



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:09 AM JST

PDB ID : 9KZH / pdb_00009kzh
EMDB ID : EMD-62663
Title : Cryo-EM structure of the RC complex from Rhodospirillum rubrum
Authors : Wang, L.; Yu, L.-J.
Deposited on : 2024-12-10
Resolution : 2.74 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

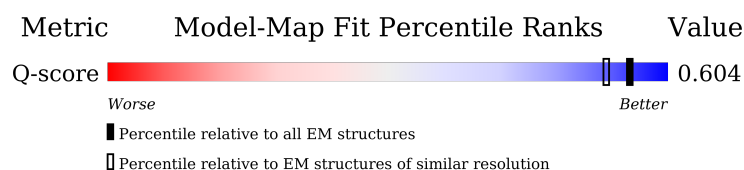
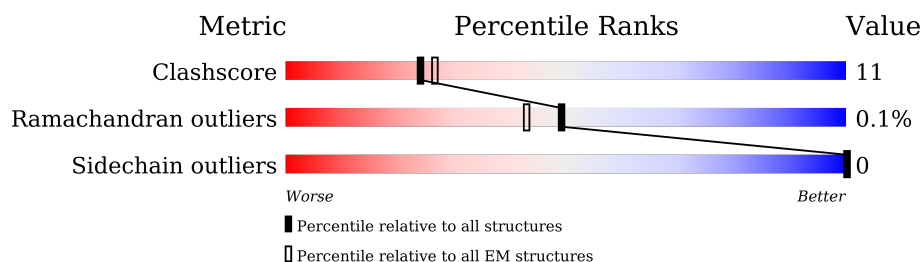
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	276	 81% 19%
2	M	306	 79% 20%
3	H	257	 5% 81% 19%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PEF	H	301	-	-	X	-
4	07D	L	301	X	-	-	-
4	07D	M	402	X	-	-	-
4	07D	M	403	X	-	-	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 8317 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	275	Total	C	N	O	S	0	0
			2169	1458	345	356	10		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	305	Total	C	N	O	S	0	0
			2425	1619	398	399	9		

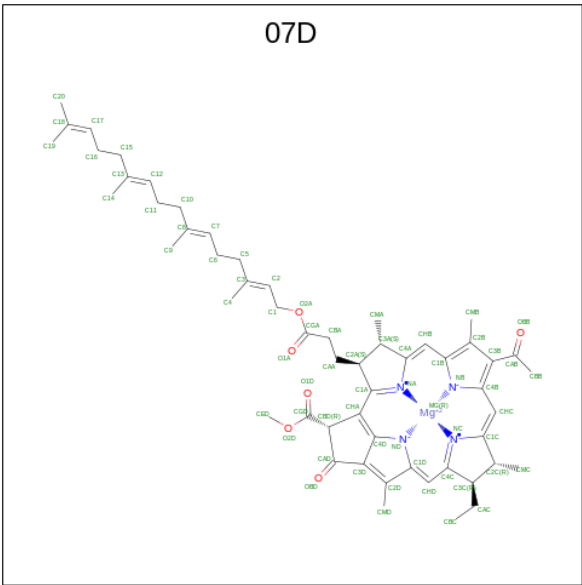
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	215	PHE	SER	conflict	UNP P10718

- Molecule 3 is a protein called Photoreaction center protein H.

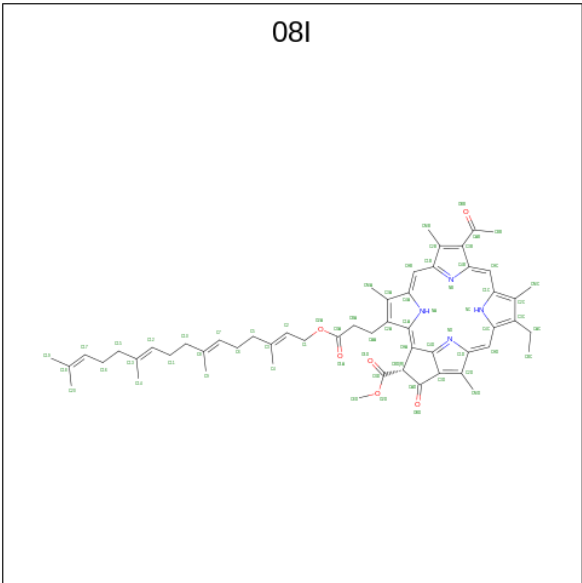
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	256	Total	C	N	O	S	0	0
			1964	1258	342	361	3		

- Molecule 4 is Trans-Geranyl BACTERIOCHLOROPHYLL A (CCD ID: 07D) (formula: $C_{55}H_{68}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



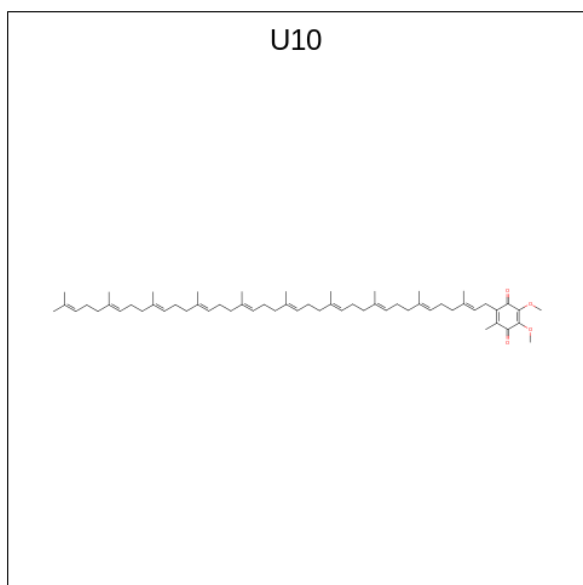
Mol	Chain	Residues	Atoms					AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 5 is Trans-Geranyl BACTERIOPHEOPHYTIN A (CCD ID: 08I) (formula: $C_{55}H_{66}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



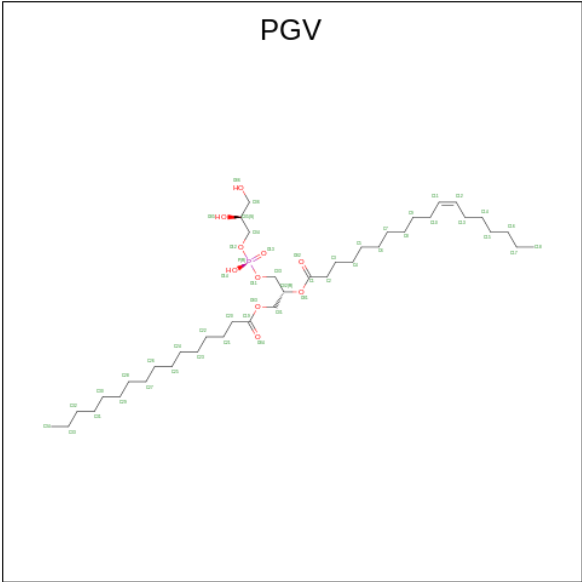
Mol	Chain	Residues	Atoms				AltConf
5	L	1	Total	C	N	O	0
			65	55	4	6	
5	M	1	Total	C	N	O	0
			65	55	4	6	

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	L	1	Total	C	O	0
			28	24	4	
6	L	1	Total	C	O	0
			18	14	4	

- Molecule 7 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



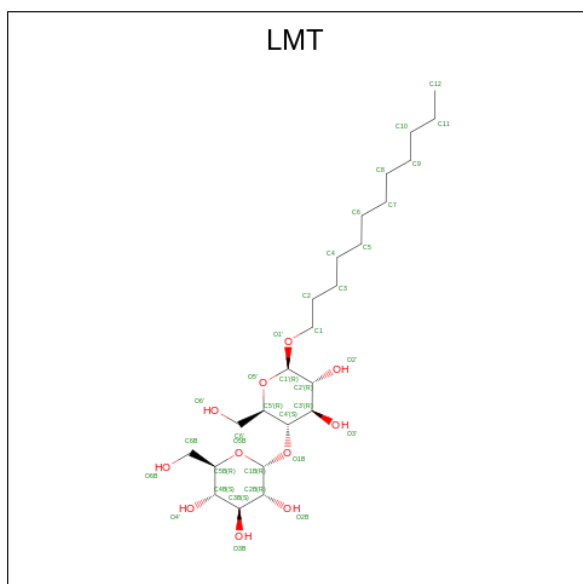
Mol	Chain	Residues	Atoms				AltConf
7	L	1	Total	C	O	P	0
			39	28	10	1	
7	L	1	Total	C	O	P	0
			33	24	8	1	
7	L	1	Total	C	O	P	0
			43	32	10	1	
7	L	1	Total	C	O	P	0
			43	32	10	1	
7	L	1	Total	C	O	P	0
			32	21	10	1	
7	L	1	Total	C	O	P	0
			40	29	10	1	
7	L	1	Total	C	O	P	0
			38	27	10	1	
7	L	1	Total	C	O	P	0
			21	12	8	1	
7	L	1	Total	C	O	P	0
			47	36	10	1	
7	M	1	Total	C	O	P	0
			40	29	10	1	
7	M	1	Total	C	O	P	0
			51	40	10	1	
7	M	1	Total	C	O	P	0
			51	40	10	1	
7	M	1	Total	C	O	P	0
			47	36	10	1	
7	M	1	Total	C	O	P	0
			34	23	10	1	

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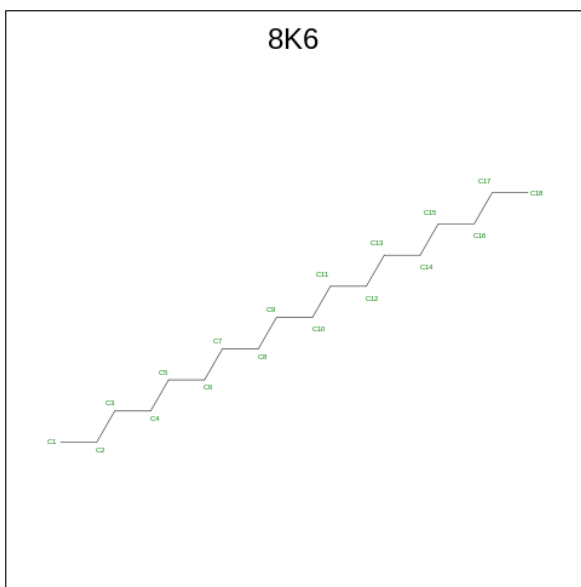
Mol	Chain	Residues	Atoms				AltConf
7	M	1	Total	C	O	P	0
			50	39	10	1	
7	M	1	Total	C	O	P	0
			26	15	10	1	
7	M	1	Total	C	O	P	0
			45	34	10	1	
7	H	1	Total	C	O	P	0
			42	31	10	1	
7	H	1	Total	C	O	P	0
			51	40	10	1	
7	H	1	Total	C	O	P	0
			36	27	8	1	

- Molecule 8 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



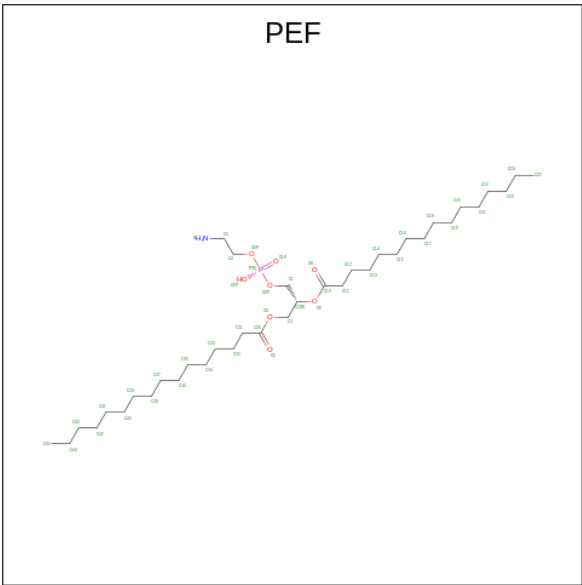
Mol	Chain	Residues	Atoms			AltConf
8	L	1	Total	C	O	0
			35	24	11	

- Molecule 9 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).



Mol	Chain	Residues	Atoms	AltConf
9	L	1	Total C 18 18	0
9	L	1	Total C 14 14	0
9	L	1	Total C 16 16	0
9	M	1	Total C 14 14	0
9	M	1	Total C 13 13	0
9	M	1	Total C 14 14	0
9	H	1	Total C 18 18	0

- Molecule 10 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).

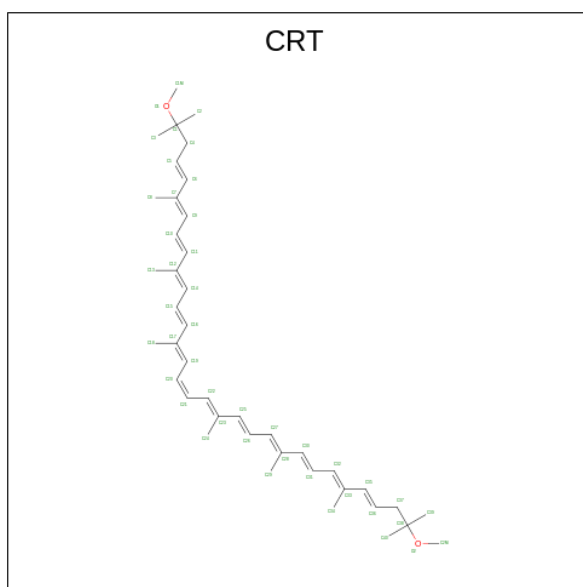


Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
10	M	1	Total	C	N	O	P	0
			40	30	1	8	1	
10	M	1	Total	C	N	O	P	0
			47	37	1	8	1	
10	M	1	Total	C	N	O	P	0
			38	28	1	8	1	
10	H	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

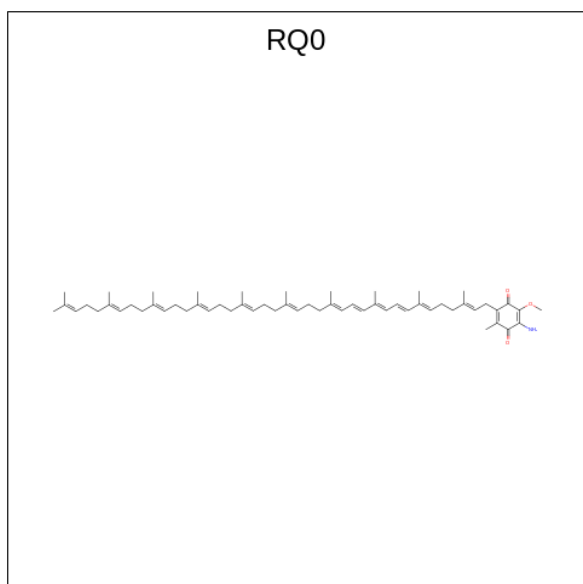
Mol	Chain	Residues	Atoms		AltConf
11	M	1	Total	Fe	0
			1	1	

- Molecule 12 is SPIRILLOXANTHIN (CCD ID: CRT) (formula: C₄₂H₆₀O₂) (labeled as "Ligand of Interest" by depositor).



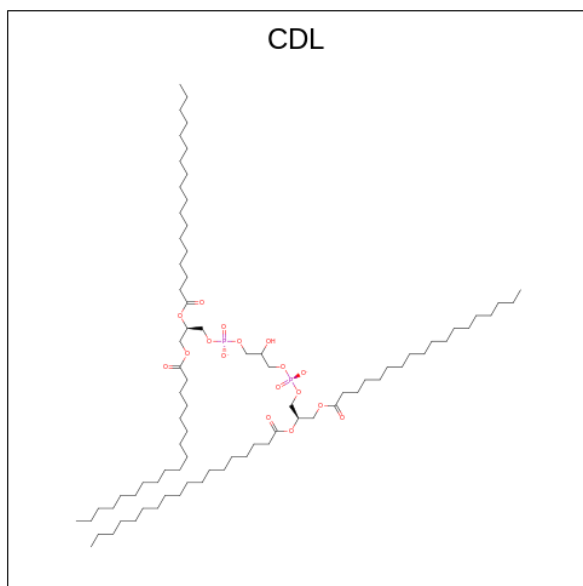
Mol	Chain	Residues	Atoms			AltConf
12	M	1	Total	C	O	0
			44	42	2	

- Molecule 13 is 2-azanyl-5-[(2 {E},6 {E},8 {E},10 {E},12 {E},14 {E},18 {E},22 {E},26 {E},30 {E},34 {E})-3,7,11,15,19,23,27,31,35,39-decamethyltetraconta-2,6,8,10,12,14,18,22,26,30,34,38-dodecaenyl]-3-methoxy-6-methyl-cyclohexa-2,5-diene-1,4-dione (CCD ID: RQ0) (formula: $C_{58}H_{85}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
13	M	1	Total	C	N	O	0
			62	58	1	3	

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



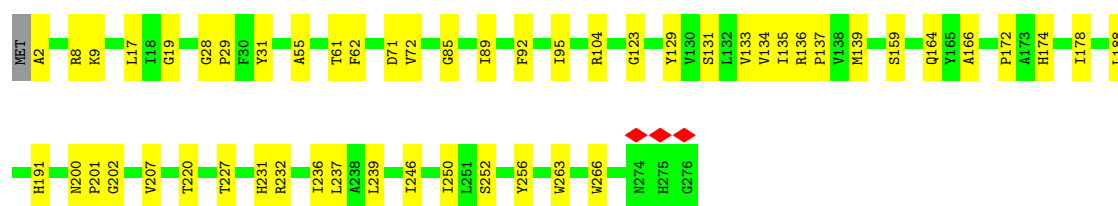
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
14	M	1	63	44	17	2	0

3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

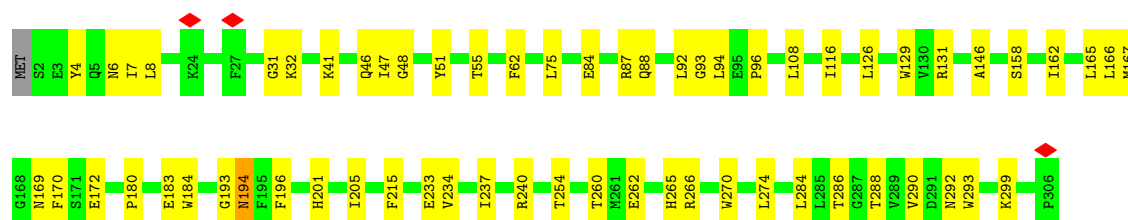
- Molecule 1: Reaction center protein L chain

Chain L: 



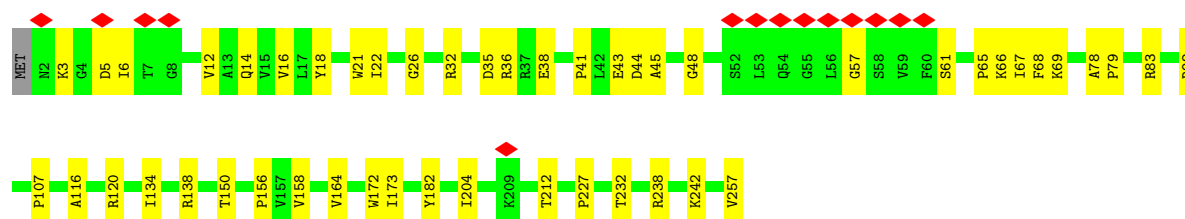
- Molecule 2: Reaction center protein M chain

Chain M: 



- Molecule 3: Photoreaction center protein H

Chain H: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118603	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.24	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.812	Depositor
Minimum map value	-1.077	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.192	Depositor
Map size ($\text{\AA}$)	323.2, 323.2, 323.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.808, 0.808, 0.808	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, LMT, PEF, RQ0, CDL, PGV, U10, 8K6, CRT, 07D, 08I

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	L	0.20	0/2253	0.37	0/3082
2	M	0.14	0/2516	0.30	0/3429
3	H	0.14	0/2006	0.30	0/2727
All	All	0.16	0/6775	0.33	0/9238

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	L	2169	0	2129	48	0
2	M	2425	0	2365	55	0
3	H	1964	0	2011	39	0
4	L	132	0	0	0	0
4	M	132	0	0	0	0
5	L	65	0	0	0	0
5	M	65	0	0	0	0
6	L	46	0	46	3	0
7	H	129	0	171	12	0
7	L	336	0	413	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	344	0	451	34	0
8	L	35	0	46	2	0
9	H	18	0	38	2	0
9	L	48	0	93	6	0
9	M	41	0	79	5	0
10	H	37	0	47	21	0
10	L	36	0	48	2	0
10	M	125	0	178	12	0
11	M	1	0	0	0	0
12	M	44	0	60	2	0
13	M	62	0	0	0	0
14	M	63	0	73	6	0
All	All	8317	0	8248	178	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 11.

All (178) 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)
7:L:310:PGV:H012	7:L:310:PGV:H062	1.52	0.91
10:M:412:PEF:H122	10:H:301:PEF:H111	1.54	0.89
1:L:231:HIS:CE1	2:M:233:GLU:OE2	2.26	0.87
2:M:233:GLU:OE1	2:M:265:HIS:CE1	2.33	0.80
3:H:67:ILE:H	10:H:301:PEF:H311	1.46	0.79
1:L:188:LEU:HD13	2:M:215:PHE:HB2	1.66	0.78
10:H:301:PEF:H321	10:H:301:PEF:H192	1.66	0.78
3:H:68:PHE:HA	10:H:301:PEF:H351	1.66	0.78
2:M:299:LYS:HB2	14:M:421:CDL:H572	1.66	0.77
1:L:139:MET:HE1	1:L:250:ILE:HG23	1.68	0.76
1:L:31:TYR:O	1:L:104:ARG:NH1	2.19	0.75
1:L:164:GLN:HA	7:L:316:PGV:H242	1.68	0.74
7:M:411:PGV:H82	10:M:413:PEF:H121	1.70	0.72
2:M:290:VAL:HA	14:M:421:CDL:H651	1.71	0.71
7:M:411:PGV:H42	10:M:413:PEF:H421	1.74	0.70
10:H:301:PEF:H142	10:H:301:PEF:H341	1.75	0.68
1:L:256:TYR:HD1	7:L:309:PGV:H011	1.59	0.68
3:H:16:VAL:HG22	7:H:302:PGV:H281	1.76	0.68
1:L:237:LEU:HD11	6:L:303:U10:H161	1.76	0.68
10:H:301:PEF:H361	10:H:301:PEF:H152	1.76	0.67
10:L:312:PEF:H132	9:L:313:8K6:H71C	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:172:GLU:HB2	9:M:420:8K6:H122	1.77	0.67
1:L:104:ARG:NH2	2:M:254:THR:O	2.28	0.67
7:L:318:PGV:H11	7:L:318:PGV:H31	1.79	0.65
2:M:240:ARG:NH1	3:H:38:GLU:OE1	2.29	0.65
2:M:266:ARG:HH22	10:M:412:PEF:H112	1.61	0.65
2:M:51:TYR:O	2:M:131:ARG:NH2	2.30	0.65
2:M:55:THR:HG23	7:M:410:PGV:H042	1.78	0.65
7:L:316:PGV:H32	2:M:194:ASN:HB2	1.80	0.63
2:M:46:GLN:NE2	2:M:48:GLY:O	2.31	0.63
1:L:133:VAL:HG23	1:L:134:VAL:HG23	1.79	0.62
1:L:236:ILE:HG12	9:L:311:8K6:H111	1.81	0.62
7:L:308:PGV:H241	7:L:308:PGV:H32	1.82	0.62
1:L:19:GLY:HA2	7:L:314:PGV:H21	1.80	0.62
2:M:169:ASN:HD21	7:M:414:PGV:H041	1.65	0.61
2:M:158:SER:HA	2:M:162:ILE:HB	1.81	0.61
1:L:28:GLY:H	7:L:306:PGV:H061	1.65	0.61
1:L:200:ASN:HB3	10:H:301:PEF:H141	1.81	0.61
10:H:301:PEF:H322	10:H:301:PEF:H121	1.83	0.61
7:M:415:PGV:H231	7:M:415:PGV:H61	1.82	0.60
2:M:183:GLU:HB2	9:M:420:8K6:H42C	1.85	0.59
7:L:315:PGV:H061	7:L:315:PGV:H31	1.84	0.58
3:H:150:THR:HG21	3:H:204:ILE:HG21	1.84	0.58
7:H:302:PGV:H51	7:H:302:PGV:H262	1.86	0.58
10:H:301:PEF:H192	10:H:301:PEF:H352	1.85	0.58
1:L:8:ARG:NH2	3:H:44:ASP:O	2.37	0.58
10:M:412:PEF:O2P	10:M:412:PEF:N	2.37	0.58
1:L:2:ALA:N	3:H:43:GLU:O	2.38	0.57
2:M:165:LEU:HB3	7:M:414:PGV:H11	1.86	0.57
1:L:172:PRO:HG2	7:L:309:PGV:H71	1.87	0.57
1:L:201:PRO:HD2	10:H:301:PEF:H152	1.86	0.57
7:L:309:PGV:H012	7:L:309:PGV:H042	1.85	0.57
2:M:47:ILE:HD12	7:M:416:PGV:H92	1.87	0.56
2:M:126:LEU:HD13	7:M:411:PGV:H232	1.86	0.56
1:L:166:ALA:HB2	7:L:316:PGV:H291	1.87	0.56
2:M:75:LEU:HD22	12:M:405:CRT:H1M1	1.88	0.56
2:M:288:THR:HB	7:M:414:PGV:H241	1.88	0.56
3:H:66:LYS:HB2	10:H:301:PEF:H331	1.88	0.56
2:M:290:VAL:HG13	14:M:421:CDL:H642	1.89	0.55
3:H:57:GLY:O	3:H:61:SER:OG	2.25	0.55
7:M:414:PGV:H251	7:H:302:PGV:H21	1.88	0.55
7:L:310:PGV:H211	7:L:310:PGV:H32	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:299:LYS:HD2	14:M:421:CDL:H612	1.88	0.54
3:H:32:ARG:HD3	9:H:304:8K6:H102	1.88	0.54
1:L:131:SER:HA	1:L:135:ILE:HB	1.89	0.53
2:M:129:TRP:NE1	2:M:146:ALA:O	2.40	0.53
10:H:301:PEF:H172	10:H:301:PEF:C38	2.39	0.53
1:L:136:ARG:NH2	1:L:252:SER:O	2.30	0.53
1:L:202:GLY:O	10:H:301:PEF:H171	2.09	0.52
3:H:45:ALA:HB1	3:H:92:ARG:HH22	1.74	0.52
1:L:62:PHE:HB3	7:H:303:PGV:H282	1.91	0.52
3:H:134:ILE:HA	3:H:173:ILE:O	2.10	0.52
1:L:129:TYR:O	1:L:133:VAL:HG22	2.10	0.52
2:M:55:THR:OG1	7:M:410:PGV:H061	2.09	0.51
3:H:41:PRO:O	3:H:83:ARG:NH2	2.38	0.51
3:H:5:ASP:N	3:H:5:ASP:OD1	2.44	0.51
1:L:8:ARG:HH22	3:H:48:GLY:HA2	1.75	0.51
7:M:411:PGV:H331	10:M:413:PEF:H381	1.93	0.51
3:H:138:ARG:NH2	3:H:232:THR:O	2.43	0.51
1:L:232:ARG:NH2	2:M:6:ASN:OD1	2.40	0.51
7:L:306:PGV:H71	9:H:304:8K6:H72C	1.92	0.51
3:H:172:TRP:HB2	3:H:182:TYR:HB2	1.93	0.51
2:M:184:TRP:CD1	9:M:420:8K6:H111	2.46	0.51
14:M:421:CDL:HA32	3:H:14:GLN:NE2	2.26	0.51
7:L:310:PGV:H51	7:L:310:PGV:H221	1.93	0.51
2:M:116:ILE:HG12	7:M:409:PGV:H72	1.92	0.50
3:H:227:PRO:HB3	3:H:242:LYS:HE3	1.94	0.50
2:M:32:LYS:HB2	7:M:418:PGV:H061	1.94	0.50
10:L:312:PEF:H171	9:L:313:8K6:H111	1.94	0.49
1:L:239:LEU:HD12	9:L:311:8K6:H131	1.93	0.49
2:M:93:GLY:HA3	2:M:180:PRO:HG2	1.94	0.49
7:M:411:PGV:H131	7:M:411:PGV:H71	1.93	0.49
1:L:61:THR:HG23	7:H:303:PGV:H332	1.94	0.49
2:M:234:VAL:HA	2:M:237:ILE:HD12	1.93	0.49
3:H:158:VAL:HG12	3:H:164:VAL:HA	1.95	0.49
1:L:9:LYS:HD2	3:H:116:ALA:HB1	1.94	0.48
1:L:8:ARG:NH1	3:H:43:GLU:OE2	2.46	0.48
3:H:36:ARG:HH21	3:H:61:SER:HA	1.79	0.48
7:L:309:PGV:H343	7:L:309:PGV:H312	1.68	0.48
2:M:84:GLU:HA	2:M:87:ARG:HB3	1.95	0.48
1:L:92:PHE:HD1	7:L:308:PGV:H12	1.78	0.47
2:M:167:MET:HE3	2:M:288:THR:HG22	1.95	0.47
2:M:260:THR:HG22	2:M:262:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:LYS:NZ	7:M:419:PGV:O02	2.38	0.47
1:L:29:PRO:HD3	7:L:306:PGV:H22	1.96	0.47
2:M:88:GLN:O	2:M:92:LEU:HG	2.13	0.47
9:L:313:8K6:H142	9:L:313:8K6:H101	1.96	0.47
3:H:32:ARG:NH1	3:H:35:ASP:OD2	2.47	0.47
3:H:120:ARG:O	3:H:238:ARG:NE	2.43	0.47
3:H:18:TYR:O	3:H:22:ILE:HG12	2.15	0.46
3:H:67:ILE:N	10:H:301:PEF:H311	2.23	0.46
1:L:55:ALA:HB3	7:L:318:PGV:H21	1.96	0.46
3:H:69:LYS:H	10:H:301:PEF:C38	2.29	0.46
1:L:263:TRP:O	1:L:266:TRP:HD1	1.99	0.46
2:M:55:THR:CG2	7:M:410:PGV:H032	2.45	0.46
10:H:301:PEF:H361	10:H:301:PEF:C15	2.45	0.46
2:M:62:PHE:HE1	7:M:410:PGV:H131	1.82	0.45
2:M:94:LEU:HA	10:M:408:PEF:H51	1.98	0.45
3:H:156:PRO:HG2	3:H:212:THR:HG22	1.99	0.45
2:M:8:LEU:H	7:M:419:PGV:H212	1.80	0.45
2:M:201:HIS:CE1	2:M:205:ILE:HD11	2.51	0.45
2:M:108:LEU:HD11	7:M:409:PGV:H222	1.98	0.45
7:M:411:PGV:H252	7:M:411:PGV:H222	1.43	0.45
2:M:193:GLY:HA3	2:M:292:ASN:OD1	2.17	0.45
1:L:174:HIS:CE1	1:L:178:ILE:HD11	2.52	0.45
2:M:284:LEU:HB3	7:M:414:PGV:H281	1.99	0.45
7:H:302:PGV:H282	7:H:302:PGV:H82	1.99	0.45
1:L:136:ARG:HB3	1:L:137:PRO:HD3	1.99	0.44
8:L:307:LMT:H3'	7:L:317:PGV:H32	1.99	0.44
2:M:286:THR:HB	2:M:293:TRP:HE1	1.81	0.44
7:M:410:PGV:H182	7:M:410:PGV:H151	1.83	0.44
7:M:411:PGV:H131	7:M:411:PGV:H102	1.54	0.44
10:M:412:PEF:H142	10:H:301:PEF:H132	1.99	0.44
1:L:71:ASP:OD1	1:L:72:VAL:N	2.50	0.44
7:L:310:PGV:H92	7:L:310:PGV:H61	1.61	0.44
7:M:419:PGV:H251	7:M:419:PGV:H222	1.78	0.44
1:L:246:ILE:O	1:L:250:ILE:HG12	2.17	0.44
10:M:412:PEF:H381	3:H:26:GLY:HA3	1.98	0.44
3:H:21:TRP:HE1	7:H:303:PGV:H21	1.82	0.44
7:M:414:PGV:H222	7:H:302:PGV:H031	2.00	0.44
8:L:307:LMT:H52	8:L:307:LMT:H82	1.70	0.43
2:M:183:GLU:HG3	9:M:420:8K6:H22C	1.99	0.43
3:H:3:LYS:HG2	7:H:302:PGV:O14	2.19	0.43
2:M:96:PRO:HB2	2:M:170:PHE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:85:GLY:O	1:L:89:ILE:HG12	2.19	0.43
14:M:421:CDL:HA62	14:M:421:CDL:H312	1.47	0.43
1:L:202:GLY:H	10:H:301:PEF:H151	1.84	0.43
2:M:7:ILE:HD12	7:M:419:PGV:H272	2.00	0.43
3:H:65:PRO:HA	3:H:79:PRO:HD2	2.00	0.43
7:M:411:PGV:H92	10:M:413:PEF:H12	2.01	0.43
1:L:159:SER:OG	7:L:316:PGV:H032	2.18	0.43
7:L:309:PGV:H302	7:L:309:PGV:H271	1.79	0.43
7:M:416:PGV:H222	7:M:416:PGV:H251	1.59	0.43
1:L:191:HIS:HA	6:L:303:U10:O2	2.18	0.42
10:M:413:PEF:H391	10:M:413:PEF:H422	1.86	0.42
1:L:227:THR:HA	6:L:303:U10:H3M2	1.99	0.42
2:M:62:PHE:CZ	7:M:410:PGV:H101	2.54	0.42
3:H:6:ILE:CD1	7:H:302:PGV:H232	2.49	0.42
1:L:123:GLY:HA3	9:L:313:8K6:H122	2.02	0.42
3:H:36:ARG:HH22	7:H:305:PGV:H101	1.84	0.42
3:H:12:VAL:HG21	7:H:302:PGV:H02	2.01	0.42
1:L:159:SER:HB2	2:M:196:PHE:CE2	2.55	0.42
2:M:166:LEU:HD23	7:M:414:PGV:H82	2.01	0.42
3:H:107:PRO:HD3	3:H:257:VAL:HG13	2.01	0.42
2:M:4:TYR:CE1	7:M:419:PGV:H211	2.55	0.41
1:L:220:THR:O	2:M:131:ARG:NH1	2.41	0.41
2:M:31:GLY:HA2	9:M:417:8K6:H101	2.02	0.41
7:M:419:PGV:H202	7:M:419:PGV:H231	1.70	0.41
10:M:413:PEF:H332	10:M:413:PEF:H362	1.85	0.41
1:L:17:LEU:O	7:L:314:PGV:H12	2.21	0.41
1:L:207:VAL:HG22	10:H:301:PEF:H371	2.02	0.41
3:H:69:LYS:HD2	10:H:301:PEF:H201	2.02	0.40
1:L:95:ILE:HG13	1:L:129:TYR:HE2	1.87	0.40
2:M:270:TRP:O	2:M:274:LEU:N	2.48	0.40
12:M:405:CRT:H82	12:M:405:CRT:H41	2.04	0.40
7:M:414:PGV:H62	7:M:414:PGV:H91	1.91	0.40
10:H:301:PEF:H321	10:H:301:PEF:H352	1.65	0.40
3:H:66:LYS:HG2	3:H:78:ALA:O	2.20	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 PDB entries followed by that with respect to all EM entries.

