# Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:50 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 13LN / pdb_000013ln |
| EMDB ID | : | EMD-77138 |
| Title | : | Structure of human TRPV3-Q580P Olmsted syndrome mutant in the inactivated state |
| Authors | : | Purohit, R.; Khau, J.; Nadezhdin, K.D.; Sobolevsky, A.I. |
| Deposited on | : | 2026-05-13 |
| Resolution | : | 3.02 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

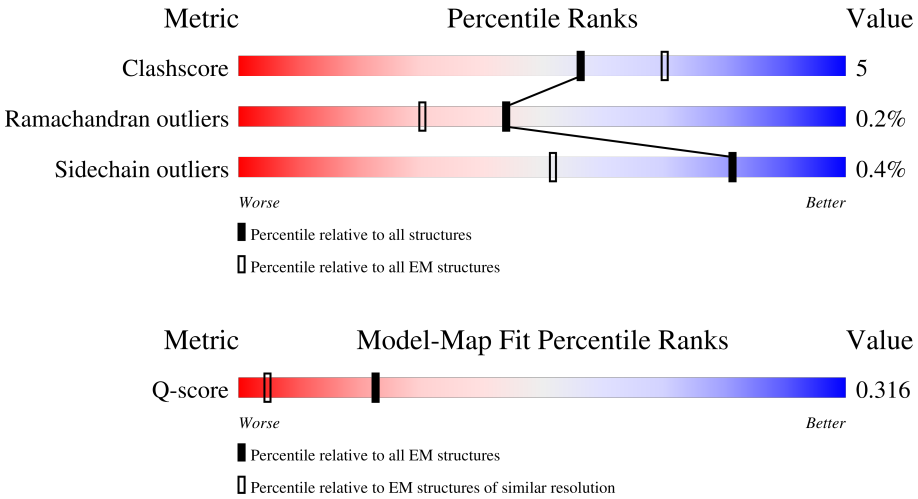
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 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) | : | 2.50 |

# 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 3.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 13913 ( 2.52 - 3.52 ) |

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 | 1052 | 10% 53% 6% 40% |
| 1 | B | 1052 | 10% 54% 6% 40% |
| 1 | C | 1052 | 9% 54% 6% 40% |
| 1 | D | 1052 | 10% 53% 6% 40% |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22147 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 Isoform 2 of Transient receptor potential cation channel subfamily V member 3,Green fluorescent protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 626 | Total | C | N | O | S | 0 | 0 |
| | | | 5094 | 3314 | 841 | 907 | 32 | | |
| 1 | B | 626 | Total | C | N | O | S | 0 | 0 |
| | | | 5094 | 3314 | 841 | 907 | 32 | | |
| 1 | C | 626 | Total | C | N | O | S | 0 | 0 |
| | | | 5094 | 3314 | 841 | 907 | 32 | | |
| 1 | D | 626 | Total | C | N | O | S | 0 | 0 |
| | | | 5094 | 3314 | 841 | 907 | 32 | | |

There are 116 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 580 | PRO | GLN | engineered mutation | UNP Q8NET8 |
| A | 792 | LEU | - | linker | UNP Q8NET8 |
| A | 793 | VAL | - | linker | UNP Q8NET8 |
| A | 794 | PRO | - | linker | UNP Q8NET8 |
| A | 795 | ARG | - | linker | UNP Q8NET8 |
| A | 796 | GLY | - | linker | UNP Q8NET8 |
| A | 797 | SER | - | linker | UNP Q8NET8 |
| A | 798 | ALA | - | linker | UNP Q8NET8 |
| A | 799 | ALA | - | linker | UNP Q8NET8 |
| A | 800 | ALA | - | linker | UNP Q8NET8 |
| A | 801 | ALA | - | linker | UNP Q8NET8 |
| A | 802 | VAL | - | linker | UNP Q8NET8 |
| A | 865 | LEU | PHE | conflict | UNP P42212 |
| A | 866 | THR | SER | conflict | UNP P42212 |
| A | 1007 | LYS | ALA | conflict | UNP P42212 |
| A | 1032 | LEU | HIS | conflict | UNP P42212 |
| A | 1040 | SER | - | expression tag | UNP P42212 |
| A | 1041 | GLY | - | expression tag | UNP P42212 |
| A | 1042 | LEU | - | expression tag | UNP P42212 |
| A | 1043 | ARG | - | expression tag | UNP P42212 |
| A | 1044 | SER | - | expression tag | UNP P42212 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1045 | TRP | - | expression tag | UNP P42212 |
| A | 1046 | SER | - | expression tag | UNP P42212 |
| A | 1047 | HIS | - | expression tag | UNP P42212 |
| A | 1048 | PRO | - | expression tag | UNP P42212 |
| A | 1049 | GLN | - | expression tag | UNP P42212 |
| A | 1050 | PHE | - | expression tag | UNP P42212 |
| A | 1051 | GLU | - | expression tag | UNP P42212 |
| A | 1052 | LYS | - | expression tag | UNP P42212 |
| B | 580 | PRO | GLN | engineered mutation | UNP Q8NET8 |
| B | 792 | LEU | - | linker | UNP Q8NET8 |
| B | 793 | VAL | - | linker | UNP Q8NET8 |
| B | 794 | PRO | - | linker | UNP Q8NET8 |
| B | 795 | ARG | - | linker | UNP Q8NET8 |
| B | 796 | GLY | - | linker | UNP Q8NET8 |
| B | 797 | SER | - | linker | UNP Q8NET8 |
| B | 798 | ALA | - | linker | UNP Q8NET8 |
| B | 799 | ALA | - | linker | UNP Q8NET8 |
| B | 800 | ALA | - | linker | UNP Q8NET8 |
| B | 801 | ALA | - | linker | UNP Q8NET8 |
| B | 802 | VAL | - | linker | UNP Q8NET8 |
| B | 865 | LEU | PHE | conflict | UNP P42212 |
| B | 866 | THR | SER | conflict | UNP P42212 |
| B | 1007 | LYS | ALA | conflict | UNP P42212 |
| B | 1032 | LEU | HIS | conflict | UNP P42212 |
| B | 1040 | SER | - | expression tag | UNP P42212 |
| B | 1041 | GLY | - | expression tag | UNP P42212 |
| B | 1042 | LEU | - | expression tag | UNP P42212 |
| B | 1043 | ARG | - | expression tag | UNP P42212 |
| B | 1044 | SER | - | expression tag | UNP P42212 |
| B | 1045 | TRP | - | expression tag | UNP P42212 |
| B | 1046 | SER | - | expression tag | UNP P42212 |
| B | 1047 | HIS | - | expression tag | UNP P42212 |
| B | 1048 | PRO | - | expression tag | UNP P42212 |
| B | 1049 | GLN | - | expression tag | UNP P42212 |
| B | 1050 | PHE | - | expression tag | UNP P42212 |
| B | 1051 | GLU | - | expression tag | UNP P42212 |
| B | 1052 | LYS | - | expression tag | UNP P42212 |
| C | 580 | PRO | GLN | engineered mutation | UNP Q8NET8 |
| C | 792 | LEU | - | linker | UNP Q8NET8 |
| C | 793 | VAL | - | linker | UNP Q8NET8 |
| C | 794 | PRO | - | linker | UNP Q8NET8 |
| C | 795 | ARG | - | linker | UNP Q8NET8 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 796 | GLY | - | linker | UNP Q8NET8 |
| C | 797 | SER | - | linker | UNP Q8NET8 |
| C | 798 | ALA | - | linker | UNP Q8NET8 |
| C | 799 | ALA | - | linker | UNP Q8NET8 |
| C | 800 | ALA | - | linker | UNP Q8NET8 |
| C | 801 | ALA | - | linker | UNP Q8NET8 |
| C | 802 | VAL | - | linker | UNP Q8NET8 |
| C | 865 | LEU | PHE | conflict | UNP P42212 |
| C | 866 | THR | SER | conflict | UNP P42212 |
| C | 1007 | LYS | ALA | conflict | UNP P42212 |
| C | 1032 | LEU | HIS | conflict | UNP P42212 |
| C | 1040 | SER | - | expression tag | UNP P42212 |
| C | 1041 | GLY | - | expression tag | UNP P42212 |
| C | 1042 | LEU | - | expression tag | UNP P42212 |
| C | 1043 | ARG | - | expression tag | UNP P42212 |
| C | 1044 | SER | - | expression tag | UNP P42212 |
| C | 1045 | TRP | - | expression tag | UNP P42212 |
| C | 1046 | SER | - | expression tag | UNP P42212 |
| C | 1047 | HIS | - | expression tag | UNP P42212 |
| C | 1048 | PRO | - | expression tag | UNP P42212 |
| C | 1049 | GLN | - | expression tag | UNP P42212 |
| C | 1050 | PHE | - | expression tag | UNP P42212 |
| C | 1051 | GLU | - | expression tag | UNP P42212 |
| C | 1052 | LYS | - | expression tag | UNP P42212 |
| D | 580 | PRO | GLN | engineered mutation | UNP Q8NET8 |
| D | 792 | LEU | - | linker | UNP Q8NET8 |
| D | 793 | VAL | - | linker | UNP Q8NET8 |
| D | 794 | PRO | - | linker | UNP Q8NET8 |
| D | 795 | ARG | - | linker | UNP Q8NET8 |
| D | 796 | GLY | - | linker | UNP Q8NET8 |
| D | 797 | SER | - | linker | UNP Q8NET8 |
| D | 798 | ALA | - | linker | UNP Q8NET8 |
| D | 799 | ALA | - | linker | UNP Q8NET8 |
| D | 800 | ALA | - | linker | UNP Q8NET8 |
| D | 801 | ALA | - | linker | UNP Q8NET8 |
| D | 802 | VAL | - | linker | UNP Q8NET8 |
| D | 865 | LEU | PHE | conflict | UNP P42212 |
| D | 866 | THR | SER | conflict | UNP P42212 |
| D | 1007 | LYS | ALA | conflict | UNP P42212 |
| D | 1032 | LEU | HIS | conflict | UNP P42212 |
| D | 1040 | SER | - | expression tag | UNP P42212 |
| D | 1041 | GLY | - | expression tag | UNP P42212 |

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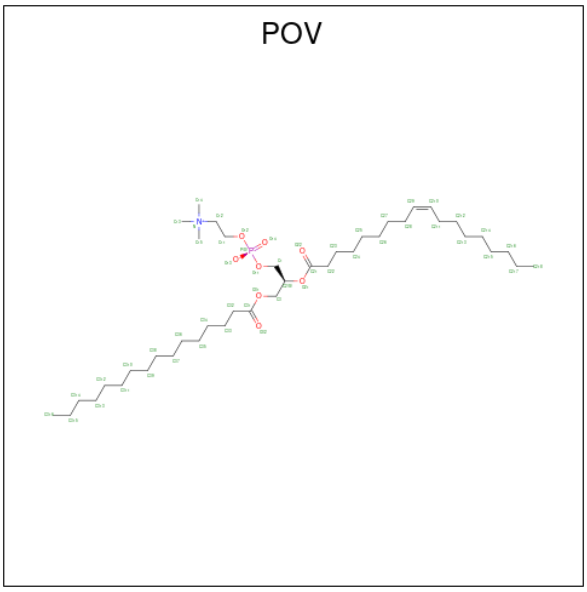
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 1042 | LEU | - | expression tag | UNP P42212 |
| D | 1043 | ARG | - | expression tag | UNP P42212 |
| D | 1044 | SER | - | expression tag | UNP P42212 |
| D | 1045 | TRP | - | expression tag | UNP P42212 |
| D | 1046 | SER | - | expression tag | UNP P42212 |
| D | 1047 | HIS | - | expression tag | UNP P42212 |
| D | 1048 | PRO | - | expression tag | UNP P42212 |
| D | 1049 | GLN | - | expression tag | UNP P42212 |
| D | 1050 | PHE | - | expression tag | UNP P42212 |
| D | 1051 | GLU | - | expression tag | UNP P42212 |
| D | 1052 | LYS | - | expression tag | UNP P42212 |

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | B | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 3 | A | 3 | Total | Na | 0 |
| | | | 3 | 3 | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 4 | A | 25 | Total | O | 0 |
| | | | 25 | 25 | |
| 4 | B | 29 | Total | O | 0 |
| | | | 29 | 29 | |
| 4 | C | 25 | Total | O | 0 |
| | | | 25 | 25 | |
| 4 | D | 25 | Total | O | 0 |
| | | | 25 | 25 | |

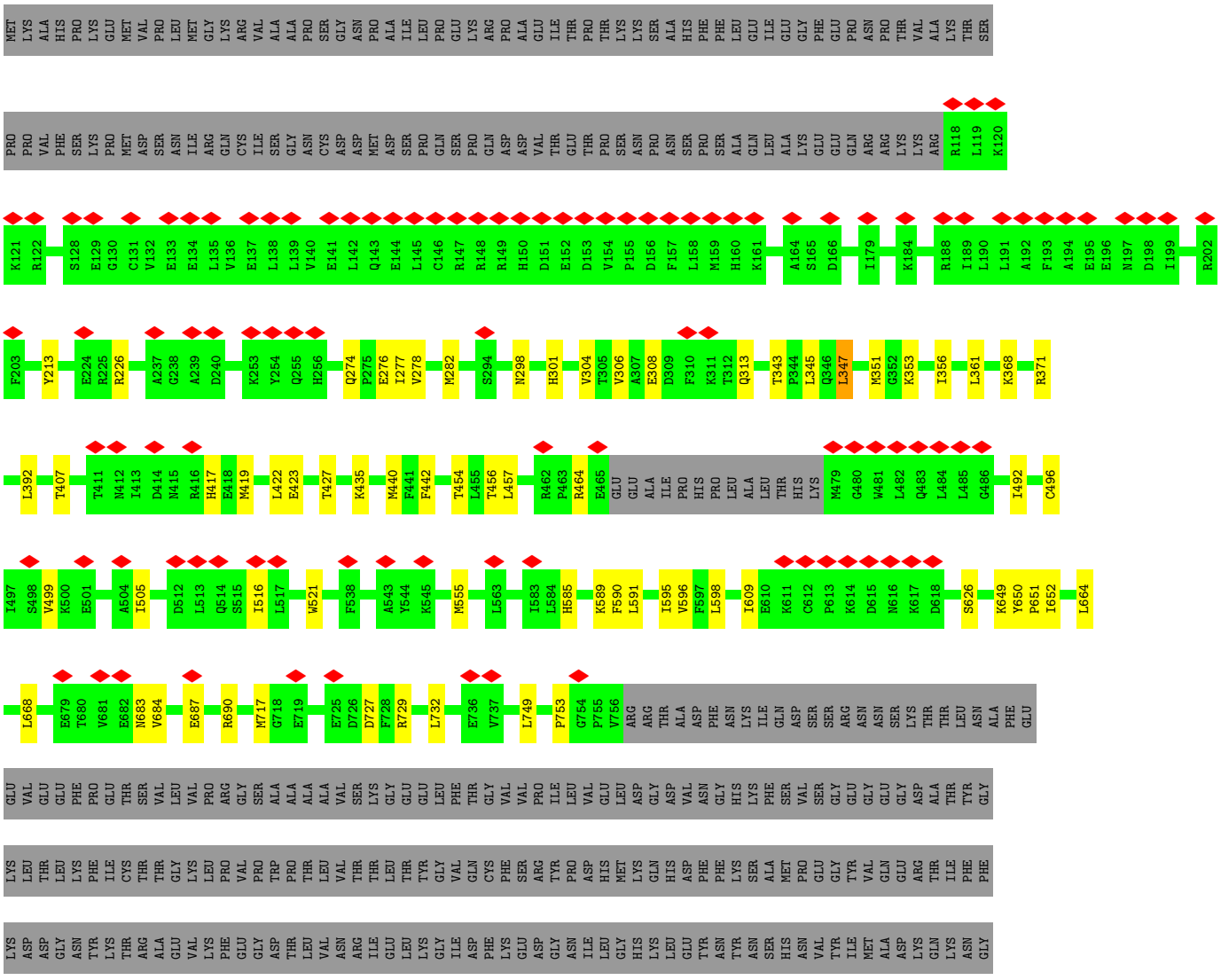
# 3 Residue-property plots (i)

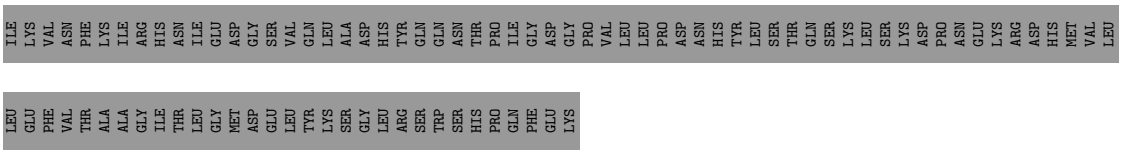
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Isoform 2 of Transient receptor potential cation channel subfamily V member 3,Green fluorescent protein

Chain A:



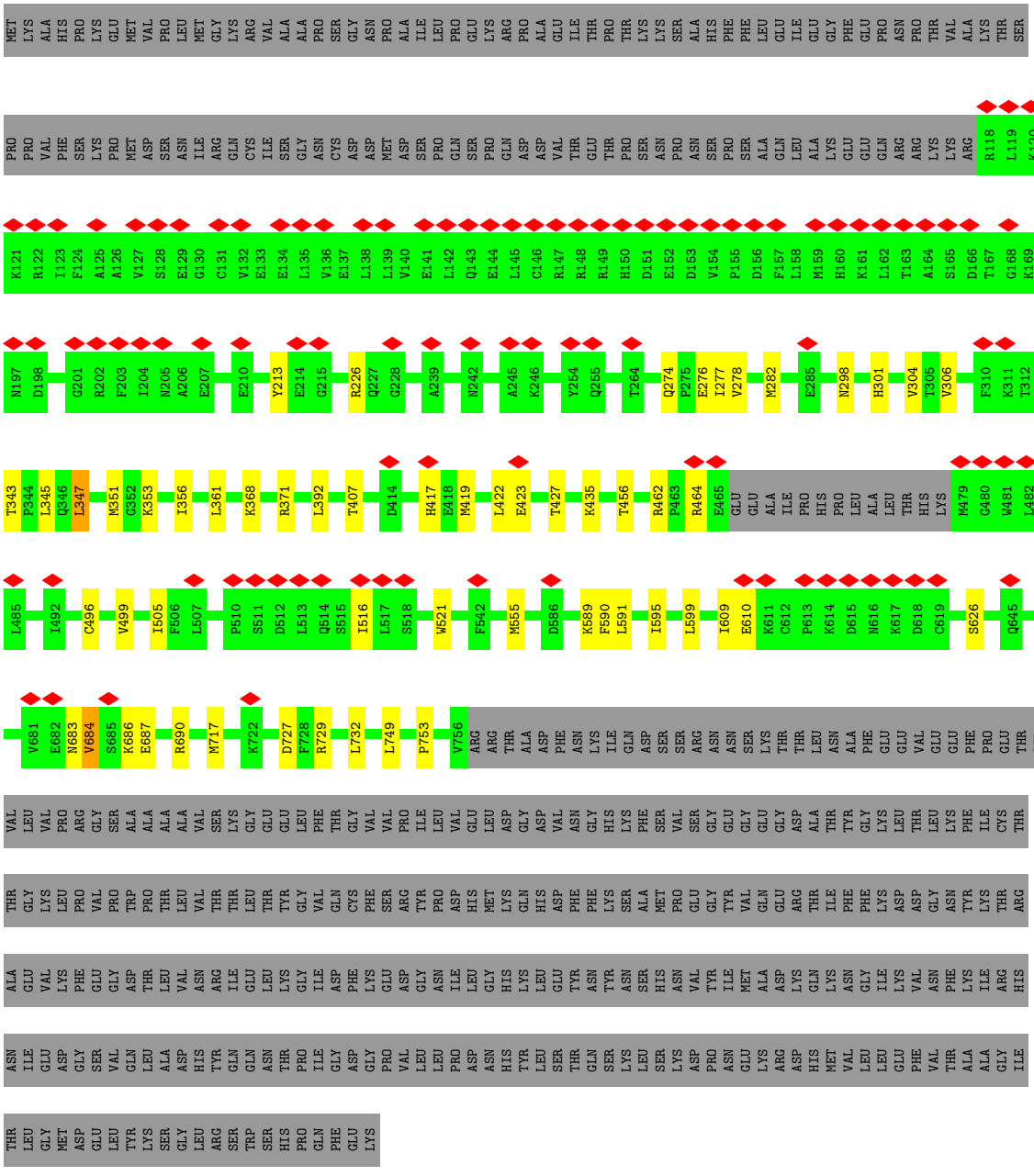




• Molecule 1: Isoform 2 of Transient receptor potential cation channel subfamily V member 3,Green fluorescent protein

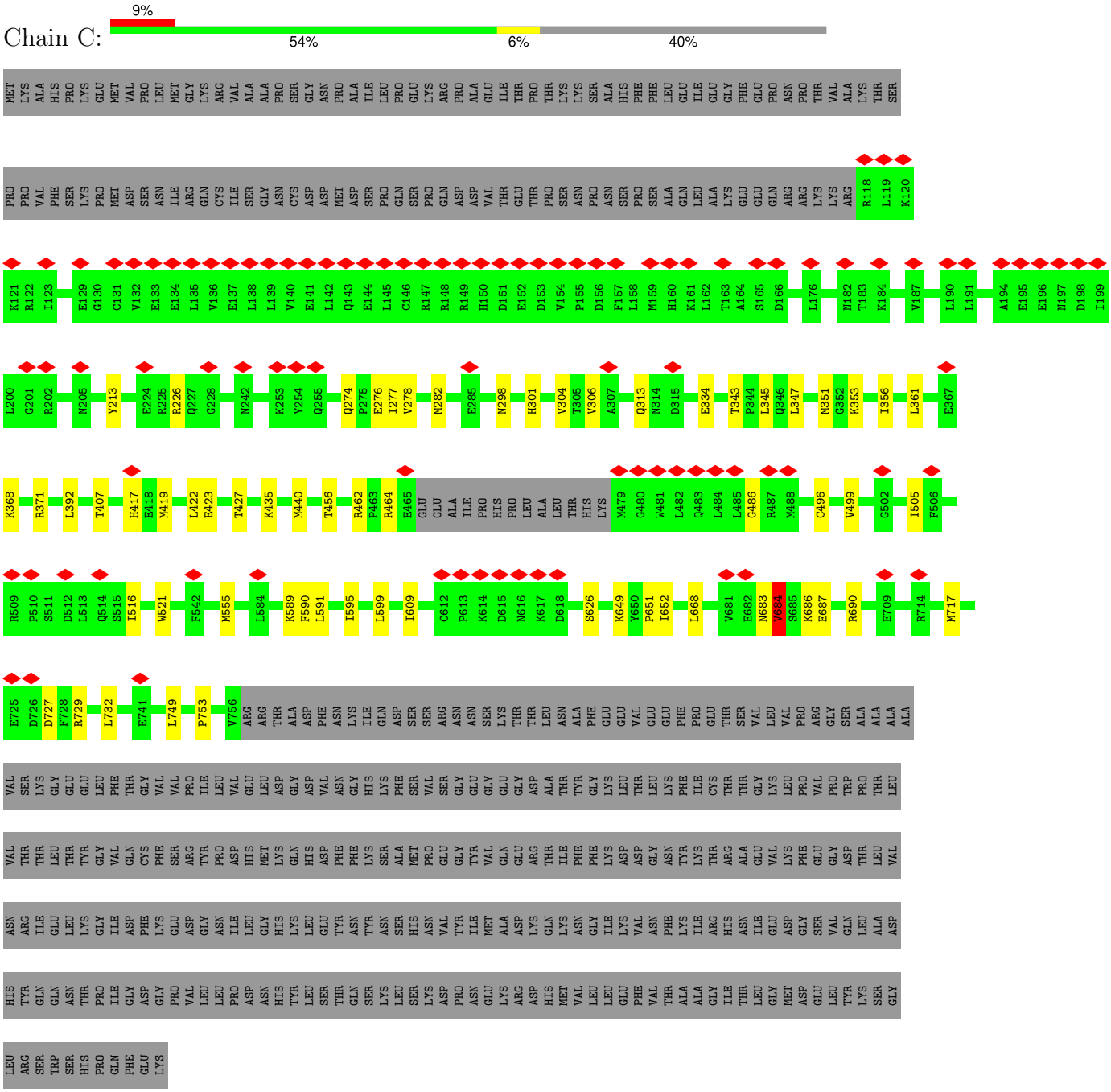
Chain B:



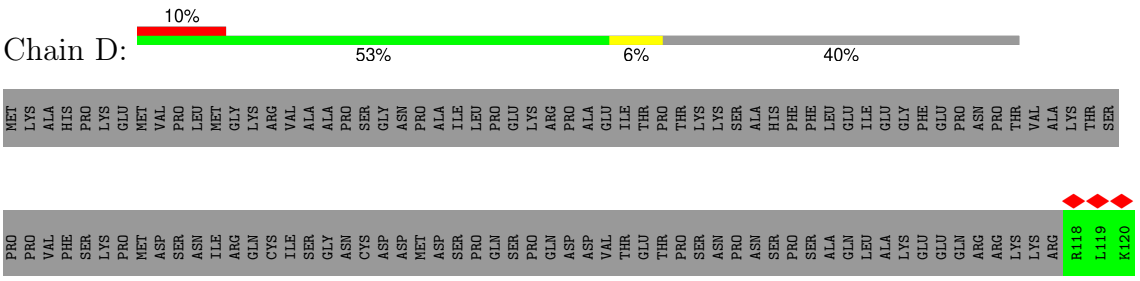
• Molecule 1: Isoform 2 of Transient receptor potential cation channel subfamily V member 3,Green fluorescent protein

