



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 11:16 am BST

PDB ID : 5MKE
EMDB ID : EMD-3523
Title : cryoEM Structure of Polycystin-2 in complex with cations and lipids
Authors : Wilkes, M.; Madej, M.G.; Ziegler, C.
Deposited on : 2016-12-04
Resolution : 4.30 Å(reported)

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

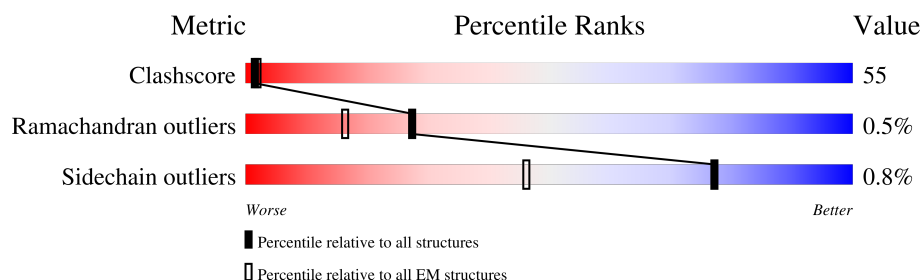
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




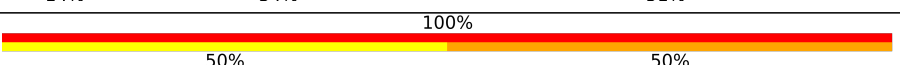
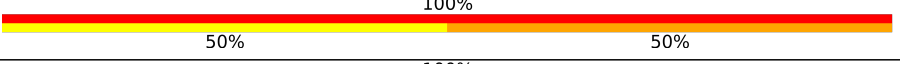

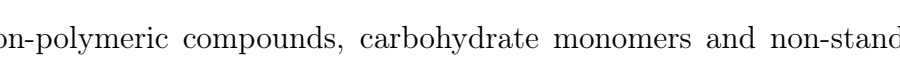
The reported resolution of this entry is 4.30 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	968	
1	B	968	
1	C	968	
1	D	968	
2	E	2	
2	F	2	
2	G	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1002	-	-	X	-
3	NAG	B	1002	-	-	X	-
3	NAG	C	1002	-	-	X	-
3	NAG	D	1002	-	-	X	-

2 Entry composition [i](#)

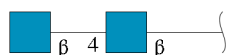
There are 7 unique types of molecules in this entry. The entry contains 16426 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	B	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	C	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	D	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		

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



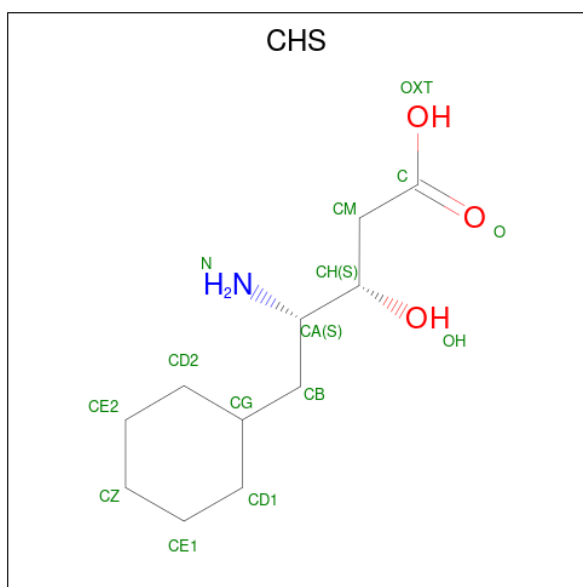
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



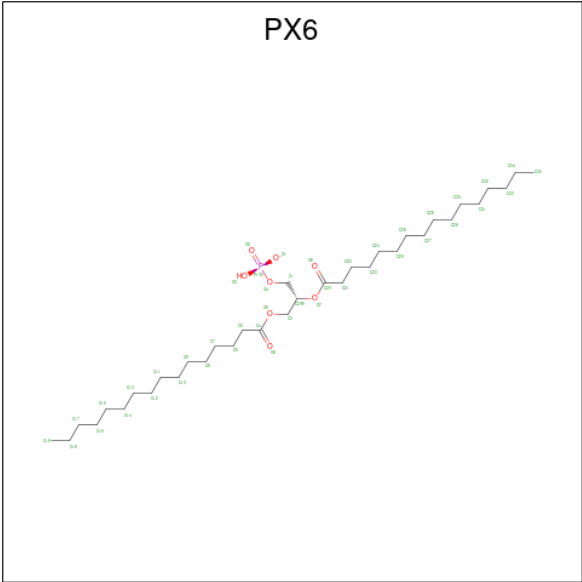
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is 4-AMINO-5-CYCLOHEXYL-3-HYDROXY-PENTANOIC ACID (three-letter code: CHS) (formula: $C_{11}H_{21}NO_3$).



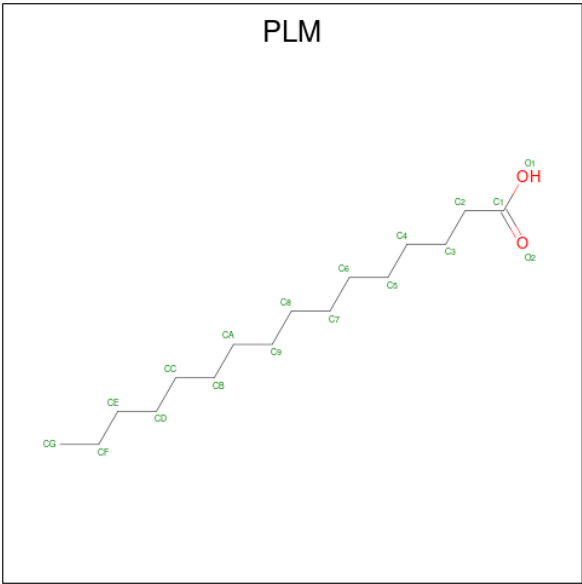
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			15	11	1	3	
4	A	1	Total	C	N	O	0
			15	11	1	3	
4	B	1	Total	C	N	O	0
			15	11	1	3	
4	B	1	Total	C	N	O	0
			15	11	1	3	
4	C	1	Total	C	N	O	0
			15	11	1	3	
4	C	1	Total	C	N	O	0
			15	11	1	3	
4	D	1	Total	C	N	O	0
			15	11	1	3	
4	D	1	Total	C	N	O	0
			15	11	1	3	

- Molecule 5 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX6) (formula: C₃₅H₆₈O₈P).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			40	31	8	1	
5	B	1	Total	C	O	P	0
			40	31	8	1	
5	C	1	Total	C	O	P	0
			40	31	8	1	
5	D	1	Total	C	O	P	0
			40	31	8	1	

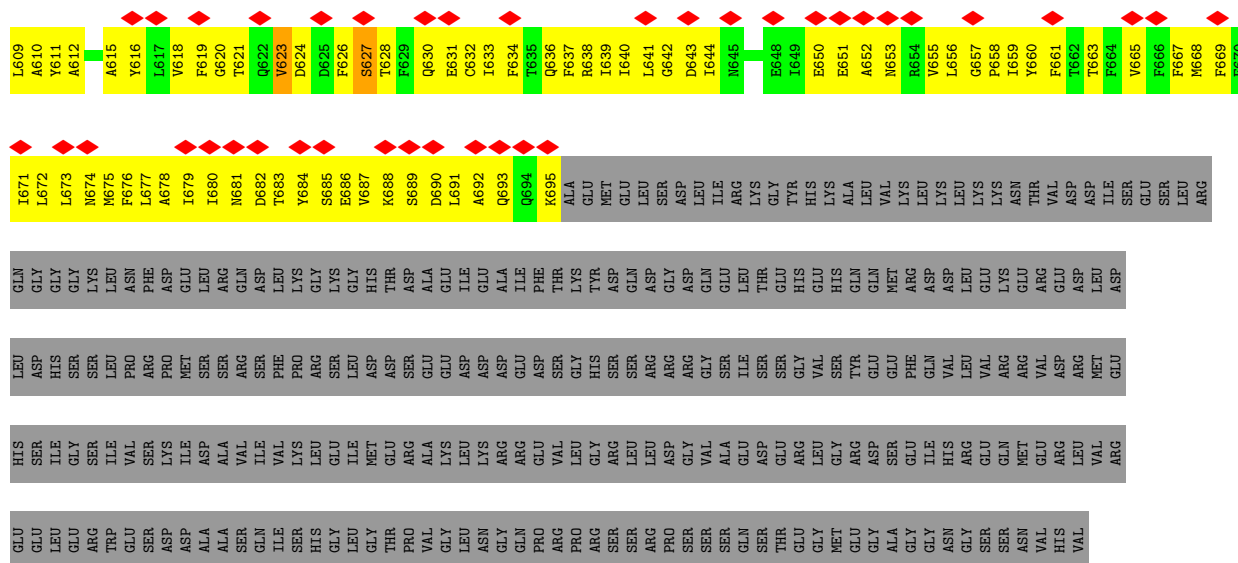
- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



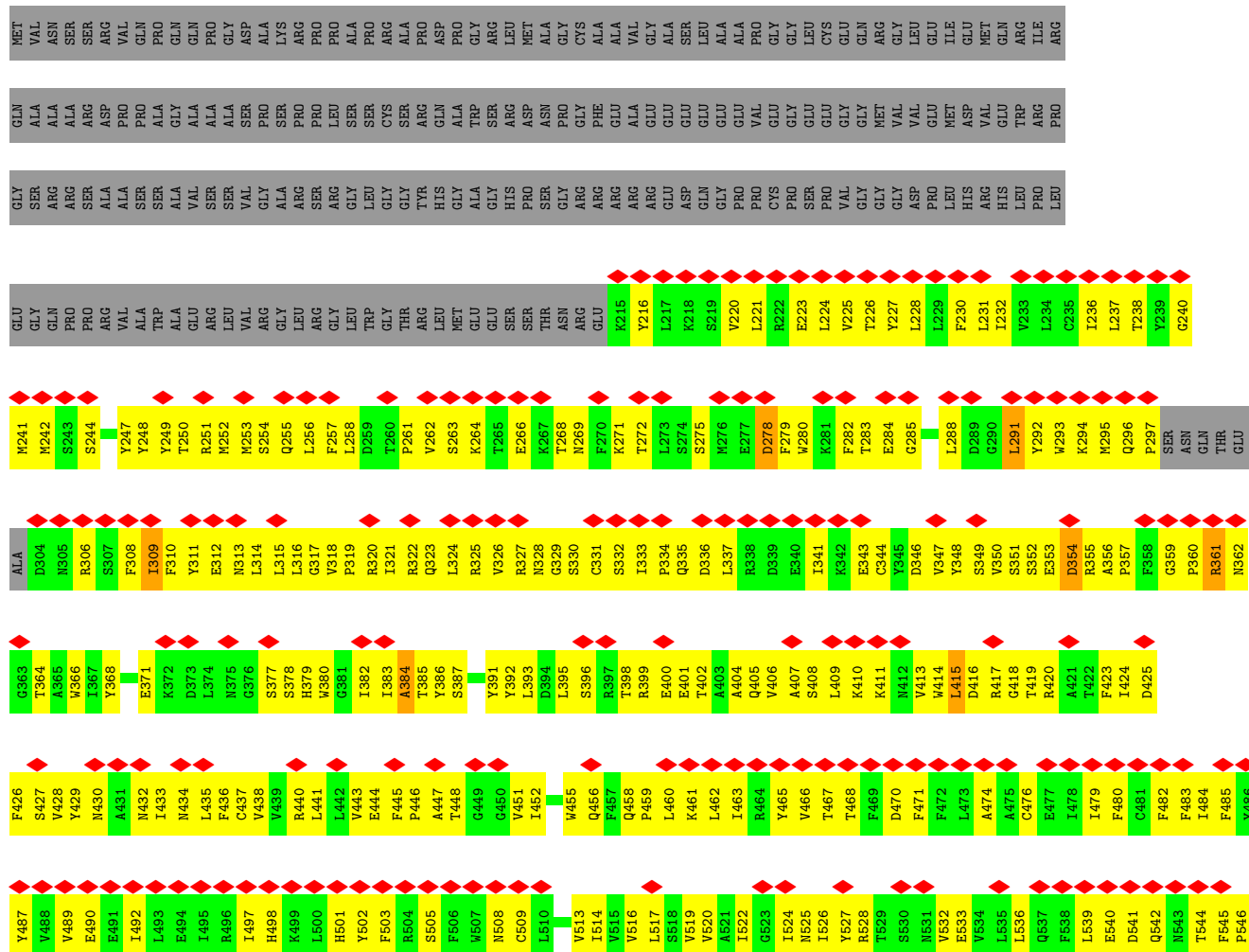
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			18	16	2	
6	A	1	Total	C	O	0
			18	16	2	
6	B	1	Total	C	O	0
			18	16	2	
6	B	1	Total	C	O	0
			18	16	2	
6	B	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			18	16	2	
6	C	1	Total	C	O	0
			18	16	2	
6	D	1	Total	C	O	0
			18	16	2	
6	D	1	Total	C	O	0
			18	16	2	
6	D	1	Total	C	O	0
			18	16	2	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