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	L	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
2	M	303/306 (99%)	292 (96%)	10 (3%)	1 (0%)	36	54
3	H	254/257 (99%)	241 (95%)	13 (5%)	0	100	100
All	All	830/839 (99%)	800 (96%)	29 (4%)	1 (0%)	49	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	194	ASN

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 PDB entries followed by that with respect to all EM entries.

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	L	219/220 (100%)	219 (100%)	0	100	100
2	M	239/240 (100%)	239 (100%)	0	100	100
3	H	203/204 (100%)	203 (100%)	0	100	100
All	All	661/664 (100%)	661 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	68	ASN
1	L	167	ASN
1	L	268	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 1 is monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PGV	H	302	-	41,41,50	1.00	2 (4%)	44,47,56	1.14	3 (6%)
9	8K6	L	313	-	13,13,17	0.08	0	12,12,16	0.12	0
10	PEF	M	412	-	46,46,46	0.29	0	49,51,51	0.36	0
7	PGV	H	305	-	35,35,50	1.13	2 (5%)	39,40,56	1.27	3 (7%)
7	PGV	H	303	-	50,50,50	0.89	2 (4%)	53,56,56	1.10	3 (5%)
9	8K6	L	311	-	17,17,17	0.09	0	16,16,16	0.10	0
7	PGV	M	415	-	33,33,50	1.11	2 (6%)	36,39,56	1.08	2 (5%)
9	8K6	H	304	-	17,17,17	0.08	0	16,16,16	0.09	0
4	07D	M	403	2	69,74,74	2.49	19 (27%)	83,115,115	2.93	34 (40%)
7	PGV	L	306	-	38,38,50	1.04	2 (5%)	41,44,56	1.14	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	8K6	M	417	-	12,12,17	0.09	0	11,11,16	0.10	0
7	PGV	L	314	-	31,31,50	0.99	2 (6%)	34,37,56	1.08	2 (5%)
10	PEF	H	301	-	36,36,46	1.08	2 (5%)	39,41,51	1.10	2 (5%)
7	PGV	L	309	-	42,42,50	0.95	2 (4%)	45,48,56	1.07	3 (6%)
9	8K6	M	407	-	13,13,17	0.08	0	12,12,16	0.09	0
4	07D	L	301	1	69,74,74	2.46	19 (27%)	83,115,115	3.01	34 (40%)
14	CDL	M	421	-	62,62,99	0.32	0	68,74,111	0.40	0
7	PGV	L	317	-	20,20,50	1.46	2 (10%)	24,25,56	1.55	4 (16%)
8	LMT	L	307	-	36,36,36	0.40	0	47,47,47	0.67	1 (2%)
9	8K6	M	420	-	13,13,17	0.09	0	12,12,16	0.11	0
4	07D	L	304	1	69,74,74	2.46	19 (27%)	83,115,115	3.02	33 (39%)
5	08I	M	404	-	60,70,70	3.75	22 (36%)	56,101,101	3.69	27 (48%)
5	08I	L	302	-	60,70,70	3.75	21 (35%)	56,101,101	3.79	31 (55%)
6	U10	L	305	-	18,18,63	1.03	2 (11%)	22,25,79	0.65	0
10	PEF	M	413	-	37,37,46	1.02	2 (5%)	40,42,51	1.25	4 (10%)
7	PGV	L	310	-	42,42,50	0.98	2 (4%)	45,48,56	1.01	2 (4%)
6	U10	L	303	-	28,28,63	0.90	2 (7%)	34,37,79	0.71	0
7	PGV	M	409	-	39,39,50	1.05	2 (5%)	41,45,56	1.10	3 (7%)
7	PGV	L	308	-	32,32,50	1.13	2 (6%)	36,37,56	1.41	5 (13%)
10	PEF	L	312	-	35,35,46	0.31	0	38,40,51	0.40	0
9	8K6	L	319	-	15,15,17	0.09	0	14,14,16	0.08	0
7	PGV	L	318	-	46,46,50	0.95	2 (4%)	49,52,56	1.05	4 (8%)
10	PEF	M	408	-	39,39,46	0.31	0	42,44,51	0.45	0
7	PGV	L	315	-	39,39,50	1.02	2 (5%)	42,45,56	1.07	4 (9%)
7	PGV	M	414	-	46,46,50	0.95	2 (4%)	49,52,56	1.03	3 (6%)
12	CRT	M	405	-	41,43,43	1.96	11 (26%)	50,54,54	1.79	14 (28%)
7	PGV	M	411	-	50,50,50	0.90	2 (4%)	53,56,56	1.06	2 (3%)
7	PGV	M	418	-	25,25,50	1.28	2 (8%)	28,31,56	1.25	3 (10%)
7	PGV	L	316	-	37,37,50	1.06	2 (5%)	40,43,56	1.11	3 (7%)
7	PGV	M	419	-	44,44,50	0.95	2 (4%)	47,50,56	1.12	5 (10%)
13	RQ0	M	406	-	62,62,62	0.92	2 (3%)	69,78,78	0.89	3 (4%)
7	PGV	M	410	-	50,50,50	0.89	2 (4%)	53,56,56	1.05	2 (3%)
4	07D	M	402	2	69,74,74	2.50	19 (27%)	83,115,115	2.91	31 (37%)
7	PGV	M	416	-	49,49,50	0.91	2 (4%)	52,55,56	1.03	3 (5%)

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
7	PGV	H	302	-	-	24/46/46/55	-
9	8K6	L	313	-	-	1/11/11/15	-
10	PEF	M	412	-	-	8/50/50/50	-
7	PGV	H	305	-	-	7/37/37/55	-
7	PGV	H	303	-	-	37/55/55/55	-
9	8K6	L	311	-	-	0/15/15/15	-
7	PGV	M	415	-	-	8/38/38/55	-
9	8K6	H	304	-	-	2/15/15/15	-
4	07D	M	403	2	1/1/21/28	18/41/137/137	-
7	PGV	L	306	-	-	5/43/43/55	-
9	8K6	M	417	-	-	1/10/10/15	-
7	PGV	L	314	-	-	10/35/35/55	-
10	PEF	H	301	-	-	19/40/40/50	-
7	PGV	L	309	-	-	30/47/47/55	-
9	8K6	M	407	-	-	1/11/11/15	-
4	07D	L	301	1	1/1/21/28	13/41/137/137	-
14	CDL	M	421	-	-	18/73/73/110	-
7	PGV	L	317	-	-	8/22/22/55	-
8	LMT	L	307	-	-	9/21/61/61	0/2/2/2
9	8K6	M	420	-	-	0/11/11/15	-
4	07D	L	304	1	-	12/41/137/137	-
5	08I	M	404	-	-	23/41/105/105	0/5/6/6
5	08I	L	302	-	-	18/41/105/105	0/5/6/6
6	U10	L	305	-	-	1/9/33/87	0/1/1/1
10	PEF	M	413	-	-	26/41/41/50	-
7	PGV	L	310	-	-	21/47/47/55	-
6	U10	L	303	-	-	5/21/45/87	0/1/1/1
7	PGV	M	409	-	-	5/44/44/55	-
7	PGV	L	308	-	-	20/34/34/55	-
10	PEF	L	312	-	-	6/39/39/50	-
9	8K6	L	319	-	-	1/13/13/15	-
7	PGV	L	318	-	-	9/51/51/55	-
10	PEF	M	408	-	-	15/43/43/50	-
7	PGV	L	315	-	-	7/44/44/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGV	M	414	-	-	5/51/51/55	-
12	CRT	M	405	-	-	5/51/51/51	-
7	PGV	M	411	-	-	28/55/55/55	-
7	PGV	M	418	-	-	6/30/30/55	-
7	PGV	L	316	-	-	14/42/42/55	-
7	PGV	M	419	-	-	15/49/49/55	-
13	RQ0	M	406	-	-	16/61/85/85	0/1/1/1
7	PGV	M	410	-	-	29/55/55/55	-
4	07D	M	402	2	1/1/21/28	15/41/137/137	-
7	PGV	M	416	-	-	11/54/54/55	-

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302	08I	C4C-C3C	10.03	1.50	1.39
5	L	302	08I	C4A-C3A	9.89	1.50	1.39
5	M	404	08I	C4A-C3A	9.86	1.50	1.39
5	M	404	08I	C4C-C3C	9.75	1.50	1.39
5	M	404	08I	C1C-C2C	9.37	1.50	1.39
5	L	302	08I	C1A-NA	-9.27	1.25	1.38
5	M	404	08I	C1A-NA	-9.16	1.25	1.38
5	L	302	08I	C1C-C2C	9.12	1.49	1.39
4	M	402	07D	C7-C8	8.49	1.53	1.33
5	M	404	08I	C12-C13	8.45	1.53	1.33
4	L	304	07D	C12-C13	8.36	1.53	1.33
4	M	402	07D	C12-C13	8.33	1.53	1.33
4	M	403	07D	C7-C8	8.25	1.52	1.33
5	M	404	08I	C7-C8	8.24	1.52	1.33
5	L	302	08I	C12-C13	8.24	1.52	1.33
4	L	301	07D	C12-C13	8.22	1.52	1.33
4	L	304	07D	C7-C8	8.20	1.52	1.33
5	L	302	08I	C7-C8	8.17	1.52	1.33
4	L	301	07D	C7-C8	8.16	1.52	1.33
4	M	403	07D	C12-C13	8.16	1.52	1.33
4	M	402	07D	C17-C18	7.20	1.53	1.32
4	L	304	07D	C17-C18	7.16	1.53	1.32
4	M	403	07D	C17-C18	7.11	1.52	1.32
5	M	404	08I	C17-C18	7.10	1.52	1.32
4	L	301	07D	C17-C18	7.10	1.52	1.32
5	L	302	08I	C17-C18	7.03	1.52	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302	08I	C1A-C2A	6.71	1.50	1.39
5	M	404	08I	C1A-C2A	6.53	1.50	1.39
5	L	302	08I	C4C-NC	-6.20	1.27	1.38
5	M	404	08I	C4C-NC	-6.15	1.27	1.38
5	L	302	08I	C2A-C3A	5.21	1.53	1.37
5	M	404	08I	C2A-C3A	5.17	1.53	1.37
4	M	403	07D	O2D-CGD	5.14	1.45	1.33
4	M	402	07D	O2D-CGD	5.12	1.45	1.33
4	L	301	07D	O2D-CGD	5.08	1.45	1.33
5	L	302	08I	O2D-CGD	5.05	1.45	1.33
5	M	404	08I	O2D-CGD	5.01	1.45	1.33
4	L	304	07D	O2D-CGD	5.00	1.45	1.33
5	L	302	08I	C3C-C2C	5.00	1.52	1.37
5	M	404	08I	C3C-C2C	4.92	1.52	1.37
4	M	403	07D	C3B-C4B	4.87	1.50	1.41
4	L	301	07D	C3B-C4B	4.70	1.49	1.41
4	M	402	07D	C3B-C4B	4.61	1.49	1.41
4	L	304	07D	C3B-C4B	4.52	1.49	1.41
4	L	301	07D	CHD-C1D	4.46	1.47	1.38
13	M	406	RQ0	C27-C19	4.45	1.41	1.35
4	M	402	07D	CHD-C1D	4.41	1.46	1.38
4	M	403	07D	CHD-C1D	4.39	1.46	1.38
4	L	304	07D	CHD-C1D	4.38	1.46	1.38
5	L	302	08I	O2A-CGA	4.32	1.46	1.33
7	L	316	PGV	O03-C19	4.27	1.45	1.33
7	M	409	PGV	O03-C19	4.26	1.45	1.33
10	H	301	PEF	O3-C30	4.25	1.45	1.33
7	H	305	PGV	O03-C19	4.24	1.45	1.33
7	M	418	PGV	O03-C19	4.24	1.45	1.33
7	L	317	PGV	O03-C19	4.23	1.45	1.33
4	L	301	07D	O2A-CGA	4.22	1.45	1.33
7	M	416	PGV	O03-C19	4.21	1.45	1.33
7	L	308	PGV	O03-C19	4.21	1.45	1.33
4	L	304	07D	O2A-CGA	4.21	1.45	1.33
7	L	315	PGV	O03-C19	4.20	1.45	1.33
7	M	415	PGV	O03-C19	4.19	1.45	1.33
7	H	305	PGV	O01-C1	4.18	1.46	1.34
7	L	318	PGV	O03-C19	4.18	1.45	1.33
4	M	402	07D	O2A-CGA	4.18	1.45	1.33
7	H	302	PGV	O03-C19	4.17	1.45	1.33
7	M	414	PGV	O03-C19	4.17	1.45	1.33
5	M	404	08I	O2A-CGA	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	403	07D	O2A-CGA	4.16	1.45	1.33
7	L	306	PGV	O03-C19	4.15	1.45	1.33
7	M	409	PGV	O01-C1	4.13	1.46	1.34
7	M	419	PGV	O03-C19	4.13	1.45	1.33
12	M	405	CRT	C22-C23	4.12	1.41	1.35
7	L	309	PGV	O03-C19	4.12	1.45	1.33
7	M	414	PGV	O01-C1	4.11	1.45	1.34
4	M	403	07D	C1D-ND	-4.10	1.32	1.37
7	L	306	PGV	O01-C1	4.10	1.45	1.34
4	M	402	07D	C1D-ND	-4.09	1.32	1.37
7	M	418	PGV	O01-C1	4.09	1.45	1.34
7	H	303	PGV	O03-C19	4.08	1.45	1.33
7	L	316	PGV	O01-C1	4.07	1.45	1.34
7	L	317	PGV	O01-C1	4.06	1.45	1.34
7	H	302	PGV	O01-C1	4.04	1.45	1.34
10	H	301	PEF	O2-C10	4.04	1.45	1.34
7	M	411	PGV	O03-C19	4.04	1.45	1.33
7	L	318	PGV	O01-C1	4.03	1.45	1.34
5	L	302	08I	C4D-CHA	4.03	1.48	1.40
7	L	315	PGV	O01-C1	4.03	1.45	1.34
7	L	314	PGV	O01-C1	4.03	1.45	1.34
12	M	405	CRT	C9-C7	4.02	1.41	1.35
4	M	403	07D	CHC-C4B	4.02	1.48	1.39
7	M	410	PGV	O01-C1	4.01	1.45	1.34
7	M	415	PGV	O01-C1	4.00	1.45	1.34
7	L	310	PGV	O01-C1	4.00	1.45	1.34
7	M	416	PGV	O01-C1	3.99	1.45	1.34
10	M	413	PEF	O3-C30	3.99	1.45	1.33
7	M	411	PGV	O01-C1	3.99	1.45	1.34
7	M	410	PGV	O03-C19	3.98	1.45	1.33
10	M	413	PEF	O2-C10	3.98	1.45	1.34
7	L	310	PGV	O03-C19	3.96	1.44	1.33
12	M	405	CRT	C27-C28	3.93	1.41	1.35
12	M	405	CRT	C32-C33	3.93	1.41	1.35
7	M	419	PGV	O01-C1	3.90	1.45	1.34
12	M	405	CRT	C19-C17	3.90	1.41	1.35
4	L	301	07D	CHC-C4B	3.90	1.48	1.39
4	M	402	07D	CHC-C4B	3.90	1.48	1.39
4	L	304	07D	CHC-C4B	3.89	1.48	1.39
7	H	303	PGV	O01-C1	3.87	1.45	1.34
5	M	404	08I	C4D-CHA	3.79	1.48	1.40
5	L	302	08I	C3B-C2B	3.74	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	304	07D	C1D-ND	-3.70	1.33	1.37
7	L	308	PGV	O01-C1	3.70	1.44	1.34
4	L	301	07D	CHB-C1B	3.68	1.47	1.39
12	M	405	CRT	C14-C12	3.67	1.40	1.35
4	M	402	07D	C3D-C2D	3.63	1.49	1.39
4	M	403	07D	CHB-C1B	3.63	1.47	1.39
7	L	309	PGV	O01-C1	3.62	1.44	1.34
4	L	304	07D	OBD-CAD	3.62	1.28	1.22
4	M	402	07D	CHB-C1B	3.62	1.47	1.39
4	L	301	07D	OBD-CAD	3.62	1.28	1.22
4	M	402	07D	OBD-CAD	3.61	1.28	1.22
5	M	404	08I	C3B-C2B	3.59	1.49	1.37
5	M	404	08I	OBD-CAD	3.59	1.28	1.22
4	M	403	07D	C1B-NB	-3.54	1.33	1.37
5	L	302	08I	OBD-CAD	3.54	1.28	1.22
4	L	301	07D	C1D-ND	-3.53	1.33	1.37
4	M	403	07D	OBD-CAD	3.51	1.28	1.22
4	L	304	07D	C3D-C2D	3.50	1.48	1.39
4	M	403	07D	C3D-C2D	3.49	1.48	1.39
5	M	404	08I	C3D-C2D	3.48	1.48	1.37
5	L	302	08I	C3D-C2D	3.46	1.48	1.37
4	M	402	07D	C4B-NB	-3.45	1.33	1.37
4	L	304	07D	CHB-C1B	3.45	1.47	1.39
4	L	301	07D	C4B-NB	-3.34	1.33	1.37
4	M	402	07D	C1B-NB	-3.31	1.33	1.37
4	L	301	07D	C1B-NB	-3.24	1.33	1.37
4	M	403	07D	C4B-NB	-3.21	1.33	1.37
4	L	301	07D	C3D-C2D	3.19	1.47	1.39
5	M	404	08I	CHA-CBD	-3.13	1.47	1.51
4	L	304	07D	C4B-NB	-3.13	1.33	1.37
5	M	404	08I	C4A-NA	-3.13	1.32	1.38
4	M	402	07D	CHD-C4C	3.06	1.47	1.39
4	L	304	07D	C1B-NB	-3.02	1.34	1.37
4	M	403	07D	CHD-C4C	2.95	1.47	1.39
5	L	302	08I	C4A-NA	-2.95	1.33	1.38
5	L	302	08I	CHA-CBD	-2.93	1.48	1.51
4	L	304	07D	CHD-C4C	2.90	1.47	1.39
5	L	302	08I	C1C-NC	-2.88	1.33	1.38
4	L	301	07D	CHD-C4C	2.79	1.47	1.39
5	M	404	08I	C1C-NC	-2.79	1.33	1.38
5	L	302	08I	C4D-C3D	-2.75	1.38	1.44
6	L	303	U10	C3-C2	-2.74	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	404	08I	C4D-C3D	-2.72	1.38	1.44
6	L	305	U10	C3-C2	-2.61	1.41	1.48
4	L	301	07D	C4D-CHA	2.58	1.47	1.38
7	L	314	PGV	O03-C19	2.52	1.45	1.33
13	M	406	RQ0	C07-C19	-2.50	1.40	1.45
4	L	301	07D	C1B-C2B	2.46	1.49	1.43
4	L	304	07D	C1B-C2B	2.43	1.49	1.43
4	M	403	07D	C4D-CHA	2.42	1.47	1.38
6	L	303	U10	C4-C5	-2.41	1.41	1.48
4	M	402	07D	C1B-C2B	2.40	1.48	1.43
12	M	405	CRT	C25-C23	-2.39	1.40	1.45
12	M	405	CRT	C16-C17	-2.37	1.40	1.45
12	M	405	CRT	C30-C28	-2.37	1.40	1.45
4	M	402	07D	C4D-CHA	2.36	1.46	1.38
4	M	402	07D	C3D-C4D	-2.36	1.38	1.44
4	L	301	07D	C3D-C4D	-2.34	1.38	1.44
12	M	405	CRT	C35-C33	-2.33	1.40	1.45
4	L	304	07D	C3D-C4D	-2.31	1.39	1.44
4	M	403	07D	C1B-C2B	2.30	1.48	1.43
4	L	304	07D	C4D-CHA	2.29	1.46	1.38
4	M	403	07D	C3D-C4D	-2.25	1.39	1.44
6	L	305	U10	C4-C5	-2.24	1.42	1.48
12	M	405	CRT	C11-C12	-2.24	1.41	1.45
4	L	301	07D	C3B-C2B	2.22	1.50	1.42
4	M	403	07D	C3B-C2B	2.21	1.49	1.42
4	M	402	07D	C3B-C2B	2.12	1.49	1.42
4	L	304	07D	C3B-C2B	2.03	1.49	1.42
5	M	404	08I	CBD-CGD	-2.00	1.49	1.52

