



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 01:43 PM UTC

PDB ID : 7MJO / pdb_00007mjo
EMDB ID : EMD-23880
Title : Vascular KATP channel: Kir6.1 SUR2B quatrefoil-like conformation 1
Authors : Sung, M.W.; Shyng, S.L.
Deposited on : 2021-04-20
Resolution : 4.00 Å(reported)
Based on initial model : 6BAA

This is a wwPDB EM Validation Summary 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:

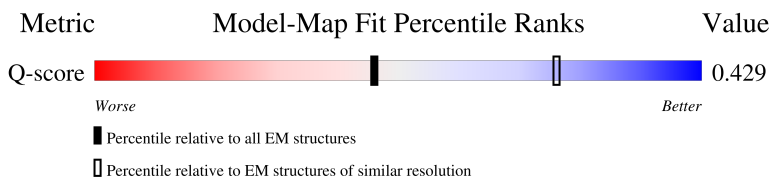
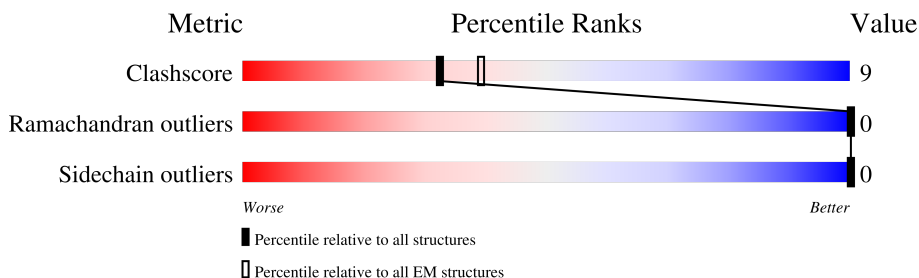
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	424	 64% 17% 19%
1	B	424	 64% 15% 21%
1	C	424	 66% 13% 21%
1	D	424	 65% 14% 21%

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Mol	Chain	Length	Quality of chain
2	E	1545	23% 83% 8% 8%
2	G	1545	12% 87%
3	F	2	50% 50%
3	N	2	100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 19977 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 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	345	Total	C	N	O	S	0	0
			2448	1571	439	425	13		
1	B	337	Total	C	N	O	S	0	0
			2426	1552	433	426	15		
1	C	337	Total	C	N	O	S	0	0
			2407	1548	430	415	14		
1	D	337	Total	C	N	O	S	0	0
			2423	1555	429	426	13		

- Molecule 2 is a protein called Isoform SUR2B of ATP-binding cassette sub-family C member 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	1420	Total	C	N	O	S	0	0
			8338	5228	1549	1546	15		
2	G	205	Total	C	N	O	S	0	0
			1261	799	231	226	5		

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

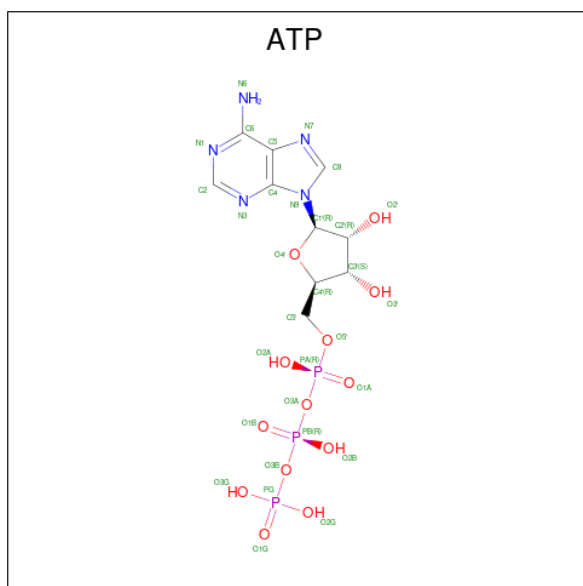


Mol	Chain	Residues	Atoms				AltConf	Trace
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

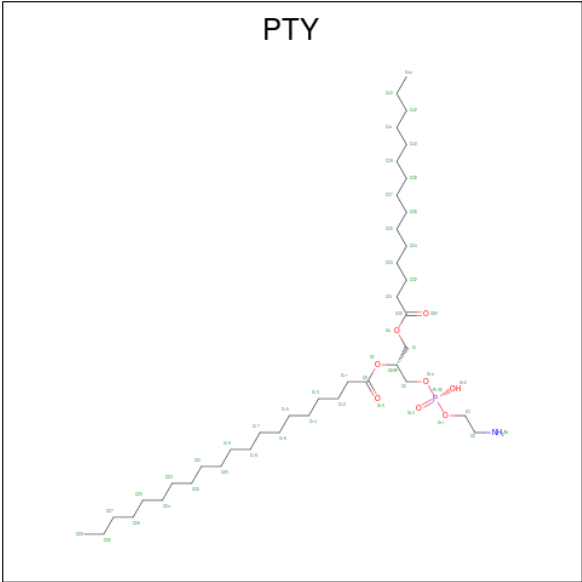
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	K	0
			2	2	

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



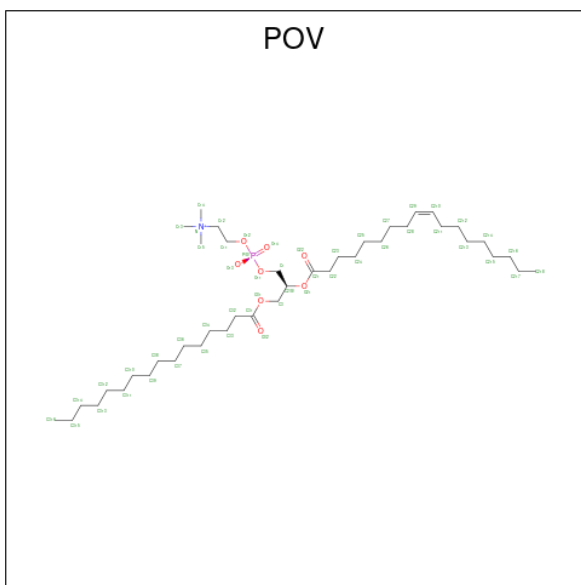
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



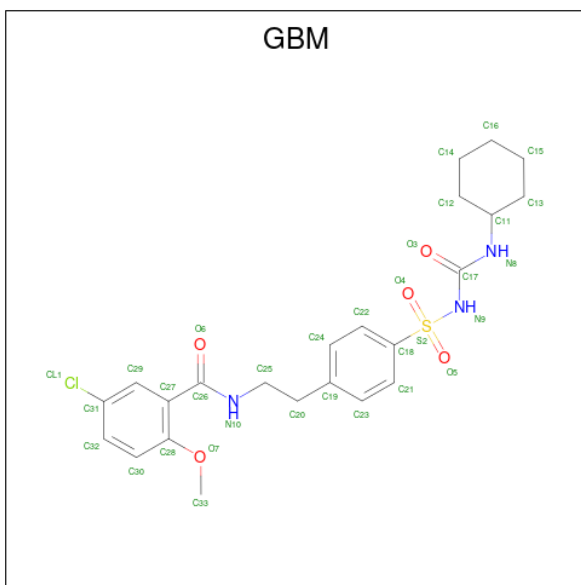
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	C	1	Total	C	N	O	P	0
			32	22	1	8	1	
6	D	1	Total	C	N	O	P	0
			32	22	1	8	1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

- Molecule 7 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



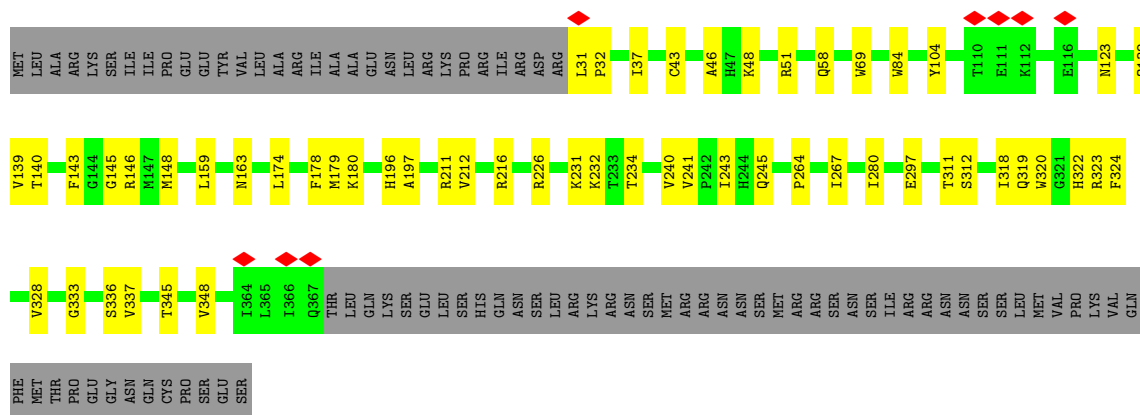
Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	C	1	Total	C	N	O	P	0
			36	26	1	8	1	
7	D	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 8 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxy benzamide (CCD ID: GBM) (formula: $C_{23}H_{28}ClN_3O_5S$) (labeled as "Ligand of Interest" by depositor).



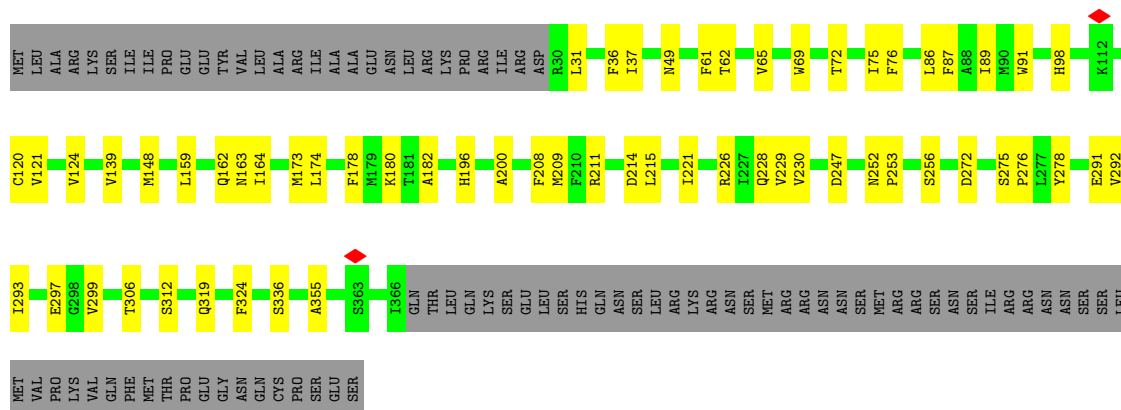
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	N	O	S	
8	E	1	33	23	1	3	5	1	0





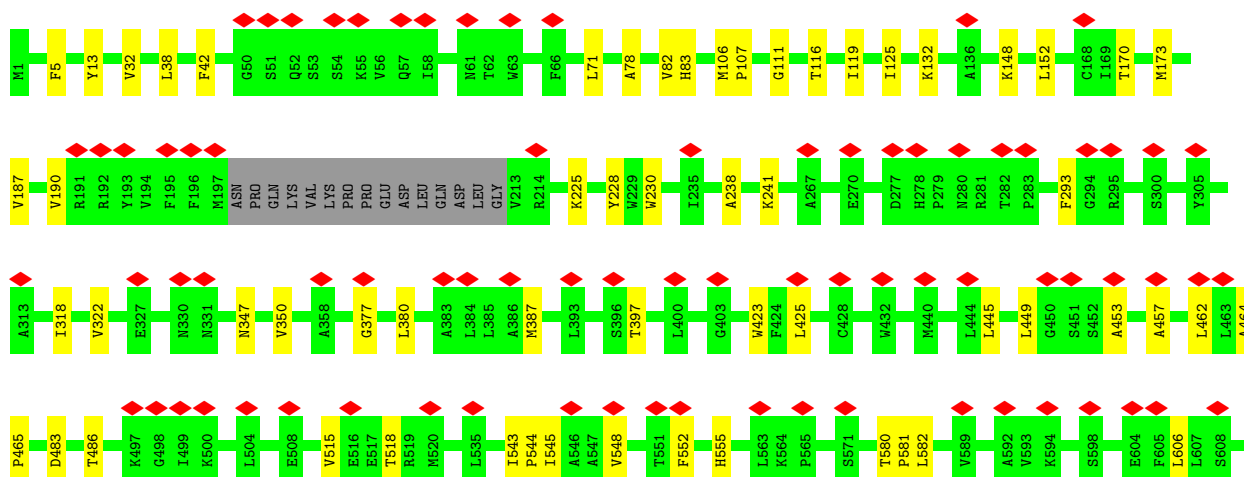
- Molecule 1: ATP-sensitive inward rectifier potassium channel 8

