



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 07:28 AM EST

PDB ID : 8SZI
EMDB ID : EMD-40917
Title : Cryo-EM structure of PAM-free human calcium-sensing receptor CaSR-Gi complex in lipid nanodiscs
Authors : He, F.; Wu, C.; Gao, Y.; Skiniotis, G.
Deposited on : 2023-05-29
Resolution : 3.50 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 : 2022.3.0, CSD as543be (2022)
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

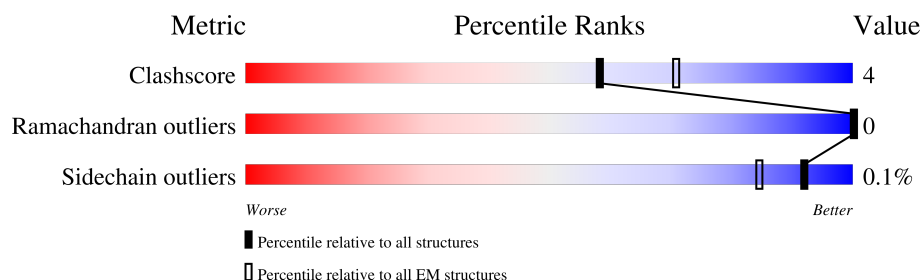
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	C	354	<div> <div>10%</div> <div>58%</div> <div>5%</div> <div>37%</div> </div>
2	D	343	<div> <div>9%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
3	E	71	<div> <div>21%</div> <div>76%</div> <div>20%</div> </div>
4	A	939	<div> <div>79%</div> <div>9%</div> <div>12%</div> </div>
5	B	959	<div> <div>74%</div> <div>9%</div> <div>16%</div> </div>
6	F	2	<div> <div>50%</div> <div>100%</div> </div>
6	G	2	<div> <div>100%</div> </div>
6	H	2	<div> <div>100%</div> </div>

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
7	PCW	A	1001	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17868 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 Guanine nucleotide-binding protein G(i) subunit alpha-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	223	Total	C	N	O	S	0	0
			1765	1126	292	335	12		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	47	ASN	SER	engineered mutation	UNP P08754
C	203	ALA	GLY	engineered mutation	UNP P08754
C	245	ALA	GLU	engineered mutation	UNP P08754
C	326	SER	ALA	engineered mutation	UNP P08754

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	338	Total	C	N	O	S	0	0
			2509	1561	449	478	21		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P62873
D	-1	SER	-	expression tag	UNP P62873
D	0	SER	-	expression tag	UNP P62873
D	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	57	Total	C	N	O	S	0	0
			408	256	71	78	3		

- Molecule 4 is a protein called Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	826	Total	C	N	O	S	1	0
			6538	4253	1072	1177	36		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ASP	-	expression tag	UNP P41180
A	10	TYR	-	expression tag	UNP P41180
A	11	LYS	-	expression tag	UNP P41180
A	12	ASP	-	expression tag	UNP P41180
A	13	ASP	-	expression tag	UNP P41180
A	14	ASP	-	expression tag	UNP P41180
A	15	ASP	-	expression tag	UNP P41180
A	16	LYS	-	expression tag	UNP P41180
A	17	ALA	-	expression tag	UNP P41180
A	18	ALA	-	expression tag	UNP P41180
A	895	THR	-	expression tag	UNP P41180
A	896	SER	-	expression tag	UNP P41180
A	897	THR	-	expression tag	UNP P41180
A	898	SER	-	expression tag	UNP P41180
A	899	VAL	-	expression tag	UNP P41180
A	900	THR	-	expression tag	UNP P41180
A	901	SER	-	expression tag	UNP P41180
A	902	VAL	-	expression tag	UNP P41180
A	903	ASN	-	expression tag	UNP P41180
A	904	GLN	-	expression tag	UNP P41180
A	905	ALA	-	expression tag	UNP P41180
A	906	SER	-	expression tag	UNP P41180
A	907	THR	-	expression tag	UNP P41180
A	908	SER	-	expression tag	UNP P41180
A	909	ARG	-	expression tag	UNP P41180
A	910	LEU	-	expression tag	UNP P41180
A	911	GLU	-	expression tag	UNP P41180
A	912	GLY	-	expression tag	UNP P41180
A	913	LEU	-	expression tag	UNP P41180
A	914	GLN	-	expression tag	UNP P41180
A	915	SER	-	expression tag	UNP P41180
A	916	GLU	-	expression tag	UNP P41180
A	917	ASN	-	expression tag	UNP P41180
A	918	HIS	-	expression tag	UNP P41180
A	919	ARG	-	expression tag	UNP P41180
A	920	LEU	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
A	921	ARG	-	expression tag	UNP P41180
A	922	MET	-	expression tag	UNP P41180
A	923	LYS	-	expression tag	UNP P41180
A	924	ILE	-	expression tag	UNP P41180
A	925	THR	-	expression tag	UNP P41180
A	926	GLU	-	expression tag	UNP P41180
A	927	LEU	-	expression tag	UNP P41180
A	928	ASP	-	expression tag	UNP P41180
A	929	LYS	-	expression tag	UNP P41180
A	930	ASP	-	expression tag	UNP P41180
A	931	LEU	-	expression tag	UNP P41180
A	932	GLU	-	expression tag	UNP P41180
A	933	GLU	-	expression tag	UNP P41180
A	934	VAL	-	expression tag	UNP P41180
A	935	THR	-	expression tag	UNP P41180
A	936	MET	-	expression tag	UNP P41180
A	937	GLN	-	expression tag	UNP P41180
A	938	LEU	-	expression tag	UNP P41180
A	939	GLN	-	expression tag	UNP P41180
A	940	ASP	-	expression tag	UNP P41180
A	941	THR	-	expression tag	UNP P41180
A	942	PRO	-	expression tag	UNP P41180
A	943	GLU	-	expression tag	UNP P41180
A	944	LYS	-	expression tag	UNP P41180
A	945	LYS	-	expression tag	UNP P41180
A	946	THR	-	expression tag	UNP P41180
A	947	ASN	-	expression tag	UNP P41180

- Molecule 5 is a protein called Extracellular calcium-sensing receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	802	Total	C	N	O	S	0	0
			6327	4110	1031	1150	36		

There are 83 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	TRP	-	expression tag	UNP P41180
B	-12	SER	-	expression tag	UNP P41180
B	-11	HIS	-	expression tag	UNP P41180
B	-10	PRO	-	expression tag	UNP P41180
B	-9	GLN	-	expression tag	UNP P41180

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	PHE	-	expression tag	UNP P41180
B	-7	GLU	-	expression tag	UNP P41180
B	-6	LYS	-	expression tag	UNP P41180
B	-5	GLY	-	expression tag	UNP P41180
B	-4	GLY	-	expression tag	UNP P41180
B	-3	GLY	-	expression tag	UNP P41180
B	-2	SER	-	expression tag	UNP P41180
B	-1	GLY	-	expression tag	UNP P41180
B	0	GLY	-	expression tag	UNP P41180
B	1	GLY	-	expression tag	UNP P41180
B	2	SER	-	expression tag	UNP P41180
B	3	GLY	-	expression tag	UNP P41180
B	4	GLY	-	expression tag	UNP P41180
B	5	SER	-	expression tag	UNP P41180
B	6	ALA	-	expression tag	UNP P41180
B	7	TRP	-	expression tag	UNP P41180
B	8	SER	-	expression tag	UNP P41180
B	9	HIS	-	expression tag	UNP P41180
B	10	PRO	-	expression tag	UNP P41180
B	11	GLN	-	expression tag	UNP P41180
B	12	PHE	-	expression tag	UNP P41180
B	13	GLU	-	expression tag	UNP P41180
B	14	LYS	-	expression tag	UNP P41180
B	15	GLY	-	expression tag	UNP P41180
B	16	SER	-	expression tag	UNP P41180
B	17	ALA	-	expression tag	UNP P41180
B	18	ALA	-	expression tag	UNP P41180
B	895	THR	-	expression tag	UNP P41180
B	896	GLY	-	expression tag	UNP P41180
B	897	SER	-	expression tag	UNP P41180
B	898	SER	-	expression tag	UNP P41180
B	899	THR	-	expression tag	UNP P41180
B	900	ASN	-	expression tag	UNP P41180
B	901	ASN	-	expression tag	UNP P41180
B	902	ASN	-	expression tag	UNP P41180
B	903	GLU	-	expression tag	UNP P41180
B	904	GLU	-	expression tag	UNP P41180
B	905	GLU	-	expression tag	UNP P41180
B	906	LYS	-	expression tag	UNP P41180
B	907	SER	-	expression tag	UNP P41180
B	908	ARG	-	expression tag	UNP P41180
B	909	LEU	-	expression tag	UNP P41180

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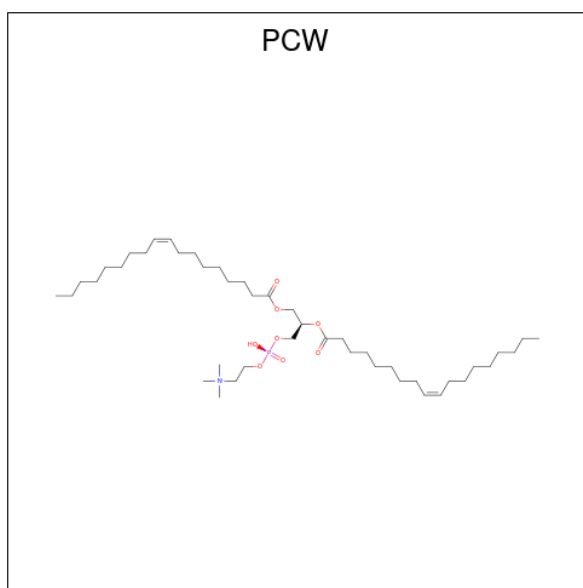
Chain	Residue	Modelled	Actual	Comment	Reference
B	910	LEU	-	expression tag	UNP P41180
B	911	GLU	-	expression tag	UNP P41180
B	912	LYS	-	expression tag	UNP P41180
B	913	GLU	-	expression tag	UNP P41180
B	914	ASN	-	expression tag	UNP P41180
B	915	ARG	-	expression tag	UNP P41180
B	916	GLU	-	expression tag	UNP P41180
B	917	LEU	-	expression tag	UNP P41180
B	918	GLU	-	expression tag	UNP P41180
B	919	LYS	-	expression tag	UNP P41180
B	920	ILE	-	expression tag	UNP P41180
B	921	ILE	-	expression tag	UNP P41180
B	922	ALA	-	expression tag	UNP P41180
B	923	GLU	-	expression tag	UNP P41180
B	924	LYS	-	expression tag	UNP P41180
B	925	GLU	-	expression tag	UNP P41180
B	926	GLU	-	expression tag	UNP P41180
B	927	ARG	-	expression tag	UNP P41180
B	928	VAL	-	expression tag	UNP P41180
B	929	SER	-	expression tag	UNP P41180
B	930	GLU	-	expression tag	UNP P41180
B	931	LEU	-	expression tag	UNP P41180
B	932	ARG	-	expression tag	UNP P41180
B	933	HIS	-	expression tag	UNP P41180
B	934	GLN	-	expression tag	UNP P41180
B	935	LEU	-	expression tag	UNP P41180
B	936	GLN	-	expression tag	UNP P41180
B	937	SER	-	expression tag	UNP P41180
B	938	ARG	-	expression tag	UNP P41180
B	939	GLN	-	expression tag	UNP P41180
B	940	GLN	-	expression tag	UNP P41180
B	941	LEU	-	expression tag	UNP P41180
B	942	LYS	-	expression tag	UNP P41180
B	943	LYS	-	expression tag	UNP P41180
B	944	THR	-	expression tag	UNP P41180
B	945	ASN	-	expression tag	UNP P41180

- Molecule 6 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
6	F	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
7	B	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

