



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 07:24 AM UTC

PDB ID : 5MKE / pdb_00005mke
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:

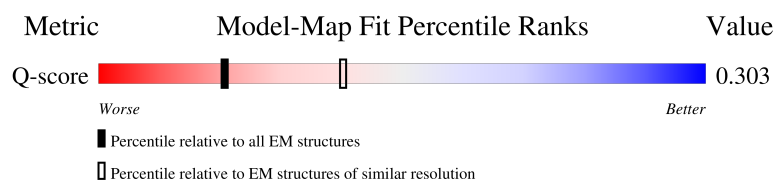
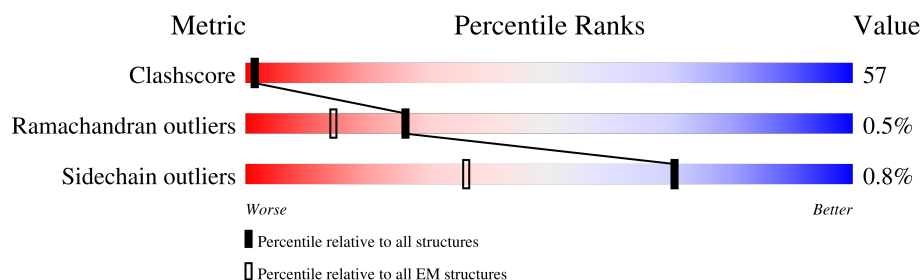
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	28% 13% 35% 51%
1	B	968	28% 13% 35% 51%
1	C	968	27% 13% 35% 51%
1	D	968	27% 14% 35% 51%

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Mol	Chain	Length	Quality of chain
2	E	2	100% 50%50%
2	F	2	100% 50%50%
2	G	2	100% 50%50%

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.



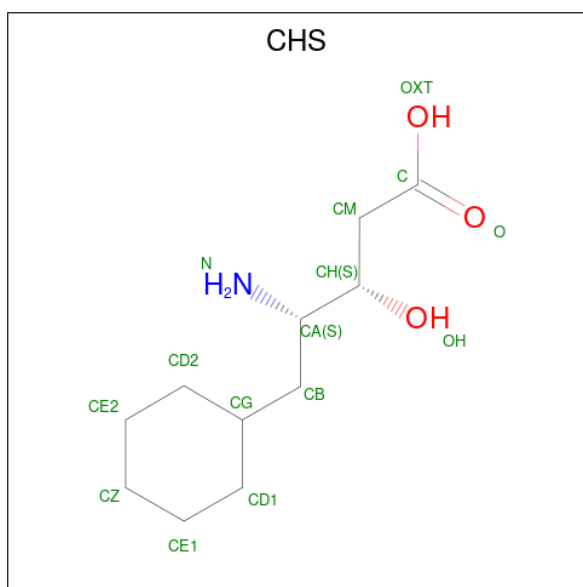
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



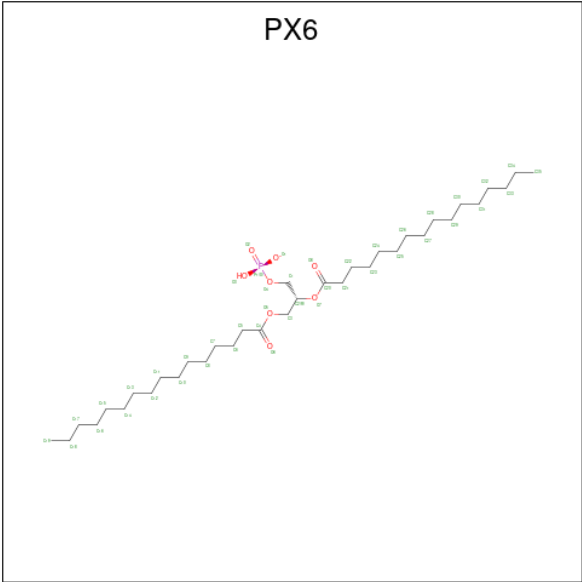
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3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

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



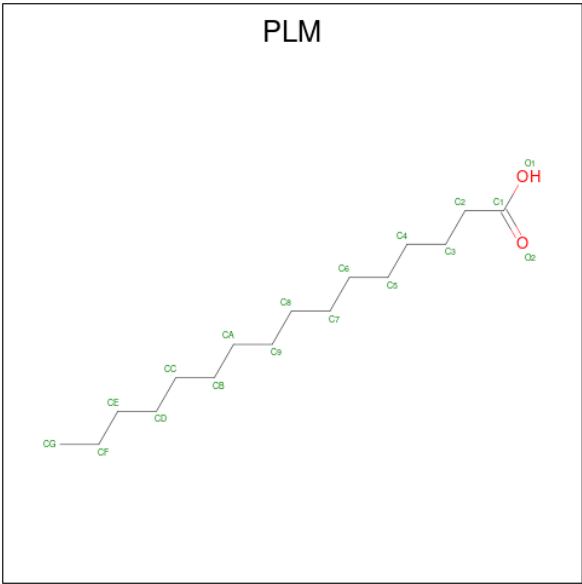
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			15	11	1	3	
4	A	1	Total	C	N	O	0
			15	11	1	3	
4	B	1	Total	C	N	O	0
			15	11	1	3	
4	B	1	Total	C	N	O	0
			15	11	1	3	
4	C	1	Total	C	N	O	0
			15	11	1	3	
4	C	1	Total	C	N	O	0
			15	11	1	3	
4	D	1	Total	C	N	O	0
			15	11	1	3	
4	D	1	Total	C	N	O	0
			15	11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

- Molecule 5 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: 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 (CCD ID: 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	

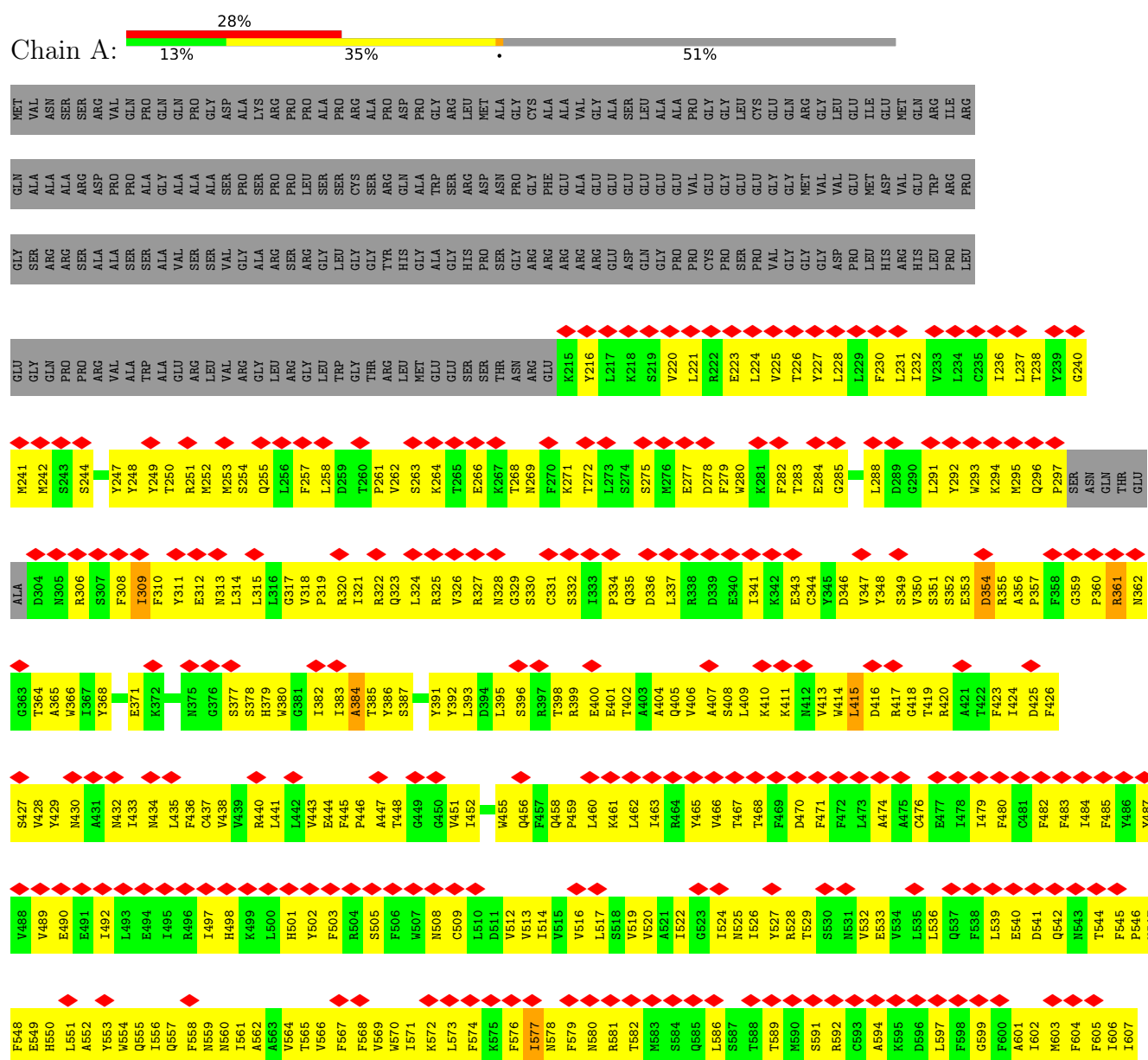
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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: Polycystin-2

