



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 09:16 AM EST

PDB ID : 7U24  
EMDB ID : EMD-26307  
Title : Cryo-EM structure of the pancreatic ATP-sensitive potassium channel bound to ATP and glibenclamide with Kir6.2-CTD in the up conformation  
Authors : Shyng, S.L.; Sung, M.W.; Driggers, C.M.  
Deposited on : 2022-02-23  
Resolution : 3.58 Å (reported)  
Based on initial models : 6PZ9, 6BAA

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

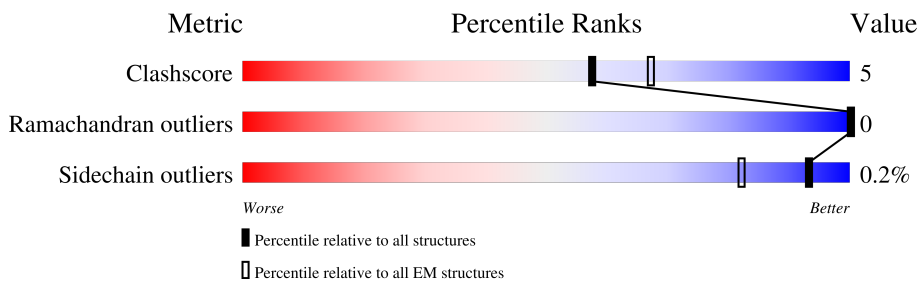
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.58 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	A	390	
1	B	390	
1	C	390	
1	D	390	
2	E	1582	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 20651 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.

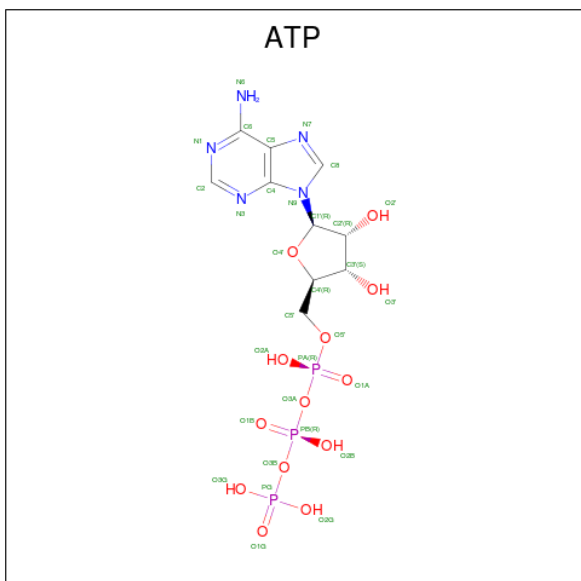
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	359	Total 2672	C 1721	N 464	O 470	S 17	0	0
1	B	328	Total 2513	C 1624	N 437	O 436	S 16	0	0
1	C	328	Total 2537	C 1636	N 441	O 443	S 17	0	0
1	D	328	Total 2508	C 1622	N 437	O 432	S 17	0	0

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

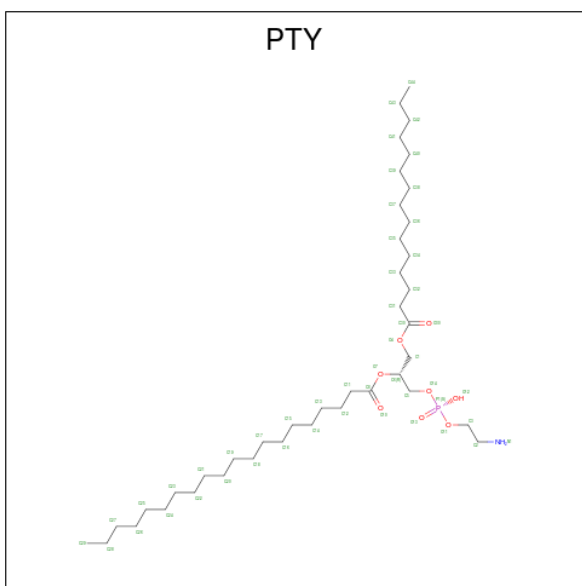
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	1427	Total 9429	C 6080	N 1678	O 1638	S 33	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



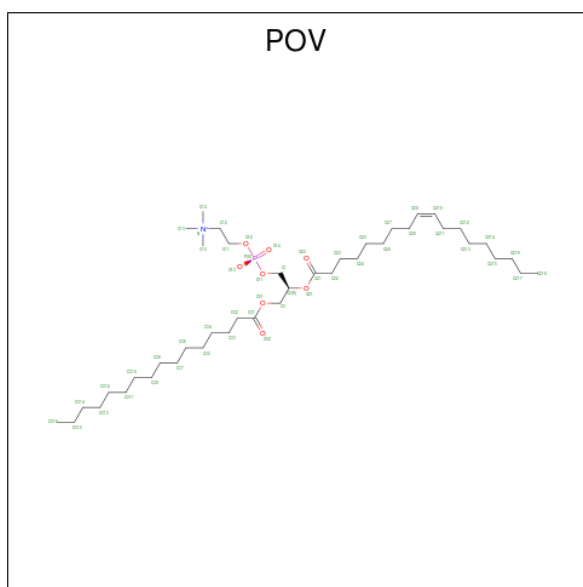
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



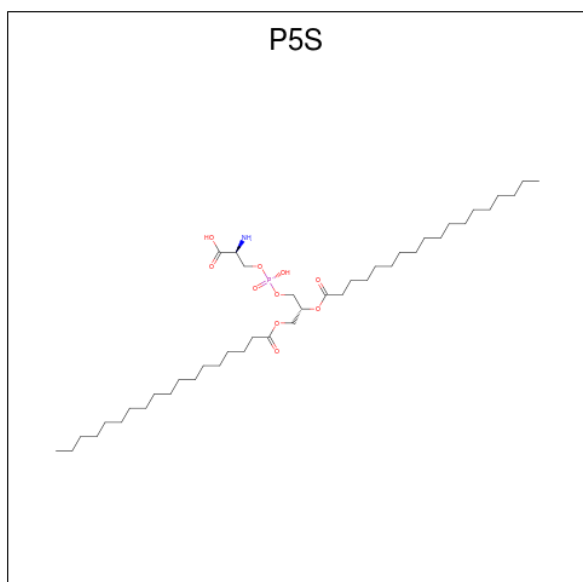
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	Total 32	C 22	N 1	O 8	P 1	0
4	E	1	Total 128	C 88	N 4	O 32	P 4	0
4	E	1	Total 128	C 88	N 4	O 32	P 4	0
4	E	1	Total 128	C 88	N 4	O 32	P 4	0
4	E	1	Total 128	C 88	N 4	O 32	P 4	0

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula:  $C_{42}H_{82}NO_8P$ ).



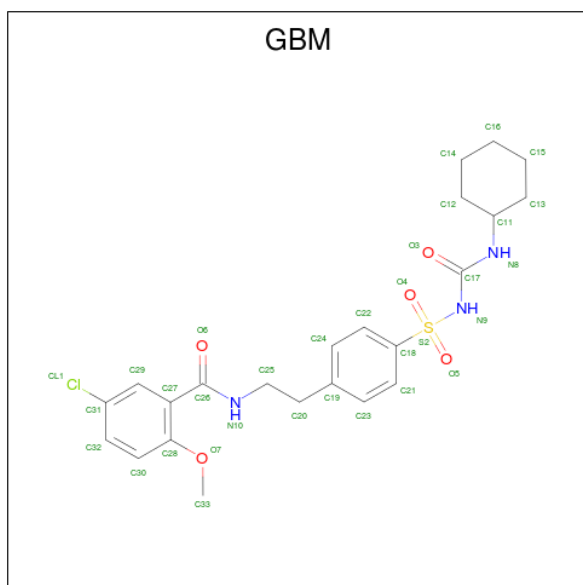
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	Total 36	C 26	N 1	O 8	P 1	0
5	B	1	Total 36	C 26	N 1	O 8	P 1	0
5	C	1	Total 36	C 26	N 1	O 8	P 1	0
5	D	1	Total 36	C 26	N 1	O 8	P 1	0

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	Total	C	N	O	P	0
			108	84	2	20	2	
6	A	1	Total	C	N	O	P	0
			108	84	2	20	2	
6	B	1	Total	C	N	O	P	0
			108	84	2	20	2	
6	B	1	Total	C	N	O	P	0
			108	84	2	20	2	
6	C	1	Total	C	N	O	P	0
			54	42	1	10	1	
6	D	1	Total	C	N	O	P	0
			162	126	3	30	3	
6	D	1	Total	C	N	O	P	0
			162	126	3	30	3	
6	D	1	Total	C	N	O	P	0
			162	126	3	30	3	
6	E	1	Total	C	N	O	P	0
			54	42	1	10	1	

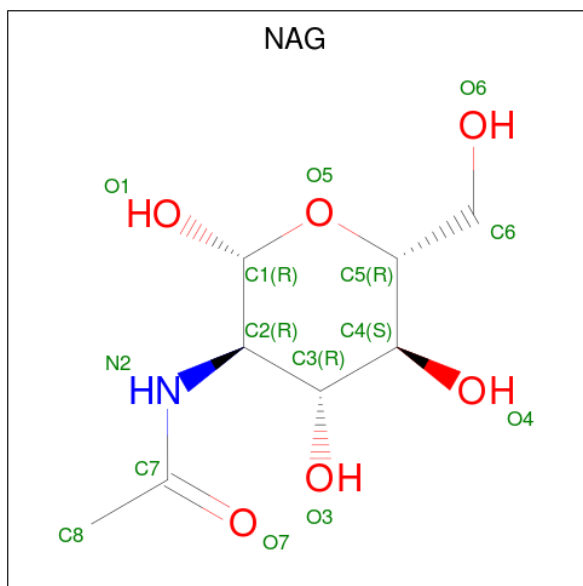
- Molecule 7 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxybenzamide (three-letter code: GBM) (formula: C<sub>23</sub>H<sub>28</sub>ClN<sub>3</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	Cl	N	O		S
7	E	1	Total	C	Cl	N	O	S	0
			33	23	1	3	5	1	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

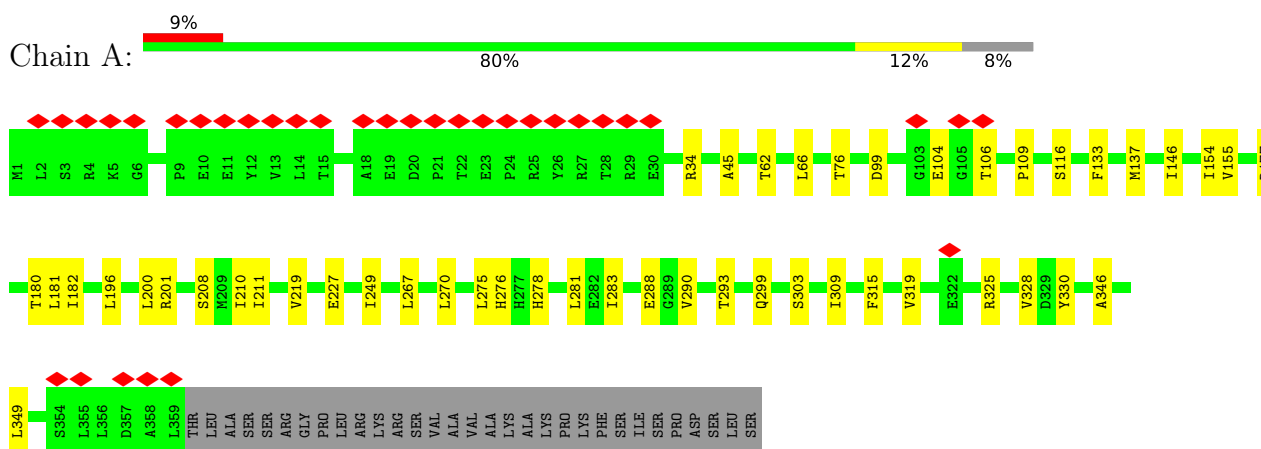


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
8	E	1	14	8	1	5	0

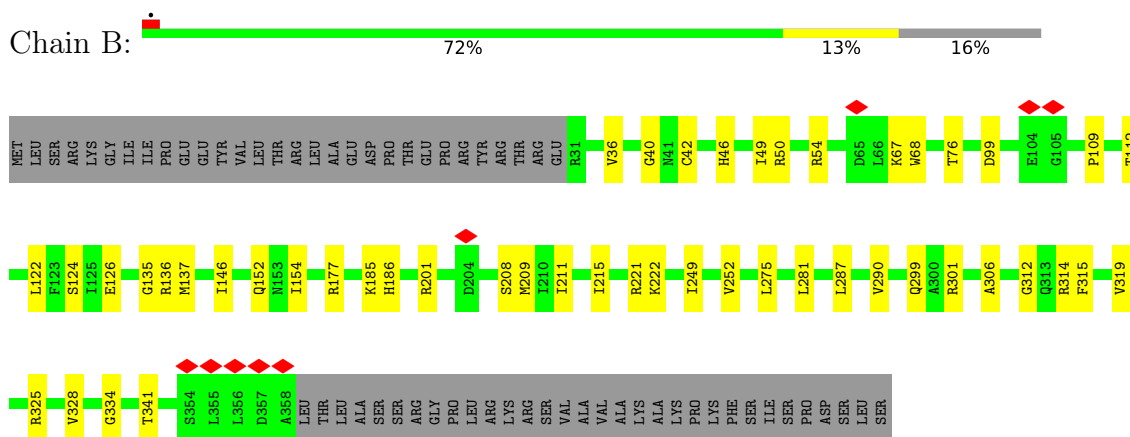
### 3 Residue-property plots [i](#)

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 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.

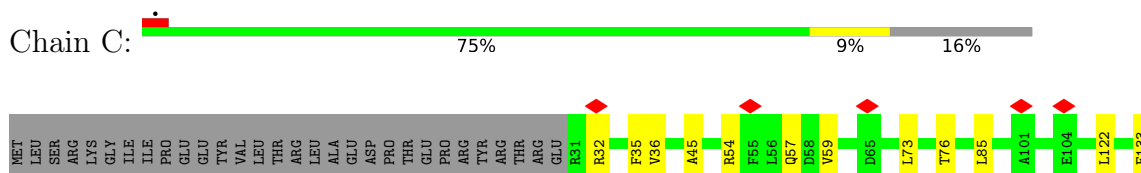
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



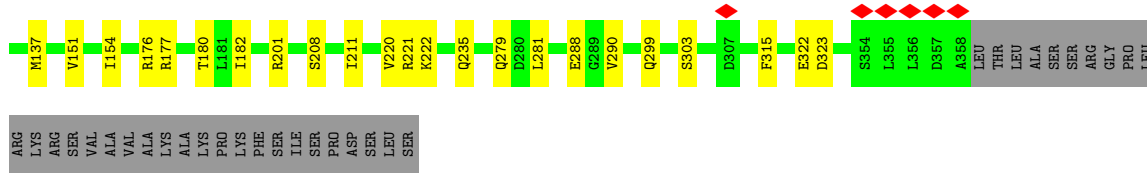
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



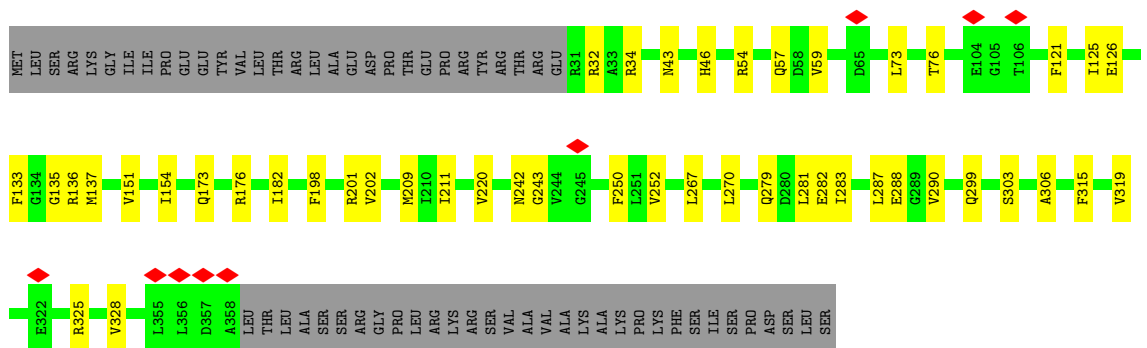
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