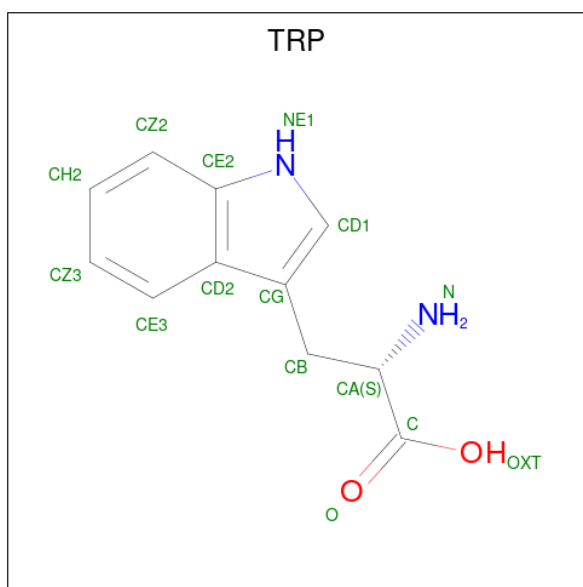


Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

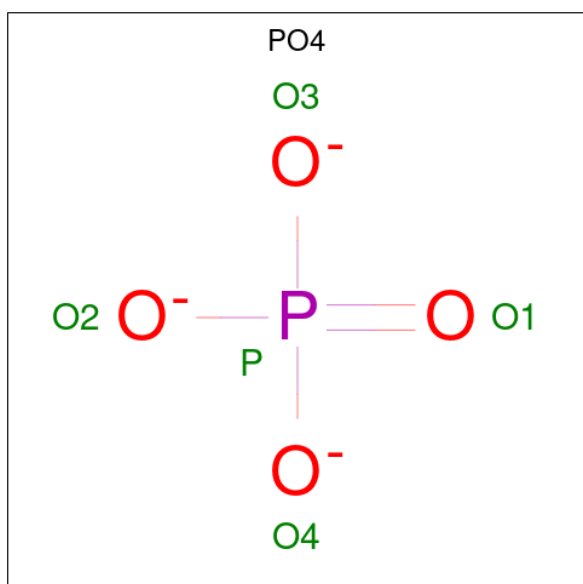
Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	Ca	0
			2	2	
9	B	2	Total	Ca	0
			2	2	

- Molecule 10 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂) (labeled as "Ligand of Interest" by depositor).



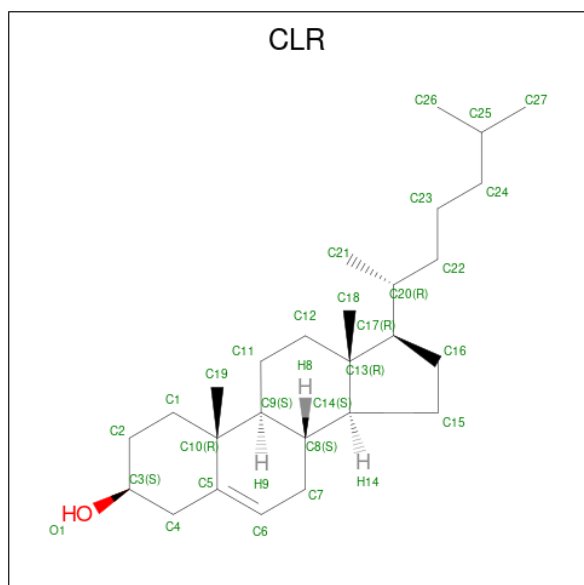
Mol	Chain	Residues	Atoms				AltConf
10	A	1	Total	C	N	O	0
			15	11	2	2	
10	A	1	Total	C	N	O	0
			15	11	2	2	
10	B	1	Total	C	N	O	0
			15	11	2	2	

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	O	P	0
			5	4	1	
11	B	1	Total	O	P	0
			5	4	1	

- Molecule 12 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

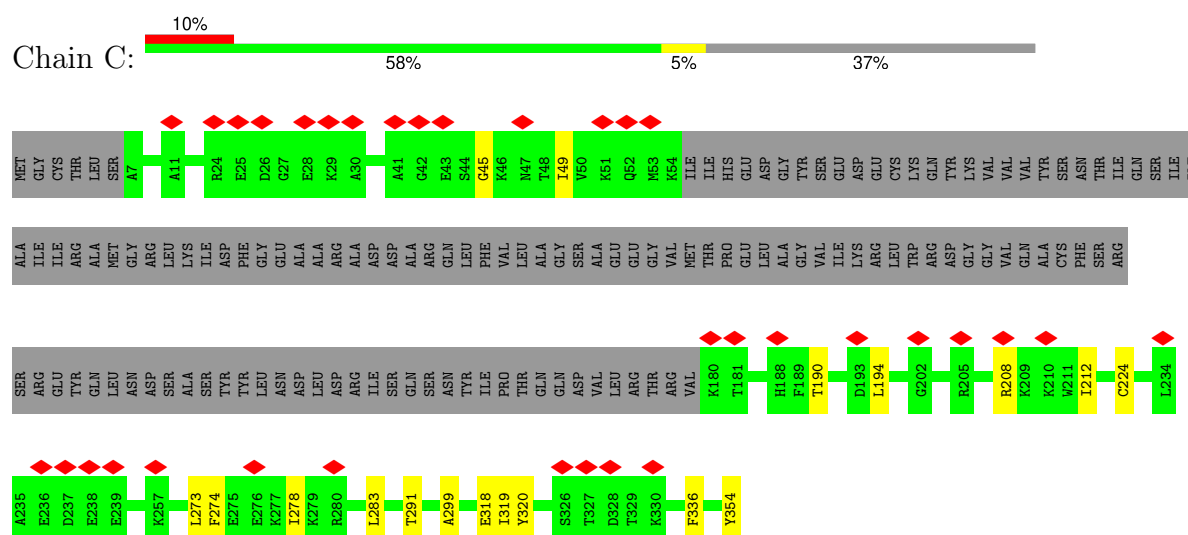


Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	C	O	0
			28	27	1	

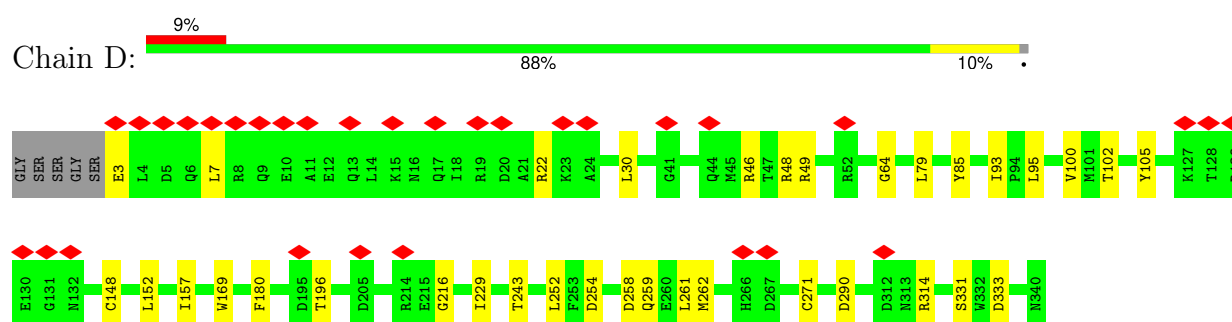
3 Residue-property plots [i](#)

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.

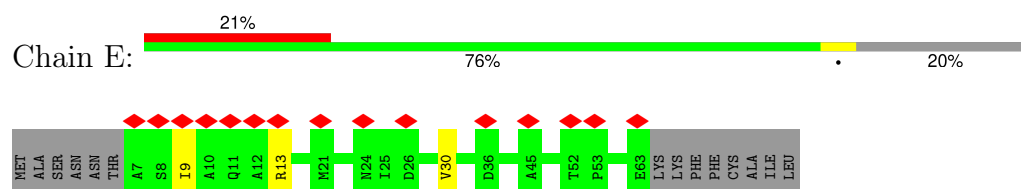
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-3




- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

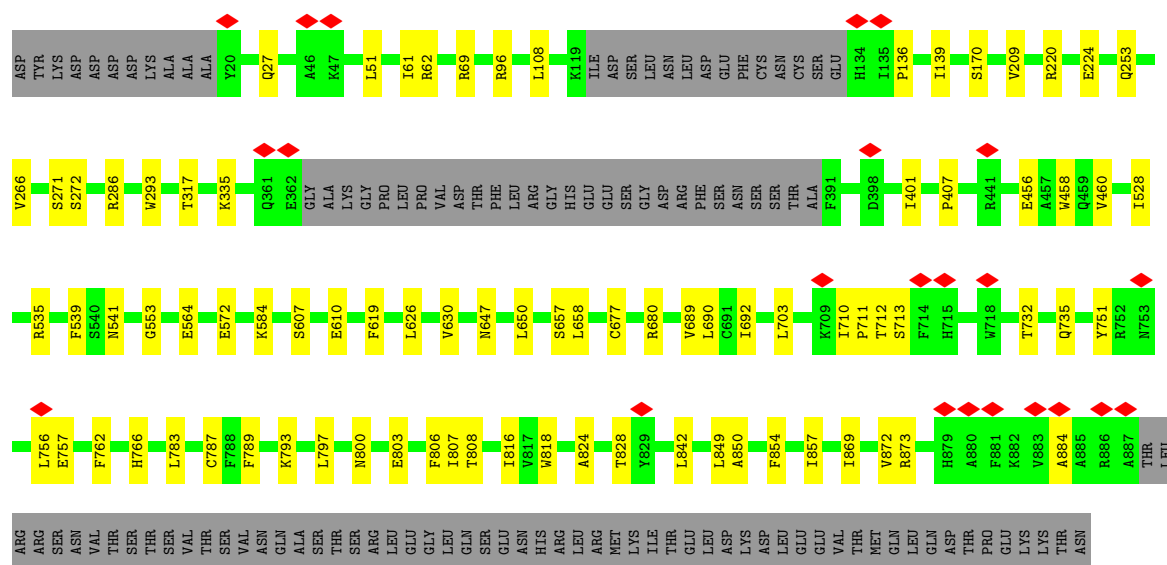


- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



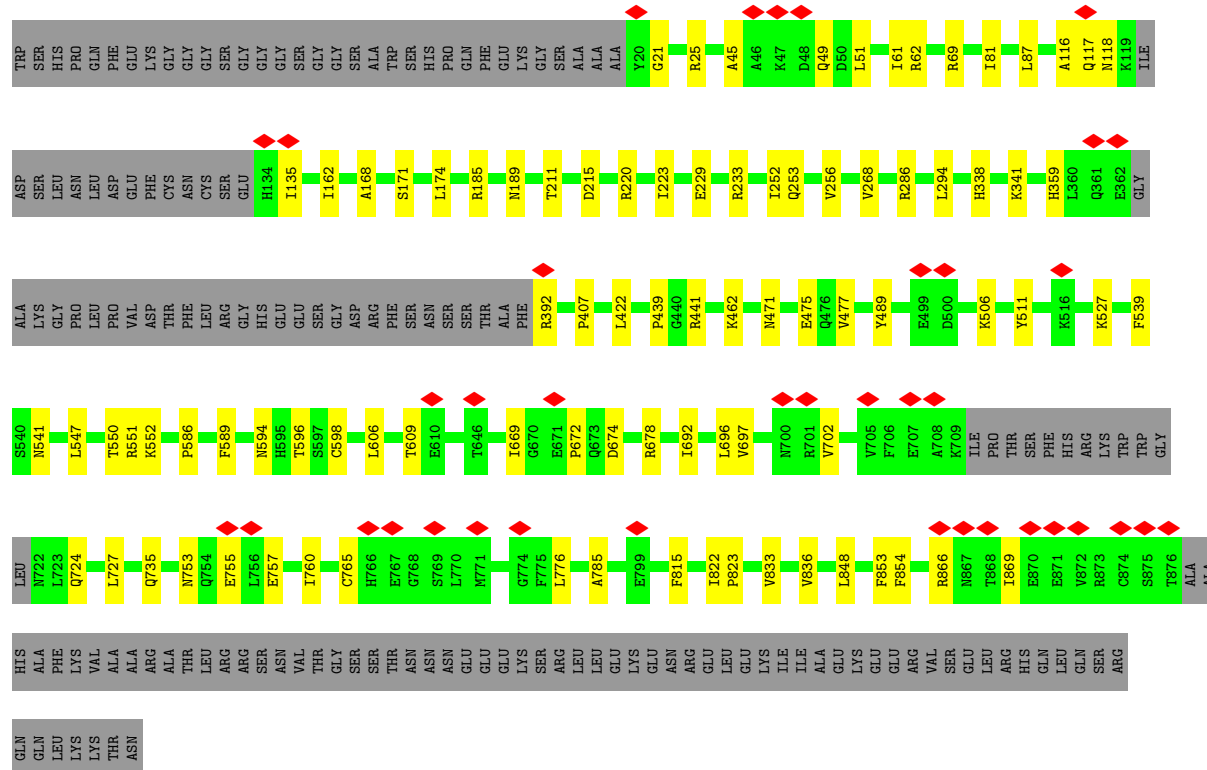
- Molecule 4: Extracellular calcium-sensing receptor

Chain A: 



• Molecule 5: Extracellular calcium-sensing receptor

Chain B: 



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	167678	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.978	Depositor
Minimum map value	-0.251	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	416.496, 416.496, 416.496	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8677, 0.8677, 0.8677	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: PCW, CLR, PO4, CA, NAG

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	C	0.39	0/1795	0.55	0/2415
2	D	0.30	0/2556	0.53	0/3473
3	E	0.37	0/414	0.50	0/562
4	A	0.36	0/6709	0.52	0/9109
5	B	0.41	0/6487	0.54	0/8807
All	All	0.38	0/17961	0.53	0/24366

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1765	0	1728	13	0
2	D	2509	0	2377	24	0
3	E	408	0	391	2	0
4	A	6538	0	6397	60	0
5	B	6327	0	6181	59	0
6	F	28	0	25	0	0
6	G	28	0	25	0	0
6	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	54	0	84	6	0
7	B	54	0	84	0	0
8	A	14	0	13	0	0
8	B	28	0	26	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	30	0	18	3	0
10	B	15	0	9	1	0
11	A	5	0	0	1	0
11	B	5	0	0	1	0
12	B	28	0	46	5	0
All	All	17868	0	17429	157	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 4.