All (276) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	07D	C2B-C1B-NB	8.84	116.16	110.23
5	L	302	08I	C3A-C4A-NA	8.29	115.25	109.53
4	M	402	07D	CHD-C1D-ND	-8.05	117.06	124.45
4	M	402	07D	C2B-C1B-NB	8.04	115.62	110.23
4	M	403	07D	C2B-C1B-NB	8.03	115.62	110.23
4	L	301	07D	C2B-C1B-NB	8.03	115.61	110.23
5	L	302	08I	C1B-C2B-C3B	-7.98	101.01	108.46
5	M	404	08I	C3A-C4A-NA	7.78	114.90	109.53
5	M	404	08I	C1B-C2B-C3B	-7.65	101.32	108.46
5	M	404	08I	CMA-C3A-C2A	-7.37	111.05	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	08I	CMA-C3A-C2A	-7.32	111.13	124.94
4	L	304	07D	C4A-NA-C1A	-7.29	103.43	106.71
5	L	302	08I	C4D-CHA-CBD	-7.28	106.72	110.42
4	M	403	07D	C6-C7-C8	-7.26	110.19	127.66
4	M	403	07D	C11-C12-C13	-7.20	110.32	127.66
5	L	302	08I	C6-C7-C8	-7.20	110.33	127.66
5	M	404	08I	O2D-CGD-CBD	7.16	120.06	111.00
4	L	304	07D	C11-C12-C13	-7.11	110.54	127.66
4	L	301	07D	C4A-NA-C1A	-7.08	103.52	106.71
4	M	402	07D	C4A-NA-C1A	-7.08	103.52	106.71
5	L	302	08I	C3C-C4C-NC	7.00	114.36	109.53
5	M	404	08I	C6-C7-C8	-6.99	110.83	127.66
5	M	404	08I	C3C-C4C-NC	6.94	114.32	109.53
5	M	404	08I	C4D-CHA-CBD	-6.84	106.95	110.42
4	L	301	07D	CHD-C1D-ND	-6.81	118.20	124.45
4	L	304	07D	CAC-C3C-C4C	6.73	127.51	112.58
5	L	302	08I	C11-C12-C13	-6.69	111.55	127.66
4	M	402	07D	C11-C12-C13	-6.65	111.64	127.66
4	L	304	07D	C6-C7-C8	-6.59	111.78	127.66
5	L	302	08I	O2D-CGD-CBD	6.59	119.35	111.00
4	M	402	07D	CAC-C3C-C4C	6.39	126.76	112.58
4	L	301	07D	CAC-C3C-C4C	6.37	126.72	112.58
5	M	404	08I	C11-C12-C13	-6.37	112.32	127.66
4	L	301	07D	C11-C12-C13	-6.33	112.43	127.66
4	L	301	07D	C15-C13-C12	-6.32	108.33	121.12
4	L	301	07D	CMC-C2C-C1C	6.26	128.61	111.77
4	M	403	07D	CHD-C1D-ND	-6.26	118.70	124.45
5	L	302	08I	C15-C13-C12	-6.19	108.60	121.12
4	L	304	07D	CMC-C2C-C1C	6.15	128.31	111.77
4	M	403	07D	CAC-C3C-C4C	6.08	126.08	112.58
5	M	404	08I	C2A-C1A-NA	6.08	116.90	110.00
5	M	404	08I	C10-C8-C7	-6.04	108.89	121.12
4	L	304	07D	C10-C8-C7	-6.01	108.95	121.12
5	L	302	08I	C10-C8-C7	-6.01	108.96	121.12
4	M	403	07D	CMC-C2C-C1C	5.99	127.86	111.77
4	M	403	07D	C10-C8-C7	-5.97	109.05	121.12
4	L	301	07D	C6-C7-C8	-5.92	113.41	127.66
4	L	301	07D	C10-C8-C7	-5.90	109.18	121.12
5	M	404	08I	CAA-C2A-C3A	-5.88	110.36	127.25
12	M	405	CRT	C5-C6-C7	5.83	134.70	125.89
4	M	402	07D	C6-C7-C8	-5.82	113.65	127.66
5	M	404	08I	C15-C13-C12	-5.69	109.61	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	302	08I	CAA-C2A-C3A	-5.68	110.94	127.25
4	M	402	07D	CMC-C2C-C1C	5.65	126.95	111.77
5	L	302	08I	C2A-C1A-NA	5.63	116.39	110.00
4	M	403	07D	C15-C13-C12	-5.63	109.73	121.12
4	L	304	07D	CHD-C1D-ND	-5.56	119.34	124.45
4	M	402	07D	C15-C13-C12	-5.52	109.94	121.12
4	L	304	07D	C15-C13-C12	-5.44	110.11	121.12
4	L	301	07D	O2D-CGD-CBD	5.30	120.69	111.27
4	M	402	07D	C10-C8-C7	-5.27	110.45	121.12
5	L	302	08I	C16-C17-C18	-5.14	110.19	127.75
4	L	304	07D	C9-C8-C7	-5.09	110.62	123.68
4	M	403	07D	C1D-CHD-C4C	-5.08	114.38	126.62
4	L	301	07D	C9-C8-C7	-5.06	110.71	123.68
5	M	404	08I	C9-C8-C7	-5.04	110.75	123.68
4	L	301	07D	C14-C13-C12	-5.02	110.81	123.68
4	M	403	07D	C14-C13-C12	-5.01	110.83	123.68
5	L	302	08I	C14-C13-C12	-5.00	110.84	123.68
5	L	302	08I	C9-C8-C7	-4.98	110.89	123.68
4	L	304	07D	C1D-CHD-C4C	-4.98	114.61	126.62
4	M	402	07D	C1D-CHD-C4C	-4.94	114.71	126.62
5	M	404	08I	C16-C17-C18	-4.88	111.08	127.75
4	L	304	07D	O2D-CGD-CBD	4.87	119.93	111.27
4	M	403	07D	C9-C8-C7	-4.85	111.22	123.68
4	L	304	07D	C14-C13-C12	-4.83	111.30	123.68
4	L	304	07D	C16-C17-C18	-4.81	111.33	127.75
4	M	402	07D	C14-C13-C12	-4.76	111.46	123.68
4	L	304	07D	C1C-NC-C4C	-4.75	104.57	106.71
4	M	402	07D	C16-C17-C18	-4.70	111.69	127.75
4	L	301	07D	C16-C17-C18	-4.67	111.80	127.75
4	M	402	07D	O2D-CGD-CBD	4.60	119.44	111.27
10	M	413	PEF	O2-C10-C11	4.55	121.31	111.50
4	M	403	07D	C16-C17-C18	-4.52	112.29	127.75
4	M	403	07D	C4A-NA-C1A	-4.48	104.69	106.71
5	M	404	08I	C14-C13-C12	-4.47	112.20	123.68
4	M	403	07D	C1C-NC-C4C	-4.41	104.72	106.71
5	L	302	08I	C2C-C1C-NC	4.41	112.57	109.53
4	M	402	07D	C9-C8-C7	-4.40	112.39	123.68
7	L	308	PGV	O01-C1-C2	4.39	120.97	111.50
7	H	305	PGV	O01-C1-C2	4.39	120.96	111.50
7	M	411	PGV	O01-C1-C2	4.36	120.91	111.50
7	M	410	PGV	O01-C1-C2	4.31	120.79	111.50
7	H	303	PGV	O01-C1-C2	4.28	120.73	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	317	PGV	O01-C1-C2	4.18	120.50	111.50
7	M	419	PGV	O01-C1-C2	4.12	120.39	111.50
4	M	403	07D	C20-C18-C17	-4.11	110.75	122.65
5	M	404	08I	C20-C18-C17	-4.11	110.75	122.65
5	L	302	08I	C20-C18-C17	-4.10	110.79	122.65
4	M	402	07D	C1D-ND-C4D	4.09	109.24	106.33
5	M	404	08I	C2C-C1C-NC	4.09	112.35	109.53
4	L	301	07D	C19-C18-C17	-4.07	110.88	122.65
7	H	302	PGV	O01-C1-C2	4.07	120.27	111.50
4	M	402	07D	C19-C18-C17	-4.06	110.92	122.65
7	L	316	PGV	O01-C1-C2	4.03	120.20	111.50
4	L	301	07D	C20-C18-C17	-4.03	111.01	122.65
4	M	403	07D	O2D-CGD-CBD	4.02	118.42	111.27
7	M	409	PGV	O01-C1-C2	4.02	120.17	111.50
5	L	302	08I	C19-C18-C17	-4.02	111.04	122.65
5	M	404	08I	C19-C18-C17	-4.00	111.08	122.65
7	M	418	PGV	O01-C1-C2	3.99	120.10	111.50
4	L	304	07D	C20-C18-C17	-3.97	111.16	122.65
5	L	302	08I	C1-C2-C3	-3.97	119.18	126.04
7	M	414	PGV	O01-C1-C2	3.96	120.04	111.50
7	L	306	PGV	O01-C1-C2	3.94	119.99	111.50
7	M	416	PGV	O01-C1-C2	3.92	119.95	111.50
4	M	403	07D	C19-C18-C17	-3.91	111.36	122.65
4	L	304	07D	C19-C18-C17	-3.87	111.45	122.65
4	L	301	07D	C1D-CHD-C4C	-3.86	117.30	126.62
4	M	402	07D	C20-C18-C17	-3.85	111.51	122.65
7	L	310	PGV	O01-C1-C2	3.84	119.78	111.50
5	M	404	08I	C1D-C2D-C3D	-3.77	104.94	108.46
7	L	318	PGV	O01-C1-C2	3.77	119.62	111.50
7	L	315	PGV	O01-C1-C2	3.75	119.58	111.50
7	M	415	PGV	O01-C1-C2	3.74	119.57	111.50
10	H	301	PEF	O2-C10-C11	3.74	119.57	111.50
7	L	309	PGV	O01-C1-C2	3.70	119.47	111.50
4	L	301	07D	CHD-C1D-C2D	-3.57	118.00	125.48
5	L	302	08I	C1D-C2D-C3D	-3.49	105.20	108.46
7	L	314	PGV	O01-C1-C2	3.44	118.92	111.50
12	M	405	CRT	C8-C7-C9	-3.44	118.11	122.92
4	L	304	07D	C2C-C3C-C4C	-3.43	96.21	101.34
7	L	317	PGV	O03-C19-C20	3.43	120.36	111.38
4	L	304	07D	C1-C2-C3	-3.41	120.14	126.04
4	L	301	07D	C4-C3-C5	3.40	120.98	115.27
4	M	403	07D	C1D-ND-C4D	3.37	108.73	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	301	07D	C1D-ND-C4D	3.32	108.70	106.33
4	M	403	07D	CMC-C2C-C3C	3.30	127.12	113.83
12	M	405	CRT	C34-C33-C32	-3.29	118.31	122.92
4	M	403	07D	C2C-C3C-C4C	-3.27	96.43	101.34
4	M	402	07D	CMC-C2C-C3C	3.25	126.93	113.83
4	L	301	07D	CBC-CAC-C3C	-3.16	106.43	113.47
4	L	301	07D	CMC-C2C-C3C	3.16	126.57	113.83
4	L	304	07D	CMC-C2C-C3C	3.16	126.57	113.83
5	M	404	08I	C1A-NA-C4A	-3.16	105.62	108.83
5	M	404	08I	C4-C3-C5	3.15	120.57	115.27
13	M	406	RQ0	C07-C19-C27	3.14	123.75	118.94
10	M	413	PEF	C2-O2-C10	-3.12	110.12	117.79
12	M	405	CRT	C29-C28-C27	-3.10	118.58	122.92
4	M	403	07D	C4B-C3B-C2B	-3.08	103.41	108.36
4	L	301	07D	C9-C8-C10	-3.07	110.10	115.27
5	L	302	08I	C1A-NA-C4A	-3.05	105.72	108.83
12	M	405	CRT	C13-C12-C14	-3.04	118.66	122.92
7	L	318	PGV	C02-O01-C1	-3.00	110.40	117.79
13	M	406	RQ0	C39-C19-C27	-2.99	118.73	122.92
4	L	301	07D	C2A-C3A-C4A	-2.96	97.09	101.87
4	M	402	07D	C14-C13-C15	-2.95	110.31	115.27
7	L	315	PGV	O03-C19-C20	2.94	121.12	111.91
4	M	402	07D	C4B-C3B-C2B	-2.93	103.65	108.36
4	L	301	07D	C1C-NC-C4C	-2.92	105.39	106.71
4	L	301	07D	C4B-C3B-C2B	-2.87	103.74	108.36
12	M	405	CRT	C35-C33-C32	2.86	123.33	118.94
7	L	308	PGV	C02-O01-C1	-2.86	110.76	117.79
4	L	304	07D	CBC-CAC-C3C	-2.85	107.11	113.47
7	L	306	PGV	O03-C19-C20	2.85	120.84	111.91
12	M	405	CRT	C24-C23-C22	-2.84	118.95	122.92
4	L	304	07D	O2A-CGA-CBA	2.84	120.82	111.91
7	M	419	PGV	O03-C19-C20	2.82	120.77	111.91
10	H	301	PEF	O3-C30-C31	2.82	120.77	111.91
7	L	308	PGV	O03-C19-C20	2.82	120.75	111.91
7	H	305	PGV	O03-C19-C20	2.79	120.65	111.91
4	M	403	07D	O2A-CGA-CBA	2.78	120.64	111.91
7	L	316	PGV	O03-C19-C20	2.77	120.60	111.91
7	L	318	PGV	O03-C19-C20	2.76	120.56	111.91
4	L	301	07D	C14-C13-C15	-2.76	110.63	115.27
4	L	301	07D	O2A-CGA-CBA	2.75	120.55	111.91
4	M	402	07D	O2A-CGA-CBA	2.72	120.43	111.91
4	L	301	07D	C3C-C4C-CHD	-2.71	117.61	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	403	07D	CHA-C1A-NA	-2.70	120.21	126.40
4	M	403	07D	CBC-CAC-C3C	-2.70	107.47	113.47
5	L	302	08I	C4-C3-C5	2.69	119.80	115.27
4	L	304	07D	C9-C8-C10	-2.69	110.75	115.27
4	M	403	07D	C14-C13-C15	-2.68	110.76	115.27
7	M	411	PGV	O03-C19-C20	2.68	120.32	111.91
4	M	402	07D	C3C-C4C-CHD	-2.68	117.67	123.39
12	M	405	CRT	C18-C17-C19	-2.66	119.20	122.92
7	L	314	PGV	C02-O01-C1	-2.66	111.25	117.79
4	M	402	07D	CHC-C4B-C3B	-2.65	122.92	132.35
7	H	303	PGV	C02-O01-C1	-2.65	111.27	117.79
4	L	304	07D	C14-C13-C15	-2.64	110.83	115.27
4	M	403	07D	C4-C3-C5	2.63	119.70	115.27
4	L	304	07D	C4-C3-C5	2.63	119.69	115.27
7	M	414	PGV	O03-C19-C20	2.63	120.16	111.91
7	M	409	PGV	O03-C19-C20	2.62	120.14	111.91
12	M	405	CRT	C30-C28-C27	2.62	122.96	118.94
4	M	402	07D	C9-C8-C10	-2.62	110.87	115.27
7	M	410	PGV	O03-C19-C20	2.60	120.08	111.91
5	L	302	08I	C9-C8-C10	-2.60	110.90	115.27
7	H	302	PGV	O03-C19-C20	2.58	119.99	111.91
4	M	402	07D	CBC-CAC-C3C	-2.57	107.74	113.47
7	M	416	PGV	C02-O01-C1	-2.57	111.47	117.79
7	L	309	PGV	O03-C19-C20	2.55	119.92	111.91
4	L	301	07D	O2D-CGD-O1D	-2.54	118.86	123.84
7	M	415	PGV	O03-C19-C20	2.53	119.83	111.91
4	L	304	07D	CHC-C4B-C3B	-2.52	123.37	132.35
7	M	416	PGV	O03-C19-C20	2.52	119.83	111.91
4	L	301	07D	CHA-C4D-ND	2.51	137.76	132.50
4	L	304	07D	C4B-C3B-C2B	-2.51	104.32	108.36
5	L	302	08I	CBA-CAA-C2A	-2.48	108.39	112.62
7	M	418	PGV	C02-O01-C1	-2.48	111.69	117.79
7	L	306	PGV	C02-O01-C1	-2.47	111.72	117.79
4	M	403	07D	CMD-C2D-C1D	2.46	129.04	124.71
4	L	304	07D	O2D-CGD-O1D	-2.44	119.06	123.84
4	M	402	07D	C4-C3-C5	2.44	119.38	115.27
7	L	317	PGV	O14-P-O13	2.44	120.22	110.68
7	M	419	PGV	C02-O01-C1	-2.44	111.80	117.79
7	H	302	PGV	C02-O01-C1	-2.43	111.81	117.79
7	H	305	PGV	O14-P-O13	2.42	120.17	110.68
7	L	310	PGV	O03-C19-C20	2.42	119.50	111.91
7	M	414	PGV	C02-O01-C1	-2.41	111.86	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	317	PGV	C02-O01-C1	-2.41	111.86	117.79
5	M	404	08I	O2D-CGD-O1D	-2.40	119.14	123.84
5	M	404	08I	O2A-CGA-CBA	2.40	119.44	111.91
4	M	402	07D	C1-C2-C3	-2.40	121.89	126.04
5	M	404	08I	O1D-CGD-CBD	-2.37	120.79	124.74
12	M	405	CRT	C20-C19-C17	2.36	130.68	127.31
4	L	301	07D	CHC-C4B-C3B	-2.35	124.00	132.35
7	M	418	PGV	O03-C19-C20	2.34	119.24	111.91
4	L	304	07D	CHA-C1A-NA	-2.34	121.05	126.40
7	L	309	PGV	C02-O01-C1	-2.33	112.05	117.79
10	M	413	PEF	O3-C30-C31	2.32	119.20	111.91
7	L	315	PGV	C02-O01-C1	-2.32	112.08	117.79
7	M	409	PGV	C02-O01-C1	-2.32	112.09	117.79
7	L	308	PGV	O14-P-O13	2.31	119.73	110.68
10	M	413	PEF	O2-C10-O4	-2.31	118.13	123.70
4	M	403	07D	CHC-C4B-C3B	-2.29	124.21	132.35
5	L	302	08I	O2D-CGD-O1D	-2.27	119.40	123.84
4	M	402	07D	O2D-CGD-O1D	-2.26	119.41	123.84
12	M	405	CRT	C11-C12-C14	2.26	122.41	118.94
4	L	304	07D	CMD-C2D-C1D	2.25	128.68	124.71
8	L	307	LMT	C1B-O1B-C4'	-2.24	112.41	117.96
4	M	403	07D	CED-O2D-CGD	2.24	121.00	115.94
7	H	303	PGV	O03-C19-C20	2.23	118.90	111.91
4	L	304	07D	CHB-C1B-C2B	-2.22	120.96	127.24
5	M	404	08I	C1-C2-C3	-2.22	122.20	126.04
4	L	304	07D	C3C-C2C-C1C	-2.20	98.31	101.87
4	L	304	07D	C1D-ND-C4D	2.20	107.90	106.33
4	M	403	07D	C3C-C4C-CHD	-2.20	118.69	123.39
4	L	301	07D	CHA-C1A-NA	-2.20	121.37	126.40
12	M	405	CRT	C6-C7-C9	2.16	122.26	118.94
4	M	402	07D	CHA-C1A-NA	-2.16	121.45	126.40
7	L	316	PGV	C02-O01-C1	-2.16	112.48	117.79
5	L	302	08I	C1-O2A-CGA	2.15	122.10	116.44
4	M	402	07D	CHA-C4D-ND	2.15	136.99	132.50
5	L	302	08I	C14-C13-C15	-2.14	111.67	115.27
12	M	405	CRT	C25-C23-C22	2.14	122.22	118.94
4	M	403	07D	C1-C2-C3	-2.13	122.36	126.04
13	M	406	RQ0	C27-C18-C14	2.12	129.84	123.22
4	M	402	07D	CMD-C2D-C1D	2.10	128.42	124.71
5	L	302	08I	O1D-CGD-CBD	-2.09	121.25	124.74
4	M	403	07D	CHB-C1B-C2B	-2.09	121.32	127.24
5	M	404	08I	CMD-C2D-C1D	2.09	128.67	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	301	07D	O2A-CGA-O1A	-2.06	118.39	123.59
5	L	302	08I	O2A-CGA-CBA	2.05	118.34	111.91
4	L	301	07D	CMD-C2D-C1D	2.05	128.32	124.71
4	M	403	07D	C3C-C2C-C1C	-2.05	98.56	101.87
7	M	419	PGV	O01-C1-O02	-2.03	118.79	123.70
7	L	308	PGV	O01-C1-O02	-2.02	118.82	123.70
5	L	302	08I	CMD-C2D-C1D	2.02	128.55	124.73
5	M	404	08I	C14-C13-C15	-2.02	111.88	115.27
7	M	419	PGV	O03-C19-O04	-2.02	118.50	123.59
7	L	315	PGV	O03-C19-O04	-2.01	118.51	123.59
4	M	403	07D	C3B-C2B-C1B	-2.01	99.93	106.39
7	L	318	PGV	O03-C19-O04	-2.01	118.53	123.59
12	M	405	CRT	C21-C22-C23	2.00	130.17	127.31
5	L	302	08I	CBC-CAC-C3C	-2.00	107.16	112.27

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	L	301	07D	ND
4	M	402	07D	ND
4	M	403	07D	ND

All (532) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	07D	C4-C3-C5-C6
4	L	301	07D	C2-C3-C5-C6
4	L	301	07D	C6-C7-C8-C9
4	L	301	07D	C12-C13-C15-C16
4	L	301	07D	C2C-C3C-CAC-CBC
4	L	301	07D	C4C-C3C-CAC-CBC
4	L	304	07D	C6-C7-C8-C9
4	L	304	07D	C2C-C3C-CAC-CBC
4	L	304	07D	C4C-C3C-CAC-CBC
4	M	402	07D	C15-C16-C17-C18
4	M	403	07D	C8-C10-C11-C12
4	M	403	07D	CHA-CBD-CGD-O1D
4	M	403	07D	CBD-CGD-O2D-CED
5	L	302	08I	C6-C7-C8-C9
5	L	302	08I	C12-C13-C15-C16
5	L	302	08I	C1A-C2A-CAA-CBA
5	L	302	08I	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
5	L	302	08I	C4B-C3B-CAB-OBB
5	M	404	08I	C4-C3-C5-C6
5	M	404	08I	C2-C3-C5-C6
5	M	404	08I	C3-C5-C6-C7
5	M	404	08I	C6-C7-C8-C10
5	M	404	08I	C6-C7-C8-C9
5	M	404	08I	C8-C10-C11-C12
5	M	404	08I	C1A-C2A-CAA-CBA
5	M	404	08I	C4B-C3B-CAB-CBB
5	M	404	08I	C4B-C3B-CAB-OBB
5	M	404	08I	C2C-C3C-CAC-CBC
7	L	306	PGV	C03-O11-P-O12
7	L	308	PGV	C03-O11-P-O12
7	L	308	PGV	C03-O11-P-O13
7	L	308	PGV	C03-O11-P-O14
7	L	308	PGV	O02-C1-O01-C02
7	L	309	PGV	C03-O11-P-O12
7	L	309	PGV	C03-O11-P-O13
7	L	309	PGV	C03-O11-P-O14
7	L	309	PGV	O12-C04-C05-C06
7	L	310	PGV	C04-O12-P-O13
7	L	310	PGV	C04-O12-P-O14
7	L	310	PGV	O02-C1-O01-C02
7	L	310	PGV	C2-C1-O01-C02
7	L	314	PGV	C03-O11-P-O12
7	L	314	PGV	C03-O11-P-O13
7	L	314	PGV	C2-C1-O01-C02
7	L	315	PGV	C03-O11-P-O14
7	L	316	PGV	C03-O11-P-O12
7	L	316	PGV	C04-O12-P-O13
7	L	317	PGV	C03-O11-P-O12
7	L	318	PGV	O02-C1-O01-C02
7	L	318	PGV	C2-C1-O01-C02
7	M	409	PGV	C03-O11-P-O13
7	M	409	PGV	C03-O11-P-O14
7	M	410	PGV	O03-C01-C02-O01
7	M	410	PGV	C04-C05-C06-O06
7	M	410	PGV	O05-C05-C06-O06
7	M	410	PGV	C2-C1-O01-C02
7	M	411	PGV	C04-O12-P-O14
7	M	414	PGV	C04-O12-P-O13
7	M	415	PGV	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
7	M	416	PGV	C03-O11-P-O12
7	M	416	PGV	C03-O11-P-O13
7	M	416	PGV	C03-O11-P-O14
7	M	416	PGV	C04-O12-P-O14
7	M	418	PGV	C04-O12-P-O13
7	M	418	PGV	C2-C1-O01-C02
7	M	419	PGV	O01-C02-C03-O11
7	H	302	PGV	C03-O11-P-O12
7	H	302	PGV	C04-O12-P-O11
7	H	302	PGV	O12-C04-C05-C06
7	H	303	PGV	C03-O11-P-O12
7	H	303	PGV	C03-O11-P-O13
7	H	303	PGV	C03-O11-P-O14
7	H	303	PGV	C04-O12-P-O11
7	H	303	PGV	O01-C02-C03-O11
7	H	303	PGV	C04-C05-C06-O06
7	H	303	PGV	C2-C1-O01-C02
7	H	305	PGV	C2-C1-O01-C02
10	M	408	PEF	C2-C1-O3P-P
10	M	412	PEF	C2-C1-O3P-P
10	M	413	PEF	O4P-C4-C5-N
10	M	413	PEF	C1-O3P-P-O1P
10	M	413	PEF	C1-O3P-P-O2P
10	M	413	PEF	C1-O3P-P-O4P
10	M	413	PEF	C4-O4P-P-O2P
10	H	301	PEF	O4P-C4-C5-N
10	H	301	PEF	C1-O3P-P-O1P
12	M	405	CRT	C32-C33-C35-C36
12	M	405	CRT	C34-C33-C35-C36
12	M	405	CRT	C35-C36-C37-C38
13	M	406	RQ0	C11-C07-C19-C27
13	M	406	RQ0	C11-C07-C19-C39
13	M	406	RQ0	C14-C23-C33-C28
14	M	421	CDL	CA2-OA2-PA1-OA3
14	M	421	CDL	OA9-CA7-OA8-CA6
14	M	421	CDL	C31-CA7-OA8-CA6
14	M	421	CDL	OB9-CB7-OB8-CB6
4	M	403	07D	O1D-CGD-O2D-CED
14	M	421	CDL	C71-CB7-OB8-CB6
4	L	301	07D	C16-C17-C18-C20
4	M	402	07D	C16-C17-C18-C20
5	L	302	08I	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
5	M	404	08I	C16-C17-C18-C20
5	M	404	08I	CBD-CGD-O2D-CED
10	M	413	PEF	O5-C30-O3-C3
7	L	314	PGV	O02-C1-O01-C02
7	M	410	PGV	O02-C1-O01-C02
7	M	418	PGV	O02-C1-O01-C02
7	H	303	PGV	O02-C1-O01-C02
7	H	305	PGV	O02-C1-O01-C02
7	L	308	PGV	C20-C19-O03-C01
10	M	413	PEF	C31-C30-O3-C3
7	L	308	PGV	C2-C1-O01-C02
4	M	403	07D	C12-C13-C15-C16
4	L	301	07D	C11-C12-C13-C14
4	L	304	07D	C11-C12-C13-C14
4	M	402	07D	C11-C12-C13-C14
4	M	403	07D	C6-C7-C8-C9
4	M	403	07D	C11-C12-C13-C14
5	L	302	08I	C11-C12-C13-C14
5	M	404	08I	C11-C12-C13-C14
4	M	402	07D	C6-C7-C8-C10
5	L	302	08I	C6-C7-C8-C10
7	L	308	PGV	O04-C19-O03-C01
7	L	310	PGV	O04-C19-O03-C01
7	L	309	PGV	O12-C04-C05-O05
7	H	303	PGV	O12-C04-C05-O05
7	L	310	PGV	C20-C19-O03-C01
7	M	411	PGV	C2-C1-O01-C02
4	L	304	07D	C16-C17-C18-C19
4	L	304	07D	CBD-CGD-O2D-CED
7	L	310	PGV	C20-C21-C22-C23
7	M	411	PGV	C20-C21-C22-C23
10	M	413	PEF	C37-C38-C39-C40
14	M	421	CDL	C1-CB2-OB2-PB2
4	L	301	07D	C16-C17-C18-C19
4	M	403	07D	C16-C17-C18-C19
5	M	404	08I	C16-C17-C18-C19
4	M	403	07D	C11-C10-C8-C9
5	L	302	08I	C4-C3-C5-C6
5	M	404	08I	C11-C10-C8-C9
4	L	304	07D	C12-C13-C15-C16
5	L	302	08I	C2-C3-C5-C6
7	M	411	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
5	L	302	08I	C3-C5-C6-C7
13	M	406	RQ0	C33-C28-C29-C35
7	M	410	PGV	C24-C25-C26-C27
7	H	303	PGV	C4-C5-C6-C7
7	M	411	PGV	C2-C3-C4-C5
7	M	411	PGV	O02-C1-O01-C02
7	L	309	PGV	C20-C19-O03-C01
7	H	303	PGV	C20-C19-O03-C01
7	H	303	PGV	C21-C22-C23-C24
7	H	302	PGV	O12-C04-C05-O05
5	M	404	08I	O1D-CGD-O2D-CED
5	L	302	08I	CBD-CGD-O2D-CED
7	H	302	PGV	C2-C1-O01-C02
7	H	302	PGV	C19-C20-C21-C22
7	H	303	PGV	O04-C19-O03-C01
7	L	310	PGV	C19-C20-C21-C22
7	H	303	PGV	O05-C05-C06-O06
7	L	309	PGV	C1-C2-C3-C4
7	L	316	PGV	C1-C2-C3-C4
7	M	410	PGV	C1-C2-C3-C4
7	H	302	PGV	C1-C2-C3-C4
7	L	310	PGV	C22-C23-C24-C25
7	L	308	PGV	C1-C2-C3-C4
7	H	303	PGV	C1-C2-C3-C4
7	M	411	PGV	C22-C23-C24-C25
7	L	309	PGV	O04-C19-O03-C01
4	L	304	07D	C8-C10-C11-C12
4	L	304	07D	C13-C15-C16-C17
5	L	302	08I	C13-C15-C16-C17
4	M	402	07D	C16-C17-C18-C19
4	M	403	07D	C16-C17-C18-C20
7	L	309	PGV	C21-C22-C23-C24
5	M	404	08I	C15-C16-C17-C18
7	L	310	PGV	C04-O12-P-O11
7	M	409	PGV	C03-O11-P-O12
7	M	411	PGV	C04-O12-P-O11
7	M	416	PGV	C04-O12-P-O11
7	M	418	PGV	C03-O11-P-O12
7	M	419	PGV	C03-O11-P-O12
7	M	419	PGV	C04-O12-P-O11
10	M	413	PEF	C4-O4P-P-O3P
10	H	301	PEF	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
4	M	402	07D	CBA-CGA-O2A-C1
7	H	302	PGV	O02-C1-O01-C02
7	L	310	PGV	C6-C7-C8-C9
7	L	309	PGV	C22-C23-C24-C25
10	H	301	PEF	C11-C10-O2-C2
5	M	404	08I	C2B-C3B-CAB-OBB
13	M	406	RQ0	C39-C19-C27-C18
10	M	413	PEF	C36-C37-C38-C39
10	H	301	PEF	O4-C10-O2-C2
7	L	308	PGV	C5-C6-C7-C8
7	L	318	PGV	C13-C14-C15-C16
7	M	410	PGV	C22-C23-C24-C25
7	M	410	PGV	C25-C26-C27-C28
7	M	411	PGV	C3-C4-C5-C6
7	L	318	PGV	C21-C22-C23-C24
7	M	411	PGV	C23-C24-C25-C26
9	L	319	8K6	C2-C3-C4-C5
7	L	314	PGV	O12-C04-C05-O05
7	M	411	PGV	C13-C14-C15-C16
10	M	413	PEF	C35-C36-C37-C38
13	M	406	RQ0	C07-C19-C27-C18
7	H	302	PGV	C26-C27-C28-C29
7	H	303	PGV	C3-C4-C5-C6
5	M	404	08I	C12-C13-C15-C16
7	L	315	PGV	C3-C4-C5-C6
7	M	419	PGV	C3-C4-C5-C6
4	M	402	07D	O1A-CGA-O2A-C1
7	M	410	PGV	C21-C22-C23-C24
7	L	309	PGV	C04-C05-C06-O06
7	H	302	PGV	C3-C4-C5-C6
7	H	303	PGV	C25-C26-C27-C28
8	L	307	LMT	C5-C6-C7-C8
7	M	411	PGV	C11-C10-C9-C8
7	M	419	PGV	C1-C2-C3-C4
7	M	411	PGV	C24-C25-C26-C27
7	L	309	PGV	C2-C3-C4-C5
7	M	411	PGV	C20-C19-O03-C01
7	H	303	PGV	C30-C31-C32-C33
8	L	307	LMT	C5'-C4'-O1B-C1B
7	L	308	PGV	C21-C22-C23-C24
7	L	309	PGV	C26-C27-C28-C29
7	L	310	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
10	M	413	PEF	C31-C32-C33-C34
10	M	413	PEF	C41-C42-C43-C44
10	H	301	PEF	C16-C17-C18-C19
4	L	304	07D	C11-C10-C8-C9
7	L	309	PGV	C20-C21-C22-C23
7	M	410	PGV	C23-C24-C25-C26
7	M	411	PGV	C4-C5-C6-C7
7	H	303	PGV	C26-C27-C28-C29
8	L	307	LMT	C6-C7-C8-C9
10	M	408	PEF	C15-C16-C17-C18
10	M	413	PEF	C12-C13-C14-C15
9	M	407	8K6	C5-C6-C7-C8
7	M	415	PGV	C2-C3-C4-C5
7	H	302	PGV	C22-C23-C24-C25
7	L	316	PGV	C27-C28-C29-C30
4	L	304	07D	O1D-CGD-O2D-CED
10	M	413	PEF	C42-C43-C44-C45
7	M	411	PGV	O04-C19-O03-C01
7	M	410	PGV	C20-C19-O03-C01
7	M	410	PGV	C6-C7-C8-C9
7	L	308	PGV	C23-C24-C25-C26
7	M	411	PGV	C1-C2-C3-C4
7	M	419	PGV	C29-C30-C31-C32
10	M	408	PEF	C14-C15-C16-C17
7	H	302	PGV	C5-C6-C7-C8
7	H	302	PGV	O03-C01-C02-O01
8	L	307	LMT	C3'-C4'-O1B-C1B
5	L	302	08I	C11-C10-C8-C9
7	M	419	PGV	C24-C25-C26-C27
4	L	304	07D	C1A-C2A-CAA-CBA
7	H	303	PGV	C27-C28-C29-C30
7	L	315	PGV	C03-O11-P-O12
7	M	415	PGV	C03-O11-P-O12
7	M	409	PGV	C1-C2-C3-C4
12	M	405	CRT	C4-C5-C6-C7
7	M	410	PGV	C01-C02-C03-O11
7	L	309	PGV	C23-C24-C25-C26
7	M	416	PGV	C11-C10-C9-C8
10	H	301	PEF	C14-C15-C16-C17
7	M	410	PGV	O04-C19-O03-C01
5	L	302	08I	O1D-CGD-O2D-CED
7	L	309	PGV	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
8	L	307	LMT	C4'-C5'-C6'-O6'
5	M	404	08I	C13-C15-C16-C17
7	L	309	PGV	C31-C32-C33-C34
5	M	404	08I	C2B-C3B-CAB-CBB
7	M	410	PGV	C7-C8-C9-C10
7	L	309	PGV	C7-C8-C9-C10
7	M	411	PGV	C31-C32-C33-C34
7	H	303	PGV	C2-C3-C4-C5
7	L	309	PGV	C05-C04-O12-P
7	L	317	PGV	C03-O11-P-O13
7	H	302	PGV	C20-C19-O03-C01
7	M	415	PGV	C1-C2-C3-C4
7	L	309	PGV	C29-C30-C31-C32
10	H	301	PEF	O3-C30-C31-C32
14	M	421	CDL	C12-C11-CA5-OA6
7	L	309	PGV	C30-C31-C32-C33
7	H	303	PGV	C20-C21-C22-C23
13	M	406	RQ0	C14-C18-C27-C19
7	H	303	PGV	C14-C15-C16-C17
9	H	304	8K6	C3-C4-C5-C6
10	M	408	PEF	C31-C30-O3-C3
7	L	308	PGV	C3-C4-C5-C6
7	L	308	PGV	C7-C8-C9-C10
7	L	315	PGV	C19-C20-C21-C22
10	M	408	PEF	O2-C10-C11-C12
7	M	419	PGV	C01-C02-C03-O11
7	H	303	PGV	C01-C02-C03-O11
10	M	413	PEF	O3P-C1-C2-C3
7	H	303	PGV	C19-C20-C21-C22
13	M	406	RQ0	C23-C14-C18-C27
10	H	301	PEF	C12-C13-C14-C15
7	M	411	PGV	C19-C20-C21-C22
10	M	413	PEF	C33-C34-C35-C36
7	H	303	PGV	C24-C25-C26-C27
7	L	318	PGV	C20-C21-C22-C23
7	H	303	PGV	C6-C7-C8-C9
7	H	302	PGV	O03-C01-C02-C03
14	M	421	CDL	CA2-OA2-PA1-OA5
7	H	302	PGV	C4-C5-C6-C7
7	H	305	PGV	C6-C7-C8-C9
7	L	317	PGV	O01-C02-C03-O11
7	M	410	PGV	O01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
10	M	413	PEF	O3P-C1-C2-O2
7	M	416	PGV	C6-C7-C8-C9
7	H	302	PGV	O04-C19-O03-C01
7	M	415	PGV	O03-C01-C02-O01
7	M	419	PGV	O03-C01-C02-O01
7	L	310	PGV	C15-C16-C17-C18
7	H	303	PGV	C22-C23-C24-C25
4	L	301	07D	C8-C10-C11-C12
7	H	303	PGV	O12-C04-C05-C06
10	L	312	PEF	O4-C10-O2-C2
10	M	408	PEF	O5-C30-O3-C3
7	M	410	PGV	C02-C03-O11-P
7	H	302	PGV	C05-C04-O12-P
7	M	416	PGV	C5-C6-C7-C8
4	M	402	07D	C4C-C3C-CAC-CBC
7	M	419	PGV	C2-C3-C4-C5
10	L	312	PEF	C11-C10-O2-C2
7	M	410	PGV	C20-C21-C22-C23
7	H	305	PGV	C11-C10-C9-C8
5	L	302	08I	C4C-C3C-CAC-CBC
10	H	301	PEF	C18-C19-C20-C21
7	L	308	PGV	C22-C23-C24-C25
7	H	302	PGV	C21-C22-C23-C24
7	M	411	PGV	C29-C30-C31-C32
7	M	416	PGV	C4-C5-C6-C7
4	M	403	07D	C4-C3-C5-C6
7	M	410	PGV	O03-C01-C02-C03
7	M	411	PGV	C02-C03-O11-P
7	H	303	PGV	C05-C04-O12-P
10	M	408	PEF	C1-C2-C3-O3
10	M	408	PEF	O3P-C1-C2-O2
10	M	412	PEF	O3P-C1-C2-O2
10	M	413	PEF	C11-C12-C13-C14
7	L	310	PGV	C13-C14-C15-C16
4	M	403	07D	CHA-CBD-CGD-O2D
7	L	315	PGV	C26-C27-C28-C29
10	H	301	PEF	C13-C14-C15-C16
7	L	309	PGV	O03-C01-C02-O01
7	L	316	PGV	C20-C19-O03-C01
7	M	411	PGV	C6-C7-C8-C9
10	M	413	PEF	C39-C40-C41-C42
7	H	303	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
7	L	309	PGV	O03-C19-C20-C21
7	H	303	PGV	C28-C29-C30-C31
10	H	301	PEF	C34-C35-C36-C37
7	M	409	PGV	C19-C20-C21-C22
7	L	314	PGV	C04-O12-P-O11
7	L	316	PGV	C04-O12-P-O11
7	M	418	PGV	C04-O12-P-O11
10	L	312	PEF	C1-O3P-P-O4P
10	M	408	PEF	C1-O3P-P-O4P
14	M	421	CDL	CA3-OA5-PA1-OA2
4	M	402	07D	C12-C13-C15-C16
7	L	306	PGV	C03-O11-P-O14
7	L	315	PGV	C03-O11-P-O13
7	L	316	PGV	C03-O11-P-O14
7	M	411	PGV	C04-O12-P-O13
7	M	415	PGV	C03-O11-P-O13
7	M	418	PGV	C03-O11-P-O13
7	M	419	PGV	C03-O11-P-O13
7	M	419	PGV	C04-O12-P-O13
7	H	302	PGV	C03-O11-P-O13
7	H	302	PGV	C04-O12-P-O14
7	H	303	PGV	C04-O12-P-O14
10	M	413	PEF	C4-O4P-P-O1P
12	M	405	CRT	C33-C35-C36-C37
7	L	309	PGV	C01-C02-C03-O11
7	L	314	PGV	C01-C02-C03-O11
7	L	317	PGV	C01-C02-C03-O11
10	M	408	PEF	O3P-C1-C2-C3
14	M	421	CDL	OB5-CB3-CB4-CB6
4	M	403	07D	CAD-CBD-CGD-O1D
10	M	412	PEF	C5-C4-O4P-P
7	L	314	PGV	O12-C04-C05-C06
7	L	309	PGV	O01-C02-C03-O11
7	L	309	PGV	C24-C25-C26-C27
7	L	309	PGV	C28-C29-C30-C31
10	M	408	PEF	O2-C2-C3-O3
14	M	421	CDL	C58-C59-C60-C61
7	L	316	PGV	C26-C27-C28-C29
7	L	316	PGV	O04-C19-O03-C01
7	L	318	PGV	C4-C5-C6-C7
10	M	412	PEF	C16-C17-C18-C19
6	L	303	U10	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
7	L	308	PGV	C01-C02-O01-C1
7	L	310	PGV	C03-C02-O01-C1
10	M	412	PEF	O3P-C1-C2-C3
5	L	302	08I	C2-C1-O2A-CGA
9	L	313	8K6	C11-C12-C13-C14
7	L	308	PGV	C02-C03-O11-P
7	M	410	PGV	C15-C16-C17-C18
7	L	314	PGV	O01-C02-C03-O11
6	L	303	U10	C12-C11-C9-C10
4	M	403	07D	C2-C3-C5-C6
10	M	413	PEF	O2-C10-C11-C12
7	L	306	PGV	C04-O12-P-O11
7	L	309	PGV	C04-O12-P-O11
7	L	318	PGV	C03-O11-P-O12
7	L	318	PGV	C04-O12-P-O11
7	M	414	PGV	C03-O11-P-O12
7	M	414	PGV	C04-O12-P-O11
10	M	408	PEF	C4-O4P-P-O3P
10	M	412	PEF	C4-O4P-P-O3P
14	M	421	CDL	CB2-OB2-PB2-OB5
14	M	421	CDL	CB3-OB5-PB2-OB2
7	M	411	PGV	O03-C01-C02-C03
13	M	406	RQ0	C09-C06-C16-C37
13	M	406	RQ0	C20-C15-C21-C40
7	M	411	PGV	O03-C19-C20-C21
7	H	302	PGV	C9-C10-C11-C12
7	M	411	PGV	C5-C6-C7-C8
7	L	309	PGV	O05-C05-C06-O06
7	H	305	PGV	C1-C2-C3-C4
8	L	307	LMT	C7-C8-C9-C10
4	L	301	07D	C11-C10-C8-C9
7	L	310	PGV	C4-C5-C6-C7
7	L	314	PGV	C7-C8-C9-C10
7	M	416	PGV	C22-C23-C24-C25
7	L	310	PGV	C7-C8-C9-C10
10	M	413	PEF	C40-C41-C42-C43
9	H	304	8K6	C5-C6-C7-C8
7	H	303	PGV	C01-C02-O01-C1
7	H	305	PGV	C03-C02-O01-C1
10	M	412	PEF	C1-C2-O2-C10
13	M	406	RQ0	C10-C05-C13-C36
10	H	301	PEF	O5-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
10	H	301	PEF	C19-C20-C21-C22
8	L	307	LMT	C3-C4-C5-C6
7	M	415	PGV	C01-C02-C03-O11
13	M	406	RQ0	C20-C15-C21-C26
10	M	413	PEF	C10-C11-C12-C13
7	L	306	PGV	C7-C8-C9-C10
10	H	301	PEF	C32-C33-C34-C35
7	M	419	PGV	C21-C22-C23-C24
4	M	403	07D	C3-C5-C6-C7
7	M	411	PGV	O12-C04-C05-C06
7	L	308	PGV	C6-C7-C8-C9
7	M	416	PGV	C30-C31-C32-C33
7	H	303	PGV	C5-C6-C7-C8
4	M	402	07D	C11-C10-C8-C9
6	L	303	U10	C12-C11-C9-C8
13	M	406	RQ0	C10-C05-C13-C22
13	M	406	RQ0	C09-C06-C16-C25
7	L	308	PGV	C11-C10-C9-C8
10	M	408	PEF	O4-C10-C11-C12
7	M	419	PGV	O03-C01-C02-C03
7	H	302	PGV	C27-C28-C29-C30
10	M	412	PEF	C18-C19-C20-C21
6	L	303	U10	C13-C14-C16-C17
7	L	310	PGV	C11-C12-C13-C14
6	L	305	U10	C2-C3-O3-C3M
14	M	421	CDL	C56-C57-C58-C59
14	M	421	CDL	C63-C64-C65-C66
14	M	421	CDL	C12-C11-CA5-OA7
10	L	312	PEF	O2-C2-C3-O3
7	L	317	PGV	C03-O11-P-O14
7	L	316	PGV	O03-C19-C20-C21
5	L	302	08I	C14-C13-C15-C16
7	L	315	PGV	C2-C3-C4-C5
13	M	406	RQ0	C12-C08-C17-C24
4	M	403	07D	C3A-C2A-CAA-CBA
8	L	307	LMT	O1'-C1-C2-C3
4	L	301	07D	CAD-CBD-CGD-O2D
7	H	303	PGV	C03-C02-O01-C1
4	L	301	07D	C2-C1-O2A-CGA
7	L	310	PGV	C3-C4-C5-C6
7	L	316	PGV	C25-C26-C27-C28
7	M	411	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
7	M	410	PGV	C11-C12-C13-C14
7	M	415	PGV	O03-C01-C02-C03
7	H	303	PGV	C15-C16-C17-C18
8	L	307	LMT	O5'-C5'-C6'-O6'
4	M	402	07D	O2A-C1-C2-C3
4	M	403	07D	O2A-C1-C2-C3
5	M	404	08I	O2A-C1-C2-C3
7	L	306	PGV	C22-C23-C24-C25
10	M	413	PEF	O3-C30-C31-C32
4	M	402	07D	CHA-CBD-CGD-O2D
7	M	410	PGV	C12-C13-C14-C15
7	M	410	PGV	C9-C10-C11-C12
7	M	410	PGV	O01-C1-C2-C3
7	M	410	PGV	O03-C19-C20-C21
5	M	404	08I	CHA-CBD-CGD-O1D
4	M	402	07D	CAA-CBA-CGA-O2A
10	H	301	PEF	O2-C10-C11-C12
7	L	317	PGV	O01-C1-C2-C3
13	M	406	RQ0	C15-C20-C32-C31
7	L	316	PGV	C29-C30-C31-C32
7	M	414	PGV	C23-C24-C25-C26
7	L	316	PGV	O04-C19-C20-C21
14	M	421	CDL	CB4-CB6-OB8-CB7
7	H	302	PGV	C25-C26-C27-C28
4	M	403	07D	C1A-C2A-CAA-CBA
7	L	316	PGV	O12-C04-C05-C06
7	L	308	PGV	C2-C3-C4-C5
10	M	413	PEF	O5-C30-C31-C32
10	L	312	PEF	C1-C2-C3-O3
7	M	410	PGV	C28-C29-C30-C31
7	L	310	PGV	O03-C19-C20-C21
7	L	317	PGV	O02-C1-O01-C02
7	L	310	PGV	C02-C03-O11-P
6	L	303	U10	C6-C7-C8-C9
7	L	318	PGV	C03-O11-P-O13
7	M	414	PGV	C03-O11-P-O13
10	M	408	PEF	C1-O3P-P-O2P
10	M	408	PEF	C4-O4P-P-O1P
10	H	301	PEF	C1-O3P-P-O2P
10	H	301	PEF	C4-O4P-P-O1P
10	H	301	PEF	C4-O4P-P-O2P
4	M	402	07D	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
7	M	410	PGV	O04-C19-C20-C21
7	M	410	PGV	O02-C1-C2-C3
7	L	309	PGV	C4-C5-C6-C7
9	M	417	8K6	C1-C2-C3-C4
7	L	317	PGV	O02-C1-C2-C3
7	L	308	PGV	O03-C19-C20-C21
7	H	305	PGV	O03-C19-C20-C21
4	M	402	07D	C8-C10-C11-C12
10	L	312	PEF	O3-C30-C31-C32
14	M	421	CDL	C32-C31-CA7-OA8
7	M	419	PGV	C22-C23-C24-C25

