



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:33 AM UTC

PDB ID : 7TYT / pdb_00007tyt
EMDB ID : EMD-26194
Title : Cryo-EM structure of the pancreatic ATP-sensitive potassium channel bound to ATP and repaglinide with Kir6.2-CTD in the down conformation
Authors : Shyng, S.L.; Sung, M.W.; Driggers, C.M.
Deposited on : 2022-02-14
Resolution : 3.60 Å (reported)
Based on initial models : 6BAA, 6PZ9

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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 EMD 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) : 2.49

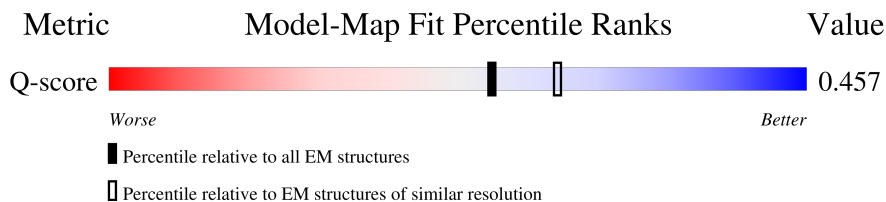
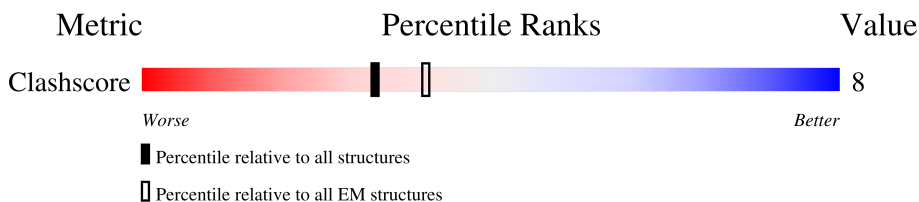
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

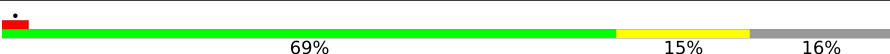
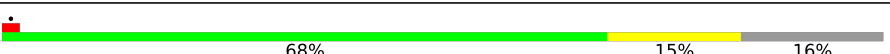
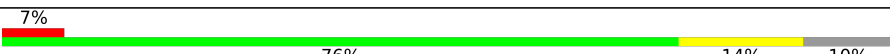
The reported resolution of this entry is 3.60 Å.

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	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	A	390	
1	B	390	
1	C	390	
1	D	390	
2	E	1582	
3	F	2	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 20349 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
1	A	356	Total	C	N	O	S	0	0
			2535	1634	446	441	14		
1	B	326	Total	C	N	O	S	0	0
			2349	1529	407	400	13		
1	C	326	Total	C	N	O	S	0	0
			2370	1542	410	403	15		
1	D	326	Total	C	N	O	S	0	0
			2395	1554	410	416	15		

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

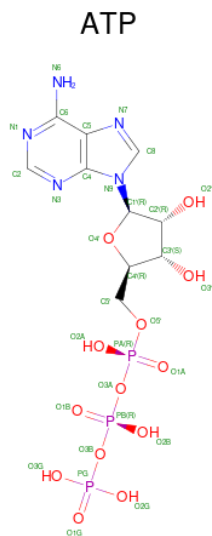
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1425	Total	C	N	O	S	0	0
			10003	6473	1737	1757	36		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

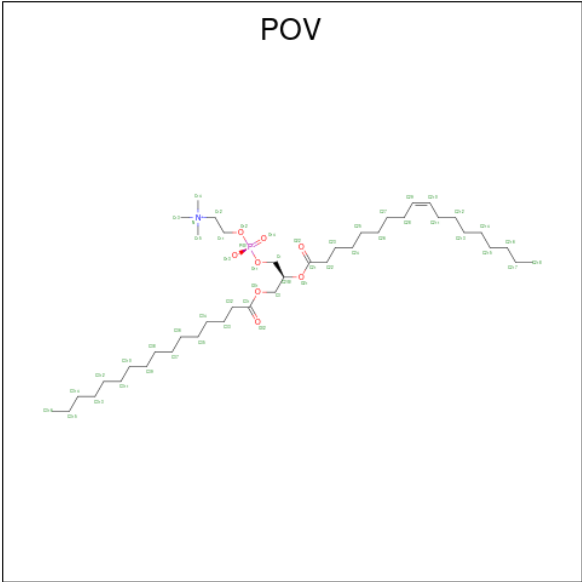


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0
4	D	1	Total 31	C 10	N 5	O 13	P 3	0
4	E	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

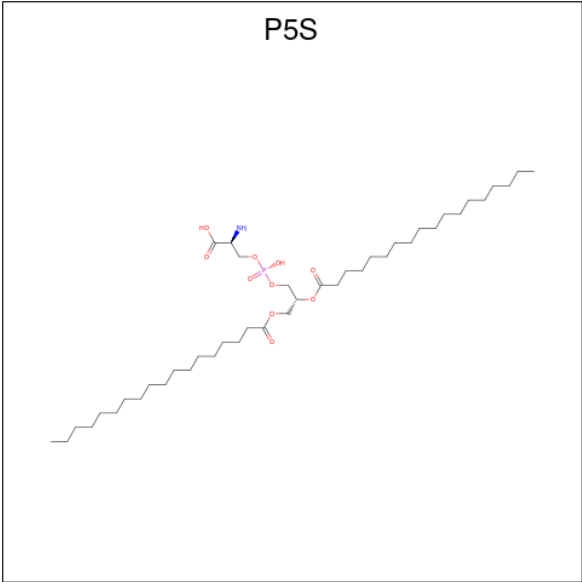
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total K 1 1	0

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



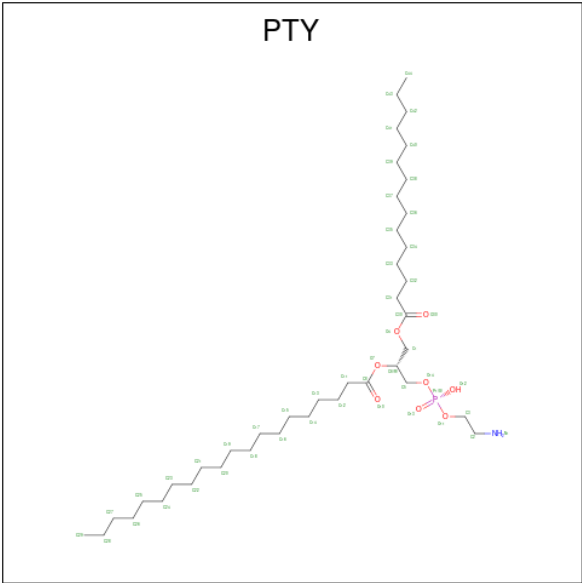
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	D	1	Total	C	N	O	P	0
			36	26	1	8	1	
6	E	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			54	42	1	10	1	
7	E	1	Total	C	N	O	P	0
			54	42	1	10	1	

- Molecule 8 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



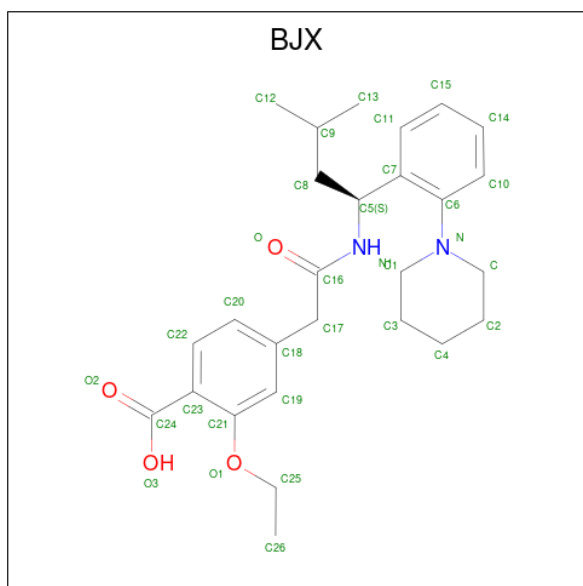
Mol	Chain	Residues	Atoms					AltConf
8	E	1	Total	C	N	O	P	0
			32	22	1	8	1	
8	E	1	Total	C	N	O	P	0
			32	22	1	8	1	

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

- Molecule 9 is Repaglinide (CCD ID: BJX) (formula: $C_{27}H_{36}N_2O_4$) (labeled as "Ligand of Interest" by depositor).

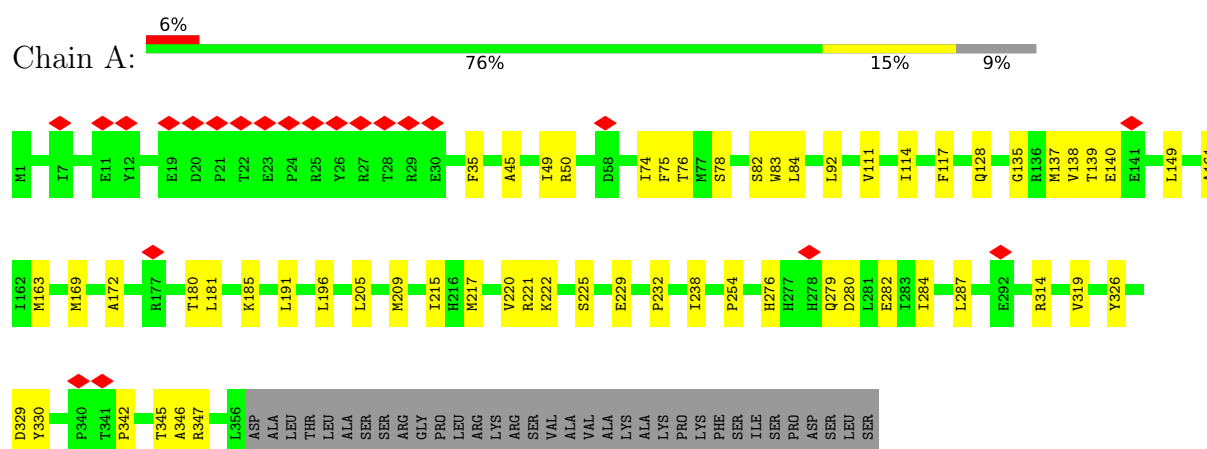


Mol	Chain	Residues	Atoms				AltConf
9	E	1	Total	C	N	O	0
			33	27	2	4	

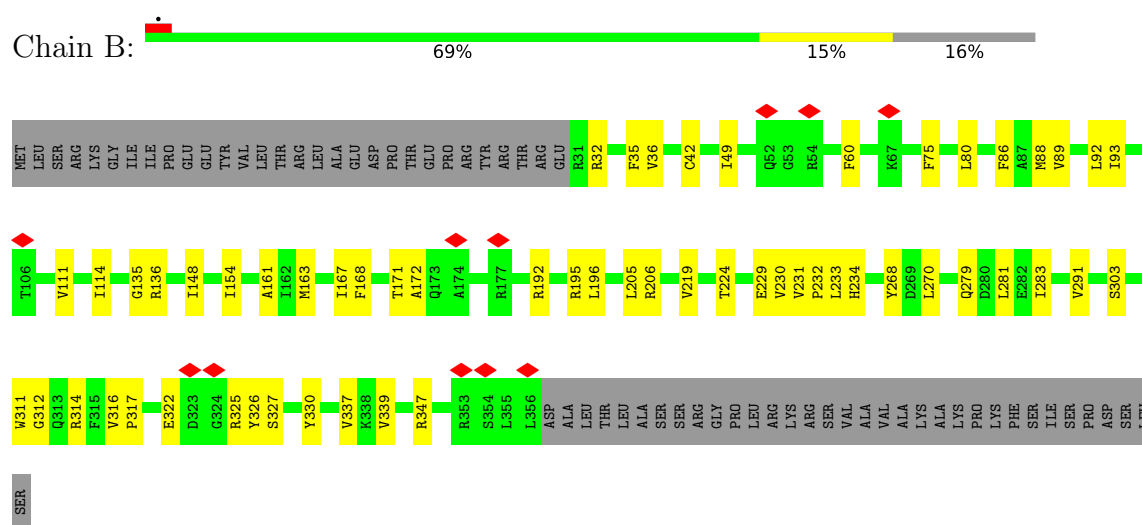
3 Residue-property plots

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: ATP-sensitive inward rectifier potassium channel 11

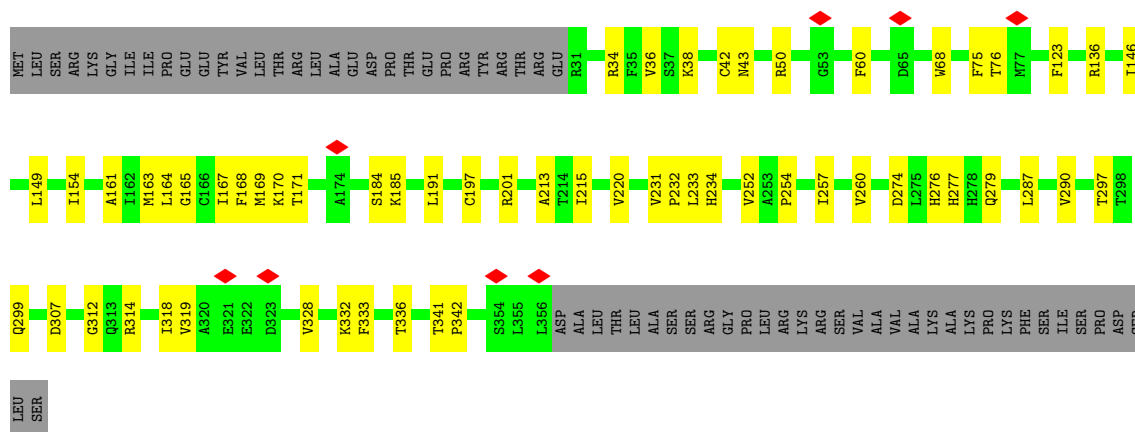


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

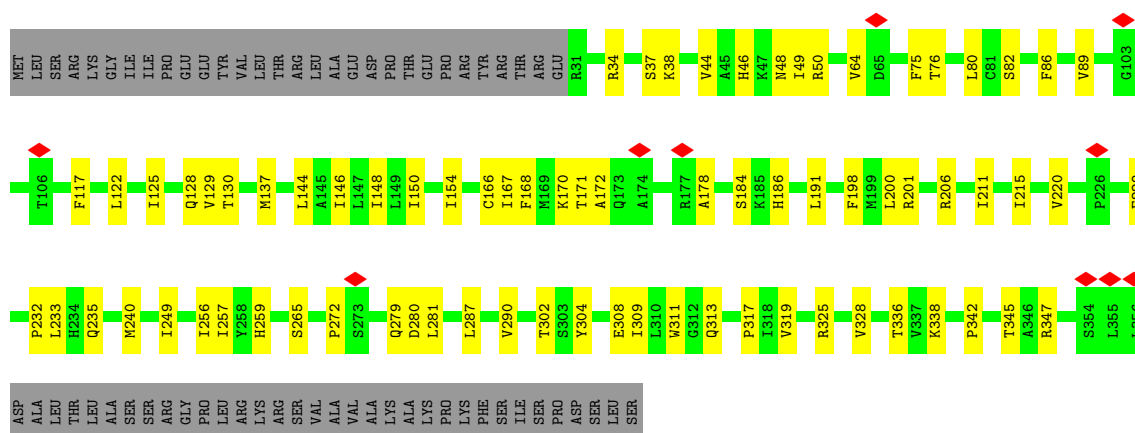


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

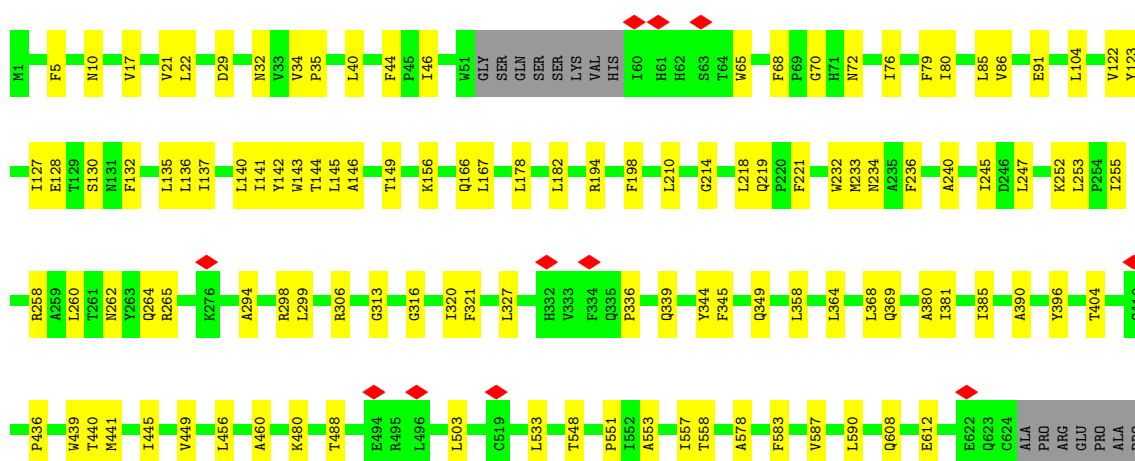
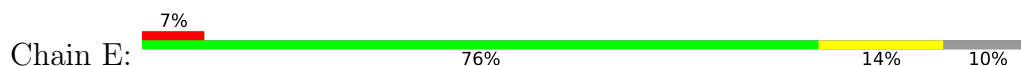