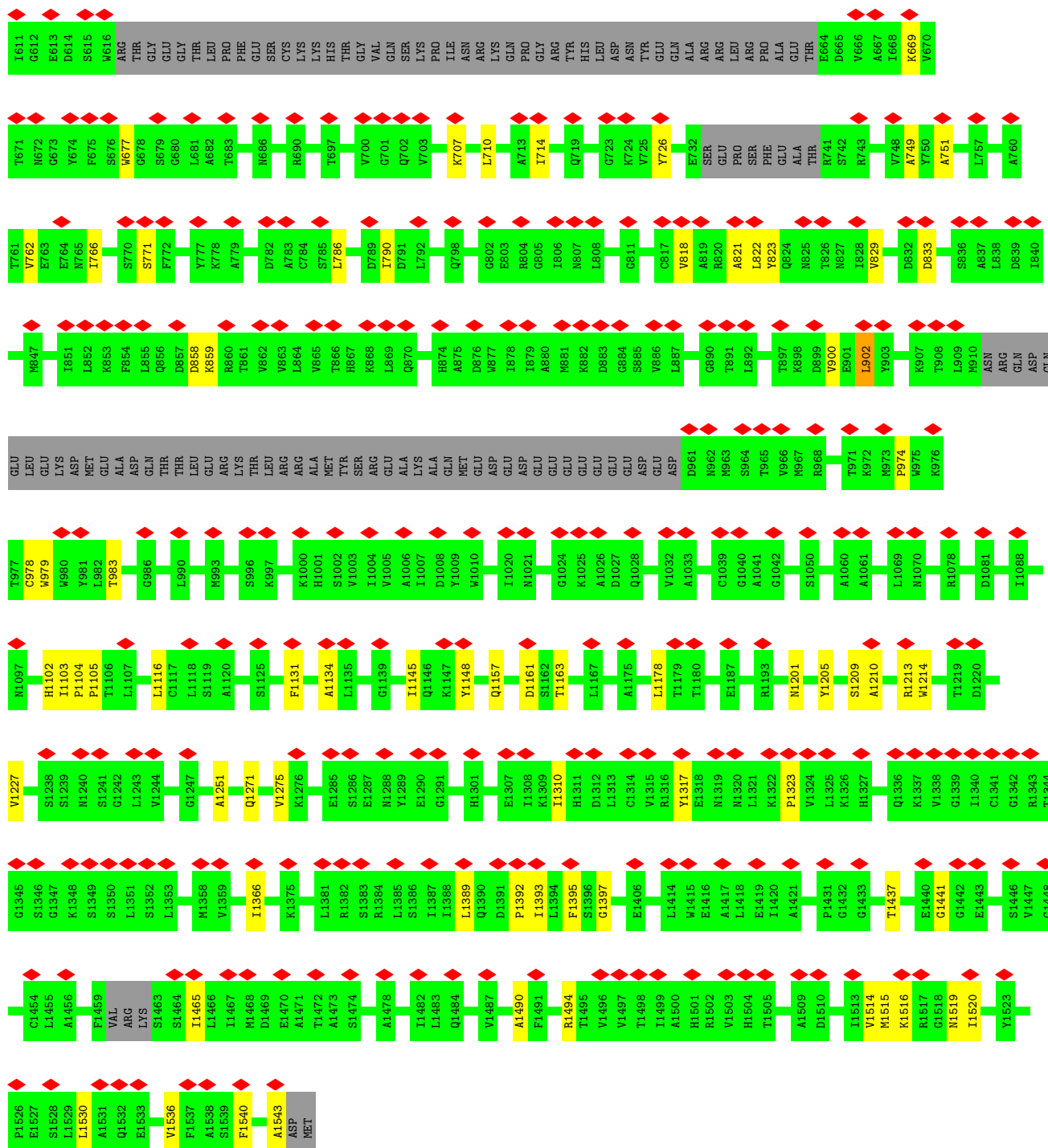
Chain D: 65% 14% 21%



- Molecule 2: Isoform SUR2B of ATP-binding cassette sub-family C member 9

Chain E: 23% 83% 8% 8%





- Molecule 2: Isoform SUR2B of ATP-binding cassette sub-family C member 9

Chain G: 12% 87%





PRO
GLU
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LYS
CYS
THR
ASP
ASP
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TRP
GLU
ALA
LEU
GLU
ILE
ALA
GLN
LEU
LYS
ASN
MET
VAL
VAL
LYS
SER
SER
LEU
PRO
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GLY
LEU
ASP
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THR
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THR
GLU
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ASN
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GLY
VAL
PHE
ALA
SER
PHE
VAL
ARG
ALA
ASP
MET

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

Chain N:

100%

MAG1
MAG2

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

Chain F:

50%

50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71880	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	13.366	Depositor
Minimum map value	-10.130	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size ($\text{\AA}$)	122.322, 161.994, 155.382	wwPDB
Map dimensions	74, 98, 94	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.653, 1.653, 1.653	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: PTY, POV, K, ATP, NAG, GBM

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	0/2499	0.48	3/3419 (0.1%)
1	B	0.25	0/2476	0.44	1/3377 (0.0%)
1	C	0.27	0/2456	0.42	0/3358
1	D	0.24	0/2472	0.42	2/3374 (0.1%)
2	E	0.21	0/8476	0.43	5/11747 (0.0%)
2	G	0.41	0/1290	0.76	8/1784 (0.4%)
All	All	0.25	0/19669	0.46	19/27059 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	203	LYS	CA-C-N	10.43	131.12	120.38
2	G	203	LYS	C-N-CA	10.43	131.12	120.38
2	E	902	LEU	N-CA-C	8.76	120.91	111.36
2	G	19	VAL	N-CA-C	7.88	118.67	110.72
2	G	189	ARG	N-CA-C	7.71	119.32	111.07

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	2448	0	2219	61	0
1	B	2426	0	2213	64	0
1	C	2407	0	2238	59	0
1	D	2423	0	2234	50	0
2	E	8338	0	5692	94	0
2	G	1261	0	895	10	0
3	F	28	0	25	1	0
3	N	28	0	25	0	0
4	A	2	0	0	0	0
5	A	31	0	12	1	0
5	B	62	0	24	6	0
5	C	31	0	12	2	0
5	E	31	0	12	0	0
6	A	128	0	148	2	0
6	C	64	0	74	6	0
6	D	32	0	37	0	0
6	E	96	0	111	1	0
7	B	36	0	45	0	0
7	C	36	0	45	1	0
7	D	36	0	45	1	0
8	E	33	0	28	5	0
All	All	19977	0	16134	308	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 9.

The worst 5 of 308 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:B:34:ALA:HB2	1:C:333:GLY:O	1.37	1.25
1:B:35:ARG:NH1	1:B:39:LYS:HG2	1.61	1.12
2:E:230:TRP:CH2	2:E:1210:ALA:CB	2.35	1.09
1:C:31:LEU:CB	1:C:32:PRO:HD2	1.82	1.08
1:C:31:LEU:CB	1:C:32:PRO:CD	2.34	1.06

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	343/424 (81%)	317 (92%)	26 (8%)	0	100	100
1	B	335/424 (79%)	300 (90%)	35 (10%)	0	100	100
1	C	335/424 (79%)	305 (91%)	30 (9%)	0	100	100
1	D	335/424 (79%)	304 (91%)	31 (9%)	0	100	100
2	E	1408/1545 (91%)	1276 (91%)	132 (9%)	0	100	100
2	G	203/1545 (13%)	191 (94%)	12 (6%)	0	100	100
All	All	2959/4786 (62%)	2693 (91%)	266 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	213/376 (57%)	213 (100%)	0	100	100
1	B	216/376 (57%)	216 (100%)	0	100	100
1	C	218/376 (58%)	218 (100%)	0	100	100
1	D	218/376 (58%)	218 (100%)	0	100	100
2	E	374/1348 (28%)	374 (100%)	0	100	100
2	G	71/1348 (5%)	71 (100%)	0	100	100
All	All	1310/4200 (31%)	1310 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	288	GLN
2	E	17	HIS
2	E	1501	HIS
1	C	44	ASN
1	C	163	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 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	2,3	14,14,15	2.69	8 (57%)	17,19,21	2.01	4 (23%)
3	NAG	F	2	3	14,14,15	2.82	7 (50%)	17,19,21	1.21	1 (5%)
3	NAG	N	1	2,3	14,14,15	2.71	8 (57%)	17,19,21	2.11	3 (17%)
3	NAG	N	2	3	14,14,15	2.77	7 (50%)	17,19,21	1.45	2 (11%)

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	2,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C5	5.65	1.54	1.43
3	N	2	NAG	O5-C5	5.35	1.53	1.43
3	F	1	NAG	O5-C5	5.30	1.53	1.43
3	N	1	NAG	O5-C5	5.16	1.53	1.43
3	N	2	NAG	C2-N2	4.71	1.54	1.46

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C4-C3-C2	5.53	119.13	111.02
3	F	1	NAG	C4-C3-C2	4.54	117.67	111.02
3	N	1	NAG	C3-C4-C5	4.26	117.96	110.23
3	N	2	NAG	C4-C3-C2	3.74	116.49	111.02
3	F	1	NAG	C1-O5-C5	-3.68	107.26	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

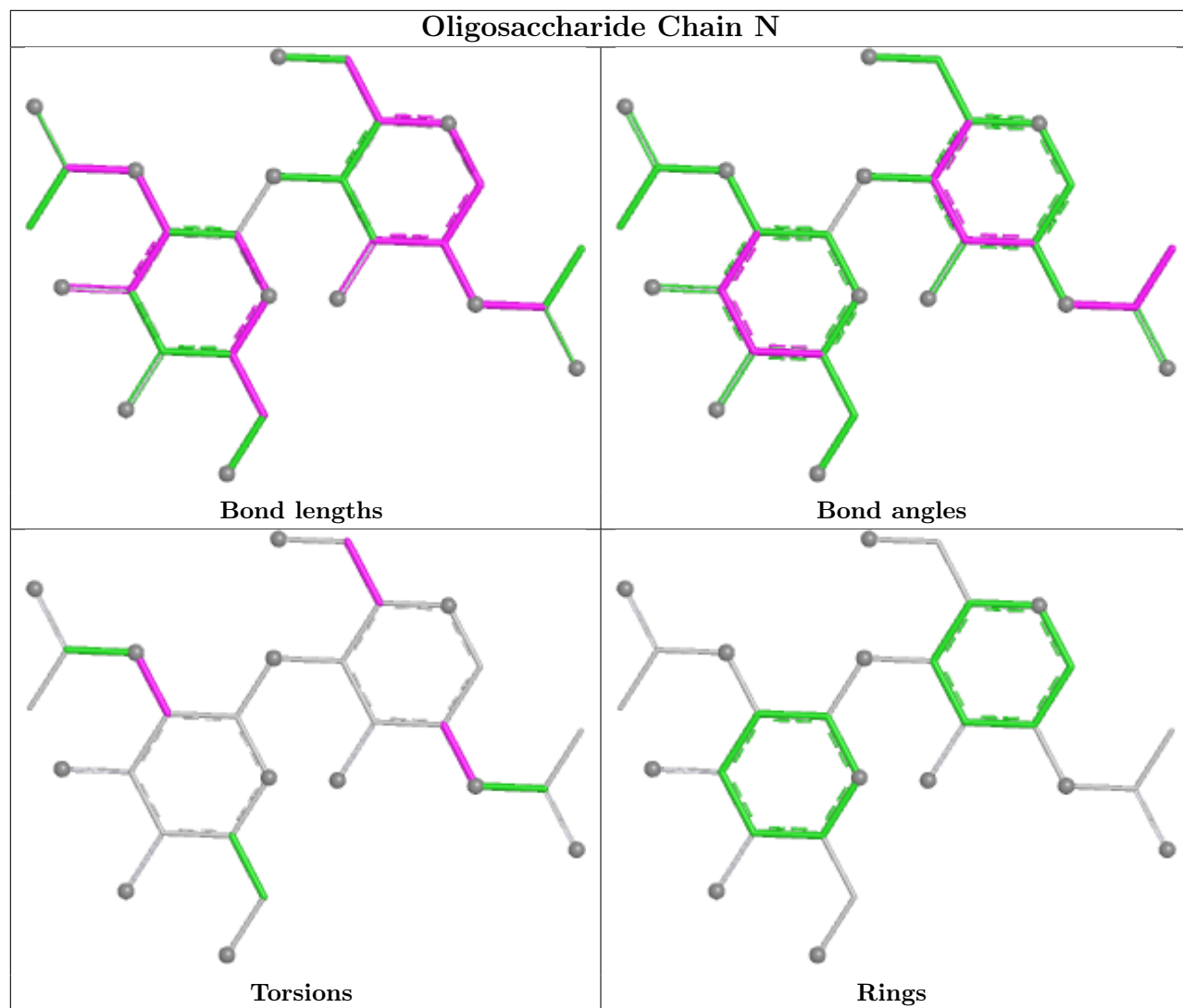
Mol	Chain	Res	Type	Atoms
3	N	2	NAG	C1-C2-N2-C7
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C4-C5-C6-O6