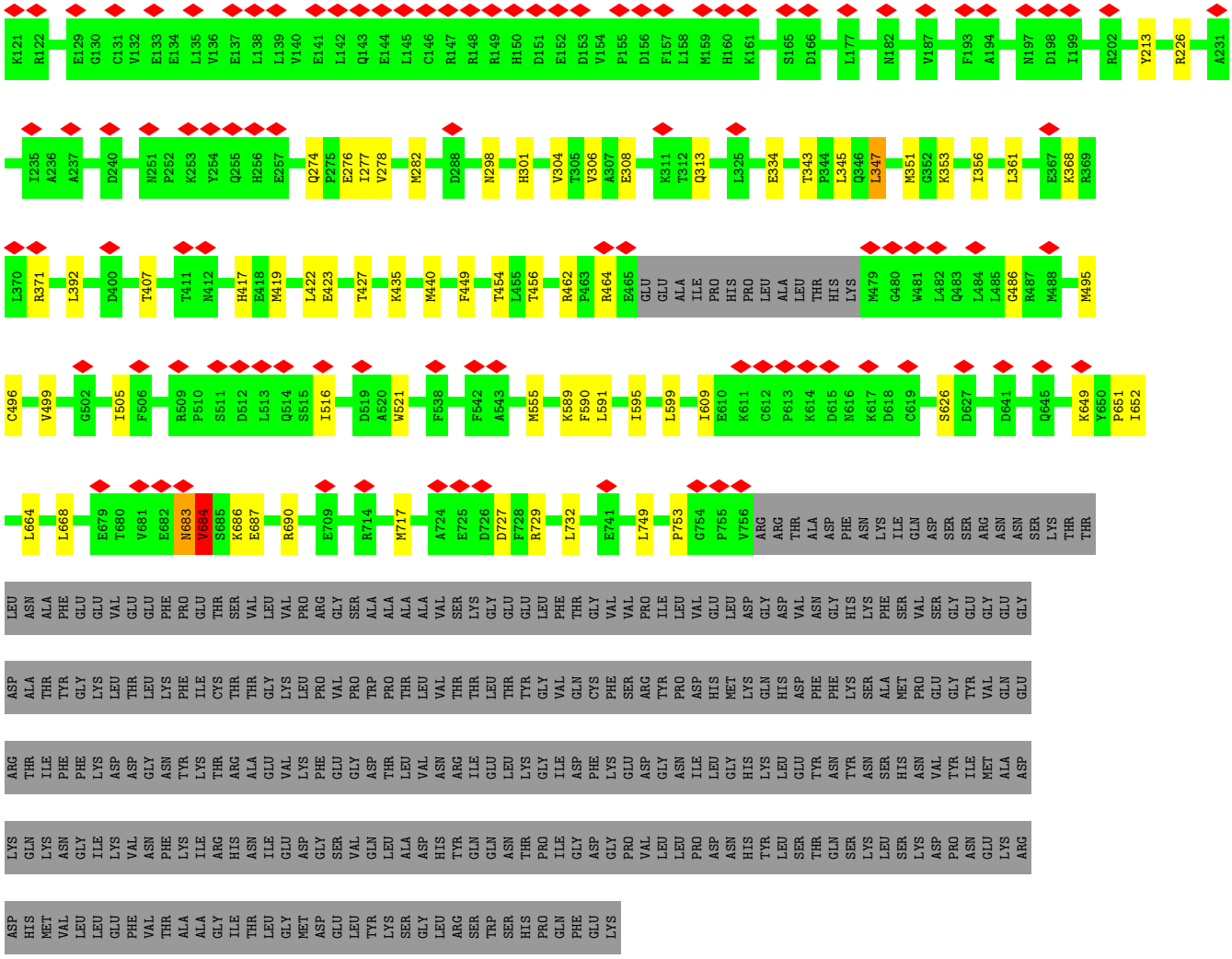
Chain C:




• Molecule 1: Isoform 2 of Transient receptor potential cation channel subfamily V member 3,Green fluorescent protein

Chain D:




K121 R122 E129 G130 C131 V132 E133 E134 L135 V136 E137 L138 L139 V140 E141 L142 Q143 E144 L145 C146 R147 R148 R149 H150 D151 E152 D153 V154 P155 D156 F157 L158 M159 H160 K161 S165 D166 L177 N182 V187 F193 A194 N197 D198 I199 R202 Y213 R226 A231
T235 A236 A237 D240 N251 P252 K253 Y254 Q255 H256 E257 Q274 P275 E276 I277 V278 M282 D288 N298 H301 V304 T305 V306 A307 E308 K311 T312 Q313 L325 E334 T343 P344 L345 Q346 L347 M351 G352 K353 I356 L361 E367 K368 R369
L370 R371 L392 D400 T407 T411 N412 H417 E418 M419 L422 E423 T427 K435 M440 F449 T454 L455 T456 R462 P463 R464 E465 GLU GLU ALA ILE PRO HIS PRO LEU ALA LEU THR HIS LYS M479 G480 W481 L482 Q483 L484 L485 G486 R487 M488 M495
C496 V499 G502 I505 F506 R509 P510 S511 D512 L513 Q514 S515 I516 D519 A520 W521 F538 F542 A543 M555 K589 F590 L591 I595 L599 I609 E610 K611 C612 P613 K614 D615 N616 K617 D618 C619 S626 D627 D641 Q645 K649 Y650 P651 I652
L664 L668 E679 T680 V681 E682 N683 V684 S685 K686 E687 R690 E709 R714 M717 A724 E725 D726 D727 F728 R729 L732 E741 L749 P753 G754 P755 V756 ARG ARG THR ALA ASP PHE ASN LYS ILE GLN ASP SER SER ARG ASN ASN SER LYS THR THR
LEU ASN ALA PHE GLU GLU VAL GLU GLU PHE PRO GLU THR SER VAL LEU VAL PRO ARG GLY SER ALA ALA ALA ALA VAL SER LYS GLY GLU GLU LEU PHE THR GLY VAL VAL PRO ILE LEU VAL GLU LEU ASP GLY ASP VAL ASN GLY HIS LYS PHE SER VAL SER GLY GLU GLY GLU GLY
ASP ALA THR TYR GLY LYS LEU THR LEU LYS PHE ILE CYS THR THR GLY LYS LEU PRO VAL PRO TRP PRO THR LEU VAL THR THR LEU THR TYR GLY VAL GLN CYS PHE SER ARG TYR PRO ASP HIS MET LYS GLN HIS ASP PHE PHE LYS SER ALA MET PRO GLU GLY TYR VAL GLN GLU
ARG THR ILE PHE PHE LYS ASP ASP GLY ASN TYR LYS THR ARG ALA GLU VAL LYS PHE GLU GLY ASP THR LEU VAL ASN ARG ILE GLU GLU LEU LYS GLY ILE ASP PHE LYS GLU ASP GLY ASN ILE LEU GLY HIS LYS LEU GLU GLU TYR ASN TYR ASN SER SER HIS ASN VAL TYR ILE MET ALA ASP
LYS GLN LYS ASN GLY PHE LYS ILE ARG HIS ASN ILE GLU GLU ASP GLY SER VAL GLN LEU ALA ASP HIS TYR GLN GLN ASN THR PRO ILE GLY ASP GLY PRO VAL LEU LEU PRO ASP ASN HIS TYR LEU SER THR GLN SER LYS LEU SER LYS ASP PRO ASN GLU LYS ARG
ASP HIS MET VAL LEU LEU GLU PHE VAL THR ALA ALA GLY ILE THR LEU GLY MET ASP GLU LEU TYR LYS SER GLY LEU ARG SER TRP SER HIS PRO GLN PHE GLU LYS

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 318748 | 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 ($e^-/Å^2$) | 60.8 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 1500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.792 | Depositor |
| Minimum map value | -0.508 | Depositor |
| Average map value | 0.002 | Depositor |
| Map value standard deviation | 0.025 | Depositor |
| Recommended contour level | 0.0557 | Depositor |
| Map size (Å) | 213.6832, 213.6832, 213.6832 | wwPDB |
| Map dimensions | 256, 256, 256 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.8347, 0.8347, 0.8347 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: POV, NA

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 | 0.25 | 0/5206 | 0.54 | 3/7043 (0.0%) |
| 1 | B | 0.25 | 0/5206 | 0.54 | 3/7043 (0.0%) |
| 1 | C | 0.25 | 0/5206 | 0.54 | 3/7043 (0.0%) |
| 1 | D | 0.25 | 0/5206 | 0.54 | 3/7043 (0.0%) |
| All | All | 0.25 | 0/20824 | 0.54 | 12/28172 (0.0%) |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 505 | ILE | N-CA-C | -6.08 | 106.88 | 112.96 |
| 1 | B | 505 | ILE | N-CA-C | -6.07 | 106.89 | 112.96 |
| 1 | A | 505 | ILE | N-CA-C | -6.05 | 106.91 | 112.96 |
| 1 | C | 505 | ILE | N-CA-C | -6.05 | 106.91 | 112.96 |
| 1 | B | 368 | LYS | CA-C-N | 5.78 | 132.58 | 121.54 |
| 1 | B | 368 | LYS | C-N-CA | 5.78 | 132.58 | 121.54 |
| 1 | C | 368 | LYS | CA-C-N | 5.77 | 132.56 | 121.54 |
| 1 | C | 368 | LYS | C-N-CA | 5.77 | 132.56 | 121.54 |
| 1 | D | 368 | LYS | CA-C-N | 5.77 | 132.55 | 121.54 |
| 1 | D | 368 | LYS | C-N-CA | 5.77 | 132.55 | 121.54 |
| 1 | A | 368 | LYS | CA-C-N | 5.76 | 132.55 | 121.54 |
| 1 | A | 368 | LYS | C-N-CA | 5.76 | 132.55 | 121.54 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5094 | 0 | 5156 | 50 | 0 |
| 1 | B | 5094 | 0 | 5156 | 44 | 0 |
| 1 | C | 5094 | 0 | 5156 | 45 | 0 |
| 1 | D | 5094 | 0 | 5156 | 53 | 0 |
| 2 | A | 468 | 0 | 738 | 35 | 0 |
| 2 | B | 364 | 0 | 574 | 16 | 0 |
| 2 | C | 468 | 0 | 738 | 32 | 0 |
| 2 | D | 364 | 0 | 574 | 27 | 0 |
| 3 | A | 3 | 0 | 0 | 0 | 0 |
| 4 | A | 25 | 0 | 0 | 0 | 0 |
| 4 | B | 29 | 0 | 0 | 0 | 0 |
| 4 | C | 25 | 0 | 0 | 0 | 0 |
| 4 | D | 25 | 0 | 0 | 0 | 0 |
| All | All | 22147 | 0 | 23248 | 222 | 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 5.

All (222) 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:753:PRO:O | 1:B:213:TYR:OH | 2.18 | 0.62 |
| 1:A:454:THR:HG23 | 2:A:1108:POV:H34 | 1.82 | 0.62 |
| 1:A:609:ILE:O | 1:D:464:ARG:NH1 | 2.34 | 0.61 |
| 1:B:464:ARG:NH1 | 1:C:609:ILE:O | 2.34 | 0.61 |
| 1:C:464:ARG:NH1 | 1:D:609:ILE:O | 2.34 | 0.59 |
| 1:A:591:LEU:HD13 | 2:A:1101:POV:H316 | 1.85 | 0.59 |
| 1:B:753:PRO:O | 1:C:213:TYR:OH | 2.22 | 0.58 |
| 1:A:464:ARG:NH1 | 1:B:609:ILE:O | 2.38 | 0.56 |
| 2:A:1103:POV:H216 | 2:A:1103:POV:H31A | 1.88 | 0.56 |
| 1:A:301:HIS:HD2 | 1:A:347:LEU:HD12 | 1.71 | 0.56 |
| 1:D:591:LEU:HD13 | 2:D:1103:POV:H316 | 1.88 | 0.56 |
| 1:C:456:THR:HA | 1:C:555:MET:HE3 | 1.89 | 0.55 |
| 1:C:753:PRO:O | 1:D:213:TYR:OH | 2.25 | 0.55 |
| 1:C:687:GLU:OE1 | 1:C:690:ARG:NE | 2.37 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:687:GLU:OE1 | 1:A:690:ARG:NE | 2.37 | 0.55 |
| 1:A:652:ILE:HG13 | 2:A:1109:POV:H1A | 1.89 | 0.55 |
| 1:D:652:ILE:HG13 | 2:D:1102:POV:H1A | 1.89 | 0.55 |
| 1:D:684:VAL:O | 1:D:686:LYS:N | 2.38 | 0.55 |
| 1:B:456:THR:HA | 1:B:555:MET:HE3 | 1.89 | 0.54 |
| 1:D:456:THR:HA | 1:D:555:MET:HE3 | 1.89 | 0.54 |
| 1:B:687:GLU:OE1 | 1:B:690:ARG:NE | 2.37 | 0.54 |
| 1:C:652:ILE:HG13 | 2:C:1101:POV:H1A | 1.90 | 0.54 |
| 1:C:591:LEU:HD13 | 2:C:1102:POV:H316 | 1.88 | 0.54 |
| 1:A:456:THR:HA | 1:A:555:MET:HE3 | 1.89 | 0.54 |
| 1:A:351:MET:HB3 | 1:A:353:LYS:HZ3 | 1.73 | 0.54 |
| 1:A:213:TYR:OH | 1:D:753:PRO:O | 2.25 | 0.53 |
| 1:D:684:VAL:C | 1:D:686:LYS:H | 2.16 | 0.53 |
| 1:B:591:LEU:HD13 | 2:B:1102:POV:H316 | 1.91 | 0.52 |
| 1:D:687:GLU:OE1 | 1:D:690:ARG:NE | 2.37 | 0.52 |
| 1:A:301:HIS:CD2 | 1:A:347:LEU:HD12 | 2.44 | 0.52 |
| 1:A:278:VAL:HG12 | 1:A:282:MET:HE2 | 1.91 | 0.52 |
| 1:C:278:VAL:HG12 | 1:C:282:MET:HE2 | 1.91 | 0.52 |
| 1:B:278:VAL:HG12 | 1:B:282:MET:HE2 | 1.91 | 0.51 |
| 1:A:664:LEU:HD11 | 2:D:1107:POV:H31H | 1.93 | 0.51 |
| 1:C:684:VAL:O | 1:C:686:LYS:HD2 | 2.11 | 0.51 |
| 1:D:278:VAL:HG12 | 1:D:282:MET:HE2 | 1.91 | 0.51 |
| 2:C:1107:POV:H31H | 1:D:664:LEU:HD11 | 1.93 | 0.50 |
| 2:A:1109:POV:H21A | 1:D:595:ILE:HD11 | 1.93 | 0.50 |
| 1:B:595:ILE:HD11 | 2:C:1101:POV:H21A | 1.92 | 0.50 |
| 1:B:496:CYS:HB3 | 2:B:1104:POV:H23A | 1.93 | 0.50 |
| 1:B:652:ILE:HG13 | 2:B:1101:POV:H1A | 1.92 | 0.50 |
| 1:C:595:ILE:HD11 | 2:D:1102:POV:H21A | 1.93 | 0.49 |
| 1:D:423:GLU:OE2 | 1:D:427:THR:OG1 | 2.31 | 0.49 |
| 1:A:419:MET:HA | 1:A:422:LEU:HD13 | 1.95 | 0.49 |
| 1:C:423:GLU:OE2 | 1:C:427:THR:OG1 | 2.31 | 0.49 |
| 1:A:727:ASP:OD2 | 1:A:729:ARG:NH1 | 2.45 | 0.49 |
| 1:C:435:LYS:HD2 | 1:C:717:MET:HE3 | 1.95 | 0.49 |
| 1:B:423:GLU:OE2 | 1:B:427:THR:OG1 | 2.31 | 0.49 |
| 1:C:407:THR:HG23 | 1:C:419:MET:HE2 | 1.95 | 0.49 |
| 1:A:435:LYS:HD2 | 1:A:717:MET:HE3 | 1.95 | 0.48 |
| 1:B:407:THR:HG23 | 1:B:419:MET:HE2 | 1.95 | 0.48 |
| 1:C:626:SER:HB3 | 2:C:1102:POV:H32A | 1.94 | 0.48 |
| 1:A:423:GLU:OE2 | 1:A:427:THR:OG1 | 2.31 | 0.48 |
| 1:D:727:ASP:OD2 | 1:D:729:ARG:NH1 | 2.45 | 0.48 |
| 1:B:343:THR:HG23 | 1:B:345:LEU:H | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:435:LYS:HD2 | 1:B:717:MET:HE3 | 1.95 | 0.48 |
| 1:C:462:ARG:HH22 | 1:D:649:LYS:HZ3 | 1.60 | 0.48 |
| 1:A:407:THR:HG23 | 1:A:419:MET:HE2 | 1.95 | 0.48 |
| 1:D:407:THR:HG23 | 1:D:419:MET:HE2 | 1.95 | 0.48 |
| 1:B:351:MET:HB3 | 1:B:353:LYS:HZ3 | 1.79 | 0.48 |
| 1:C:419:MET:HA | 1:C:422:LEU:HD13 | 1.95 | 0.48 |
| 1:C:727:ASP:OD2 | 1:C:729:ARG:NH1 | 2.45 | 0.48 |
| 1:D:419:MET:HA | 1:D:422:LEU:HD13 | 1.95 | 0.48 |
| 1:A:649:LYS:HZ3 | 1:D:462:ARG:HH22 | 1.61 | 0.48 |
| 1:C:343:THR:HG23 | 1:C:345:LEU:H | 1.79 | 0.48 |
| 1:C:496:CYS:HB3 | 2:C:1105:POV:H23A | 1.95 | 0.48 |
| 2:A:1102:POV:H22A | 2:A:1102:POV:H2 | 1.65 | 0.48 |
| 2:A:1103:POV:H28 | 1:D:456:THR:HG21 | 1.95 | 0.48 |
| 2:D:1104:POV:H22A | 2:D:1104:POV:H2 | 1.66 | 0.48 |
| 1:A:683:ASN:HA | 1:A:687:GLU:HG3 | 1.96 | 0.47 |
| 2:A:1105:POV:H31F | 2:A:1106:POV:H212 | 1.96 | 0.47 |
| 1:D:496:CYS:HB3 | 2:D:1105:POV:H23A | 1.97 | 0.47 |
| 1:B:462:ARG:HH22 | 1:C:649:LYS:HZ3 | 1.61 | 0.47 |
| 1:D:343:THR:HG23 | 1:D:345:LEU:H | 1.79 | 0.47 |
| 1:B:419:MET:HA | 1:B:422:LEU:HD13 | 1.95 | 0.47 |
| 1:A:496:CYS:HB3 | 2:A:1104:POV:H23A | 1.97 | 0.47 |
| 1:C:599:LEU:HB2 | 2:C:1104:POV:H21A | 1.96 | 0.47 |
| 1:D:626:SER:HB3 | 2:D:1103:POV:H32A | 1.96 | 0.47 |
| 2:A:1107:POV:H21A | 1:B:599:LEU:HB2 | 1.97 | 0.47 |
| 1:B:727:ASP:OD2 | 1:B:729:ARG:NH1 | 2.45 | 0.47 |
| 2:C:1108:POV:H32A | 2:D:1103:POV:H34A | 1.96 | 0.47 |
| 1:D:435:LYS:HD2 | 1:D:717:MET:HE3 | 1.95 | 0.47 |
| 1:A:343:THR:HG23 | 1:A:345:LEU:H | 1.79 | 0.47 |
| 2:A:1107:POV:H32A | 2:B:1102:POV:H34A | 1.96 | 0.47 |
| 2:C:1104:POV:H32 | 2:C:1104:POV:H3 | 1.43 | 0.47 |
| 2:C:1107:POV:H11A | 1:D:652:ILE:HB | 1.96 | 0.47 |
| 2:C:1108:POV:H21A | 1:D:599:LEU:HB2 | 1.96 | 0.46 |
| 1:A:596:VAL:HG12 | 2:A:1103:POV:H212 | 1.96 | 0.46 |
| 2:A:1106:POV:H11A | 1:B:652:ILE:HB | 1.96 | 0.46 |
| 1:B:626:SER:HB3 | 2:B:1102:POV:H32A | 1.97 | 0.46 |
| 2:C:1102:POV:H34A | 2:C:1104:POV:H32A | 1.96 | 0.46 |
| 1:D:486:GLY:HA3 | 2:D:1101:POV:H33A | 1.98 | 0.46 |
| 1:C:351:MET:HB3 | 1:C:353:LYS:HZ3 | 1.79 | 0.46 |
| 1:C:599:LEU:HB3 | 2:C:1104:POV:H29 | 1.98 | 0.46 |
| 2:C:1103:POV:H2 | 2:C:1103:POV:H22A | 1.67 | 0.46 |
| 1:C:684:VAL:C | 1:C:686:LYS:H | 2.24 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:683:ASN:HA | 1:A:687:GLU:CG | 2.45 | 0.46 |
| 2:B:1106:POV:H11A | 1:C:652:ILE:HB | 1.97 | 0.46 |
| 1:A:361:LEU:HD22 | 1:A:422:LEU:HD23 | 1.98 | 0.46 |
| 2:A:1101:POV:H28 | 2:D:1101:POV:H211 | 1.98 | 0.46 |
| 1:B:226:ARG:HD2 | 1:B:274:GLN:HE21 | 1.81 | 0.46 |
| 1:D:651:PRO:HG2 | 2:D:1102:POV:H13B | 1.97 | 0.45 |
| 1:D:440:MET:HE3 | 2:D:1105:POV:H35A | 1.98 | 0.45 |
| 1:C:226:ARG:HD2 | 1:C:274:GLN:HE21 | 1.81 | 0.45 |
| 1:A:226:ARG:HD2 | 1:A:274:GLN:HE21 | 1.81 | 0.45 |
| 1:A:652:ILE:HB | 2:D:1107:POV:H11A | 1.98 | 0.45 |
| 2:B:1105:POV:H2 | 2:B:1105:POV:H22A | 1.48 | 0.45 |
| 1:A:499:VAL:HB | 2:A:1104:POV:H210 | 1.97 | 0.45 |
| 2:A:1107:POV:H29 | 1:B:599:LEU:HB3 | 1.99 | 0.45 |
| 1:B:361:LEU:HD22 | 1:B:422:LEU:HD23 | 1.98 | 0.45 |
| 1:B:683:ASN:HA | 1:B:687:GLU:HG3 | 1.98 | 0.45 |
| 1:C:499:VAL:HB | 2:C:1105:POV:H210 | 1.97 | 0.45 |
| 1:B:304:VAL:HG22 | 1:B:356:ILE:HG21 | 1.98 | 0.45 |
| 2:C:1109:POV:H211 | 2:D:1103:POV:H28 | 1.99 | 0.45 |
| 1:A:371:ARG:HH22 | 1:A:749:LEU:HD12 | 1.82 | 0.45 |
| 1:C:440:MET:HE3 | 2:C:1105:POV:H35A | 1.99 | 0.45 |
| 1:D:226:ARG:HD2 | 1:D:274:GLN:HE21 | 1.81 | 0.45 |
| 2:A:1108:POV:H211 | 2:B:1102:POV:H28 | 1.99 | 0.45 |
| 1:B:651:PRO:HG2 | 2:B:1101:POV:H13B | 1.97 | 0.45 |
| 2:C:1108:POV:H29 | 1:D:599:LEU:HB3 | 1.99 | 0.45 |
| 2:C:1108:POV:H32 | 2:C:1108:POV:H3 | 1.47 | 0.45 |
| 1:A:304:VAL:HG22 | 1:A:356:ILE:HG21 | 1.98 | 0.45 |
| 2:B:1107:POV:H211 | 2:C:1102:POV:H28 | 1.99 | 0.45 |
| 1:D:351:MET:HB3 | 1:D:353:LYS:HZ3 | 1.82 | 0.44 |
| 1:C:304:VAL:HG22 | 1:C:356:ILE:HG21 | 1.98 | 0.44 |
| 1:D:371:ARG:HH22 | 1:D:749:LEU:HD12 | 1.82 | 0.44 |
| 1:A:590:PHE:HE1 | 1:A:668:LEU:HB3 | 1.83 | 0.44 |
| 1:B:610:GLU:HG2 | 1:B:649:LYS:HZ1 | 1.82 | 0.44 |
| 1:D:499:VAL:HB | 2:D:1105:POV:H210 | 1.98 | 0.44 |
| 1:C:361:LEU:HD22 | 1:C:422:LEU:HD23 | 1.98 | 0.44 |
| 1:B:371:ARG:HH22 | 1:B:749:LEU:HD12 | 1.82 | 0.44 |
| 1:B:590:PHE:HE1 | 1:B:668:LEU:HB3 | 1.83 | 0.44 |
| 1:C:371:ARG:HH22 | 1:C:749:LEU:HD12 | 1.82 | 0.44 |
| 1:C:651:PRO:HG2 | 2:C:1101:POV:H13B | 1.99 | 0.44 |
| 1:D:361:LEU:HD22 | 1:D:422:LEU:HD23 | 1.98 | 0.44 |
| 2:A:1101:POV:H34A | 2:A:1103:POV:H32A | 2.00 | 0.44 |
| 1:D:304:VAL:HG22 | 1:D:356:ILE:HG21 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:590:PHE:HE1 | 1:D:668:LEU:HB3 | 1.83 | 0.44 |
| 2:D:1101:POV:H31C | 2:D:1101:POV:H39A | 1.73 | 0.44 |
| 1:A:440:MET:HE3 | 2:A:1104:POV:H35A | 1.99 | 0.44 |
| 1:B:276:GLU:HG2 | 1:B:277:ILE:HG13 | 2.00 | 0.44 |
| 1:B:499:VAL:HB | 2:B:1104:POV:H210 | 2.00 | 0.44 |
| 1:D:298:ASN:H | 1:D:301:HIS:HB2 | 1.83 | 0.44 |
| 2:A:1104:POV:H32A | 2:A:1104:POV:H3A | 1.61 | 0.43 |
| 2:A:1104:POV:H14B | 2:A:1104:POV:H11 | 1.82 | 0.43 |
| 1:C:276:GLU:HG2 | 1:C:277:ILE:HG13 | 2.00 | 0.43 |
| 1:C:298:ASN:H | 1:C:301:HIS:HB2 | 1.83 | 0.43 |
| 1:B:298:ASN:H | 1:B:301:HIS:HB2 | 1.83 | 0.43 |
| 1:C:516:ILE:HG12 | 1:C:521:TRP:HB2 | 2.01 | 0.43 |
| 1:C:684:VAL:O | 1:C:686:LYS:N | 2.51 | 0.43 |
| 2:A:1108:POV:H39A | 2:A:1108:POV:H31C | 1.80 | 0.43 |
| 1:D:392:LEU:HD11 | 1:D:732:LEU:HB2 | 2.01 | 0.43 |
| 2:D:1106:POV:H31F | 2:D:1107:POV:H212 | 2.00 | 0.43 |
| 1:A:276:GLU:HG2 | 1:A:277:ILE:HG13 | 2.00 | 0.43 |
| 1:A:589:LYS:HG3 | 2:A:1105:POV:H25A | 2.00 | 0.43 |
| 1:B:516:ILE:HG12 | 1:B:521:TRP:HB2 | 2.01 | 0.43 |
| 1:C:392:LEU:HD11 | 1:C:732:LEU:HB2 | 2.01 | 0.43 |
| 1:D:684:VAL:O | 1:D:686:LYS:HD2 | 2.18 | 0.43 |
| 1:A:298:ASN:H | 1:A:301:HIS:HB2 | 1.83 | 0.43 |
| 2:C:1105:POV:H32A | 2:C:1105:POV:H3A | 1.62 | 0.43 |
| 1:D:454:THR:HG23 | 2:D:1101:POV:H34 | 1.99 | 0.43 |
| 1:D:589:LYS:HG3 | 2:D:1106:POV:H25A | 2.00 | 0.43 |
| 1:A:392:LEU:HD11 | 1:A:732:LEU:HB2 | 2.01 | 0.43 |
| 2:B:1104:POV:H3A | 2:B:1104:POV:H32A | 1.63 | 0.43 |
| 1:C:590:PHE:HE1 | 1:C:668:LEU:HB3 | 1.83 | 0.43 |
| 1:A:585:HIS:HA | 2:A:1105:POV:H25 | 2.00 | 0.43 |
| 2:C:1106:POV:H31F | 2:C:1107:POV:H212 | 2.01 | 0.42 |
| 2:D:1105:POV:H14B | 2:D:1105:POV:H11 | 1.82 | 0.42 |
| 1:B:347:LEU:HD23 | 1:B:347:LEU:HA | 1.87 | 0.42 |
| 1:A:651:PRO:HG2 | 2:A:1109:POV:H13B | 2.00 | 0.42 |
| 1:B:392:LEU:HD11 | 1:B:732:LEU:HB2 | 2.01 | 0.42 |
| 1:D:417:HIS:HB3 | 1:D:690:ARG:HG3 | 2.01 | 0.42 |
| 1:C:417:HIS:HB3 | 1:C:690:ARG:HG3 | 2.01 | 0.42 |
| 1:D:276:GLU:HG2 | 1:D:277:ILE:HG13 | 2.00 | 0.42 |
| 2:A:1103:POV:H31F | 2:A:1105:POV:H21H | 2.01 | 0.42 |
| 1:A:417:HIS:HB3 | 1:A:690:ARG:HG3 | 2.01 | 0.42 |
| 2:C:1105:POV:H14B | 2:C:1105:POV:H11 | 1.82 | 0.42 |
| 1:A:650:TYR:HD1 | 2:D:1107:POV:H12A | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:347:LEU:HD23 | 1:D:347:LEU:HA | 1.91 | 0.42 |
| 1:A:442:PHE:HD1 | 2:A:1102:POV:H28A | 1.85 | 0.42 |
| 1:A:516:ILE:HG12 | 1:A:521:TRP:HB2 | 2.01 | 0.42 |
| 2:A:1105:POV:H22A | 2:A:1105:POV:H2 | 1.48 | 0.42 |
| 2:A:1106:POV:H14B | 2:A:1106:POV:H11 | 1.88 | 0.42 |
| 1:B:684:VAL:C | 1:B:686:LYS:H | 2.27 | 0.42 |
| 2:A:1105:POV:H21H | 2:A:1105:POV:H215 | 1.93 | 0.42 |
| 1:D:306:VAL:O | 1:D:313:GLN:NE2 | 2.53 | 0.42 |
| 1:D:516:ILE:HG12 | 1:D:521:TRP:HB2 | 2.01 | 0.42 |
| 1:D:683:ASN:HA | 1:D:687:GLU:HG3 | 2.02 | 0.42 |
| 2:D:1101:POV:H34A | 2:D:1101:POV:H37 | 1.81 | 0.41 |
| 1:B:417:HIS:HB3 | 1:B:690:ARG:HG3 | 2.01 | 0.41 |
| 1:B:651:PRO:HB2 | 2:B:1101:POV:H11A | 2.01 | 0.41 |
| 1:C:486:GLY:HA3 | 2:C:1109:POV:H33A | 2.00 | 0.41 |
| 1:C:589:LYS:HG3 | 2:C:1106:POV:H25A | 2.00 | 0.41 |
| 1:D:684:VAL:C | 1:D:686:LYS:N | 2.78 | 0.41 |
| 2:B:1103:POV:H2 | 2:B:1103:POV:H22A | 1.68 | 0.41 |
| 2:D:1105:POV:H32A | 2:D:1105:POV:H3A | 1.61 | 0.41 |
| 1:C:595:ILE:HD12 | 2:C:1102:POV:H31B | 2.01 | 0.41 |
| 2:C:1107:POV:H14B | 2:C:1107:POV:H11 | 1.89 | 0.41 |
| 1:A:306:VAL:O | 1:A:313:GLN:NE2 | 2.53 | 0.41 |
| 2:D:1106:POV:H21H | 2:D:1106:POV:H215 | 1.93 | 0.41 |
| 1:B:589:LYS:HG3 | 2:B:1105:POV:H25A | 2.02 | 0.41 |
| 1:B:683:ASN:HA | 1:B:687:GLU:CG | 2.50 | 0.41 |
| 1:C:306:VAL:O | 1:C:313:GLN:NE2 | 2.53 | 0.41 |
| 1:D:308:GLU:HB2 | 1:D:313:GLN:HG3 | 2.02 | 0.41 |
| 1:A:595:ILE:HD12 | 2:A:1101:POV:H31B | 2.02 | 0.41 |
| 2:C:1109:POV:H37 | 2:C:1109:POV:H34A | 1.92 | 0.41 |
| 1:A:492:ILE:HG23 | 2:A:1104:POV:H21G | 2.02 | 0.40 |
| 1:A:626:SER:HB3 | 2:A:1101:POV:H32A | 2.02 | 0.40 |
| 1:B:334:GLU:O | 1:B:343:THR:OG1 | 2.39 | 0.40 |
| 2:C:1109:POV:H31C | 2:C:1109:POV:H39A | 1.90 | 0.40 |
| 1:A:308:GLU:HB2 | 1:A:313:GLN:HG3 | 2.02 | 0.40 |
| 1:A:598:LEU:HD21 | 2:B:1101:POV:H28 | 2.03 | 0.40 |
| 1:B:306:VAL:O | 1:B:313:GLN:NE2 | 2.53 | 0.40 |
| 1:C:334:GLU:O | 1:C:343:THR:OG1 | 2.39 | 0.40 |
| 2:C:1106:POV:H2 | 2:C:1106:POV:H22A | 1.48 | 0.40 |
| 1:D:449:PHE:HZ | 2:D:1101:POV:H216 | 1.86 | 0.40 |
| 1:D:495:MET:HB3 | 2:D:1105:POV:H214 | 2.03 | 0.40 |
| 2:D:1106:POV:H22A | 2:D:1106:POV:H2 | 1.48 | 0.40 |
| 1:A:457:LEU:HB3 | 2:A:1108:POV:H3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:1103:POV:H32A | 2:A:1103:POV:H35A | 1.92 | 0.40 |
| 2:C:1108:POV:H32A | 2:C:1108:POV:H35A | 1.90 | 0.40 |
| 1:D:334:GLU:O | 1:D:343:THR:OG1 | 2.39 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 622/1052 (59%) | 580 (93%) | 41 (7%) | 1 (0%) | 43 | 75 |
| 1 | B | 622/1052 (59%) | 580 (93%) | 41 (7%) | 1 (0%) | 43 | 75 |
| 1 | C | 622/1052 (59%) | 580 (93%) | 41 (7%) | 1 (0%) | 43 | 75 |
| 1 | D | 622/1052 (59%) | 580 (93%) | 41 (7%) | 1 (0%) | 43 | 75 |
| All | All | 2488/4208 (59%) | 2320 (93%) | 164 (7%) | 4 (0%) | 44 | 75 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 684 | VAL |
| 1 | D | 684 | VAL |
| 1 | A | 684 | VAL |
| 1 | B | 684 | VAL |