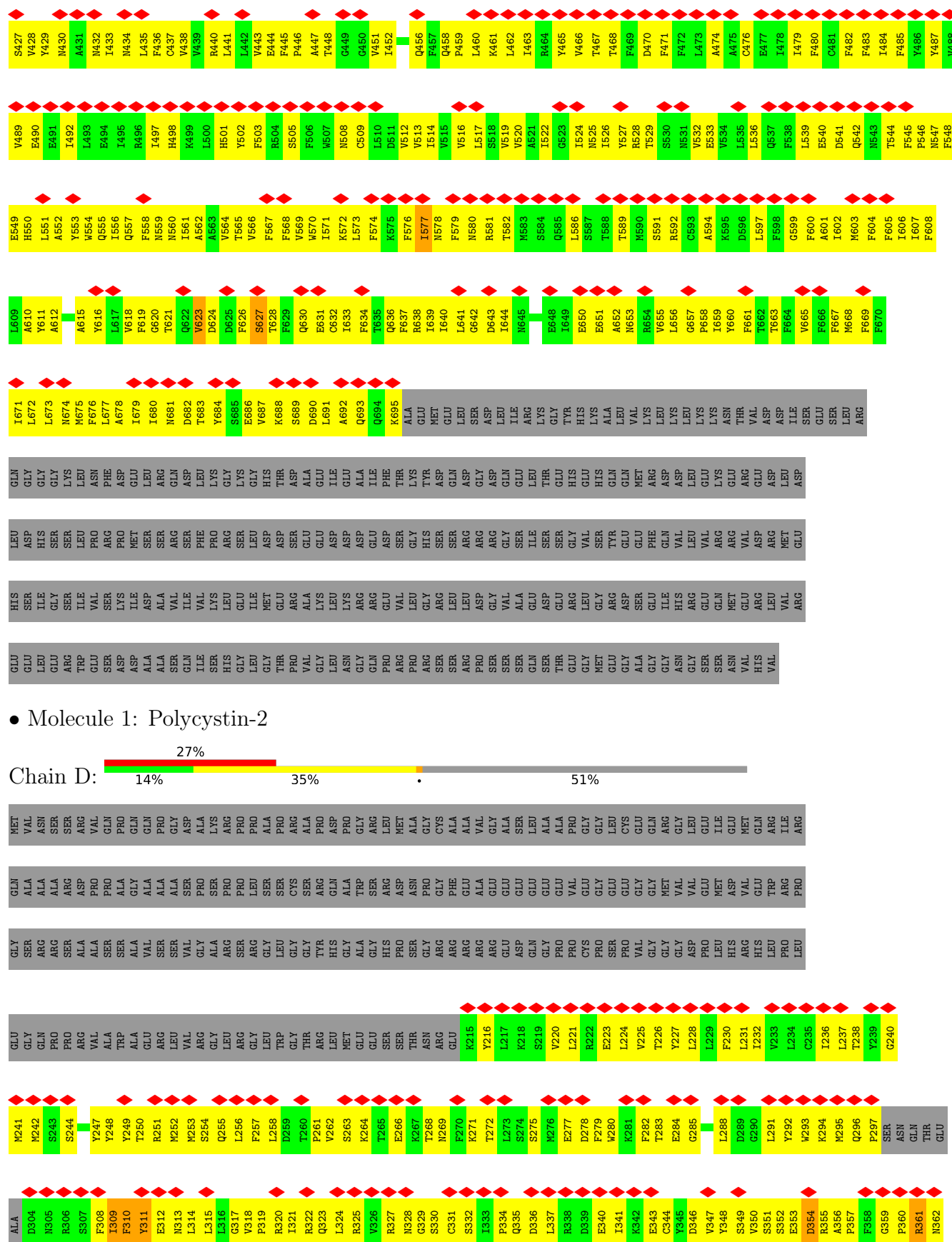


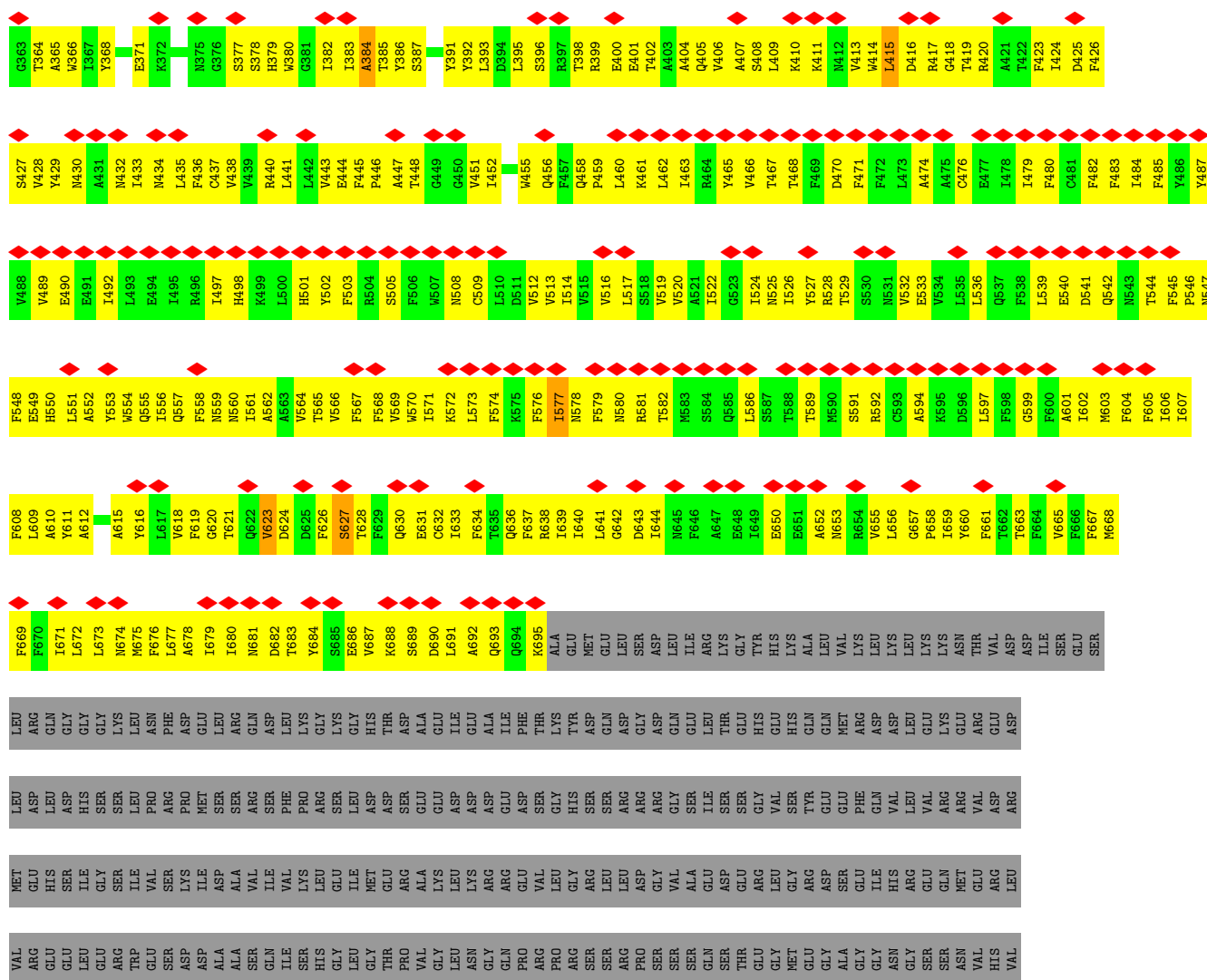
F608	L609	A610	Y611	A612	A615	Y616	L617	V618	F619	G620	T621	Q622	D624	D625	F626	S627	T628	F629	Q630	E631	C632	I633	F634	T635	Q636	F637	R638	I639	I640	L641	G642	D643	I644	N645	E648	I649	E650	E651	A652	N653	R654	V655	L656	G657	P658	I659	Y660	F661	T662	F663	V664	V665	F666	F667	M668	F669			
F670	L671	L672	L673	N674	M675	F676	L677	A678	I679	I680	N681	D682	T683	Y684	S685	E686	V687	K688	S689	D690	L691	A692	Q693	Q694	K695	ALA	GLU	MET	GLU	GLU	LEU	SER	ASP	LEU	ILE	ARG	LYS	TYR	HIS	LYS	ALA	LEU	VAL	LYS	L656	G657	P658	I659	THR	VAL	F661	T662	ASP	ASP	ILE	SER	GLU	SER	LEU
ARG	GLN	GLY	GLY	LYS	LEU	ASN	PHE	ASP	GLU	LEU	GLN	ASP	LEU	LYS	GLY	LYS	GLY	HIS	THR	ASP	ALA	GLU	ILE	PHE	THR	LYS	TYR	ASP	GLN	ASP	GLY	GLY	GLN	ILE	ARG	LYS	THR	GLU	HIS	GLY	GLU	GLN	GLN	ASP	LEU	LYS	LYS	GLY	ASN	ARG	GLU	THR	VAL	ASP	GLU	ASP	LEU		
ASP	LEU	ASP	HIS	SER	SER	PRO	ARG	PRO	MET	SER	ARG	SER	PHE	PRO	ARG	SER	LEU	ASP	SER	GLU	ASP	ASP	GLU	ASP	SER	SER	GLY	HIS	SER	GLN	ARG	ARG	GLY	ARG	ILE	SER	SER	GLY	VAL	VAL	GLY	LEU	VAL	GLU	GLY	ARG	VAL	ARG	GLU	VAL	ARG	VAL	ASP	ARG	MET				
GLU	HIS	GLU	ILE	GLY	SER	ILE	VAL	SER	LYS	ILE	VAL	ALA	VAL	LYS	GLU	ILE	MET	GLU	ARG	ALA	LYS	LEU	LYS	ARG	GLU	VAL	LEU	GLY	LEU	ASP	GLN	ASP	VAL	ALA	GLY	ASP	GLY	THR	GLU	ARG	GLY	HIS	GLY	VAL	GLY	GLU	GLN	GLY	ASN	GLY	GLY	VAL	HIS	VAL					
ARG	GLU	GLU	LEU	LEU	ARG	TRP	GLU	SER	ASP	ALA	SER	GLN	ILE	GLY	HIS	GLY	LEU	THR	PRO	VAL	GLY	ASN	GLY	GLN	PRO	ARG	ARG	PRO	GLY	SER	ARG	GLY	GLY	GLN	SER	SER	GLY	VAL	SER	GLY	GLY	GLY	ASN	GLY	GLY	SER	GLY	GLY	ASN	VAL	HIS	VAL							

• Molecule 1: Polycystin-2



Y487	F426	G363	ALA	M241	GLU	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
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- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	0/4031	0.66	2/5469 (0.0%)
1	B	0.41	0/4031	0.66	2/5469 (0.0%)
1	C	0.41	0/4031	0.66	2/5469 (0.0%)
1	D	0.41	0/4031	0.66	2/5469 (0.0%)
All	All	0.41	0/16124	0.66	8/21876 (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 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ALA	CA-C-N	7.17	134.60	121.70
1	A	384	ALA	C-N-CA	7.17	134.60	121.70
1	C	384	ALA	CA-C-N	7.14	134.55	121.70
1	C	384	ALA	C-N-CA	7.14	134.55	121.70
1	B	384	ALA	CA-C-N	7.13	134.53	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	508	0
1	B	3926	0	3880	513	0
1	C	3926	0	3880	494	0
1	D	3926	0	3880	513	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	1885	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 57.

The worst 5 of 1885 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	66
1	B	471/968 (49%)	383 (81%)	86 (18%)	2 (0%)	30	66
1	C	471/968 (49%)	381 (81%)	88 (19%)	2 (0%)	30	66
1	D	471/968 (49%)	381 (81%)	87 (18%)	3 (1%)	21	58
All	All	1884/3872 (49%)	1527 (81%)	348 (18%)	9 (0%)	26	62

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%)	76	79
1	B	429/837 (51%)	426 (99%)	3 (1%)	76	79
1	C	429/837 (51%)	425 (99%)	4 (1%)	70	76
1	D	429/837 (51%)	425 (99%)	4 (1%)	70	76
All	All	1716/3348 (51%)	1702 (99%)	14 (1%)	70	77

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	309	ILE
1	C	415	LEU
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 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	458	GLN
1	C	550	HIS
1	D	550	HIS
1	C	537	GLN
1	C	622	GLN

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	2,1	14,14,15	0.52	0	17,19,21	1.16	2 (11%)
2	NAG	E	2	2	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
2	NAG	F	1	2,1	14,14,15	0.54	0	17,19,21	1.15	2 (11%)
2	NAG	F	2	2	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
2	NAG	G	1	2,1	14,14,15	0.49	0	17,19,21	1.14	2 (11%)
2	NAG	G	2	2	14,14,15	0.43	0	17,19,21	1.17	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	2,1	-	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	2,1	-	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	2,1	-	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	2.38	120.07	116.12
2	E	1	NAG	C8-C7-N2	2.37	120.05	116.12
2	E	2	NAG	C8-C7-N2	2.36	120.04	116.12
2	F	2	NAG	C8-C7-N2	2.36	120.03	116.12
2	F	1	NAG	C8-C7-N2	2.35	120.01	116.12

There are no chirality outliers.

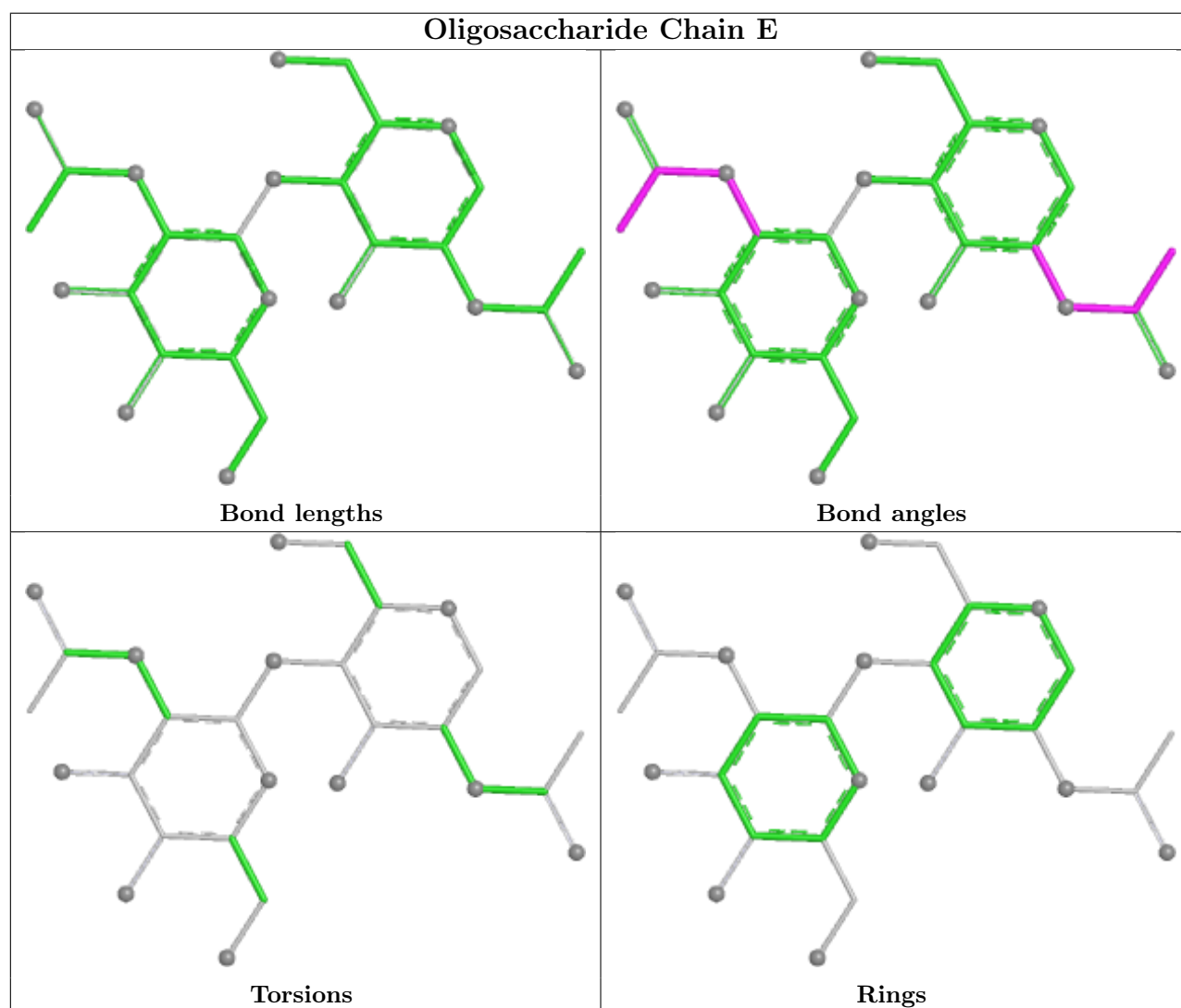
There are no torsion outliers.