The worst 5 of 157 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)
5:B:854:PHE:CD2	12:B:1401:CLR:H183	1.73	1.22
4:A:787:CYS:SG	4:A:807:ILE:CG2	2.37	1.12
5:B:854:PHE:CD2	12:B:1401:CLR:C18	2.49	0.95
4:A:756:LEU:HD23	4:A:757:GLU:HG2	1.53	0.91
4:A:787:CYS:SG	4:A:807:ILE:HG22	2.08	0.91

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	C	219/354 (62%)	214 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	336/343 (98%)	323 (96%)	13 (4%)	0	100	100
3	E	55/71 (78%)	55 (100%)	0	0	100	100
4	A	821/939 (87%)	803 (98%)	18 (2%)	0	100	100
5	B	794/959 (83%)	769 (97%)	25 (3%)	0	100	100
All	All	2225/2666 (84%)	2164 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	188/310 (61%)	188 (100%)	0	100	100
2	D	256/284 (90%)	256 (100%)	0	100	100
3	E	38/58 (66%)	38 (100%)	0	100	100
4	A	701/817 (86%)	701 (100%)	0	100	100
5	B	683/827 (83%)	683 (100%)	0	100	100
All	All	1866/2296 (81%)	1866 (100%)	0	92	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	117	GLN
5	B	753	ASN
5	B	800	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
6	NAG	F	1	4,6	14,14,15	0.27	0	17,19,21	0.49	0
6	NAG	F	2	6	14,14,15	0.24	0	17,19,21	0.42	0
6	NAG	G	1	4,6	14,14,15	0.36	0	17,19,21	0.41	0
6	NAG	G	2	6	14,14,15	0.23	0	17,19,21	0.45	0
6	NAG	H	1	5,6	14,14,15	0.29	0	17,19,21	0.57	0
6	NAG	H	2	6	14,14,15	0.27	0	17,19,21	0.66	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
6	NAG	F	1	4,6	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	NAG	G	1	4,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	NAG	H	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

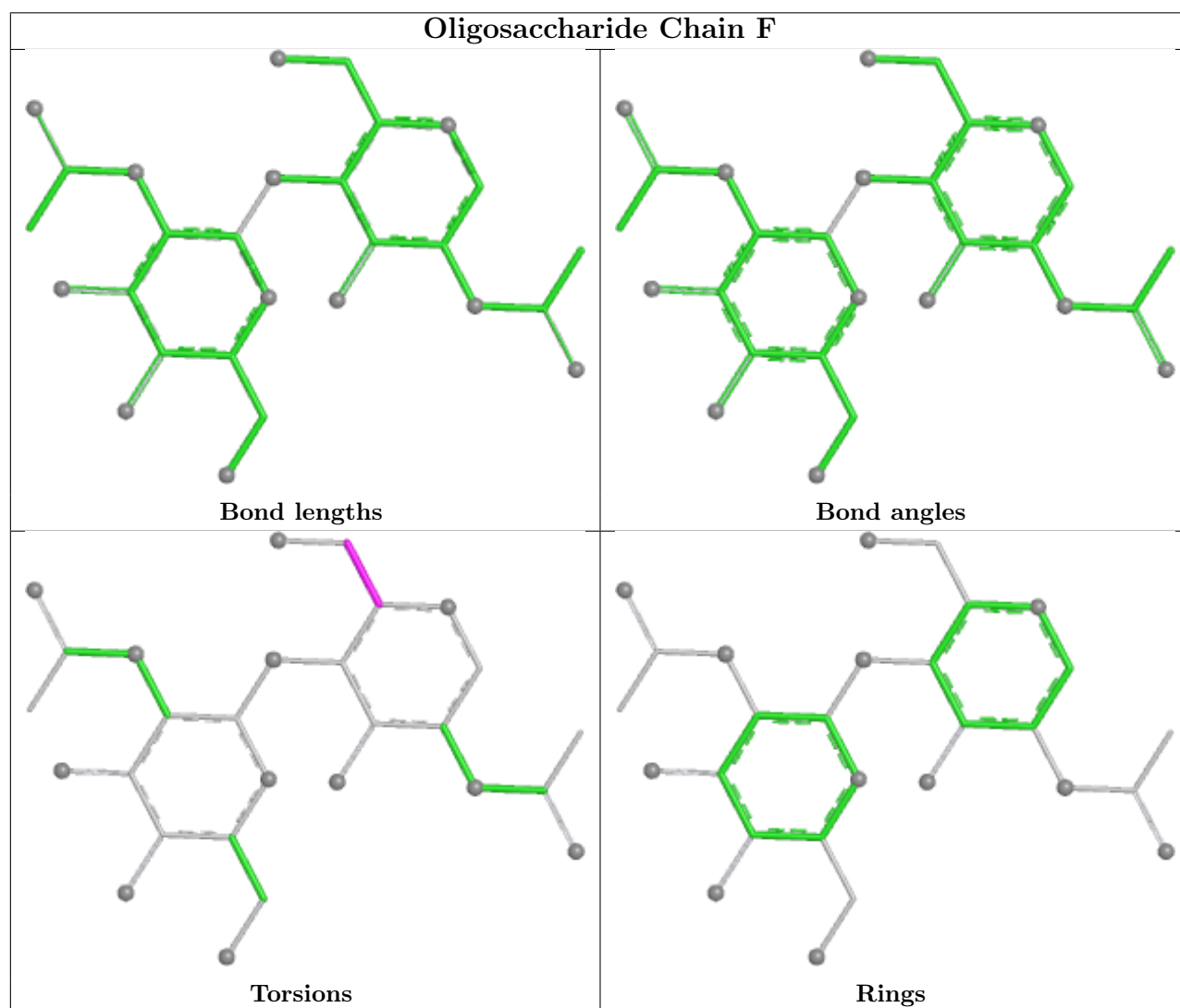
5 of 6 torsion outliers are listed below:

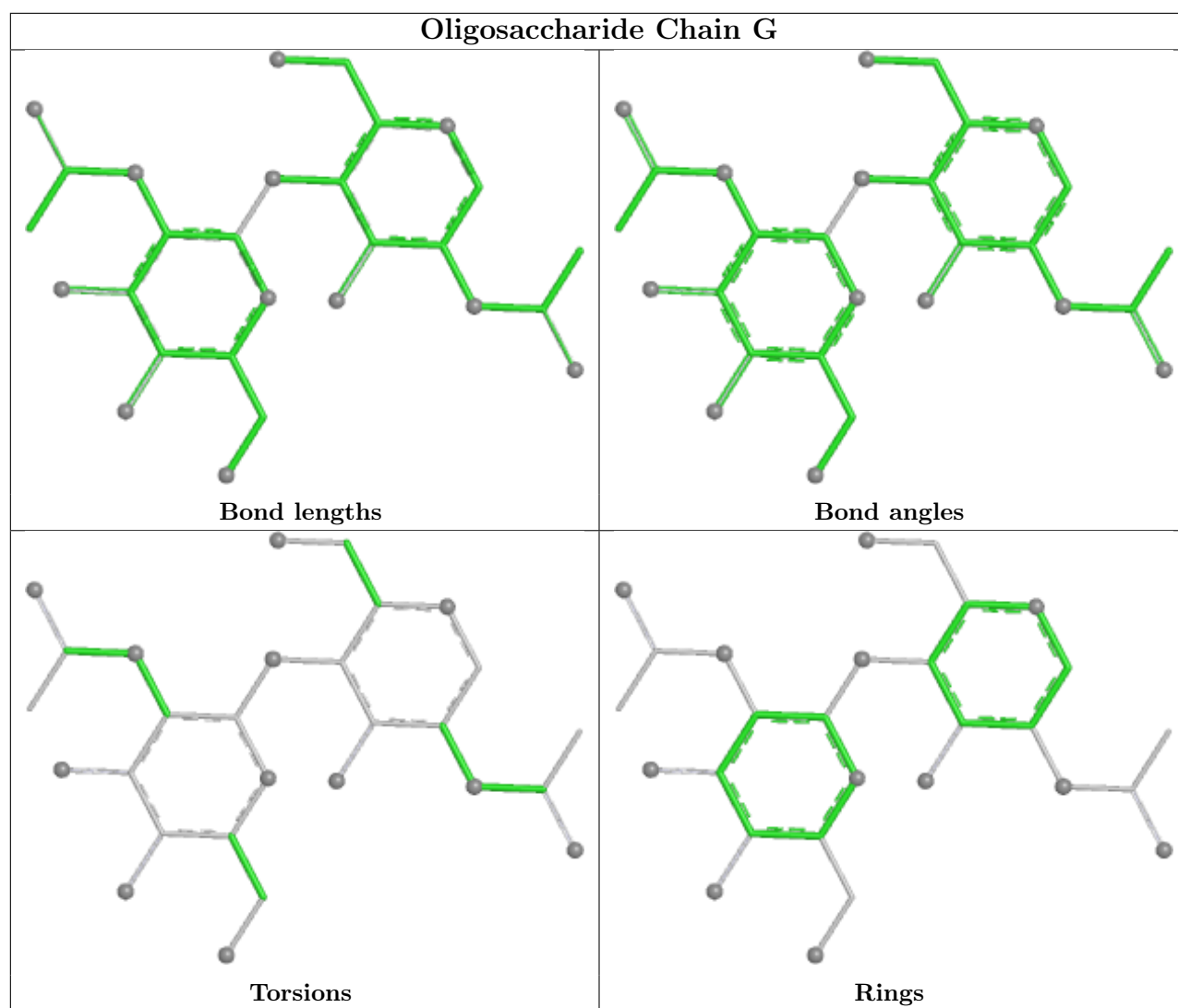
Mol	Chain	Res	Type	Atoms
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
6	H	1	NAG	C8-C7-N2-C2
6	H	1	NAG	O7-C7-N2-C2
6	F	1	NAG	C4-C5-C6-O6

