# WORLDWIDE wwPDB PROTEIN DATA BANK

# Full wwPDB EM Validation Report (i)

May 20, 2025 – 02:20 AM EDT

|  |  |  |
|---|---|---|
| PDB ID | : | 9B2A / pdb_00009b2a |
| EMDB ID | : | EMD-44102 |
| Title | : | Cryo-EM structure of the mouse TRPM3 alpha 2 channel in complex with the neurosteroid pregnenolone sulfate and the synthetic agonist CIM 0216 |
| Authors | : | Yin, Y.; Park, C.G.; Feng, S.; Zhang, F.; Guan, Z.; Sharma, K.; Borgnia, M.J.; Im, W.; Lee, S.-Y. |
| Deposited on | : | 2024-03-14 |
| Resolution | : | 3.82 Å(reported) |

# 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 3.82 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.
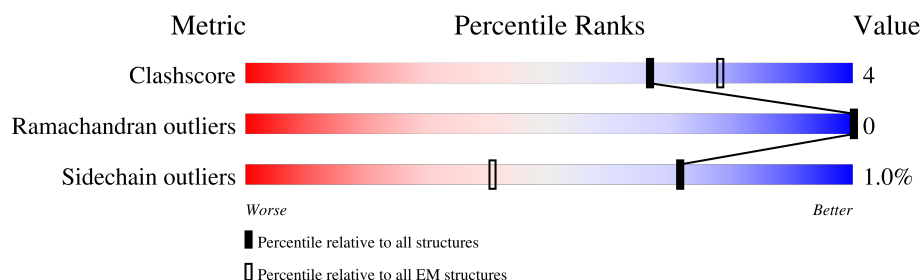


| Metric | Whole archive (#Entries) | EM structures (#Entries) |
| --- | --- | --- |
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 <=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 | 1739 | 44%　　·　53% |
| 1 | B | 1739 | 44%　　·　53% |
| 1 | C | 1739 | 44%　　·　53% |
| 1 | D | 1739 | 44%　　·　53% |

# 2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 41384 atoms, of which 18808 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 Transient receptor potential cation channel, subfamily M, member 3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|-----|---------|-------|
| 1 | A | 817 | Total | C | H | N | O | S | 0 | 0 |
| | | | 10182 | 3580 | 4619 | 966 | 986 | 31 | | |
| 1 | B | 817 | Total | C | H | N | O | S | 0 | 0 |
| | | | 10182 | 3580 | 4619 | 966 | 986 | 31 | | |
| 1 | C | 817 | Total | C | H | N | O | S | 0 | 0 |
| | | | 10182 | 3580 | 4619 | 966 | 986 | 31 | | |
| 1 | D | 817 | Total | C | H | N | O | S | 0 | 0 |
| | | | 10182 | 3580 | 4619 | 966 | 986 | 31 | | |

There are 120 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 1710 | SER | - | expression tag | UNP Q5F4S7 |
| A | 1711 | ASN | - | expression tag | UNP Q5F4S7 |
| A | 1712 | SER | - | expression tag | UNP Q5F4S7 |
| A | 1713 | LEU | - | expression tag | UNP Q5F4S7 |
| A | 1714 | GLU | - | expression tag | UNP Q5F4S7 |
| A | 1715 | VAL | - | expression tag | UNP Q5F4S7 |
| A | 1716 | LEU | - | expression tag | UNP Q5F4S7 |
| A | 1717 | PHE | - | expression tag | UNP Q5F4S7 |
| A | 1718 | GLN | - | expression tag | UNP Q5F4S7 |
| A | 1719 | GLY | - | expression tag | UNP Q5F4S7 |
| A | 1720 | PRO | - | expression tag | UNP Q5F4S7 |
| A | 1721 | ASP | - | expression tag | UNP Q5F4S7 |
| A | 1722 | TYR | - | expression tag | UNP Q5F4S7 |
| A | 1723 | LYS | - | expression tag | UNP Q5F4S7 |
| A | 1724 | ASP | - | expression tag | UNP Q5F4S7 |
| A | 1725 | ASP | - | expression tag | UNP Q5F4S7 |
| A | 1726 | ASP | - | expression tag | UNP Q5F4S7 |
| A | 1727 | ASP | - | expression tag | UNP Q5F4S7 |
| A | 1728 | LYS | - | expression tag | UNP Q5F4S7 |
| A | 1729 | ALA | - | expression tag | UNP Q5F4S7 |
| A | 1730 | HIS | - | expression tag | UNP Q5F4S7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:-:|:-:|:-:|:-:|:-:|:-:|
| A | 1731 | HIS | - | expression tag | UNP Q5F4S7 |
| A | 1732 | HIS | - | expression tag | UNP Q5F4S7 |
| A | 1733 | HIS | - | expression tag | UNP Q5F4S7 |
| A | 1734 | HIS | - | expression tag | UNP Q5F4S7 |
| A | 1735 | HIS | - | expression tag | UNP Q5F4S7 |
| A | 1736 | HIS | - | expression tag | UNP Q5F4S7 |
| A | 1737 | HIS | - | expression tag | UNP Q5F4S7 |
| A | 1738 | HIS | - | expression tag | UNP Q5F4S7 |
| A | 1739 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1710 | SER | - | expression tag | UNP Q5F4S7 |
| B | 1711 | ASN | - | expression tag | UNP Q5F4S7 |
| B | 1712 | SER | - | expression tag | UNP Q5F4S7 |
| B | 1713 | LEU | - | expression tag | UNP Q5F4S7 |
| B | 1714 | GLU | - | expression tag | UNP Q5F4S7 |
| B | 1715 | VAL | - | expression tag | UNP Q5F4S7 |
| B | 1716 | LEU | - | expression tag | UNP Q5F4S7 |
| B | 1717 | PHE | - | expression tag | UNP Q5F4S7 |
| B | 1718 | GLN | - | expression tag | UNP Q5F4S7 |
| B | 1719 | GLY | - | expression tag | UNP Q5F4S7 |
| B | 1720 | PRO | - | expression tag | UNP Q5F4S7 |
| B | 1721 | ASP | - | expression tag | UNP Q5F4S7 |
| B | 1722 | TYR | - | expression tag | UNP Q5F4S7 |
| B | 1723 | LYS | - | expression tag | UNP Q5F4S7 |
| B | 1724 | ASP | - | expression tag | UNP Q5F4S7 |
| B | 1725 | ASP | - | expression tag | UNP Q5F4S7 |
| B | 1726 | ASP | - | expression tag | UNP Q5F4S7 |
| B | 1727 | ASP | - | expression tag | UNP Q5F4S7 |
| B | 1728 | LYS | - | expression tag | UNP Q5F4S7 |
| B | 1729 | ALA | - | expression tag | UNP Q5F4S7 |
| B | 1730 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1731 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1732 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1733 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1734 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1735 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1736 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1737 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1738 | HIS | - | expression tag | UNP Q5F4S7 |
| B | 1739 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1710 | SER | - | expression tag | UNP Q5F4S7 |
| C | 1711 | ASN | - | expression tag | UNP Q5F4S7 |
| C | 1712 | SER | - | expression tag | UNP Q5F4S7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|:---:|:---:|:---:|:---:|:---:|:---:|
| C | 1713 | LEU | - | expression tag | UNP Q5F4S7 |
| C | 1714 | GLU | - | expression tag | UNP Q5F4S7 |
| C | 1715 | VAL | - | expression tag | UNP Q5F4S7 |
| C | 1716 | LEU | - | expression tag | UNP Q5F4S7 |
| C | 1717 | PHE | - | expression tag | UNP Q5F4S7 |
| C | 1718 | GLN | - | expression tag | UNP Q5F4S7 |
| C | 1719 | GLY | - | expression tag | UNP Q5F4S7 |
| C | 1720 | PRO | - | expression tag | UNP Q5F4S7 |
| C | 1721 | ASP | - | expression tag | UNP Q5F4S7 |
| C | 1722 | TYR | - | expression tag | UNP Q5F4S7 |
| C | 1723 | LYS | - | expression tag | UNP Q5F4S7 |
| C | 1724 | ASP | - | expression tag | UNP Q5F4S7 |
| C | 1725 | ASP | - | expression tag | UNP Q5F4S7 |
| C | 1726 | ASP | - | expression tag | UNP Q5F4S7 |
| C | 1727 | ASP | - | expression tag | UNP Q5F4S7 |
| C | 1728 | LYS | - | expression tag | UNP Q5F4S7 |
| C | 1729 | ALA | - | expression tag | UNP Q5F4S7 |
| C | 1730 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1731 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1732 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1733 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1734 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1735 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1736 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1737 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1738 | HIS | - | expression tag | UNP Q5F4S7 |
| C | 1739 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1710 | SER | - | expression tag | UNP Q5F4S7 |
| D | 1711 | ASN | - | expression tag | UNP Q5F4S7 |
| D | 1712 | SER | - | expression tag | UNP Q5F4S7 |
| D | 1713 | LEU | - | expression tag | UNP Q5F4S7 |
| D | 1714 | GLU | - | expression tag | UNP Q5F4S7 |
| D | 1715 | VAL | - | expression tag | UNP Q5F4S7 |
| D | 1716 | LEU | - | expression tag | UNP Q5F4S7 |
| D | 1717 | PHE | - | expression tag | UNP Q5F4S7 |
| D | 1718 | GLN | - | expression tag | UNP Q5F4S7 |
| D | 1719 | GLY | - | expression tag | UNP Q5F4S7 |
| D | 1720 | PRO | - | expression tag | UNP Q5F4S7 |
| D | 1721 | ASP | - | expression tag | UNP Q5F4S7 |
| D | 1722 | TYR | - | expression tag | UNP Q5F4S7 |
| D | 1723 | LYS | - | expression tag | UNP Q5F4S7 |
| D | 1724 | ASP | - | expression tag | UNP Q5F4S7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| D | 1725 | ASP | - | expression tag | UNP Q5F4S7 |
| D | 1726 | ASP | - | expression tag | UNP Q5F4S7 |
| D | 1727 | ASP | - | expression tag | UNP Q5F4S7 |
| D | 1728 | LYS | - | expression tag | UNP Q5F4S7 |
| D | 1729 | ALA | - | expression tag | UNP Q5F4S7 |
| D | 1730 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1731 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1732 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1733 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1734 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1735 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1736 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1737 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1738 | HIS | - | expression tag | UNP Q5F4S7 |
| D | 1739 | HIS | - | expression tag | UNP Q5F4S7 |

- Molecule 2 is (2S)-2-(3,4-dihydroquinolin-1(2H)-yl)-N-(5-methyl-1,2-oxazol-3-yl)-2-phenylacetamide (CCD ID: A1AIB) (formula: $C_{21}H_{21}N_3O_2$) (labeled as "Ligand of Interest" by depositor).
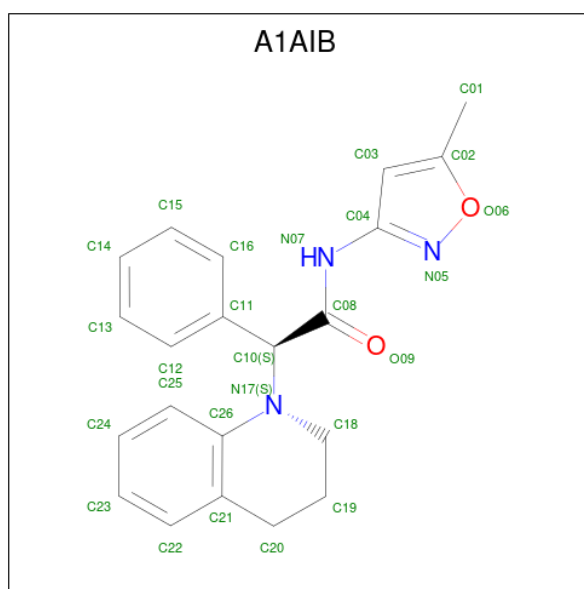


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 2 | A | 1 | Total | C | H | N | O | 0 |
| | | | 47 | 21 | 21 | 3 | 2 | |
| 2 | B | 1 | Total | C | H | N | O | 0 |
| | | | 47 | 21 | 21 | 3 | 2 | |
| 2 | C | 1 | Total | C | H | N | O | 0 |
| | | | 47 | 21 | 21 | 3 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 2 | D | 1 | Total | C | H | N | O | 0 |
| | | | 47 | 21 | 21 | 3 | 2 | |

- Molecule 3 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-prop an-2-yl] ( {Z})-octadec-9-enoate (CCD ID: 6OU) (formula: $C_{39}H_{76}NO_8P$).



6OU
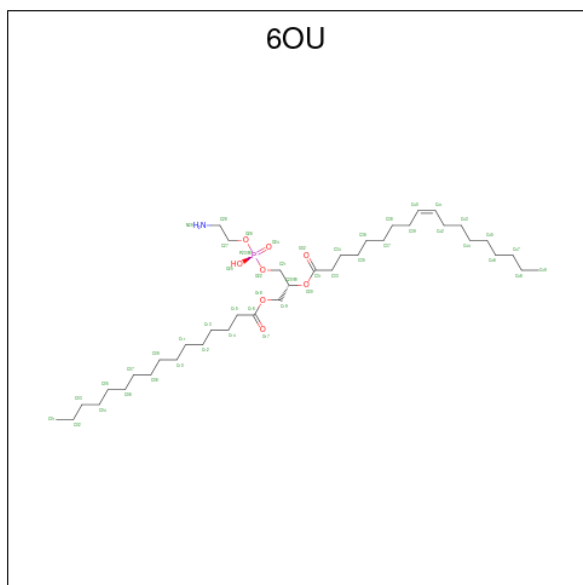
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---|---|---------|
| 3 | A | 1 | Total | C | H | N | O | P | 0 |
| | | | 59 | 18 | 31 | 1 | 8 | 1 | |
| 3 | B | 1 | Total | C | H | N | O | P | 0 |
| | | | 59 | 18 | 31 | 1 | 8 | 1 | |
| 3 | C | 1 | Total | C | H | N | O | P | 0 |
| | | | 59 | 18 | 31 | 1 | 8 | 1 | |
| 3 | D | 1 | Total | C | H | N | O | P | 0 |
| | | | 59 | 18 | 31 | 1 | 8 | 1 | |

- Molecule 4 is Pregnenolone sulfate (CCD ID: A8W) (formula: $C_{21}H_{32}O_5S$) (labeled as "Ligand of Interest" by depositor).