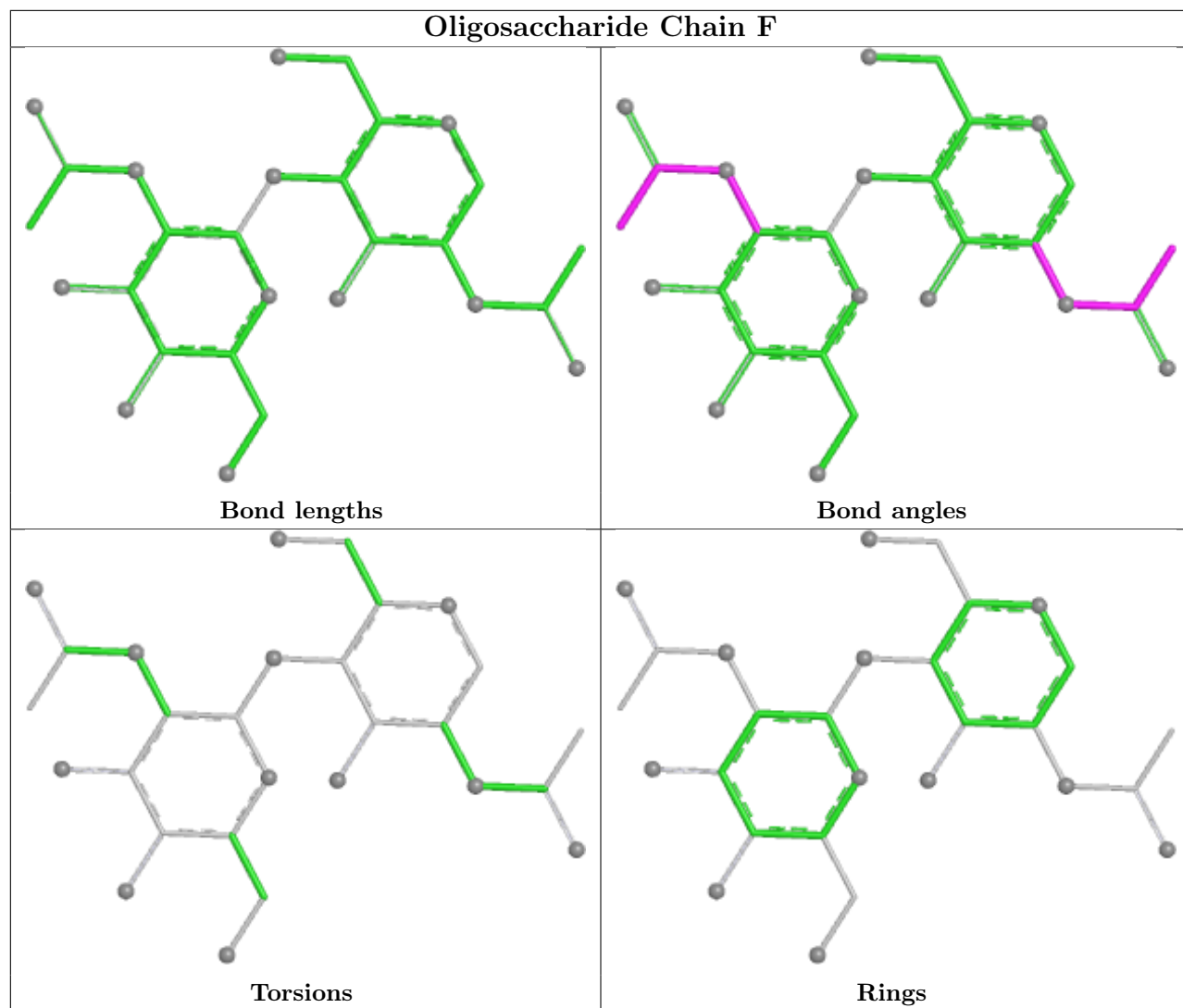
There are no ring outliers.

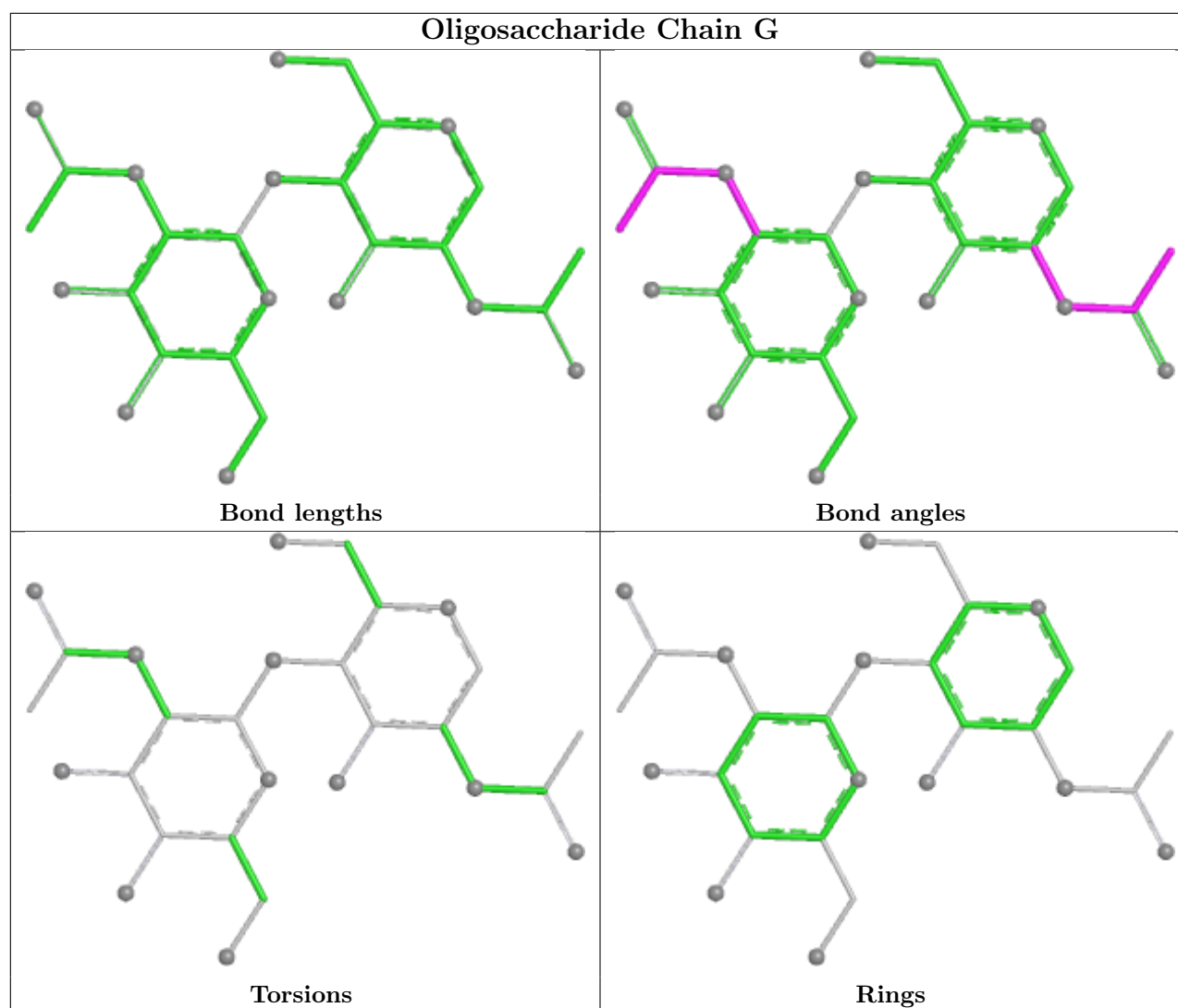
3 monomers are involved in 6 short contacts:

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	$\# Z > 2$
3	NAG	D	1004	-	14,14,15	0.43	0	17,19,21	1.17	2 (11%)
6	PLM	C	1009	-	17,17,17	0.51	0	17,17,17	0.96	0
3	NAG	D	1003	1	14,14,15	0.45	0	17,19,21	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	1001	1	14,14,15	0.93	1 (7%)	17,19,21	0.83	1 (5%)
4	CHS	C	1005	-	15,15,15	0.51	0	15,19,19	0.81	0
3	NAG	A	1001	1	14,14,15	0.73	1 (7%)	17,19,21	0.86	1 (5%)
4	CHS	B	1005	-	15,15,15	0.53	0	15,19,19	0.82	0
6	PLM	D	1008	-	17,17,17	0.58	0	17,17,17	0.74	0
4	CHS	A	1005	-	15,15,15	0.52	0	15,19,19	0.82	0
5	PX6	B	1007	-	39,39,43	1.48	6 (15%)	42,44,48	1.58	4 (9%)
3	NAG	A	1002	1	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
4	CHS	D	1006	-	15,15,15	0.60	0	15,19,19	0.97	1 (6%)
6	PLM	A	1009	-	17,17,17	0.51	0	17,17,17	0.97	0
4	CHS	B	1006	-	15,15,15	0.59	0	15,19,19	1.02	1 (6%)
6	PLM	C	1008	-	17,17,17	0.57	0	17,17,17	0.75	0
6	PLM	D	1010	-	17,17,17	0.53	0	17,17,17	0.77	0
4	CHS	C	1006	-	15,15,15	0.60	0	15,19,19	1.00	1 (6%)
4	CHS	D	1005	-	15,15,15	0.52	0	15,19,19	0.82	0
6	PLM	B	1010	-	17,17,17	0.54	0	17,17,17	0.77	0
5	PX6	D	1007	-	39,39,43	1.48	6 (15%)	42,44,48	1.58	4 (9%)
5	PX6	C	1007	-	39,39,43	1.48	6 (15%)	42,44,48	1.55	4 (9%)
3	NAG	B	1001	1	14,14,15	0.63	1 (7%)	17,19,21	0.83	1 (5%)
6	PLM	C	1010	-	17,17,17	0.53	0	17,17,17	0.77	0
5	PX6	A	1007	-	39,39,43	1.47	6 (15%)	42,44,48	1.58	5 (11%)
3	NAG	D	1002	1	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
3	NAG	C	1001	1	14,14,15	0.58	0	17,19,21	0.71	1 (5%)
6	PLM	A	1008	-	17,17,17	0.58	0	17,17,17	0.74	0
6	PLM	D	1009	-	17,17,17	0.51	0	17,17,17	0.96	0
6	PLM	B	1008	-	17,17,17	0.58	0	17,17,17	0.75	0
4	CHS	A	1006	-	15,15,15	0.60	0	15,19,19	0.99	1 (6%)
6	PLM	B	1009	-	17,17,17	0.52	0	17,17,17	0.96	0
3	NAG	C	1002	1	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
6	PLM	A	1010	-	17,17,17	0.53	0	17,17,17	0.77	0
3	NAG	B	1002	1	14,14,15	0.42	0	17,19,21	1.15	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	D	1004	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PLM	C	1009	-	-	6/15/15/15	-
3	NAG	D	1003	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1001	1	-	2/6/23/26	0/1/1/1
4	CHS	C	1005	-	-	5/12/20/20	0/1/1/1
3	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
4	CHS	B	1005	-	-	5/12/20/20	0/1/1/1
6	PLM	D	1008	-	-	11/15/15/15	-
4	CHS	A	1005	-	-	5/12/20/20	0/1/1/1
5	PX6	B	1007	-	-	18/41/41/45	-
3	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
4	CHS	D	1006	-	-	6/12/20/20	0/1/1/1
6	PLM	A	1009	-	-	7/15/15/15	-
4	CHS	B	1006	-	-	6/12/20/20	0/1/1/1
6	PLM	C	1008	-	-	11/15/15/15	-
6	PLM	D	1010	-	-	12/15/15/15	-
4	CHS	C	1006	-	-	5/12/20/20	0/1/1/1
4	CHS	D	1005	-	-	5/12/20/20	0/1/1/1
6	PLM	B	1010	-	-	12/15/15/15	-
5	PX6	D	1007	-	-	18/41/41/45	-
5	PX6	C	1007	-	-	18/41/41/45	-
3	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
6	PLM	C	1010	-	-	12/15/15/15	-
5	PX6	A	1007	-	-	17/41/41/45	-
3	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1001	1	-	2/6/23/26	0/1/1/1
6	PLM	A	1008	-	-	11/15/15/15	-
6	PLM	D	1009	-	-	6/15/15/15	-
6	PLM	B	1008	-	-	11/15/15/15	-
4	CHS	A	1006	-	-	5/12/20/20	0/1/1/1
6	PLM	B	1009	-	-	6/15/15/15	-
3	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
6	PLM	A	1010	-	-	12/15/15/15	-
3	NAG	B	1002	1	-	0/6/23/26	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1007	PX6	P1-O2	4.82	1.65	1.50
5	D	1007	PX6	P1-O2	4.82	1.65	1.50
5	A	1007	PX6	P1-O2	4.80	1.65	1.50
5	C	1007	PX6	P1-O2	4.78	1.65	1.50
5	A	1007	PX6	O7-C2	-3.32	1.38	1.46

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1007	PX6	O5-C3-C2	7.68	130.54	108.40
5	D	1007	PX6	O5-C3-C2	7.64	130.42	108.40
5	A	1007	PX6	O5-C3-C2	7.63	130.40	108.40
5	C	1007	PX6	O5-C3-C2	7.60	130.30	108.40
3	A	1001	NAG	C1-O5-C5	2.92	116.09	112.19

There are no chirality outliers.