There are no ring outliers.

34 monomers are involved in 119 short contacts:

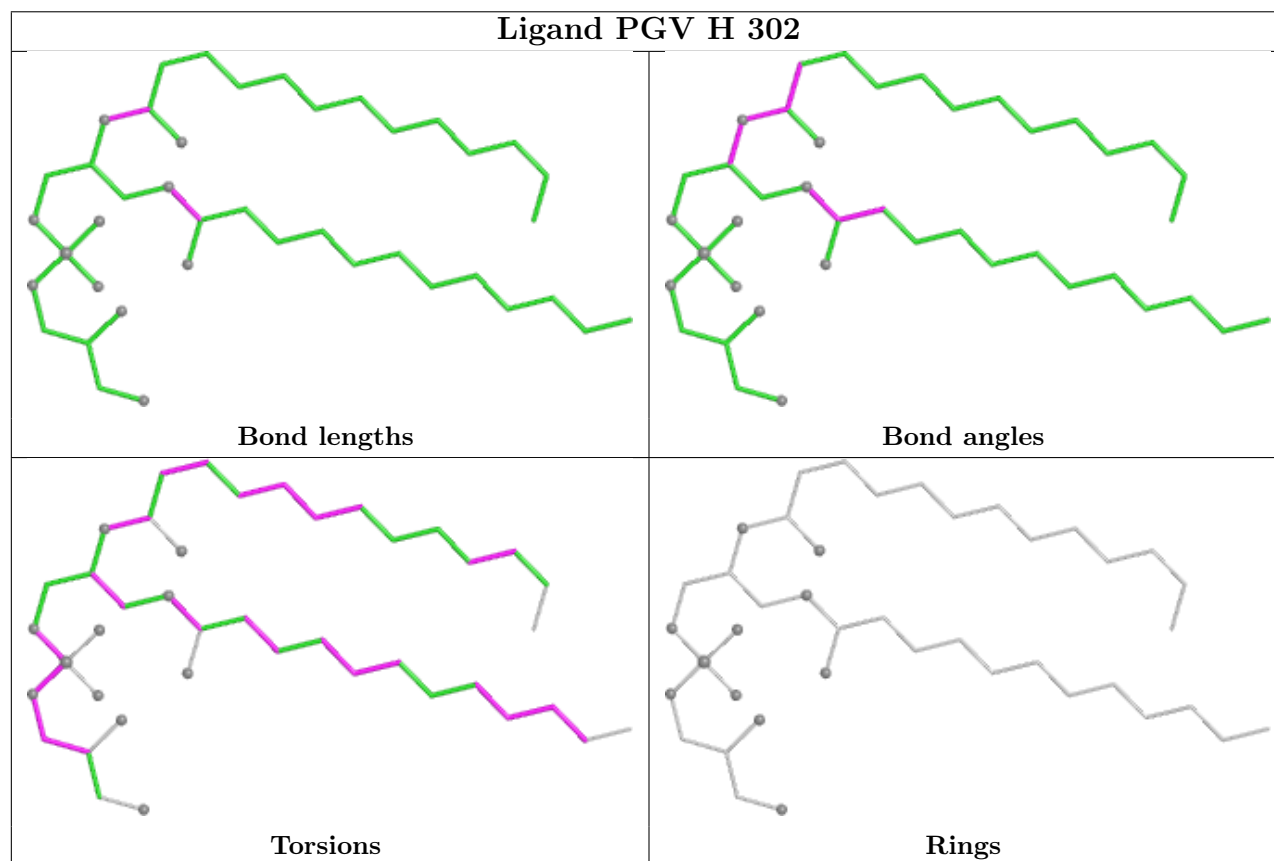
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	302	PGV	8	0
9	L	313	8K6	4	0
10	M	412	PEF	5	0
7	H	305	PGV	1	0
7	H	303	PGV	3	0
9	L	311	8K6	2	0
7	M	415	PGV	1	0
9	H	304	8K6	2	0
7	L	306	PGV	3	0
9	M	417	8K6	1	0
7	L	314	PGV	2	0
10	H	301	PEF	21	0
7	L	309	PGV	5	0
14	M	421	CDL	6	0
7	L	317	PGV	1	0
8	L	307	LMT	2	0
9	M	420	8K6	4	0
10	M	413	PEF	6	0
7	L	310	PGV	4	0
6	L	303	U10	3	0
7	M	409	PGV	2	0
7	L	308	PGV	2	0
10	L	312	PEF	2	0
7	L	318	PGV	2	0
10	M	408	PEF	1	0
7	L	315	PGV	1	0

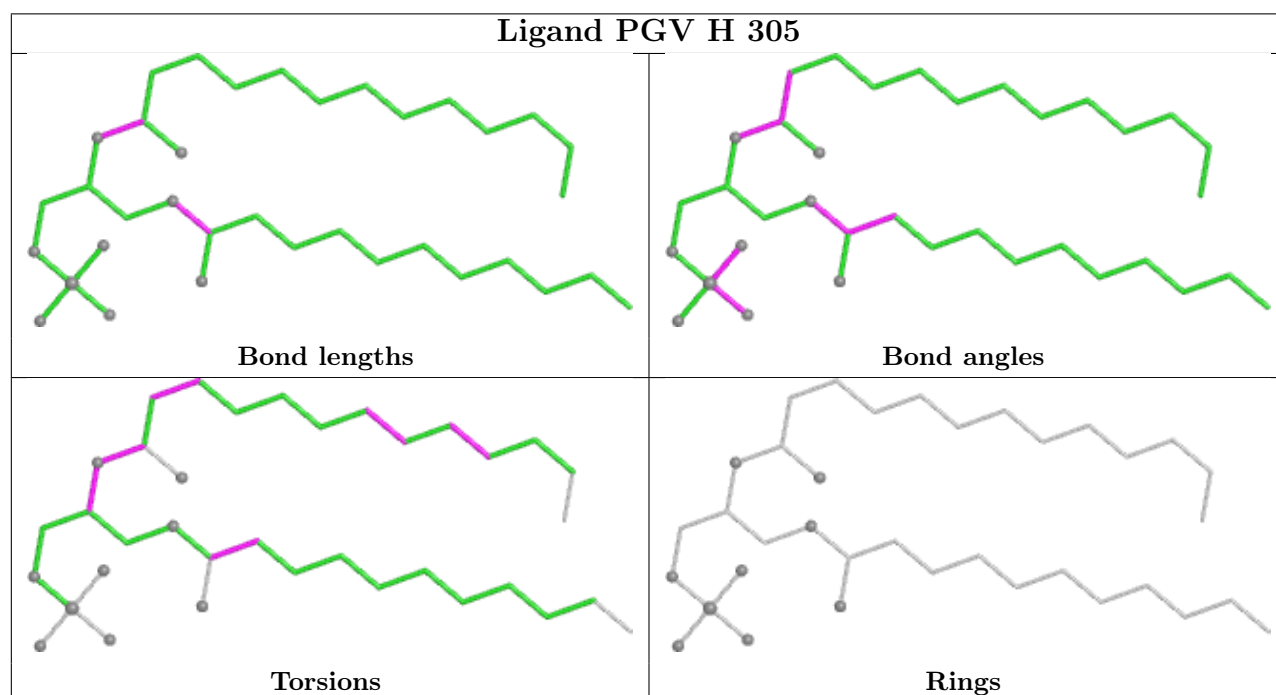
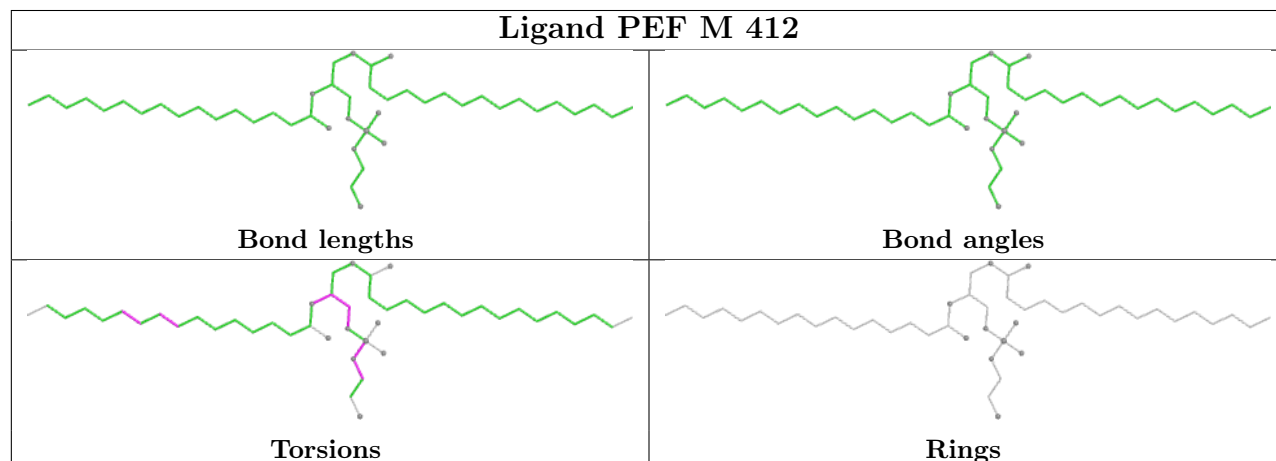
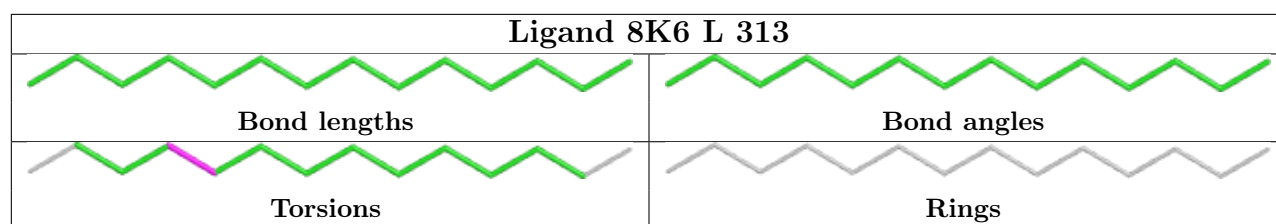
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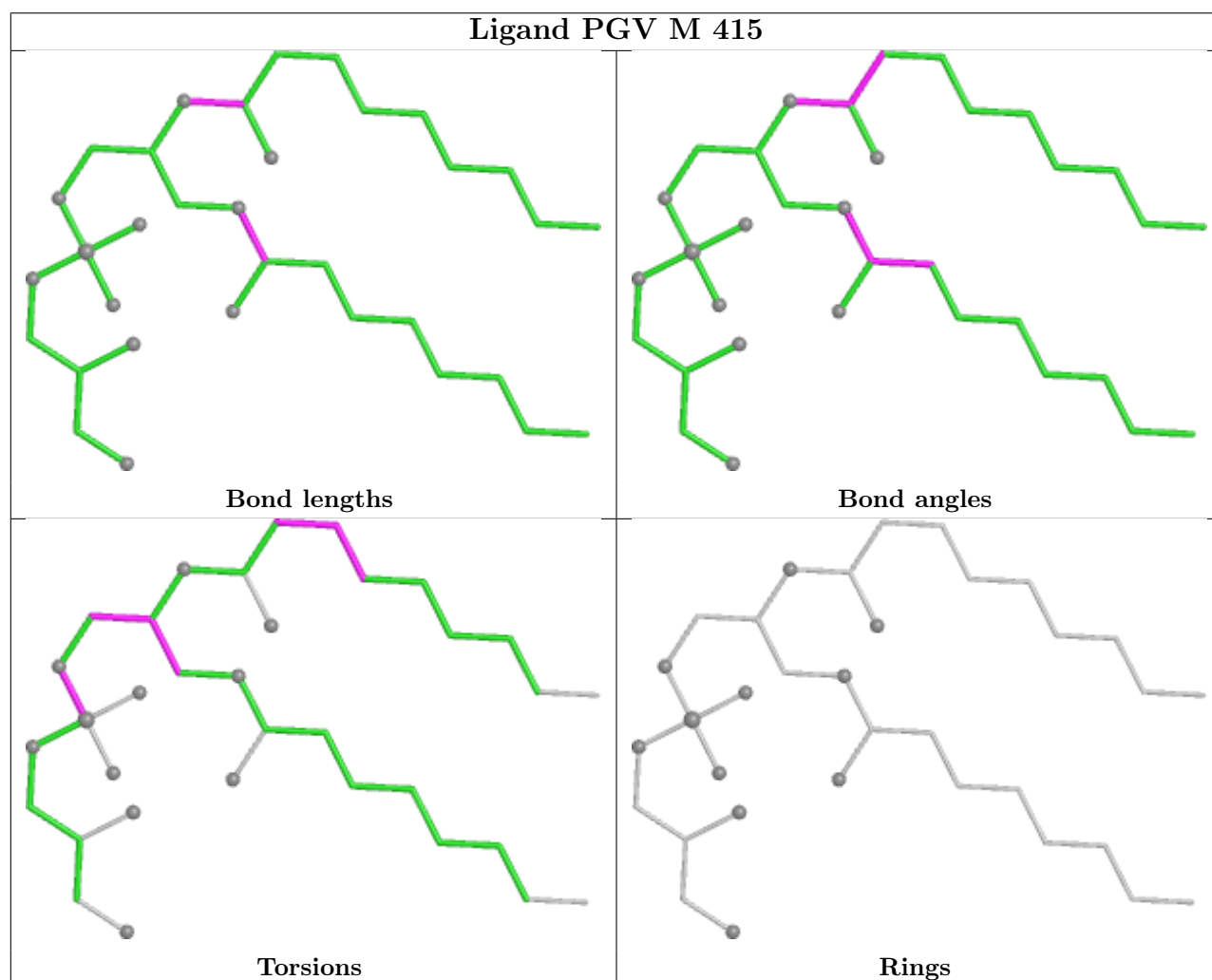
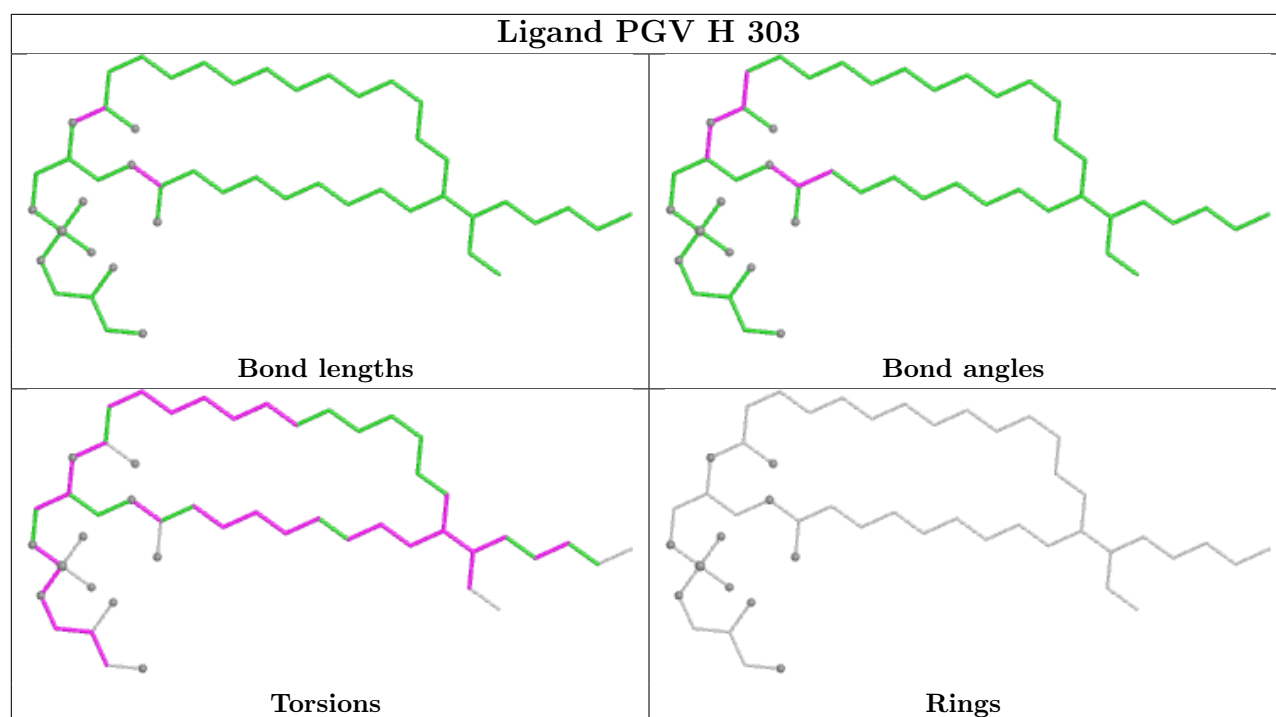
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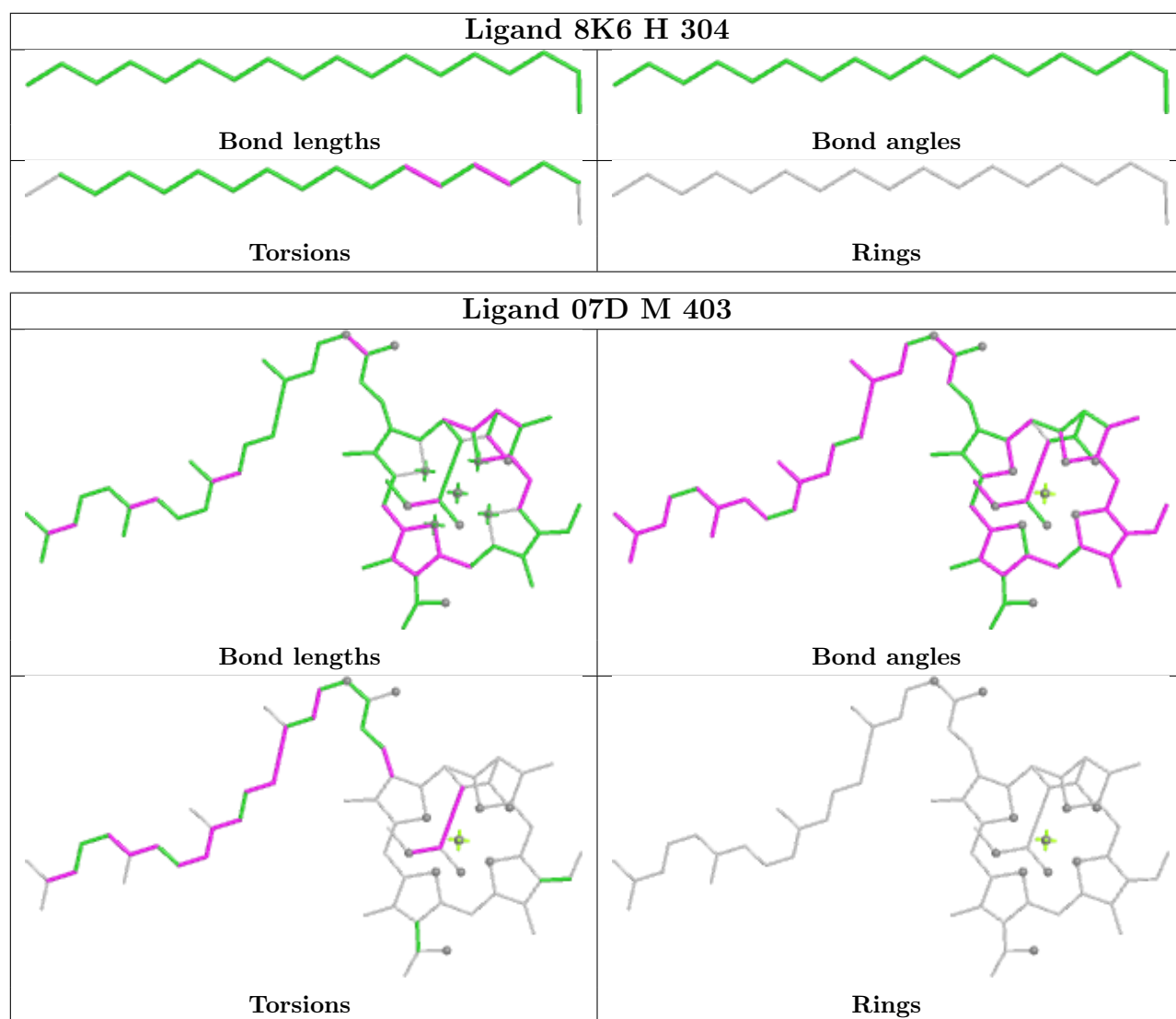
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	414	PGV	8	0
12	M	405	CRT	2	0
7	M	411	PGV	8	0
7	M	418	PGV	1	0
7	L	316	PGV	4	0
7	M	419	PGV	6	0
7	M	410	PGV	6	0
7	M	416	PGV	2	0

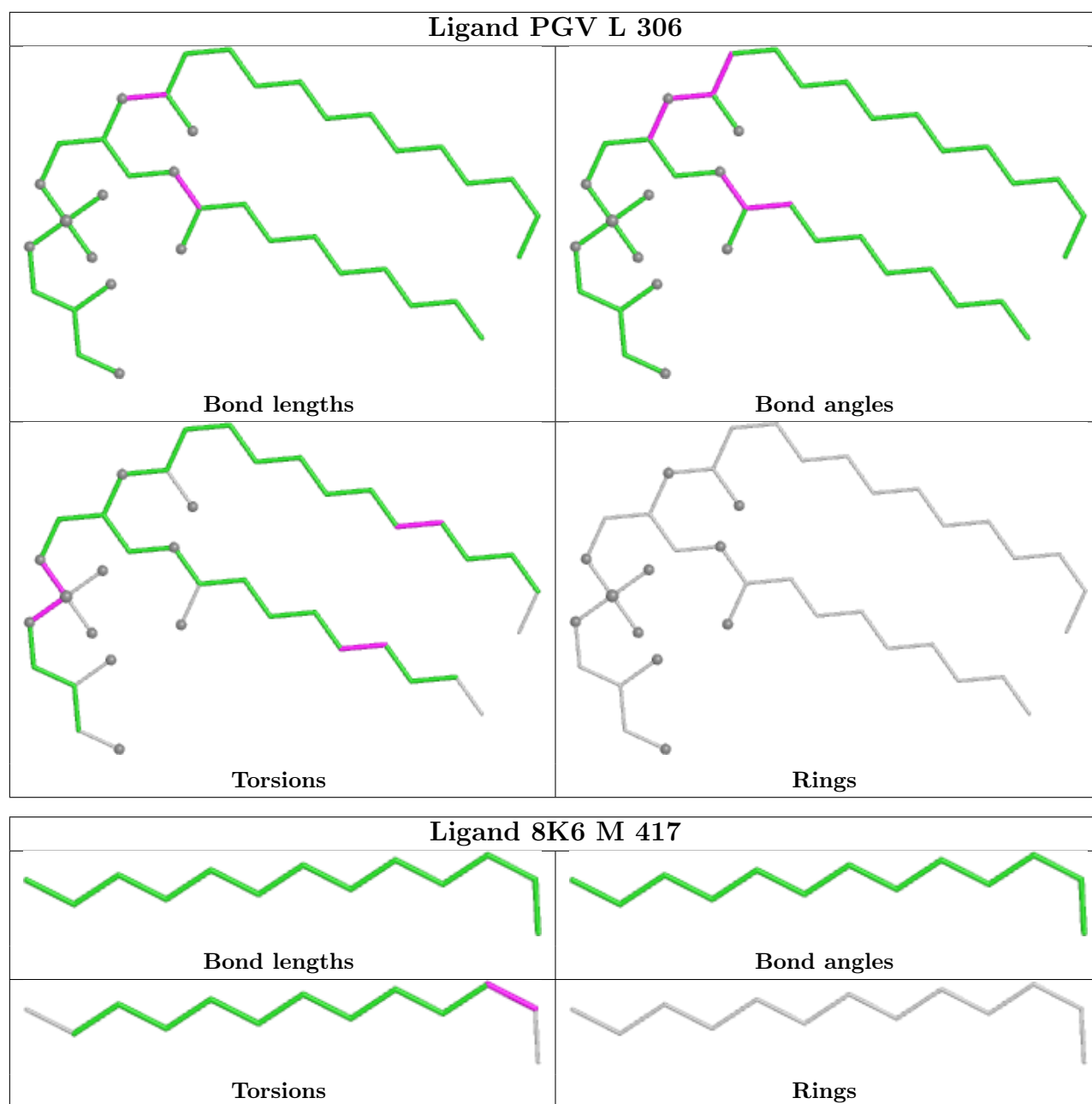
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