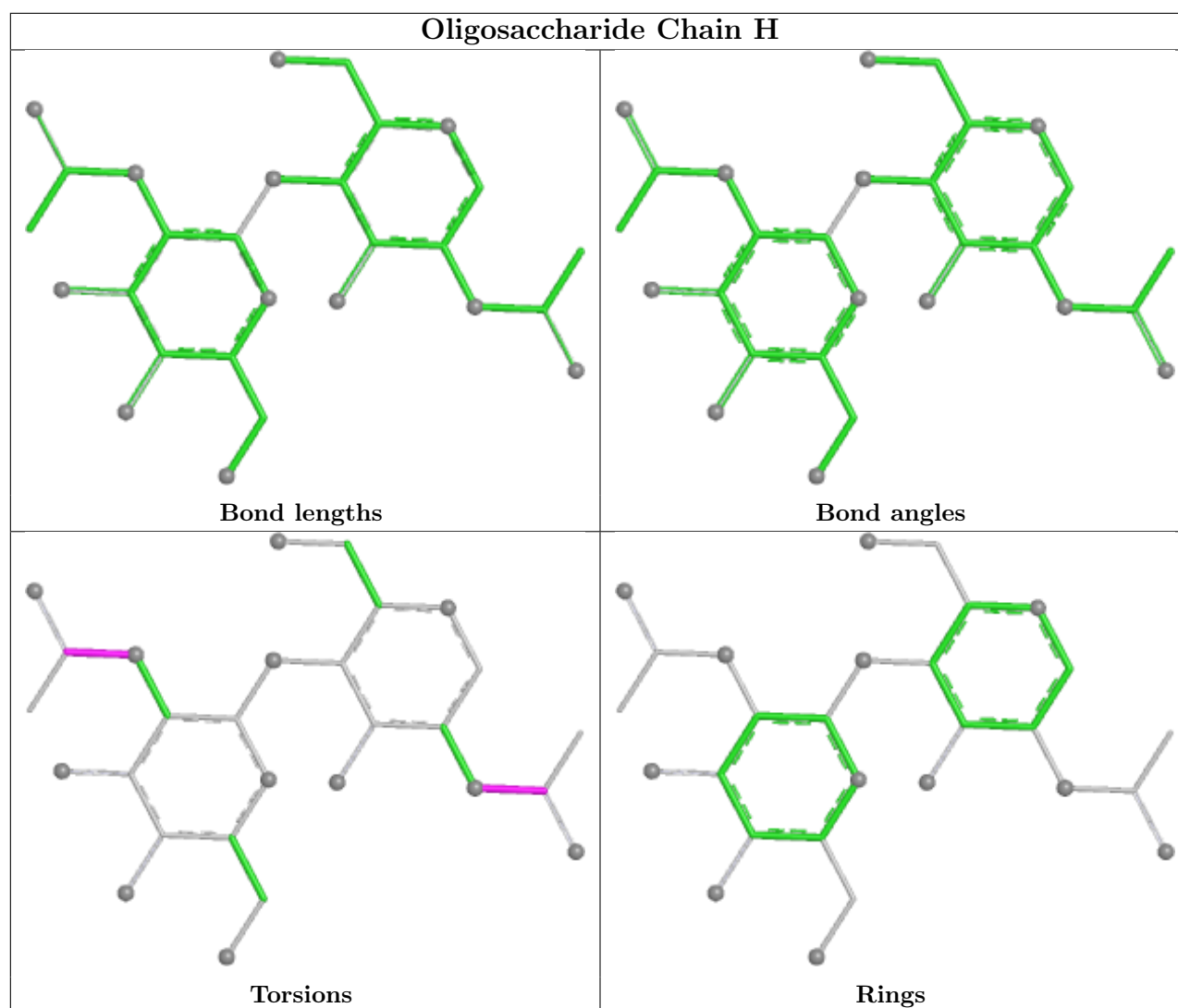
There are no ring outliers.

No monomer is involved in short contacts.

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 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	$\# Z > 2$
7	PCW	A	1001	-	53,53,53	1.52	8 (15%)	59,61,61	0.98	3 (5%)
10	TRP	A	1005	-	14,16,16	0.92	1 (7%)	13,22,22	1.18	1 (7%)
11	PO4	A	1006	-	4,4,4	1.08	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	A	1002	4	14,14,15	0.23	0	17,19,21	0.43	0
8	NAG	B	1403	5	14,14,15	0.30	0	17,19,21	0.64	0
10	TRP	B	1407	-	14,16,16	0.92	1 (7%)	13,22,22	1.13	1 (7%)
11	PO4	B	1408	-	4,4,4	1.06	0	6,6,6	0.44	0
12	CLR	B	1401	-	31,31,31	0.66	1 (3%)	48,48,48	1.52	9 (18%)
7	PCW	B	1402	-	53,53,53	1.54	8 (15%)	59,61,61	0.99	3 (5%)
8	NAG	B	1404	5	14,14,15	0.28	0	17,19,21	0.51	0
10	TRP	A	1007	-	14,16,16	0.85	1 (7%)	13,22,22	0.88	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
7	PCW	A	1001	-	1/1/5/9	29/57/57/57	-
10	TRP	A	1005	-	-	2/7/8/8	0/2/2/2
8	NAG	A	1002	4	-	1/6/23/26	0/1/1/1
8	NAG	B	1403	5	-	2/6/23/26	0/1/1/1
10	TRP	B	1407	-	-	1/7/8/8	0/2/2/2
12	CLR	B	1401	-	-	6/10/68/68	0/4/4/4
7	PCW	B	1402	-	-	24/57/57/57	-
8	NAG	B	1404	5	-	1/6/23/26	0/1/1/1
10	TRP	A	1007	-	-	6/7/8/8	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1402	PCW	O2-C31	5.29	1.49	1.34
7	A	1001	PCW	O2-C31	5.19	1.48	1.34
7	B	1402	PCW	C32-C31	3.43	1.60	1.50
7	A	1001	PCW	C32-C31	3.43	1.60	1.50
7	B	1402	PCW	O3-C11	3.03	1.42	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1401	CLR	C13-C17-C20	-4.13	113.12	119.50
7	B	1402	PCW	O2-C31-C32	4.01	120.16	111.48
7	A	1001	PCW	O2-C31-C32	3.78	119.66	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1401	CLR	C19-C10-C9	-3.78	107.42	111.66
7	B	1402	PCW	C18-C19-C20	3.74	152.88	124.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1001	PCW	C2

5 of 72 torsion outliers are listed below:

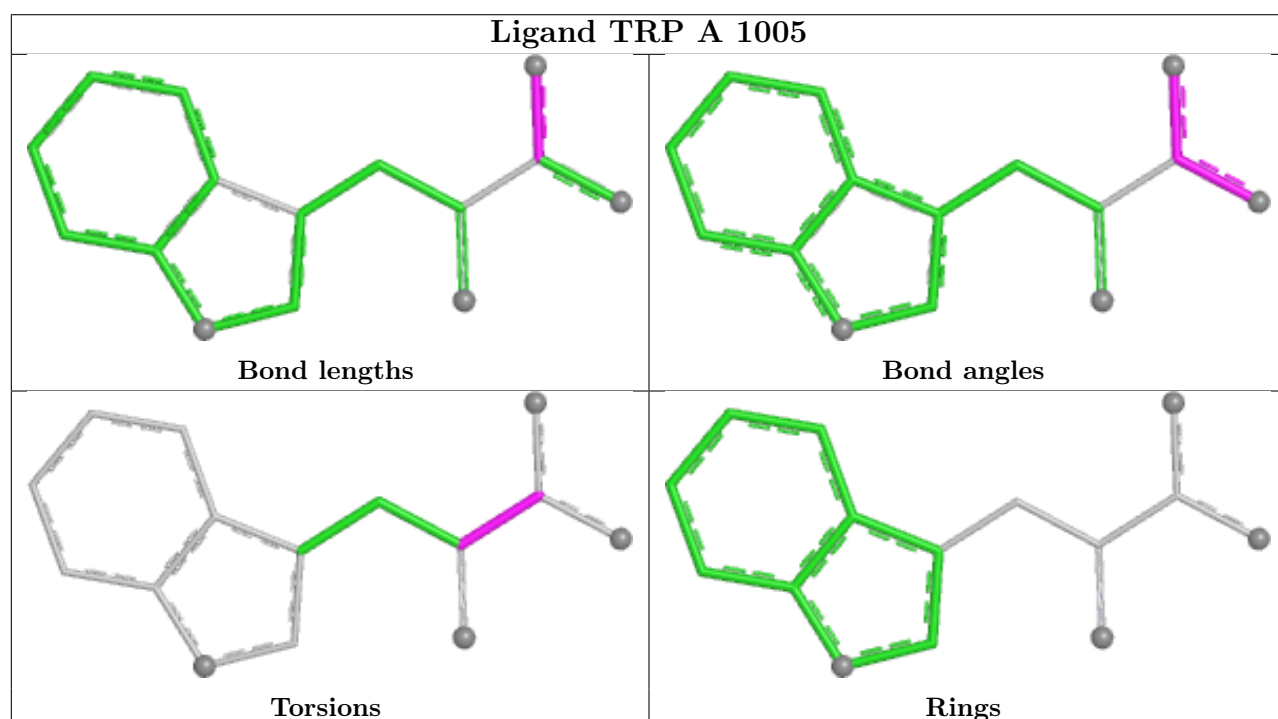
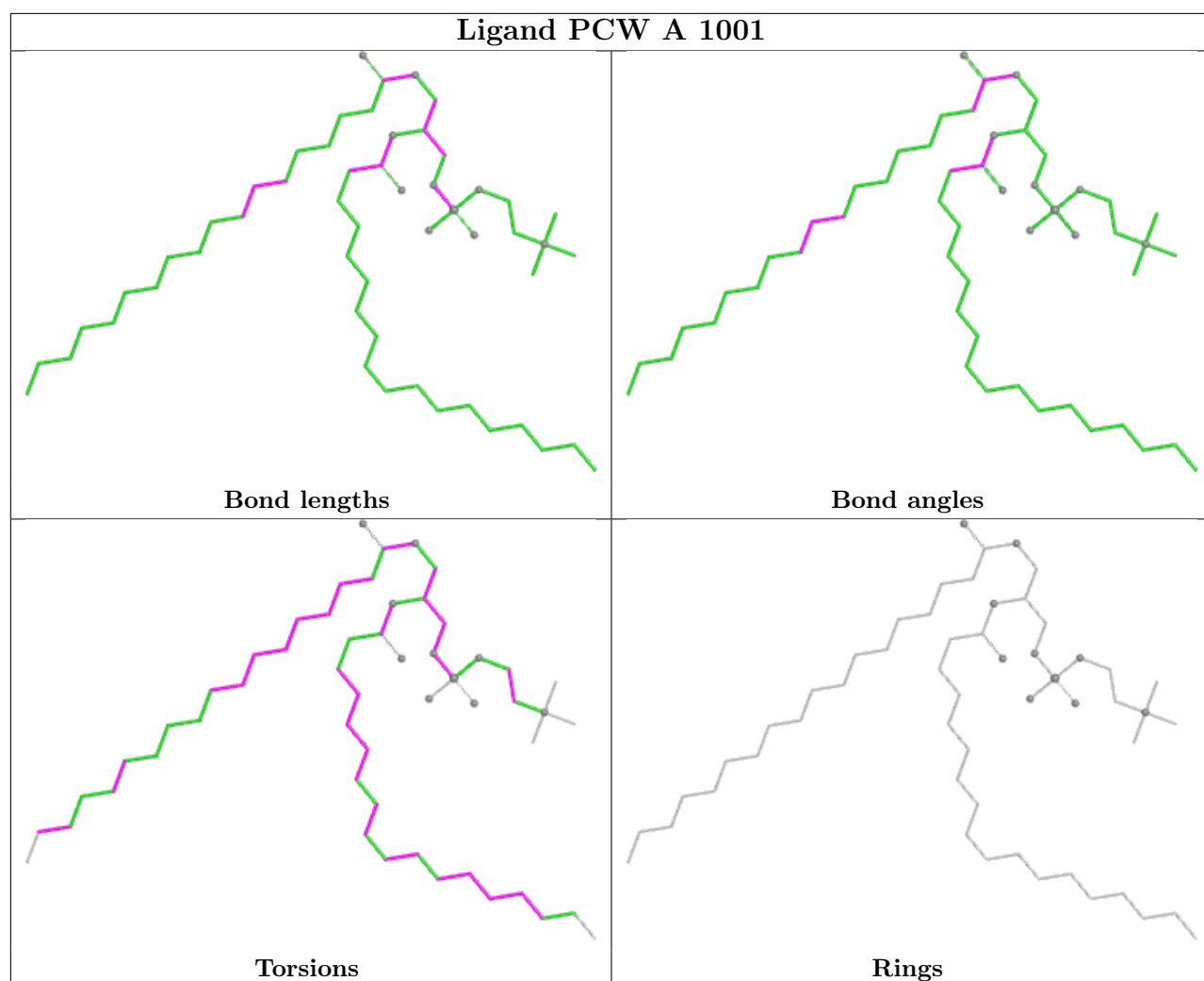
Mol	Chain	Res	Type	Atoms
7	A	1001	PCW	O4P-C4-C5-N
7	A	1001	PCW	C32-C31-O2-C2
7	B	1402	PCW	C1-O3P-P-O1P
7	B	1402	PCW	C1-O3P-P-O2P
7	B	1402	PCW	C1-O3P-P-O4P