A8W
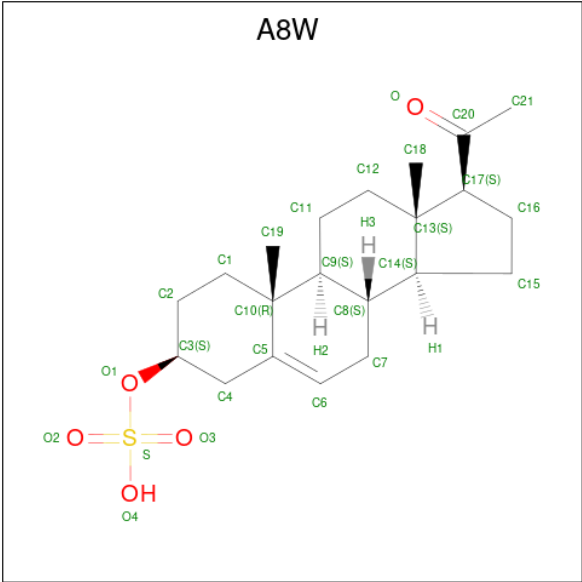


| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 4 | A | 1 | Total | C | H | O | S | 0 |
| | | | 58 | 21 | 31 | 5 | 1 | |
| 4 | B | 1 | Total | C | H | O | S | 0 |
| | | | 58 | 21 | 31 | 5 | 1 | |
| 4 | C | 1 | Total | C | H | O | S | 0 |
| | | | 58 | 21 | 31 | 5 | 1 | |
| 4 | D | 1 | Total | C | H | O | S | 0 |
| | | | 58 | 21 | 31 | 5 | 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: Transient receptor potential cation channel, subfamily M, member 3

PHE ILE THR **D1187** **K1245** ALA SER LEU GLN THR VAL ASP ILE ARG LEU ALA GLN LEU GLU ASP LEU GLY ARG MET ALA THR ALA LEU GLU GLU ASN LYS ILE ARG SER ARG THR SER SER ASP CYS THR ASP ALA ALA TYR ILE VAL ARG

GLN SER SER PHE ASN SER GLN GLU GLY ASN GLY THR PHE LYS GLU GLN GLU SER ILE ASP GLU SER ILE GLU ASP PRO ALA GLY GLU GLU THR ILE SER PRO THR SER PRO THR LEU ALA LEU GLU LEU THR MET PRO ARG MET ARG SER HIS SER PHE TYR SER VAL ASN VAL LYS ASP LYS GLY ILE GLU LEU GLU HIS CYS ASP ILE GLU GLU PRO LEU PHE

LYS GLU ARG SER LEU SER LEU HIS ARG ALA THR SER SER HIS SER VAL ALA LYS GLU PRO LYS ALA PRO ALA THR LEU ALA VAL PRO ASP ARG ARG PRO SER ASN CYS ILE ASP TYR VAL SER ALA MET ASP GLU LEU GLU HIS CYS ASP ILE GLU PRO LEU

ASP ASN SER MET ASN ILE LEU GLY LEU GLU GLY PRO SER PHE ALA LEU ALA PRO SER THR PRO SER SER ALA TYR ALA THR LEU ALA PRO THR ASP ARG PRO ARG SER ILE ASP PHE GLU ASP THR MET ASP ARG PHE SER ASP TYR THR

HIS LEU PRO CYS GLN ASN PRO TRP ASP THR ASP PRO THR HIS VAL ILE GLU ARG LYS SER SER ARG TYR LEU ALA THR THR PRO PHE LEU LEU GLU GLU ALA PRO ILE VAL LYS SER HIS SER PHE MET PHE SER PRO SER ARG GLU TYR TYR ALA PHE GLY VAL

PRO VAL LYS ALA GLU TYR THR SER ILE THR ASP CYS ILE ASP THR ARG CYS ASN VAL ASN SER ALA PRO GLN ALA ILE ALA ASP ALA ALA THR PHE PRO GLY LEU GLY LEU GLU GLU ALA PRO ILE VAL LYS GLU ASP LEU SER CYS HIS PRO GLU ARG GLU ALA GLU LEU HIS PRO SER SER ASP SER

GLU GLU ASN ALA ARG GLY GLN ARG ALA ALA ASN PRO ILE SER GLN GLU ALA GLU GLU ALA ASP ARG ALA ALA THR PRO GLY LEU GLY LEU GLU LEU GLY ASP VAL GLU LEU SER CYS TYR ALA GLU GLU PRO ASN TYR ALA HIS THR LYS SER PHE ILE SER

ASP LYS LEU ASP ARG GLN ASN ASP THR ALA SER LEU ASP ASN PRO PHE GLN ASP ARG SER LYS SER LYS PRO GLU GLY ARG ASP SER LEU MET ARG ARG LEU SER ARG THR SER ALA PHE HIS SER PHE GLU GLU SER LYS HIS ASN ASN SER LEU GLU VAL LEU PHE GLN GLY

PRO ASP TYR LYS ASP ASP ASP LYS ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

Chain B:



44% 53%

MET GLY LYS LYS TRP ARG ASP ALA GLY GLU GLU LEU GLU ARG GLY CYS SER ASP ARG GLU GLU ALA GLU SER ARG ARG ARG SER ARG SER ALA GLU GLY ARG PHE ALA GLU GLU SER TRP LYS ARG LEU SER GLU LYS GLN GLY SER THR LYS ARG SER LEU PRO ALA GLN GLN THR

PRO ALA GLN LYS SER TRP ILE GLU LEU ARG ALA PHE TYR LYS ARG GLU VAL CYS VAL HIS ILE ILE PRO SER THR LYS ASP PRO HIS ARG CYS CYS GLY ARG LEU ILE GLY LEU GLN GLN HIS VAL GLY LEU THR PRO SER ILE SER VAL LEU GLN ASN GLU LYS ASN GLU SER ARG GLU ILE SER ARG ASN

ASP ILE GLN SER GLU GLU LYS SER TRP SER ILE SER LYS HIS THR GLN LEU SER PRO THR ASP ALA PHE GLY THR ILE GLU PHE GLN GLY GLY GLY HIS SER ASN LYS **A155** **M156** **Y157** VAL ARG VAL SER PHE ASP THR **K165** **T174** **Q178** **L179** GLU LEU PRO LYS **L184** **G190** GLY LEU GLN

ASN PHE GLU LEU GLN PRO LYS LEU LYS **Q203** **D239** **S242** **K243** SER ARG **G246** SER **I258** **V259** **I266** GLY ARG ASP VAL VAL ARG PRO TYR GLN THR MET SER ASN PRO MET SER LYS LEU THR VAL LEU ASN SER MET **H291** **F294** ILE LEU ALA ASP ASN GLY THR THR GLY LYS

TYR GLY ALA **E308** **K323** ILE ASN THR ARG ILE GLY GLN GLY VAL **V334** PRO **E340** GLY GLY PRO ASN **V345** ARG **R354** SER **C364** **D365** LEU **L374** **V380** SER GLU GLU GLY GLY LEU ILE LEU ASN GLU **S390** LYS **T398** ILE GLN LYS SER THR PHE THR TYR THR ARG THR **Q409** **L413** **F414** **I415**

**I416** **L417** **M418** **M432** GLY SER GLU GLY HIS GLN ASP ASP **I440** ALA **A447** **N453** ALA **S455** LEU **L506** ASP **N510** ASP PRO GLU **L526** **T529** **P533** SER ASN **T536** **L537** **K545** LYS GLY ASN LEU **P550** PRO **L567** LEU **N587** LEU PHE GLY PRO LYS ARG PRO LYS ALA PRO LYS LEU LEU LEU GLY MET GLU

ASP ASP ILE PRO LEU ARG ARG GLY ARG LYS THR LYS LYS ARG GLU GLU VAL VAL ASP ILE ASP LEU ASP ASP PRO GLU **I631** **W644** **M648** **L674** **A682** SER GLU ASN ASP MET VAL ASP **D690** **V742** **I750** **S755** **M764** **M769** **N794** LYS ASP ASP MET

• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

Chain C:

44% 53%

TYR GLY ALA E308 K323 ILE ASN THR ARG ILE GLY GLN GLY VAL PRO V334 E340 GLY GLY PRO ASN V345 R354 C364 D365 L374 Y380 SER GLU GLU GLY GLY LEU ILE ASN GLU S390 T398 ILE GLN LYS THR PHE THR TYR THR ARG THR Q409 L413 F414 I415

I416 L417 M418 M432 GLY SER GLU GLY HIS GLN ASP I440 A447 N453 ALA S455 L506 N510 L526 T529 P533 ASN T536 L537 K545 LYS GLY ASN LEU P550 L567 N587 LEU PHE GLY PRO LYS ARG PRO LYS ALA LEU LYS LEU LEU GLY MET GLU

ASP ASP ILE PRO LEU ARG ARG GLY ARG LYS THR THR LYS LYS ARG GLU GLU GLU VAL ASP ILE LEU ASP LEU ASP PRO GLU I631 W644 M648 L674 A682 SER GLU ASN ASP MET VAL ASP D690 L729 N734 V742 I750 S755 M764 M769 N794

LYS ASP ASP MET PRO TYR MET THR GLN ALA GLN GLU ILE GLU HIS LEU GLU LYS PRO GLU PRO GLU GLU LYS PRO THR LYS GLU LYS ASP GLU ASP ASP MET GLU LEU THR ALA MET LEU GLY ARG SER ASN GLY GLU SER ARG LYS ASP GLU GLU VAL GLN SER ARG

HIS ARG LEU ILE PRO VAL G861 F867 V873 F877 V895 K896 Q904 T914 L915 M920 I923 E927 P928 W938 I951 C976 V977 N978 I979 W982 G997 P998 M1002 F1024 W1040 K1041 L1042 Y1048 I1054 Y1055 V1058 F1059 ALA ASP

GLN ILE ASP PRO PRO CYS GLY GLN ASN GLU THR ARG ASP GLY LYS THR ILE GLN LEU PRO PRO CYS K1085 L1099 L1105 L1109 N1115 I1124 V1128 Y1134 P1148 P1149 L1150 I1151 I1152 H1162 VAL CYS CYS ARG TRP ARG LYS HIS GLU SER ASP GLN ASP GLU

ARG ASP TYR GLY LEU LYS LYS LEU PHE ILE THR D1187 K1245 ALA SER LEU GLN THR VAL ASP ILE ARG LEU ALA GLN LEU GLU ASP GLY LYS THR ILE GLN LEU PRO PRO CYS ARG MET ALA THR ALA LEU GLU ARG LEU THR GLY LEU GLU ARG ALA GLU GLU SER SER ASN LYS ILE ALA SER ARG SER ARG THR SER SER ASP CYS THR

ASP ALA ALA TYR VAL ILE ARG GLN SER SER PHE ASN SER GLN GLU GLY ASN THR PHE LYS LEU GLN LEU SER ILE ASP SER ILE GLU ASN PRO ALA GLY LEU GLU THR SER PRO ALA ASN THR LEU ILE VAL PRO ASP SER ARG MET ARG MET SER HIS SER PHE TYR SER VAL ASN VAL LYS ASP GLY GLY ILE

GLU LYS LEU GLU SER ILE PHE LYS GLU ARG SER LEU SER LEU HIS ARG ALA THR SER HIS SER VAL ALA LYS GLU PRO ALA PRO ALA PRO ALA ASN THR LEU ALA ILE VAL PRO ASP SER ARG ARG PRO SER ARG SER CYS ILE ASP ILE TYR VAL SER ALA MET ASP GLU LEU

HIS CYS ASP ILE PRO LEU ASP ASN SER MET ASN ILE LEU GLY GLU GLY PRO SER PHE SER ALA LEU ALA PRO THR THR PRO SER ALA TYR ALA THR LEU ALA PRO THR ASP ARG PRO SER ARG SER ILE ASP PHE GLU ASP THR SER MET ASP THR ARG

SER PHE SER ASP TYR THR THR HIS LEU PRO GLU CYS GLN ASN PRO TRP ASP THR ASP PRO THR HIS LEU THR GLU ILE GLU ARG SER LYS SER ARG ALA TYR ALA THR THR PRO PHE LEU GLU LEU GLY ALA PRO LYS VAL GLU ASP SER LEU SER HIS SER SER MET PHE PRO SER ARG SER

TYR TYR ALA ASN PHE GLY VAL PRO VAL LYS THR ALA GLU TYR THR SER ILE ASP ASP CYS ILE ASP THR ARG CYS VAL ASN ALA PRO GLN GLN ILE ALA ASP ARG ALA THR THR PRO GLY LEU GLY LEU ASP LYS GLU LYS VAL GLU ASP LEU SER CYS HIS PRO GLU ARG GLU ALA GLU LEU

SER HIS PRO SER ASP SER GLU GLU ASN ALA ARG GLY GLN ARG ASN THR ALA ALA ASN PRO ILE SER SER GLN GLU ALA GLU ASP THR LEU SER ASN ILE THR VAL PRO GLY LEU GLY ASP LYS ARG ALA ALA ASN THR LEU SER MET ARG ARG LEU SER ARG THR SER TYR SER HIS THR

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

LEU GLU VAL LEU PHE GLN GLY PRO ASP TYR LYS ASP ASP ASP ASP LYS ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: Transient receptor potential cation channel, subfamily M, member 3

Chain D:

MET GLY LYS LYS TRP ARG ASP ALA GLY LEU GLU LEU ARG GLY CYS SER ASP ARG GLU ASP SER ALA GLU SER ARG ARG SER ARG SER ALA SER GLY ARG PHE ALA GLU GLU TRP LYS ARG LEU SER LYS GLN SER SER THR LYS ARG SER GLY LEU PRO ALA GLN GLN THR

PRO ALA GLN SER TRP ILE GLU ARG ALA PHE TYR LYS ARG GLU CYS VAL HIS ILE ILE PRO SER THR LYS ASP PRO HIS ARG CYS CYS GLY ARG LEU ILE GLY GLN HIS VAL GLY LEU THR PRO SER ILE SER VAL LEU GLN ASN GLU LYS ASN GLU SER ARG LEU SER ARG ASN

ASP ILE GLN SER GLU LYS TRP SER ILE SER LYS HIS THR GLN LEU SER PRO THR ASP ALA PHE GLY THR ILE GLU PHE GLN GLY GLY GLY HIS SER ASN LYS A155 M156 Y157 VAL ARG VAL SER PHE ASP THR K165 T174 Q178 L179 GLU LEU PRO LYS L184 G190 GLY LEU GLN

ASN PHE GLU LEU GLN PRO LEU LYS LEU LYS Q203 ASP VAL ARG TYR GLN MET SER ASN PRO MET SER LEU LYS LEU THR VAL LEU ASN SER MET H291 GLU F294 ILE LEU ALA ASP ASN GLY THR GLY LYS D239 S242 K243 SER ARG G246 I258 V259 I266 GLY ARG

TYR GLY ALA E308 K323 ILE ASN THR ARG ILE GLY GLN GLY VAL PRO V334 E340 GLY GLY PRO ASN V345 R354 C364 D365 L374 Y380 SER GLU GLY GLY LEU ILE ASN GLU S390 T398 ILE GLN LYS THR PHE THR TYR THR ARG THR Q409 L413 F414 I415

I416 L417 M418 M432 GLY SER GLU HIS GLN ASP I440 A447 N453 ALA S465 L506 N510 L526 T529 P533 SER ASN T536 L537 K545 GLY ASN LEU GLU P550 L567 N587 PHE GLY PRO LYS ARG LYS ALA LEU LYS LEU LEU GLY MET GLU