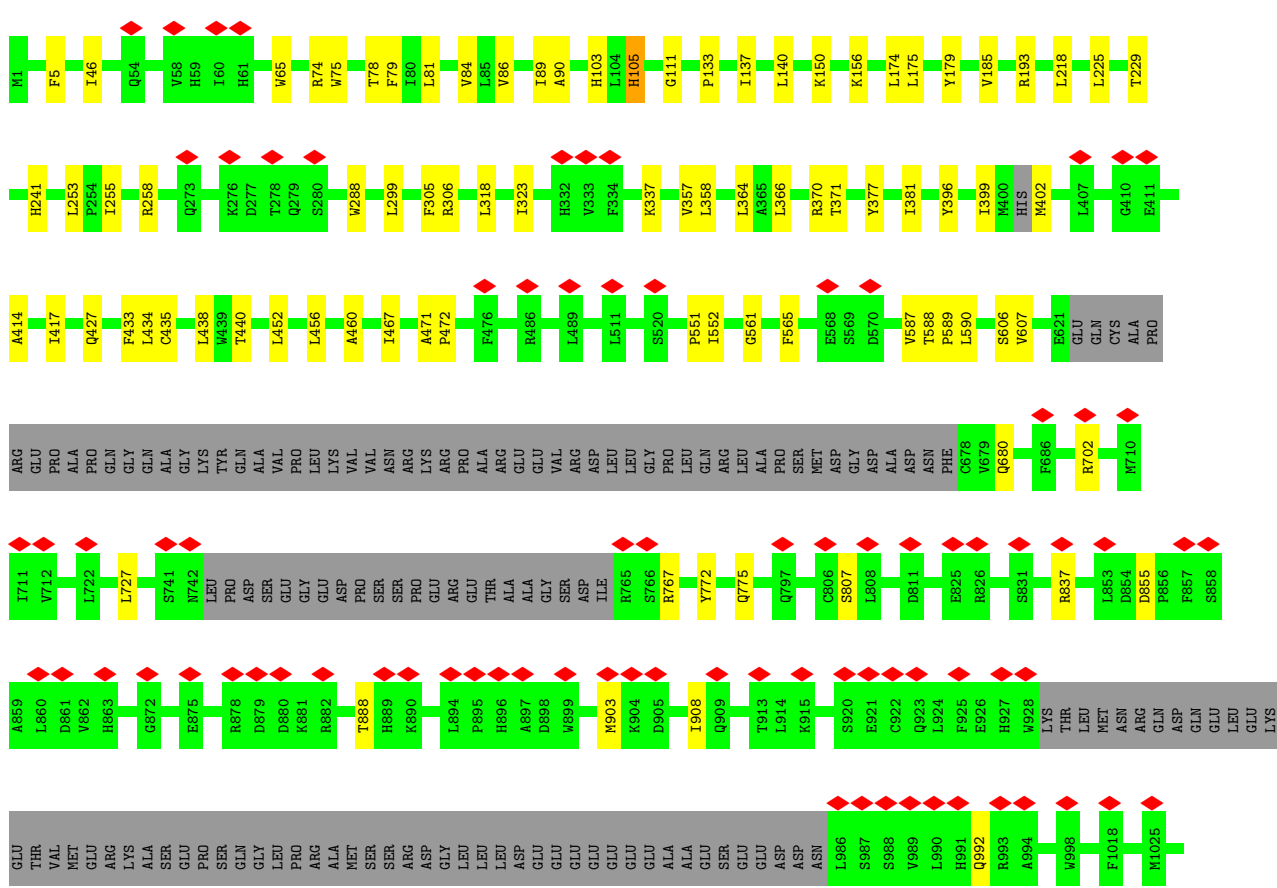
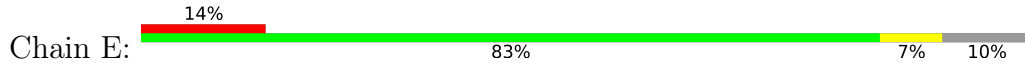


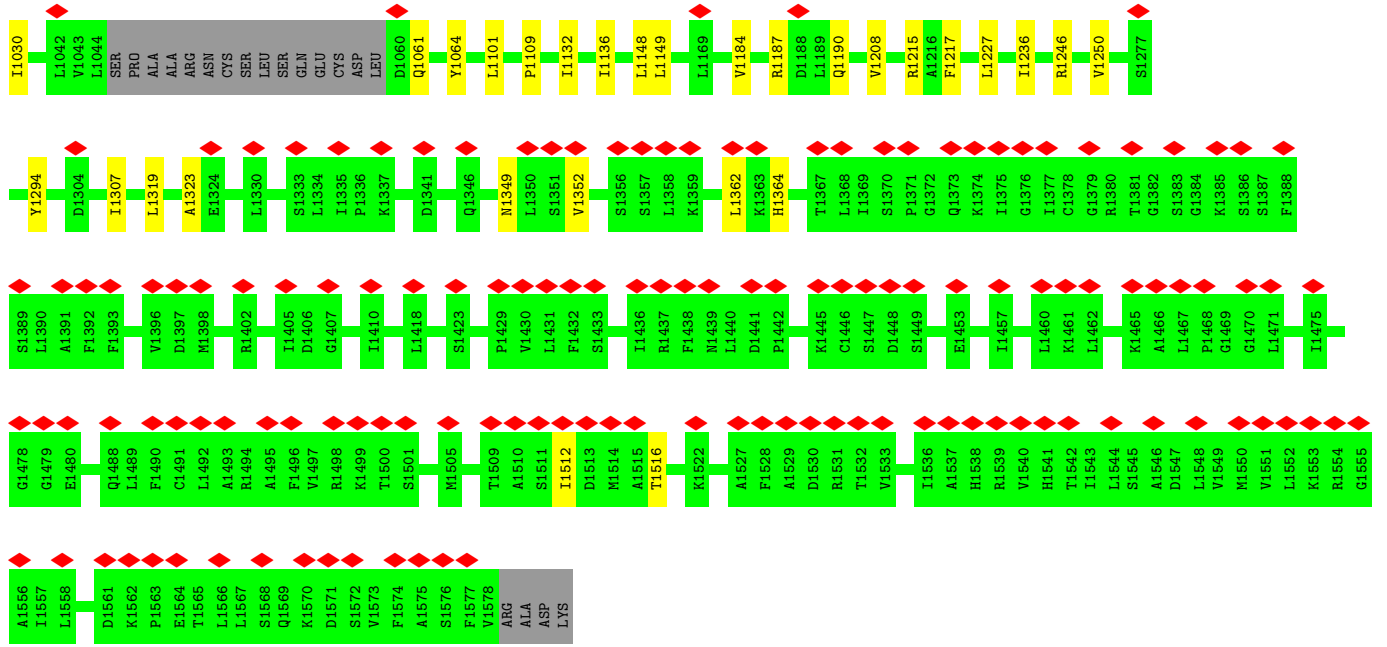


• Molecule 1: ATP-sensitive inward rectifier potassium channel 11



• Molecule 2: ATP-binding cassette sub-family C member 8





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.285	Depositor
Minimum map value	-10.068	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.0	Depositor
Map size ( $\text{\AA}$ )	180.47101, 121.713005, 151.09201	wwPDB
Map dimensions	108, 87, 129	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.399, 1.399, 1.399	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: GBM, P5S, PTY, POV, NAG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/2732	0.48	0/3730
1	B	0.24	0/2570	0.47	0/3500
1	C	0.24	0/2594	0.48	0/3529
1	D	0.24	0/2565	0.47	0/3494
2	E	0.24	0/9636	0.42	0/13254
All	All	0.24	0/20097	0.45	0/27507

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	A	2672	0	2598	38	0
1	B	2513	0	2526	35	0
1	C	2537	0	2560	28	0
1	D	2508	0	2519	35	0
2	E	9429	0	7797	69	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	2	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	31	0	12	1	0
3	E	31	0	12	1	0
4	A	32	0	37	0	0
4	E	128	0	148	1	0
5	A	36	0	45	1	0
5	B	36	0	45	0	0
5	C	36	0	45	0	0
5	D	36	0	45	1	0
6	A	108	0	160	6	0
6	B	108	0	160	12	0
6	C	54	0	80	3	0
6	D	162	0	240	9	0
6	E	54	0	80	6	0
7	E	33	0	28	4	0
8	E	14	0	13	0	0
All	All	20651	0	19186	199	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 5.

All (199) 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)
6:B:404:P5S:HN	1:C:176:ARG:HH12	1.36	0.71
1:D:201:ARG:HH21	1:D:315:PHE:HB3	1.55	0.71
1:C:201:ARG:HH21	1:C:315:PHE:HB3	1.55	0.70
1:A:201:ARG:HH21	1:A:315:PHE:HB3	1.58	0.67
1:B:201:ARG:HH21	1:B:315:PHE:HB3	1.59	0.67
1:B:299:GLN:HG3	1:C:211:ILE:HG23	1.76	0.66
1:A:319:VAL:HG22	1:A:328:VAL:HG22	1.77	0.66
1:D:281:LEU:HB2	1:D:306:ALA:HB2	1.76	0.66
1:A:177:ARG:NH1	1:A:208:SER:OG	2.28	0.65
1:D:176:ARG:HH21	6:D:404:P5S:HB	1.60	0.65
2:E:452:LEU:HG	2:E:460:ALA:HB1	1.78	0.65
2:E:992:GLN:O	2:E:1187:ARG:NH1	2.30	0.65
6:A:404:P5S:H53	1:D:151:VAL:HG22	1.79	0.64
1:C:182:ILE:HD12	3:C:401:ATP:H1'	1.79	0.64
1:A:293:THR:O	1:D:173:GLN:NE2	2.31	0.63
2:E:551:PRO:HB3	2:E:587:VAL:HG21	1.80	0.63
6:B:403:P5S:H22	6:B:403:P5S:H40	1.80	0.63
1:D:32:ARG:NH1	1:D:279:GLN:O	2.31	0.62

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:VAL:HG22	1:D:328:VAL:HG22	1.82	0.62
1:C:45:ALA:HB2	1:D:325:ARG:HD3	1.80	0.62
2:E:306:ARG:NH2	7:E:2001:GBM:CL1	2.69	0.62
6:A:405:P5S:H48A	6:B:403:P5S:H28	1.81	0.62
1:C:137:MET:HG2	1:D:133:PHE:HB3	1.82	0.61
1:A:133:PHE:HB3	1:D:137:MET:HG2	1.81	0.61
6:C:403:P5S:H41A	6:C:403:P5S:H45	1.83	0.61
2:E:552:ILE:HD11	2:E:1030:ILE:HD13	1.82	0.60
2:E:680:GLN:HA	2:E:702:ARG:HG2	1.82	0.60
1:B:319:VAL:HG22	1:B:328:VAL:HG22	1.84	0.59
1:A:146:ILE:HG12	1:B:122:LEU:HD21	1.86	0.58
1:C:59:VAL:HG11	6:D:405:P5S:H41A	1.85	0.58
6:A:405:P5S:H41	2:E:46:ILE:HD11	1.86	0.58
1:B:126:GLU:OE2	1:B:136:ARG:NH1	2.36	0.58
2:E:103:HIS:HB3	2:E:105:HIS:HD2	1.68	0.58
2:E:306:ARG:HG3	2:E:440:THR:HG21	1.87	0.57
2:E:807:SER:O	2:E:837:ARG:NH1	2.38	0.57
1:C:177:ARG:NH1	1:C:208:SER:OG	2.38	0.57
2:E:775:GLN:NE2	3:E:2002:ATP:O2B	2.37	0.56
1:B:177:ARG:NH1	1:B:208:SER:OG	2.39	0.56
1:A:276:HIS:NE2	1:A:278:HIS:O	2.39	0.55
1:A:288:GLU:HG2	1:A:299:GLN:HG2	1.88	0.55
2:E:1109:PRO:HD3	2:E:1323:ALA:HB3	1.88	0.55
2:E:305:PHE:HZ	6:E:2008:P5S:H1A	1.71	0.55
1:D:267:LEU:HD22	1:D:270:LEU:HD11	1.88	0.55
1:A:155:VAL:HG22	6:B:403:P5S:H31	1.87	0.55
6:A:404:P5S:H23	6:A:404:P5S:H48A	1.88	0.54
2:E:137:ILE:HA	2:E:140:LEU:HD23	1.89	0.54
2:E:229:THR:HA	2:E:1250:VAL:HG11	1.90	0.54
2:E:1190:GLN:HG2	2:E:1307:ILE:HD13	1.89	0.54
1:A:180:THR:HG22	1:D:54:ARG:HD2	1.90	0.54
1:D:126:GLU:OE2	1:D:136:ARG:NH1	2.41	0.54
2:E:255:ILE:HD13	2:E:258:ARG:HD2	1.89	0.53
2:E:103:HIS:HB3	2:E:105:HIS:CD2	2.43	0.53
1:A:76:THR:HG23	1:D:154:ILE:HD13	1.89	0.53
1:C:73:LEU:HD21	6:C:403:P5S:H53	1.91	0.53
1:A:182:ILE:HD12	3:A:401:ATP:H1'	1.91	0.53
1:A:211:ILE:HB	1:A:290:VAL:HG13	1.91	0.53
2:E:1352:VAL:HG12	2:E:1362:LEU:H	1.74	0.52
1:C:154:ILE:HD13	1:D:76:THR:HG23	1.91	0.52
1:A:219:VAL:HG22	1:A:283:ILE:HD12	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:402:MET:O	2:E:1215:ARG:NH1	2.43	0.52
1:D:54:ARG:HA	1:D:57:GLN:HB2	1.91	0.52
2:E:1349:ASN:HA	2:E:1364:HIS:HA	1.92	0.51
2:E:371:THR:HG21	6:E:2008:P5S:H46	1.91	0.51
2:E:427:GLN:NE2	2:E:606:SER:OG	2.44	0.51
1:B:186:HIS:NE2	1:B:334:GLY:O	2.43	0.51
2:E:241:HIS:HA	2:E:1184:VAL:HG11	1.93	0.51
1:C:221:ARG:HG2	1:C:222:LYS:H	1.75	0.50
2:E:561:GLY:HA2	2:E:565:PHE:HD2	1.76	0.50
1:B:112:THR:HG1	1:B:137:MET:H	1.58	0.50
1:C:151:VAL:HG22	6:D:404:P5S:H34	1.92	0.50
1:B:112:THR:OG1	1:B:137:MET:N	2.40	0.50
1:C:32:ARG:NH1	1:C:279:GLN:O	2.31	0.50
1:B:36:VAL:HG12	1:B:42:CYS:HA	1.93	0.50
2:E:456:LEU:HB3	2:E:460:ALA:HB2	1.94	0.50
6:E:2008:P5S:H29	6:E:2008:P5S:H34	1.92	0.50
1:A:267:LEU:HD22	1:A:270:LEU:HD11	1.93	0.50
1:D:59:VAL:HG11	6:D:401:P5S:H40A	1.92	0.50
6:B:404:P5S:H31	6:C:403:P5S:H44	1.94	0.49
1:A:227:GLU:O	1:B:314:ARG:NH2	2.45	0.49
2:E:855:ASP:HA	2:E:888:THR:HB	1.94	0.49
1:A:346:ALA:HA	1:A:349:LEU:HD13	1.95	0.49
1:D:34:ARG:NH2	1:D:303:SER:OG	2.45	0.49
2:E:323:ILE:HG13	2:E:358:LEU:HD23	1.94	0.49
2:E:396:TYR:HA	2:E:399:ILE:HD12	1.95	0.49
1:D:211:ILE:HB	1:D:290:VAL:HG13	1.95	0.49
1:D:220:VAL:HB	1:D:282:GLU:HB3	1.95	0.49
2:E:1246:ARG:NH1	7:E:2001:GBM:H18	2.28	0.48
1:C:288:GLU:HG2	1:C:299:GLN:HG2	1.95	0.48
2:E:305:PHE:CZ	6:E:2008:P5S:H1A	2.48	0.48
2:E:1149:LEU:HD23	2:E:1294:TYR:CZ	2.48	0.48
1:D:57:GLN:NE2	6:D:401:P5S:O15	2.36	0.48
1:B:124:SER:HA	1:B:152:GLN:HE22	1.79	0.48
6:E:2008:P5S:H1	6:E:2008:P5S:H20A	1.60	0.47
1:B:67:LYS:HZ2	6:B:403:P5S:HNA	1.62	0.47
1:A:275:LEU:HD21	1:A:309:ILE:HB	1.96	0.47
2:E:1512:ILE:O	2:E:1516:THR:N	2.44	0.47
1:A:45:ALA:HB2	1:B:325:ARG:HD2	1.95	0.47
1:A:270:LEU:HD21	1:A:281:LEU:HD11	1.95	0.47
2:E:337:LYS:HA	2:E:337:LYS:HE2	1.97	0.47
1:B:54:ARG:HD3	1:C:180:THR:HG22	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:ARG:HH21	2:E:185:VAL:HG12	1.80	0.47
2:E:253:LEU:HB3	2:E:1236:ILE:HD13	1.97	0.47
2:E:5:PHE:O	2:E:105:HIS:HB3	2.15	0.46
1:A:154:ILE:HD13	1:B:76:THR:HG23	1.97	0.46
1:B:99:ASP:HB2	1:B:109:PRO:HB3	1.97	0.46
1:D:182:ILE:HD12	3:D:402:ATP:H1'	1.97	0.46
1:A:325:ARG:NH1	1:D:43:ASN:OD1	2.49	0.46
1:C:35:PHE:HE2	1:D:250:PHE:HE2	1.63	0.46
2:E:417:ILE:HG21	2:E:1208:VAL:HG21	1.97	0.46
2:E:1061:GLN:HA	2:E:1064:TYR:HD2	1.81	0.46
1:C:299:GLN:HG3	1:D:211:ILE:HG23	1.97	0.46
2:E:65:TRP:CH2	2:E:218:LEU:HD22	2.51	0.46
2:E:84:VAL:HG11	2:E:174:LEU:HD22	1.97	0.46
2:E:86:VAL:HG11	2:E:364:LEU:HD11	1.97	0.46
1:C:36:VAL:HG23	1:C:303:SER:HB3	1.98	0.46
1:A:275:LEU:HD23	1:A:275:LEU:O	2.17	0.45
1:D:198:PHE:CE2	1:D:283:ILE:HG21	2.51	0.45
2:E:79:PHE:CZ	2:E:225:LEU:HD13	2.52	0.45
1:B:312:GLY:HA3	1:B:341:THR:HG21	1.98	0.45
1:B:50:ARG:NH2	3:C:401:ATP:O3G	2.43	0.45
1:D:73:LEU:HD11	6:D:405:P5S:H32A	1.98	0.45
2:E:772:TYR:H	2:E:1217:PHE:HE1	1.63	0.45
1:B:215:ILE:HG12	1:B:287:LEU:HD13	1.99	0.44
1:B:154:ILE:HD13	1:C:76:THR:HG23	1.99	0.44
6:B:404:P5S:H20	6:B:404:P5S:H23A	1.78	0.44
2:E:377:TYR:O	2:E:381:ILE:HG12	2.18	0.44
1:B:46:HIS:HB3	1:B:49:ILE:HD11	1.99	0.44
2:E:150:LYS:HZ1	2:E:179:TYR:HE2	1.65	0.44
2:E:1132:ILE:HA	2:E:1136:ILE:HD12	1.98	0.44
1:A:330:TYR:HH	1:D:46:HIS:CE1	2.35	0.44
6:A:404:P5S:H32	6:A:404:P5S:H55A	2.00	0.44
6:B:403:P5S:H1	6:B:403:P5S:H39A	1.99	0.44
2:E:1101:LEU:HA	2:E:1319:LEU:HD21	1.99	0.44
2:E:81:LEU:HA	2:E:84:VAL:HG22	2.00	0.44
1:A:196:LEU:HD23	1:A:346:ALA:HB2	2.00	0.44
5:D:403:POV:H24	5:D:403:POV:H27	1.68	0.44
2:E:467:ILE:HG22	2:E:590:LEU:HG	2.00	0.44
7:E:2001:GBM:H19	7:E:2001:GBM:H21	1.83	0.43
6:D:405:P5S:H34A	6:D:405:P5S:H31A	1.63	0.43
2:E:435:CYS:O	2:E:438:LEU:HG	2.17	0.43
1:A:62:THR:O	1:A:66:LEU:HG	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:404:P5S:H1A	6:D:401:P5S:H39	1.99	0.43
2:E:366:LEU:O	2:E:370:ARG:HG2	2.18	0.43
1:B:146:ILE:HG12	1:C:122:LEU:HD21	2.00	0.43
1:B:249:ILE:HD12	1:B:249:ILE:HA	1.93	0.43
1:D:121:PHE:O	1:D:125:ILE:HG12	2.19	0.43
2:E:727:LEU:HA	2:E:767:ARG:HH12	1.84	0.43
6:B:403:P5S:H1	6:B:403:P5S:H20	1.83	0.42
1:A:200:LEU:HD23	1:A:201:ARG:N	2.34	0.42
1:C:322:GLU:HG2	1:C:323:ASP:N	2.33	0.42
1:D:242:ASN:OD1	1:D:243:GLY:N	2.49	0.42
1:A:34:ARG:NH2	1:A:303:SER:OG	2.53	0.42
1:C:85:LEU:HD23	6:D:405:P5S:H56B	2.00	0.42
1:D:202:VAL:HG21	1:D:287:LEU:HD22	2.01	0.42
2:E:75:TRP:O	2:E:78:THR:OG1	2.31	0.42
2:E:90:ALA:HB1	2:E:357:VAL:HG22	2.02	0.42
2:E:588:THR:HB	2:E:589:PRO:HD3	2.01	0.42
1:A:99:ASP:HB2	1:A:109:PRO:HB3	2.02	0.42
1:B:281:LEU:HB2	1:B:306:ALA:HB2	2.02	0.42
1:B:209:MET:SD	1:B:252:VAL:HG22	2.60	0.42
2:E:381:ILE:HA	2:E:433:PHE:CE1	2.54	0.42
6:E:2008:P5S:H29A	6:E:2008:P5S:H25	2.02	0.42
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.93	0.41
1:B:40:GLY:HA2	1:B:301:ARG:HB2	2.02	0.41
1:A:104:GLU:HG2	1:A:106:THR:H	1.84	0.41
1:B:67:LYS:HE3	1:B:67:LYS:HB3	1.86	0.41
6:B:403:P5S:H41	6:B:403:P5S:H44A	1.57	0.41
2:E:156:LYS:HD3	2:E:156:LYS:HA	1.77	0.41
2:E:299:LEU:HD21	2:E:435:CYS:SG	2.60	0.41
2:E:414:ALA:HA	2:E:417:ILE:HG22	2.02	0.41
6:B:403:P5S:H27	6:B:403:P5S:H30	1.94	0.41
1:C:281:LEU:HD23	1:C:281:LEU:HA	1.95	0.41
2:E:133:PRO:HG3	2:E:193:ARG:HE	1.85	0.41
2:E:396:TYR:CD2	2:E:1227:LEU:HD22	2.55	0.41
1:B:185:LYS:HB2	3:B:401:ATP:H5'1	2.02	0.41
2:E:471:ALA:HB3	2:E:472:PRO:HD3	2.03	0.41
2:E:903:MET:HA	2:E:908:ILE:HA	2.02	0.41
1:A:116:SER:HB2	5:A:403:POV:O14	2.20	0.41
1:A:249:ILE:HD12	1:A:249:ILE:HA	1.95	0.41
1:A:181:LEU:HD21	1:A:210:ILE:HD12	2.02	0.41
1:A:299:GLN:HG3	1:B:211:ILE:HG23	2.02	0.41
1:B:221:ARG:HG2	1:B:222:LYS:N	2.36	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ARG:HA	1:C:57:GLN:HB2	2.02	0.41
2:E:89:ILE:HD11	2:E:111:GLY:N	2.36	0.41
2:E:434:LEU:HD23	7:E:2001:GBM:H21	2.03	0.41
1:B:68:TRP:HD1	6:B:403:P5S:H3	1.86	0.41
1:C:211:ILE:HB	1:C:290:VAL:HG13	2.02	0.41
1:D:288:GLU:HG2	1:D:299:GLN:HG2	2.02	0.41
2:E:318:LEU:HD13	4:E:2007:PTY:H172	2.03	0.40
1:A:201:ARG:NH2	1:A:315:PHE:HB3	2.29	0.40
1:A:137:MET:SD	1:B:135:GLY:HA3	2.61	0.40
1:B:211:ILE:HB	1:B:290:VAL:HG13	2.02	0.40
2:E:288:TRP:HZ3	2:E:607:VAL:HG21	1.87	0.40
1:A:211:ILE:HG23	1:D:299:GLN:HG3	2.02	0.40
1:D:209:MET:SD	1:D:252:VAL:HG22	2.61	0.40
1:B:137:MET:HG2	1:C:133:PHE:HB3	2.03	0.40
1:C:137:MET:SD	1:D:135:GLY:HA3	2.61	0.40
1:C:220:VAL:HG22	1:C:235:GLN:HG2	2.04	0.40
2:E:1148:LEU:HD12	2:E:1148:LEU:HA	1.91	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	A	357/390 (92%)	340 (95%)	17 (5%)	0	100	100
1	B	326/390 (84%)	308 (94%)	18 (6%)	0	100	100
1	C	326/390 (84%)	318 (98%)	8 (2%)	0	100	100
1	D	326/390 (84%)	312 (96%)	14 (4%)	0	100	100
2	E	1415/1582 (89%)	1348 (95%)	67 (5%)	0	100	100
All	All	2750/3142 (88%)	2626 (96%)	124 (4%)	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 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	A	272/341 (80%)	272 (100%)	0	100	100
1	B	269/341 (79%)	268 (100%)	1 (0%)	91	97
1	C	275/341 (81%)	275 (100%)	0	100	100
1	D	267/341 (78%)	267 (100%)	0	100	100
2	E	665/1373 (48%)	663 (100%)	2 (0%)	92	98
All	All	1748/2737 (64%)	1745 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	275	LEU
2	E	105	HIS
2	E	175	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