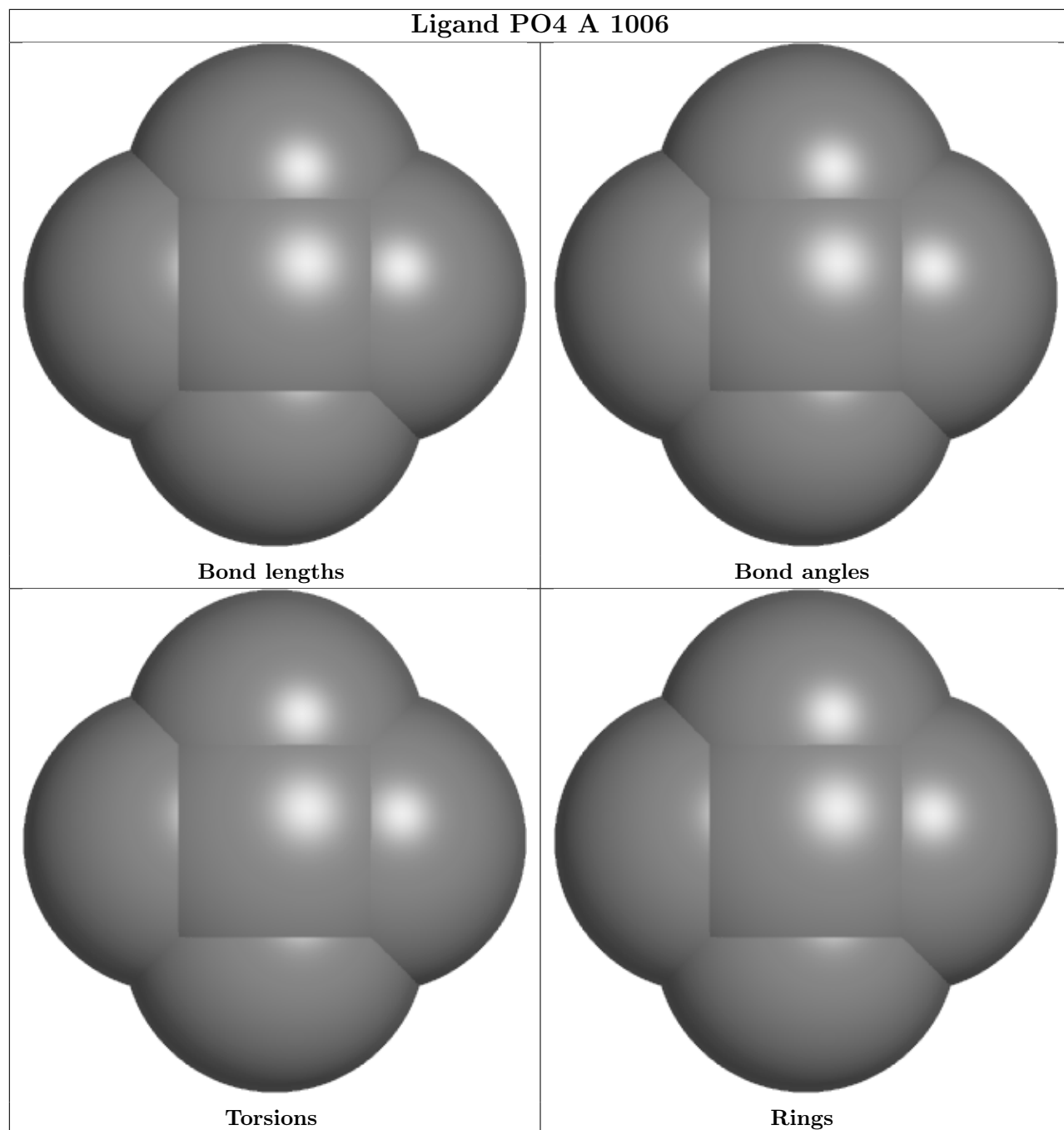
There are no ring outliers.

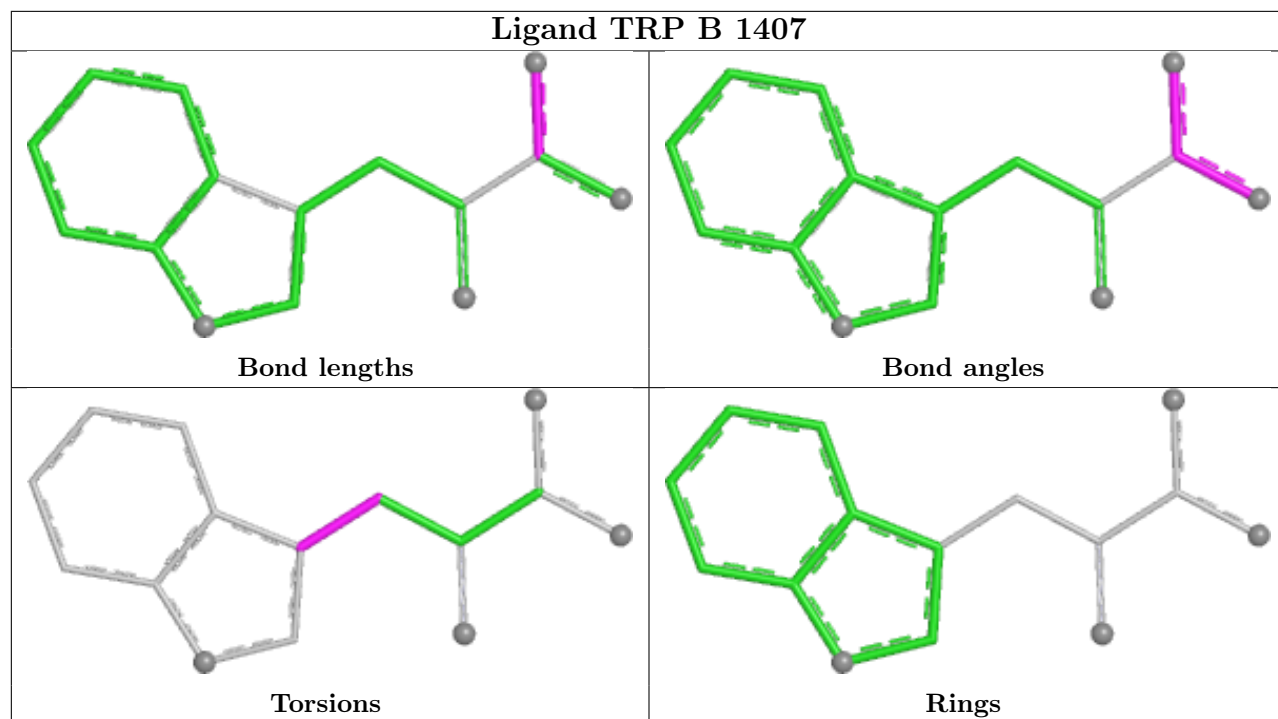
7 monomers are involved in 16 short contacts:

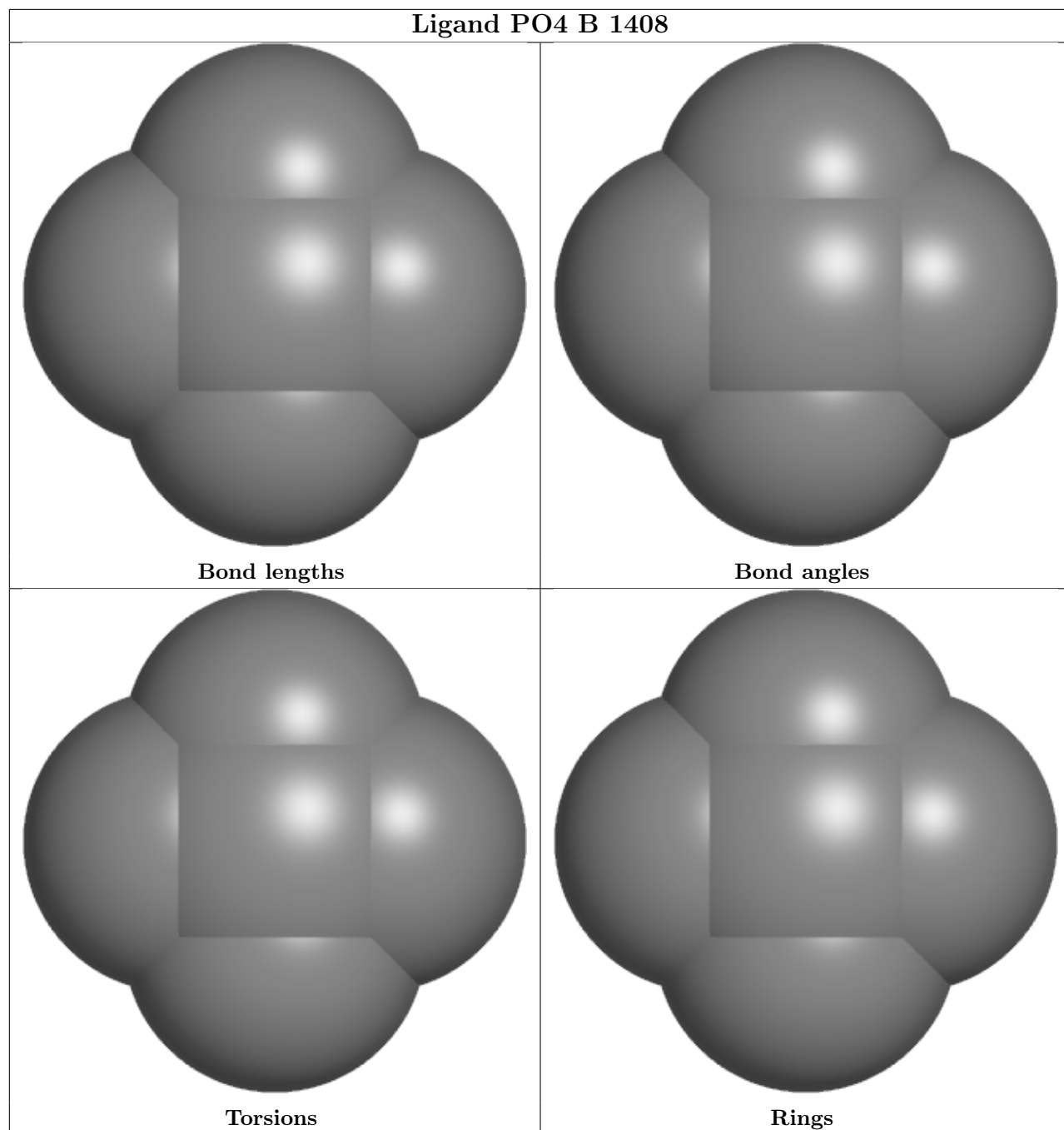
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1001	PCW	6	0
10	A	1005	TRP	1	0
11	A	1006	PO4	1	0
10	B	1407	TRP	1	0
11	B	1408	PO4	1	0
12	B	1401	CLR	5	0
10	A	1007	TRP	2	0