ASP ASP ILE LEU ARG ARG GLY ARG LYS THR THR LYS LYS ARG GLU GLU GLU LYS GLU VAL ASP ILE ASP LEU ASP ASP PRO GLU I631 W644 M648 L674 A682 SER GLU ASN ASP MET VAL ASP D690 L729 N734 V742 I750 S755 M764 M769 N794

LYS ASP ASP MET PRO TYR MET THR GLN ALA GLN GLU ILE HIS LEU GLU GLY LYS ARG GLU GLU GLU THR LYS GLU ASP GLU ASP GLU MET GLU LEU THR ALA MET LEU GLY ARG ASN GLY SER ARG LYS ASP GLU GLU VAL GLN SER ARG

HIS ARG LEU ILE PRO VAL G861 F867 V873 F877 Y882 V895 K896 Q904 T914 L915 M920 I923 L924 E927 P928 W938 I951 C976 V977 N978 I979 W982 G997 P998 M1002 F1024 W1040 K1041 L1042 Y1048 I1054 Y1055 V1058

F1059 ALA ASP GLN ILE ASP PRO PRO CYS GLY GLN ASN GLU THR ARG GLU ASP GLY LYS THR ILE GLN LEU PRO PRO CYS K1085 L1099 L1105 L1109 N1115 I1124 V1128 Y1134 P1148 P1149 L1150 I1151 I1152 H1162 VAL CYS CYS ARG TRP ARG LYS HIS GLU VAL GLN SER ASP

GLN ASP GLU ARG ASP TYR GLY LEU LYS LEU LEU PHE ILE THR D1187 K1245 ALA SER LEU GLN THR VAL ASP ILE LEU ALA GLN LEU ASP LEU ASP GLU LEU GLY ARG MET ALA THR ALA LEU GLU ARG LEU THR GLY LEU GLU GLU ARG ALA GLU SER ASN LYS ILE ARG SER ARG THR SER SER

ASP CYS THR ASP ALA ALA TYR ILE VAL ARG GLN SER SER PHE ASN SER GLN GLU GLY ASN THR PHE LYS LEU GLN GLU GLU SER ILE GLY GLU PRO ALA GLY LYS GLU ILE SER PRO THR SER PRO ARG MET ALA MET ARG HIS SER PHE TYR SER VAL ASN VAL LYS ASP LYS

GLY GLY ILE GLU LYS LEU GLU SER ILE PHE LYS GLU ARG SER LEU HIS ARG ALA THR SER HIS SER VAL ALA LEU ALA PRO THR SER SER SER ALA ILE ALA PRO ALA ASN ASP ARG ARG PRO SER CYS ILE ASP PHE GLU ASP LEU THR SER VAL ALA MET

ASP GLU LEU CYS ASP ILE GLU PRO LEU ASP ASN MET ASN ILE LEU GLY LEU GLY PRO SER PHE SER ALA LEU LYS ALA PRO THR SER PRO SER ALA THR PRO PHE ASP ARG PRO SER ARG PRO SER ARG ILE ASP PHE GLU ASP LEU THR SER MET

ASP THR ARG PHE SER ASP TYR THR HIS LEU PRO GLU CYS GLN ASN PRO TRP ASP THR ASP PRO THR HIS SER THR ILE GLU ARG SER LYS SER SER ARG TYR ALA ASP THR LEU ALA THR PRO PHE GLU LEU GLU GLY ALA PRO LYS GLU ILE ASP PHE GLU ASP THR SER MET

SER ARG SER TYR ALA ASN PHE GLY VAL PRO VAL THR LYS LEU ASP ARG GLY GLN GLN TYR THR ILE SER VAL GLU PRO ALA ALA ILE ALA ASP ARG ALA THR PHE GLY LEU GLU LEU GLY LEU ASP LYS VAL GLU LEU SER HIS SER MET PHE SER PRO ASP GLU GLY ARG GLU

ALA GLU LEU LEU HIS PRO SER ASP GLU GLU ALA GLY ILE ALA ARG GLY GLN ASN ARG ALA ALA LEU ASN ILE THR VAL PRO LYS ILE GLU GLY ARG ASP SER ASN VAL GLU TYR SER ALA GLU GLU PRO ASN VAL PRO TYR

ALA HIS THR ARG LYS SER SER ILE SER ASP ASP LYS ASP ARG ASN THR ALA LEU ASN ASP LEU THR LYS SER GLU LEU SER ASN MET ARG LEU SER THR SER ALA PHE HIS SER SER PHE GLU GLU SER LYS HIS ASN

SER ASN SER LEU GLU VAL LEU PHE GLN GLY PRO ASP TYR LYS ASP ASP ASP LYS ALA HIS HIS HIS HIS HIS HIS HIS HIS

# 4 Experimental information (i)

| Property | Value | Source |
| --- | --- | --- |
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 25649 | 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 $(e^-/\text{Å}^2)$ | 60 | Depositor |
| Minimum defocus (nm) | 700 | Depositor |
| Maximum defocus (nm) | 2200 | Depositor |
| Magnification | 81000 | Depositor |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.932 | Depositor |
| Minimum map value | -0.436 | Depositor |
| Average map value | 0.007 | Depositor |
| Map value standard deviation | 0.044 | Depositor |
| Recommended contour level | 0.2 | Depositor |
| Map size (Å) | 345.6, 345.6, 345.6 | wwPDB |
| Map dimensions | 320, 320, 320 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.08, 1.08, 1.08 | Depositor |

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A8W, 6OU, A1AIB

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 | 0.08 | 0/5666 | 0.23 | 0/7740 |
| 1 | B | 0.08 | 0/5666 | 0.23 | 0/7740 |
| 1 | C | 0.08 | 0/5666 | 0.23 | 0/7740 |
| 1 | D | 0.08 | 0/5666 | 0.23 | 0/7740 |
| All | All | 0.08 | 0/22664 | 0.23 | 0/30960 |

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 | 5563 | 4619 | 4645 | 37 | 0 |
| 1 | B | 5563 | 4619 | 4645 | 40 | 0 |
| 1 | C | 5563 | 4619 | 4645 | 40 | 0 |
| 1 | D | 5563 | 4619 | 4645 | 42 | 0 |
| 2 | A | 26 | 21 | 0 | 0 | 0 |
| 2 | B | 26 | 21 | 0 | 0 | 0 |
| 2 | C | 26 | 21 | 0 | 0 | 0 |
| 2 | D | 26 | 21 | 0 | 0 | 0 |
| 3 | A | 28 | 31 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | B | 28 | 31 | 0 | 0 | 0 |
| 3 | C | 28 | 31 | 0 | 0 | 0 |
| 3 | D | 28 | 31 | 0 | 0 | 0 |
| 4 | A | 27 | 31 | 0 | 0 | 0 |
| 4 | B | 27 | 31 | 0 | 0 | 0 |
| 4 | C | 27 | 31 | 0 | 0 | 0 |
| 4 | D | 27 | 31 | 0 | 0 | 0 |
| All | All | 22576 | 18808 | 18580 | 151 | 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.