25 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
4	PTY	E	2004	-	31,31,49	0.57	0	34,36,54	0.62	0
4	PTY	E	2007	-	31,31,49	0.55	0	34,36,54	0.54	0
3	ATP	D	402	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
6	P5S	A	404	-	52,53,53	0.54	0	56,60,60	0.83	1 (1%)
6	P5S	D	404	-	52,53,53	0.52	0	56,60,60	0.77	1 (1%)
3	ATP	B	401	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
5	POV	B	402	-	35,35,51	0.59	0	41,43,59	0.51	0
6	P5S	B	403	-	52,53,53	0.53	0	56,60,60	0.98	3 (5%)
7	GBM	E	2001	-	35,35,35	1.88	11 (31%)	48,48,48	1.23	5 (10%)
8	NAG	E	2003	2	14,14,15	0.60	1 (7%)	17,19,21	1.07	1 (5%)
6	P5S	B	404	-	52,53,53	0.53	0	56,60,60	0.84	1 (1%)
4	PTY	A	402	-	31,31,49	0.56	0	34,36,54	0.45	0
6	P5S	D	405	-	52,53,53	0.54	0	56,60,60	0.81	1 (1%)
3	ATP	C	401	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
4	PTY	E	2005	-	31,31,49	0.55	0	34,36,54	0.54	0
4	PTY	E	2006	-	31,31,49	0.55	0	34,36,54	0.48	0
3	ATP	A	401	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
5	POV	C	402	-	35,35,51	0.60	0	41,43,59	0.53	0
6	P5S	C	403	-	52,53,53	0.52	0	56,60,60	0.80	1 (1%)
6	P5S	A	405	-	52,53,53	0.53	0	56,60,60	0.83	1 (1%)
5	POV	A	403	-	35,35,51	0.59	0	41,43,59	0.57	0
5	POV	D	403	-	35,35,51	0.59	0	41,43,59	0.50	0
6	P5S	E	2008	-	52,53,53	0.54	0	56,60,60	0.86	1 (1%)
6	P5S	D	401	-	52,53,53	0.53	0	56,60,60	0.79	1 (1%)
3	ATP	E	2002	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)

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
4	PTY	E	2004	-	-	12/35/35/53	-
4	PTY	E	2007	-	-	15/35/35/53	-
3	ATP	D	402	-	-	11/18/38/38	0/3/3/3
6	P5S	A	404	-	-	23/59/59/59	-
6	P5S	D	404	-	-	28/59/59/59	-
3	ATP	B	401	-	-	8/18/38/38	0/3/3/3
5	POV	B	402	-	-	15/39/39/55	-
6	P5S	B	403	-	-	27/59/59/59	-
7	GBM	E	2001	-	-	5/27/35/35	0/3/3/3
8	NAG	E	2003	2	-	3/6/23/26	0/1/1/1
6	P5S	B	404	-	-	24/59/59/59	-
4	PTY	A	402	-	-	10/35/35/53	-
6	P5S	D	405	-	-	28/59/59/59	-
3	ATP	C	401	-	-	12/18/38/38	0/3/3/3
4	PTY	E	2005	-	-	18/35/35/53	-
4	PTY	E	2006	-	-	13/35/35/53	-
3	ATP	A	401	-	-	3/18/38/38	0/3/3/3
5	POV	C	402	-	-	15/39/39/55	-
6	P5S	C	403	-	-	28/59/59/59	-
6	P5S	A	405	-	-	25/59/59/59	-
5	POV	A	403	-	-	16/39/39/55	-
5	POV	D	403	-	-	12/39/39/55	-
6	P5S	E	2008	-	-	28/59/59/59	-
6	P5S	D	401	-	-	25/59/59/59	-
3	ATP	E	2002	-	-	2/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	2001	GBM	C26-N10	5.41	1.45	1.33
7	E	2001	GBM	C17-N8	4.63	1.45	1.35
7	E	2001	GBM	C18-S2	3.60	1.82	1.76
7	E	2001	GBM	S2-N9	3.36	1.71	1.64
7	E	2001	GBM	O4-S2	3.01	1.46	1.43
7	E	2001	GBM	O5-S2	2.98	1.46	1.43

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	2001	GBM	C17-N9	2.80	1.45	1.39
7	E	2001	GBM	O6-C26	-2.17	1.18	1.23
7	E	2001	GBM	O3-C17	-2.15	1.18	1.23
8	E	2003	NAG	O5-C1	2.11	1.47	1.43
7	E	2001	GBM	C31-CL1	2.04	1.78	1.74
7	E	2001	GBM	O7-C28	2.02	1.40	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	404	P5S	OG-CB-CA	4.57	112.05	108.06
6	A	405	P5S	OG-CB-CA	4.44	111.93	108.06
6	D	405	P5S	OG-CB-CA	4.28	111.79	108.06
6	A	404	P5S	OG-CB-CA	4.25	111.76	108.06
6	B	403	P5S	OG-CB-CA	4.22	111.73	108.06
6	E	2008	P5S	OG-CB-CA	4.19	111.71	108.06
6	D	401	P5S	OG-CB-CA	4.13	111.66	108.06
8	E	2003	NAG	C1-O5-C5	4.03	117.66	112.19
6	D	404	P5S	OG-CB-CA	4.02	111.56	108.06
6	C	403	P5S	OG-CB-CA	3.46	111.07	108.06
7	E	2001	GBM	C28-C27-C26	-3.38	120.00	126.16
6	B	403	P5S	C2-O37-C38	3.15	125.56	117.79
7	E	2001	GBM	O5-S2-O4	-2.50	116.47	119.55
3	E	2002	ATP	C5-C6-N6	2.30	123.84	120.35
3	C	401	ATP	C5-C6-N6	2.29	123.84	120.35
3	B	401	ATP	C5-C6-N6	2.29	123.83	120.35
3	D	402	ATP	C5-C6-N6	2.29	123.83	120.35
3	A	401	ATP	C5-C6-N6	2.28	123.82	120.35
7	E	2001	GBM	O7-C28-C30	-2.27	120.48	124.37
7	E	2001	GBM	C11-N8-C17	-2.23	118.31	123.02
7	E	2001	GBM	O7-C28-C27	2.20	119.75	116.55
6	B	403	P5S	O37-C38-C39	2.18	116.19	111.50
3	A	401	ATP	PB-O3B-PG	2.07	139.93	132.83
3	B	401	ATP	PB-O3B-PG	2.05	139.87	132.83
3	C	401	ATP	PB-O3B-PG	2.05	139.87	132.83
3	D	402	ATP	PB-O3B-PG	2.05	139.87	132.83
3	E	2002	ATP	PB-O3B-PG	2.05	139.86	132.83

There are no chirality outliers.