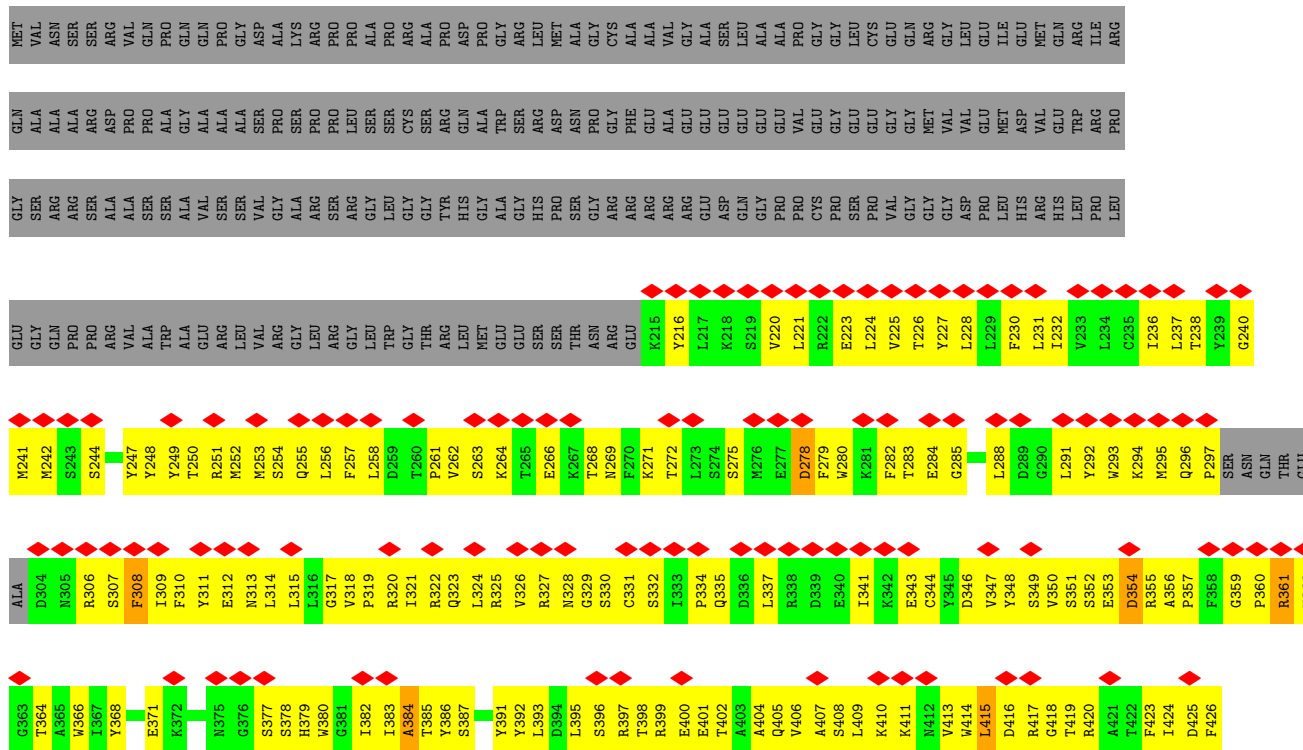
Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Ca	0
			2	2	

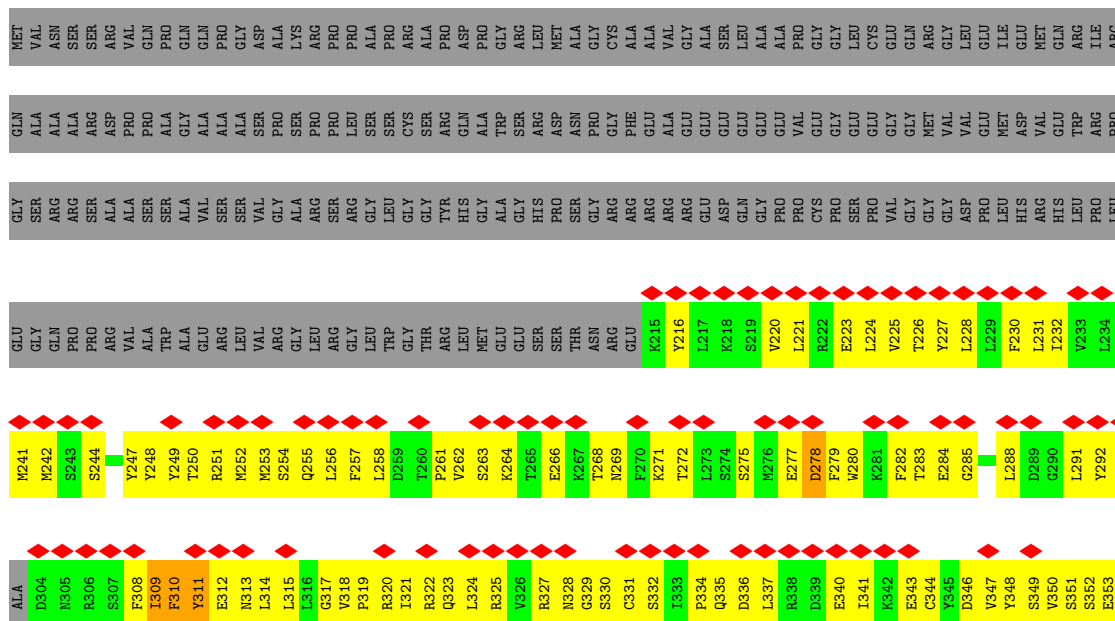


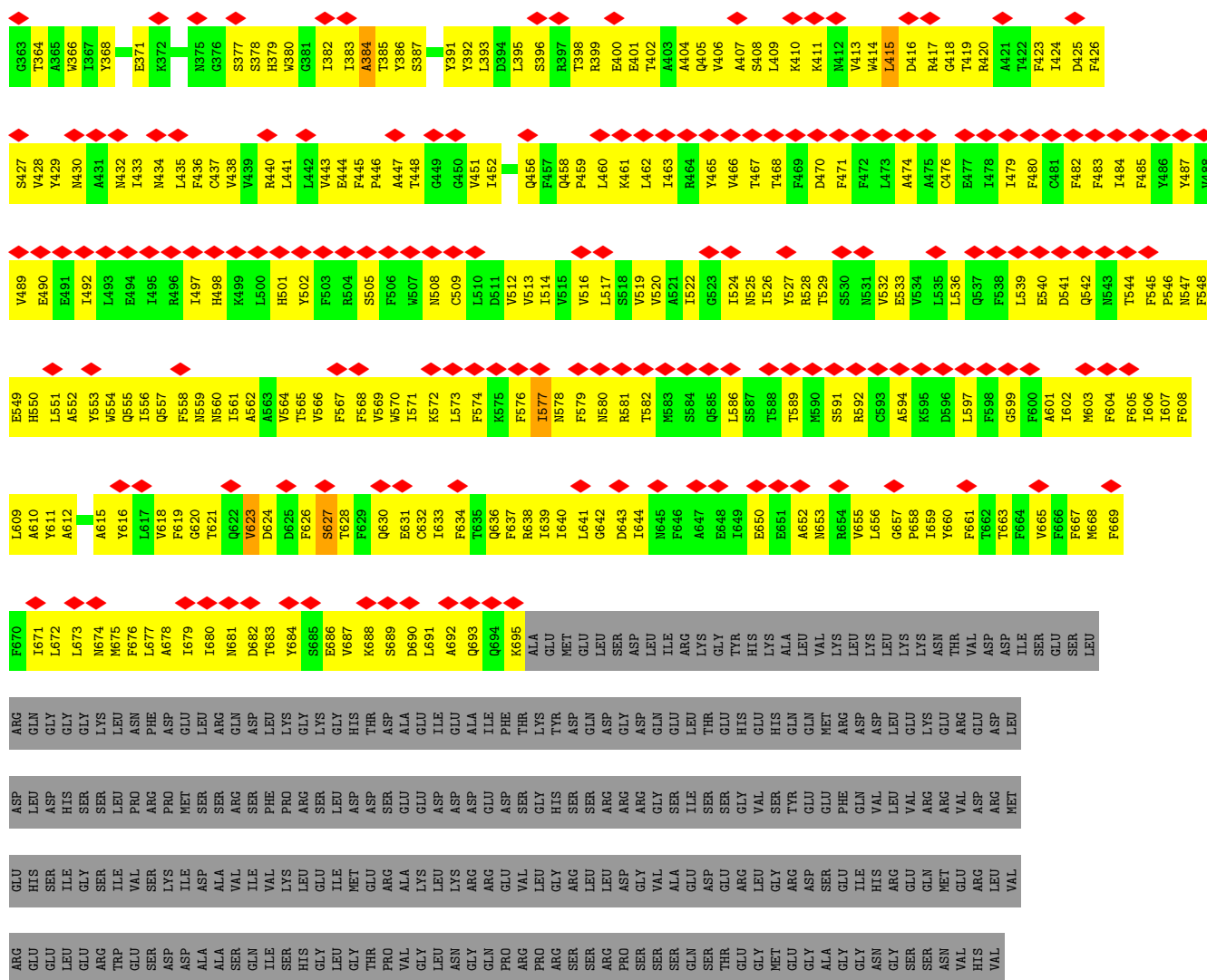
• Molecule 1: Polycystin-2



- Molecule 1: Polycystin-2







- Molecule 2: 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, C4	Depositor
Number of particles used	42268	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0345	Depositor
Map size (Å)	191.52, 191.52, 191.52	wwPDB
Map dimensions	168, 168, 168	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, PX6, CHS, PLM

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	0.49	0/4031	0.62	2/5469 (0.0%)
1	B	0.49	0/4031	0.62	3/5469 (0.1%)
1	C	0.49	0/4031	0.62	3/5469 (0.1%)
1	D	0.49	0/4031	0.63	2/5469 (0.0%)
All	All	0.49	0/16124	0.62	10/21876 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	278	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	278	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	278	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	384	ALA	C-N-CA	5.16	134.60	121.70

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	LEU	Peptide
1	A	354	ASP	Peptide
1	A	361	ARG	Peptide
1	A	578	ASN	Peptide
1	A	627	SER	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3926	0	3880	489	0
1	B	3926	0	3880	496	0
1	C	3926	0	3880	476	0
1	D	3926	0	3880	490	0
2	E	28	0	25	2	0
2	F	28	0	25	2	0
2	G	28	0	25	2	0
3	A	28	0	26	8	0
3	B	28	0	26	8	0
3	C	28	0	26	8	0
3	D	56	0	51	16	0
4	A	30	0	40	3	0
4	B	30	0	40	4	0
4	C	30	0	40	5	0
4	D	30	0	40	4	0
5	A	40	0	56	3	0
5	B	40	0	56	6	0
5	C	40	0	56	4	0
5	D	40	0	56	4	0
6	A	54	0	93	9	0
6	B	54	0	93	8	0
6	C	54	0	93	9	0
6	D	54	0	93	6	0
7	A	2	0	0	0	0
All	All	16426	0	16480	1816	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 55.

The worst 5 of 1816 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:606:ILE:CD1	1:D:573:LEU:HD11	1.21	1.66
1:A:606:ILE:HD11	1:D:573:LEU:CD1	1.26	1.63
1:A:573:LEU:CD1	1:B:606:ILE:HD11	1.17	1.62
1:C:573:LEU:HD11	1:D:606:ILE:CD1	1.18	1.58
1:B:573:LEU:CD1	1:C:606:ILE:HD11	1.15	1.57

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	471/968 (49%)	382 (81%)	87 (18%)	2 (0%)	30	67
1	B	471/968 (49%)	383 (81%)	86 (18%)	2 (0%)	30	67
1	C	471/968 (49%)	381 (81%)	88 (19%)	2 (0%)	30	67
1	D	471/968 (49%)	381 (81%)	87 (18%)	3 (1%)	22	59
All	All	1884/3872 (49%)	1527 (81%)	348 (18%)	9 (0%)	27	63

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	311	TYR
1	A	258	LEU
1	B	258	LEU
1	C	258	LEU
1	D	258	LEU

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	429/837 (51%)	426 (99%)	3 (1%)	81	87
1	B	429/837 (51%)	426 (99%)	3 (1%)	81	87
1	C	429/837 (51%)	426 (99%)	3 (1%)	81	87
1	D	429/837 (51%)	425 (99%)	4 (1%)	75	83
All	All	1716/3348 (51%)	1703 (99%)	13 (1%)	77	85

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	415	LEU
1	C	577	ILE
1	D	577	ILE
1	D	310	PHE
1	D	415	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	550	HIS
1	D	622	GLN
1	B	622	GLN
1	B	550	HIS
1	D	653	ASN

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

6 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$
2	NAG	E	1	1,2	14,14,15	0.51	0	17,19,21	1.15	2 (11%)
2	NAG	E	2	2	14,14,15	0.40	0	17,19,21	1.17	2 (11%)
2	NAG	F	1	1,2	14,14,15	0.52	0	17,19,21	1.14	2 (11%)
2	NAG	F	2	2	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
2	NAG	G	1	1,2	14,14,15	0.47	0	17,19,21	1.14	2 (11%)
2	NAG	G	2	2	14,14,15	0.42	0	17,19,21	1.18	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C8-C7-N2	2.35	120.07	116.10
2	E	1	NAG	C8-C7-N2	2.33	120.05	116.10
2	E	2	NAG	C8-C7-N2	2.33	120.04	116.10
2	F	2	NAG	C8-C7-N2	2.32	120.03	116.10
2	F	1	NAG	C8-C7-N2	2.31	120.01	116.10

There are no chirality outliers.