### 5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 555/929 (60%) | 554 (100%) | 1 (0%) | 87 91 |
| 1 | B | 555/929 (60%) | 554 (100%) | 1 (0%) | 87 91 |
| 1 | C | 555/929 (60%) | 552 (100%) | 3 (0%) | 81 88 |
| 1 | D | 555/929 (60%) | 552 (100%) | 3 (0%) | 81 88 |
| All | All | 2220/3716 (60%) | 2212 (100%) | 8 (0%) | 81 89 |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 347 | LEU |
| 1 | B | 347 | LEU |
| 1 | C | 347 | LEU |
| 1 | C | 683 | ASN |
| 1 | C | 684 | VAL |
| 1 | D | 347 | LEU |
| 1 | D | 683 | ASN |
| 1 | D | 684 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 150 | HIS |
| 1 | A | 298 | ASN |
| 1 | A | 483 | GLN |
| 1 | A | 745 | HIS |
| 1 | B | 150 | HIS |
| 1 | B | 483 | GLN |
| 1 | B | 745 | HIS |
| 1 | C | 150 | HIS |
| 1 | C | 178 | ASN |
| 1 | C | 279 | GLN |
| 1 | C | 483 | GLN |
| 1 | C | 745 | HIS |
| 1 | D | 150 | HIS |
| 1 | D | 483 | GLN |
| 1 | D | 745 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 3 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | POV | C | 1106 | - | 51,51,51 | 0.32 | 0 | 57,59,59 | 0.40 | 0 |
| 2 | POV | C | 1103 | - | 51,51,51 | 0.33 | 0 | 57,59,59 | 0.45 | 0 |
| 2 | POV | B | 1104 | - | 51,51,51 | 0.31 | 0 | 57,59,59 | 0.43 | 0 |
| 2 | POV | C | 1104 | - | 51,51,51 | 0.32 | 0 | 57,59,59 | 0.45 | 0 |
| 2 | POV | C | 1109 | - | 51,51,51 | 0.31 | 0 | 57,59,59 | 0.37 | 0 |
| 2 | POV | A | 1105 | - | 51,51,51 | 0.33 | 0 | 57,59,59 | 0.39 | 0 |
| 2 | POV | A | 1103 | - | 51,51,51 | 0.32 | 0 | 57,59,59 | 0.47 | 0 |
| 2 | POV | B | 1107 | - | 51,51,51 | 0.31 | 0 | 57,59,59 | 0.38 | 0 |
| 2 | POV | D | 1101 | - | 51,51,51 | 0.31 | 0 | 57,59,59 | 0.37 | 0 |
| 2 | POV | D | 1104 | - | 51,51,51 | 0.34 | 0 | 57,59,59 | 0.45 | 0 |
| 2 | POV | A | 1104 | - | 51,51,51 | 0.31 | 0 | 57,59,59 | 0.41 | 0 |
| 2 | POV | B | 1101 | - | 51,51,51 | 0.30 | 0 | 57,59,59 | 0.41 | 0 |
| 2 | POV | D | 1102 | - | 51,51,51 | 0.29 | 0 | 57,59,59 | 0.40 | 0 |
| 2 | POV | A | 1102 | - | 51,51,51 | 0.34 | 0 | 57,59,59 | 0.46 | 0 |
| 2 | POV | A | 1109 | - | 51,51,51 | 0.30 | 0 | 57,59,59 | 0.40 | 0 |
| 2 | POV | C | 1105 | - | 51,51,51 | 0.32 | 0 | 57,59,59 | 0.42 | 0 |
| 2 | POV | D | 1107 | - | 51,51,51 | 0.34 | 0 | 57,59,59 | 0.56 | 1 (1%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | POV | B | 1105 | - | 51,51,51 | 0.32 | 0 | 57,59,59 | 0.39 | 0 |
| 2 | POV | A | 1107 | - | 51,51,51 | 0.32 | 0 | 57,59,59 | 0.44 | 0 |
| 2 | POV | A | 1106 | - | 51,51,51 | 0.33 | 0 | 57,59,59 | 0.56 | 1 (1%) |
| 2 | POV | B | 1103 | - | 51,51,51 | 0.33 | 0 | 57,59,59 | 0.44 | 0 |
| 2 | POV | D | 1105 | - | 51,51,51 | 0.32 | 0 | 57,59,59 | 0.41 | 0 |
| 2 | POV | C | 1107 | - | 51,51,51 | 0.34 | 0 | 57,59,59 | 0.56 | 1 (1%) |
| 2 | POV | C | 1108 | - | 51,51,51 | 0.32 | 0 | 57,59,59 | 0.45 | 0 |
| 2 | POV | D | 1106 | - | 51,51,51 | 0.33 | 0 | 57,59,59 | 0.40 | 0 |
| 2 | POV | B | 1102 | - | 51,51,51 | 0.28 | 0 | 57,59,59 | 0.27 | 0 |
| 2 | POV | C | 1101 | - | 51,51,51 | 0.29 | 0 | 57,59,59 | 0.40 | 0 |
| 2 | POV | D | 1103 | - | 51,51,51 | 0.28 | 0 | 57,59,59 | 0.28 | 0 |
| 2 | POV | A | 1108 | - | 51,51,51 | 0.31 | 0 | 57,59,59 | 0.37 | 0 |
| 2 | POV | A | 1101 | - | 51,51,51 | 0.28 | 0 | 57,59,59 | 0.28 | 0 |
| 2 | POV | C | 1102 | - | 51,51,51 | 0.28 | 0 | 57,59,59 | 0.27 | 0 |
| 2 | POV | B | 1106 | - | 51,51,51 | 0.33 | 0 | 57,59,59 | 0.56 | 1 (1%) |

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 | POV | C | 1106 | - | - | 11/55/55/55 | - |
| 2 | POV | C | 1103 | - | - | 21/55/55/55 | - |
| 2 | POV | B | 1104 | - | - | 20/55/55/55 | - |
| 2 | POV | C | 1104 | - | - | 14/55/55/55 | - |
| 2 | POV | C | 1109 | - | - | 19/55/55/55 | - |
| 2 | POV | A | 1105 | - | - | 12/55/55/55 | - |
| 2 | POV | A | 1103 | - | - | 17/55/55/55 | - |
| 2 | POV | B | 1107 | - | - | 21/55/55/55 | - |
| 2 | POV | D | 1101 | - | - | 19/55/55/55 | - |
| 2 | POV | D | 1104 | - | - | 23/55/55/55 | - |
| 2 | POV | A | 1104 | - | - | 20/55/55/55 | - |
| 2 | POV | B | 1101 | - | - | 15/55/55/55 | - |
| 2 | POV | D | 1102 | - | - | 14/55/55/55 | - |
| 2 | POV | A | 1102 | - | - | 23/55/55/55 | - |
| 2 | POV | A | 1109 | - | - | 14/55/55/55 | - |
| 2 | POV | C | 1105 | - | - | 20/55/55/55 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | POV | D | 1107 | - | - | 21/55/55/55 | - |
| 2 | POV | B | 1105 | - | - | 11/55/55/55 | - |
| 2 | POV | A | 1107 | - | - | 14/55/55/55 | - |
| 2 | POV | A | 1106 | - | - | 22/55/55/55 | - |
| 2 | POV | B | 1103 | - | - | 25/55/55/55 | - |
| 2 | POV | D | 1105 | - | - | 20/55/55/55 | - |
| 2 | POV | C | 1107 | - | - | 22/55/55/55 | - |
| 2 | POV | C | 1108 | - | - | 14/55/55/55 | - |
| 2 | POV | D | 1106 | - | - | 10/55/55/55 | - |
| 2 | POV | B | 1102 | - | - | 15/55/55/55 | - |
| 2 | POV | C | 1101 | - | - | 14/55/55/55 | - |
| 2 | POV | D | 1103 | - | - | 16/55/55/55 | - |
| 2 | POV | A | 1108 | - | - | 15/55/55/55 | - |
| 2 | POV | A | 1101 | - | - | 16/55/55/55 | - |
| 2 | POV | C | 1102 | - | - | 16/55/55/55 | - |
| 2 | POV | B | 1106 | - | - | 23/55/55/55 | - |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 1106 | POV | C2-O21-C21 | 2.65 | 124.14 | 117.80 |
| 2 | D | 1107 | POV | C2-O21-C21 | 2.65 | 124.14 | 117.80 |
| 2 | C | 1107 | POV | C2-O21-C21 | 2.63 | 124.08 | 117.80 |
| 2 | B | 1106 | POV | C2-O21-C21 | 2.63 | 124.08 | 117.80 |

There are no chirality outliers.

