67	0.42
1:M:58:LYS:O	1:M:86:PRO:HB3	2.20	0.42
1:H:7:VAL:HB	1:N:50:PHE:CZ	2.54	0.42
1:I:86:PRO:O	1:J:195:LYS:HE2	2.19	0.42
1:I:179:GLU:HB3	2:I:204:PEG:H41	2.01	0.42
1:J:163:GLU:H	1:J:163:GLU:CD	2.28	0.42
1:L:8:ILE:HD13	1:L:17:ALA:HA	2.02	0.42
1:J:58:LYS:O	1:J:86:PRO:HB3	2.20	0.41
1:K:58:LYS:O	1:K:86:PRO:HB3	2.21	0.41
1:M:66:SER:C	1:M:95:MET:HE3	2.46	0.41
1:I:152:ARG:O	1:I:156:GLU:HG3	2.20	0.41
1:L:85:LYS:N	1:L:86:PRO:CD	2.84	0.41
1:K:32:LEU:HD11	1:K:36:ILE:HG12	2.03	0.41
1:I:76:ALA:HB1	1:J:93:ILE:HG22	2.03	0.41
1:J:8:ILE:HA	1:J:16:ARG:O	2.21	0.41
1:K:7:VAL:HG11	1:K:20:ILE:HD12	2.03	0.41
1:I:85:LYS:N	1:I:86:PRO:CD	2.84	0.41
1:M:76:ALA:HB1	1:N:93:ILE:HG23	2.02	0.41
1:K:65:ASN:HB2	1:K:93:ILE:HG13	2.03	0.41
1:K:85:LYS:N	1:K:86:PRO:CD	2.84	0.41
1:M:152:ARG:HB3	1:M:152:ARG:CZ	2.50	0.40
2:N:203:PEG:H11	2:N:203:PEG:H32	1.70	0.40
1:H:7:VAL:HG11	1:H:20:ILE:HD12	2.04	0.40
1:H:190:MET:HB2	1:H:190:MET:HE3	1.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:ASN:ND2	1:K:33:GLY:HA3	2.37	0.40

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	H	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	I	189/196 (96%)	183 (97%)	6 (3%)	0	100	100
1	J	193/196 (98%)	189 (98%)	4 (2%)	0	100	100
1	K	187/196 (95%)	181 (97%)	6 (3%)	0	100	100
1	L	191/196 (97%)	186 (97%)	5 (3%)	0	100	100
1	M	190/196 (97%)	184 (97%)	6 (3%)	0	100	100
1	N	188/196 (96%)	182 (97%)	6 (3%)	0	100	100
All	All	1324/1372 (96%)	1286 (97%)	38 (3%)	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	H	147/164 (90%)	143 (97%)	4 (3%)	39	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	150/164 (92%)	147 (98%)	3 (2%)	48	61
1	J	151/164 (92%)	149 (99%)	2 (1%)	61	74
1	K	151/164 (92%)	148 (98%)	3 (2%)	48	61
1	L	149/164 (91%)	148 (99%)	1 (1%)	76	86
1	M	156/164 (95%)	153 (98%)	3 (2%)	50	63
1	N	149/164 (91%)	148 (99%)	1 (1%)	76	86
All	All	1053/1148 (92%)	1036 (98%)	17 (2%)	59	68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	27	ASP
1	H	95[A]	MET
1	H	95[B]	MET
1	H	130	GLN
1	I	27	ASP
1	I	95[A]	MET
1	I	95[B]	MET
1	J	145	LYS
1	J	193	GLU
1	K	27	ASP
1	K	145	LYS
1	K	182	GLU
1	L	191	VAL
1	M	16	ARG
1	M	181	LYS
1	M	182	GLU
1	N	2	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	54	GLN
1	H	65	ASN
1	H	89	GLN
1	I	47	GLN
1	I	65	ASN
1	I	89	GLN
1	I	151	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	166	GLN
1	J	35	GLN
1	J	42	ASN
1	J	47	GLN
1	J	65	ASN
1	J	89	GLN
1	K	47	GLN
1	K	65	ASN
1	K	89	GLN
1	L	42	ASN
1	L	52	GLN
1	L	83	HIS
1	L	89	GLN
1	L	166	GLN
1	M	65	ASN
1	M	89	GLN
1	N	65	ASN
1	N	89	GLN
1	N	123	HIS

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 ⓘ

31 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	A1EDS	K	205	-	38,38,38	5.81	14 (36%)	44,54,54	2.26	8 (18%)
3	A1EDS	L	205	-	38,38,38	5.82	13 (34%)	44,54,54	2.17	9 (20%)
3	A1EDS	N	205	-	38,38,38	5.82	15 (39%)	44,54,54	2.39	10 (22%)
2	PEG	I	201	-	6,6,6	0.49	0	5,5,5	0.23	0
2	PEG	J	201	-	6,6,6	0.49	0	5,5,5	0.32	0
2	PEG	N	201	-	6,6,6	0.51	0	5,5,5	0.27	0
2	PEG	L	201	-	6,6,6	0.49	0	5,5,5	0.30	0
2	PEG	H	202	-	6,6,6	0.48	0	5,5,5	0.37	0
2	PEG	N	203	-	6,6,6	0.48	0	5,5,5	0.39	0
2	PEG	K	202	-	6,6,6	0.49	0	5,5,5	0.45	0
2	PEG	N	202	-	6,6,6	0.50	0	5,5,5	0.31	0
2	PEG	H	201	-	6,6,6	0.50	0	5,5,5	0.27	0
3	A1EDS	I	205	-	38,38,38	5.81	14 (36%)	44,54,54	3.03	10 (22%)
3	A1EDS	M	203	-	38,38,38	5.79	14 (36%)	44,54,54	2.32	11 (25%)
2	PEG	L	204	-	6,6,6	0.49	0	5,5,5	0.27	0
2	PEG	J	203	-	6,6,6	0.49	0	5,5,5	0.41	0
2	PEG	I	203	-	6,6,6	0.47	0	5,5,5	0.30	0
2	PEG	K	204	-	6,6,6	0.51	0	5,5,5	0.32	0
2	PEG	L	202	-	6,6,6	0.51	0	5,5,5	0.20	0
2	PEG	I	202	-	6,6,6	0.53	0	5,5,5	0.28	0
2	PEG	I	204	-	6,6,6	0.51	0	5,5,5	0.30	0
2	PEG	H	203	-	6,6,6	0.54	0	5,5,5	0.34	0
3	A1EDS	H	204	-	38,38,38	5.78	13 (34%)	44,54,54	2.05	6 (13%)
3	A1EDS	J	204	-	38,38,38	5.71	14 (36%)	44,54,54	2.41	13 (29%)
2	PEG	K	203	-	6,6,6	0.48	0	5,5,5	0.30	0
2	PEG	L	203	-	6,6,6	0.52	0	5,5,5	0.41	0
2	PEG	M	202	-	6,6,6	0.51	0	5,5,5	0.29	0
2	PEG	N	204	-	6,6,6	0.49	0	5,5,5	0.29	0
2	PEG	J	202	-	6,6,6	0.48	0	5,5,5	0.30	0
2	PEG	K	201	-	6,6,6	0.49	0	5,5,5	0.31	0
2	PEG	M	201	-	6,6,6	0.50	0	5,5,5	0.28	0

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	A1EDS	K	205	-	-	1/12/30/30	0/5/5/5
3	A1EDS	L	205	-	-	2/12/30/30	0/5/5/5
3	A1EDS	N	205	-	-	2/12/30/30	0/5/5/5
2	PEG	I	201	-	-	0/4/4/4	-
2	PEG	J	201	-	-	0/4/4/4	-
2	PEG	N	201	-	-	0/4/4/4	-
2	PEG	L	201	-	-	2/4/4/4	-
2	PEG	H	202	-	-	2/4/4/4	-
2	PEG	N	203	-	-	1/4/4/4	-
2	PEG	K	202	-	-	2/4/4/4	-
2	PEG	N	202	-	-	2/4/4/4	-
2	PEG	H	201	-	-	2/4/4/4	-
3	A1EDS	I	205	-	-	0/12/30/30	0/5/5/5
3	A1EDS	M	203	-	-	1/12/30/30	0/5/5/5
2	PEG	L	204	-	-	3/4/4/4	-
2	PEG	J	203	-	-	2/4/4/4	-
2	PEG	I	203	-	-	3/4/4/4	-
2	PEG	K	204	-	-	1/4/4/4	-
2	PEG	L	202	-	-	0/4/4/4	-
2	PEG	I	202	-	-	0/4/4/4	-
2	PEG	I	204	-	-	1/4/4/4	-
2	PEG	H	203	-	-	1/4/4/4	-
3	A1EDS	H	204	-	-	0/12/30/30	0/5/5/5
3	A1EDS	J	204	-	-	2/12/30/30	0/5/5/5
2	PEG	K	203	-	-	2/4/4/4	-
2	PEG	L	203	-	-	1/4/4/4	-
2	PEG	M	202	-	-	1/4/4/4	-
2	PEG	N	204	-	-	2/4/4/4	-
2	PEG	J	202	-	-	2/4/4/4	-
2	PEG	K	201	-	-	2/4/4/4	-
2	PEG	M	201	-	-	0/4/4/4	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	205	A1EDS	C30-N31	24.75	1.47	1.28
3	L	205	A1EDS	C30-N31	24.73	1.47	1.28
3	N	205	A1EDS	C30-N31	24.56	1.47	1.28
3	M	203	A1EDS	C30-N31	24.53	1.47	1.28
3	H	204	A1EDS	C30-N31	24.40	1.47	1.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	204	A1EDS	C30-N31	24.39	1.47	1.28
3	I	205	A1EDS	C30-N31	24.08	1.47	1.28
3	N	205	A1EDS	C11-N10	-13.48	1.24	1.47
3	L	205	A1EDS	C05-N10	-13.24	1.26	1.48
3	N	205	A1EDS	C05-N10	-13.23	1.26	1.48
3	M	203	A1EDS	C05-N10	-13.08	1.26	1.48
3	H	204	A1EDS	C05-N10	-13.06	1.26	1.48
3	I	205	A1EDS	C06-C07	-13.04	1.33	1.50
3	K	205	A1EDS	C05-N10	-13.02	1.26	1.48
3	M	203	A1EDS	C11-N10	-12.94	1.25	1.47
3	L	205	A1EDS	C11-N10	-12.86	1.25	1.47
3	H	204	A1EDS	C11-N10	-12.86	1.25	1.47
3	K	205	A1EDS	C11-N10	-12.85	1.25	1.47
3	I	205	A1EDS	C05-N10	-12.53	1.27	1.48
3	I	205	A1EDS	C11-N10	-12.51	1.26	1.47
3	J	204	A1EDS	C05-N10	-12.41	1.27	1.48
3	J	204	A1EDS	C11-N10	-12.32	1.26	1.47
3	H	204	A1EDS	C06-C07	-10.88	1.36	1.50
3	K	205	A1EDS	C06-C07	-10.57	1.36	1.50
3	L	205	A1EDS	C06-C07	-10.48	1.36	1.50
3	M	203	A1EDS	C06-C07	-10.44	1.36	1.50
3	N	205	A1EDS	C06-C07	-10.23	1.37	1.50
3	J	204	A1EDS	C06-C07	-9.83	1.37	1.50
3	J	204	A1EDS	C06-C05	7.22	1.67	1.53
3	M	203	A1EDS	C06-C05	6.88	1.66	1.53
3	L	205	A1EDS	C06-C05	6.81	1.66	1.53
3	K	205	A1EDS	C06-C05	6.76	1.66	1.53
3	N	205	A1EDS	C06-C05	6.67	1.66	1.53
3	J	204	A1EDS	C19-C08	6.48	1.60	1.44
3	H	204	A1EDS	C19-C08	6.44	1.59	1.44
3	I	205	A1EDS	C06-C05	6.43	1.65	1.53
3	L	205	A1EDS	C19-C08	6.42	1.59	1.44
3	K	205	A1EDS	C19-C08	6.42	1.59	1.44
3	M	203	A1EDS	C19-C08	6.37	1.59	1.44
3	H	204	A1EDS	C06-C05	6.34	1.65	1.53
3	I	205	A1EDS	C19-C08	6.31	1.59	1.44
3	N	205	A1EDS	C19-C08	6.01	1.58	1.44
3	I	205	A1EDS	C19-N21	5.59	1.50	1.40
3	J	204	A1EDS	C09-C08	-5.38	1.43	1.51
3	H	204	A1EDS	C19-N21	5.30	1.49	1.40
3	L	205	A1EDS	C19-N21	5.25	1.49	1.40
3	K	205	A1EDS	C19-N21	5.23	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	204	A1EDS	C19-N21	5.22	1.49	1.40
3	N	205	A1EDS	C19-N21	5.17	1.49	1.40
3	M	203	A1EDS	C09-C08	-5.16	1.43	1.51
3	N	205	A1EDS	C09-C08	-5.04	1.43	1.51
3	H	204	A1EDS	C07-C08	5.03	1.49	1.36
3	M	203	A1EDS	C19-N21	4.98	1.49	1.40
3	L	205	A1EDS	C09-C08	-4.93	1.43	1.51
3	N	205	A1EDS	C07-C08	4.90	1.49	1.36
3	K	205	A1EDS	C09-C08	-4.88	1.43	1.51
3	I	205	A1EDS	C09-N10	4.82	1.58	1.47
3	I	205	A1EDS	C09-C08	-4.81	1.44	1.51
3	J	204	A1EDS	C09-N10	4.76	1.58	1.47
3	K	205	A1EDS	C07-C08	4.73	1.48	1.36
3	L	205	A1EDS	C07-C08	4.72	1.48	1.36
3	M	203	A1EDS	C07-C08	4.70	1.48	1.36
3	H	204	A1EDS	C09-N10	4.68	1.58	1.47
3	J	204	A1EDS	C07-C08	4.50	1.48	1.36
3	K	205	A1EDS	C09-N10	4.41	1.58	1.47
3	L	205	A1EDS	C09-N10	4.39	1.57	1.47
3	M	203	A1EDS	C09-N10	4.35	1.57	1.47
3	I	205	A1EDS	C07-C08	4.32	1.47	1.36
3	H	204	A1EDS	C09-C08	-4.23	1.44	1.51
3	N	205	A1EDS	C09-N10	4.15	1.57	1.47
3	N	205	A1EDS	C30-N21	3.83	1.45	1.38
3	L	205	A1EDS	C30-N21	3.74	1.45	1.38
3	K	205	A1EDS	C30-N21	3.70	1.45	1.38
3	H	204	A1EDS	C30-N21	3.60	1.45	1.38
3	M	203	A1EDS	C30-N21	3.60	1.45	1.38
3	J	204	A1EDS	C30-N21	3.56	1.45	1.38
3	I	205	A1EDS	C30-N21	3.53	1.45	1.38
3	J	204	A1EDS	C32-N31	-2.70	1.43	1.47
3	H	204	A1EDS	C32-N31	-2.68	1.43	1.47
3	I	205	A1EDS	O20-C19	-2.60	1.17	1.23
3	N	205	A1EDS	C07-N34	2.59	1.44	1.39
3	I	205	A1EDS	C32-N31	-2.58	1.43	1.47
3	L	205	A1EDS	C32-N31	-2.55	1.43	1.47
3	M	203	A1EDS	O20-C19	-2.53	1.17	1.23
3	H	204	A1EDS	O20-C19	-2.50	1.18	1.23
3	K	205	A1EDS	O20-C19	-2.50	1.18	1.23
3	J	204	A1EDS	O20-C19	-2.48	1.18	1.23
3	M	203	A1EDS	C32-N31	-2.48	1.43	1.47
3	N	205	A1EDS	C32-N31	-2.44	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	205	A1EDS	O20-C19	-2.44	1.18	1.23
3	K	205	A1EDS	C32-N31	-2.40	1.43	1.47
3	J	204	A1EDS	C07-N34	2.15	1.43	1.39
3	I	205	A1EDS	O03-C04	-2.14	1.36	1.42
3	M	203	A1EDS	C07-N34	2.09	1.43	1.39
3	N	205	A1EDS	C30-N34	2.06	1.42	1.38
3	N	205	A1EDS	O20-C19	-2.05	1.18	1.23
3	K	205	A1EDS	C07-N34	2.02	1.43	1.39

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	205	A1EDS	C06-C05-C04	-15.73	88.70	112.46
3	J	204	A1EDS	C32-C33-N34	9.46	108.13	101.30
3	N	205	A1EDS	C32-C33-N34	8.93	107.75	101.30
3	M	203	A1EDS	C32-C33-N34	8.84	107.69	101.30
3	K	205	A1EDS	C32-C33-N34	8.74	107.61	101.30
3	L	205	A1EDS	C32-C33-N34	8.65	107.55	101.30
3	H	204	A1EDS	C32-C33-N34	8.51	107.45	101.30
3	I	205	A1EDS	C32-C33-N34	7.91	107.02	101.30
3	K	205	A1EDS	C06-C05-C04	-7.03	101.84	112.46
3	M	203	A1EDS	C06-C05-C04	-6.38	102.82	112.46
3	L	205	A1EDS	C06-C05-C04	-6.05	103.32	112.46
3	N	205	A1EDS	C06-C05-C04	-5.95	103.47	112.46
3	N	205	A1EDS	C06-C07-N34	5.86	126.03	116.85
3	J	204	A1EDS	C06-C07-N34	5.54	125.53	116.85
3	H	204	A1EDS	C06-C05-C04	-5.42	104.27	112.46
3	J	204	A1EDS	C08-C07-N34	-5.06	115.04	120.59
3	M	203	A1EDS	C06-C07-N34	5.00	124.69	116.85
3	H	204	A1EDS	C06-C07-N34	4.85	124.44	116.85
3	K	205	A1EDS	C06-C07-N34	4.53	123.95	116.85
3	N	205	A1EDS	C11-N10-C05	-4.39	105.53	112.18
3	L	205	A1EDS	C06-C07-N34	4.35	123.66	116.85
3	M	203	A1EDS	C08-C07-N34	-4.04	116.16	120.59
3	I	205	A1EDS	O03-C04-C05	3.59	120.64	109.50
3	I	205	A1EDS	C22-N21-C19	3.54	122.71	117.72
3	N	205	A1EDS	C08-C07-N34	-3.49	116.77	120.59
3	J	204	A1EDS	C06-C05-C04	-3.43	107.27	112.46
3	J	204	A1EDS	C22-N21-C19	3.41	122.53	117.72
3	J	204	A1EDS	C11-N10-C09	-3.40	105.41	111.51
3	K	205	A1EDS	C08-C07-N34	-3.36	116.91	120.59
3	L	205	A1EDS	C08-C07-N34	-3.35	116.92	120.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	205	A1EDS	C11-N10-C09	-3.25	105.68	111.51
3	K	205	A1EDS	C06-C05-N10	3.13	117.32	109.26
3	L	205	A1EDS	C06-C05-N10	3.05	117.12	109.26
3	H	204	A1EDS	C08-C07-N34	-3.01	117.29	120.59
3	M	203	A1EDS	C06-C05-N10	2.94	116.85	109.26
3	H	204	A1EDS	C22-N21-C19	2.94	121.86	117.72
3	J	204	A1EDS	C08-C09-N10	2.91	115.52	110.85
3	K	205	A1EDS	C22-N21-C19	2.88	121.78	117.72
3	N	205	A1EDS	C06-C05-N10	2.88	116.69	109.26
3	K	205	A1EDS	C11-N10-C09	-2.88	106.35	111.51
3	M	203	A1EDS	C12-C11-N10	-2.78	108.21	112.73
3	I	205	A1EDS	C06-C07-N34	2.71	121.09	116.85
3	L	205	A1EDS	C22-N21-C19	2.70	121.53	117.72
3	M	203	A1EDS	C22-N21-C19	2.70	121.53	117.72
3	J	204	A1EDS	C15-C14-C13	-2.69	119.68	123.23
3	M	203	A1EDS	C11-N10-C09	-2.67	106.72	111.51
3	N	205	A1EDS	C22-N21-C30	2.63	121.37	117.95
3	M	203	A1EDS	C23-C22-N21	2.58	117.42	113.09
3	I	205	A1EDS	C22-C23-C24	-2.58	116.00	120.75
3	L	205	A1EDS	C12-C11-N10	-2.52	108.64	112.73
3	L	205	A1EDS	C15-C14-C13	-2.46	119.98	123.23
3	K	205	A1EDS	C15-C14-C13	-2.42	120.04	123.23
3	L	205	A1EDS	C11-N10-C09	-2.42	107.17	111.51
3	I	205	A1EDS	C06-C05-N10	2.41	115.47	109.26
3	I	205	A1EDS	C11-N10-C09	-2.39	107.21	111.51
3	J	204	A1EDS	C11-N10-C05	2.37	115.76	112.18
3	H	204	A1EDS	C15-C14-C13	-2.28	120.22	123.23
3	M	203	A1EDS	C15-C14-C13	-2.26	120.25	123.23
3	N	205	A1EDS	C15-C14-C13	-2.26	120.25	123.23
3	J	204	A1EDS	C12-C11-N10	-2.17	109.19	112.73
3	I	205	A1EDS	C02-O03-C04	-2.17	101.91	113.17
3	I	205	A1EDS	C15-C14-C13	-2.16	120.38	123.23
3	N	205	A1EDS	O20-C19-C08	-2.10	121.06	125.06
3	J	204	A1EDS	C06-C05-N10	2.07	114.60	109.26
3	J	204	A1EDS	O03-C04-C05	2.07	115.92	109.50
3	J	204	A1EDS	O20-C19-C08	-2.06	121.15	125.06
3	M	203	A1EDS	C22-N21-C30	2.04	120.60	117.95