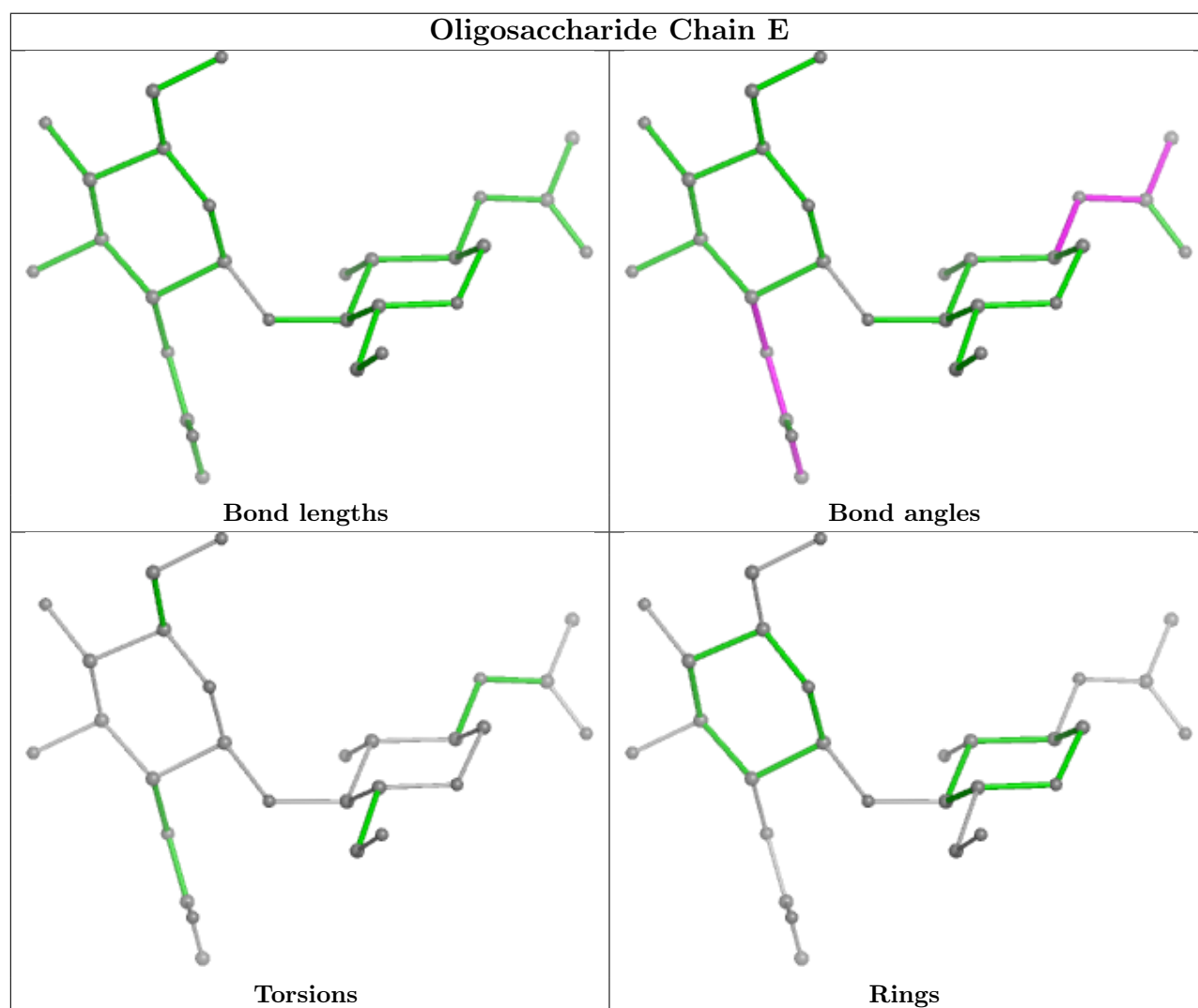
There are no torsion outliers.

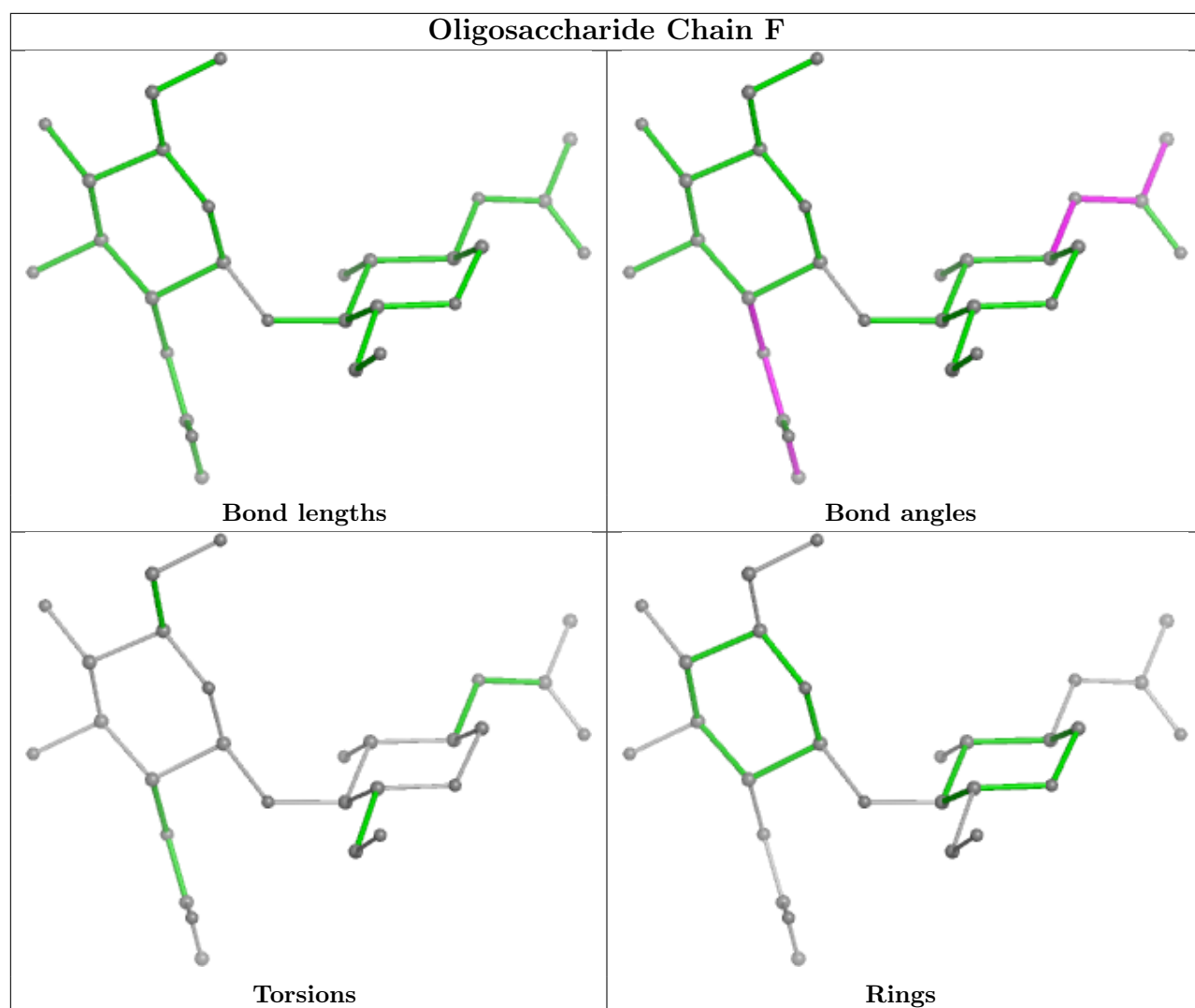
There are no ring outliers.

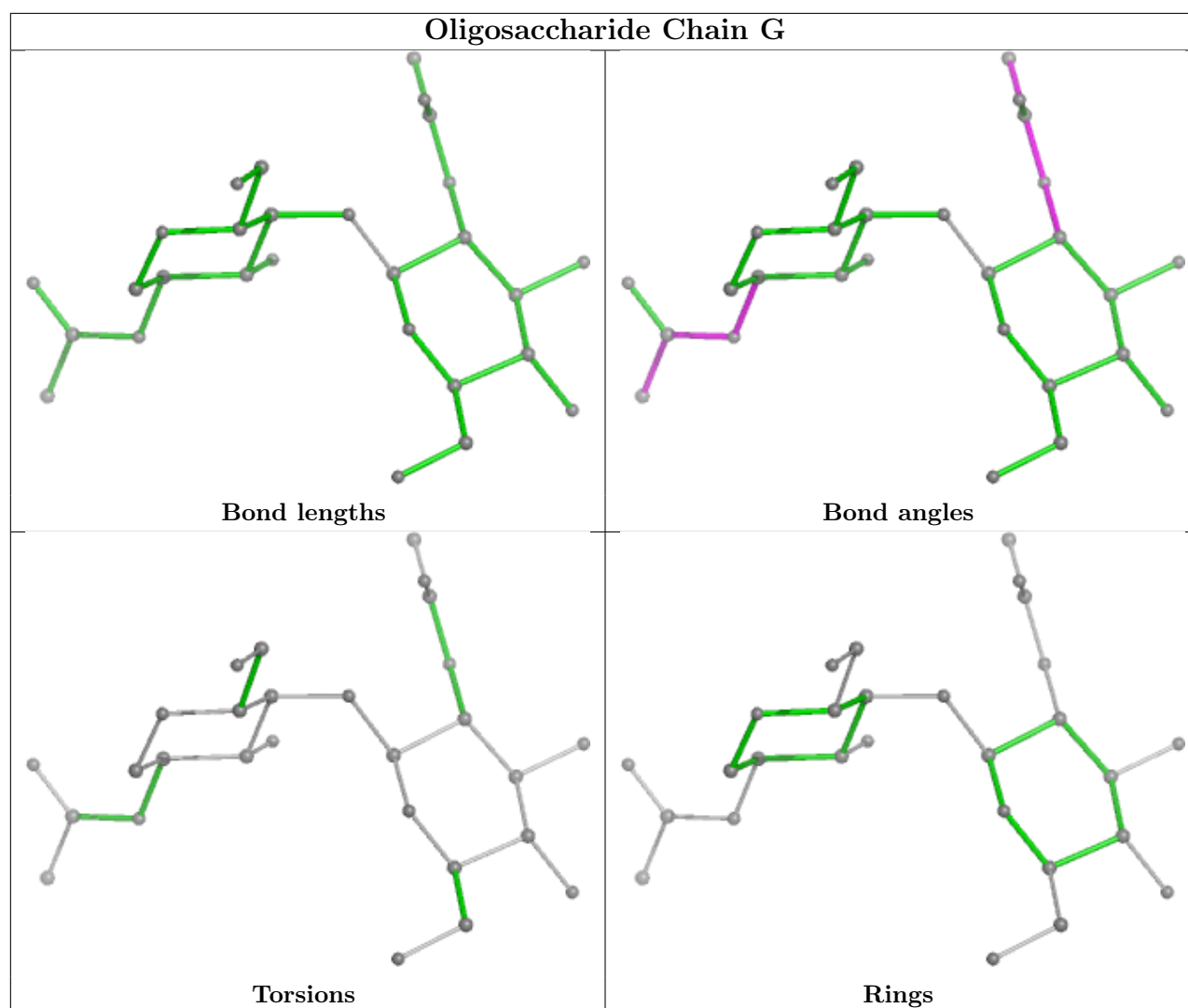
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	2	0
2	G	2	NAG	2	0
2	F	2	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 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	CHS	A	1005	-	15,15,15	0.52	0	15,19,19	0.83	0
6	PLM	A	1008	-	17,17,17	0.57	0	17,17,17	0.74	0
6	PLM	A	1009	-	17,17,17	0.50	0	17,17,17	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHS	A	1006	-	15,15,15	0.59	0	15,19,19	1.01	1 (6%)
3	NAG	C	1002	1	14,14,15	0.40	0	17,19,21	1.16	2 (11%)
4	CHS	D	1006	-	15,15,15	0.59	0	15,19,19	0.99	1 (6%)
3	NAG	A	1002	1	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
3	NAG	D	1001	1	14,14,15	0.86	1 (7%)	17,19,21	0.82	1 (5%)
6	PLM	C	1009	-	17,17,17	0.50	0	17,17,17	0.97	0
5	PX6	A	1007	-	39,39,43	1.43	6 (15%)	43,44,48	1.54	3 (6%)
6	PLM	D	1010	-	17,17,17	0.52	0	17,17,17	0.77	0
3	NAG	B	1002	1	14,14,15	0.41	0	17,19,21	1.16	2 (11%)
3	NAG	C	1001	1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
4	CHS	B	1006	-	15,15,15	0.57	0	15,19,19	1.03	1 (6%)
4	CHS	C	1005	-	15,15,15	0.51	0	15,19,19	0.82	0
5	PX6	C	1007	-	39,39,43	1.43	6 (15%)	43,44,48	1.51	4 (9%)
5	PX6	B	1007	-	39,39,43	1.43	6 (15%)	43,44,48	1.54	4 (9%)
3	NAG	A	1001	1	14,14,15	0.70	1 (7%)	17,19,21	0.85	1 (5%)
6	PLM	D	1009	-	17,17,17	0.50	0	17,17,17	0.96	0
6	PLM	D	1008	-	17,17,17	0.57	0	17,17,17	0.74	0
3	NAG	D	1004	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)
4	CHS	D	1005	-	15,15,15	0.51	0	15,19,19	0.83	0
6	PLM	B	1009	-	17,17,17	0.51	0	17,17,17	0.97	0
3	NAG	D	1002	1	14,14,15	0.40	0	17,19,21	1.16	2 (11%)
6	PLM	C	1008	-	17,17,17	0.56	0	17,17,17	0.75	0
6	PLM	A	1010	-	17,17,17	0.52	0	17,17,17	0.77	0
4	CHS	B	1005	-	15,15,15	0.52	0	15,19,19	0.84	0
4	CHS	C	1006	-	15,15,15	0.58	0	15,19,19	1.01	1 (6%)
6	PLM	B	1008	-	17,17,17	0.57	0	17,17,17	0.75	0
6	PLM	B	1010	-	17,17,17	0.53	0	17,17,17	0.77	0
3	NAG	D	1003	1	14,14,15	0.44	0	17,19,21	1.18	2 (11%)
6	PLM	C	1010	-	17,17,17	0.52	0	17,17,17	0.77	0
5	PX6	D	1007	-	39,39,43	1.43	6 (15%)	43,44,48	1.54	4 (9%)
3	NAG	B	1001	1	14,14,15	0.60	0	17,19,21	0.82	1 (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
4	CHS	A	1005	-	-	5/12/20/20	0/1/1/1
6	PLM	A	1008	-	-	11/15/15/15	-
6	PLM	A	1009	-	-	7/15/15/15	-
4	CHS	A	1006	-	-	4/12/20/20	0/1/1/1
3	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
4	CHS	D	1006	-	-	5/12/20/20	0/1/1/1
3	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1001	1	-	2/6/23/26	0/1/1/1
6	PLM	C	1009	-	-	6/15/15/15	-
5	PX6	A	1007	-	-	17/41/41/45	-
6	PLM	D	1010	-	-	12/15/15/15	-
3	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1001	1	-	2/6/23/26	0/1/1/1
4	CHS	B	1006	-	-	5/12/20/20	0/1/1/1
4	CHS	C	1005	-	-	5/12/20/20	0/1/1/1
5	PX6	C	1007	-	-	17/41/41/45	-
5	PX6	B	1007	-	-	19/41/41/45	-
3	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
6	PLM	D	1009	-	-	6/15/15/15	-
6	PLM	D	1008	-	-	11/15/15/15	-
3	NAG	D	1004	-	-	0/6/23/26	0/1/1/1
4	CHS	D	1005	-	-	5/12/20/20	0/1/1/1
6	PLM	B	1009	-	-	6/15/15/15	-
3	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
6	PLM	C	1008	-	-	11/15/15/15	-
6	PLM	A	1010	-	-	12/15/15/15	-
4	CHS	B	1005	-	-	5/12/20/20	0/1/1/1
4	CHS	C	1006	-	-	4/12/20/20	0/1/1/1
6	PLM	B	1008	-	-	11/15/15/15	-
6	PLM	B	1010	-	-	12/15/15/15	-
3	NAG	D	1003	1	-	0/6/23/26	0/1/1/1
6	PLM	C	1010	-	-	12/15/15/15	-
5	PX6	D	1007	-	-	19/41/41/45	-
3	NAG	B	1001	1	-	2/6/23/26	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1007	PX6	P1-O2	4.62	1.65	1.50
5	D	1007	PX6	P1-O2	4.62	1.65	1.50
5	A	1007	PX6	P1-O2	4.61	1.65	1.50
5	C	1007	PX6	P1-O2	4.59	1.65	1.50
5	A	1007	PX6	O7-C2	-3.11	1.38	1.46