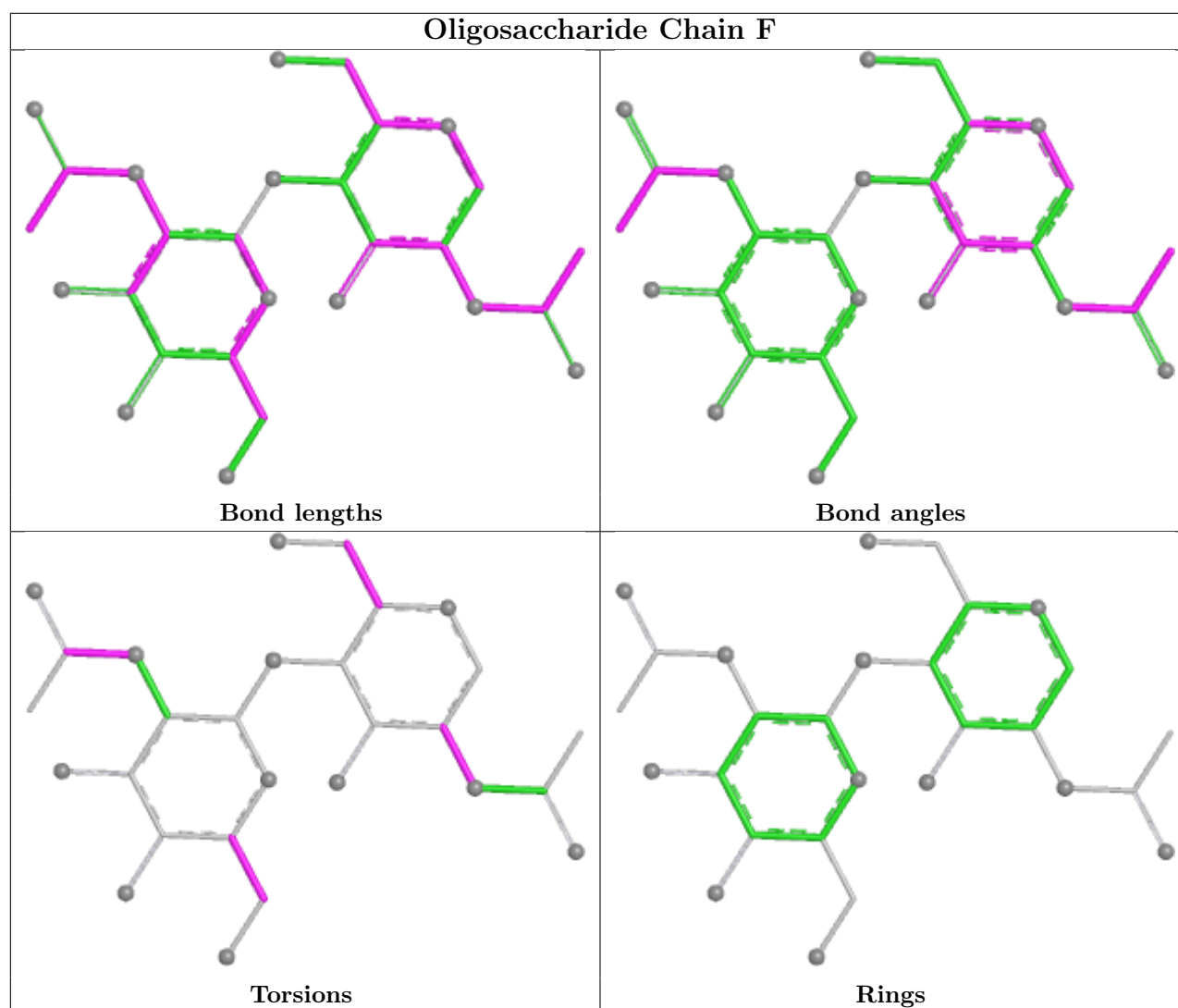
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	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 21 ligands modelled in this entry, 2 are 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	$\# Z > 2$
8	GBM	E	1602	-	35,35,35	4.82	8 (22%)	48,48,48	1.95	8 (16%)
6	PTY	C	502	-	31,31,49	1.09	4 (12%)	34,36,54	1.08	2 (5%)
5	ATP	B	501	-	32,33,33	1.34	5 (15%)	48,52,52	1.79	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PTY	E	1605	-	31,31,49	1.10	4 (12%)	34,36,54	1.06	2 (5%)
5	ATP	E	1601	-	32,33,33	1.39	4 (12%)	48,52,52	1.76	9 (18%)
7	POV	D	801	-	35,35,51	1.46	4 (11%)	41,43,59	1.15	3 (7%)
6	PTY	C	503	-	31,31,49	1.09	4 (12%)	34,36,54	1.06	2 (5%)
6	PTY	A	505	-	31,31,49	1.10	4 (12%)	34,36,54	1.01	2 (5%)
5	ATP	B	502	-	32,33,33	1.35	5 (15%)	48,52,52	1.75	8 (16%)
6	PTY	A	504	-	31,31,49	1.11	4 (12%)	34,36,54	1.06	2 (5%)
6	PTY	E	1603	-	31,31,49	1.10	4 (12%)	34,36,54	1.07	2 (5%)
7	POV	B	503	-	35,35,51	1.46	4 (11%)	41,43,59	1.19	4 (9%)
5	ATP	C	501	-	32,33,33	1.33	5 (15%)	48,52,52	1.75	10 (20%)
6	PTY	A	506	-	31,31,49	1.11	4 (12%)	34,36,54	1.02	2 (5%)
7	POV	C	504	-	35,35,51	1.46	4 (11%)	41,43,59	1.16	4 (9%)
6	PTY	A	507	-	31,31,49	1.12	3 (9%)	34,36,54	1.11	3 (8%)
6	PTY	E	1604	-	31,31,49	1.09	4 (12%)	34,36,54	1.08	2 (5%)
5	ATP	A	503	-	32,33,33	1.36	5 (15%)	48,52,52	1.72	9 (18%)
6	PTY	D	802	-	31,31,49	1.11	4 (12%)	34,36,54	1.04	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GBM	E	1602	-	-	13/27/35/35	0/3/3/3
6	PTY	C	502	-	-	18/35/35/53	-
5	ATP	B	501	-	-	5/22/38/38	0/3/3/3
6	PTY	E	1605	-	-	16/35/35/53	-
5	ATP	E	1601	-	-	1/22/38/38	0/3/3/3
7	POV	D	801	-	-	13/39/39/55	-
6	PTY	C	503	-	-	14/35/35/53	-
6	PTY	A	505	-	-	21/35/35/53	-
5	ATP	B	502	-	-	6/22/38/38	0/3/3/3
6	PTY	A	504	-	-	13/35/35/53	-
6	PTY	E	1603	-	-	16/35/35/53	-
7	POV	B	503	-	-	18/39/39/55	-
5	ATP	C	501	-	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PTY	A	506	-	-	14/35/35/53	-
7	POV	C	504	-	-	17/39/39/55	-
6	PTY	A	507	-	-	15/35/35/53	-
6	PTY	E	1604	-	-	13/35/35/53	-
5	ATP	A	503	-	-	6/22/38/38	0/3/3/3
6	PTY	D	802	-	-	13/35/35/53	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	1602	GBM	O4-S2	19.04	1.65	1.43
8	E	1602	GBM	O5-S2	18.91	1.65	1.43
8	E	1602	GBM	C26-N10	5.66	1.46	1.33
5	E	1601	ATP	C5-C4	4.65	1.47	1.39
5	B	501	ATP	C5-C4	4.48	1.47	1.39

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	1602	GBM	O5-S2-O4	-8.02	109.79	119.52
5	B	501	ATP	C5-C4-N3	-5.78	118.76	126.72
5	E	1601	ATP	C5-C4-N3	-5.76	118.79	126.72
5	B	502	ATP	C5-C4-N3	-5.73	118.82	126.72
5	C	501	ATP	C5-C4-N3	-5.66	118.93	126.72

There are no chirality outliers.

5 of 236 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	ATP	C5'-O5'-PA-O3A
5	B	501	ATP	C5'-O5'-PA-O3A
5	B	502	ATP	C5'-O5'-PA-O2A
5	B	502	ATP	O4'-C4'-C5'-O5'
5	C	501	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

11 monomers are involved in 25 short contacts:

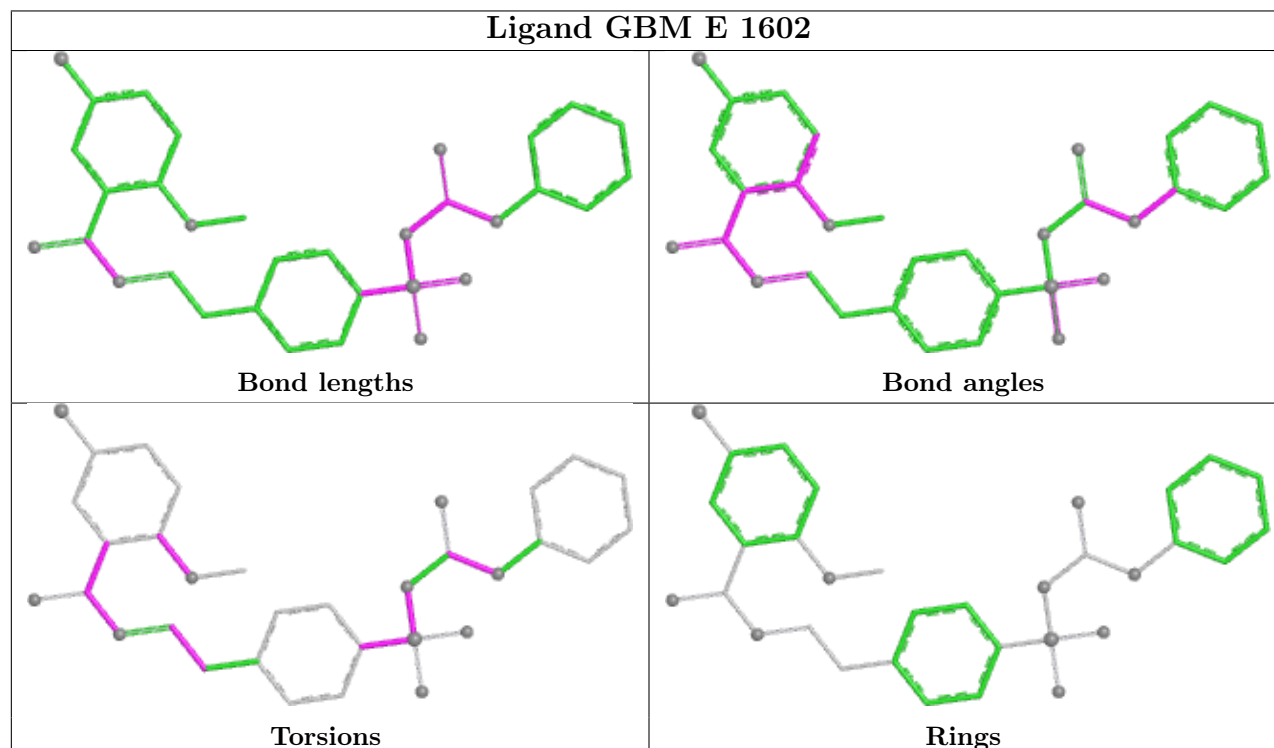
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	1602	GBM	5	0

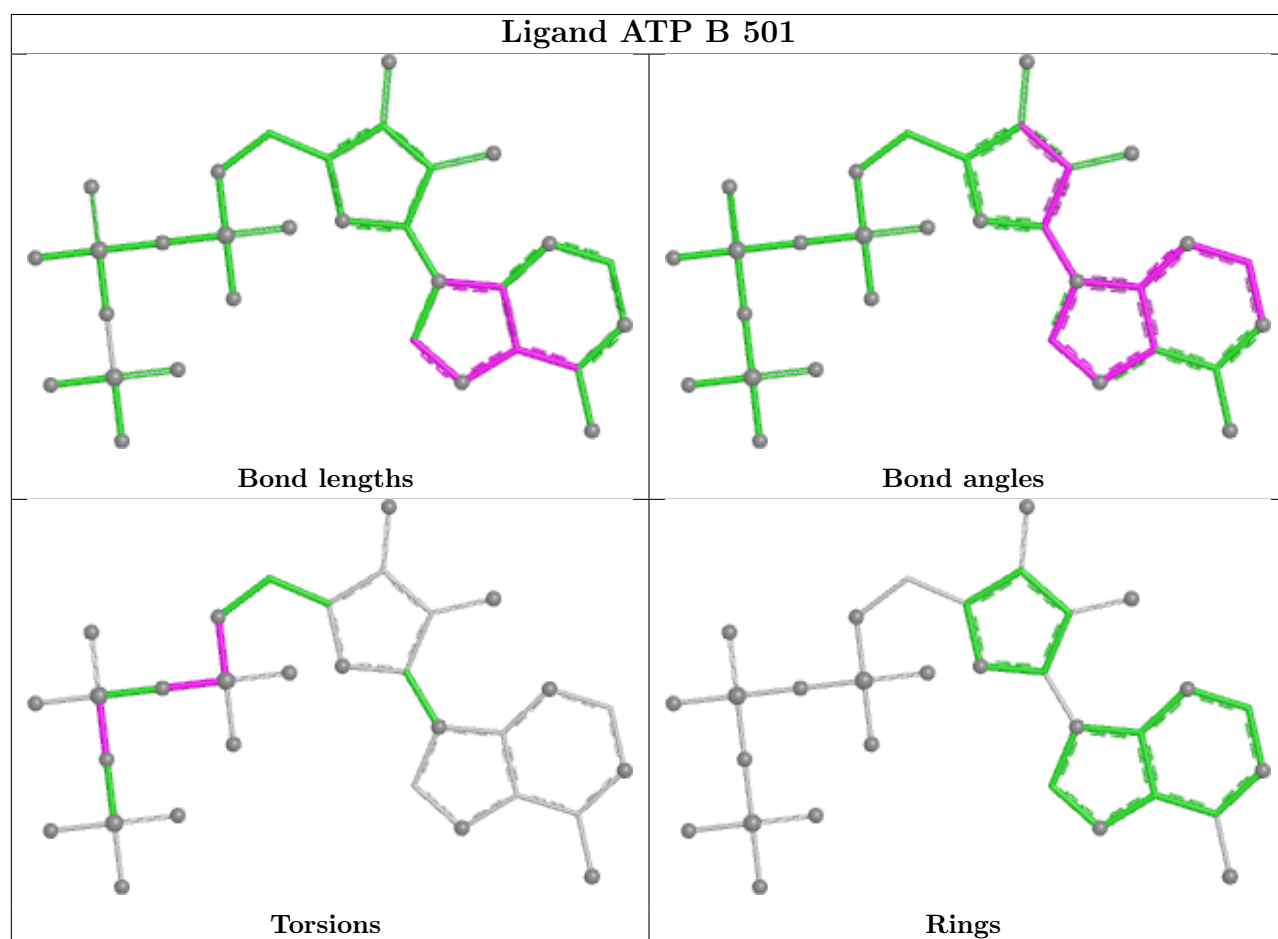
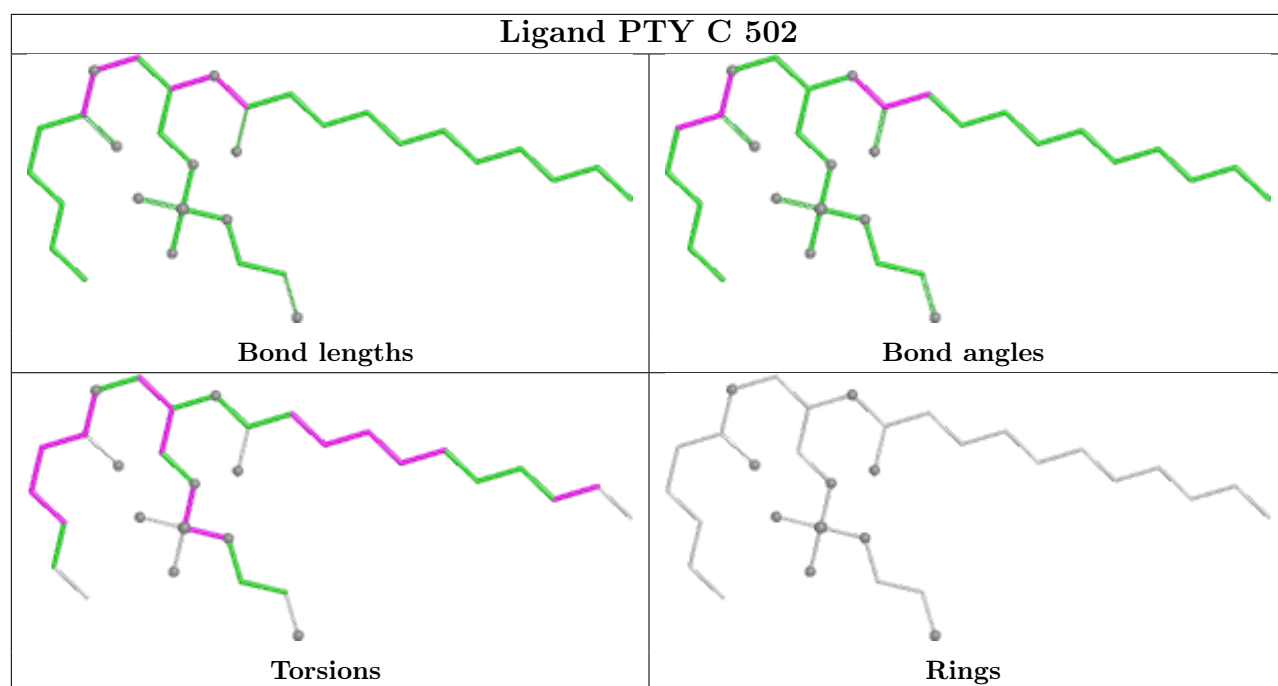
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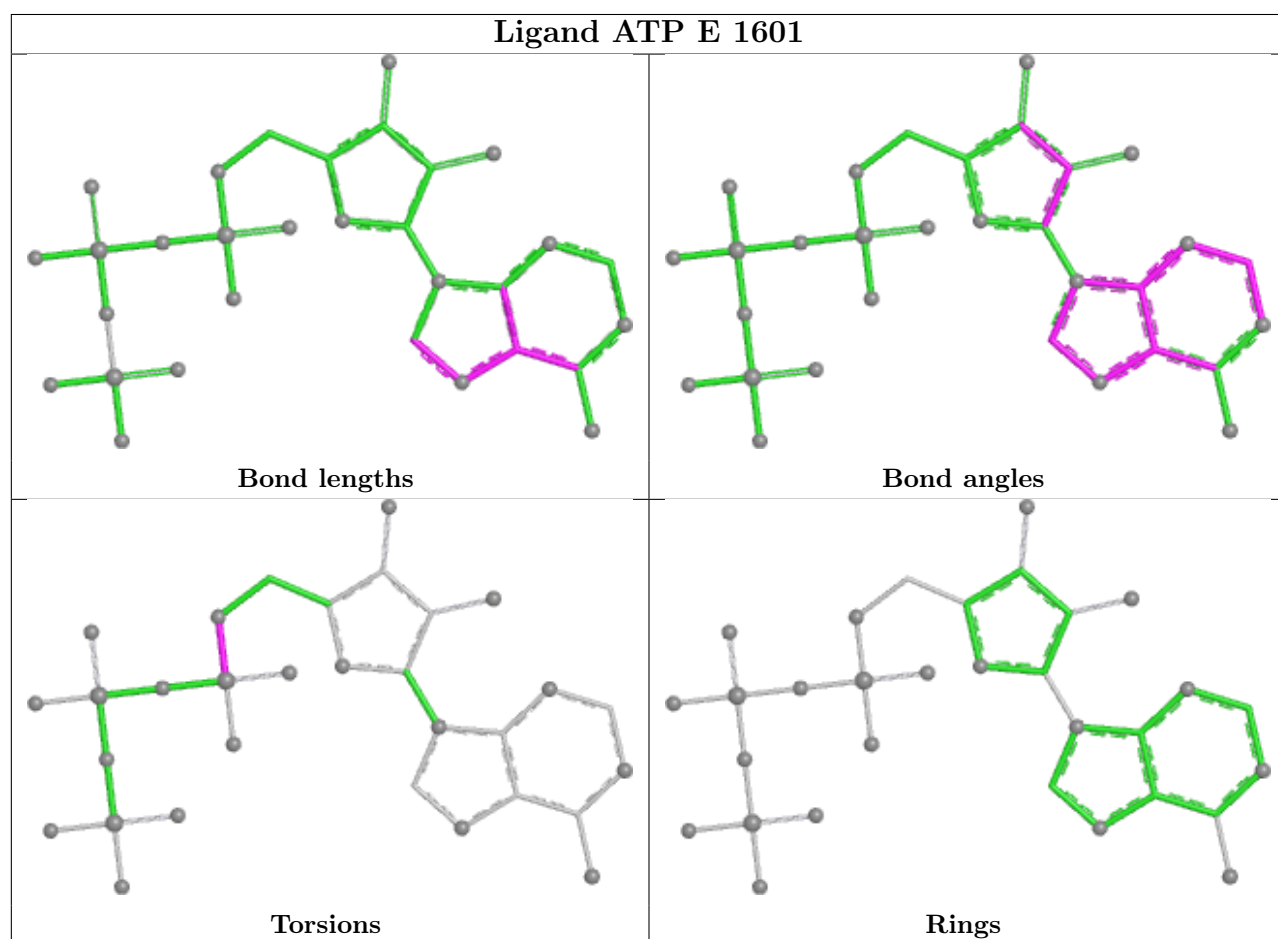
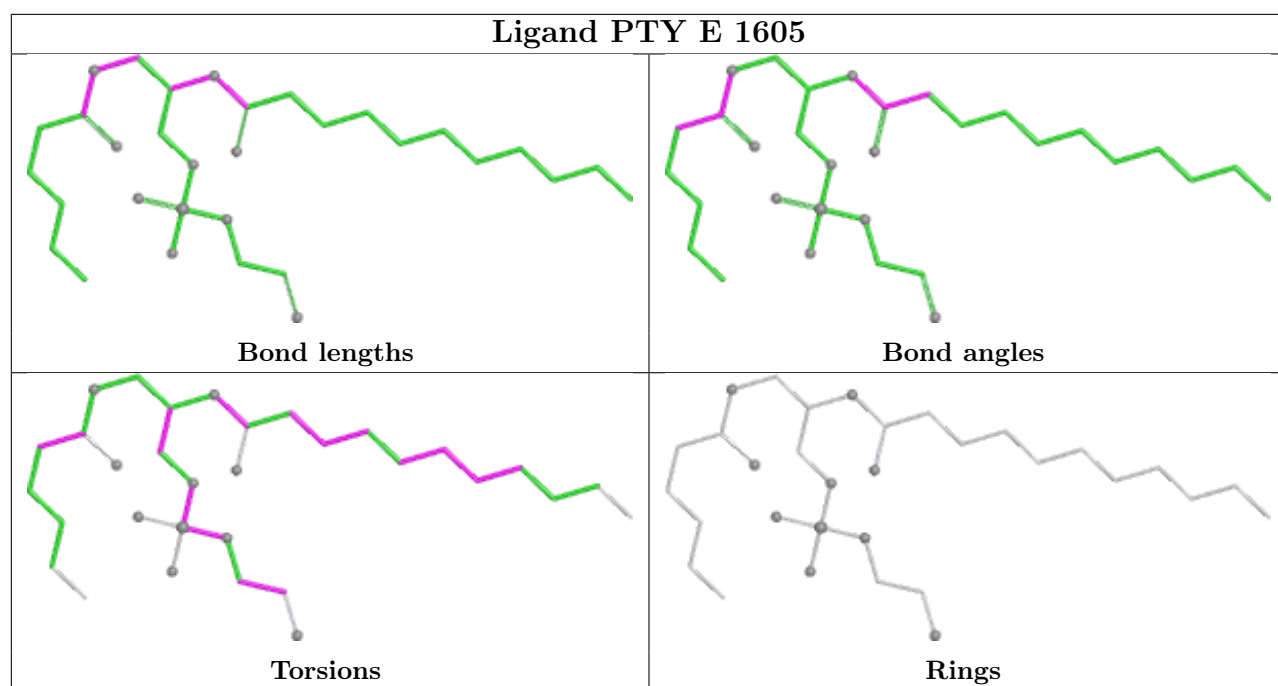
Continued from previous page...

