



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 02:28 AM UTC

PDB ID : 9FAV / pdb\_00009fav  
EMDB ID : EMD-50283  
Title : CryoEM structure of human full-length beta3gamma2 GABA(A) receptor in complex with GARLH4, the TMD of Neuroligin2 and Megabody25, in a closed state (StateC2)  
Authors : Kasaragod, V.B.; Aricescu, A.R.  
Deposited on : 2024-05-10  
Resolution : 3.20 Å (reported)  
Based on initial model : 7QNB

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

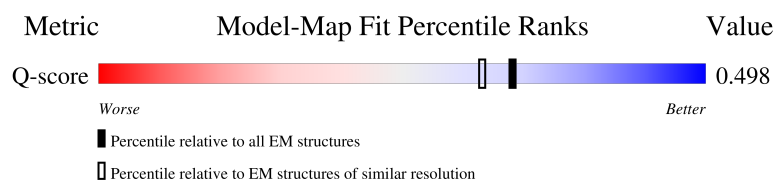
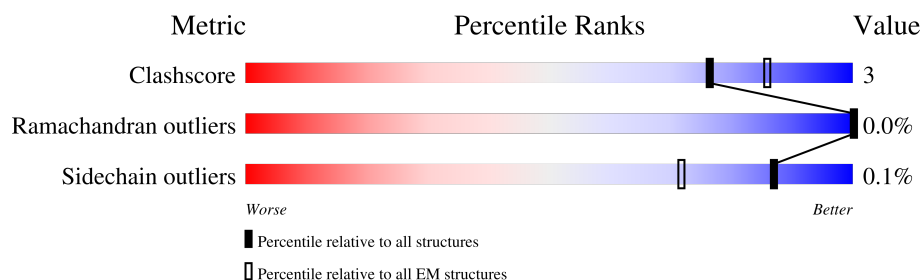
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.20 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.



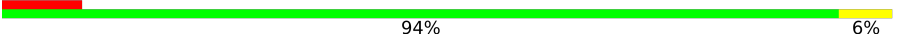
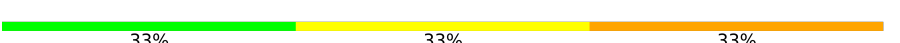
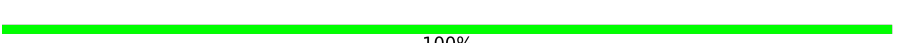
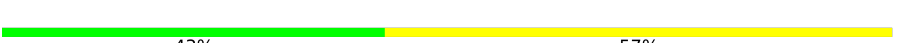
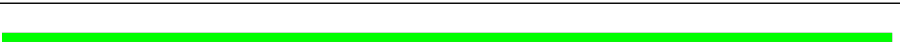
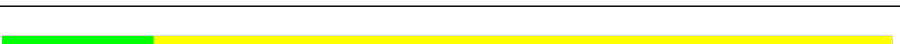
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 15020 ( 2.70 - 3.70 )                                    |

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  $\geq 3$ , 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     | 439    |  |
| 1   | B     | 439    |  |
| 1   | D     | 439    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 439    |    |
| 2   | C     | 405    |    |
| 3   | H     | 33     |    |
| 4   | L     | 185    |    |
| 5   | F     | 522    |    |
| 5   | K     | 522    |    |
| 5   | O     | 522    |    |
| 6   | G     | 3      |    |
| 6   | N     | 3      |    |
| 7   | I     | 7      |    |
| 8   | J     | 2      |    |
| 8   | Q     | 2      |    |
| 9   | M     | 6      |  |
| 10  | P     | 8      |  |
| 11  | R     | 5      |  |

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 18975 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 Gamma-aminobutyric acid receptor subunit beta-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | B     | 330      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2712  | 1777 | 442 | 477 | 16 |         |       |
| 1   | E     | 331      | Total | C    | N   | O   | S  | 3       | 0     |
|     |       |          | 2745  | 1805 | 444 | 480 | 16 |         |       |
| 1   | A     | 330      | Total | C    | N   | O   | S  | 2       | 0     |
|     |       |          | 2731  | 1792 | 446 | 477 | 16 |         |       |
| 1   | D     | 330      | Total | C    | N   | O   | S  | 2       | 0     |
|     |       |          | 2732  | 1795 | 443 | 478 | 16 |         |       |

- Molecule 2 is a protein called Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | C     | 352      | Total | C    | N   | O   | S  | 2       | 0     |
|     |       |          | 2951  | 1935 | 480 | 516 | 20 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 429     | GLY      | -      | expression tag | UNP P18507 |

- Molecule 3 is a protein called Neuroligin-2.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 3   | H     | 33       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 255   | 168 | 38 | 49 |         |       |

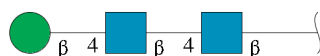
- Molecule 4 is a protein called LHFPL tetraspan subfamily member 4 protein.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 4   | L     | 185      | Total | C   | N   | O   | S  | 1       | 0     |
|     |       |          | 1432  | 953 | 226 | 238 | 15 |         |       |

- Molecule 5 is a protein called Megabody25.

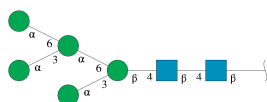
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | K     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 912   | 575 | 156 | 177 | 4 |         |       |
| 5   | O     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 902   | 570 | 154 | 174 | 4 |         |       |
| 5   | F     | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 912   | 575 | 156 | 177 | 4 |         |       |

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 6   | G     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 6   | N     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



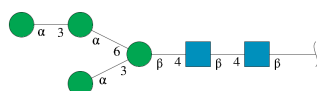
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 7   | I     | 7        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 83    | 46 | 2 | 35 |         |       |

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



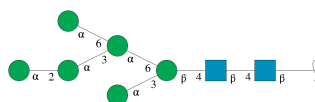
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 8   | J     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 8   | Q     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



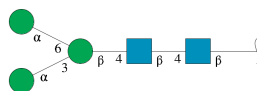
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 9   | M     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



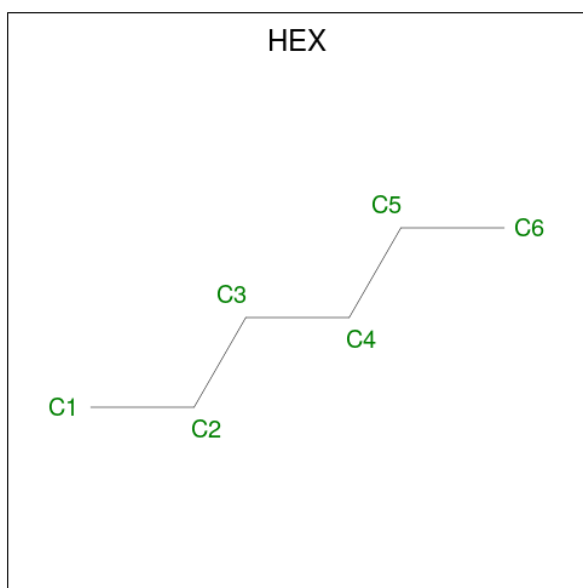
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 10  | P     | 8        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 94    | 52 | 2 | 40 |         |       |

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



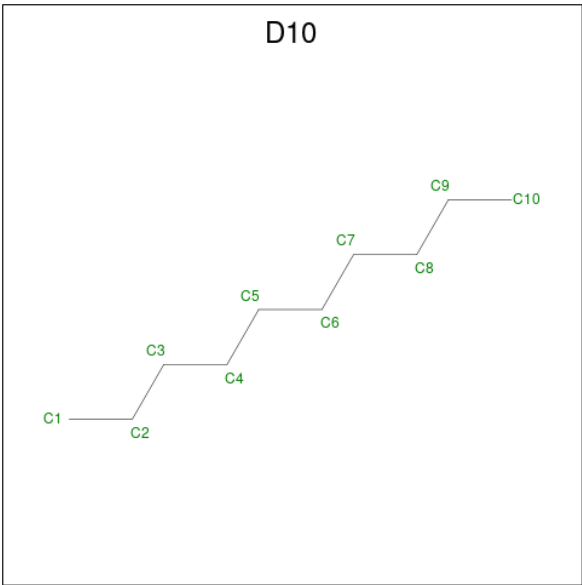
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 11  | R     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |

- Molecule 12 is HEXANE (CCD ID: HEX) (formula:  $C_6H_{14}$ ).



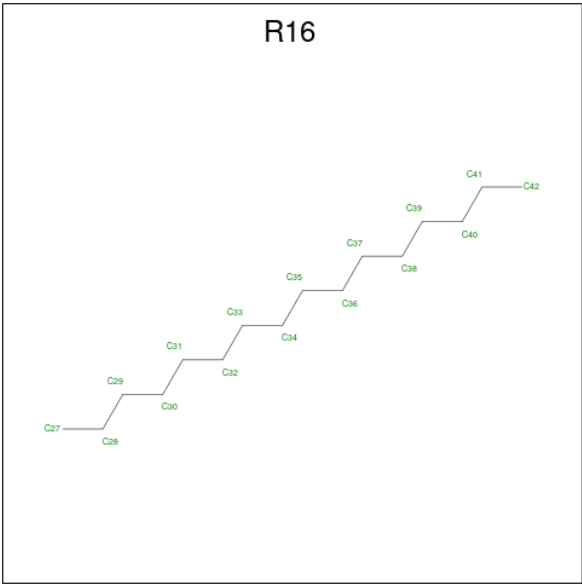
| Mol | Chain | Residues | Atoms          | AltConf |
|-----|-------|----------|----------------|---------|
| 12  | B     | 1        | Total C<br>6 6 | 0       |
| 12  | B     | 1        | Total C<br>6 6 | 0       |
| 12  | E     | 1        | Total C<br>6 6 | 0       |
| 12  | E     | 1        | Total C<br>6 6 | 0       |
| 12  | A     | 1        | Total C<br>6 6 | 0       |

- Molecule 13 is DECANE (CCD ID: D10) (formula:  $C_{10}H_{22}$ ).



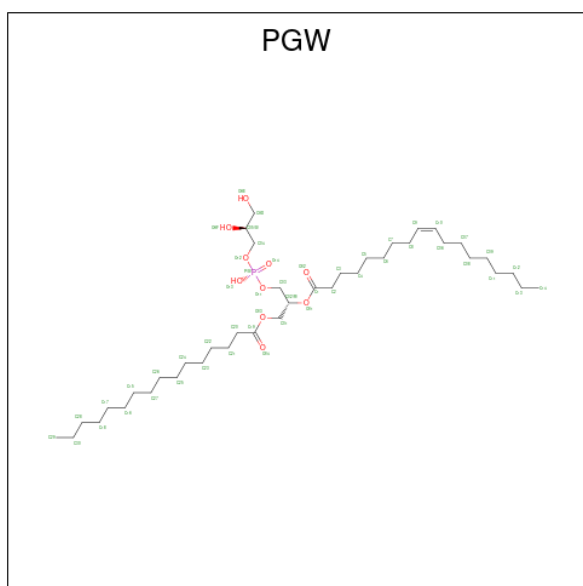
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 13  | B     | 1        | Total | C  | 0       |
|     |       |          | 10    | 10 |         |
| 13  | E     | 1        | Total | C  | 0       |
|     |       |          | 10    | 10 |         |
| 13  | A     | 1        | Total | C  | 0       |
|     |       |          | 10    | 10 |         |
| 13  | C     | 1        | Total | C  | 0       |
|     |       |          | 10    | 10 |         |

- Molecule 14 is HEXADECANE (CCD ID: R16) (formula: C<sub>16</sub>H<sub>34</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 14  | B     | 1        | Total | C  | 0       |
|     |       |          | 16    | 16 |         |
| 14  | C     | 1        | Total | C  | 0       |
|     |       |          | 16    | 16 |         |
| 14  | C     | 1        | Total | C  | 0       |
|     |       |          | 16    | 16 |         |

- Molecule 15 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula:  $C_{40}H_{77}O_{10}P$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 15  | B     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |

- Molecule 16 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula:  $C_{27}H_{52}O_8P$ ).



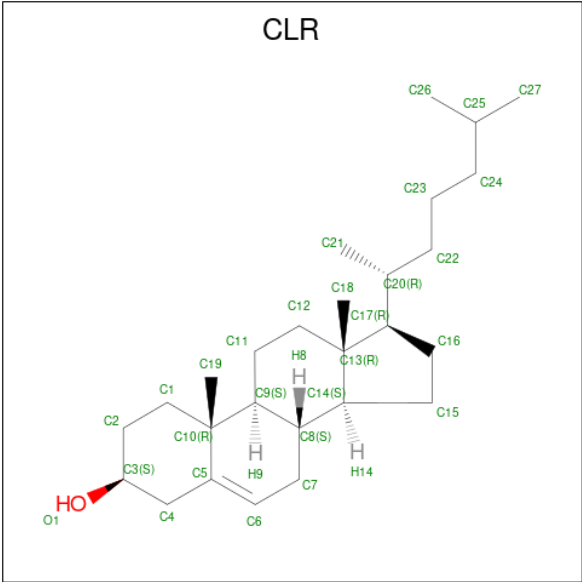
| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 16  | D     | 1        | Total | C  | O | P | 0       |
|     |       |          | 36    | 27 | 8 | 1 |         |

- Molecule 17 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $\text{C}_8\text{H}_{15}\text{NO}_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 17  | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

- Molecule 18 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ) (labeled as "Ligand of Interest" by depositor).

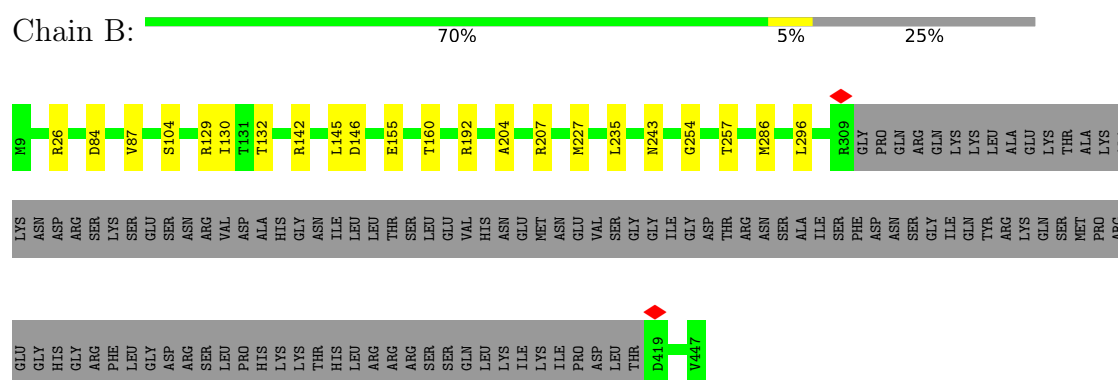


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 18  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 27 | 1 |         |

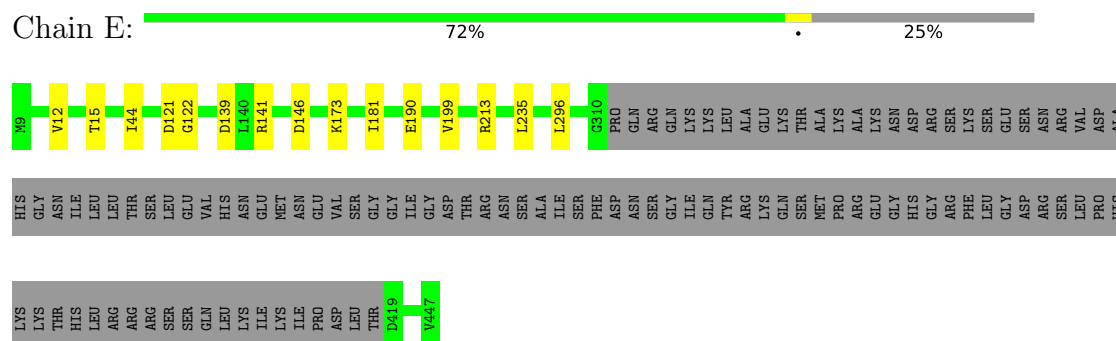
### 3 Residue-property plots

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.