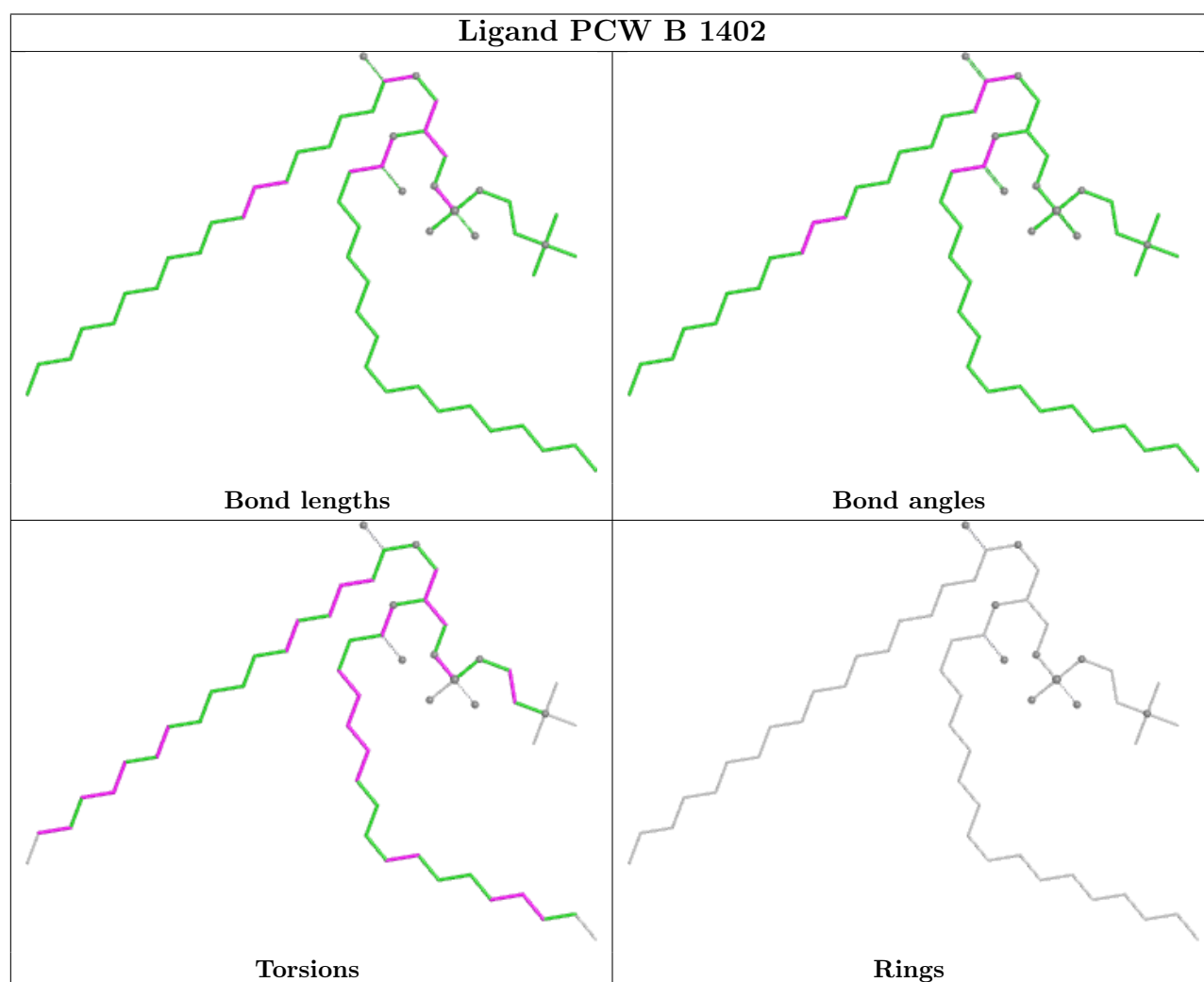
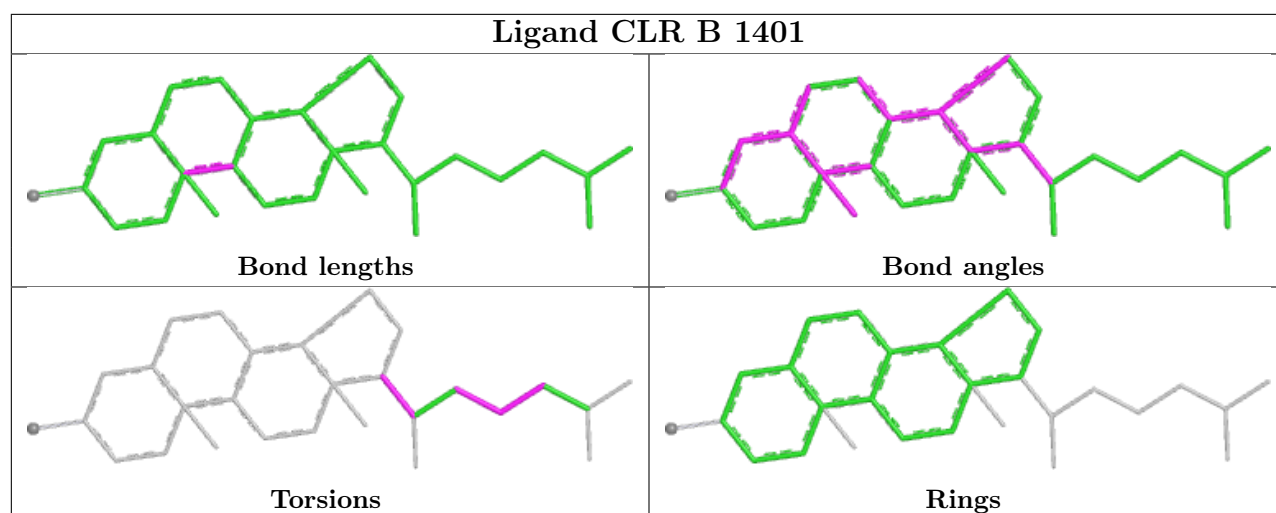
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

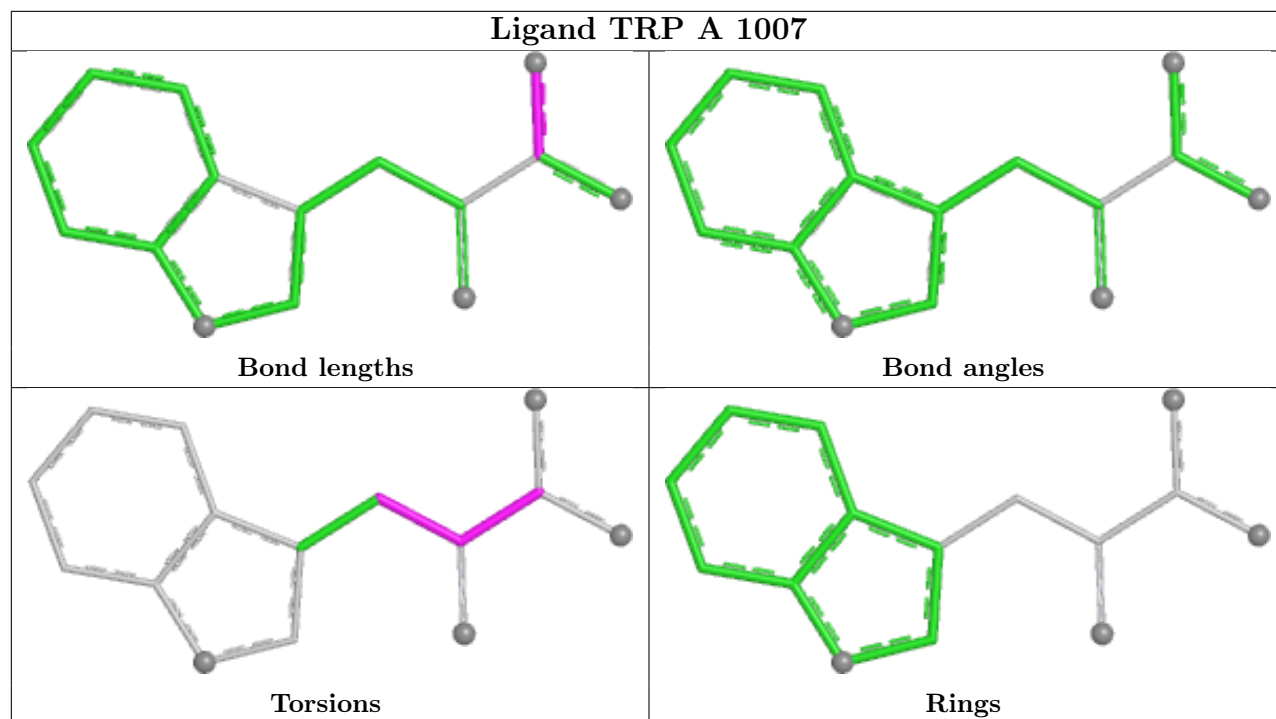












5.7 Other polymers [i](#)

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-40917. These allow visual inspection of the internal detail of the map and identification of artifacts.

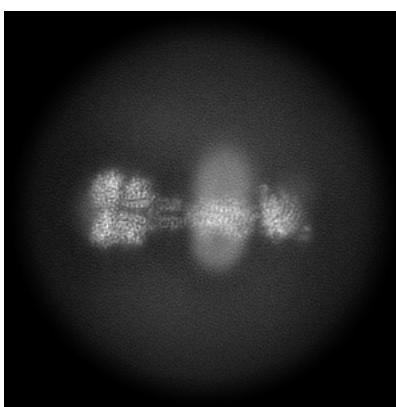
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

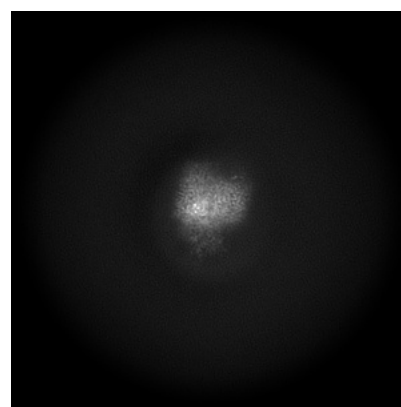
6.1.1 Primary map



X



Y

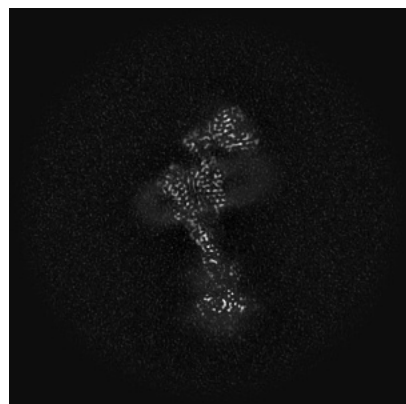


Z

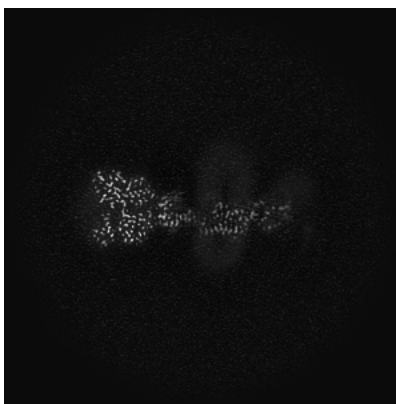
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

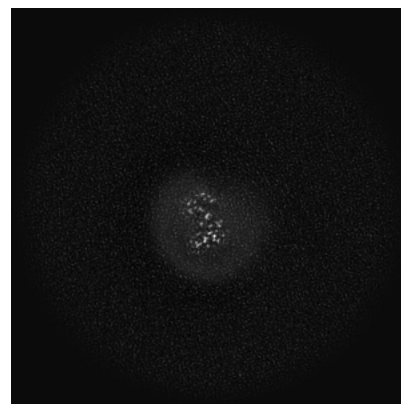
6.2.1 Primary map



X Index: 240



Y Index: 240

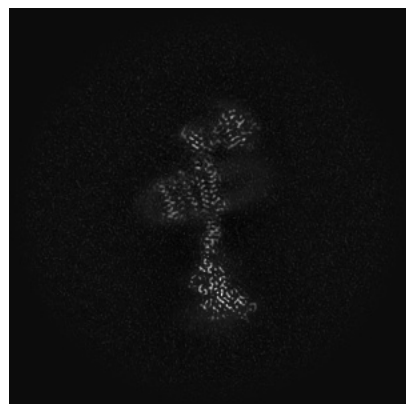


Z Index: 240

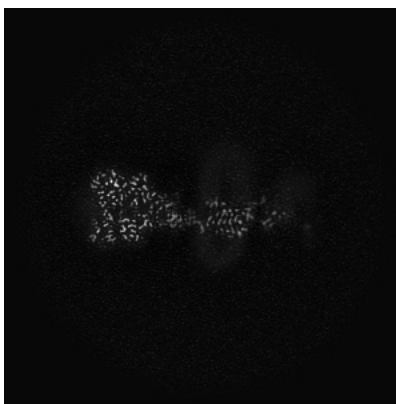
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

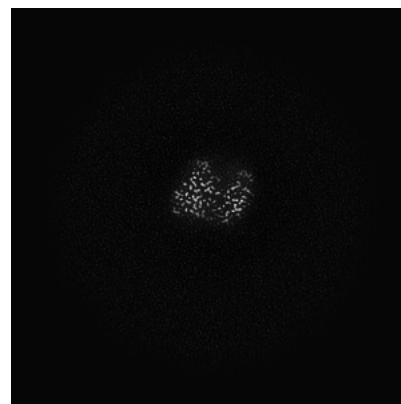
6.3.1 Primary map



X Index: 225



Y Index: 243



Z Index: 123

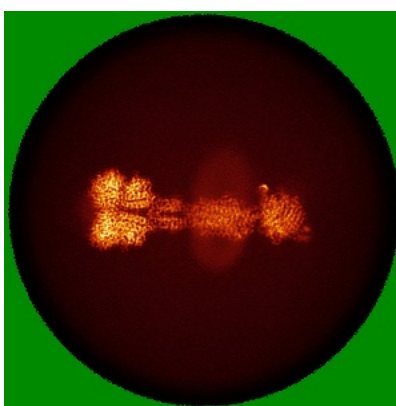
The images above show the largest variance slices of the map in three orthogonal directions.