All (151) 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:B:1002:MET:HE2 | 1:C:1109:LEU:HD13 | 1.60 | 0.83 |
| 1:C:1002:MET:HE2 | 1:D:1109:LEU:HD13 | 1.61 | 0.83 |
| 1:A:1109:LEU:HD13 | 1:D:1002:MET:HE2 | 1.61 | 0.80 |
| 1:A:1002:MET:HE2 | 1:B:1109:LEU:HD13 | 1.62 | 0.80 |
| 1:C:1115:ASN:C | 1:C:1115:ASN:HD22 | 1.98 | 0.72 |
| 1:B:1115:ASN:C | 1:B:1115:ASN:HD22 | 1.98 | 0.72 |
| 1:C:1048:TYR:O | 1:D:1055:TYR:OH | 2.07 | 0.72 |
| 1:D:1115:ASN:HD22 | 1:D:1115:ASN:C | 1.98 | 0.71 |
| 1:A:1115:ASN:HD22 | 1:A:1115:ASN:C | 1.98 | 0.71 |
| 1:B:1048:TYR:O | 1:C:1055:TYR:OH | 2.07 | 0.71 |
| 1:A:1048:TYR:O | 1:B:1055:TYR:OH | 2.08 | 0.70 |
| 1:D:1054:ILE:O | 1:D:1058:VAL:HG23 | 1.93 | 0.69 |
| 1:A:1054:ILE:O | 1:A:1058:VAL:HG23 | 1.93 | 0.69 |
| 1:C:1054:ILE:O | 1:C:1058:VAL:HG23 | 1.93 | 0.68 |
| 1:A:1055:TYR:OH | 1:D:1048:TYR:O | 2.10 | 0.68 |
| 1:B:1054:ILE:O | 1:B:1058:VAL:HG23 | 1.93 | 0.68 |
| 1:C:904:GLN:OE1 | 1:C:904:GLN:N | 2.31 | 0.64 |
| 1:B:904:GLN:N | 1:B:904:GLN:OE1 | 2.31 | 0.64 |
| 1:D:904:GLN:N | 1:D:904:GLN:OE1 | 2.31 | 0.64 |
| 1:A:904:GLN:N | 1:A:904:GLN:OE1 | 2.31 | 0.62 |
| 1:B:742:VAL:HG21 | 1:B:1134:TYR:CD2 | 2.35 | 0.61 |
| 1:C:742:VAL:HG21 | 1:C:1134:TYR:CD2 | 2.36 | 0.61 |
| 1:A:742:VAL:HG21 | 1:A:1134:TYR:CD2 | 2.35 | 0.61 |
| 1:D:742:VAL:HG21 | 1:D:1134:TYR:CD2 | 2.35 | 0.61 |
| 1:C:978:ASN:OD1 | 1:C:982:TRP:NE1 | 2.37 | 0.57 |
| 1:C:1058:VAL:HG12 | 1:C:1059:PHE:CD2 | 2.40 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1058:VAL:HG12 | 1:D:1059:PHE:CD2 | 2.39 | 0.57 |
| 1:A:1058:VAL:HG12 | 1:A:1059:PHE:CD2 | 2.39 | 0.57 |
| 1:B:1058:VAL:HG12 | 1:B:1059:PHE:CD2 | 2.39 | 0.57 |
| 1:A:526:LEU:O | 1:A:529:THR:HG22 | 2.05 | 0.56 |
| 1:B:526:LEU:O | 1:B:529:THR:HG22 | 2.05 | 0.56 |
| 1:D:978:ASN:OD1 | 1:D:982:TRP:NE1 | 2.37 | 0.56 |
| 1:C:526:LEU:O | 1:C:529:THR:HG22 | 2.05 | 0.56 |
| 1:D:526:LEU:O | 1:D:529:THR:HG22 | 2.05 | 0.56 |
| 1:B:1124:ILE:HG22 | 1:B:1128:VAL:HG23 | 1.88 | 0.56 |
| 1:A:978:ASN:OD1 | 1:A:982:TRP:NE1 | 2.37 | 0.56 |
| 1:B:978:ASN:OD1 | 1:B:982:TRP:NE1 | 2.37 | 0.55 |
| 1:B:742:VAL:HG21 | 1:B:1134:TYR:CE2 | 2.42 | 0.55 |
| 1:A:742:VAL:HG21 | 1:A:1134:TYR:CE2 | 2.42 | 0.55 |
| 1:A:1124:ILE:HG22 | 1:A:1128:VAL:HG23 | 1.88 | 0.55 |
| 1:C:742:VAL:HG21 | 1:C:1134:TYR:CE2 | 2.42 | 0.55 |
| 1:C:1124:ILE:HG22 | 1:C:1128:VAL:HG23 | 1.88 | 0.55 |
| 1:D:1124:ILE:HG22 | 1:D:1128:VAL:HG23 | 1.88 | 0.54 |
| 1:D:742:VAL:HG21 | 1:D:1134:TYR:CE2 | 2.42 | 0.53 |
| 1:A:174:THR:O | 1:A:178:GLN:N | 2.41 | 0.53 |
| 1:D:750:ILE:O | 1:D:755:SER:OG | 2.26 | 0.53 |
| 1:D:927:GLU:N | 1:D:928:PRO:HD2 | 2.24 | 0.52 |
| 1:A:915:LEU:CD2 | 1:A:951:ILE:HD11 | 2.40 | 0.52 |
| 1:B:915:LEU:CD2 | 1:B:951:ILE:HD11 | 2.40 | 0.52 |
| 1:A:927:GLU:N | 1:A:928:PRO:HD2 | 2.24 | 0.52 |
| 1:D:915:LEU:CD2 | 1:D:951:ILE:HD11 | 2.40 | 0.52 |
| 1:C:927:GLU:N | 1:C:928:PRO:HD2 | 2.24 | 0.52 |
| 1:C:915:LEU:CD2 | 1:C:951:ILE:HD11 | 2.40 | 0.52 |
| 1:A:895:VAL:HG13 | 1:A:896:LYS:N | 2.25 | 0.52 |
| 1:C:644:TRP:NE1 | 1:C:648:MET:SD | 2.83 | 0.52 |
| 1:B:927:GLU:N | 1:B:928:PRO:HD2 | 2.24 | 0.51 |
| 1:D:895:VAL:HG13 | 1:D:896:LYS:N | 2.26 | 0.51 |
| 1:D:644:TRP:NE1 | 1:D:648:MET:SD | 2.83 | 0.51 |
| 1:C:895:VAL:HG13 | 1:C:896:LYS:N | 2.26 | 0.51 |
| 1:C:1042:LEU:HD22 | 1:C:1042:LEU:N | 2.26 | 0.51 |
| 1:B:644:TRP:NE1 | 1:B:648:MET:SD | 2.83 | 0.50 |
| 1:B:750:ILE:O | 1:B:755:SER:OG | 2.26 | 0.50 |
| 1:D:174:THR:O | 1:D:178:GLN:N | 2.41 | 0.50 |
| 1:B:895:VAL:HG13 | 1:B:896:LYS:N | 2.26 | 0.50 |
| 1:B:1042:LEU:HD22 | 1:B:1042:LEU:N | 2.26 | 0.50 |
| 1:A:644:TRP:NE1 | 1:A:648:MET:SD | 2.83 | 0.50 |
| 1:A:1042:LEU:N | 1:A:1042:LEU:HD22 | 2.26 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1042:LEU:HD22 | 1:D:1042:LEU:N | 2.26 | 0.49 |
| 1:D:1115:ASN:C | 1:D:1115:ASN:ND2 | 2.69 | 0.48 |
| 1:C:174:THR:O | 1:C:178:GLN:N | 2.41 | 0.48 |
| 1:A:1115:ASN:C | 1:A:1115:ASN:ND2 | 2.69 | 0.47 |
| 1:D:1024:PHE:HB2 | 1:D:1099:LEU:HD21 | 1.96 | 0.47 |
| 1:B:174:THR:O | 1:B:178:GLN:N | 2.41 | 0.47 |
| 1:B:1024:PHE:HB2 | 1:B:1099:LEU:HD21 | 1.96 | 0.47 |
| 1:C:1024:PHE:HB2 | 1:C:1099:LEU:HD21 | 1.96 | 0.47 |
| 1:D:567:LEU:HD23 | 1:D:674:LEU:HD23 | 1.97 | 0.47 |
| 1:A:1024:PHE:HB2 | 1:A:1099:LEU:HD21 | 1.96 | 0.47 |
| 1:C:567:LEU:HD23 | 1:C:674:LEU:HD23 | 1.97 | 0.47 |
| 1:A:567:LEU:HD23 | 1:A:674:LEU:HD23 | 1.97 | 0.47 |
| 1:B:567:LEU:HD23 | 1:B:674:LEU:HD23 | 1.97 | 0.46 |
| 1:A:1151:ILE:HD12 | 1:A:1152:ILE:N | 2.31 | 0.46 |
| 1:C:1151:ILE:HD12 | 1:C:1152:ILE:N | 2.31 | 0.46 |
| 1:B:1151:ILE:HD12 | 1:B:1152:ILE:N | 2.31 | 0.46 |
| 1:C:506:LEU:O | 1:C:510:ASN:N | 2.49 | 0.46 |
| 1:D:506:LEU:O | 1:D:510:ASN:N | 2.49 | 0.46 |
| 1:A:537:LEU:C | 1:A:537:LEU:HD13 | 2.41 | 0.45 |
| 1:B:537:LEU:C | 1:B:537:LEU:HD13 | 2.41 | 0.45 |
| 1:C:750:ILE:O | 1:C:755:SER:OG | 2.26 | 0.45 |
| 1:D:1151:ILE:HD12 | 1:D:1152:ILE:N | 2.31 | 0.45 |
| 1:D:537:LEU:C | 1:D:537:LEU:HD13 | 2.41 | 0.45 |
| 1:C:537:LEU:C | 1:C:537:LEU:HD13 | 2.41 | 0.45 |
| 1:A:506:LEU:O | 1:A:510:ASN:N | 2.49 | 0.44 |
| 1:B:506:LEU:O | 1:B:510:ASN:N | 2.49 | 0.44 |
| 1:B:976:CYS:O | 1:B:979:ILE:HG22 | 2.18 | 0.44 |
| 1:A:882:TYR:OH | 1:A:982:TRP:O | 2.32 | 0.44 |
| 1:C:914:THR:HB | 1:C:1151:ILE:HD11 | 2.01 | 0.43 |
| 1:D:914:THR:HB | 1:D:1151:ILE:HD11 | 2.01 | 0.43 |
| 1:D:976:CYS:O | 1:D:979:ILE:HG22 | 2.18 | 0.43 |
| 1:A:976:CYS:O | 1:A:979:ILE:HG22 | 2.18 | 0.43 |
| 1:C:1124:ILE:HG22 | 1:C:1124:ILE:O | 2.19 | 0.43 |
| 1:C:923:ILE:HD11 | 1:C:938:TRP:CZ2 | 2.54 | 0.43 |
| 1:C:1105:LEU:C | 1:C:1105:LEU:HD23 | 2.43 | 0.43 |
| 1:A:1105:LEU:C | 1:A:1105:LEU:HD23 | 2.43 | 0.43 |
| 1:B:1115:ASN:C | 1:B:1115:ASN:ND2 | 2.69 | 0.43 |
| 1:C:976:CYS:O | 1:C:979:ILE:HG22 | 2.18 | 0.43 |
| 1:C:764:MET:HE2 | 1:C:769:MET:O | 2.19 | 0.43 |
| 1:A:764:MET:HE2 | 1:A:769:MET:O | 2.19 | 0.43 |
| 1:A:923:ILE:HD11 | 1:A:938:TRP:CZ2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:923:ILE:HD11 | 1:B:938:TRP:CZ2 | 2.54 | 0.42 |
| 1:B:914:THR:HB | 1:B:1151:ILE:HD11 | 2.01 | 0.42 |
| 1:B:997:GLY:N | 1:B:998:PRO:CD | 2.83 | 0.42 |
| 1:B:1124:ILE:HG22 | 1:B:1124:ILE:O | 2.19 | 0.42 |
| 1:A:997:GLY:N | 1:A:998:PRO:CD | 2.83 | 0.42 |
| 1:D:1124:ILE:HG22 | 1:D:1124:ILE:O | 2.19 | 0.42 |
| 1:A:914:THR:HB | 1:A:1151:ILE:HD11 | 2.00 | 0.42 |
| 1:D:923:ILE:HD11 | 1:D:938:TRP:CZ2 | 2.54 | 0.42 |
| 1:D:867:PHE:O | 1:D:873:VAL:HG21 | 2.20 | 0.42 |
| 1:D:915:LEU:HD22 | 1:D:951:ILE:HD11 | 2.02 | 0.42 |
| 1:D:1105:LEU:C | 1:D:1105:LEU:HD23 | 2.43 | 0.42 |
| 1:B:764:MET:HE2 | 1:B:769:MET:O | 2.19 | 0.42 |
| 1:C:1115:ASN:C | 1:C:1115:ASN:ND2 | 2.69 | 0.42 |
| 1:D:764:MET:HE2 | 1:D:769:MET:O | 2.19 | 0.42 |
| 1:A:1124:ILE:HG22 | 1:A:1124:ILE:O | 2.19 | 0.42 |
| 1:B:1105:LEU:C | 1:B:1105:LEU:HD23 | 2.43 | 0.42 |
| 1:C:997:GLY:N | 1:C:998:PRO:CD | 2.83 | 0.42 |
| 1:D:997:GLY:N | 1:D:998:PRO:CD | 2.83 | 0.42 |
| 1:A:915:LEU:HD22 | 1:A:951:ILE:HD11 | 2.02 | 0.42 |
| 1:B:867:PHE:O | 1:B:873:VAL:HG21 | 2.20 | 0.42 |
| 1:D:882:TYR:OH | 1:D:982:TRP:O | 2.32 | 0.42 |
| 1:B:1148:PRO:N | 1:B:1149:PRO:HD2 | 2.35 | 0.42 |
| 1:C:915:LEU:HD22 | 1:C:951:ILE:HD11 | 2.02 | 0.42 |
| 1:C:1148:PRO:N | 1:C:1149:PRO:HD2 | 2.35 | 0.42 |
| 1:C:895:VAL:HG13 | 1:C:896:LYS:H | 1.85 | 0.41 |
| 1:D:729:LEU:O | 1:D:734:ASN:N | 2.49 | 0.41 |
| 1:C:923:ILE:HD11 | 1:C:938:TRP:CH2 | 2.56 | 0.41 |
| 1:A:867:PHE:O | 1:A:873:VAL:HG21 | 2.20 | 0.41 |
| 1:B:895:VAL:HG13 | 1:B:896:LYS:H | 1.85 | 0.41 |
| 1:D:1148:PRO:N | 1:D:1149:PRO:HD2 | 2.35 | 0.41 |
| 1:B:915:LEU:HD22 | 1:B:951:ILE:HD11 | 2.02 | 0.41 |
| 1:D:923:ILE:HD11 | 1:D:938:TRP:CH2 | 2.56 | 0.41 |
| 1:A:1148:PRO:N | 1:A:1149:PRO:HD2 | 2.35 | 0.41 |
| 1:C:867:PHE:O | 1:C:873:VAL:HG21 | 2.20 | 0.41 |
| 1:A:923:ILE:HD11 | 1:A:938:TRP:CH2 | 2.56 | 0.41 |
| 1:B:923:ILE:HD11 | 1:B:938:TRP:CH2 | 2.55 | 0.41 |
| 1:C:729:LEU:O | 1:C:734:ASN:N | 2.49 | 0.41 |
| 1:C:927:GLU:N | 1:C:928:PRO:CD | 2.84 | 0.40 |
| 1:D:895:VAL:HG13 | 1:D:896:LYS:H | 1.85 | 0.40 |
| 1:B:882:TYR:OH | 1:B:982:TRP:O | 2.32 | 0.40 |
| 1:B:927:GLU:N | 1:B:928:PRO:CD | 2.84 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:924:LEU:HD13 | 1:D:924:LEU:C | 2.47 | 0.40 |
| 1:D:927:GLU:N | 1:D:928:PRO:CD | 2.84 | 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 | 777/1739 (45%) | 761 (98%) | 16 (2%) | 0 | 100 | 100 |
| 1 | B | 777/1739 (45%) | 761 (98%) | 16 (2%) | 0 | 100 | 100 |
| 1 | C | 777/1739 (45%) | 761 (98%) | 16 (2%) | 0 | 100 | 100 |
| 1 | D | 777/1739 (45%) | 761 (98%) | 16 (2%) | 0 | 100 | 100 |
| All | All | 3108/6956 (45%) | 3044 (98%) | 64 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 421/1545 (27%) | 417 (99%) | 4 (1%) | 73 | 81 |
| 1 | B | 421/1545 (27%) | 417 (99%) | 4 (1%) | 73 | 81 |
| 1 | C | 421/1545 (27%) | 417 (99%) | 4 (1%) | 73 | 81 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|:---:|:---:|:---:|:---:|:---:|:---:|:---:|
| 1 | D | 421/1545 (27%) | 417 (99%) | 4 (1%) | 73 | 81 |
| All | All | 1684/6180 (27%) | 1668 (99%) | 16 (1%) | 71 | 81 |

All (16) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|:---:|:---:|:---:|:---:|
| 1 | A | 877 | PHE |
| 1 | A | 920 | MET |
| 1 | A | 1040 | TRP |
| 1 | A | 1115 | ASN |
| 1 | B | 877 | PHE |
| 1 | B | 920 | MET |
| 1 | B | 1040 | TRP |
| 1 | B | 1115 | ASN |
| 1 | C | 877 | PHE |
| 1 | C | 920 | MET |
| 1 | C | 1040 | TRP |
| 1 | C | 1115 | ASN |
| 1 | D | 877 | PHE |
| 1 | D | 920 | MET |
| 1 | D | 1040 | TRP |
| 1 | D | 1115 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|:---:|:---:|:---:|:---:|
| 1 | A | 752 | HIS |
| 1 | A | 965 | GLN |
| 1 | A | 1029 | GLN |
| 1 | A | 1115 | ASN |
| 1 | A | 1141 | HIS |
| 1 | B | 752 | HIS |
| 1 | B | 965 | GLN |
| 1 | B | 1029 | GLN |
| 1 | B | 1115 | ASN |
| 1 | B | 1141 | HIS |
| 1 | C | 752 | HIS |
| 1 | C | 965 | GLN |
| 1 | C | 1029 | GLN |
| 1 | C | 1115 | ASN |
| 1 | C | 1141 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 752 | HIS |
| 1 | D | 890 | ASN |
| 1 | D | 965 | GLN |
| 1 | D | 1029 | GLN |
| 1 | D | 1115 | ASN |
| 1 | D | 1141 | HIS |

### 5.3.3 RNA ⓘ

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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 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 | $\#\|Z\| > 2$ |
| 2 | A1AIB | C | 1801 | - | 25,29,29 | 1.82 | 6 (24%) | 31,40,40 | 1.57 | 4 (12%) |
| 4 | A8W | B | 1803 | - | 30,30,30 | 1.10 | 2 (6%) | 45,49,49 | 1.30 | 6 (13%) |
| 2 | A1AIB | A | 1801 | - | 25,29,29 | 1.81 | 6 (24%) | 31,40,40 | 1.56 | 4 (12%) |
| 4 | A8W | C | 1803 | - | 30,30,30 | 1.10 | 2 (6%) | 45,49,49 | 1.29 | 6 (13%) |
| 3 | 6OU | D | 1802 | - | 27,27,48 | 1.11 | 3 (11%) | 30,32,53 | 1.05 | 1 (3%) |
| 4 | A8W | D | 1803 | - | 30,30,30 | 1.10 | 2 (6%) | 45,49,49 | 1.29 | 6 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|---------|--------|------|---------|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 2 | A1AIB | B | 1801 | - | 25,29,29 | 1.82 | 6 (24%) | 31,40,40 | 1.57 | 4 (12%) |
| 4 | A8W | A | 1803 | - | 30,30,30 | 1.10 | 2 (6%) | 45,49,49 | 1.29 | 6 (13%) |
| 2 | A1AIB | D | 1801 | - | 25,29,29 | 1.81 | 6 (24%) | 31,40,40 | 1.56 | 4 (12%) |
| 3 | 6OU | C | 1802 | - | 27,27,48 | 1.12 | 3 (11%) | 30,32,53 | 1.05 | 1 (3%) |
| 3 | 6OU | B | 1802 | - | 27,27,48 | 1.12 | 3 (11%) | 30,32,53 | 1.05 | 1 (3%) |
| 3 | 6OU | A | 1802 | - | 27,27,48 | 1.12 | 3 (11%) | 30,32,53 | 1.05 | 1 (3%) |

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 | A1AIB | C | 1801 | - | - | 8/15/26/26 | 0/4/4/4 |
| 4 | A8W | B | 1803 | - | - | 4/9/67/67 | 0/4/4/4 |
| 2 | A1AIB | A | 1801 | - | - | 8/15/26/26 | 0/4/4/4 |
| 4 | A8W | C | 1803 | - | - | 4/9/67/67 | 0/4/4/4 |
| 3 | 6OU | D | 1802 | - | - | 13/30/30/52 | - |
| 4 | A8W | D | 1803 | - | - | 4/9/67/67 | 0/4/4/4 |
| 2 | A1AIB | B | 1801 | - | - | 8/15/26/26 | 0/4/4/4 |
| 4 | A8W | A | 1803 | - | - | 4/9/67/67 | 0/4/4/4 |
| 2 | A1AIB | D | 1801 | - | - | 8/15/26/26 | 0/4/4/4 |
| 3 | 6OU | C | 1802 | - | - | 13/30/30/52 | - |
| 3 | 6OU | B | 1802 | - | - | 13/30/30/52 | - |
| 3 | 6OU | A | 1802 | - | - | 13/30/30/52 | - |