All (406) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ATP	O4'-C4'-C5'-O5'
3	A	401	ATP	C3'-C4'-C5'-O5'
3	B	401	ATP	C5'-O5'-PA-O3A
3	B	401	ATP	O4'-C4'-C5'-O5'
3	B	401	ATP	C3'-C4'-C5'-O5'
3	C	401	ATP	C5'-O5'-PA-O3A
3	C	401	ATP	O4'-C4'-C5'-O5'
3	C	401	ATP	C3'-C4'-C5'-O5'
3	D	402	ATP	C5'-O5'-PA-O3A
3	D	402	ATP	O4'-C4'-C5'-O5'
3	D	402	ATP	C3'-C4'-C5'-O5'
4	E	2004	PTY	C11-C8-O7-C6
4	E	2004	PTY	C5-O14-P1-O12
4	E	2004	PTY	C5-O14-P1-O13
4	E	2005	PTY	N1-C2-C3-O11
4	E	2005	PTY	C5-O14-P1-O11
4	E	2005	PTY	C5-O14-P1-O12
4	E	2005	PTY	C5-O14-P1-O13
4	E	2006	PTY	C3-O11-P1-O12
4	E	2006	PTY	C3-O11-P1-O13
4	E	2006	PTY	C3-O11-P1-O14
4	E	2006	PTY	C5-O14-P1-O12
4	E	2007	PTY	O4-C1-C6-O7
4	E	2007	PTY	N1-C2-C3-O11
4	E	2007	PTY	C3-O11-P1-O14
5	A	403	POV	C1-O11-P-O13
5	A	403	POV	O12-C11-C12-N
5	B	402	POV	C1-O11-P-O12
5	B	402	POV	C1-O11-P-O13
5	B	402	POV	C1-O11-P-O14
5	D	403	POV	C1-O11-P-O13
6	A	404	P5S	N-CA-CB-OG
6	A	404	P5S	CB-OG-P12-O13
6	A	405	P5S	O-C-CA-CB
6	A	405	P5S	OXT-C-CA-CB
6	A	405	P5S	O19-C1-C2-O37
6	B	403	P5S	O-C-CA-CB
6	B	403	P5S	OXT-C-CA-CB
6	B	403	P5S	O37-C2-C3-O16
6	B	403	P5S	C-CA-CB-OG
6	B	403	P5S	N-CA-CB-OG
6	B	403	P5S	CA-CB-OG-P12
6	B	403	P5S	C20-C17-O19-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	B	403	P5S	C39-C38-O37-C2
6	B	403	P5S	O47-C38-O37-C2
6	B	404	P5S	O-C-CA-CB
6	B	404	P5S	OXT-C-CA-CB
6	B	404	P5S	C2-C3-O16-P12
6	B	404	P5S	CB-OG-P12-O13
6	C	403	P5S	C-CA-CB-OG
6	C	403	P5S	N-CA-CB-OG
6	C	403	P5S	CB-OG-P12-O15
6	C	403	P5S	C3-O16-P12-O13
6	C	403	P5S	C39-C38-O37-C2
6	D	401	P5S	C-CA-CB-OG
6	D	401	P5S	N-CA-CB-OG
6	D	401	P5S	C3-O16-P12-O15
6	D	404	P5S	C2-C3-O16-P12
6	D	404	P5S	CB-OG-P12-O13
6	D	404	P5S	C3-O16-P12-OG
6	D	404	P5S	C39-C38-O37-C2
6	D	405	P5S	CA-CB-OG-P12
6	D	405	P5S	CB-OG-P12-O16
6	E	2008	P5S	O-C-CA-CB
6	E	2008	P5S	C-CA-CB-OG
6	E	2008	P5S	N-CA-CB-OG
6	E	2008	P5S	CA-CB-OG-P12
6	E	2008	P5S	CB-OG-P12-O16
6	E	2008	P5S	O18-C17-O19-C1
6	E	2008	P5S	C20-C17-O19-C1
6	B	403	P5S	O18-C17-O19-C1
4	E	2004	PTY	O10-C8-O7-C6
6	C	403	P5S	O47-C38-O37-C2
6	D	404	P5S	O47-C38-O37-C2
6	C	403	P5S	O18-C17-O19-C1
6	C	403	P5S	C20-C17-O19-C1
6	A	405	P5S	OXT-C-CA-N
7	E	2001	GBM	O6-C26-C27-C28
4	E	2006	PTY	C31-C30-O4-C1
6	B	403	P5S	C41-C42-C43-C44
7	E	2001	GBM	N10-C26-C27-C28
6	C	403	P5S	C21-C22-C23-C24
6	C	403	P5S	C44-C45-C46-C48
6	E	2008	P5S	C25-C26-C27-C28
4	E	2006	PTY	O30-C30-O4-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	402	POV	C22-C23-C24-C25
5	D	403	POV	C34-C35-C36-C37
6	D	405	P5S	C31-C32-C33-C34
6	E	2008	P5S	C48-C49-C50-C51
4	E	2005	PTY	C31-C30-O4-C1
4	E	2007	PTY	C31-C30-O4-C1
5	C	402	POV	C32-C31-O31-C3
6	A	405	P5S	C20-C17-O19-C1
5	B	402	POV	C32-C33-C34-C35
6	D	404	P5S	C25-C26-C27-C28
6	D	401	P5S	C26-C27-C28-C29
8	E	2003	NAG	C8-C7-N2-C2
8	E	2003	NAG	O7-C7-N2-C2
6	B	404	P5S	C39-C40-C41-C42
6	A	404	P5S	O19-C1-C2-O37
6	B	404	P5S	O19-C1-C2-O37
5	D	403	POV	C24-C25-C26-C27
5	B	402	POV	C21-C22-C23-C24
4	E	2005	PTY	O30-C30-O4-C1
4	E	2007	PTY	O30-C30-O4-C1
6	A	405	P5S	O18-C17-O19-C1
5	A	403	POV	C31-C32-C33-C34
3	E	2002	ATP	O4'-C4'-C5'-O5'
3	E	2002	ATP	C3'-C4'-C5'-O5'
5	D	403	POV	C32-C33-C34-C35
6	D	405	P5S	C26-C27-C28-C29
5	D	403	POV	C21-C22-C23-C24
6	D	404	P5S	C38-C39-C40-C41
5	C	402	POV	O32-C31-O31-C3
6	B	404	P5S	C20-C21-C22-C23
4	E	2004	PTY	C3-O11-P1-O14
4	E	2004	PTY	C5-O14-P1-O11
4	E	2006	PTY	C5-O14-P1-O11
5	A	403	POV	C1-O11-P-O12
5	D	403	POV	C1-O11-P-O12
6	B	404	P5S	C3-O16-P12-OG
6	C	403	P5S	CB-OG-P12-O16
6	D	401	P5S	C3-O16-P12-OG
6	D	404	P5S	CB-OG-P12-O16
6	E	2008	P5S	C3-O16-P12-OG
6	B	403	P5S	OXT-C-CA-N
4	E	2004	PTY	C8-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	C	402	POV	C24-C25-C26-C27
4	E	2005	PTY	C16-C17-C18-C19
4	E	2007	PTY	C12-C13-C14-C15
6	A	404	P5S	C50-C51-C52-C53
4	E	2007	PTY	C15-C16-C17-C18
6	B	404	P5S	C21-C22-C23-C24
6	C	403	P5S	C3-C2-O37-C38
6	A	404	P5S	C30-C31-C32-C33
5	C	402	POV	C25-C26-C27-C28
6	C	403	P5S	C43-C44-C45-C46
6	E	2008	P5S	C20-C21-C22-C23
6	D	405	P5S	C44-C45-C46-C48
5	D	403	POV	C31-C32-C33-C34
4	E	2005	PTY	C12-C13-C14-C15
4	A	402	PTY	C14-C15-C16-C17
6	E	2008	P5S	C31-C32-C33-C34
6	A	404	P5S	C42-C43-C44-C45
6	D	404	P5S	C20-C21-C22-C23
5	D	403	POV	C25-C26-C27-C28
6	A	405	P5S	C24-C25-C26-C27
4	E	2004	PTY	C14-C15-C16-C17
6	C	403	P5S	C49-C50-C51-C52
6	B	403	P5S	C46-C48-C49-C50
6	D	404	P5S	O19-C1-C2-C3
6	B	403	P5S	C50-C51-C52-C53
6	E	2008	P5S	C50-C51-C52-C53
6	A	405	P5S	C39-C40-C41-C42
6	E	2008	P5S	C42-C43-C44-C45
4	E	2005	PTY	C11-C8-O7-C6
6	D	404	P5S	C49-C50-C51-C52
6	D	405	P5S	C39-C40-C41-C42
6	D	401	P5S	O47-C38-O37-C2
6	D	405	P5S	O47-C38-O37-C2
6	D	405	P5S	C-CA-CB-OG
6	A	404	P5S	C40-C41-C42-C43
6	D	405	P5S	C42-C43-C44-C45
6	D	401	P5S	C39-C38-O37-C2
6	D	405	P5S	C39-C38-O37-C2
6	B	403	P5S	C30-C31-C32-C33
6	B	403	P5S	C40-C41-C42-C43
4	E	2005	PTY	O10-C8-O7-C6
5	B	402	POV	C25-C26-C27-C28

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
6	D	401	P5S	O19-C1-C2-O37
5	B	402	POV	C32-C31-O31-C3
6	E	2008	P5S	C21-C22-C23-C24
4	A	402	PTY	C12-C13-C14-C15
6	D	401	P5S	C46-C48-C49-C50
6	B	403	P5S	C38-C39-C40-C41
6	C	403	P5S	O-C-CA-CB
6	E	2008	P5S	OXT-C-CA-CB
6	B	404	P5S	C23-C24-C25-C26
6	A	404	P5S	CB-OG-P12-O16
6	A	405	P5S	C3-O16-P12-OG
4	E	2005	PTY	O14-C5-C6-C1
4	E	2007	PTY	O14-C5-C6-C1
6	D	405	P5S	C1-C2-C3-O16
6	A	404	P5S	C24-C25-C26-C27
6	B	403	P5S	C42-C43-C44-C45
6	D	404	P5S	C39-C40-C41-C42
6	C	403	P5S	C25-C26-C27-C28
6	D	405	P5S	C20-C17-O19-C1
6	E	2008	P5S	C45-C46-C48-C49
5	C	402	POV	C1-C2-C3-O31
6	A	404	P5S	O19-C1-C2-C3
6	A	405	P5S	O19-C1-C2-C3
6	D	405	P5S	C41-C42-C43-C44
6	D	401	P5S	C43-C44-C45-C46
4	E	2005	PTY	C30-C31-C32-C33
6	B	404	P5S	C46-C48-C49-C50
6	D	405	P5S	C45-C46-C48-C49
6	D	401	P5S	C27-C28-C29-C30
6	D	405	P5S	C50-C51-C52-C53
5	A	403	POV	C35-C36-C37-C38
6	B	404	P5S	C42-C43-C44-C45
6	D	405	P5S	C23-C24-C25-C26
6	B	404	P5S	C50-C51-C52-C53
6	C	403	P5S	O37-C2-C3-O16
4	E	2004	PTY	C11-C12-C13-C14
5	B	402	POV	O32-C31-O31-C3
6	A	404	P5S	C23-C24-C25-C26
6	D	405	P5S	C29-C30-C31-C32
4	E	2005	PTY	C17-C18-C19-C20
4	E	2005	PTY	C11-C12-C13-C14
6	C	403	P5S	C39-C40-C41-C42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	D	405	P5S	C48-C49-C50-C51
5	A	403	POV	C25-C26-C27-C28
3	C	401	ATP	PB-O3A-PA-O1A
3	D	402	ATP	PB-O3A-PA-O1A
6	A	405	P5S	C53-C54-C55-C56
6	D	405	P5S	O18-C17-O19-C1
4	E	2006	PTY	C16-C17-C18-C19
6	D	404	P5S	C22-C23-C24-C25
6	B	403	P5S	C1-C2-C3-O16
6	B	404	P5S	C1-C2-C3-O16
6	D	404	P5S	C24-C25-C26-C27
6	D	401	P5S	C17-C20-C21-C22
6	D	401	P5S	C38-C39-C40-C41
6	A	404	P5S	C26-C27-C28-C29
5	C	402	POV	C33-C34-C35-C36
4	E	2007	PTY	O4-C1-C6-C5
6	B	404	P5S	O19-C1-C2-C3
6	C	403	P5S	O19-C1-C2-C3
6	D	401	P5S	O19-C1-C2-C3
6	D	404	P5S	C33-C34-C35-C36
4	E	2004	PTY	C12-C13-C14-C15
6	B	403	P5S	C3-O16-P12-OG
6	C	403	P5S	C3-O16-P12-OG
6	E	2008	P5S	C33-C34-C35-C36
4	E	2007	PTY	O14-C5-C6-O7
6	D	401	P5S	O37-C2-C3-O16
6	D	405	P5S	O37-C2-C3-O16
4	E	2007	PTY	C31-C32-C33-C34
6	D	404	P5S	C48-C49-C50-C51
4	E	2006	PTY	O4-C1-C6-O7
6	A	405	P5S	C30-C31-C32-C33
6	C	403	P5S	C31-C32-C33-C34
6	A	405	P5S	O-C-CA-N
6	B	403	P5S	O-C-CA-N
6	D	404	P5S	C27-C28-C29-C30
6	E	2008	P5S	C22-C23-C24-C25
5	C	402	POV	C32-C33-C34-C35
6	A	404	P5S	C39-C40-C41-C42
7	E	2001	GBM	C23-C19-C20-C25
6	A	405	P5S	C31-C32-C33-C34
6	C	403	P5S	C1-C2-C3-O16
3	C	401	ATP	PB-O3B-PG-O1G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	E	2001	GBM	C24-C19-C20-C25
6	A	405	P5S	C22-C23-C24-C25
6	A	404	P5S	C53-C54-C55-C56
5	D	403	POV	C26-C27-C28-C29
6	A	405	P5S	C33-C34-C35-C36
6	A	405	P5S	O37-C2-C3-O16
6	B	404	P5S	O19-C17-C20-C21
5	A	403	POV	C32-C31-O31-C3
6	D	405	P5S	C32-C33-C34-C35
3	D	402	ATP	PB-O3B-PG-O2G
6	E	2008	P5S	C52-C53-C54-C55
5	A	403	POV	C21-C22-C23-C24
6	D	404	P5S	O19-C1-C2-O37
6	A	405	P5S	CA-CB-OG-P12
6	D	404	P5S	CA-CB-OG-P12
6	E	2008	P5S	C28-C29-C30-C31
5	A	403	POV	C22-C21-O21-C2
6	C	403	P5S	OXT-C-CA-CB
5	A	403	POV	O22-C21-O21-C2
6	B	403	P5S	C2-C1-O19-C17
6	D	404	P5S	C29-C30-C31-C32
3	B	401	ATP	PA-O3A-PB-O2B
3	C	401	ATP	PA-O3A-PB-O2B
3	D	402	ATP	PA-O3A-PB-O2B
4	A	402	PTY	C13-C14-C15-C16
6	D	404	P5S	N-CA-CB-OG
6	D	405	P5S	N-CA-CB-OG
4	A	402	PTY	C5-O14-P1-O11
6	D	404	P5S	C40-C41-C42-C43
3	B	401	ATP	C5'-O5'-PA-O1A
3	B	401	ATP	C5'-O5'-PA-O2A
3	C	401	ATP	C5'-O5'-PA-O1A
3	C	401	ATP	C5'-O5'-PA-O2A
3	D	402	ATP	C5'-O5'-PA-O1A
3	D	402	ATP	C5'-O5'-PA-O2A
4	E	2004	PTY	C3-O11-P1-O13
4	E	2007	PTY	C3-O11-P1-O13
5	C	402	POV	C1-O11-P-O13
6	A	405	P5S	C3-O16-P12-O15
6	B	404	P5S	C3-O16-P12-O13
6	D	404	P5S	C3-O16-P12-O15
6	D	405	P5S	CB-OG-P12-O15

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
6	E	2008	P5S	CB-OG-P12-O13
6	E	2008	P5S	C3-O16-P12-O13
6	E	2008	P5S	C3-O16-P12-O15
6	A	405	P5S	C1-C2-C3-O16
5	B	402	POV	C27-C28-C29-C210
6	B	404	P5S	C22-C23-C24-C25
4	E	2007	PTY	C16-C17-C18-C19
4	E	2005	PTY	O14-C5-C6-O7
4	E	2005	PTY	C8-C11-C12-C13
6	B	404	P5S	O37-C2-C3-O16
5	A	403	POV	O32-C31-O31-C3
6	A	405	P5S	O19-C17-C20-C21
6	B	404	P5S	C24-C25-C26-C27
6	E	2008	P5S	C23-C24-C25-C26
8	E	2003	NAG	C4-C5-C6-O6
5	B	402	POV	O12-C11-C12-N
6	D	401	P5S	C52-C53-C54-C55
6	D	401	P5S	O19-C17-C20-C21
6	B	403	P5S	C2-C3-O16-P12
6	A	405	P5S	C21-C22-C23-C24
4	E	2005	PTY	C31-C32-C33-C34
6	D	401	P5S	O18-C17-O19-C1
6	D	405	P5S	C40-C41-C42-C43
4	E	2005	PTY	C1-C6-O7-C8
6	D	401	P5S	C1-C2-C3-O16
6	A	405	P5S	C42-C43-C44-C45
5	A	403	POV	C32-C33-C34-C35
6	D	401	P5S	C20-C17-O19-C1
5	C	402	POV	O11-C1-C2-O21
5	A	403	POV	C33-C34-C35-C36
6	C	403	P5S	C53-C54-C55-C56
6	C	403	P5S	O19-C1-C2-O37
6	D	405	P5S	C27-C28-C29-C30
4	A	402	PTY	C3-O11-P1-O14
4	E	2007	PTY	C5-O14-P1-O11
5	A	403	POV	C11-O12-P-O11
5	B	402	POV	C11-O12-P-O11
5	C	402	POV	C11-O12-P-O11
5	D	403	POV	C11-O12-P-O11
6	B	404	P5S	CB-OG-P12-O16
6	B	404	P5S	C29-C30-C31-C32
4	E	2006	PTY	O4-C1-C6-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	401	ATP	PB-O3A-PA-O2A
5	B	402	POV	C22-C23-C24-C25
4	E	2006	PTY	C13-C14-C15-C16
6	D	401	P5S	C21-C22-C23-C24
5	A	403	POV	C34-C35-C36-C37
4	E	2006	PTY	C31-C32-C33-C34
4	E	2007	PTY	C17-C18-C19-C20
5	B	402	POV	O21-C2-C3-O31
6	A	404	P5S	C2-C3-O16-P12
6	B	403	P5S	C51-C52-C53-C54
6	D	401	P5S	C53-C54-C55-C56
6	D	405	P5S	C51-C52-C53-C54
5	C	402	POV	O21-C2-C3-O31
6	A	405	P5S	C40-C41-C42-C43
6	B	403	P5S	C24-C25-C26-C27
6	D	404	P5S	O19-C17-C20-C21
6	A	404	P5S	C51-C52-C53-C54
3	B	401	ATP	PB-O3A-PA-O1A
3	C	401	ATP	PB-O3A-PA-O2A
3	D	402	ATP	PB-O3A-PA-O2A
4	A	402	PTY	O14-C5-C6-O7
6	A	404	P5S	C46-C48-C49-C50
5	A	403	POV	C27-C28-C29-C210
6	D	405	P5S	C3-O16-P12-OG
4	A	402	PTY	C12-C11-C8-O7
4	E	2006	PTY	C12-C13-C14-C15
6	D	404	P5S	C50-C51-C52-C53
6	D	401	P5S	C22-C23-C24-C25
4	A	402	PTY	O4-C30-C31-C32
6	B	403	P5S	O37-C38-C39-C40
3	C	401	ATP	PB-O3B-PG-O2G
3	C	401	ATP	PB-O3B-PG-O3G
3	D	402	ATP	PB-O3B-PG-O3G
5	C	402	POV	O11-C1-C2-C3
6	A	404	P5S	C49-C50-C51-C52
6	A	405	P5S	C29-C30-C31-C32
6	D	404	P5S	C42-C43-C44-C45
5	C	402	POV	C34-C35-C36-C37
6	A	404	P5S	O37-C38-C39-C40
6	B	404	P5S	O37-C38-C39-C40
6	A	404	P5S	CA-CB-OG-P12
6	C	403	P5S	CA-CB-OG-P12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	D	404	P5S	O37-C38-C39-C40
3	B	401	ATP	PA-O3A-PB-O1B
3	C	401	ATP	PA-O3A-PB-O1B
3	D	402	ATP	PA-O3A-PB-O1B
6	B	403	P5S	O47-C38-C39-C40
4	A	402	PTY	C12-C11-C8-O10
5	D	403	POV	C33-C34-C35-C36
5	B	402	POV	C33-C34-C35-C36
4	A	402	PTY	O30-C30-C31-C32
6	E	2008	P5S	O37-C38-C39-C40
6	A	404	P5S	C25-C26-C27-C28
6	C	403	P5S	C48-C49-C50-C51
5	B	402	POV	C11-O12-P-O14
5	C	402	POV	C11-O12-P-O14
5	D	403	POV	C11-O12-P-O14
6	A	404	P5S	CB-OG-P12-O15
6	D	405	P5S	C3-O16-P12-O13
6	D	404	P5S	O47-C38-C39-C40
6	A	404	P5S	O47-C38-C39-C40
6	E	2008	P5S	C41-C42-C43-C44
6	B	404	P5S	O47-C38-C39-C40
6	D	401	P5S	C40-C41-C42-C43
6	D	401	P5S	C49-C50-C51-C52
7	E	2001	GBM	C21-C18-S2-O5
4	E	2004	PTY	C17-C18-C19-C20
6	C	403	P5S	C27-C28-C29-C30
6	E	2008	P5S	O47-C38-C39-C40

There are no ring outliers.