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	204	A1EDS	O03-C04-C05-C06
3	L	205	A1EDS	O03-C04-C05-C06
2	N	203	PEG	C1-C2-O2-C3
2	K	204	PEG	O1-C1-C2-O2
2	H	201	PEG	O2-C3-C4-O4
2	I	203	PEG	O1-C1-C2-O2
2	L	201	PEG	O1-C1-C2-O2
2	L	203	PEG	O1-C1-C2-O2
2	H	203	PEG	O2-C3-C4-O4
2	J	202	PEG	O2-C3-C4-O4
2	H	202	PEG	O1-C1-C2-O2
2	J	203	PEG	O1-C1-C2-O2
2	K	203	PEG	O1-C1-C2-O2
2	N	202	PEG	O2-C3-C4-O4
2	I	203	PEG	O2-C3-C4-O4
3	J	204	A1EDS	C01-C02-O03-C04
2	L	204	PEG	O2-C3-C4-O4
2	L	204	PEG	C1-C2-O2-C3
2	M	202	PEG	C1-C2-O2-C3
2	H	201	PEG	O1-C1-C2-O2
2	K	202	PEG	O2-C3-C4-O4
2	J	203	PEG	C4-C3-O2-C2
2	N	204	PEG	C4-C3-O2-C2
2	K	201	PEG	O2-C3-C4-O4
2	K	203	PEG	C1-C2-O2-C3
2	N	202	PEG	C1-C2-O2-C3
2	I	203	PEG	C1-C2-O2-C3
2	K	201	PEG	C1-C2-O2-C3
2	L	204	PEG	O1-C1-C2-O2
3	M	203	A1EDS	C01-C02-O03-C04
2	N	204	PEG	C1-C2-O2-C3
2	L	201	PEG	C1-C2-O2-C3
3	K	205	A1EDS	C01-C02-O03-C04
2	J	202	PEG	C4-C3-O2-C2
3	N	205	A1EDS	C01-C02-O03-C04
3	N	205	A1EDS	C12-C11-N10-C09
3	L	205	A1EDS	C01-C02-O03-C04
2	H	202	PEG	O2-C3-C4-O4
2	K	202	PEG	C1-C2-O2-C3
2	I	204	PEG	O2-C3-C4-O4

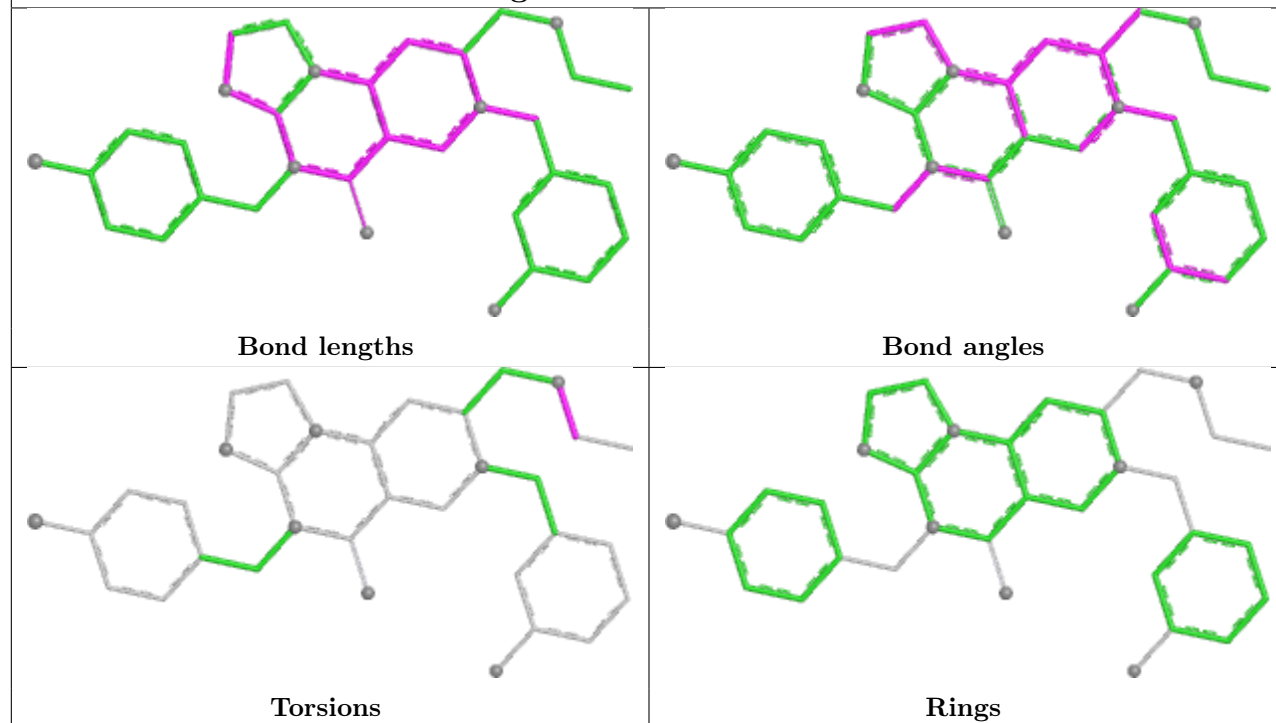
There are no ring outliers.

14 monomers are involved in 19 short contacts:

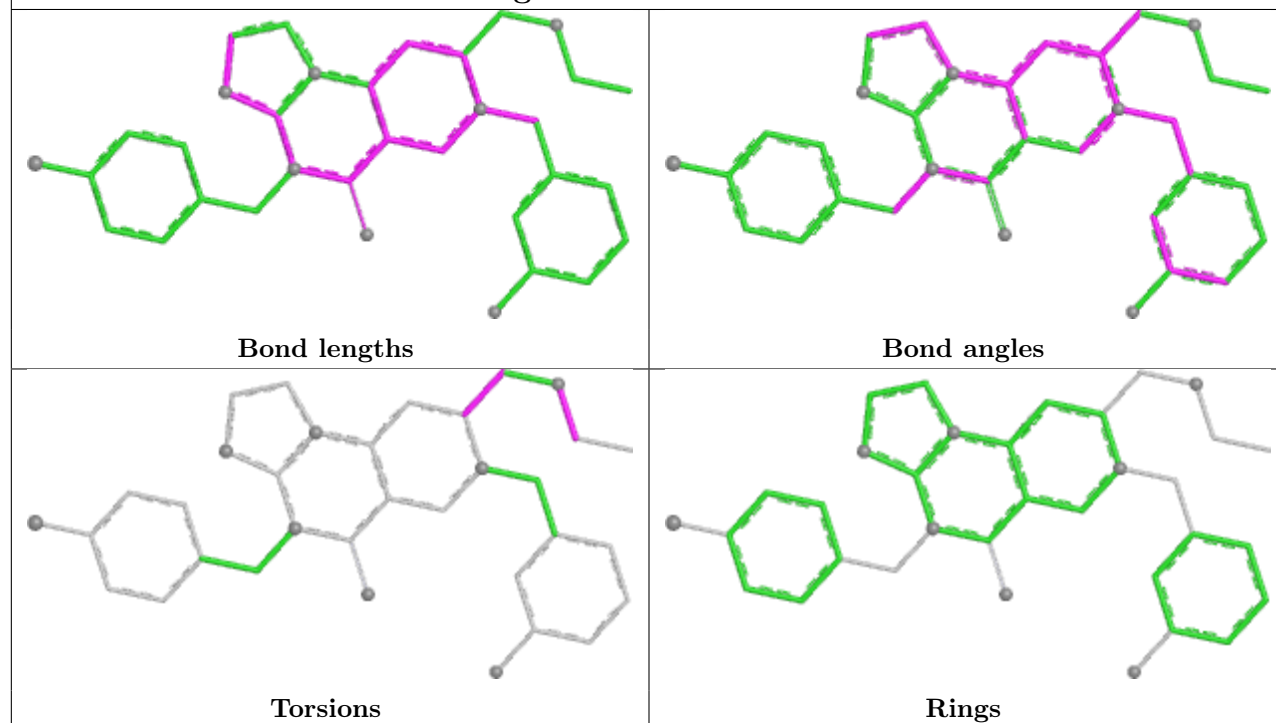
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	205	A1EDS	1	0
3	N	205	A1EDS	1	0
2	N	203	PEG	1	0
2	K	202	PEG	1	0
2	H	201	PEG	1	0
3	I	205	A1EDS	1	0
3	M	203	A1EDS	1	0
2	L	204	PEG	2	0
2	K	204	PEG	2	0
2	L	202	PEG	1	0
2	I	204	PEG	1	0
2	H	203	PEG	4	0
3	H	204	A1EDS	1	0
2	M	201	PEG	1	0

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.

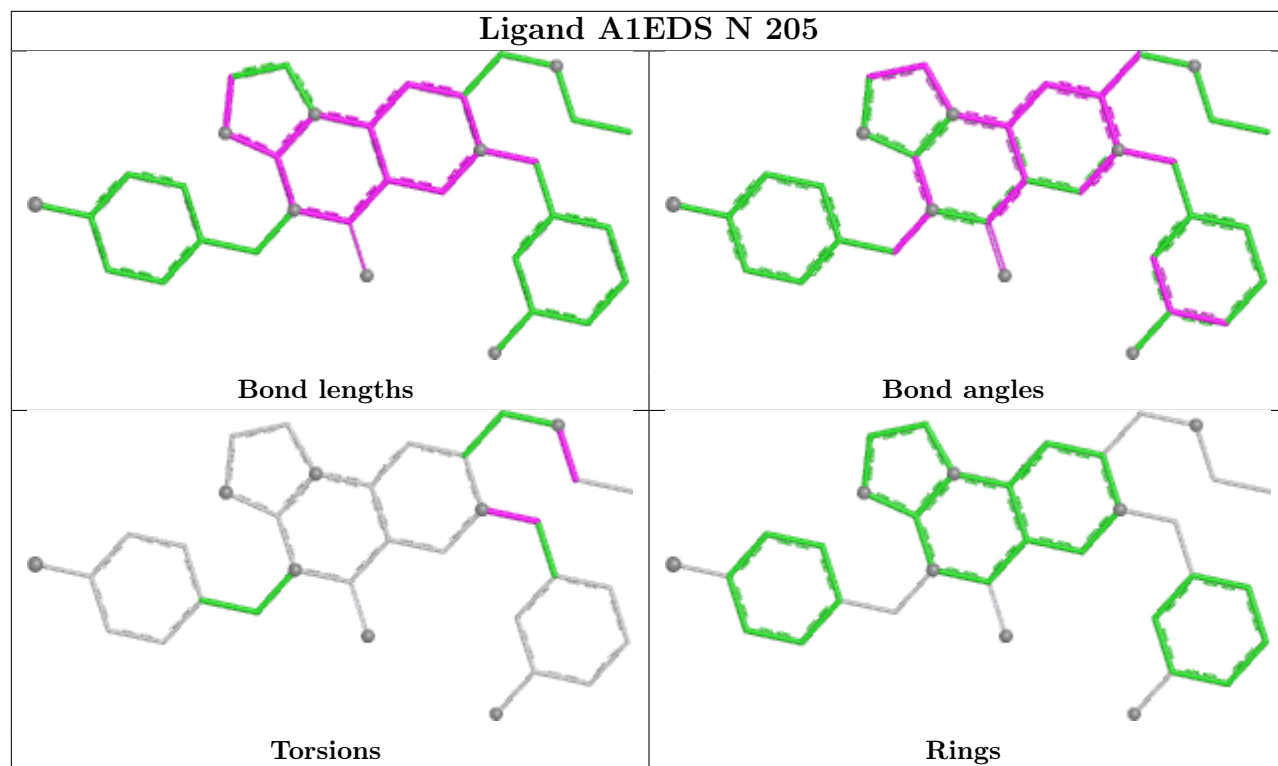
Ligand A1EDS K 205



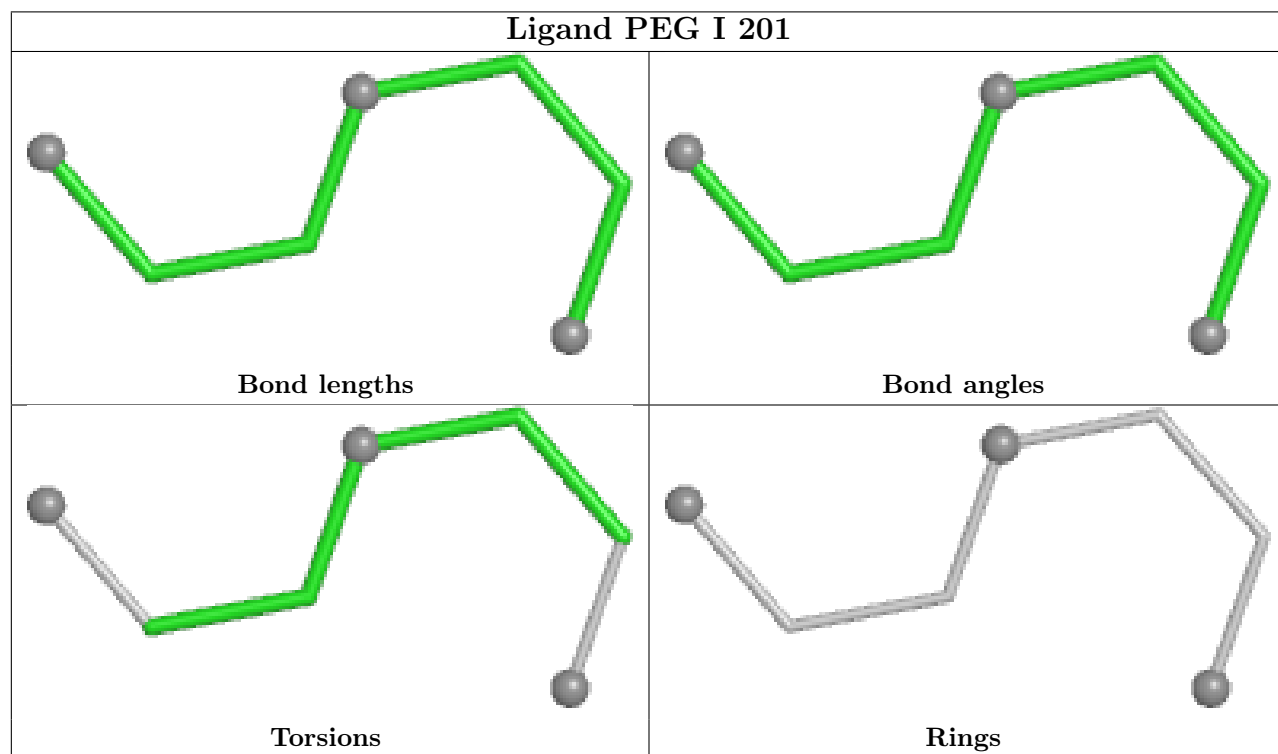
Ligand A1EDS L 205

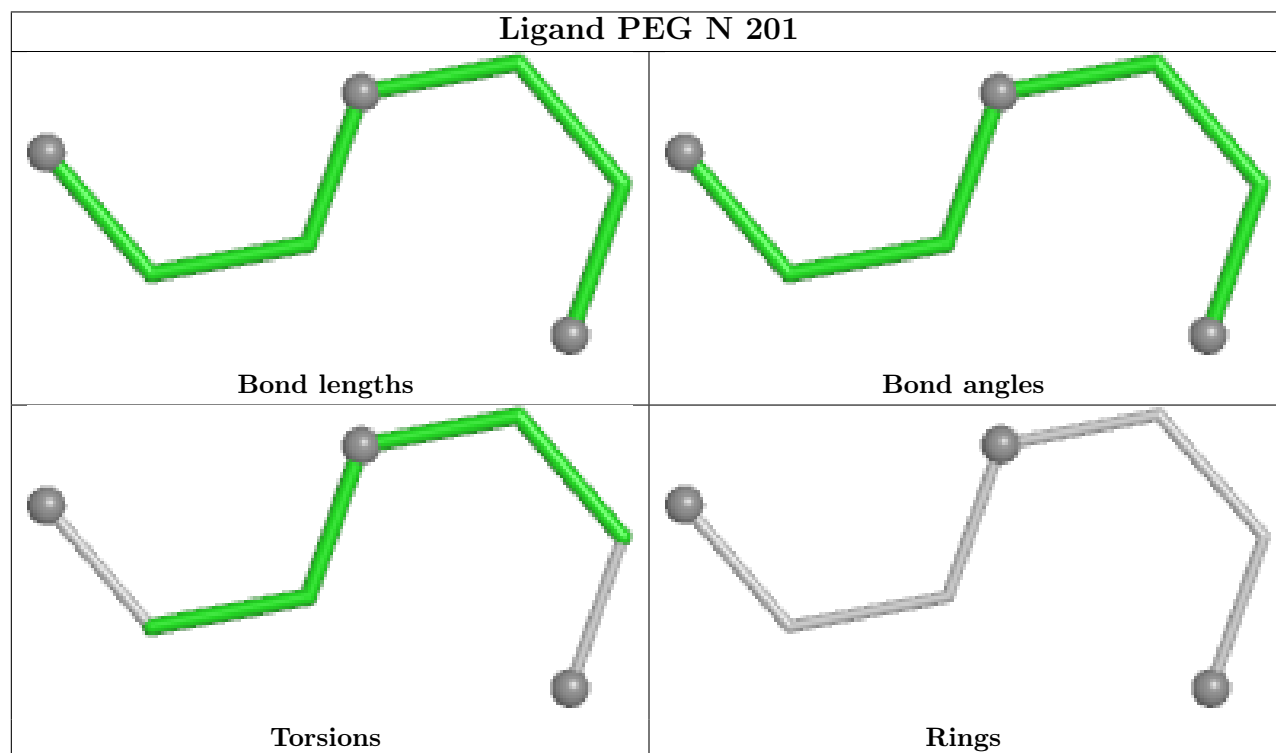
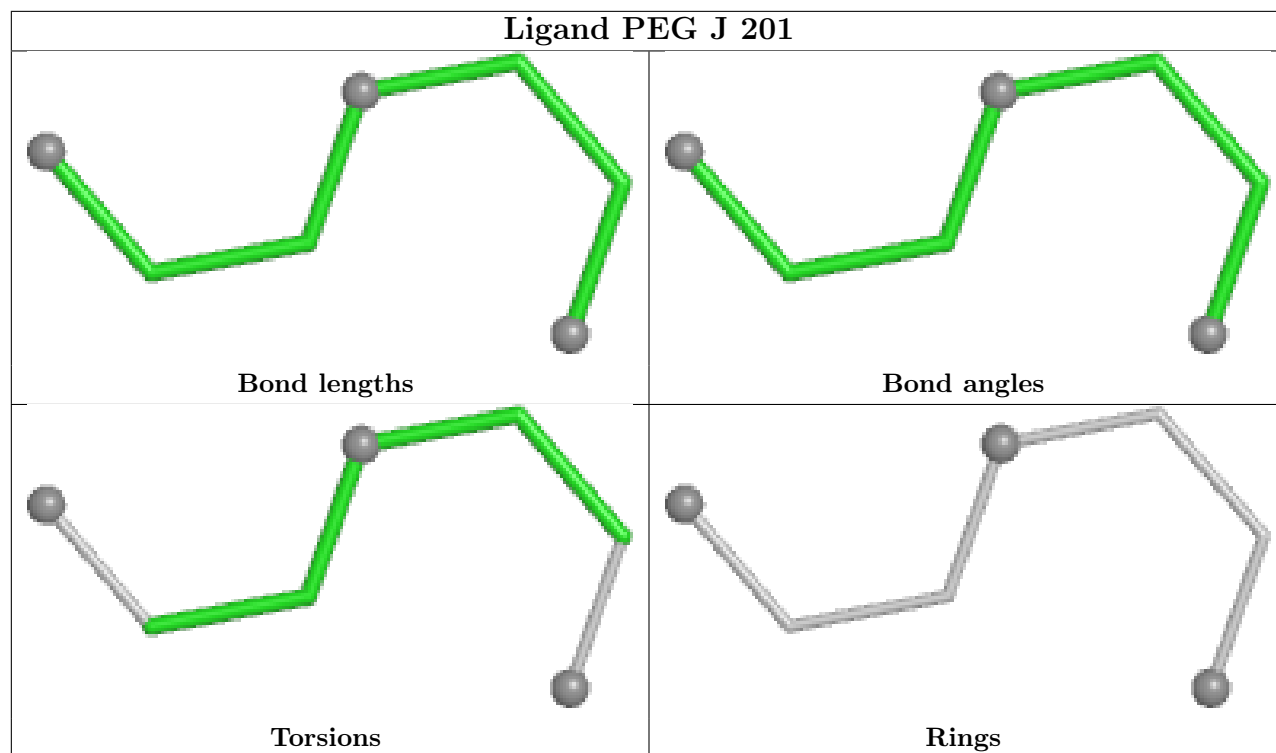


