



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 08:56 PM UTC

PDB ID : 5MKF / pdb_00005mkf
EMDB ID : EMD-3524
Title : cryoEM Structure of Polycystin-2 in complex with calcium and lipids
Authors : Wilkes, M.; Madej, M.G.; Ziegler, C.
Deposited on : 2016-12-04
Resolution : 4.20 Å (reported)

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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:

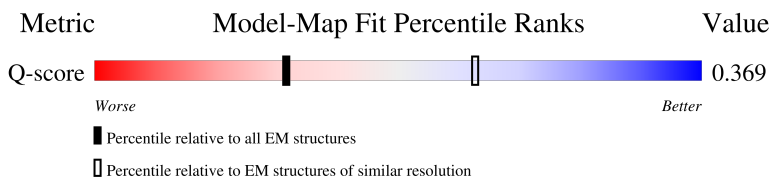
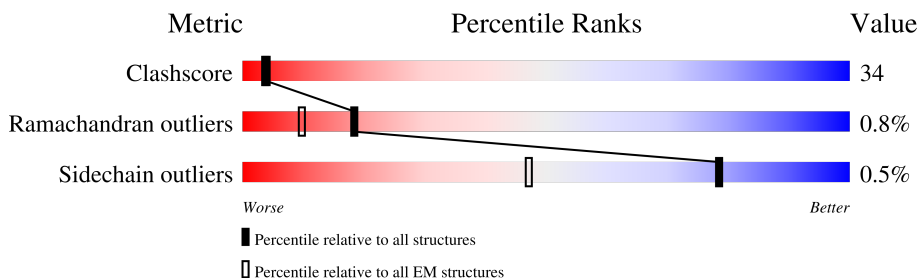
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.20 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	5410 (3.70 - 4.70)

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	<p>16% (red), 20% (orange), 29% (yellow), 50% (grey)</p>
1	B	968	<p>15% (red), 20% (orange), 29% (yellow), 50% (grey)</p>
1	C	968	<p>15% (red), 20% (orange), 29% (yellow), 50% (grey)</p>
1	D	968	<p>16% (red), 19% (orange), 30% (yellow), 50% (grey)</p>

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

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 16620 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
			Total	C	N	O	S		
1	A	481	Total 3962	C 2612	N 629	O 702	S 19	0	0
1	B	481	Total 3959	C 2610	N 629	O 702	S 18	0	0
1	C	481	Total 3959	C 2610	N 629	O 702	S 18	0	0
1	D	481	Total 3959	C 2610	N 629	O 702	S 18	0	0

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



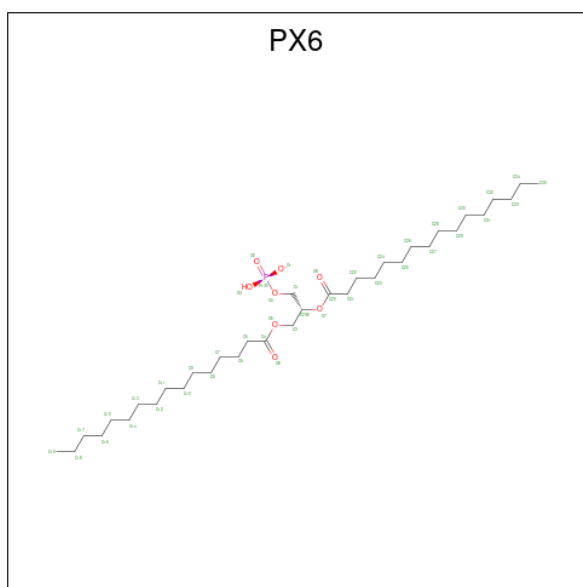
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	E	2	Total 28	C 16	N 2	O 10	0	0
2	F	2	Total 28	C 16	N 2	O 10	0	0
2	G	2	Total 28	C 16	N 2	O 10	0	0
2	H	2	Total 28	C 16	N 2	O 10	0	0

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



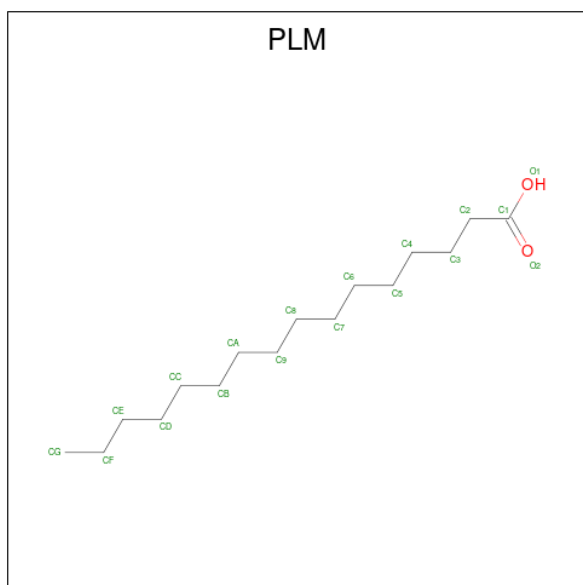
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	A	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	B	1	Total 14	8	1	5	0
3	C	1	Total 14	8	1	5	0
3	C	1	Total 14	8	1	5	0
3	C	1	Total 14	8	1	5	0
3	D	1	Total 14	8	1	5	0
3	D	1	Total 14	8	1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

- Molecule 4 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX6) (formula: C₃₅H₆₈O₈P).



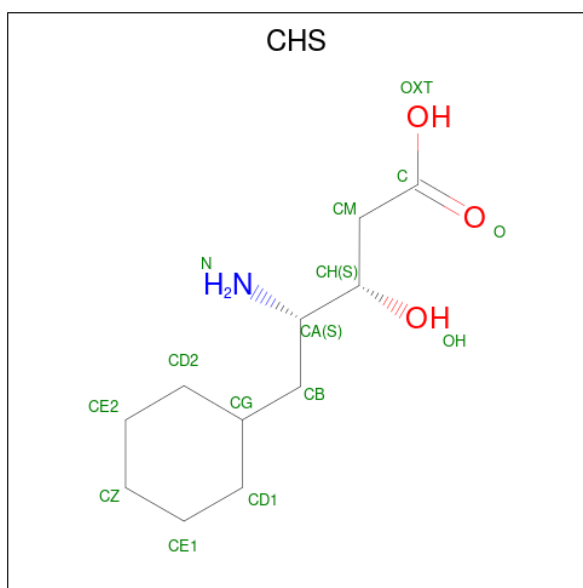
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	A	1	Total 40	C 31	O 8	P 1	0
4	B	1	Total 40	C 31	O 8	P 1	0
4	C	1	Total 40	C 31	O 8	P 1	0
4	D	1	Total 40	C 31	O 8	P 1	0

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



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

- Molecule 6 is 4-AMINO-5-CYCLOHEXYL-3-HYDROXY-PENTANOIC ACID (CCD ID: CHS) (formula: $C_{11}H_{21}NO_3$).



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

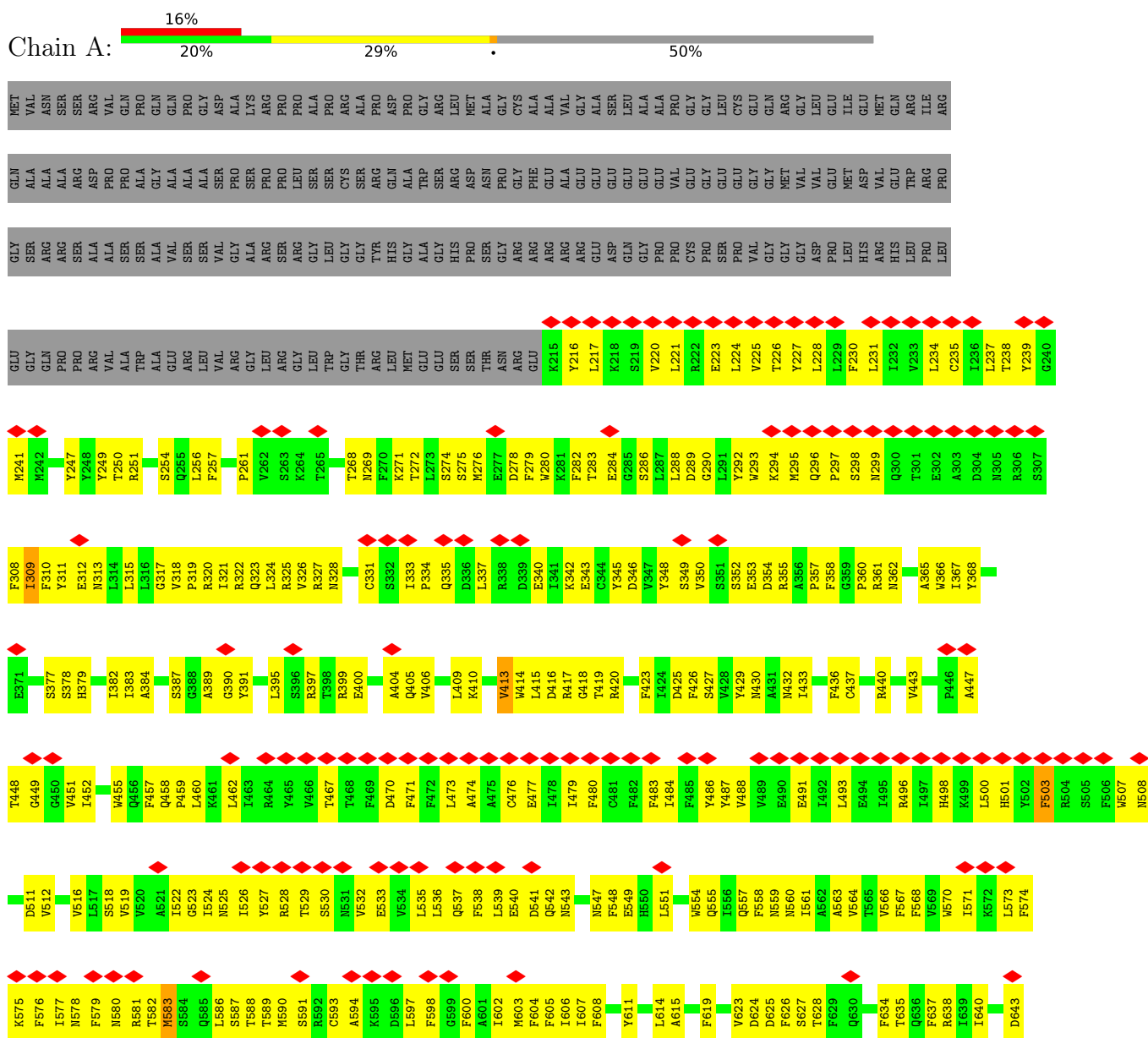
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total	Ca	0
			4	4	
7	B	1	Total	Ca	0
			1	1	