All (557) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 1101 | POV | C1-O11-P-O12 |
| 2 | A | 1101 | POV | C1-O11-P-O13 |
| 2 | A | 1101 | POV | C11-O12-P-O11 |
| 2 | A | 1102 | POV | C1-O11-P-O12 |
| 2 | A | 1102 | POV | C1-O11-P-O13 |
| 2 | A | 1102 | POV | C1-O11-P-O14 |
| 2 | A | 1102 | POV | C11-O12-P-O11 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 1102 | POV | C22-C21-O21-C2 |
| 2 | A | 1102 | POV | O22-C21-O21-C2 |
| 2 | A | 1102 | POV | C32-C31-O31-C3 |
| 2 | A | 1102 | POV | O32-C31-O31-C3 |
| 2 | A | 1103 | POV | C1-O11-P-O12 |
| 2 | A | 1103 | POV | C1-O11-P-O13 |
| 2 | A | 1103 | POV | C11-O12-P-O11 |
| 2 | A | 1103 | POV | C22-C21-O21-C2 |
| 2 | A | 1103 | POV | O22-C21-O21-C2 |
| 2 | A | 1103 | POV | C32-C31-O31-C3 |
| 2 | A | 1103 | POV | O32-C31-O31-C3 |
| 2 | A | 1104 | POV | C1-O11-P-O12 |
| 2 | A | 1104 | POV | C1-O11-P-O13 |
| 2 | A | 1104 | POV | C11-O12-P-O11 |
| 2 | A | 1104 | POV | O12-C11-C12-N |
| 2 | A | 1104 | POV | C32-C31-O31-C3 |
| 2 | A | 1104 | POV | O32-C31-O31-C3 |
| 2 | A | 1105 | POV | C22-C21-O21-C2 |
| 2 | A | 1105 | POV | O22-C21-O21-C2 |
| 2 | A | 1106 | POV | C1-O11-P-O12 |
| 2 | A | 1106 | POV | C1-O11-P-O14 |
| 2 | A | 1106 | POV | C11-O12-P-O13 |
| 2 | A | 1106 | POV | O12-C11-C12-N |
| 2 | A | 1106 | POV | C22-C21-O21-C2 |
| 2 | A | 1106 | POV | C32-C31-O31-C3 |
| 2 | A | 1106 | POV | O32-C31-O31-C3 |
| 2 | A | 1107 | POV | C1-O11-P-O12 |
| 2 | A | 1107 | POV | C1-O11-P-O13 |
| 2 | A | 1107 | POV | C11-O12-P-O11 |
| 2 | A | 1107 | POV | C22-C21-O21-C2 |
| 2 | A | 1107 | POV | O22-C21-O21-C2 |
| 2 | A | 1107 | POV | C32-C31-O31-C3 |
| 2 | A | 1107 | POV | O32-C31-O31-C3 |
| 2 | A | 1108 | POV | C1-O11-P-O12 |
| 2 | A | 1108 | POV | C32-C31-O31-C3 |
| 2 | A | 1108 | POV | O32-C31-O31-C3 |
| 2 | A | 1109 | POV | C11-O12-P-O11 |
| 2 | A | 1109 | POV | C22-C21-O21-C2 |
| 2 | A | 1109 | POV | O22-C21-O21-C2 |
| 2 | B | 1101 | POV | C11-O12-P-O11 |
| 2 | B | 1101 | POV | C22-C21-O21-C2 |
| 2 | B | 1101 | POV | O22-C21-O21-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | B | 1102 | POV | C1-O11-P-O12 |
| 2 | B | 1102 | POV | C1-O11-P-O13 |
| 2 | B | 1102 | POV | C11-O12-P-O11 |
| 2 | B | 1103 | POV | C1-O11-P-O12 |
| 2 | B | 1103 | POV | C1-O11-P-O14 |
| 2 | B | 1103 | POV | C22-C21-O21-C2 |
| 2 | B | 1103 | POV | O22-C21-O21-C2 |
| 2 | B | 1103 | POV | C32-C31-O31-C3 |
| 2 | B | 1103 | POV | O32-C31-O31-C3 |
| 2 | B | 1104 | POV | C1-O11-P-O12 |
| 2 | B | 1104 | POV | C1-O11-P-O13 |
| 2 | B | 1104 | POV | C11-O12-P-O11 |
| 2 | B | 1104 | POV | O12-C11-C12-N |
| 2 | B | 1104 | POV | C32-C31-O31-C3 |
| 2 | B | 1104 | POV | O32-C31-O31-C3 |
| 2 | B | 1105 | POV | C22-C21-O21-C2 |
| 2 | B | 1105 | POV | O22-C21-O21-C2 |
| 2 | B | 1106 | POV | C1-O11-P-O12 |
| 2 | B | 1106 | POV | C1-O11-P-O14 |
| 2 | B | 1106 | POV | C11-O12-P-O13 |
| 2 | B | 1106 | POV | O12-C11-C12-N |
| 2 | B | 1106 | POV | C22-C21-O21-C2 |
| 2 | B | 1106 | POV | C32-C31-O31-C3 |
| 2 | B | 1106 | POV | O32-C31-O31-C3 |
| 2 | B | 1107 | POV | C1-O11-P-O12 |
| 2 | B | 1107 | POV | C32-C31-O31-C3 |
| 2 | B | 1107 | POV | O32-C31-O31-C3 |
| 2 | C | 1101 | POV | C11-O12-P-O11 |
| 2 | C | 1101 | POV | C22-C21-O21-C2 |
| 2 | C | 1101 | POV | O22-C21-O21-C2 |
| 2 | C | 1102 | POV | C1-O11-P-O12 |
| 2 | C | 1102 | POV | C1-O11-P-O13 |
| 2 | C | 1102 | POV | C11-O12-P-O11 |
| 2 | C | 1103 | POV | C1-O11-P-O12 |
| 2 | C | 1103 | POV | C1-O11-P-O14 |
| 2 | C | 1103 | POV | C22-C21-O21-C2 |
| 2 | C | 1103 | POV | O22-C21-O21-C2 |
| 2 | C | 1103 | POV | C32-C31-O31-C3 |
| 2 | C | 1103 | POV | O32-C31-O31-C3 |
| 2 | C | 1104 | POV | C1-O11-P-O12 |
| 2 | C | 1104 | POV | C1-O11-P-O13 |
| 2 | C | 1104 | POV | C11-O12-P-O11 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | C | 1104 | POV | C22-C21-O21-C2 |
| 2 | C | 1104 | POV | O22-C21-O21-C2 |
| 2 | C | 1104 | POV | C32-C31-O31-C3 |
| 2 | C | 1104 | POV | O32-C31-O31-C3 |
| 2 | C | 1105 | POV | C1-O11-P-O12 |
| 2 | C | 1105 | POV | C1-O11-P-O13 |
| 2 | C | 1105 | POV | C11-O12-P-O11 |
| 2 | C | 1105 | POV | O12-C11-C12-N |
| 2 | C | 1105 | POV | C32-C31-O31-C3 |
| 2 | C | 1105 | POV | O32-C31-O31-C3 |
| 2 | C | 1106 | POV | C22-C21-O21-C2 |
| 2 | C | 1106 | POV | O22-C21-O21-C2 |
| 2 | C | 1107 | POV | C1-O11-P-O12 |
| 2 | C | 1107 | POV | C1-O11-P-O14 |
| 2 | C | 1107 | POV | C11-O12-P-O13 |
| 2 | C | 1107 | POV | O12-C11-C12-N |
| 2 | C | 1107 | POV | C22-C21-O21-C2 |
| 2 | C | 1107 | POV | C32-C31-O31-C3 |
| 2 | C | 1107 | POV | O32-C31-O31-C3 |
| 2 | C | 1108 | POV | C1-O11-P-O12 |
| 2 | C | 1108 | POV | C1-O11-P-O13 |
| 2 | C | 1108 | POV | C11-O12-P-O11 |
| 2 | C | 1108 | POV | C22-C21-O21-C2 |
| 2 | C | 1108 | POV | O22-C21-O21-C2 |
| 2 | C | 1108 | POV | C32-C31-O31-C3 |
| 2 | C | 1108 | POV | O32-C31-O31-C3 |
| 2 | C | 1109 | POV | C1-O11-P-O12 |
| 2 | C | 1109 | POV | C32-C31-O31-C3 |
| 2 | C | 1109 | POV | O32-C31-O31-C3 |
| 2 | D | 1101 | POV | C1-O11-P-O12 |
| 2 | D | 1101 | POV | C32-C31-O31-C3 |
| 2 | D | 1101 | POV | O32-C31-O31-C3 |
| 2 | D | 1102 | POV | C11-O12-P-O11 |
| 2 | D | 1102 | POV | C22-C21-O21-C2 |
| 2 | D | 1102 | POV | O22-C21-O21-C2 |
| 2 | D | 1103 | POV | C1-O11-P-O12 |
| 2 | D | 1103 | POV | C1-O11-P-O13 |
| 2 | D | 1103 | POV | C11-O12-P-O11 |
| 2 | D | 1104 | POV | C1-O11-P-O12 |
| 2 | D | 1104 | POV | C1-O11-P-O13 |
| 2 | D | 1104 | POV | C1-O11-P-O14 |
| 2 | D | 1104 | POV | C11-O12-P-O11 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | D | 1104 | POV | C22-C21-O21-C2 |
| 2 | D | 1104 | POV | O22-C21-O21-C2 |
| 2 | D | 1104 | POV | C32-C31-O31-C3 |
| 2 | D | 1104 | POV | O32-C31-O31-C3 |
| 2 | D | 1105 | POV | C1-O11-P-O12 |
| 2 | D | 1105 | POV | C1-O11-P-O13 |
| 2 | D | 1105 | POV | C11-O12-P-O11 |
| 2 | D | 1105 | POV | O12-C11-C12-N |
| 2 | D | 1105 | POV | C32-C31-O31-C3 |
| 2 | D | 1105 | POV | O32-C31-O31-C3 |
| 2 | D | 1106 | POV | C22-C21-O21-C2 |
| 2 | D | 1106 | POV | O22-C21-O21-C2 |
| 2 | D | 1107 | POV | C1-O11-P-O12 |
| 2 | D | 1107 | POV | C1-O11-P-O14 |
| 2 | D | 1107 | POV | C11-O12-P-O11 |
| 2 | D | 1107 | POV | C11-O12-P-O13 |
| 2 | D | 1107 | POV | O12-C11-C12-N |
| 2 | D | 1107 | POV | C22-C21-O21-C2 |
| 2 | D | 1107 | POV | C32-C31-O31-C3 |
| 2 | D | 1107 | POV | O32-C31-O31-C3 |
| 2 | A | 1106 | POV | O22-C21-O21-C2 |
| 2 | B | 1106 | POV | O22-C21-O21-C2 |
| 2 | C | 1107 | POV | O22-C21-O21-C2 |
| 2 | D | 1107 | POV | O22-C21-O21-C2 |
| 2 | B | 1106 | POV | C11-C12-N-C14 |
| 2 | A | 1104 | POV | C11-C12-N-C14 |
| 2 | A | 1106 | POV | C11-C12-N-C14 |
| 2 | B | 1104 | POV | C11-C12-N-C14 |
| 2 | B | 1106 | POV | C11-C12-N-C15 |
| 2 | C | 1105 | POV | C11-C12-N-C14 |
| 2 | C | 1107 | POV | C11-C12-N-C14 |
| 2 | D | 1105 | POV | C11-C12-N-C14 |
| 2 | D | 1107 | POV | C11-C12-N-C14 |
| 2 | C | 1104 | POV | C31-C32-C33-C34 |
| 2 | A | 1106 | POV | C11-C12-N-C15 |
| 2 | B | 1104 | POV | C11-C12-N-C13 |
| 2 | A | 1107 | POV | C31-C32-C33-C34 |
| 2 | C | 1108 | POV | C31-C32-C33-C34 |
| 2 | A | 1104 | POV | C11-C12-N-C13 |
| 2 | C | 1105 | POV | C11-C12-N-C13 |
| 2 | D | 1105 | POV | C11-C12-N-C13 |
| 2 | D | 1107 | POV | C11-C12-N-C13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | D | 1107 | POV | C11-C12-N-C15 |
| 2 | C | 1107 | POV | C11-C12-N-C15 |
| 2 | A | 1103 | POV | C31-C32-C33-C34 |
| 2 | A | 1108 | POV | C25-C26-C27-C28 |
| 2 | B | 1105 | POV | C214-C215-C216-C217 |
| 2 | C | 1104 | POV | C311-C312-C313-C314 |
| 2 | C | 1106 | POV | C214-C215-C216-C217 |
| 2 | D | 1106 | POV | C214-C215-C216-C217 |
| 2 | A | 1105 | POV | C214-C215-C216-C217 |
| 2 | A | 1107 | POV | C311-C312-C313-C314 |
| 2 | B | 1103 | POV | C213-C214-C215-C216 |
| 2 | C | 1108 | POV | C311-C312-C313-C314 |
| 2 | B | 1107 | POV | C25-C26-C27-C28 |
| 2 | D | 1101 | POV | C25-C26-C27-C28 |
| 2 | C | 1109 | POV | C25-C26-C27-C28 |
| 2 | A | 1103 | POV | C311-C312-C313-C314 |
| 2 | C | 1105 | POV | C211-C212-C213-C214 |
| 2 | D | 1103 | POV | C22-C23-C24-C25 |
| 2 | A | 1104 | POV | C211-C212-C213-C214 |
| 2 | A | 1106 | POV | C11-C12-N-C13 |
| 2 | B | 1104 | POV | C11-C12-N-C15 |
| 2 | B | 1106 | POV | C11-C12-N-C13 |
| 2 | C | 1107 | POV | C11-C12-N-C13 |
| 2 | B | 1105 | POV | C310-C311-C312-C313 |
| 2 | C | 1106 | POV | C310-C311-C312-C313 |
| 2 | D | 1105 | POV | C211-C212-C213-C214 |
| 2 | A | 1101 | POV | C22-C23-C24-C25 |
| 2 | B | 1102 | POV | C22-C23-C24-C25 |
| 2 | C | 1102 | POV | C22-C23-C24-C25 |
| 2 | D | 1106 | POV | C310-C311-C312-C313 |
| 2 | C | 1109 | POV | C35-C36-C37-C38 |
| 2 | B | 1104 | POV | C211-C212-C213-C214 |
| 2 | D | 1102 | POV | C25-C26-C27-C28 |
| 2 | A | 1102 | POV | C22-C23-C24-C25 |
| 2 | B | 1107 | POV | C35-C36-C37-C38 |
| 2 | A | 1109 | POV | C25-C26-C27-C28 |
| 2 | C | 1102 | POV | C33-C34-C35-C36 |
| 2 | C | 1101 | POV | C25-C26-C27-C28 |
| 2 | C | 1102 | POV | C35-C36-C37-C38 |
| 2 | B | 1104 | POV | C22-C23-C24-C25 |
| 2 | B | 1102 | POV | C33-C34-C35-C36 |
| 2 | A | 1104 | POV | C11-C12-N-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | C | 1105 | POV | C11-C12-N-C15 |
| 2 | D | 1105 | POV | C11-C12-N-C15 |
| 2 | C | 1105 | POV | C22-C23-C24-C25 |
| 2 | D | 1105 | POV | C22-C23-C24-C25 |
| 2 | A | 1103 | POV | O11-C1-C2-O21 |
| 2 | A | 1105 | POV | C310-C311-C312-C313 |
| 2 | A | 1104 | POV | C22-C23-C24-C25 |
| 2 | D | 1104 | POV | C22-C23-C24-C25 |
| 2 | C | 1105 | POV | C26-C27-C28-C29 |
| 2 | B | 1102 | POV | C35-C36-C37-C38 |
| 2 | C | 1109 | POV | C311-C310-C39-C38 |
| 2 | B | 1107 | POV | C311-C310-C39-C38 |
| 2 | D | 1103 | POV | C33-C34-C35-C36 |
| 2 | A | 1104 | POV | C26-C27-C28-C29 |
| 2 | B | 1104 | POV | C26-C27-C28-C29 |
| 2 | D | 1105 | POV | C26-C27-C28-C29 |
| 2 | B | 1107 | POV | O11-C1-C2-C3 |
| 2 | D | 1101 | POV | O11-C1-C2-C3 |
| 2 | C | 1103 | POV | C22-C23-C24-C25 |
| 2 | D | 1103 | POV | C31-C32-C33-C34 |
| 2 | C | 1101 | POV | C24-C25-C26-C27 |
| 2 | A | 1109 | POV | C24-C25-C26-C27 |
| 2 | D | 1102 | POV | C24-C25-C26-C27 |
| 2 | C | 1105 | POV | C34-C35-C36-C37 |
| 2 | A | 1101 | POV | C1-C2-C3-O31 |
| 2 | B | 1102 | POV | C1-C2-C3-O31 |
| 2 | B | 1106 | POV | C1-C2-C3-O31 |
| 2 | C | 1102 | POV | C1-C2-C3-O31 |
| 2 | C | 1107 | POV | C1-C2-C3-O31 |
| 2 | D | 1104 | POV | C1-C2-C3-O31 |
| 2 | A | 1103 | POV | C26-C27-C28-C29 |
| 2 | C | 1102 | POV | C210-C211-C212-C213 |
| 2 | D | 1103 | POV | C210-C211-C212-C213 |
| 2 | B | 1104 | POV | C34-C35-C36-C37 |
| 2 | D | 1105 | POV | C34-C35-C36-C37 |
| 2 | A | 1104 | POV | C34-C35-C36-C37 |
| 2 | B | 1103 | POV | C22-C23-C24-C25 |
| 2 | A | 1101 | POV | C31-C32-C33-C34 |
| 2 | A | 1101 | POV | C210-C211-C212-C213 |
| 2 | B | 1102 | POV | C210-C211-C212-C213 |
| 2 | A | 1103 | POV | C27-C28-C29-C210 |
| 2 | C | 1103 | POV | O21-C2-C3-O31 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | D | 1103 | POV | C35-C36-C37-C38 |
| 2 | B | 1102 | POV | C31-C32-C33-C34 |
| 2 | A | 1106 | POV | C2-C1-O11-P |
| 2 | B | 1106 | POV | C2-C1-O11-P |
| 2 | B | 1107 | POV | C2-C1-O11-P |
| 2 | C | 1107 | POV | C2-C1-O11-P |
| 2 | C | 1109 | POV | C2-C1-O11-P |
| 2 | D | 1101 | POV | C2-C1-O11-P |
| 2 | D | 1107 | POV | C2-C1-O11-P |
| 2 | D | 1107 | POV | C35-C36-C37-C38 |
| 2 | A | 1108 | POV | O11-C1-C2-C3 |
| 2 | C | 1109 | POV | O11-C1-C2-C3 |
| 2 | B | 1103 | POV | C24-C25-C26-C27 |
| 2 | C | 1103 | POV | C24-C25-C26-C27 |
| 2 | A | 1106 | POV | C35-C36-C37-C38 |
| 2 | D | 1104 | POV | C24-C25-C26-C27 |
| 2 | A | 1105 | POV | C1-C2-C3-O31 |
| 2 | B | 1105 | POV | C1-C2-C3-O31 |
| 2 | D | 1106 | POV | C1-C2-C3-O31 |
| 2 | D | 1107 | POV | C1-C2-C3-O31 |
| 2 | C | 1107 | POV | C35-C36-C37-C38 |
| 2 | A | 1105 | POV | C39-C310-C311-C312 |
| 2 | C | 1102 | POV | C31-C32-C33-C34 |
| 2 | C | 1109 | POV | O11-C1-C2-O21 |
| 2 | A | 1102 | POV | C2-C1-O11-P |
| 2 | A | 1108 | POV | C2-C1-O11-P |
| 2 | D | 1104 | POV | C2-C1-O11-P |
| 2 | A | 1104 | POV | C23-C24-C25-C26 |
| 2 | B | 1106 | POV | C35-C36-C37-C38 |
| 2 | A | 1101 | POV | O21-C2-C3-O31 |
| 2 | A | 1105 | POV | O21-C2-C3-O31 |
| 2 | B | 1102 | POV | O21-C2-C3-O31 |
| 2 | D | 1103 | POV | O21-C2-C3-O31 |
| 2 | D | 1104 | POV | O21-C2-C3-O31 |
| 2 | A | 1102 | POV | C24-C25-C26-C27 |
| 2 | A | 1108 | POV | C11-C12-N-C14 |
| 2 | B | 1107 | POV | C11-C12-N-C14 |
| 2 | C | 1109 | POV | C11-C12-N-C14 |
| 2 | D | 1101 | POV | C11-C12-N-C14 |
| 2 | D | 1105 | POV | C23-C24-C25-C26 |
| 2 | A | 1101 | POV | C33-C34-C35-C36 |
| 2 | B | 1103 | POV | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | D | 1104 | POV | C210-C211-C212-C213 |
| 2 | A | 1104 | POV | C21-C22-C23-C24 |
| 2 | C | 1105 | POV | C23-C24-C25-C26 |
| 2 | B | 1106 | POV | C312-C313-C314-C315 |
| 2 | B | 1106 | POV | C1-C2-O21-C21 |
| 2 | A | 1102 | POV | C210-C211-C212-C213 |
| 2 | D | 1105 | POV | C21-C22-C23-C24 |
| 2 | A | 1108 | POV | O11-C1-C2-O21 |
| 2 | C | 1108 | POV | O11-C1-C2-O21 |
| 2 | A | 1106 | POV | C1-C2-C3-O31 |
| 2 | A | 1109 | POV | C1-C2-C3-O31 |
| 2 | B | 1101 | POV | C1-C2-C3-O31 |
| 2 | C | 1101 | POV | C1-C2-C3-O31 |
| 2 | C | 1106 | POV | C1-C2-C3-O31 |
| 2 | D | 1102 | POV | C1-C2-C3-O31 |
| 2 | D | 1103 | POV | C1-C2-C3-O31 |
| 2 | A | 1109 | POV | C39-C310-C311-C312 |
| 2 | A | 1101 | POV | C12-C11-O12-P |
| 2 | B | 1102 | POV | C12-C11-O12-P |
| 2 | C | 1102 | POV | C12-C11-O12-P |
| 2 | D | 1103 | POV | C12-C11-O12-P |
| 2 | C | 1101 | POV | C39-C310-C311-C312 |
| 2 | A | 1109 | POV | O21-C2-C3-O31 |
| 2 | B | 1101 | POV | O21-C2-C3-O31 |
| 2 | B | 1101 | POV | C26-C27-C28-C29 |
| 2 | C | 1101 | POV | O21-C2-C3-O31 |
| 2 | C | 1102 | POV | O21-C2-C3-O31 |
| 2 | C | 1103 | POV | C210-C211-C212-C213 |
| 2 | C | 1106 | POV | O21-C2-C3-O31 |
| 2 | D | 1102 | POV | O21-C2-C3-O31 |
| 2 | A | 1108 | POV | C11-C12-N-C13 |
| 2 | B | 1107 | POV | C11-C12-N-C13 |
| 2 | C | 1109 | POV | C11-C12-N-C13 |
| 2 | D | 1101 | POV | C11-C12-N-C13 |
| 2 | A | 1103 | POV | C2-C1-O11-P |
| 2 | D | 1102 | POV | C39-C310-C311-C312 |
| 2 | A | 1101 | POV | O12-C11-C12-N |
| 2 | A | 1102 | POV | O12-C11-C12-N |
| 2 | A | 1109 | POV | O12-C11-C12-N |
| 2 | B | 1101 | POV | O12-C11-C12-N |
| 2 | B | 1102 | POV | O12-C11-C12-N |
| 2 | B | 1103 | POV | O12-C11-C12-N |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | C | 1101 | POV | O12-C11-C12-N |
| 2 | C | 1102 | POV | O12-C11-C12-N |
| 2 | C | 1103 | POV | O12-C11-C12-N |
| 2 | D | 1102 | POV | O12-C11-C12-N |
| 2 | D | 1103 | POV | O12-C11-C12-N |
| 2 | D | 1104 | POV | O12-C11-C12-N |
| 2 | B | 1104 | POV | C23-C24-C25-C26 |
| 2 | A | 1103 | POV | O11-C1-C2-C3 |
| 2 | B | 1101 | POV | C312-C313-C314-C315 |
| 2 | C | 1108 | POV | C2-C1-O11-P |
| 2 | B | 1107 | POV | O11-C1-C2-O21 |
| 2 | D | 1101 | POV | O11-C1-C2-O21 |
| 2 | B | 1103 | POV | C214-C215-C216-C217 |
| 2 | A | 1102 | POV | O21-C2-C3-O31 |
| 2 | A | 1106 | POV | O21-C2-C3-O31 |
| 2 | B | 1103 | POV | O21-C2-C3-O31 |
| 2 | B | 1105 | POV | O21-C2-C3-O31 |
| 2 | B | 1106 | POV | O21-C2-C3-O31 |
| 2 | C | 1107 | POV | O21-C2-C3-O31 |
| 2 | D | 1106 | POV | O21-C2-C3-O31 |
| 2 | C | 1105 | POV | C21-C22-C23-C24 |
| 2 | A | 1102 | POV | C1-C2-C3-O31 |
| 2 | B | 1103 | POV | C1-C2-C3-O31 |
| 2 | C | 1103 | POV | C1-C2-C3-O31 |
| 2 | D | 1101 | POV | C34-C35-C36-C37 |
| 2 | D | 1101 | POV | C36-C37-C38-C39 |
| 2 | C | 1109 | POV | C31-C32-C33-C34 |
| 2 | A | 1101 | POV | C1-O11-P-O14 |
| 2 | A | 1101 | POV | C11-O12-P-O14 |
| 2 | A | 1102 | POV | C11-O12-P-O14 |
| 2 | A | 1103 | POV | C11-O12-P-O14 |
| 2 | A | 1104 | POV | C1-O11-P-O14 |
| 2 | A | 1104 | POV | C11-O12-P-O14 |
| 2 | A | 1106 | POV | C11-O12-P-O11 |
| 2 | A | 1107 | POV | C11-O12-P-O14 |
| 2 | A | 1108 | POV | C11-C12-N-C15 |
| 2 | A | 1108 | POV | C1-O11-P-O14 |
| 2 | A | 1109 | POV | C11-O12-P-O14 |
| 2 | B | 1101 | POV | C11-O12-P-O14 |
| 2 | B | 1102 | POV | C1-O11-P-O14 |
| 2 | B | 1102 | POV | C11-O12-P-O14 |
| 2 | B | 1103 | POV | C1-O11-P-O13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | B | 1104 | POV | C1-O11-P-O14 |
| 2 | B | 1104 | POV | C11-O12-P-O14 |
| 2 | B | 1106 | POV | C1-O11-P-O13 |
| 2 | B | 1106 | POV | C11-O12-P-O11 |
| 2 | B | 1107 | POV | C11-C12-N-C15 |
| 2 | B | 1107 | POV | C1-O11-P-O14 |
| 2 | C | 1101 | POV | C11-O12-P-O14 |
| 2 | C | 1102 | POV | C1-O11-P-O14 |
| 2 | C | 1102 | POV | C11-O12-P-O14 |
| 2 | C | 1103 | POV | C1-O11-P-O13 |
| 2 | C | 1104 | POV | C11-O12-P-O14 |
| 2 | C | 1105 | POV | C1-O11-P-O14 |
| 2 | C | 1105 | POV | C11-O12-P-O14 |
| 2 | C | 1107 | POV | C1-O11-P-O13 |
| 2 | C | 1107 | POV | C11-O12-P-O11 |
| 2 | C | 1107 | POV | C11-O12-P-O14 |
| 2 | C | 1108 | POV | C11-O12-P-O14 |
| 2 | C | 1109 | POV | C11-C12-N-C15 |
| 2 | C | 1109 | POV | C1-O11-P-O14 |
| 2 | D | 1101 | POV | C11-C12-N-C15 |
| 2 | D | 1101 | POV | C1-O11-P-O14 |
| 2 | D | 1102 | POV | C11-O12-P-O14 |
| 2 | D | 1103 | POV | C1-O11-P-O14 |
| 2 | D | 1103 | POV | C11-O12-P-O14 |
| 2 | D | 1104 | POV | C11-O12-P-O14 |
| 2 | D | 1105 | POV | C1-O11-P-O14 |
| 2 | D | 1105 | POV | C11-O12-P-O14 |
| 2 | D | 1107 | POV | C11-O12-P-O14 |
| 2 | B | 1103 | POV | C2-C1-O11-P |
| 2 | C | 1103 | POV | C2-C1-O11-P |
| 2 | C | 1104 | POV | C2-C1-O11-P |
| 2 | B | 1101 | POV | C39-C310-C311-C312 |
| 2 | B | 1101 | POV | C27-C28-C29-C210 |
| 2 | B | 1101 | POV | C24-C25-C26-C27 |
| 2 | A | 1106 | POV | C1-C2-O21-C21 |
| 2 | C | 1107 | POV | C1-C2-O21-C21 |
| 2 | D | 1107 | POV | C1-C2-O21-C21 |
| 2 | A | 1104 | POV | C24-C25-C26-C27 |
| 2 | B | 1107 | POV | C36-C37-C38-C39 |
| 2 | A | 1107 | POV | O11-C1-C2-O21 |
| 2 | D | 1105 | POV | C24-C25-C26-C27 |
| 2 | C | 1105 | POV | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | B | 1107 | POV | C31-C32-C33-C34 |
| 2 | A | 1107 | POV | C2-C1-O11-P |
| 2 | D | 1107 | POV | O21-C2-C3-O31 |
| 2 | A | 1101 | POV | C35-C36-C37-C38 |
| 2 | B | 1107 | POV | C34-C35-C36-C37 |
| 2 | A | 1109 | POV | C312-C313-C314-C315 |
| 2 | B | 1104 | POV | C24-C25-C26-C27 |
| 2 | B | 1104 | POV | C21-C22-C23-C24 |
| 2 | B | 1103 | POV | C210-C211-C212-C213 |
| 2 | C | 1104 | POV | O11-C1-C2-O21 |
| 2 | A | 1103 | POV | C29-C210-C211-C212 |
| 2 | B | 1103 | POV | C32-C33-C34-C35 |
| 2 | A | 1108 | POV | C36-C37-C38-C39 |
| 2 | A | 1101 | POV | C211-C212-C213-C214 |
| 2 | D | 1104 | POV | C32-C33-C34-C35 |
| 2 | C | 1101 | POV | C312-C313-C314-C315 |
| 2 | D | 1102 | POV | C312-C313-C314-C315 |
| 2 | C | 1109 | POV | C36-C37-C38-C39 |
| 2 | B | 1103 | POV | C29-C210-C211-C212 |
| 2 | C | 1109 | POV | C34-C35-C36-C37 |
| 2 | A | 1102 | POV | C32-C33-C34-C35 |
| 2 | D | 1103 | POV | C211-C212-C213-C214 |
| 2 | C | 1102 | POV | C211-C212-C213-C214 |
| 2 | A | 1105 | POV | C27-C28-C29-C210 |
| 2 | D | 1104 | POV | C27-C28-C29-C210 |
| 2 | B | 1102 | POV | C211-C212-C213-C214 |
| 2 | B | 1105 | POV | C27-C28-C29-C210 |
| 2 | C | 1103 | POV | C32-C33-C34-C35 |
| 2 | C | 1108 | POV | O11-C1-C2-C3 |
| 2 | D | 1101 | POV | C39-C310-C311-C312 |
| 2 | C | 1103 | POV | C27-C28-C29-C210 |
| 2 | C | 1106 | POV | C27-C28-C29-C210 |
| 2 | B | 1104 | POV | C25-C26-C27-C28 |
| 2 | C | 1105 | POV | C25-C26-C27-C28 |
| 2 | B | 1103 | POV | C27-C28-C29-C210 |
| 2 | D | 1106 | POV | C27-C28-C29-C210 |
| 2 | C | 1106 | POV | C35-C36-C37-C38 |
| 2 | B | 1101 | POV | C310-C311-C312-C313 |
| 2 | C | 1101 | POV | C310-C311-C312-C313 |
| 2 | A | 1104 | POV | C25-C26-C27-C28 |
| 2 | A | 1109 | POV | C310-C311-C312-C313 |
| 2 | D | 1105 | POV | C25-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | C | 1106 | POV | C215-C216-C217-C218 |
| 2 | D | 1102 | POV | C310-C311-C312-C313 |
| 2 | A | 1105 | POV | C215-C216-C217-C218 |
| 2 | D | 1106 | POV | C215-C216-C217-C218 |
| 2 | B | 1105 | POV | C215-C216-C217-C218 |
| 2 | A | 1102 | POV | C27-C28-C29-C210 |
| 2 | B | 1107 | POV | C27-C28-C29-C210 |
| 2 | A | 1107 | POV | C32-C33-C34-C35 |
| 2 | C | 1104 | POV | C32-C33-C34-C35 |
| 2 | C | 1109 | POV | C27-C28-C29-C210 |
| 2 | D | 1101 | POV | C27-C28-C29-C210 |
| 2 | D | 1104 | POV | C29-C210-C211-C212 |
| 2 | A | 1108 | POV | C27-C28-C29-C210 |
| 2 | C | 1103 | POV | C29-C210-C211-C212 |
| 2 | D | 1104 | POV | C21-C22-C23-C24 |
| 2 | A | 1109 | POV | C2-C1-O11-P |
| 2 | C | 1101 | POV | C2-C1-O11-P |
| 2 | D | 1102 | POV | C2-C1-O11-P |
| 2 | B | 1103 | POV | C26-C27-C28-C29 |
| 2 | C | 1106 | POV | C31-C32-C33-C34 |
| 2 | A | 1106 | POV | C27-C28-C29-C210 |
| 2 | B | 1107 | POV | C24-C25-C26-C27 |
| 2 | D | 1101 | POV | C32-C33-C34-C35 |
| 2 | A | 1102 | POV | C29-C210-C211-C212 |
| 2 | C | 1107 | POV | C27-C28-C29-C210 |
| 2 | D | 1107 | POV | C27-C28-C29-C210 |
| 2 | A | 1102 | POV | O21-C21-C22-C23 |
| 2 | A | 1107 | POV | O11-C1-C2-C3 |
| 2 | C | 1104 | POV | O11-C1-C2-C3 |
| 2 | D | 1104 | POV | O21-C21-C22-C23 |
| 2 | B | 1106 | POV | C211-C212-C213-C214 |
| 2 | B | 1101 | POV | C2-C1-O11-P |
| 2 | B | 1103 | POV | C311-C312-C313-C314 |
| 2 | B | 1103 | POV | O21-C21-C22-C23 |
| 2 | C | 1103 | POV | O21-C21-C22-C23 |
| 2 | C | 1108 | POV | C32-C33-C34-C35 |
| 2 | B | 1106 | POV | C27-C28-C29-C210 |
| 2 | B | 1103 | POV | C21-C22-C23-C24 |
| 2 | A | 1104 | POV | C312-C313-C314-C315 |
| 2 | C | 1107 | POV | C211-C212-C213-C214 |
| 2 | C | 1103 | POV | C21-C22-C23-C24 |
| 2 | C | 1105 | POV | C312-C313-C314-C315 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 1102 | POV | C21-C22-C23-C24 |
| 2 | D | 1101 | POV | C24-C25-C26-C27 |
| 2 | A | 1106 | POV | C312-C313-C314-C315 |
| 2 | A | 1102 | POV | C214-C215-C216-C217 |
| 2 | A | 1105 | POV | O31-C31-C32-C33 |
| 2 | C | 1103 | POV | C214-C215-C216-C217 |
| 2 | D | 1105 | POV | C312-C313-C314-C315 |
| 2 | B | 1101 | POV | C311-C312-C313-C314 |
| 2 | B | 1107 | POV | C39-C310-C311-C312 |
| 2 | D | 1107 | POV | C211-C212-C213-C214 |
| 2 | C | 1109 | POV | C39-C310-C311-C312 |
| 2 | A | 1108 | POV | O21-C21-C22-C23 |
| 2 | D | 1106 | POV | O31-C31-C32-C33 |
| 2 | A | 1105 | POV | C24-C25-C26-C27 |
| 2 | D | 1104 | POV | C214-C215-C216-C217 |
| 2 | C | 1101 | POV | C311-C312-C313-C314 |
| 2 | B | 1103 | POV | O22-C21-C22-C23 |
| 2 | A | 1108 | POV | O31-C31-C32-C33 |
| 2 | B | 1104 | POV | C312-C313-C314-C315 |
| 2 | C | 1106 | POV | C24-C25-C26-C27 |
| 2 | A | 1101 | POV | C313-C314-C315-C316 |
| 2 | A | 1103 | POV | C25-C26-C27-C28 |
| 2 | D | 1102 | POV | C311-C312-C313-C314 |
| 2 | A | 1106 | POV | C211-C212-C213-C214 |
| 2 | B | 1106 | POV | C22-C23-C24-C25 |
| 2 | C | 1107 | POV | C22-C23-C24-C25 |
| 2 | D | 1106 | POV | C24-C25-C26-C27 |
| 2 | A | 1102 | POV | O22-C21-C22-C23 |
| 2 | B | 1107 | POV | O31-C31-C32-C33 |
| 2 | A | 1109 | POV | C311-C312-C313-C314 |
| 2 | D | 1104 | POV | O22-C21-C22-C23 |
| 2 | A | 1106 | POV | C22-C23-C24-C25 |
| 2 | B | 1105 | POV | C35-C36-C37-C38 |
| 2 | D | 1101 | POV | O31-C31-C32-C33 |
| 2 | D | 1107 | POV | C22-C23-C24-C25 |
| 2 | C | 1103 | POV | O22-C21-C22-C23 |
| 2 | B | 1106 | POV | O31-C31-C32-C33 |
| 2 | C | 1109 | POV | O31-C31-C32-C33 |
| 2 | C | 1102 | POV | C313-C314-C315-C316 |
| 2 | A | 1105 | POV | O32-C31-C32-C33 |
| 2 | B | 1107 | POV | O21-C21-C22-C23 |
| 2 | D | 1103 | POV | C313-C314-C315-C316 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 1106 | POV | O31-C31-C32-C33 |
| 2 | B | 1105 | POV | O31-C31-C32-C33 |
| 2 | B | 1105 | POV | C24-C25-C26-C27 |
| 2 | D | 1101 | POV | O21-C21-C22-C23 |