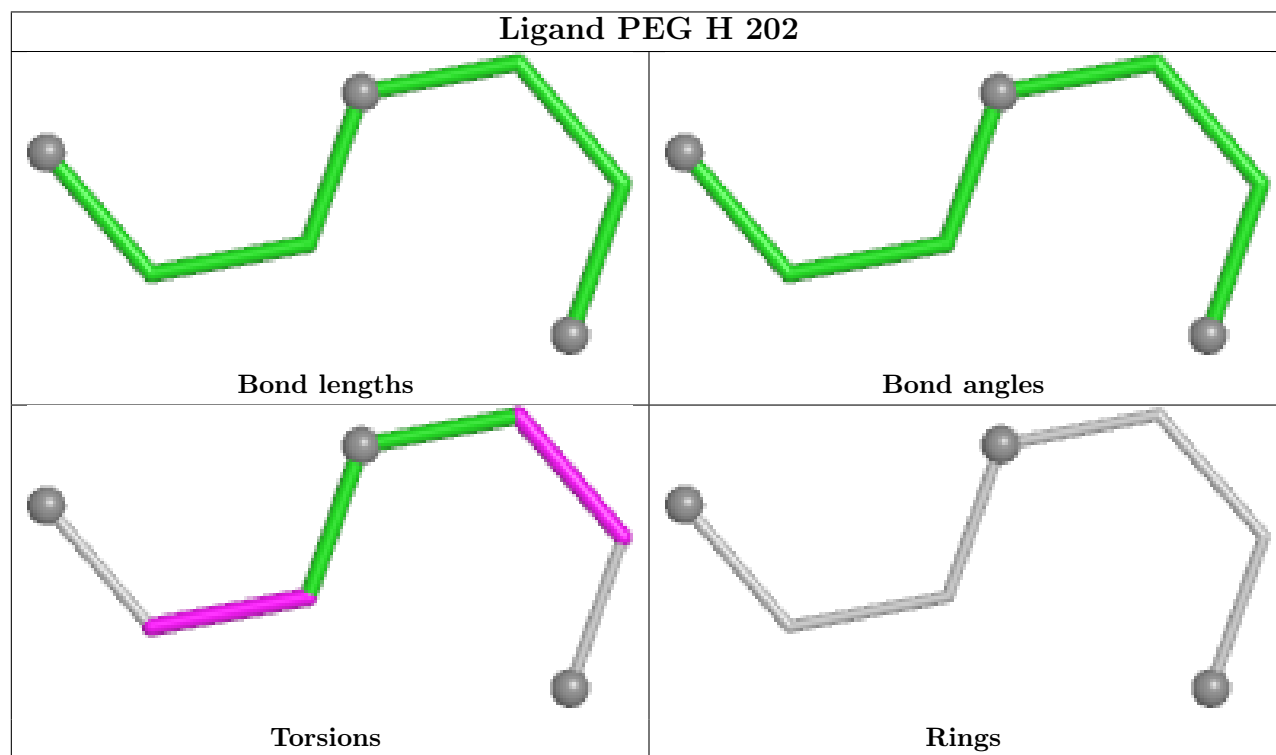
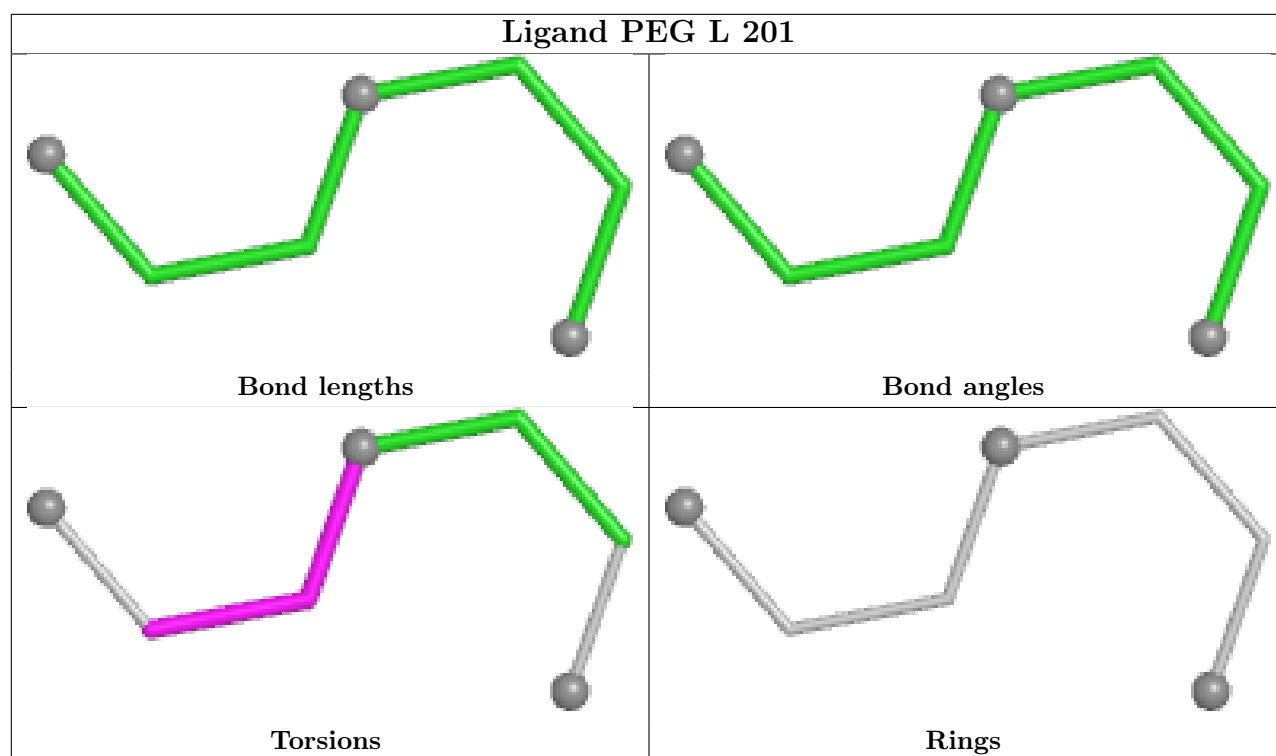
Ligand A1EDS N 205

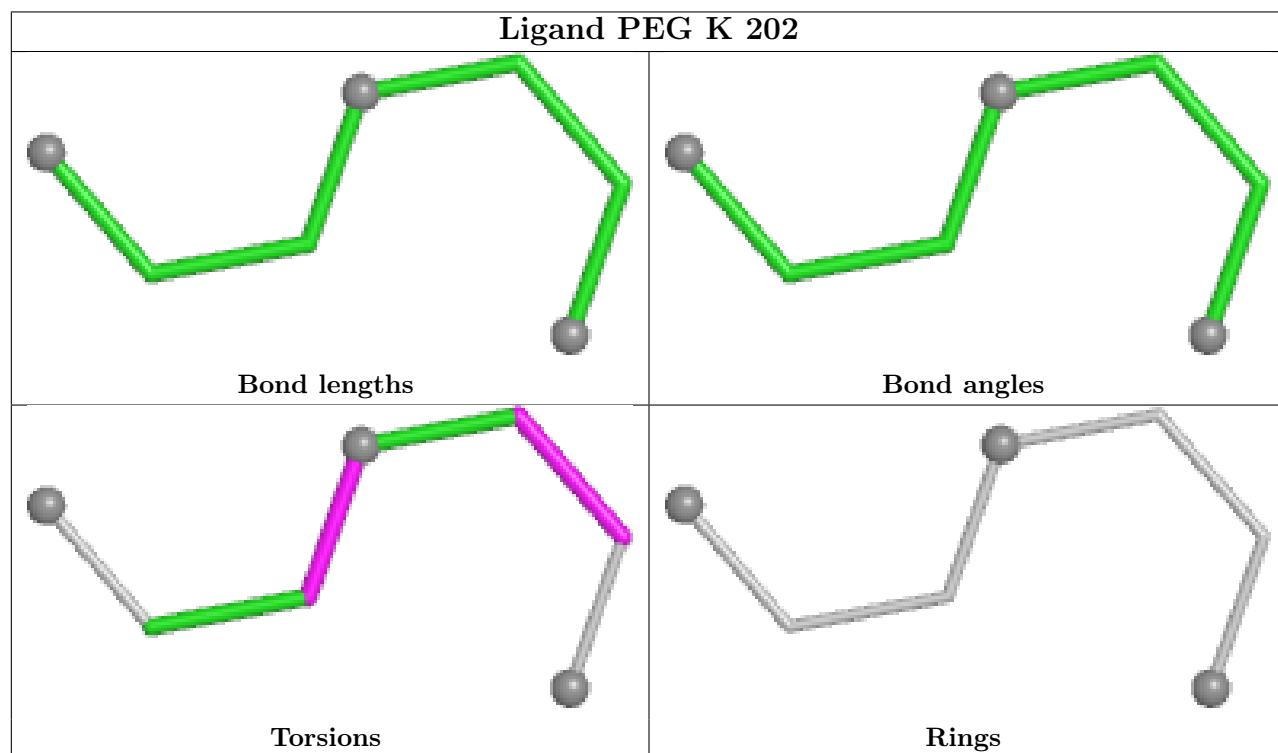
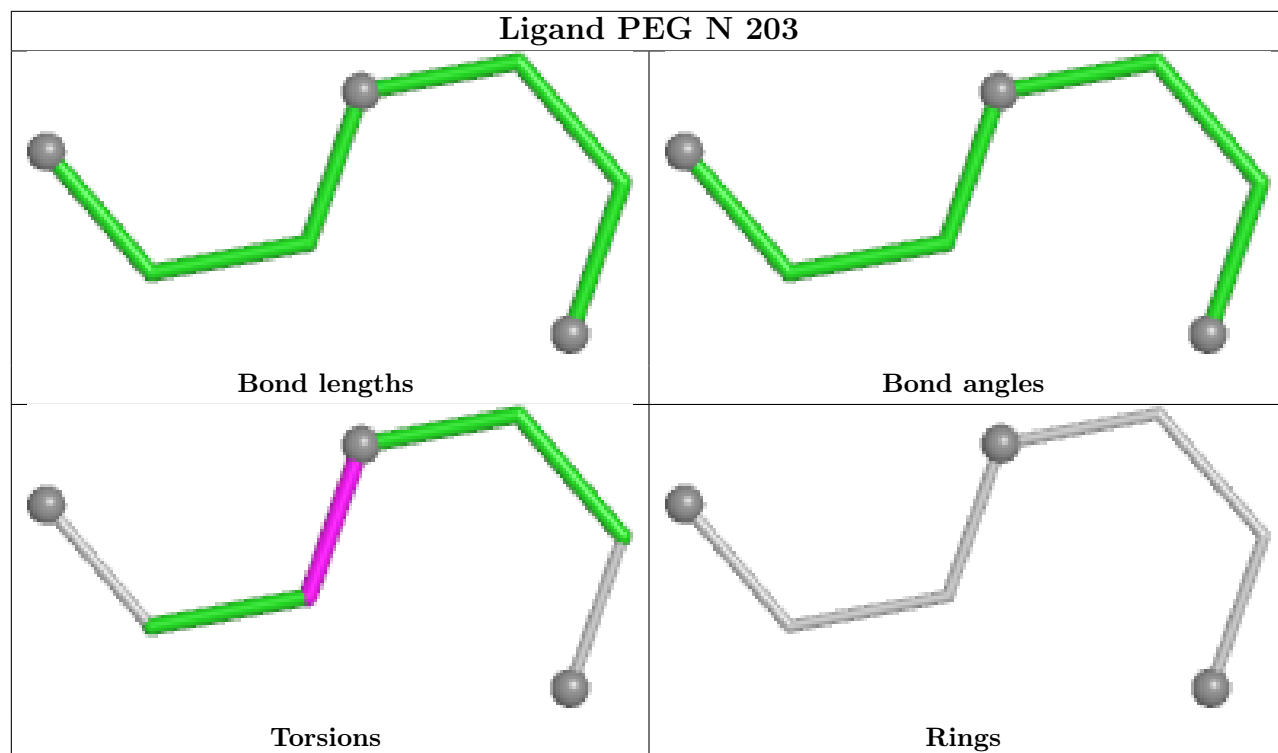


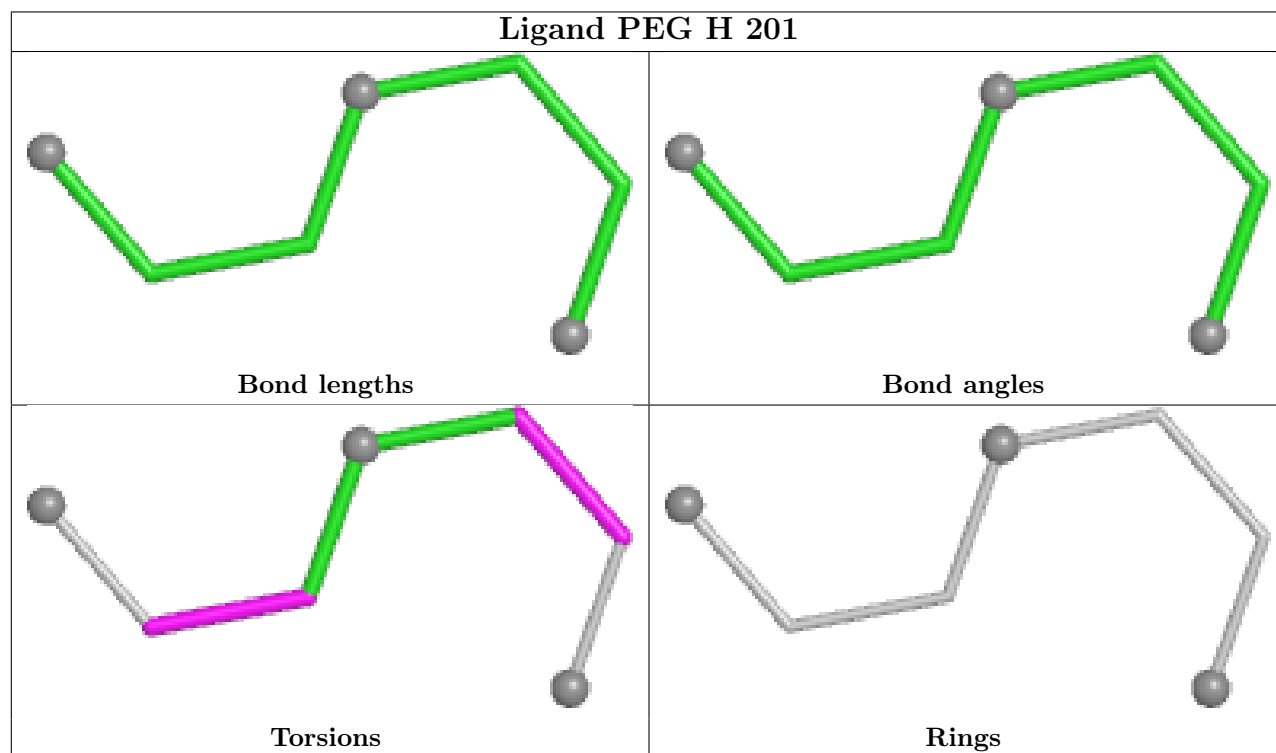
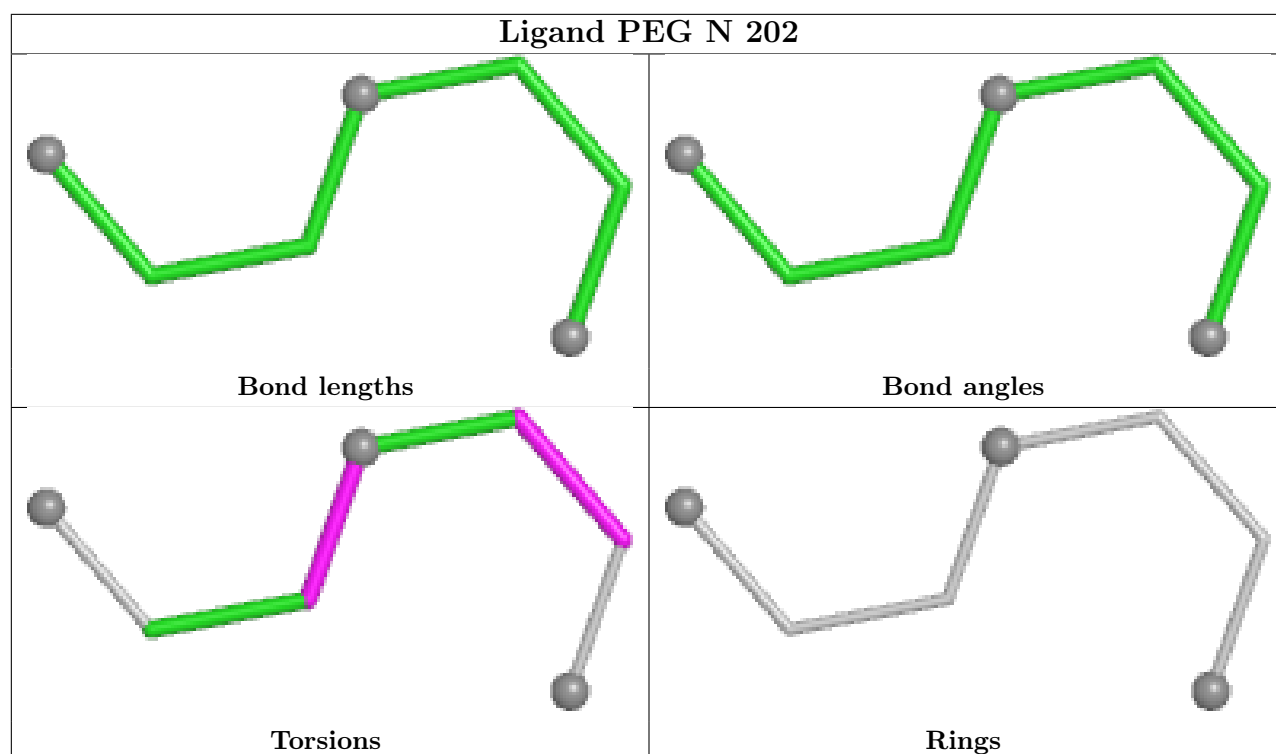
Ligand PEG I 201

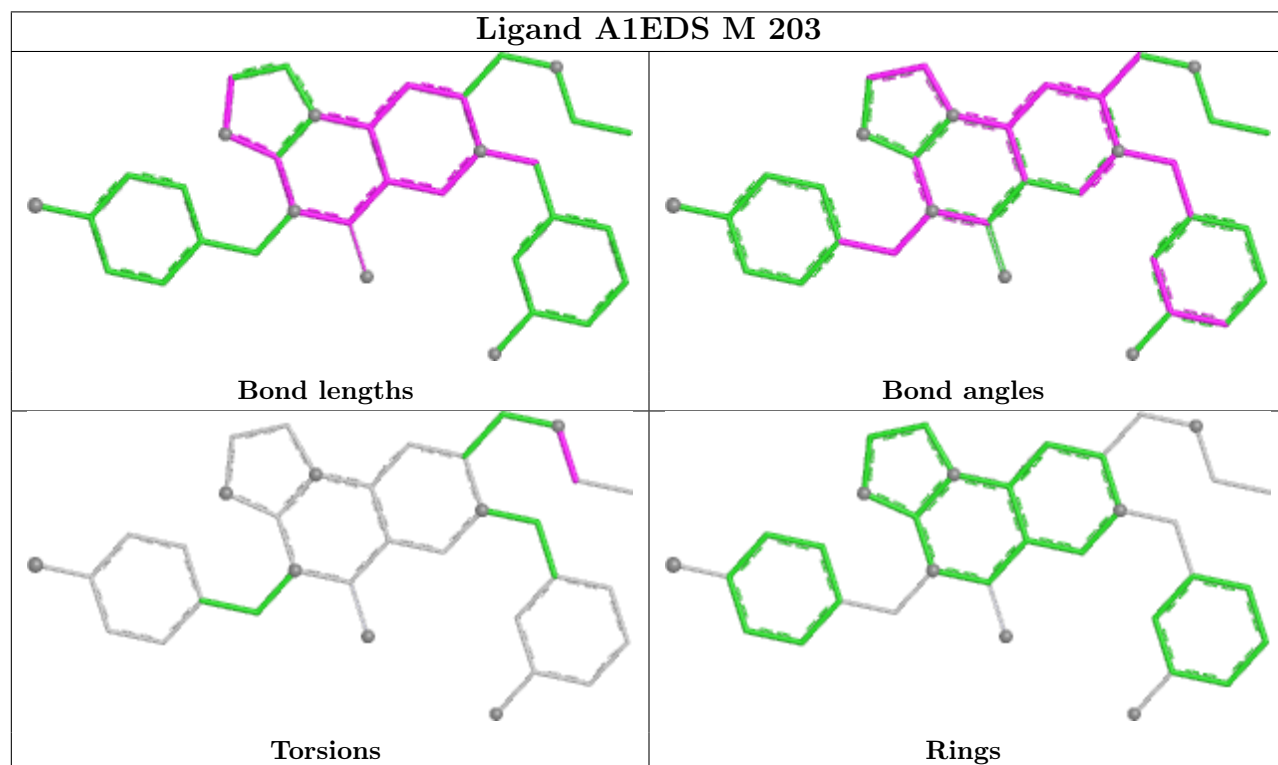
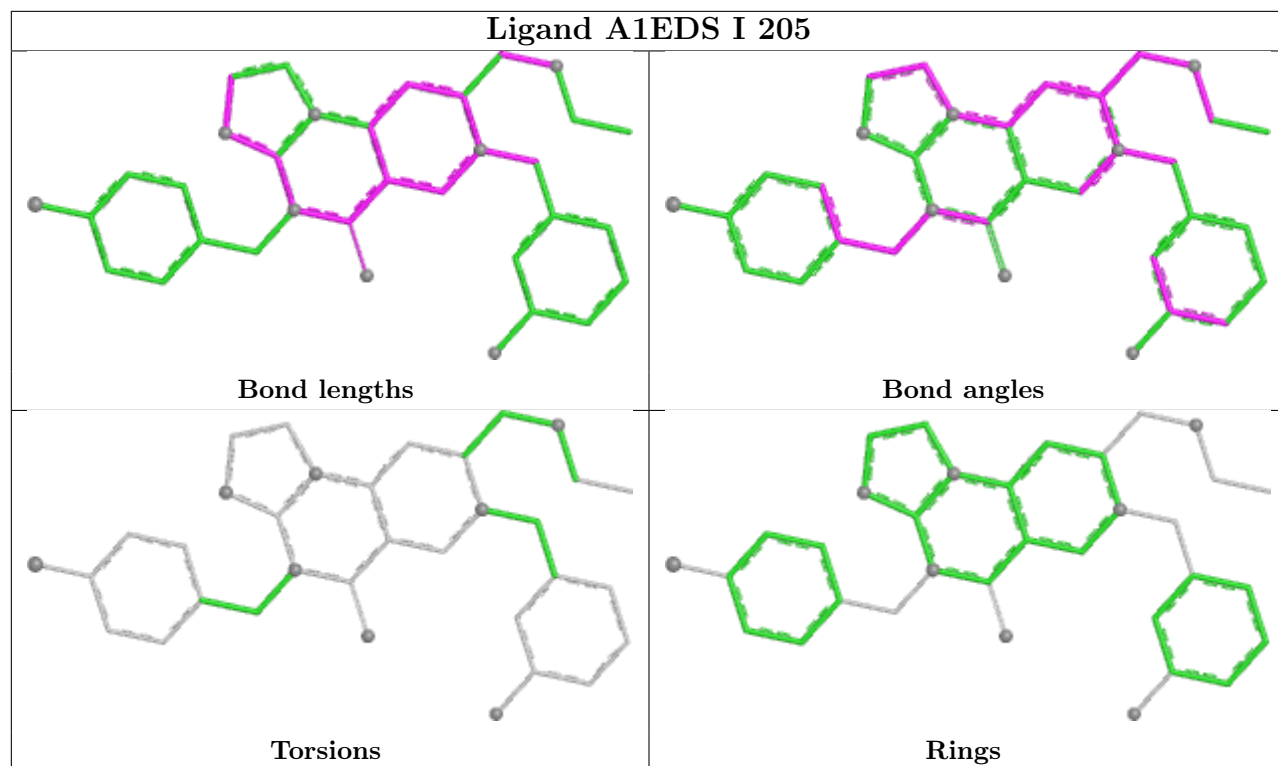