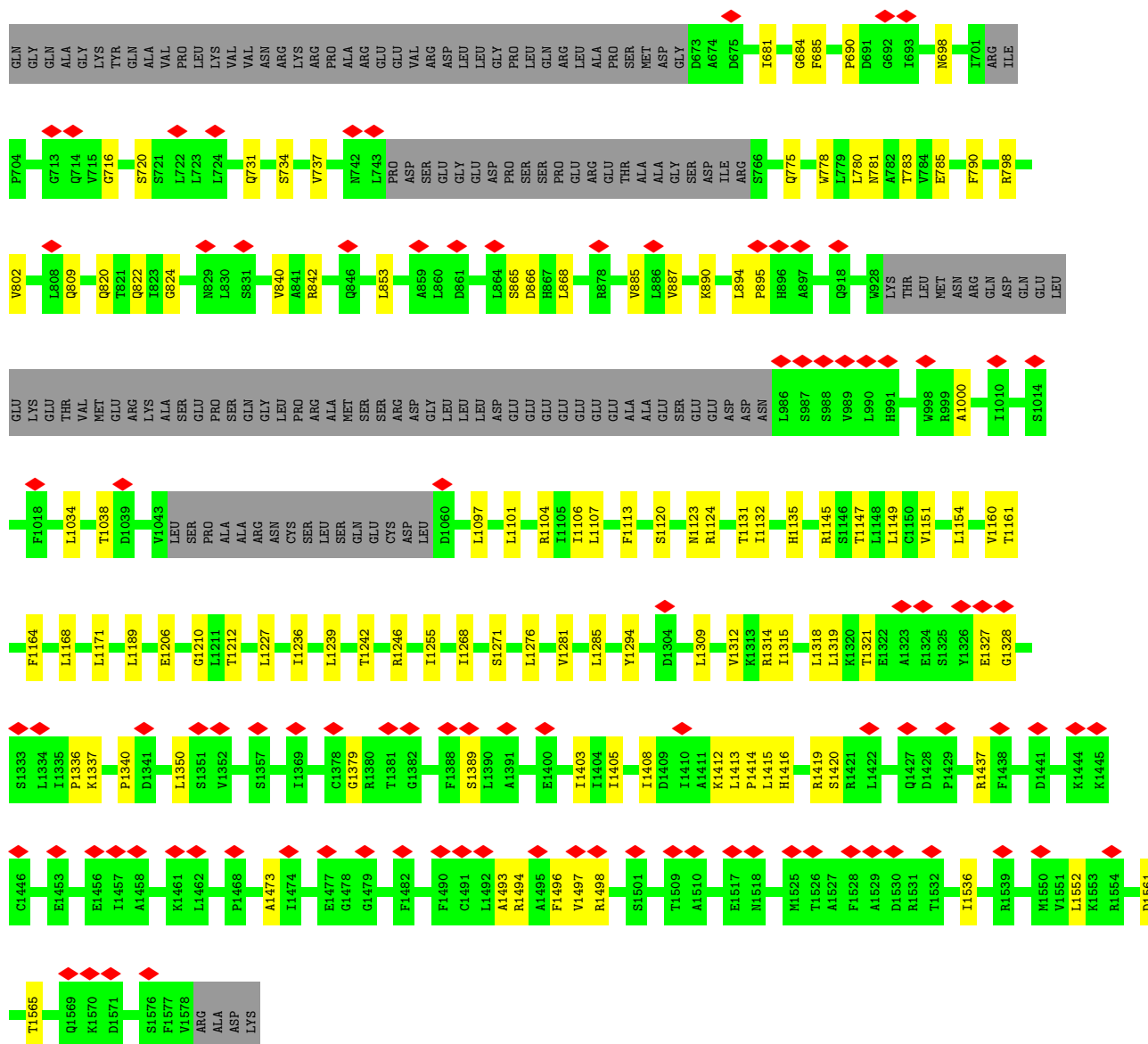


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



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





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36042	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	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	14.074	Depositor
Minimum map value	-9.463	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	166.155, 109.725, 149.435	wwPDB
Map dimensions	143, 105, 159	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	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: P5S, K, PTY, POV, ATP, NAG, BJX

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	0.16	0/2592	0.29	0/3551
1	B	0.16	0/2402	0.31	0/3287
1	C	0.18	0/2424	0.32	0/3315
1	D	0.17	0/2451	0.30	0/3355
2	E	0.15	0/10215	0.31	0/13997
All	All	0.16	0/20084	0.31	0/27505

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	2535	0	2344	52	0
1	B	2349	0	2249	46	0
1	C	2370	0	2286	52	0
1	D	2395	0	2297	61	0
2	E	10003	0	9134	150	0
3	F	28	0	25	1	0
4	A	31	0	12	5	0
4	B	62	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	31	0	12	1	0
4	E	31	0	12	4	0
5	A	1	0	0	0	0
6	A	36	0	45	2	0
6	B	36	0	45	1	0
6	C	36	0	45	0	0
6	D	36	0	45	2	0
6	E	36	0	45	1	0
7	B	54	0	80	1	0
7	E	54	0	80	5	0
8	E	192	0	222	7	0
9	E	33	0	0	1	0
All	All	20349	0	19002	328	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 8.