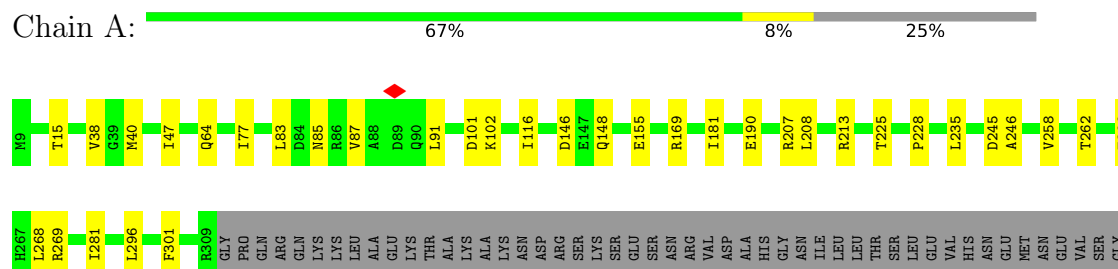
- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3



- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3



- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3



GLY  
ILE  
GLY  
ASP  
THR  
ARG  
ASN  
SER  
ALA  
ILE  
SER  
PHE  
ASP  
ASN  
GLY  
ILE  
GLN  
TVR  
ARG  
LYS  
GLN  
SER  
MET  
PRO  
ARG  
GLY  
GLY  
HIS  
GLY  
ARG  
PHE  
LEU  
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ASP  
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SER  
LEU  
PRO  
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LYS  
LYS  
THR  
HIS  
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ARG  
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SER  
SER  
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LEU  
LYS  
ILE  
LYS  
PRO  
ASP  
LEU  
THR

D419  
S427  
V430  
V447

- Molecule 1: Gamma-aminobutyric acid receptor subunit beta-3

Chain D:  70% 5% 25%

H9  
L19  
L27  
Y62  
Y74  
D84  
N85  
R86  
V87  
S104  
M115  
D121  
G122  
T123  
L128  
D146  
E147  
Q148  
E179  
R180  
I181  
E182  
I188  
R192  
A201  
T202  
L235  
R269  
E270  
I275  
L296  
A300  
R309  
GLY  
PRO  
GLN  
GLN  
ARG  
GLY  
LYS  
LYS

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ALA  
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GLU  
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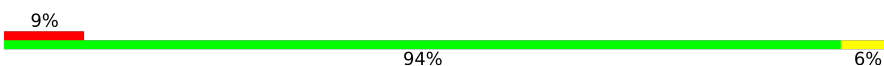
- Molecule 2: Isoform 2 of Gamma-aminobutyric acid receptor subunit gamma-2

Chain C:  80% 7% 13%

G25  
D26  
V27  
R43  
P44  
D45  
G63  
N66  
N69  
T73  
I74  
D75  
S116  
I124  
T125  
M135  
D136  
Y174  
I179  
R185  
L250  
V253  
T305  
L311  
N323  
K324  
K325  
PRO  
LYS  
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ARG  
ALA  
THR  
ILE  
GLN  
MET  
ASN  
ASN  
ALA  
THR  
HIS  
HIS  
LEU  
GLN  
GLU  
ASP  
GLU  
C369  
L370  
D371  
G372  
K373  
D374  
C380  
C381  
C385  
ARG  
THR  
GLY  
ALA  
TRP  
ARG  
HIS  
GLY  
ARG  
ILE  
E396  
I408  
S424  
L428  
Q429

- Molecule 3: Neuroligin-2

Chain H:  9% 94% 6%

D668  
G683  
F688  
L689  
N690  
A695  
Y699  
K700

- Molecule 4: LHFPL tetraspan subfamily member 4 protein

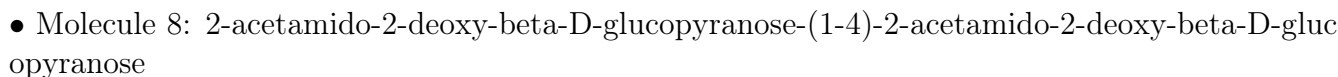
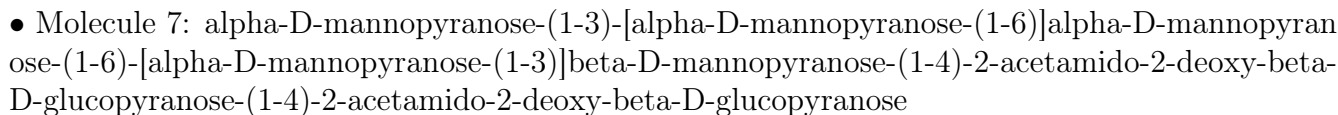
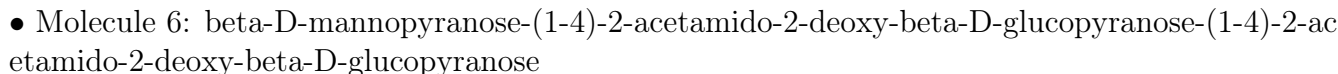
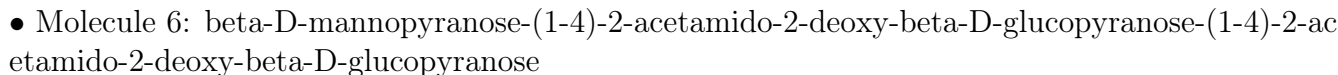
Chain L:  90% 10%

R17  
A21  
L25  
F29  
A34  
I42  
S50  
T53  
G67  
S68  
G69  
L70  
A71  
G72  
R73  
E74  
L75  
I87  
A95  
V99  
I110  
T111  
S114  
L133  
L137  
I182  
L190  
Q201

- Molecule 5: Megabody25

Chain K:  21% 78%





Chain J:  100%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

MAG1  
MAG2

- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  17% 83%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5  
MAN6

- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 38% 12%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8

- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  20% 40% 60%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 26047                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 45.28                                   | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | 165000                                  | Depositor |
| Image detector                       | TFS FALCON 4i (4k x 4k)                 | Depositor |
| Maximum map value                    | 0.591                                   | Depositor |
| Minimum map value                    | -0.226                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.016                                   | Depositor |
| Recommended contour level            | 0.09                                    | Depositor |
| Map size (Å)                         | 338.25598, 338.25598, 338.25598         | wwPDB     |
| Map dimensions                       | 464, 464, 464                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.729, 0.729, 0.729                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, R16, MAN, HEX, CLR, BMA, PX2, P1L, PGW, D10

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     | 0.18         | 0/2811      | 0.42        | 0/3824      |
| 1   | B     | 0.17         | 0/2784      | 0.39        | 0/3787      |
| 1   | D     | 0.16         | 0/2813      | 0.38        | 0/3828      |
| 1   | E     | 0.17         | 0/2830      | 0.41        | 0/3851      |
| 2   | C     | 0.30         | 0/2964      | 0.54        | 0/4024      |
| 3   | H     | 0.17         | 0/259       | 0.36        | 0/352       |
| 4   | L     | 0.17         | 0/1474      | 0.36        | 0/2003      |
| 5   | F     | 0.16         | 0/935       | 0.38        | 0/1266      |
| 5   | K     | 0.17         | 0/935       | 0.35        | 0/1266      |
| 5   | O     | 0.18         | 0/925       | 0.39        | 0/1253      |
| All | All   | 0.20         | 0/18730     | 0.42        | 0/25454     |

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

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     | 2731  | 0        | 2728     | 30      | 0            |
| 1   | B     | 2712  | 0        | 2705     | 19      | 0            |
| 1   | D     | 2732  | 0        | 2724     | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 2745  | 0        | 2736     | 10      | 0            |
| 2   | C     | 2951  | 0        | 2967     | 23      | 0            |
| 3   | H     | 255   | 0        | 256      | 2       | 0            |
| 4   | L     | 1432  | 0        | 1446     | 12      | 0            |
| 5   | F     | 912   | 0        | 856      | 5       | 0            |
| 5   | K     | 912   | 0        | 856      | 5       | 0            |
| 5   | O     | 902   | 0        | 848      | 9       | 0            |
| 6   | G     | 39    | 0        | 34       | 1       | 0            |
| 6   | N     | 39    | 0        | 34       | 0       | 0            |
| 7   | I     | 83    | 0        | 70       | 1       | 0            |
| 8   | J     | 28    | 0        | 25       | 0       | 0            |
| 8   | Q     | 28    | 0        | 25       | 0       | 0            |
| 9   | M     | 72    | 0        | 61       | 1       | 0            |
| 10  | P     | 94    | 0        | 79       | 1       | 0            |
| 11  | R     | 61    | 0        | 52       | 1       | 0            |
| 12  | A     | 6     | 0        | 14       | 0       | 0            |
| 12  | B     | 12    | 0        | 28       | 0       | 0            |
| 12  | E     | 12    | 0        | 28       | 0       | 0            |
| 13  | A     | 10    | 0        | 22       | 1       | 0            |
| 13  | B     | 10    | 0        | 22       | 0       | 0            |
| 13  | C     | 10    | 0        | 22       | 2       | 0            |
| 13  | E     | 10    | 0        | 22       | 0       | 0            |
| 14  | B     | 16    | 0        | 34       | 0       | 0            |
| 14  | C     | 32    | 0        | 68       | 0       | 0            |
| 15  | B     | 51    | 0        | 76       | 0       | 0            |
| 16  | D     | 36    | 0        | 52       | 0       | 0            |
| 17  | C     | 14    | 0        | 13       | 0       | 0            |
| 18  | C     | 28    | 0        | 46       | 0       | 0            |
| All | All   | 18975 | 0        | 18949    | 114     | 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 3.

All (114) 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:225:THR:HG23 | 1:A:268:LEU:CD1  | 1.81                     | 1.11              |
| 1:A:225:THR:HG21 | 1:A:281:ILE:HD11 | 1.38                     | 1.00              |
| 1:A:225:THR:HG23 | 1:A:268:LEU:HD11 | 1.54                     | 0.89              |
| 1:E:296:LEU:HD23 | 1:D:235:LEU:HD22 | 1.63                     | 0.80              |
| 2:C:428:LEU:HD13 | 4:L:42:ILE:HD12  | 1.70                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:26:ARG:HE    | 1:A:83:LEU:HD12  | 1.55                     | 0.71              |
| 1:E:190:GLU:OE1  | 1:E:213:ARG:NH2  | 2.24                     | 0.70              |
| 1:D:146:ASP:OD2  | 1:D:148:GLN:NE2  | 2.24                     | 0.70              |
| 1:B:160:THR:OG1  | 1:B:204:ALA:O    | 2.13                     | 0.67              |
| 1:D:62[B]:TYR:OH | 1:D:115:MET:SD   | 2.50                     | 0.67              |
| 1:A:146:ASP:OD2  | 1:A:148:GLN:NE2  | 2.28                     | 0.66              |
| 1:A:225:THR:HG23 | 1:A:268:LEU:HD13 | 1.76                     | 0.65              |
| 5:K:426:GLN:NE2  | 5:K:430:LYS:O    | 2.29                     | 0.65              |
| 5:O:439:SER:O    | 5:O:459:ARG:NE   | 2.32                     | 0.63              |
| 1:D:84:ASP:OD2   | 1:D:86:ARG:NH2   | 2.32                     | 0.62              |
| 2:C:43:ARG:NH1   | 2:C:45:ASP:O     | 2.32                     | 0.62              |
| 1:A:225:THR:CG2  | 1:A:268:LEU:CD1  | 2.71                     | 0.62              |
| 1:A:87:VAL:HG13  | 1:A:91:LEU:HD13  | 1.81                     | 0.61              |
| 1:B:26:ARG:NH1   | 1:A:85:ASN:OD1   | 2.34                     | 0.61              |
| 1:E:44:ILE:HG21  | 1:E:181:ILE:HD11 | 1.83                     | 0.61              |
| 1:D:128:LEU:CD1  | 2:C:125:THR:HG23 | 2.31                     | 0.59              |
| 2:C:66:ASN:ND2   | 2:C:69:ASN:OD1   | 2.36                     | 0.58              |
| 1:B:296:LEU:HD23 | 1:A:235:LEU:HD22 | 1.86                     | 0.58              |
| 1:E:235:LEU:HD22 | 1:A:296:LEU:HD23 | 1.85                     | 0.57              |
| 5:K:6:GLU:OE2    | 5:K:504:GLN:N    | 2.38                     | 0.57              |
| 2:C:63:GLY:N     | 2:C:73:THR:O     | 2.39                     | 0.56              |
| 1:D:104:SER:HB2  | 2:C:124:ILE:HD11 | 1.87                     | 0.56              |
| 5:O:478:THR:HG22 | 5:O:510:VAL:H    | 1.71                     | 0.54              |
| 1:A:87:VAL:HG11  | 1:A:116:ILE:HG21 | 1.90                     | 0.53              |
| 5:F:6:GLU:OE2    | 5:F:483:CYS:N    | 2.41                     | 0.53              |
| 1:B:26:ARG:NE    | 1:A:83:LEU:HD12  | 2.22                     | 0.53              |
| 5:F:438:ILE:HD13 | 5:F:445:THR:HG22 | 1.90                     | 0.52              |
| 2:C:408:ILE:HD11 | 13:C:504:D10:H52 | 1.92                     | 0.51              |
| 1:D:104:SER:CB   | 2:C:124:ILE:HD11 | 2.41                     | 0.51              |
| 1:D:270:GLU:N    | 1:D:270:GLU:OE2  | 2.45                     | 0.50              |
| 1:B:104:SER:CB   | 1:B:132:THR:HG22 | 2.41                     | 0.50              |
| 5:O:450:SER:O    | 5:O:454:ARG:NH2  | 2.43                     | 0.50              |
| 1:A:190:GLU:OE1  | 1:A:213:ARG:NH2  | 2.44                     | 0.50              |
| 1:A:101:ASP:OD1  | 1:A:102:LYS:N    | 2.45                     | 0.50              |
| 1:B:235:LEU:HD22 | 2:C:311:LEU:HD23 | 1.93                     | 0.49              |
| 1:A:245:ASP:OD1  | 1:A:246:ALA:N    | 2.46                     | 0.49              |
| 1:A:258:VAL:O    | 1:A:262:THR:HG23 | 2.13                     | 0.48              |
| 1:B:130:ILE:HG22 | 1:B:132:THR:HG23 | 1.95                     | 0.48              |
| 1:B:155:GLU:OE1  | 1:B:207:ARG:NH2  | 2.46                     | 0.48              |
| 1:D:300:ALA:HB2  | 2:C:253:VAL:HG13 | 1.96                     | 0.48              |
| 1:B:84:ASP:O     | 1:B:87:VAL:HG12  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:104:SER:HB3  | 1:B:132:THR:HG22 | 1.96                     | 0.48              |
| 1:B:227:MET:CE   | 2:C:305:ILE:HD11 | 2.44                     | 0.48              |
| 1:A:301:PHE:CE1  | 13:A:501:D10:H22 | 2.49                     | 0.47              |
| 1:A:47:ILE:HG22  | 1:A:47:ILE:O     | 2.13                     | 0.47              |
| 2:C:408:ILE:HD11 | 13:C:504:D10:C5  | 2.44                     | 0.47              |
| 1:B:142:ARG:O    | 1:B:145:LEU:N    | 2.47                     | 0.47              |
| 4:L:67:GLY:HA2   | 4:L:75:LEU:HD23  | 1.96                     | 0.47              |
| 5:F:438:ILE:HD13 | 5:F:445:THR:CG2  | 2.44                     | 0.47              |
| 1:E:121:ASP:OD1  | 1:E:122:GLY:N    | 2.47                     | 0.47              |
| 1:E:199:VAL:HG21 | 5:O:497:THR:HG21 | 1.97                     | 0.47              |
| 1:A:64:GLN:OE1   | 1:A:169:ARG:NH2  | 2.46                     | 0.47              |
| 1:A:155:GLU:OE1  | 1:A:207:ARG:NH2  | 2.44                     | 0.47              |
| 1:D:182:GLU:OE1  | 1:D:182:GLU:N    | 2.47                     | 0.47              |
| 5:F:504:GLN:OE1  | 5:F:504:GLN:N    | 2.45                     | 0.47              |
| 2:C:135:ASN:OD1  | 2:C:136:ASP:N    | 2.49                     | 0.46              |
| 2:C:424:SER:HA   | 2:C:428:LEU:HD11 | 1.97                     | 0.46              |
| 4:L:111:THR:O    | 4:L:114:SER:OG   | 2.32                     | 0.46              |
| 1:D:296:LEU:HD23 | 2:C:250:LEU:HD22 | 1.96                     | 0.46              |
| 4:L:34:ALA:HB2   | 4:L:110:ILE:HD11 | 1.98                     | 0.46              |
| 2:C:373:LYS:O    | 2:C:374:ASP:C    | 2.58                     | 0.46              |
| 2:C:428:LEU:CD1  | 4:L:42:ILE:HD12  | 2.43                     | 0.46              |
| 1:A:38:VAL:HG12  | 1:A:40:MET:HE2   | 1.97                     | 0.46              |
| 1:A:47:ILE:HD12  | 1:A:181:ILE:HG12 | 1.98                     | 0.46              |
| 5:O:500:ASP:N    | 5:O:500:ASP:OD1  | 2.49                     | 0.46              |
| 1:A:40:MET:HG3   | 1:A:208:LEU:HD22 | 1.97                     | 0.46              |
| 3:H:683:GLY:HA3  | 4:L:182:ILE:HD13 | 1.98                     | 0.46              |
| 2:C:174:TYR:CG   | 2:C:179:ILE:HD12 | 2.50                     | 0.45              |
| 4:L:133:LEU:O    | 4:L:137:LEU:HD23 | 2.16                     | 0.45              |
| 6:G:2:NAG:H83    | 6:G:2:NAG:H3     | 1.99                     | 0.45              |
| 1:D:19:LEU:HD21  | 1:D:74:TYR:HB3   | 1.98                     | 0.45              |
| 1:B:243:ASN:OD1  | 2:C:323:ASN:ND2  | 2.50                     | 0.45              |
| 1:E:139:ASP:OD1  | 1:E:141:ARG:NH1  | 2.50                     | 0.45              |
| 5:F:431:GLU:N    | 5:F:431:GLU:OE1  | 2.49                     | 0.45              |
| 1:A:225:THR:CG2  | 1:A:268:LEU:HD13 | 2.42                     | 0.45              |
| 1:D:121:ASP:OD1  | 1:D:123:THR:HG22 | 2.17                     | 0.44              |
| 5:K:470:MET:HB3  | 5:K:473:LEU:HD21 | 1.97                     | 0.44              |
| 1:D:84:ASP:O     | 1:D:87:VAL:HG12  | 2.17                     | 0.44              |
| 1:B:129:ARG:NH2  | 2:C:116:SER:O    | 2.48                     | 0.44              |
| 1:B:146:ASP:OD1  | 1:B:146:ASP:N    | 2.51                     | 0.44              |
| 1:B:286:MET:HE1  | 1:A:228:PRO:HG3  | 1.98                     | 0.44              |
| 1:A:15:THR:HG21  | 1:A:77:ILE:HD12  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:254:GLY:O    | 1:B:257:THR:OG1  | 2.28                     | 0.43              |
| 2:C:370:LEU:C    | 2:C:372:GLY:H    | 2.25                     | 0.43              |
| 5:O:439:SER:OG   | 5:O:440:TRP:N    | 2.50                     | 0.43              |
| 1:B:192:ARG:HG3  | 7:I:1:NAG:H83    | 1.99                     | 0.43              |
| 5:O:421:MET:HE2  | 5:O:459:ARG:HH22 | 1.82                     | 0.43              |
| 4:L:95:ALA:O     | 4:L:99:VAL:HG23  | 2.19                     | 0.43              |
| 1:D:146:ASP:OD1  | 1:D:146:ASP:N    | 2.52                     | 0.43              |
| 1:A:225:THR:HG21 | 1:A:281:ILE:CD1  | 2.28                     | 0.43              |
| 1:A:266:THR:HG23 | 1:A:269:ARG:HH22 | 1.83                     | 0.43              |
| 1:D:179:GLU:HG3  | 5:O:493:LEU:HD11 | 2.00                     | 0.42              |
| 1:D:181:ILE:HG21 | 1:D:188:ILE:HD11 | 2.00                     | 0.42              |
| 1:E:173:LYS:NZ   | 5:K:449:ASP:OD2  | 2.52                     | 0.42              |
| 1:D:104:SER:OG   | 2:C:124:ILE:HD11 | 2.20                     | 0.42              |
| 3:H:690:ASN:HD21 | 4:L:29:PHE:HB3   | 1.85                     | 0.42              |
| 10:P:3:BMA:H62   | 10:P:4:MAN:H2    | 1.60                     | 0.42              |
| 4:L:21:ALA:O     | 4:L:25:LEU:HD23  | 2.20                     | 0.41              |
| 9:M:1:NAG:O3     | 9:M:2:NAG:O5     | 2.33                     | 0.41              |
| 4:L:50:SER:N     | 4:L:53:THR:OG1   | 2.53                     | 0.41              |
| 5:K:6:GLU:OE2    | 5:K:505:GLY:N    | 2.45                     | 0.41              |
| 1:D:275:ILE:O    | 1:D:275:ILE:HG23 | 2.20                     | 0.41              |
| 1:E:12:VAL:O     | 1:E:15:THR:HG22  | 2.20                     | 0.41              |
| 1:A:427:SER:HA   | 1:A:430:VAL:HG12 | 2.03                     | 0.41              |
| 1:D:192:ARG:NH2  | 11:R:1:NAG:O3    | 2.50                     | 0.41              |
| 4:L:29:PHE:HB2   | 4:L:190:LEU:HD21 | 2.02                     | 0.41              |
| 1:E:146:ASP:OD1  | 1:E:146:ASP:N    | 2.55                     | 0.40              |
| 1:D:27:LEU:HD11  | 2:C:27:VAL:HG21  | 2.03                     | 0.40              |
| 5:O:419:PRO:HG2  | 5:O:420:ILE:HD12 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 328/439 (75%)   | 315 (96%)  | 13 (4%) | 0        | 100         | 100 |
| 1   | B     | 326/439 (74%)   | 309 (95%)  | 17 (5%) | 0        | 100         | 100 |
| 1   | D     | 328/439 (75%)   | 313 (95%)  | 15 (5%) | 0        | 100         | 100 |
| 1   | E     | 330/439 (75%)   | 320 (97%)  | 10 (3%) | 0        | 100         | 100 |
| 2   | C     | 346/405 (85%)   | 326 (94%)  | 19 (6%) | 1 (0%)   | 36          | 68  |
| 3   | H     | 31/33 (94%)     | 30 (97%)   | 1 (3%)  | 0        | 100         | 100 |
| 4   | L     | 184/185 (100%)  | 179 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 5   | F     | 113/522 (22%)   | 107 (95%)  | 6 (5%)  | 0        | 100         | 100 |
| 5   | K     | 113/522 (22%)   | 109 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 5   | O     | 111/522 (21%)   | 104 (94%)  | 7 (6%)  | 0        | 100         | 100 |
| All | All   | 2210/3945 (56%) | 2112 (96%) | 97 (4%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 63  | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 299/392 (76%)  | 299 (100%) | 0        | 100         | 100 |
| 1   | B     | 297/392 (76%)  | 297 (100%) | 0        | 100         | 100 |
| 1   | D     | 299/392 (76%)  | 299 (100%) | 0        | 100         | 100 |
| 1   | E     | 300/392 (76%)  | 300 (100%) | 0        | 100         | 100 |
| 2   | C     | 322/366 (88%)  | 320 (99%)  | 2 (1%)   | 78          | 84  |
| 3   | H     | 27/27 (100%)   | 27 (100%)  | 0        | 100         | 100 |
| 4   | L     | 152/151 (101%) | 152 (100%) | 0        | 100         | 100 |
| 5   | F     | 94/430 (22%)   | 94 (100%)  | 0        | 100         | 100 |
| 5   | K     | 94/430 (22%)   | 94 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 5   | O     | 93/430 (22%)    | 93 (100%)   | 0        | 100         | 100 |
| All | All   | 1977/3402 (58%) | 1975 (100%) | 2 (0%)   | 87          | 91  |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 75  | ASP  |
| 2   | C     | 370 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 54  | ASN  |
| 2   | C     | 318 | HIS  |
| 3   | H     | 690 | ASN  |
| 5   | F     | 414 | HIS  |
| 5   | F     | 426 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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   | P1L  | C     | 385 | 2    | 21,22,23     | 1.12 | 1 (4%)   | 19,23,25    | 1.45 | 2 (10%)  |
| 2   | P1L  | C     | 381 | 2    | 21,22,23     | 0.63 | 0        | 19,23,25    | 1.90 | 3 (15%)  |
| 2   | P1L  | C     | 380 | 2    | 21,22,23     | 1.12 | 1 (4%)   | 19,23,25    | 1.51 | 3 (15%)  |