5 of 238 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:

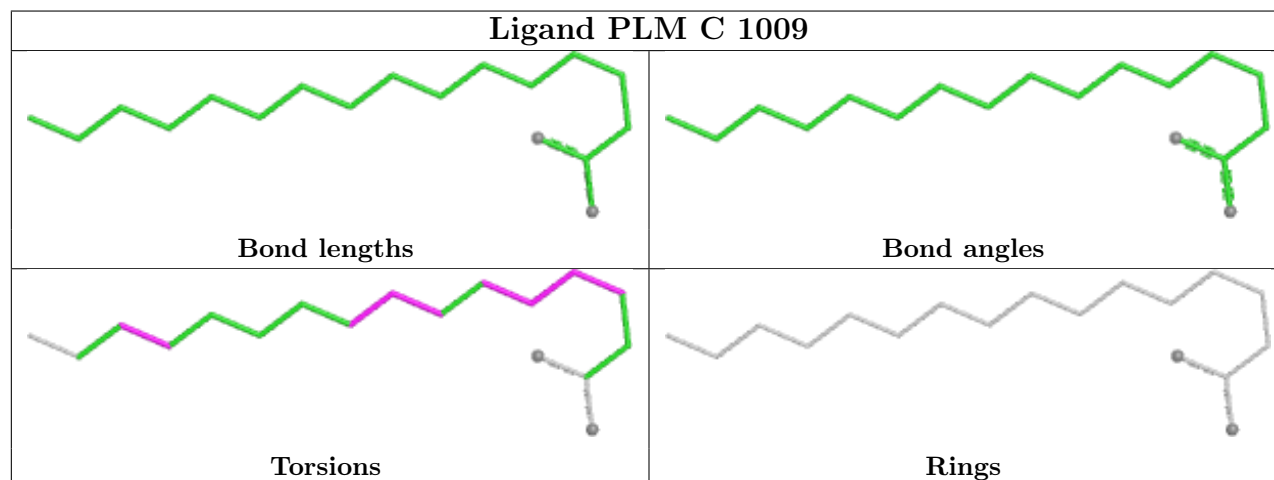
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1004	NAG	2	0
6	C	1009	PLM	4	0
3	D	1001	NAG	6	0
4	C	1005	CHS	4	0
4	B	1005	CHS	3	0
6	D	1008	PLM	2	0
4	A	1005	CHS	2	0
5	B	1007	PX6	6	0
3	A	1002	NAG	8	0
4	D	1006	CHS	2	0
6	A	1009	PLM	4	0
4	B	1006	CHS	3	0
6	C	1008	PLM	2	0

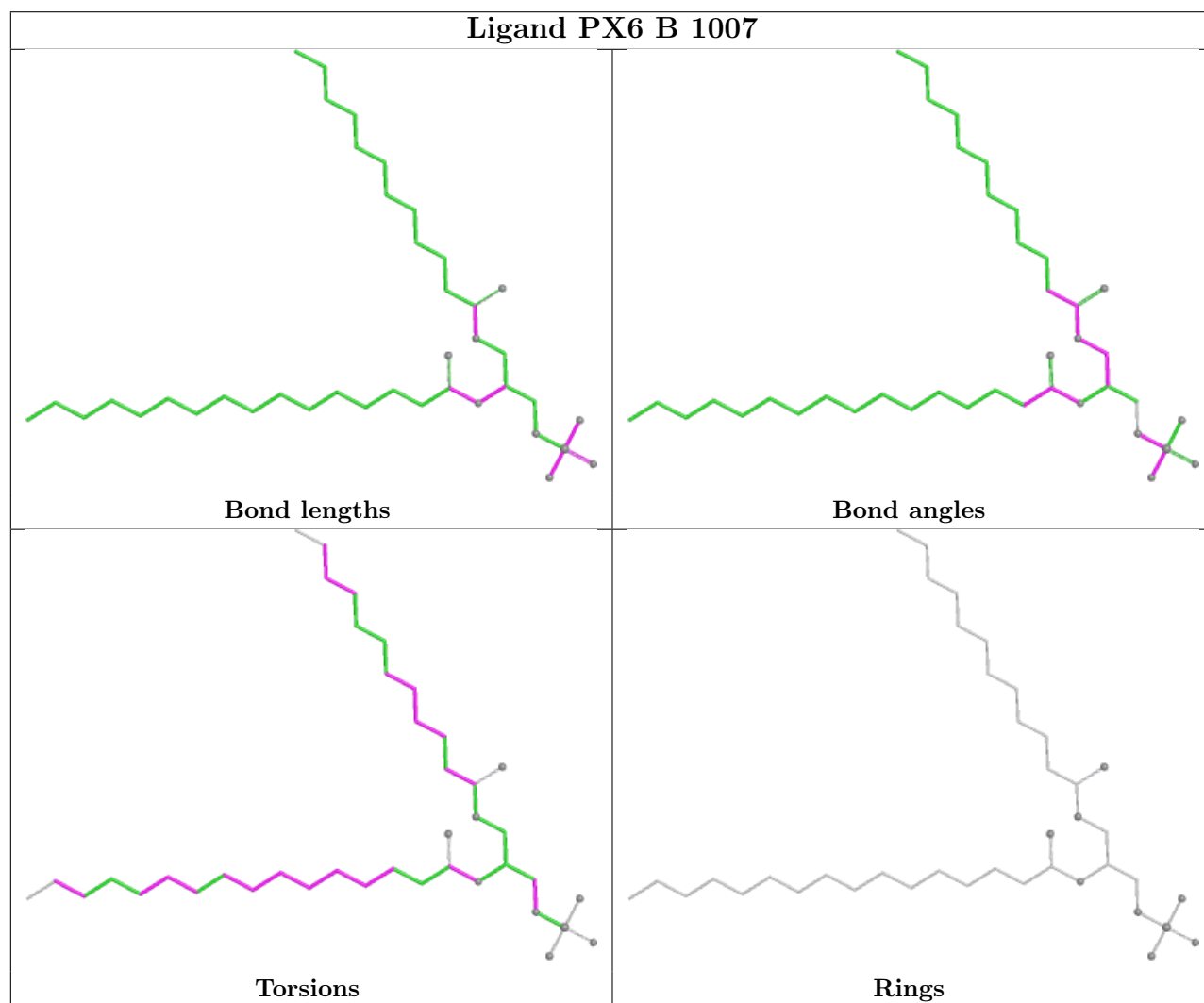
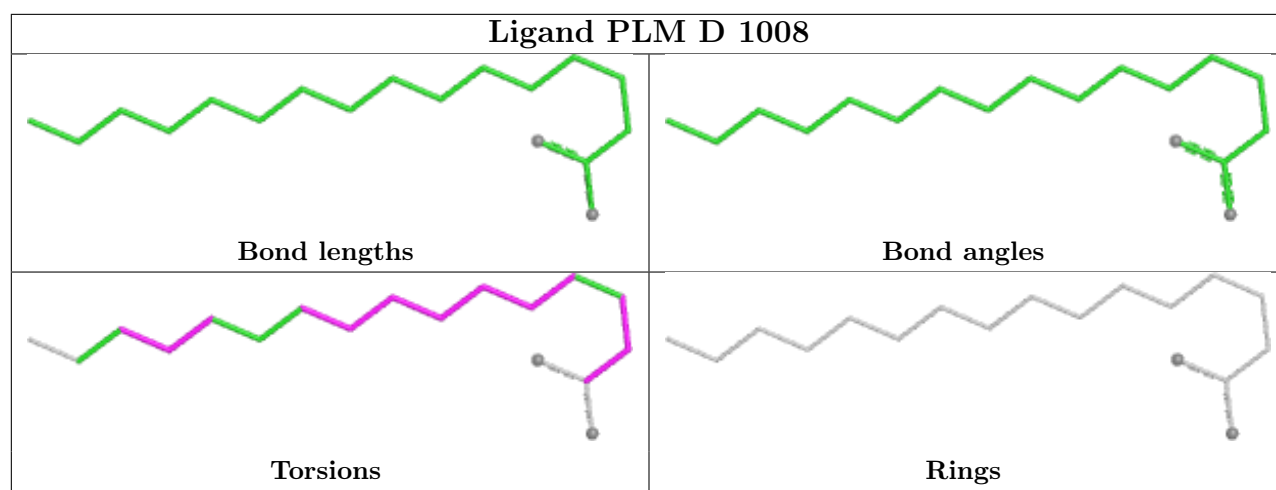
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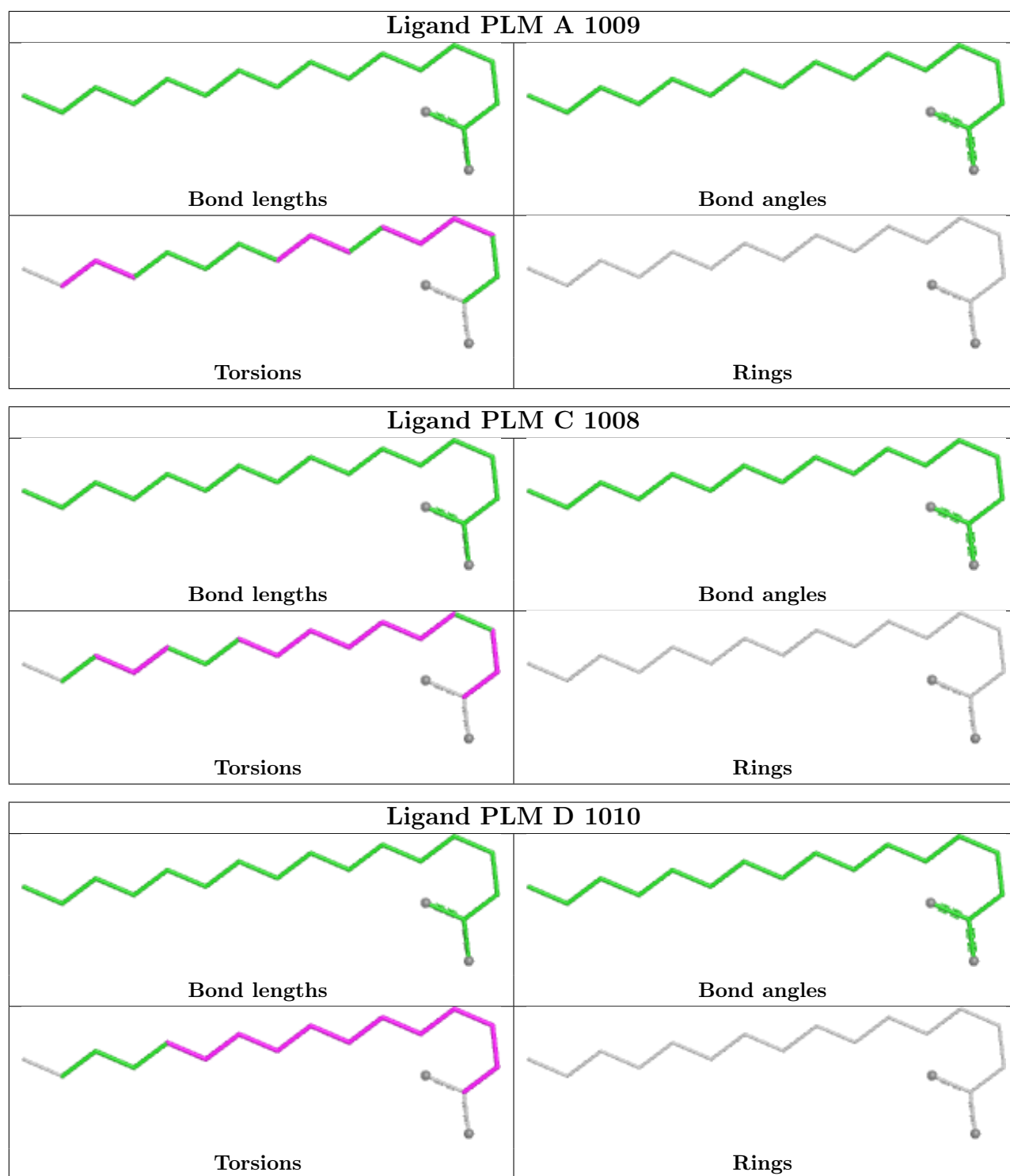
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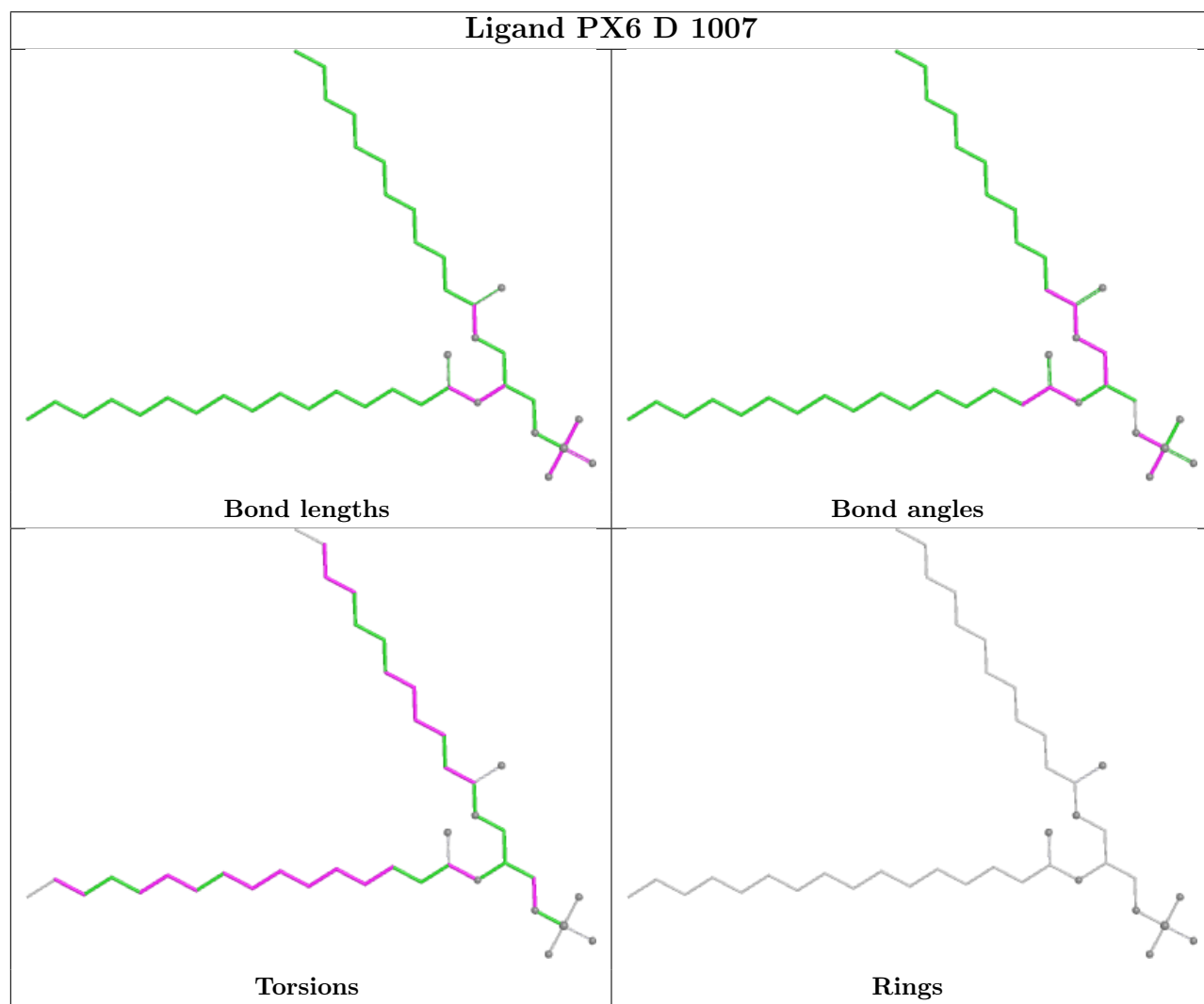
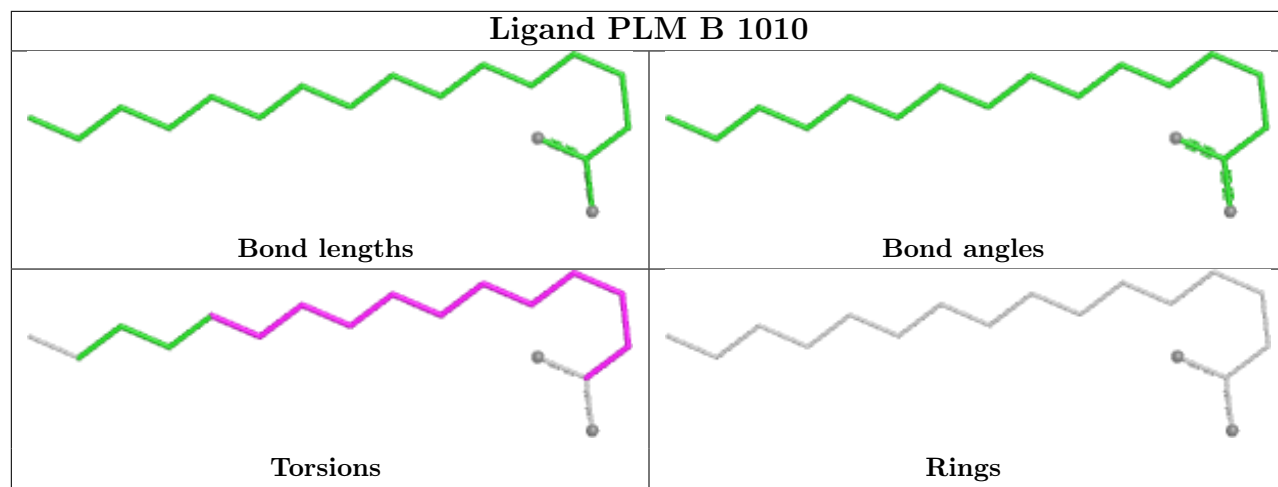
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1010	PLM	3	0
4	C	1006	CHS	3	0
4	D	1005	CHS	3	0
6	B	1010	PLM	3	0
5	D	1007	PX6	4	0
5	C	1007	PX6	4	0
6	C	1010	PLM	3	0
5	A	1007	PX6	3	0
3	D	1002	NAG	8	0
6	A	1008	PLM	2	0
6	D	1009	PLM	1	0
6	B	1008	PLM	2	0
4	A	1006	CHS	2	0
6	B	1009	PLM	3	0
3	C	1002	NAG	8	0
6	A	1010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