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1007	PX6	O5-C3-C2	7.59	130.54	108.43
5	D	1007	PX6	O5-C3-C2	7.55	130.42	108.43
5	A	1007	PX6	O5-C3-C2	7.55	130.40	108.43
5	C	1007	PX6	O5-C3-C2	7.51	130.30	108.43
5	D	1007	PX6	O7-C20-C21	2.90	117.74	111.50

There are no chirality outliers.

5 of 235 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1005	CHS	N-CA-CB-CG
4	A	1005	CHS	N-CA-CH-CM
4	A	1005	CHS	CB-CA-CH-CM
4	B	1005	CHS	N-CA-CB-CG
4	B	1005	CHS	N-CA-CH-CM

There are no ring outliers.

30 monomers are involved in 95 short contacts:

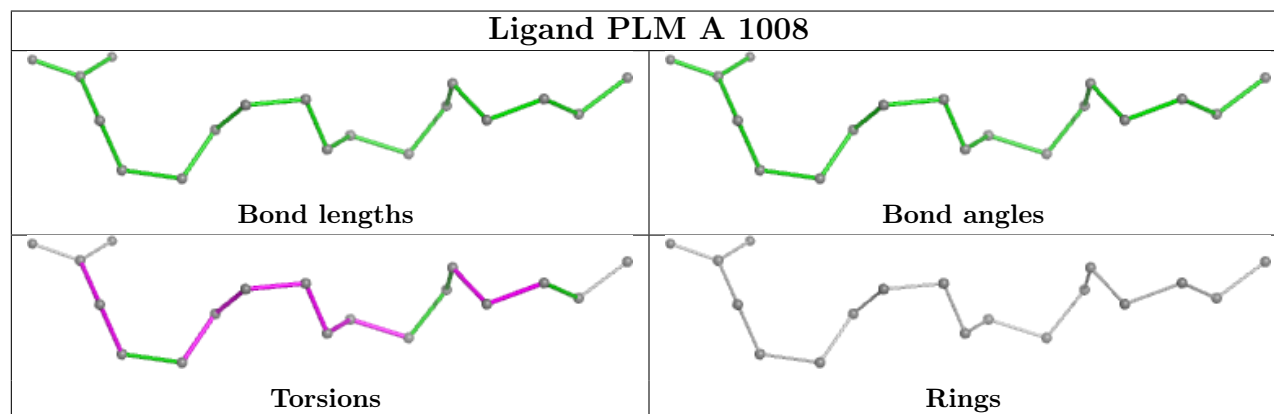
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	CHS	2	0
6	A	1008	PLM	2	0
6	A	1009	PLM	4	0
4	A	1006	CHS	2	0
3	C	1002	NAG	8	0
4	D	1006	CHS	2	0
3	A	1002	NAG	8	0
3	D	1001	NAG	6	0
6	C	1009	PLM	4	0
5	A	1007	PX6	3	0
6	D	1010	PLM	3	0
3	B	1002	NAG	8	0
4	B	1006	CHS	3	0

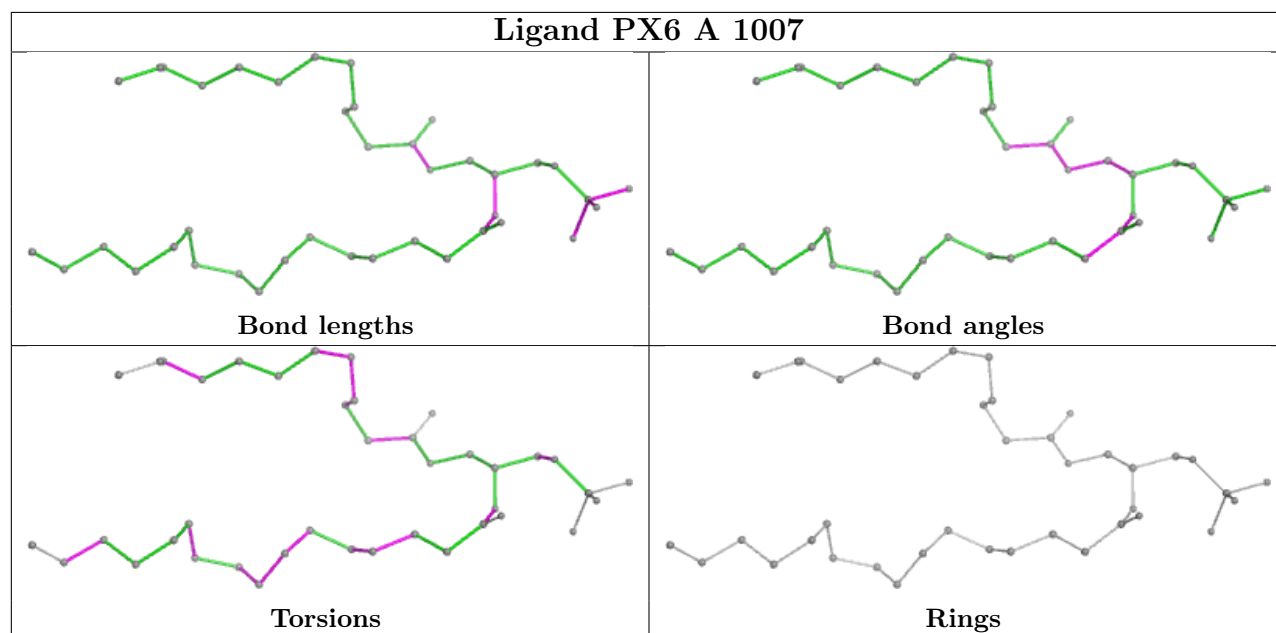
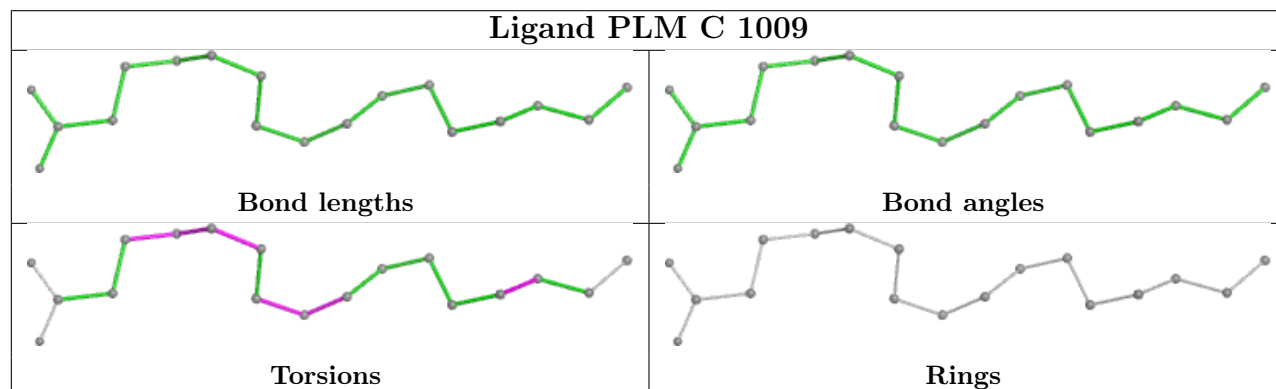
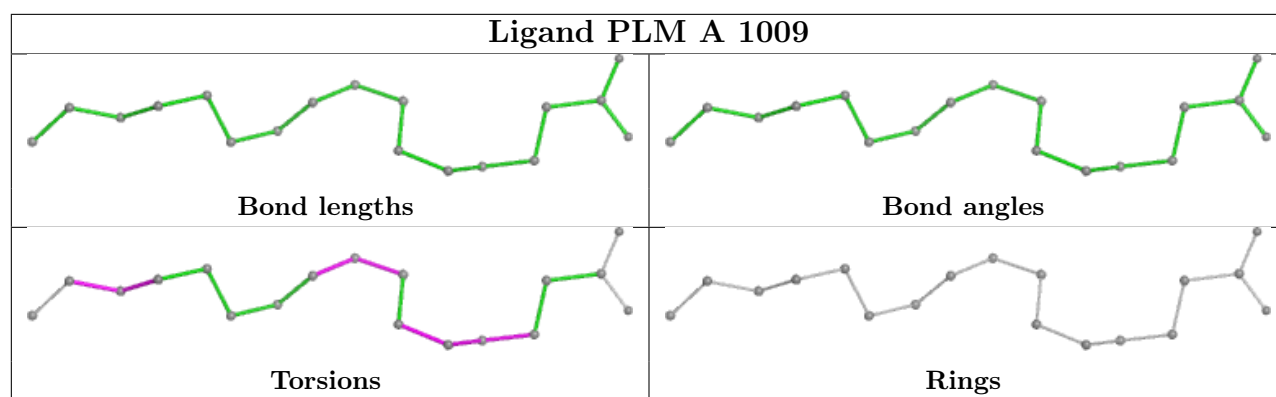
Continued on next page...