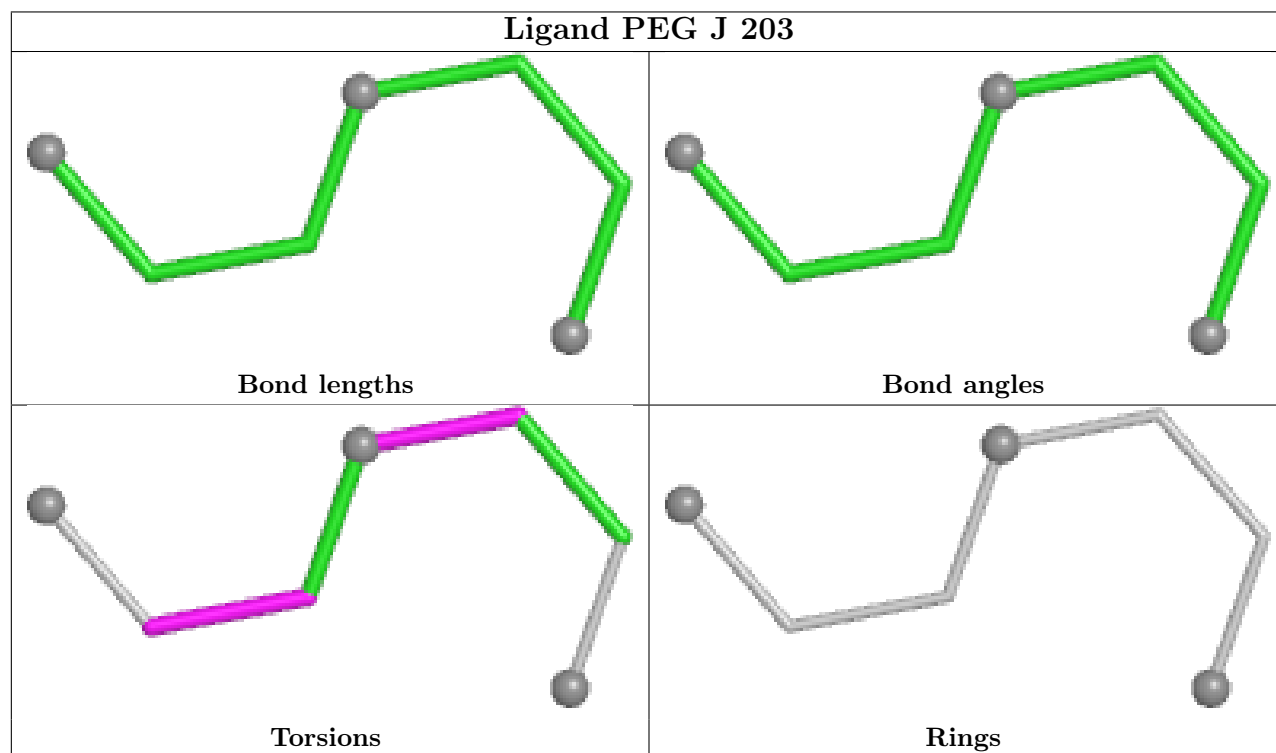
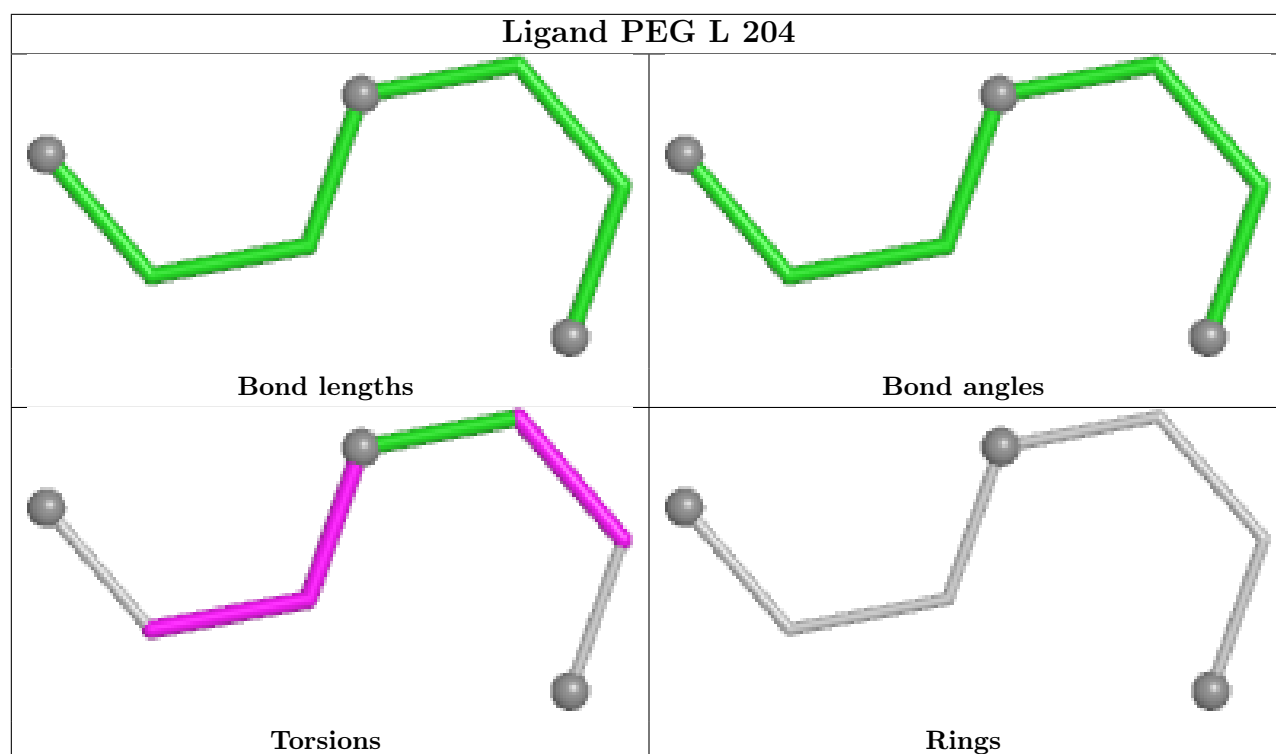


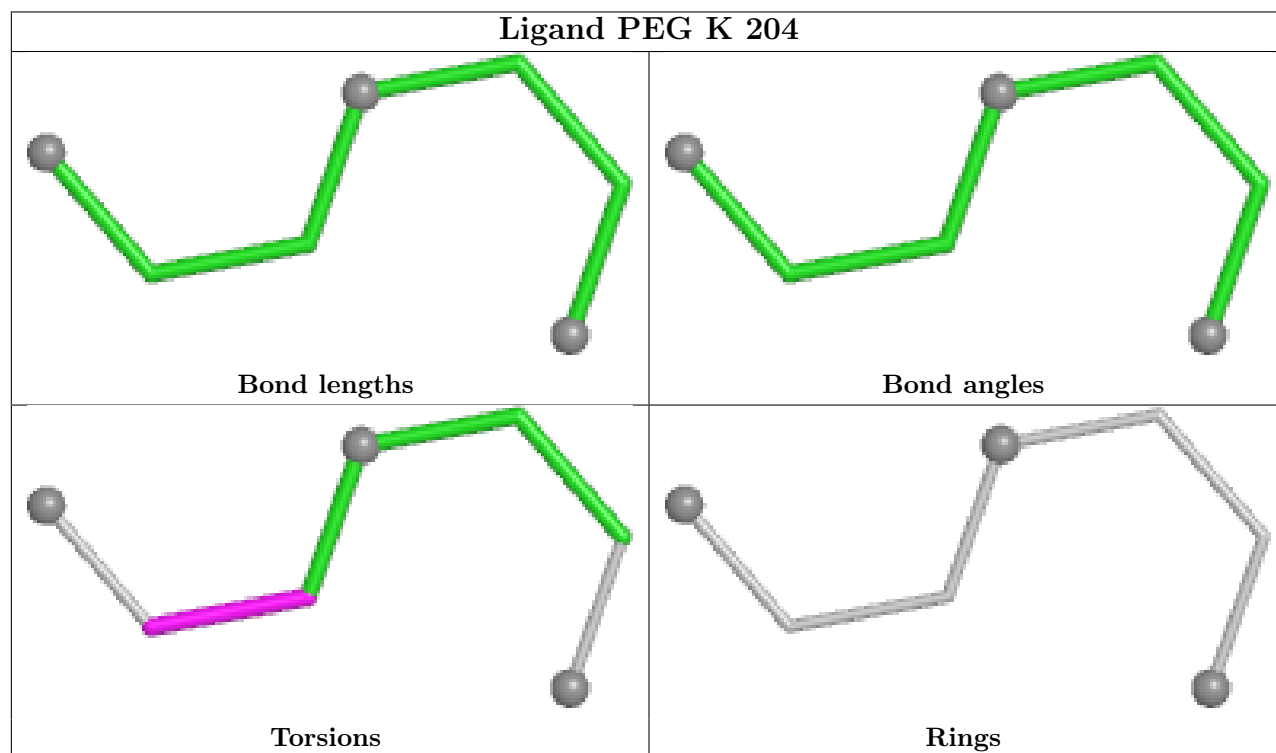
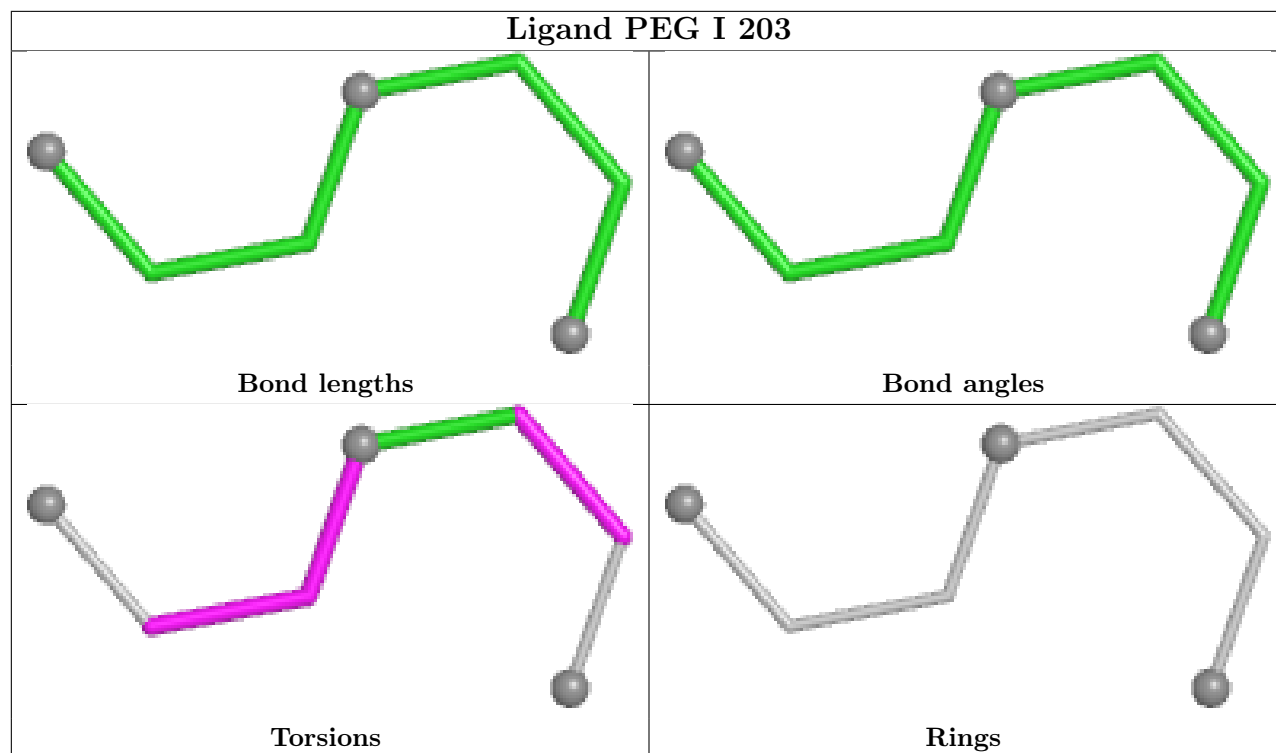


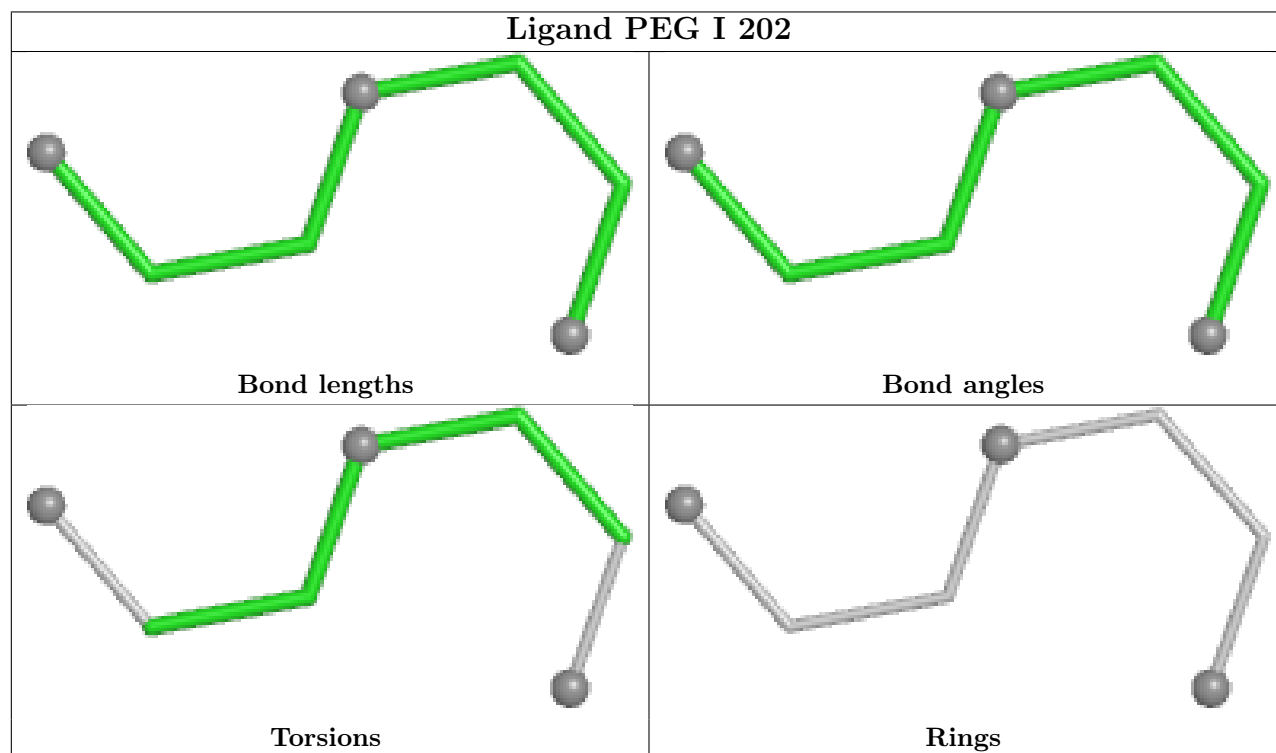
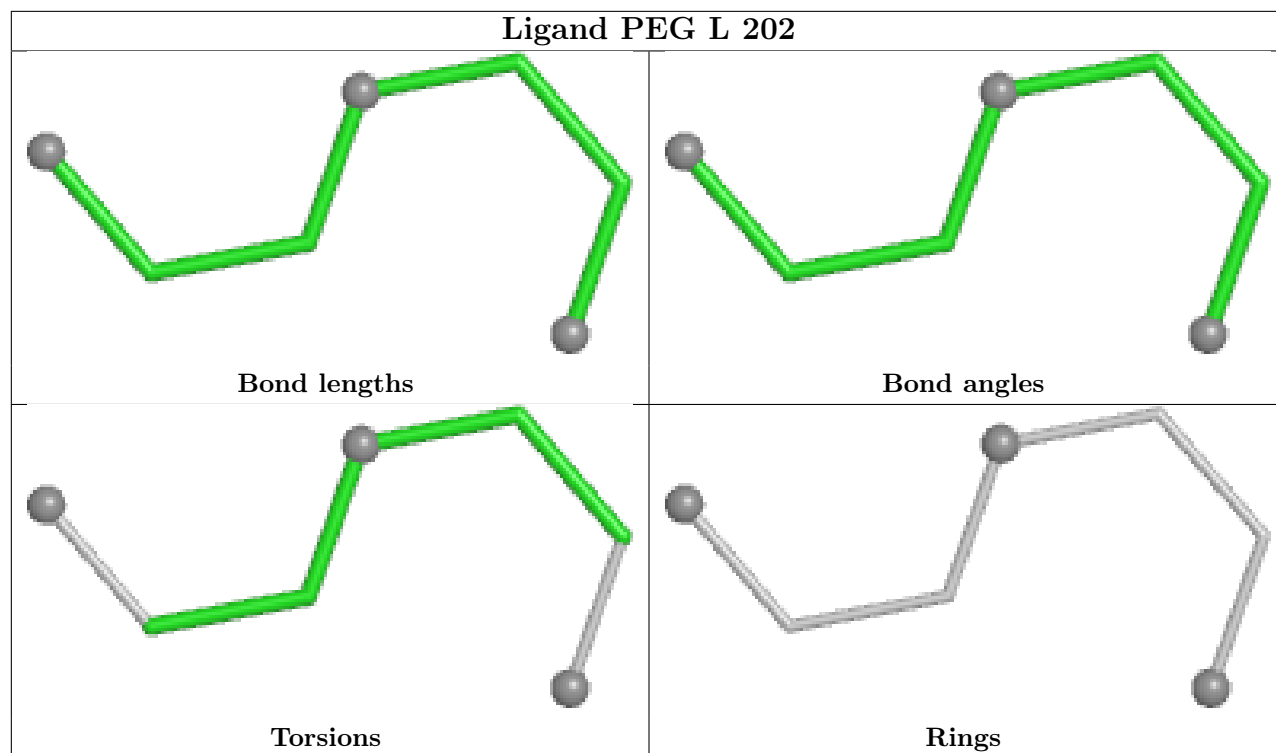


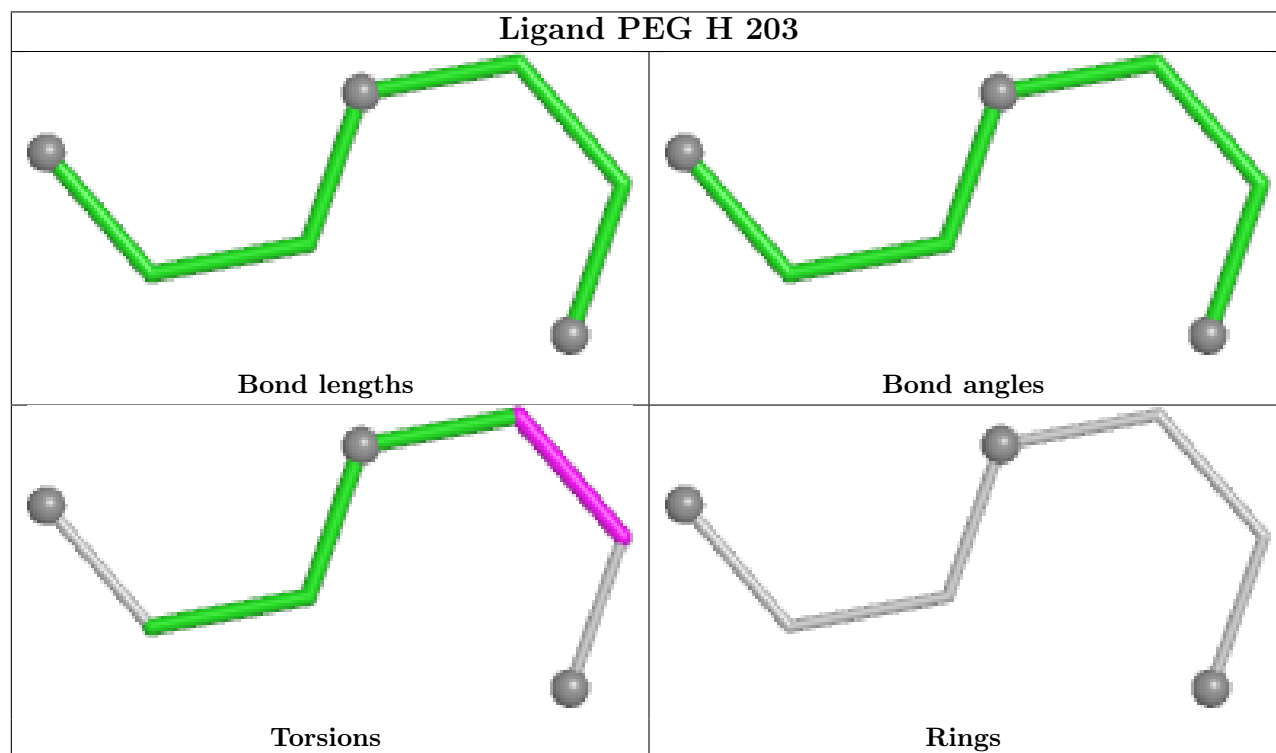
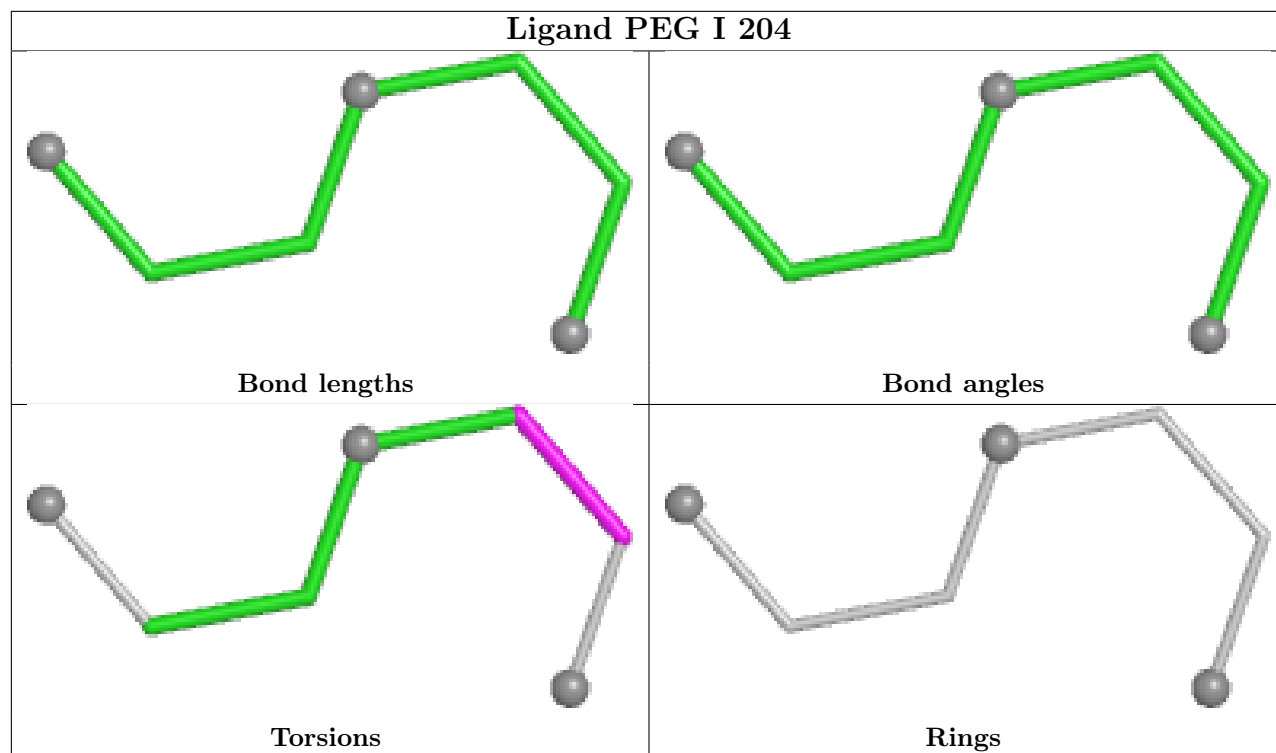