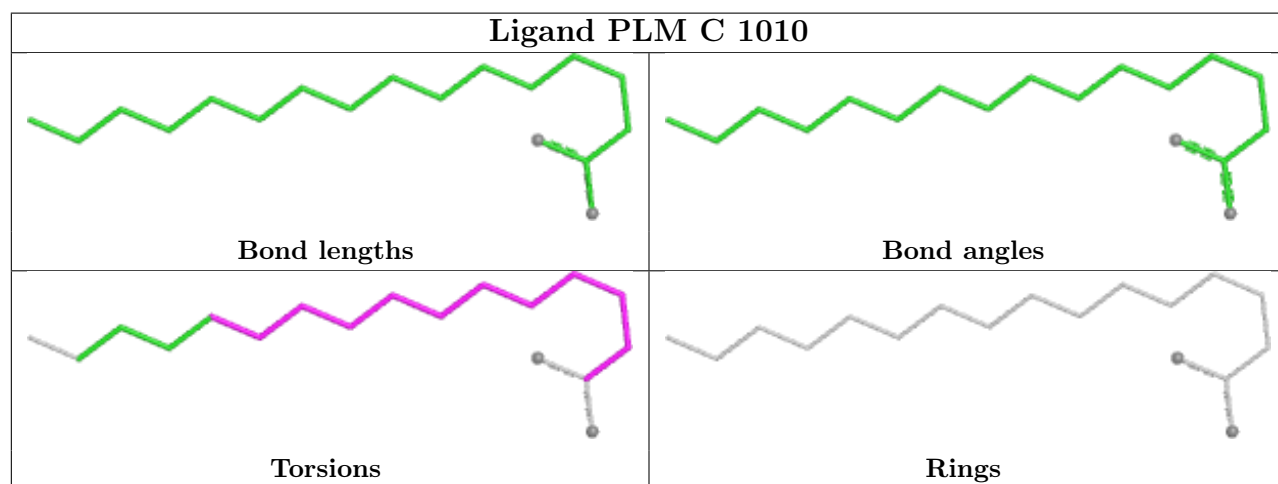
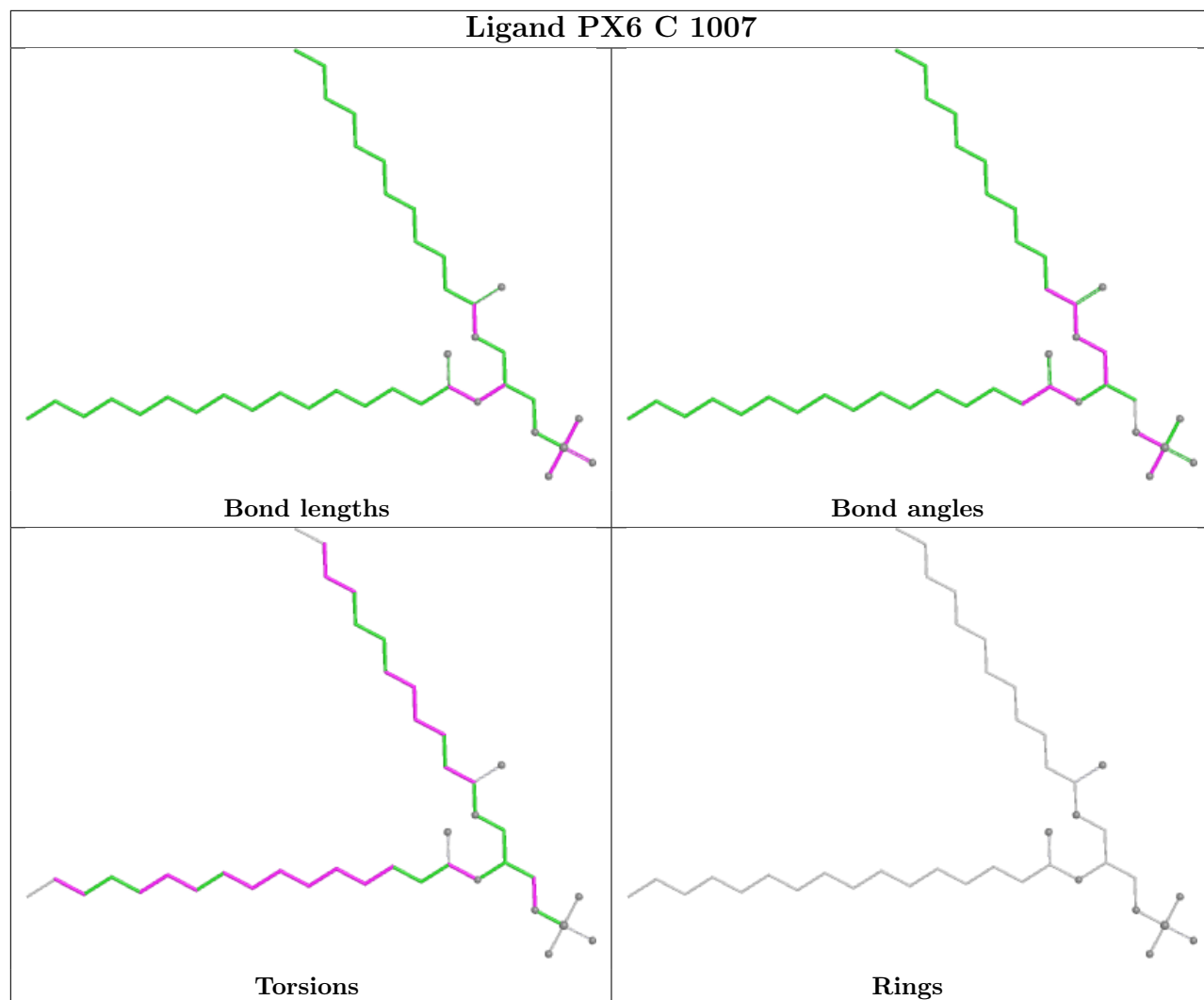
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