All (328) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:SER:HB3	1:A:229:GLU:HB2	1.67	0.75
2:E:781:ASN:ND2	2:E:1206:GLU:OE2	2.22	0.73
1:A:181:LEU:HD21	1:A:287:LEU:HD22	1.70	0.72
2:E:775:GLN:NE2	4:E:1603:ATP:O2G	2.25	0.69
2:E:690:PRO:HA	2:E:731:GLN:HG2	1.74	0.69
1:B:49:ILE:HA	4:B:404:ATP:HN62	1.58	0.68
1:B:161:ALA:HB1	1:C:167:ILE:HG21	1.75	0.67
1:C:68:TRP:HD1	1:C:170:LYS:HE3	1.59	0.67
2:E:127:ILE:HG21	2:E:136:LEU:HG	1.76	0.66
2:E:234:ASN:ND2	8:E:1606:PTY:O10	2.28	0.66
1:B:311:TRP:HD1	1:B:312:GLY:H	1.44	0.66
1:C:274:ASP:OD2	1:C:279:GLN:NE2	2.29	0.66
1:C:201:ARG:NH2	1:C:318:ILE:HG13	2.11	0.66
1:D:178:ALA:O	1:D:206:ARG:NH2	2.28	0.66
1:C:232:PRO:HG3	1:D:317:PRO:HB3	1.79	0.65
2:E:1104:ARG:NH1	2:E:1319:LEU:O	2.29	0.65
2:E:1101:LEU:HD11	2:E:1318:LEU:HD23	1.77	0.65
1:B:224:THR:HG22	1:B:230:VAL:HG22	1.78	0.65
2:E:1271:SER:HA	2:E:1276:LEU:H	1.60	0.65
1:C:184:SER:HB3	1:C:201:ARG:HB3	1.78	0.65
1:B:36:VAL:HA	1:B:42:CYS:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:219:GLN:OE1	2:E:232:TRP:NE1	2.27	0.64
1:A:185:LYS:NZ	4:A:401:ATP:O1G	2.28	0.64
1:A:221:ARG:NH1	1:A:280:ASP:O	2.31	0.64
1:B:233:LEU:HD12	1:C:319:VAL:HG11	1.80	0.63
2:E:1104:ARG:NH2	2:E:1321:THR:O	2.25	0.63
1:A:222:LYS:HG3	1:A:232:PRO:HA	1.80	0.63
1:C:312:GLY:HA3	1:C:341:THR:HG21	1.80	0.63
2:E:866:ASP:HB3	2:E:890:LYS:HE2	1.81	0.63
1:A:326:TYR:HB2	1:D:44:VAL:HG13	1.81	0.62
1:C:36:VAL:HG12	1:C:42:CYS:HA	1.81	0.62
1:C:232:PRO:HB2	1:D:319:VAL:HB	1.80	0.62
1:A:329:ASP:OD1	1:D:48:ASN:ND2	2.34	0.61
2:E:1171:LEU:HD22	2:E:1255:ILE:HG23	1.82	0.61
1:C:146:ILE:HG12	1:D:122:LEU:HD21	1.83	0.61
2:E:1160:VAL:HG12	2:E:1161:THR:HG23	1.82	0.61
1:B:36:VAL:HG13	1:B:303:SER:HB2	1.82	0.61
2:E:80:ILE:HG22	7:E:1607:P5S:H30A	1.82	0.60
1:C:299:GLN:HB2	1:D:211:ILE:HD12	1.83	0.60
1:D:279:GLN:HG3	1:D:281:LEU:H	1.65	0.60
1:A:314:ARG:HH12	1:D:229:GLU:HA	1.67	0.59
1:A:45:ALA:N	1:B:326:TYR:O	2.33	0.59
1:D:34:ARG:NH2	1:D:308:GLU:OE1	2.36	0.59
2:E:123:TYR:OH	2:E:135:LEU:O	2.20	0.59
2:E:265:ARG:NH2	2:E:294:ALA:O	2.35	0.59
4:A:401:ATP:N6	1:D:48:ASN:O	2.35	0.59
1:B:229:GLU:OE1	1:C:314:ARG:NH1	2.37	0.58
2:E:778:TRP:CE2	2:E:1210:GLY:HA3	2.38	0.58
1:B:111:VAL:HG23	1:B:114:ILE:HG13	1.86	0.57
1:D:184:SER:HB3	1:D:201:ARG:HB3	1.86	0.57
1:A:138:VAL:HG21	1:A:149:LEU:HD22	1.86	0.57
1:A:117:PHE:N	6:A:403:POV:O14	2.37	0.56
1:C:168:PHE:O	1:C:171:THR:OG1	2.21	0.56
2:E:364:LEU:HD22	7:E:1607:P5S:H56A	1.86	0.56
1:C:34:ARG:HH12	1:C:38:LYS:HG2	1.71	0.55
1:A:45:ALA:HB3	1:B:327:SER:HA	1.88	0.55
1:C:191:LEU:HD11	1:C:342:PRO:HD2	1.87	0.55
2:E:1494:ARG:HA	2:E:1497:VAL:HB	1.88	0.55
2:E:488:THR:HG21	2:E:533:LEU:HD13	1.88	0.55
2:E:798:ARG:O	2:E:802:VAL:HG23	2.07	0.55
4:B:404:ATP:H5'2	1:C:185:LYS:HB2	1.89	0.54
2:E:306:ARG:HG3	2:E:440:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:VAL:HG22	1:B:337:VAL:HG13	1.89	0.54
2:E:1561:ASP:H	2:E:1565:THR:HA	1.72	0.54
2:E:298:ARG:NH1	7:E:1607:P5S:O15	2.36	0.54
2:E:441:MET:O	2:E:445:ILE:HG13	2.08	0.54
1:B:32:ARG:NH1	1:B:279:GLN:O	2.41	0.54
4:A:401:ATP:HN62	1:D:49:ILE:HA	1.73	0.53
1:C:277:HIS:HB2	1:C:307:ASP:HB3	1.90	0.53
2:E:178:LEU:O	2:E:182:LEU:HG	2.09	0.53
2:E:218:LEU:H	2:E:218:LEU:HD23	1.74	0.53
1:B:168:PHE:HD2	1:C:168:PHE:HB2	1.73	0.53
1:C:146:ILE:HG21	6:D:402:POV:H27A	1.90	0.53
1:B:75:PHE:CZ	1:B:163:MET:HA	2.44	0.53
1:A:191:LEU:HD12	1:A:342:PRO:HD2	1.91	0.53
2:E:349:GLN:OE1	2:E:349:GLN:N	2.28	0.53
2:E:1034:LEU:O	2:E:1038:THR:OG1	2.24	0.53
2:E:684:GLY:O	2:E:698:ASN:N	2.42	0.52
1:B:195:ARG:NH1	1:B:196:LEU:H	2.08	0.52
1:C:215:ILE:HG21	1:C:257:ILE:HG21	1.91	0.52
2:E:456:LEU:HB2	2:E:460:ALA:HB2	1.92	0.52
1:C:213:ALA:HB1	1:C:287:LEU:HD11	1.90	0.52
1:A:169:MET:HE1	1:B:172:ALA:N	2.25	0.52
1:D:272:PRO:HB3	1:D:311:TRP:CD1	2.45	0.52
1:C:201:ARG:NH1	1:C:333:PHE:O	2.43	0.52
2:E:1416:HIS:O	2:E:1420:SER:OG	2.23	0.52
1:B:167:ILE:O	1:B:171:THR:OG1	2.24	0.52
1:C:50:ARG:NH1	4:D:401:ATP:O1B	2.37	0.52
1:C:231:VAL:HG11	1:C:234:HIS:CD2	2.45	0.52
1:B:206:ARG:HH21	1:B:291:VAL:HG11	1.75	0.51
2:E:1124:ARG:HD2	2:E:1314:ARG:HB3	1.91	0.51
1:A:196:LEU:HD12	1:A:346:ALA:HB2	1.92	0.51
2:E:551:PRO:HG3	2:E:587:VAL:HG21	1.92	0.51
2:E:840:VAL:HG23	2:E:853:LEU:HD22	1.93	0.51
2:E:70:GLY:HA2	6:E:1608:POV:H2	1.91	0.51
2:E:86:VAL:HG11	2:E:364:LEU:HD11	1.91	0.51
2:E:783:THR:HB	2:E:820:GLN:HA	1.92	0.51
2:E:65:TRP:HZ3	8:E:1604:PTY:HC21	1.76	0.51
1:B:60:PHE:HB2	1:C:68:TRP:HH2	1.76	0.51
1:A:49:ILE:HD11	1:B:205:LEU:HD13	1.93	0.50
2:E:445:ILE:HD13	2:E:590:LEU:HD23	1.92	0.50
1:C:201:ARG:HH22	1:C:318:ILE:HG13	1.75	0.50
1:D:86:PHE:HA	1:D:89:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:LEU:O	2:E:44:PHE:HB2	2.11	0.50
1:A:74:ILE:O	1:A:78:SER:OG	2.21	0.50
1:C:75:PHE:CZ	1:C:163:MET:HA	2.47	0.50
1:A:83:TRP:HZ3	1:D:150:ILE:HG23	1.77	0.50
2:E:316:GLY:O	2:E:320:ILE:HG13	2.11	0.49
2:E:558:THR:HG21	2:E:583:PHE:HZ	1.75	0.49
2:E:809:GLN:OE1	2:E:809:GLN:N	2.45	0.49
1:B:88:MET:HE1	6:B:402:POV:H36	1.94	0.49
2:E:716:GLY:HA2	4:E:1603:ATP:H5'2	1.95	0.49
1:D:75:PHE:HZ	1:D:166:CYS:HB3	1.77	0.49
1:A:82:SER:OG	1:A:128:GLN:NE2	2.45	0.49
1:B:314:ARG:HG3	1:B:339:VAL:HG11	1.95	0.49
2:E:29:ASP:HA	2:E:32:ASN:HD22	1.77	0.49
1:C:154:ILE:HD13	1:D:76:THR:HG23	1.94	0.49
1:D:345:THR:HG22	1:D:347:ARG:H	1.78	0.49
1:A:220:VAL:HG23	1:A:282:GLU:HB3	1.95	0.49
1:B:42:CYS:SG	1:C:252:VAL:HG21	2.53	0.49
2:E:339:GLN:N	2:E:339:GLN:OE1	2.45	0.49
1:A:161:ALA:HB1	1:B:167:ILE:HG13	1.95	0.48
1:B:35:PHE:CD1	1:B:233:LEU:HD13	2.48	0.48
2:E:142:TYR:O	2:E:146:ALA:N	2.43	0.48
1:C:161:ALA:HB1	1:D:167:ILE:HG13	1.95	0.48
2:E:790:PHE:HB2	2:E:842:ARG:HD2	1.94	0.48
2:E:445:ILE:O	2:E:449:VAL:HG12	2.13	0.48
2:E:553:ALA:O	2:E:557:ILE:HG12	2.13	0.48
2:E:396:TYR:CG	2:E:1227:LEU:HD22	2.49	0.48
2:E:1389:SER:HB3	2:E:1536:ILE:HD13	1.95	0.48
1:D:129:VAL:O	1:D:130:THR:OG1	2.24	0.48
1:A:140:GLU:N	1:A:140:GLU:OE1	2.47	0.48
2:E:122:VAL:HG22	8:E:1610:PTY:H112	1.96	0.48
2:E:156:LYS:HA	2:E:156:LYS:HD3	1.54	0.48
1:A:35:PHE:CZ	1:A:220:VAL:HG11	2.49	0.47
1:B:311:TRP:CD1	1:B:312:GLY:H	2.30	0.47
1:C:43:ASN:OD1	1:D:325:ARG:NE	2.31	0.47
1:C:319:VAL:HG22	1:C:328:VAL:HG22	1.94	0.47
1:D:211:ILE:HB	1:D:290:VAL:HG13	1.95	0.47
2:E:785:GLU:OE2	2:E:820:GLN:NE2	2.35	0.47
2:E:1415:LEU:HD22	2:E:1419:ARG:HH12	1.79	0.47
2:E:1337:LYS:HZ2	2:E:1408:ILE:HD13	1.79	0.47
1:A:135:GLY:HA3	1:D:137:MET:HE1	1.96	0.47
2:E:68:PHE:CE1	2:E:128:GLU:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD11	2:E:34:VAL:HG21	1.97	0.47
1:D:215:ILE:HG23	1:D:240:MET:HG3	1.96	0.47
2:E:1101:LEU:HD22	2:E:1315:ILE:HG23	1.97	0.47
1:A:172:ALA:HB2	1:D:168:PHE:HZ	1.80	0.47
2:E:141:ILE:O	2:E:145:LEU:HB2	2.15	0.47
2:E:1350:LEU:HD13	2:E:1403:ILE:HD11	1.96	0.47
4:A:401:ATP:H2'	1:D:50:ARG:HH12	1.79	0.47
1:B:270:LEU:HD23	1:B:270:LEU:HA	1.82	0.46
1:D:313:GLN:OE1	1:D:336:THR:OG1	2.25	0.46
2:E:91:GLU:HG3	2:E:167:LEU:HD23	1.97	0.46
2:E:327:LEU:HD23	2:E:1281:VAL:HG21	1.97	0.46
2:E:439:TRP:N	2:E:439:TRP:CD1	2.84	0.46
1:A:209:MET:SD	1:A:209:MET:N	2.82	0.46
2:E:1106:ILE:HG23	2:E:1107:LEU:HD23	1.95	0.46
1:B:205:LEU:HD11	4:B:401:ATP:H2	1.80	0.46
1:A:232:PRO:HD3	1:B:317:PRO:HB3	1.98	0.46
1:A:217:MET:HA	1:A:284:ILE:O	2.16	0.46
1:A:345:THR:HG22	1:A:347:ARG:H	1.81	0.46
1:B:322:GLU:HB2	1:B:325:ARG:O	2.15	0.46
1:D:215:ILE:HB	1:D:287:LEU:HD13	1.97	0.46
2:E:368:LEU:HD21	7:E:1607:P5S:H29A	1.98	0.46
1:A:180:THR:HB	1:A:205:LEU:HB2	1.97	0.46
2:E:143:TRP:HA	2:E:143:TRP:CE3	2.51	0.46
1:D:38:LYS:O	1:D:302:THR:OG1	2.33	0.46
1:C:290:VAL:HG12	1:C:297:THR:HG22	1.98	0.46
2:E:404:THR:HG21	2:E:1212:THR:HG22	1.98	0.46
2:E:608:GLN:O	2:E:612:GLU:HG3	2.16	0.46
1:A:84:LEU:HD21	6:A:403:POV:H36A	1.97	0.46
1:D:200:LEU:HD11	1:D:304:TYR:CE2	2.51	0.46
2:E:5:PHE:HA	2:E:104:LEU:HB3	1.98	0.46
1:C:220:VAL:HG13	1:C:233:LEU:HD22	1.96	0.45
2:E:385:ILE:HG21	2:E:1239:LEU:HG	1.97	0.45
2:E:1097:LEU:HD21	2:E:1315:ILE:HG21	1.98	0.45
1:B:268:TYR:CZ	1:B:347:ARG:HA	2.52	0.45
1:A:139:THR:HG22	1:A:140:GLU:H	1.81	0.45
2:E:22:LEU:HD23	2:E:22:LEU:HA	1.78	0.45
2:E:865:SER:HA	2:E:868:LEU:HD12	1.99	0.45
1:C:149:LEU:HD21	1:D:125:ILE:HG21	1.99	0.45
1:C:254:PRO:HB3	1:C:333:PHE:HE2	1.82	0.45
1:D:191:LEU:HD11	1:D:342:PRO:HD2	1.99	0.45
1:D:259:HIS:NE2	1:D:265:SER:OG	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1337:LYS:HE2	2:E:1340:PRO:HA	1.98	0.45
1:A:191:LEU:HD23	1:A:196:LEU:HD23	1.98	0.45
1:A:319:VAL:HB	1:D:232:PRO:HB2	1.99	0.45
2:E:79:PHE:HB2	7:E:1607:P5S:H27	1.98	0.45
8:E:1604:PTY:H312	8:E:1604:PTY:HC12	1.78	0.45
2:E:145:LEU:O	2:E:149:THR:HG22	2.17	0.45
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.78	0.45
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.74	0.45
2:E:65:TRP:NE1	2:E:221:PHE:O	2.46	0.45
1:A:75:PHE:CZ	1:A:163:MET:HA	2.52	0.44
1:D:82:SER:HB2	1:D:128:GLN:NE2	2.32	0.44
2:E:32:ASN:O	2:E:35:PRO:HD2	2.17	0.44
2:E:720:SER:OG	4:E:1603:ATP:O2B	2.35	0.44
1:A:319:VAL:O	1:D:232:PRO:HB3	2.18	0.44
1:C:197:CYS:SG	1:C:260:VAL:HG22	2.57	0.44
2:E:65:TRP:CZ3	8:E:1604:PTY:HC21	2.51	0.44
1:C:231:VAL:HG21	1:C:234:HIS:HD2	1.81	0.44
2:E:320:ILE:HG12	2:E:1285:LEU:HD23	1.98	0.44
2:E:1494:ARG:O	2:E:1498:ARG:N	2.47	0.44
2:E:240:ALA:HB2	2:E:245:ILE:HD11	1.99	0.44
2:E:720:SER:OG	4:E:1603:ATP:O1A	2.30	0.44
1:A:330:TYR:HB3	4:A:401:ATP:N6	2.32	0.44
1:D:80:LEU:HD12	1:D:80:LEU:HA	1.79	0.44
1:D:249:ILE:HD12	1:D:249:ILE:HA	1.90	0.44
2:E:380:ALA:HB2	2:E:436:PRO:HG2	1.99	0.44
2:E:681:ILE:HG23	2:E:737:VAL:HG22	1.99	0.44
1:A:215:ILE:HD11	1:A:287:LEU:HD12	2.00	0.44
1:D:233:LEU:HD13	1:D:233:LEU:HA	1.64	0.44
1:D:117:PHE:N	6:D:402:POV:O14	2.50	0.44
1:D:186:HIS:HB2	1:D:308:GLU:O	2.17	0.44
1:A:276:HIS:CD2	1:A:279:GLN:HB2	2.53	0.44
1:C:314:ARG:O	1:C:336:THR:HB	2.18	0.43
2:E:313:GLY:N	2:E:369:GLN:HG3	2.33	0.43
2:E:381:ILE:HG21	2:E:1242:THR:HG21	2.00	0.43
2:E:1123:ASN:HB3	2:E:1124:ARG:NH1	2.32	0.43
1:B:281:LEU:HD12	1:B:281:LEU:HA	1.89	0.43
1:D:220:VAL:HG22	1:D:235:GLN:HG2	1.99	0.43
2:E:247:LEU:HD12	2:E:247:LEU:HA	1.86	0.43
1:C:123:PHE:HB2	1:C:136:ARG:HD2	2.00	0.43
2:E:10:ASN:HB3	3:F:1:NAG:O5	2.18	0.43
2:E:780:LEU:O	2:E:824:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:GLN:HG2	1:D:338:LYS:HA	2.00	0.43
2:E:1000:ALA:HB1	2:E:1309:LEU:HD22	2.00	0.43
1:B:154:ILE:HD13	1:C:76:THR:HG23	1.99	0.43
2:E:358:LEU:HD12	2:E:358:LEU:HA	1.78	0.43
2:E:1164:PHE:O	2:E:1168:LEU:N	2.52	0.43
2:E:1327:GLU:HA	2:E:1414:PRO:HB3	2.00	0.43
1:B:192:ARG:HB3	1:B:192:ARG:NH1	2.34	0.43
2:E:17:VAL:HG13	2:E:21:VAL:HB	1.99	0.43
2:E:1132:ILE:HD11	2:E:1312:VAL:HG22	2.01	0.43
2:E:1493:ALA:HA	2:E:1496:PHE:HD2	1.83	0.43
2:E:1147:THR:O	2:E:1151:VAL:HG12	2.18	0.43
1:D:200:LEU:O	1:D:256:ILE:HA	2.19	0.43
1:D:220:VAL:HG13	1:D:233:LEU:HD12	2.01	0.43
2:E:233:MET:HE3	2:E:233:MET:O	2.19	0.43
1:A:76:THR:HG23	1:D:154:ILE:HD13	2.01	0.43
1:A:50:ARG:HD3	4:B:401:ATP:C5	2.54	0.42
2:E:214:GLY:O	2:E:252:LYS:HG2	2.19	0.42
1:A:217:MET:HG2	1:A:238:ILE:HG13	2.00	0.42
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.92	0.42
1:B:330:TYR:O	4:B:401:ATP:N6	2.52	0.42
1:D:279:GLN:OE1	1:D:280:ASP:N	2.51	0.42
2:E:72:ASN:O	2:E:76:ILE:HG23	2.19	0.42
2:E:194:ARG:HD3	2:E:198:PHE:CE1	2.54	0.42
2:E:1145:ARG:NH1	2:E:1145:ARG:HG3	2.34	0.42
2:E:1309:LEU:HD23	2:E:1309:LEU:HA	1.84	0.42
1:A:35:PHE:HE1	1:A:220:VAL:HG21	1.84	0.42
1:A:138:VAL:O	1:B:136:ARG:NH2	2.52	0.42
2:E:327:LEU:HD11	2:E:1268:ILE:HG23	2.01	0.42
1:D:319:VAL:HG22	1:D:328:VAL:HG12	1.99	0.42
2:E:85:LEU:HD23	2:E:85:LEU:HA	1.79	0.42
2:E:143:TRP:CE2	2:E:182:LEU:HD13	2.55	0.42
1:D:64:VAL:O	1:D:170:LYS:NZ	2.52	0.42
2:E:1328:GLY:HA3	2:E:1412:LYS:O	2.19	0.42
1:A:137:MET:SD	1:B:135:GLY:HA3	2.59	0.42
1:A:225:SER:N	1:A:229:GLU:O	2.52	0.42
1:C:169:MET:HE1	1:D:172:ALA:N	2.35	0.42
1:D:34:ARG:HD3	1:D:37:SER:HA	2.01	0.42
1:D:198:PHE:HE1	1:D:309:ILE:HD12	1.84	0.42
2:E:135:LEU:C	2:E:137:ILE:H	2.27	0.42
2:E:336:PRO:HG2	2:E:344:TYR:HD2	1.85	0.42
2:E:685:PHE:HB2	2:E:734:SER:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:233:MET:HE1	2:E:236:PHE:HD2	1.85	0.42
2:E:262:ASN:HB3	2:E:390:ALA:HB2	2.02	0.42
2:E:480:LYS:HE3	2:E:480:LYS:HB3	1.91	0.42
2:E:1405:ILE:O	2:E:1408:ILE:HG12	2.19	0.42
1:B:232:PRO:HB2	1:C:319:VAL:HB	2.02	0.42
1:C:60:PHE:HE2	1:D:171:THR:HG22	1.84	0.42
2:E:720:SER:HB3	2:E:775:GLN:NE2	2.35	0.42
2:E:1124:ARG:HH11	2:E:1314:ARG:HH11	1.66	0.42
1:B:219:VAL:HG22	1:B:283:ILE:HD13	2.01	0.42
1:B:231:VAL:HG11	1:B:234:HIS:ND1	2.34	0.42
1:D:272:PRO:HB3	1:D:311:TRP:CG	2.55	0.42
1:C:34:ARG:NH1	1:C:38:LYS:HG2	2.33	0.42
2:E:236:PHE:CZ	2:E:245:ILE:HD12	2.55	0.42
2:E:1154:LEU:HD12	2:E:1164:PHE:HE2	1.85	0.42
2:E:1336:PRO:HB3	2:E:1413:LEU:HD11	2.02	0.42
8:E:1606:PTY:H151	8:E:1606:PTY:H181	1.72	0.42
2:E:130:SER:O	2:E:132:PHE:N	2.51	0.41
2:E:253:LEU:HB3	2:E:1236:ILE:HD12	2.02	0.41
1:D:44:VAL:HB	1:D:46:HIS:CE1	2.55	0.41
2:E:260:LEU:O	2:E:264:GLN:HG2	2.20	0.41
2:E:46:ILE:HD13	2:E:46:ILE:HA	1.89	0.41
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.87	0.41
1:C:332:LYS:HB3	1:C:332:LYS:HE3	1.83	0.41
1:D:146:ILE:O	1:D:150:ILE:HG13	2.20	0.41
2:E:299:LEU:HD12	2:E:299:LEU:HA	1.83	0.41
2:E:1246:ARG:NH1	9:E:1602:BJX:O3	2.47	0.41
1:B:93:ILE:HD11	1:B:148:ILE:HD13	2.02	0.41
2:E:255:ILE:HA	2:E:258:ARG:HG3	2.02	0.41
2:E:822:GLN:HE21	2:E:822:GLN:HB3	1.66	0.41
2:E:1149:LEU:HD13	2:E:1294:TYR:CZ	2.56	0.41
2:E:1189:LEU:HD23	2:E:1189:LEU:HA	1.84	0.41
8:E:1604:PTY:H112	8:E:1610:PTY:H122	2.02	0.41
1:B:86:PHE:HA	1:B:89:VAL:HG12	2.03	0.41
1:D:82:SER:HB2	1:D:128:GLN:HE22	1.84	0.41
2:E:194:ARG:HB3	2:E:198:PHE:CG	2.55	0.41
2:E:885:VAL:HG12	2:E:887:VAL:HG23	2.02	0.41
7:B:403:P5S:H30A	7:B:403:P5S:H33	1.97	0.41
2:E:140:LEU:O	2:E:144:THR:HG22	2.21	0.41
1:A:254:PRO:HG3	1:A:330:TYR:CE1	2.56	0.41
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.82	0.41
1:C:165:GLY:HA2	1:C:168:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ILE:HD13	1:C:167:ILE:HA	1.94	0.41
2:E:210:LEU:O	2:E:210:LEU:HG	2.21	0.41
2:E:558:THR:HG21	2:E:583:PHE:CZ	2.54	0.41
2:E:321:PHE:HB2	2:E:578:ALA:CB	2.51	0.41
2:E:1379:GLY:HA3	2:E:1552:LEU:O	2.21	0.41
2:E:166:GLN:HB3	2:E:345:PHE:HD2	1.84	0.40
2:E:503:LEU:HD23	2:E:503:LEU:HA	1.88	0.40
2:E:894:LEU:HB3	2:E:895:PRO:HD3	2.03	0.40
1:C:254:PRO:HB3	1:C:333:PHE:CE2	2.56	0.40
2:E:503:LEU:HD22	2:E:1113:PHE:HE2	1.85	0.40
2:E:548:THR:HG22	2:E:1145:ARG:CZ	2.52	0.40
2:E:1120:SER:O	2:E:1124:ARG:HG2	2.21	0.40
1:D:144:LEU:O	1:D:148:ILE:HG22	2.22	0.40
2:E:1437:ARG:H	2:E:1473:ALA:HB3	1.86	0.40
1:A:330:TYR:HE2	1:D:46:HIS:HB3	1.85	0.40
1:C:276:HIS:O	1:C:279:GLN:HB3	2.21	0.40
1:D:215:ILE:HD13	1:D:257:ILE:HG13	2.04	0.40
1:A:83:TRP:HE1	1:A:128:GLN:HG2	1.87	0.40
1:A:111:VAL:HB	1:A:114:ILE:HG13	2.03	0.40
2:E:1131:THR:HA	2:E:1135:HIS:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	F	1	3,2	14,14,15	0.42	0	17,19,21	0.57	0
3	NAG	F	2	3	14,14,15	0.31	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