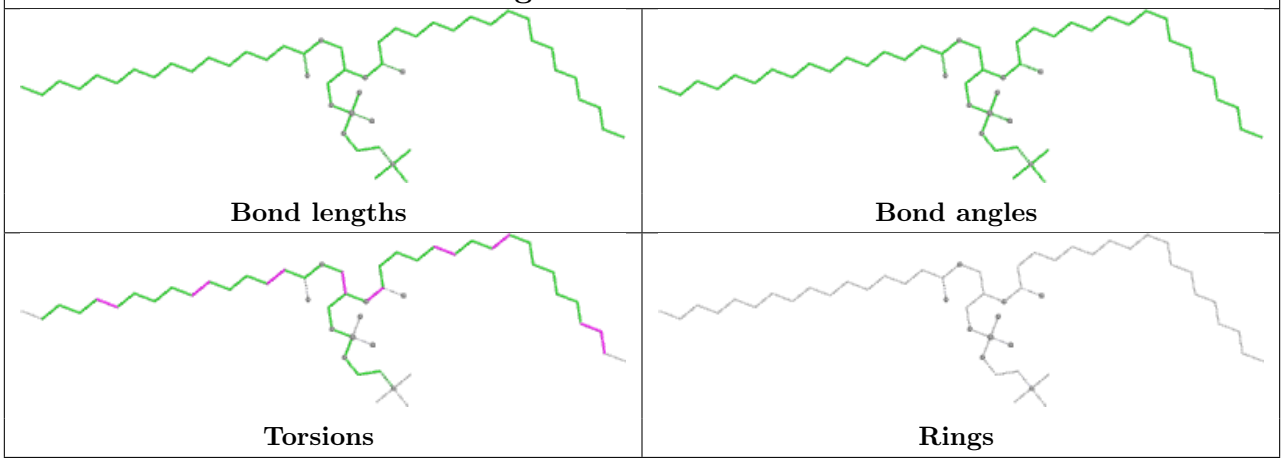
There are no ring outliers.

32 monomers are involved in 104 short contacts:

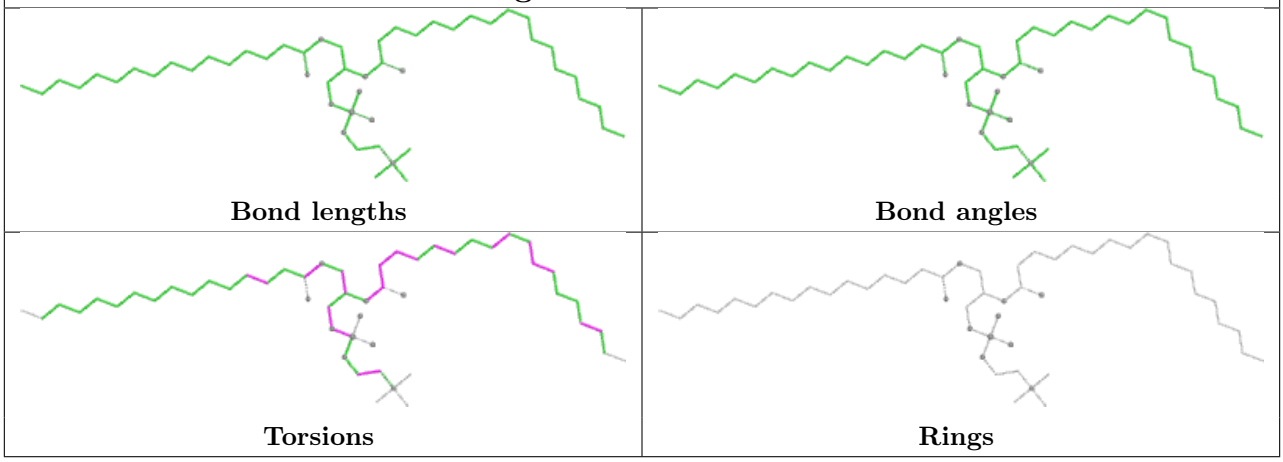
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | C | 1106 | POV | 3 | 0 |
| 2 | C | 1103 | POV | 1 | 0 |
| 2 | B | 1104 | POV | 3 | 0 |
| 2 | C | 1104 | POV | 4 | 0 |
| 2 | C | 1109 | POV | 4 | 0 |
| 2 | A | 1105 | POV | 6 | 0 |
| 2 | A | 1103 | POV | 6 | 0 |
| 2 | B | 1107 | POV | 1 | 0 |
| 2 | D | 1101 | POV | 6 | 0 |
| 2 | D | 1104 | POV | 1 | 0 |
| 2 | A | 1104 | POV | 6 | 0 |
| 2 | B | 1101 | POV | 4 | 0 |
| 2 | D | 1102 | POV | 3 | 0 |
| 2 | A | 1102 | POV | 2 | 0 |
| 2 | A | 1109 | POV | 3 | 0 |
| 2 | C | 1105 | POV | 5 | 0 |
| 2 | D | 1107 | POV | 4 | 0 |
| 2 | B | 1105 | POV | 2 | 0 |
| 2 | A | 1107 | POV | 3 | 0 |
| 2 | A | 1106 | POV | 3 | 0 |
| 2 | B | 1103 | POV | 1 | 0 |
| 2 | D | 1105 | POV | 6 | 0 |
| 2 | C | 1107 | POV | 4 | 0 |
| 2 | C | 1108 | POV | 5 | 0 |
| 2 | D | 1106 | POV | 4 | 0 |
| 2 | B | 1102 | POV | 4 | 0 |
| 2 | C | 1101 | POV | 3 | 0 |
| 2 | D | 1103 | POV | 4 | 0 |
| 2 | A | 1108 | POV | 4 | 0 |
| 2 | A | 1101 | POV | 5 | 0 |
| 2 | C | 1102 | POV | 5 | 0 |
| 2 | B | 1106 | POV | 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 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.