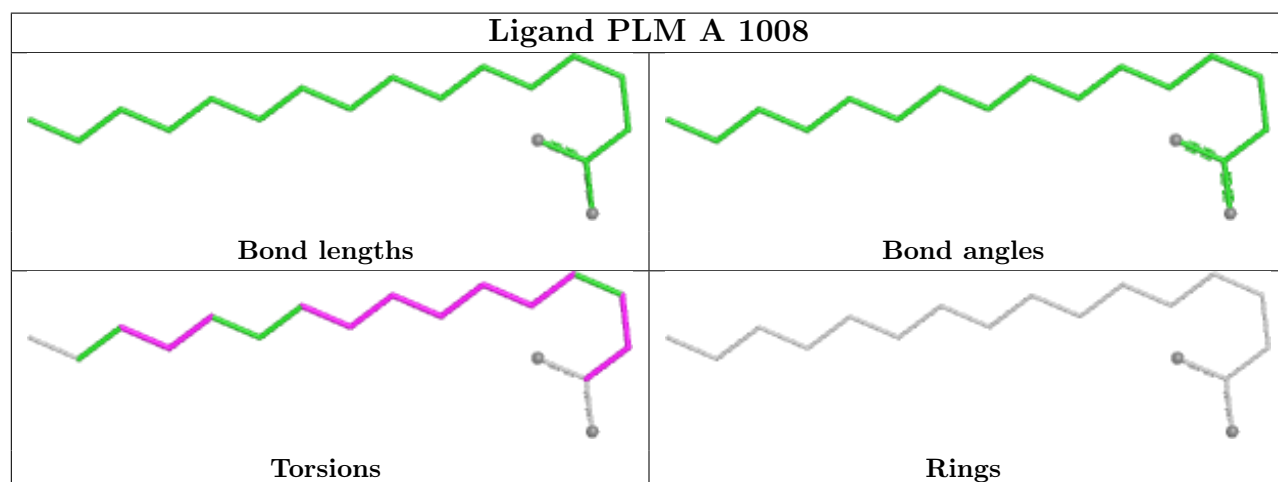
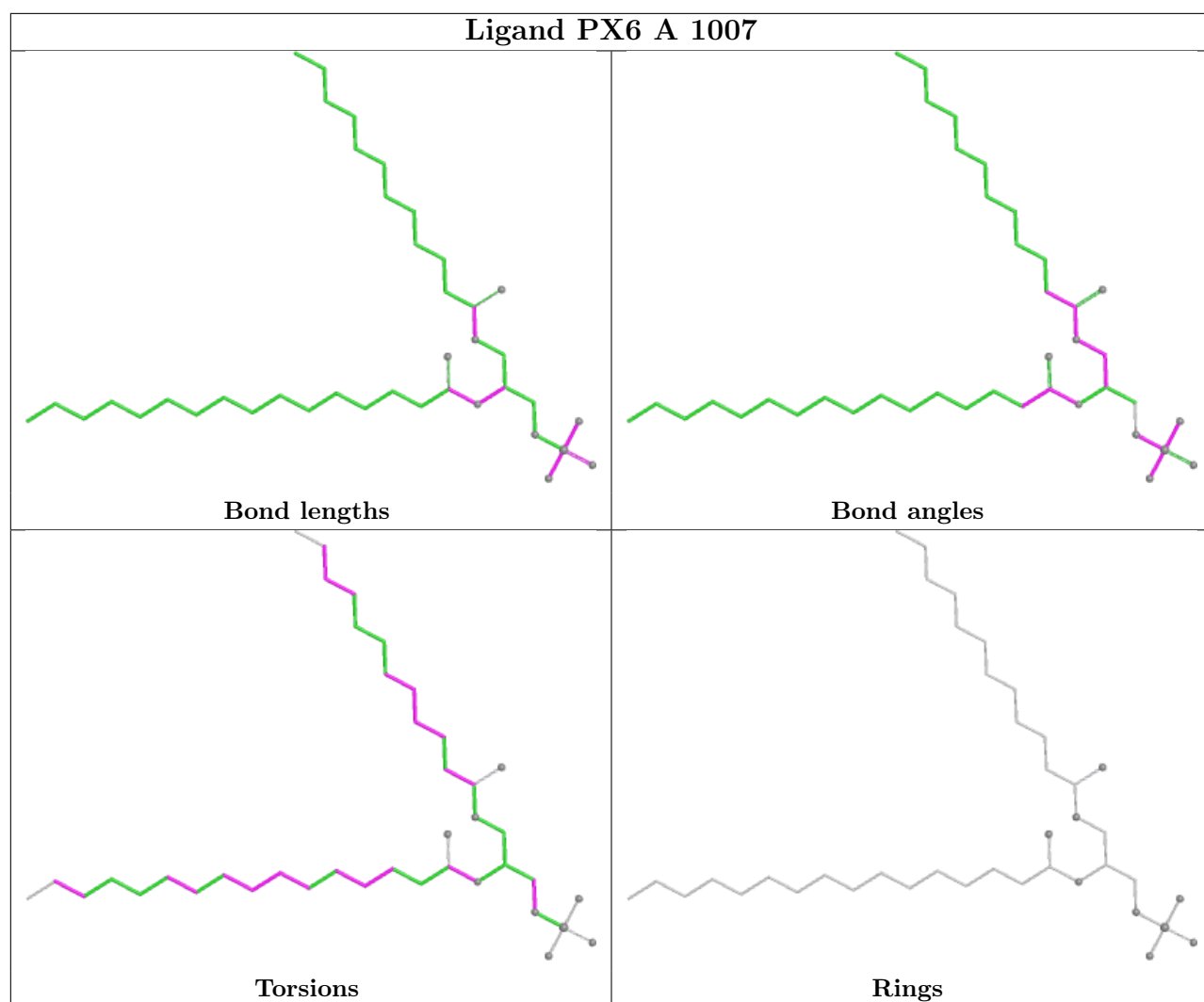


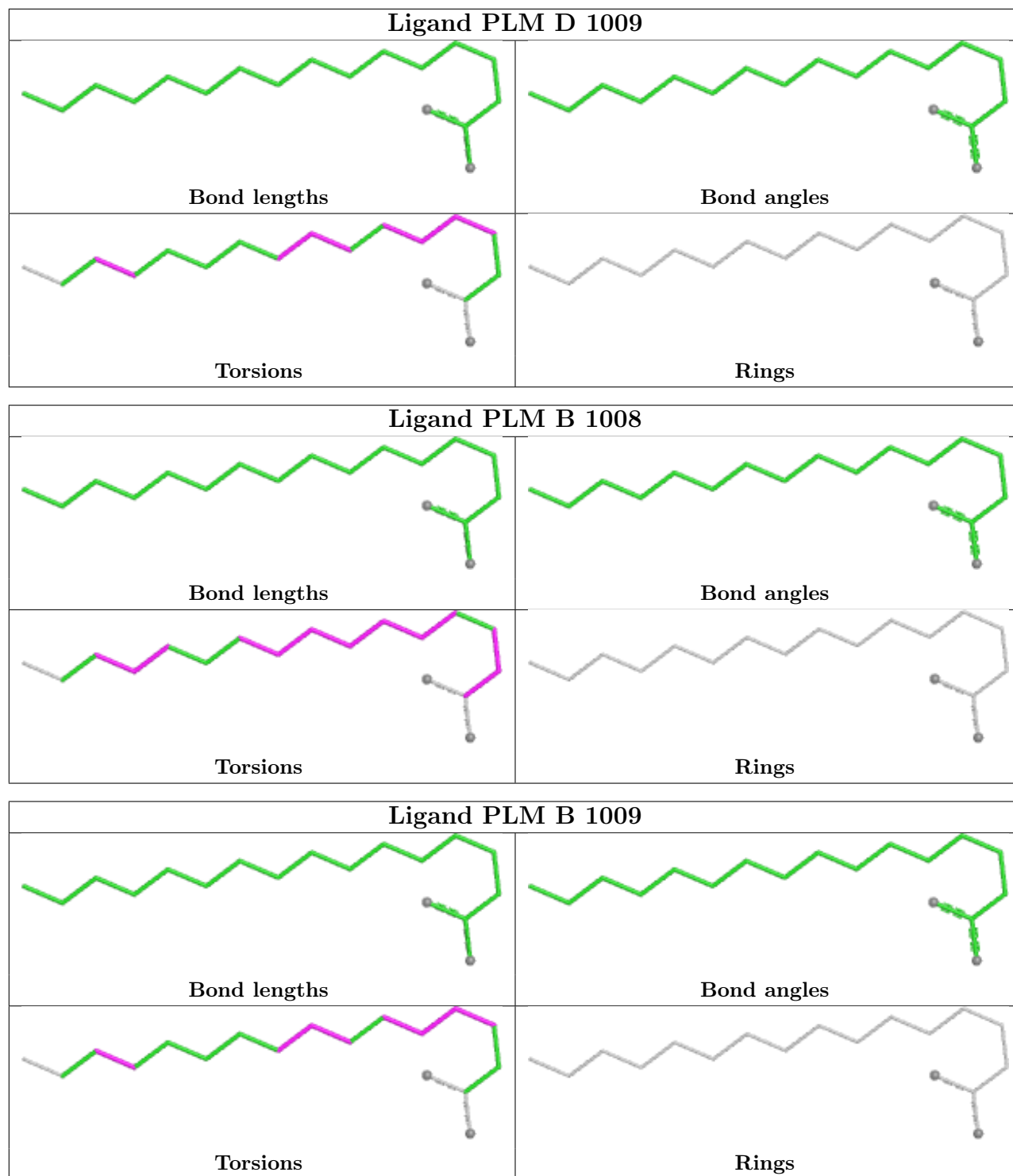


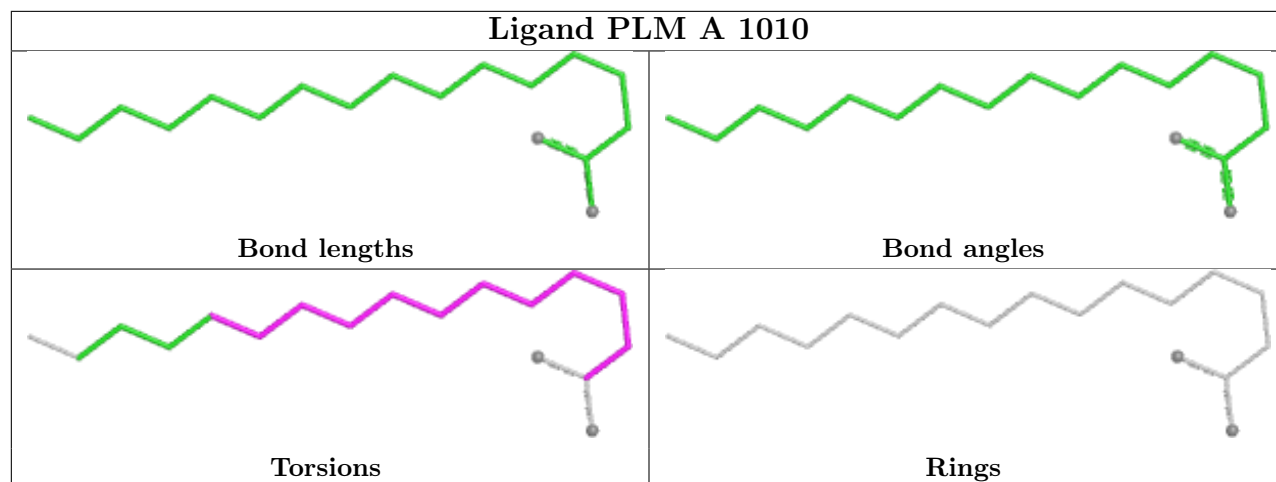












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

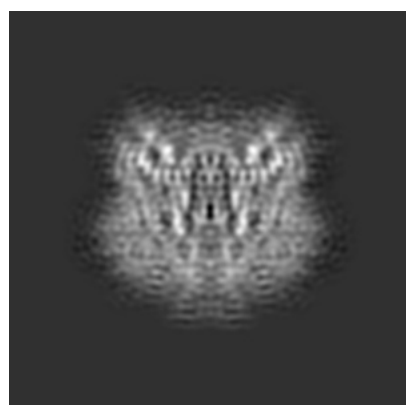
6 Map visualisation [i](#)

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.