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

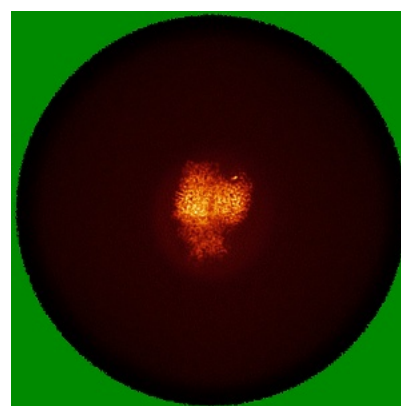
6.4.1 Primary map



X



Y

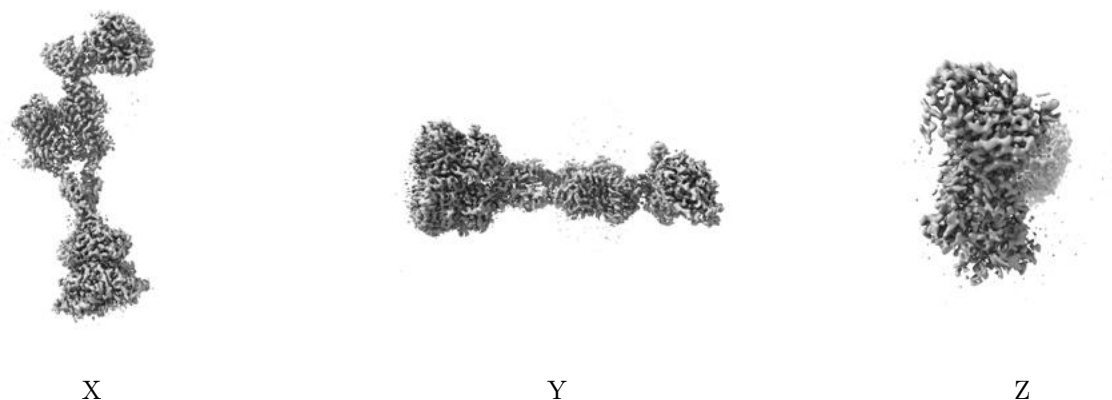


Z

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

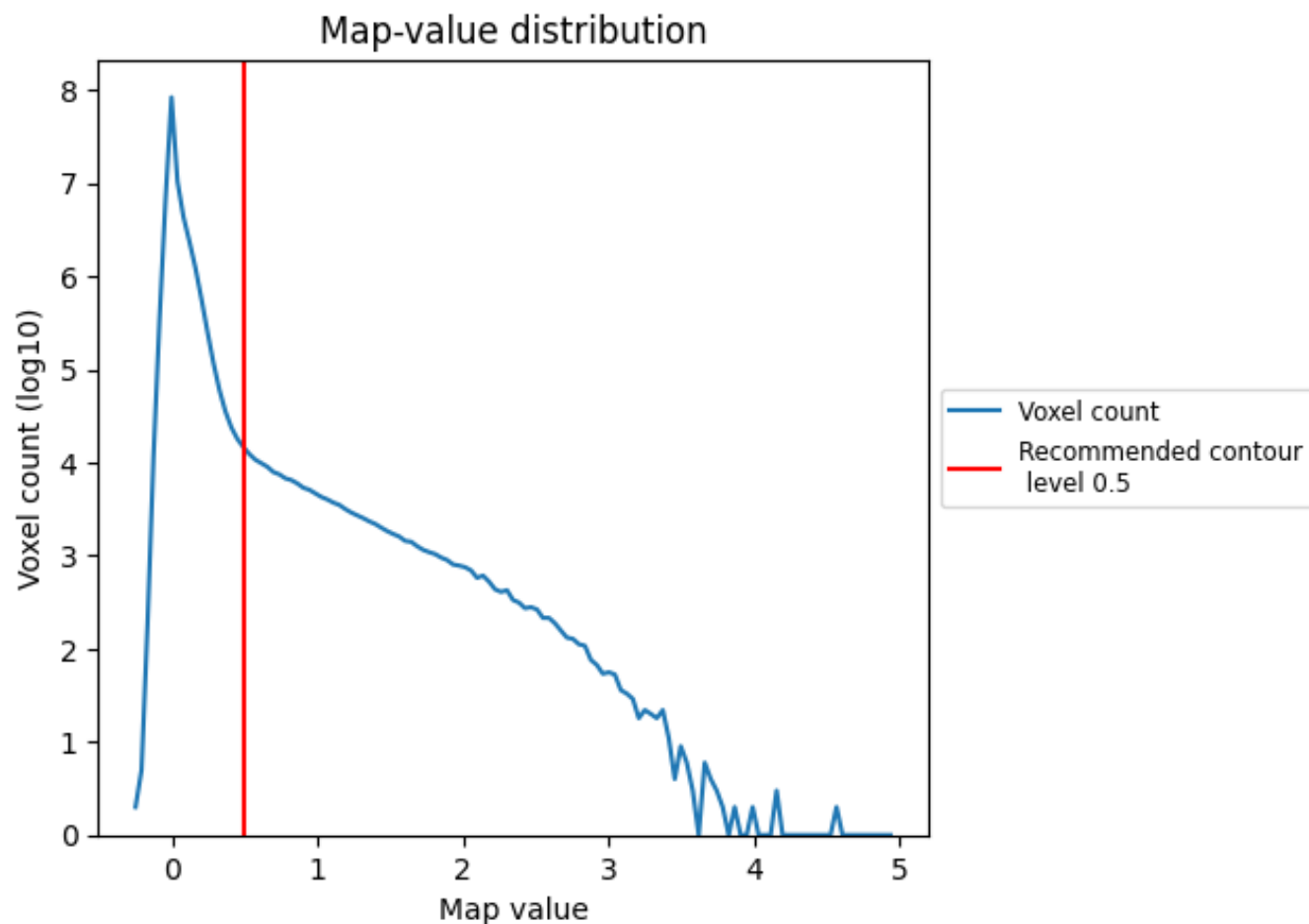
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

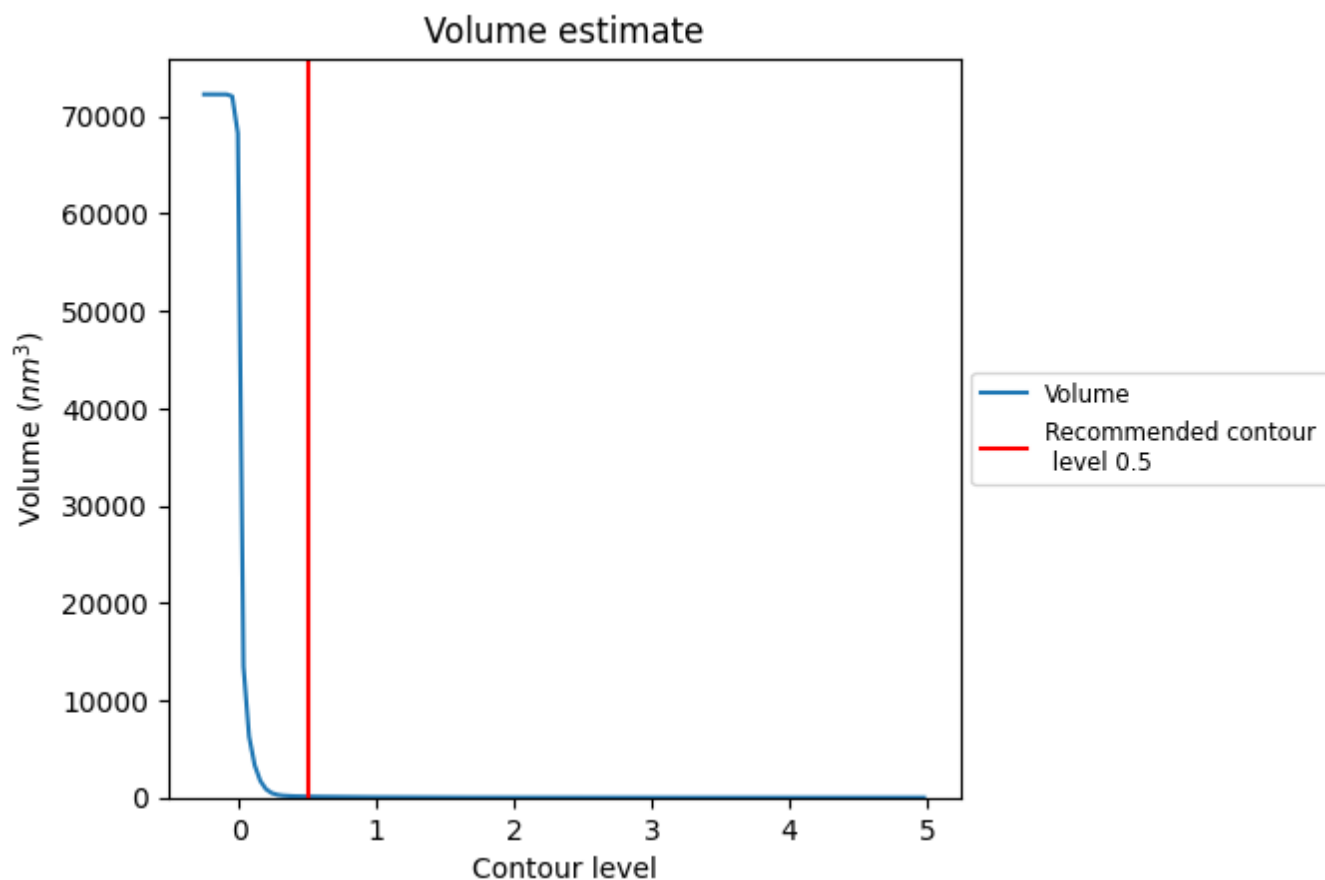
This section contains the results of statistical analysis of the map.

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.