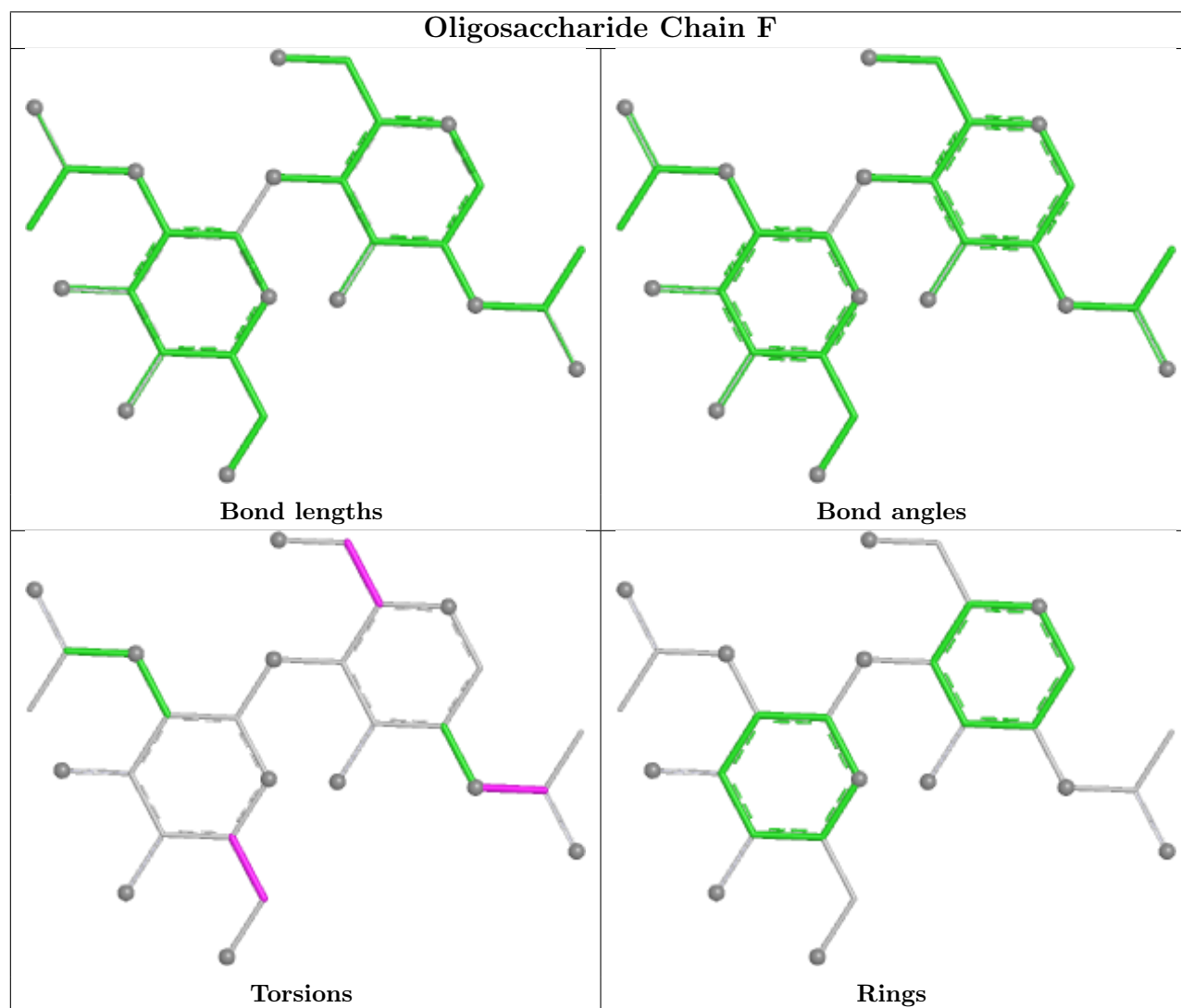
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	$\# Z > 2$
4	ATP	B	404	-	32,33,33	0.34	0	48,52,52	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PTY	E	1609	-	31,31,49	0.56	0	34,36,54	0.59	0
8	PTY	E	1606	-	31,31,49	0.56	0	34,36,54	0.46	0
4	ATP	D	401	-	32,33,33	0.29	0	48,52,52	0.28	0
8	PTY	E	1605	-	31,31,49	0.56	0	34,36,54	0.46	0
6	POV	C	401	-	35,35,51	0.60	0	41,43,59	0.51	0
4	ATP	E	1603	-	32,33,33	0.35	0	48,52,52	0.30	0
4	ATP	A	401	-	32,33,33	0.28	0	48,52,52	0.28	0
4	ATP	B	401	-	32,33,33	0.40	0	48,52,52	0.30	0
7	P5S	B	403	-	52,53,53	0.53	0	54,60,60	0.82	1 (1%)
8	PTY	E	1601	-	31,31,49	0.57	0	34,36,54	0.44	0
6	POV	A	403	-	35,35,51	0.62	0	41,43,59	0.51	0
9	BJX	E	1602	-	35,35,35	2.67	13 (37%)	45,47,47	1.78	7 (15%)
6	POV	D	402	-	35,35,51	0.61	0	41,43,59	0.51	0
8	PTY	E	1610	-	31,31,49	0.56	0	34,36,54	0.52	0
8	PTY	E	1604	-	31,31,49	0.55	0	34,36,54	0.55	0
6	POV	E	1608	-	35,35,51	0.59	0	41,43,59	0.54	0
7	P5S	E	1607	-	52,53,53	0.53	0	54,60,60	0.79	1 (1%)
6	POV	B	402	-	35,35,51	0.61	0	41,43,59	0.54	1 (2%)

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	ATP	B	404	-	-	2/22/38/38	0/3/3/3
8	PTY	E	1609	-	-	7/35/35/53	-
8	PTY	E	1606	-	-	14/35/35/53	-
4	ATP	D	401	-	-	8/22/38/38	0/3/3/3
8	PTY	E	1605	-	-	4/35/35/53	-
6	POV	C	401	-	-	12/39/39/55	-
4	ATP	E	1603	-	-	3/22/38/38	0/3/3/3
4	ATP	A	401	-	-	5/22/38/38	0/3/3/3
4	ATP	B	401	-	-	4/22/38/38	0/3/3/3
7	P5S	B	403	-	-	30/59/59/59	-
8	PTY	E	1601	-	-	8/35/35/53	-
6	POV	A	403	-	-	10/39/39/55	-
9	BJX	E	1602	-	-	15/27/35/35	0/3/3/3
6	POV	D	402	-	-	12/39/39/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PTY	E	1610	-	-	9/35/35/53	-
8	PTY	E	1604	-	-	11/35/35/53	-
6	POV	E	1608	-	-	9/39/39/55	-
7	P5S	E	1607	-	-	32/59/59/59	-
6	POV	B	402	-	-	18/39/39/55	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	1602	BJX	C8-C5	7.34	1.60	1.53
9	E	1602	BJX	C6-N	5.69	1.53	1.41
9	E	1602	BJX	C16-N1	5.57	1.45	1.34
9	E	1602	BJX	C6-C7	5.00	1.45	1.40
9	E	1602	BJX	C5-N1	4.53	1.52	1.46
9	E	1602	BJX	C7-C5	4.32	1.58	1.52
9	E	1602	BJX	C-N	2.79	1.51	1.46
9	E	1602	BJX	C23-C24	2.77	1.55	1.49
9	E	1602	BJX	O1-C21	2.62	1.42	1.37
9	E	1602	BJX	C17-C18	2.40	1.55	1.51
9	E	1602	BJX	C19-C21	2.28	1.42	1.38
9	E	1602	BJX	O2-C24	2.14	1.29	1.22
9	E	1602	BJX	C1-N	2.08	1.50	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1602	BJX	C5-N1-C16	7.21	134.20	123.44
7	B	403	P5S	OG-CB-CA	4.45	111.94	108.06
7	E	1607	P5S	OG-CB-CA	3.90	111.46	108.06
9	E	1602	BJX	C8-C5-N1	3.38	115.32	109.71
9	E	1602	BJX	C7-C6-N	2.99	123.91	119.32
9	E	1602	BJX	C17-C16-N1	2.76	120.18	115.88
9	E	1602	BJX	C10-C6-N	-2.61	118.33	122.42
9	E	1602	BJX	C7-C5-N1	-2.12	107.26	111.44
6	B	402	POV	O13-P-O14	2.09	122.15	112.44
9	E	1602	BJX	C-N-C1	-2.08	106.89	111.57

There are no chirality outliers.

All (213) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	ATP	O4'-C4'-C5'-O5'
4	B	401	ATP	O4'-C4'-C5'-O5'
4	D	401	ATP	C5'-O5'-PA-O1A
4	D	401	ATP	C5'-O5'-PA-O2A
4	D	401	ATP	C5'-O5'-PA-O3A
4	D	401	ATP	O4'-C4'-C5'-O5'
6	A	403	POV	C11-O12-P-O11
6	A	403	POV	C11-O12-P-O14
6	B	402	POV	C1-O11-P-O12
6	B	402	POV	C1-O11-P-O13
6	B	402	POV	C1-O11-P-O14
6	B	402	POV	C11-O12-P-O11
6	B	402	POV	O21-C2-C3-O31
6	B	402	POV	C12-C11-O12-P
6	C	401	POV	C1-O11-P-O12
6	C	401	POV	C1-O11-P-O13
6	C	401	POV	C11-O12-P-O11
6	C	401	POV	C11-O12-P-O13
6	C	401	POV	C12-C11-O12-P
6	D	402	POV	C11-O12-P-O14
6	D	402	POV	O12-C11-C12-N
6	E	1608	POV	C1-O11-P-O13
6	E	1608	POV	C11-O12-P-O11
6	E	1608	POV	C11-O12-P-O14
7	B	403	P5S	O19-C1-C2-O37
7	B	403	P5S	N-CA-CB-OG
7	B	403	P5S	CB-OG-P12-O16
7	E	1607	P5S	O-C-CA-CB
7	E	1607	P5S	OXT-C-CA-CB
7	E	1607	P5S	C-CA-CB-OG
7	E	1607	P5S	N-CA-CB-OG
7	E	1607	P5S	CB-OG-P12-O15
7	E	1607	P5S	CB-OG-P12-O16
8	E	1601	PTY	O10-C8-O7-C6
8	E	1601	PTY	C11-C8-O7-C6
8	E	1601	PTY	C5-O14-P1-O13
8	E	1604	PTY	C5-O14-P1-O13
8	E	1606	PTY	C2-C3-O11-P1
8	E	1606	PTY	C11-C8-O7-C6
8	E	1606	PTY	C3-O11-P1-O12
8	E	1606	PTY	C3-O11-P1-O14
8	E	1609	PTY	C11-C8-O7-C6
8	E	1610	PTY	C11-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
8	E	1610	PTY	C3-O11-P1-O12
8	E	1610	PTY	C5-O14-P1-O13
9	E	1602	BJX	N1-C5-C7-C6
9	E	1602	BJX	C8-C5-N1-C16
9	E	1602	BJX	C21-C23-C24-O2
9	E	1602	BJX	C21-C23-C24-O3
7	E	1607	P5S	O18-C17-O19-C1
7	E	1607	P5S	C20-C17-O19-C1
8	E	1604	PTY	O30-C30-O4-C1
8	E	1606	PTY	O10-C8-O7-C6
8	E	1609	PTY	O10-C8-O7-C6
8	E	1610	PTY	O10-C8-O7-C6
8	E	1604	PTY	C31-C30-O4-C1
8	E	1609	PTY	O30-C30-O4-C1
8	E	1609	PTY	C31-C30-O4-C1
7	B	403	P5S	C39-C38-O37-C2
8	E	1604	PTY	C11-C8-O7-C6
4	A	401	ATP	C3'-C4'-C5'-O5'
4	B	401	ATP	C3'-C4'-C5'-O5'
4	D	401	ATP	C3'-C4'-C5'-O5'
6	A	403	POV	C34-C35-C36-C37
8	E	1604	PTY	O10-C8-O7-C6
7	B	403	P5S	C17-C20-C21-C22
6	B	402	POV	C11-C12-N-C15
9	E	1602	BJX	N1-C5-C8-C9
7	B	403	P5S	O47-C38-O37-C2
6	D	402	POV	C23-C24-C25-C26
7	E	1607	P5S	C2-C3-O16-P12
7	E	1607	P5S	OXT-C-CA-N
8	E	1609	PTY	C5-C6-O7-C8
8	E	1605	PTY	C31-C32-C33-C34
7	B	403	P5S	C26-C27-C28-C29
7	E	1607	P5S	C30-C31-C32-C33
6	C	401	POV	C31-C32-C33-C34
7	E	1607	P5S	C39-C40-C41-C42
8	E	1606	PTY	C12-C13-C14-C15
7	B	403	P5S	C30-C31-C32-C33
7	E	1607	P5S	C51-C52-C53-C54
8	E	1601	PTY	C13-C14-C15-C16
7	E	1607	P5S	C39-C38-O37-C2
7	E	1607	P5S	C29-C30-C31-C32
6	B	402	POV	C11-C12-N-C14

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Mol	Chain	Res	Type	Atoms
6	D	402	POV	O11-C1-C2-O21
6	D	402	POV	C22-C21-O21-C2
7	B	403	P5S	C-CA-CB-OG
6	A	403	POV	O21-C2-C3-O31
7	E	1607	P5S	O19-C1-C2-O37
7	B	403	P5S	C38-C39-C40-C41
7	E	1607	P5S	O47-C38-O37-C2
8	E	1606	PTY	C15-C16-C17-C18
7	B	403	P5S	C41-C42-C43-C44
6	B	402	POV	C11-C12-N-C13
9	E	1602	BJX	C23-C21-O1-C25
6	E	1608	POV	O11-C1-C2-C3
7	E	1607	P5S	C1-C2-C3-O16
6	B	402	POV	C23-C24-C25-C26
6	E	1608	POV	C22-C21-O21-C2
7	B	403	P5S	O19-C1-C2-C3
6	B	402	POV	C22-C23-C24-C25
6	B	402	POV	C24-C25-C26-C27
7	B	403	P5S	C31-C32-C33-C34
7	B	403	P5S	C3-C2-O37-C38
8	E	1604	PTY	C1-C6-O7-C8
7	E	1607	P5S	C43-C44-C45-C46
9	E	1602	BJX	C19-C21-O1-C25
6	C	401	POV	C32-C31-O31-C3
7	B	403	P5S	C42-C43-C44-C45
8	E	1606	PTY	C17-C18-C19-C20
7	E	1607	P5S	C38-C39-C40-C41
6	A	403	POV	C1-C2-C3-O31
6	B	402	POV	C1-C2-C3-O31
7	E	1607	P5S	O19-C1-C2-C3
8	E	1604	PTY	O4-C1-C6-C5
7	E	1607	P5S	O-C-CA-N
4	D	401	ATP	PG-O3B-PB-O3A
6	D	402	POV	O22-C21-O21-C2
8	E	1604	PTY	O4-C1-C6-O7
8	E	1609	PTY	C11-C12-C13-C14
9	E	1602	BJX	C8-C5-C7-C11
7	B	403	P5S	C24-C25-C26-C27
6	D	402	POV	C21-C22-C23-C24
8	E	1606	PTY	C13-C14-C15-C16
6	C	401	POV	O11-C1-C2-C3
7	E	1607	P5S	C50-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
6	A	403	POV	C25-C26-C27-C28
6	E	1608	POV	O22-C21-O21-C2
7	E	1607	P5S	C3-C2-O37-C38
6	C	401	POV	O32-C31-O31-C3
7	B	403	P5S	C39-C40-C41-C42
6	C	401	POV	O11-C1-C2-O21
7	E	1607	P5S	O37-C2-C3-O16
8	E	1610	PTY	C2-C3-O11-P1
9	E	1602	BJX	C7-C5-C8-C9
7	E	1607	P5S	C24-C25-C26-C27
9	E	1602	BJX	C22-C23-C24-O2
7	E	1607	P5S	C27-C28-C29-C30
8	E	1606	PTY	C14-C15-C16-C17
6	D	402	POV	C35-C36-C37-C38
4	A	401	ATP	PB-O3A-PA-O2A
4	D	401	ATP	PB-O3A-PA-O1A
4	E	1603	ATP	PA-O3A-PB-O2B
6	A	403	POV	O12-C11-C12-N
6	E	1608	POV	O12-C11-C12-N
7	E	1607	P5S	C25-C26-C27-C28
7	B	403	P5S	CA-CB-OG-P12
7	E	1607	P5S	CA-CB-OG-P12
6	D	402	POV	C22-C23-C24-C25
6	D	402	POV	O11-C1-C2-C3
9	E	1602	BJX	C22-C23-C24-O3
8	E	1605	PTY	C14-C15-C16-C17
6	E	1608	POV	O11-C1-C2-O21
8	E	1605	PTY	O4-C1-C6-C5
7	B	403	P5S	C23-C24-C25-C26
7	B	403	P5S	C43-C44-C45-C46
6	B	402	POV	C32-C33-C34-C35
6	A	403	POV	C1-O11-P-O14
6	B	402	POV	C11-O12-P-O14
6	C	401	POV	C1-O11-P-O14
6	E	1608	POV	C1-O11-P-O12
7	B	403	P5S	CB-OG-P12-O13
8	E	1601	PTY	C3-O11-P1-O13
8	E	1609	PTY	C5-O14-P1-O13
9	E	1602	BJX	O-C16-C17-C18
8	E	1605	PTY	C6-C5-O14-P1
8	E	1604	PTY	C8-C11-C12-C13
8	E	1606	PTY	C8-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
8	E	1610	PTY	O14-C5-C6-O7
7	E	1607	P5S	C53-C54-C55-C56
8	E	1601	PTY	O4-C1-C6-O7
4	B	401	ATP	PB-O3A-PA-O2A
8	E	1606	PTY	C11-C12-C13-C14
8	E	1601	PTY	C32-C33-C34-C35
7	B	403	P5S	O18-C17-O19-C1
9	E	1602	BJX	C26-C25-O1-C21
7	E	1607	P5S	C40-C41-C42-C43
6	B	402	POV	C21-C22-C23-C24
6	A	403	POV	C21-C22-C23-C24
7	E	1607	P5S	C48-C49-C50-C51
7	B	403	P5S	C20-C17-O19-C1
7	B	403	P5S	C48-C49-C50-C51
8	E	1610	PTY	C15-C16-C17-C18
8	E	1610	PTY	C6-C5-O14-P1
8	E	1604	PTY	O14-C5-C6-O7
6	A	403	POV	C23-C24-C25-C26
8	E	1604	PTY	O14-C5-C6-C1
7	B	403	P5S	C2-C3-O16-P12
7	B	403	P5S	C40-C41-C42-C43
4	E	1603	ATP	PB-O3B-PG-O3G
9	E	1602	BJX	C8-C5-C7-C6
6	C	401	POV	C24-C25-C26-C27
4	A	401	ATP	PA-O3A-PB-O2B
4	A	401	ATP	PB-O3A-PA-O1A
4	B	404	ATP	PA-O3A-PB-O1B
4	B	404	ATP	PA-O3A-PB-O2B
4	E	1603	ATP	PA-O3A-PB-O1B
9	E	1602	BJX	N1-C16-C17-C18
8	E	1606	PTY	C12-C11-C8-O7
6	D	402	POV	O21-C21-C22-C23
6	B	402	POV	O11-C1-C2-O21
8	E	1601	PTY	C12-C11-C8-O7
6	B	402	POV	C25-C26-C27-C28
7	B	403	P5S	C22-C23-C24-C25
7	B	403	P5S	O37-C38-C39-C40
7	B	403	P5S	C45-C46-C48-C49
7	B	403	P5S	OXT-C-CA-N
8	E	1606	PTY	C12-C11-C8-O10
8	E	1610	PTY	O14-C5-C6-C1
4	B	401	ATP	PB-O3A-PA-O1A