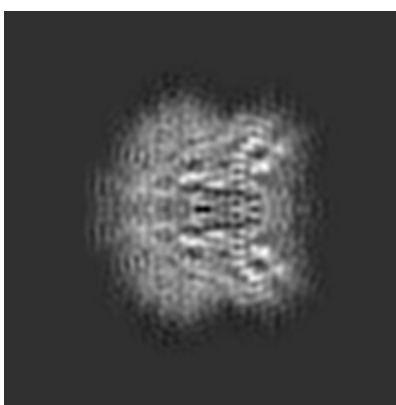
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

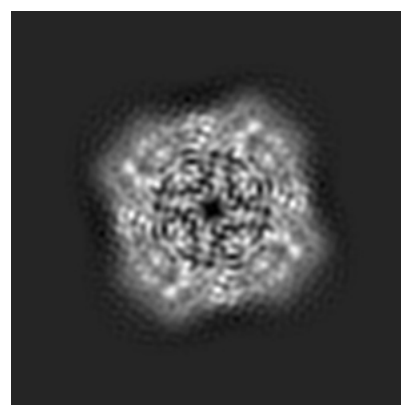
6.1.1 Primary map



X



Y

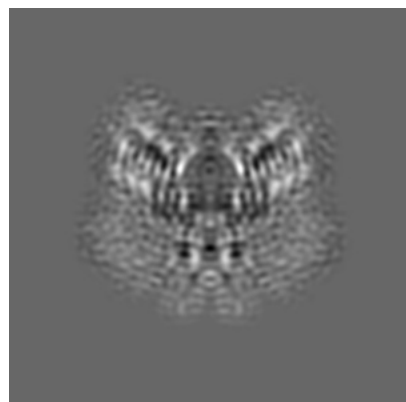


Z

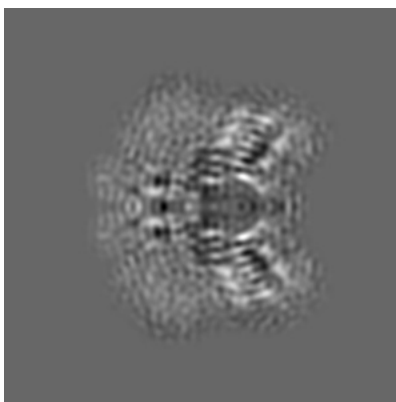
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

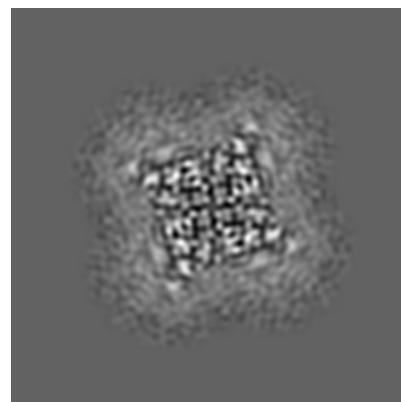
6.2.1 Primary map



X Index: 84



Y Index: 84

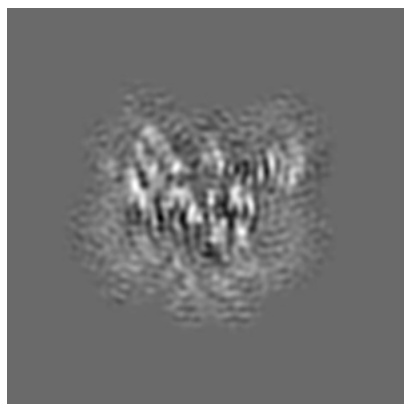


Z Index: 84

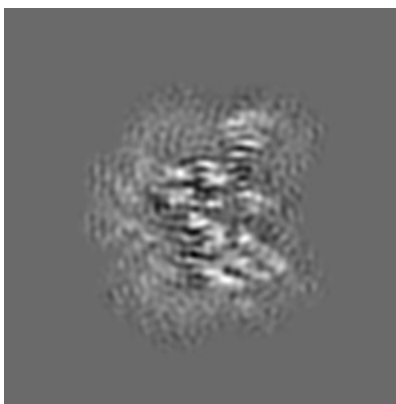
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

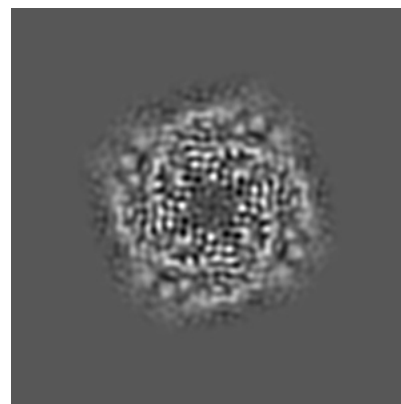
6.3.1 Primary map



X Index: 74



Y Index: 94

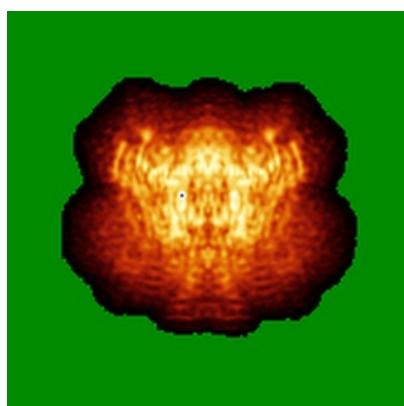


Z Index: 100

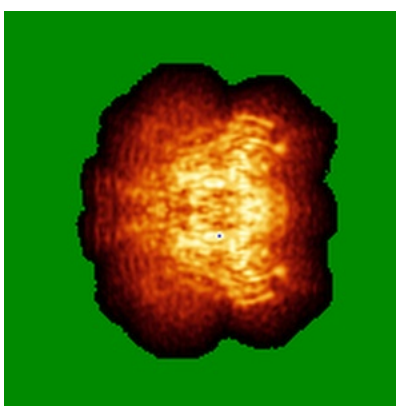
The images above show the largest variance slices of the map in three orthogonal directions.

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

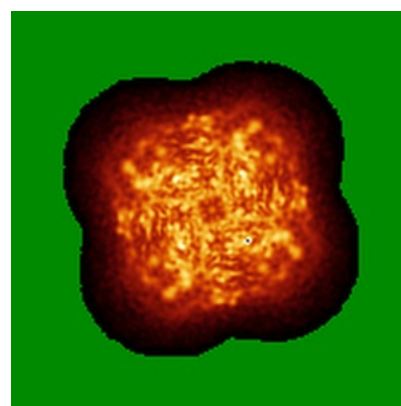
6.4.1 Primary map



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.

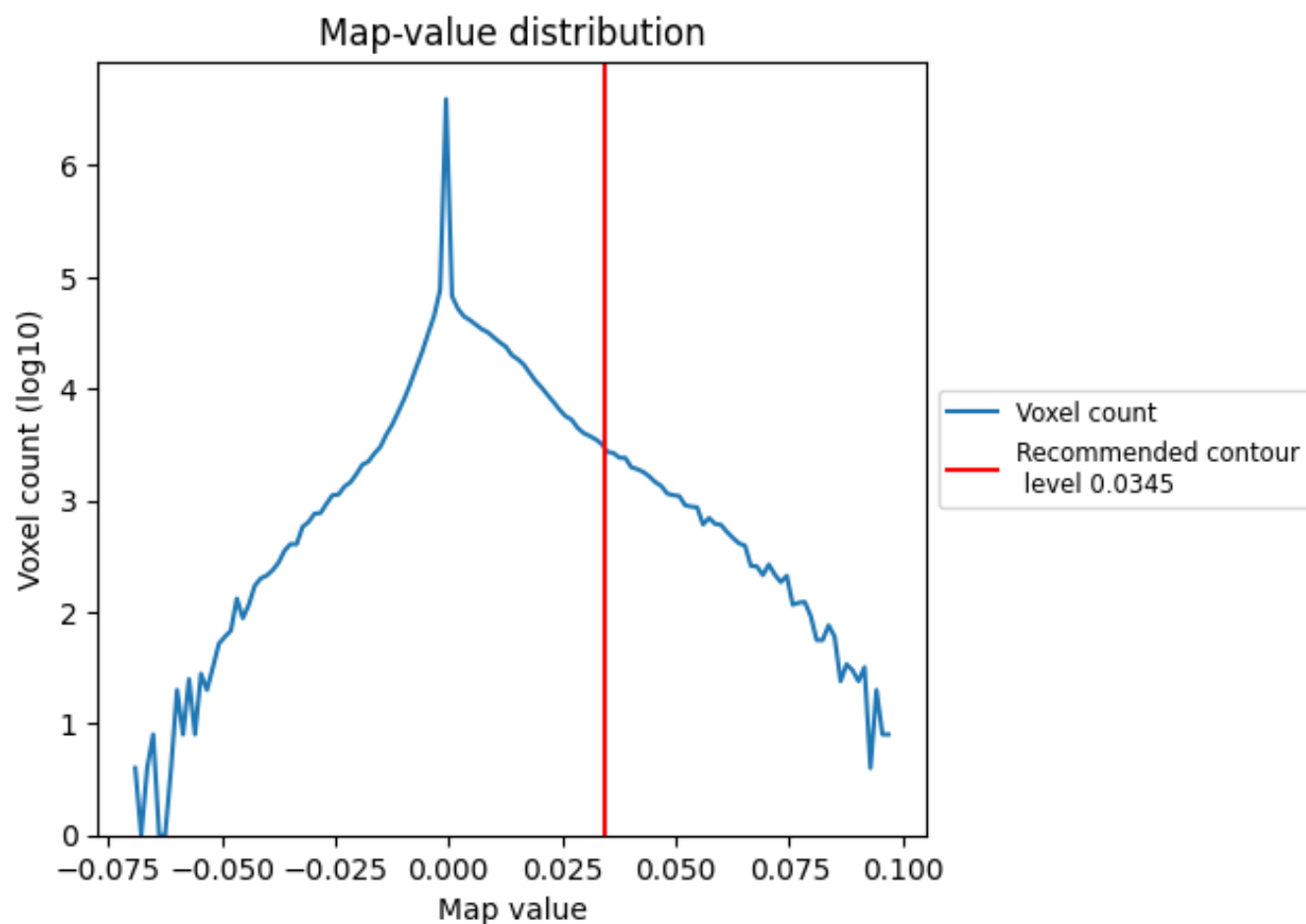
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

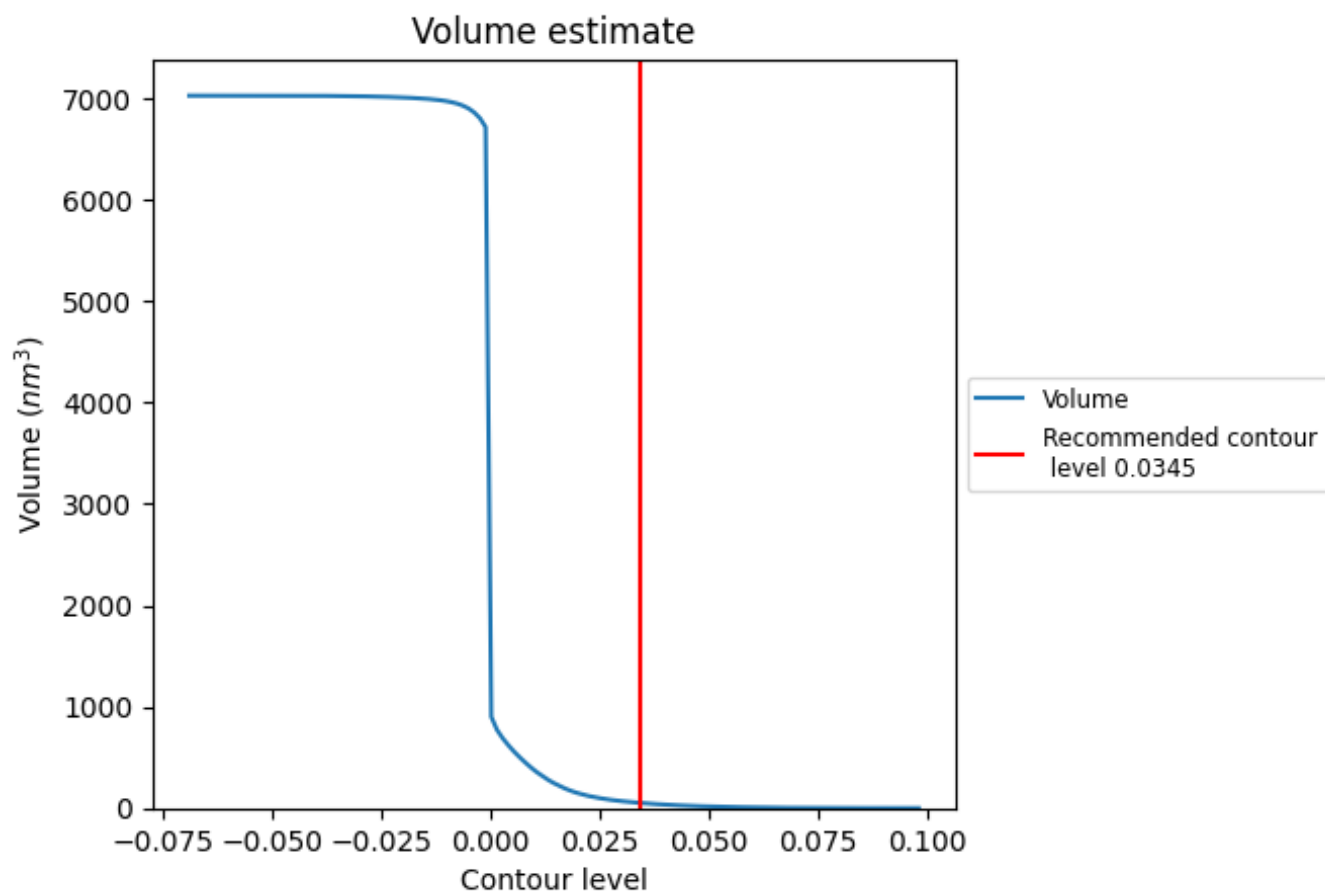
This section contains the results of statistical analysis of the map.

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.