All (44) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | B | 1801 | A1AIB | C08-N07 | 4.52 | 1.45 | 1.35 |
| 2 | A | 1801 | A1AIB | C08-N07 | 4.52 | 1.45 | 1.35 |
| 2 | D | 1801 | A1AIB | C08-N07 | 4.51 | 1.45 | 1.35 |
| 2 | C | 1801 | A1AIB | C08-N07 | 4.51 | 1.45 | 1.35 |
| 2 | B | 1801 | A1AIB | C01-C02 | 3.77 | 1.53 | 1.48 |
| 2 | C | 1801 | A1AIB | C01-C02 | 3.77 | 1.53 | 1.48 |
| 2 | D | 1801 | A1AIB | C01-C02 | 3.77 | 1.53 | 1.48 |
| 2 | A | 1801 | A1AIB | C01-C02 | 3.73 | 1.53 | 1.48 |
| 2 | C | 1801 | A1AIB | C20-C21 | 3.29 | 1.56 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 2 | D | 1801 | A1AIB | C20-C21 | 3.29 | 1.56 | 1.51 |
| 2 | B | 1801 | A1AIB | C20-C21 | 3.27 | 1.56 | 1.51 |
| 2 | B | 1801 | A1AIB | C26-N17 | 3.27 | 1.47 | 1.40 |
| 2 | A | 1801 | A1AIB | C20-C21 | 3.26 | 1.56 | 1.51 |
| 2 | C | 1801 | A1AIB | C26-N17 | 3.26 | 1.47 | 1.40 |
| 2 | D | 1801 | A1AIB | C26-N17 | 3.26 | 1.47 | 1.40 |
| 2 | A | 1801 | A1AIB | C26-N17 | 3.25 | 1.47 | 1.40 |
| 3 | B | 1802 | 6OU | O30-C20 | -2.72 | 1.40 | 1.46 |
| 3 | C | 1802 | 6OU | O30-C20 | -2.72 | 1.40 | 1.46 |
| 3 | A | 1802 | 6OU | O30-C20 | -2.69 | 1.40 | 1.46 |
| 3 | D | 1802 | 6OU | O30-C20 | -2.68 | 1.40 | 1.46 |
| 4 | B | 1803 | A8W | O1-S | -2.57 | 1.49 | 1.57 |
| 4 | A | 1803 | A8W | O1-S | -2.53 | 1.49 | 1.57 |
| 4 | C | 1803 | A8W | O1-S | -2.52 | 1.49 | 1.57 |
| 4 | D | 1803 | A8W | O1-S | -2.51 | 1.49 | 1.57 |
| 2 | B | 1801 | A1AIB | O09-C08 | -2.45 | 1.18 | 1.23 |
| 2 | B | 1801 | A1AIB | C04-N07 | 2.44 | 1.46 | 1.40 |
| 2 | C | 1801 | A1AIB | C04-N07 | 2.44 | 1.46 | 1.40 |
| 2 | D | 1801 | A1AIB | C04-N07 | 2.44 | 1.46 | 1.40 |
| 2 | A | 1801 | A1AIB | C04-N07 | 2.43 | 1.45 | 1.40 |
| 2 | A | 1801 | A1AIB | O09-C08 | -2.43 | 1.18 | 1.23 |
| 2 | C | 1801 | A1AIB | O09-C08 | -2.41 | 1.18 | 1.23 |
| 2 | D | 1801 | A1AIB | O09-C08 | -2.39 | 1.18 | 1.23 |
| 4 | C | 1803 | A8W | O1-C3 | -2.27 | 1.43 | 1.48 |
| 4 | A | 1803 | A8W | O1-C3 | -2.25 | 1.43 | 1.48 |
| 4 | D | 1803 | A8W | O1-C3 | -2.25 | 1.43 | 1.48 |
| 4 | B | 1803 | A8W | O1-C3 | -2.24 | 1.43 | 1.48 |
| 3 | C | 1802 | 6OU | O18-C19 | -2.19 | 1.40 | 1.45 |
| 3 | A | 1802 | 6OU | O18-C19 | -2.18 | 1.40 | 1.45 |
| 3 | D | 1802 | 6OU | O18-C19 | -2.14 | 1.40 | 1.45 |
| 3 | B | 1802 | 6OU | O18-C19 | -2.14 | 1.40 | 1.45 |
| 3 | B | 1802 | 6OU | O30-C31 | 2.09 | 1.40 | 1.34 |
| 3 | A | 1802 | 6OU | O30-C31 | 2.07 | 1.40 | 1.34 |
| 3 | C | 1802 | 6OU | O30-C31 | 2.07 | 1.40 | 1.34 |
| 3 | D | 1802 | 6OU | O30-C31 | 2.07 | 1.40 | 1.34 |

All (44) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 2 | B | 1801 | A1AIB | C04-N07-C08 | -5.29 | 120.03 | 127.52 |
| 2 | C | 1801 | A1AIB | C04-N07-C08 | -5.27 | 120.05 | 127.52 |
| 2 | D | 1801 | A1AIB | C04-N07-C08 | -5.25 | 120.08 | 127.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 2 | A | 1801 | A1AIB | C04-N07-C08 | -5.25 | 120.08 | 127.52 |
| 3 | C | 1802 | 6OU | O30-C31-C33 | 3.90 | 119.91 | 111.48 |
| 3 | B | 1802 | 6OU | O30-C31-C33 | 3.88 | 119.88 | 111.48 |
| 3 | D | 1802 | 6OU | O30-C31-C33 | 3.87 | 119.85 | 111.48 |
| 3 | A | 1802 | 6OU | O30-C31-C33 | 3.87 | 119.85 | 111.48 |
| 2 | D | 1801 | A1AIB | C03-C04-N07 | -3.39 | 126.44 | 131.11 |
| 2 | C | 1801 | A1AIB | C03-C04-N07 | -3.37 | 126.47 | 131.11 |
| 2 | B | 1801 | A1AIB | C03-C04-N07 | -3.35 | 126.50 | 131.11 |
| 2 | A | 1801 | A1AIB | C03-C04-N07 | -3.34 | 126.51 | 131.11 |
| 2 | A | 1801 | A1AIB | C21-C26-N17 | -3.16 | 117.17 | 120.47 |
| 2 | B | 1801 | A1AIB | C21-C26-N17 | -3.15 | 117.18 | 120.47 |
| 2 | C | 1801 | A1AIB | C21-C26-N17 | -3.15 | 117.19 | 120.47 |
| 2 | D | 1801 | A1AIB | C21-C26-N17 | -3.15 | 117.19 | 120.47 |
| 4 | C | 1803 | A8W | C7-C6-C5 | -2.68 | 120.50 | 125.02 |
| 4 | D | 1803 | A8W | C7-C6-C5 | -2.68 | 120.50 | 125.02 |
| 4 | B | 1803 | A8W | C7-C6-C5 | -2.67 | 120.52 | 125.02 |
| 4 | A | 1803 | A8W | C7-C6-C5 | -2.66 | 120.53 | 125.02 |
| 4 | B | 1803 | A8W | C13-C17-C20 | -2.57 | 111.38 | 114.95 |
| 4 | C | 1803 | A8W | C13-C17-C20 | -2.54 | 111.42 | 114.95 |
| 4 | D | 1803 | A8W | C13-C17-C20 | -2.53 | 111.44 | 114.95 |
| 4 | A | 1803 | A8W | C13-C17-C20 | -2.52 | 111.45 | 114.95 |
| 4 | A | 1803 | A8W | C8-C7-C6 | -2.45 | 109.36 | 112.76 |
| 4 | B | 1803 | A8W | C8-C7-C6 | -2.44 | 109.39 | 112.76 |
| 4 | D | 1803 | A8W | C8-C7-C6 | -2.43 | 109.40 | 112.76 |
| 4 | C | 1803 | A8W | C8-C7-C6 | -2.41 | 109.42 | 112.76 |
| 2 | B | 1801 | A1AIB | C19-C18-N17 | 2.37 | 115.31 | 110.91 |
| 2 | A | 1801 | A1AIB | C19-C18-N17 | 2.36 | 115.29 | 110.91 |
| 2 | C | 1801 | A1AIB | C19-C18-N17 | 2.36 | 115.29 | 110.91 |
| 2 | D | 1801 | A1AIB | C19-C18-N17 | 2.36 | 115.29 | 110.91 |
| 4 | C | 1803 | A8W | C4-C5-C10 | 2.14 | 119.16 | 116.42 |
| 4 | B | 1803 | A8W | C4-C5-C10 | 2.14 | 119.16 | 116.42 |
| 4 | D | 1803 | A8W | C4-C5-C10 | 2.13 | 119.16 | 116.42 |
| 4 | A | 1803 | A8W | C15-C14-C8 | -2.12 | 115.71 | 119.10 |
| 4 | C | 1803 | A8W | C15-C14-C8 | -2.11 | 115.73 | 119.10 |
| 4 | A | 1803 | A8W | C4-C5-C10 | 2.10 | 119.12 | 116.42 |
| 4 | B | 1803 | A8W | C15-C14-C8 | -2.10 | 115.75 | 119.10 |
| 4 | D | 1803 | A8W | C15-C14-C8 | -2.08 | 115.78 | 119.10 |
| 4 | D | 1803 | A8W | C4-C5-C6 | -2.05 | 117.79 | 120.57 |
| 4 | B | 1803 | A8W | C4-C5-C6 | -2.03 | 117.81 | 120.57 |
| 4 | C | 1803 | A8W | C4-C5-C6 | -2.03 | 117.81 | 120.57 |
| 4 | A | 1803 | A8W | C4-C5-C6 | -2.03 | 117.82 | 120.57 |

There are no chirality outliers.

All (100) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 1801 | A1AIB | C03-C04-N07-C08 |
| 2 | A | 1801 | A1AIB | N07-C08-C10-C11 |
| 2 | B | 1801 | A1AIB | C03-C04-N07-C08 |
| 2 | B | 1801 | A1AIB | N07-C08-C10-C11 |
| 2 | C | 1801 | A1AIB | C03-C04-N07-C08 |
| 2 | C | 1801 | A1AIB | N07-C08-C10-C11 |
| 2 | D | 1801 | A1AIB | C03-C04-N07-C08 |
| 2 | D | 1801 | A1AIB | N07-C08-C10-C11 |
| 3 | A | 1802 | 6OU | O26-C27-C28-N29 |
| 3 | A | 1802 | 6OU | C33-C31-O30-C20 |
| 3 | B | 1802 | 6OU | O26-C27-C28-N29 |
| 3 | B | 1802 | 6OU | C33-C31-O30-C20 |
| 3 | C | 1802 | 6OU | O26-C27-C28-N29 |
| 3 | C | 1802 | 6OU | C33-C31-O30-C20 |
| 3 | D | 1802 | 6OU | O26-C27-C28-N29 |
| 3 | D | 1802 | 6OU | C33-C31-O30-C20 |
| 3 | A | 1802 | 6OU | O32-C31-O30-C20 |
| 3 | B | 1802 | 6OU | O32-C31-O30-C20 |
| 3 | C | 1802 | 6OU | O32-C31-O30-C20 |
| 3 | D | 1802 | 6OU | O32-C31-O30-C20 |
| 4 | A | 1803 | A8W | C13-C17-C20-C21 |
| 4 | B | 1803 | A8W | C13-C17-C20-C21 |
| 4 | C | 1803 | A8W | C13-C17-C20-C21 |
| 4 | D | 1803 | A8W | C13-C17-C20-C21 |
| 3 | A | 1802 | 6OU | C31-C33-C34-C35 |
| 3 | B | 1802 | 6OU | C31-C33-C34-C35 |
| 3 | C | 1802 | 6OU | C31-C33-C34-C35 |
| 3 | D | 1802 | 6OU | C31-C33-C34-C35 |
| 3 | A | 1802 | 6OU | C15-C16-O18-C19 |
| 3 | C | 1802 | 6OU | C15-C16-O18-C19 |
| 3 | D | 1802 | 6OU | C15-C16-O18-C19 |
| 3 | B | 1802 | 6OU | C15-C16-O18-C19 |
| 2 | A | 1801 | A1AIB | O09-C08-C10-C11 |
| 2 | B | 1801 | A1AIB | O09-C08-C10-C11 |
| 2 | C | 1801 | A1AIB | O09-C08-C10-C11 |
| 2 | D | 1801 | A1AIB | O09-C08-C10-C11 |
| 3 | B | 1802 | 6OU | C36-C37-C38-C39 |
| 3 | A | 1802 | 6OU | C36-C37-C38-C39 |
| 3 | C | 1802 | 6OU | C36-C37-C38-C39 |
| 3 | D | 1802 | 6OU | C36-C37-C38-C39 |
| 3 | D | 1802 | 6OU | C34-C35-C36-C37 |
| 3 | A | 1802 | 6OU | C34-C35-C36-C37 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------|
| 3 | B | 1802 | 6OU | C34-C35-C36-C37 |
| 3 | C | 1802 | 6OU | C34-C35-C36-C37 |
| 2 | A | 1801 | A1AIB | C08-C10-C11-C12 |
| 2 | B | 1801 | A1AIB | C08-C10-C11-C12 |
| 2 | C | 1801 | A1AIB | C08-C10-C11-C12 |
| 2 | D | 1801 | A1AIB | C08-C10-C11-C12 |
| 3 | A | 1802 | 6OU | C37-C38-C39-C40 |
| 3 | B | 1802 | 6OU | C37-C38-C39-C40 |
| 3 | C | 1802 | 6OU | C37-C38-C39-C40 |
| 3 | D | 1802 | 6OU | C37-C38-C39-C40 |
| 4 | A | 1803 | A8W | C16-C17-C20-O |
| 4 | A | 1803 | A8W | C16-C17-C20-C21 |
| 4 | B | 1803 | A8W | C16-C17-C20-O |
| 4 | B | 1803 | A8W | C16-C17-C20-C21 |
| 4 | C | 1803 | A8W | C16-C17-C20-O |
| 4 | C | 1803 | A8W | C16-C17-C20-C21 |
| 4 | D | 1803 | A8W | C16-C17-C20-O |
| 4 | D | 1803 | A8W | C16-C17-C20-C21 |
| 3 | A | 1802 | 6OU | C33-C34-C35-C36 |
| 3 | B | 1802 | 6OU | C33-C34-C35-C36 |
| 3 | D | 1802 | 6OU | C33-C34-C35-C36 |
| 3 | C | 1802 | 6OU | C33-C34-C35-C36 |
| 4 | A | 1803 | A8W | C13-C17-C20-O |
| 4 | B | 1803 | A8W | C13-C17-C20-O |
| 4 | C | 1803 | A8W | C13-C17-C20-O |
| 4 | D | 1803 | A8W | C13-C17-C20-O |
| 2 | A | 1801 | A1AIB | C08-C10-C11-C16 |
| 2 | B | 1801 | A1AIB | C08-C10-C11-C16 |
| 2 | C | 1801 | A1AIB | C08-C10-C11-C16 |
| 2 | D | 1801 | A1AIB | C08-C10-C11-C16 |
| 3 | A | 1802 | 6OU | O17-C16-O18-C19 |
| 3 | B | 1802 | 6OU | O17-C16-O18-C19 |
| 3 | C | 1802 | 6OU | O17-C16-O18-C19 |
| 3 | D | 1802 | 6OU | O17-C16-O18-C19 |
| 2 | A | 1801 | A1AIB | N07-C08-C10-N17 |
| 2 | B | 1801 | A1AIB | N07-C08-C10-N17 |
| 2 | C | 1801 | A1AIB | N07-C08-C10-N17 |
| 2 | D | 1801 | A1AIB | N07-C08-C10-N17 |
| 2 | A | 1801 | A1AIB | C08-C10-N17-C18 |
| 2 | B | 1801 | A1AIB | C08-C10-N17-C18 |
| 2 | C | 1801 | A1AIB | C08-C10-N17-C18 |
| 2 | D | 1801 | A1AIB | C08-C10-N17-C18 |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | A | 1802 | 6OU | C21-O22-P23-O24 |
| 3 | B | 1802 | 6OU | C21-O22-P23-O24 |
| 3 | C | 1802 | 6OU | C21-O22-P23-O24 |
| 3 | D | 1802 | 6OU | C21-O22-P23-O24 |
| 2 | A | 1801 | A1AIB | O09-C08-C10-N17 |
| 2 | B | 1801 | A1AIB | O09-C08-C10-N17 |
| 2 | C | 1801 | A1AIB | O09-C08-C10-N17 |
| 2 | D | 1801 | A1AIB | O09-C08-C10-N17 |
| 3 | A | 1802 | 6OU | O30-C31-C33-C34 |
| 3 | B | 1802 | 6OU | O30-C31-C33-C34 |
| 3 | C | 1802 | 6OU | O30-C31-C33-C34 |
| 3 | D | 1802 | 6OU | O30-C31-C33-C34 |
| 3 | C | 1802 | 6OU | O32-C31-C33-C34 |
| 3 | A | 1802 | 6OU | O32-C31-C33-C34 |
| 3 | B | 1802 | 6OU | O32-C31-C33-C34 |
| 3 | D | 1802 | 6OU | O32-C31-C33-C34 |

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 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 then 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.