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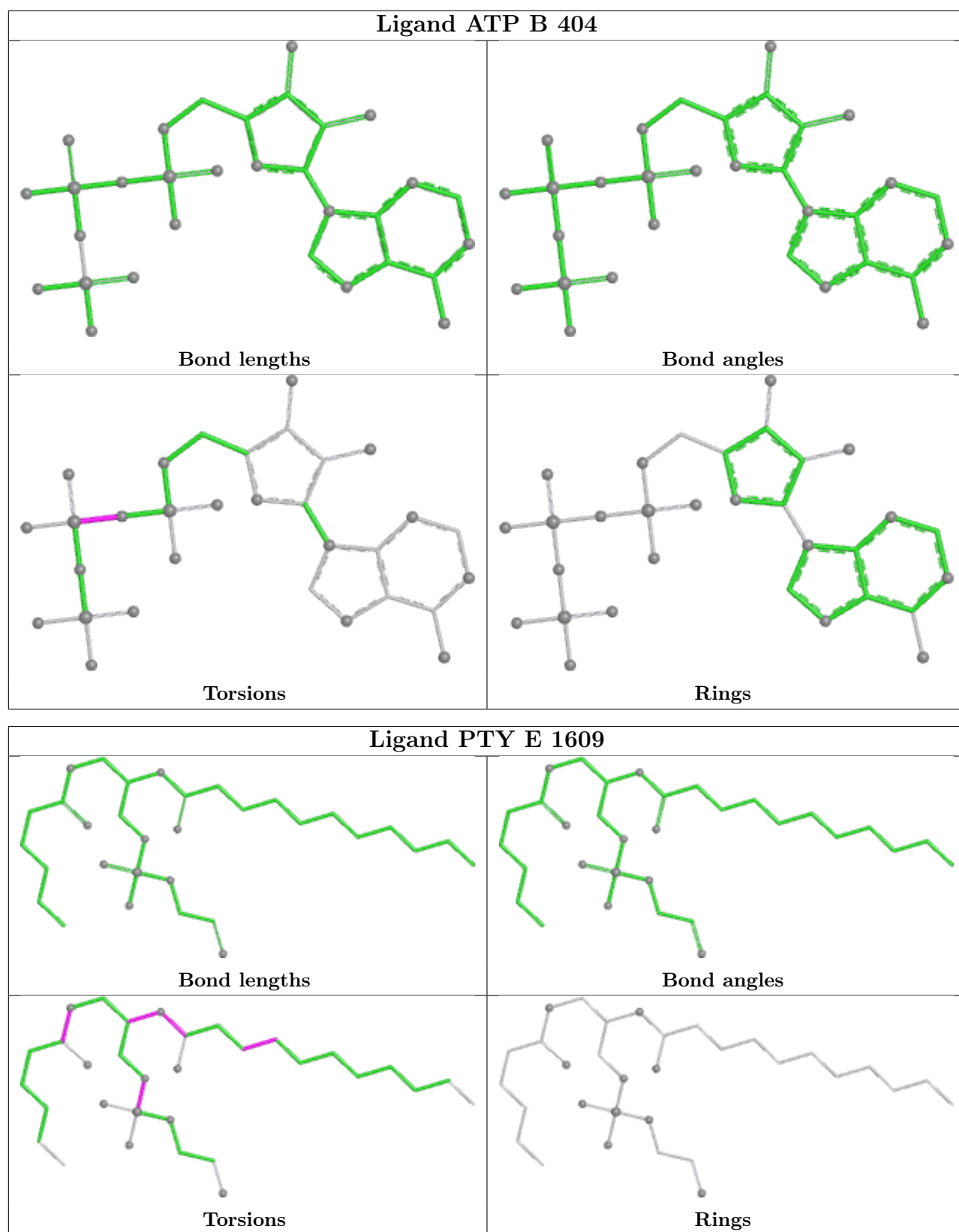
Mol	Chain	Res	Type	Atoms
4	D	401	ATP	PB-O3A-PA-O2A
6	D	402	POV	O22-C21-C22-C23

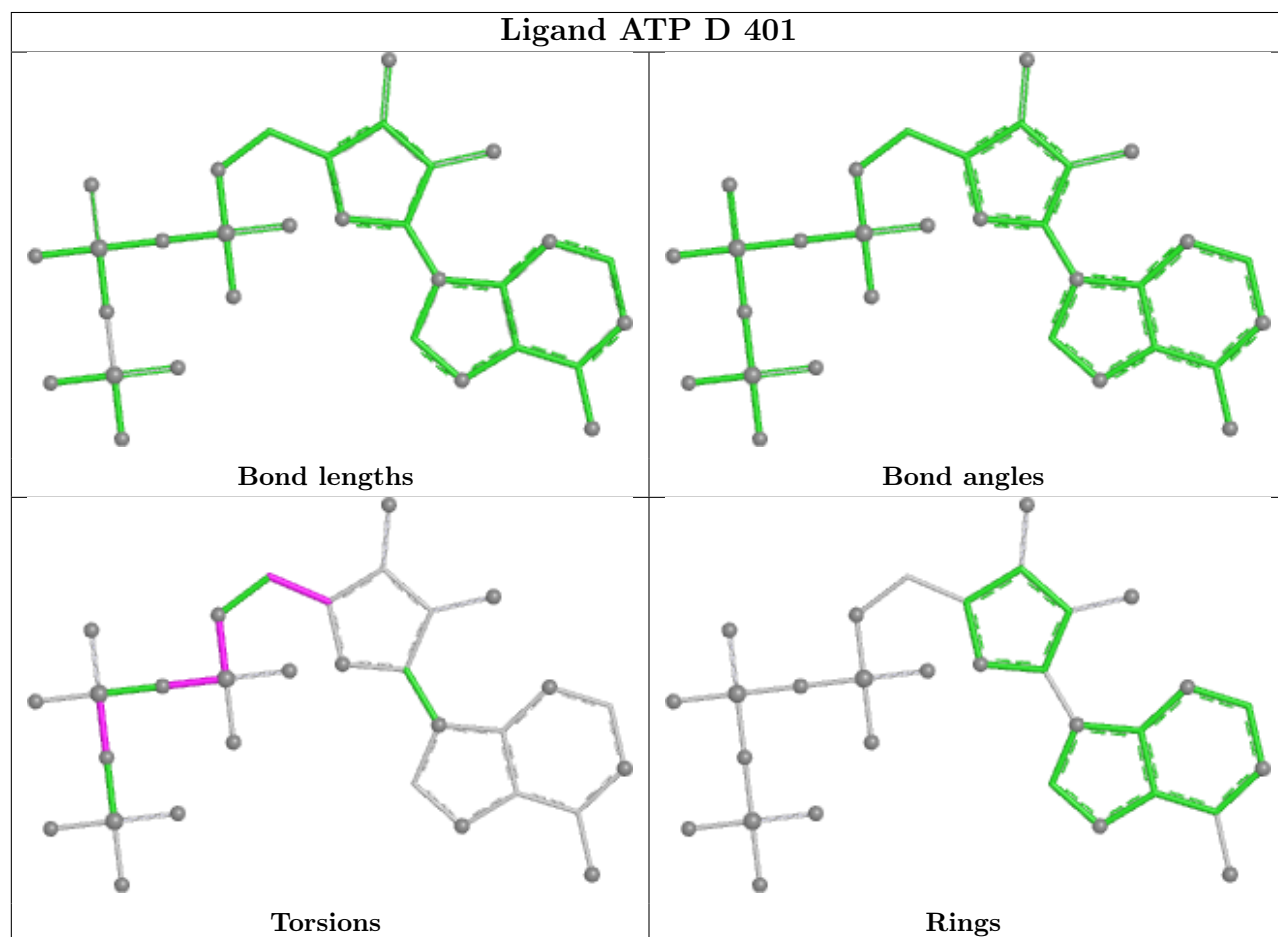
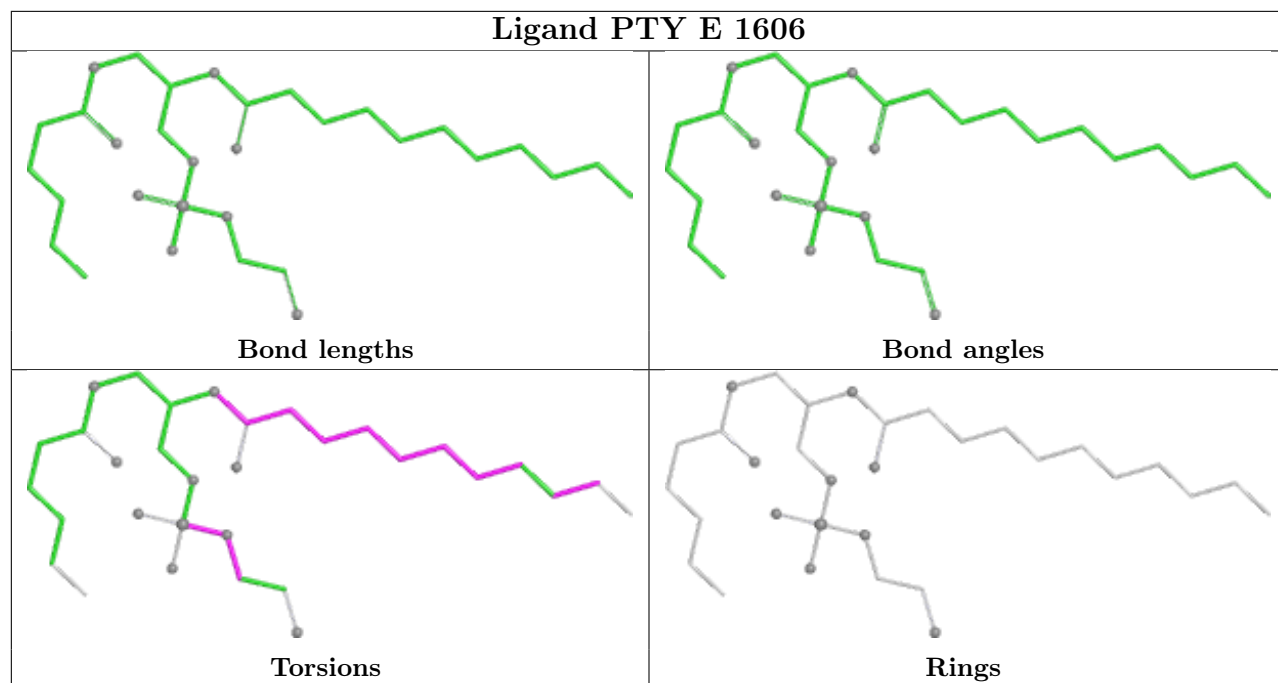
There are no ring outliers.

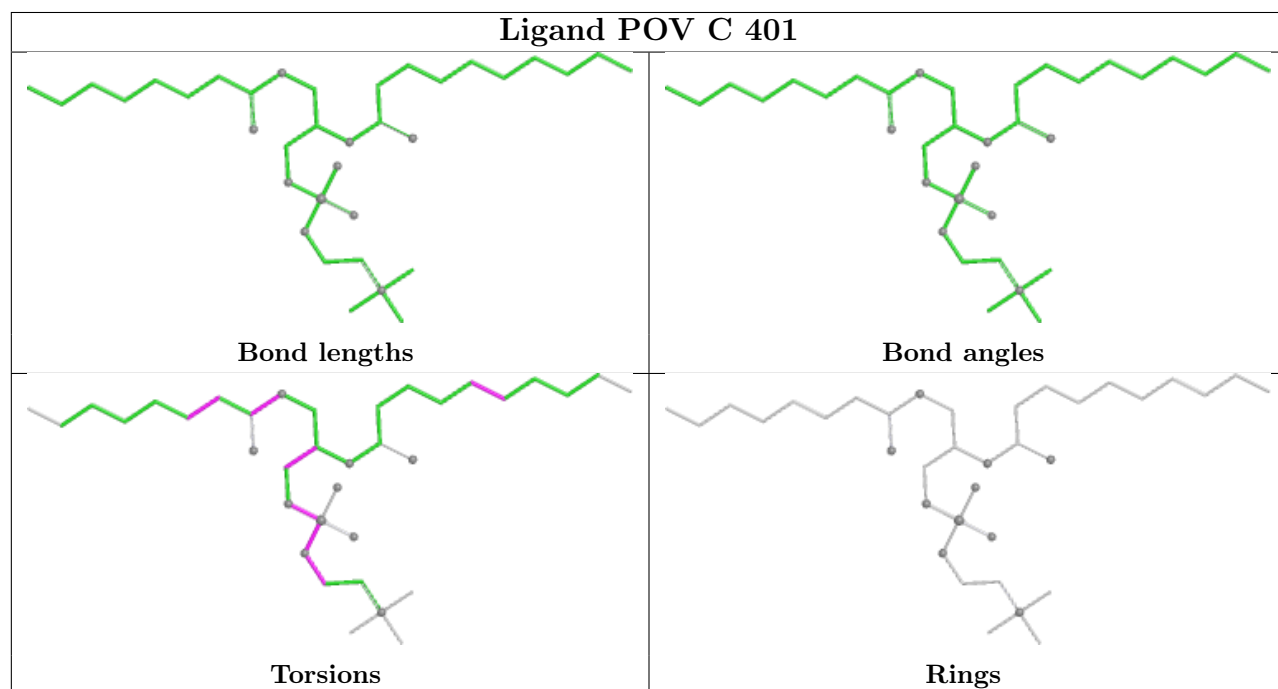
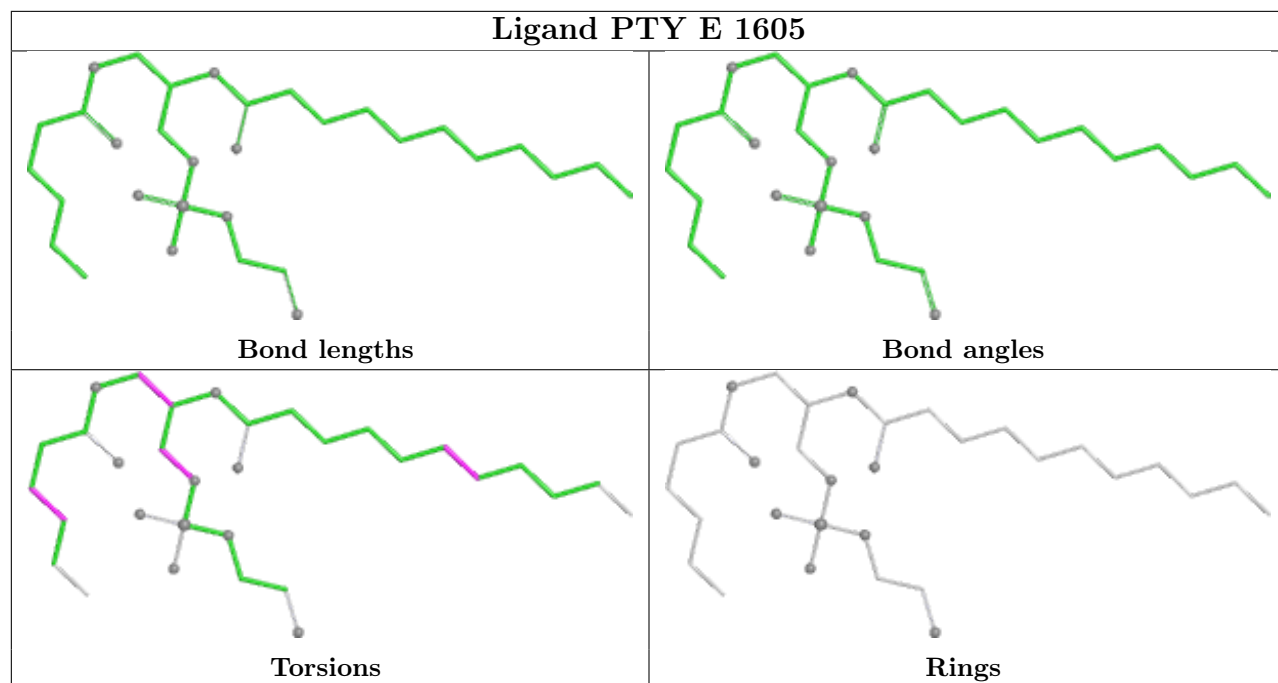
15 monomers are involved in 35 short contacts:

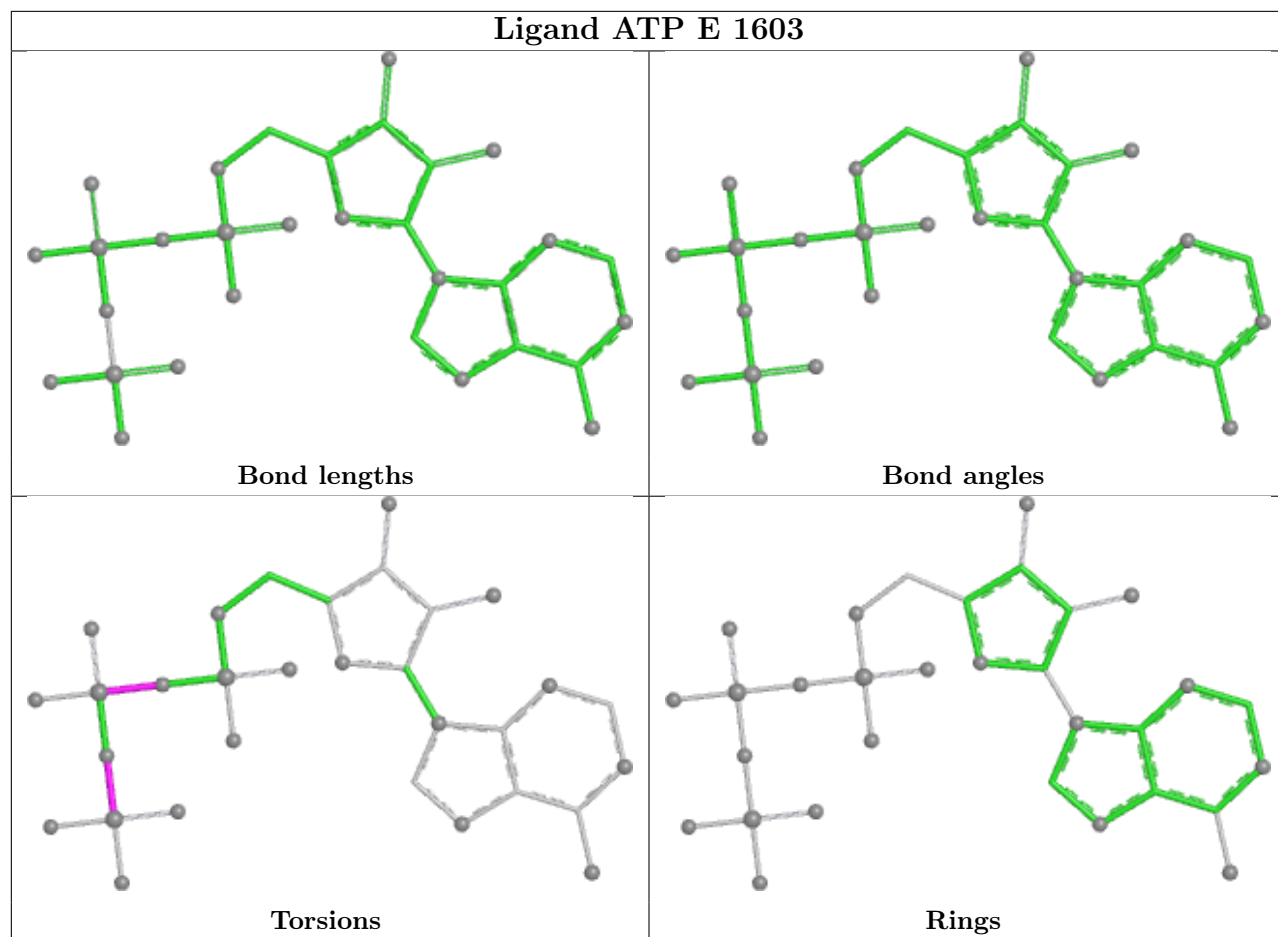
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	ATP	2	0
8	E	1606	PTY	2	0
4	D	401	ATP	1	0
4	E	1603	ATP	4	0
4	A	401	ATP	5	0
4	B	401	ATP	3	0
7	B	403	P5S	1	0
6	A	403	POV	2	0
9	E	1602	BJX	1	0
6	D	402	POV	2	0
8	E	1610	PTY	2	0
8	E	1604	PTY	4	0
6	E	1608	POV	1	0
7	E	1607	P5S	5	0
6	B	402	POV	1	0

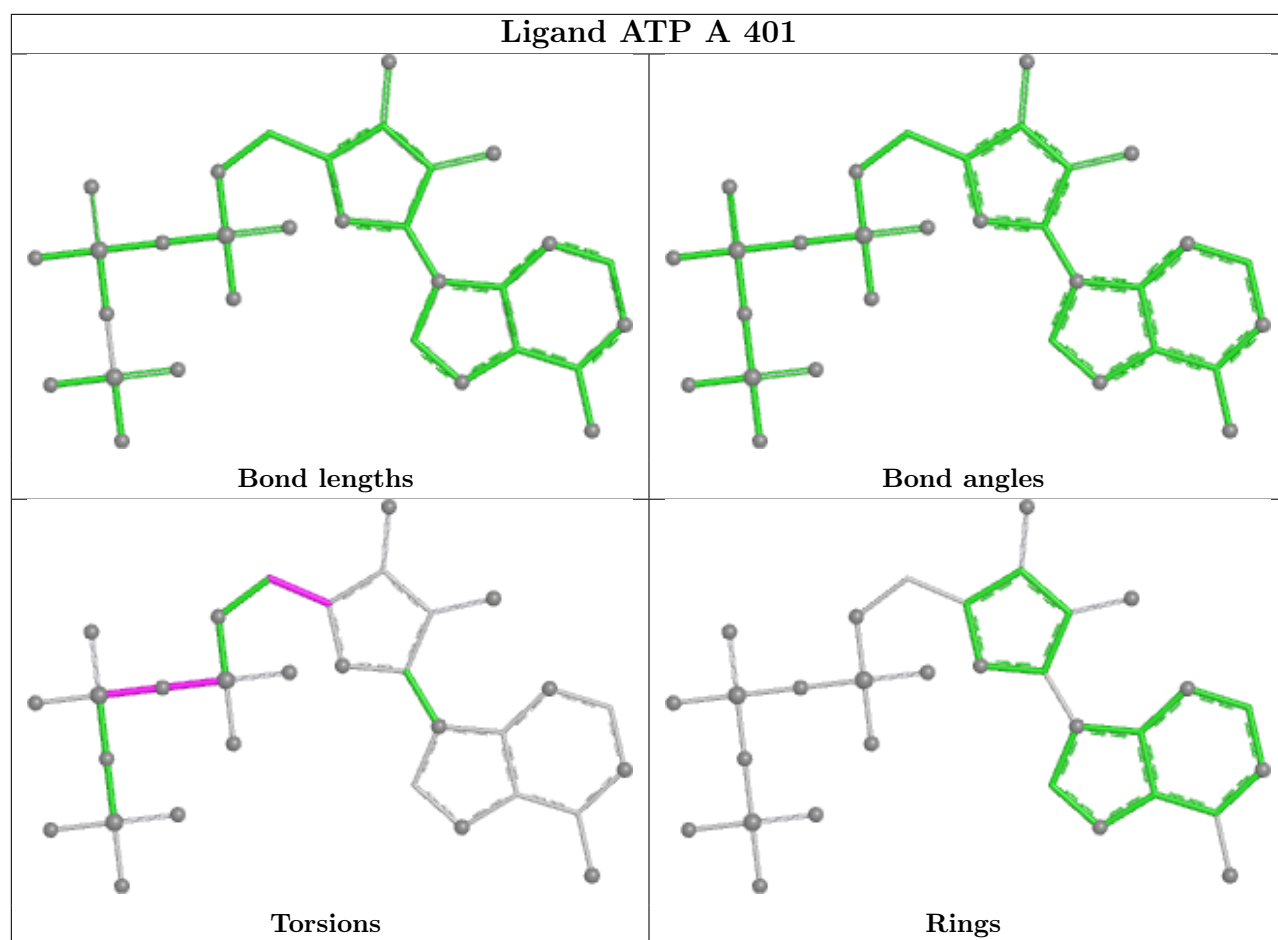
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

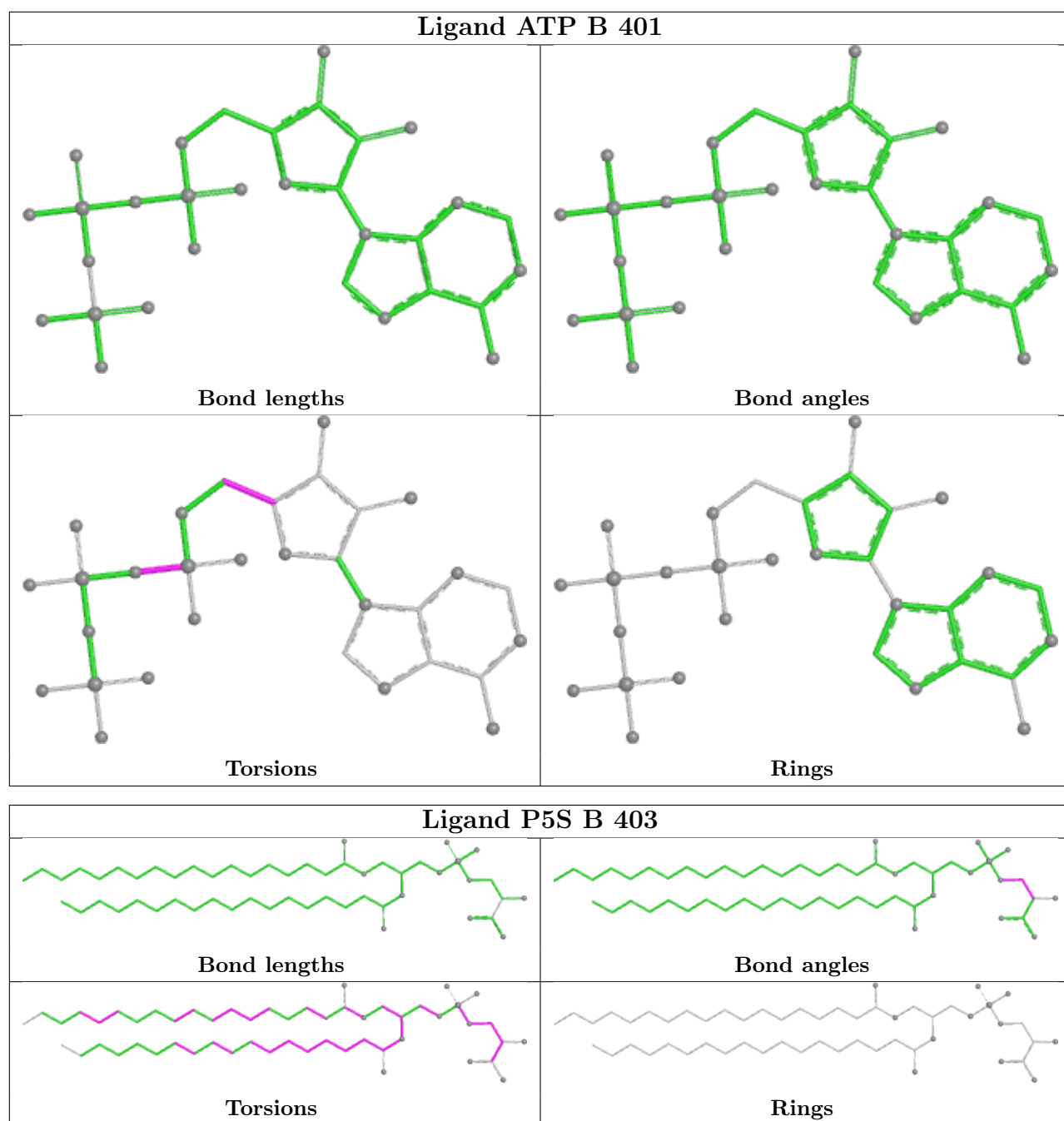


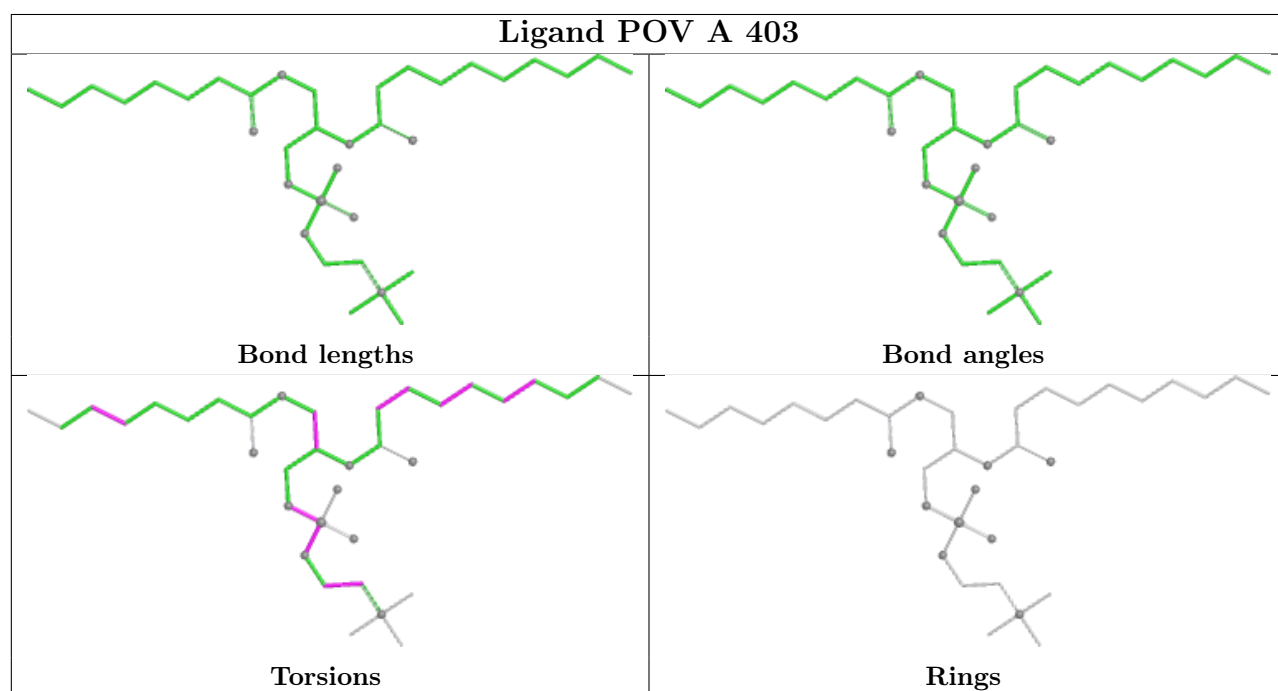
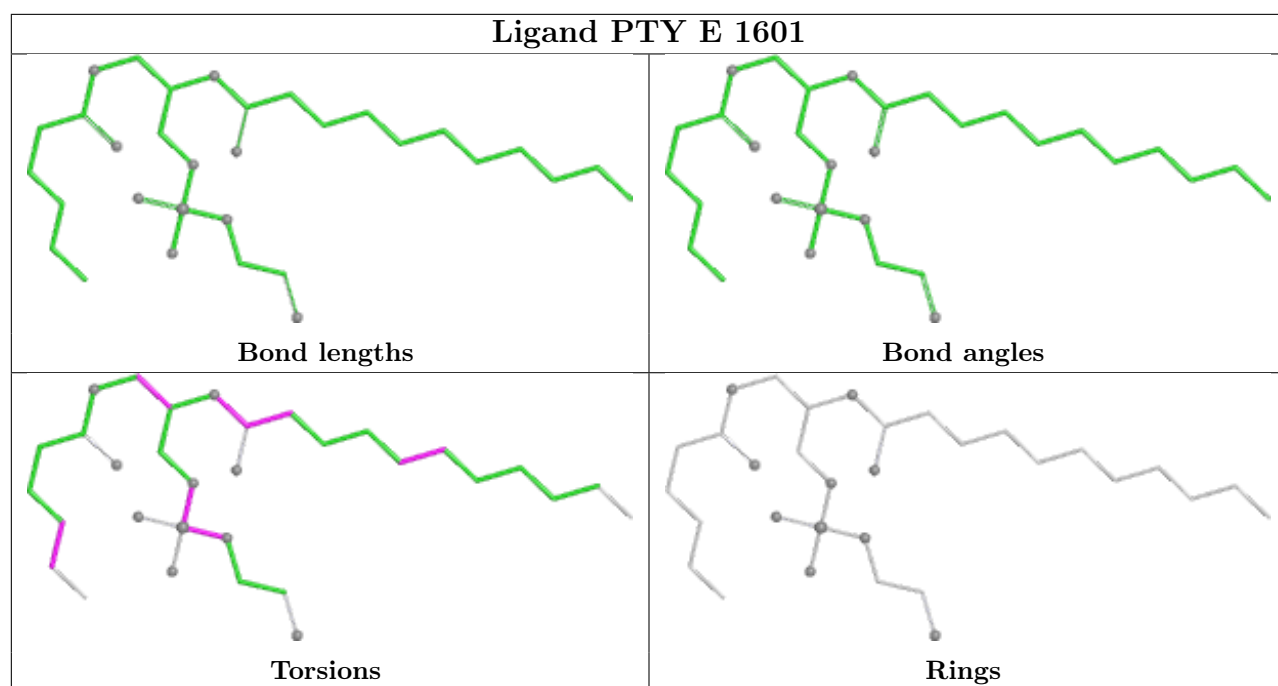