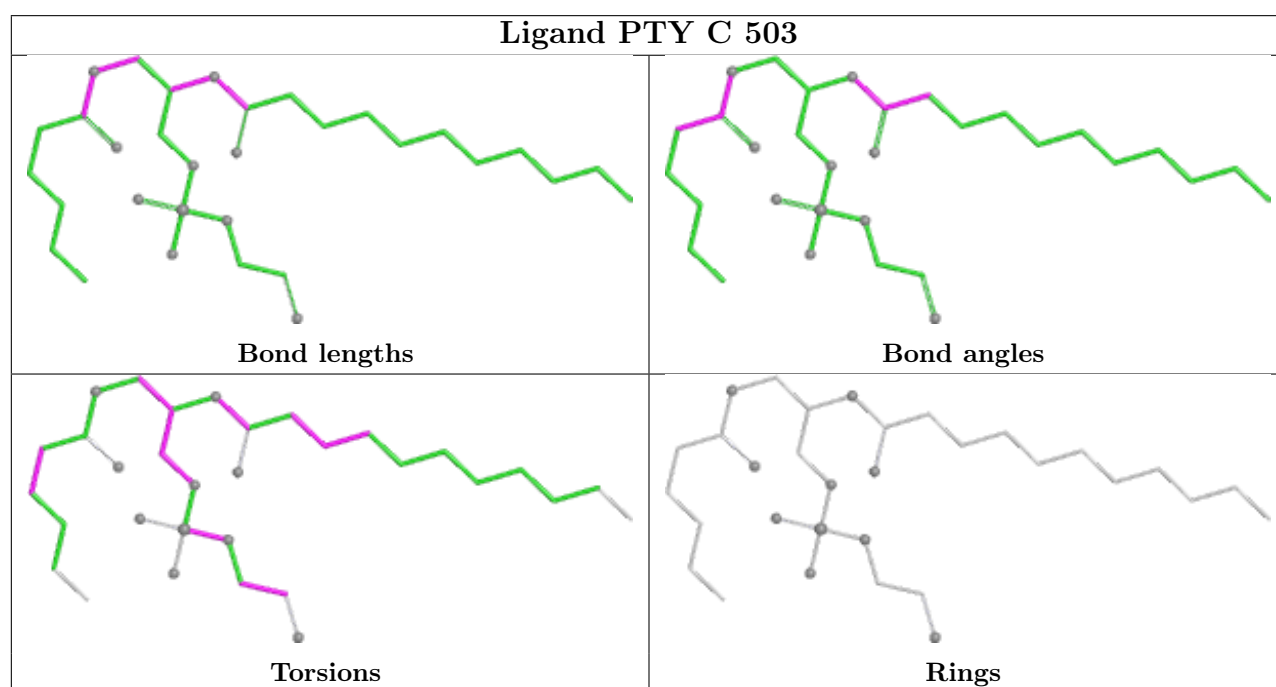
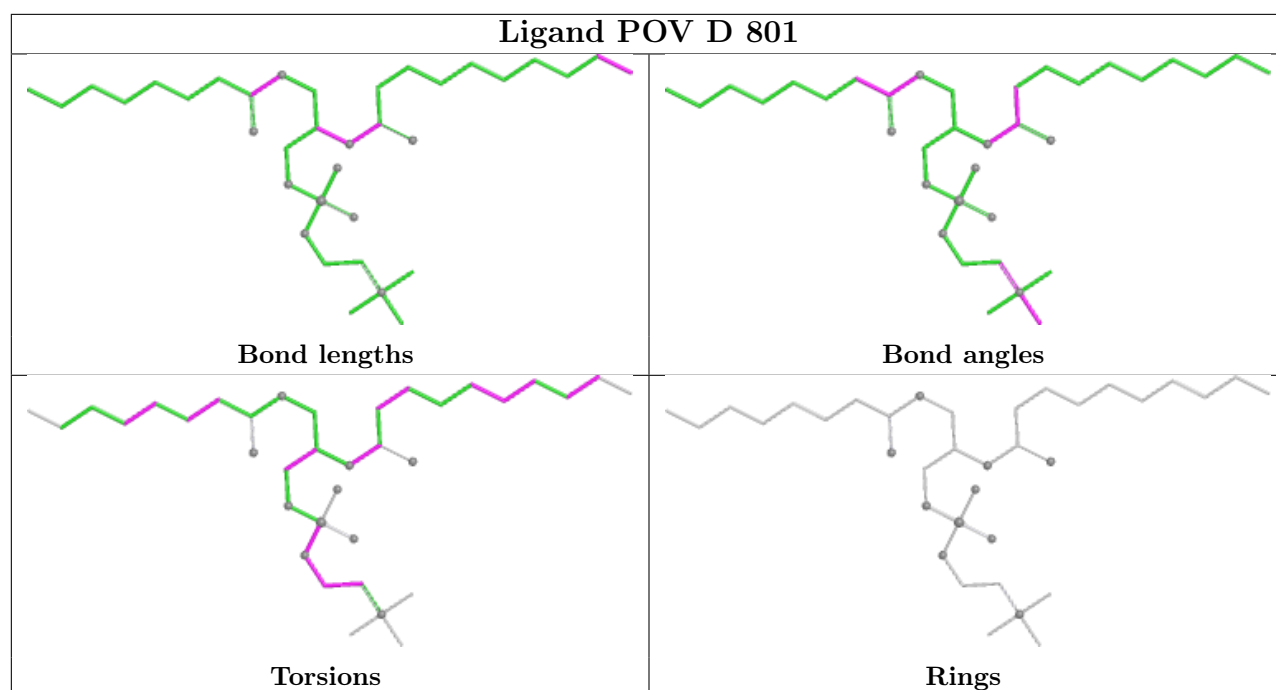
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	502	PTY	5	0
5	B	501	ATP	4	0
7	D	801	POV	1	0
6	C	503	PTY	1	0
5	B	502	ATP	2	0
6	E	1603	PTY	1	0
5	C	501	ATP	2	0
7	C	504	POV	1	0
6	A	507	PTY	2	0
5	A	503	ATP	1	0