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   | P1L  | C     | 385 | 2    | -       | 10/20/22/24 | -     |
| 2   | P1L  | C     | 381 | 2    | -       | 5/20/22/24  | -     |
| 2   | P1L  | C     | 380 | 2    | -       | 5/20/22/24  | -     |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | C     | 385 | P1L  | O-C   | 4.34 | 1.36        | 1.20     |
| 2   | C     | 380 | P1L  | O-C   | 4.29 | 1.36        | 1.20     |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | C     | 381 | P1L  | CB-SG-C7 | 6.78  | 110.08      | 100.76   |
| 2   | C     | 385 | P1L  | CB-SG-C7 | 5.21  | 107.93      | 100.76   |
| 2   | C     | 380 | P1L  | CB-SG-C7 | 4.42  | 106.84      | 100.76   |
| 2   | C     | 380 | P1L  | C8-C7-SG | -3.69 | 109.01      | 113.40   |
| 2   | C     | 381 | P1L  | C8-C7-SG | -3.16 | 109.63      | 113.40   |
| 2   | C     | 381 | P1L  | O7-C7-SG | 2.88  | 126.35      | 122.68   |
| 2   | C     | 380 | P1L  | O7-C7-SG | 2.61  | 126.00      | 122.68   |
| 2   | C     | 385 | P1L  | O7-C7-SG | 2.12  | 125.38      | 122.68   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 380 | P1L  | N-CA-CB-SG      |
| 2   | C     | 380 | P1L  | C-CA-CB-SG      |
| 2   | C     | 381 | P1L  | CA-CB-SG-C7     |
| 2   | C     | 381 | P1L  | O7-C7-SG-CB     |
| 2   | C     | 381 | P1L  | C8-C7-SG-CB     |
| 2   | C     | 385 | P1L  | O7-C7-SG-CB     |
| 2   | C     | 385 | P1L  | C8-C7-SG-CB     |
| 2   | C     | 380 | P1L  | C16-C17-C18-C19 |
| 2   | C     | 380 | P1L  | C14-C15-C16-C17 |
| 2   | C     | 385 | P1L  | C11-C12-C13-C14 |
| 2   | C     | 380 | P1L  | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | C     | 381 | P1L  | C11-C10-C9-C8   |
| 2   | C     | 385 | P1L  | SG-C7-C8-C9     |
| 2   | C     | 385 | P1L  | O7-C7-C8-C9     |
| 2   | C     | 385 | P1L  | C19-C20-C21-C22 |
| 2   | C     | 385 | P1L  | C11-C10-C9-C8   |
| 2   | C     | 385 | P1L  | C12-C13-C14-C15 |
| 2   | C     | 385 | P1L  | C9-C10-C11-C12  |
| 2   | C     | 381 | P1L  | C18-C19-C20-C21 |
| 2   | C     | 385 | P1L  | C7-C8-C9-C10    |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

36 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  | G     | 1   | 6    | 14,14,15     | 0.86 | 1 (7%)      | 17,19,21    | 1.20 | 1 (5%)      |
| 6   | NAG  | G     | 2   | 6    | 14,14,15     | 0.28 | 0           | 17,19,21    | 1.43 | 2 (11%)     |
| 6   | BMA  | G     | 3   | 6    | 11,11,12     | 0.58 | 0           | 15,15,17    | 0.70 | 0           |
| 7   | NAG  | I     | 1   | 1,7  | 14,14,15     | 0.28 | 0           | 17,19,21    | 0.41 | 0           |
| 7   | NAG  | I     | 2   | 7    | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.41 | 0           |
| 7   | BMA  | I     | 3   | 7    | 11,11,12     | 0.56 | 0           | 15,15,17    | 0.74 | 0           |
| 7   | MAN  | I     | 4   | 7    | 11,11,12     | 0.41 | 0           | 15,15,17    | 0.77 | 1 (6%)      |
| 7   | MAN  | I     | 5   | 7    | 11,11,12     | 0.24 | 0           | 15,15,17    | 0.64 | 0           |
| 7   | MAN  | I     | 6   | 7    | 11,11,12     | 0.31 | 0           | 15,15,17    | 0.83 | 1 (6%)      |
| 7   | MAN  | I     | 7   | 7    | 11,11,12     | 0.64 | 0           | 15,15,17    | 1.02 | 2 (13%)     |
| 8   | NAG  | J     | 1   | 8    | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.44 | 0           |
| 8   | NAG  | J     | 2   | 8    | 14,14,15     | 0.20 | 0           | 17,19,21    | 0.43 | 0           |
| 9   | NAG  | M     | 1   | 9    | 14,14,15     | 0.26 | 0           | 17,19,21    | 0.39 | 0           |
| 9   | NAG  | M     | 2   | 9    | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.44 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | BMA  | M     | 3   | 9    | 11,11,12     | 0.55 | 0        | 15,15,17    | 0.72 | 0        |
| 9   | MAN  | M     | 4   | 9    | 11,11,12     | 0.67 | 0        | 15,15,17    | 0.97 | 2 (13%)  |
| 9   | MAN  | M     | 5   | 9    | 11,11,12     | 0.65 | 0        | 15,15,17    | 0.98 | 2 (13%)  |
| 9   | MAN  | M     | 6   | 9    | 11,11,12     | 0.62 | 0        | 15,15,17    | 0.99 | 2 (13%)  |
| 6   | NAG  | N     | 1   | 1,6  | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.52 | 0        |
| 6   | NAG  | N     | 2   | 6    | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.43 | 0        |
| 6   | BMA  | N     | 3   | 6    | 11,11,12     | 0.57 | 0        | 15,15,17    | 0.73 | 0        |
| 10  | NAG  | P     | 1   | 1,10 | 14,14,15     | 0.41 | 0        | 17,19,21    | 1.28 | 2 (11%)  |
| 10  | NAG  | P     | 2   | 10   | 14,14,15     | 0.42 | 0        | 17,19,21    | 0.55 | 0        |
| 10  | BMA  | P     | 3   | 10   | 11,11,12     | 0.57 | 0        | 15,15,17    | 0.53 | 0        |
| 10  | MAN  | P     | 4   | 10   | 11,11,12     | 0.45 | 0        | 15,15,17    | 1.07 | 1 (6%)   |
| 10  | MAN  | P     | 5   | 10   | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 0.97 | 1 (6%)   |
| 10  | MAN  | P     | 6   | 10   | 11,11,12     | 0.22 | 0        | 15,15,17    | 0.71 | 0        |
| 10  | MAN  | P     | 7   | 10   | 11,11,12     | 0.39 | 0        | 15,15,17    | 0.72 | 0        |
| 10  | MAN  | P     | 8   | 10   | 11,11,12     | 0.35 | 0        | 15,15,17    | 0.54 | 0        |
| 8   | NAG  | Q     | 1   | 1,8  | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.64 | 0        |
| 8   | NAG  | Q     | 2   | 8    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.48 | 0        |
| 11  | NAG  | R     | 1   | 11   | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.42 | 0        |
| 11  | NAG  | R     | 2   | 11   | 14,14,15     | 0.18 | 0        | 17,19,21    | 0.43 | 0        |
| 11  | BMA  | R     | 3   | 11   | 11,11,12     | 0.57 | 0        | 15,15,17    | 0.71 | 0        |
| 11  | MAN  | R     | 4   | 11   | 11,11,12     | 0.65 | 0        | 15,15,17    | 0.99 | 2 (13%)  |
| 11  | MAN  | R     | 5   | 11   | 11,11,12     | 0.63 | 0        | 15,15,17    | 0.97 | 2 (13%)  |

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  | G     | 1   | 6    | -       | 4/6/23/26 | 0/1/1/1 |
| 6   | NAG  | G     | 2   | 6    | -       | 4/6/23/26 | 0/1/1/1 |
| 6   | BMA  | G     | 3   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | I     | 1   | 1,7  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | I     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | I     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | I     | 4   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | I     | 5   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | I     | 6   | 7    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | MAN  | I     | 7   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | J     | 1   | 8    | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 8   | NAG  | J     | 2   | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | M     | 1   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | M     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | M     | 3   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | M     | 4   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | M     | 5   | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 9   | MAN  | M     | 6   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | N     | 1   | 1,6  | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | NAG  | N     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | BMA  | N     | 3   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | NAG  | P     | 1   | 1,10 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | P     | 2   | 10   | -       | 0/6/23/26 | 0/1/1/1 |
| 10  | BMA  | P     | 3   | 10   | -       | 1/2/19/22 | 0/1/1/1 |
| 10  | MAN  | P     | 4   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | P     | 5   | 10   | -       | 1/2/19/22 | 0/1/1/1 |
| 10  | MAN  | P     | 6   | 10   | -       | 1/2/19/22 | 0/1/1/1 |
| 10  | MAN  | P     | 7   | 10   | -       | 1/2/19/22 | 0/1/1/1 |
| 10  | MAN  | P     | 8   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | Q     | 1   | 1,8  | -       | 4/6/23/26 | 0/1/1/1 |
| 8   | NAG  | Q     | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | R     | 1   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | NAG  | R     | 2   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | R     | 3   | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | MAN  | R     | 4   | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | MAN  | R     | 5   | 11   | -       | 0/2/19/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 6   | G     | 1   | NAG  | O5-C1 | 2.89 | 1.48        | 1.43     |
| 10  | P     | 5   | MAN  | C1-C2 | 2.36 | 1.57        | 1.52     |

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 6   | G     | 2   | NAG  | C2-N2-C7 | 4.77 | 129.30      | 122.90   |
| 6   | G     | 1   | NAG  | C1-O5-C5 | 4.14 | 117.73      | 112.19   |
| 10  | P     | 1   | NAG  | C1-C2-N2 | 3.88 | 116.55      | 110.43   |
| 10  | P     | 5   | MAN  | O2-C2-C1 | 2.82 | 115.68      | 109.22   |
| 10  | P     | 4   | MAN  | C1-C2-C3 | 2.78 | 113.69      | 109.64   |
| 10  | P     | 1   | NAG  | C2-N2-C7 | 2.45 | 126.18      | 122.90   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | I     | 7   | MAN  | C1-O5-C5 | 2.40  | 115.40      | 112.19   |
| 6   | G     | 2   | NAG  | C1-C2-N2 | 2.39  | 114.19      | 110.43   |
| 11  | R     | 5   | MAN  | C1-O5-C5 | 2.35  | 115.34      | 112.19   |
| 7   | I     | 6   | MAN  | C1-O5-C5 | 2.34  | 115.32      | 112.19   |
| 11  | R     | 4   | MAN  | C1-O5-C5 | 2.31  | 115.29      | 112.19   |
| 9   | M     | 5   | MAN  | C1-O5-C5 | 2.30  | 115.27      | 112.19   |
| 9   | M     | 6   | MAN  | C1-O5-C5 | 2.27  | 115.23      | 112.19   |
| 7   | I     | 7   | MAN  | O2-C2-C3 | -2.21 | 105.56      | 110.15   |
| 9   | M     | 4   | MAN  | O2-C2-C3 | -2.20 | 105.60      | 110.15   |
| 11  | R     | 4   | MAN  | O2-C2-C3 | -2.19 | 105.62      | 110.15   |
| 9   | M     | 5   | MAN  | O2-C2-C3 | -2.18 | 105.64      | 110.15   |
| 7   | I     | 4   | MAN  | C1-O5-C5 | 2.16  | 115.08      | 112.19   |
| 9   | M     | 6   | MAN  | O2-C2-C3 | -2.13 | 105.73      | 110.15   |
| 11  | R     | 5   | MAN  | O2-C2-C3 | -2.12 | 105.76      | 110.15   |
| 9   | M     | 4   | MAN  | C1-O5-C5 | 2.07  | 114.96      | 112.19   |

There are no chirality outliers.

All (29) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 9   | M     | 4   | MAN  | O5-C5-C6-O6 |
| 9   | M     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | M     | 4   | MAN  | C4-C5-C6-O6 |
| 9   | M     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | G     | 1   | NAG  | C8-C7-N2-C2 |
| 6   | G     | 1   | NAG  | O7-C7-N2-C2 |
| 6   | G     | 2   | NAG  | C8-C7-N2-C2 |
| 6   | G     | 2   | NAG  | O7-C7-N2-C2 |
| 8   | Q     | 1   | NAG  | C8-C7-N2-C2 |
| 8   | Q     | 1   | NAG  | O7-C7-N2-C2 |
| 8   | Q     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | P     | 3   | BMA  | O5-C5-C6-O6 |
| 10  | P     | 7   | MAN  | O5-C5-C6-O6 |
| 7   | I     | 6   | MAN  | O5-C5-C6-O6 |
| 10  | P     | 5   | MAN  | O5-C5-C6-O6 |
| 10  | P     | 6   | MAN  | O5-C5-C6-O6 |
| 9   | M     | 5   | MAN  | O5-C5-C6-O6 |
| 10  | P     | 1   | NAG  | C3-C2-N2-C7 |
| 7   | I     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | G     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | Q     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | G     | 2   | NAG  | C1-C2-N2-C7 |