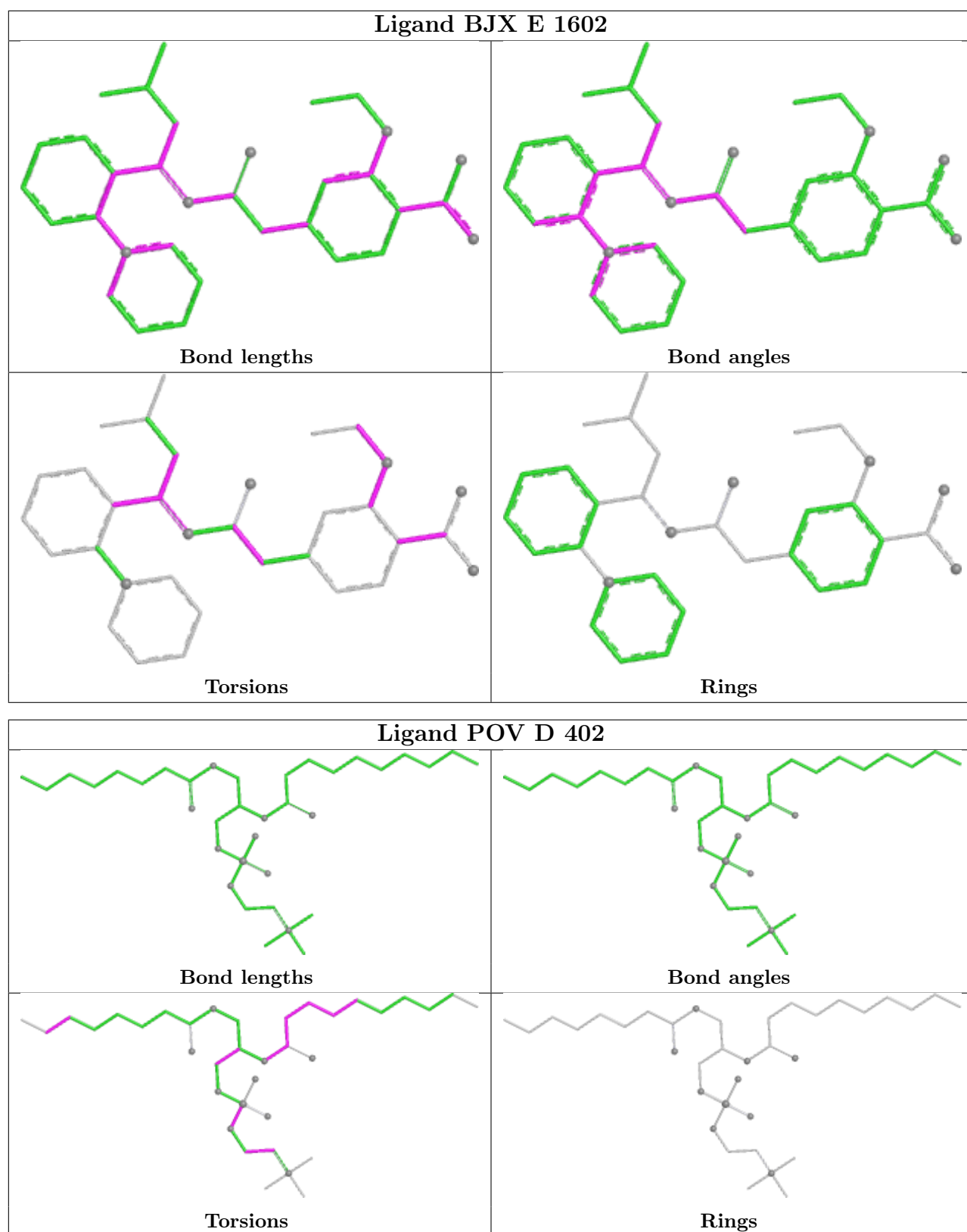


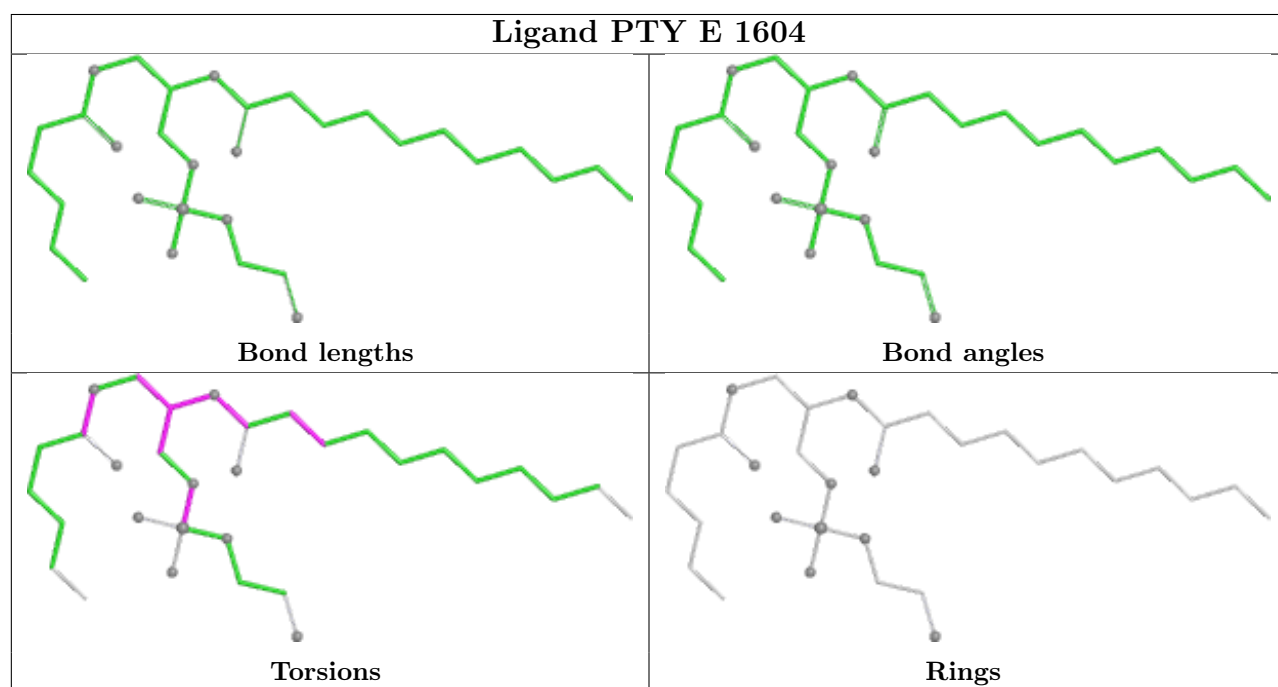
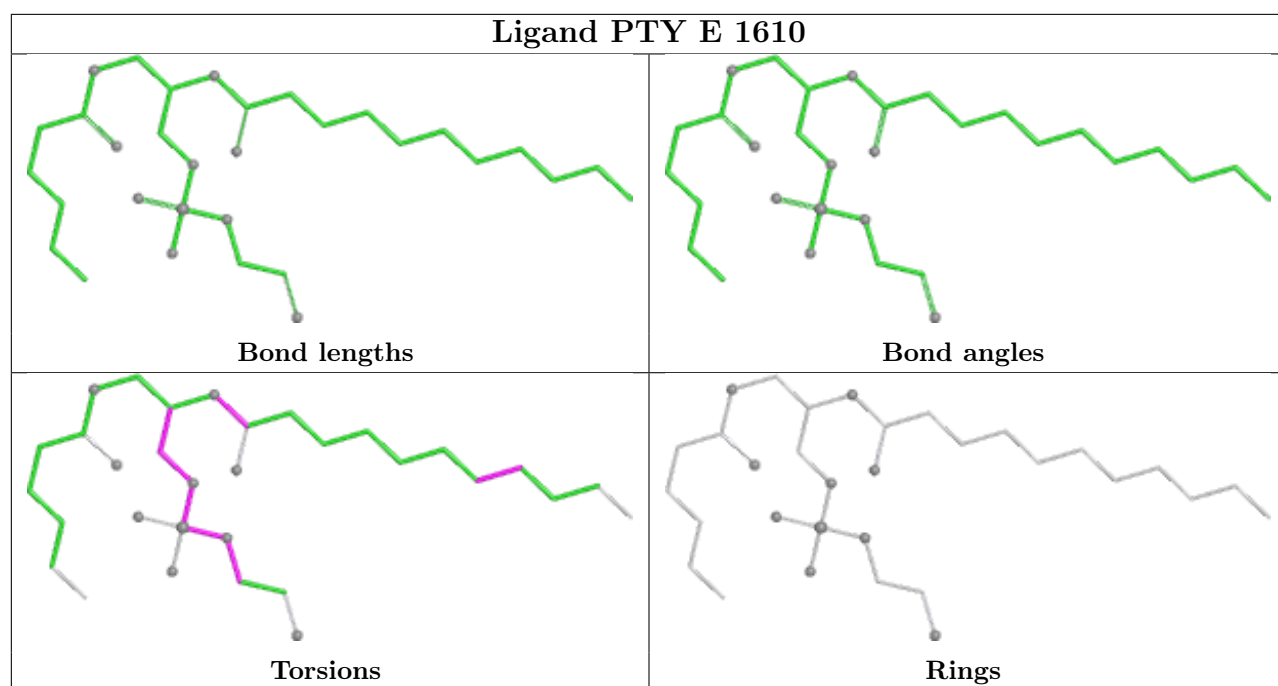


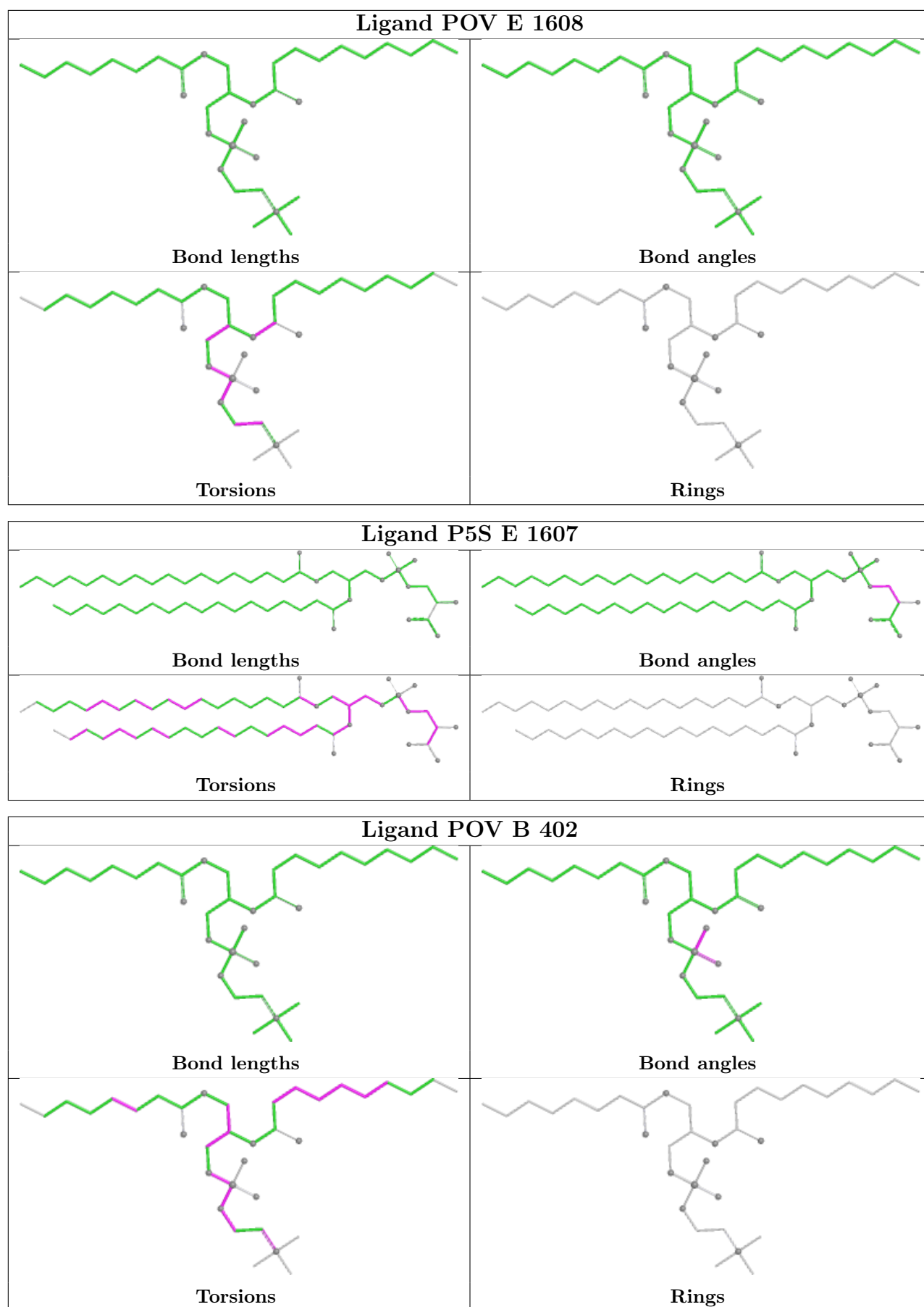












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

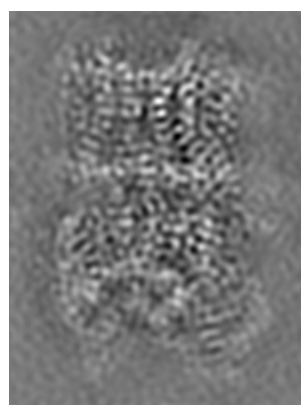
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26194. These allow visual inspection of the internal detail of the map and identification of artifacts.

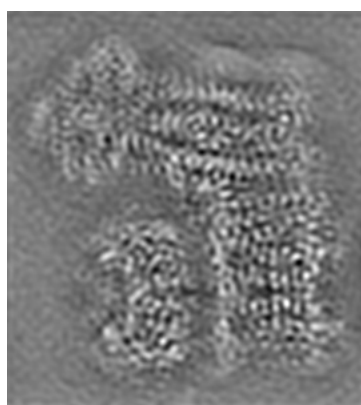
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

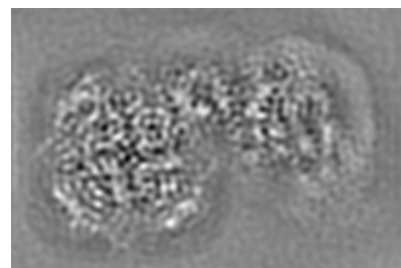
6.1.1 Primary map



X



Y

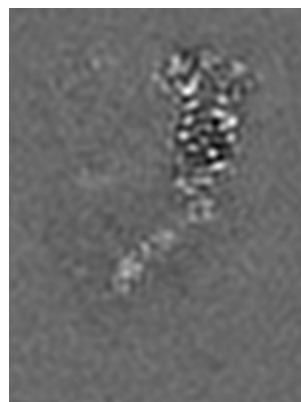


Z

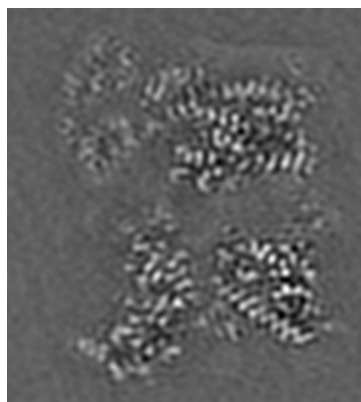
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

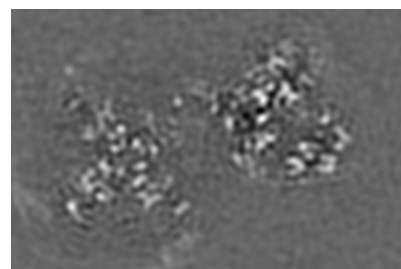
6.2.1 Primary map



X Index: 79



Y Index: 52

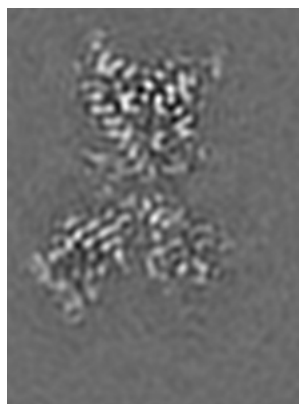


Z Index: 71

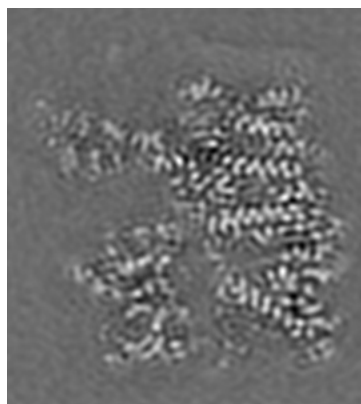
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

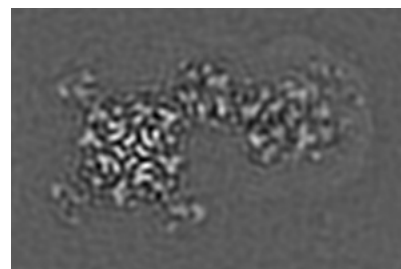
6.3.1 Primary map



X Index: 41



Y Index: 64

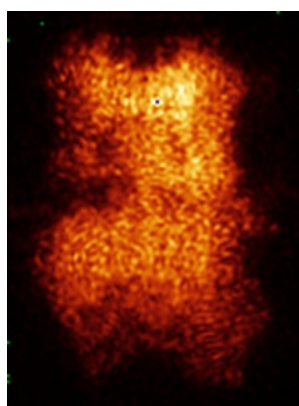


Z Index: 110

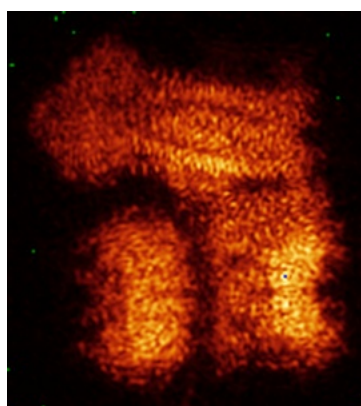
The images above show the largest variance slices of the map in three orthogonal directions.