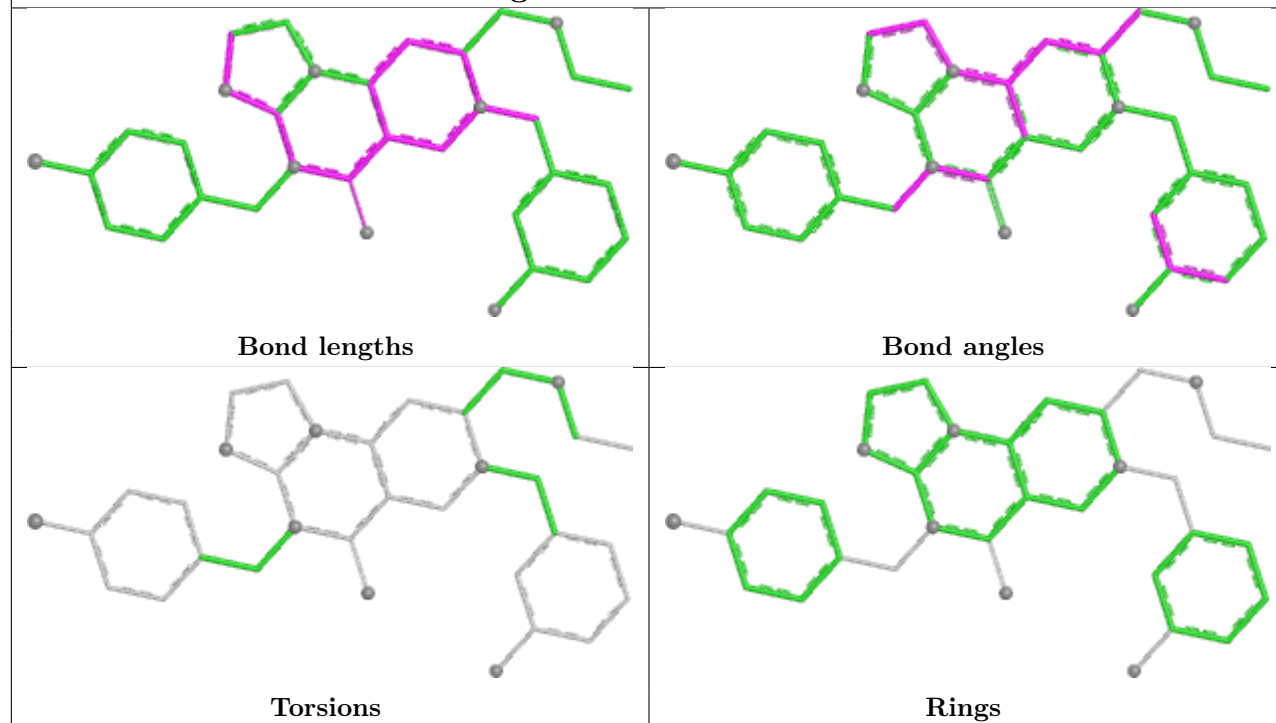




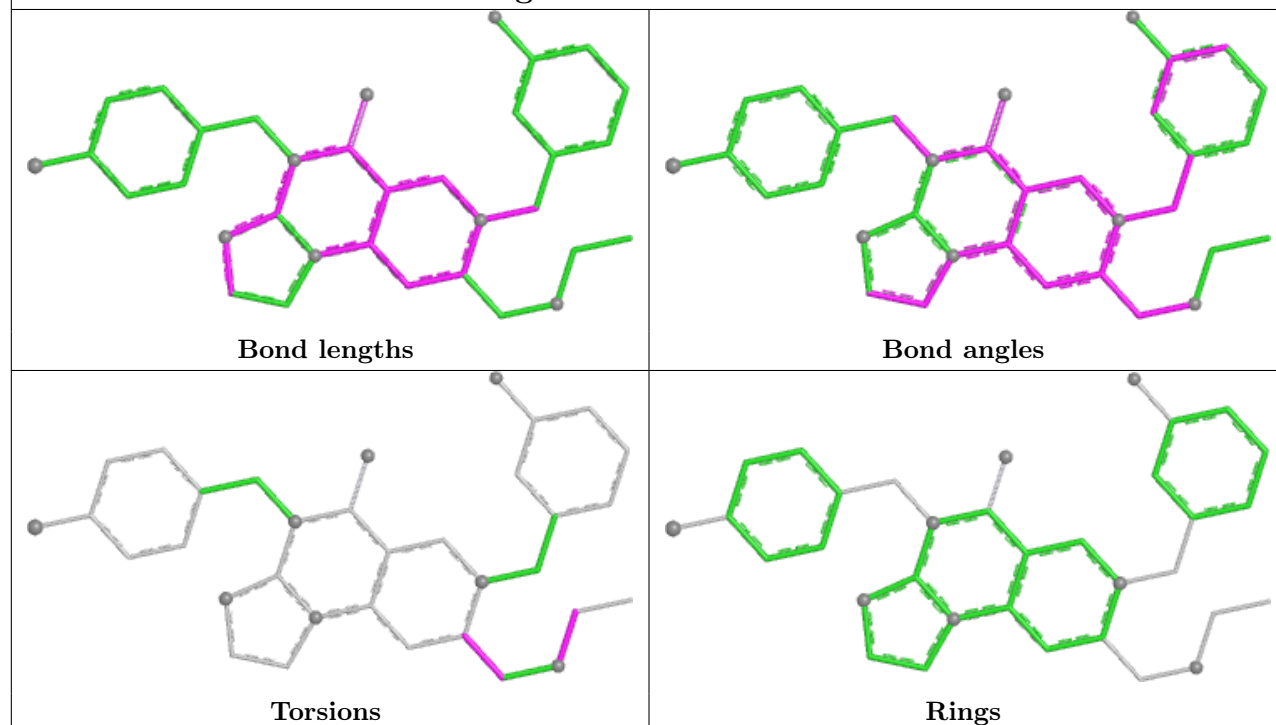


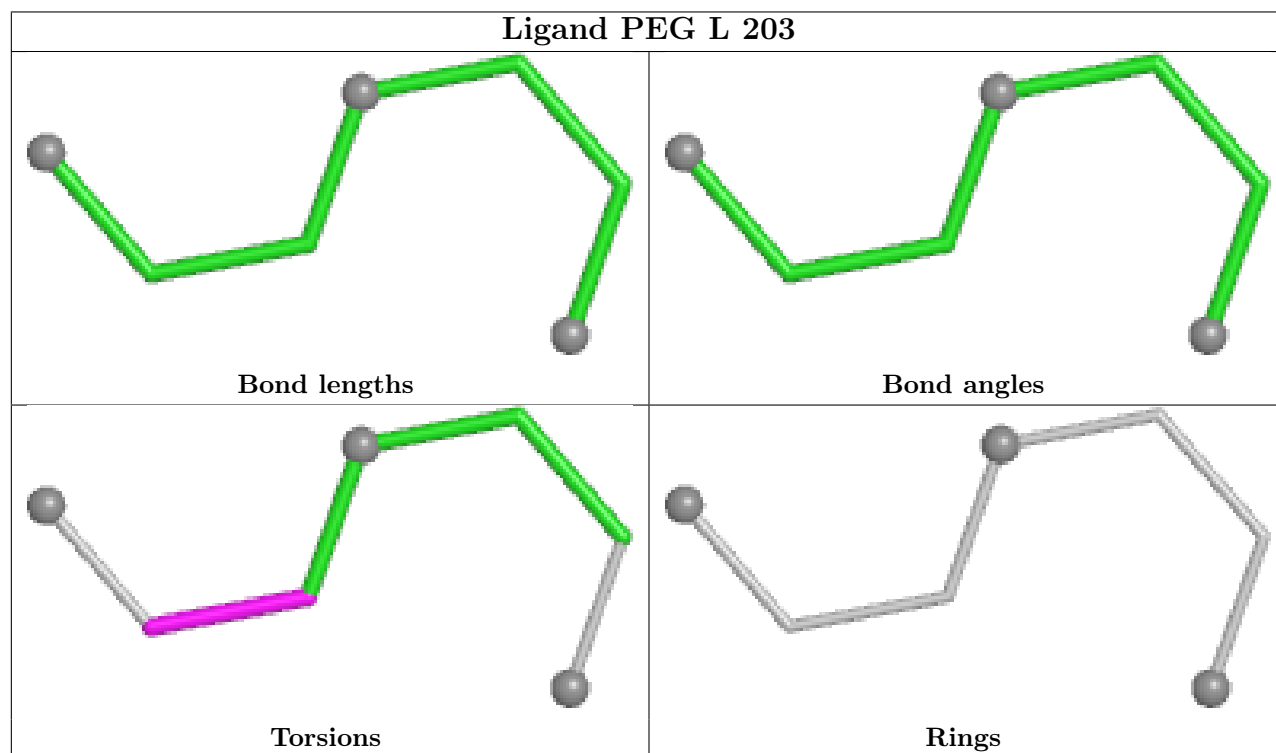
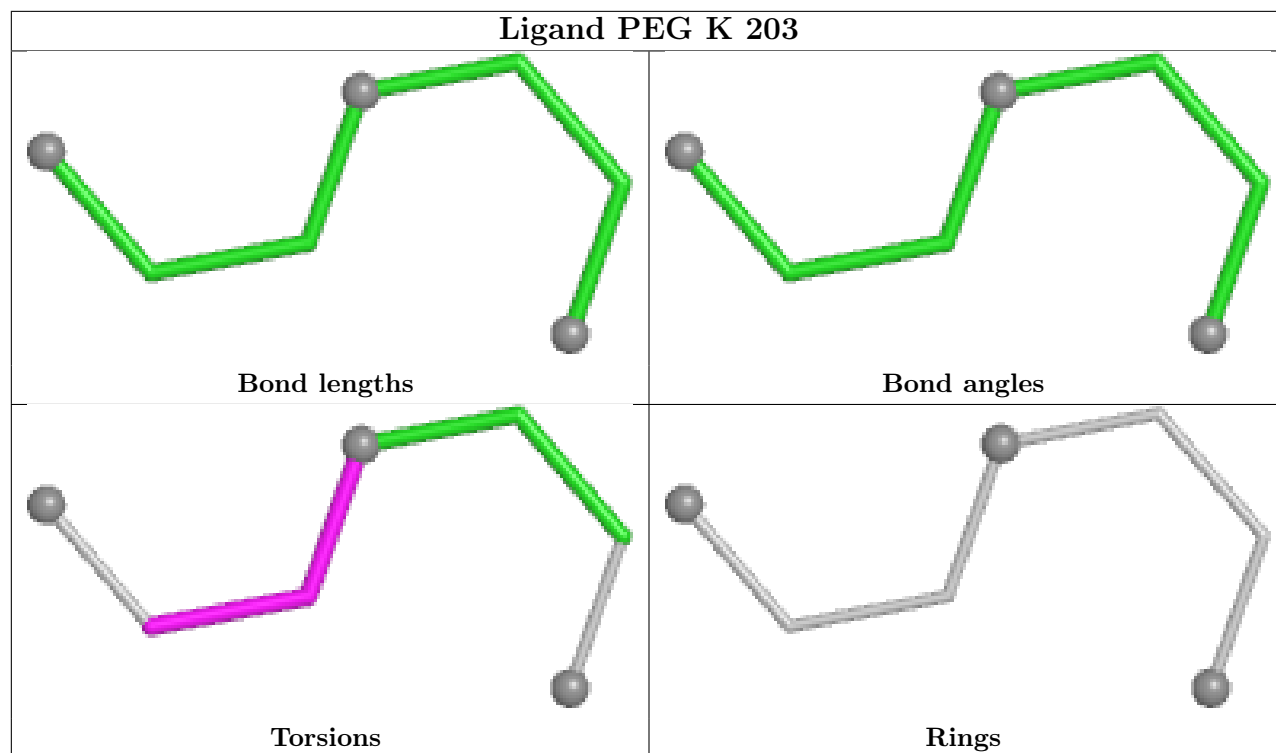


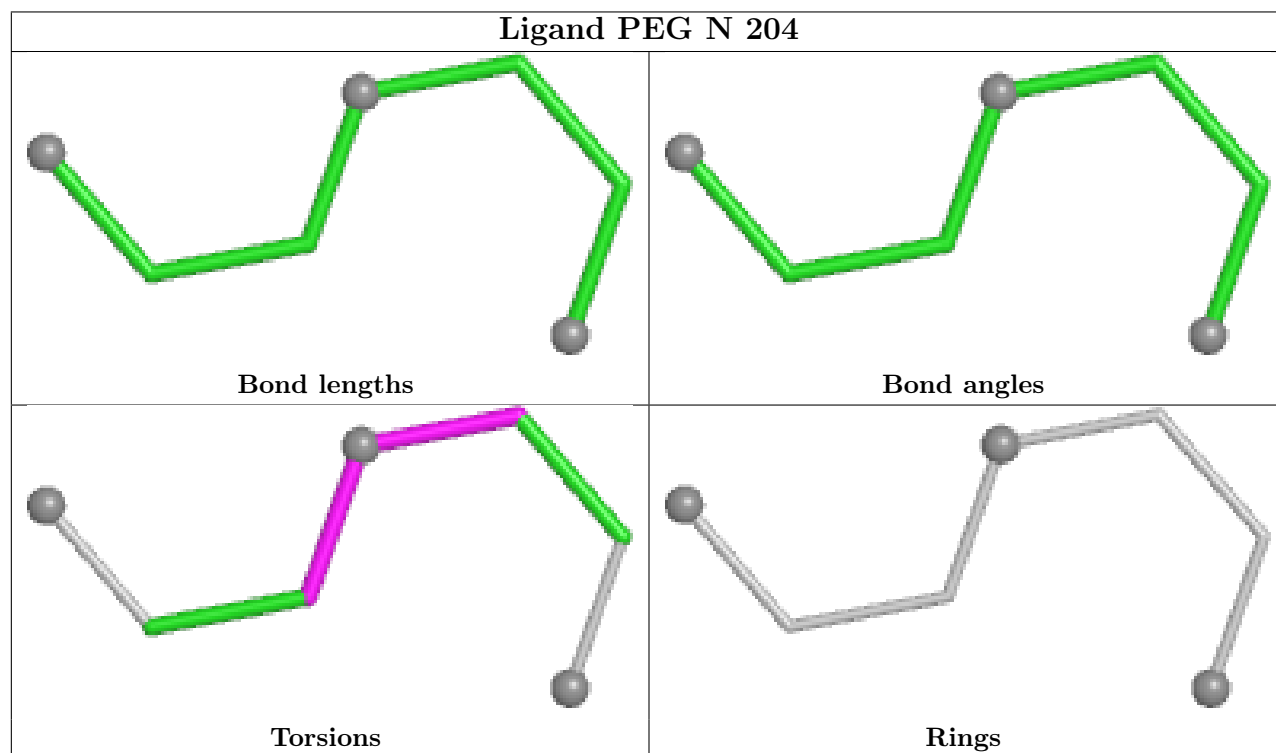
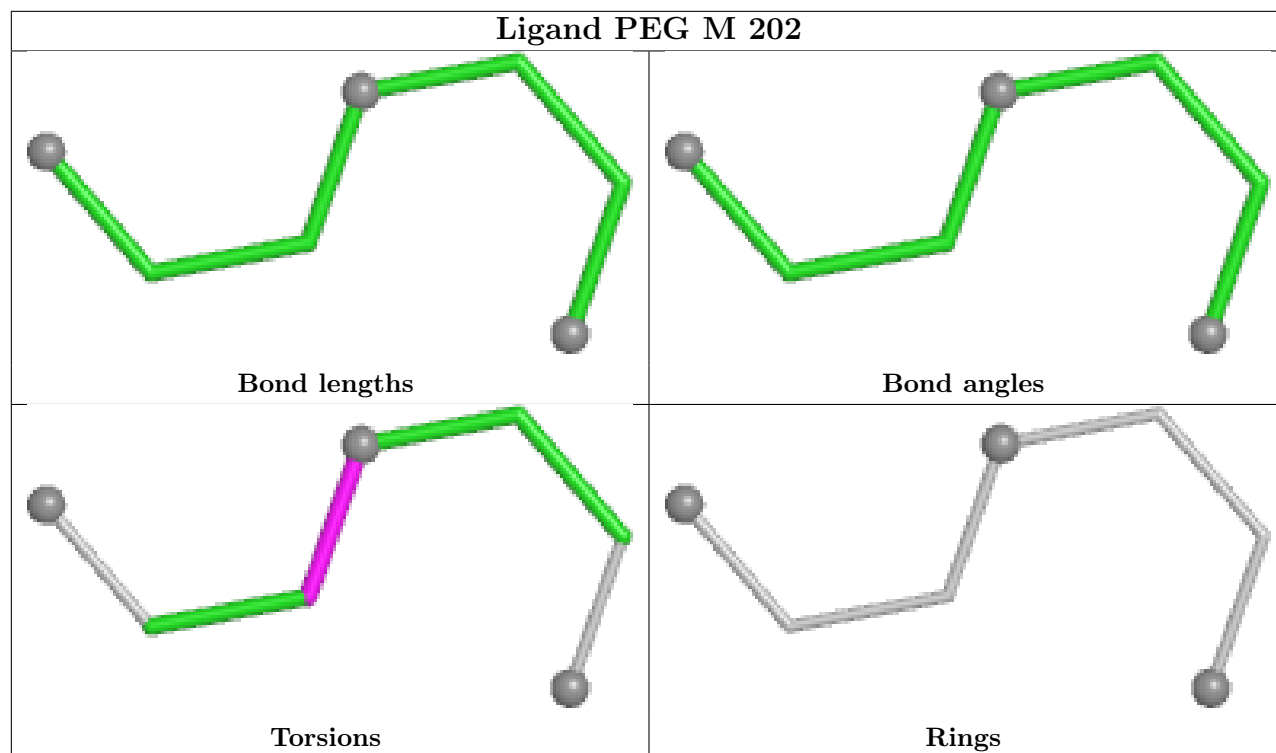
Ligand A1EDS H 204