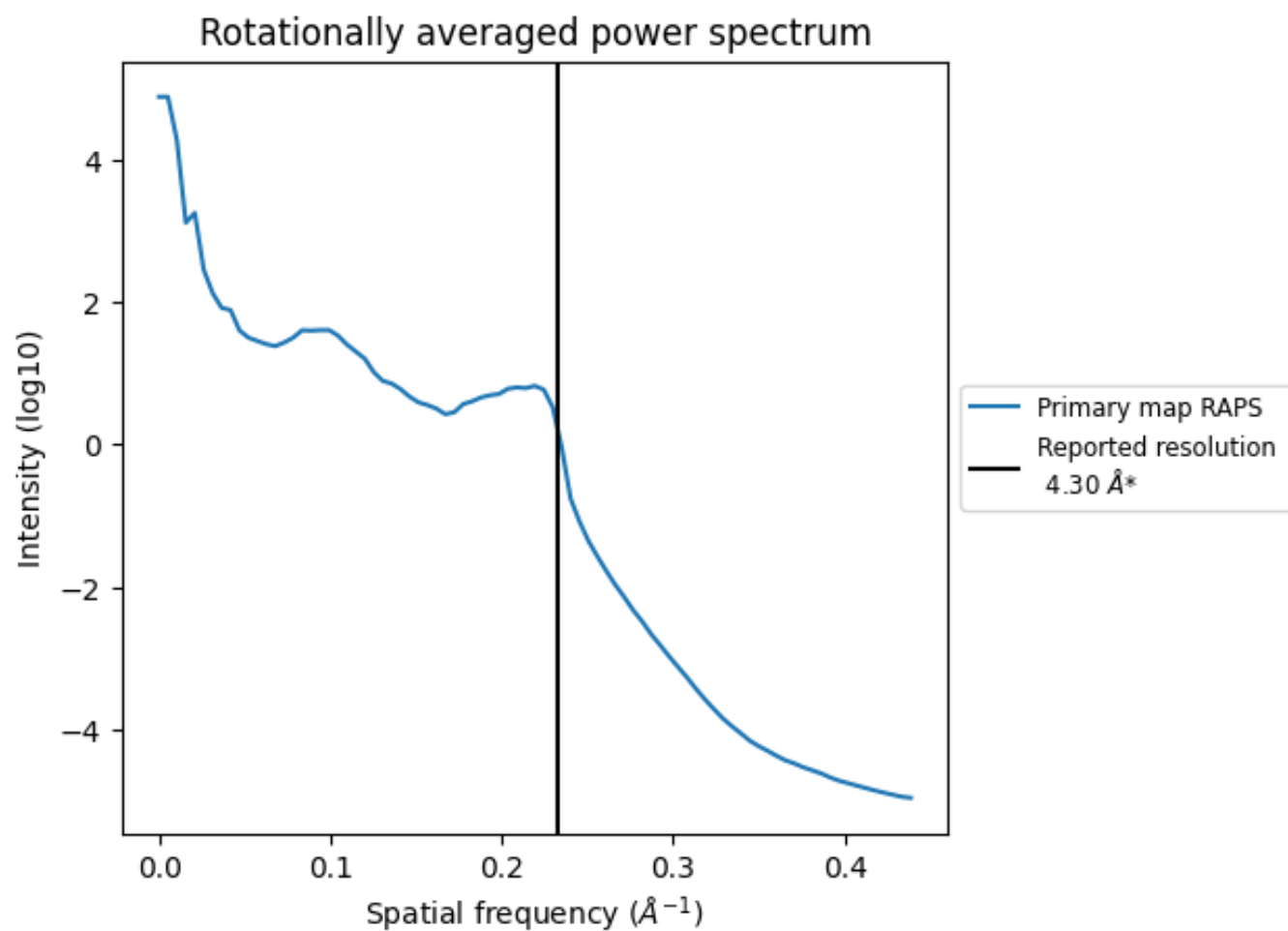
7.2 Volume estimate [i](#)



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

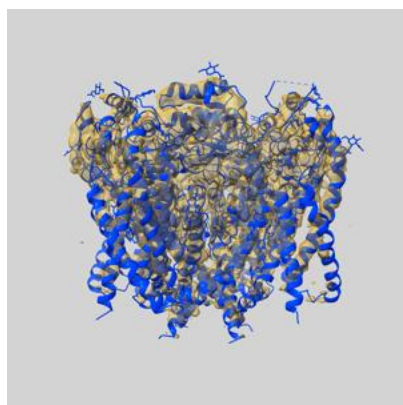
8 Fourier-Shell correlation

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

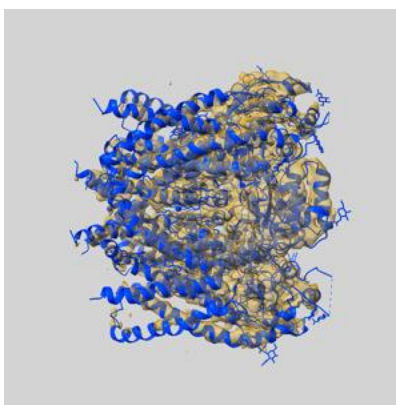
9 Map-model fit [i](#)

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](#).

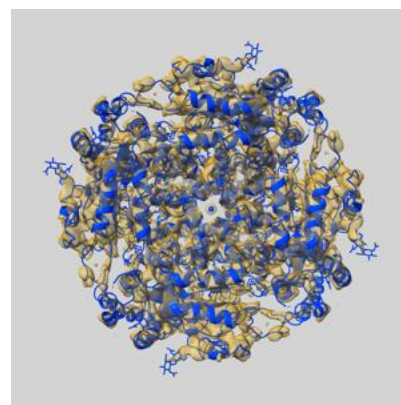
9.1 Map-model overlay [i](#)



X



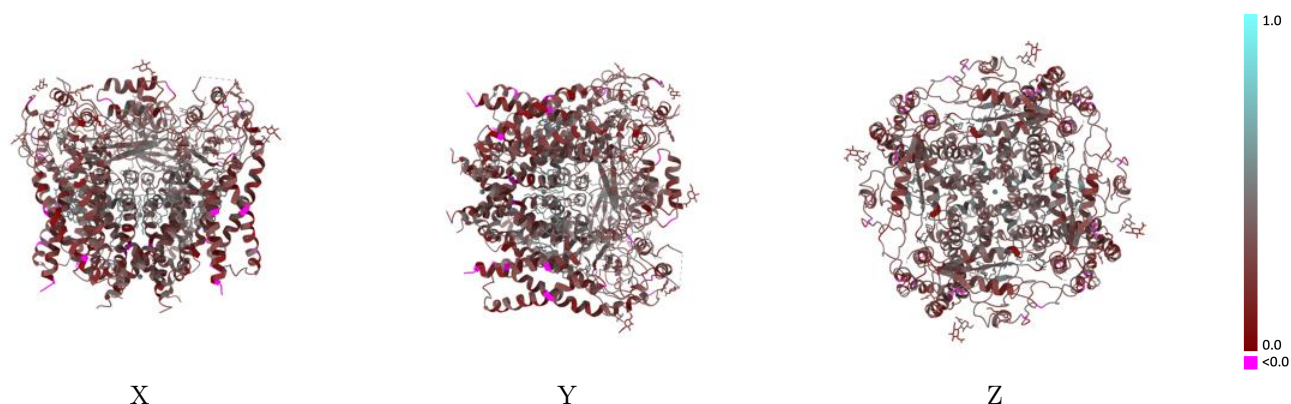
Y



Z

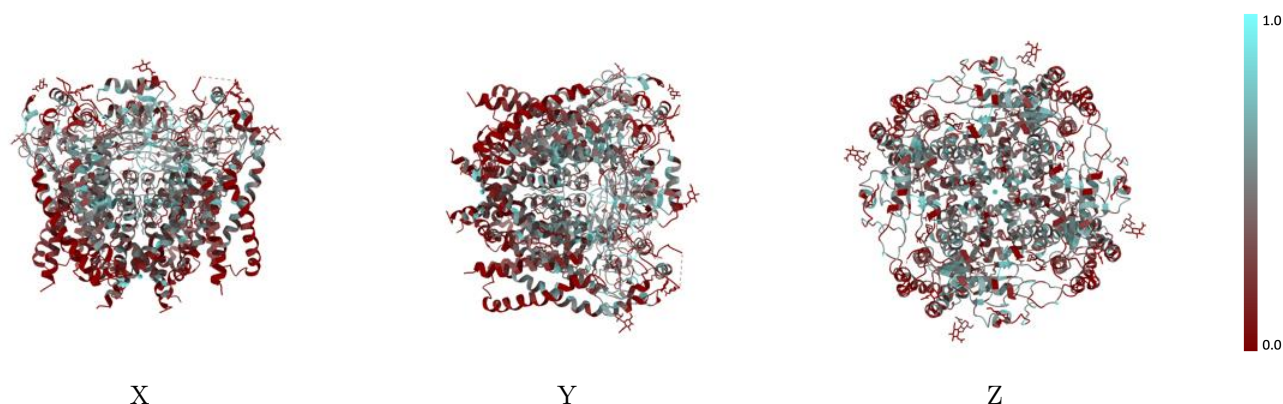
The images above show the 3D surface view of the map at the recommended contour level 0.0345 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



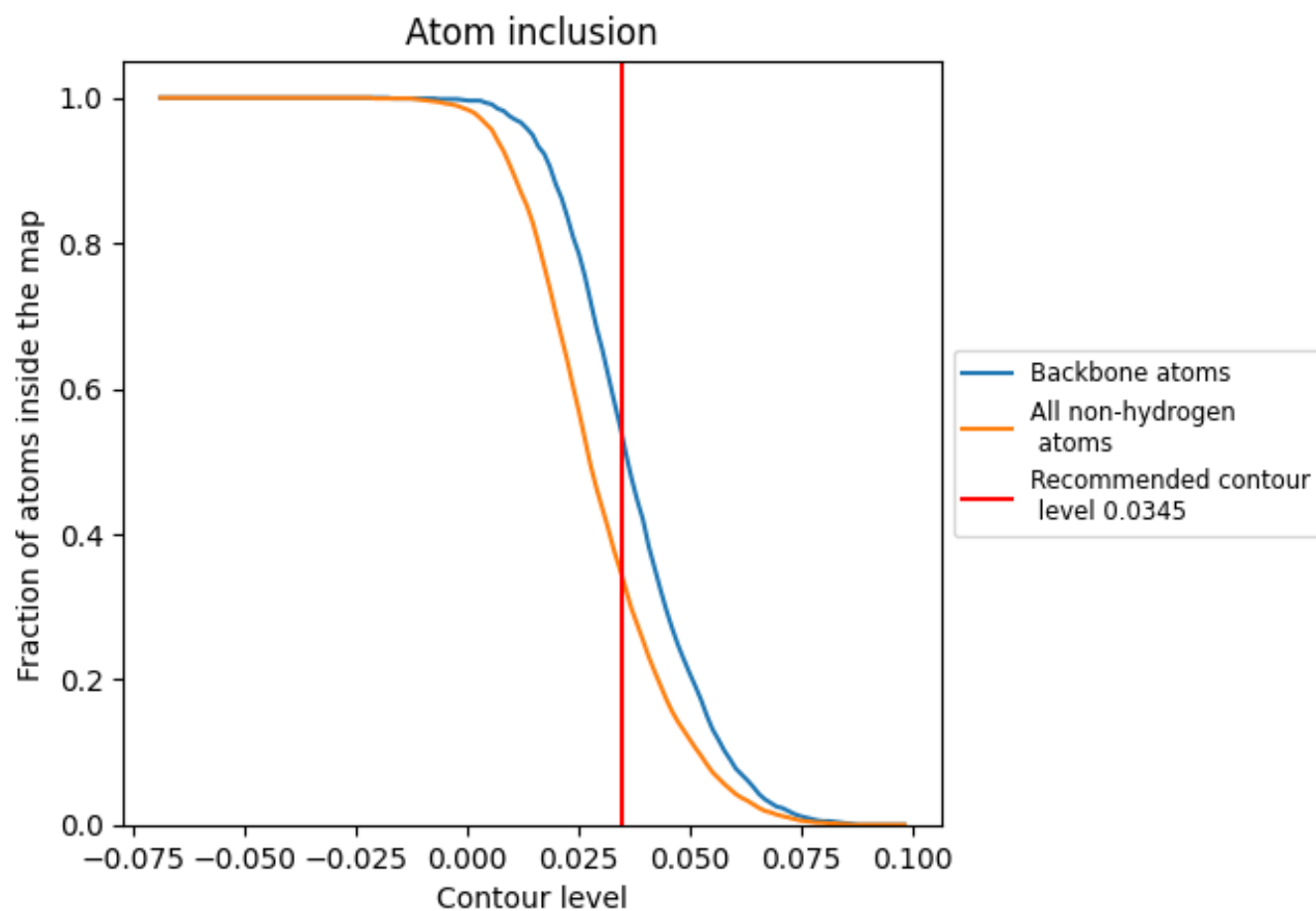
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.3460	0.3030
A	0.3460	0.3040
B	0.3480	0.3040
C	0.3460	0.3020
D	0.3470	0.3030
E	0.1070	0.2280
F	0.0710	0.2390
G	0.1070	0.2180

1.0

0.0

<0.0