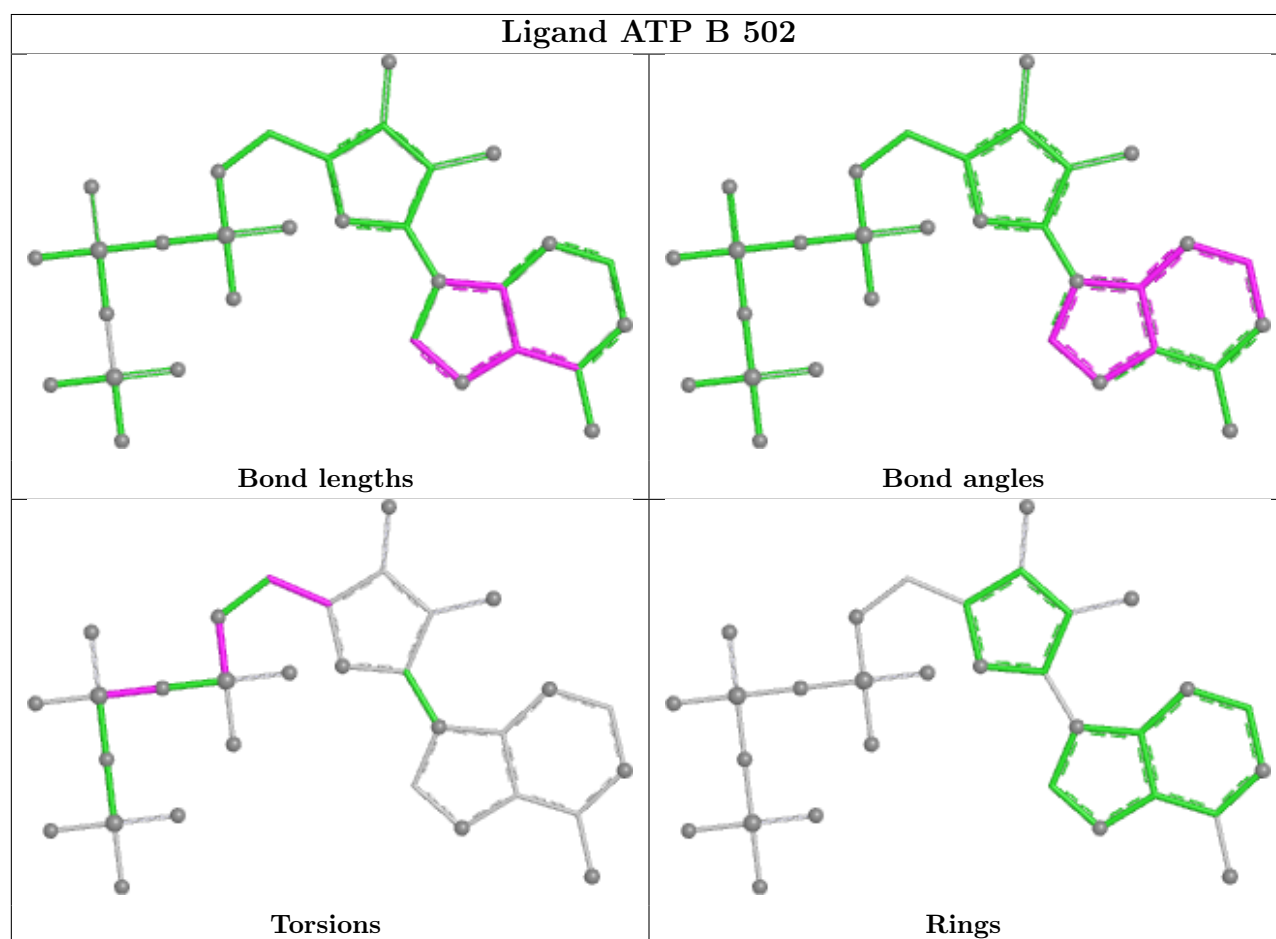
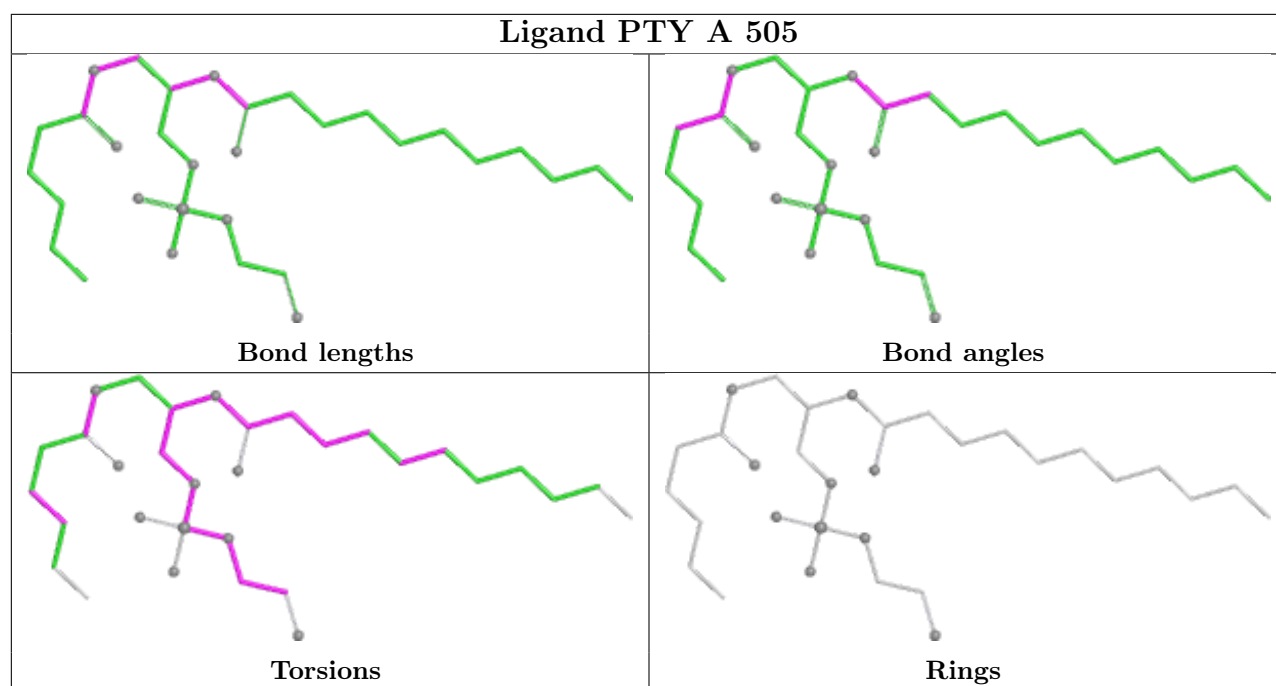
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

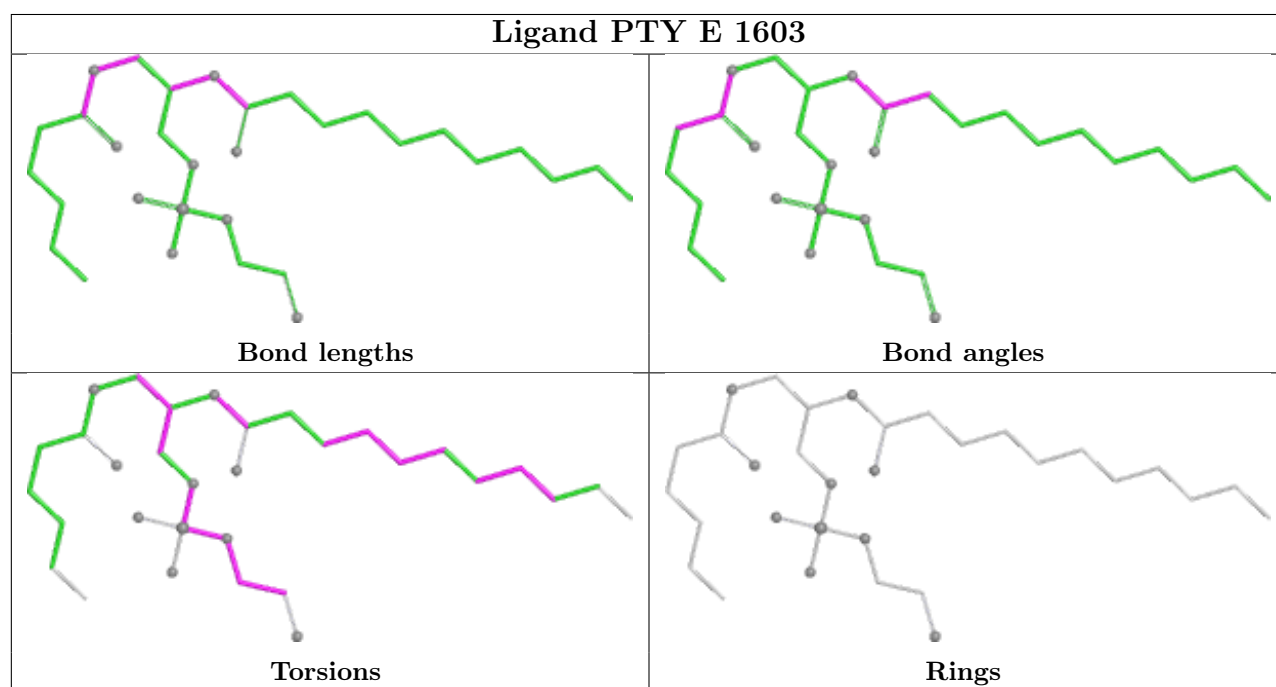
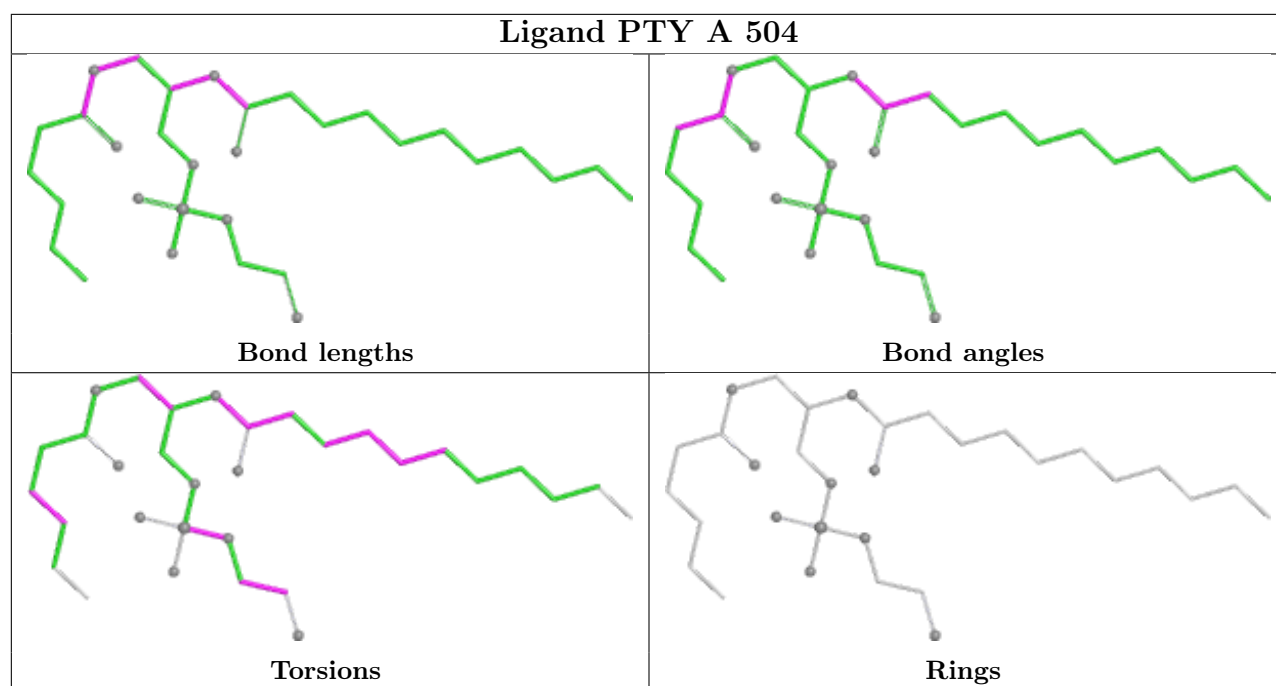


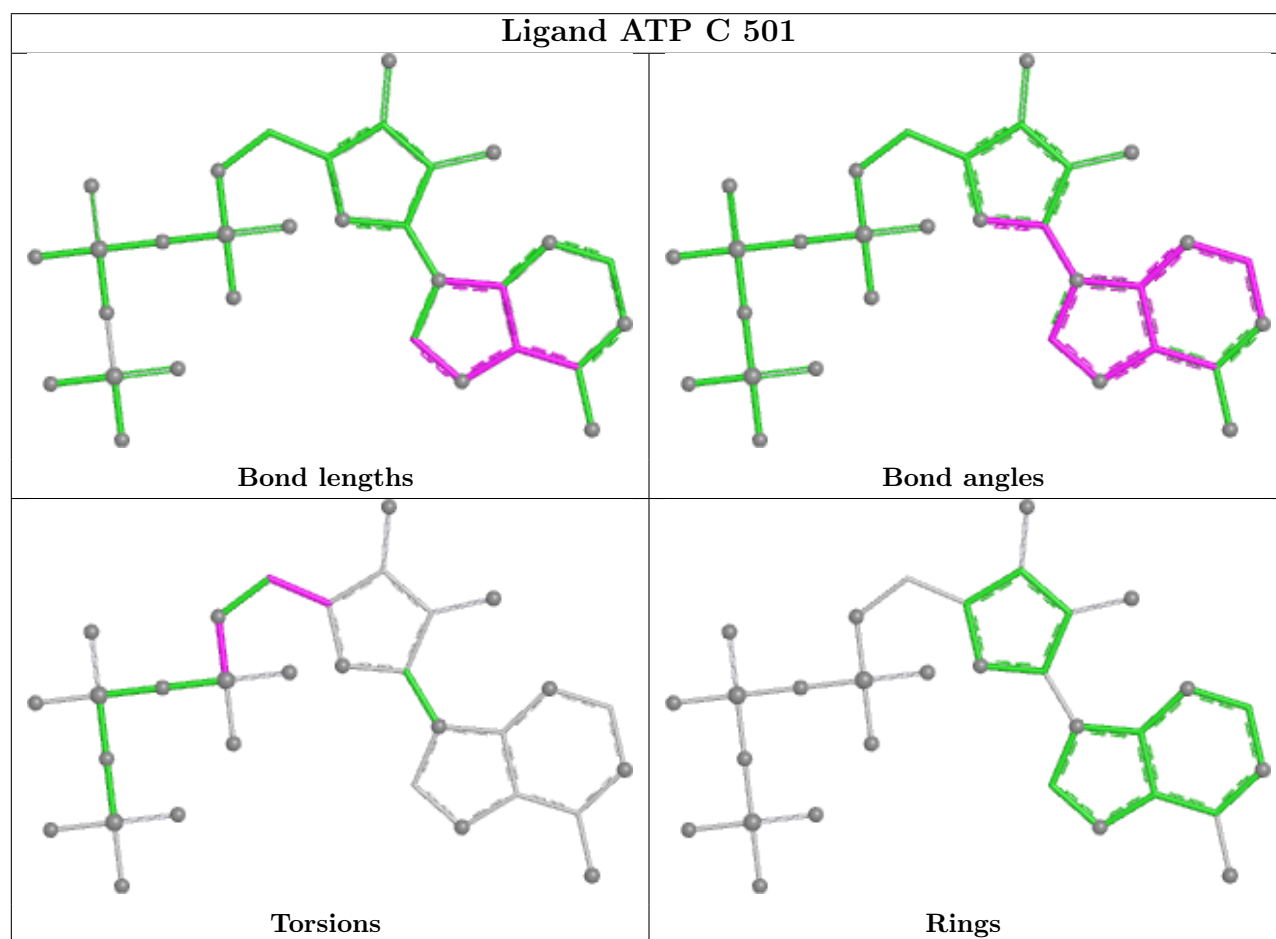
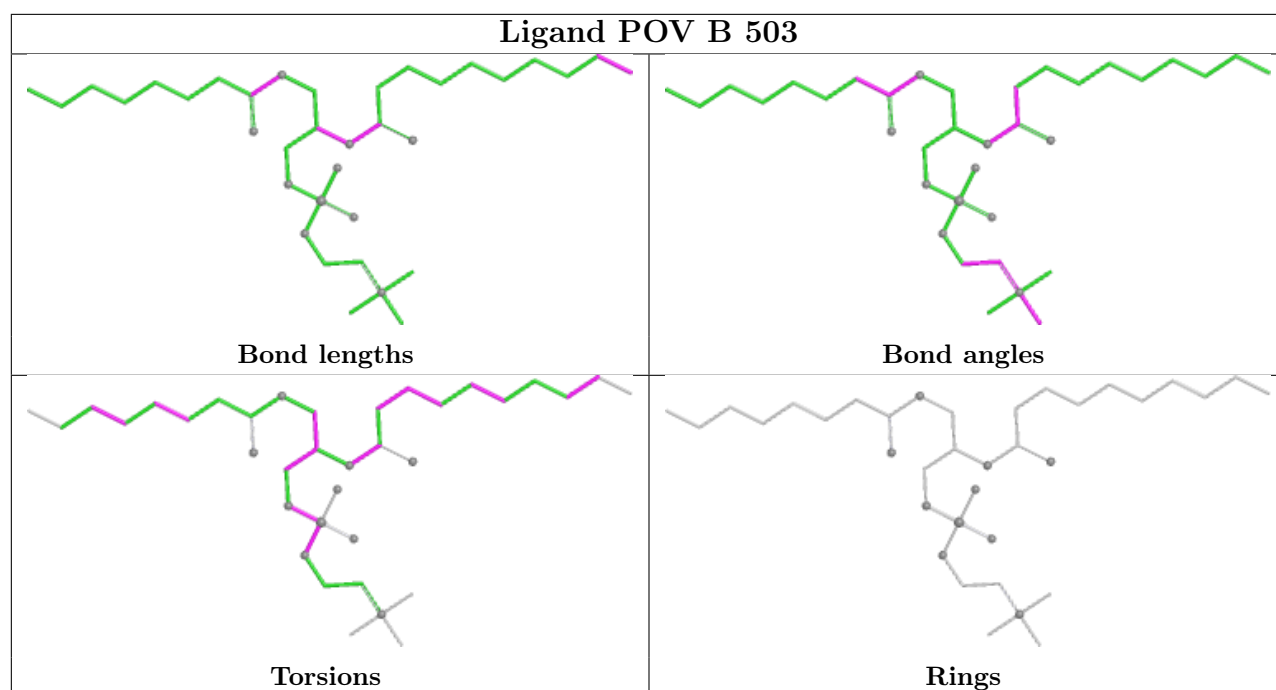