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

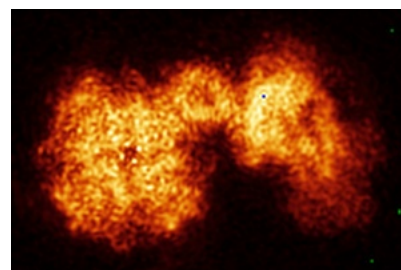
6.4.1 Primary map



X



Y

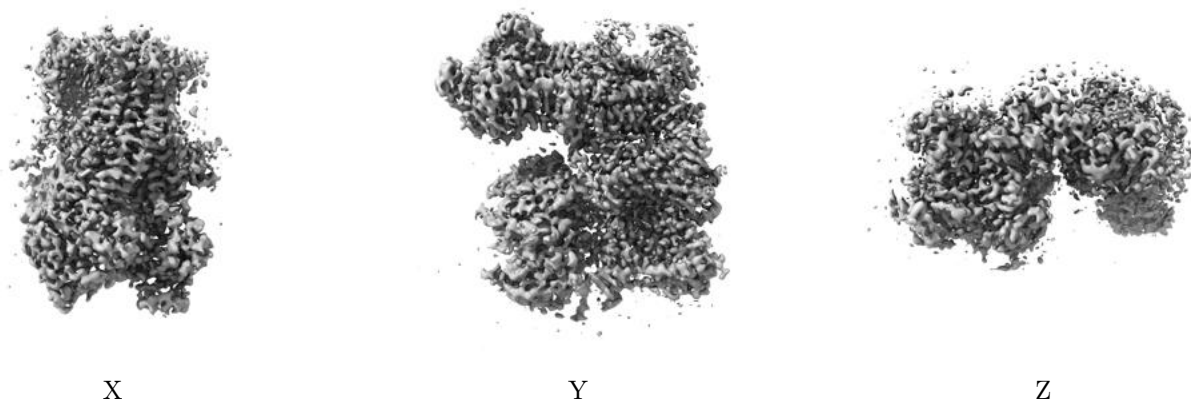


Z

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

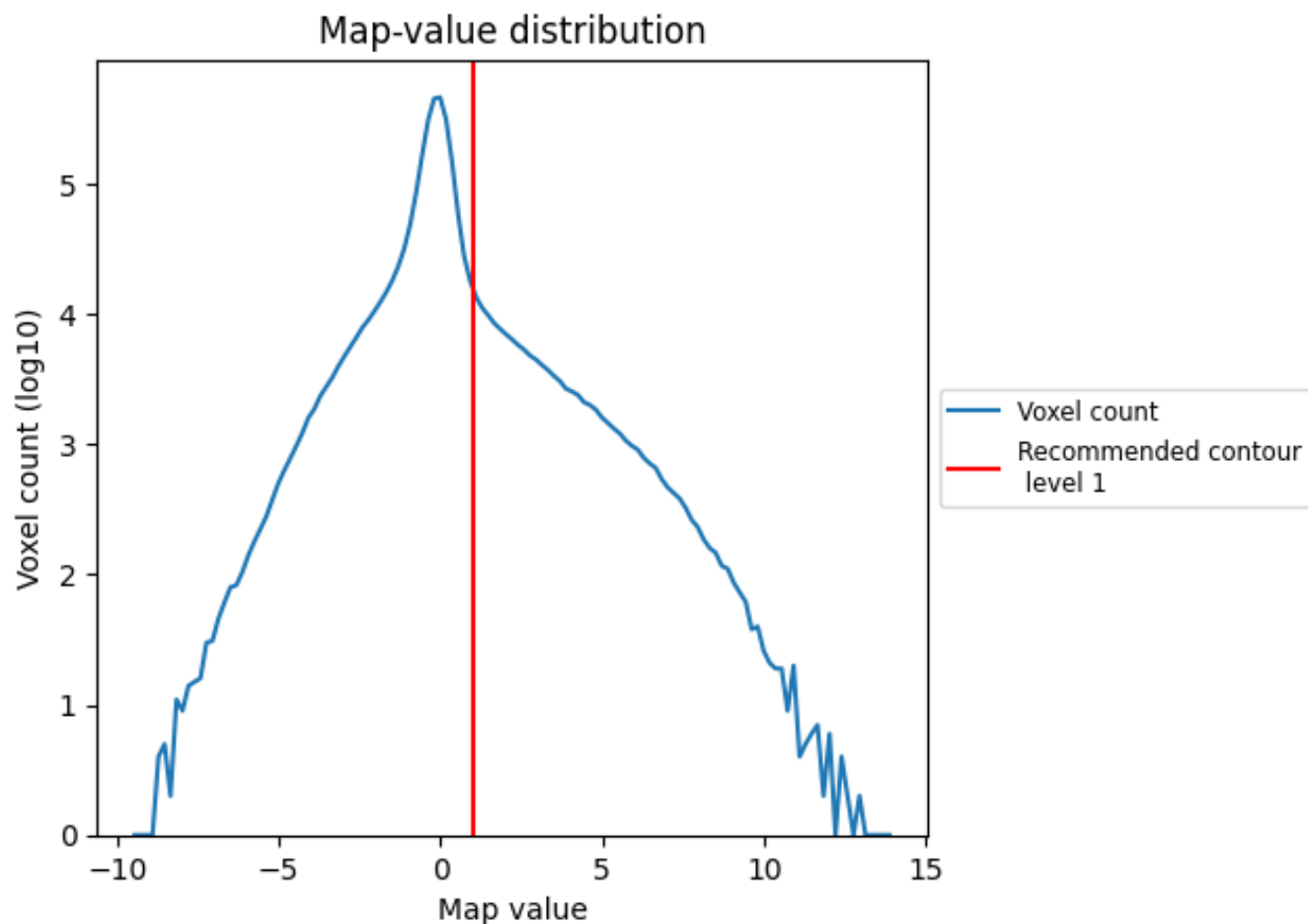
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

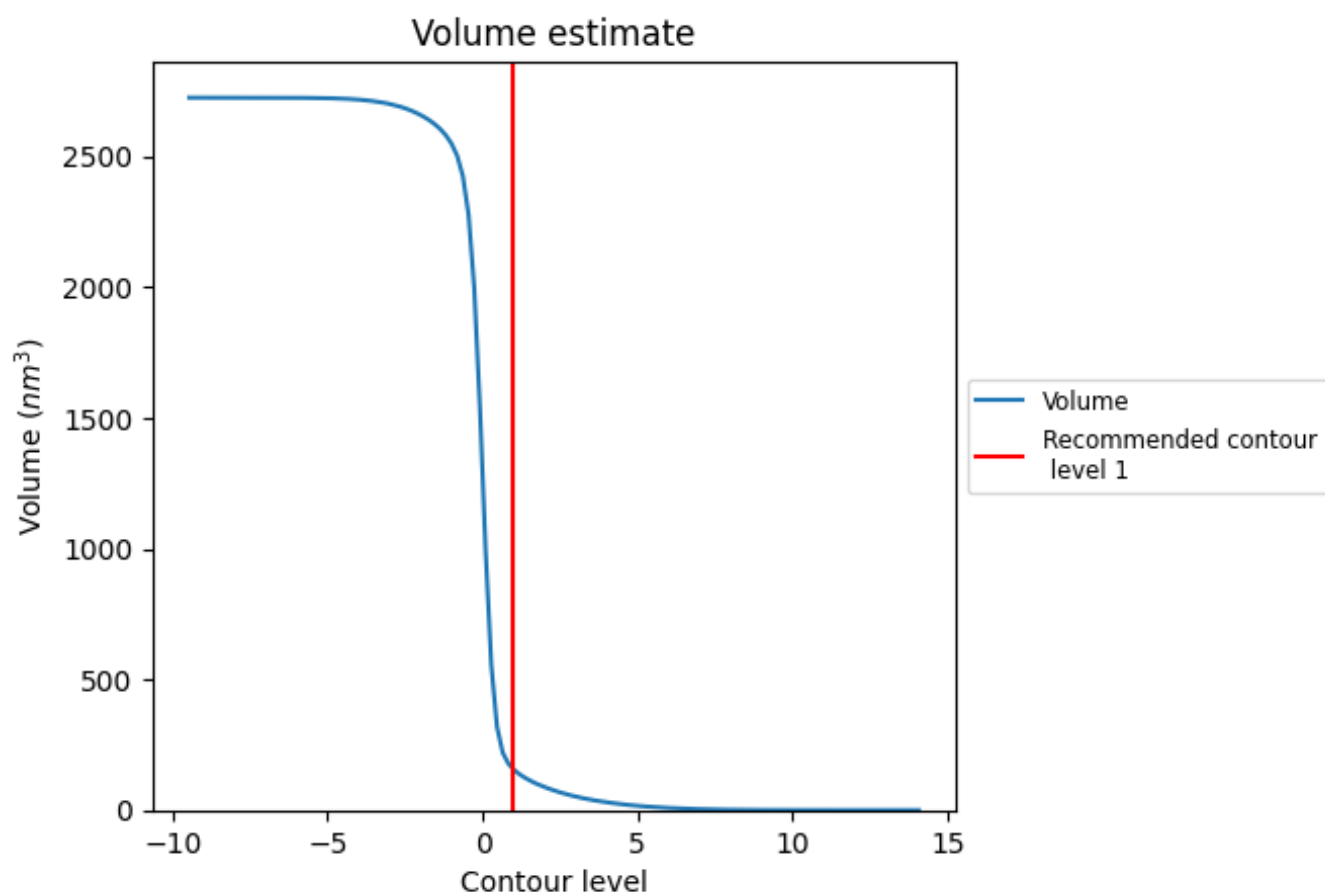
This section contains the results of statistical analysis of the map.

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 156 nm³; this corresponds to an approximate mass of 141 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.

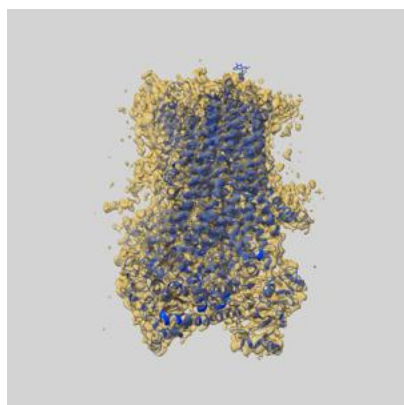
8 Fourier-Shell correlation ⓘ

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

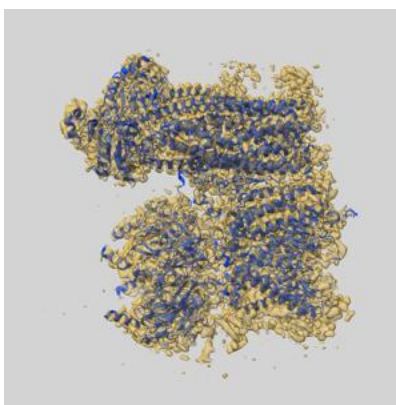
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26194 and PDB model 7TYT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

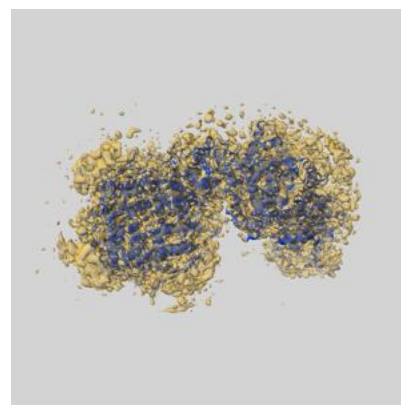
9.1 Map-model overlay [i](#)



X



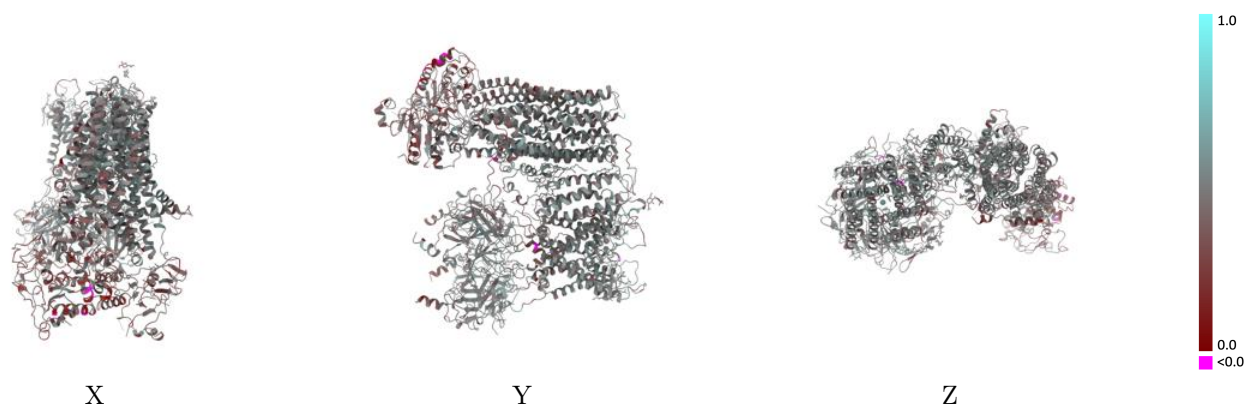
Y



Z

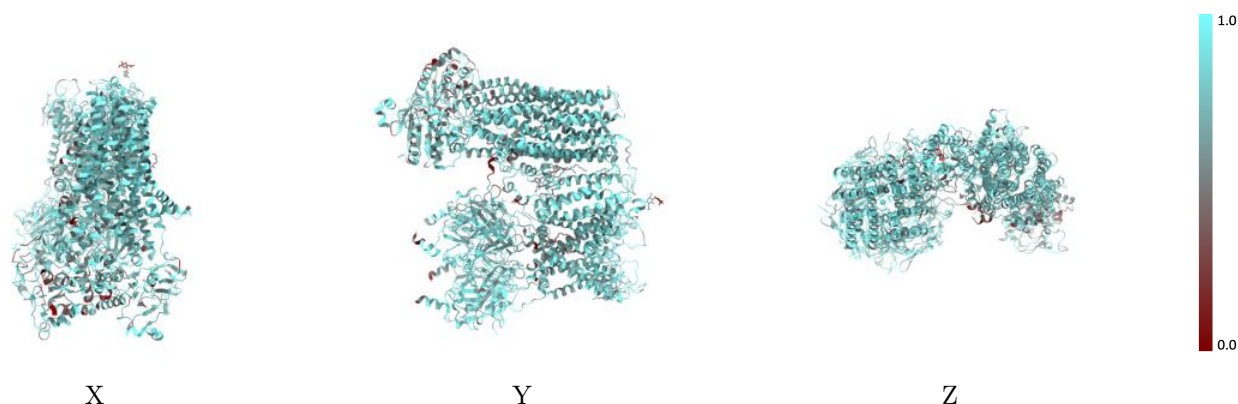
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



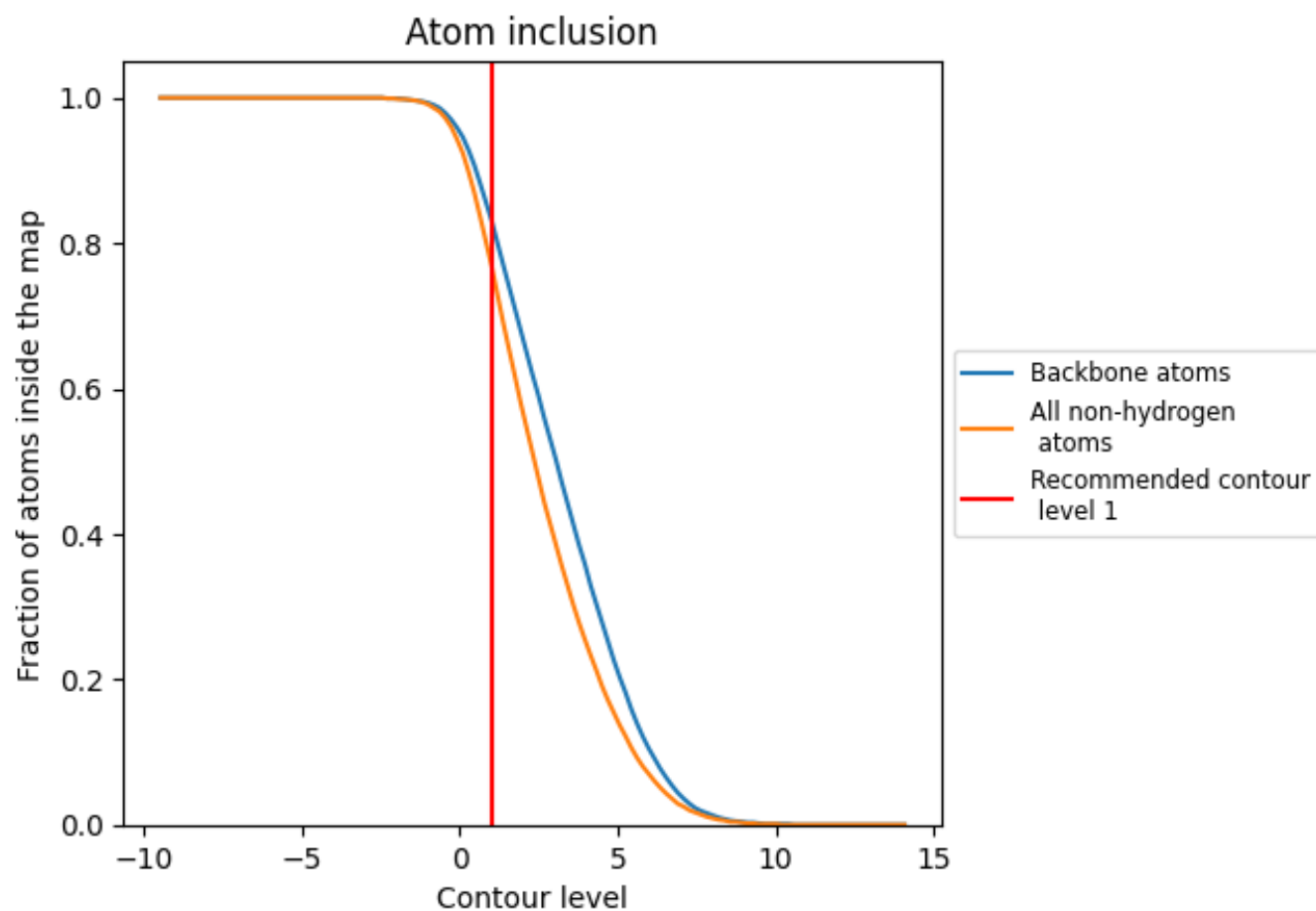
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7710	0.4570
A	0.7690	0.4590
B	0.7900	0.4760
C	0.8010	0.4740
D	0.8040	0.4760
E	0.7520	0.4430
F	0.2500	0.3710

1.0

0.0

<0.0