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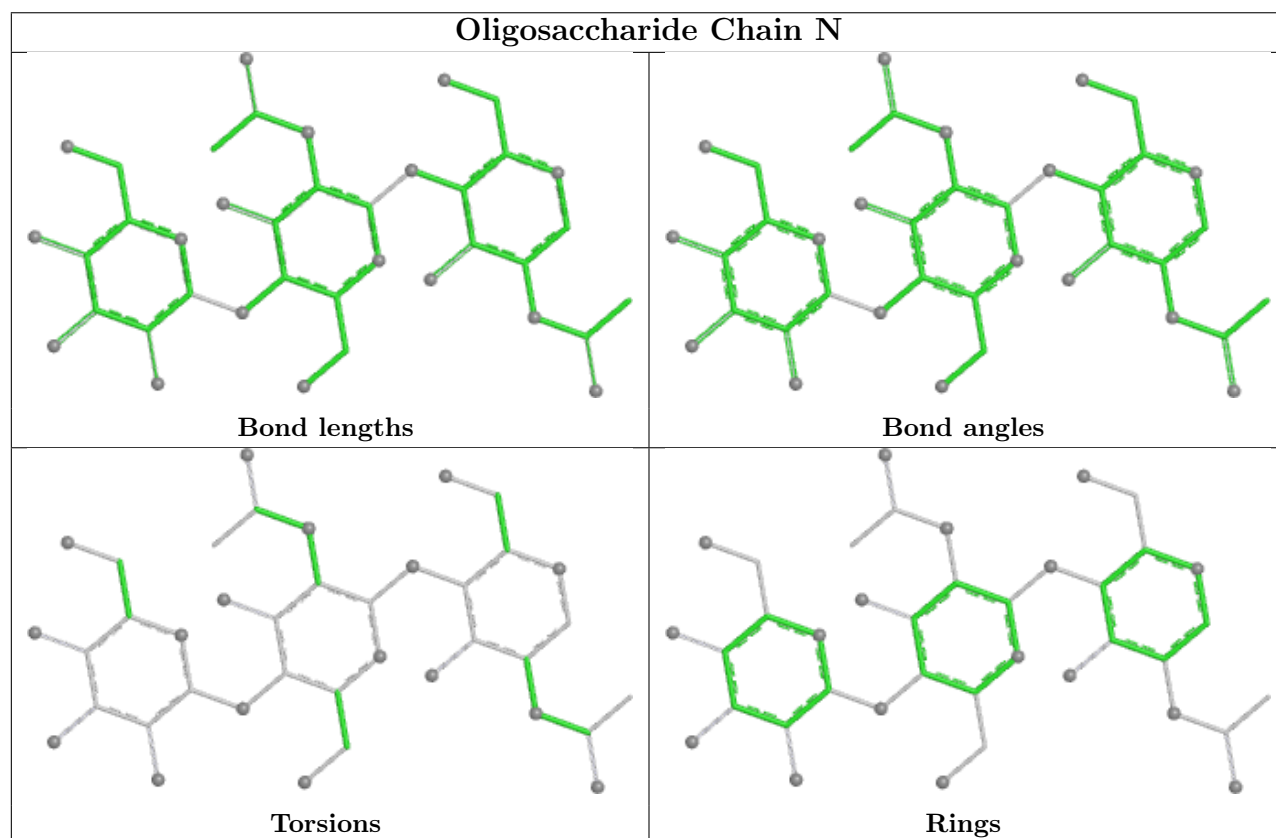
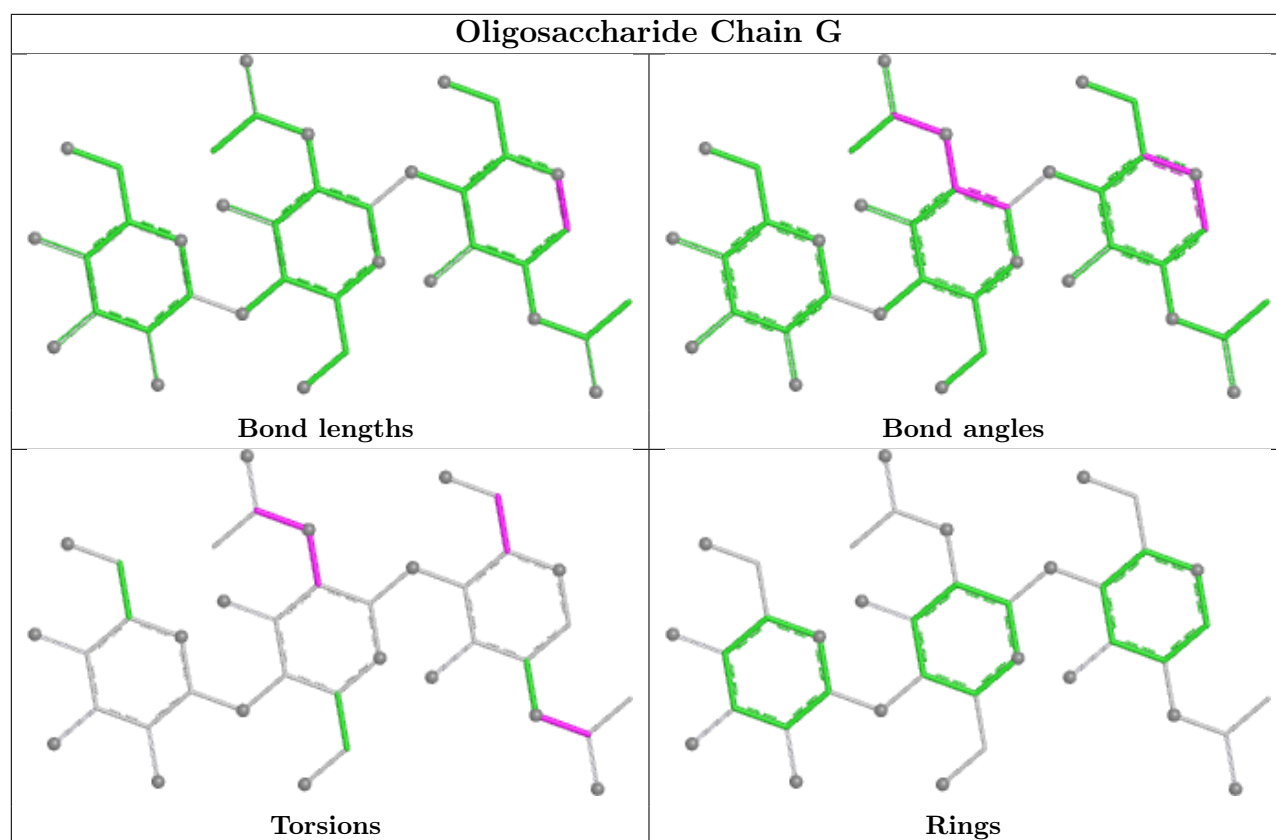
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | Q     | 2   | NAG  | C1-C2-N2-C7 |
| 10  | P     | 1   | NAG  | C1-C2-N2-C7 |
| 8   | Q     | 2   | NAG  | C3-C2-N2-C7 |
| 9   | M     | 1   | NAG  | C1-C2-N2-C7 |
| 6   | G     | 2   | NAG  | C3-C2-N2-C7 |
| 9   | M     | 1   | NAG  | C3-C2-N2-C7 |
| 6   | G     | 1   | NAG  | O5-C5-C6-O6 |

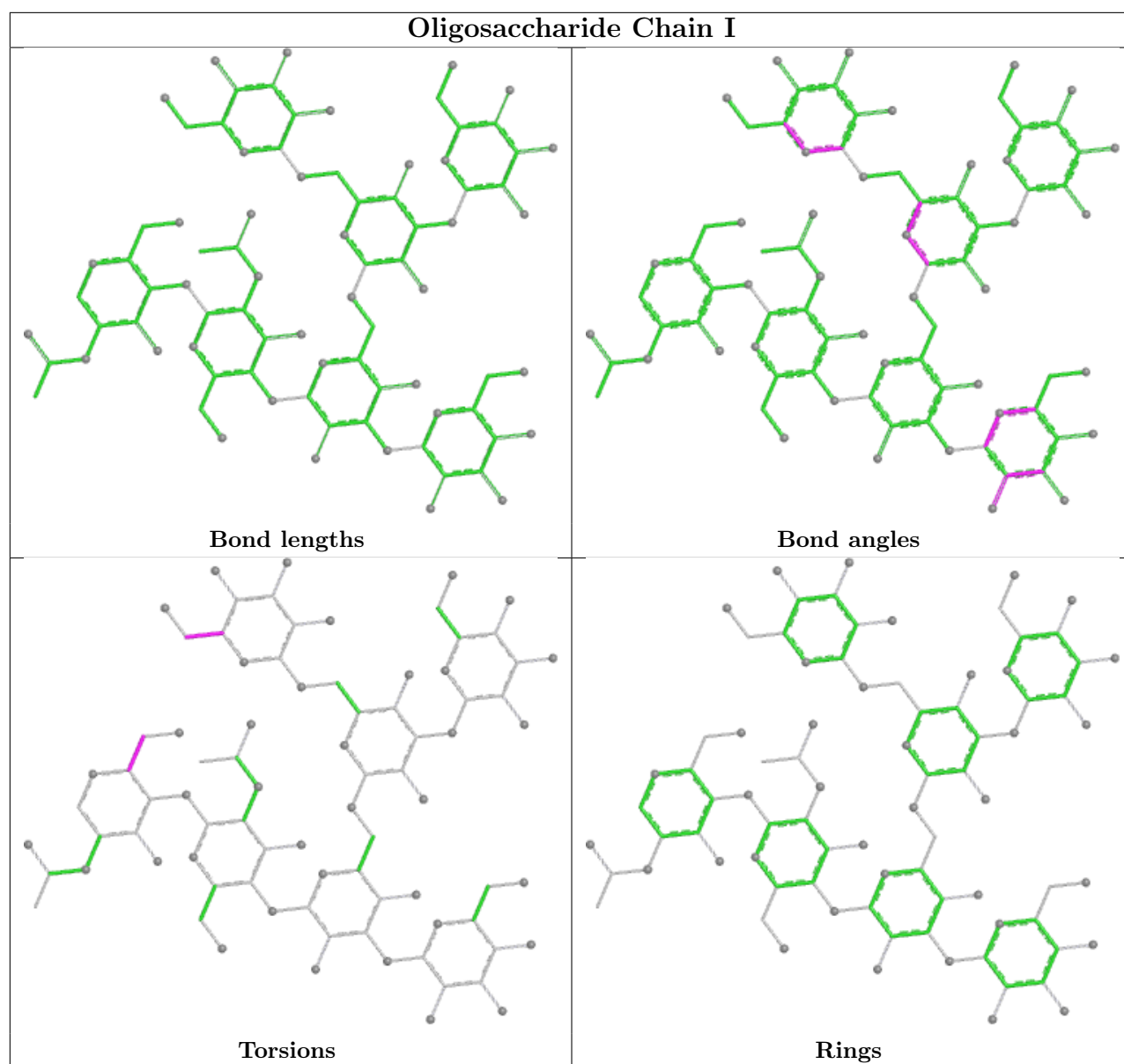
There are no ring outliers.

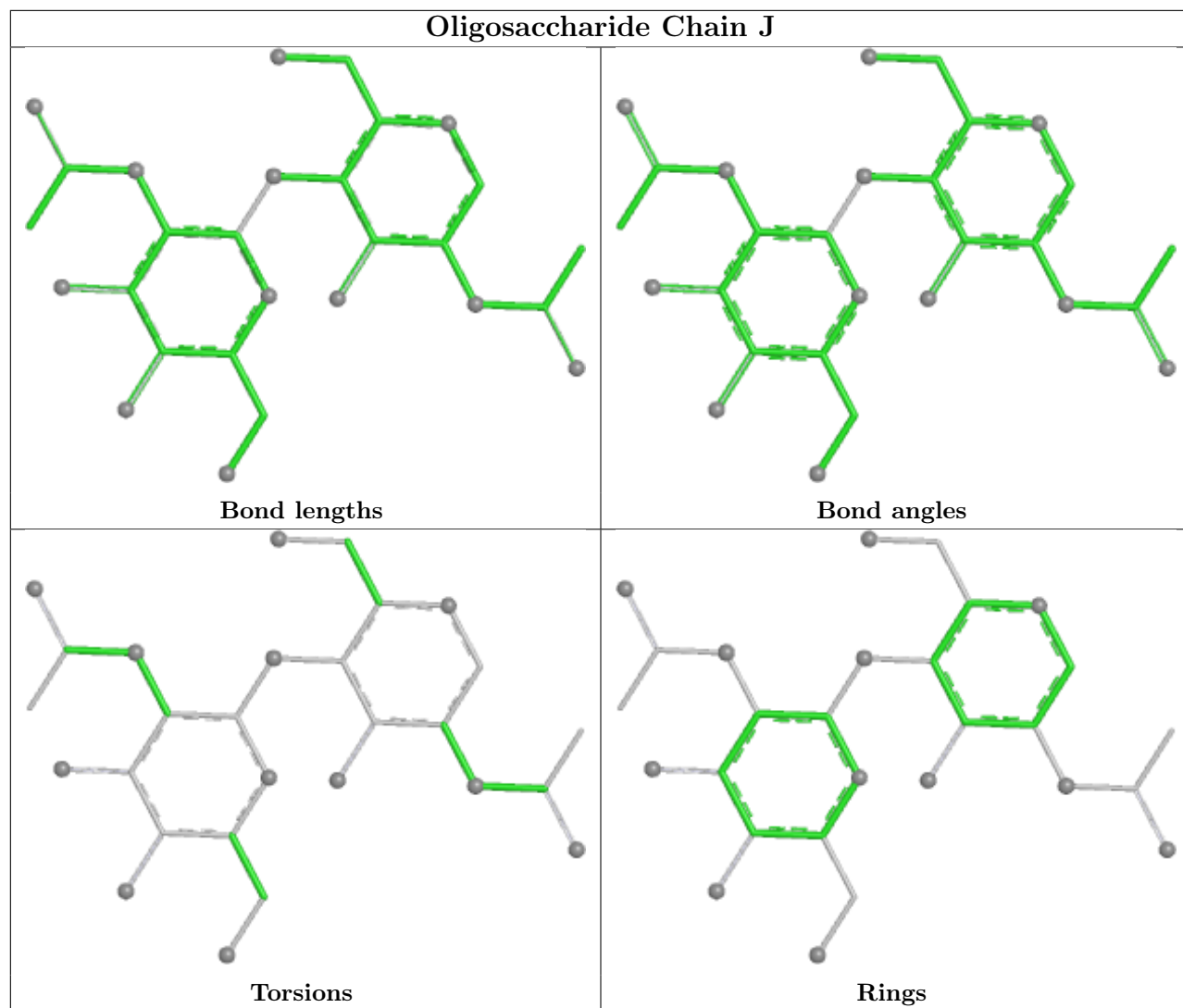
7 monomers are involved in 5 short contacts:

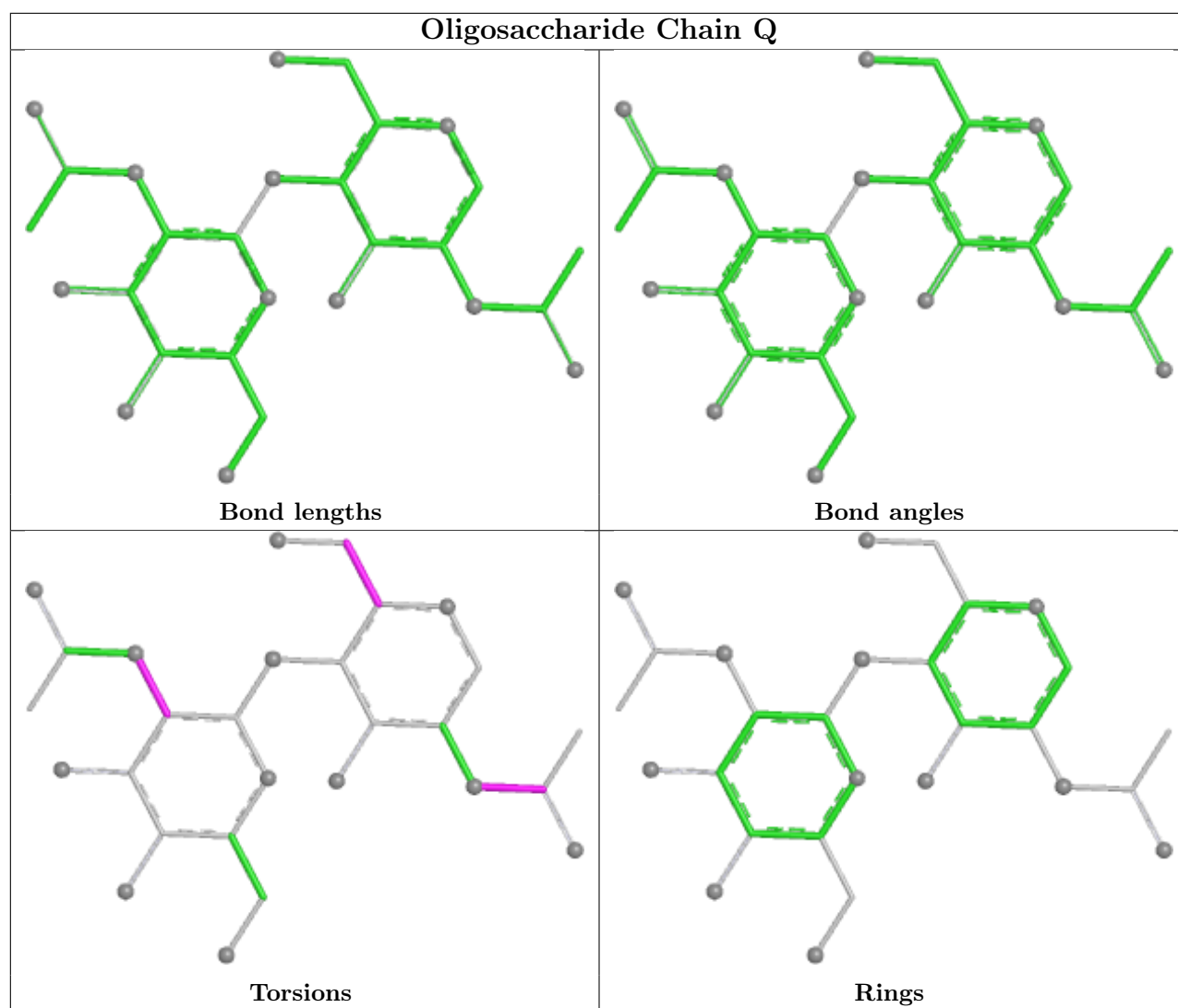
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 10  | P     | 3   | BMA  | 1       | 0            |
| 10  | P     | 4   | MAN  | 1       | 0            |
| 7   | I     | 1   | NAG  | 1       | 0            |
| 9   | M     | 2   | NAG  | 1       | 0            |
| 6   | G     | 2   | NAG  | 1       | 0            |
| 11  | R     | 1   | NAG  | 1       | 0            |
| 9   | M     | 1   | NAG  | 1       | 0            |