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

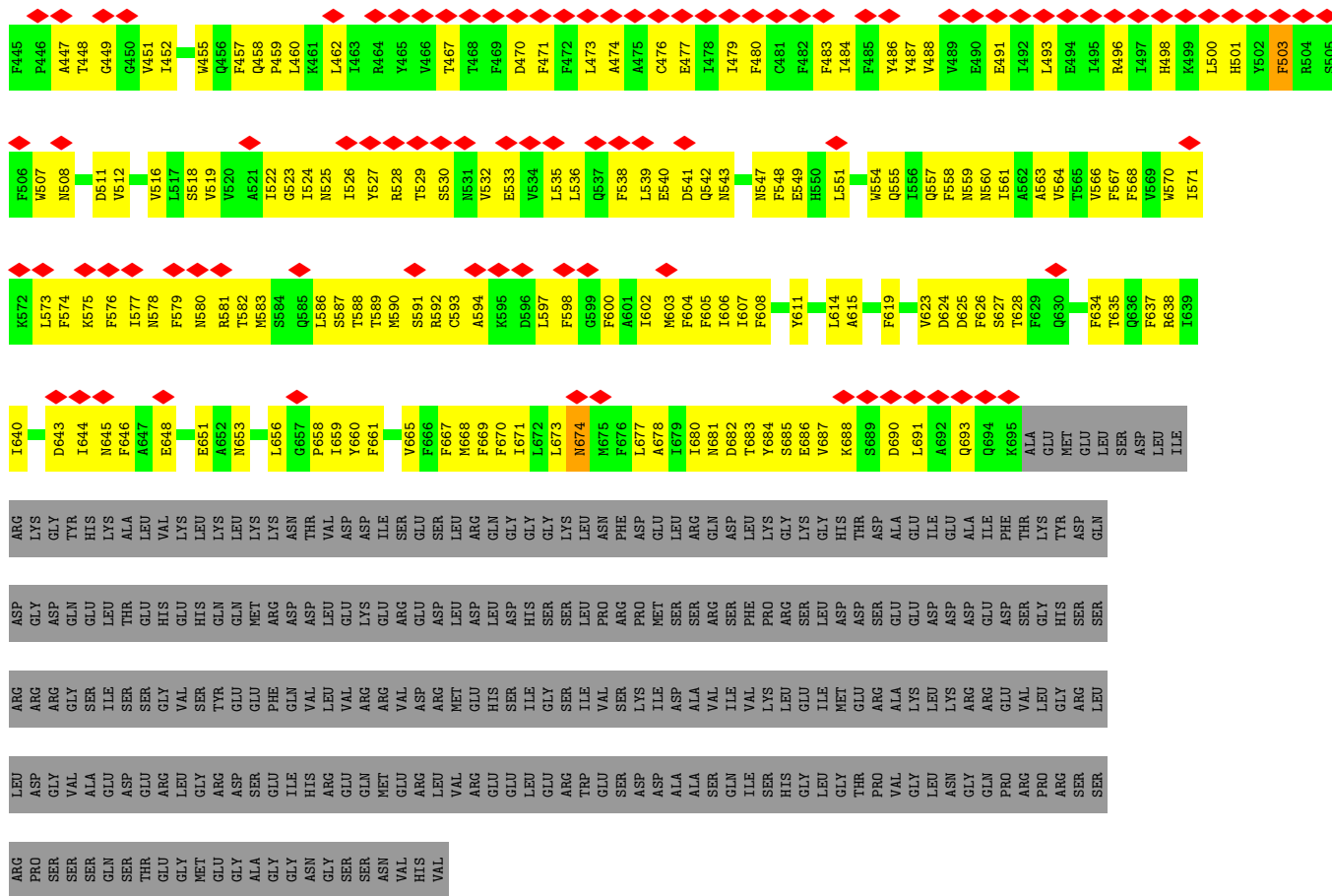


M508	F574	I644	VAL	SER	GLY	GLN	TYR
D511	K575	N645	ALA	SER	SER	GLU	HIS
V512	F576	F646	ASP	GLN	GLN	LEU	LYS
I577	I577	A647	THR	THR	THR	THR	ALA
V516	N578	E648	ARG	GLU	GLU	GLU	VAL
L517	F579	E651	GLY	VAL	VAL	VAL	LYS
S518	N580	A652	LEU	SER	SER	SER	LEU
V519	R581	N653	ARG	ARG	ARG	ARG	LEU
V520	R582	L656	GLY	GLY	GLY	GLY	LEU
A521	T582	G657	ALA	ALA	ALA	ALA	LEU
I522	S583	G658	GLY	GLY	GLY	GLY	LEU
G523	M584	P658	ASN	ASN	ASN	ASN	LEU
G524	Q585	I659	THR	THR	THR	THR	LEU
N525	L586	I660	GLY	GLY	GLY	GLY	LEU
I526	S587	Y660	VAL	VAL	VAL	VAL	LEU
I527	T588	F661	ARG	ARG	ARG	ARG	LEU
Y527	T589	F665	MET	MET	MET	MET	LEU
R528	M590	V665	GLY	VAL	VAL	VAL	LEU
T529	S591	F667	ARG	ARG	ARG	ARG	LEU
S530	R592	F668	PRO	PRO	PRO	PRO	LEU
N531	C593	M668	VAL	VAL	VAL	VAL	LEU
V532	A594	F669	ARG	ARG	ARG	ARG	LEU
E533	K595	F670	GLY	HIS	HIS	HIS	LEU
V534	D596	I671	GLU	GLU	GLU	GLU	LEU
L535	L597	L672	LEU	LEU	LEU	LEU	LEU
L536	F598	M674	GLU	GLU	GLU	GLU	LEU
Q537	G599	M675	TRP	TRP	TRP	TRP	LEU
F538	F600	F676	SER	SER	SER	SER	LEU
L539	I602	A678	ASP	ASP	ASP	ASP	LEU
E540	I603	L677	PRO	PRO	PRO	PRO	LEU
D541	M603	I679	ALA	ALA	ALA	ALA	LEU
Q542	F604	N681	VAL	VAL	VAL	VAL	LEU
N543	F605	D682	GLN	GLN	GLN	GLN	LEU
N547	I606	T683	ILE	ILE	ILE	ILE	LEU
E549	I607	Y684	SER	SER	SER	SER	LEU
H550	I608	S685	PRO	PRO	PRO	PRO	LEU
L551	Y611	E686	HIS	HIS	HIS	HIS	LEU
V554	L614	V687	THR	THR	THR	THR	LEU
Q555	A615	K688	PRO	PRO	PRO	PRO	LEU
Q557	F619	S689	ASP	ASP	ASP	ASP	LEU
F558	V623	D690	VAL	VAL	VAL	VAL	LEU
N559	D624	L691	GLY	GLY	GLY	GLY	LEU
N560	D625	A692	LEU	LEU	LEU	LEU	LEU
N561	D626	Q693	ASP	ASP	ASP	ASP	LEU
I561	S627	Q694	GLY	GLY	GLY	GLY	LEU
A562	T628	K695	GLN	GLN	GLN	GLN	LEU
A563	T628	ALA	PRO	PRO	PRO	PRO	LEU
V564	F629	GLU	ARG	ARG	ARG	ARG	LEU
T565	A563	MET	PRO	PRO	PRO	PRO	LEU
V566	V564	GLU	THR	THR	THR	THR	LEU
F567	T565	LEU	GLY	GLY	GLY	GLY	LEU
F568	T566	SER	TYR	TYR	TYR	TYR	LEU
V569	F567	ASP	ASP	ASP	ASP	ASP	LEU
I570	F568	LEU	GLN	GLN	GLN	GLN	LEU
I571	V569	ILE	SER	SER	SER	SER	LEU
K572	I570	ARG	ARG	ARG	ARG	ARG	LEU
L573	I571	LYS	ILE	ILE	ILE	ILE	LEU
	D643	GLY	GLY	GLY	GLY	GLY	LEU

● Molecule 1: Polycystin-2



M241	F308	E371	GLY	GLY	GLU	GLN	MET
M242	I309	L374	SER	GLY	VAL	ALA	VAL
Y247	F310	S377	ARG	GLN	ASN	ALA	ALA
Y248	Y311	H378	ARG	PRO	ARG	ALA	ASP
Y249	E312	S379	ALA	SER	ARG	ASP	ARG
T250	N313	H379	ALA	VAL	ASP	VAL	VAL
R251	L314	S379	ALA	ALA	PRO	GLN	VAL
S254	L315	T382	SER	TRP	PRO	PRO	GLY
Q255	G317	I383	VAL	ALA	ALA	GLN	ARG
L256	V318	A384	VAL	ALA	ASP	GLY	LEU
F257	F319	S387	SER	ARG	GLY	ILE	VAL
P261	R320	G388	VAL	THR	ASP	VAL	VAL
V262	R322	A389	ARG	GLY	ALA	ARG	ARG
S263	Q323	G390	ALA	GLY	GLY	LYS	LEU
K264	L324	Y391	PRO	LEU	PRO	ARG	PRO
T265	R325	L395	LEU	GLY	PRO	PRO	PRO
T268	V326	S396	ALA	LEU	ALA	ALA	ALA
M269	R327	R397	SER	LEU	PRO	PRO	PRO
F270	N328	T398	LEU	TRP	PRO	ARG	ARG
K271	C331	R398	GLY	GLY	ARG	CYS	VAL
L272	M269	R399	TYR	GLY	SER	SER	ARG
L273	F270	E400	ARG	THR	ARG	GLY	ALA
S274	K271	A404	GLN	LEU	ARG	GLY	GLY
S275	T272	Q405	ALA	ALA	ASP	ASP	ASP
M276	G273	V406	PRO	TRP	PRO	PRO	PRO
E277	L273	L409	ASN	GLY	ASN	ASN	ALA
D278	R274	K410	PRO	GLY	PRO	PRO	GLY
F279	F279	E413	GLY	CYS	GLY	CYS	GLY
W280	M280	V414	ARG	ALA	ALA	ALA	ALA
K281	T341	L415	ALA	VAL	VAL	VAL	VAL
F282	K342	D416	VAL	GLY	GLY	GLY	GLY
T283	E343	R417	GLY	GLY	GLY	GLY	GLY
C344	C344	G418	ASP	ALA	ALA	ALA	ALA
E284	Y345	T419	SER	SER	SER	SER	SER
G285	D346	R420	LEU	LEU	LEU	LEU	LEU
S286	V347	F423	GLY	GLY	GLY	GLY	GLY
L287	V347	I424	PRO	PRO	PRO	PRO	PRO
L221	V220	D425	PRO	PRO	PRO	PRO	PRO
R222	L221	F426	CYS	CYS	CYS	CYS	CYS
E223	R222	S427	PRO	PRO	PRO	PRO	PRO
L224	E223	V428	SER	SER	SER	SER	SER
V225	L224	N430	VAL	VAL	VAL	VAL	VAL
T226	V225	A431	GLY	GLY	GLY	GLY	GLY
Y227	T226	N432	GLY	GLY	GLY	GLY	GLY
L228	M295	I433	ASP	ASP	ASP	ASP	ASP
L229	Q296	F436	VAL	VAL	VAL	VAL	VAL
F230	P297	C437	GLU	GLU	GLU	GLU	GLU
L231	S298	R440	LEU	LEU	LEU	LEU	LEU
L232	N299	V443	HIS	HIS	HIS	HIS	HIS
V233	Q300	E444	ASP	ASP	ASP	ASP	ASP
L234	T301		VAL	VAL	VAL	VAL	VAL
C235	E302		GLY	GLY	GLY	GLY	GLY
L236	A303		LEU	LEU	LEU	LEU	LEU
L237	D304		LEU	LEU	LEU	LEU	LEU
T238	N305		TRP	TRP	TRP	TRP	TRP
Y239	R306		PRO	PRO	PRO	PRO	PRO
G240	S307		LEU	LEU	LEU	LEU	LEU



- 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





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

Chain H:
100%
100%

A horizontal bar representing validation metrics for Chain H. The bar is divided into two segments: a red segment on the left and a yellow segment on the right. The red segment is labeled '100%' above it, and the yellow segment is labeled '100%' below it.



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	35318	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	0.135	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0354	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: PLM, NAG, CHS, CA, 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	0.44	0/4068	0.61	0/5521
1	B	0.44	0/4065	0.60	0/5518
1	C	0.44	0/4065	0.60	0/5518
1	D	0.44	0/4065	0.60	0/5518
All	All	0.44	0/16263	0.61	0/22075

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	PHE	Peptide
1	B	579	PHE	Peptide
1	C	579	PHE	Peptide
1	D	579	PHE	Peptide

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	3962	0	3898	291	0
1	B	3959	0	3891	288	0
1	C	3959	0	3891	283	0
1	D	3959	0	3891	286	0
2	E	28	0	25	0	0
2	F	28	0	25	3	0
2	G	28	0	25	3	0
2	H	28	0	25	1	0
3	A	42	0	39	15	0
3	B	42	0	39	15	0
3	C	42	0	39	15	0
3	D	42	0	39	15	0
4	A	40	0	56	2	0
4	B	40	0	56	4	0
4	C	40	0	56	5	0
4	D	40	0	56	4	0
5	A	54	0	93	5	0
5	B	54	0	93	5	0
5	C	54	0	93	4	0
5	D	54	0	93	4	0
6	A	30	0	40	2	0
6	B	30	0	40	2	0
6	C	30	0	40	1	0
6	D	30	0	40	1	0
7	A	4	0	0	0	0
7	B	1	0	0	0	0
All	All	16620	0	16583	1113	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 34.

The worst 5 of 1113 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:D:299:ASN:HD22	3:D:1005:NAG:C1	1.10	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ASN:HD22	3:C:1005:NAG:C1	1.17	1.58
1:C:375:ASN:ND2	2:G:1:NAG:C1	1.68	1.56
1:B:299:ASN:HD22	3:B:1005:NAG:C1	1.17	1.55
1:B:375:ASN:ND2	2:F:1:NAG:C1	1.68	1.55

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	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	16	52
1	B	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	16	52
1	C	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	16	52
1	D	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	16	52
All	All	1916/3872 (50%)	1676 (88%)	224 (12%)	16 (1%)	18	52

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	THR
1	B	628	THR
1	C	628	THR
1	D	628	THR
1	A	674	ASN

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	432/837 (52%)	429 (99%)	3 (1%)	76	78
1	B	431/837 (52%)	429 (100%)	2 (0%)	81	81
1	C	431/837 (52%)	429 (100%)	2 (0%)	81	81
1	D	431/837 (52%)	429 (100%)	2 (0%)	81	81
All	All	1725/3348 (52%)	1716 (100%)	9 (0%)	78	81

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	503	PHE
1	D	623	VAL
1	B	503	PHE
1	B	623	VAL
1	C	503	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	379	HIS
1	C	430	ASN
1	D	630	GLN
1	D	379	HIS
1	D	430	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 [i](#)

8 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	14,14,15	0.33	0	17,19,21	0.61	0
2	NAG	E	2	2	14,14,15	1.00	1 (7%)	17,19,21	0.64	0
2	NAG	F	1	2	14,14,15	0.34	0	17,19,21	0.60	0
2	NAG	F	2	2	14,14,15	1.01	1 (7%)	17,19,21	0.65	0
2	NAG	G	1	2	14,14,15	0.34	0	17,19,21	0.61	0
2	NAG	G	2	2	14,14,15	1.00	1 (7%)	17,19,21	0.64	0
2	NAG	H	1	2	14,14,15	0.34	0	17,19,21	0.60	0
2	NAG	H	2	2	14,14,15	1.01	1 (7%)	17,19,21	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	NAG	C1-C2	3.36	1.56	1.52
2	H	2	NAG	C1-C2	3.32	1.56	1.52
2	E	2	NAG	C1-C2	3.31	1.56	1.52
2	G	2	NAG	C1-C2	3.28	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