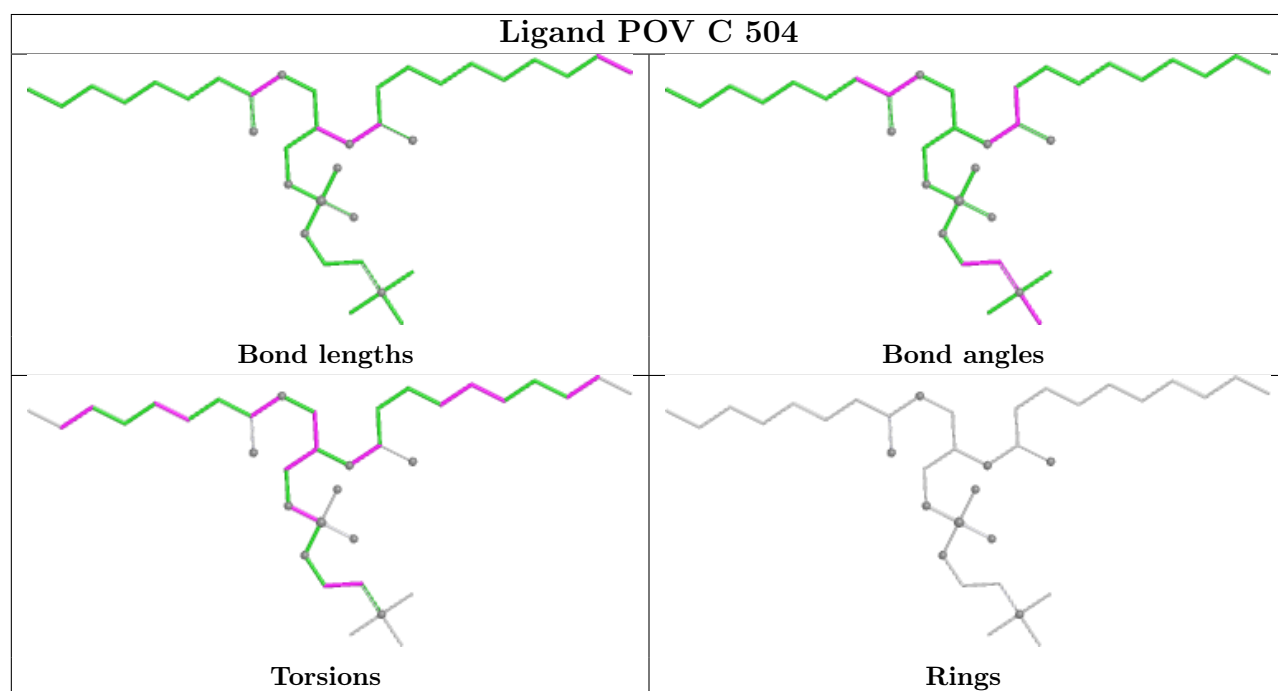
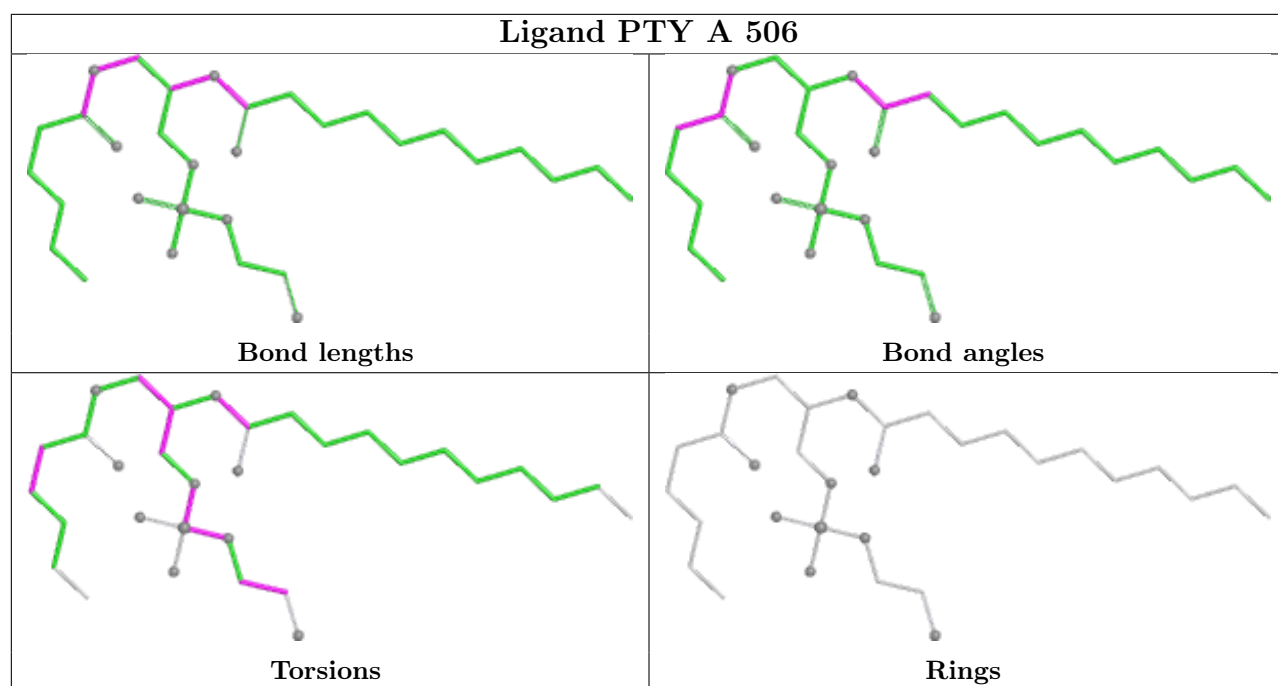


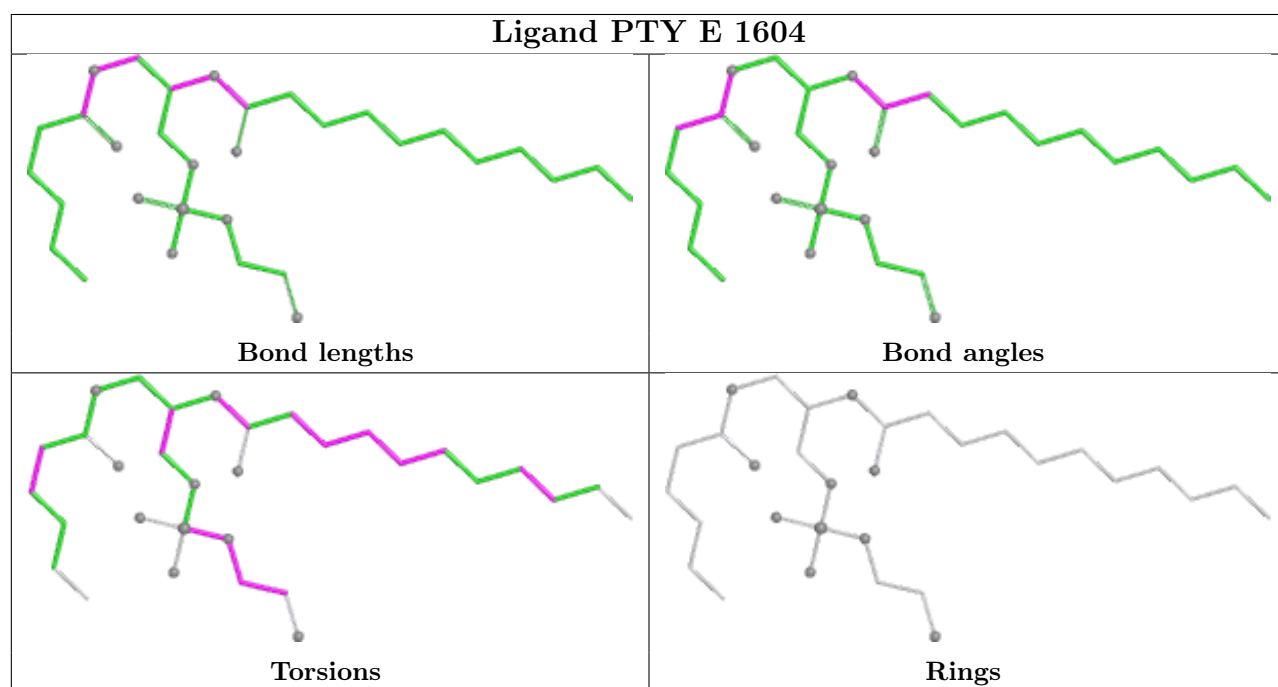
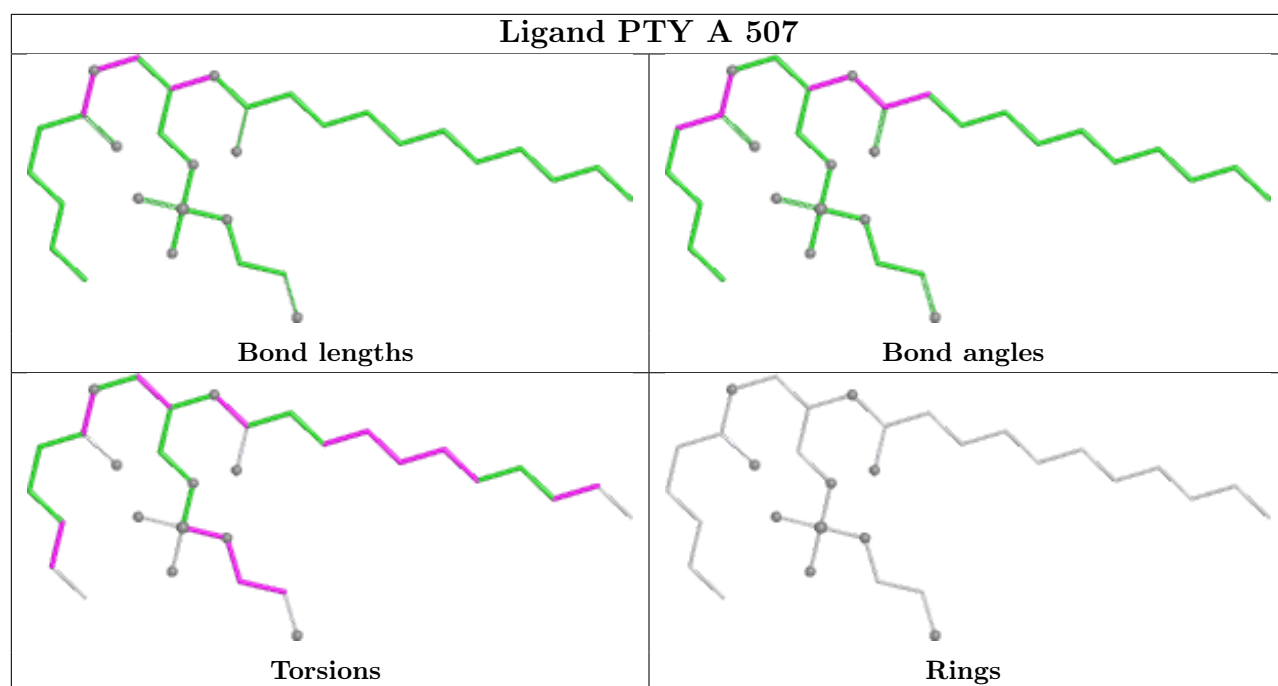