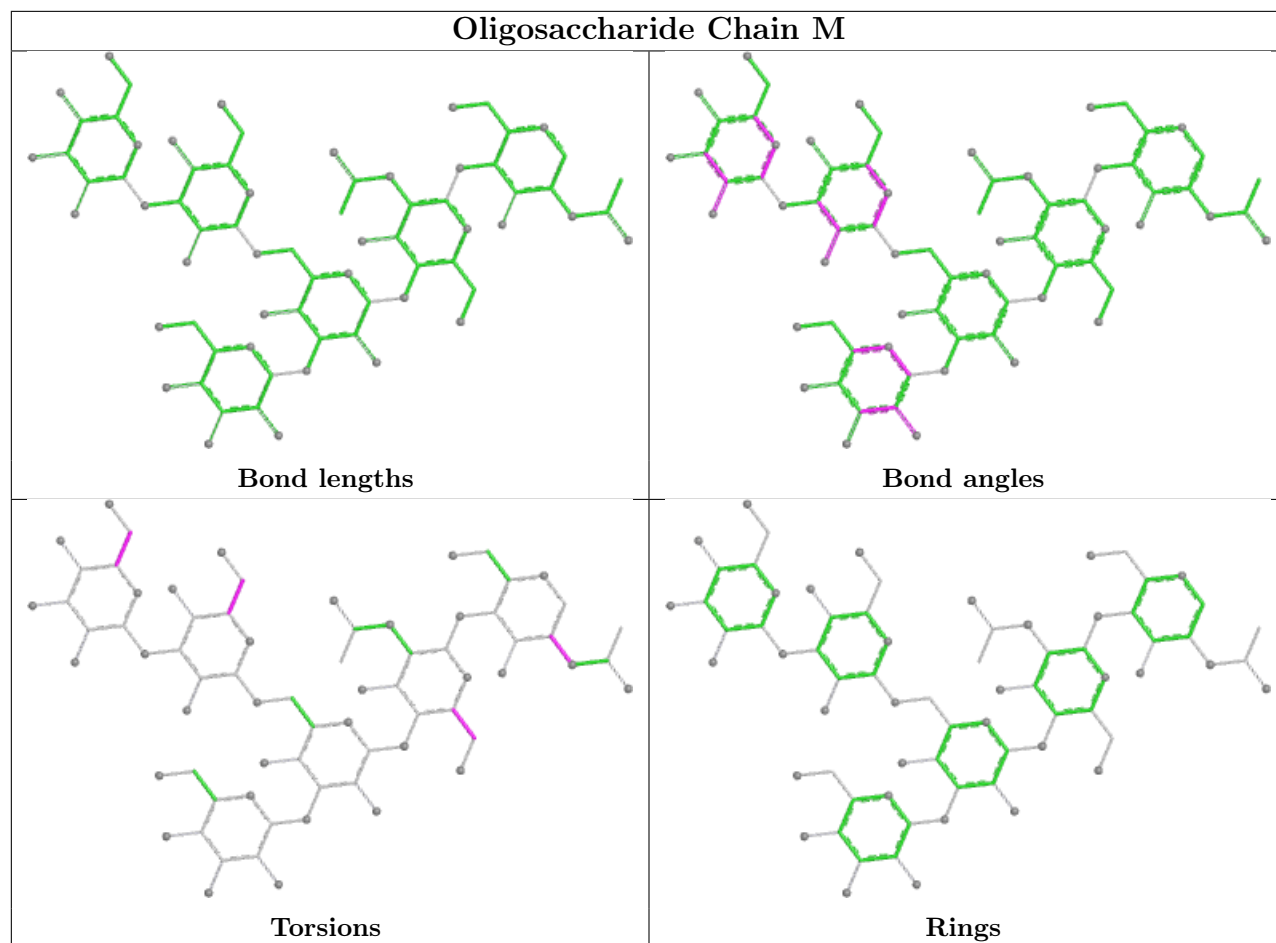
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

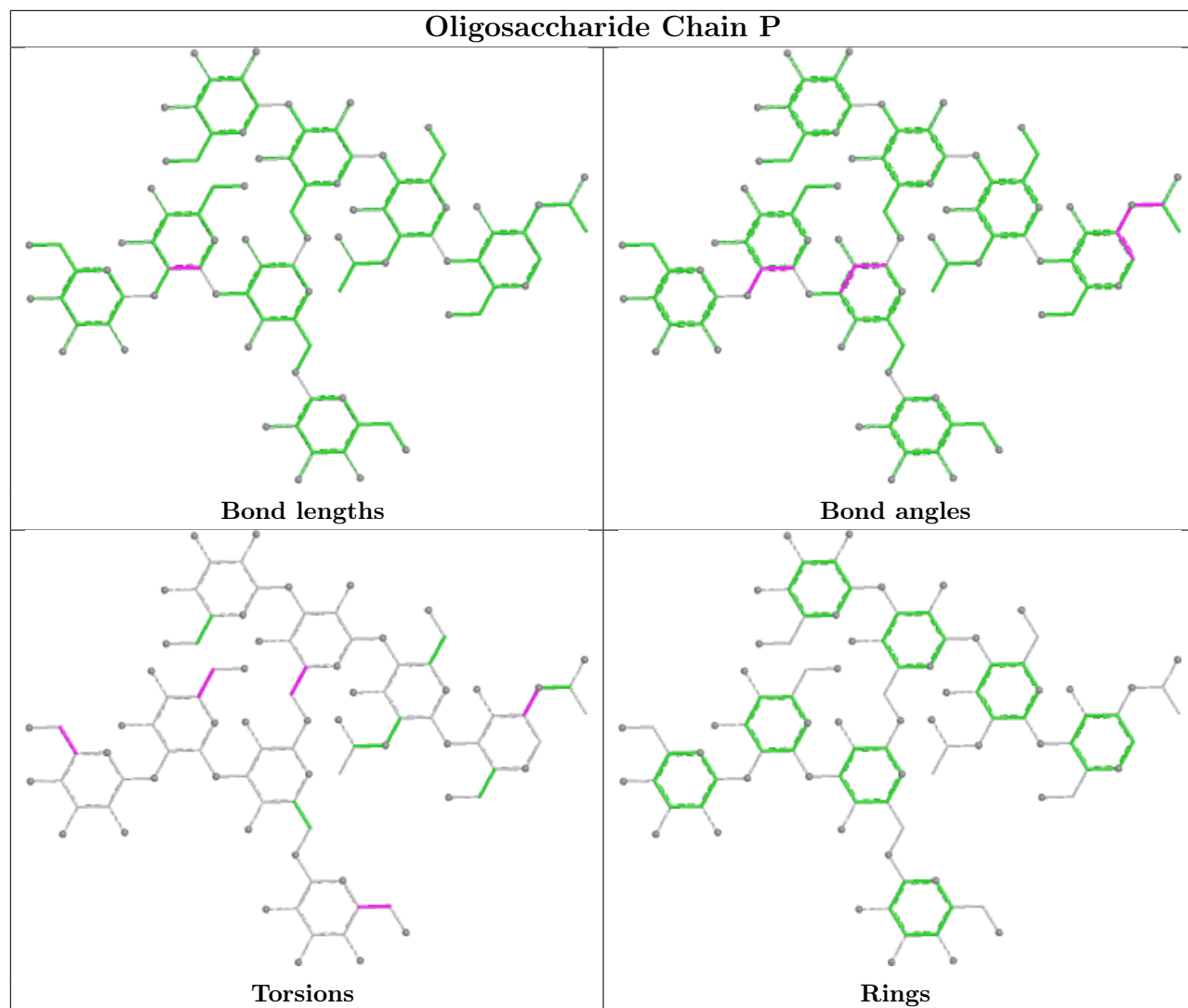


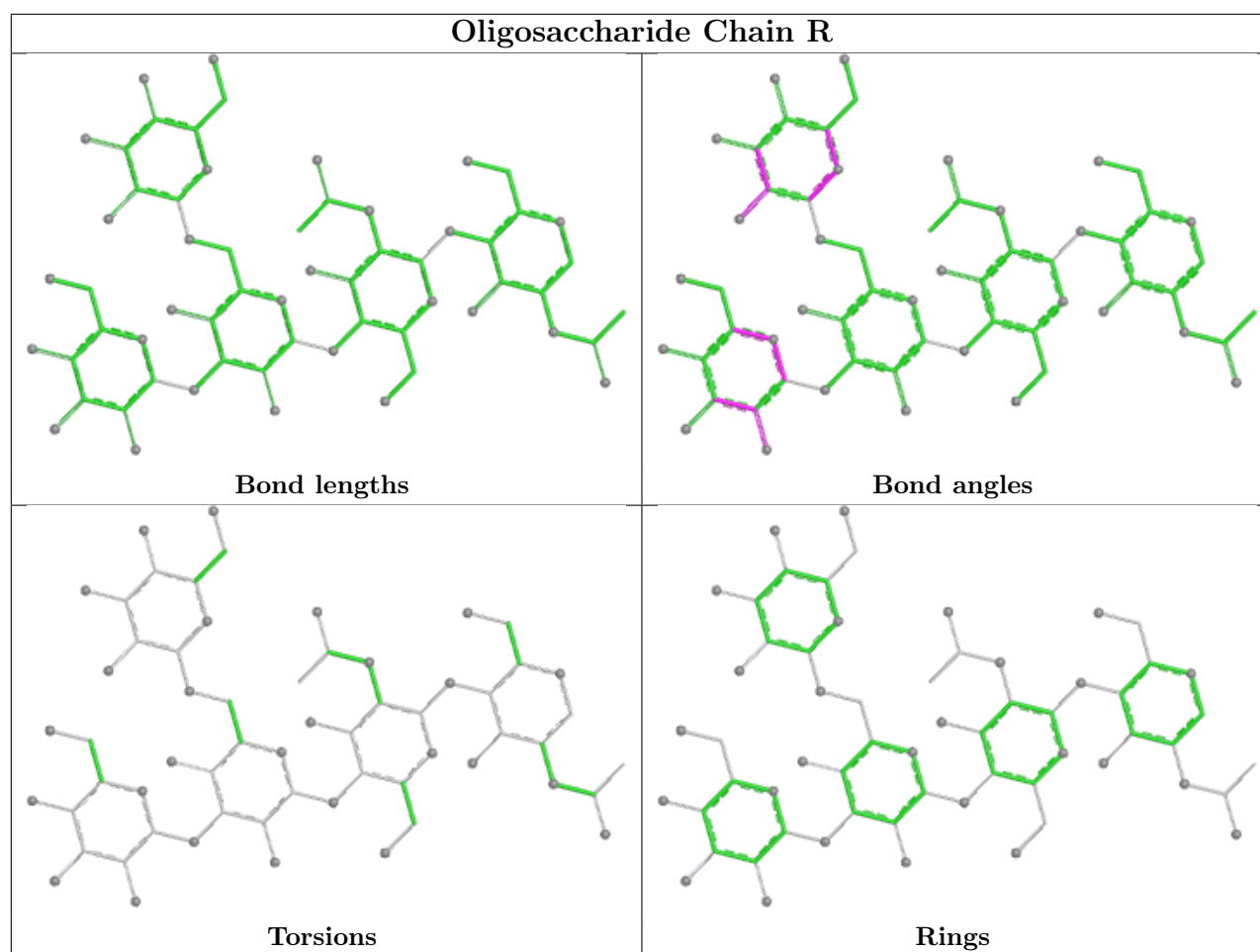












## 5.6 Ligand geometry [i](#)

16 ligands 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 | $\# Z  > 2$ |
| 12  | HEX  | B     | 502 | -    | 5,5,5        | 0.32 | 0           | 4,4,4       | 0.59 | 0           |
| 12  | HEX  | B     | 501 | -    | 5,5,5        | 0.31 | 0           | 4,4,4       | 0.59 | 0           |
| 12  | HEX  | E     | 502 | -    | 5,5,5        | 0.32 | 0           | 4,4,4       | 0.59 | 0           |
| 14  | R16  | B     | 504 | -    | 15,15,15     | 0.31 | 0           | 14,14,14    | 0.84 | 0           |
| 14  | R16  | C     | 503 | -    | 15,15,15     | 0.34 | 0           | 14,14,14    | 0.68 | 0           |
| 16  | PX2  | D     | 501 | -    | 35,35,35     | 1.03 | 3 (8%)      | 38,40,40    | 1.25 | 2 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | D10  | E     | 503 | -    | 9,9,9        | 0.30 | 0        | 8,8,8       | 0.77 | 0        |
| 14  | R16  | C     | 502 | -    | 15,15,15     | 0.33 | 0        | 14,14,14    | 0.72 | 0        |
| 15  | PGW  | B     | 505 | -    | 50,50,50     | 1.00 | 2 (4%)   | 53,56,56    | 0.94 | 2 (3%)   |
| 12  | HEX  | A     | 502 | -    | 5,5,5        | 0.13 | 0        | 4,4,4       | 0.09 | 0        |
| 18  | CLR  | C     | 505 | -    | 31,31,31     | 0.18 | 0        | 48,48,48    | 0.34 | 0        |
| 13  | D10  | B     | 503 | -    | 9,9,9        | 0.32 | 0        | 8,8,8       | 0.74 | 0        |
| 13  | D10  | C     | 504 | -    | 9,9,9        | 0.19 | 0        | 8,8,8       | 0.11 | 0        |
| 17  | NAG  | C     | 501 | -    | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.49 | 0        |
| 12  | HEX  | E     | 501 | -    | 5,5,5        | 0.31 | 0        | 4,4,4       | 0.62 | 0        |
| 13  | D10  | A     | 501 | -    | 9,9,9        | 0.16 | 0        | 8,8,8       | 0.12 | 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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 12  | HEX  | B     | 502 | -    | -       | 0/3/3/3     | -       |
| 12  | HEX  | B     | 501 | -    | -       | 0/3/3/3     | -       |
| 12  | HEX  | E     | 502 | -    | -       | 0/3/3/3     | -       |
| 14  | R16  | B     | 504 | -    | -       | 6/13/13/13  | -       |
| 14  | R16  | C     | 503 | -    | -       | 2/13/13/13  | -       |
| 16  | PX2  | D     | 501 | -    | -       | 19/37/37/37 | -       |
| 13  | D10  | E     | 503 | -    | -       | 3/7/7/7     | -       |
| 14  | R16  | C     | 502 | -    | -       | 3/13/13/13  | -       |
| 15  | PGW  | B     | 505 | -    | -       | 19/55/55/55 | -       |
| 12  | HEX  | A     | 502 | -    | -       | 0/3/3/3     | -       |
| 18  | CLR  | C     | 505 | -    | -       | 0/10/68/68  | 0/4/4/4 |
| 13  | D10  | B     | 503 | -    | -       | 2/7/7/7     | -       |
| 13  | D10  | C     | 504 | -    | -       | 2/7/7/7     | -       |
| 17  | NAG  | C     | 501 | -    | -       | 4/6/23/26   | 0/1/1/1 |
| 12  | HEX  | E     | 501 | -    | -       | 0/3/3/3     | -       |
| 13  | D10  | A     | 501 | -    | -       | 0/7/7/7     | -       |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 15  | B     | 505 | PGW  | O03-C19 | 2.91 | 1.41        | 1.33     |
| 15  | B     | 505 | PGW  | O01-C1  | 2.82 | 1.42        | 1.34     |
| 16  | D     | 501 | PX2  | O5-C4   | 2.81 | 1.41        | 1.33     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | D     | 501 | PX2  | O7-C16 | 2.44  | 1.41        | 1.34     |
| 16  | D     | 501 | PX2  | O7-C2  | -2.32 | 1.41        | 1.46     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 16  | D     | 501 | PX2  | O7-C16-C17  | 4.78 | 121.82      | 111.48   |
| 15  | B     | 505 | PGW  | O01-C1-C2   | 3.80 | 119.69      | 111.48   |
| 15  | B     | 505 | PGW  | O03-C19-C20 | 2.88 | 120.60      | 111.83   |
| 16  | D     | 501 | PX2  | O5-C4-C5    | 2.51 | 119.47      | 111.83   |

There are no chirality outliers.

All (60) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 16  | D     | 501 | PX2  | C1-O4-P1-O1     |
| 16  | D     | 501 | PX2  | C1-O4-P1-O3     |
| 16  | D     | 501 | PX2  | O8-C16-O7-C2    |
| 16  | D     | 501 | PX2  | C17-C16-O7-C2   |
| 15  | B     | 505 | PGW  | C20-C19-O03-C01 |
| 15  | B     | 505 | PGW  | O04-C19-O03-C01 |
| 17  | C     | 501 | NAG  | O5-C5-C6-O6     |
| 17  | C     | 501 | NAG  | C4-C5-C6-O6     |
| 14  | C     | 503 | R16  | C34-C35-C36-C37 |
| 15  | B     | 505 | PGW  | C24-C25-C26-C27 |
| 16  | D     | 501 | PX2  | C22-C23-C24-C25 |
| 14  | C     | 502 | R16  | C38-C39-C40-C41 |
| 16  | D     | 501 | PX2  | C5-C6-C7-C8     |
| 15  | B     | 505 | PGW  | C5-C6-C7-C8     |
| 15  | B     | 505 | PGW  | C2-C1-O01-C02   |
| 14  | C     | 502 | R16  | C31-C32-C33-C34 |
| 13  | C     | 504 | D10  | C4-C5-C6-C7     |
| 16  | D     | 501 | PX2  | C18-C19-C20-C21 |
| 13  | E     | 503 | D10  | C4-C5-C6-C7     |
| 15  | B     | 505 | PGW  | O02-C1-O01-C02  |
| 16  | D     | 501 | PX2  | C1-O4-P1-O2     |
| 15  | B     | 505 | PGW  | C23-C24-C25-C26 |
| 16  | D     | 501 | PX2  | C5-C4-O5-C3     |
| 14  | B     | 504 | R16  | C33-C34-C35-C36 |
| 16  | D     | 501 | PX2  | C4-C5-C6-C7     |
| 16  | D     | 501 | PX2  | C11-C10-C9-C8   |
| 15  | B     | 505 | PGW  | C16-C15-C27-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | B     | 505 | PGW  | C27-C15-C16-C17 |
| 16  | D     | 501 | PX2  | O6-C4-O5-C3     |
| 14  | B     | 504 | R16  | C37-C38-C39-C40 |
| 15  | B     | 505 | PGW  | O01-C02-C03-O11 |
| 14  | B     | 504 | R16  | C32-C33-C34-C35 |
| 15  | B     | 505 | PGW  | C02-C03-O11-P   |
| 14  | B     | 504 | R16  | C28-C29-C30-C31 |
| 17  | C     | 501 | NAG  | C1-C2-N2-C7     |
| 14  | B     | 504 | R16  | C35-C36-C37-C38 |
| 16  | D     | 501 | PX2  | C10-C11-C12-C13 |
| 15  | B     | 505 | PGW  | C01-C02-C03-O11 |
| 14  | B     | 504 | R16  | C36-C37-C38-C39 |
| 16  | D     | 501 | PX2  | C16-C17-C18-C19 |
| 15  | B     | 505 | PGW  | C07-C06-C10-C9  |
| 14  | C     | 502 | R16  | C28-C29-C30-C31 |
| 15  | B     | 505 | PGW  | C03-O11-P-O14   |
| 15  | B     | 505 | PGW  | C04-O12-P-O11   |
| 15  | B     | 505 | PGW  | C04-O12-P-O13   |
| 15  | B     | 505 | PGW  | C04-O12-P-O14   |
| 17  | C     | 501 | NAG  | C3-C2-N2-C7     |
| 15  | B     | 505 | PGW  | C05-C04-O12-P   |
| 16  | D     | 501 | PX2  | C3-C2-O7-C16    |
| 16  | D     | 501 | PX2  | C21-C22-C23-C24 |
| 13  | B     | 503 | D10  | C2-C3-C4-C5     |
| 15  | B     | 505 | PGW  | C3-C4-C5-C6     |
| 13  | E     | 503 | D10  | C1-C2-C3-C4     |
| 13  | E     | 503 | D10  | C2-C3-C4-C5     |
| 13  | C     | 504 | D10  | C2-C3-C4-C5     |
| 13  | B     | 503 | D10  | C1-C2-C3-C4     |
| 16  | D     | 501 | PX2  | O7-C16-C17-C18  |
| 16  | D     | 501 | PX2  | C7-C8-C9-C10    |
| 14  | C     | 503 | R16  | C28-C29-C30-C31 |
| 16  | D     | 501 | PX2  | O8-C16-C17-C18  |