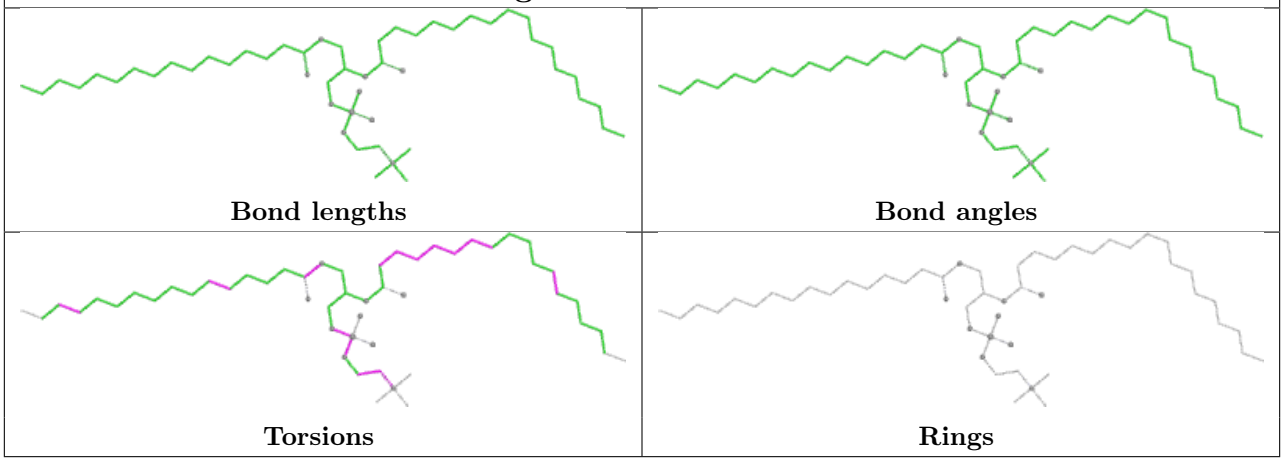
**Ligand POV C 1106**



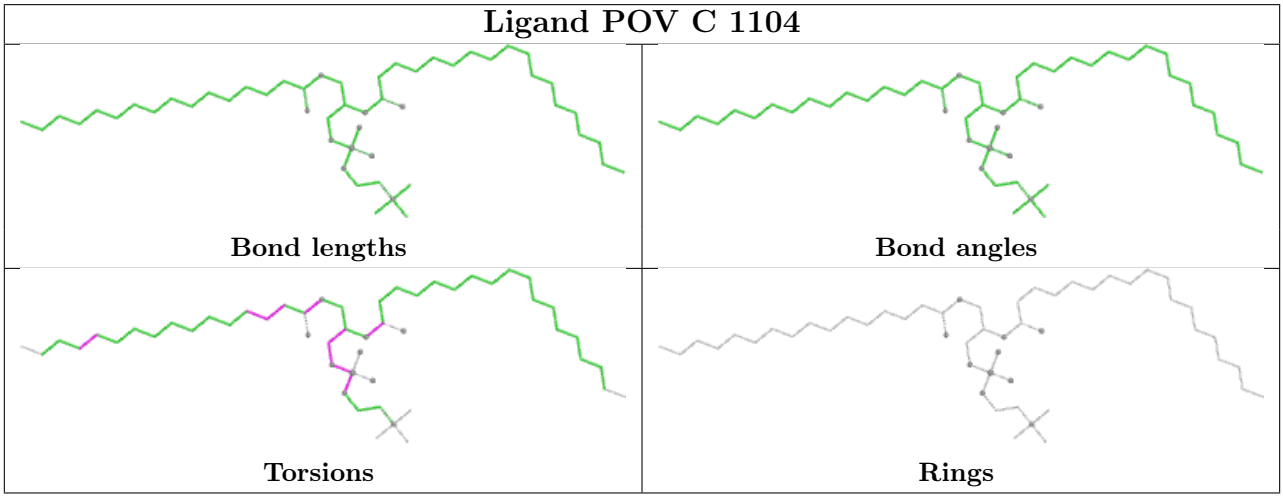

**Ligand POV C 1103**



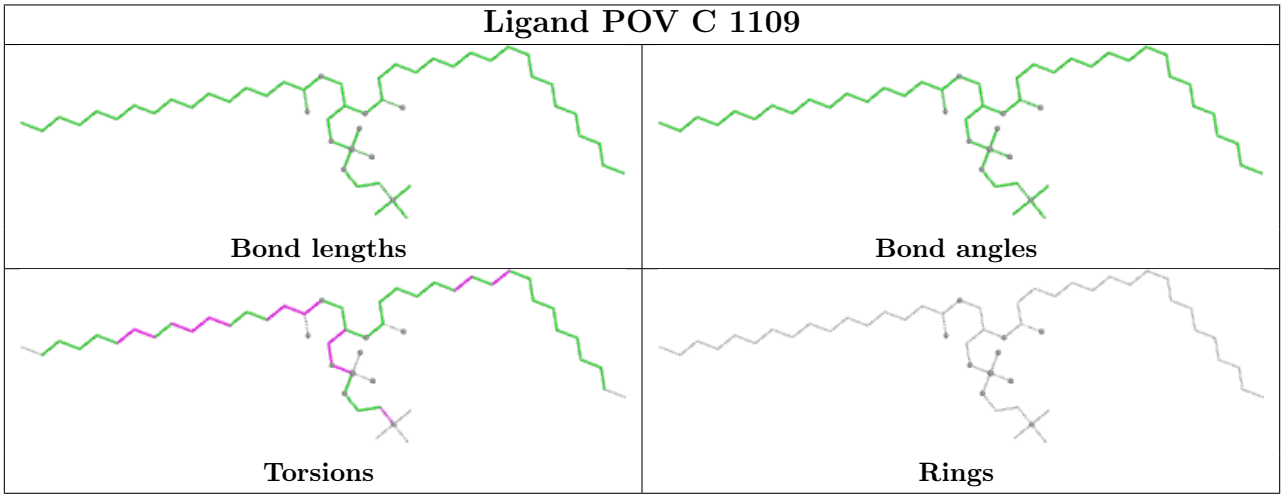
## Ligand POV B 1104



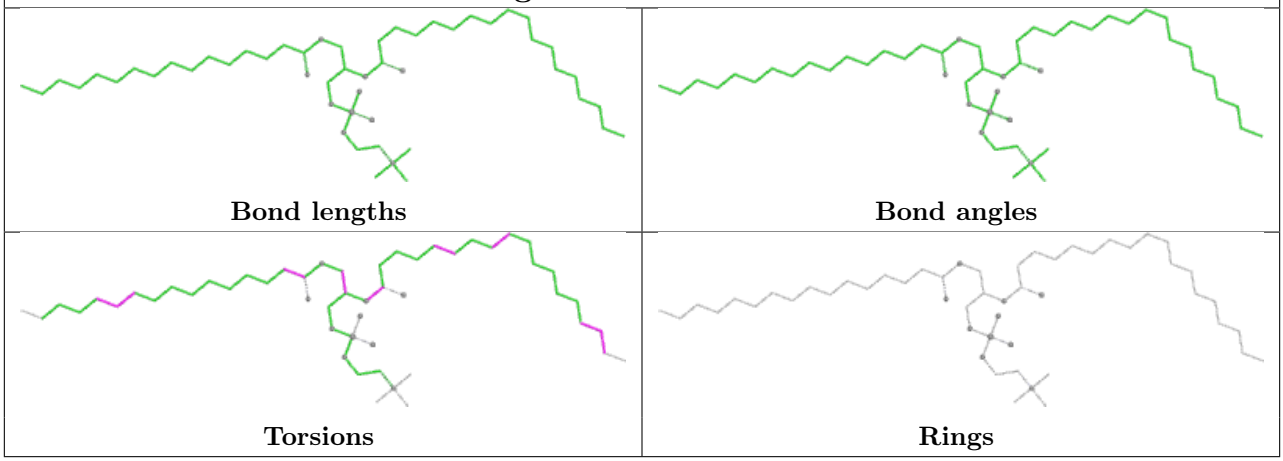

## Ligand POV C 1104



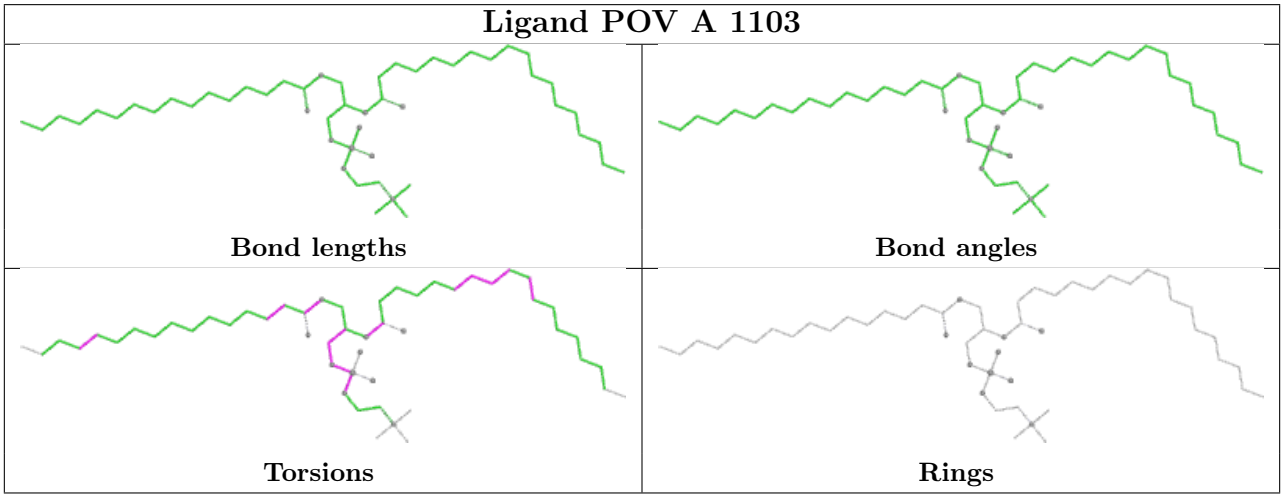

## Ligand POV C 1109



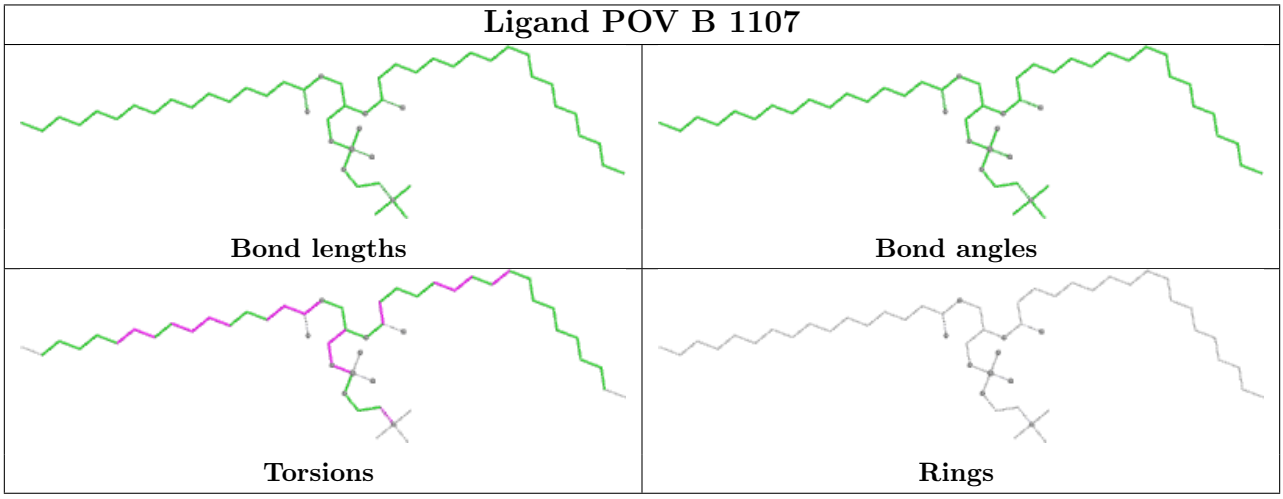
**Ligand POV A 1105**



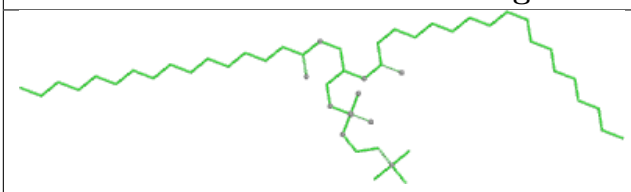

**Ligand POV A 1103**

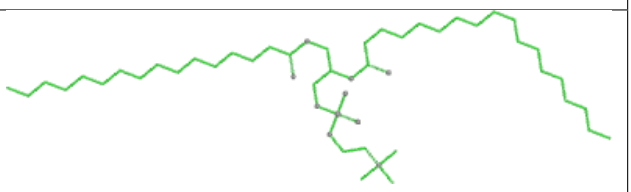


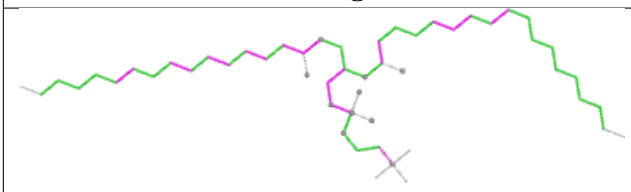

**Ligand POV B 1107**

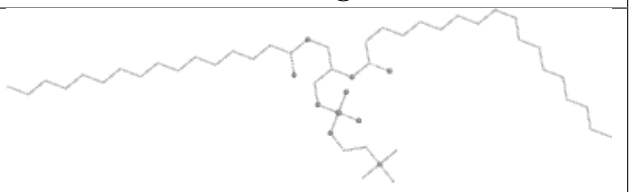


## Ligand POV D 1101

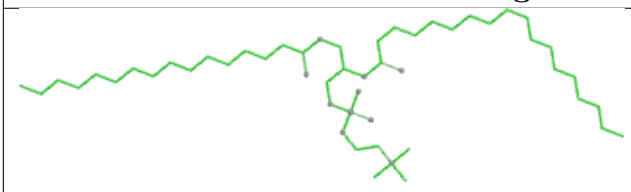

Bond lengths

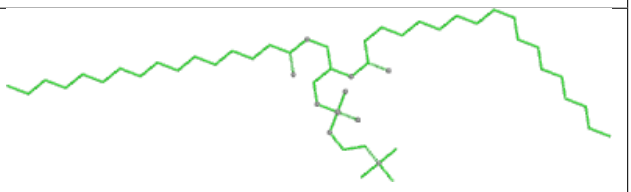

Bond angles

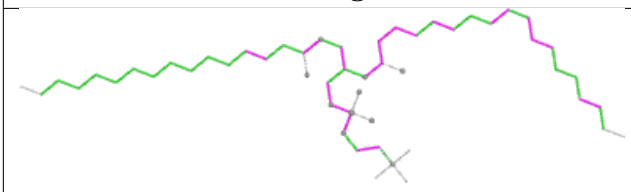

Torsions

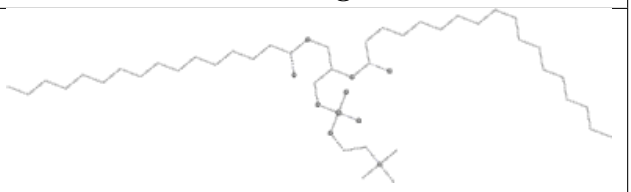

Rings

## Ligand POV D 1104

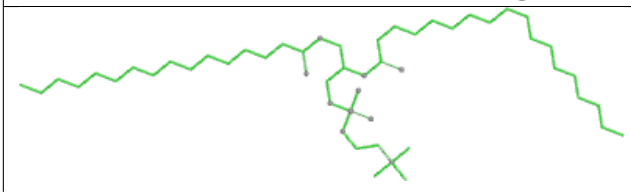

Bond lengths

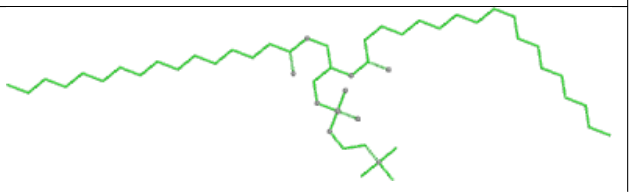

Bond angles

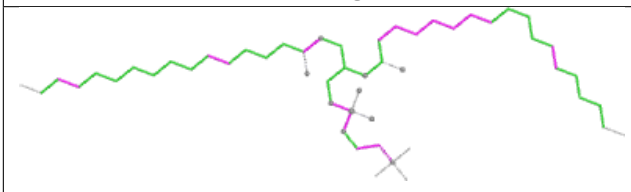

Torsions

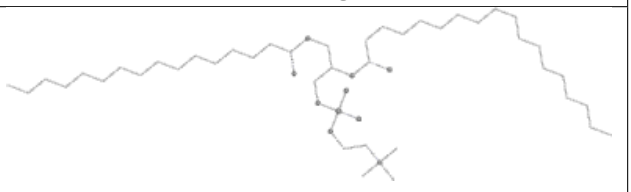

Rings

## Ligand POV A 1104

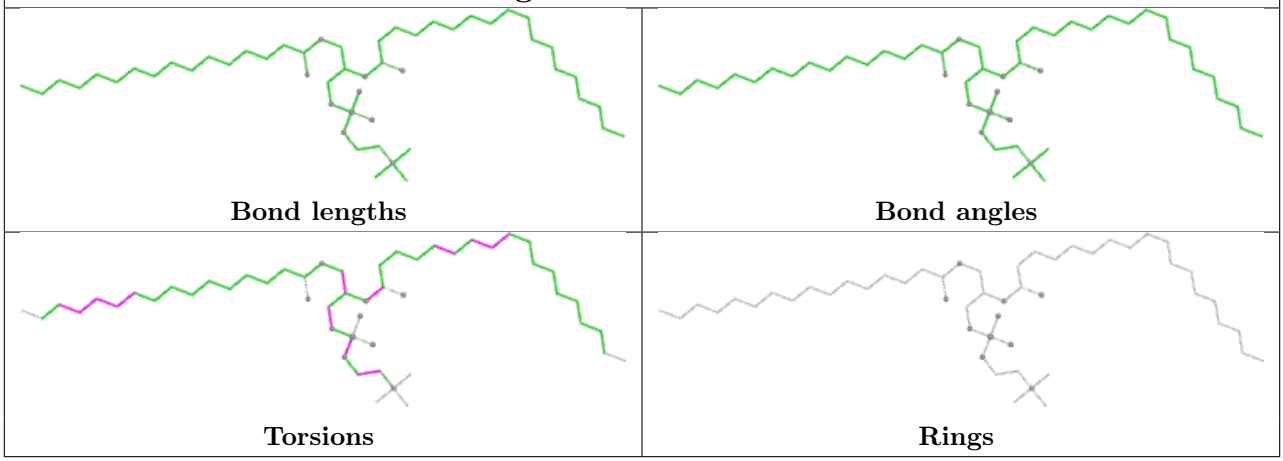

Bond lengths


Bond angles

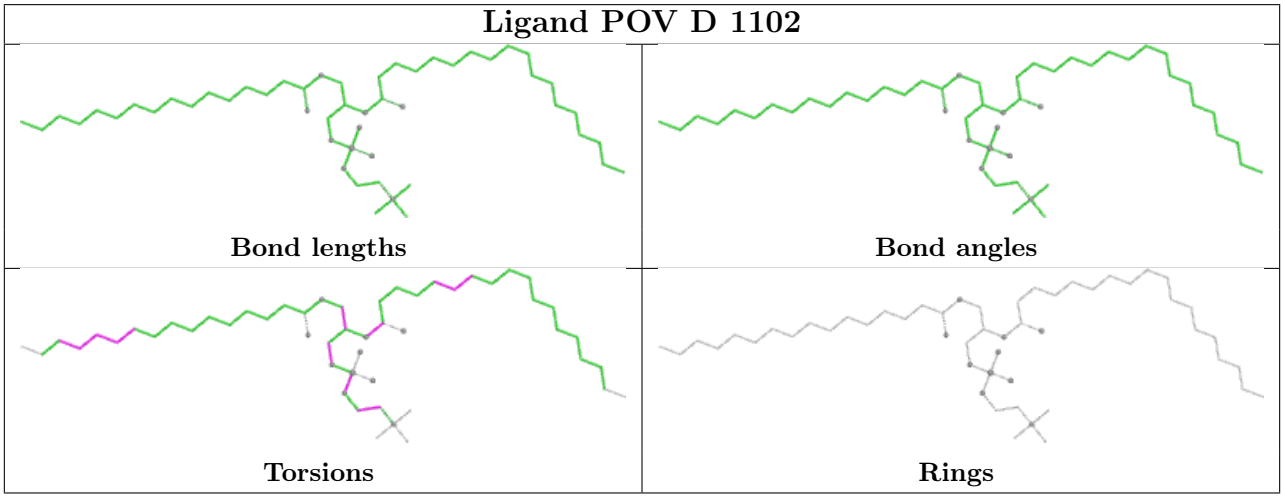

Torsions


Rings

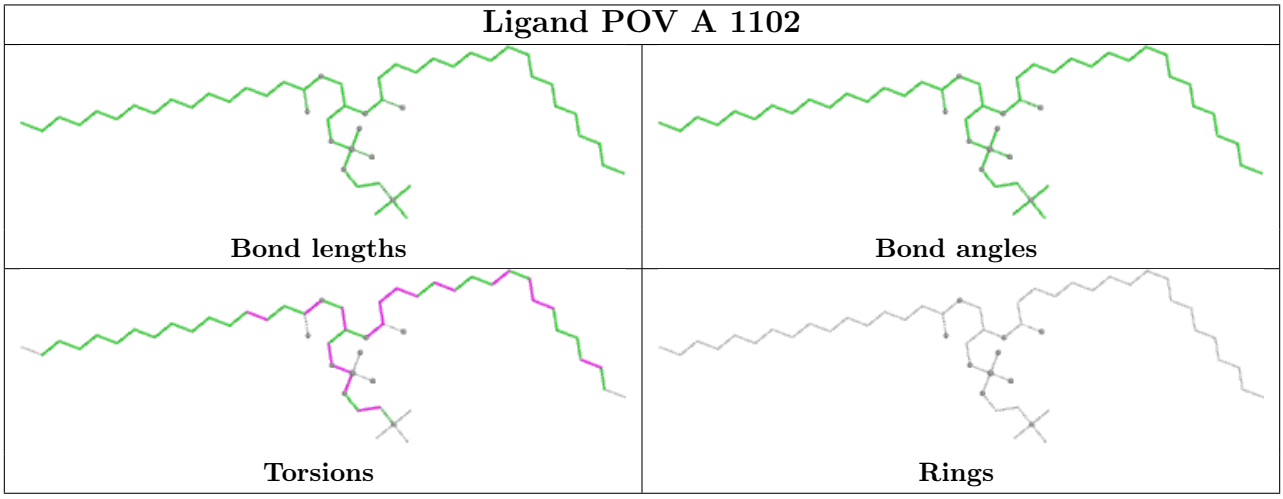
## Ligand POV B 1101



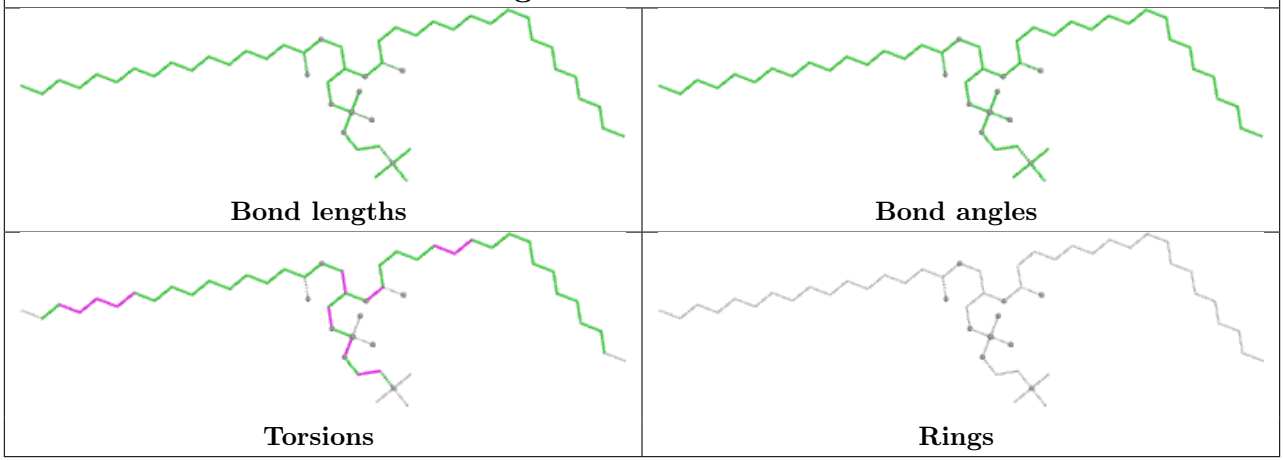

## Ligand POV D 1102



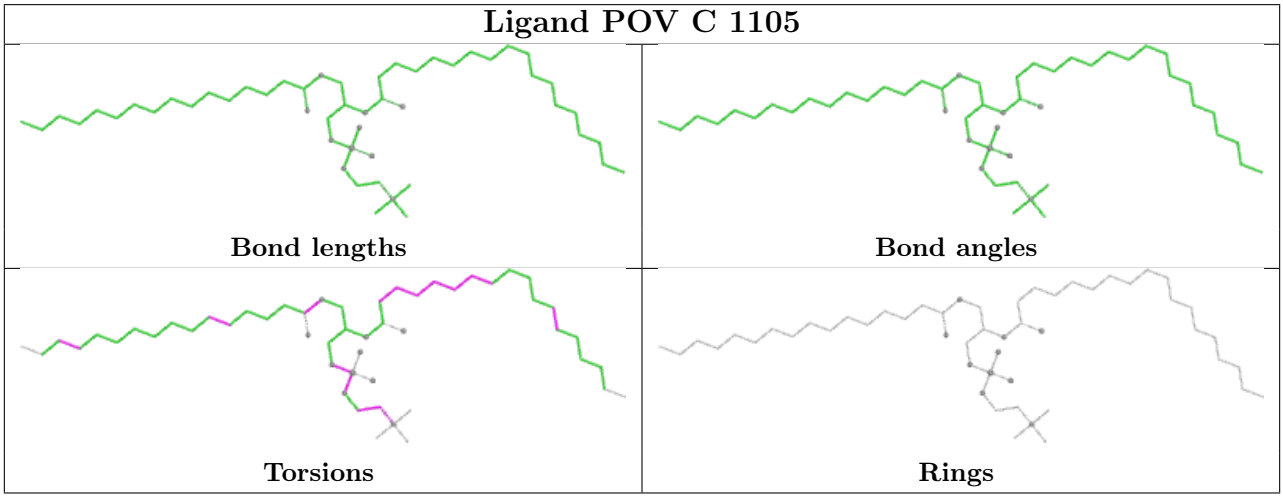

## Ligand POV A 1102



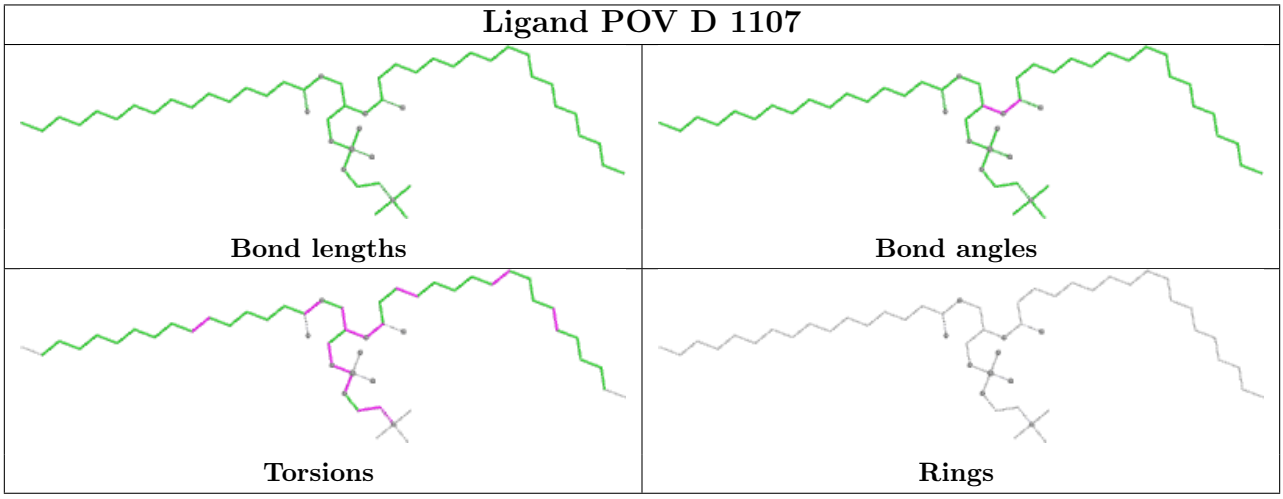
## Ligand POV A 1109



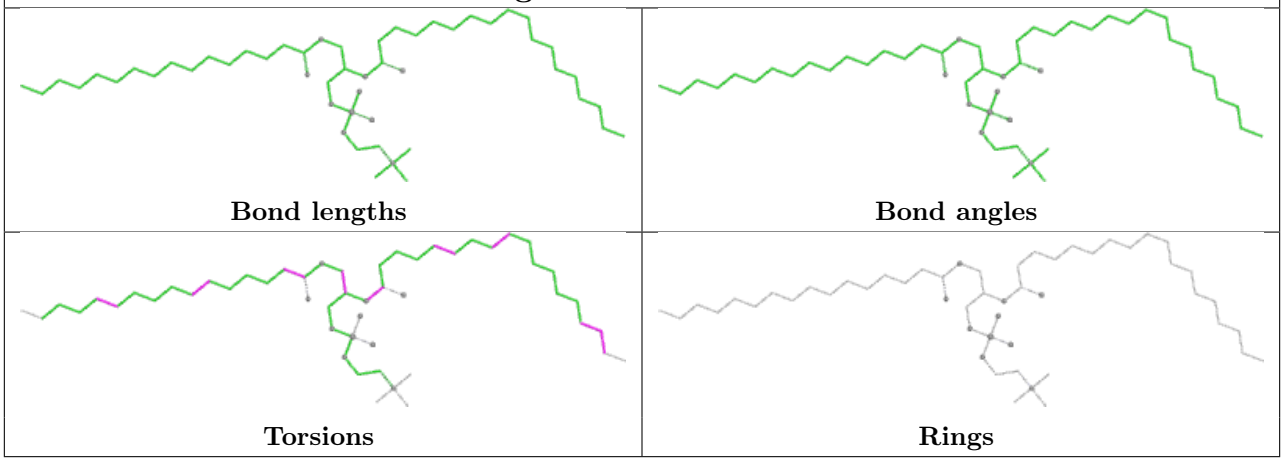

## Ligand POV C 1105



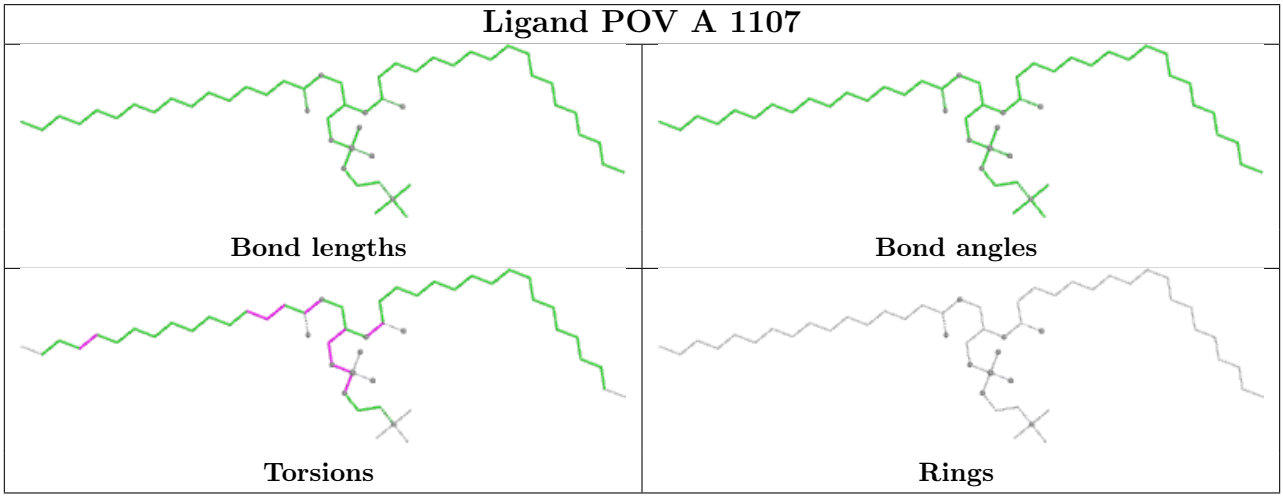

## Ligand POV D 1107



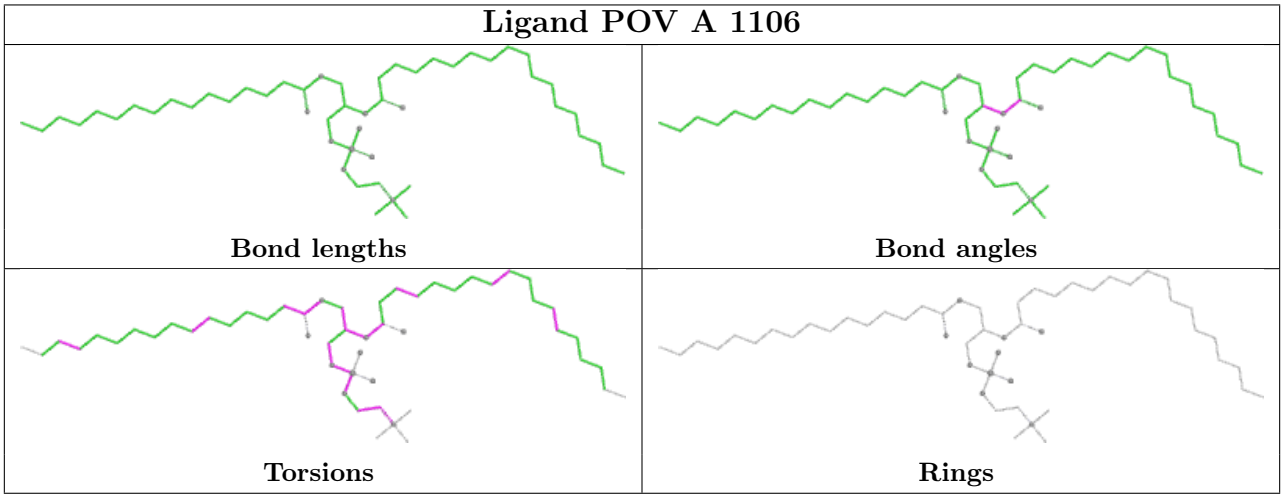
**Ligand POV B 1105**



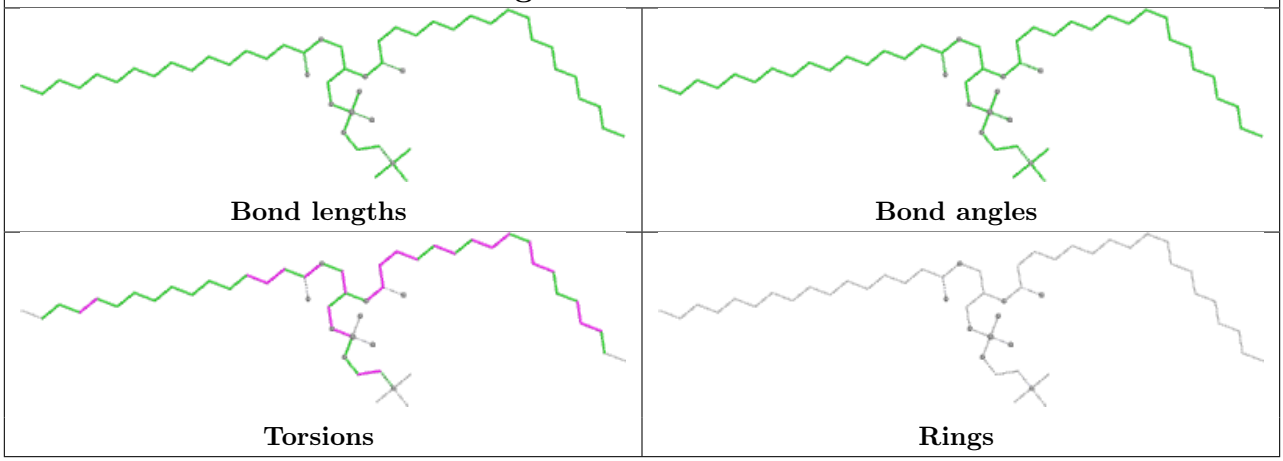

**Ligand POV A 1107**



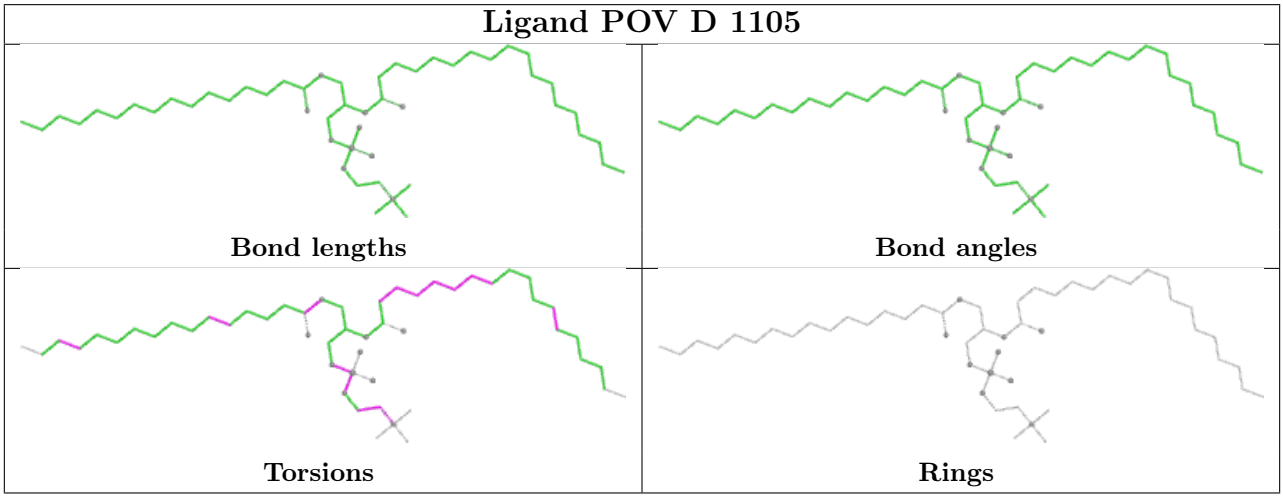

**Ligand POV A 1106**



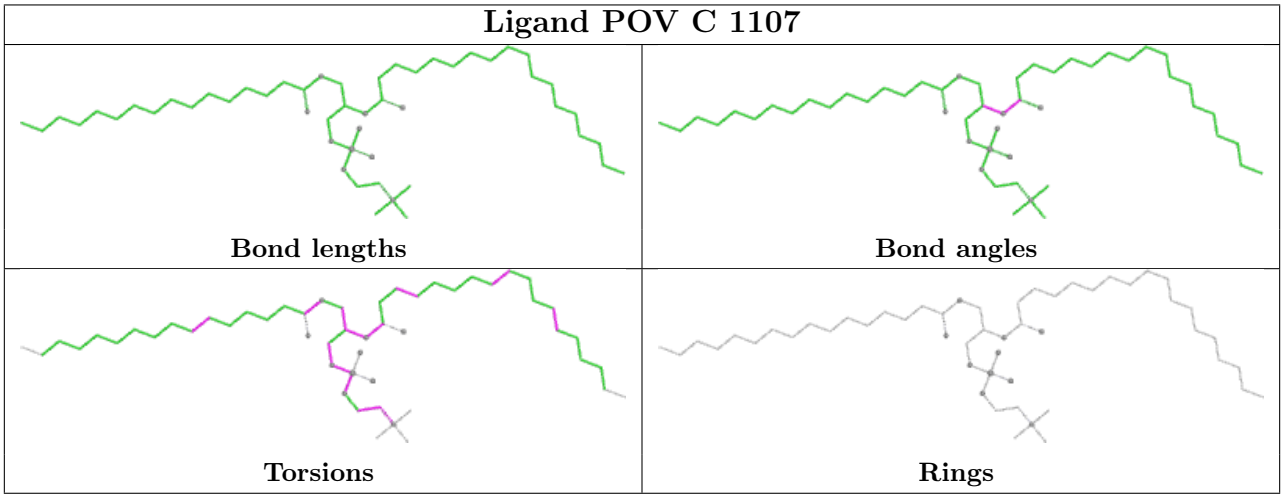
## Ligand POV B 1103



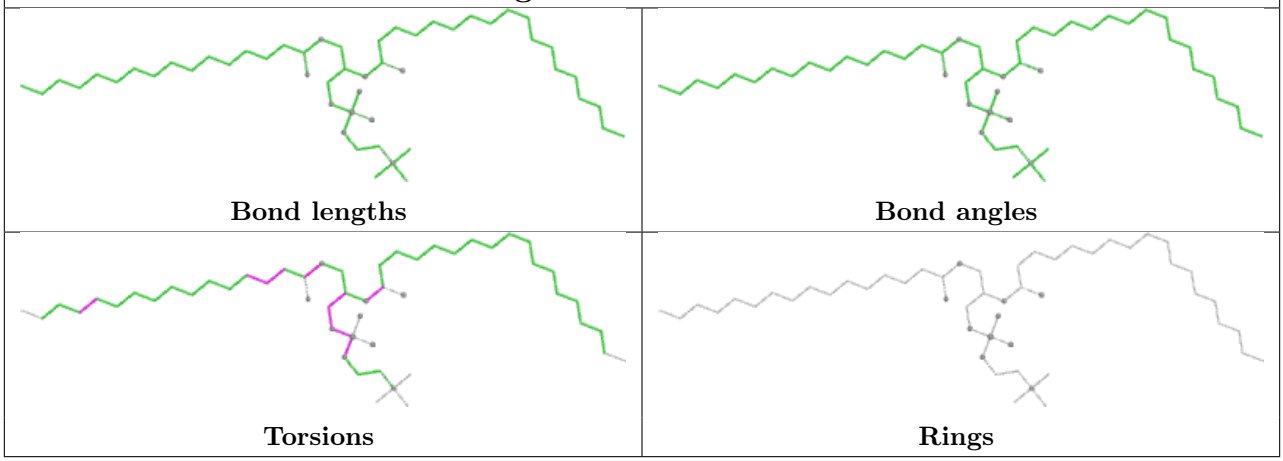

## Ligand POV D 1105



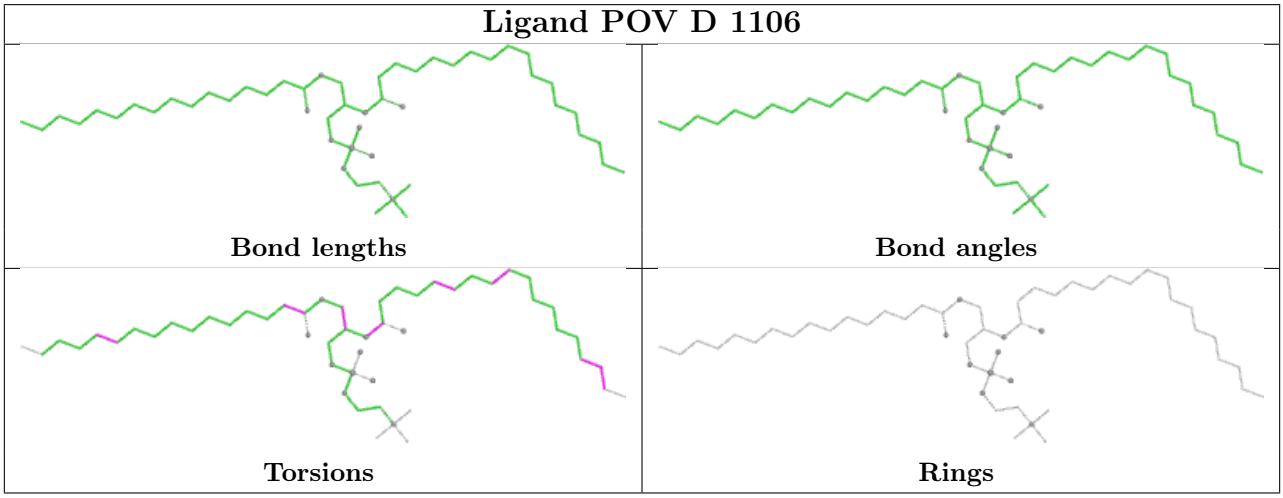

## Ligand POV C 1107



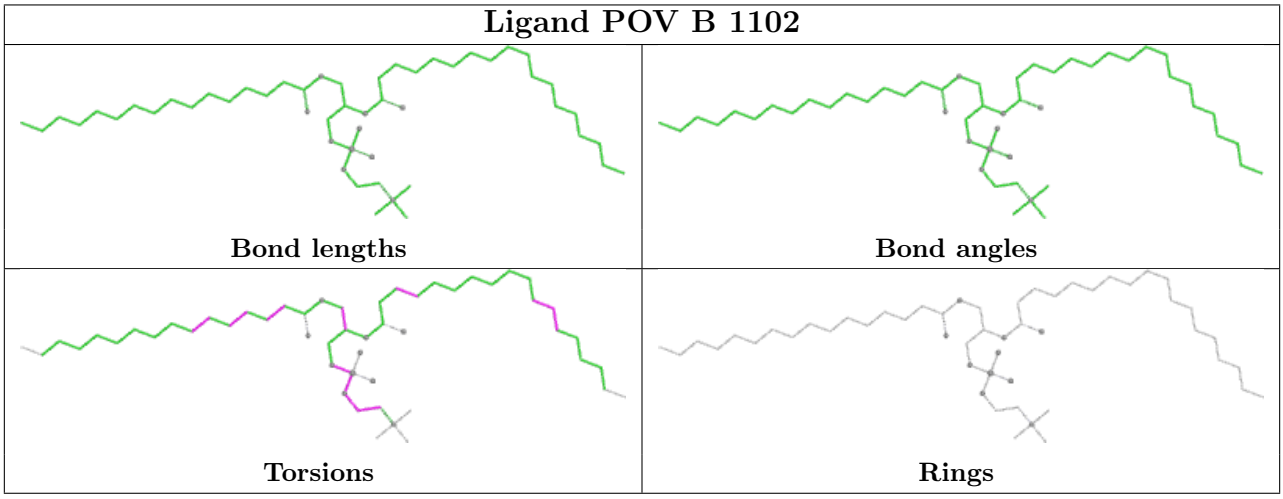
## Ligand POV C 1108



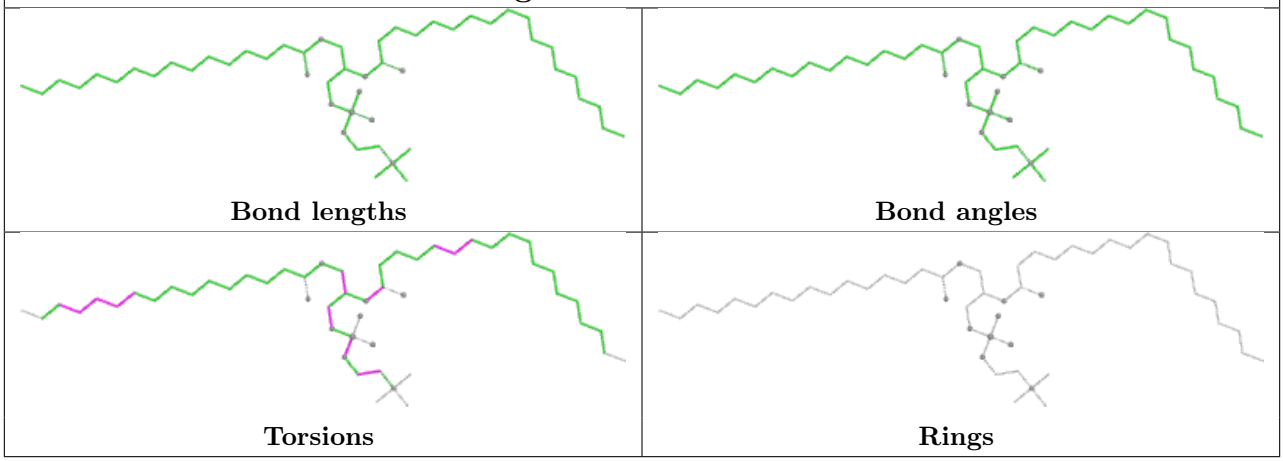

## Ligand POV D 1106



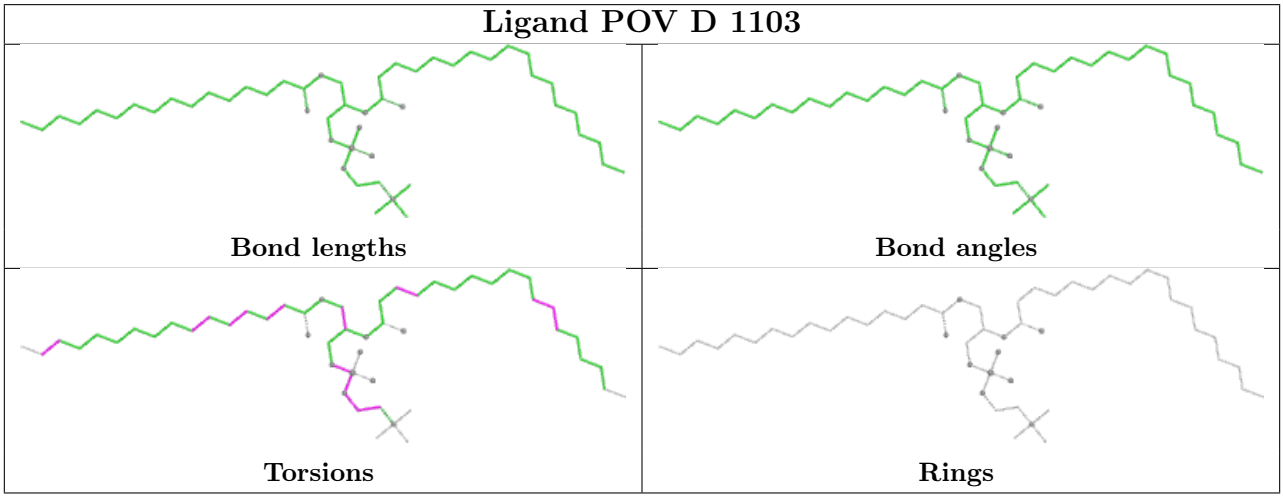

## Ligand POV B 1102



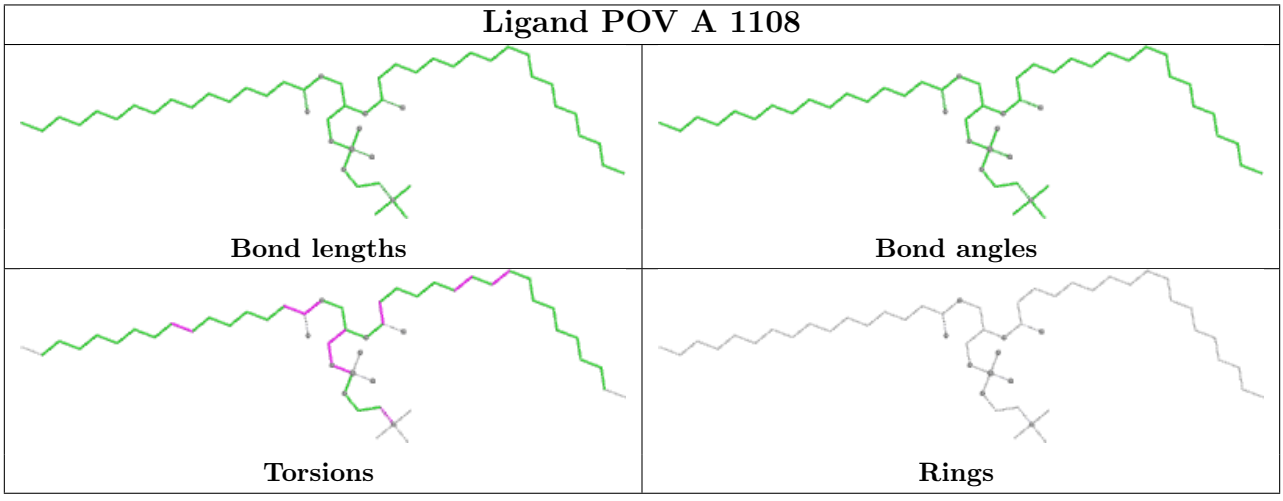