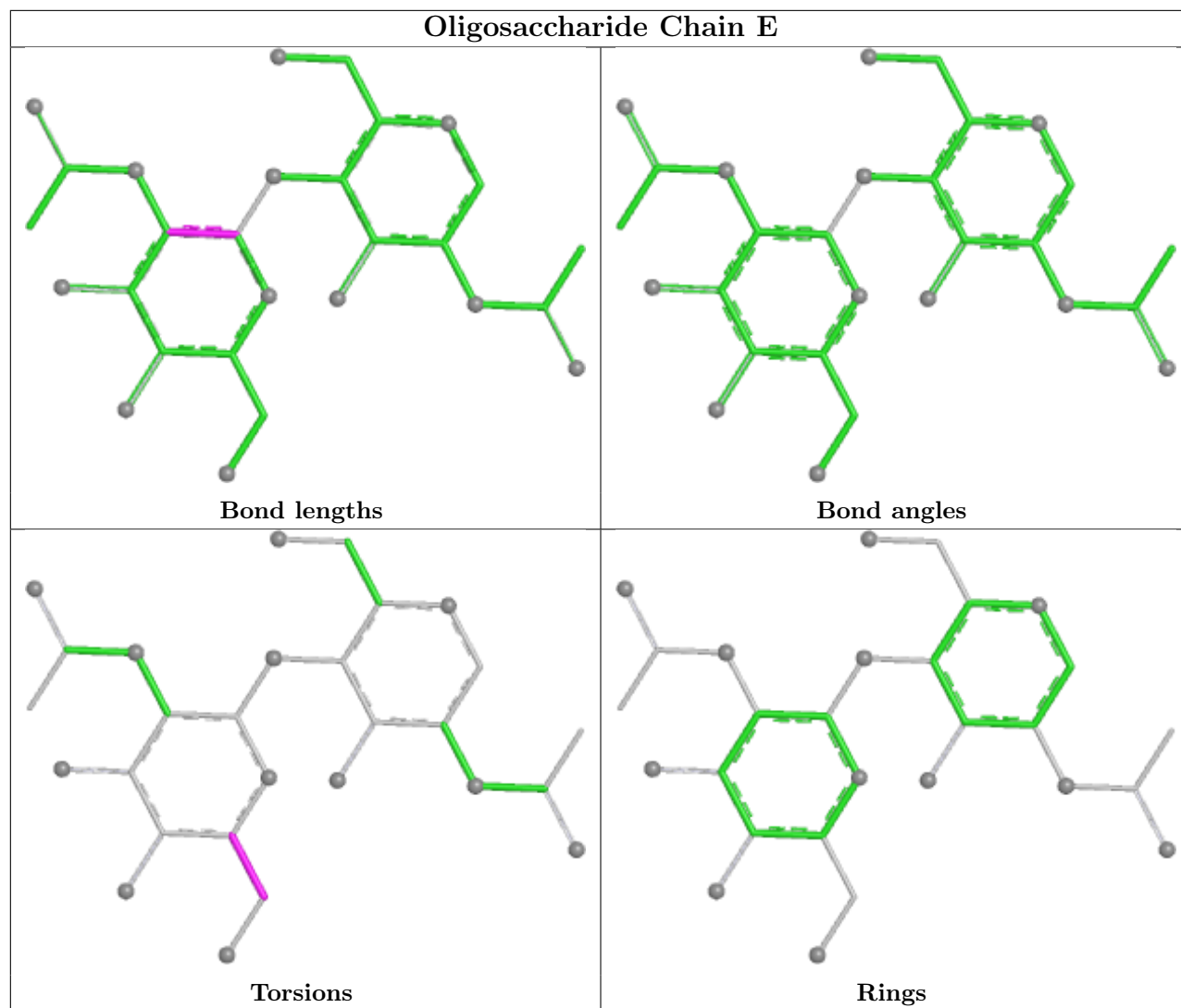
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

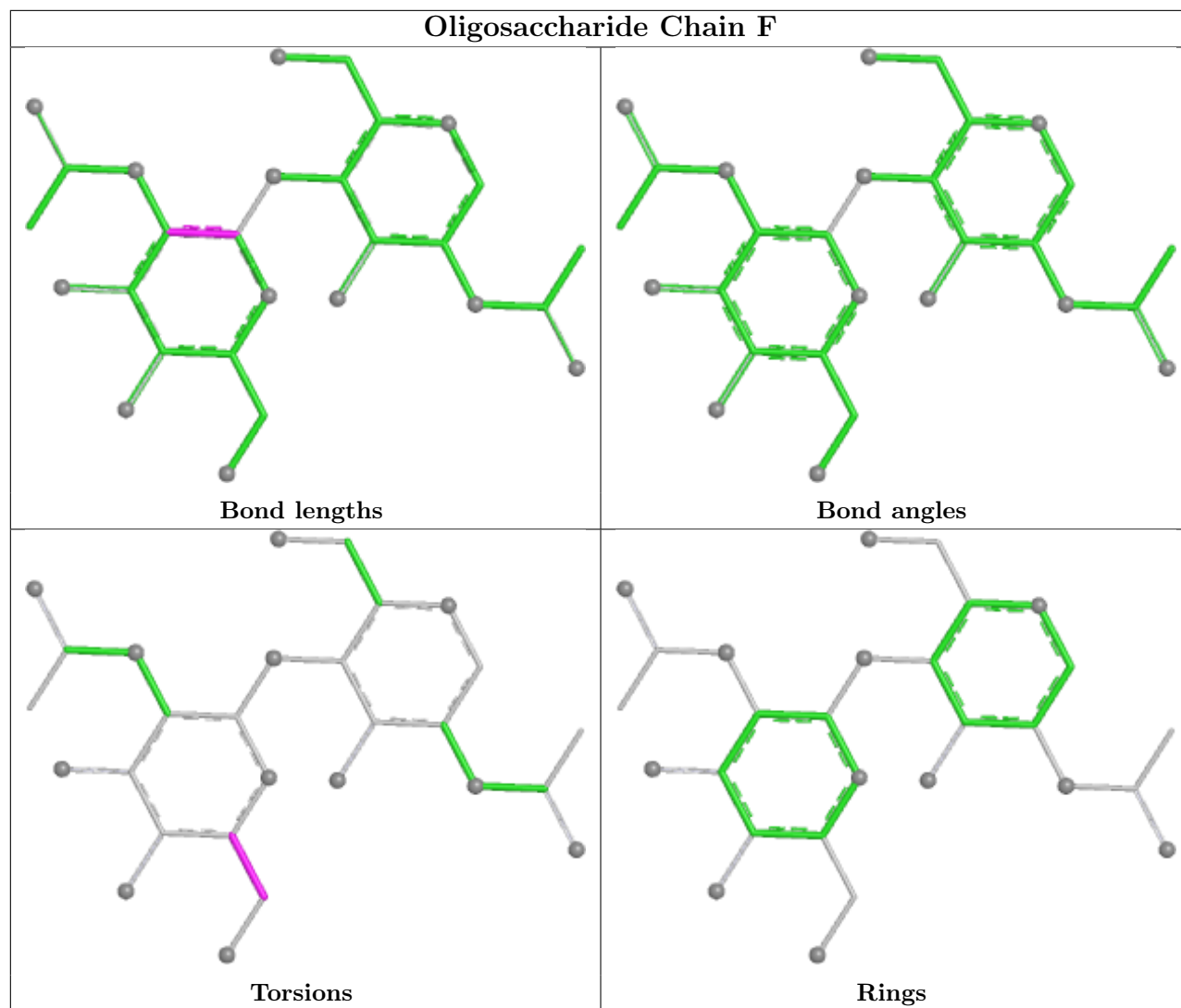
There are no ring outliers.

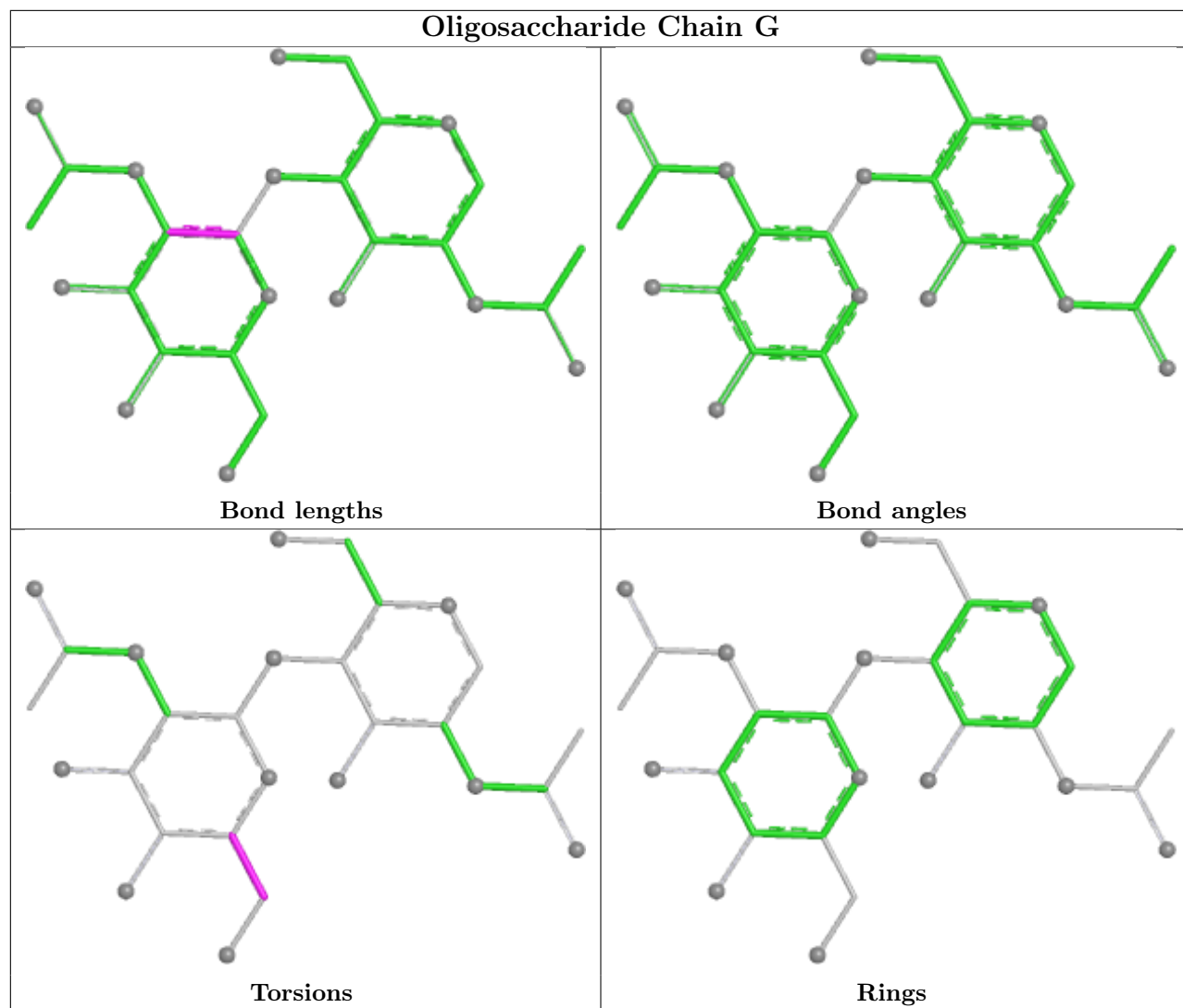
3 monomers are involved in 7 short contacts:

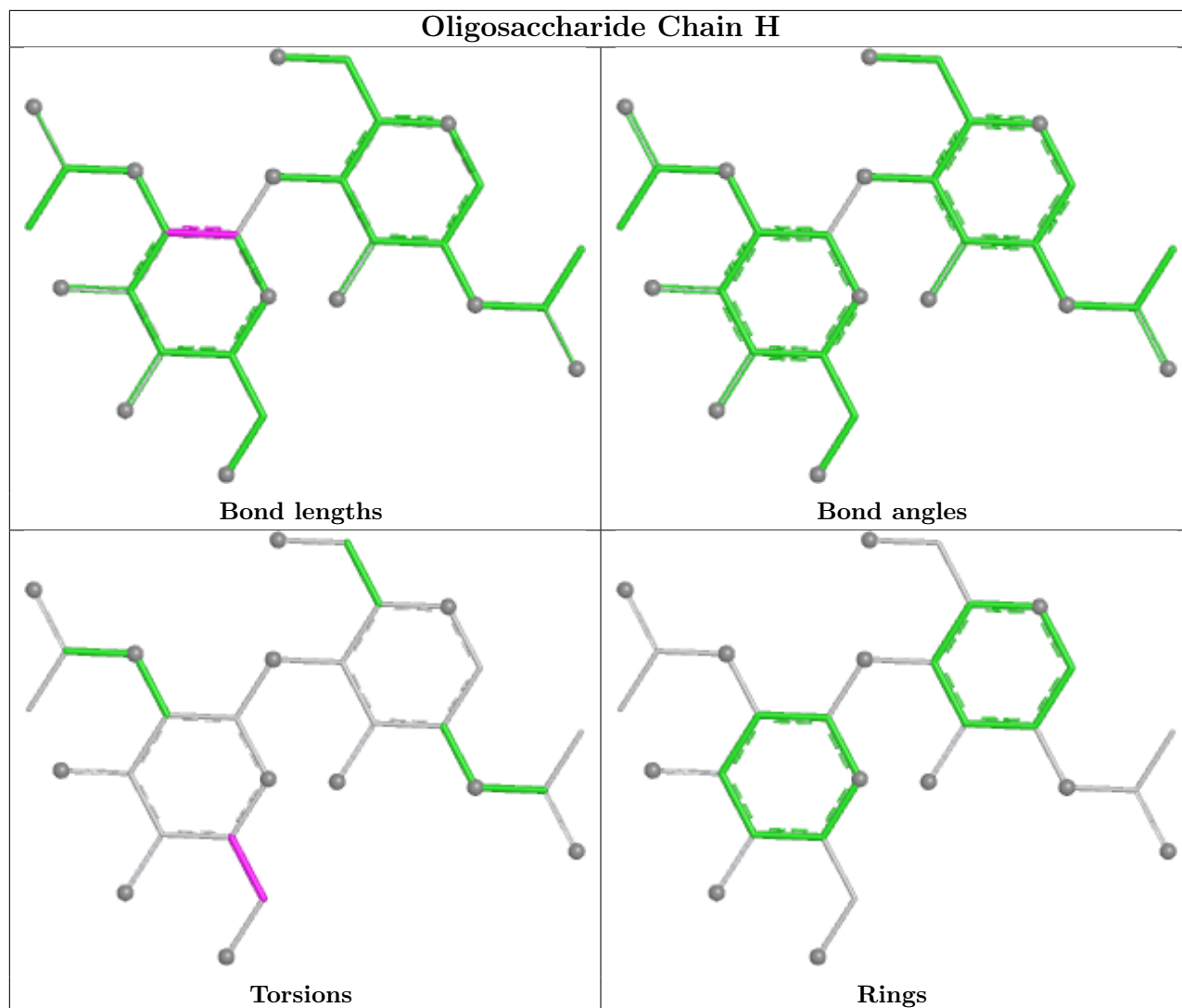
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	G	1	NAG	3	0
2	F	1	NAG	3	0