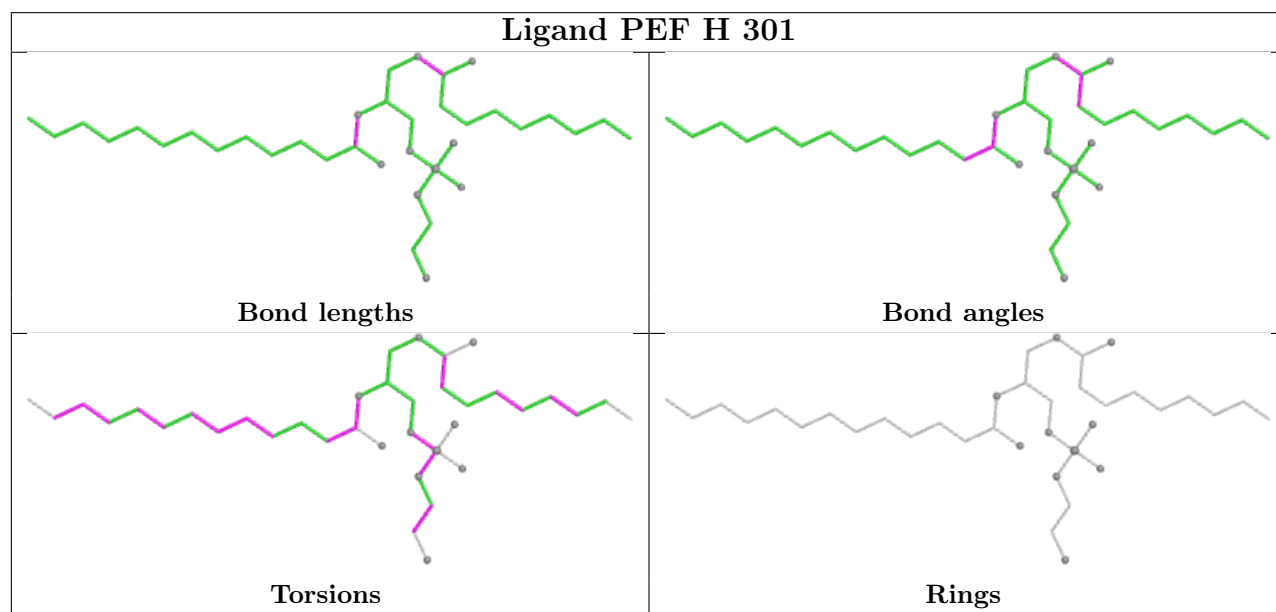
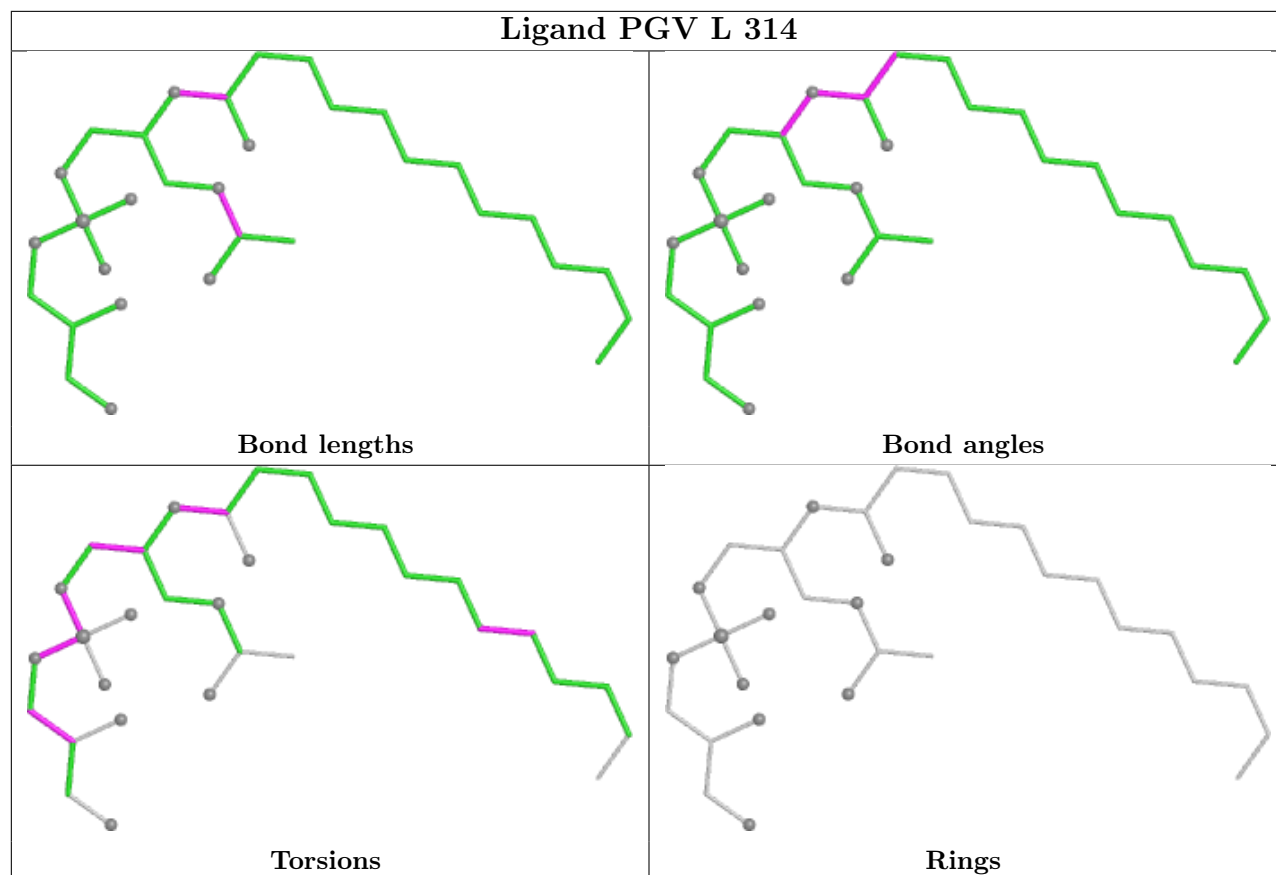


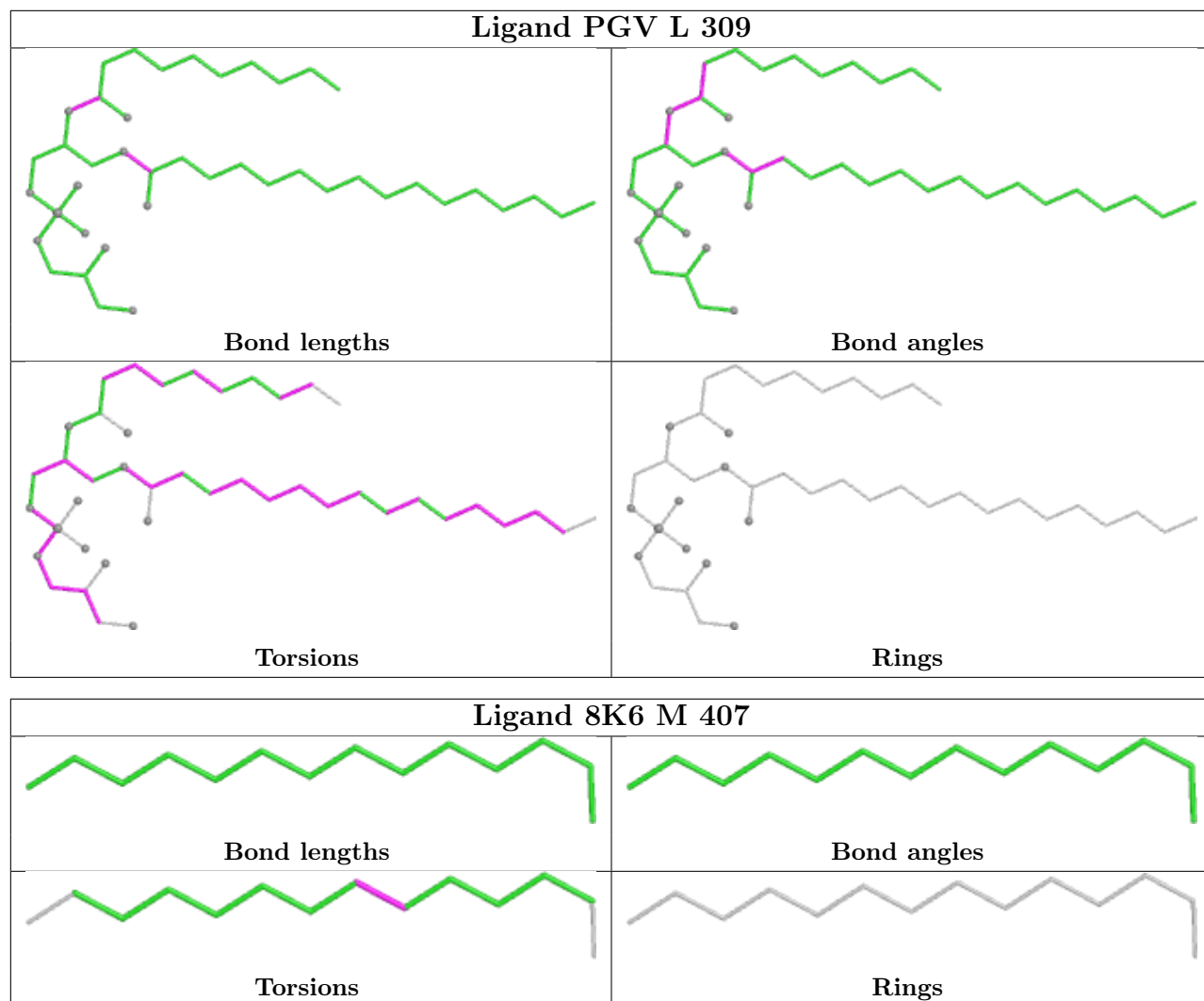


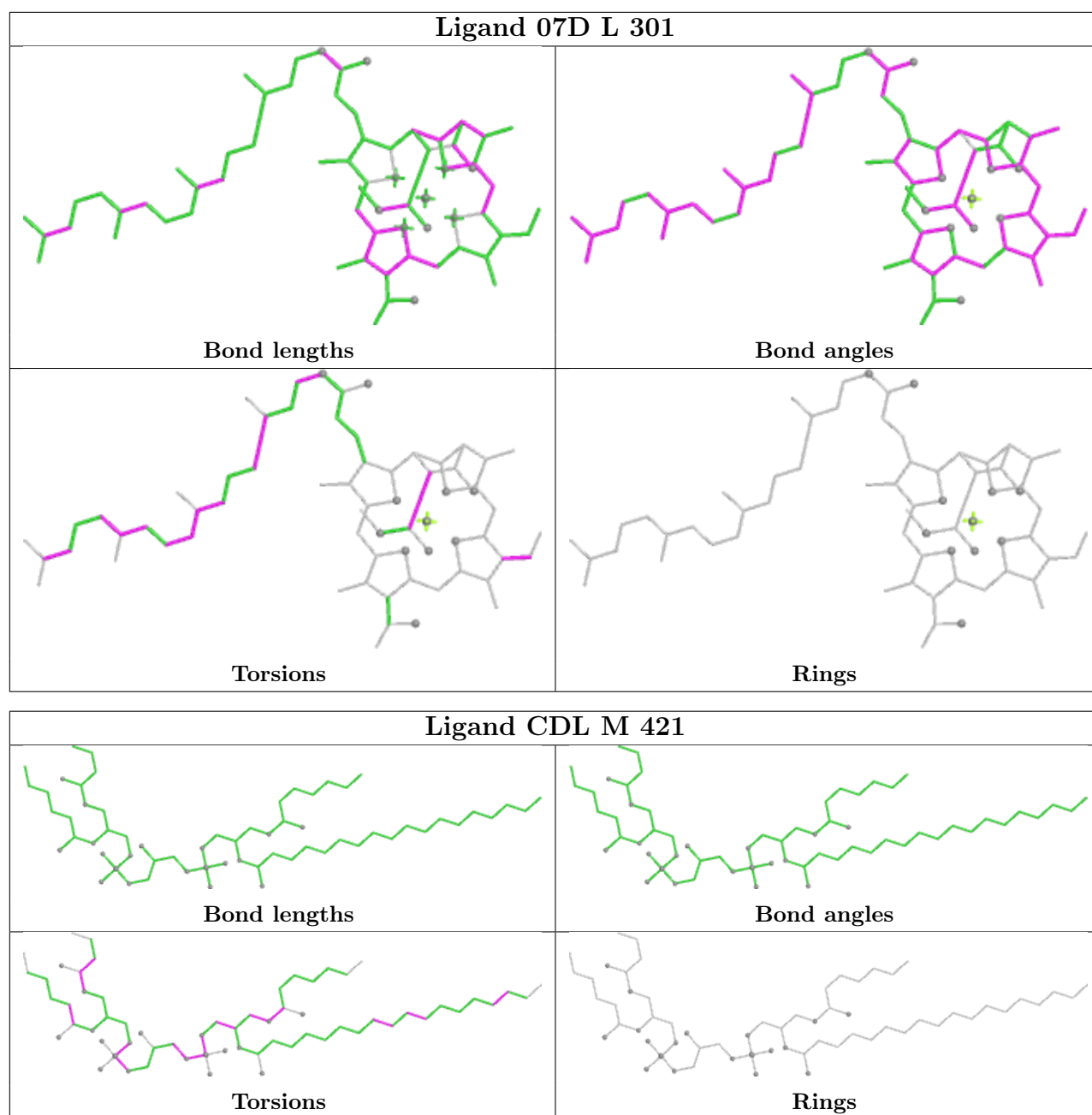


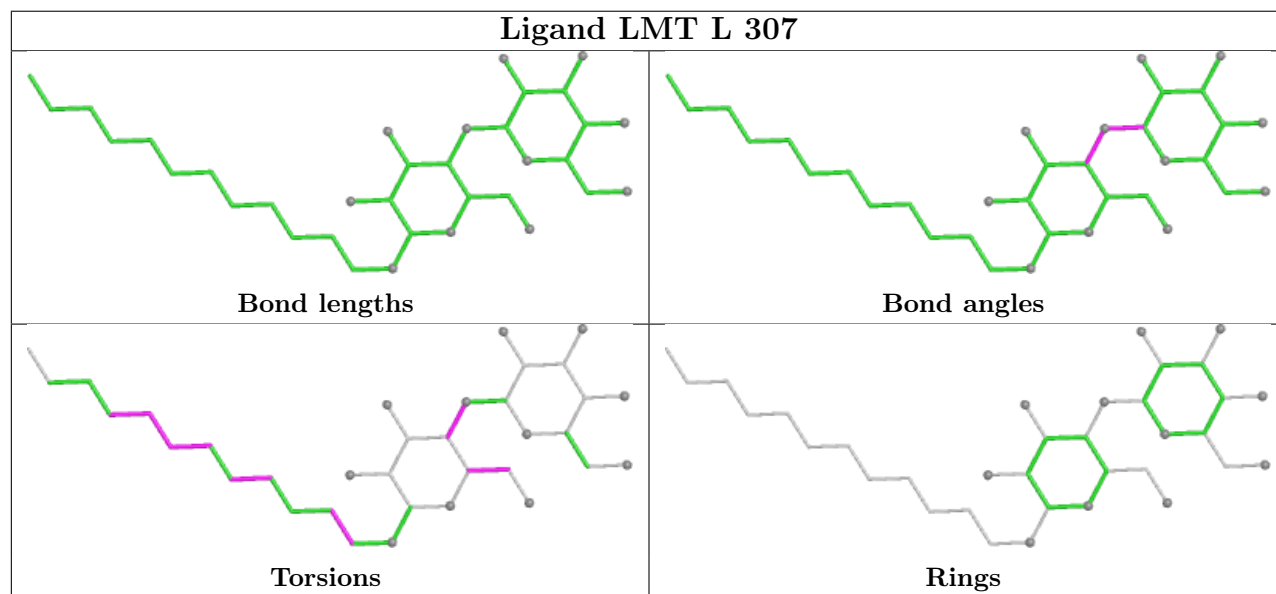
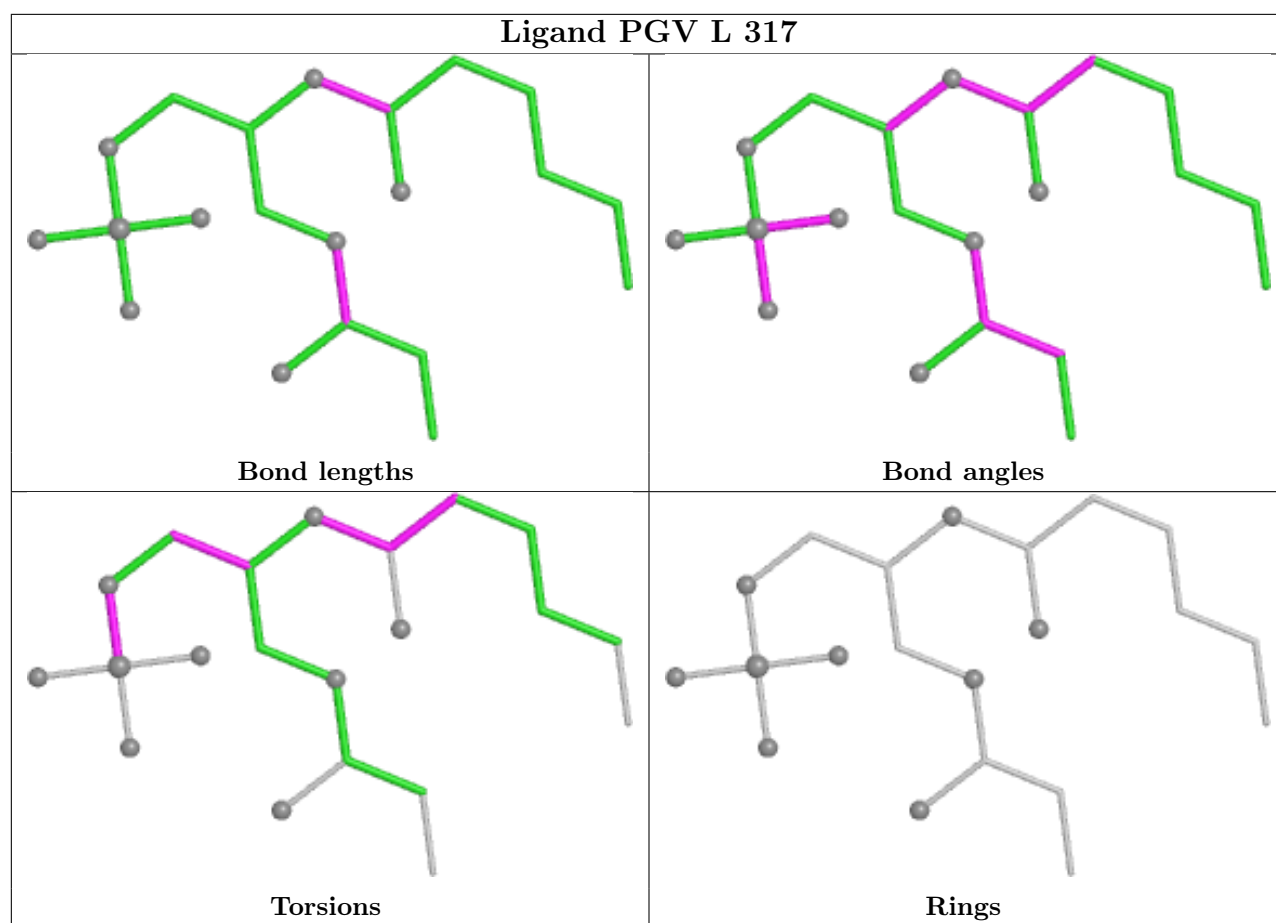


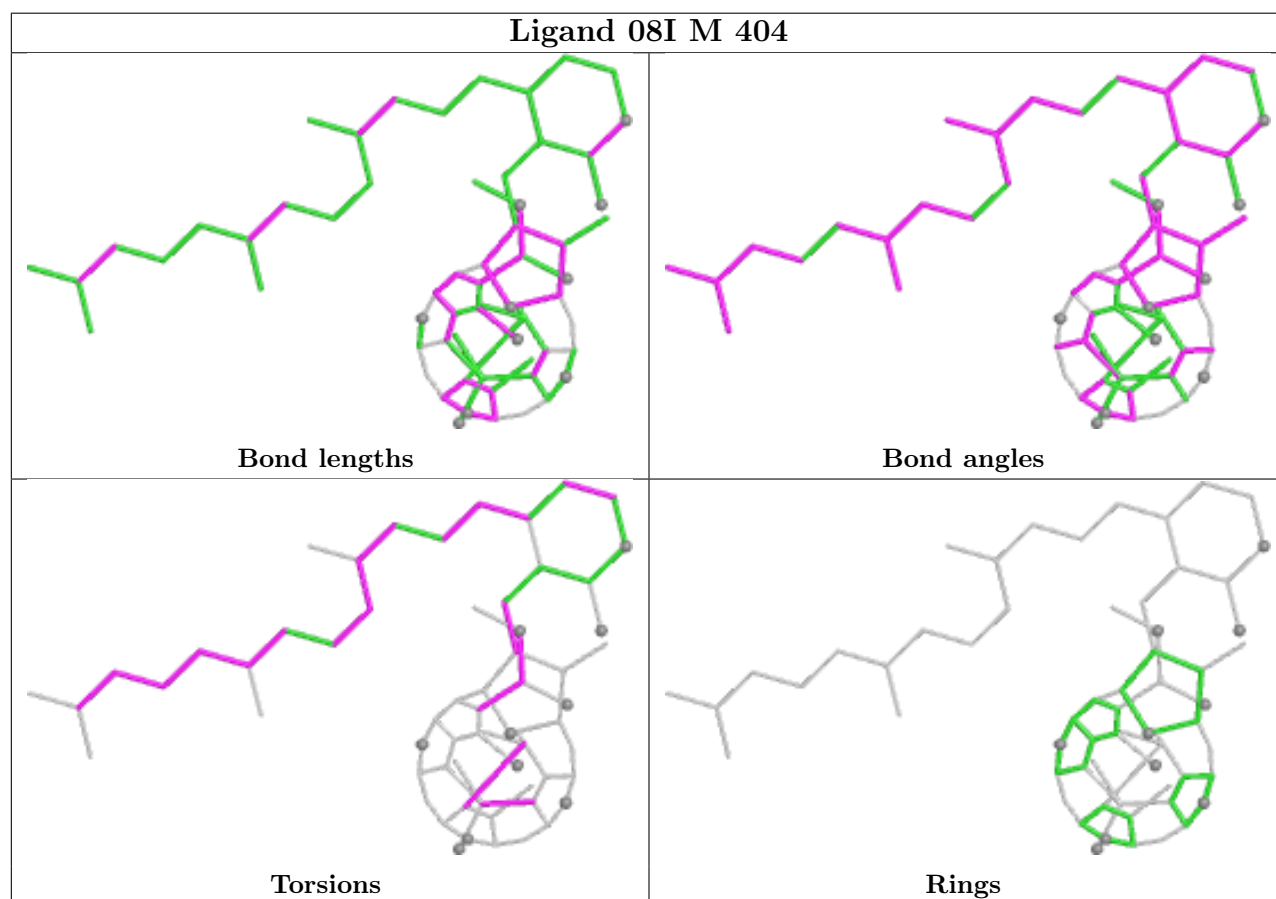
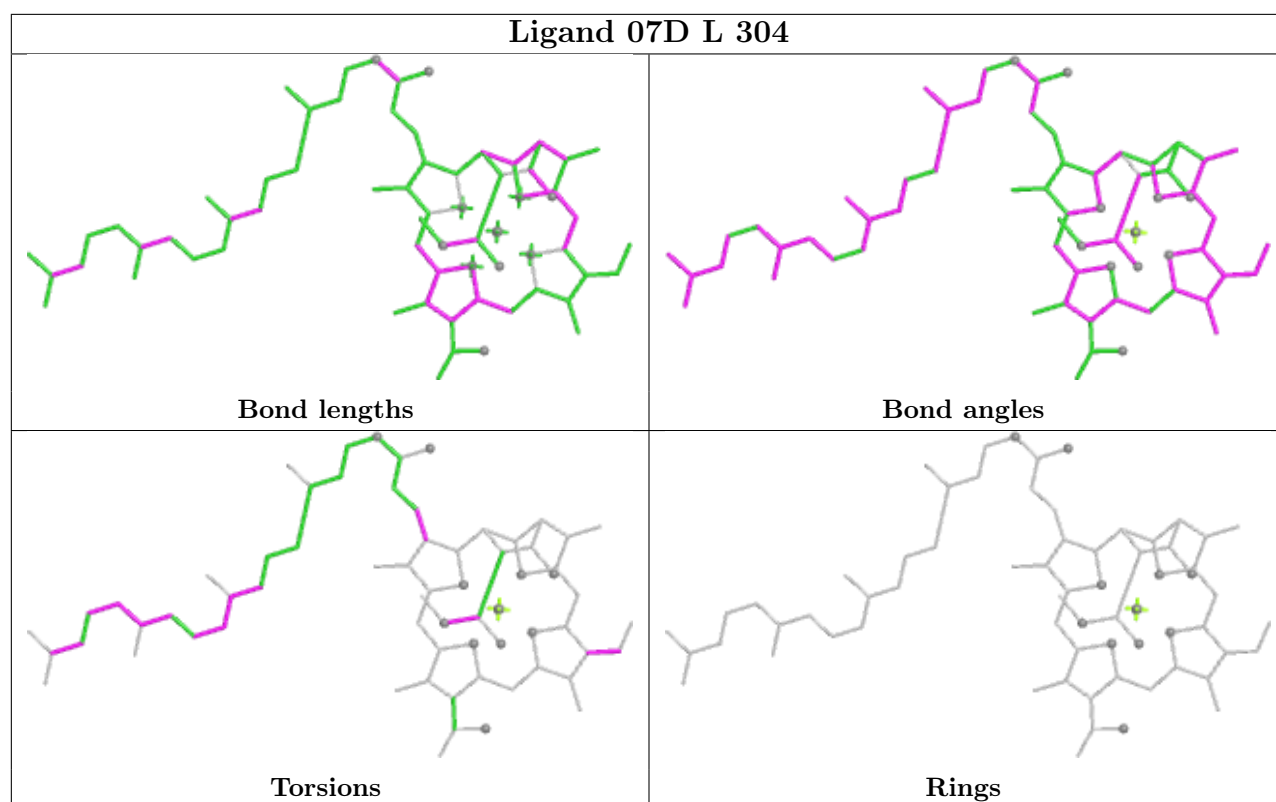