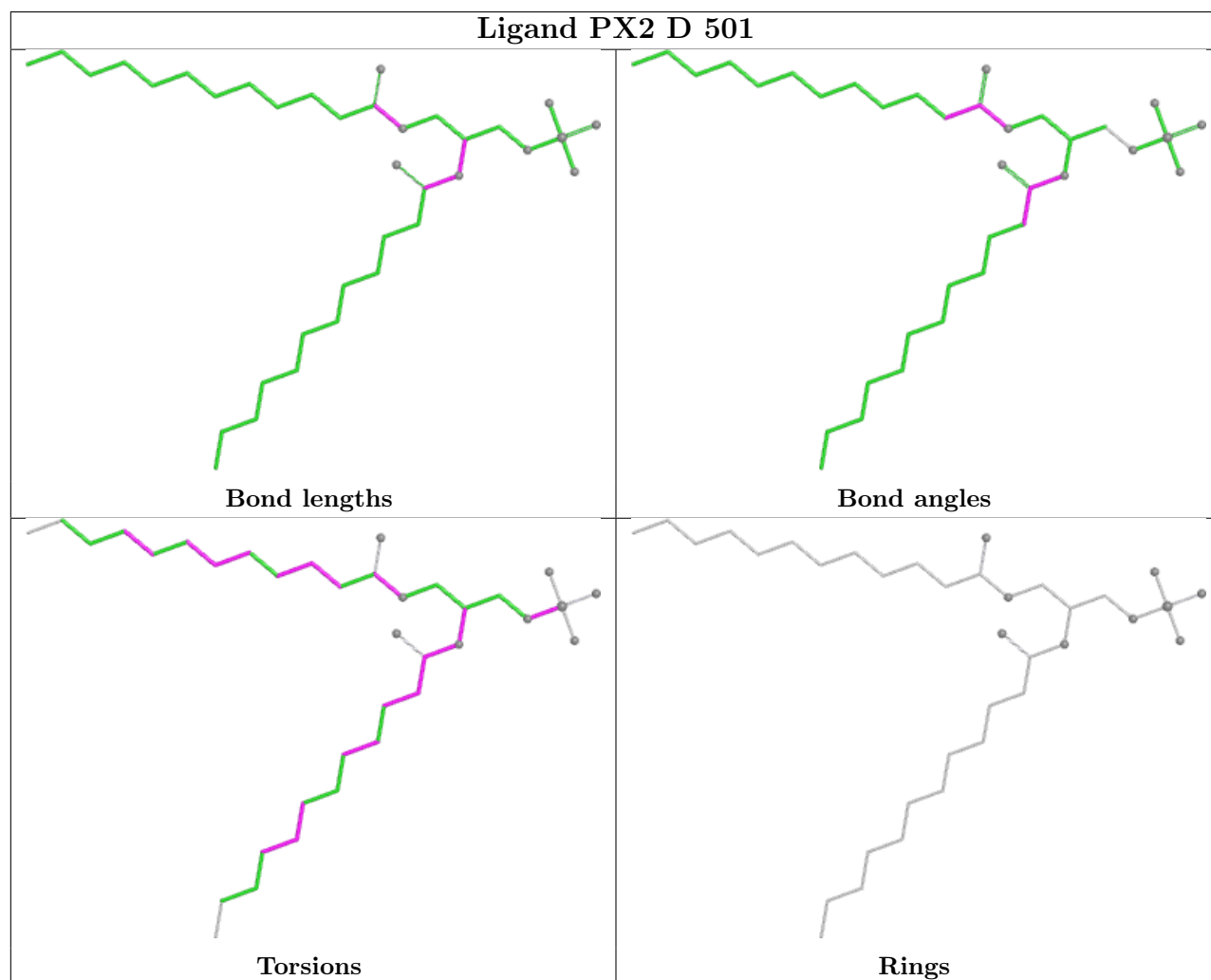
There are no ring outliers.

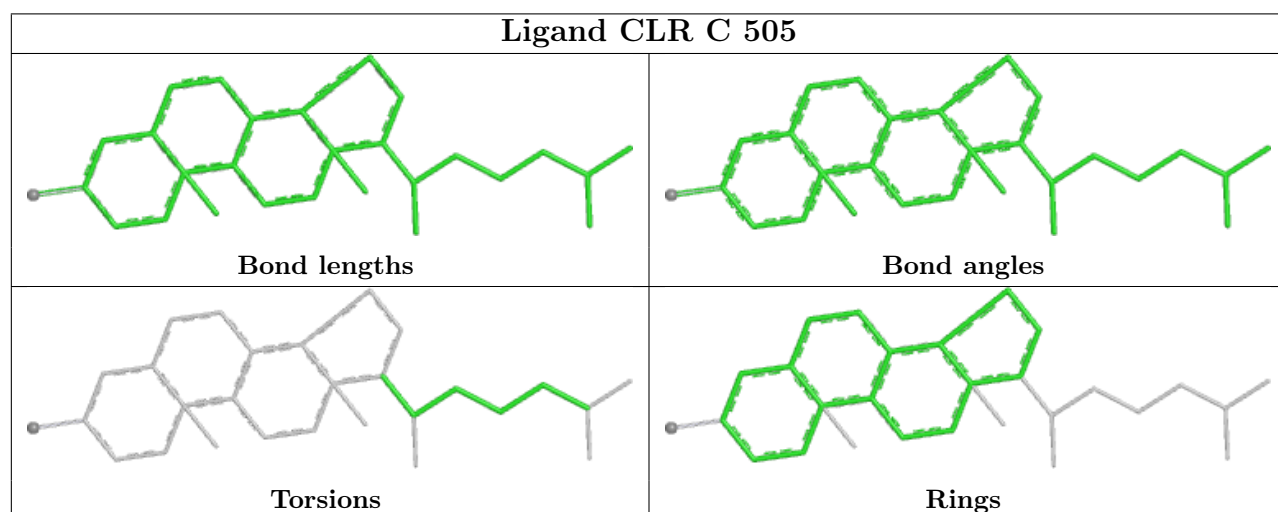
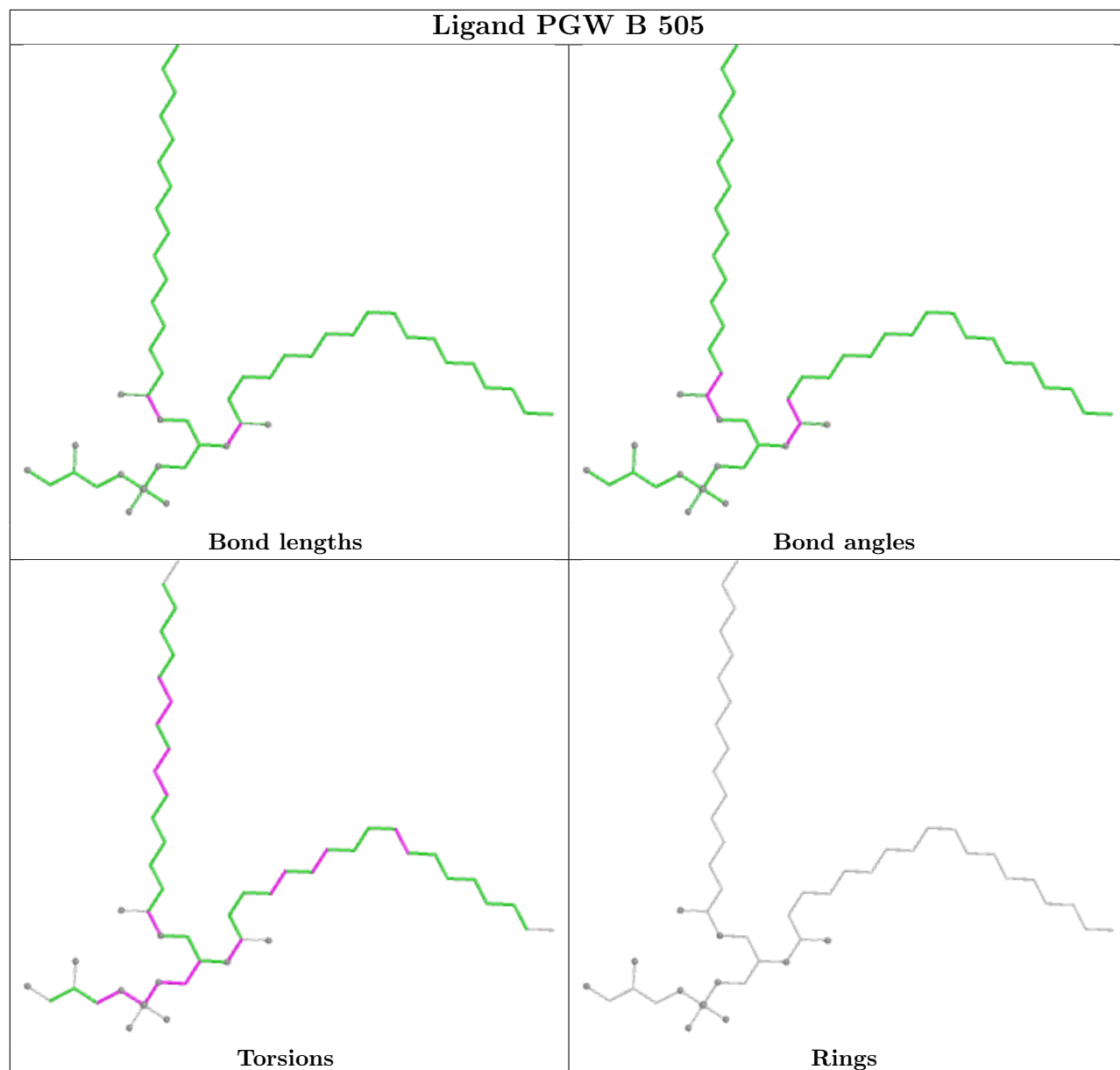
2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | C     | 504 | D10  | 2       | 0            |
| 13  | A     | 501 | D10  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

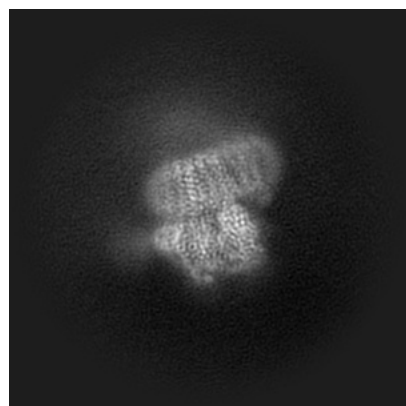
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50283. These allow visual inspection of the internal detail of the map and identification of artifacts.

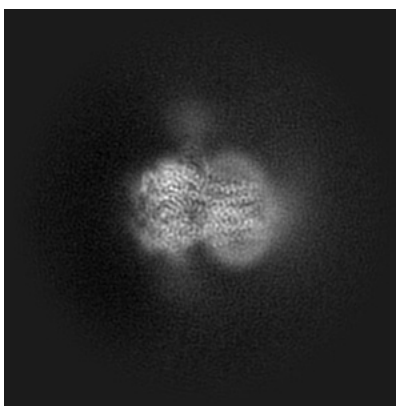
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

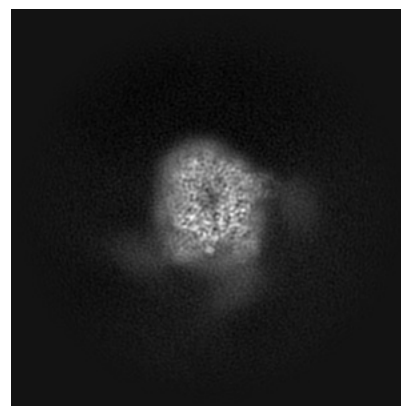
#### 6.1.1 Primary map



X

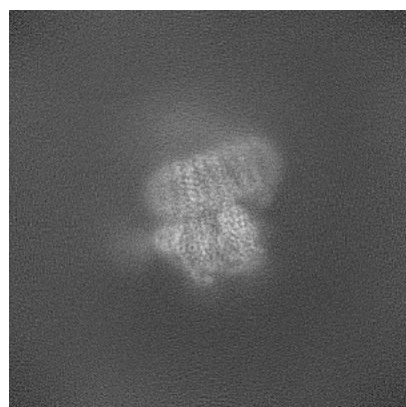


Y

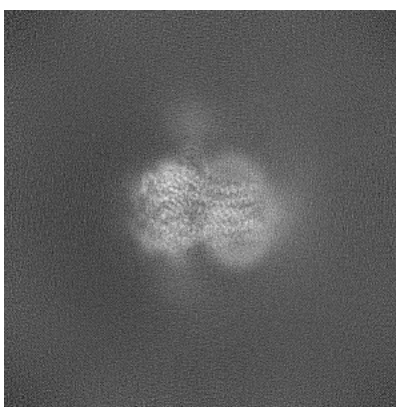


Z

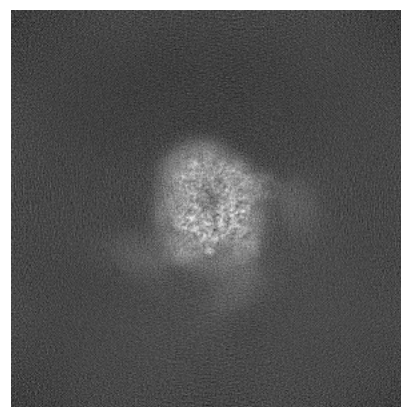
#### 6.1.2 Raw map



X



Y

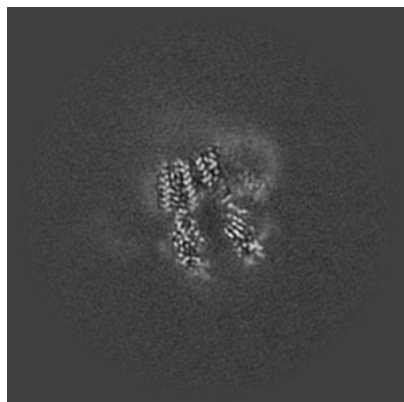


Z

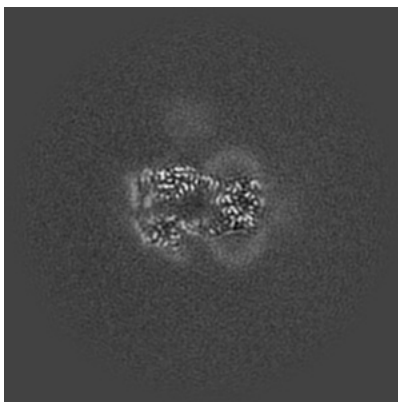
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

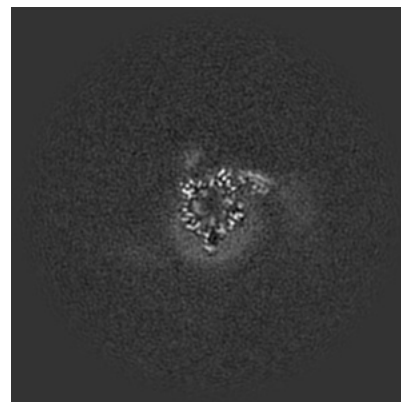
### 6.2.1 Primary map



X Index: 232

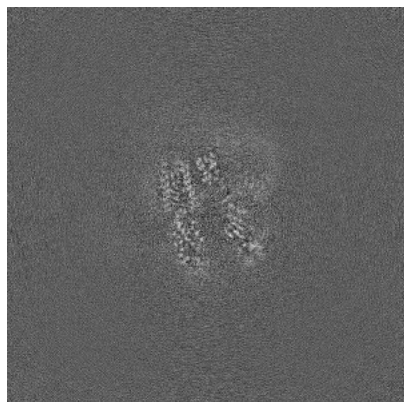


Y Index: 232

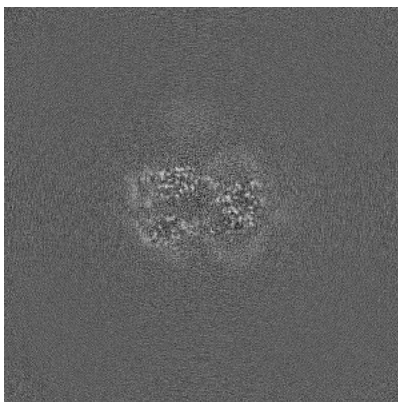


Z Index: 232

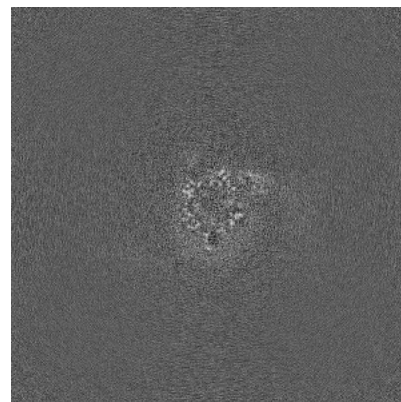
### 6.2.2 Raw map



X Index: 232



Y Index: 232

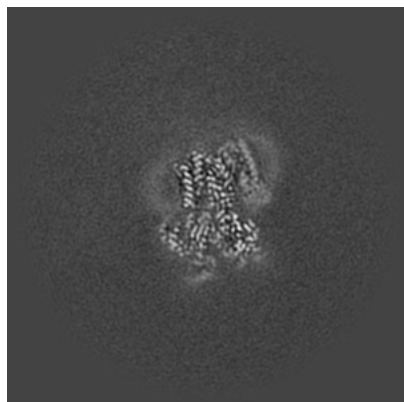


Z Index: 232

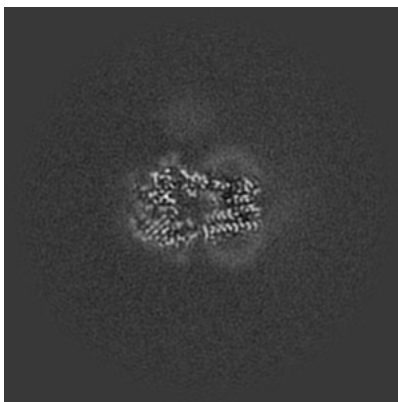
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