## Ligand A1AIB C 1801



Bond lengths



Bond angles



Torsions



Rings

## Ligand A8W B 1803



Bond lengths



Bond angles



Torsions



Rings

## Ligand A1AIB A 1801



**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

## Ligand A8W C 1803



**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

## Ligand 6OU D 1802



Bond lengths



Bond angles



Torsions



Rings

## Ligand A8W D 1803



Bond lengths



Bond angles



Torsions



Rings

## Ligand A1AIB B 1801



Bond lengths



Bond angles



Torsions



Rings

## Ligand A8W A 1803



Bond lengths



Bond angles



Torsions



Rings

**Ligand A1AIB D 1801**



Bond lengths



Bond angles



Torsions



Rings

**Ligand 6OU C 1802**



Bond lengths



Bond angles



Torsions



Rings

**Ligand 6OU B 1802**


Bond lengths


Bond angles


Torsions


Rings

**Ligand 6OU A 1802**


Bond lengths


Bond angles


Torsions


Rings

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-44102. 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 ⓘ
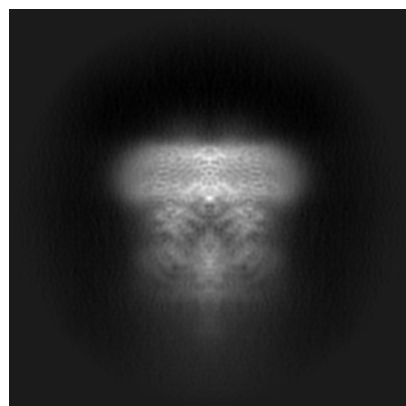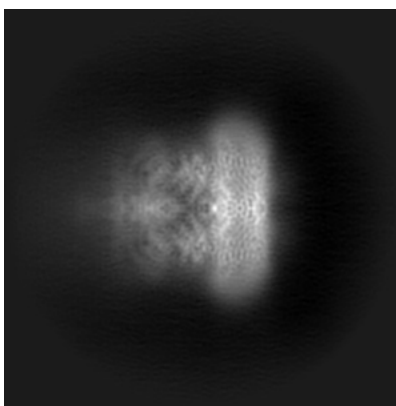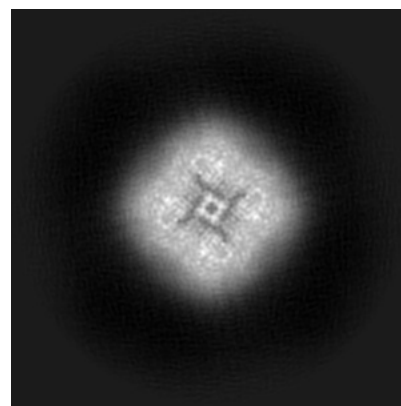
### 6.1.1 Primary map



| X | Y | Z |

### 6.1.2 Raw map



| X | Y | Z |
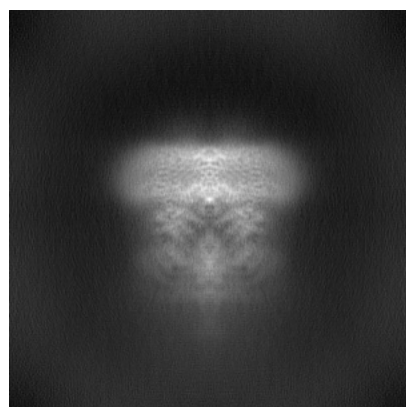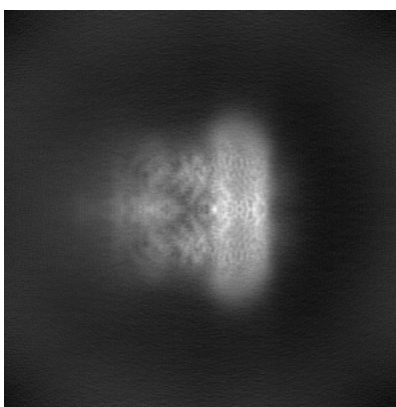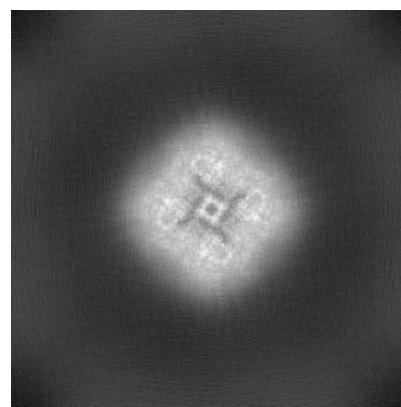
The images above show the map projected in three orthogonal directions.

## 6.2　Central slices ⓘ
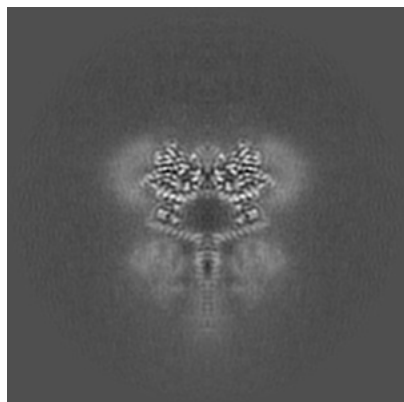
### 6.2.1　Primary map
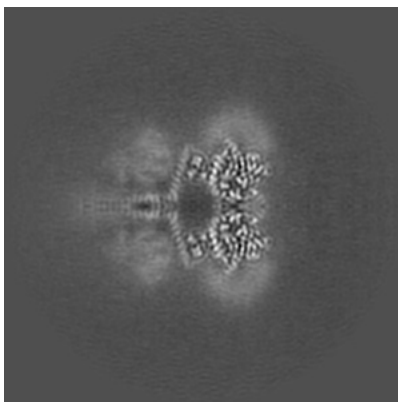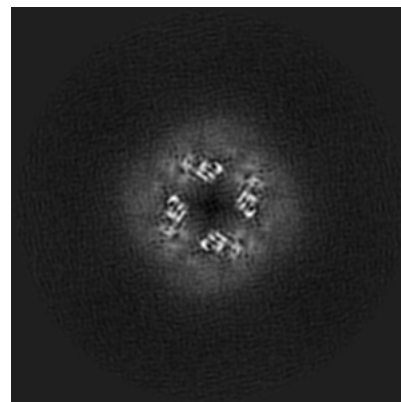


| X Index: 160 | Y Index: 160 | Z Index: 160 |

### 6.2.2　Raw map
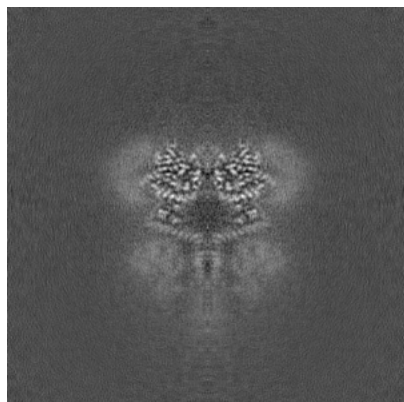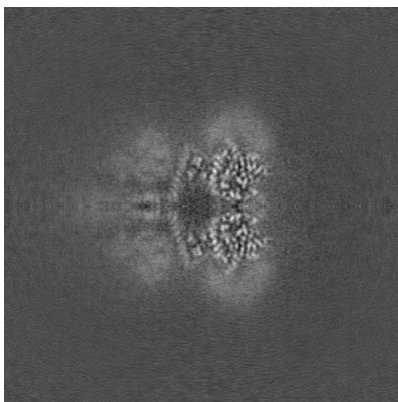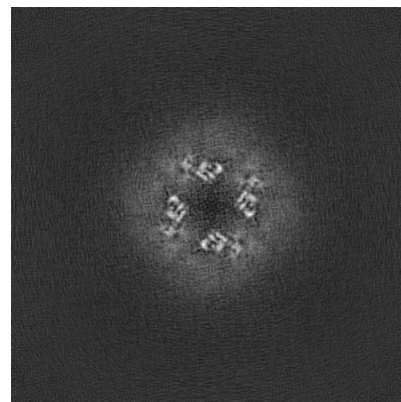


| X Index: 160 | Y Index: 160 | Z Index: 160 |

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

## 6.3   Largest variance slices   ⓘ

### 6.3.1   Primary map
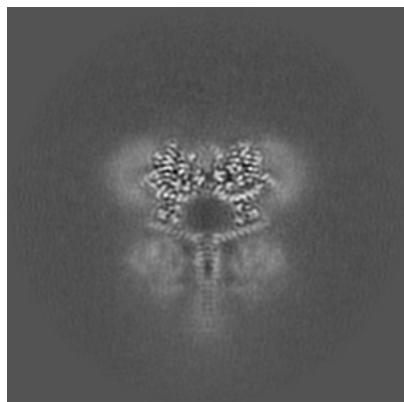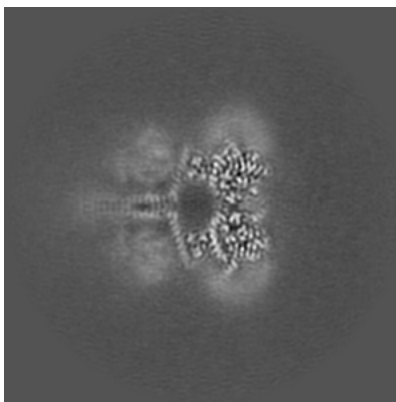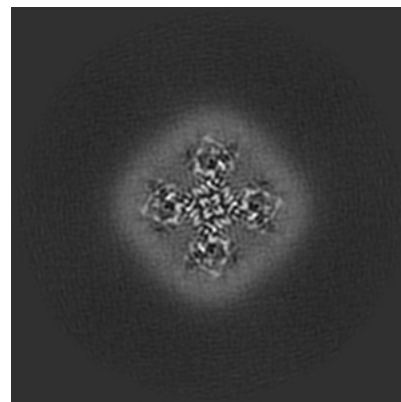


X Index: 159      Y Index: 159      Z Index: 178

### 6.3.2   Raw map
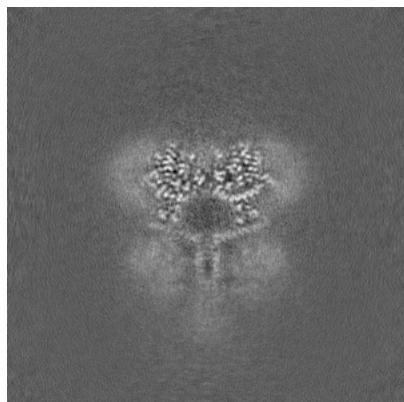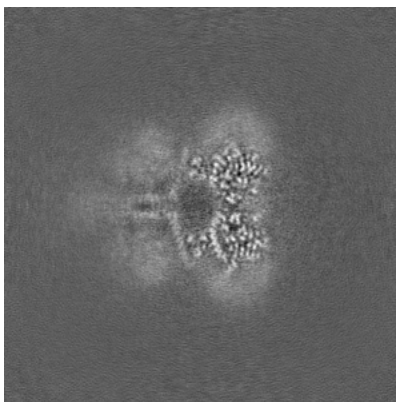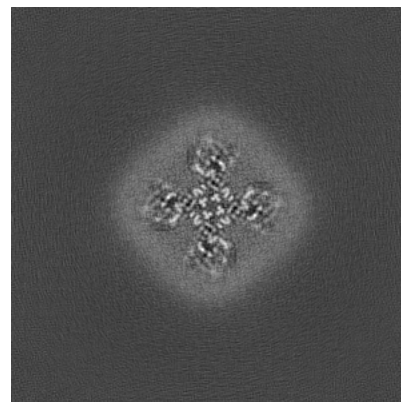


X Index: 159      Y Index: 159      Z Index: 179

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

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

### 6.4.1 Primary map
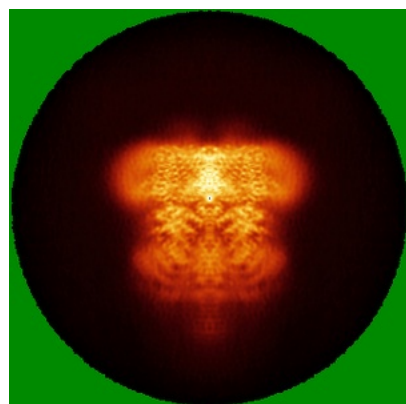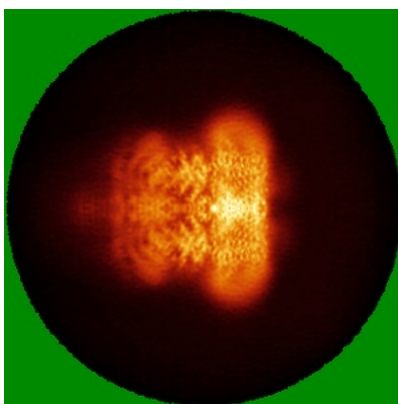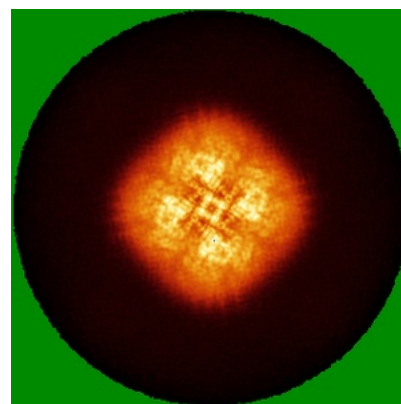


|  |  |  |
|---|---|---|
| X | Y | Z |

### 6.4.2 Raw map



|  |  |  |
|---|---|---|
| X | Y | Z |
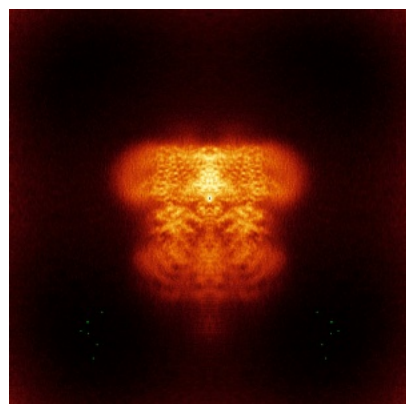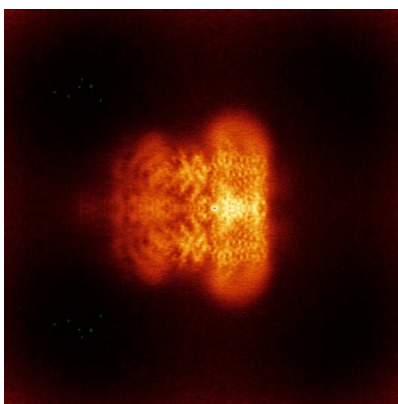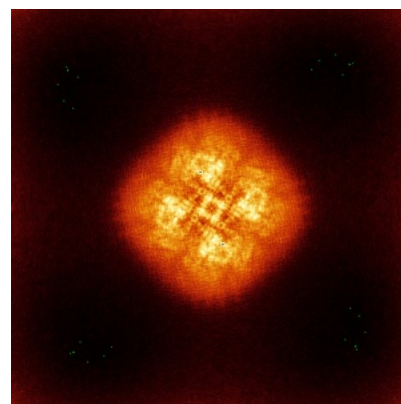
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views ⓘ