18 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2007	PTY	1	0
3	D	402	ATP	1	0
6	A	404	P5S	4	0
6	D	404	P5S	2	0
3	B	401	ATP	1	0
6	B	403	P5S	9	0
7	E	2001	GBM	4	0
6	B	404	P5S	3	0
6	D	405	P5S	4	0
3	C	401	ATP	2	0

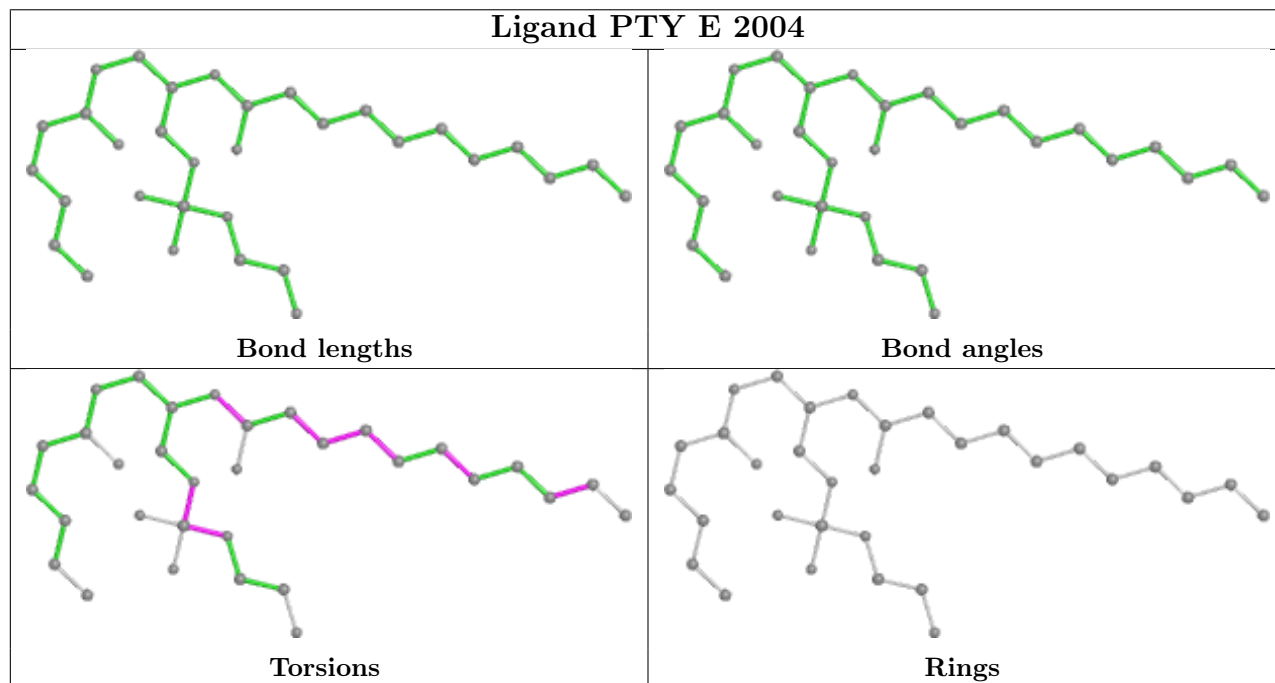
*Continued on next page...*

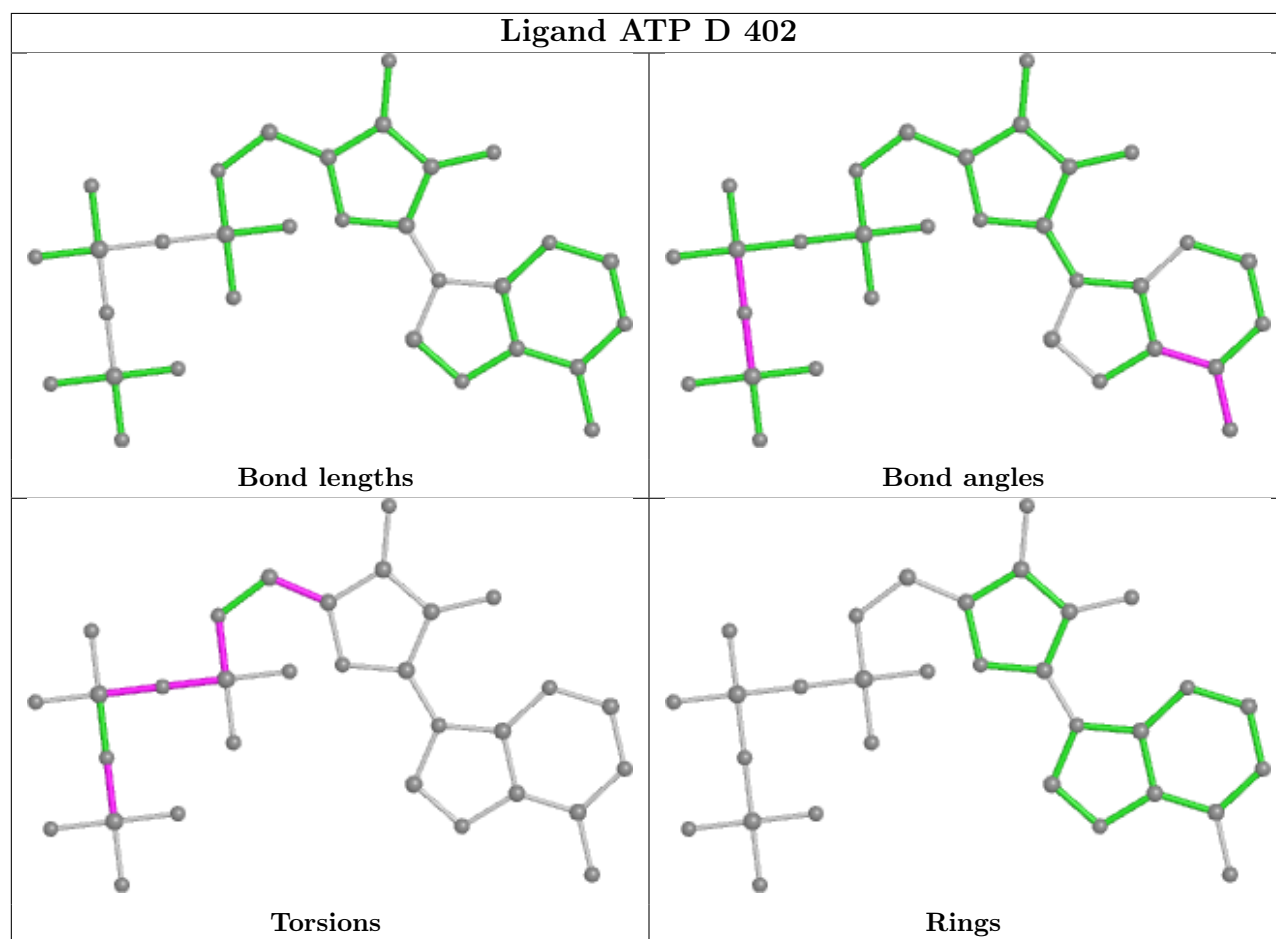
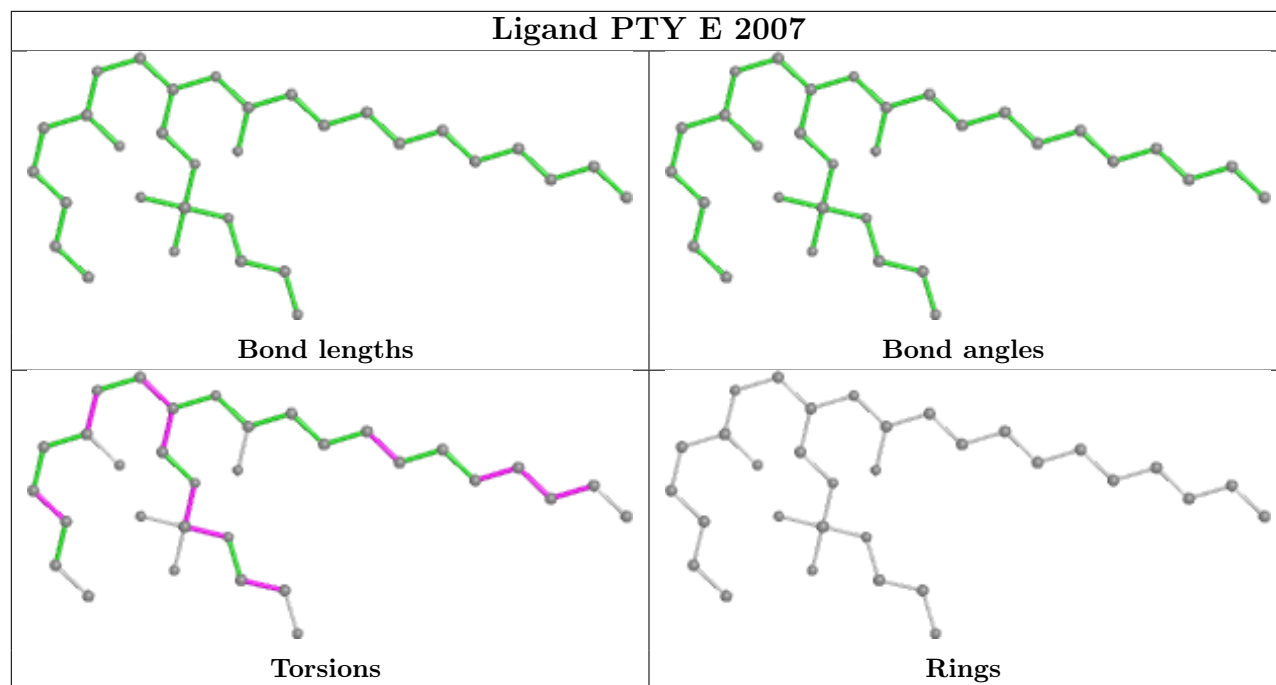


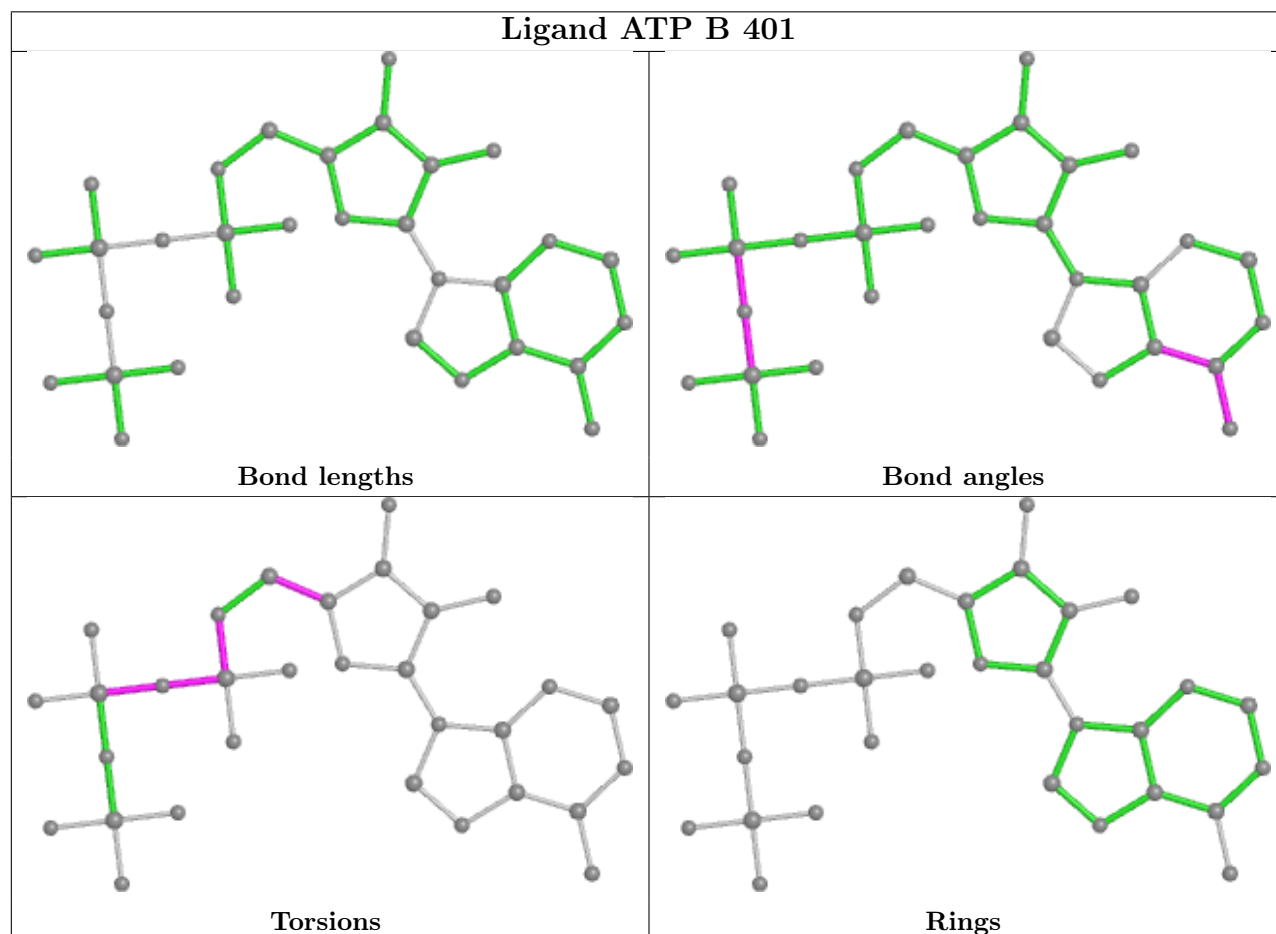
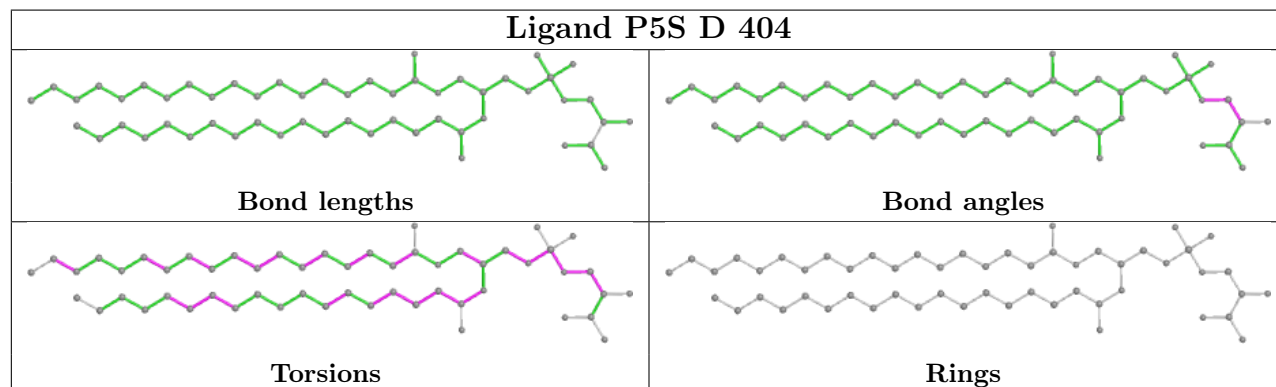
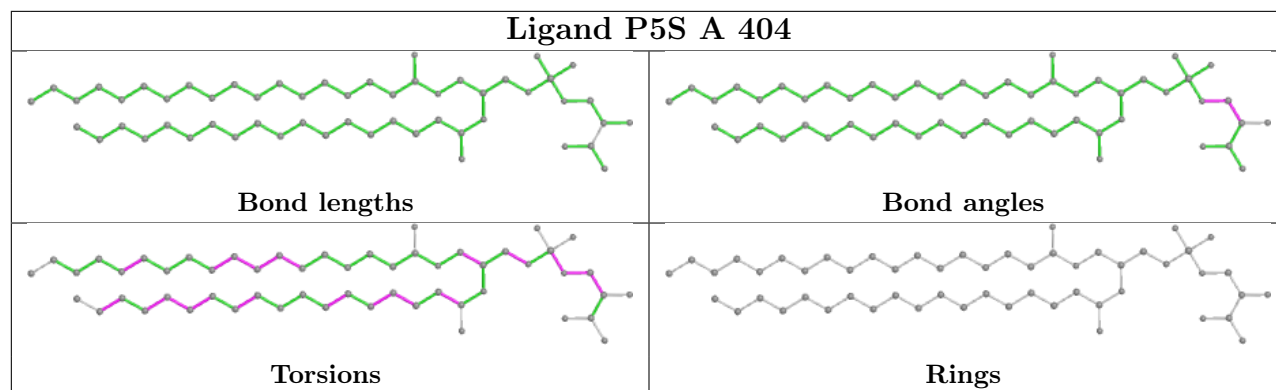
Continued from previous page...