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 41 ligands modelled in this entry, 5 are monoatomic - leaving 36 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	$\# Z > 2$
5	PLM	C	1008	-	17,17,17	0.52	0	17,17,17	0.89	0
3	NAG	C	1001	1	14,14,15	0.34	0	17,19,21	0.49	0
5	PLM	B	1008	-	17,17,17	0.52	0	17,17,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PLM	D	1007	-	17,17,17	0.55	0	17,17,17	0.78	1 (5%)
3	NAG	C	1005	-	14,14,15	0.31	0	17,19,21	0.38	0
4	PX6	A	1006	-	39,39,43	1.46	6 (15%)	42,44,48	1.49	3 (7%)
6	CHS	D	1010	-	15,15,15	0.65	0	15,19,19	0.90	1 (6%)
6	CHS	D	1011	-	15,15,15	0.59	0	15,19,19	0.94	1 (6%)
3	NAG	C	1002	1	14,14,15	0.37	0	17,19,21	0.36	0
5	PLM	A	1008	-	17,17,17	0.52	0	17,17,17	0.90	0
6	CHS	A	1011	-	15,15,15	0.58	0	15,19,19	0.94	1 (6%)
5	PLM	D	1009	-	17,17,17	0.55	0	17,17,17	0.76	0
3	NAG	A	1001	1	14,14,15	0.34	0	17,19,21	0.48	0
3	NAG	B	1002	1	14,14,15	0.38	0	17,19,21	0.36	0
3	NAG	B	1005	-	14,14,15	0.31	0	17,19,21	0.38	0
5	PLM	A	1009	-	17,17,17	0.55	0	17,17,17	0.77	0
6	CHS	A	1010	-	15,15,15	0.66	0	15,19,19	0.90	0
4	PX6	B	1006	-	39,39,43	1.47	6 (15%)	42,44,48	1.48	3 (7%)
4	PX6	C	1006	-	39,39,43	1.47	6 (15%)	42,44,48	1.48	3 (7%)
5	PLM	B	1007	-	17,17,17	0.55	0	17,17,17	0.77	1 (5%)
3	NAG	A	1002	1	14,14,15	0.38	0	17,19,21	0.36	0
5	PLM	B	1009	-	17,17,17	0.55	0	17,17,17	0.76	0
3	NAG	D	1005	-	14,14,15	0.31	0	17,19,21	0.38	0
6	CHS	C	1011	-	15,15,15	0.58	0	15,19,19	0.95	1 (6%)
5	PLM	C	1009	-	17,17,17	0.56	0	17,17,17	0.76	0
5	PLM	A	1007	-	17,17,17	0.55	0	17,17,17	0.78	1 (5%)
3	NAG	B	1001	1	14,14,15	0.34	0	17,19,21	0.47	0
4	PX6	D	1006	-	39,39,43	1.47	6 (15%)	42,44,48	1.48	3 (7%)
5	PLM	C	1007	-	17,17,17	0.56	0	17,17,17	0.78	1 (5%)
5	PLM	D	1008	-	17,17,17	0.52	0	17,17,17	0.89	0
3	NAG	D	1002	1	14,14,15	0.38	0	17,19,21	0.36	0
6	CHS	B	1010	-	15,15,15	0.65	0	15,19,19	0.90	1 (6%)
6	CHS	B	1011	-	15,15,15	0.57	0	15,19,19	0.93	1 (6%)
3	NAG	D	1001	1	14,14,15	0.34	0	17,19,21	0.48	0
6	CHS	C	1010	-	15,15,15	0.65	0	15,19,19	0.90	0
3	NAG	A	1005	-	14,14,15	0.33	0	17,19,21	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PLM	C	1008	-	-	7/15/15/15	-
3	NAG	C	1001	1	-	2/6/23/26	0/1/1/1
5	PLM	B	1008	-	-	6/15/15/15	-
5	PLM	D	1007	-	-	11/15/15/15	-
3	NAG	C	1005	-	-	2/6/23/26	0/1/1/1
4	PX6	A	1006	-	-	19/41/41/45	-
6	CHS	D	1010	-	-	3/12/20/20	0/1/1/1
6	CHS	D	1011	-	-	2/12/20/20	0/1/1/1
3	NAG	C	1002	1	-	3/6/23/26	0/1/1/1
5	PLM	A	1008	-	-	6/15/15/15	-
6	CHS	A	1011	-	-	2/12/20/20	0/1/1/1
5	PLM	D	1009	-	-	8/15/15/15	-
3	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1002	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1005	-	-	2/6/23/26	0/1/1/1
5	PLM	A	1009	-	-	6/15/15/15	-
6	CHS	A	1010	-	-	3/12/20/20	0/1/1/1
4	PX6	B	1006	-	-	19/41/41/45	-
4	PX6	C	1006	-	-	18/41/41/45	-
5	PLM	B	1007	-	-	11/15/15/15	-
3	NAG	A	1002	1	-	3/6/23/26	0/1/1/1
5	PLM	B	1009	-	-	8/15/15/15	-
3	NAG	D	1005	-	-	2/6/23/26	0/1/1/1
6	CHS	C	1011	-	-	2/12/20/20	0/1/1/1
5	PLM	C	1009	-	-	8/15/15/15	-
5	PLM	A	1007	-	-	11/15/15/15	-
3	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
4	PX6	D	1006	-	-	18/41/41/45	-
5	PLM	C	1007	-	-	11/15/15/15	-
5	PLM	D	1008	-	-	6/15/15/15	-
3	NAG	D	1002	1	-	3/6/23/26	0/1/1/1
6	CHS	B	1010	-	-	3/12/20/20	0/1/1/1
6	CHS	B	1011	-	-	4/12/20/20	0/1/1/1
3	NAG	D	1001	1	-	2/6/23/26	0/1/1/1
6	CHS	C	1010	-	-	3/12/20/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1005	-	-	2/6/23/26	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1006	PX6	P1-O2	4.79	1.65	1.50
4	D	1006	PX6	P1-O2	4.78	1.65	1.50
4	B	1006	PX6	P1-O2	4.78	1.65	1.50
4	A	1006	PX6	P1-O2	4.77	1.65	1.50
4	C	1006	PX6	O7-C2	-3.26	1.38	1.46

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1006	PX6	O5-C3-C2	7.08	128.82	108.40
4	D	1006	PX6	O5-C3-C2	7.07	128.78	108.40
4	B	1006	PX6	O5-C3-C2	7.05	128.73	108.40
4	C	1006	PX6	O5-C3-C2	7.04	128.70	108.40
4	A	1006	PX6	O7-C20-C21	3.36	118.76	111.48

There are no chirality outliers.

5 of 223 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	NAG	C3-C2-N2-C7
3	B	1002	NAG	C3-C2-N2-C7
3	C	1002	NAG	C3-C2-N2-C7
3	D	1002	NAG	C3-C2-N2-C7
4	A	1006	PX6	O7-C2-C3-O5

There are no ring outliers.

30 monomers are involved in 99 short contacts:

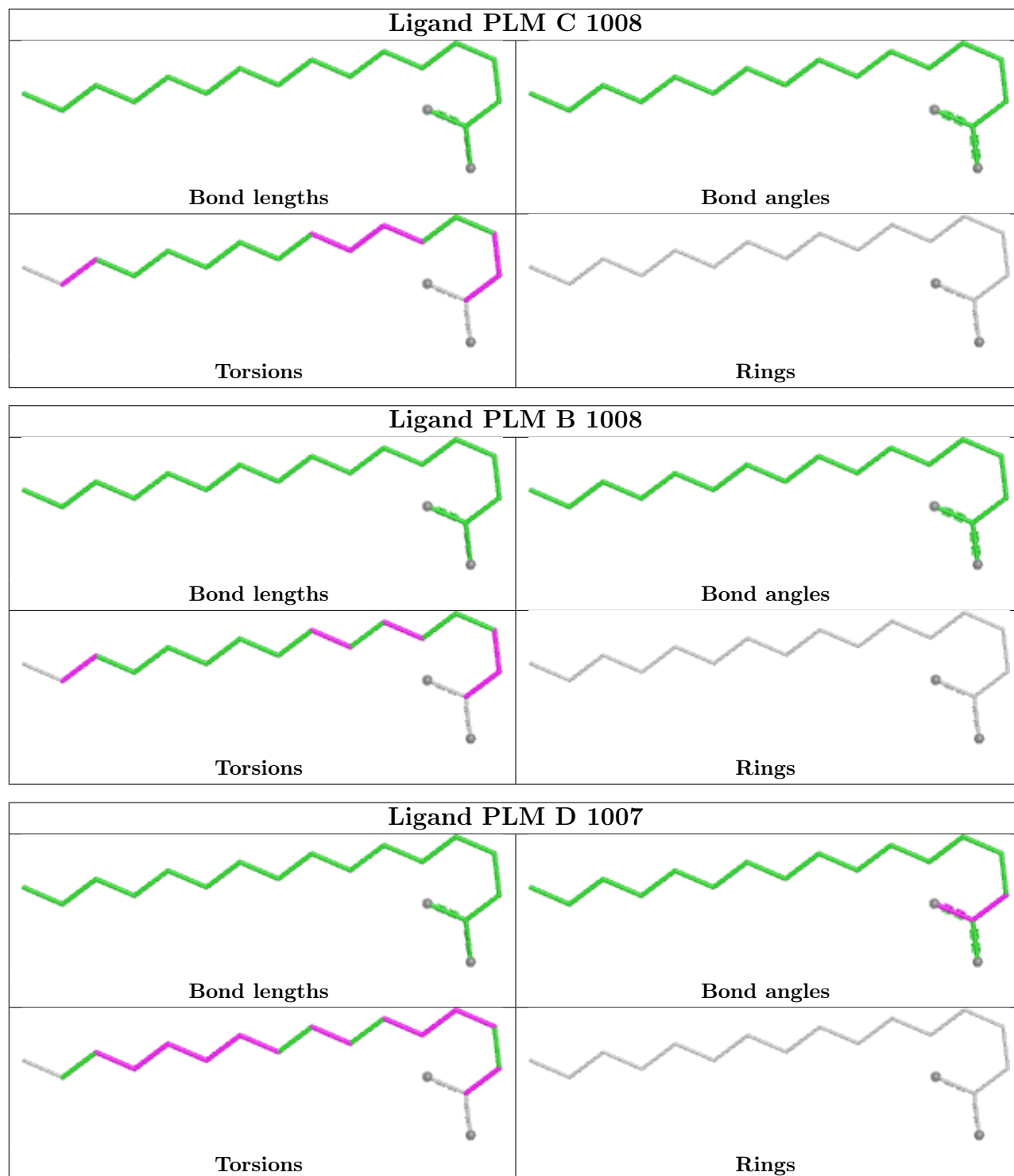
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1008	PLM	1	0
3	C	1001	NAG	3	0
5	B	1008	PLM	1	0
5	D	1007	PLM	3	0
3	C	1005	NAG	2	0
4	A	1006	PX6	2	0
6	D	1010	CHS	1	0