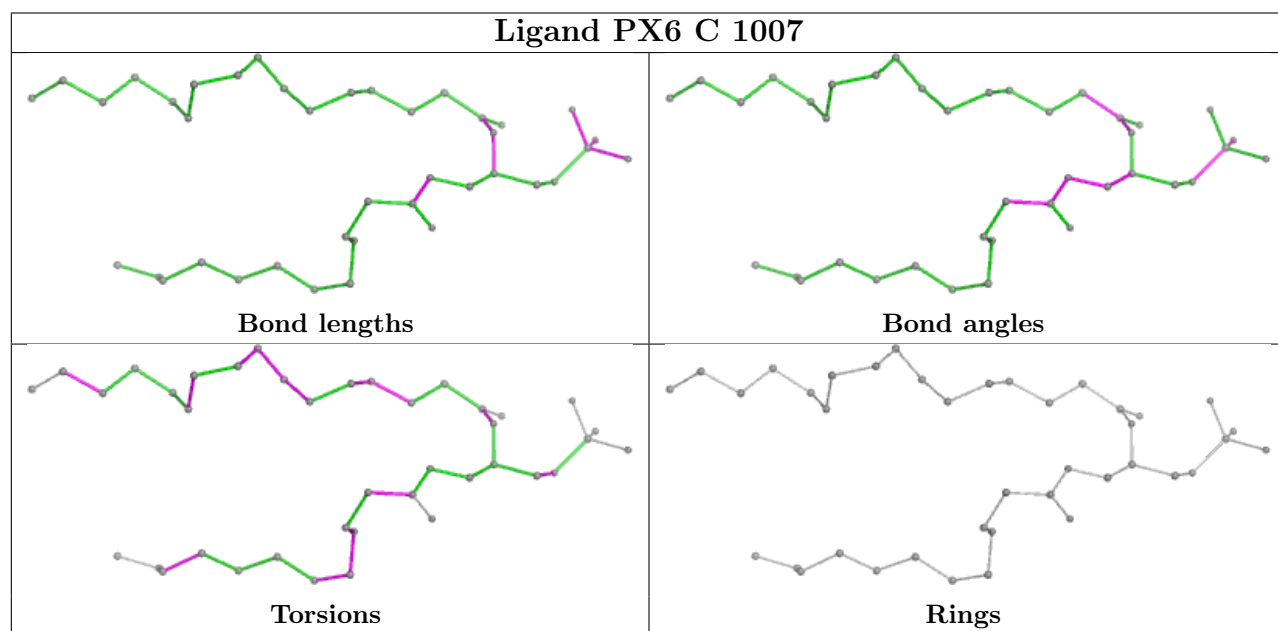
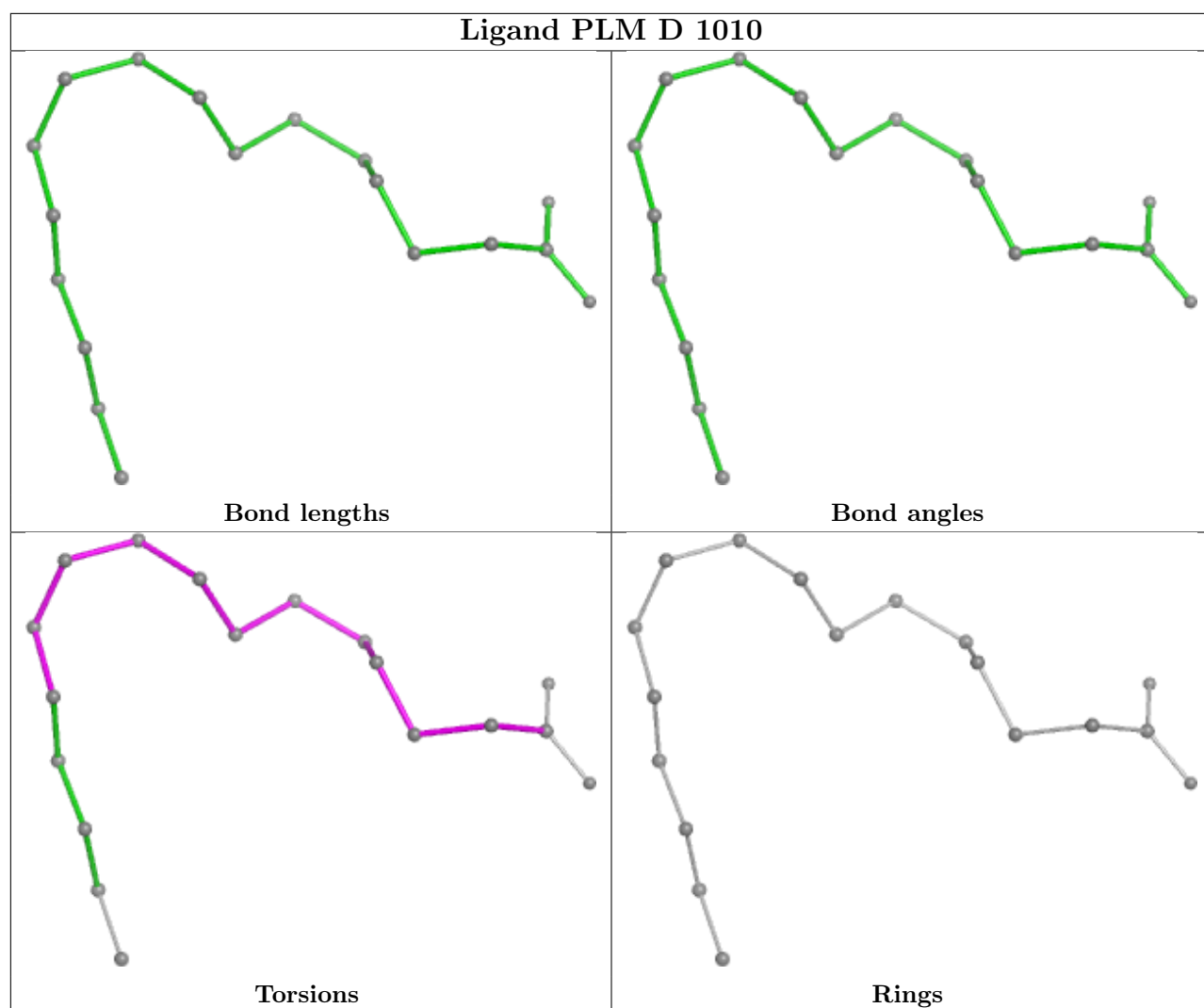
Continued from previous page...

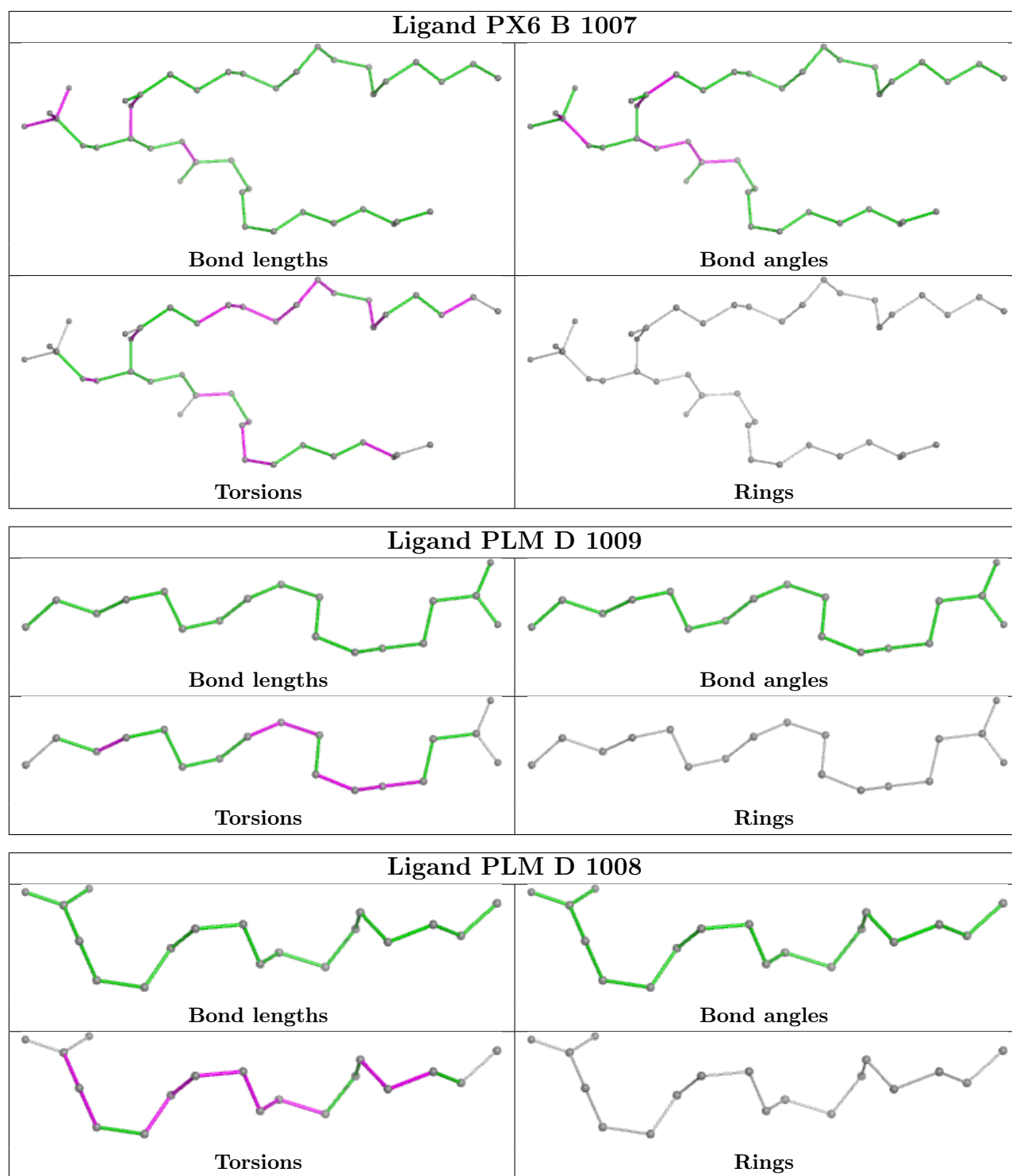
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1005	CHS	4	0
5	C	1007	PX6	4	0
5	B	1007	PX6	6	0
6	D	1009	PLM	1	0
6	D	1008	PLM	2	0
3	D	1004	NAG	2	0
4	D	1005	CHS	3	0
6	B	1009	PLM	3	0
3	D	1002	NAG	8	0
6	C	1008	PLM	2	0
6	A	1010	PLM	3	0
4	B	1005	CHS	3	0
4	C	1006	CHS	3	0
6	B	1008	PLM	2	0
6	B	1010	PLM	3	0
6	C	1010	PLM	3	0
5	D	1007	PX6	4	0

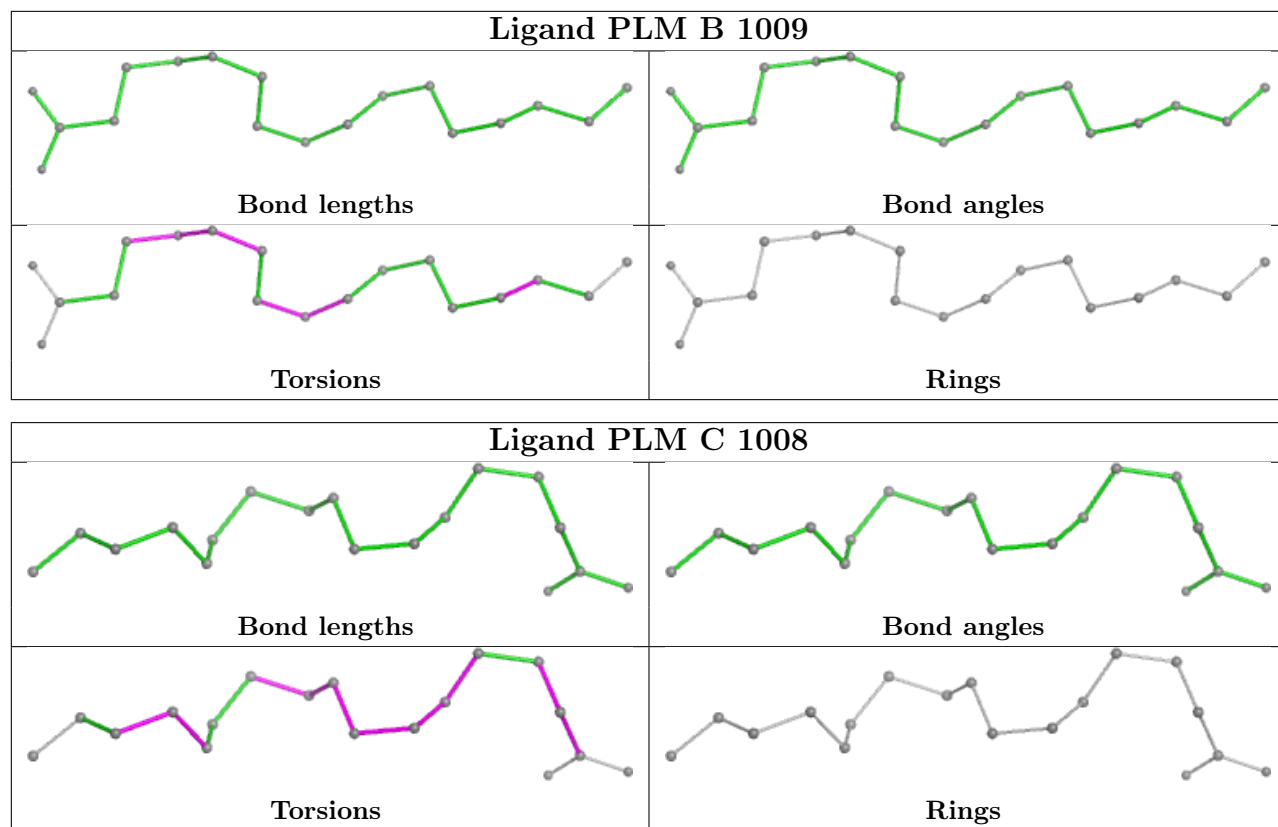
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