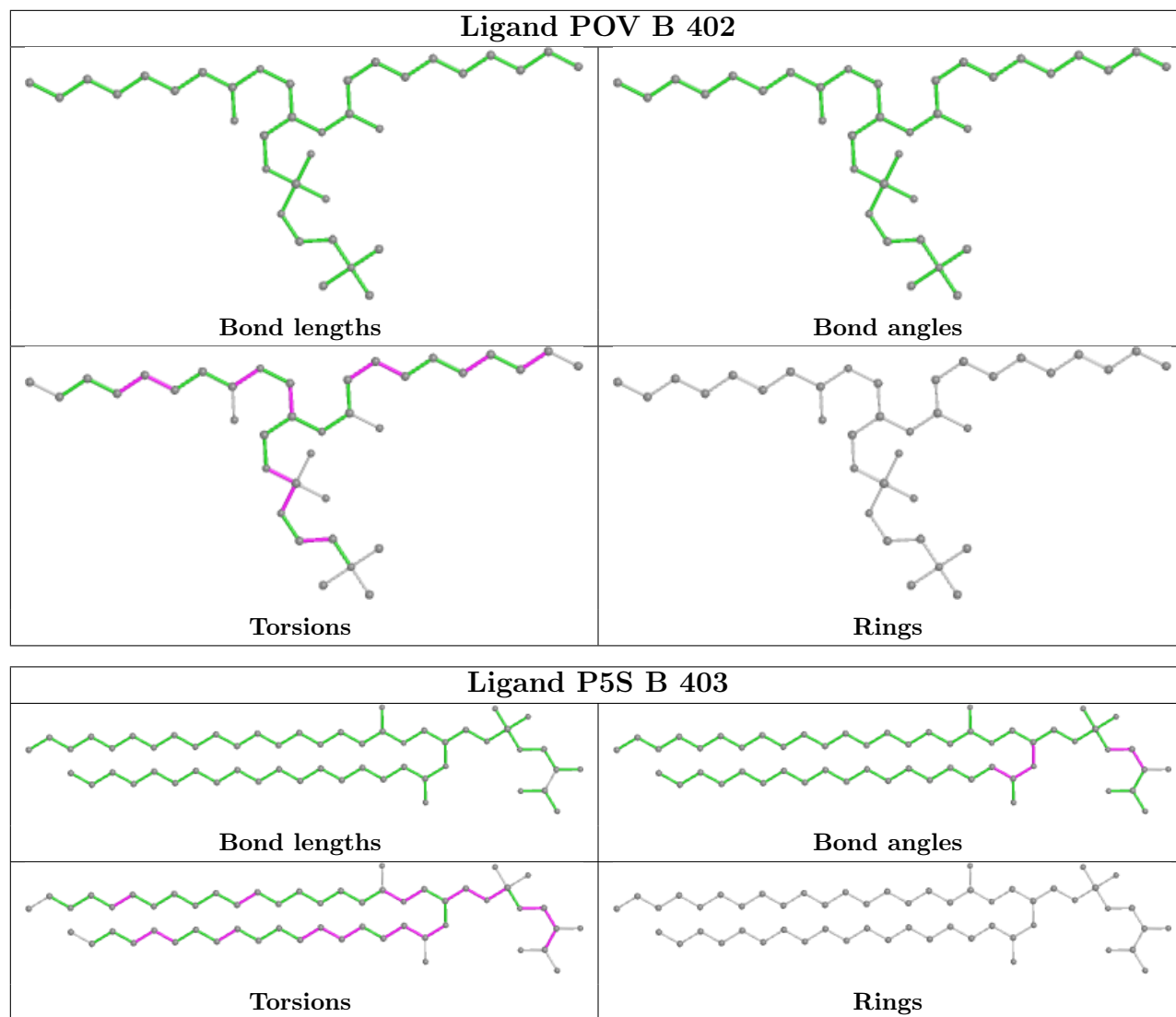
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ATP	1	0
6	C	403	P5S	3	0
6	A	405	P5S	2	0
5	A	403	POV	1	0
5	D	403	POV	1	0
6	E	2008	P5S	6	0
6	D	401	P5S	3	0
3	E	2002	ATP	1	0

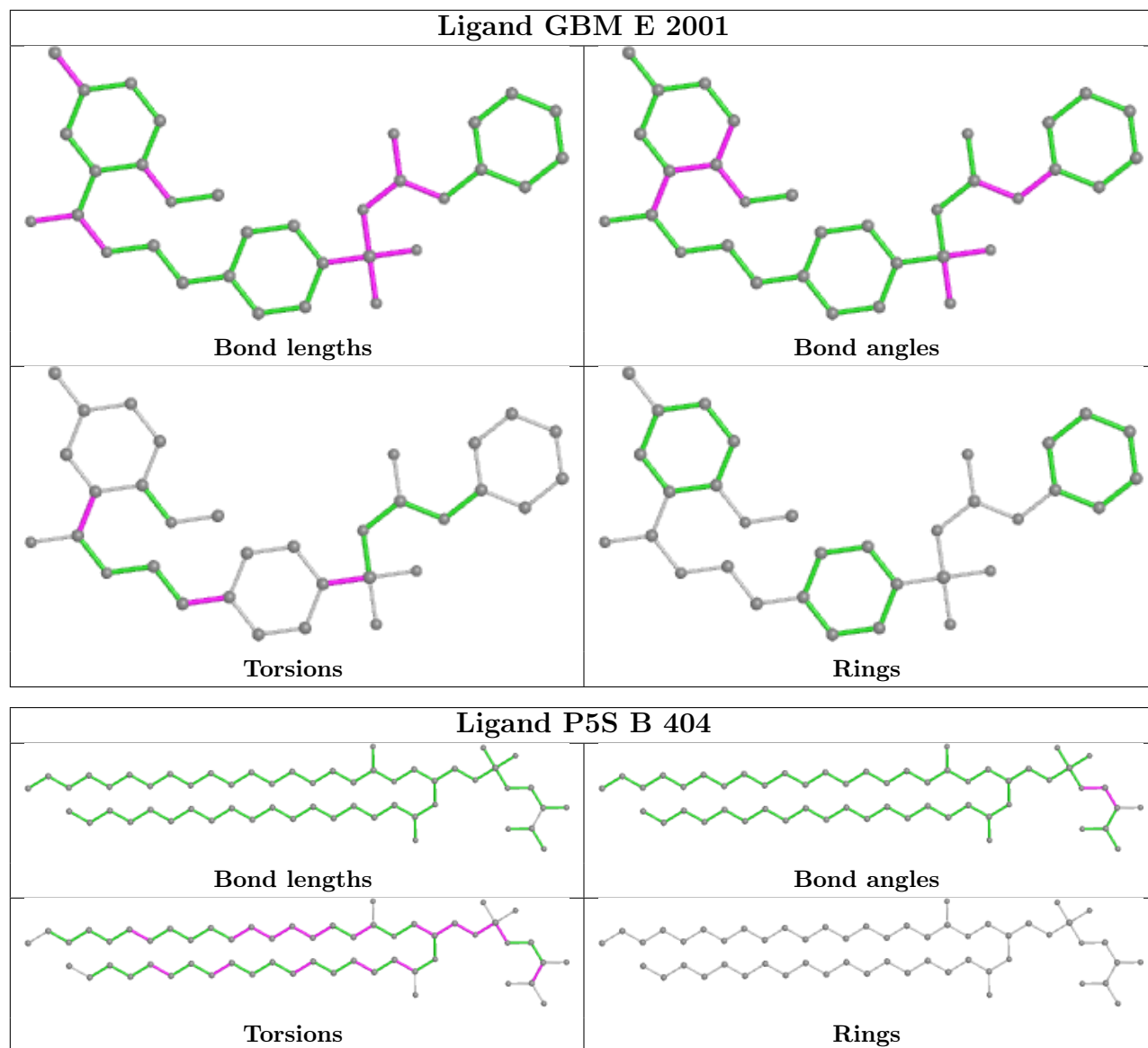
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