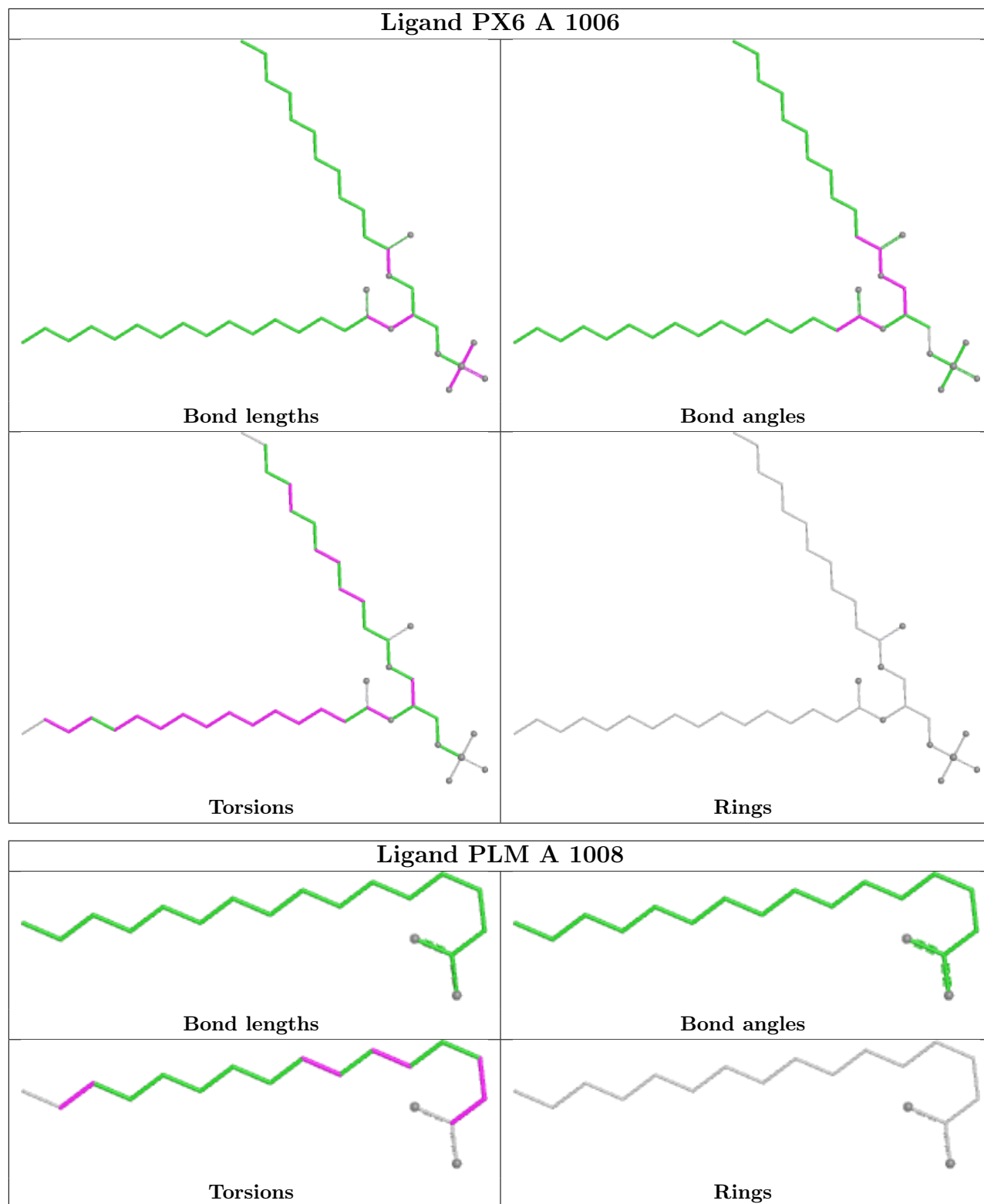
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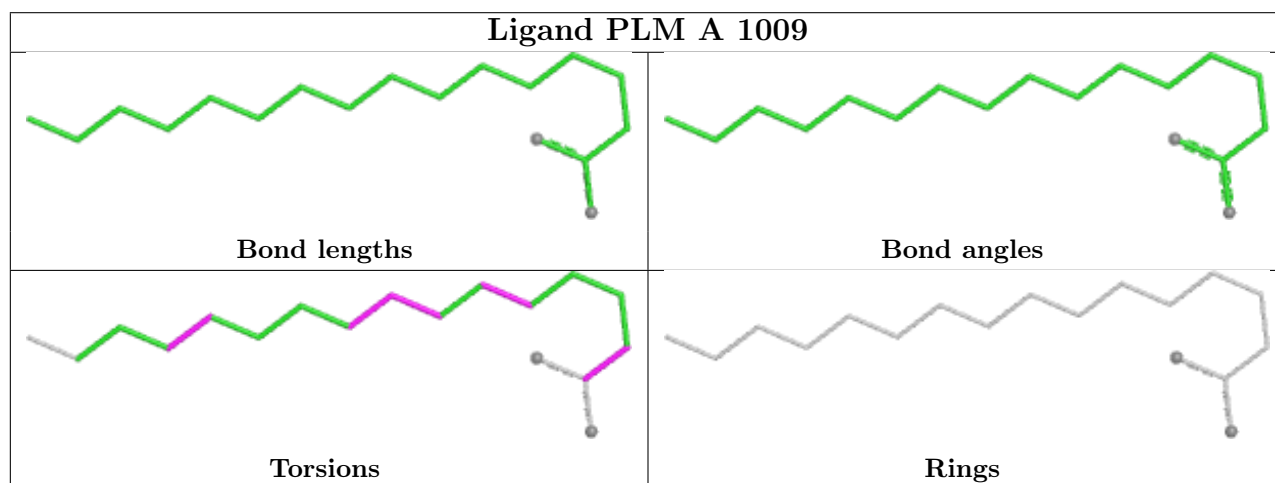
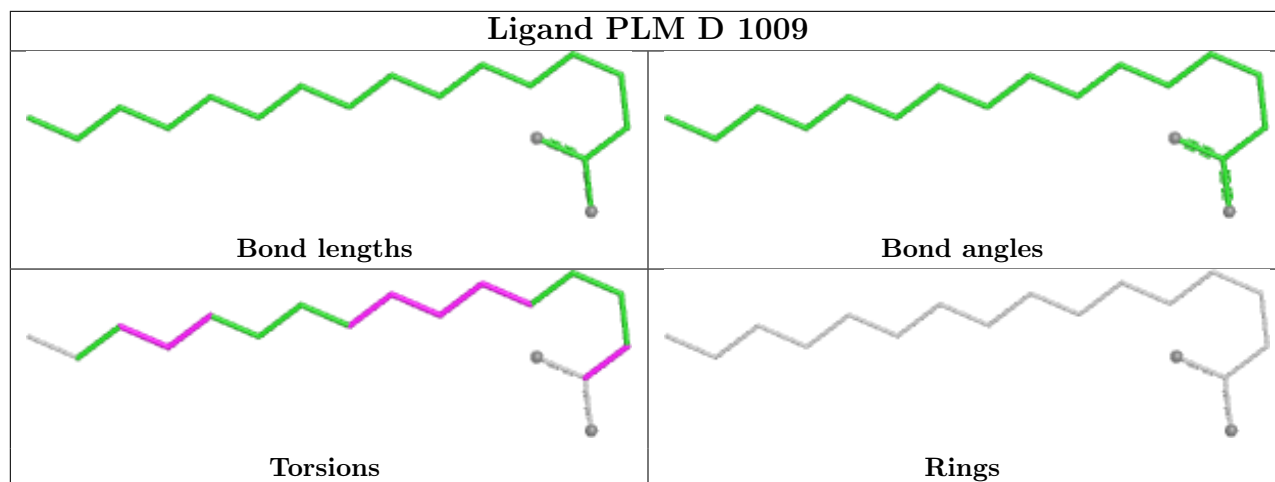
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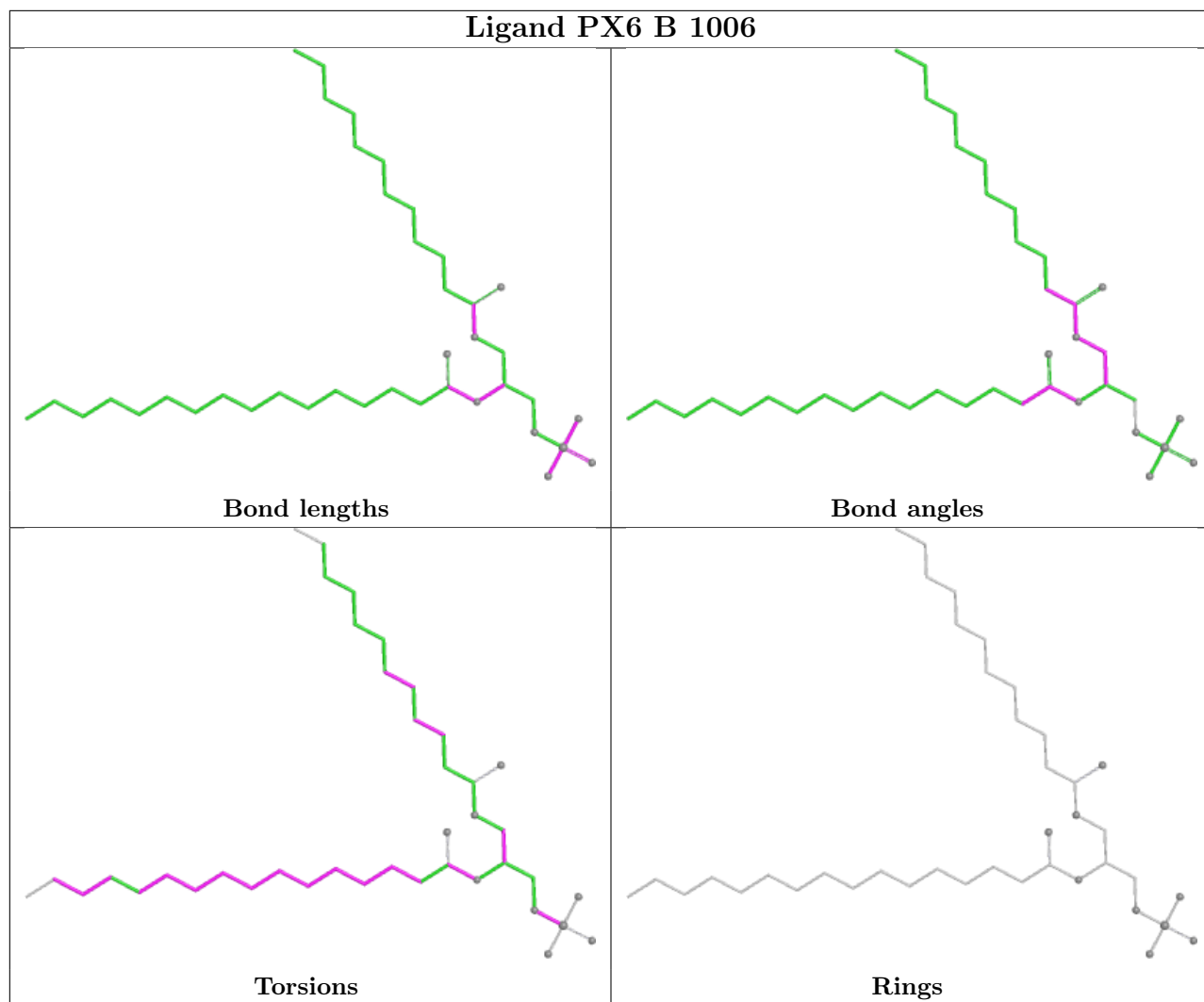
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	NAG	10	0
5	A	1008	PLM	1	0
6	A	1011	CHS	1	0
5	D	1009	PLM	1	0
3	A	1001	NAG	3	0
3	B	1002	NAG	10	0
3	B	1005	NAG	2	0
6	A	1010	CHS	1	0
4	B	1006	PX6	4	0
4	C	1006	PX6	5	0
5	B	1007	PLM	4	0
3	A	1002	NAG	10	0
3	D	1005	NAG	2	0
5	A	1007	PLM	4	0
3	B	1001	NAG	3	0
4	D	1006	PX6	4	0
5	C	1007	PLM	3	0
3	D	1002	NAG	10	0
6	B	1010	CHS	1	0
6	B	1011	CHS	1	0
3	D	1001	NAG	3	0
6	C	1010	CHS	1	0
3	A	1005	NAG	2	0

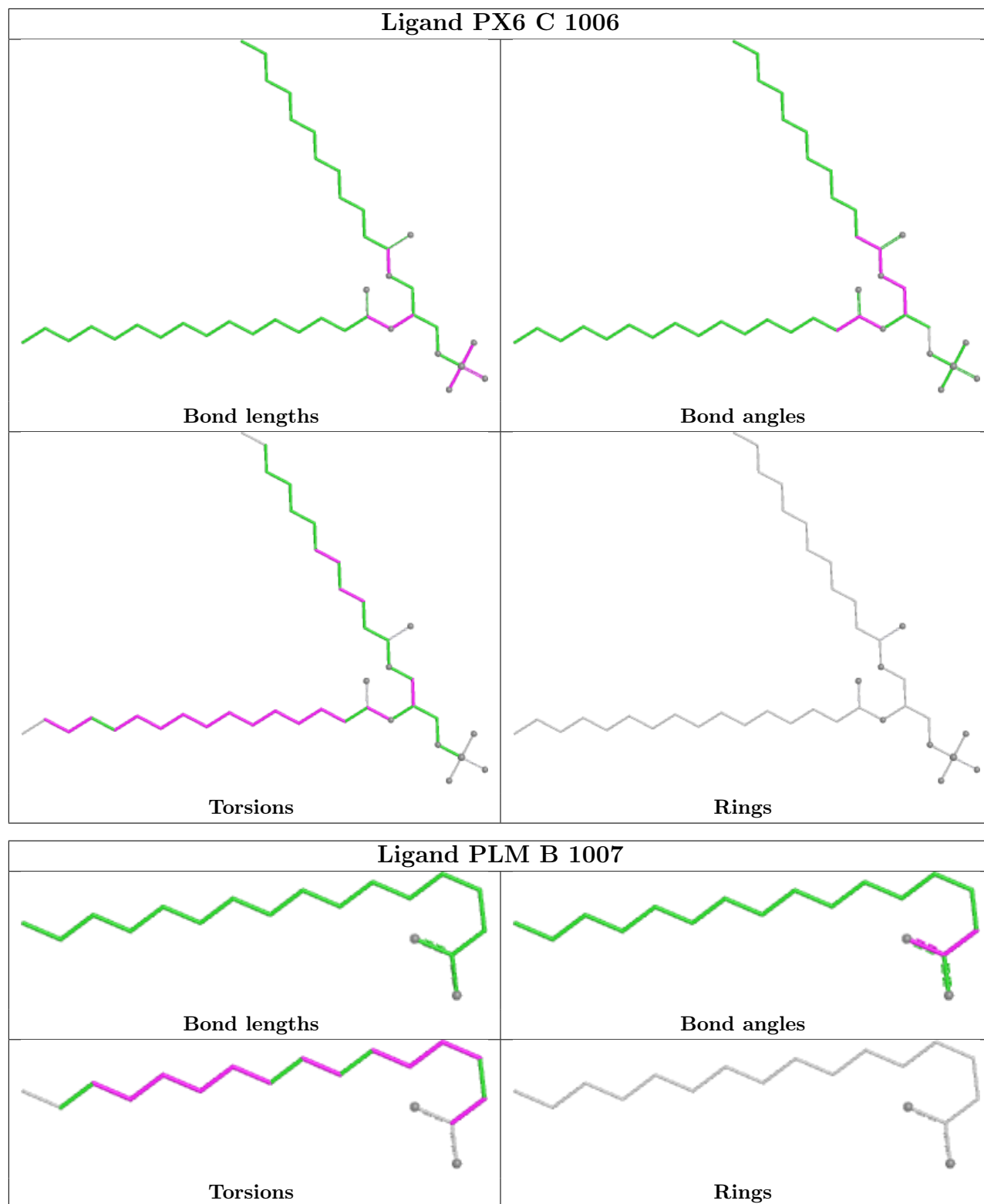
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