### 6.5.1 Primary map



X          Y          Z
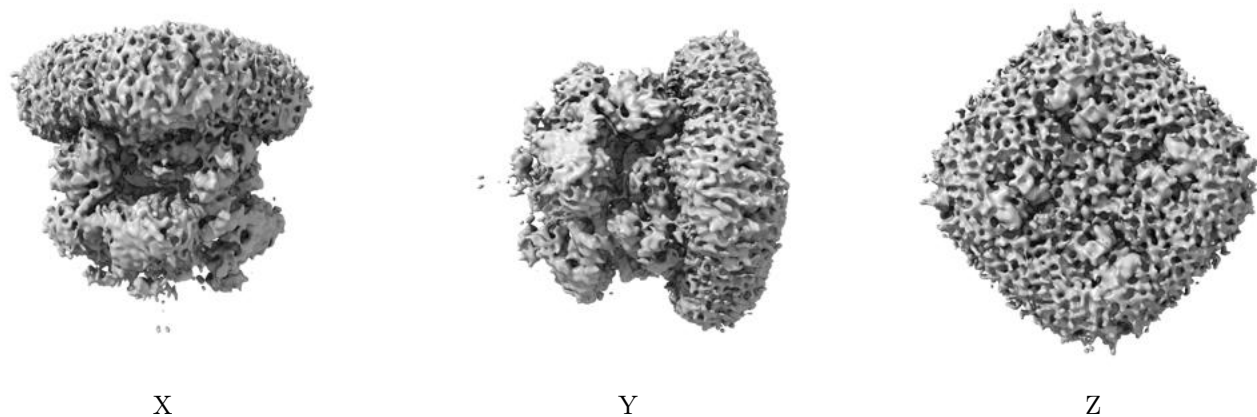
The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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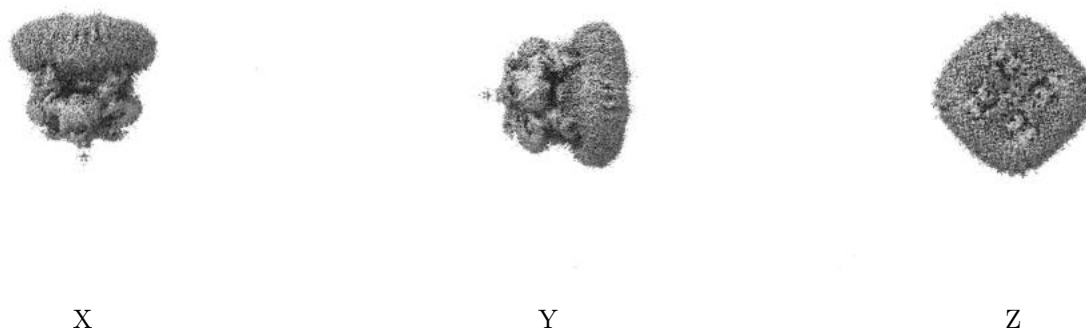
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation ⓘ

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

# 7 Map analysis ⓘ

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

## 7.1 Map-value distribution ⓘ
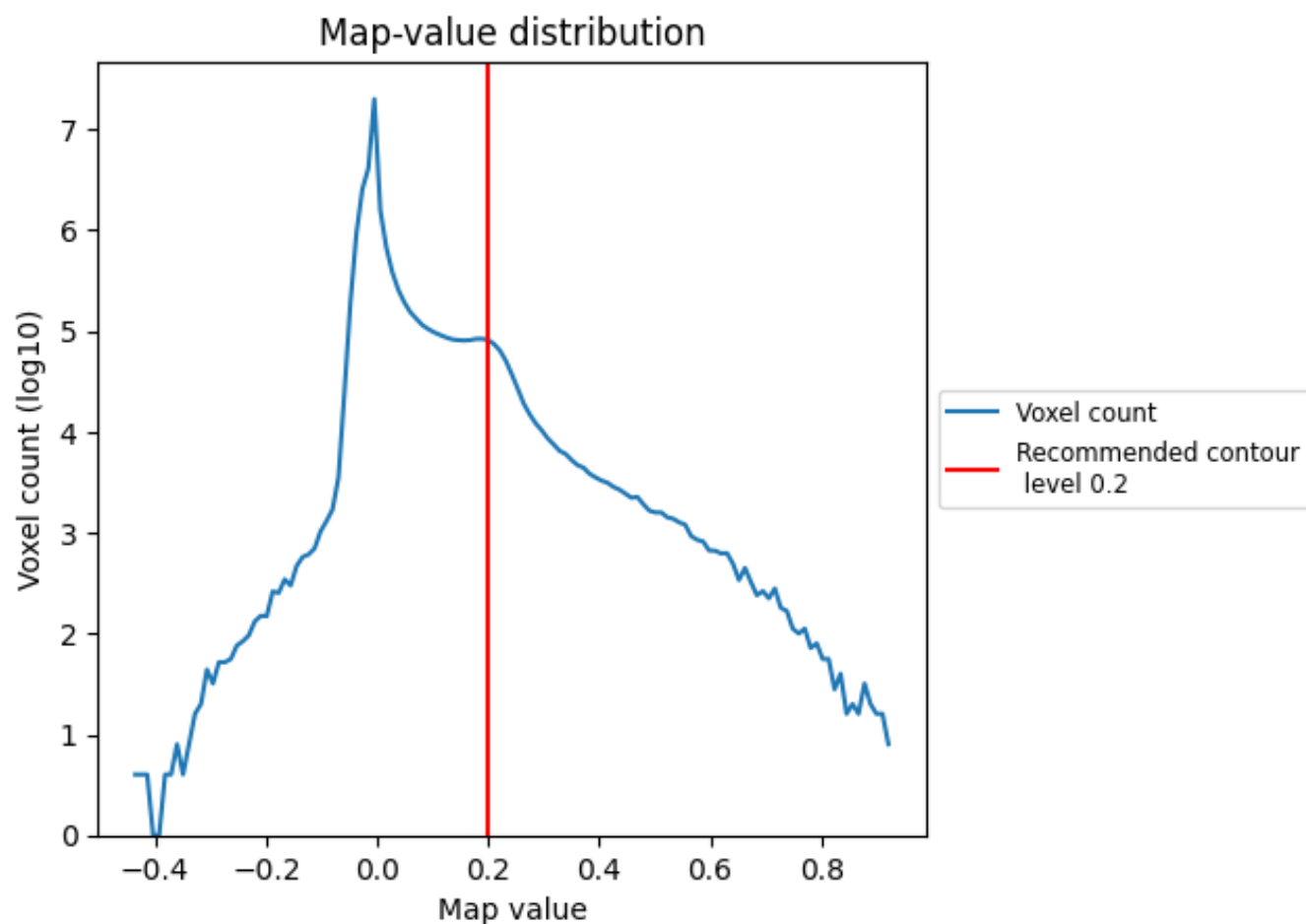


The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate ⓘ
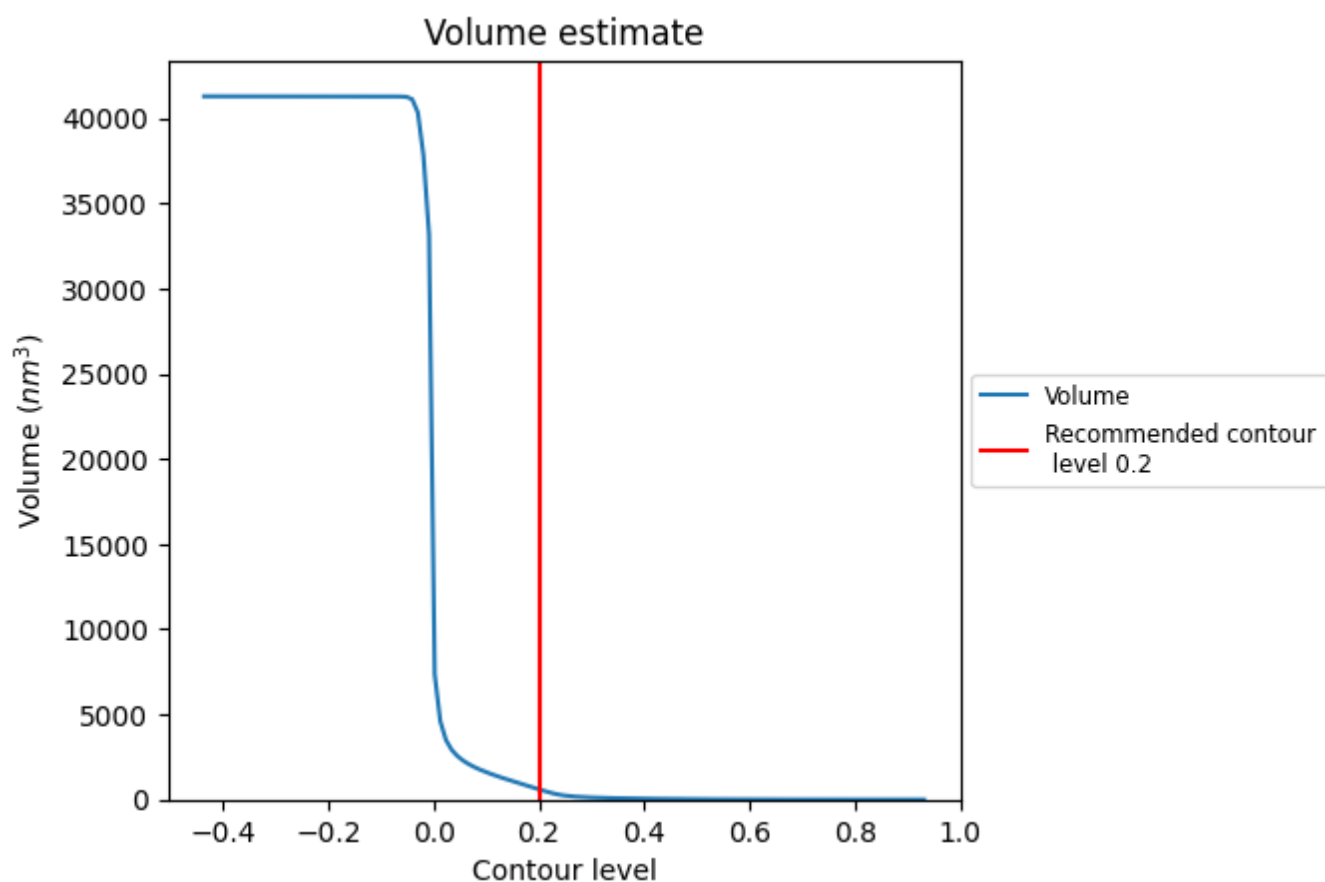


The volume at the recommended contour level is 603 nm$^3$; this corresponds to an approximate mass of 545 kDa.

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 ⓘ
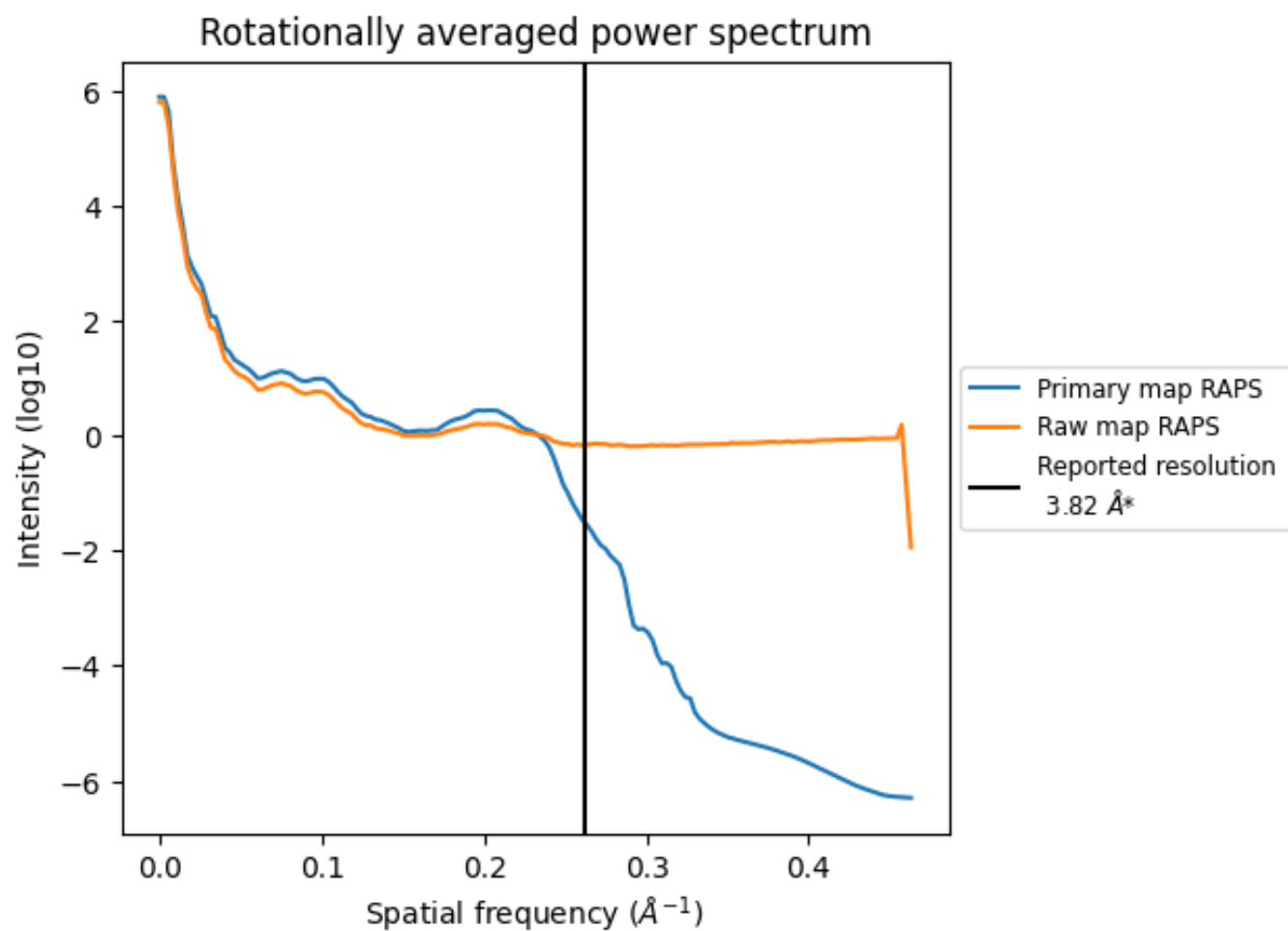