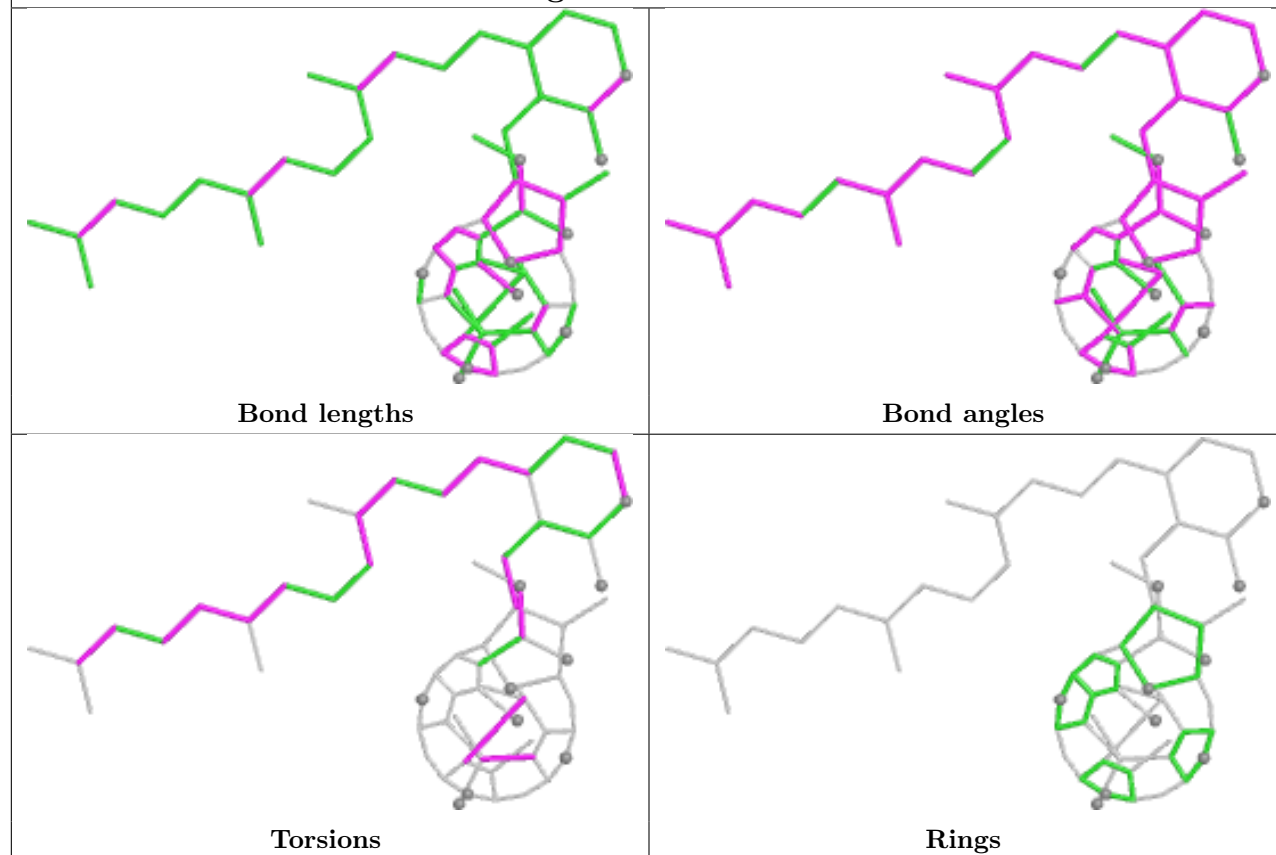




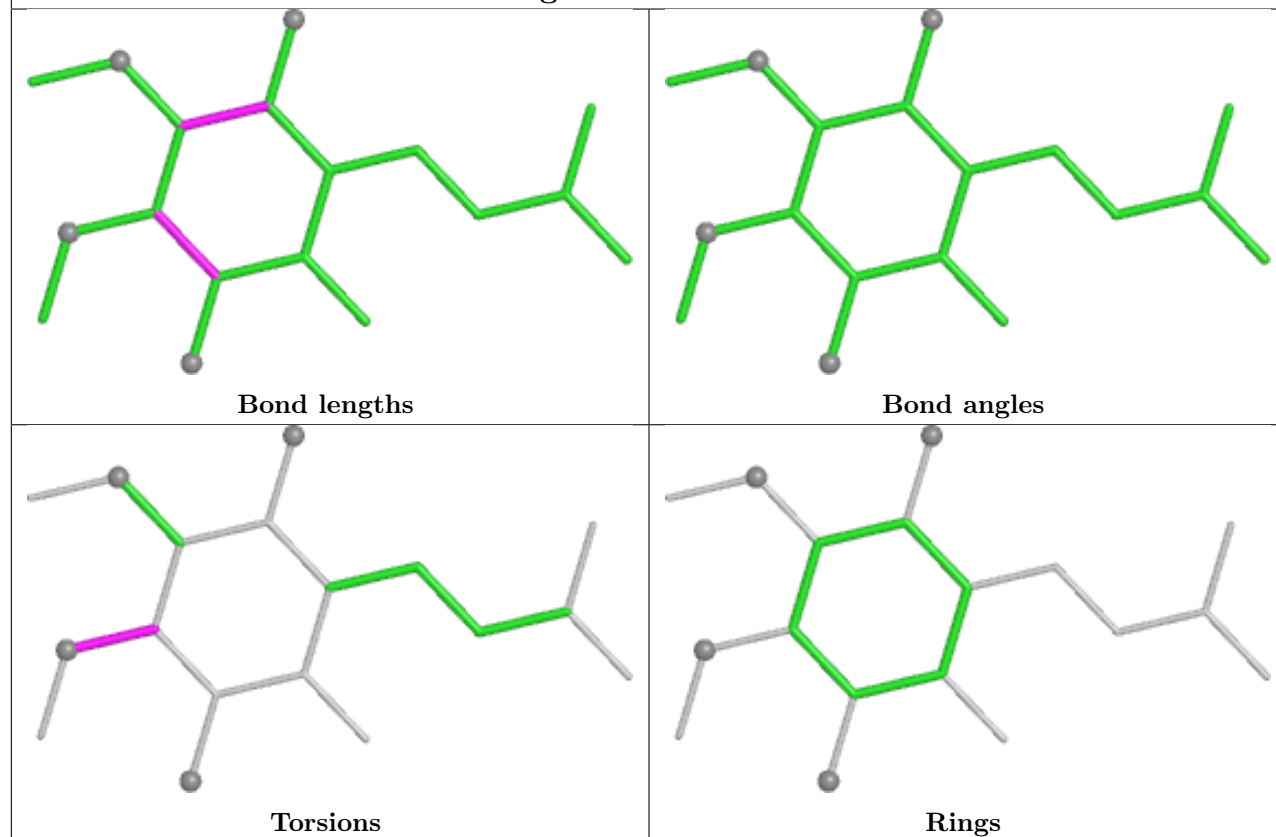


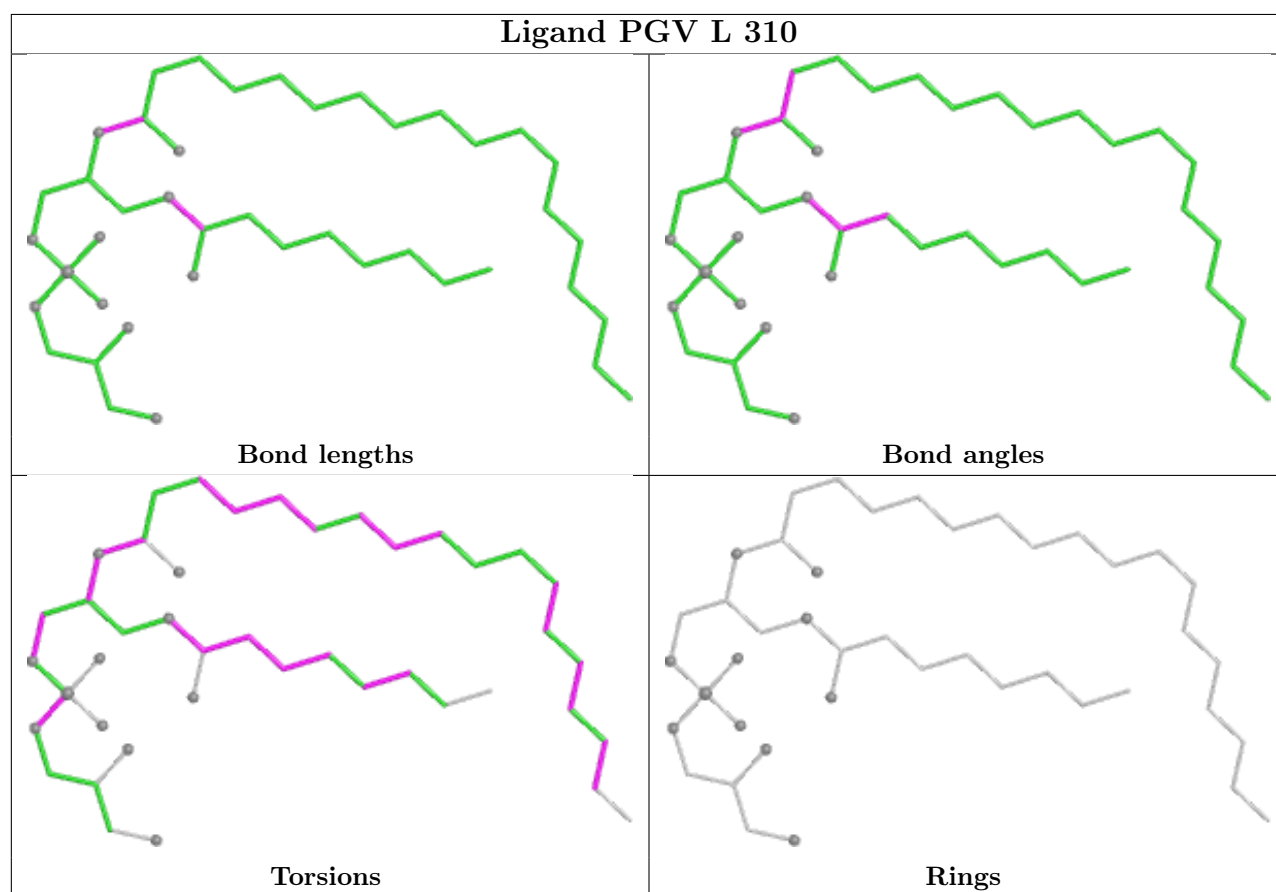
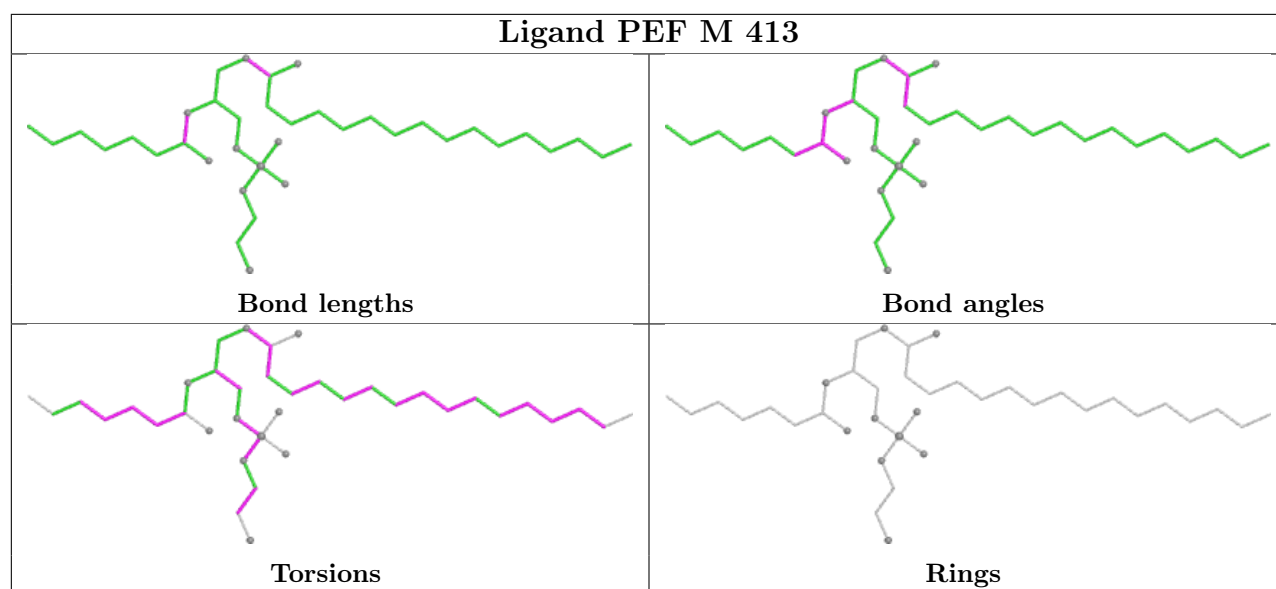


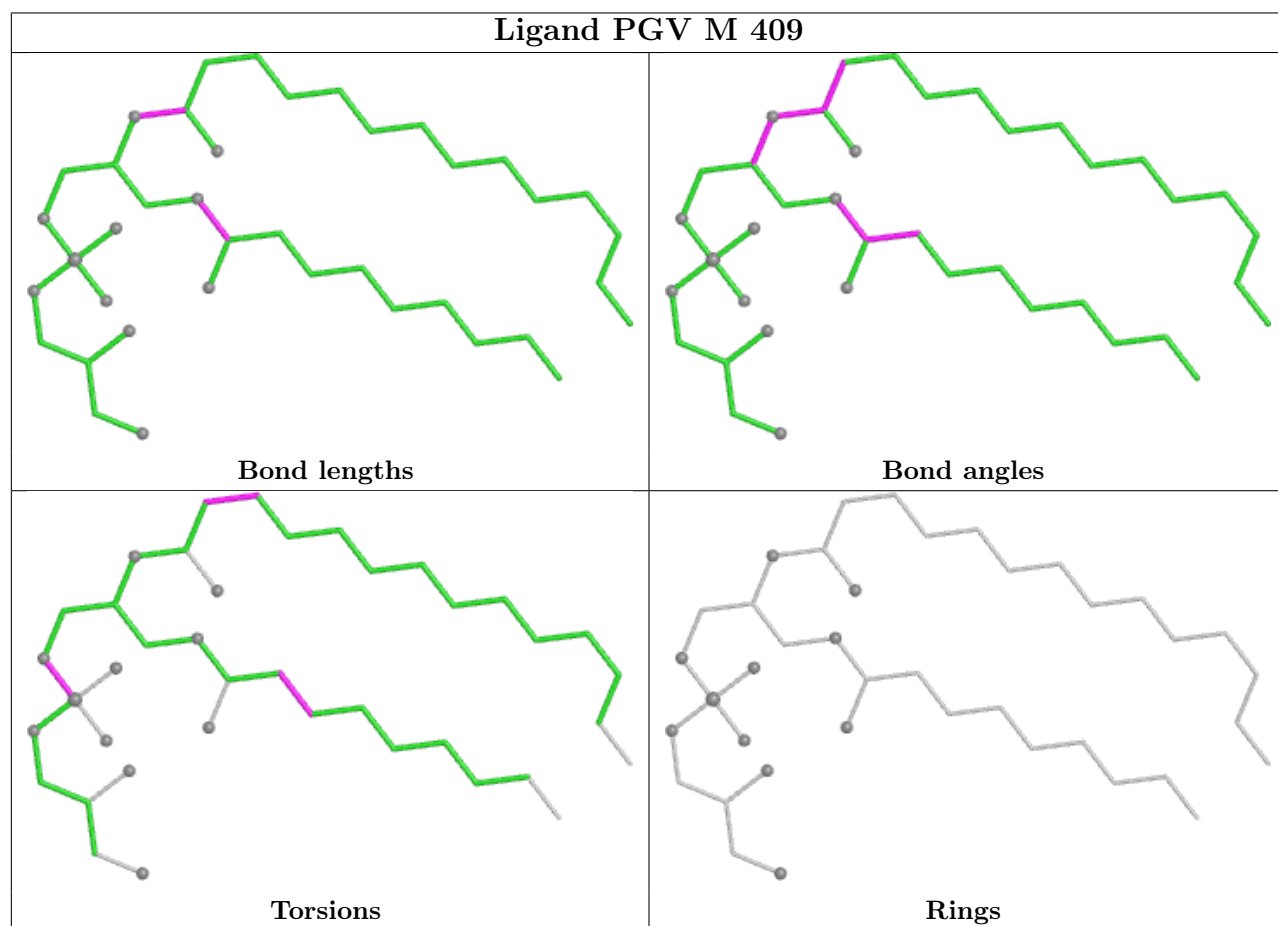
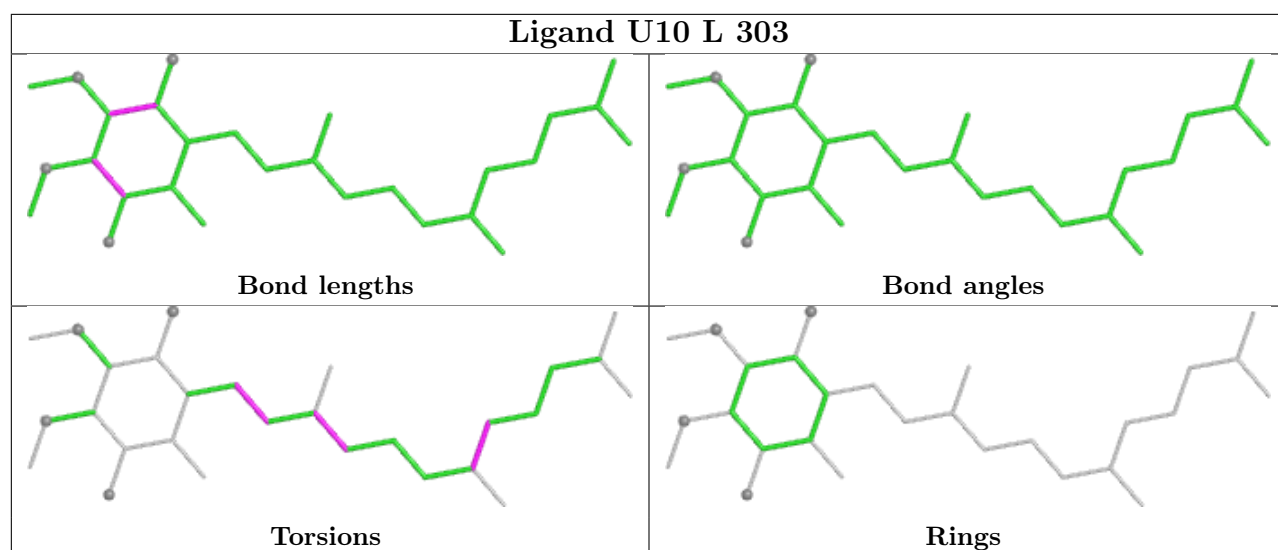
Ligand 08I L 302

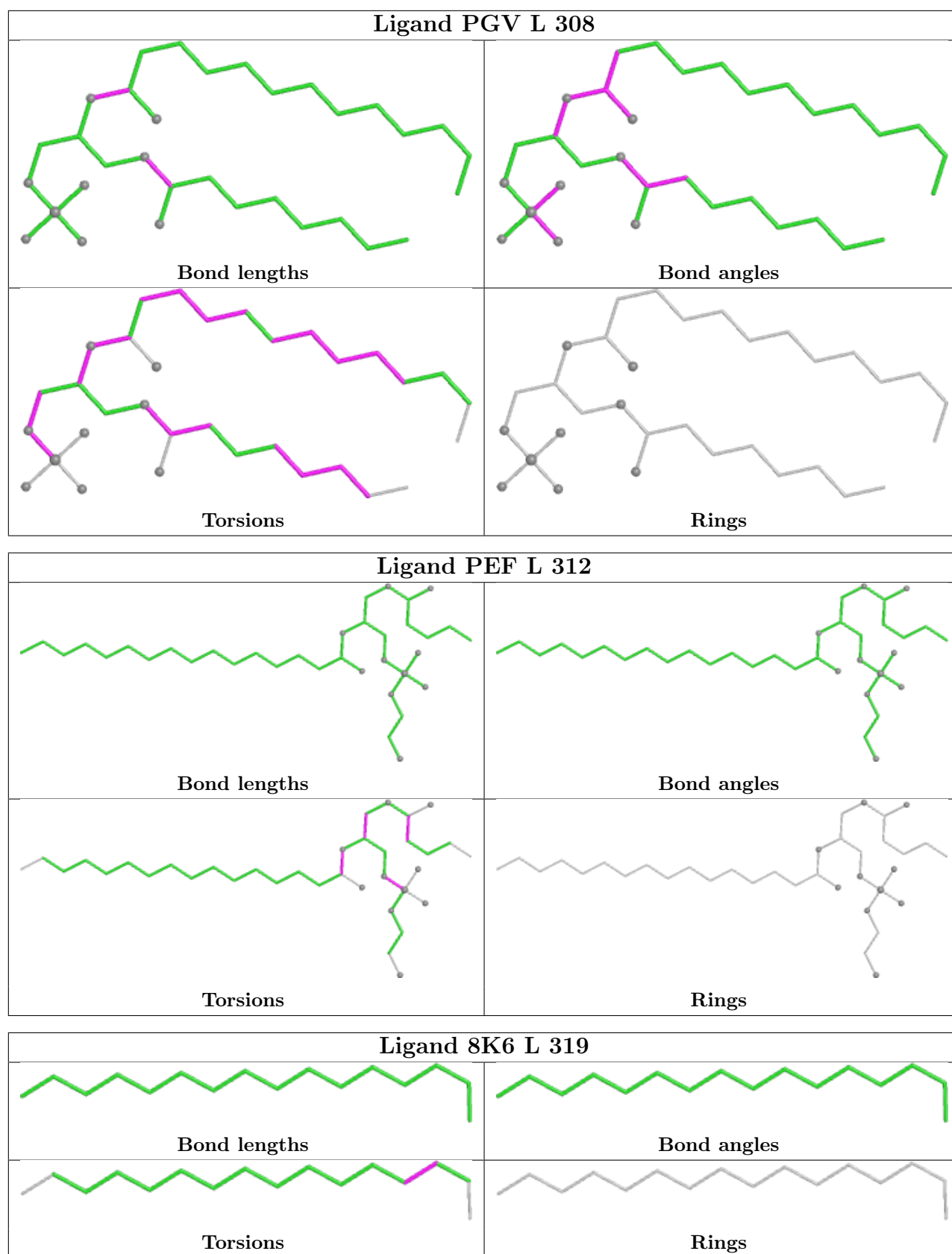


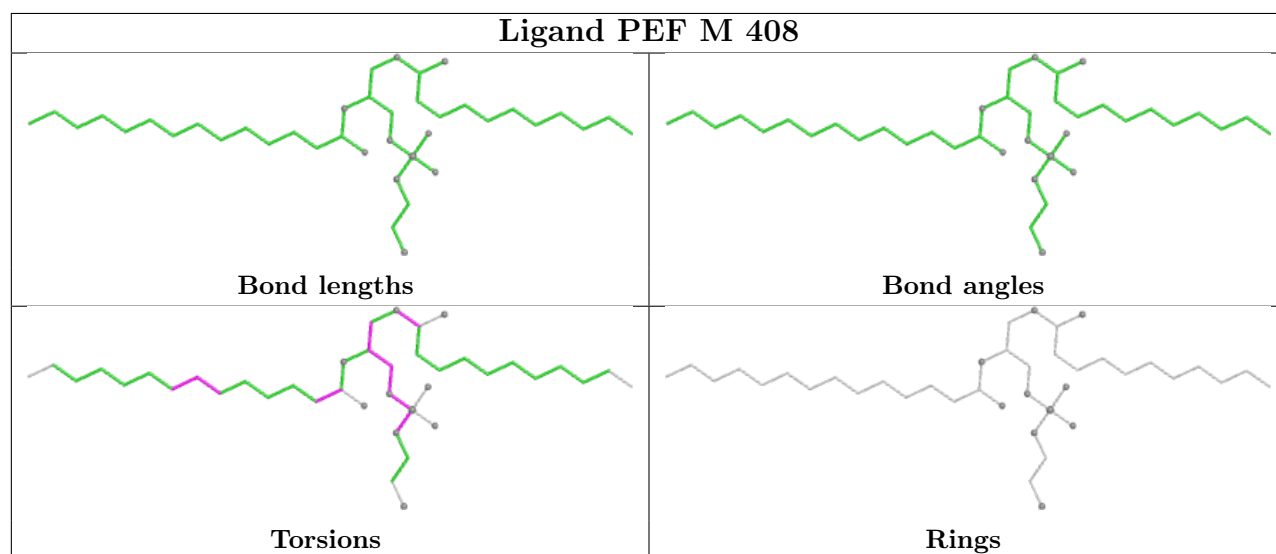
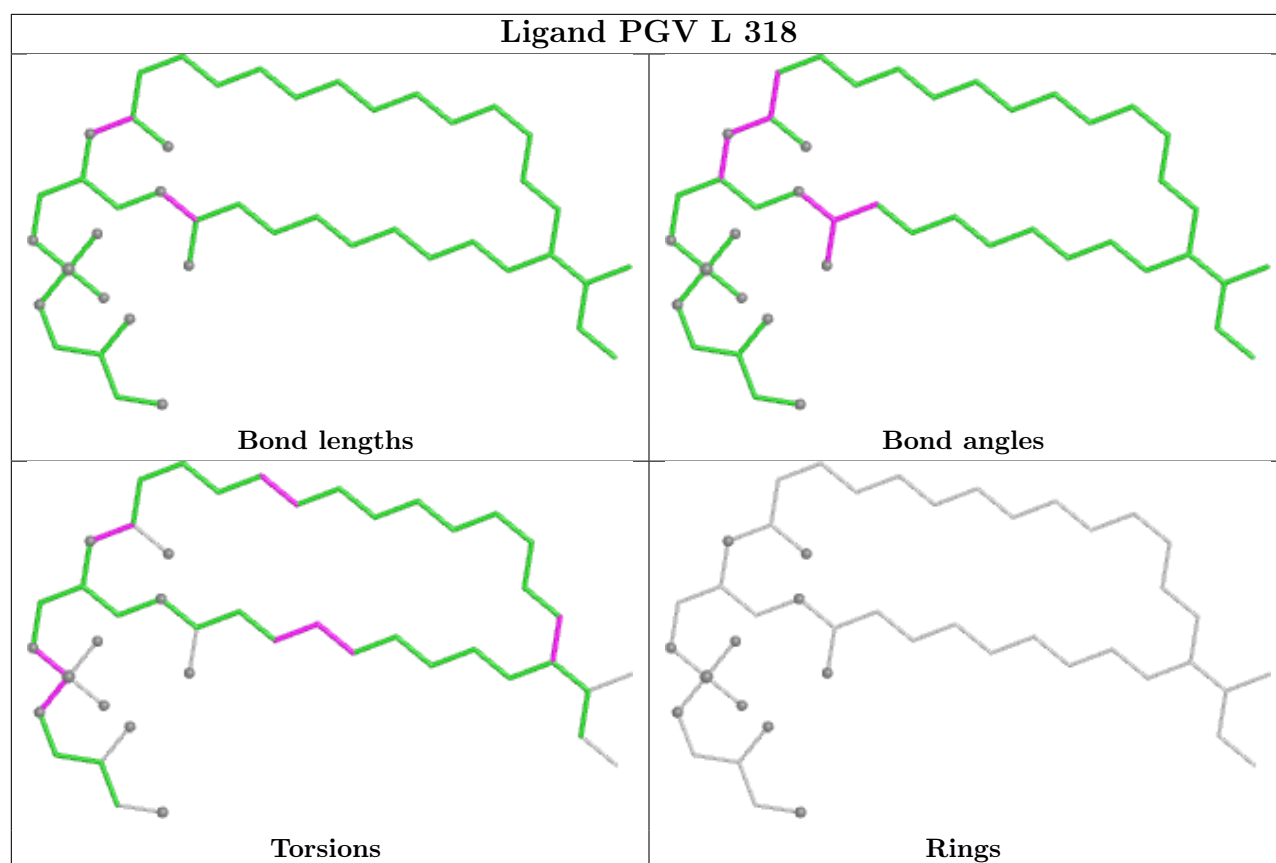
Ligand U10 L 305

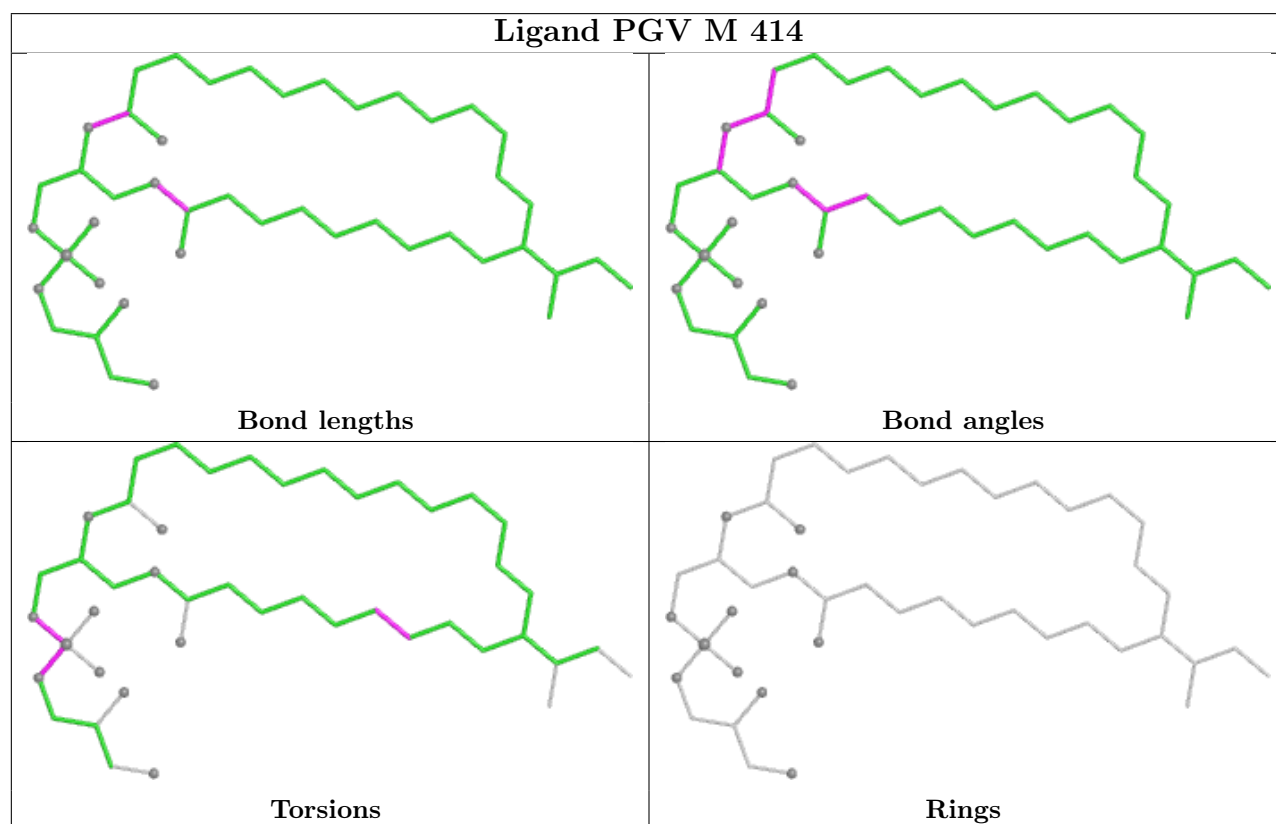
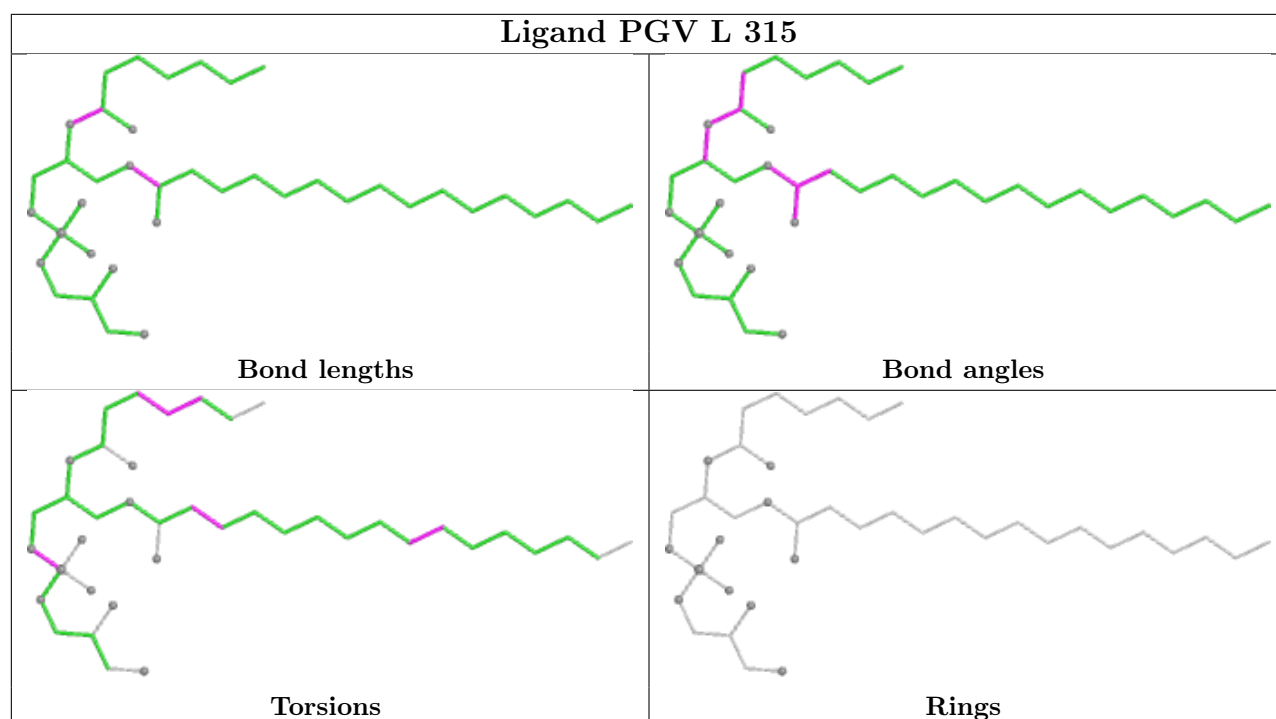


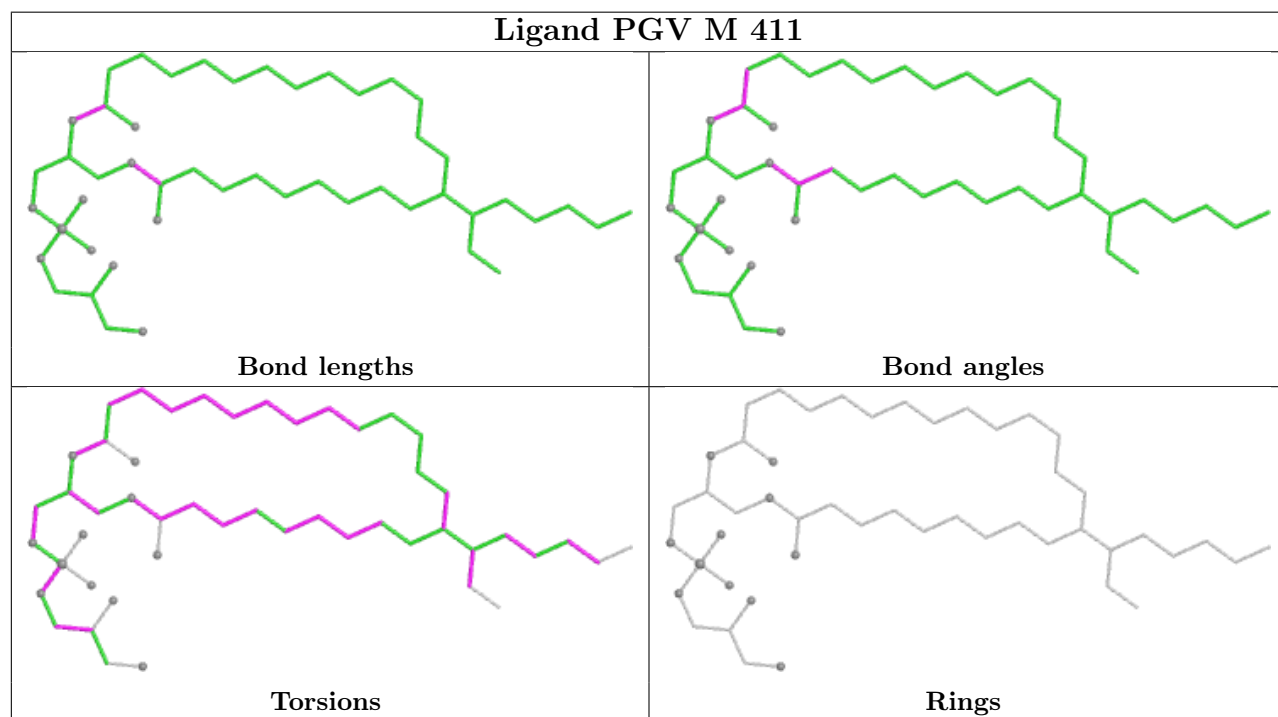
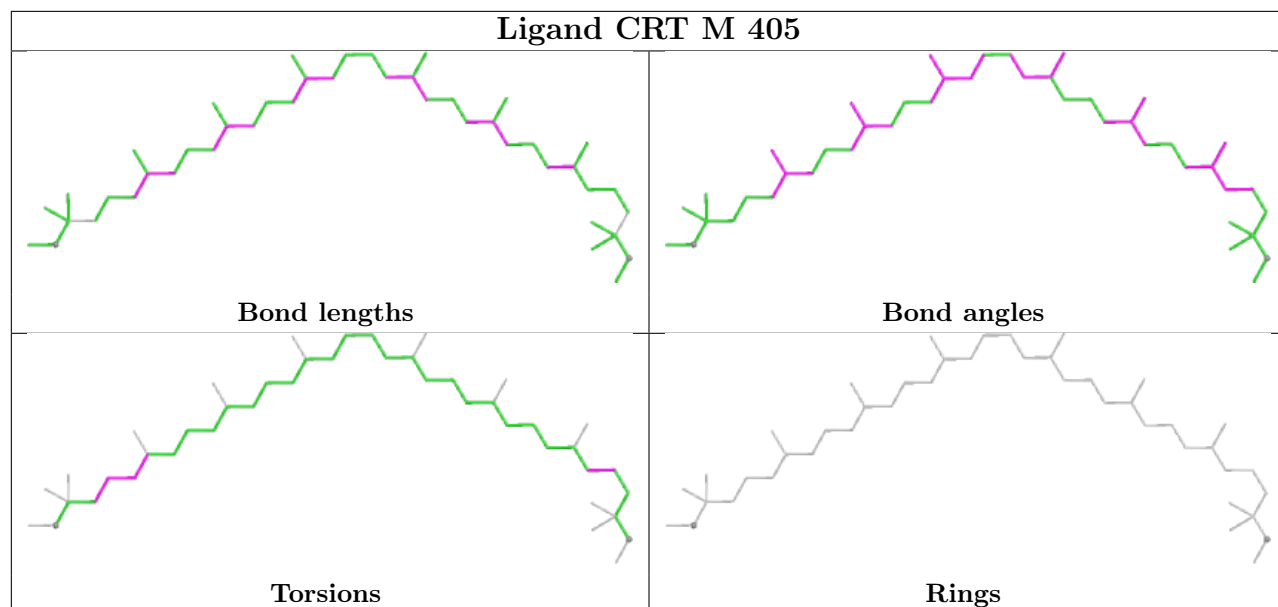