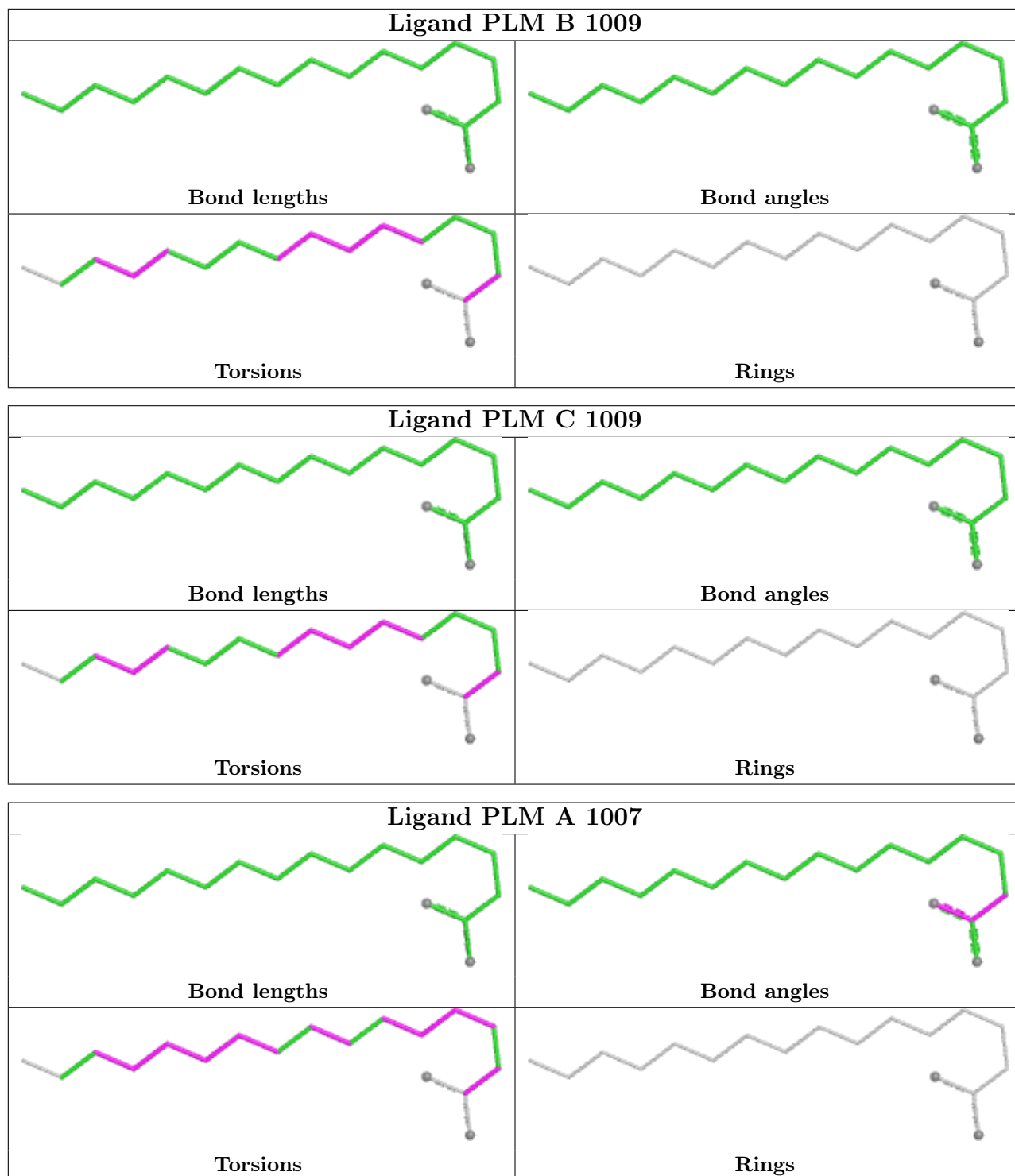


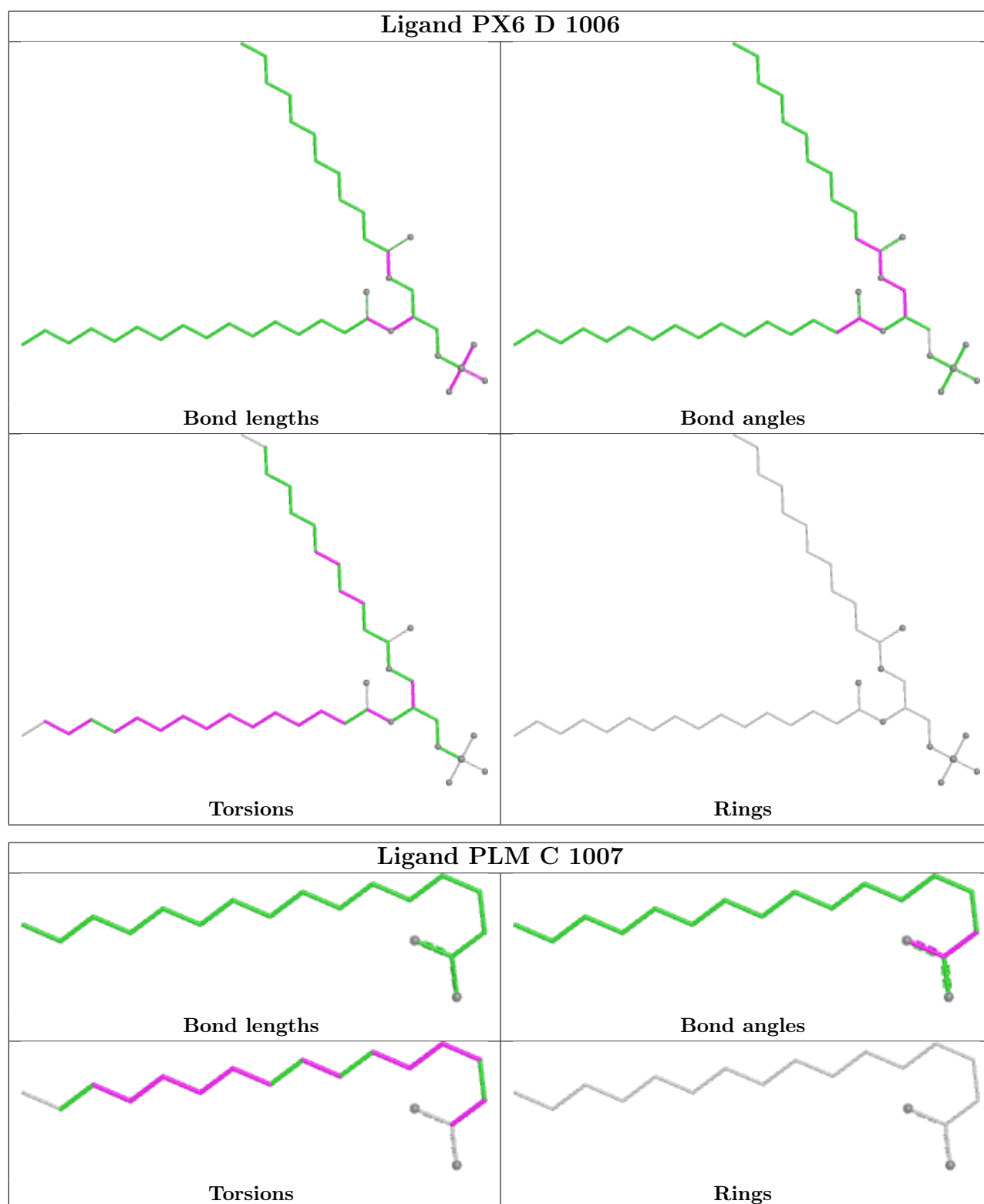


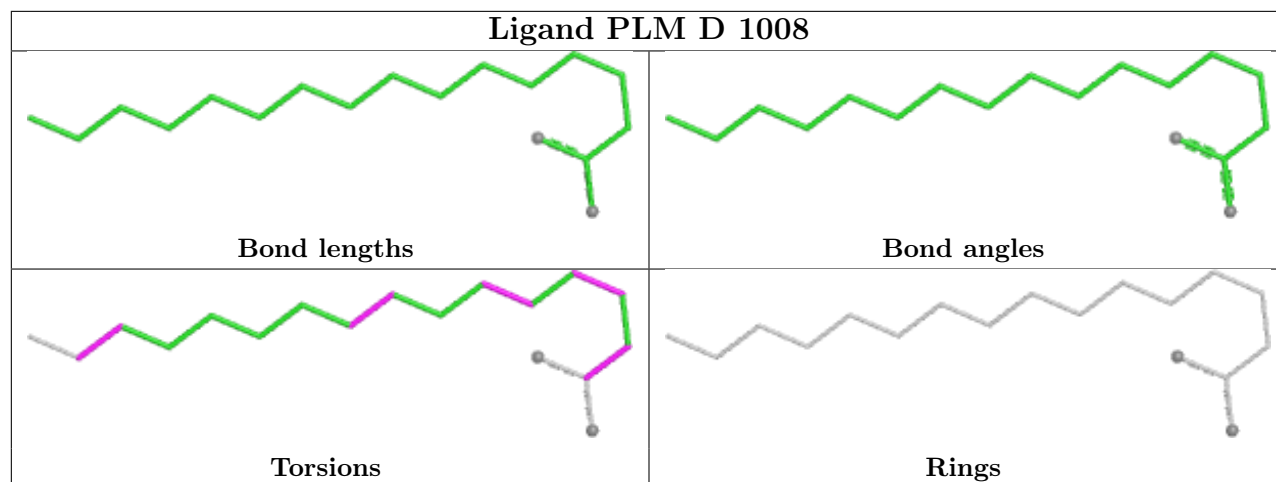












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

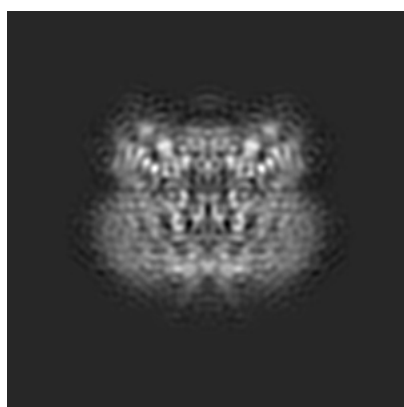
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3524. These allow visual inspection of the internal detail of the map and identification of artifacts.

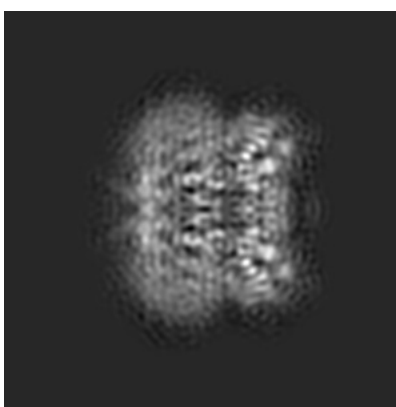
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

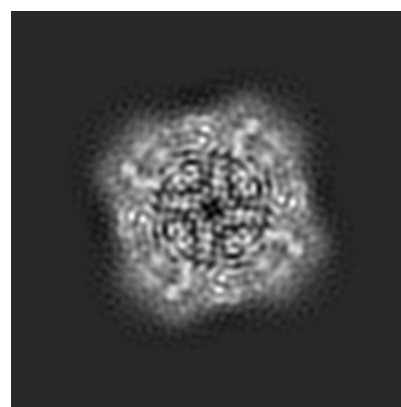
6.1.1 Primary map



X



Y



Z

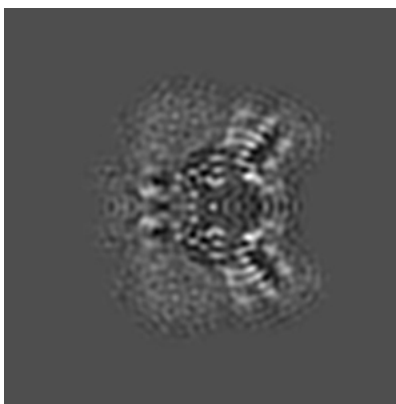
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

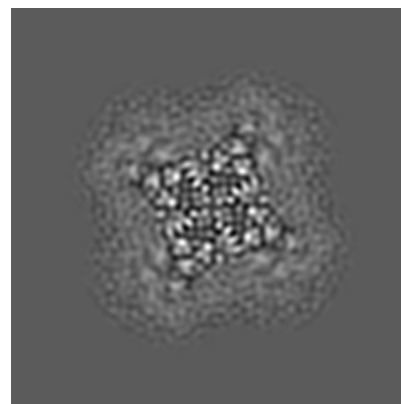
6.2.1 Primary map



X Index: 84



Y Index: 84

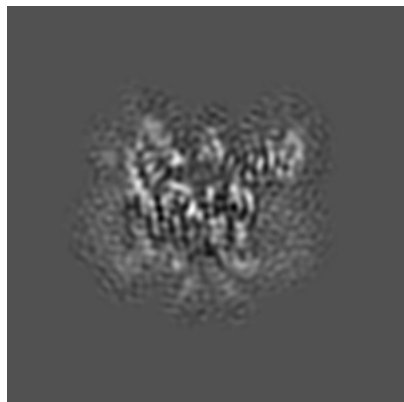


Z Index: 84

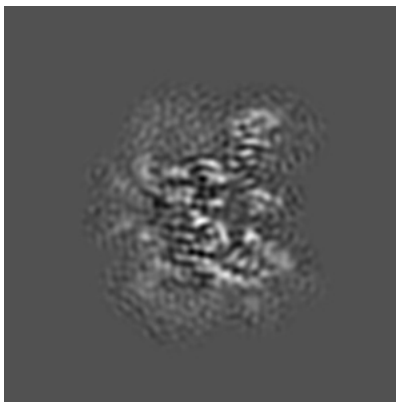
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

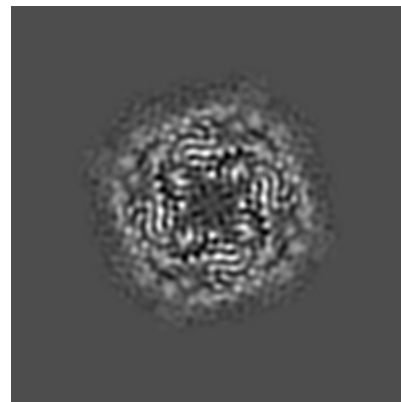
6.3.1 Primary map



X Index: 74



Y Index: 94

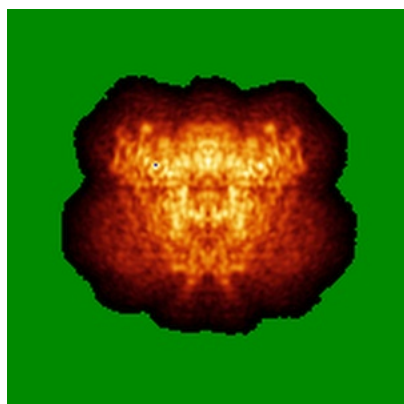


Z Index: 102

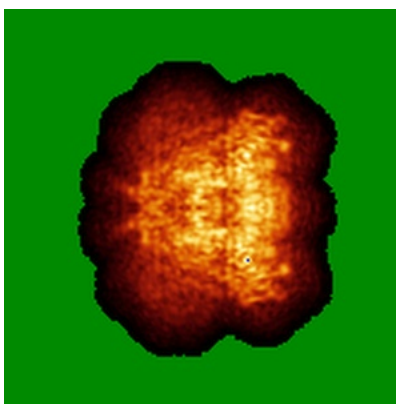
The images above show the largest variance slices of the map in three orthogonal directions.