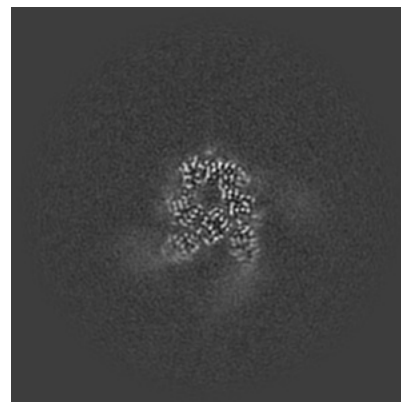
### 6.3.1 Primary map



X Index: 212

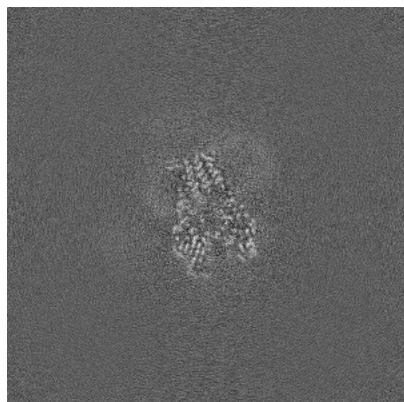


Y Index: 223

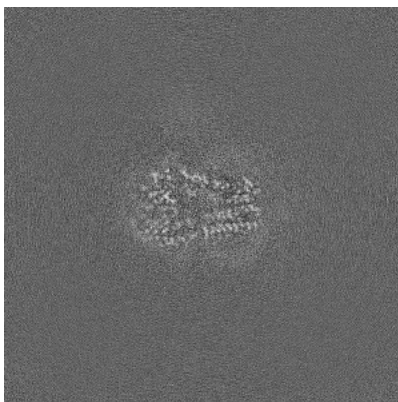


Z Index: 195

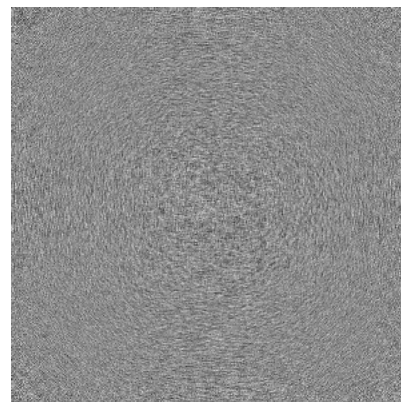
### 6.3.2 Raw map



X Index: 244



Y Index: 223

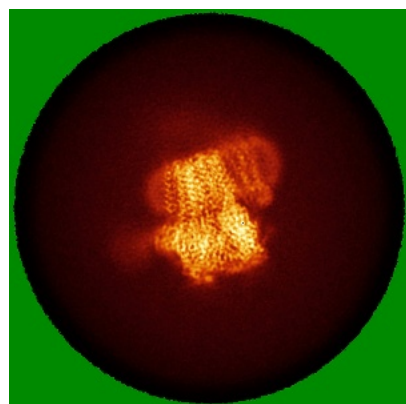


Z Index: 0

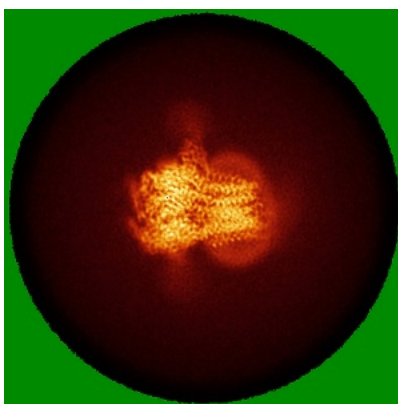
The images above show the largest variance slices of the map in three orthogonal directions.

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

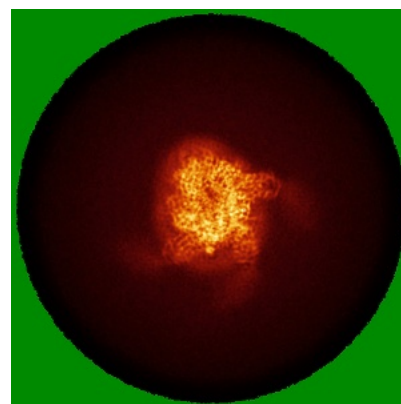
### 6.4.1 Primary map



X

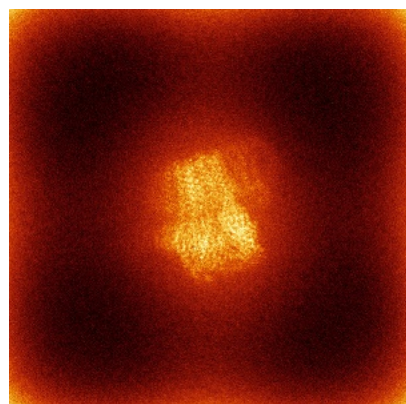


Y

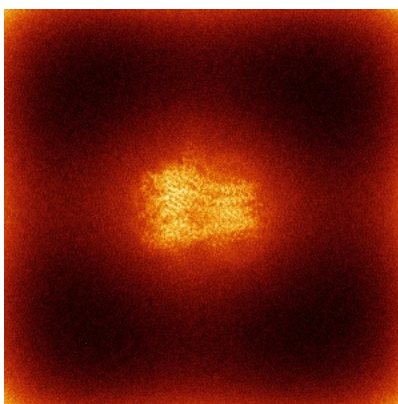


Z

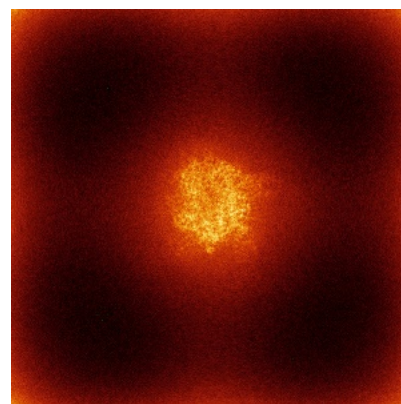
### 6.4.2 Raw map



X



Y

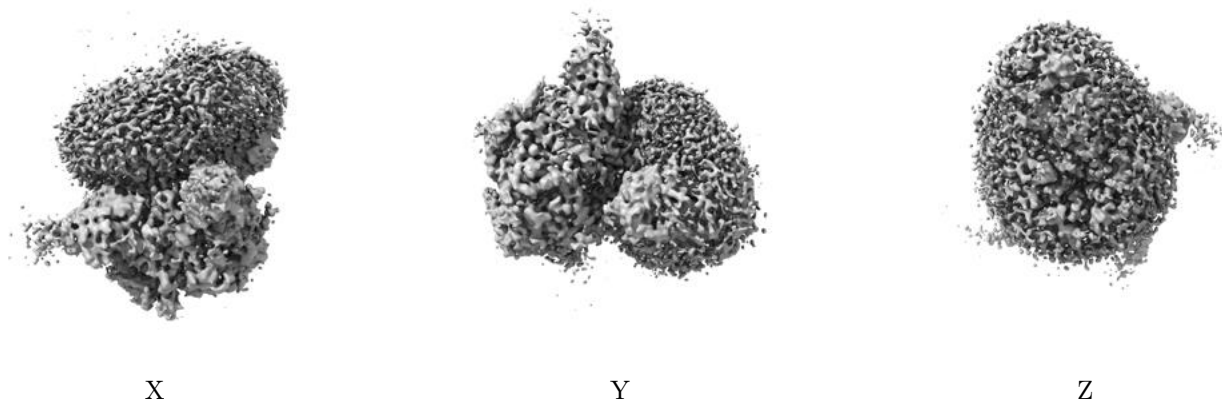


Z

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.

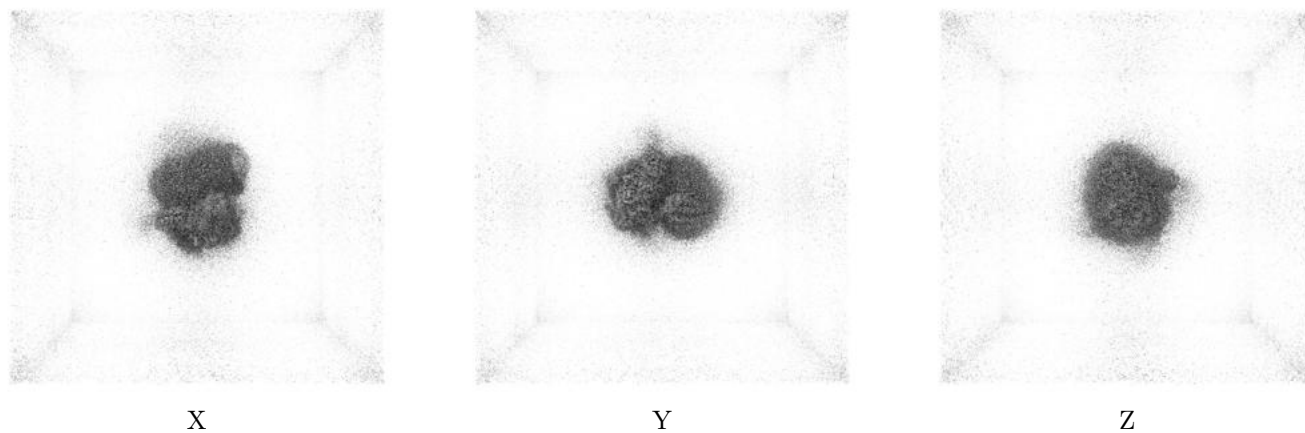
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

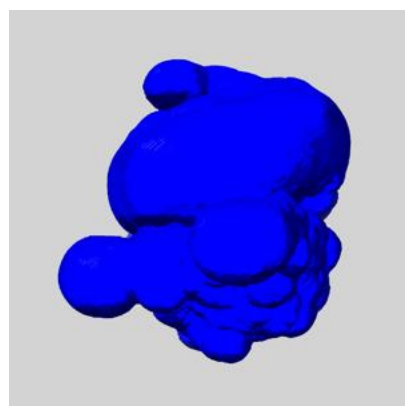
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

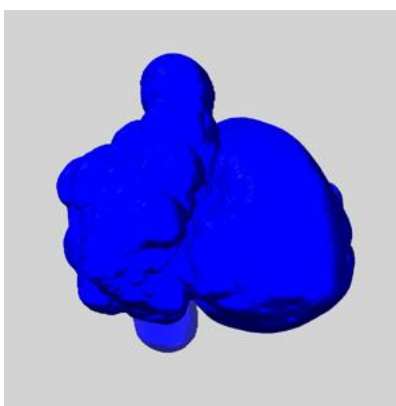
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

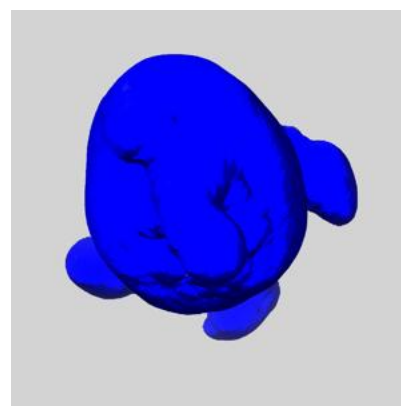
### 6.6.1 emd\_50283\_msk\_1.map [i](#)



X



Y

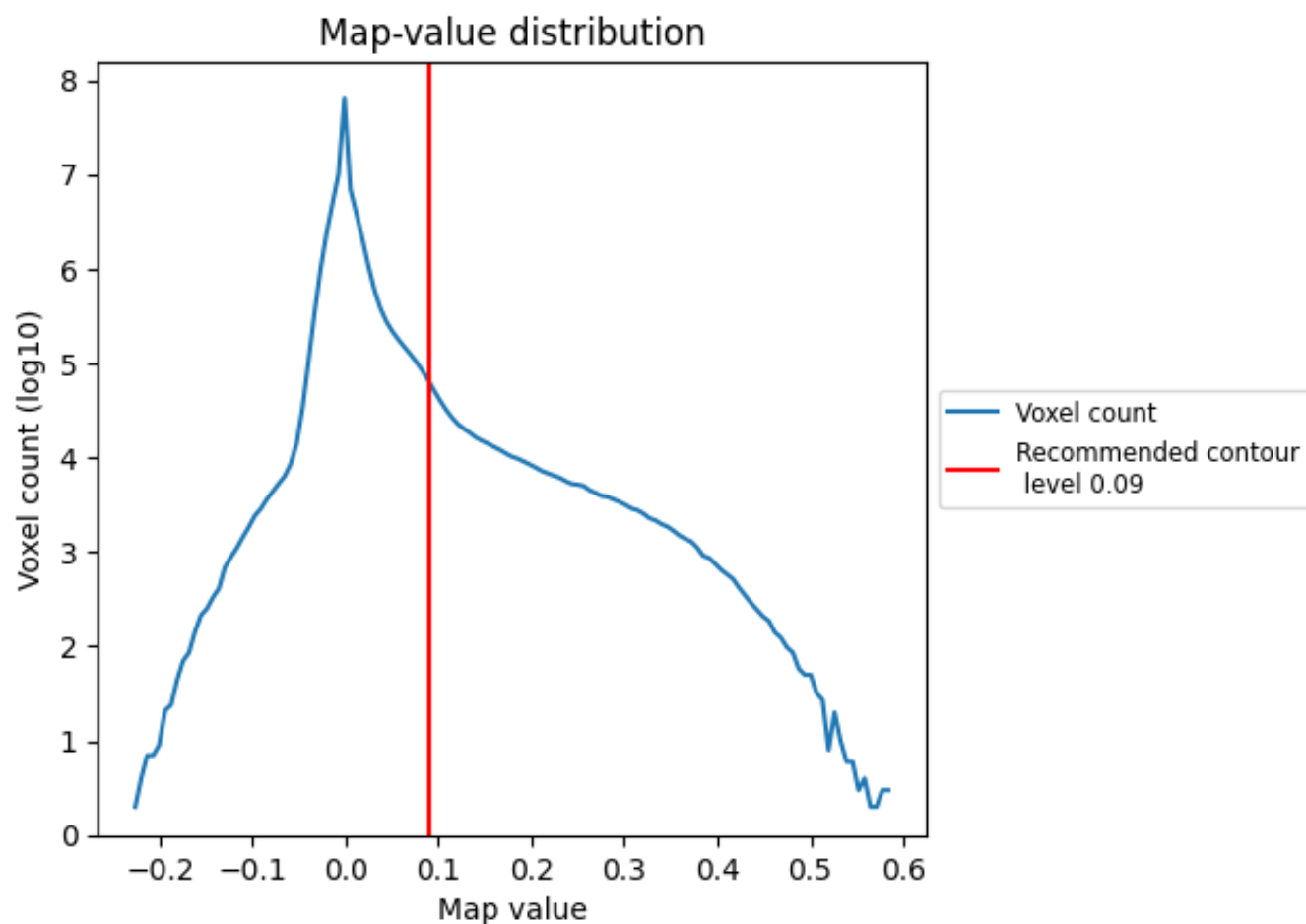


Z

## 7 Map analysis [i](#)

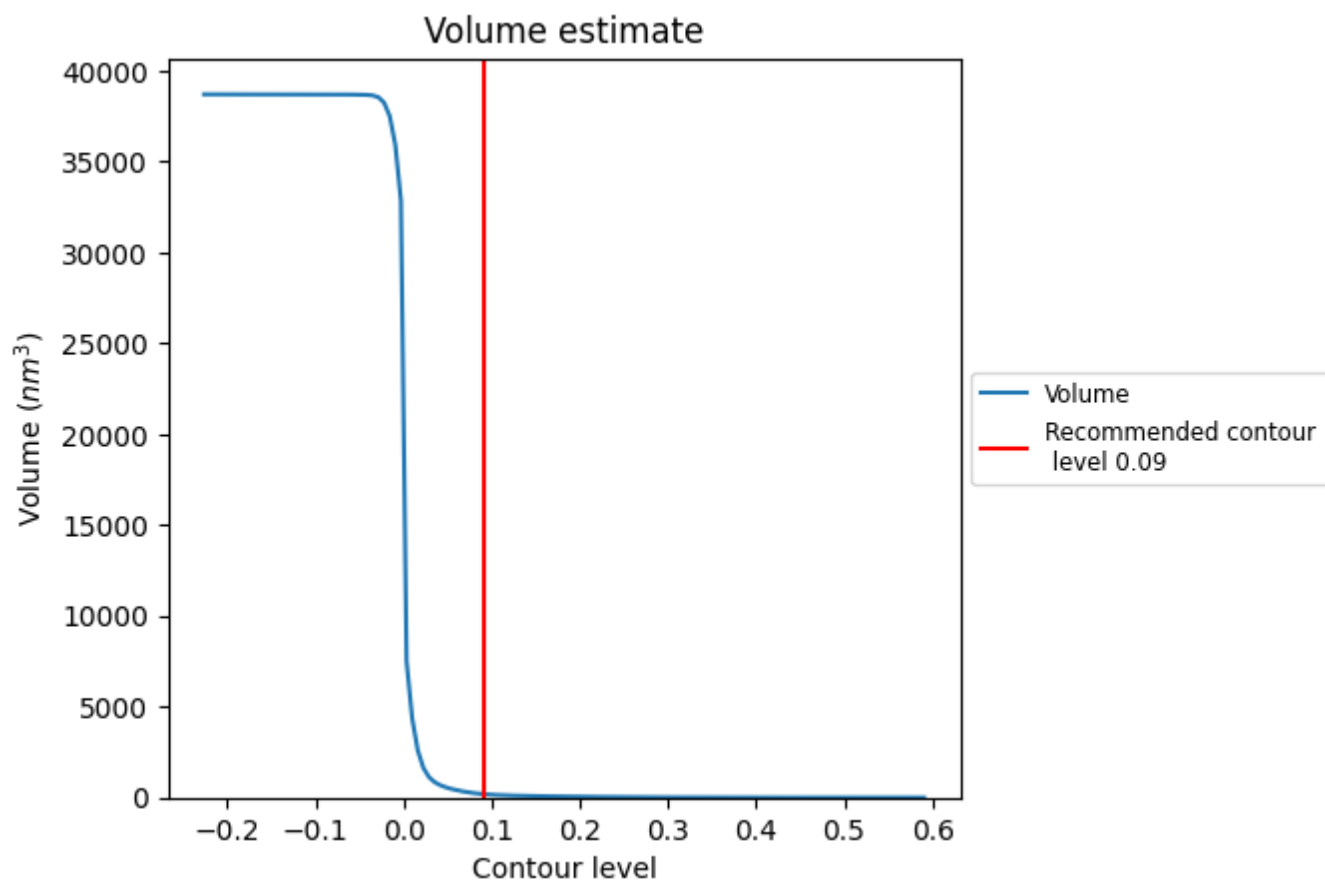
This section contains the results of statistical analysis of the map.