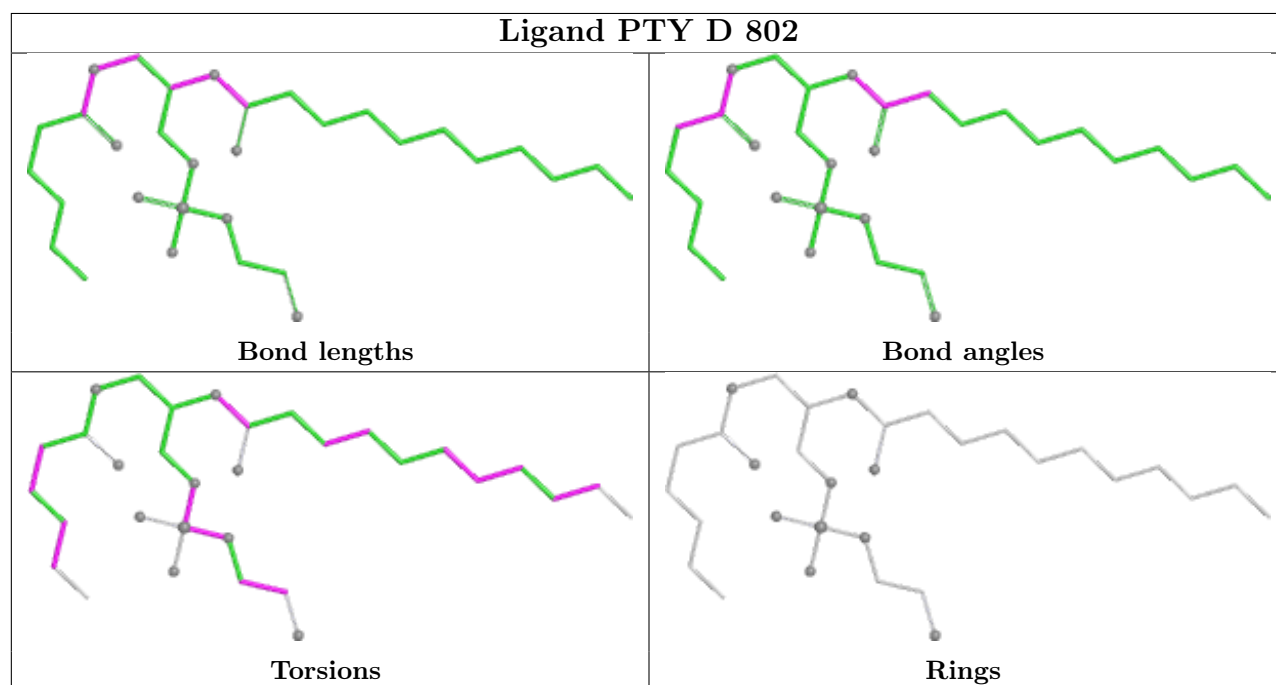
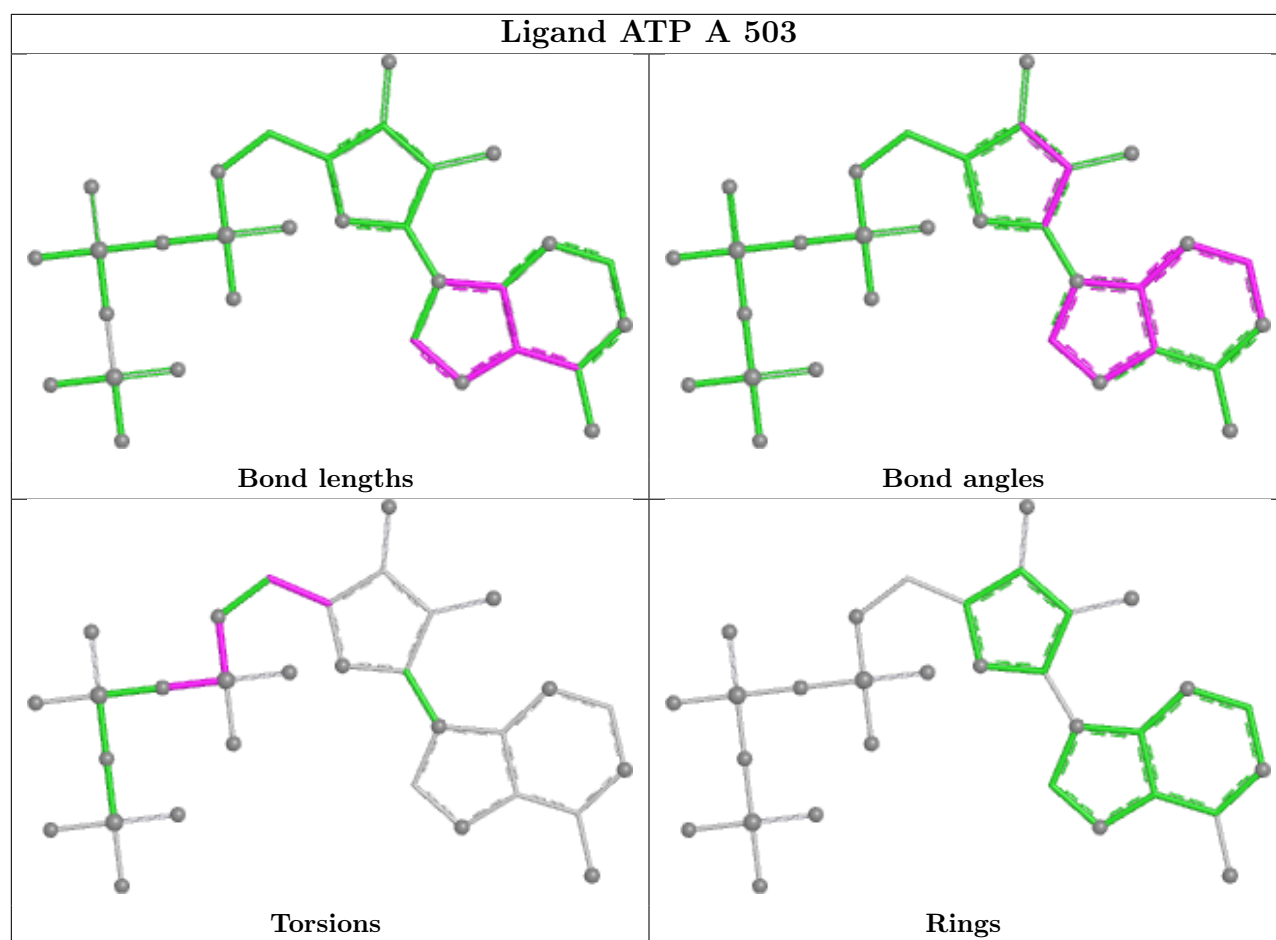












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

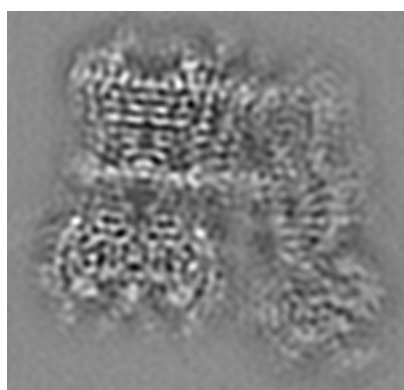
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23880. These allow visual inspection of the internal detail of the map and identification of artifacts.

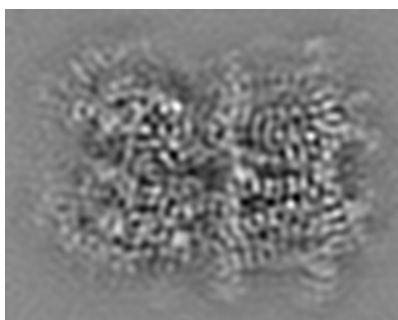
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

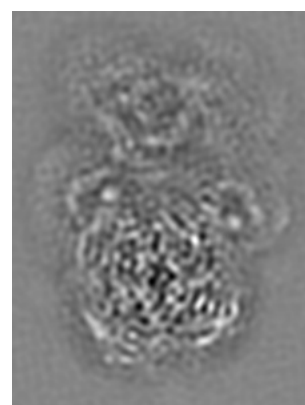
6.1.1 Primary map



X



Y

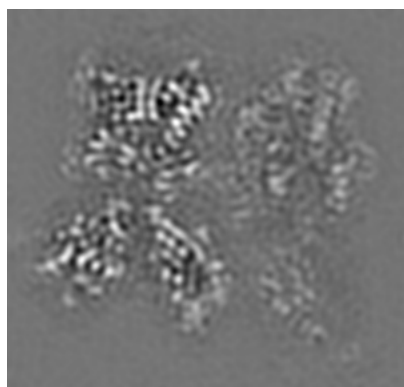


Z

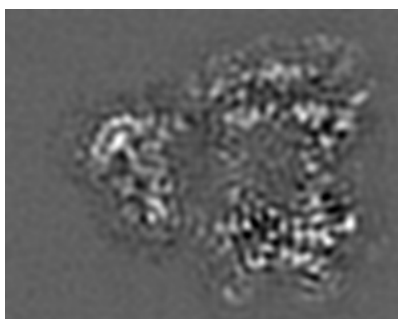
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

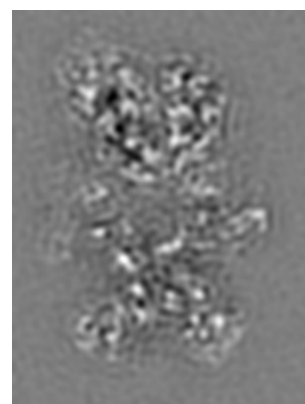
6.2.1 Primary map



X Index: 37



Y Index: 49

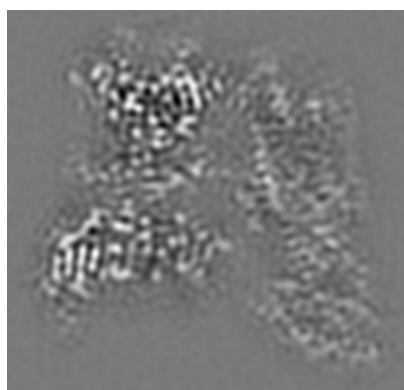


Z Index: 47

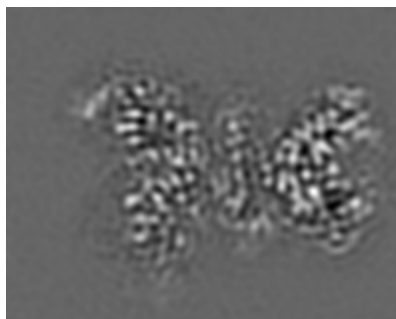
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

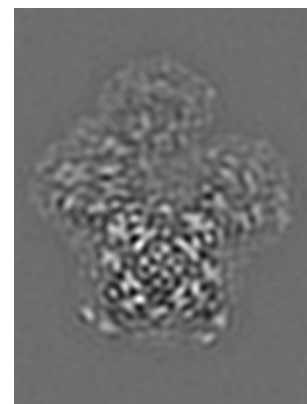
6.3.1 Primary map



X Index: 29



Y Index: 26

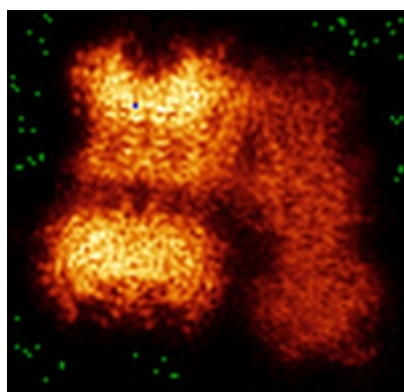


Z Index: 72

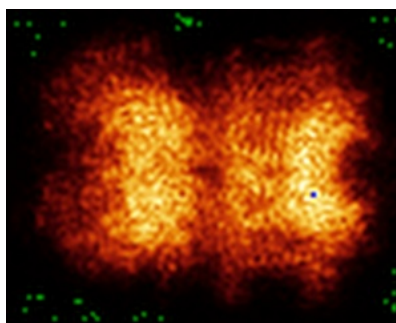
The images above show the largest variance slices of the map in three orthogonal directions.

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

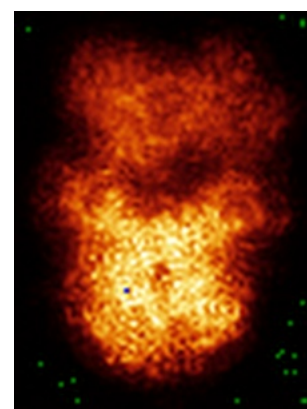
6.4.1 Primary map



X



Y

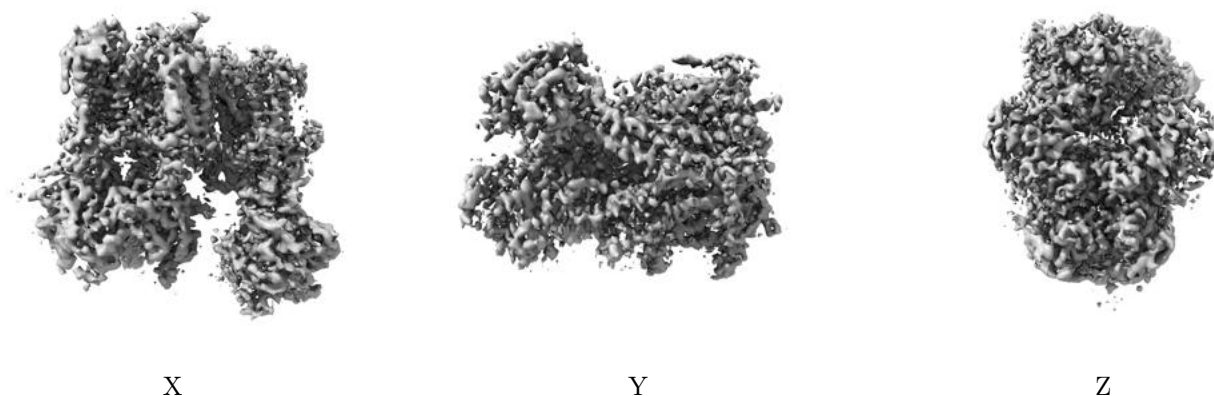


Z

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.

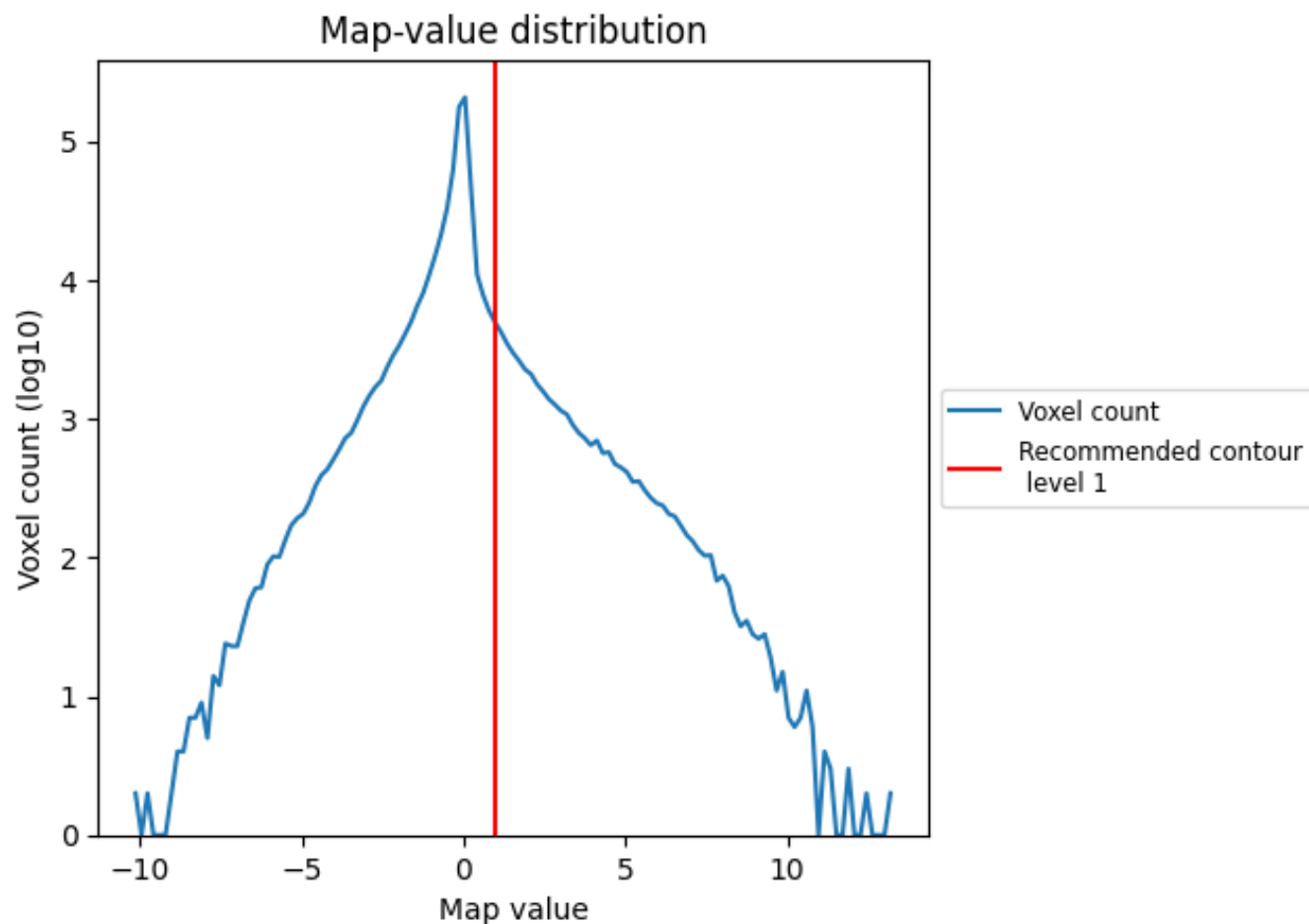
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