## Ligand POV C 1101

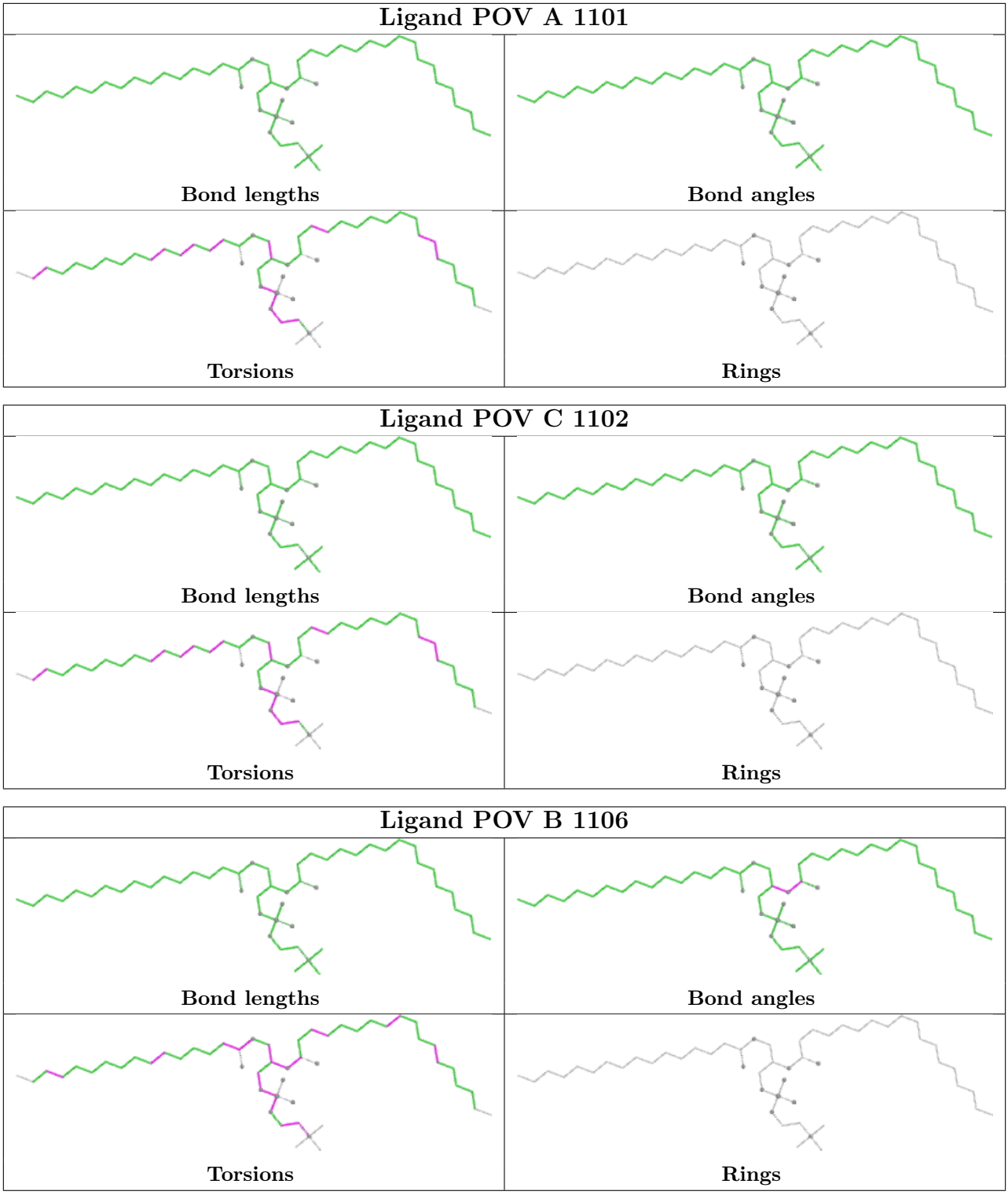



## Ligand POV D 1103




## Ligand POV A 1108






## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

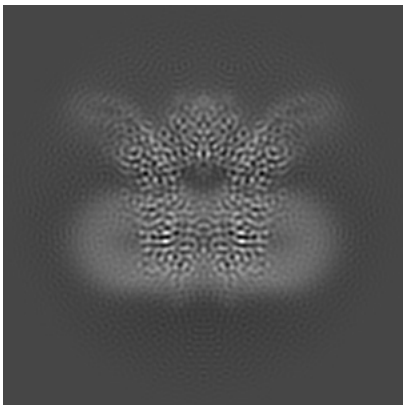
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-77138. These allow visual inspection of the internal detail of the map and identification of artifacts.

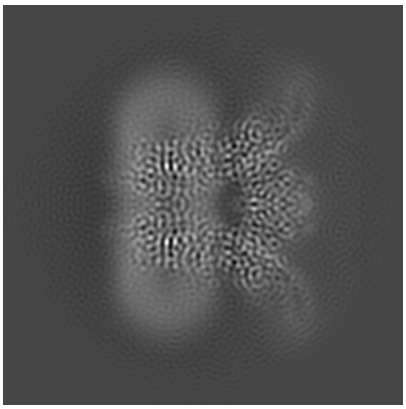
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

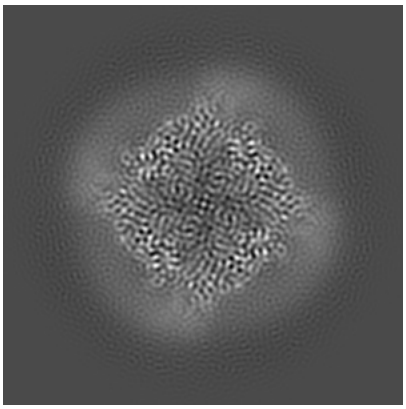
### 6.1.1 Primary map



X

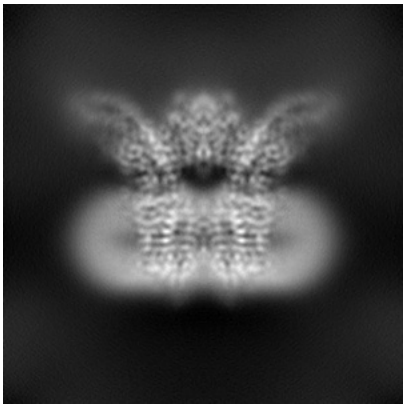


Y

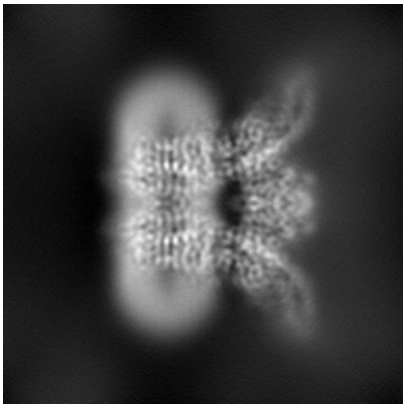


Z

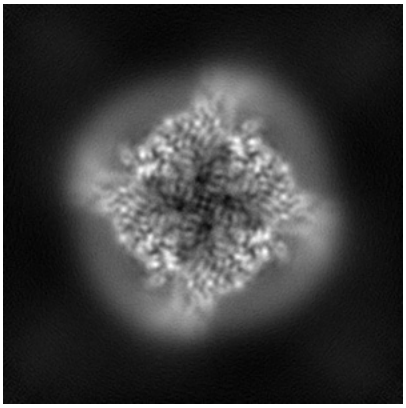
### 6.1.2 Raw map



X



Y

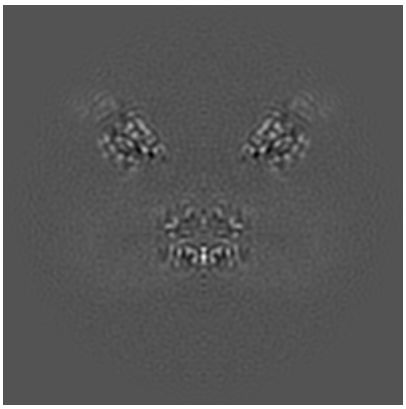


Z

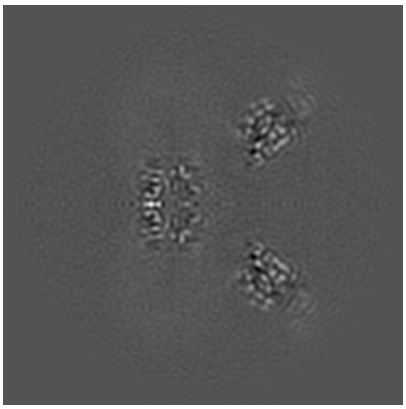
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

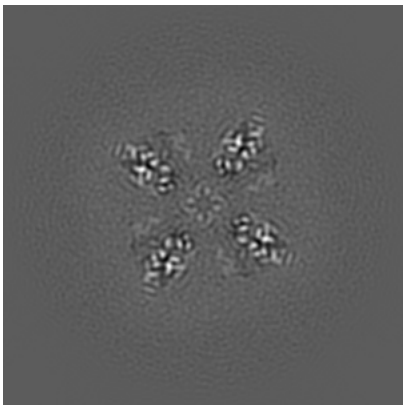
### 6.2.1 Primary map



X Index: 128

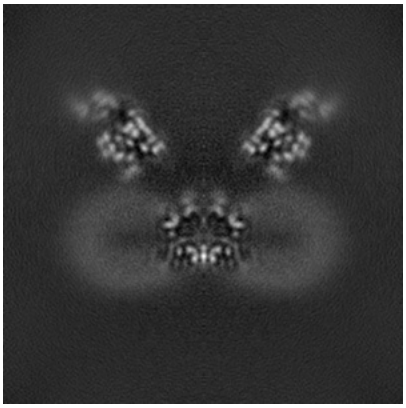


Y Index: 128

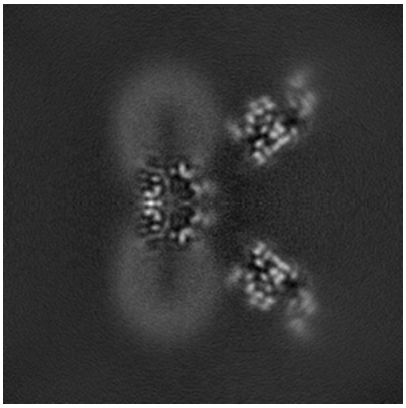


Z Index: 128

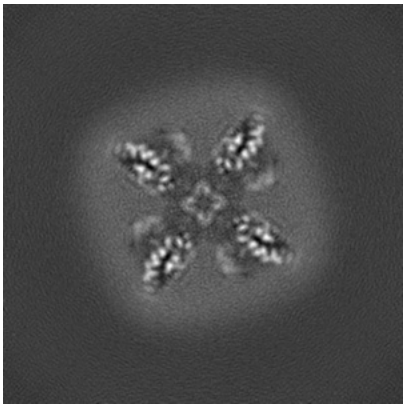
### 6.2.2 Raw map



X Index: 128



Y Index: 128

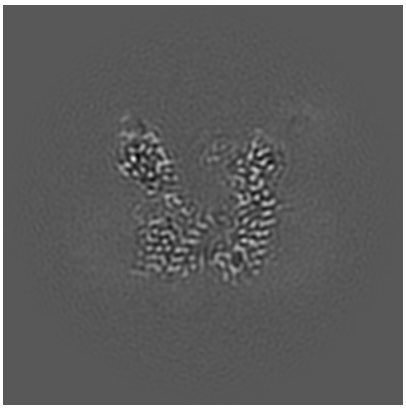


Z Index: 128

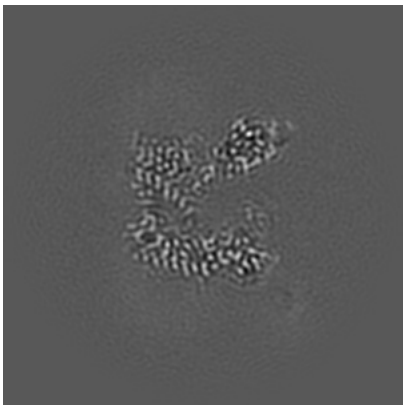
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

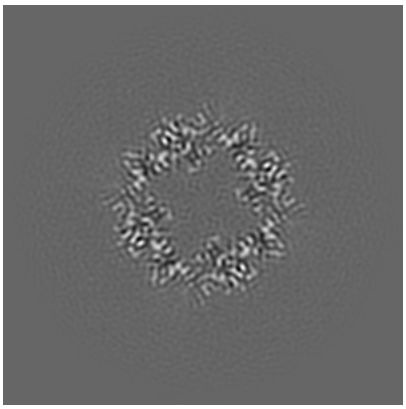
### 6.3.1 Primary map



X Index: 151

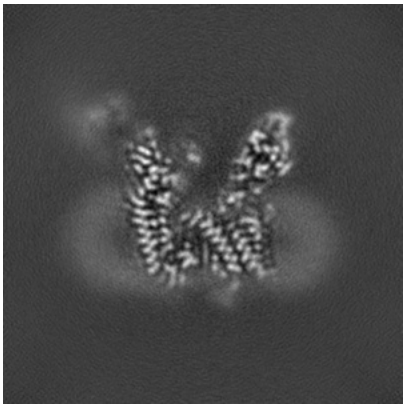


Y Index: 151

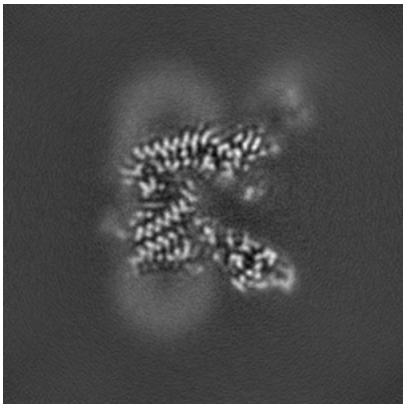


Z Index: 158

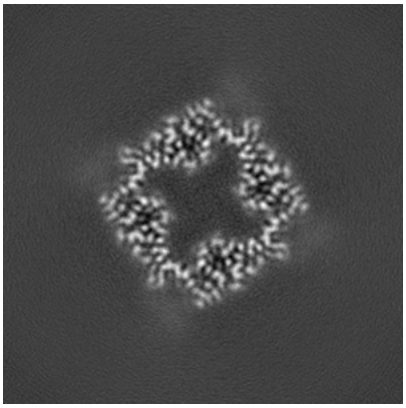
### 6.3.2 Raw map



X Index: 106



Y Index: 106

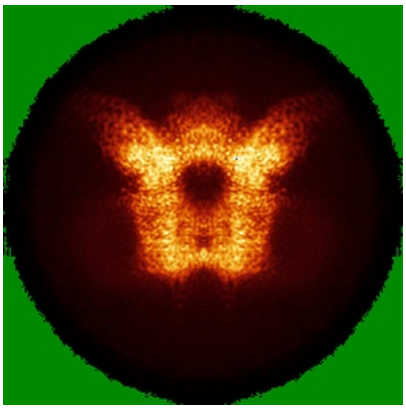


Z Index: 163

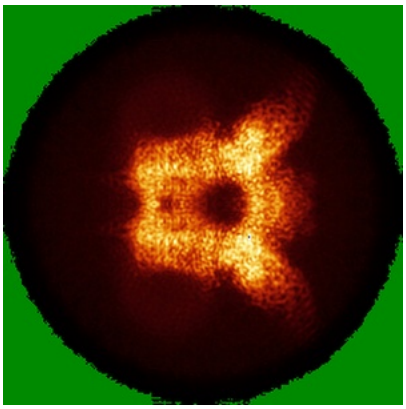
The images above show the largest variance slices of the map in three orthogonal directions.

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

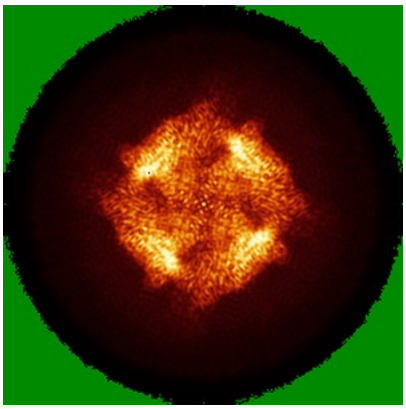
### 6.4.1 Primary map



X

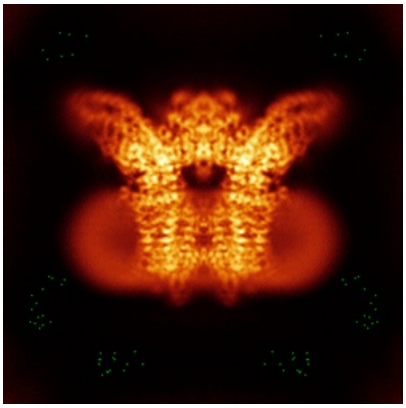


Y

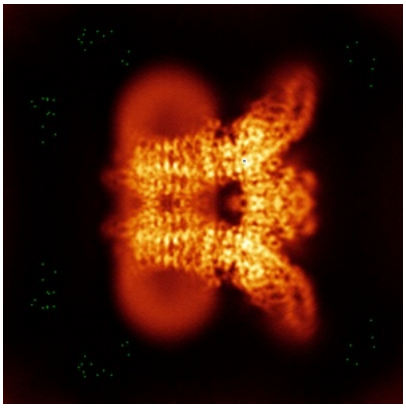


Z

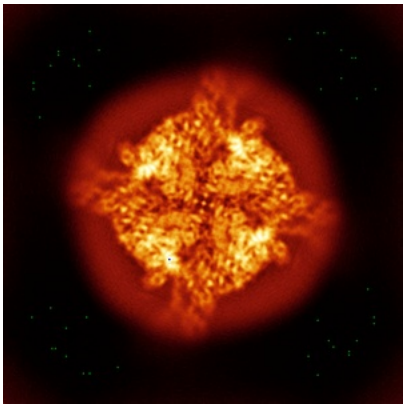
### 6.4.2 Raw map



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)

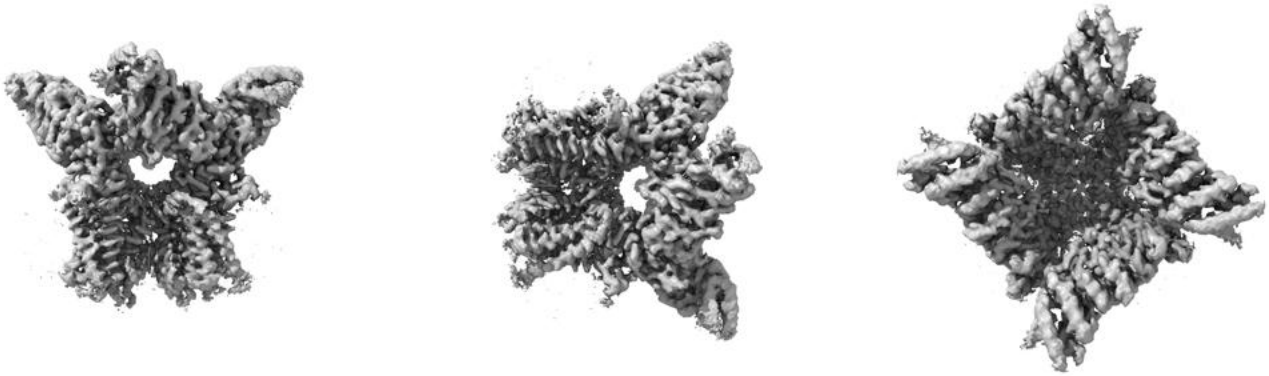
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0557. 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.