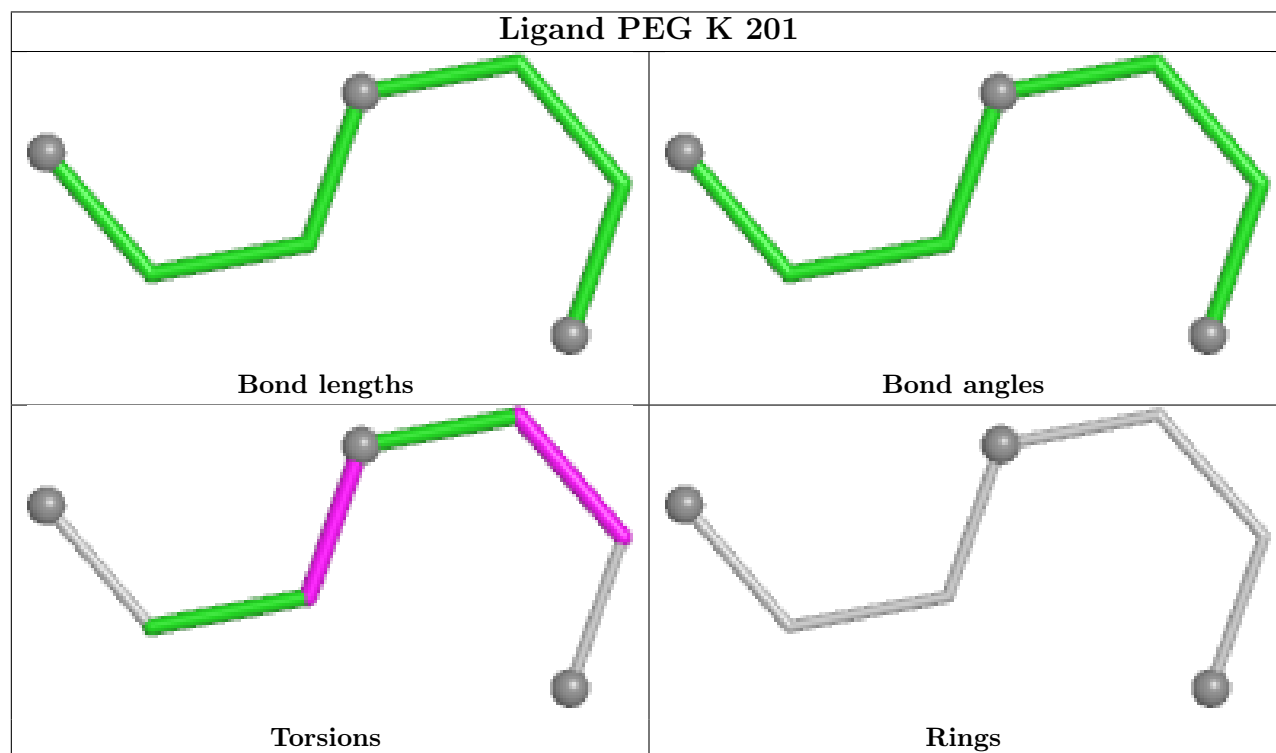
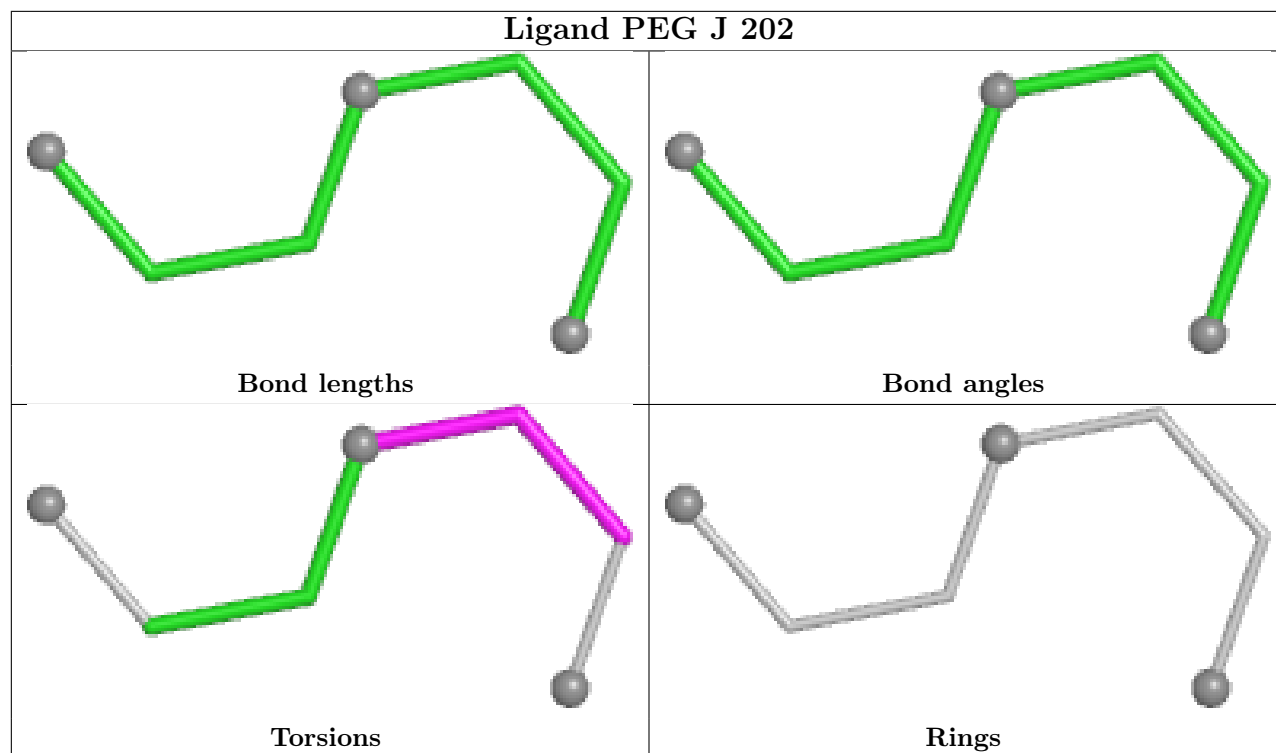


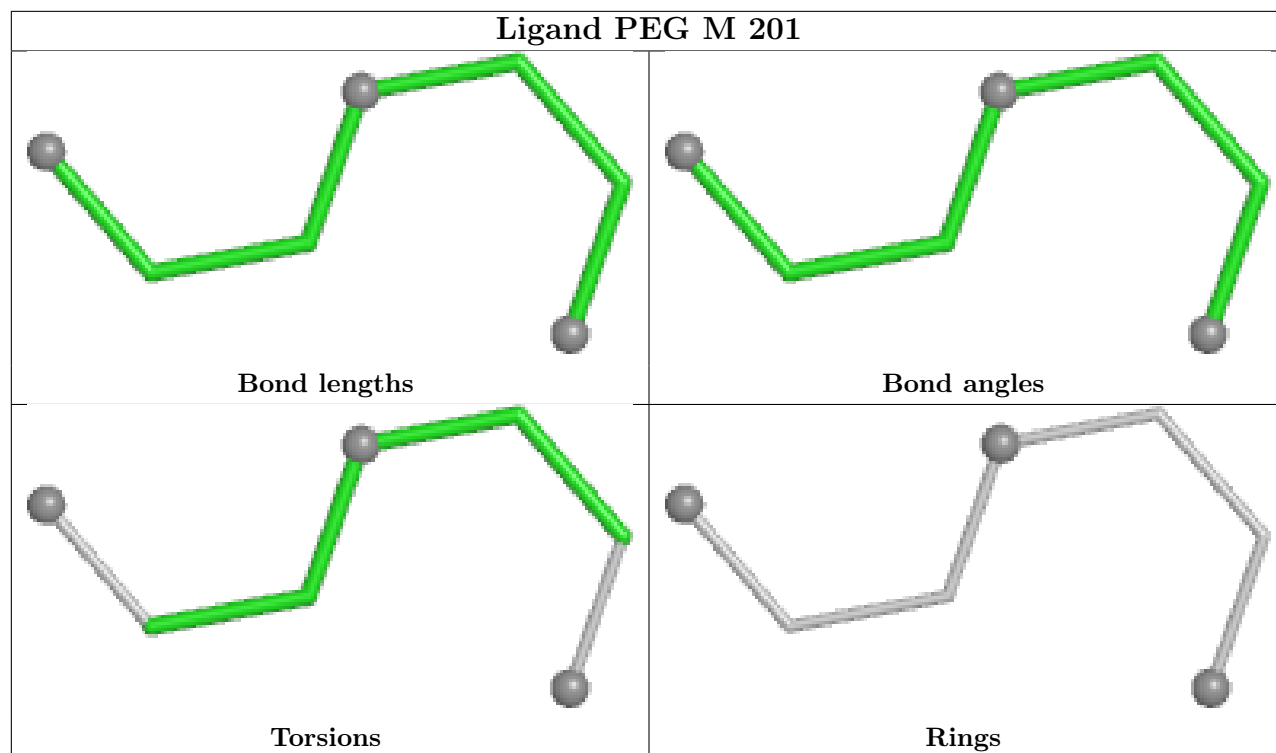
Ligand A1EDS J 204











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	H	189/196 (96%)	0.16	10 (5%)	32	31	17, 33, 70, 107	1 (0%)
1	I	190/196 (96%)	0.17	16 (8%)	17	16	15, 33, 72, 100	3 (1%)
1	J	193/196 (98%)	0.24	19 (9%)	13	12	17, 35, 83, 113	2 (1%)
1	K	190/196 (96%)	0.27	15 (7%)	18	18	19, 39, 67, 96	1 (0%)
1	L	193/196 (98%)	0.49	16 (8%)	17	16	32, 45, 74, 106	0
1	M	192/196 (97%)	0.47	10 (5%)	33	32	33, 42, 65, 100	0
1	N	190/196 (96%)	0.18	17 (8%)	15	14	17, 35, 74, 112	2 (1%)
All	All	1337/1372 (97%)	0.28	103 (7%)	19	18	15, 38, 74, 113	9 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	194	THR	7.6
1	I	3	LEU	5.8
1	M	3	LEU	5.4
1	M	183	TYR	5.4
1	I	195	LYS	5.3
1	M	194	THR	5.3
1	H	8	ILE	5.1
1	L	10	THR	5.0
1	K	3	LEU	4.9
1	L	3	LEU	4.7
1	I	10	THR	4.7
1	J	194	THR	4.7
1	H	14	GLY	4.5
1	M	181	LYS	4.5
1	I	194	THR	4.4
1	J	15	GLU	4.4
1	I	9	GLU	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	8	ILE	4.3
1	L	192	PRO	4.2
1	J	195	LYS	4.1
1	H	194	THR	4.1
1	N	3	LEU	4.0
1	J	12	ASN	4.0
1	N	194	THR	4.0
1	J	14	GLY	4.0
1	J	13	ARG	3.9
1	I	14	GLY	3.9
1	N	14	GLY	3.8
1	J	4	ILE	3.8
1	J	16	ARG	3.8
1	K	10	THR	3.8
1	L	4	ILE	3.7
1	K	194	THR	3.7
1	H	130	GLN	3.6
1	K	11	THR	3.6
1	H	9	GLU	3.5
1	K	15	GLU	3.5
1	M	16	ARG	3.4
1	K	8	ILE	3.4
1	N	8	ILE	3.4
1	L	191	VAL	3.3
1	I	18	TYR	3.2
1	M	182	GLU	3.1
1	L	2	ASN	3.1
1	K	195	LYS	3.0
1	N	130	GLN	3.0
1	L	193	GLU	3.0
1	I	7	VAL	3.0
1	H	3	LEU	3.0
1	J	11	THR	2.9
1	M	18	TYR	2.9
1	N	15	GLU	2.9
1	J	3	LEU	2.9
1	J	8	ILE	2.9
1	J	10	THR	2.9
1	H	13	ARG	2.8
1	N	195	LYS	2.8
1	L	14	GLY	2.8
1	K	17	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	93	ILE	2.8
1	K	16	ARG	2.8
1	I	15	GLU	2.8
1	M	93	ILE	2.8
1	M	15	GLU	2.7
1	N	9	GLU	2.7
1	H	15	GLU	2.7
1	J	17	ALA	2.6
1	M	193	GLU	2.6
1	J	193	GLU	2.6
1	K	192	PRO	2.6
1	L	11	THR	2.6
1	I	95[A]	MET	2.6
1	L	6	THR	2.6
1	N	17	ALA	2.6
1	L	13	ARG	2.5
1	L	130	GLN	2.5
1	I	127	GLY	2.4
1	J	130	GLN	2.3
1	K	4	ILE	2.3
1	I	191	VAL	2.3
1	L	9	GLU	2.3
1	K	6	THR	2.3
1	N	2	ASN	2.3
1	K	193	GLU	2.3
1	N	4	ILE	2.2
1	I	16	ARG	2.2
1	L	12	ASN	2.2
1	J	123	HIS	2.2
1	N	16	ARG	2.2
1	J	192	PRO	2.1
1	I	17	ALA	2.1
1	H	18	TYR	2.1
1	J	18	TYR	2.1
1	H	192	PRO	2.1
1	N	129	ALA	2.1
1	N	18	TYR	2.1
1	I	4	ILE	2.1
1	L	7	VAL	2.1
1	N	191	VAL	2.1
1	J	5	PRO	2.1
1	K	121	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	123	HIS	2.0
1	N	123	HIS	2.0

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
2	PEG	L	204	7/7	0.68	0.17	66,82,87,88	0
2	PEG	K	201	7/7	0.78	0.16	64,70,81,81	0
2	PEG	L	203	7/7	0.80	0.17	61,66,75,80	0
2	PEG	I	203	7/7	0.81	0.15	65,67,73,76	0
2	PEG	N	204	7/7	0.81	0.12	48,56,67,76	0
2	PEG	J	203	7/7	0.82	0.18	60,67,70,74	0
2	PEG	H	202	7/7	0.82	0.19	52,53,59,61	0
2	PEG	L	201	7/7	0.82	0.15	66,70,74,79	0
2	PEG	I	204	7/7	0.83	0.15	61,64,72,72	0
2	PEG	H	203	7/7	0.84	0.15	51,54,57,62	0
2	PEG	J	202	7/7	0.84	0.15	68,73,75,77	0
2	PEG	K	203	7/7	0.86	0.13	54,59,65,68	0
2	PEG	M	201	7/7	0.87	0.13	62,73,76,76	0
2	PEG	I	201	7/7	0.88	0.15	52,57,59,67	0
2	PEG	M	202	7/7	0.88	0.13	53,55,57,58	0
2	PEG	N	202	7/7	0.88	0.15	51,55,61,63	0
2	PEG	K	202	7/7	0.88	0.11	67,72,80,80	0
3	A1EDS	M	203	34/34	0.88	0.14	44,53,65,72	0
3	A1EDS	J	204	34/34	0.89	0.11	30,39,47,51	0
3	A1EDS	I	205	34/34	0.89	0.11	30,37,44,56	0
2	PEG	H	201	7/7	0.90	0.11	46,48,50,50	0

Continued on next page...

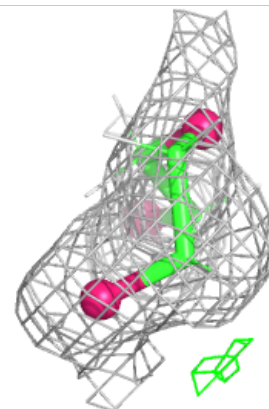
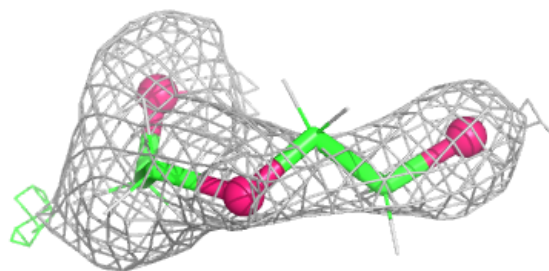
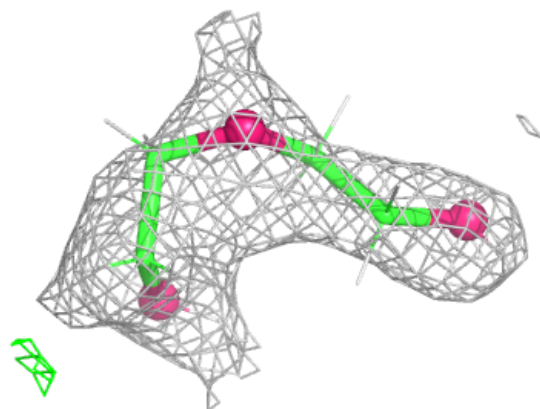
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	N	203	7/7	0.90	0.13	44,47,51,54	0
3	A1EDS	K	205	34/34	0.90	0.10	35,45,56,67	0
3	A1EDS	L	205	34/34	0.90	0.11	43,49,66,72	0
2	PEG	L	202	7/7	0.90	0.12	56,56,57,58	0
3	A1EDS	N	205	34/34	0.91	0.10	39,47,58,64	0
2	PEG	J	201	7/7	0.92	0.11	46,46,50,53	0
2	PEG	N	201	7/7	0.93	0.09	46,49,50,54	0
2	PEG	I	202	7/7	0.93	0.11	46,48,50,56	0
3	A1EDS	H	204	34/34	0.93	0.09	30,39,49,56	0
2	PEG	K	204	7/7	0.94	0.10	49,52,53,57	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.

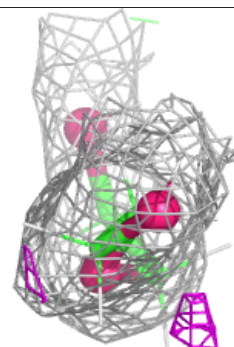
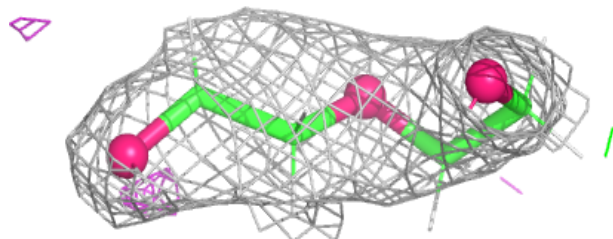
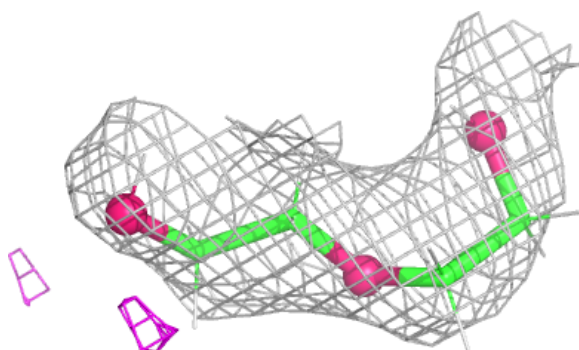
Electron density around PEG L 204:

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

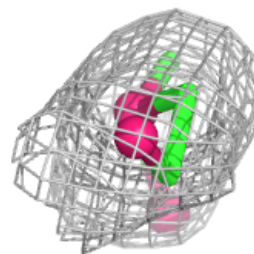
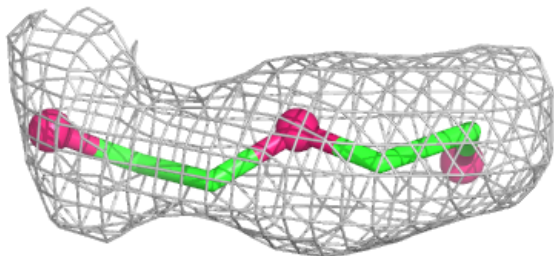
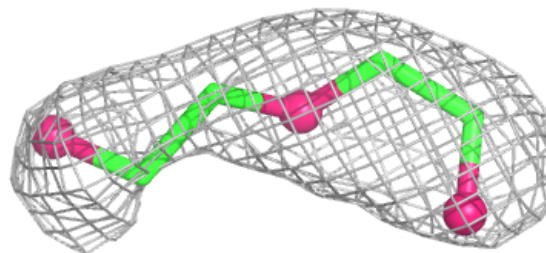


Electron density around PEG K 201:

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

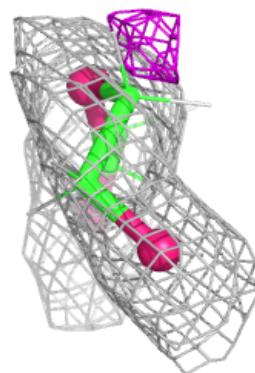
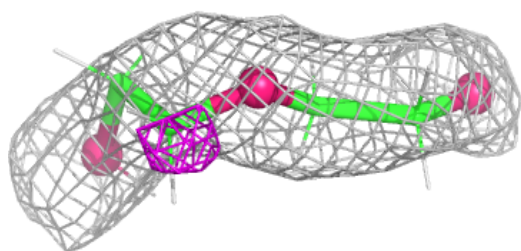
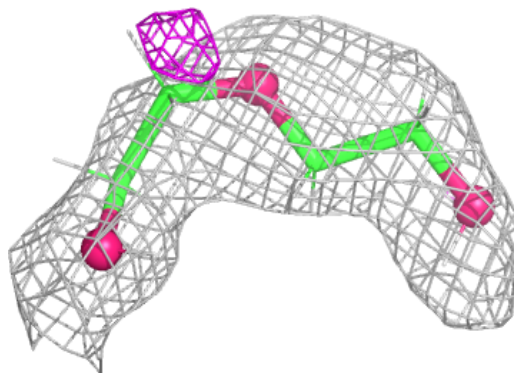
**Electron density around PEG L 203:**

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

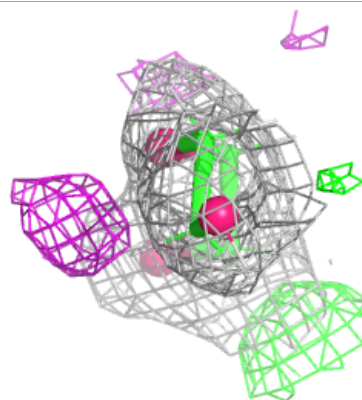
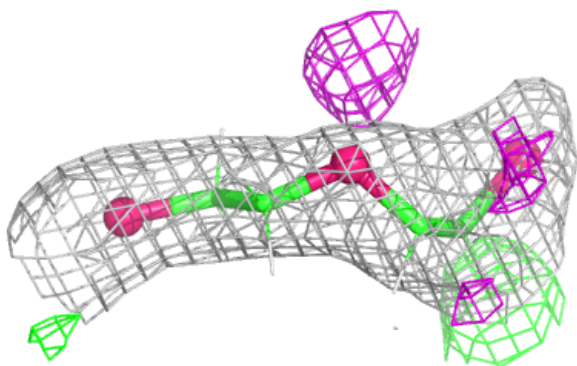
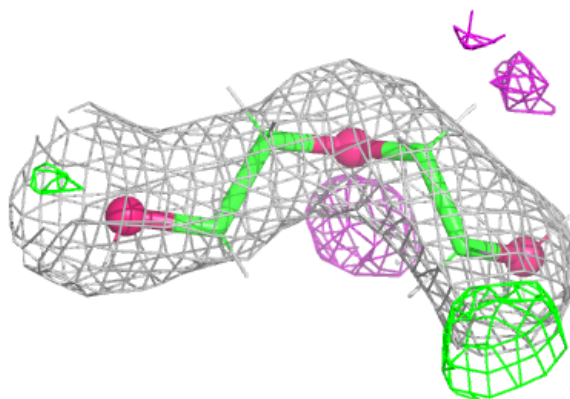


Electron density around PEG I 203:

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

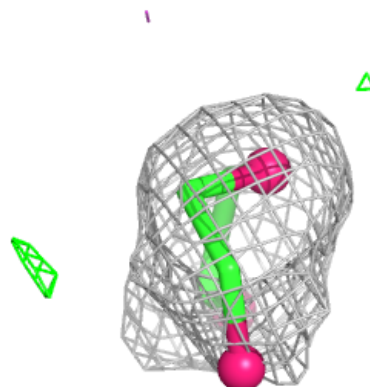
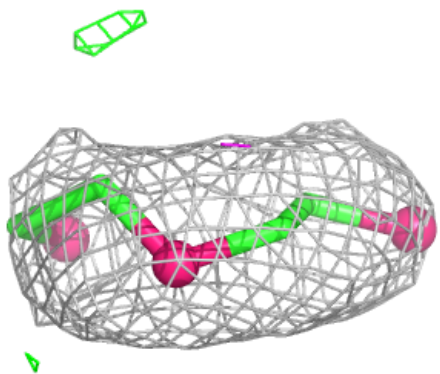
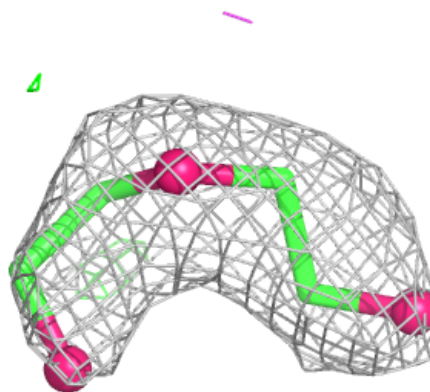
**Electron density around PEG N 204:**