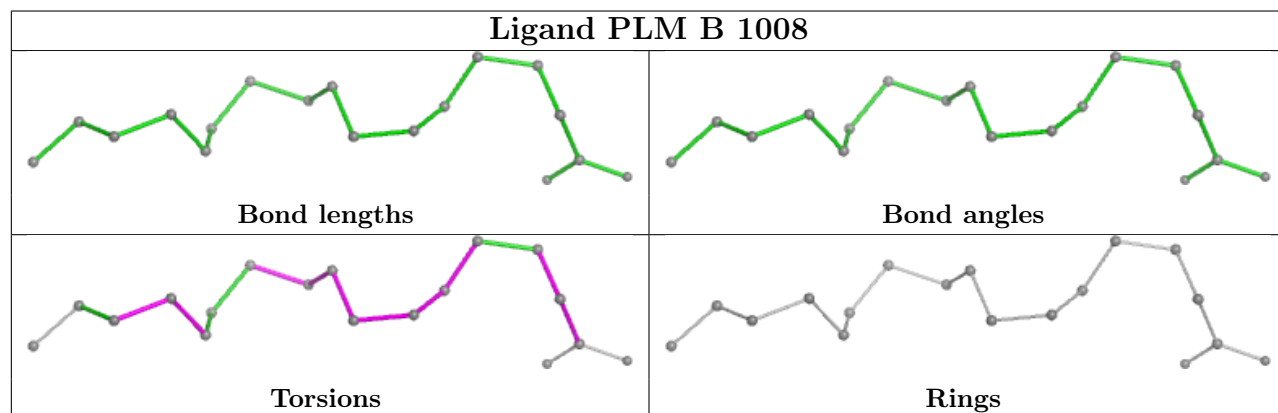
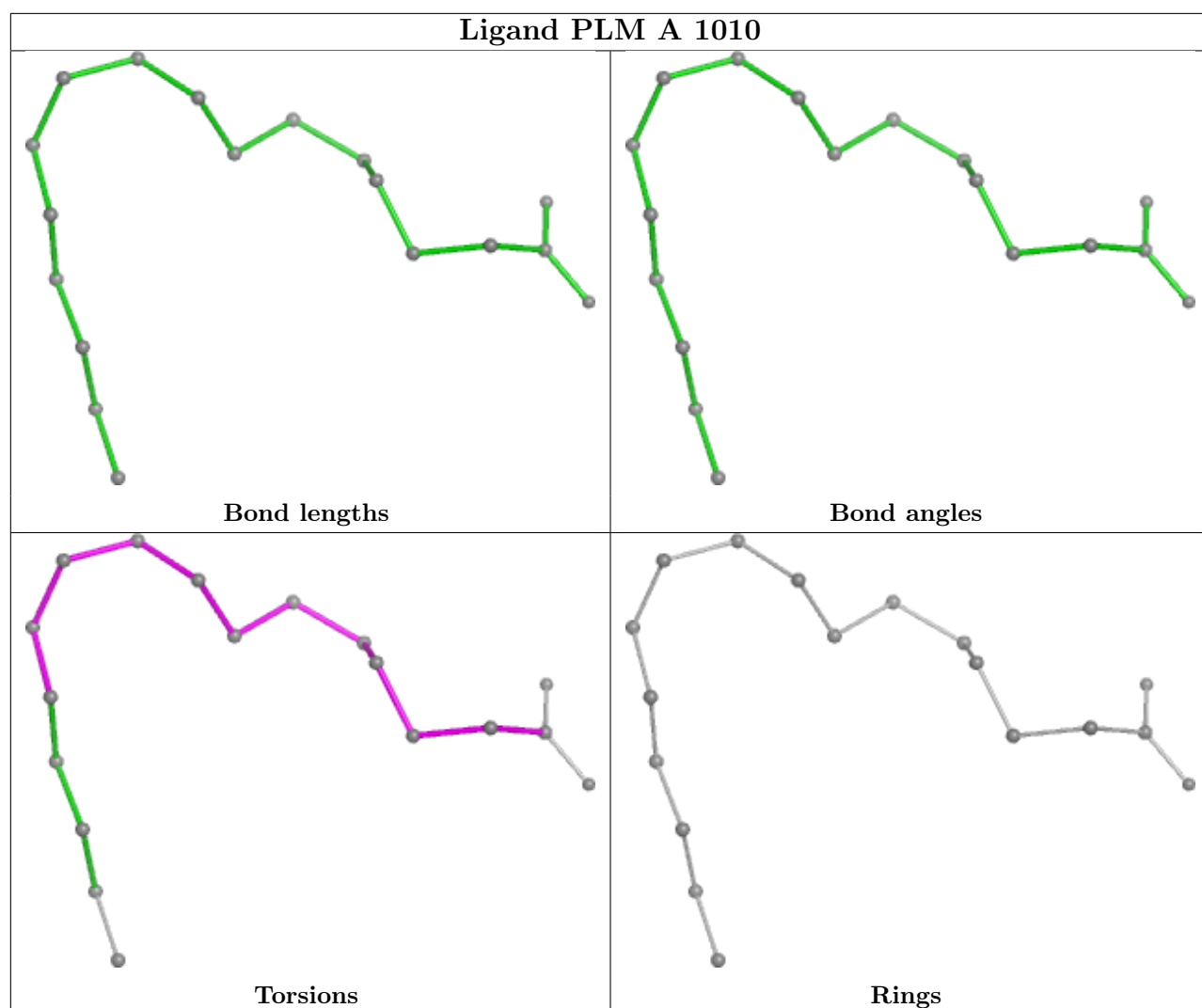


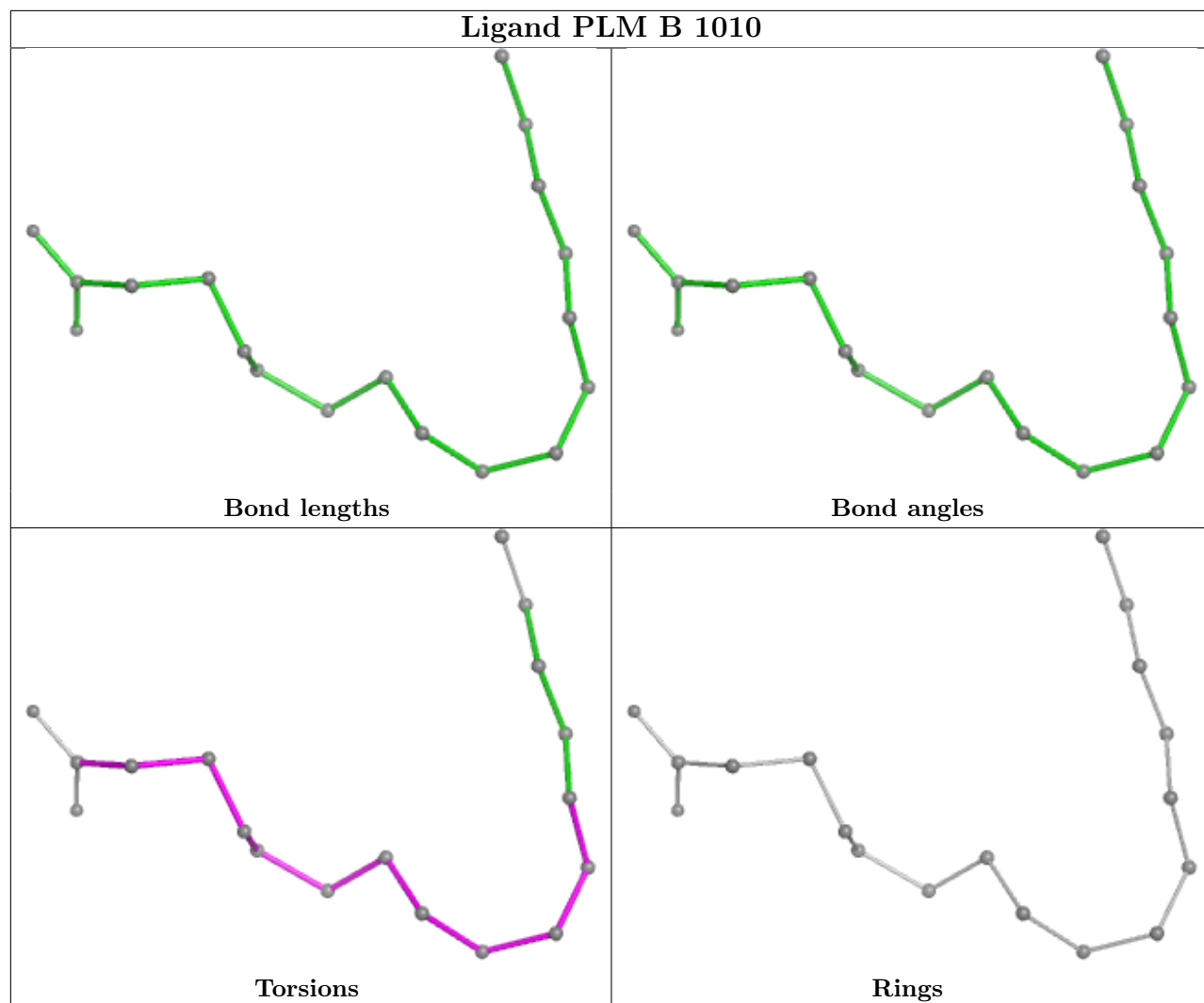


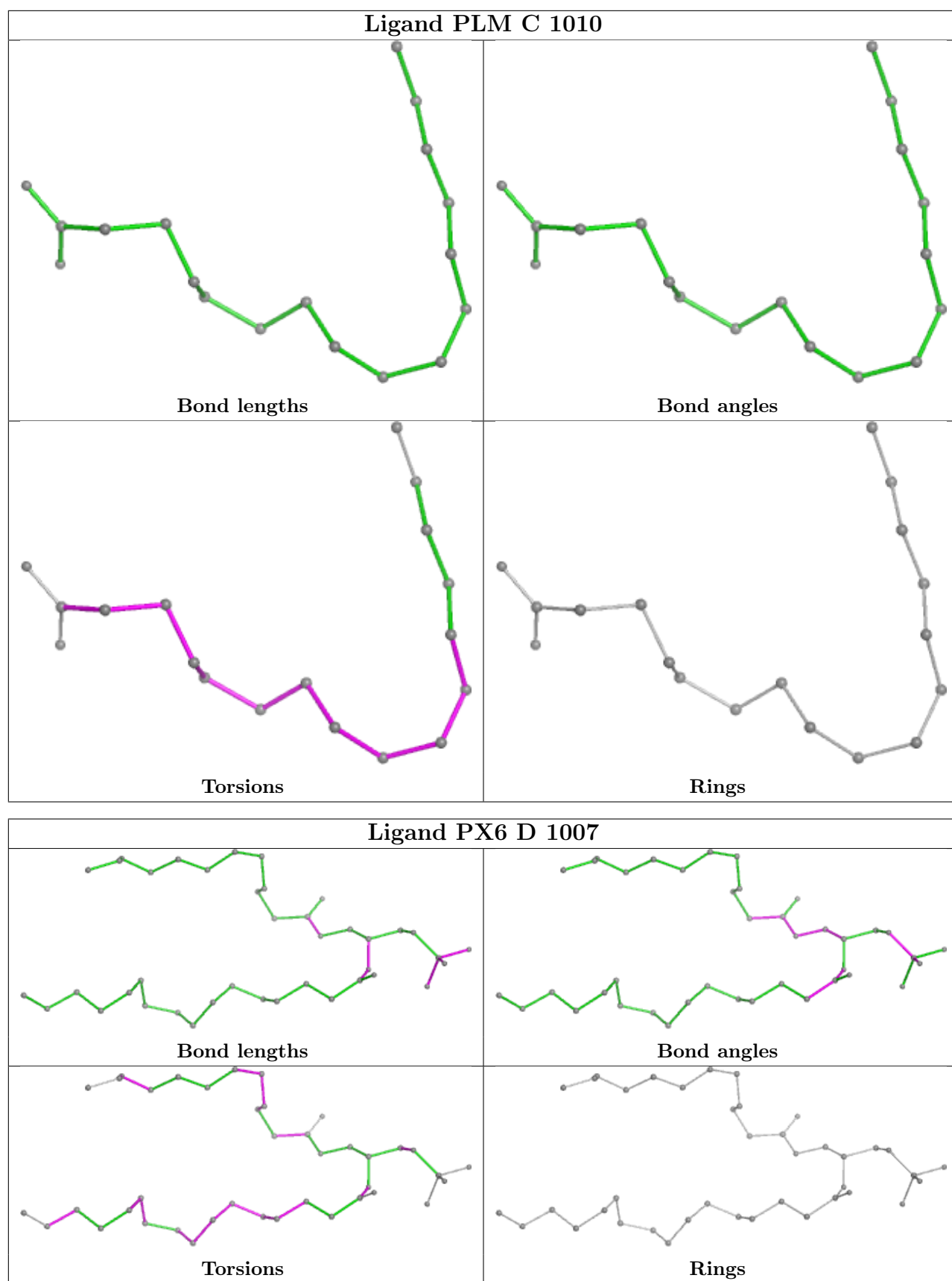












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

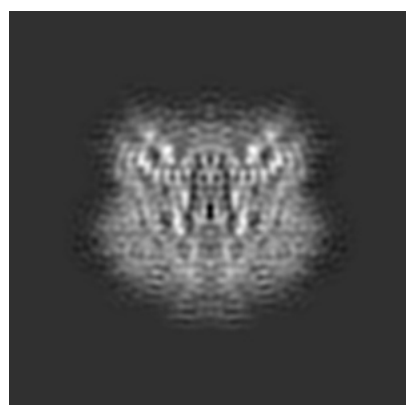
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3523. These allow visual inspection of the internal detail of the map and identification of artifacts.