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

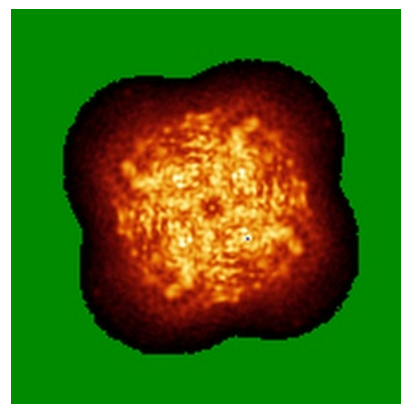
6.4.1 Primary map



X



Y

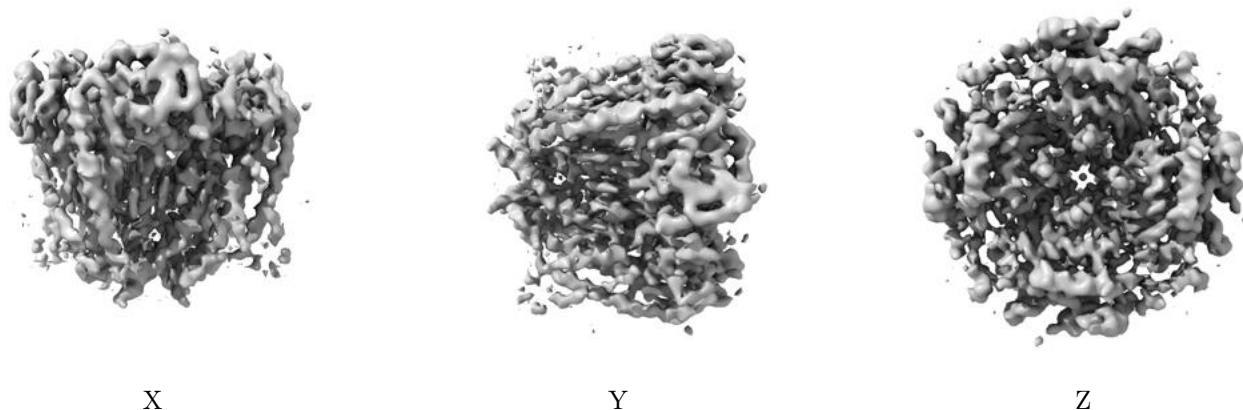


Z

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 0.0354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

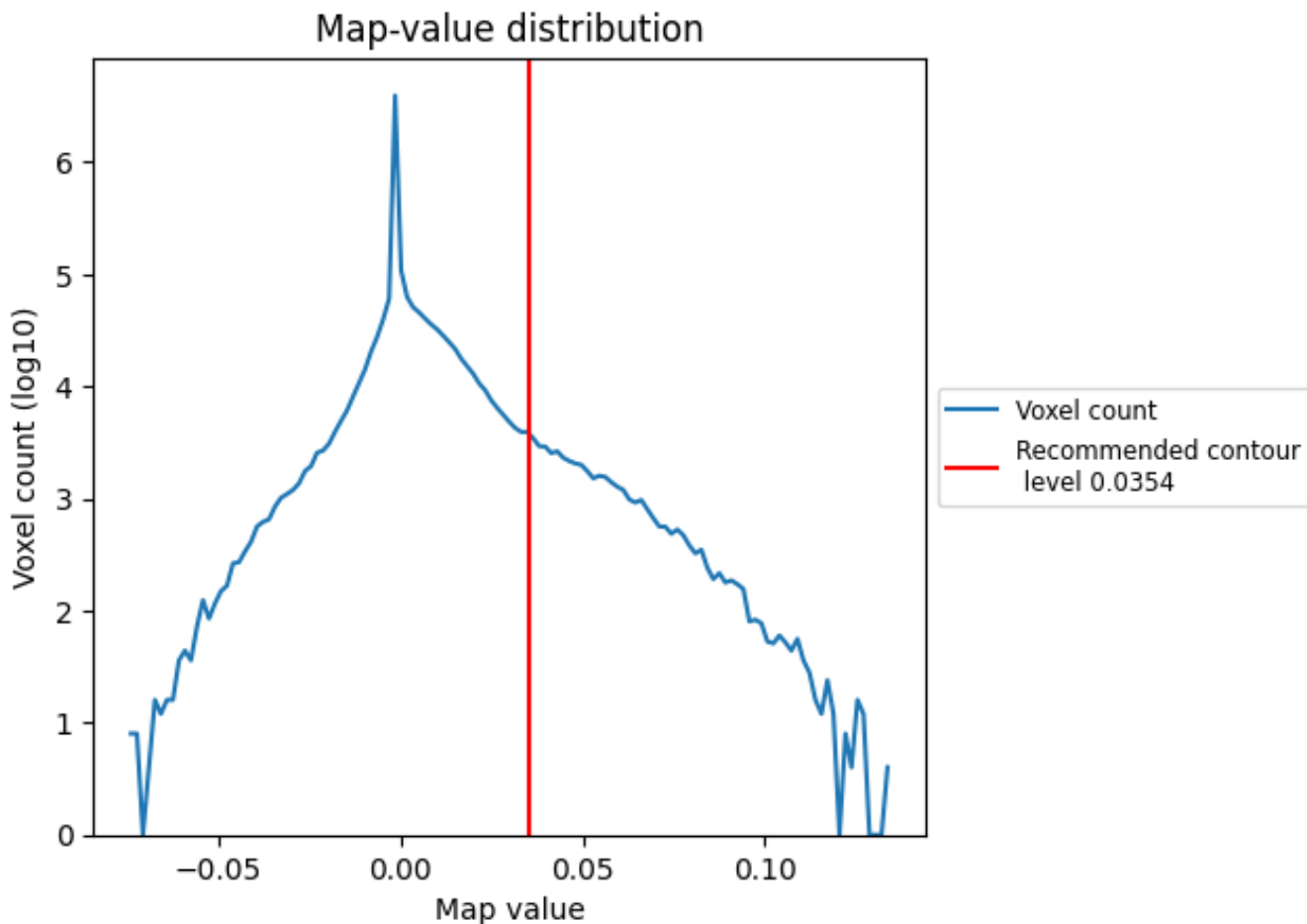
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

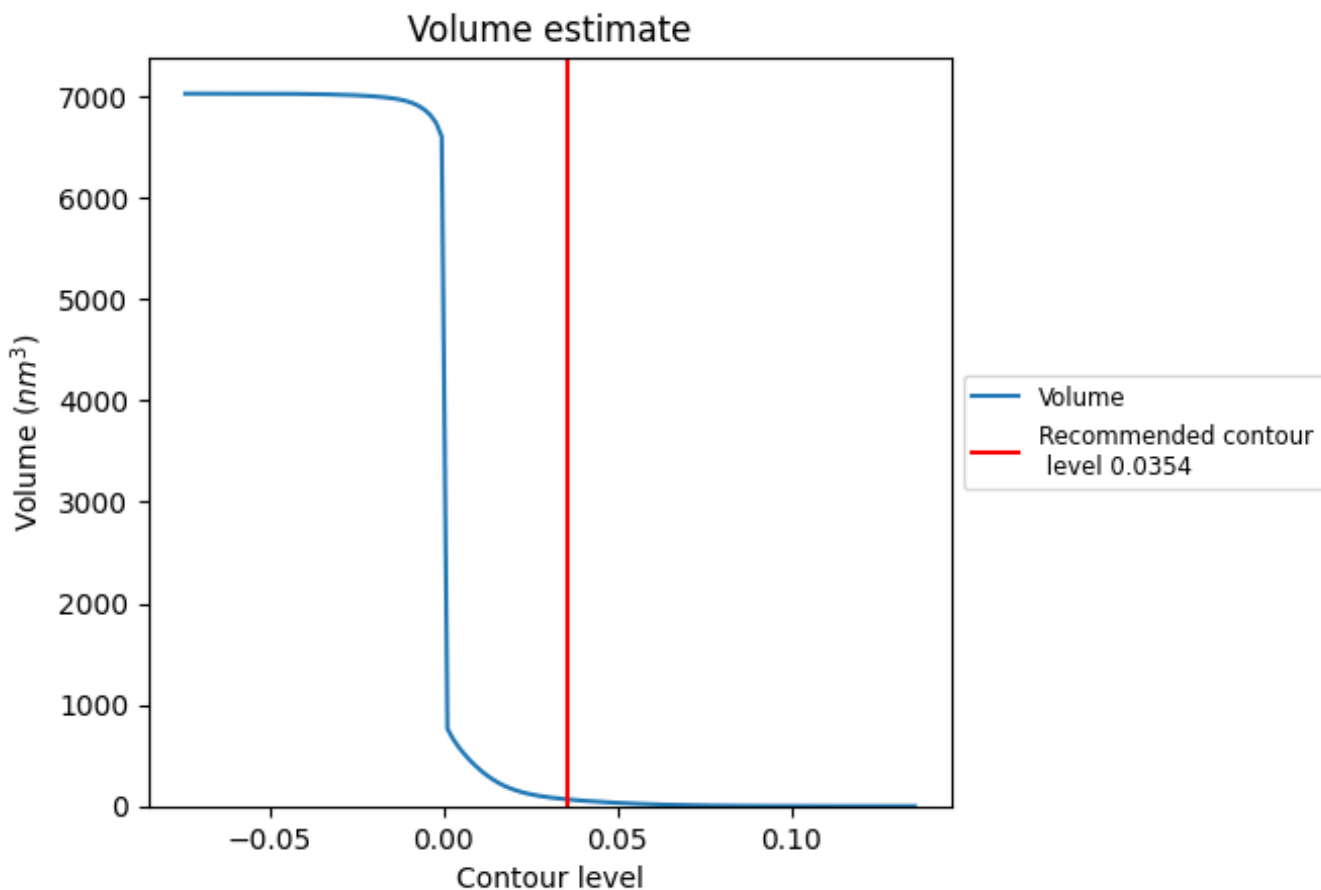
This section contains the results of statistical analysis of the map.

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.

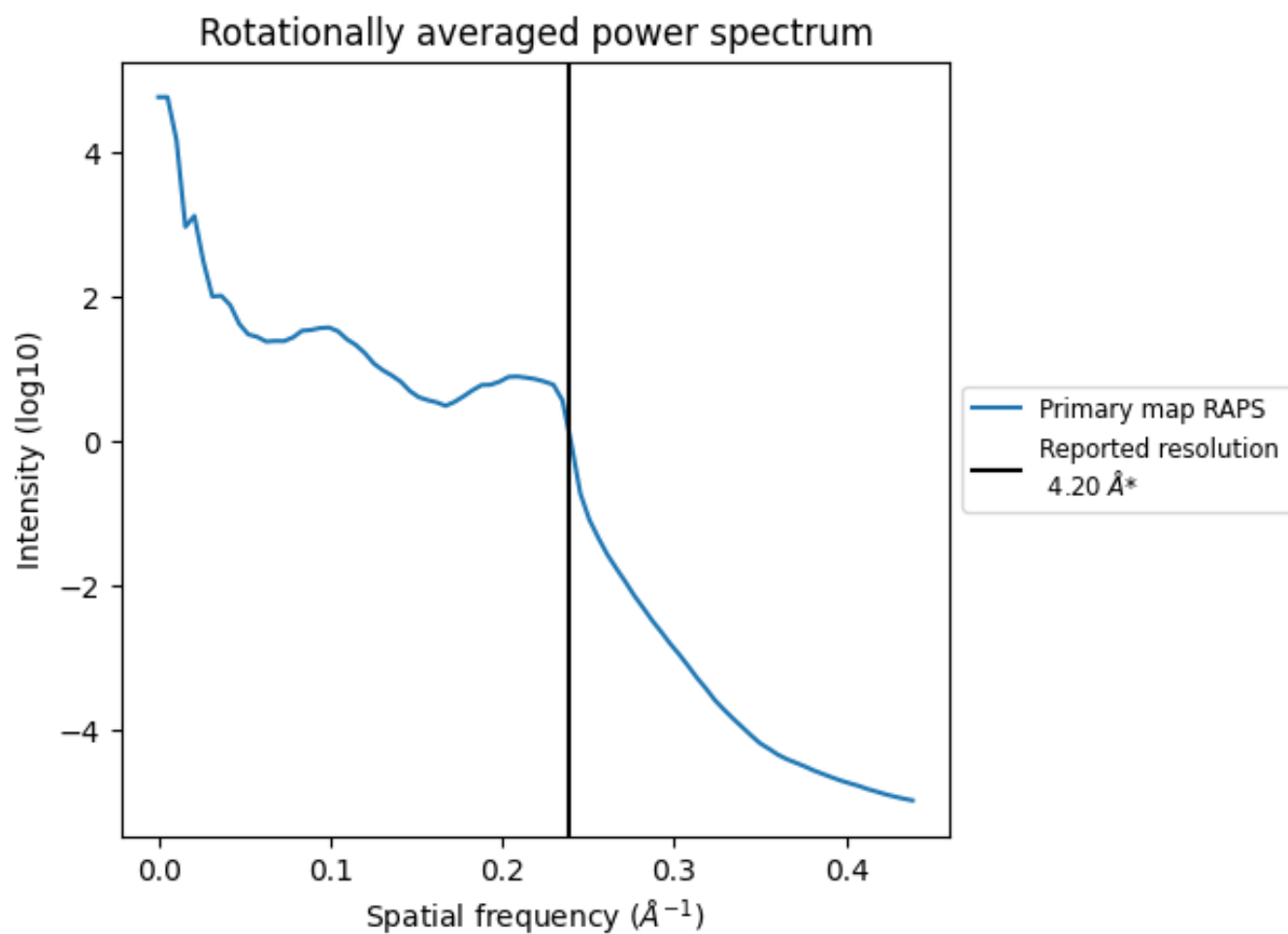
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 68 nm³; this corresponds to an approximate mass of 61 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](#)