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

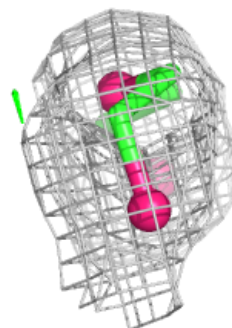
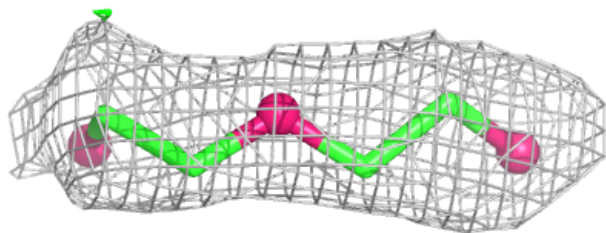
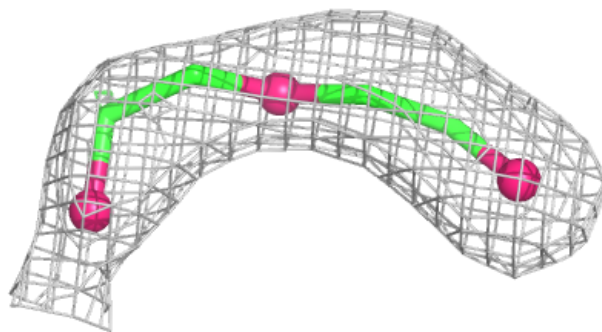


Electron density around PEG J 203:

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

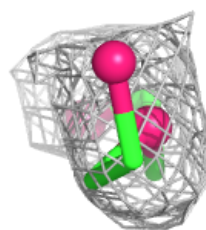
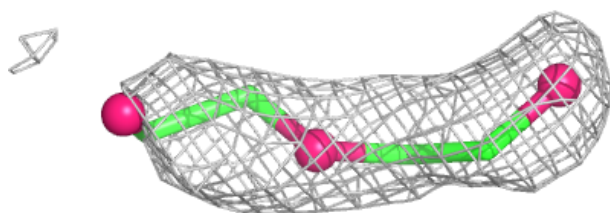
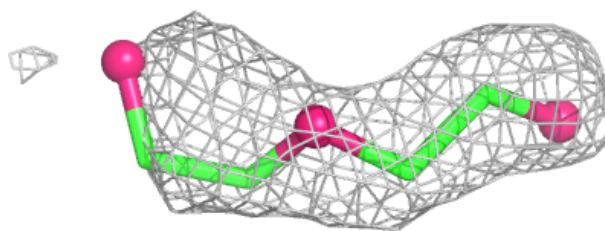
**Electron density around PEG H 202:**

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

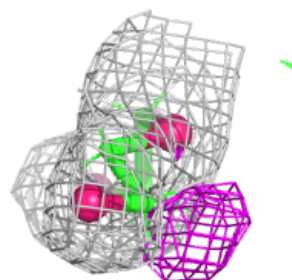
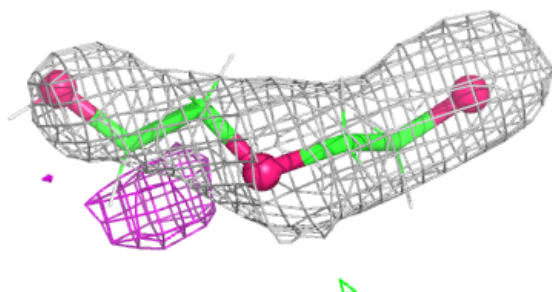
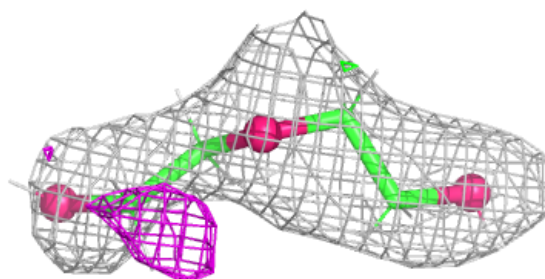


Electron density around PEG L 201:

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

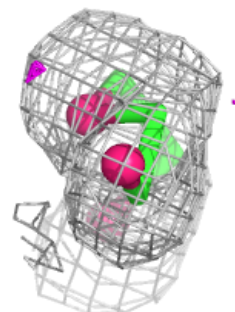
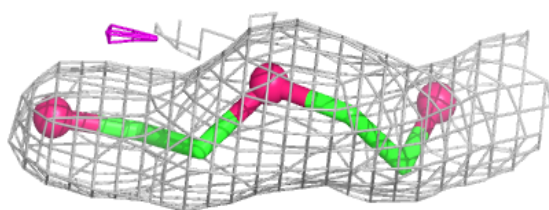
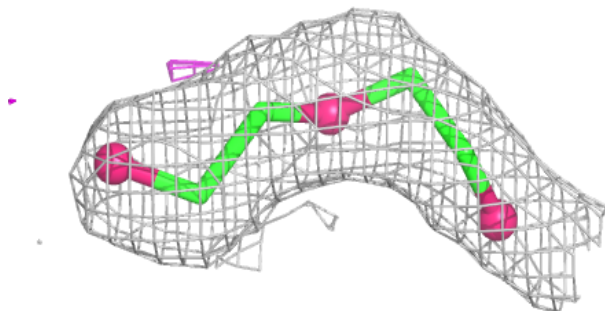
**Electron density around PEG I 204:**

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

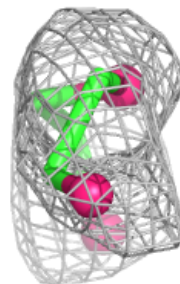
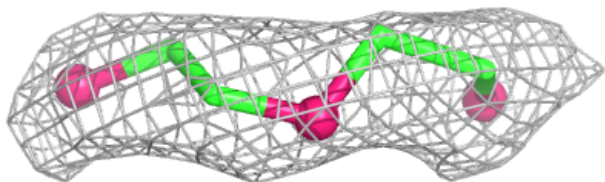
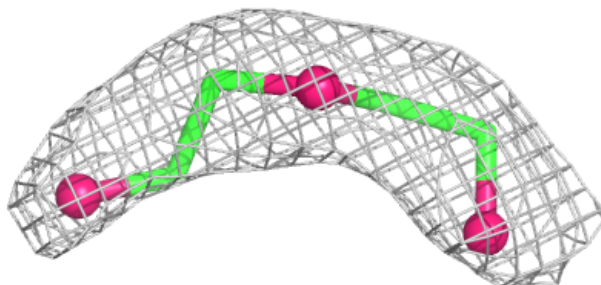


Electron density around PEG H 203:

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

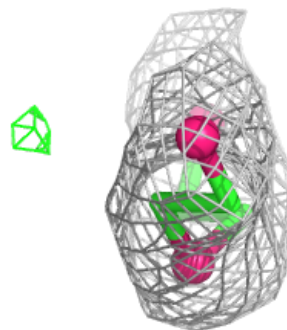
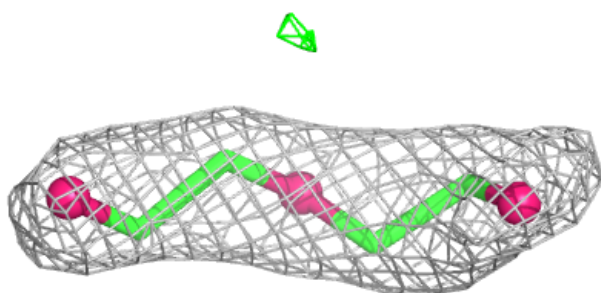
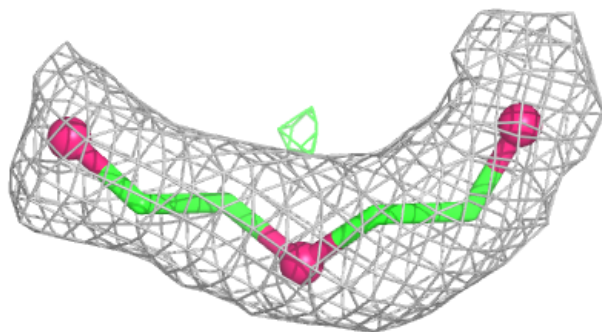
**Electron density around PEG J 202:**

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

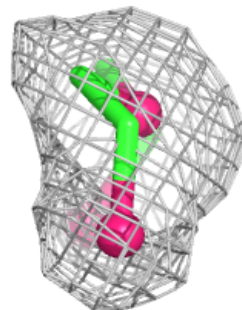
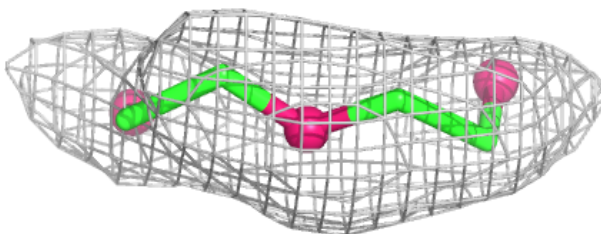
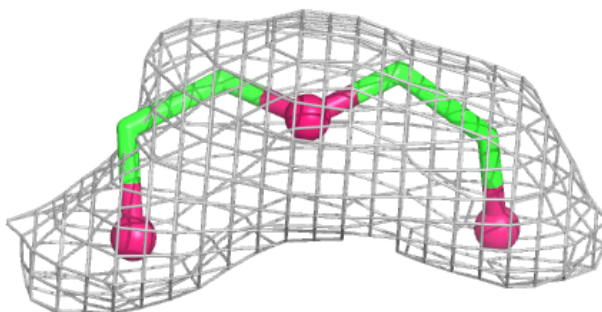


Electron density around PEG K 203:

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

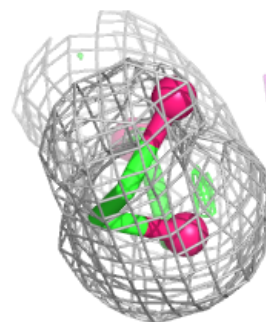
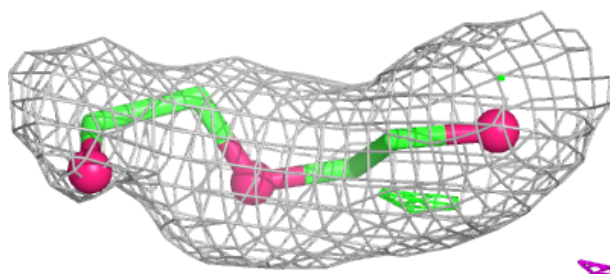
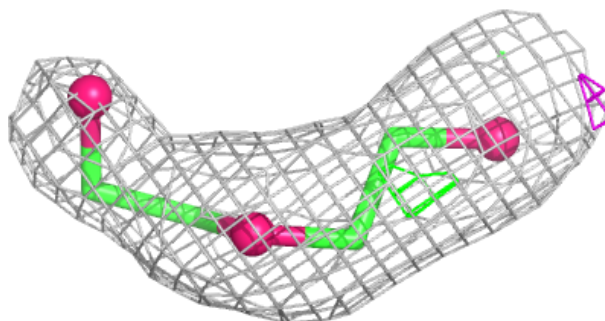
**Electron density around PEG M 201:**

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

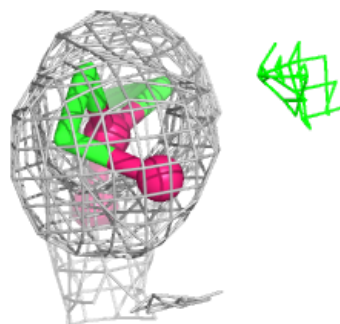
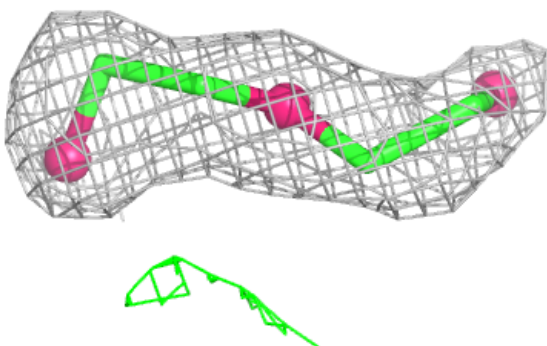
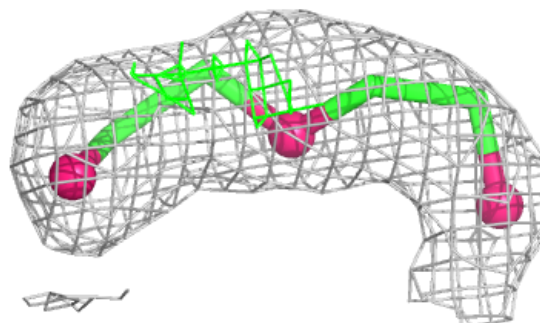


Electron density around PEG I 201:

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

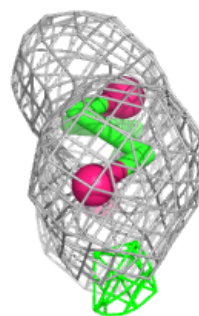
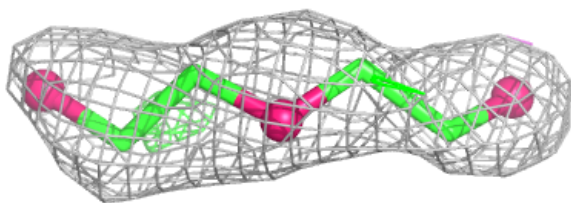
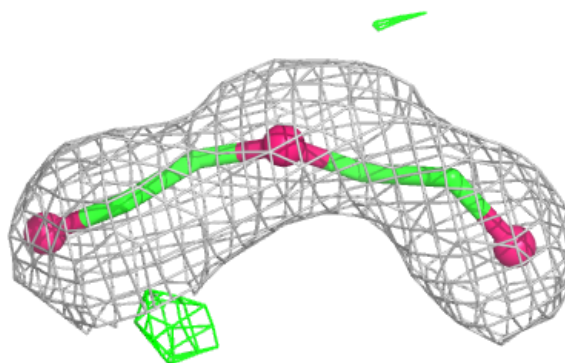
**Electron density around PEG M 202:**

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

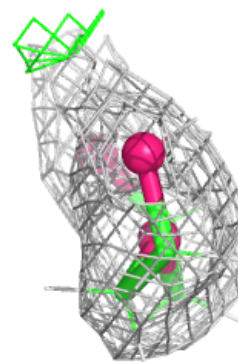
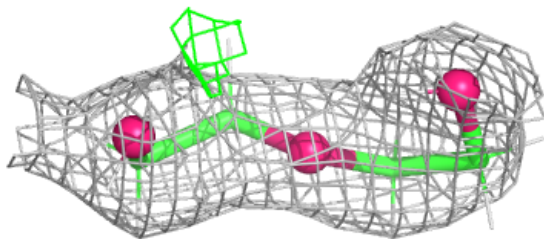
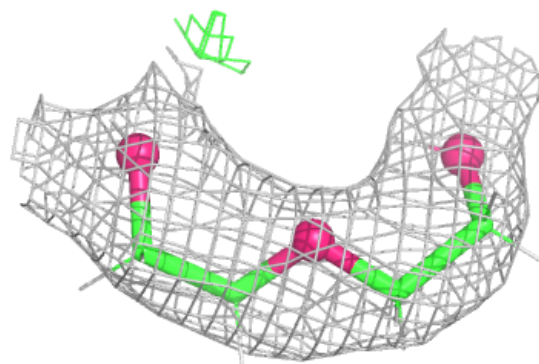


Electron density around PEG N 202:

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

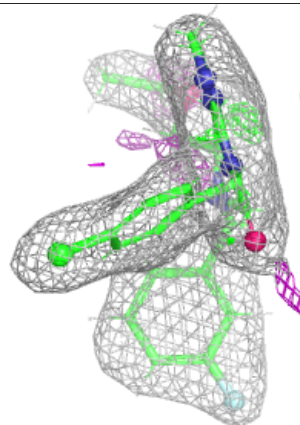
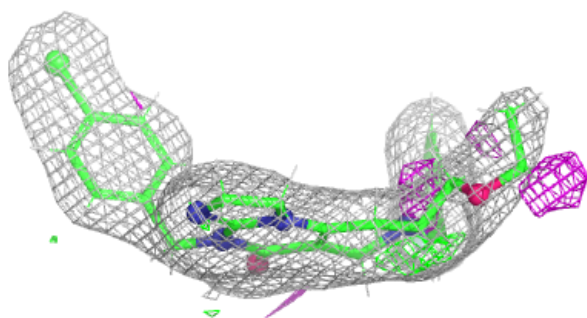
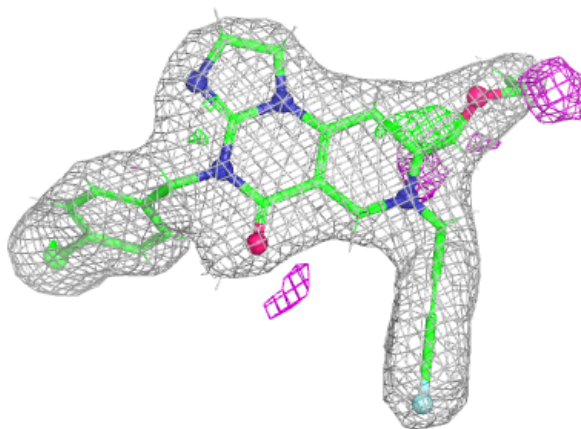
**Electron density around PEG K 202:**

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



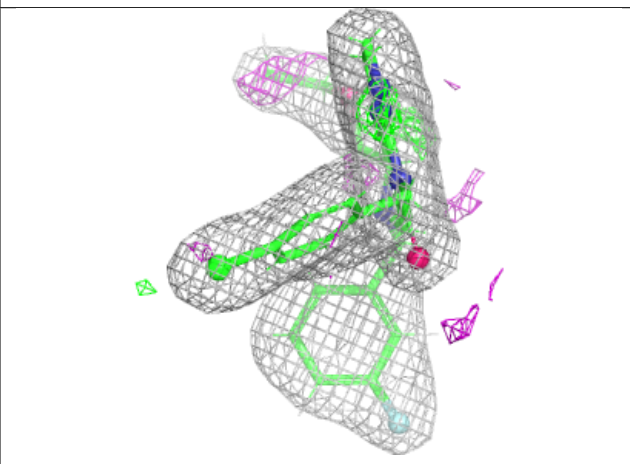
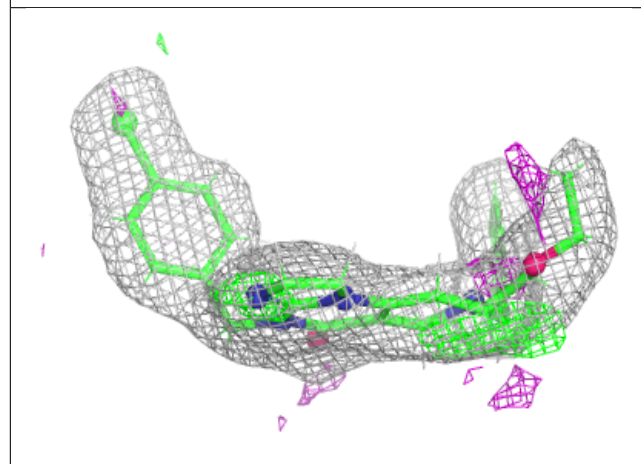
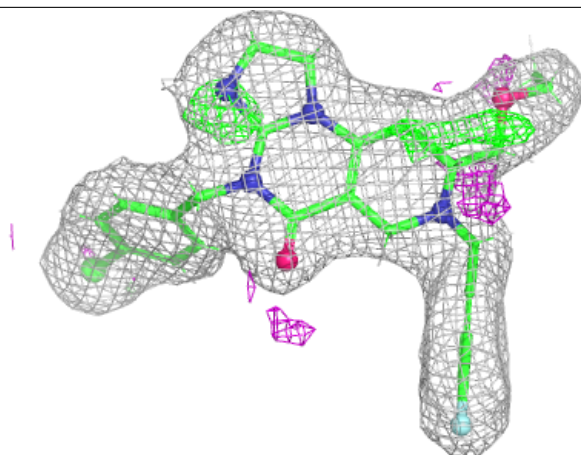
Electron density around A1EDS M 203:

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



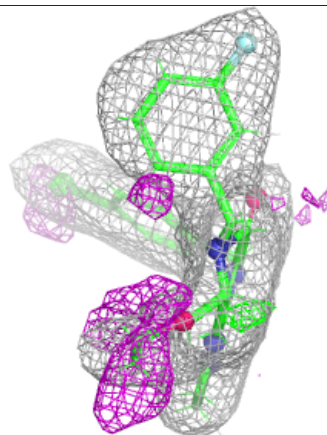
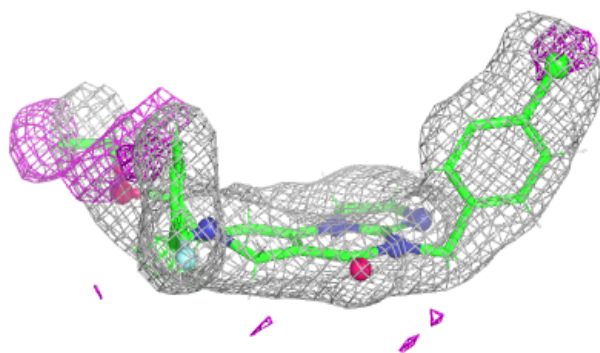
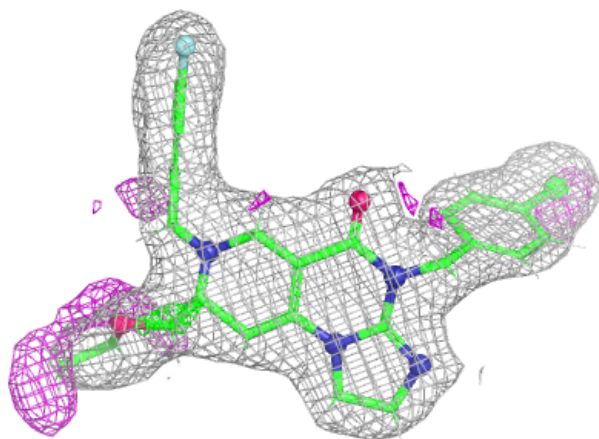
Electron density around A1EDS J 204:

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



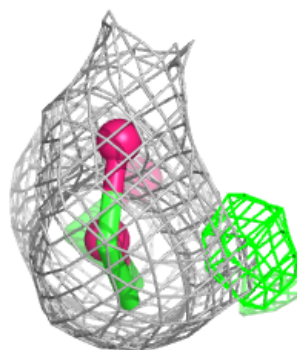
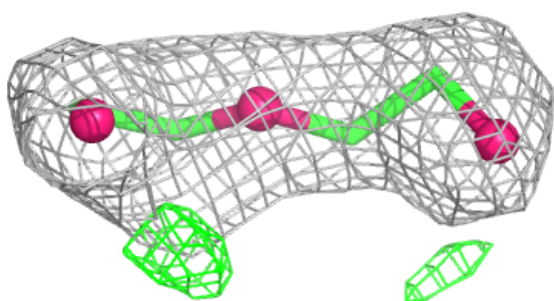
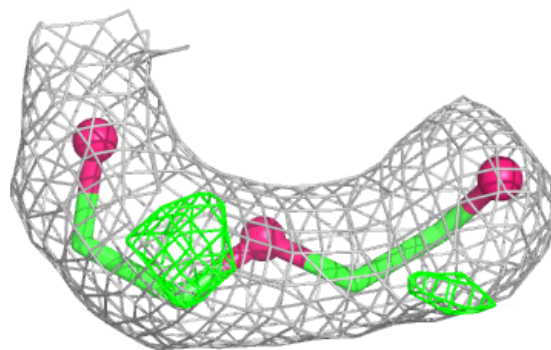
Electron density around A1EDS I 205:

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

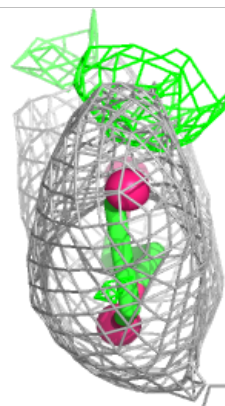
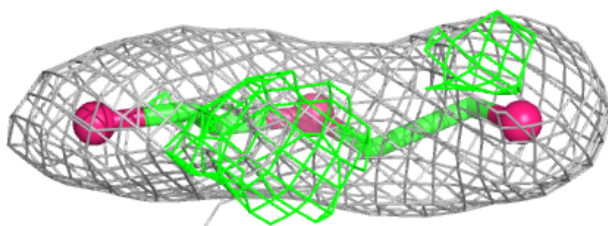
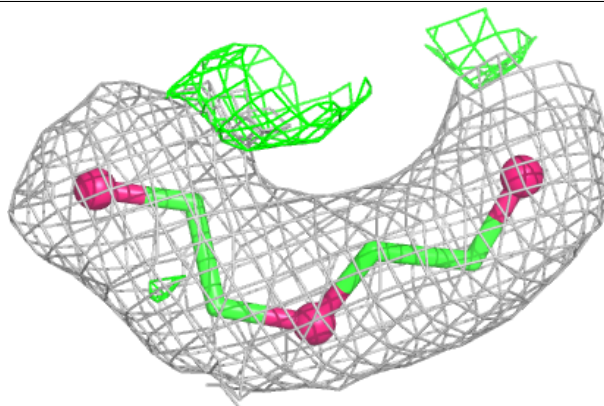


Electron density around PEG H 201:

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

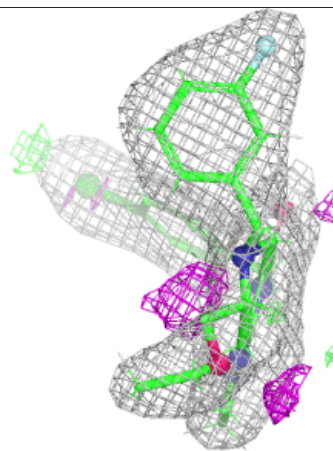
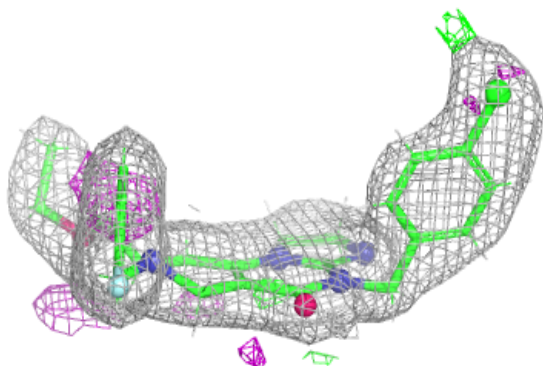
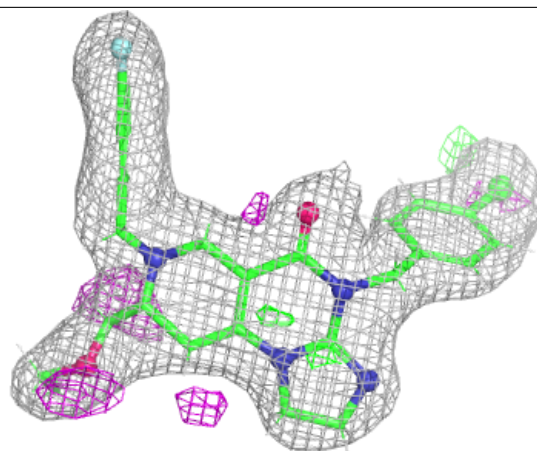
**Electron density around PEG N 203:**

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



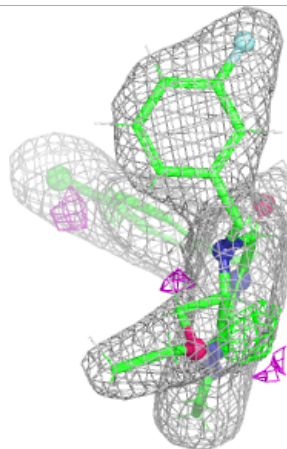
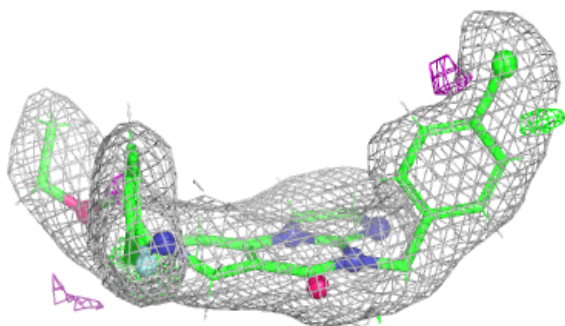
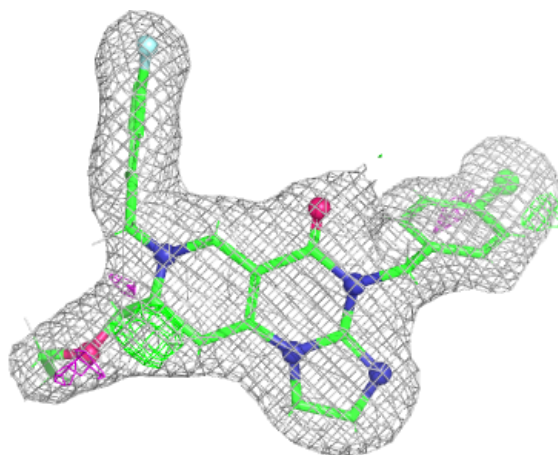
Electron density around A1EDS K 205:

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



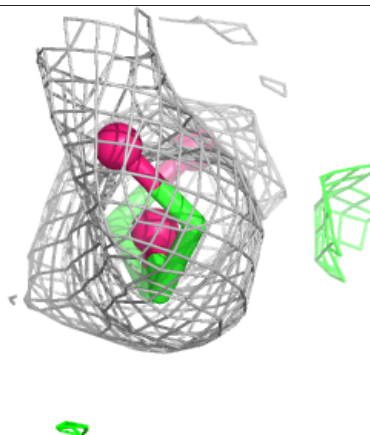
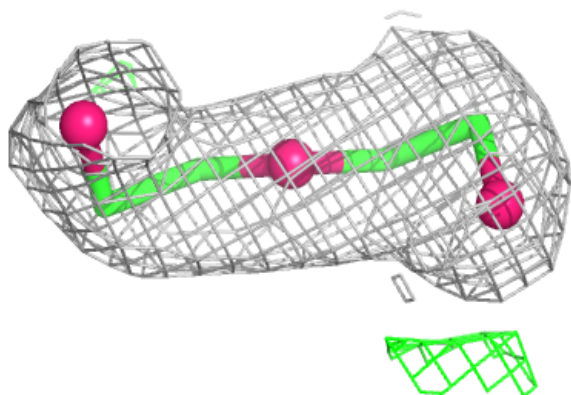
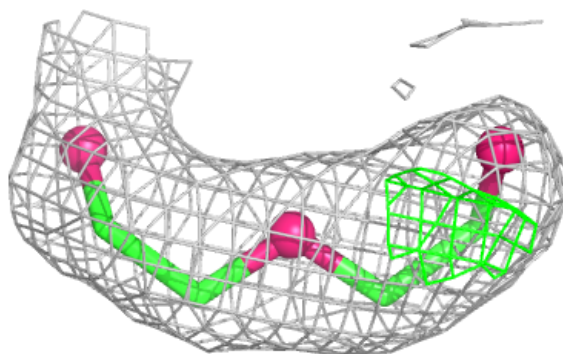
Electron density around A1EDS L 205:

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



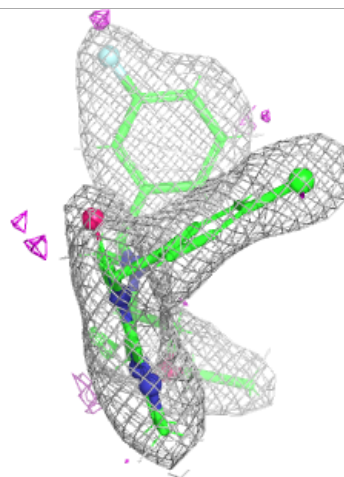
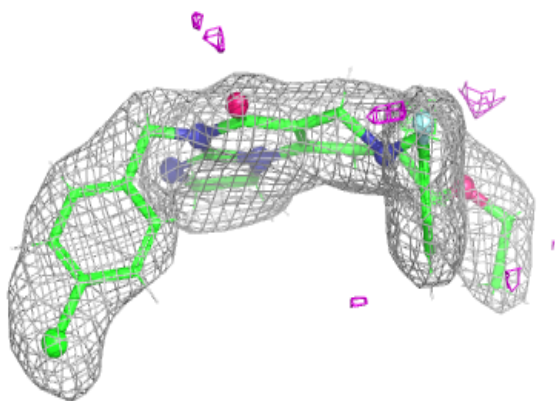
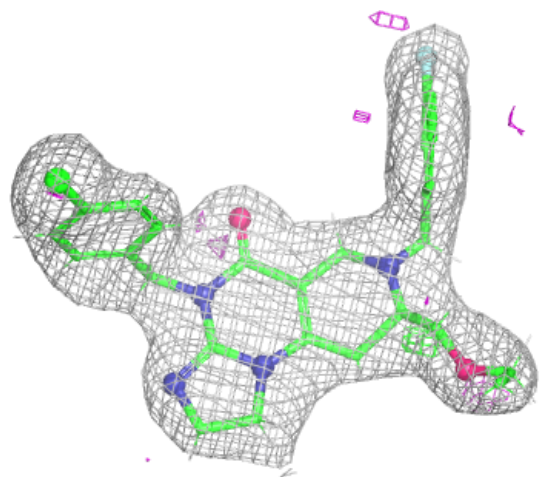
Electron density around PEG L 202:

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



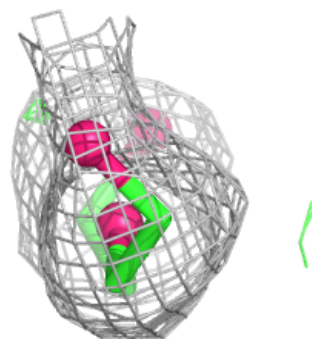
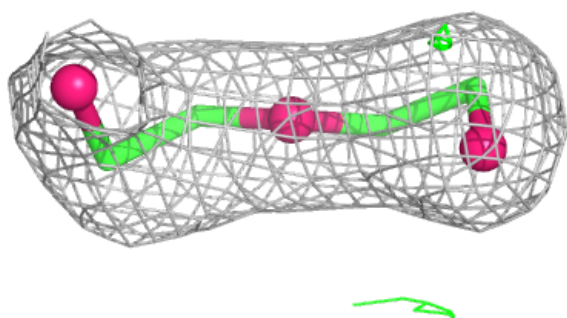
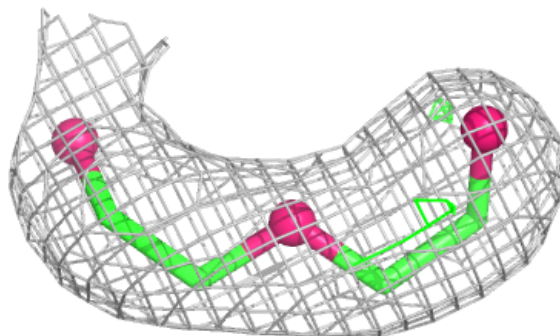
Electron density around A1EDS N 205:

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

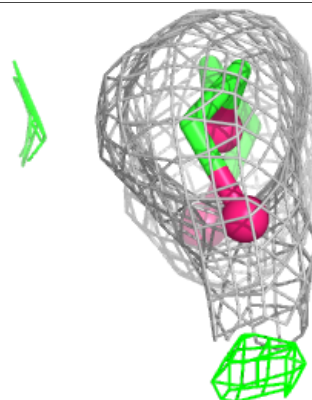
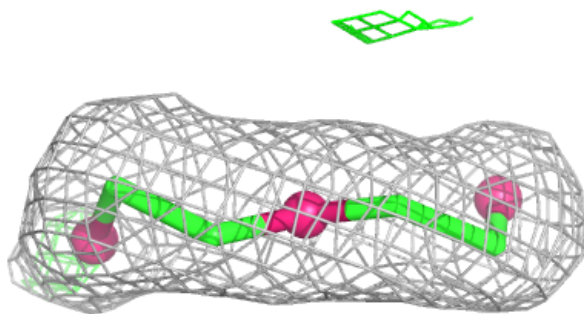
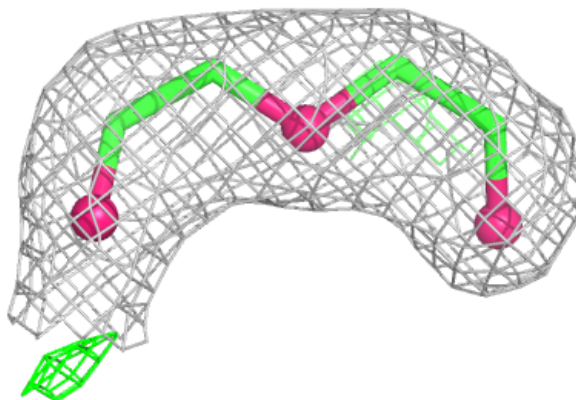


Electron density around PEG J 201:

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

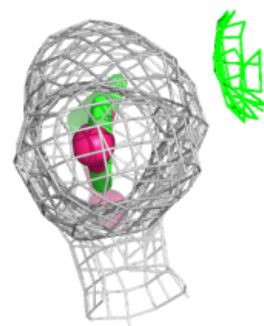
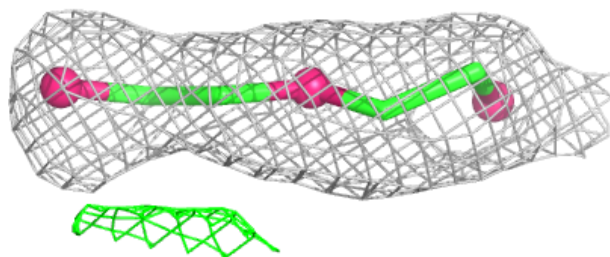
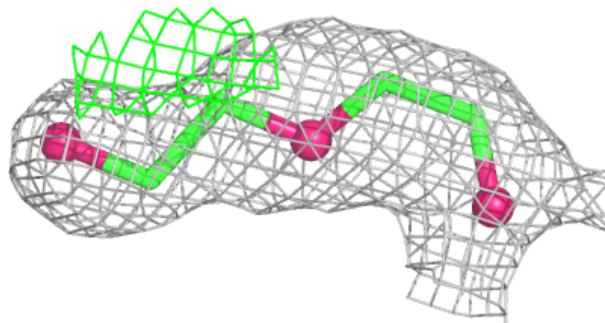
**Electron density around PEG N 201:**

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



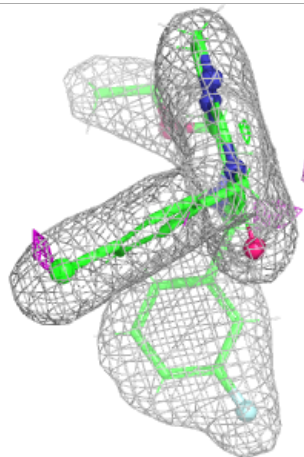
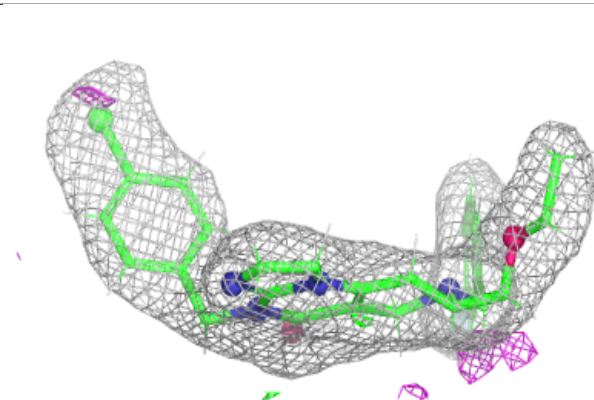
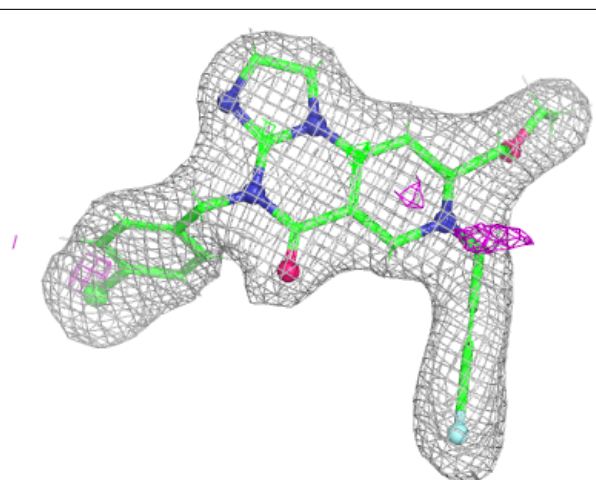
Electron density around PEG I 202:

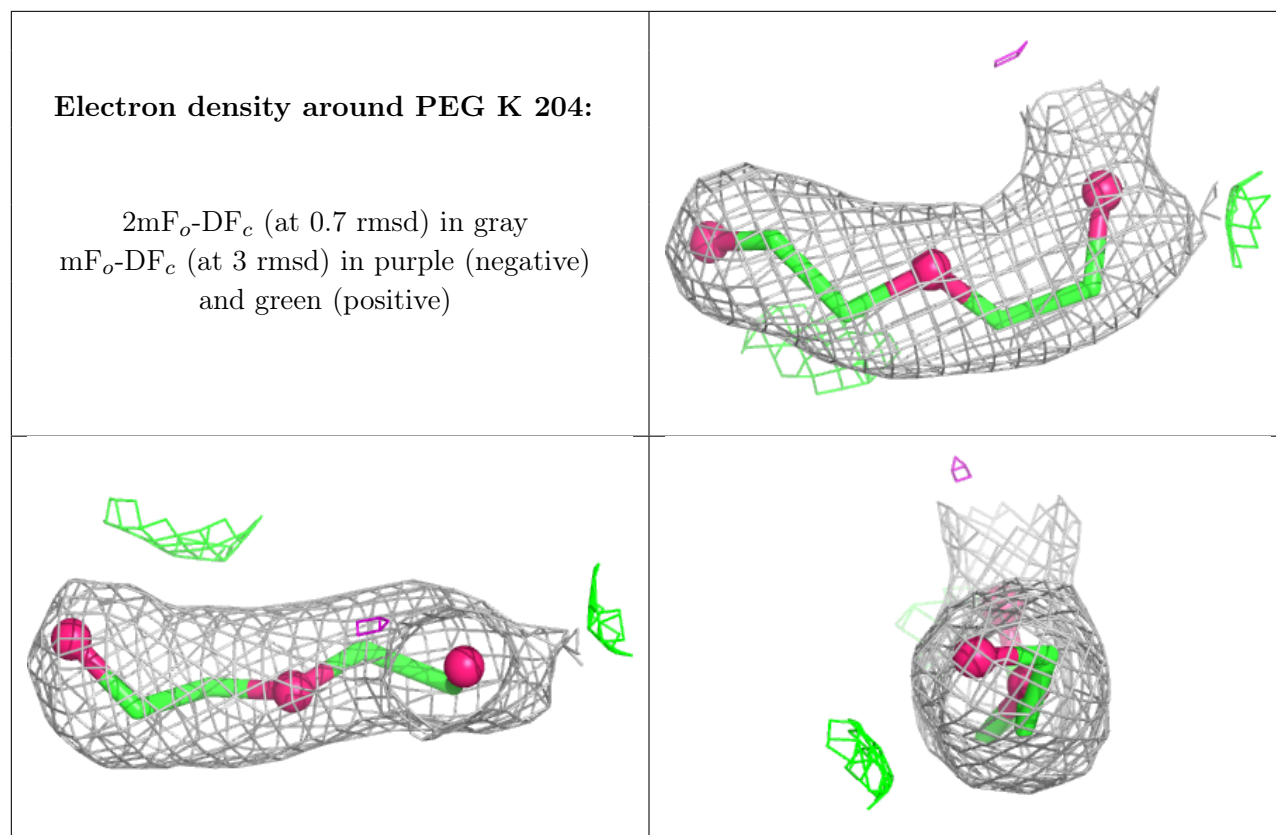
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1EDS H 204:

$2mF_o-DF_c$ (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.