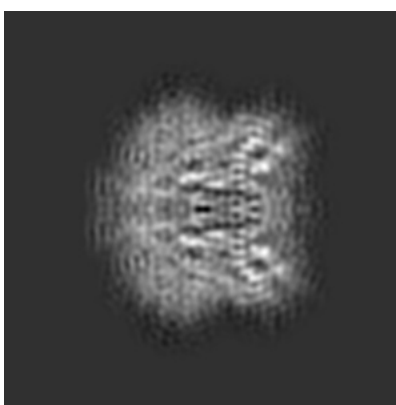
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

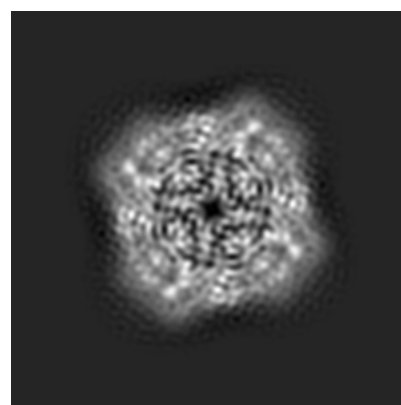
6.1.1 Primary map



X



Y

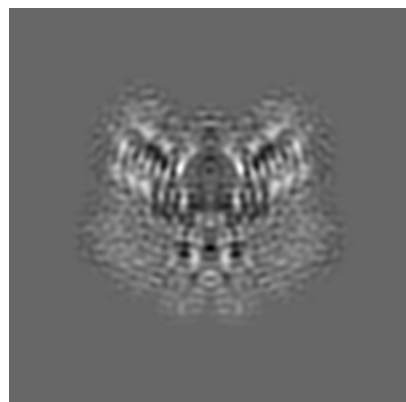


Z

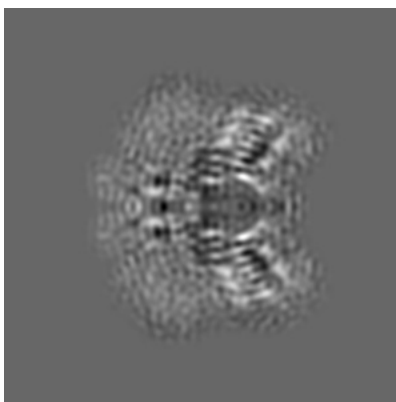
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

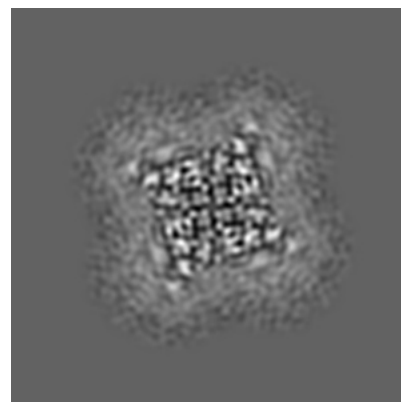
6.2.1 Primary map



X Index: 84



Y Index: 84

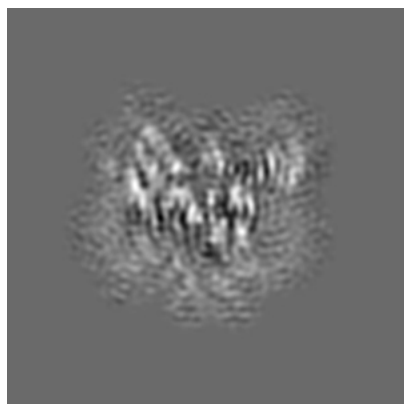


Z Index: 84

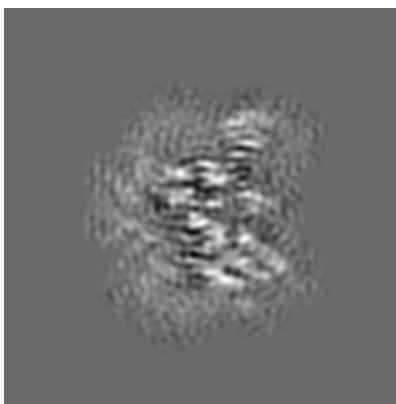
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

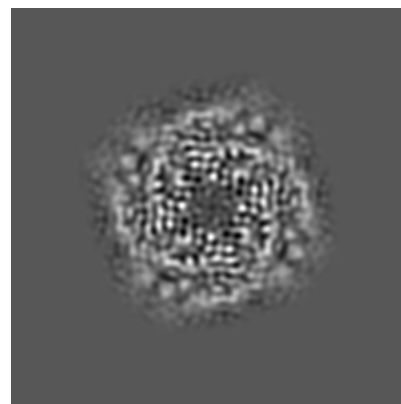
6.3.1 Primary map



X Index: 74



Y Index: 94

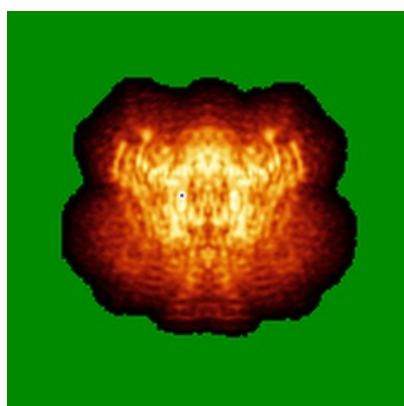


Z Index: 100

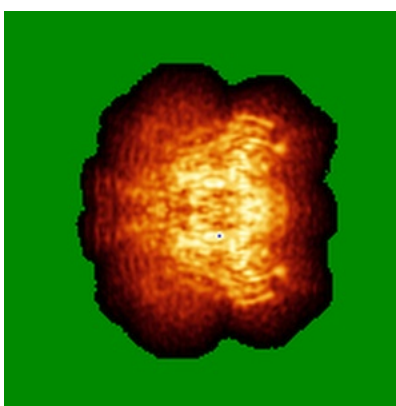
The images above show the largest variance slices of the map in three orthogonal directions.

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

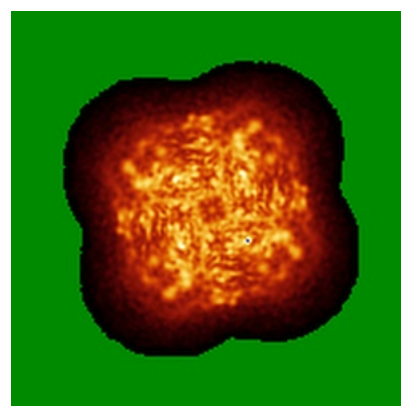
6.4.1 Primary map



X



Y

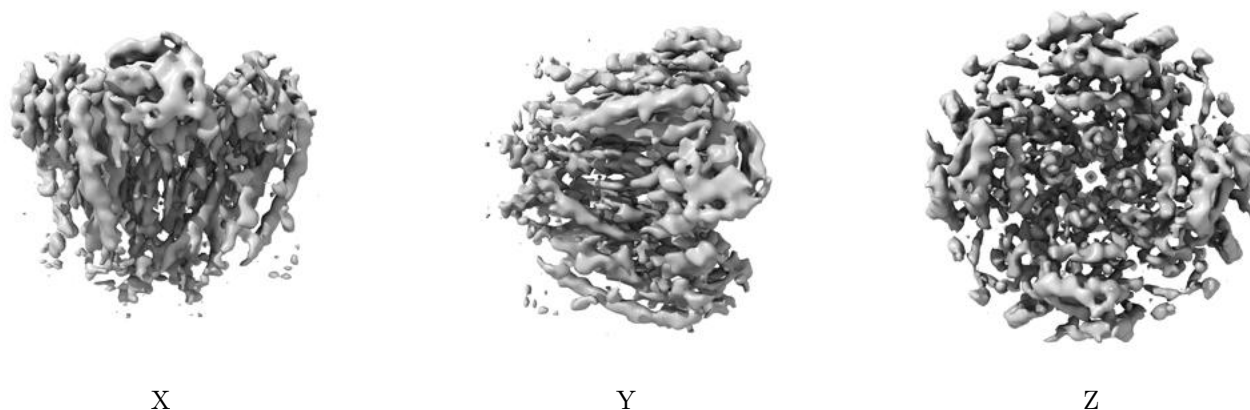


Z

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 0.0345. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

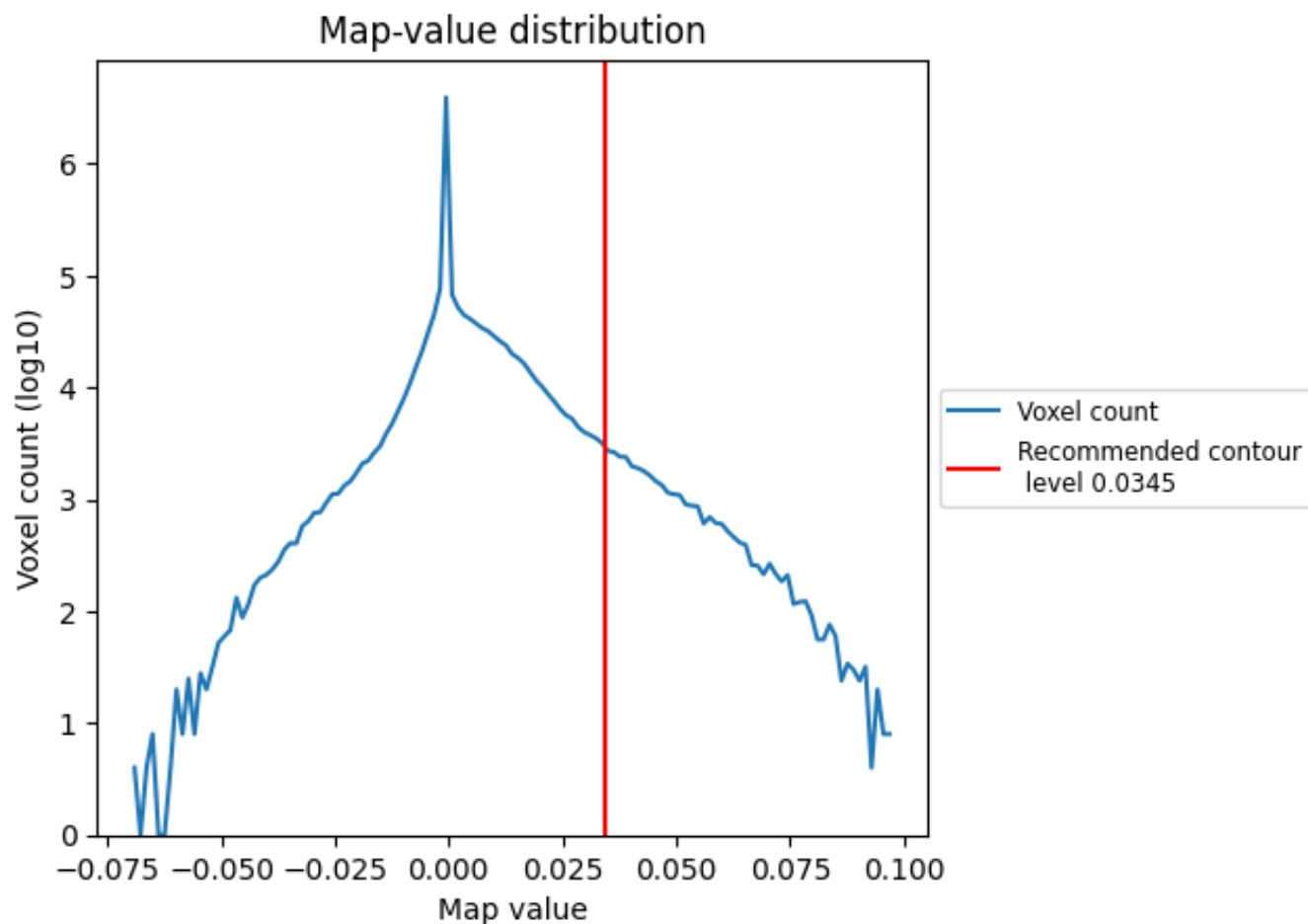
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

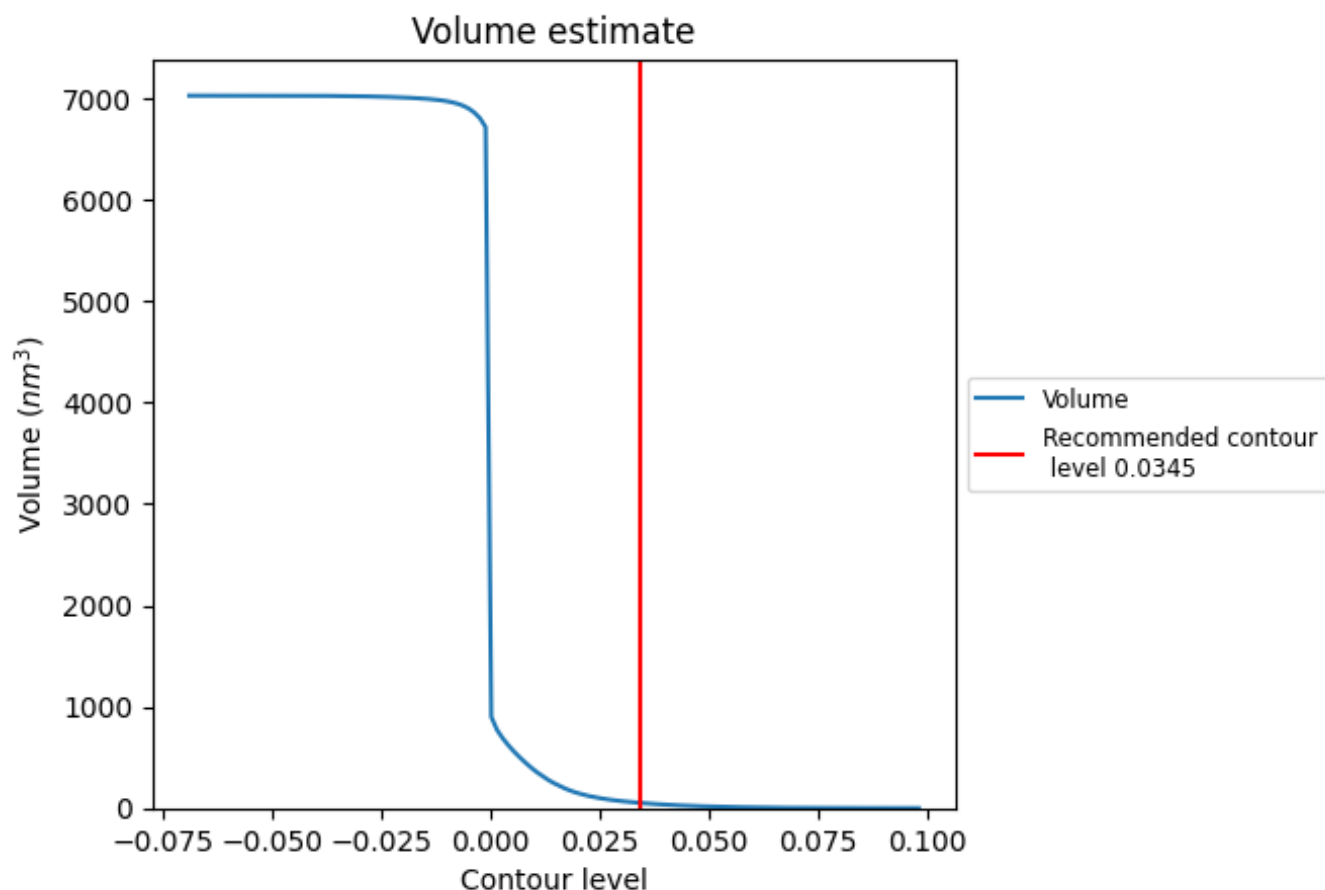
This section contains the results of statistical analysis of the map.