### 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.

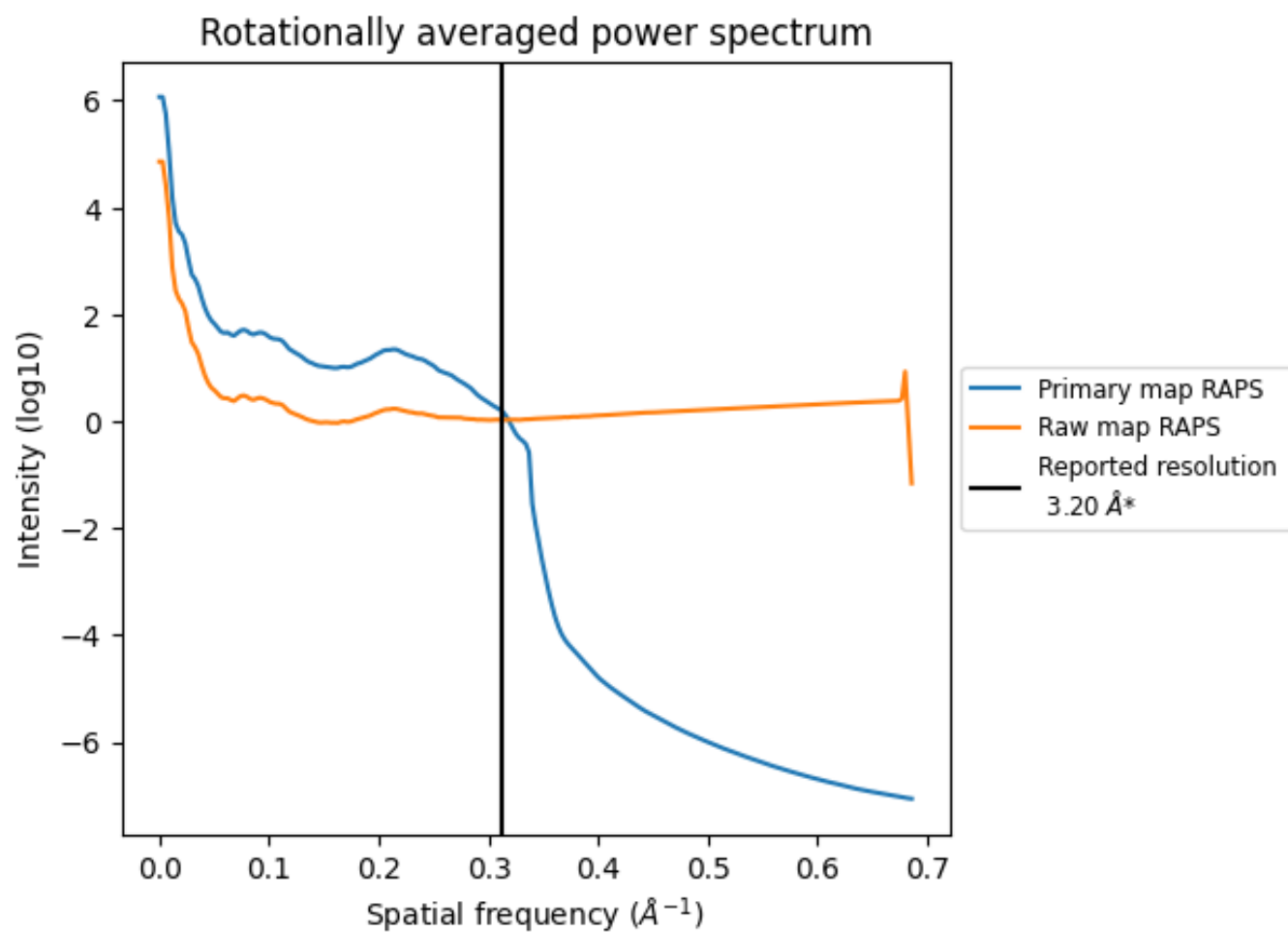
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192  $\text{nm}^3$ ; this corresponds to an approximate mass of 174 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 ⓘ

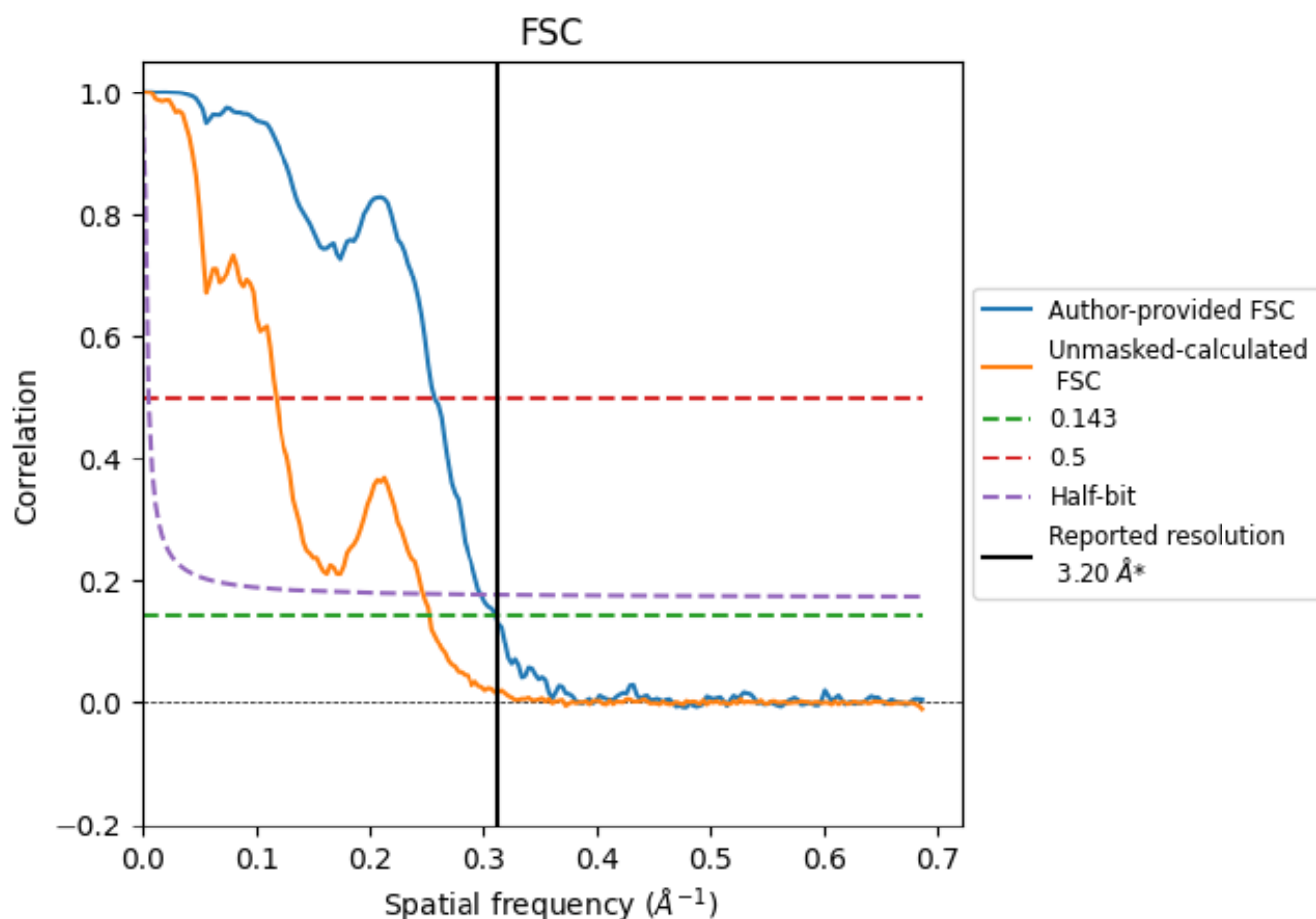


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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  $0.312 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

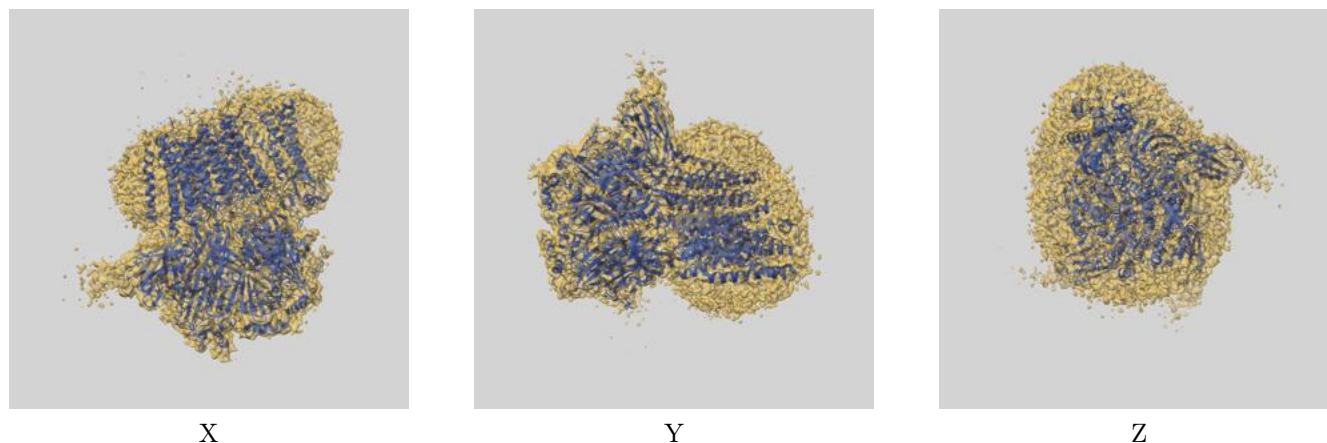
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.20                               | -    | -        |
| Author-provided FSC curve | 3.21                               | 3.89 | 3.35     |
| Unmasked-calculated*      | 3.96                               | 8.50 | 4.05     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

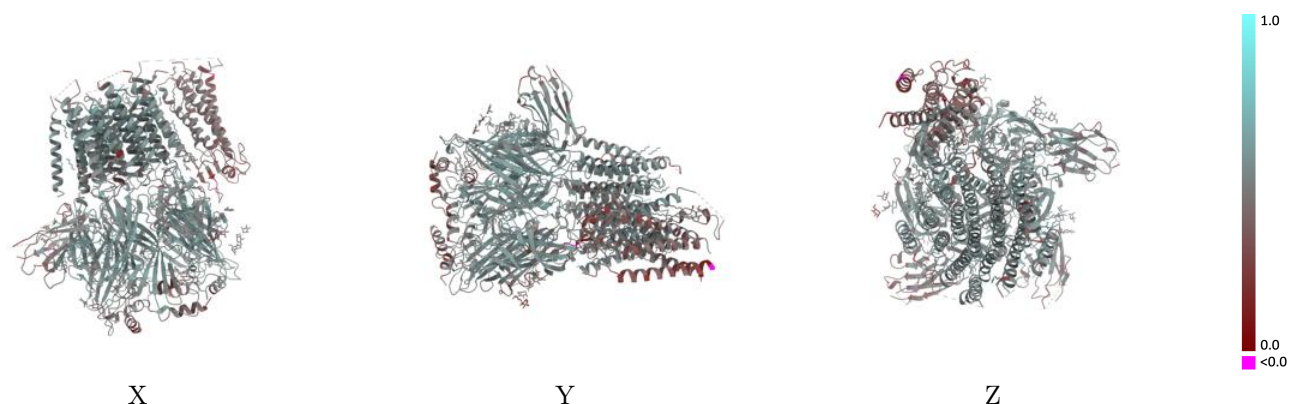
This section contains information regarding the fit between EMDB map EMD-50283 and PDB model 9FAV. Per-residue inclusion information can be found in section [3](#) on page [12](#).

### 9.1 Map-model overlay [i](#)



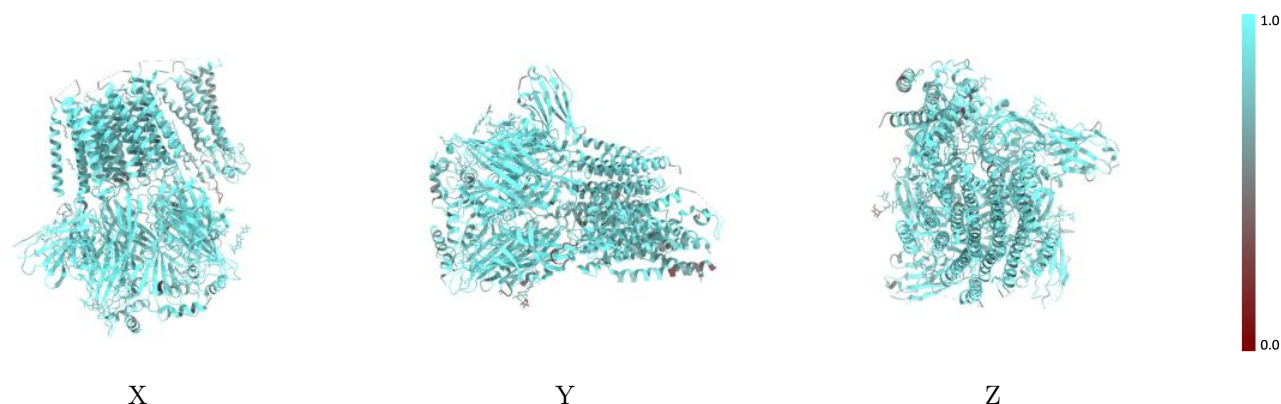
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



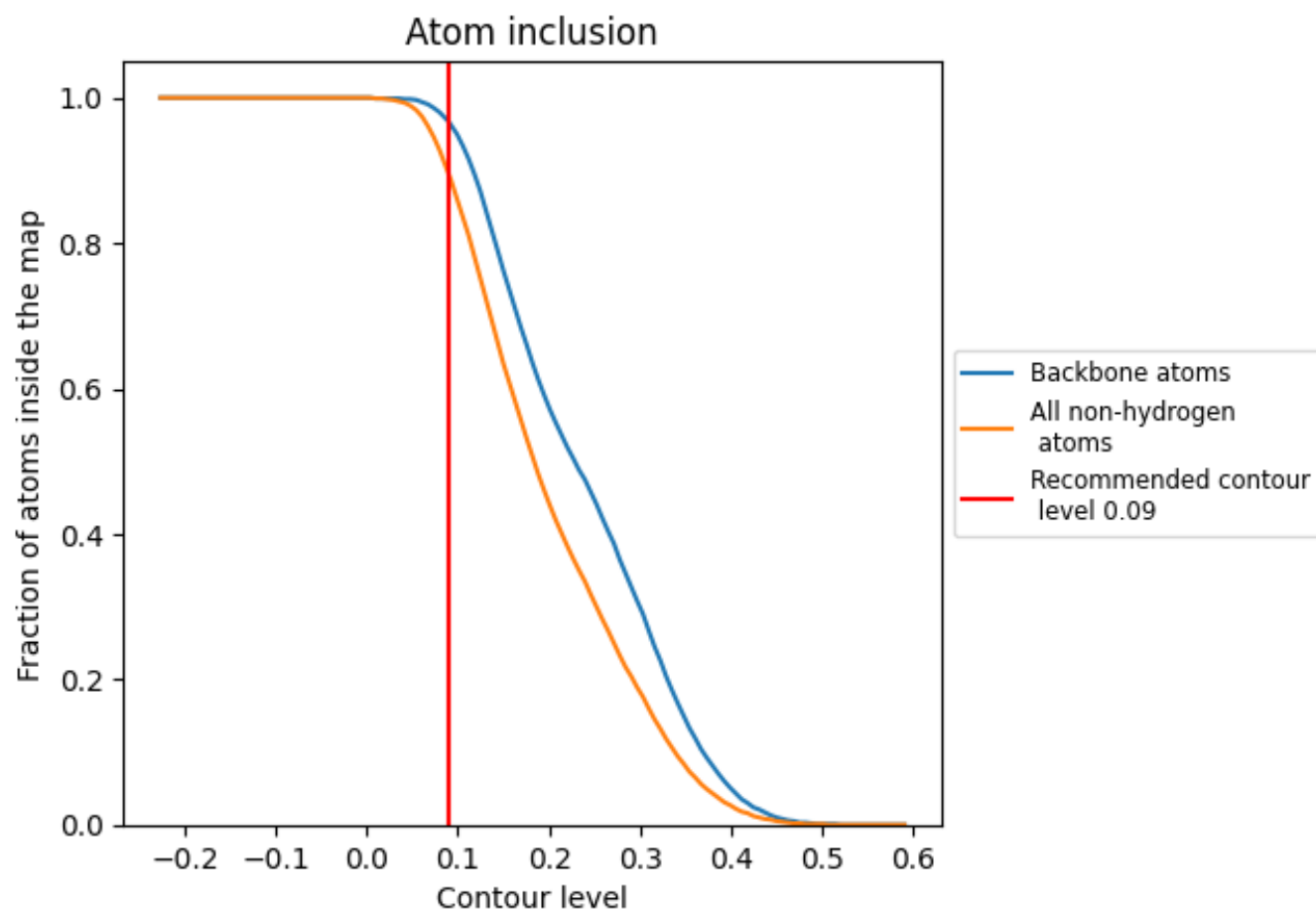
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.09) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8950   |  0.4980   |
| A     |  0.9190   |  0.5200   |
| B     |  0.9270   |  0.5360   |
| C     |  0.9010   |  0.5170   |
| D     |  0.8990   |  0.5080   |
| E     |  0.9200   |  0.5180   |
| F     |  0.8850   |  0.4970   |
| G     |  0.8720   |  0.4550   |
| H     |  0.6960   |  0.2720   |
| I     |  0.9520   |  0.5040   |
| J     |  0.7860   |  0.4190   |
| K     |  0.9010   |  0.4830   |
| L     |  0.7980   |  0.3800   |
| M     |  0.9720   |  0.5010   |
| N     |  0.7690  |  0.4140  |
| O     |  0.8530 |  0.4360 |
| P     |  0.9250 |  0.5000 |
| Q     |  0.7500 |  0.3750 |
| R     |  0.6720 |  0.3870 |