*Reported resolution corresponds to spatial frequency of 0.262 Å$^{-1}$

# 8　Fourier-Shell correlation ⓘ

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 ⓘ
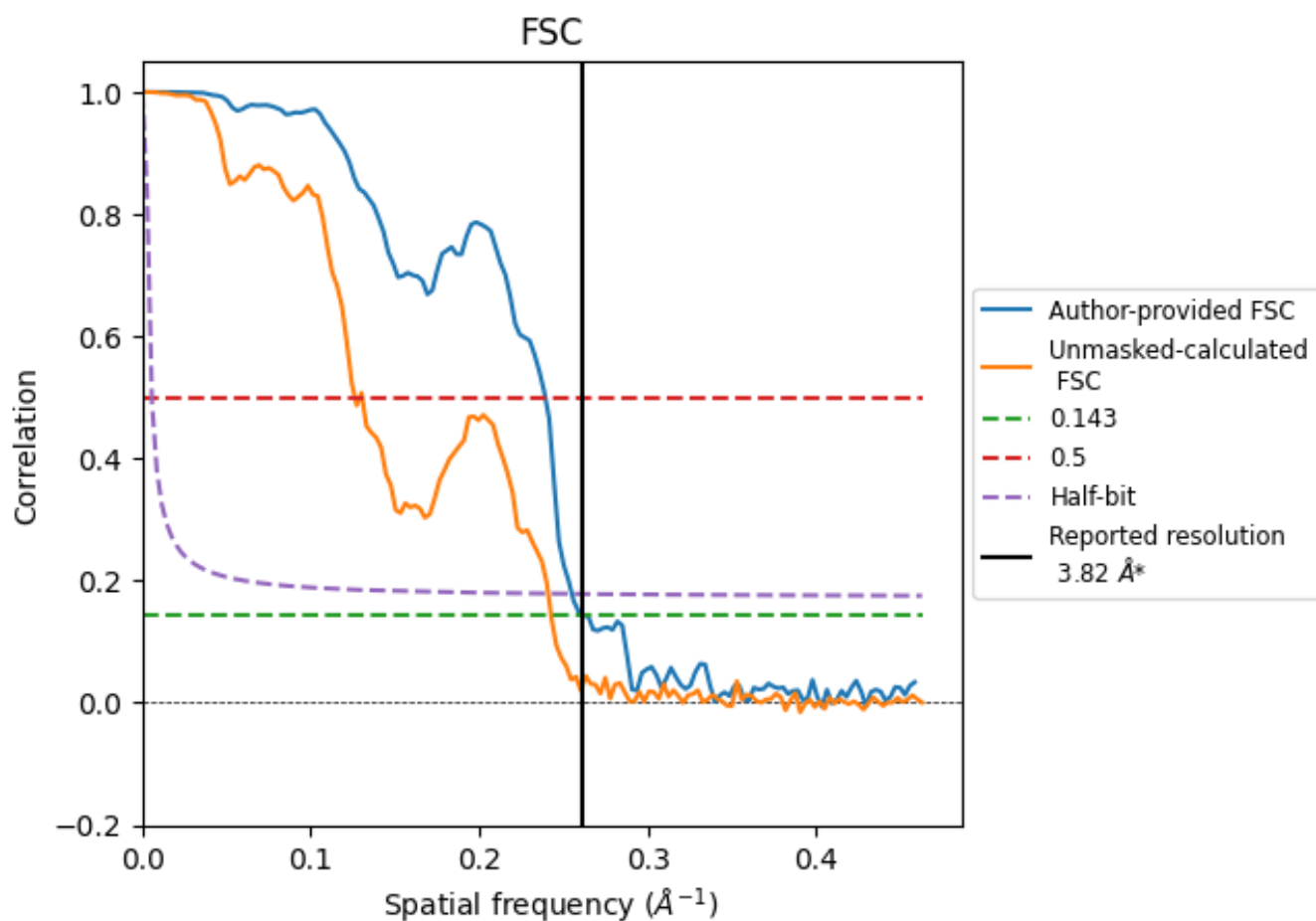


*Reported resolution corresponds to spatial frequency of 0.262 Å$^{-1}$

## 8.2 Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.82 | - | - |
| Author-provided FSC curve | 3.82 | 4.18 | 3.92 |
| Unmasked-calculated* | 4.12 | 7.92 | 4.15 |

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

# 9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-44102 and PDB model 9B2A. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1 Map-model overlay ⓘ
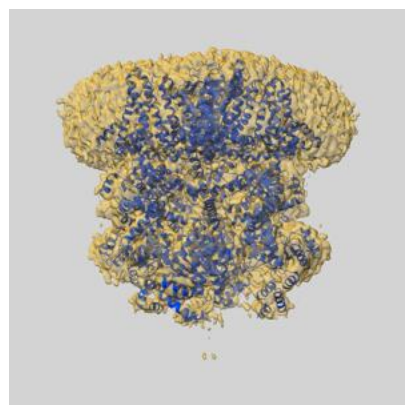


|    |    |    |
|:--:|:--:|:--:|
| X  | Y  | Z  |
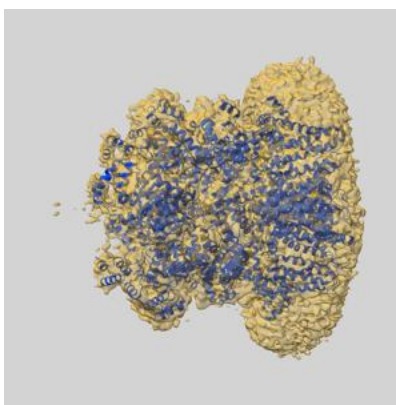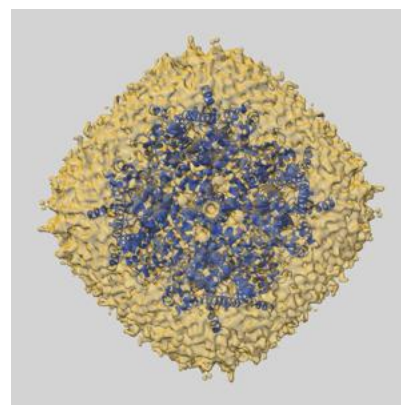
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model ⓘ



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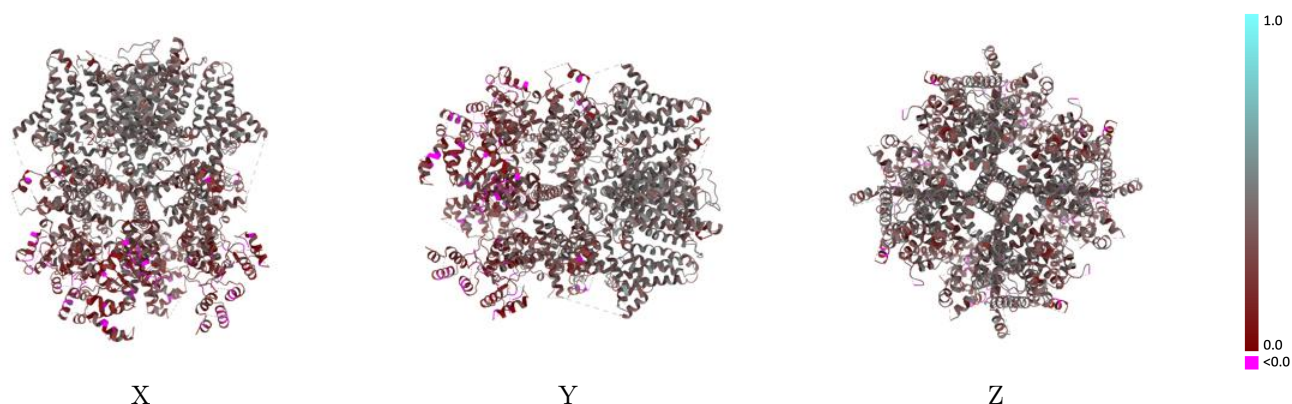
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



X        Y        Z
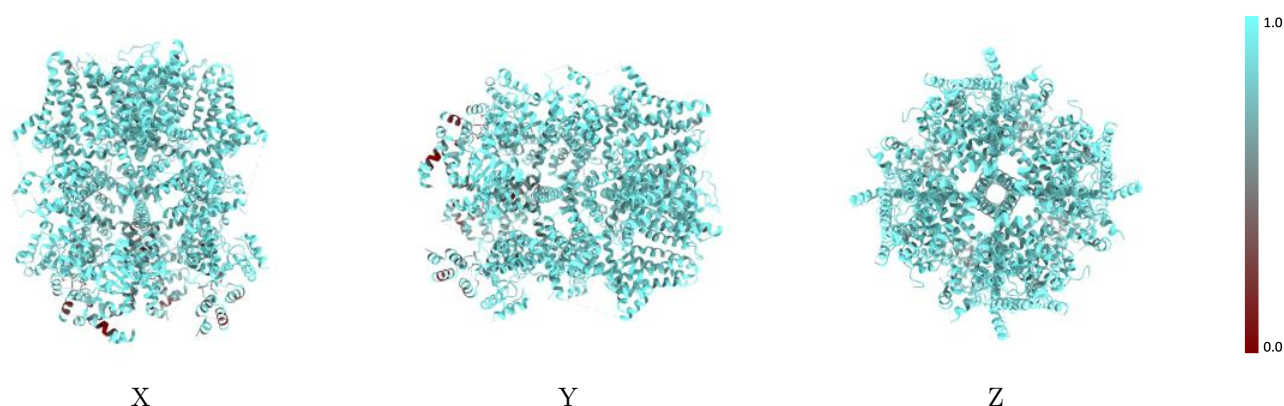
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

## 9.4 Atom inclusion ⓘ
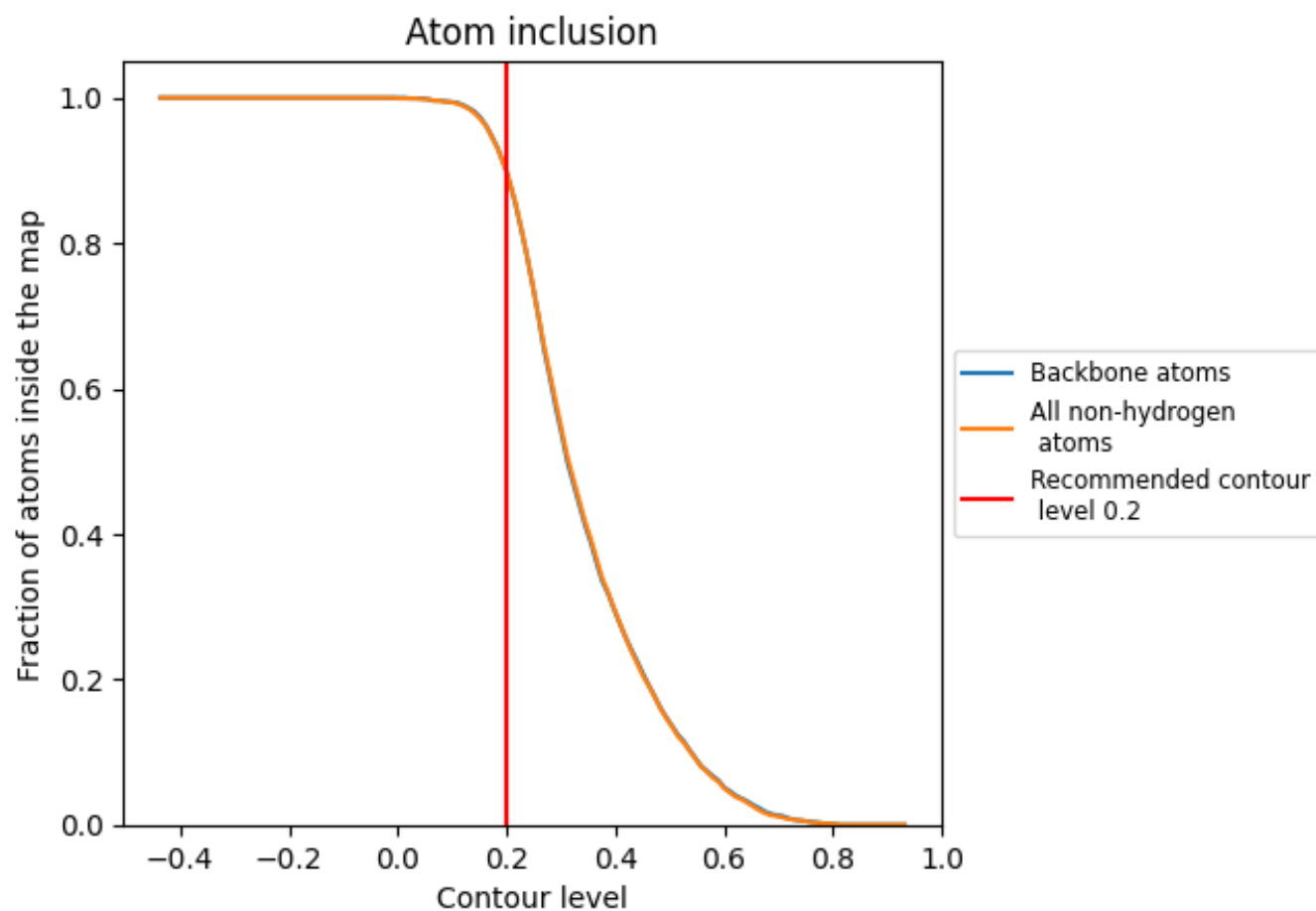


At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

## 9.5  Map-model fit summary  ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for
the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|:-----:|:--------------:|:-------:|
| All | 0.8990 | 0.3400 |
| A | 0.9020 | 0.3400 |
| B | 0.9020 | 0.3410 |
| C | 0.9020 | 0.3400 |
| D | 0.9020 | 0.3400 |