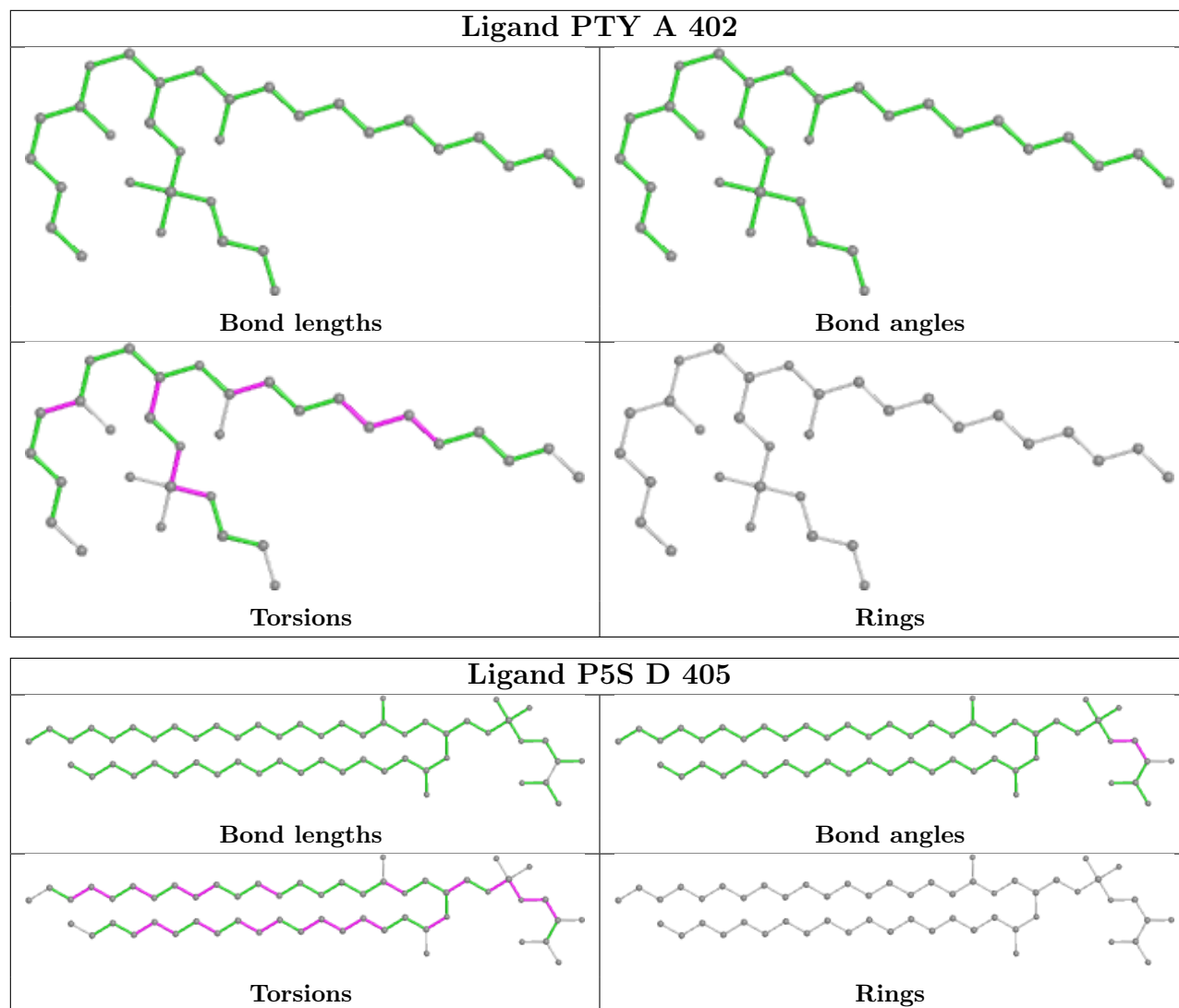


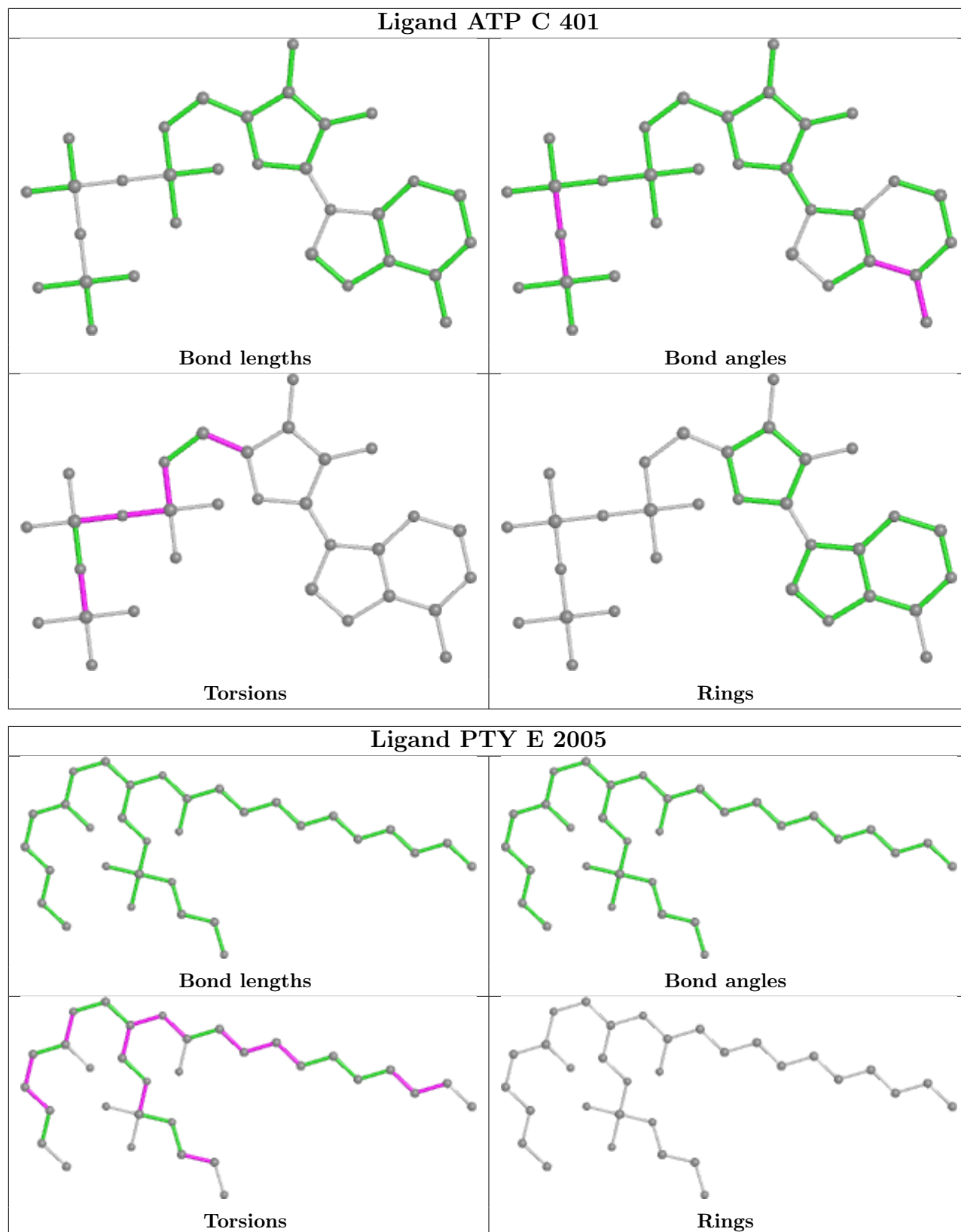


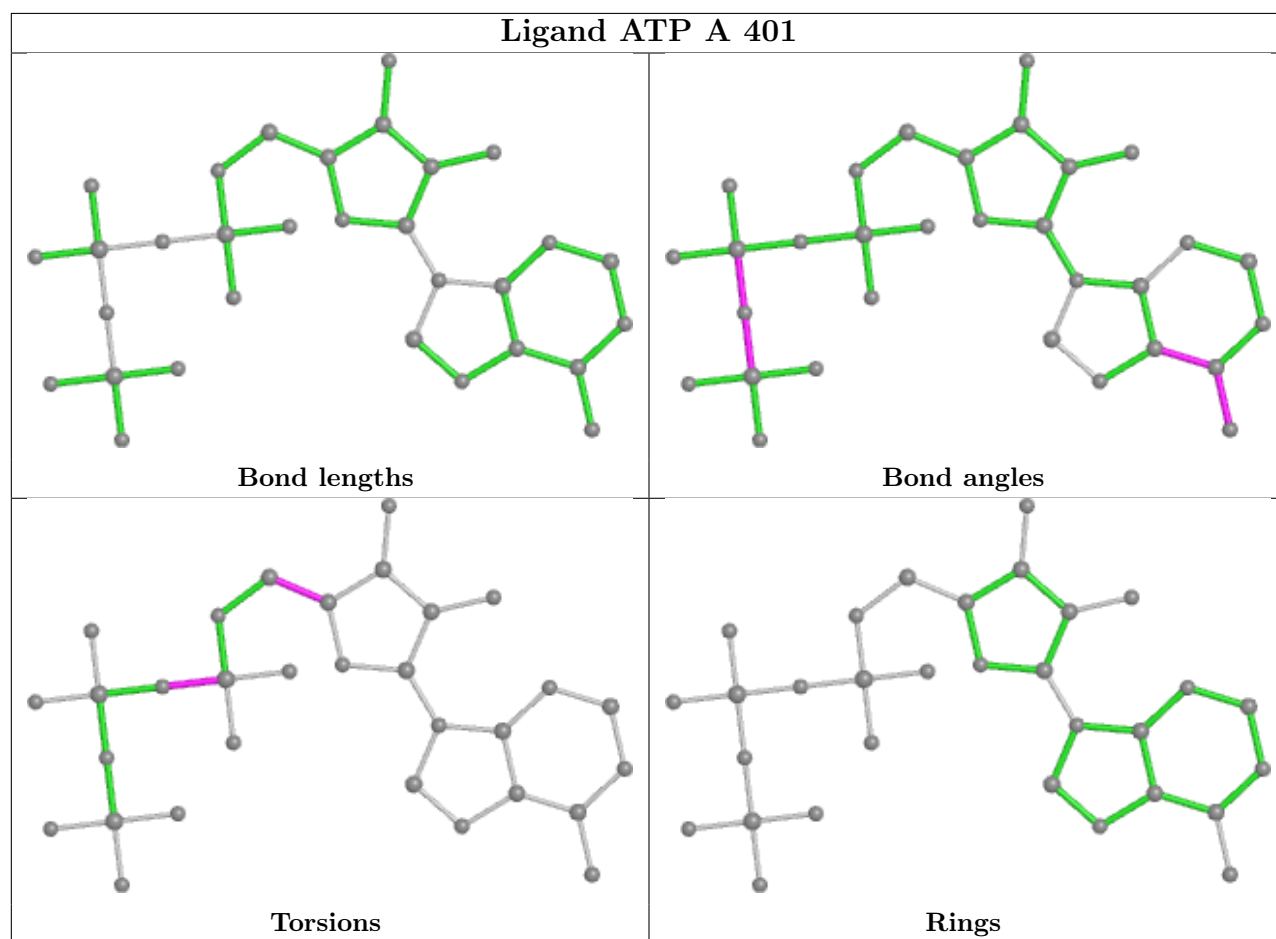
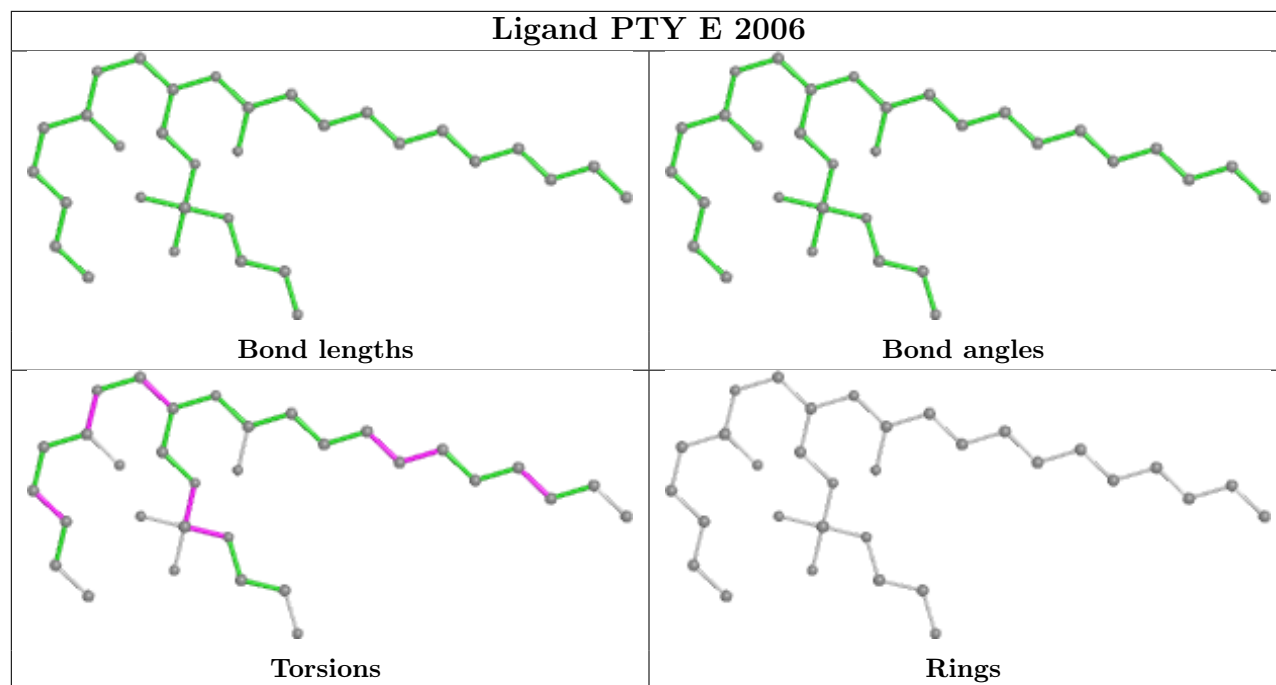




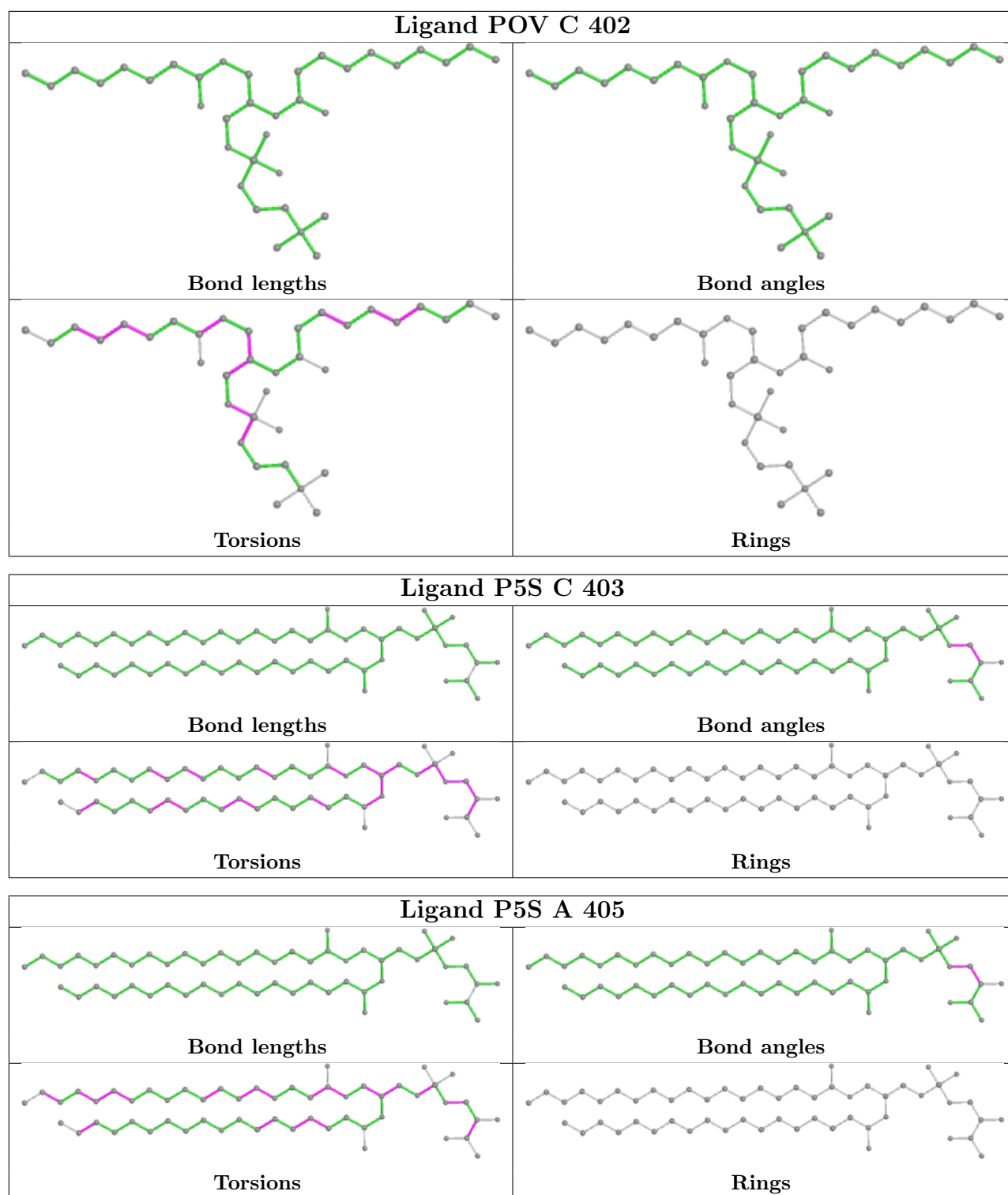


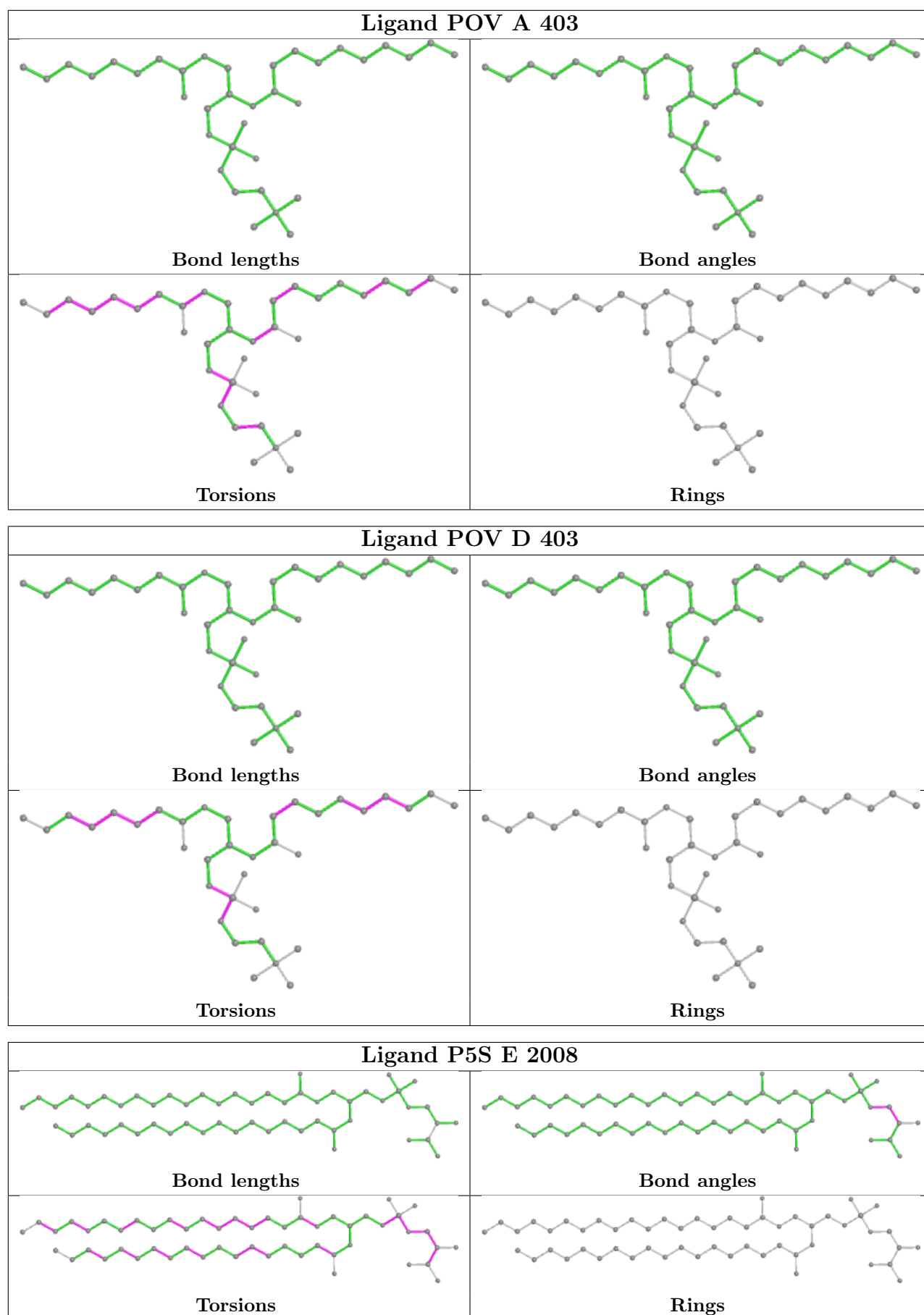


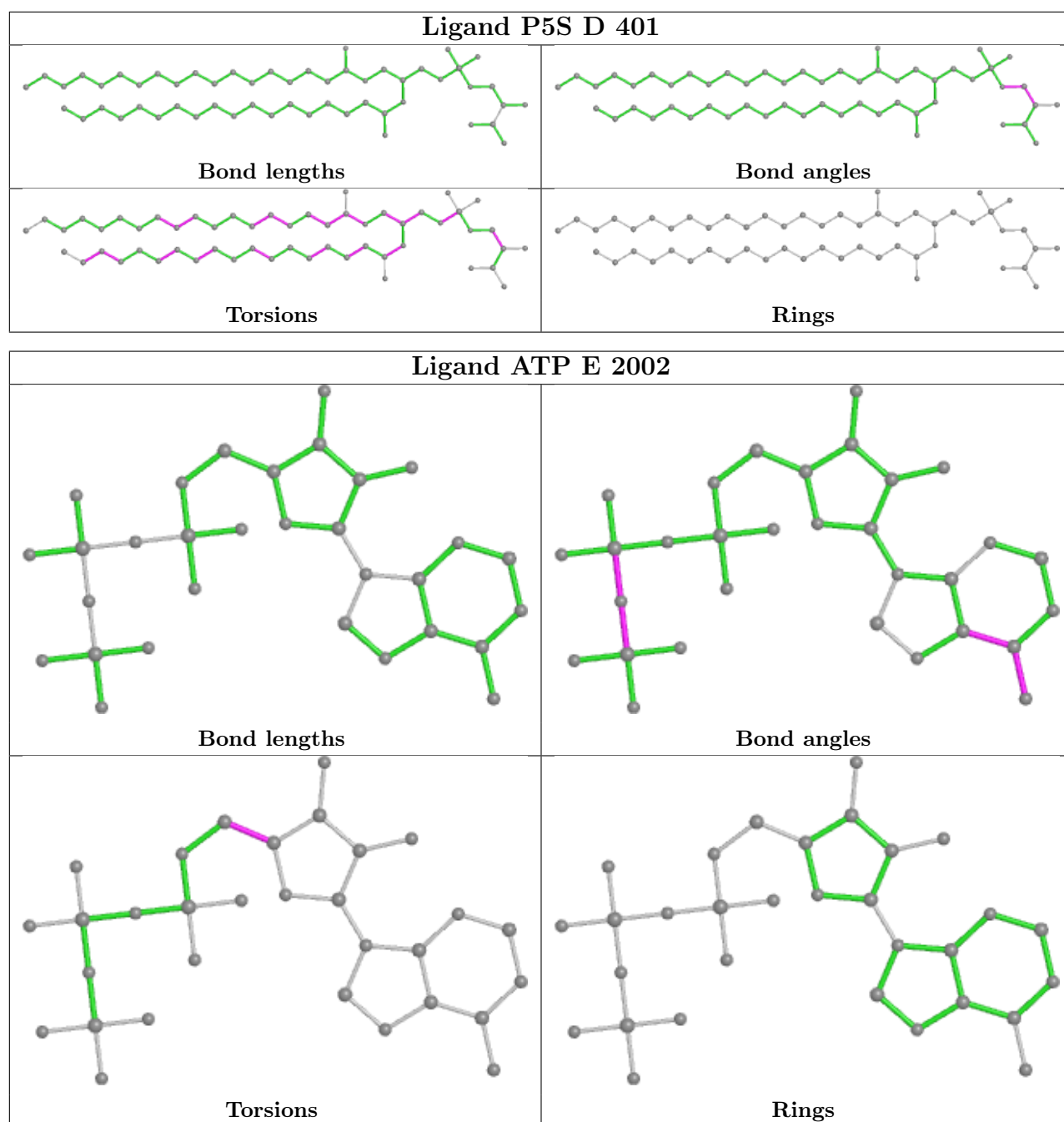












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

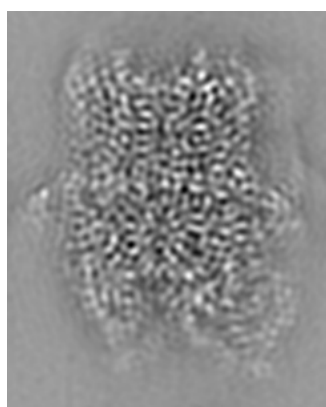
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26307. These allow visual inspection of the internal detail of the map and identification of artifacts.