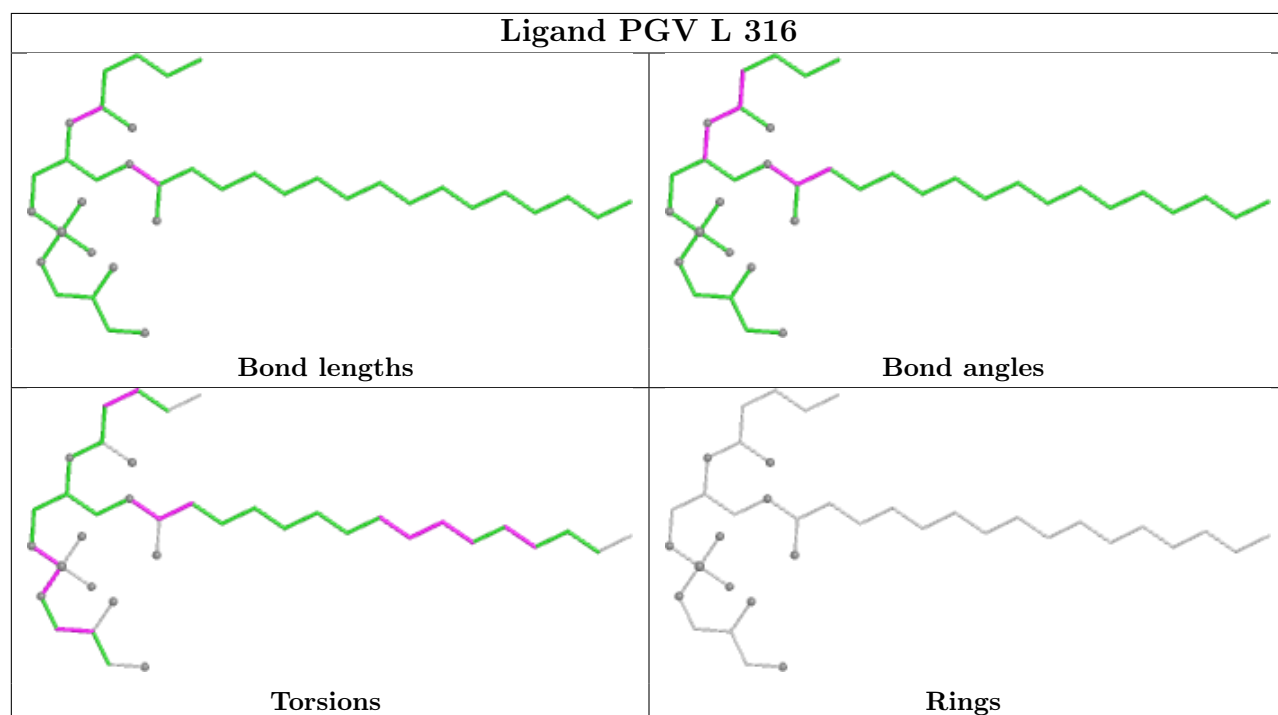
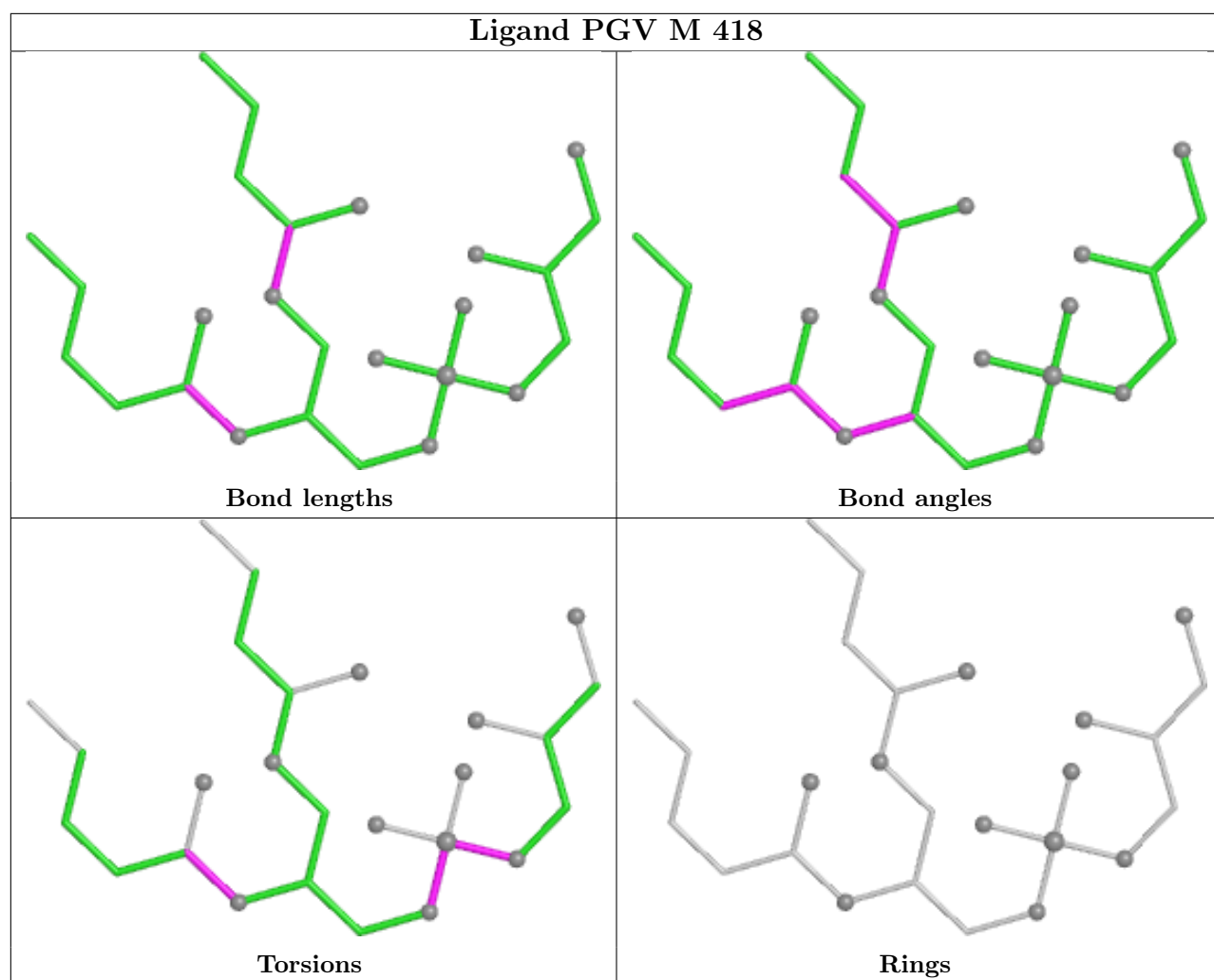


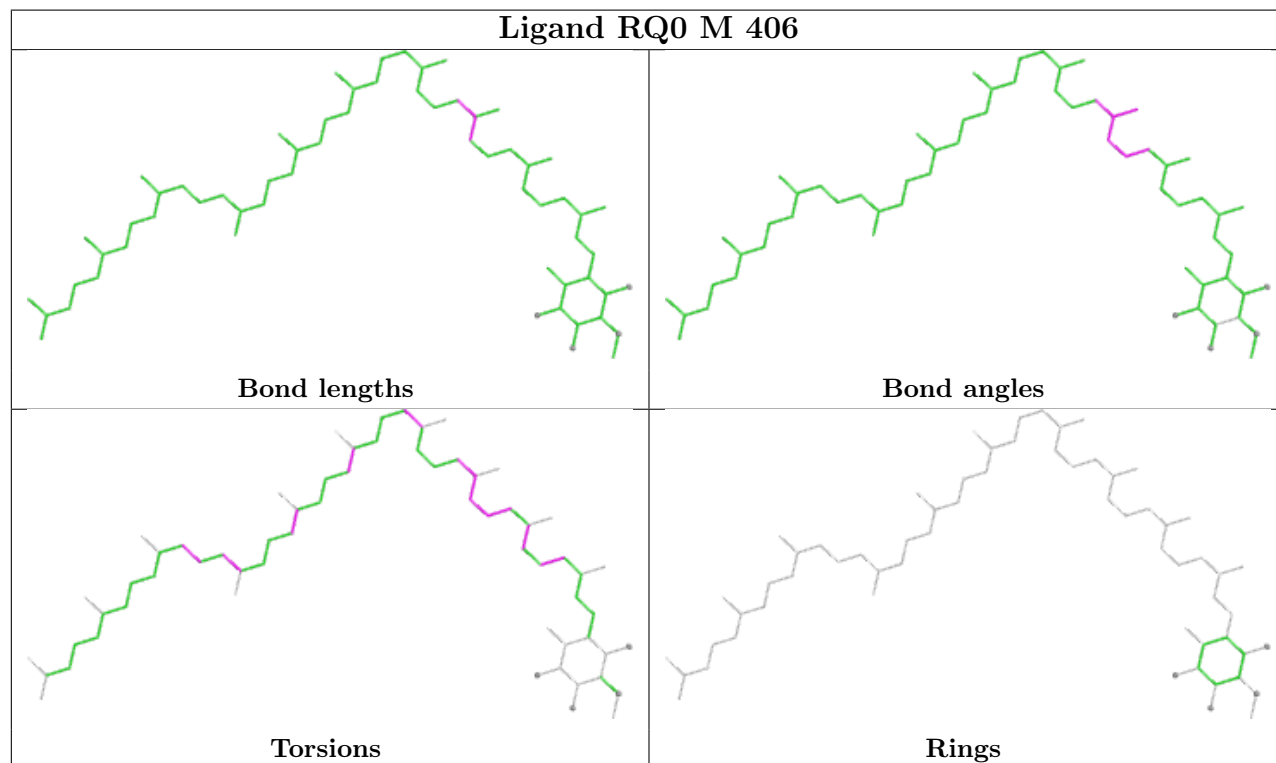
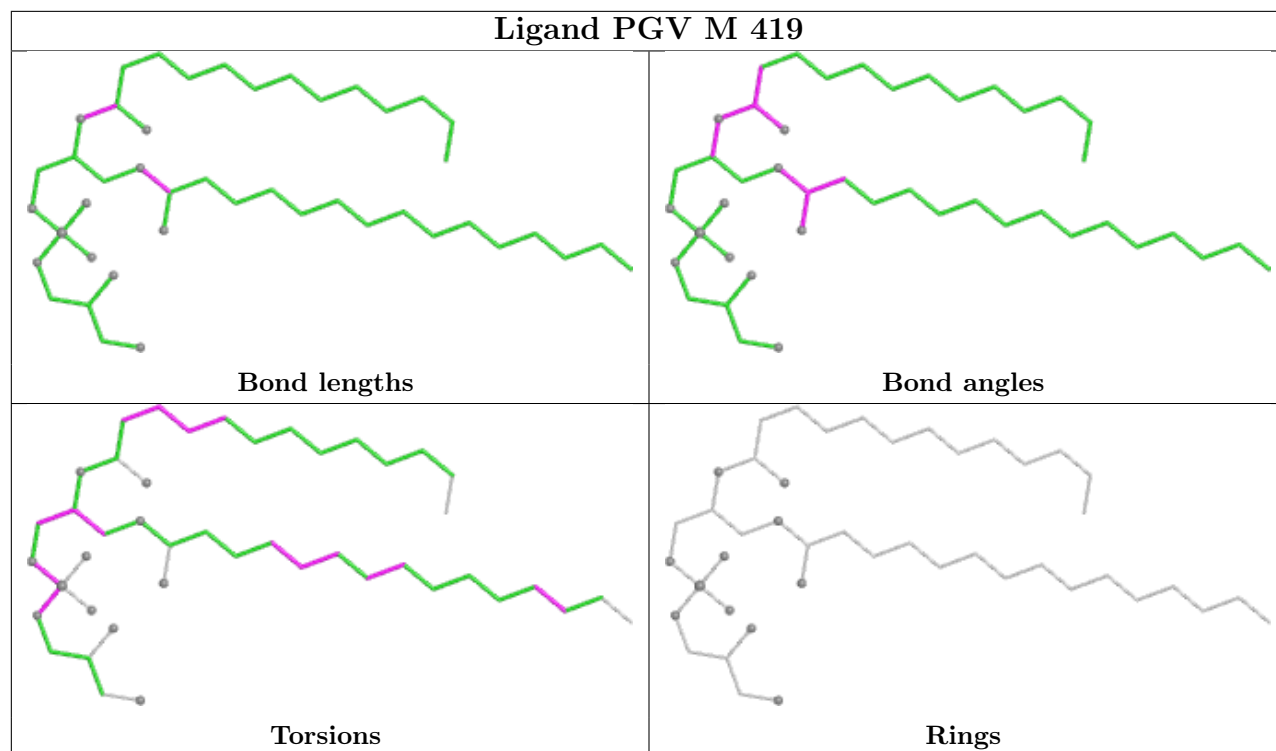


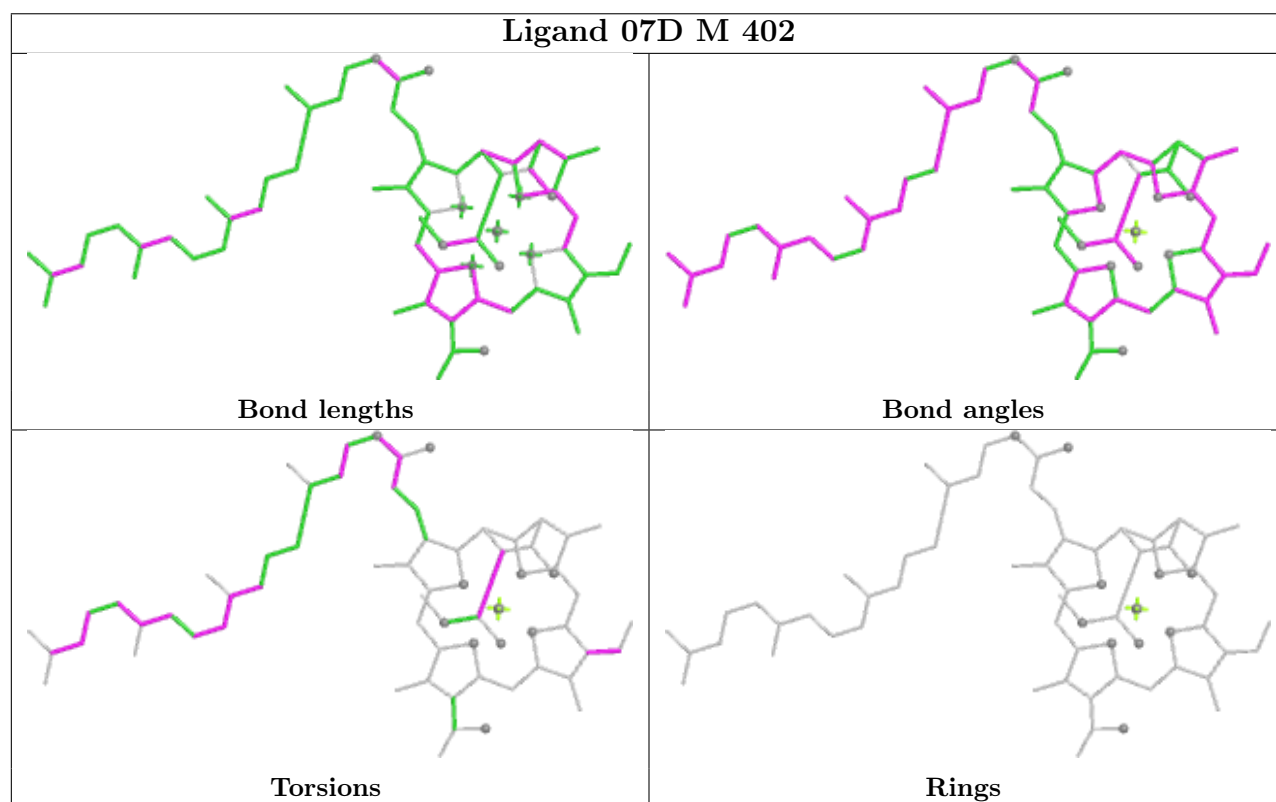
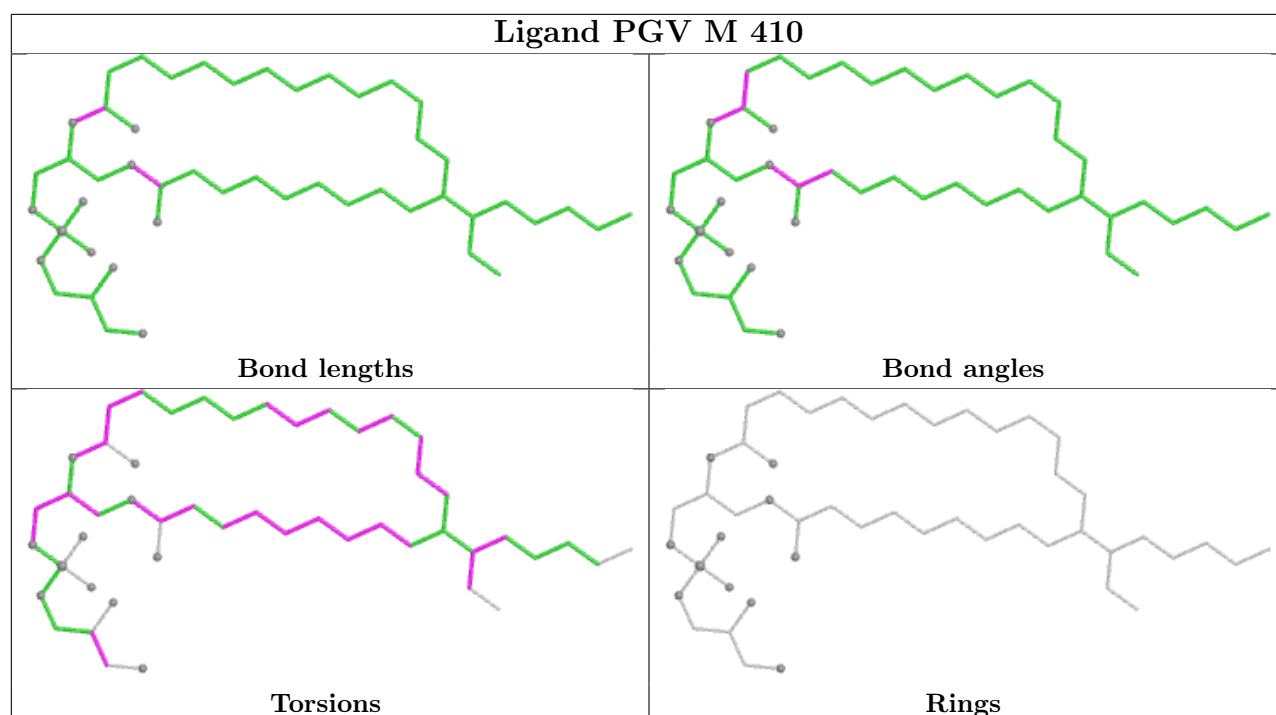


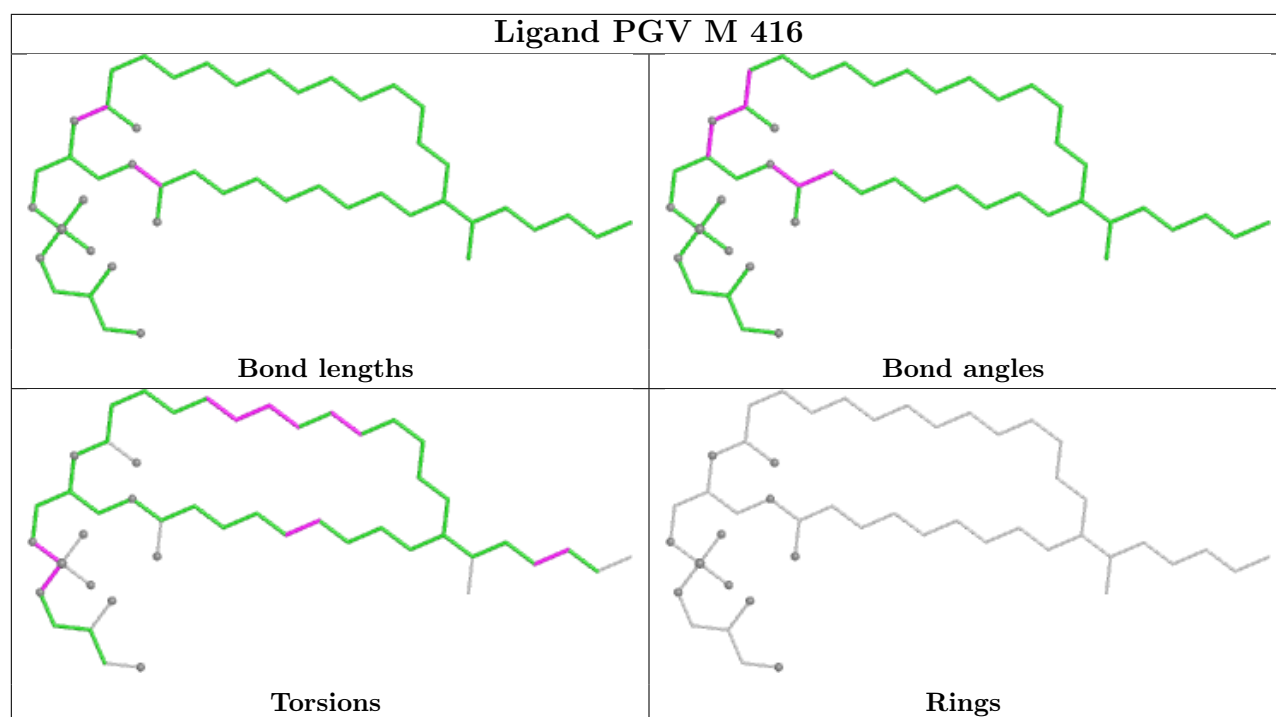












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

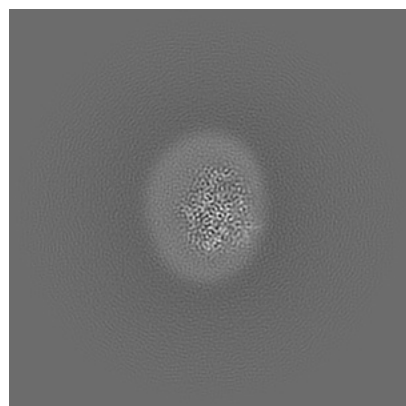
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62663. These allow visual inspection of the internal detail of the map and identification of artifacts.

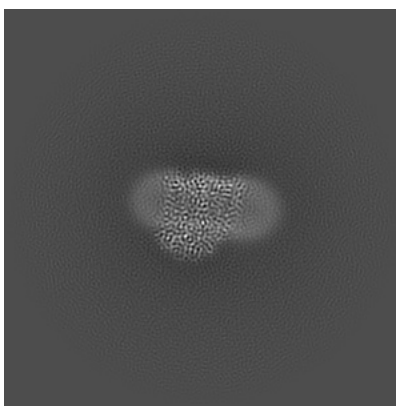
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

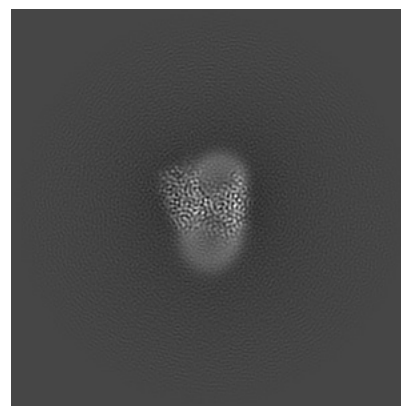
6.1.1 Primary map



X

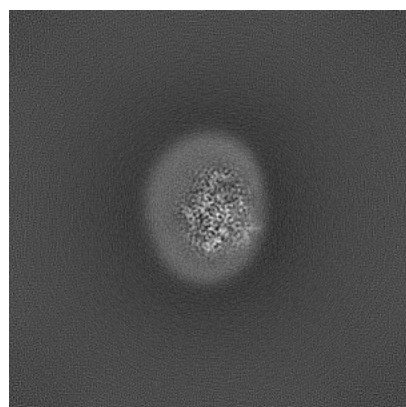


Y

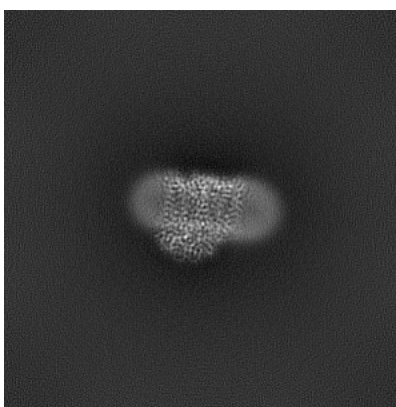


Z

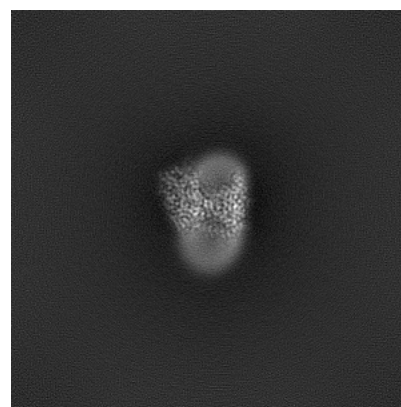
6.1.2 Raw map



X



Y

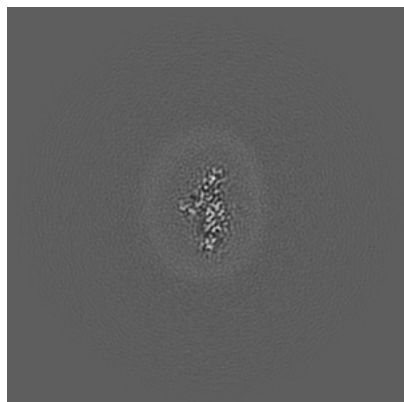


Z

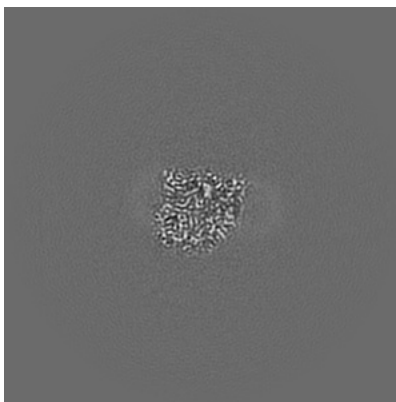
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

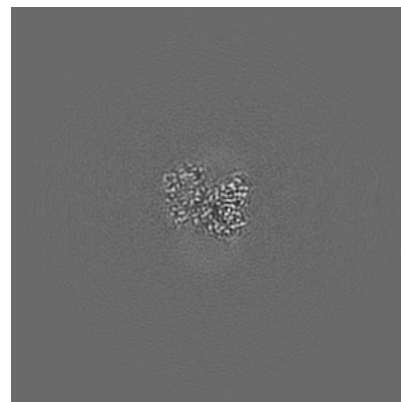
6.2.1 Primary map



X Index: 200

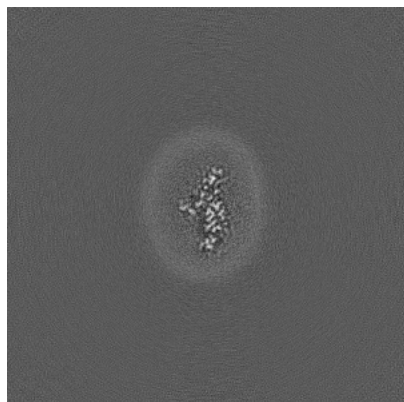


Y Index: 200

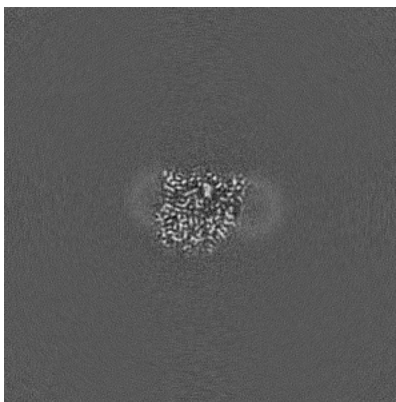


Z Index: 200

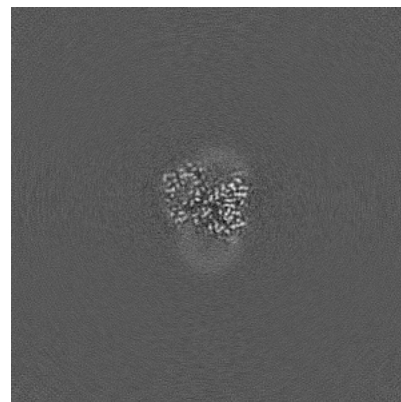
6.2.2 Raw map



X Index: 200



Y Index: 200

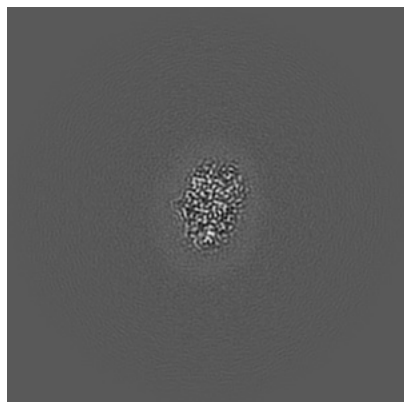


Z Index: 200

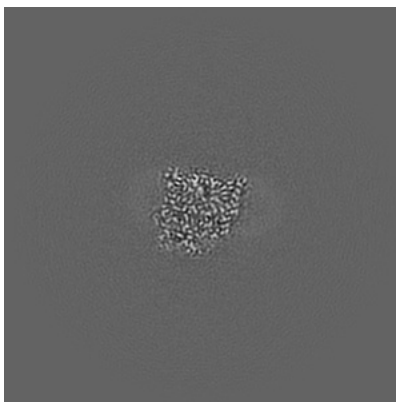
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