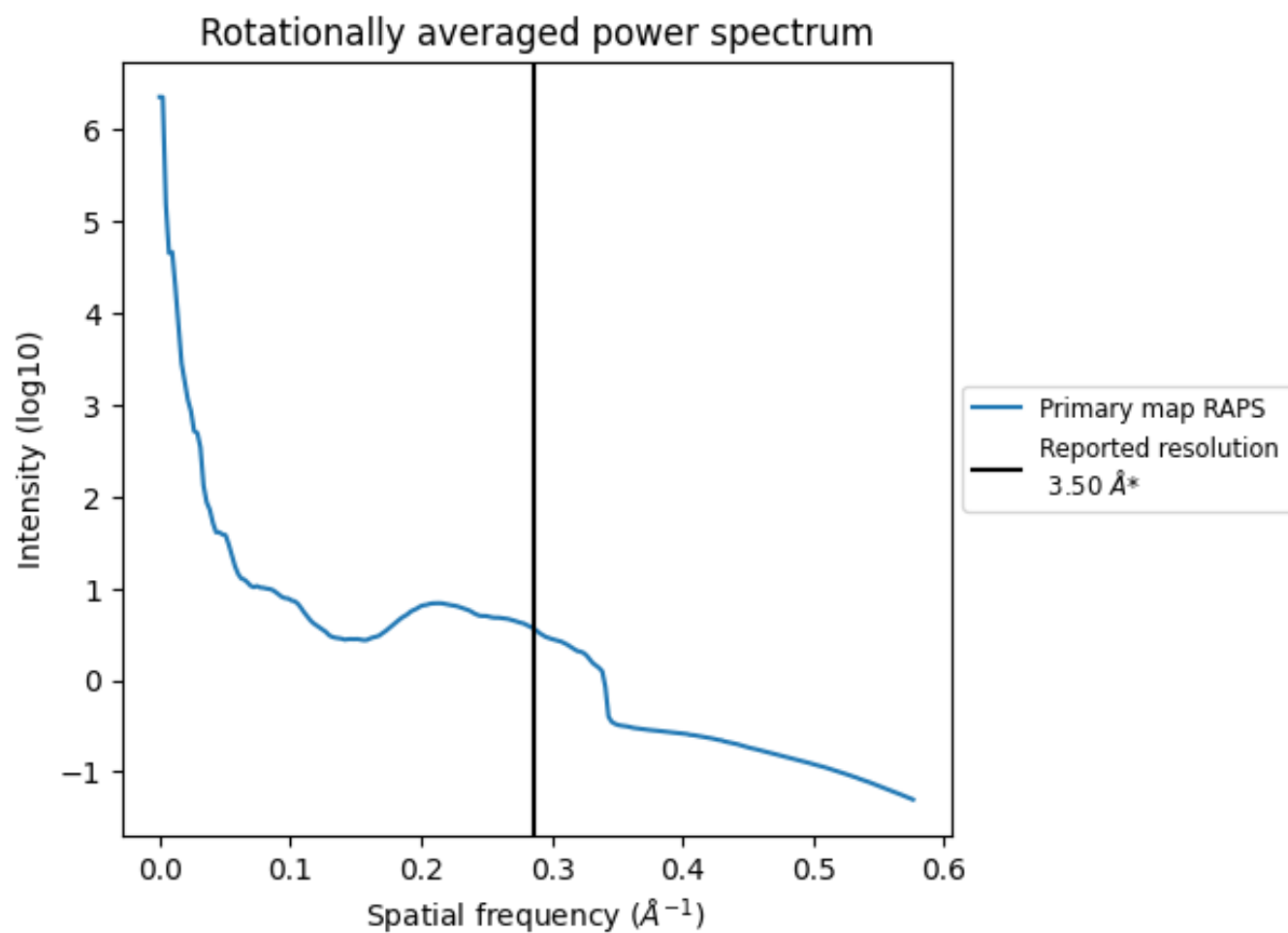
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm^3 ; this corresponds to an approximate mass of 94 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 0.286 Å⁻¹

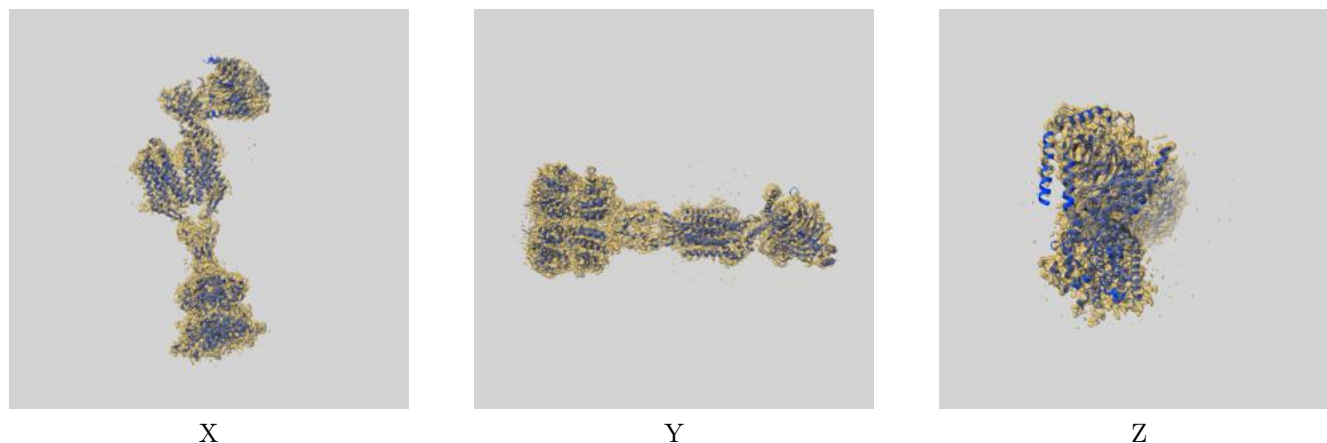
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

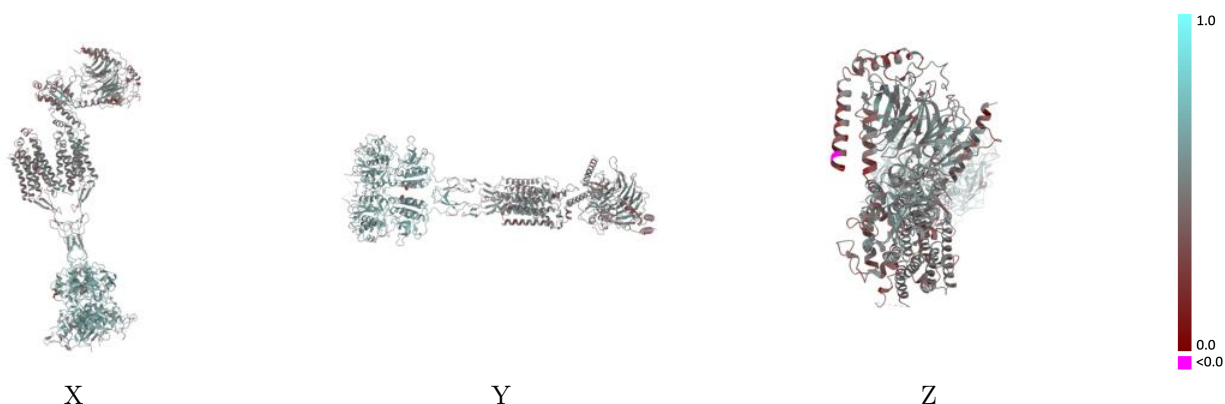
This section contains information regarding the fit between EMDB map EMD-40917 and PDB model 8SZI. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



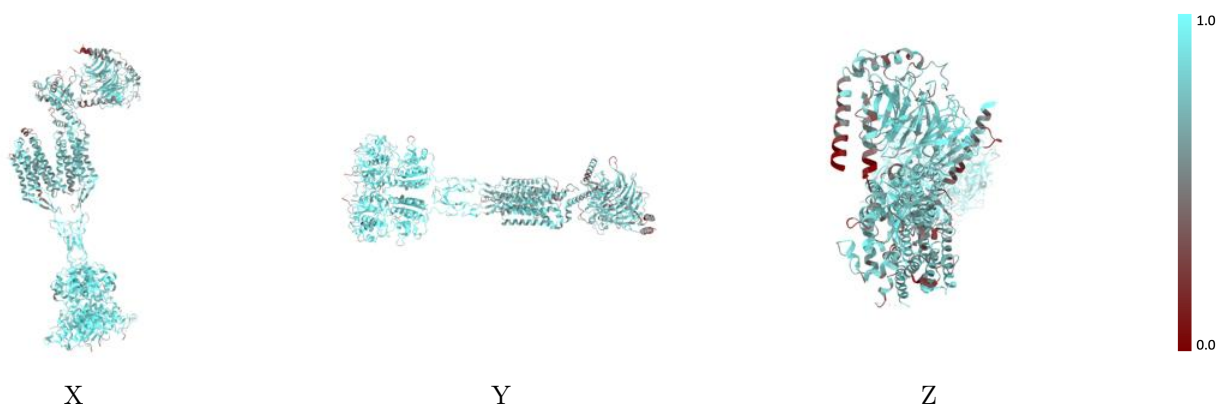
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



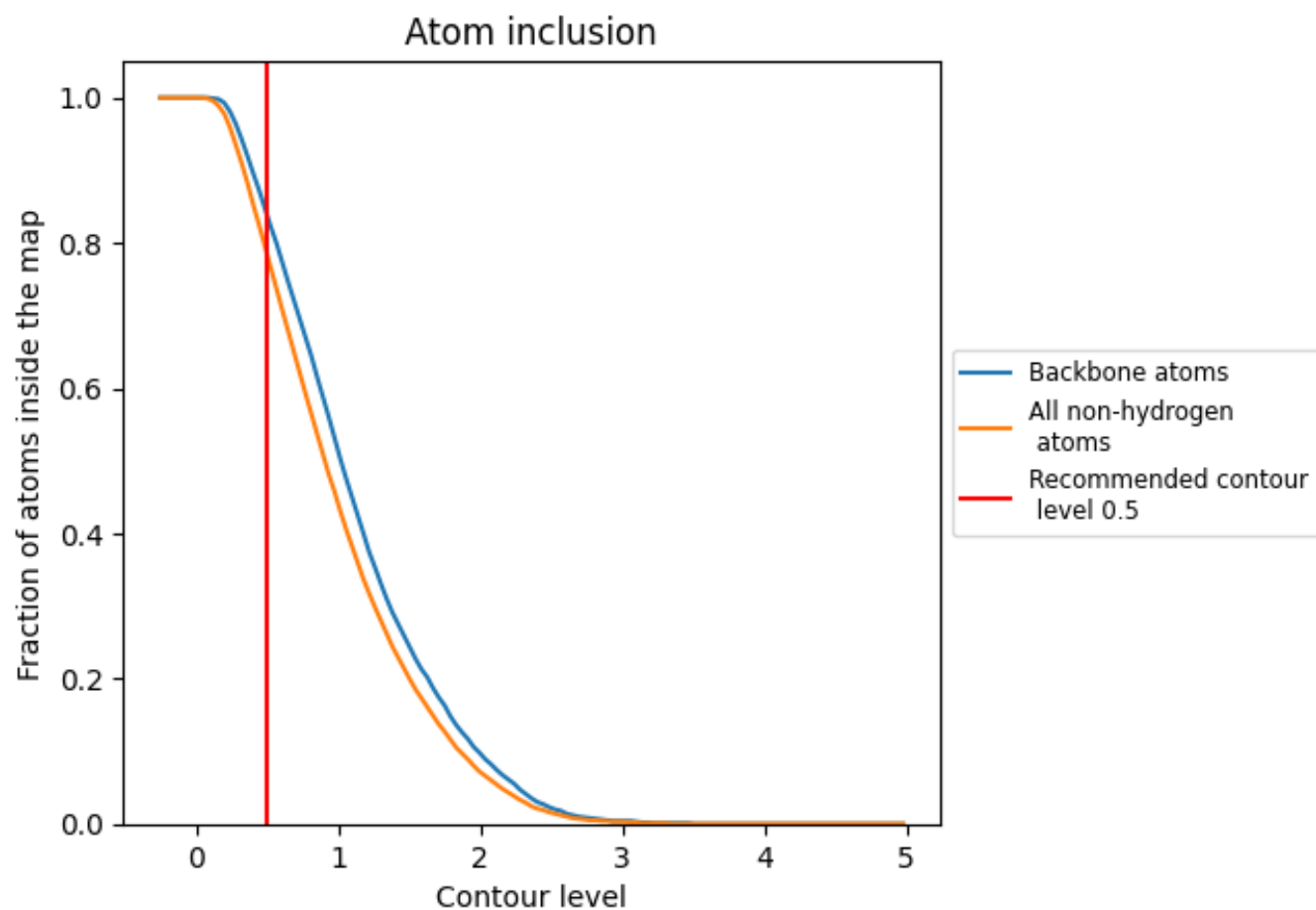
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 78% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7840	<div></div> 0.5100
A	<div></div> 0.8270	<div></div> 0.5340
B	<div></div> 0.8150	<div></div> 0.5260
C	<div></div> 0.6580	<div></div> 0.4460
D	<div></div> 0.7260	<div></div> 0.4700
E	<div></div> 0.5280	<div></div> 0.3920
F	<div></div> 0.5360	<div></div> 0.3990
G	<div></div> 0.6790	<div></div> 0.5050
H	<div></div> 0.6070	<div></div> 0.3740