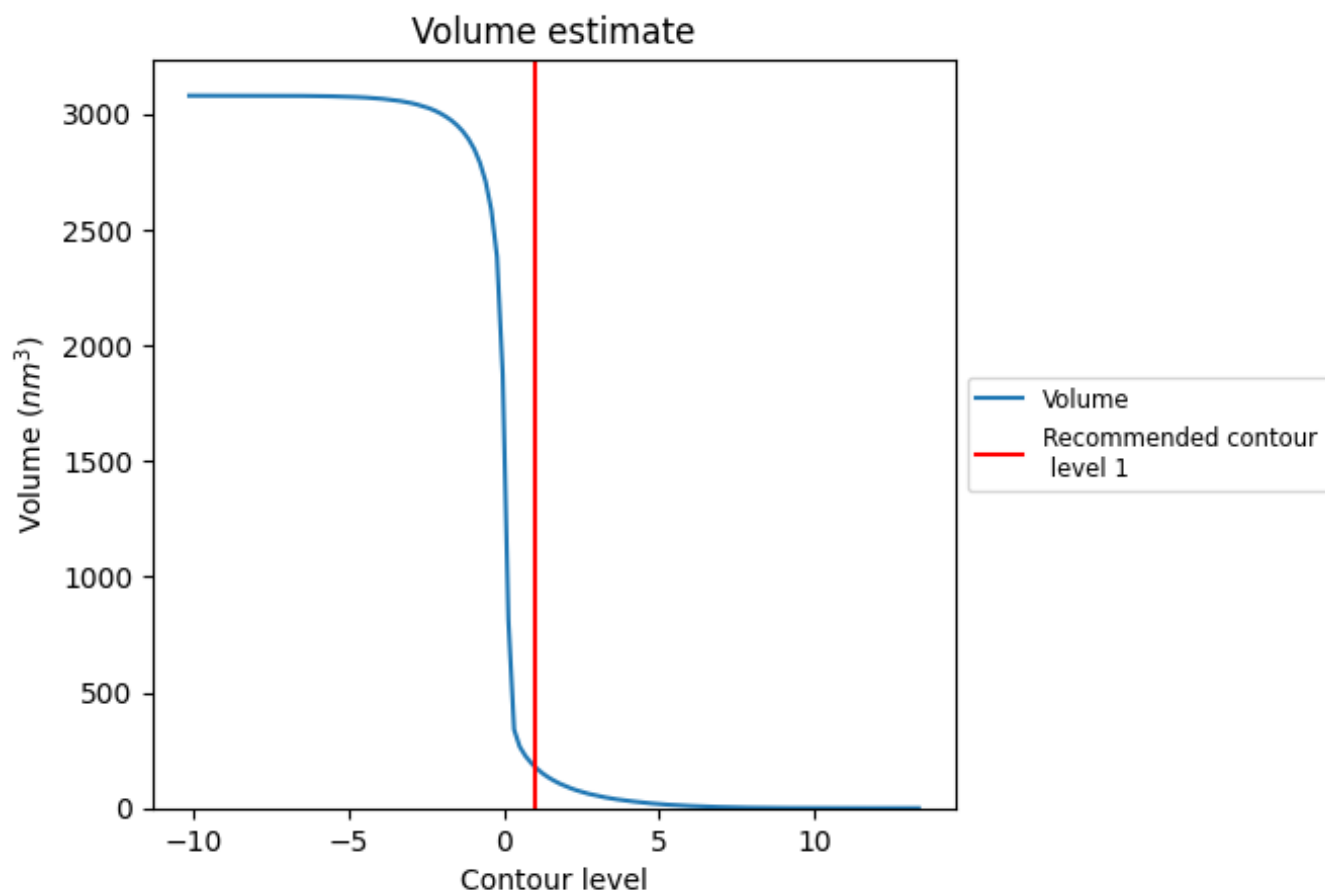
This section contains the results of statistical analysis of the map.

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 180 nm³; this corresponds to an approximate mass of 162 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.

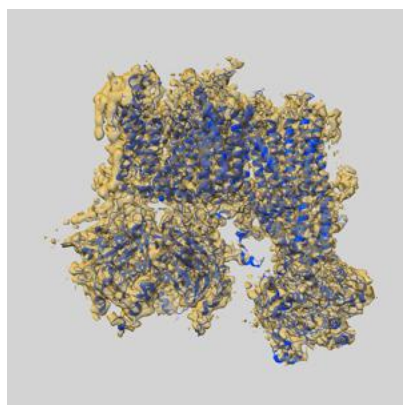
8 Fourier-Shell correlation

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

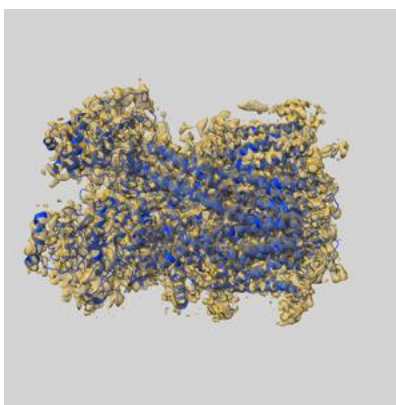
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23880 and PDB model 7MJO. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

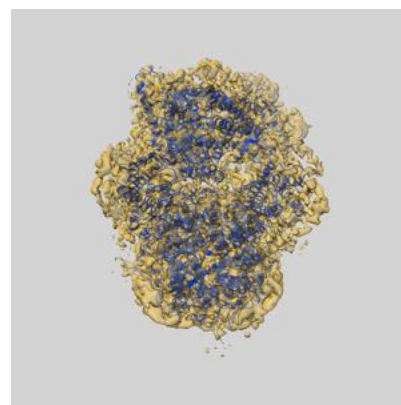
9.1 Map-model overlay [i](#)



X



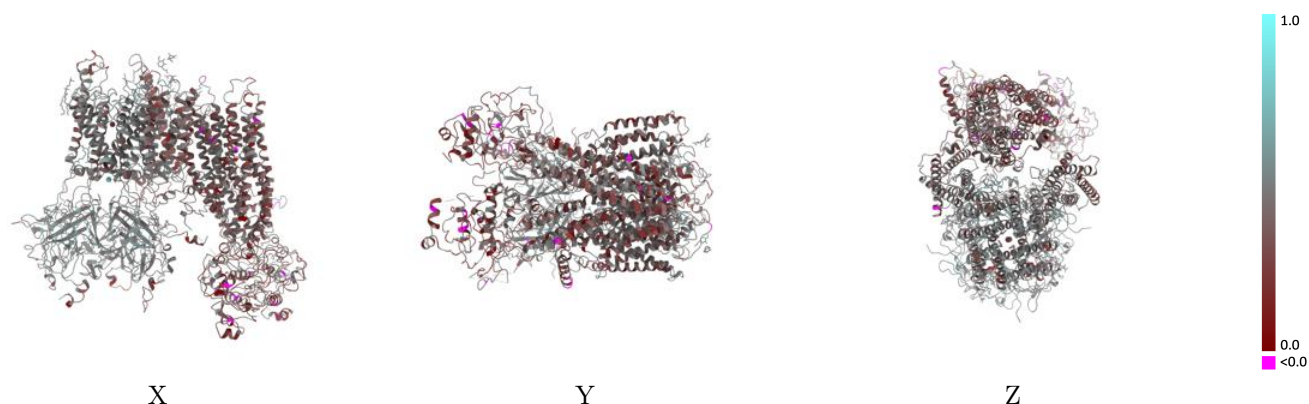
Y



Z

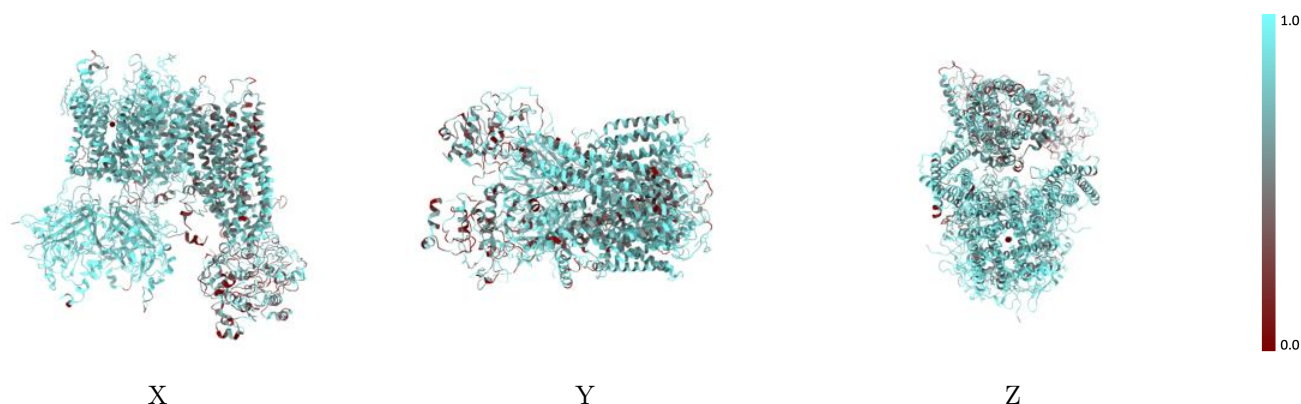
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



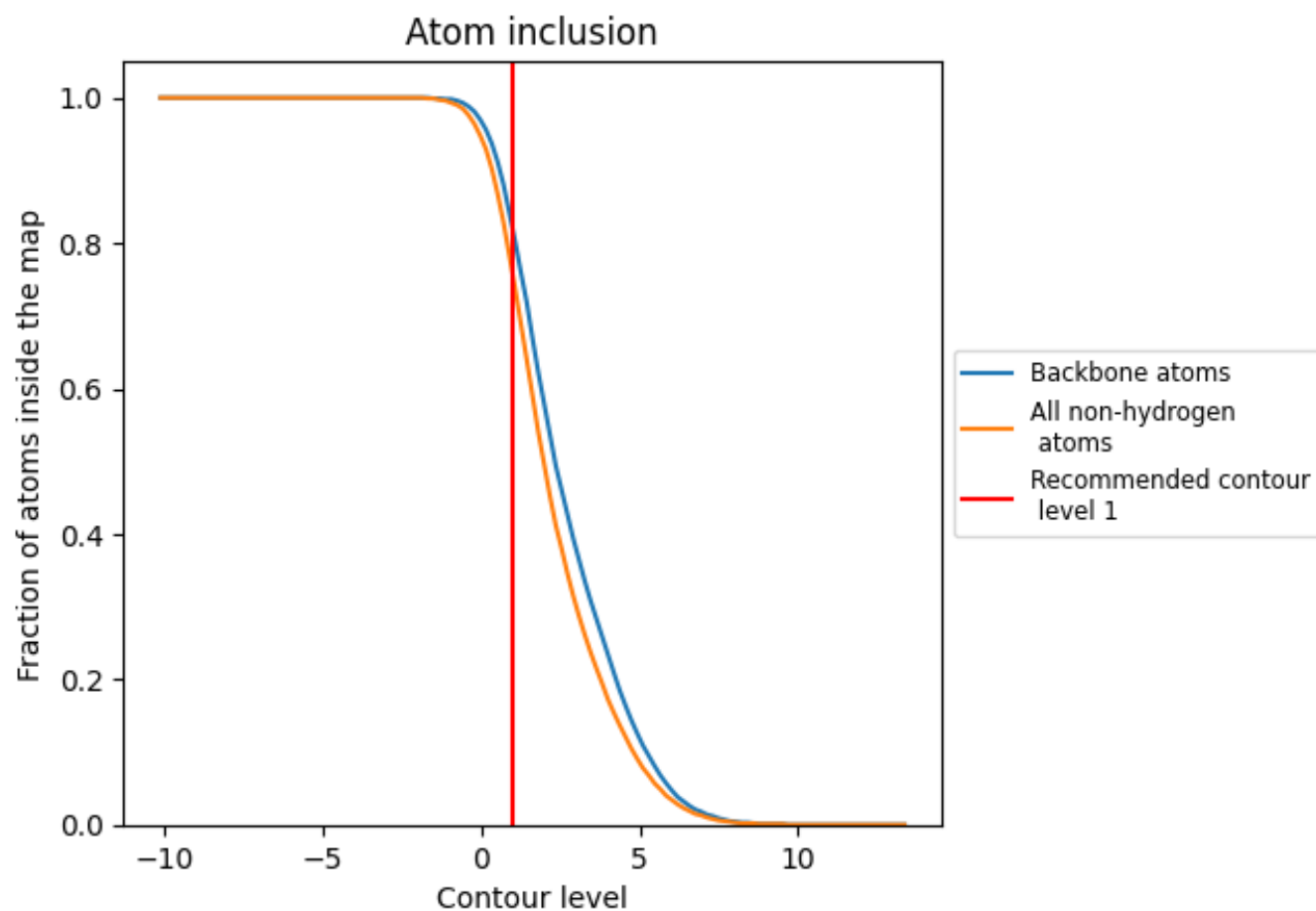
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 82% of all backbone atoms, 75% 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	0.7540	0.4290
A	0.8150	0.4730
B	0.8540	0.4770
C	0.8430	0.4800
D	0.8400	0.4800
E	0.6520	0.3720
F	0.7860	0.4890
G	0.7740	0.4210
N	0.8210	0.4570