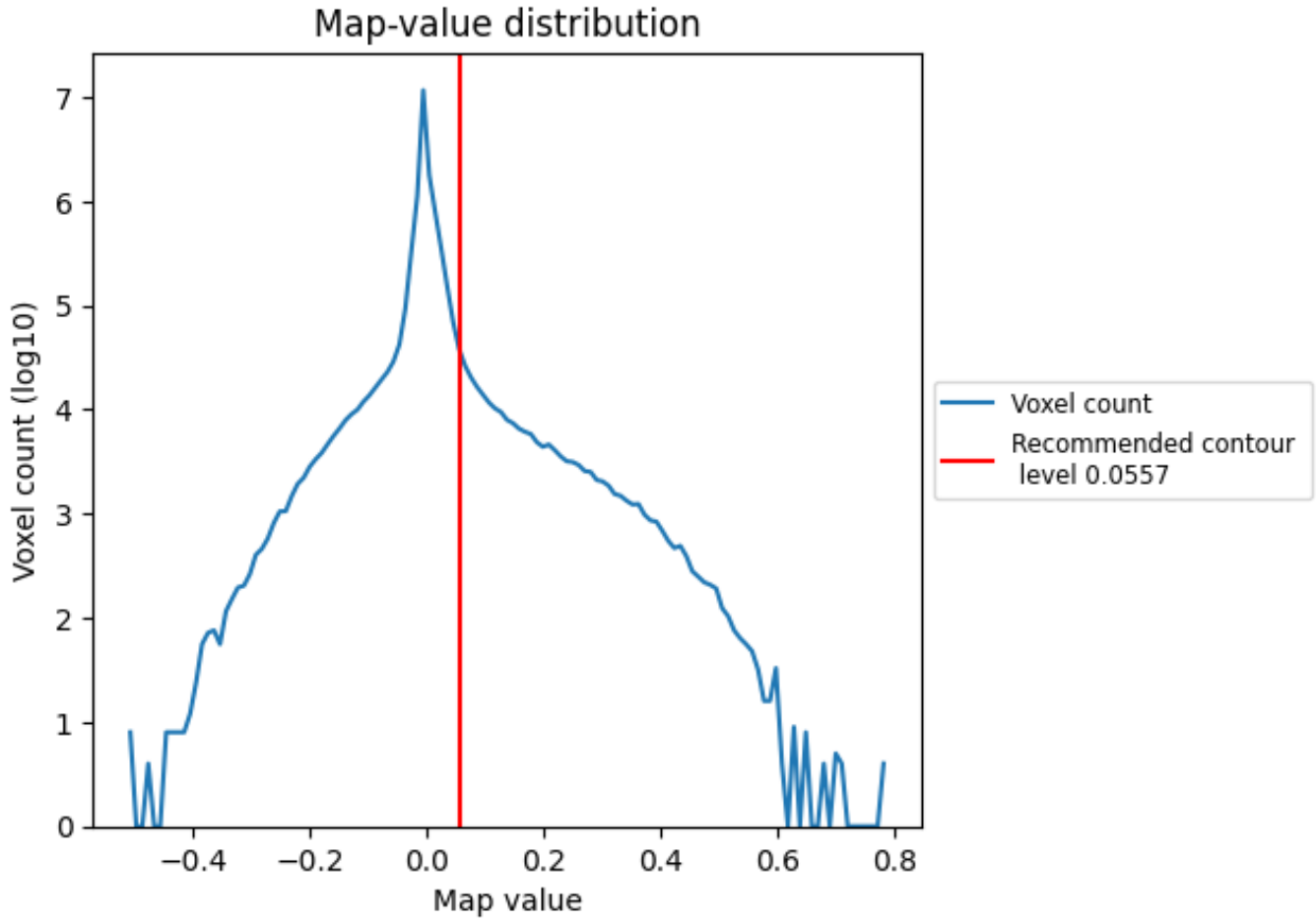
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

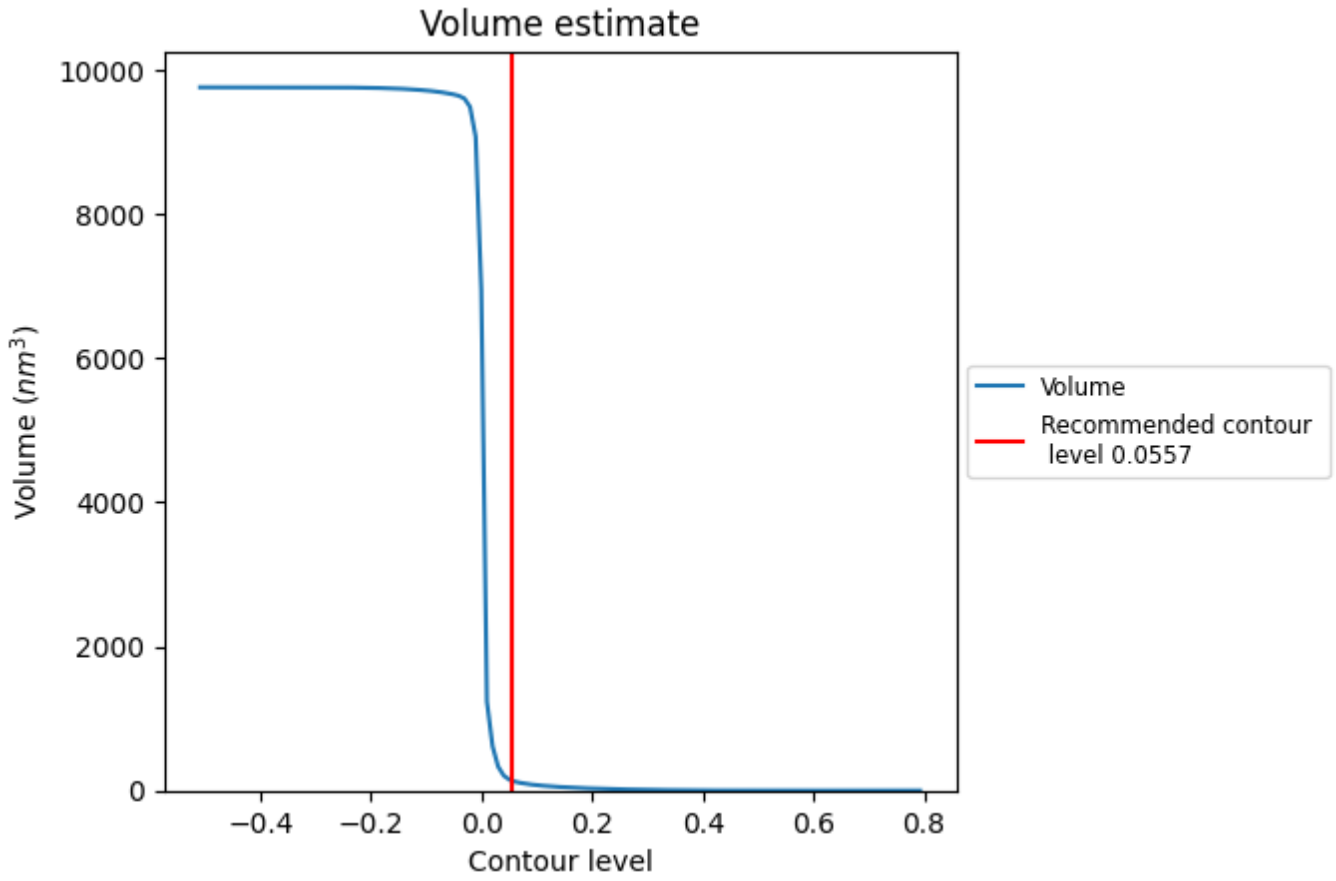
This section contains the results of statistical analysis of the map.

## 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.

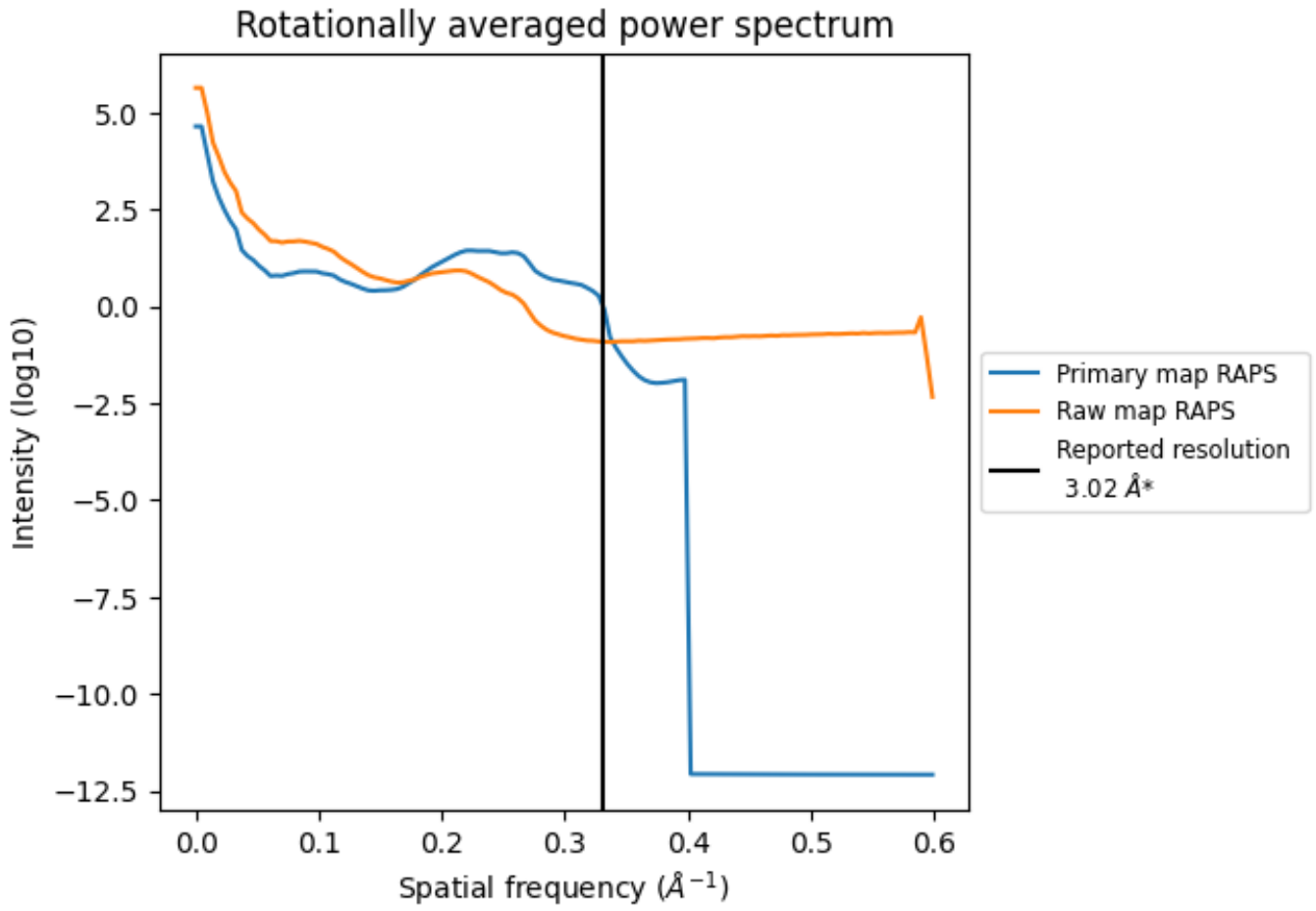
## 7.2 Volume estimate




The volume at the recommended contour level is 137 $nm^3$; this corresponds to an approximate mass of 124 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)

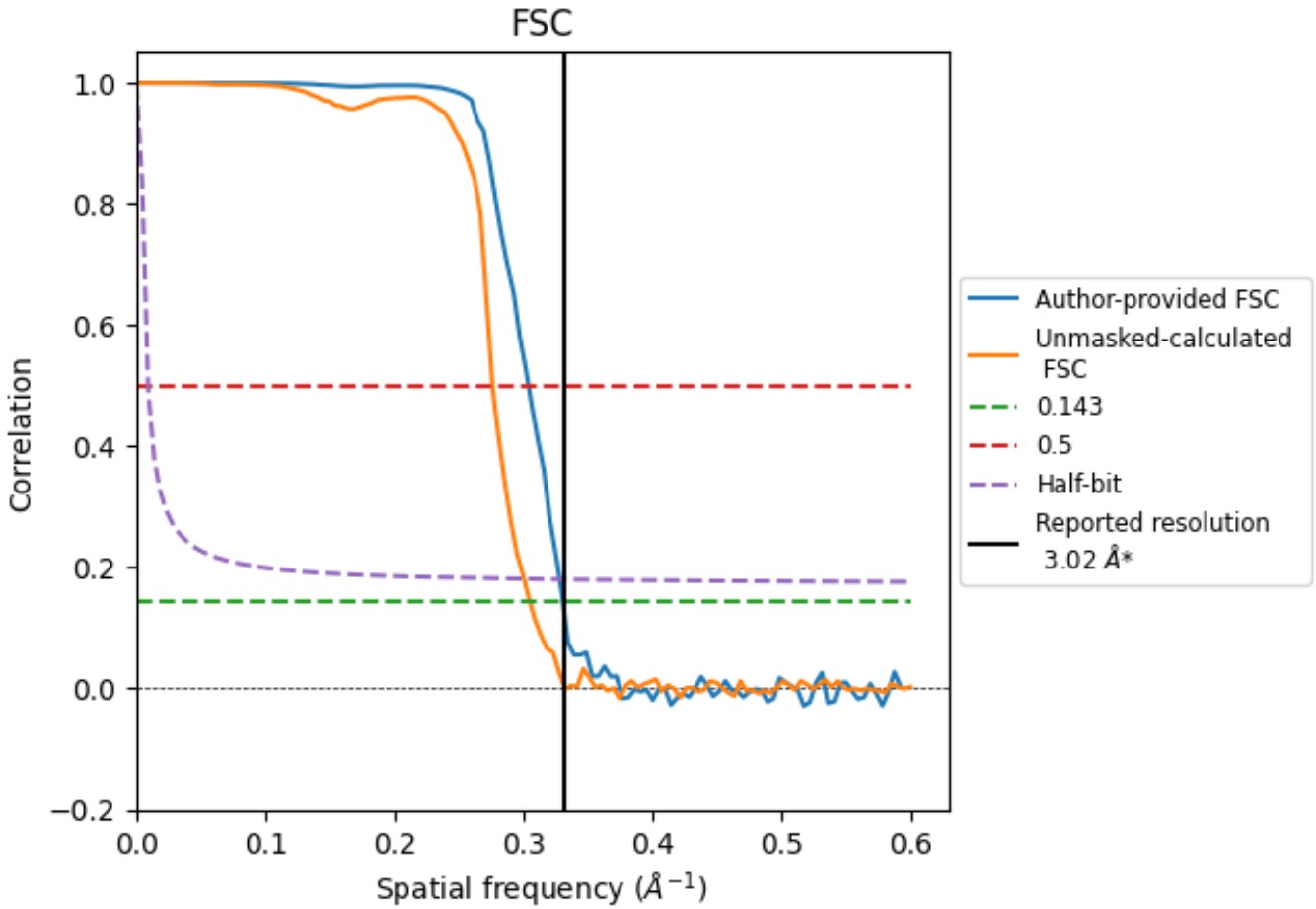



*Reported resolution corresponds to spatial frequency of 0.331 $Å^{-1}$

# 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 0.331 Å$^{-1}$

## 8.2 Resolution estimates (i)

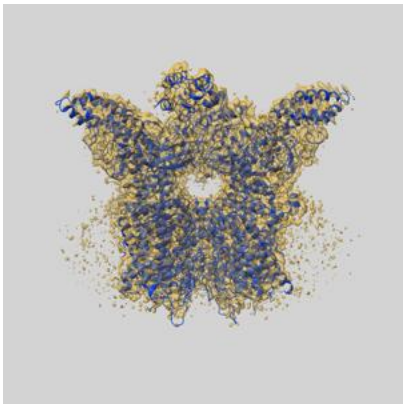
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.02 | - | - |
| Author-provided FSC curve | 3.02 | 3.29 | 3.05 |
| Unmasked-calculated* | 3.28 | 3.62 | 3.33 |

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

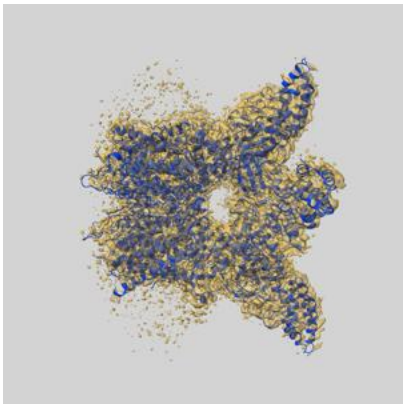
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-77138 and PDB model 13LN. Per-residue inclusion information can be found in section 3 on page 9.

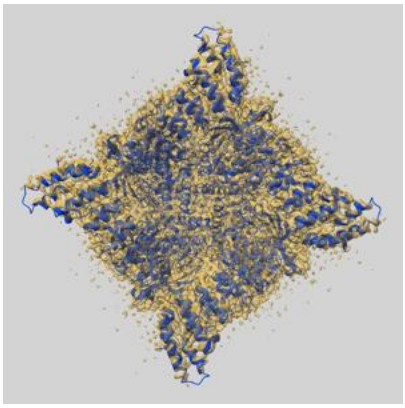
## 9.1 Map-model overlay



X



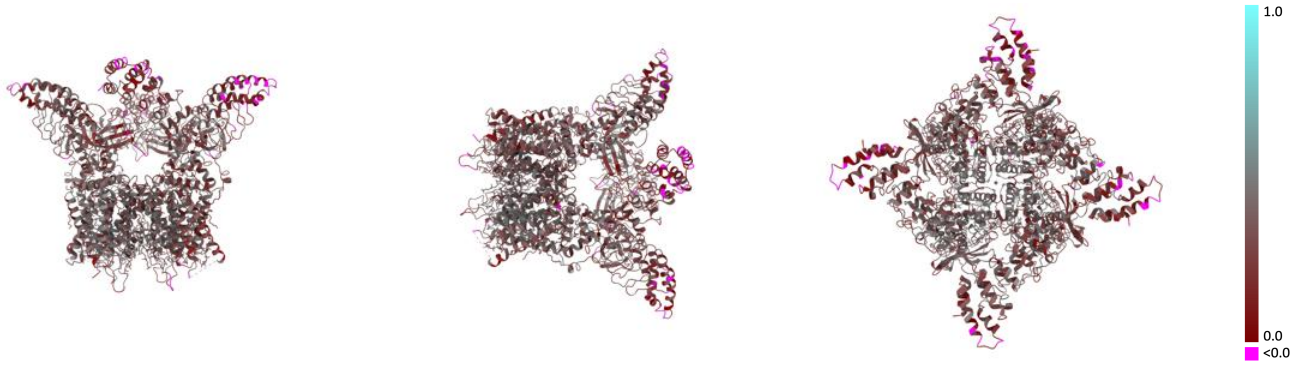
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0557 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.

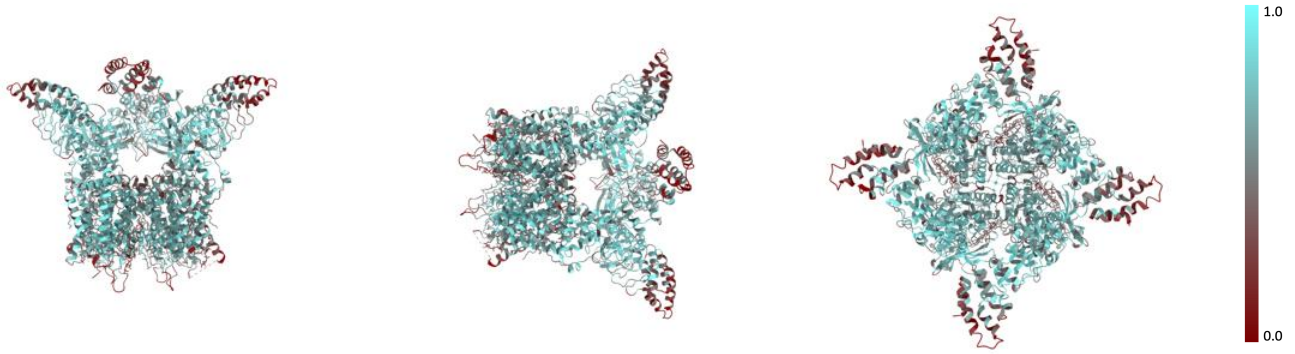
## 9.2 Q-score mapped to coordinate model (i)




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.

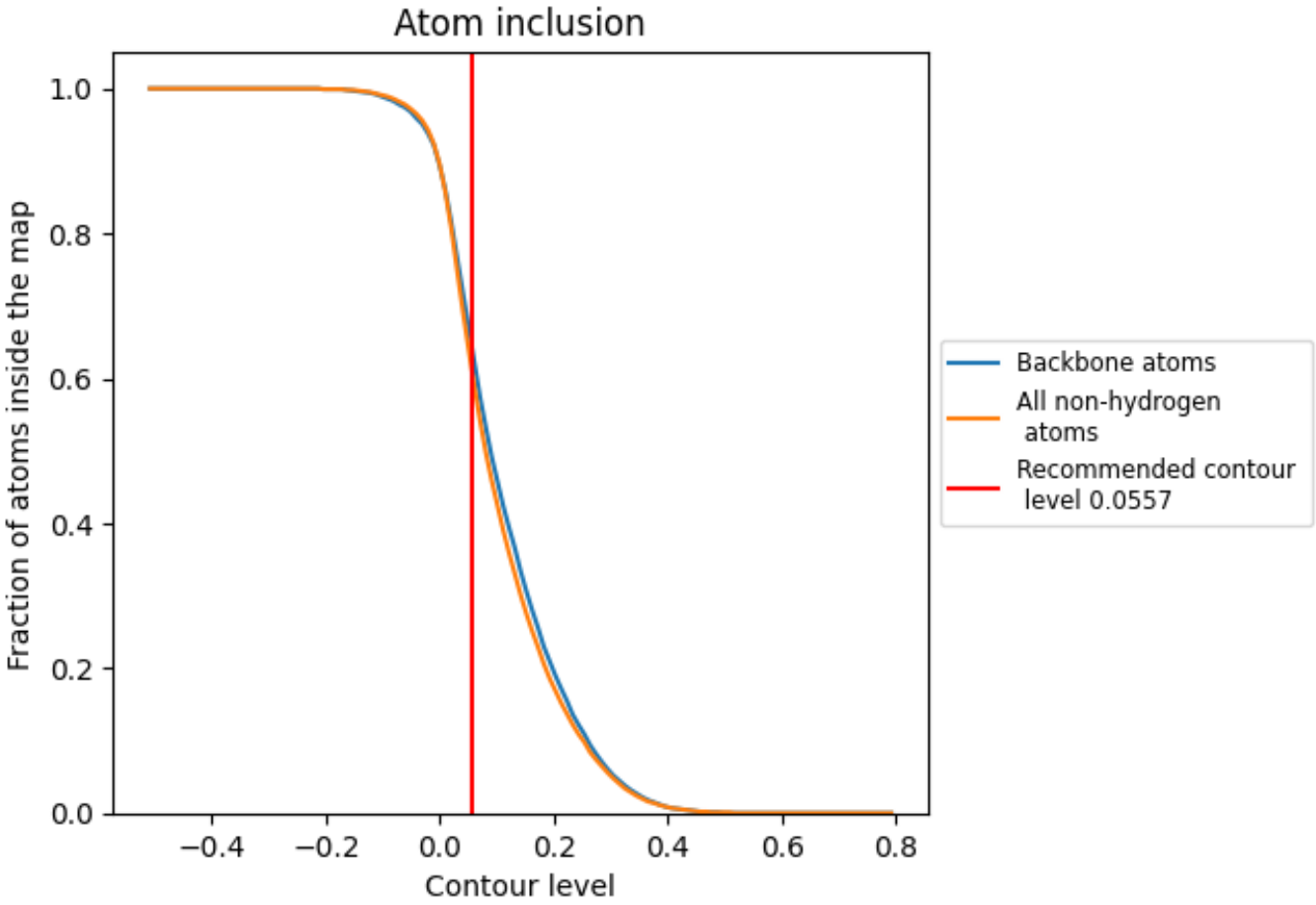
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.0557).

## 9.4 Atom inclusion (i)




At the recommended contour level, 65% of all backbone atoms, 61% 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 (0.0557) and Q-score for the entire model and for each chain.




| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.6140 | 0.3160 |
| A | 0.6030 | 0.3060 |
| B | 0.6070 | 0.2970 |
| C | 0.6340 | 0.3340 |
| D | 0.6260 | 0.3270 |