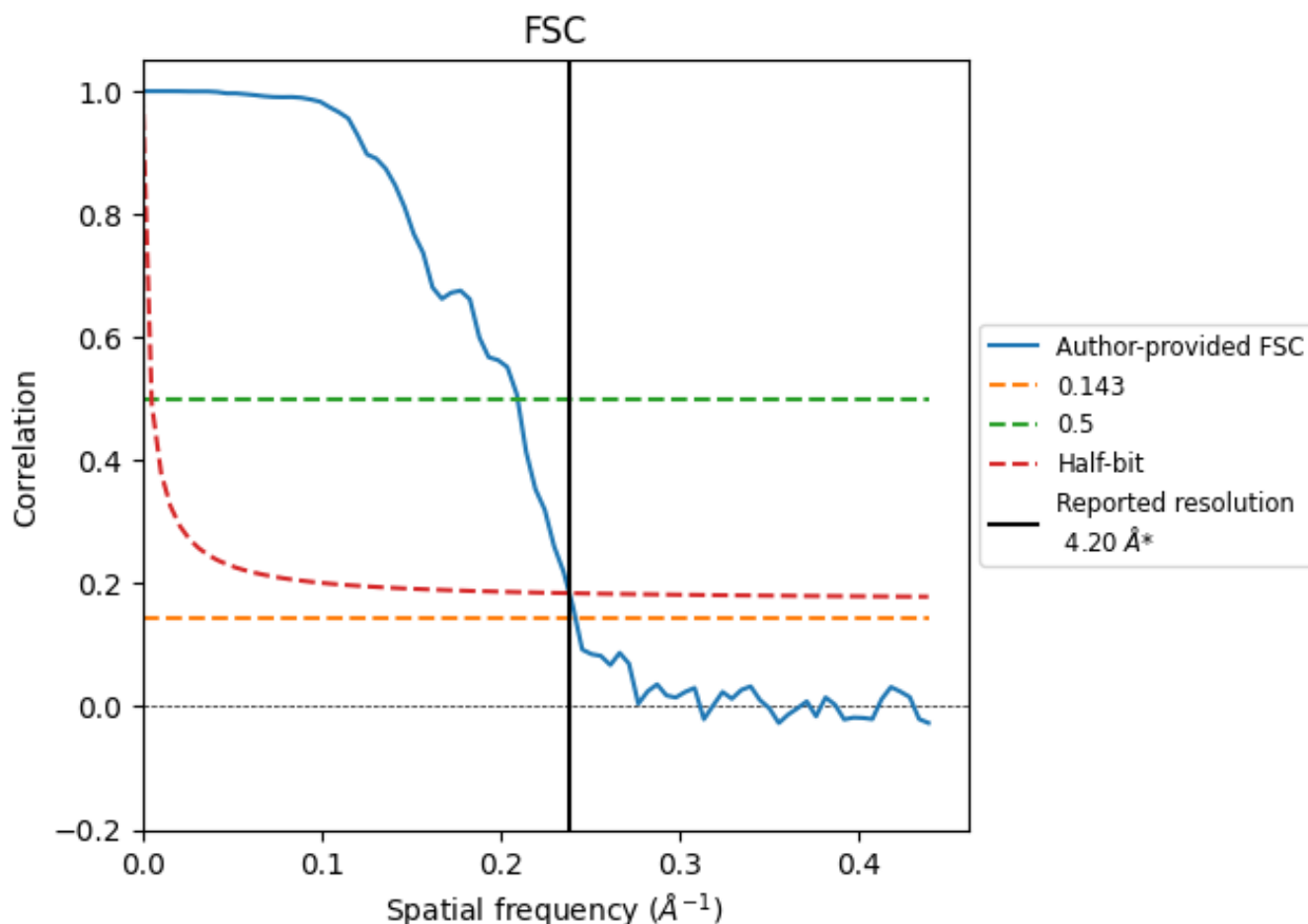


*Reported resolution corresponds to spatial frequency of 0.238\AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

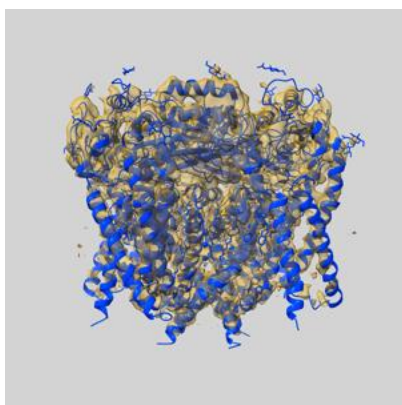
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.14	4.78	4.20
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

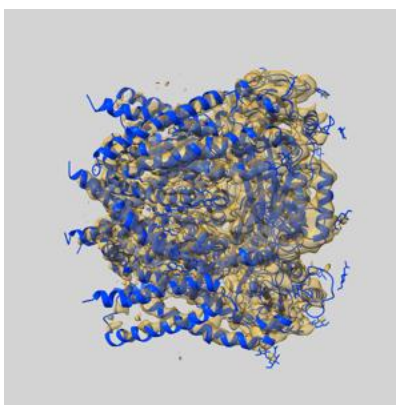
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3524 and PDB model 5MKF. Per-residue inclusion information can be found in section [3](#) on page [9](#).

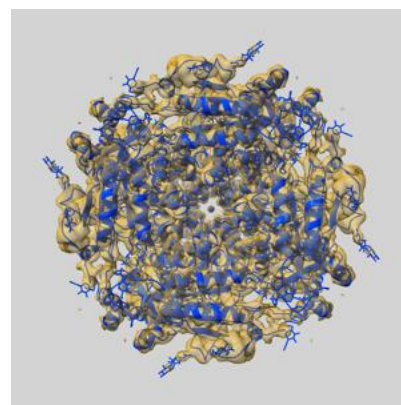
9.1 Map-model overlay [i](#)



X



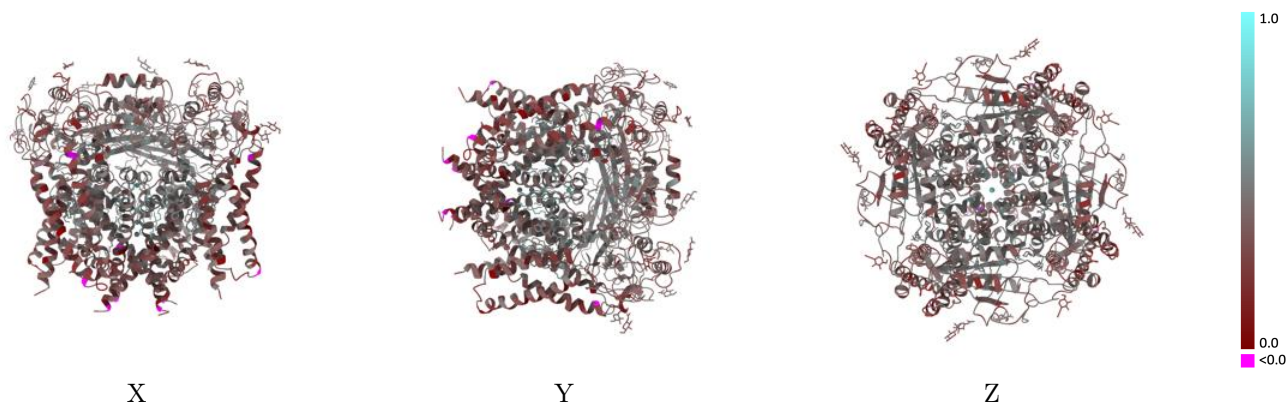
Y



Z

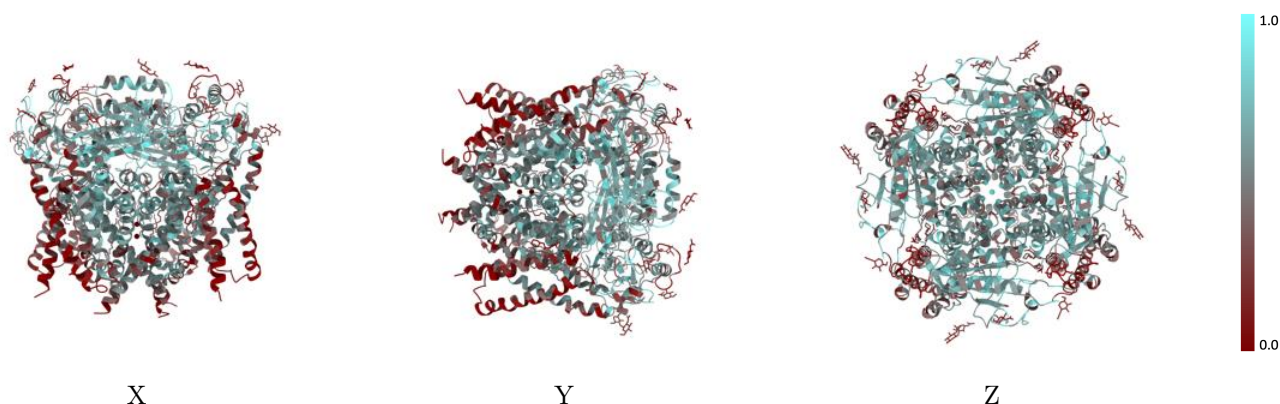
The images above show the 3D surface view of the map at the recommended contour level 0.0354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



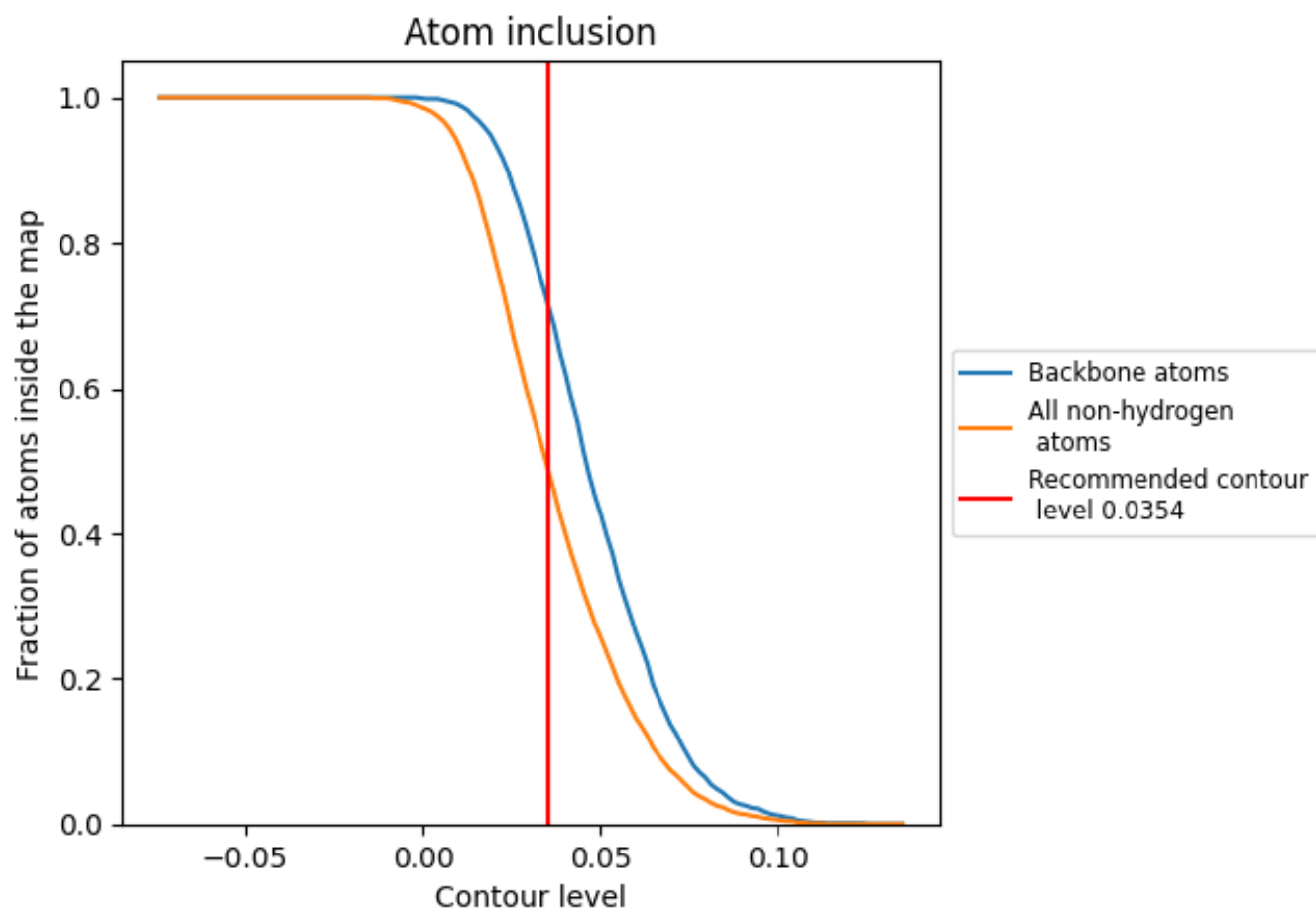
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0354).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 49% 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 (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4890	 0.3690
A	 0.4900	 0.3690
B	 0.4910	 0.3710
C	 0.4910	 0.3680
D	 0.4900	 0.3680
E	 0.2140	 0.3220
F	 0.2140	 0.3130
G	 0.2140	 0.3010
H	 0.2140	 0.3180