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.

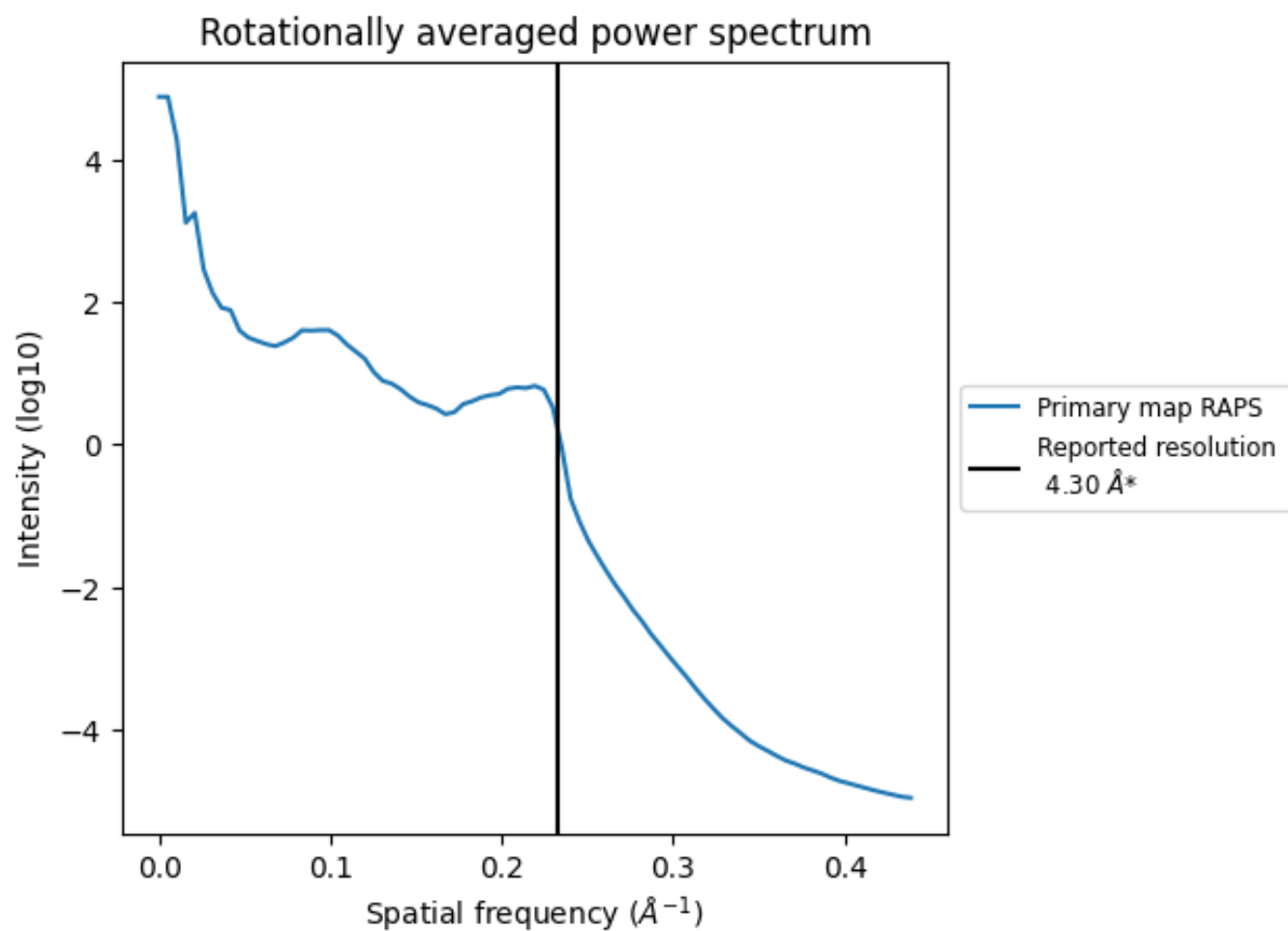
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm³; this corresponds to an approximate mass of 46 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

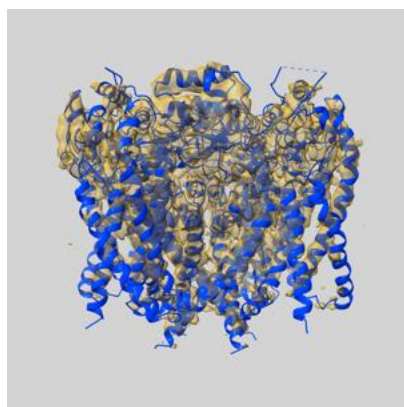
8 Fourier-Shell correlation

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

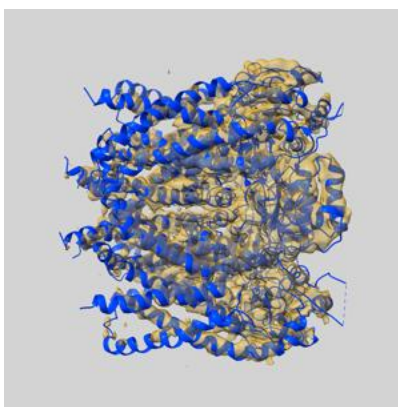
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3523 and PDB model 5MKE. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

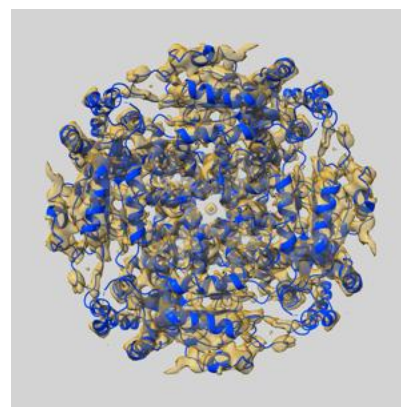
9.1 Map-model overlay [i](#)



X



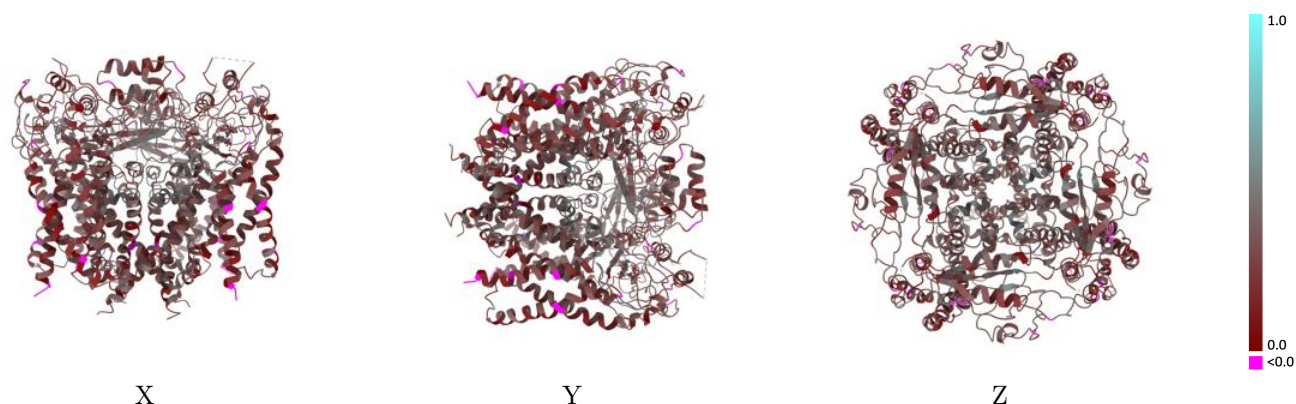
Y



Z

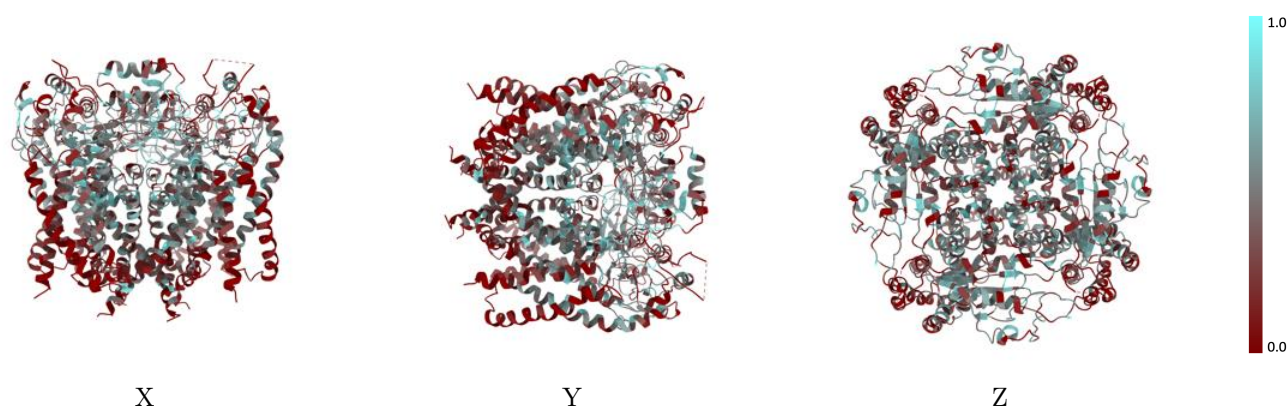
The images above show the 3D surface view of the map at the recommended contour level 0.0345 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



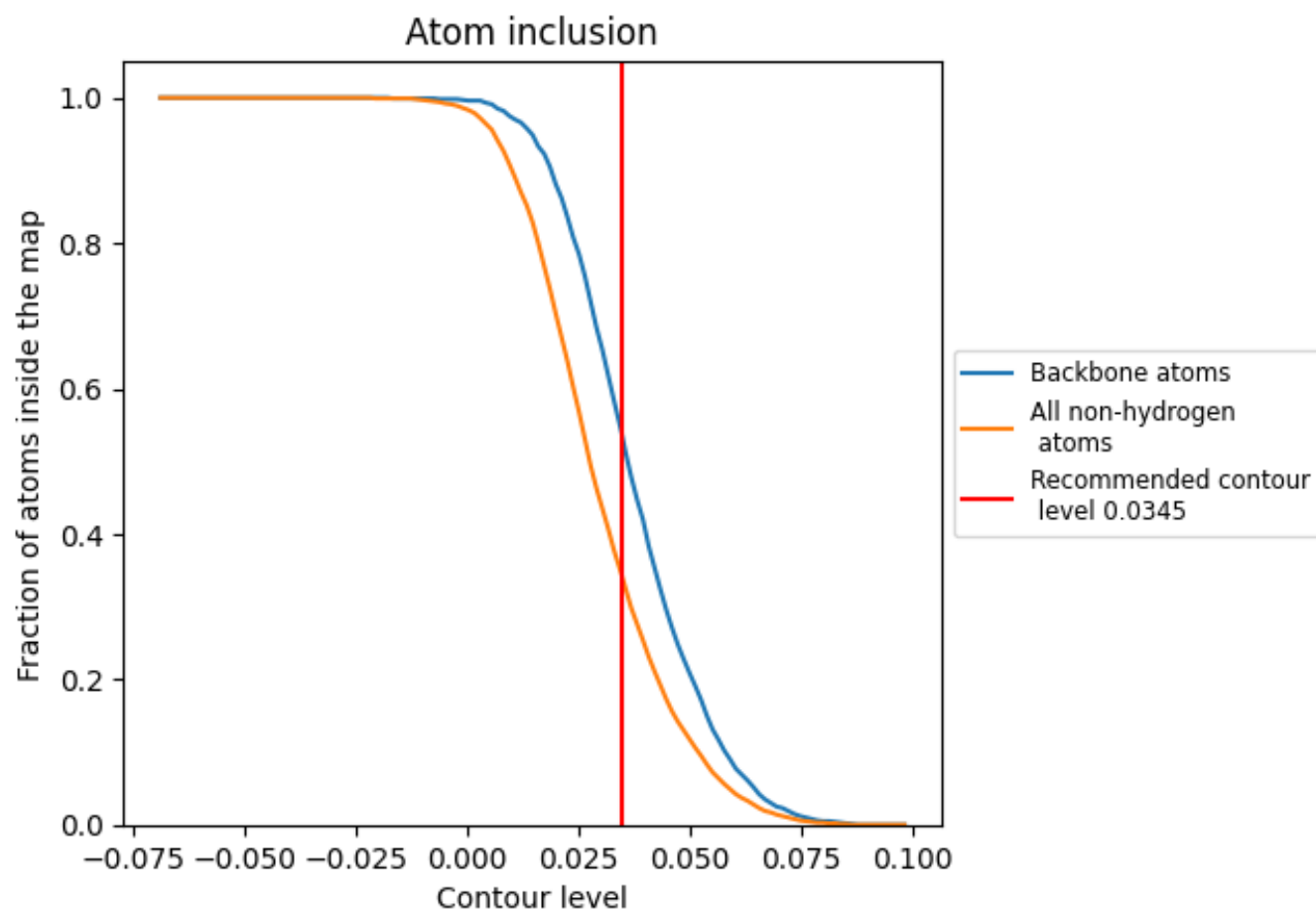
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0345).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 35% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0345) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.3460</div>	<div><div></div>0.3030</div>
A	<div><div></div>0.3460</div>	<div><div></div>0.3040</div>
B	<div><div></div>0.3480</div>	<div><div></div>0.3040</div>
C	<div><div></div>0.3460</div>	<div><div></div>0.3020</div>
D	<div><div></div>0.3470</div>	<div><div></div>0.3030</div>
E	<div><div></div>0.1070</div>	<div><div></div>0.2280</div>
F	<div><div></div>0.0710</div>	<div><div></div>0.2390</div>
G	<div><div></div>0.1070</div>	<div><div></div>0.2180</div>

1.0

0.0

<0.0