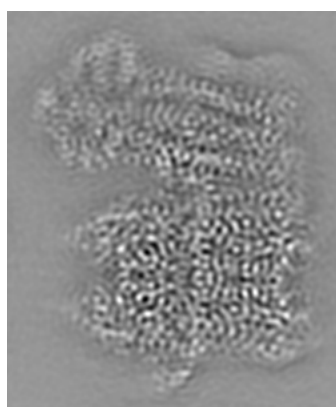
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

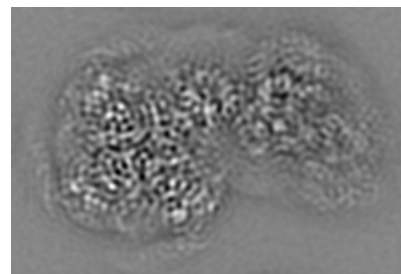
#### 6.1.1 Primary map



X



Y



Z

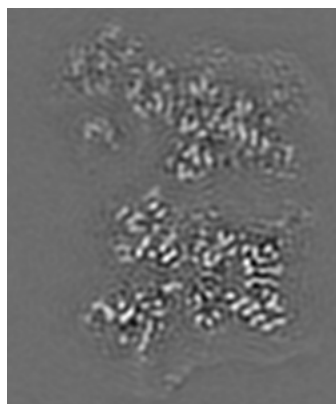
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

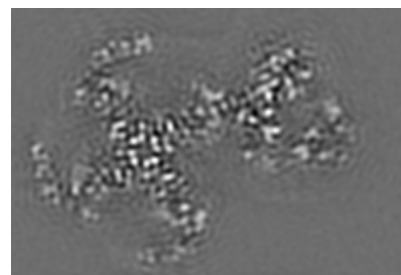
#### 6.2.1 Primary map



X Index: 64



Y Index: 43

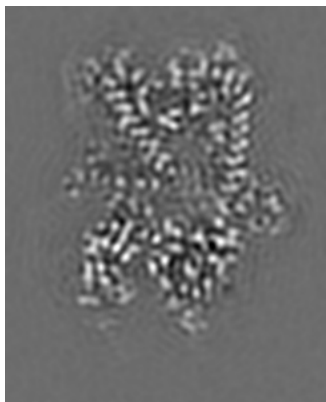


Z Index: 54

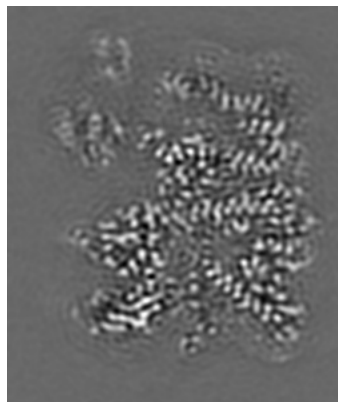
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

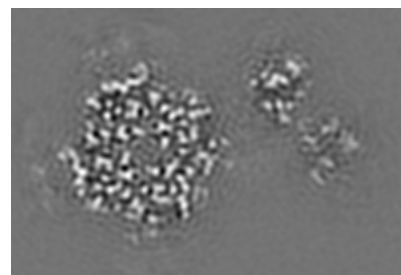
### 6.3.1 Primary map



X Index: 30



Y Index: 53



Z Index: 46

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

## 6.4 Orthogonal surface views [i](#)

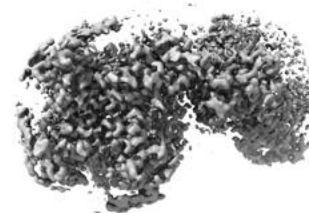
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

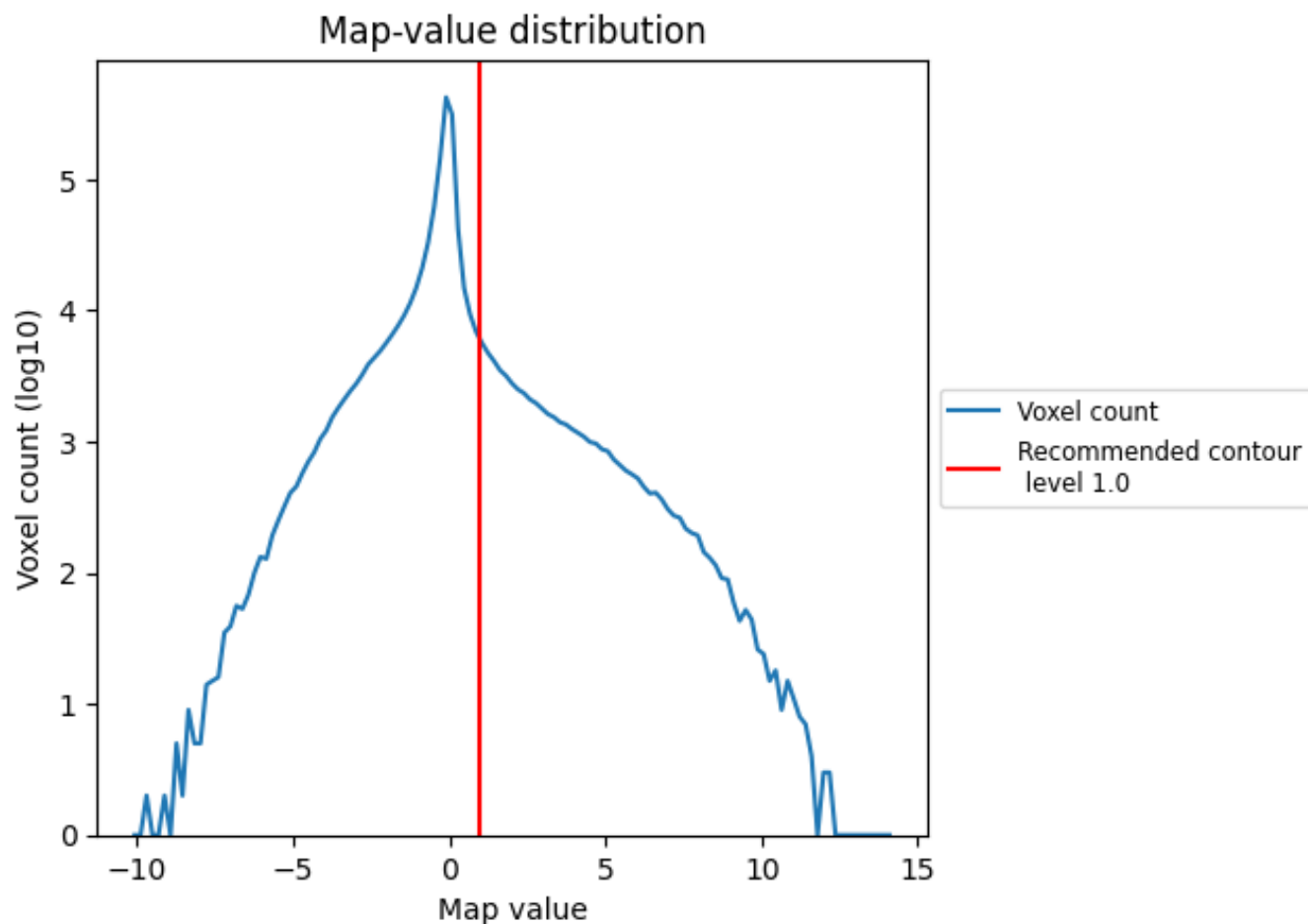
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

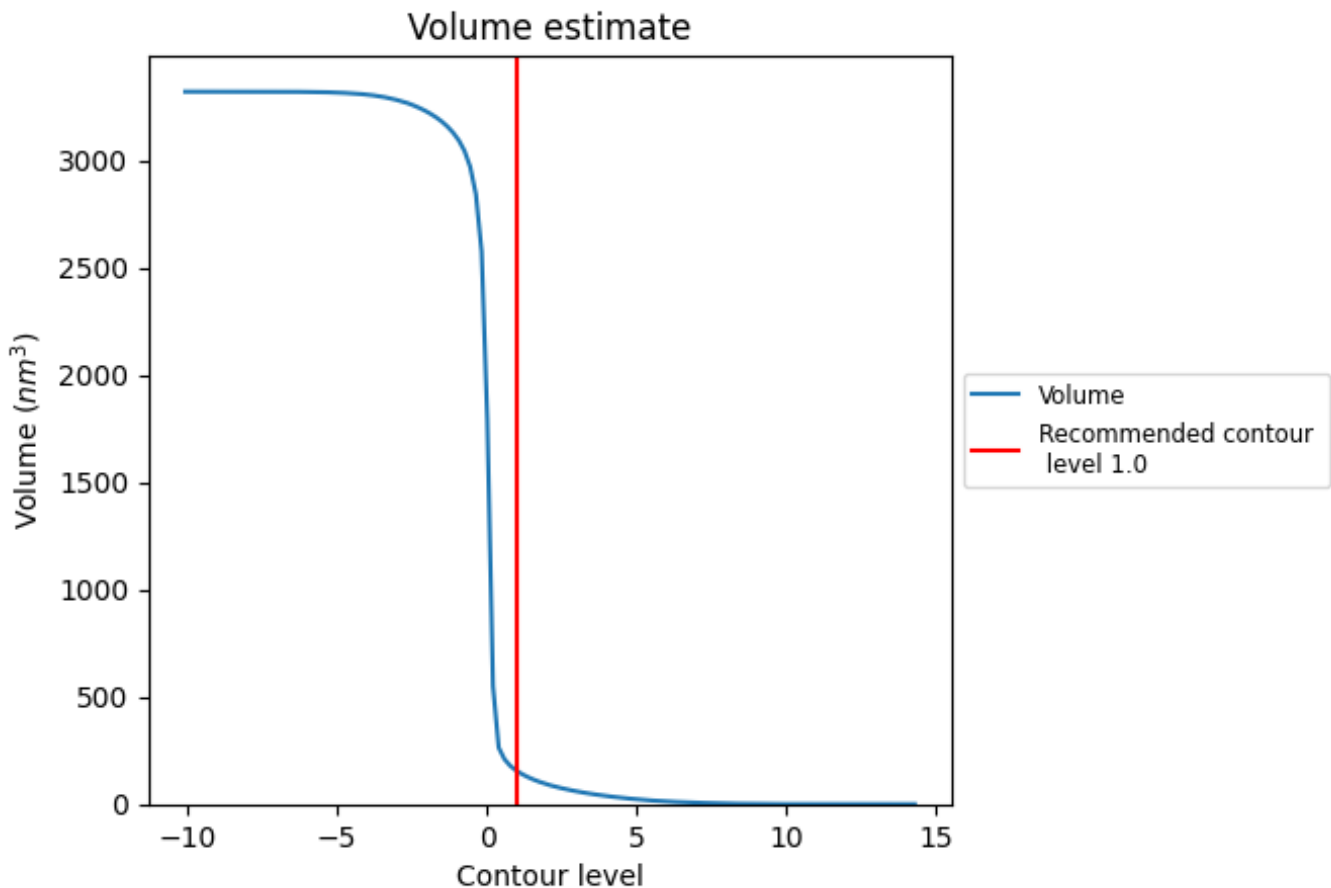
This section contains the results of statistical analysis of the map.

### 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 155 nm<sup>3</sup>; this corresponds to an approximate mass of 140 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.



## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

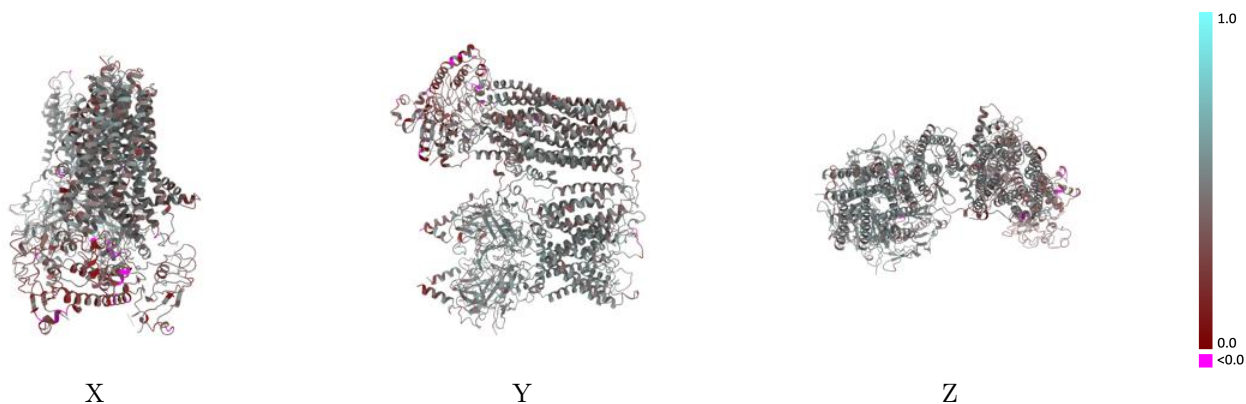
This section contains information regarding the fit between EMDB map EMD-26307 and PDB model 7U24. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



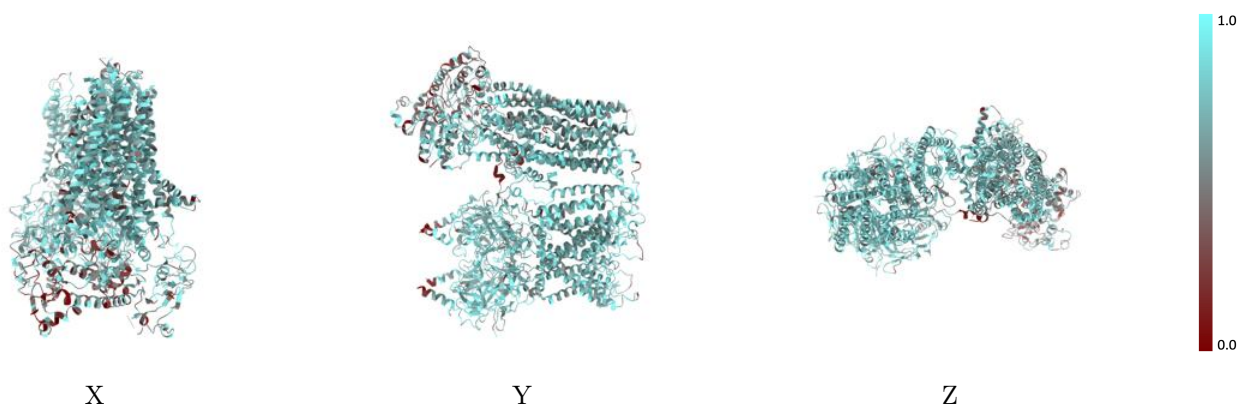
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



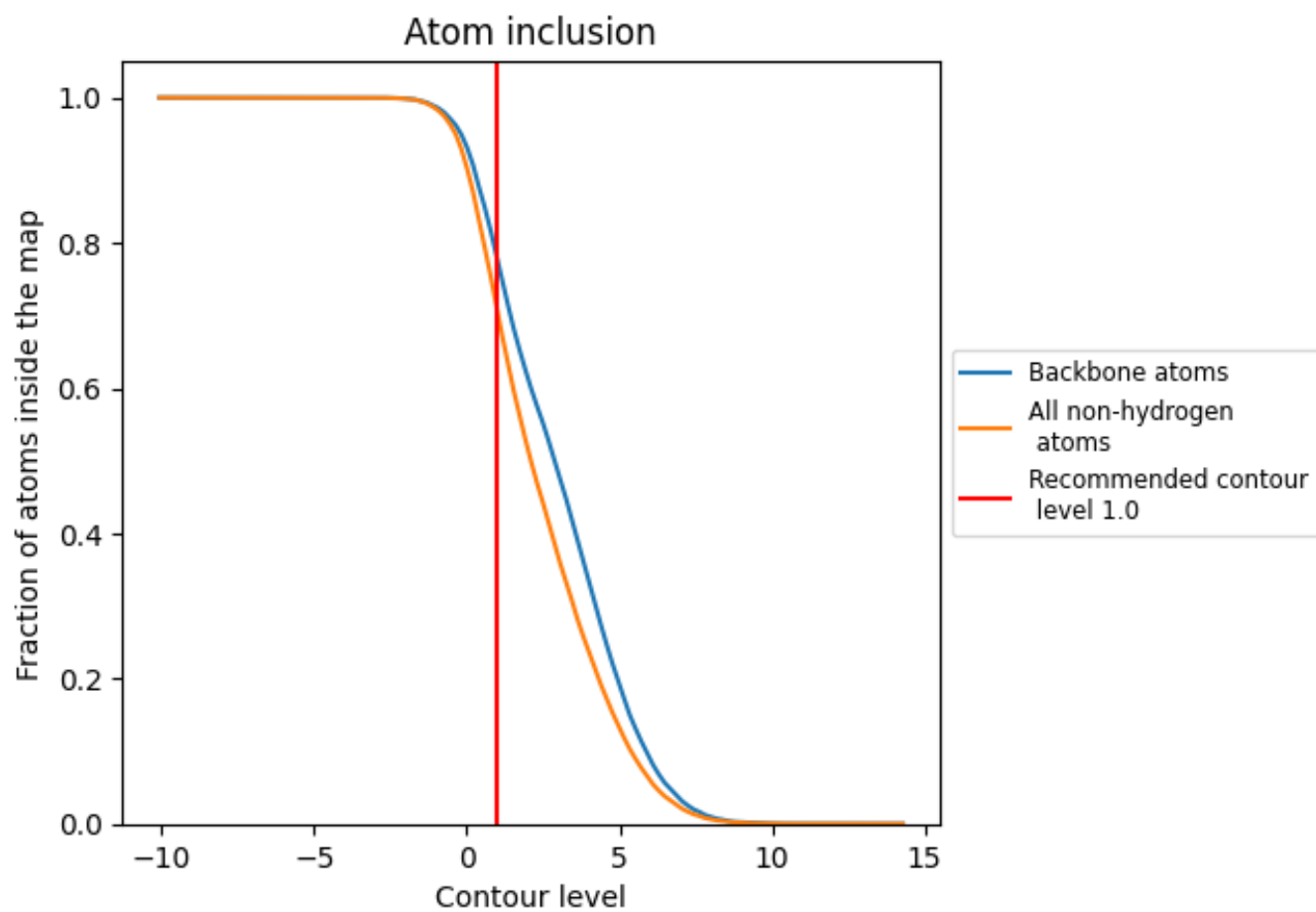
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.0).













## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 71% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7069	 0.4520
A	 0.7076	 0.4740
B	 0.7445	 0.4820
C	 0.7494	 0.4810
D	 0.7347	 0.4860
E	 0.6768	 0.4200