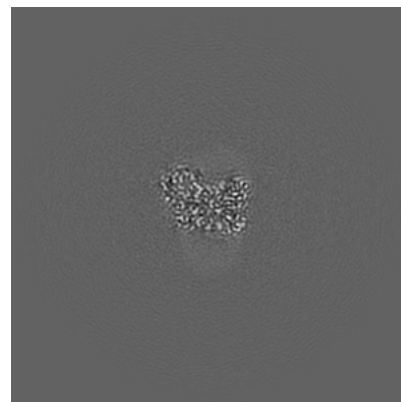
6.3.1 Primary map



X Index: 223

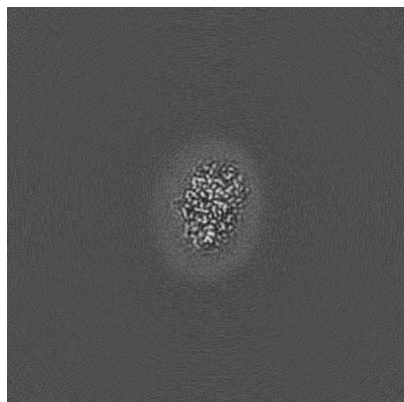


Y Index: 203

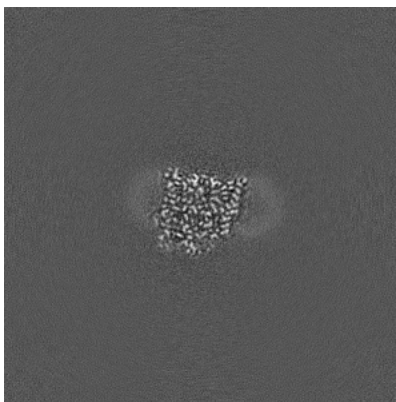


Z Index: 194

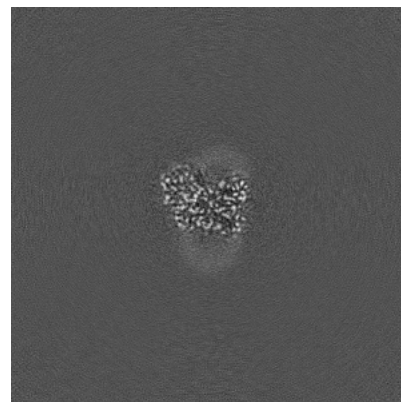
6.3.2 Raw map



X Index: 223



Y Index: 203

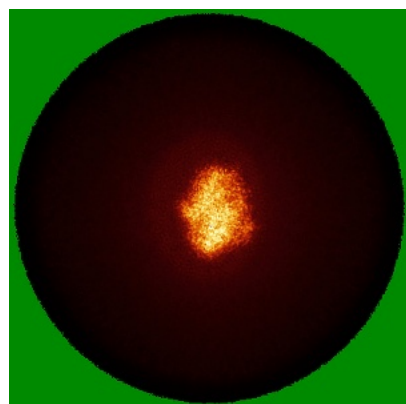


Z Index: 195

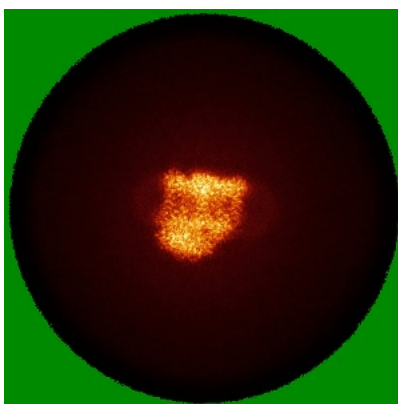
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

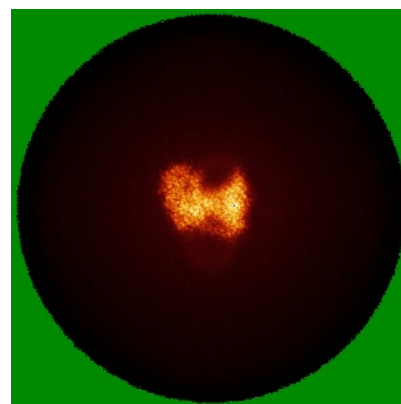
6.4.1 Primary map



X

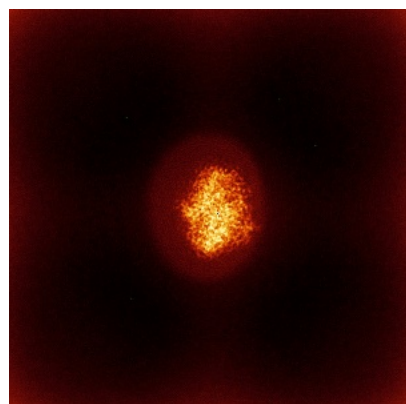


Y

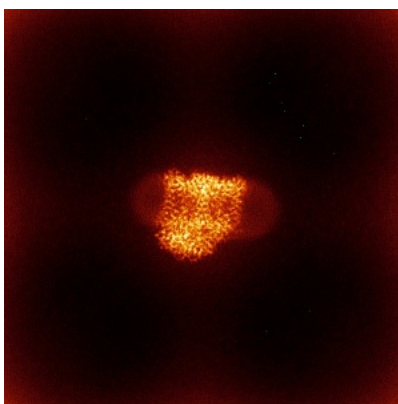


Z

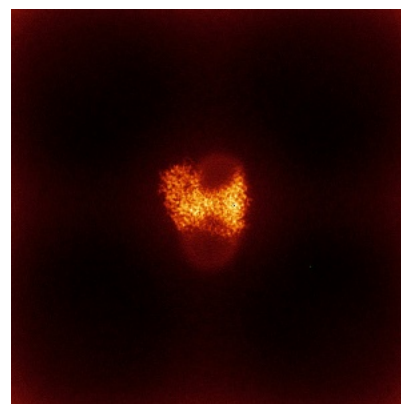
6.4.2 Raw map



X



Y

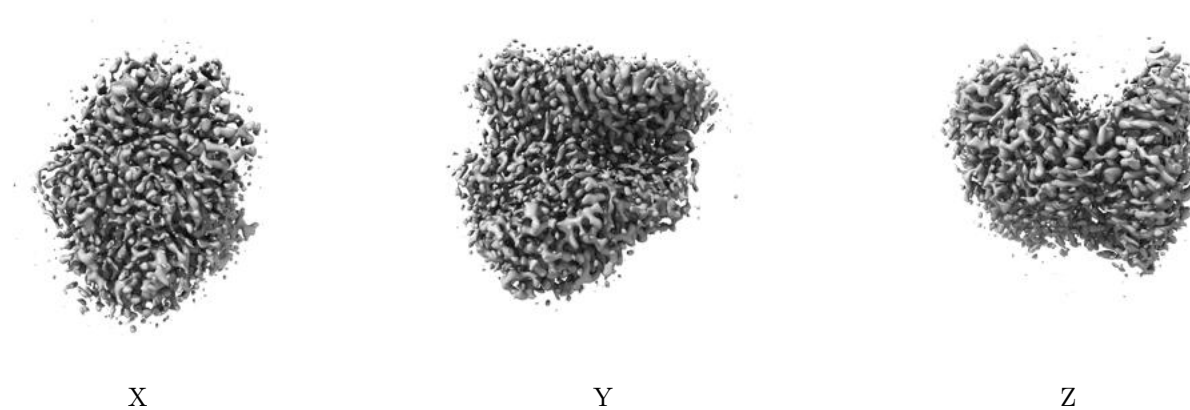


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

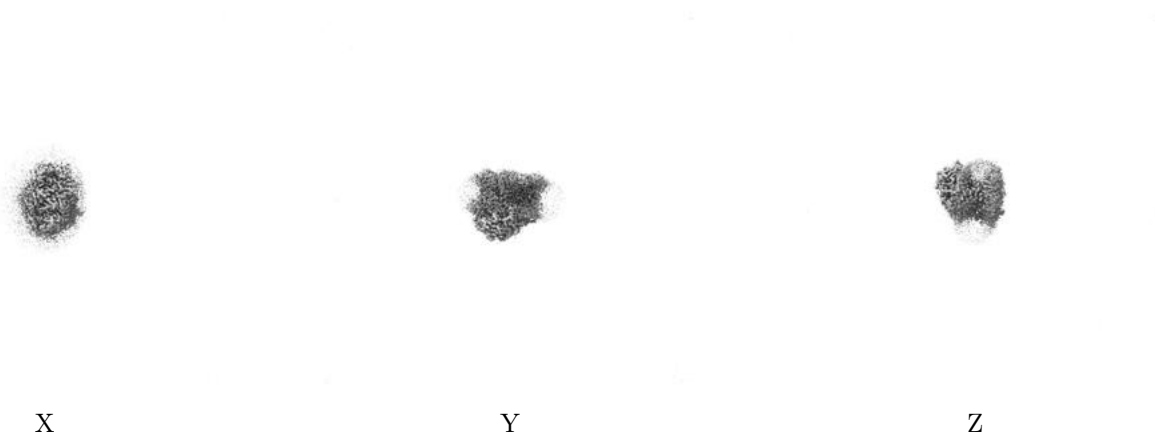
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.192. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

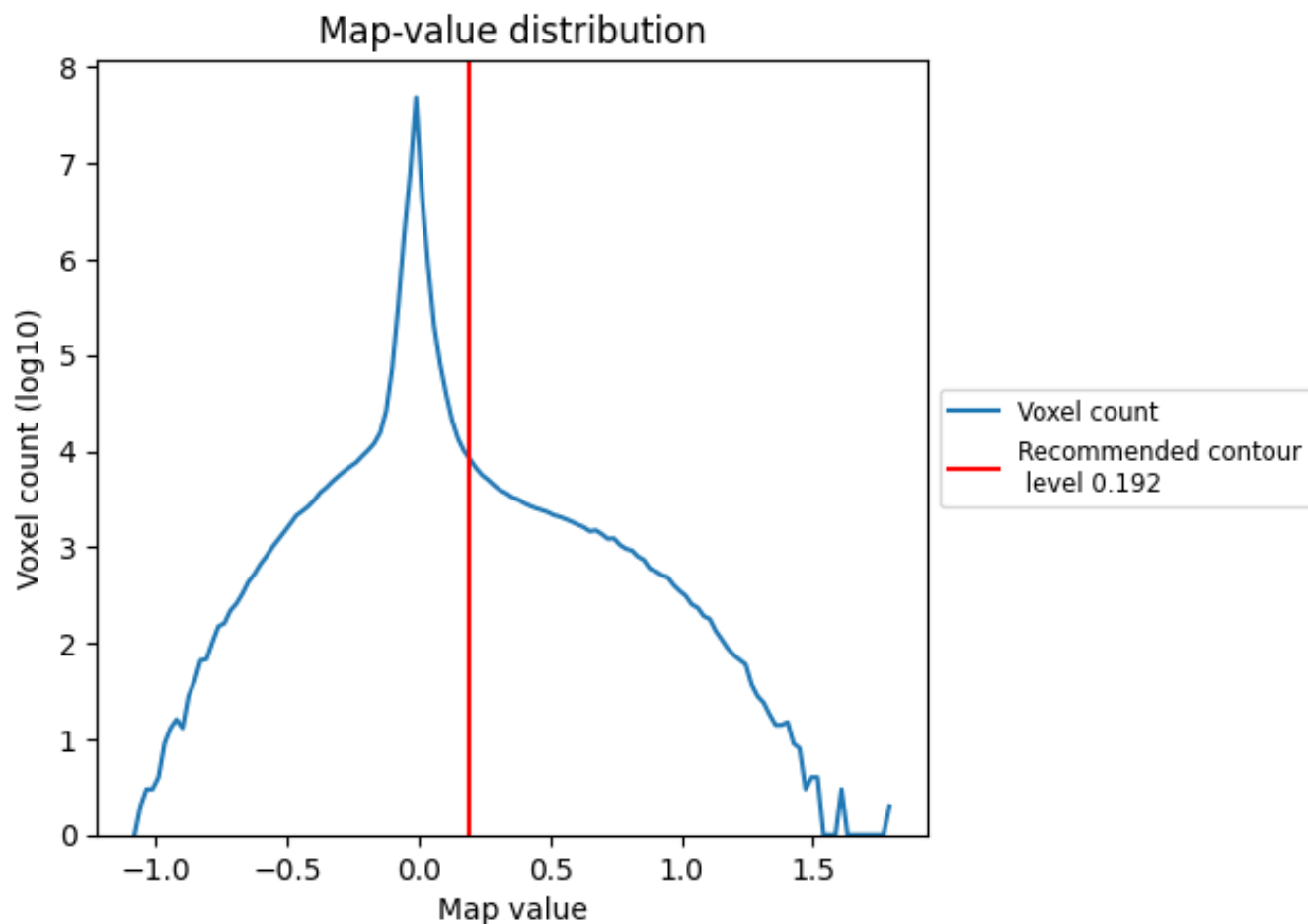
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

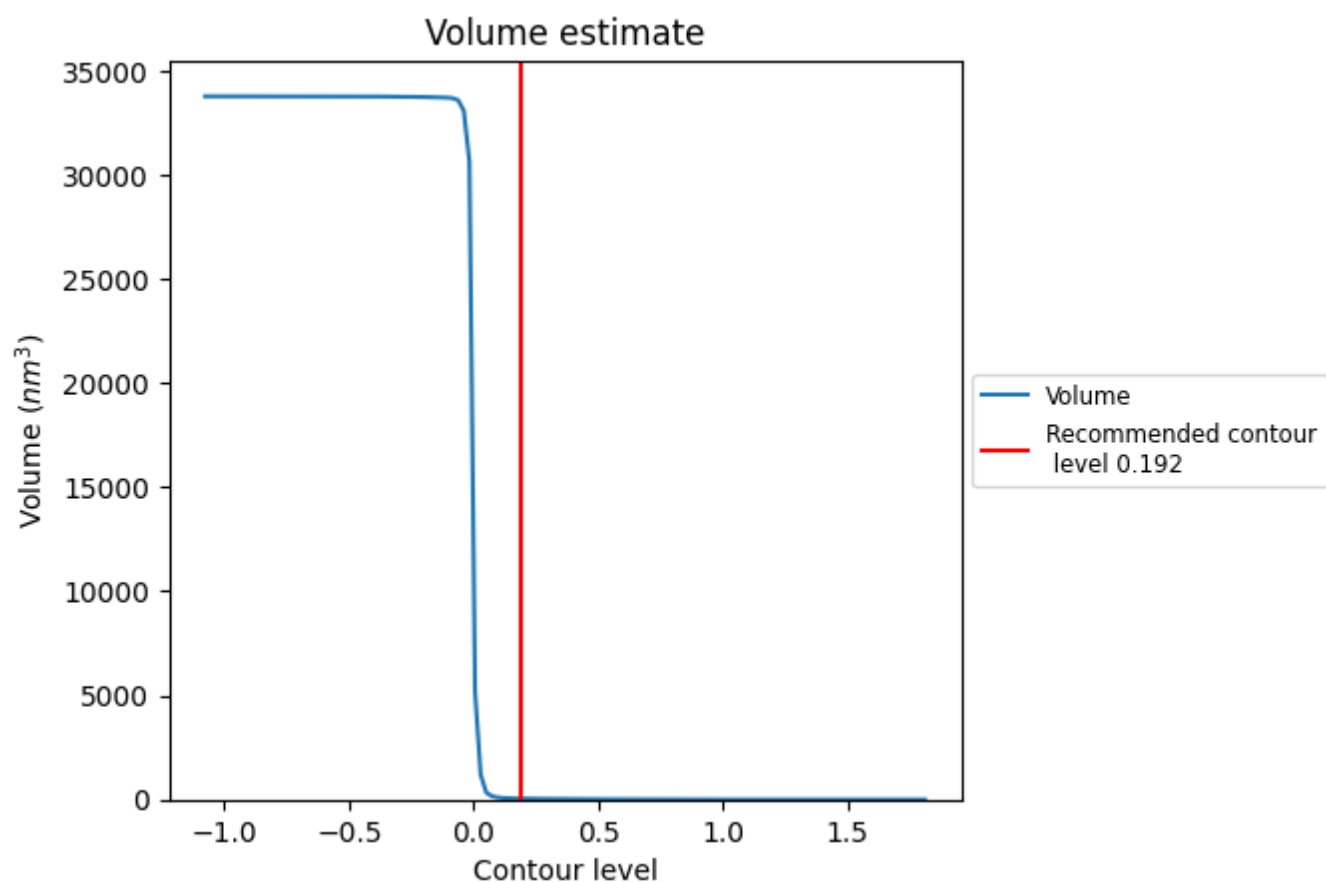
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

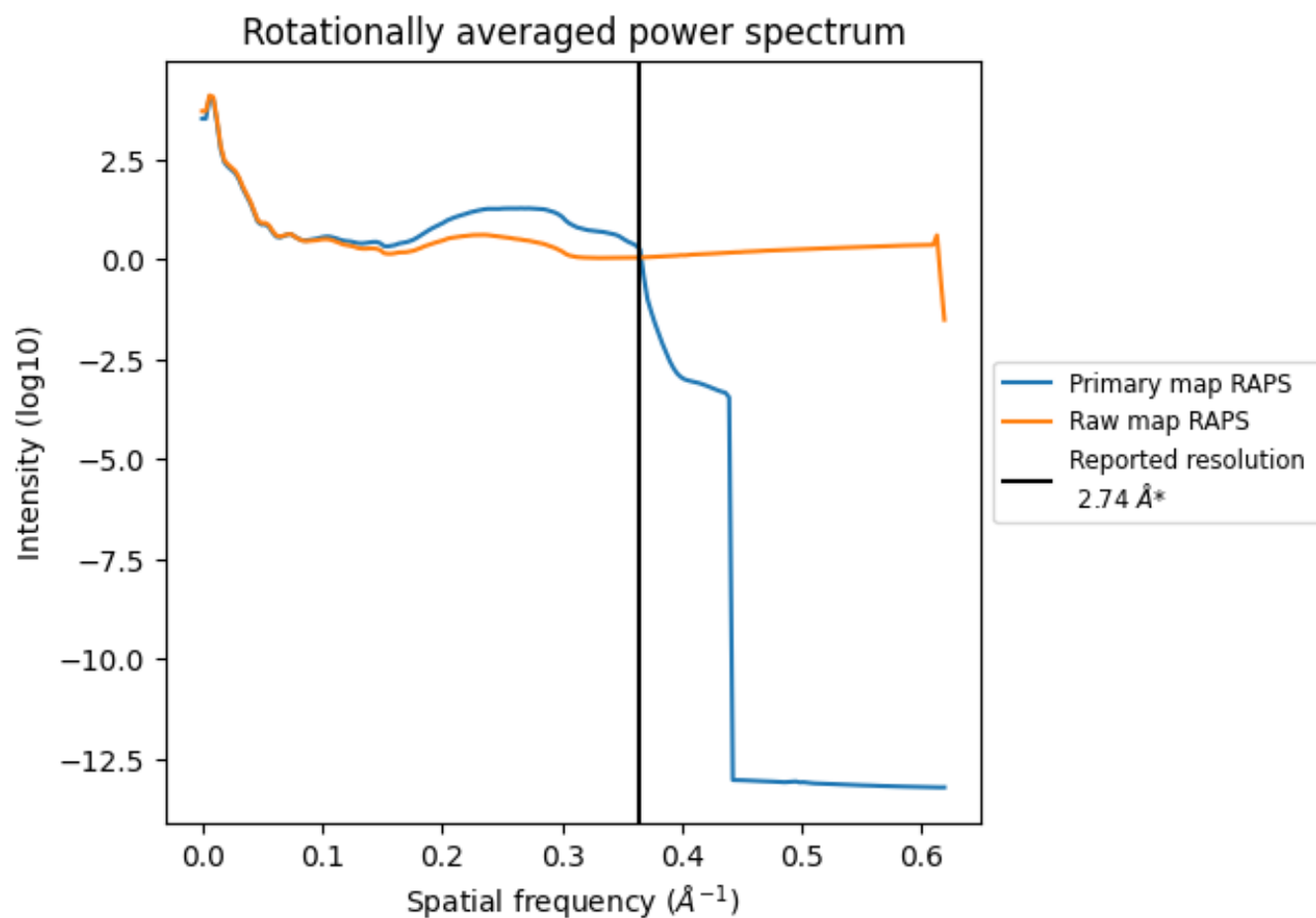
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 41 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

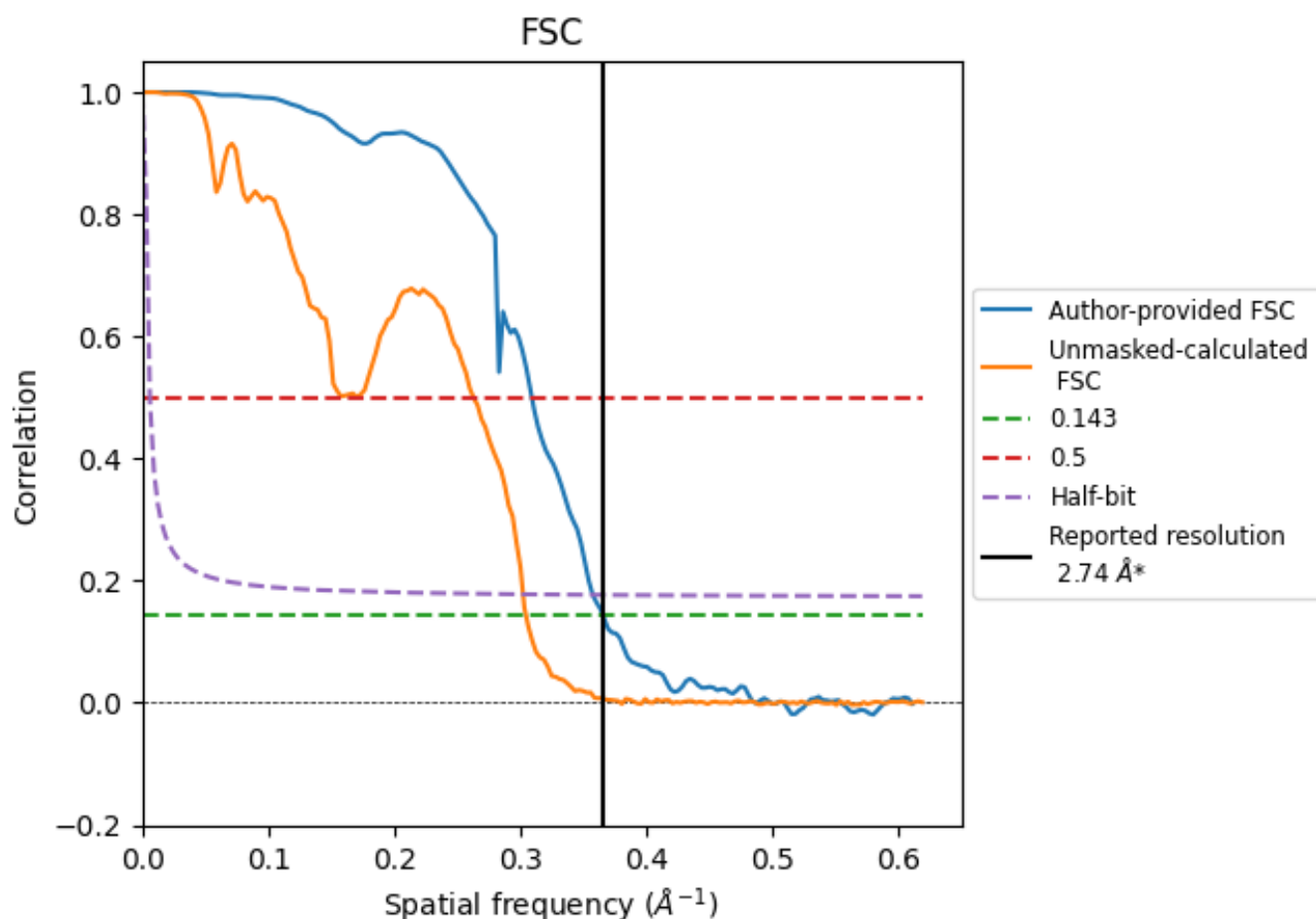


*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.365 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

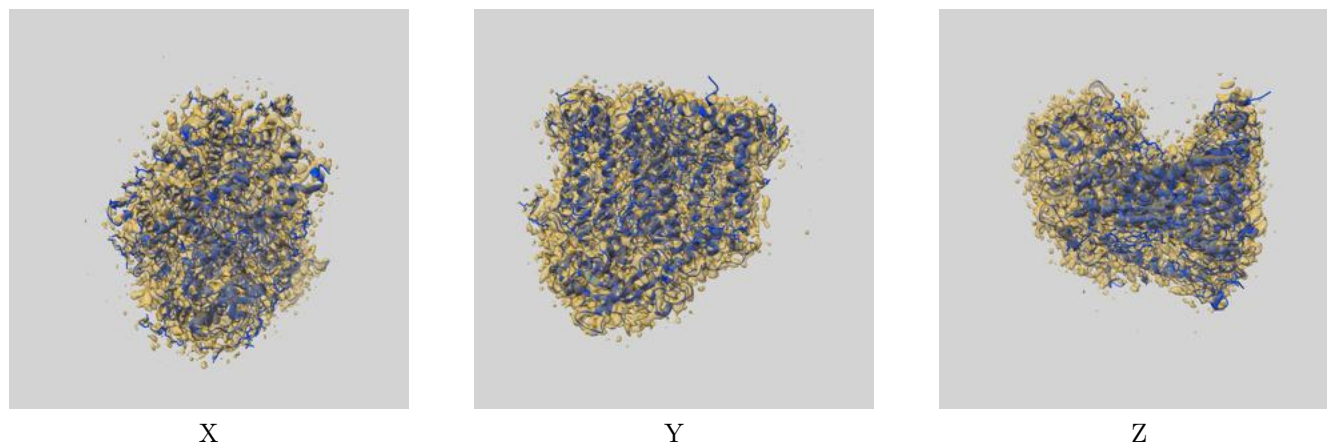
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.74	3.24	2.80
Unmasked-calculated*	3.28	3.81	3.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

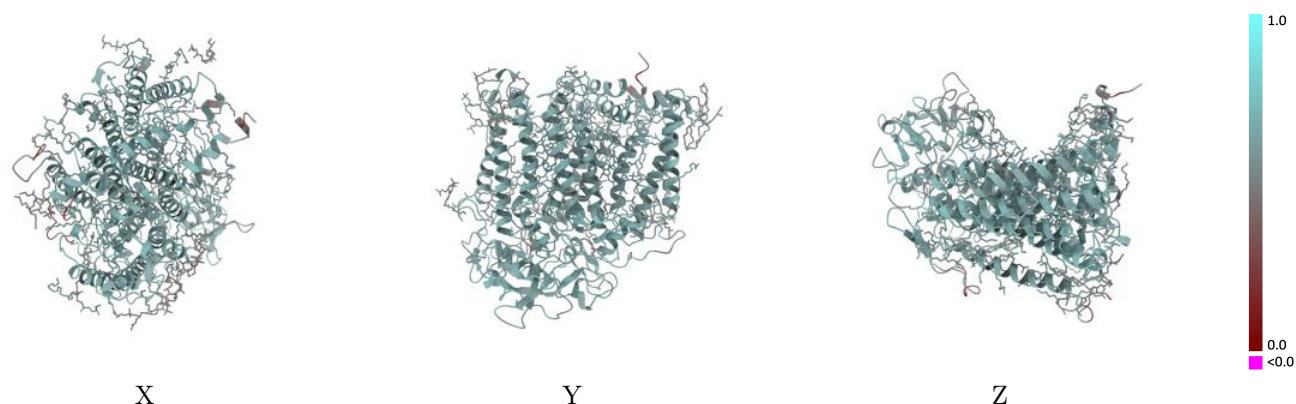
This section contains information regarding the fit between EMDB map EMD-62663 and PDB model 9KZH. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



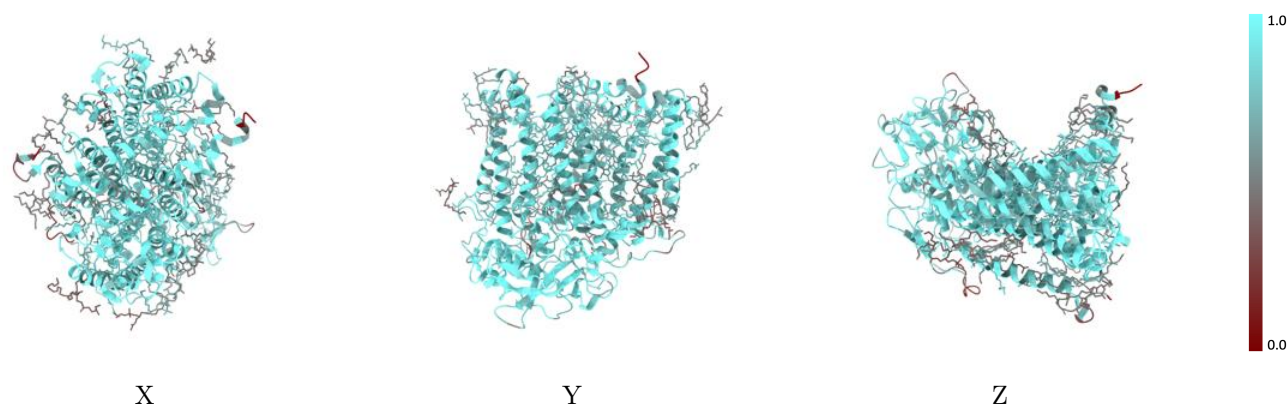
The images above show the 3D surface view of the map at the recommended contour level 0.192 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



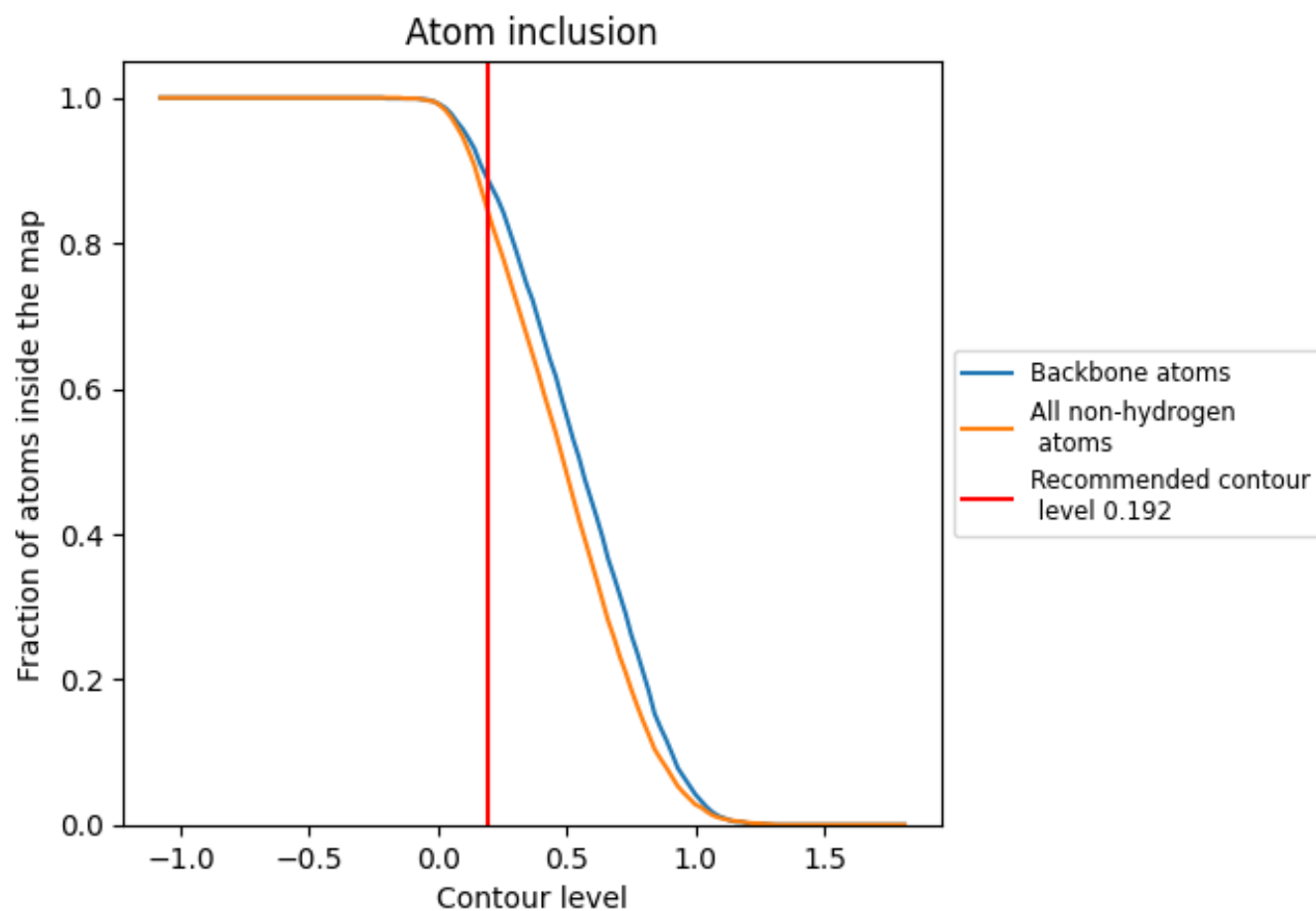
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.192).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.192) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.6040
H	0.8150	0.5870
L	0.8610	0.6080
M	0.8550	0.6110

