# Full wwPDB EM Validation Report ⓘ

May 4, 2024 – 06:18 pm BST

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|---|---|---|
| PDB ID | : | 6GNI |
| EMDB ID | : | EMD-0044 |
| Title | : | Cryo-tomography and subtomogram averaging of Sar1-Sec23-Sec24 - fitted model. |
| Authors | : | Hutchings, J.; Zanetti, G. |
| Deposited on | : | 2018-05-30 |
| Resolution | : | 4.90 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.dev92 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

PERCENTILES INFOmissingINFO

# 1 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12937 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 Protein transport protein SEC23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 733 | 5780 | 3679 | 969 | 1109 | 23 | 0 | 0 |

- Molecule 2 is a protein called Protein transport protein SEC24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | E | 735 | 5823 | 3702 | 999 | 1084 | 38 | 0 | 0 |

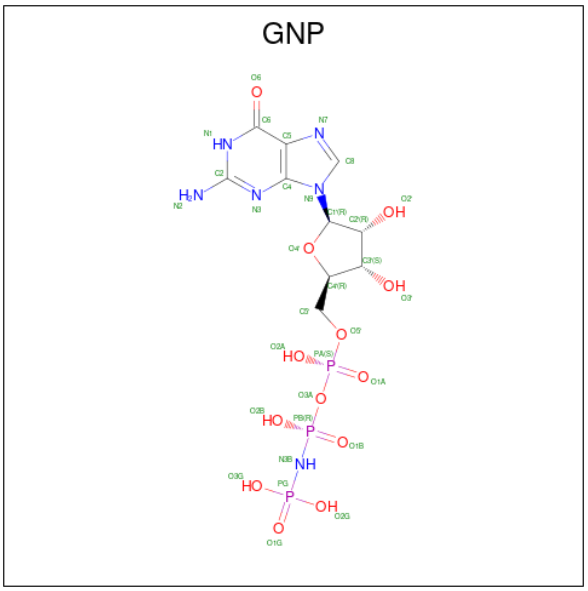
- Molecule 3 is a protein called Small COPII coat GTPase SAR1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | B | 164 | 1299 | 836 | 220 | 239 | 4 | 0 | 0 |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 4 | A | 1 | 1 | 1 | 0 |
| 4 | E | 1 | 1 | 1 | 0 |

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 5 | B | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 6 | 13 | 3 | |

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 6 | B | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

SEQUENCE-PLOTS INFOmissingINFO

# 2 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SUBTOMOGRAM AVERAGING | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of subtomograms used | 87000 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 3.5 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |

# 3 Model quality

## 3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, ZN, MG

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 | 0.38 | 0/5915 | 0.62 | 0/8052 |
| 2 | E | 0.39 | 0/5943 | 0.68 | 1/8064 (0.0%) |
| 3 | B | 0.34 | 0/1327 | 0.61 | 0/1800 |
| All | All | 0.38 | 0/13185 | 0.65 | 1/17916 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | E | 768 | LEU | CA-CB-CG | 5.33 | 127.57 | 115.30 |

There are no chirality outliers.

There are no planarity outliers.

## 3.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5780 | 0 | 5663 | 180 | 0 |
| 2 | E | 5823 | 0 | 5853 | 282 | 0 |
| 3 | B | 1299 | 0 | 1288 | 63 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | E | 1 | 0 | 0 | 0 | 0 |
| 5 | B | 32 | 0 | 13 | 6 | 0 |
| 6 | B | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 12937 | 0 | 12817 | 508 | 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 20.

All (508) 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) |
|---|---|---|---|
| 2:E:147:LEU:HB3 | 2:E:148:PRO:HD2 | 1.16 | 1.13 |
| 2:E:907:ILE:HG22 | 2:E:908:LEU:HG | 1.35 | 1.05 |
| 1:A:176:ILE:CD1 | 2:E:413:ILE:HG12 | 1.87 | 1.03 |
| 1:A:651:ASN:H | 1:A:651:ASN:HD22 | 1.05 | 0.95 |
| 2:E:147:LEU:CB | 2:E:148:PRO:HD2 | 1.97 | 0.94 |
| 2:E:147:LEU:HB3 | 2:E:148:PRO:CD | 2.02 | 0.89 |
| 2:E:441:LYS:HE2 | 2:E:498:ASP:OD2 | 1.72 | 0.88 |
| 2:E:459:ARG:HG2 | 2:E:459:ARG:HH11 | 1.39 | 0.88 |
| 1:A:176:ILE:HD11 | 2:E:413:ILE:HG12 | 1.57 | 0.85 |
| 2:E:352:ASN:HD22 | 2:E:353:ALA:N | 1.75 | 0.85 |
| 2:E:375:MET:HE1 | 2:E:413:ILE:HG21 | 1.57 | 0.84 |
| 2:E:333:LEU:HB2 | 2:E:400:ARG:NH2 | 1.93 | 0.83 |
| 1:A:722:ARG:HD3 | 5:B:201:GNP:H5'1 | 1.59 | 0.83 |
| 1:A:96:LEU:HG | 1:A:97:SER:H | 1.43 | 0.83 |
| 1:A:616:GLU:HG3 | 1:A:620:ASN:HB2 | 1.63 | 0.80 |
| 2:E:919:ILE:O | 2:E:923:ARG:HG3 | 1.83 | 0.79 |
| 2:E:147:LEU:HD13 | 2:E:914:ARG:NH1 | 1.97 | 0.78 |
| 1:A:164:ASN:N | 1:A:164:ASN:HD22 | 1.81 | 0.78 |
| 2:E:680:GLN:HG3 | 2:E:920:MET:HE1 | 1.65 | 0.78 |
| 3:B:140:VAL:HG12 | 3:B:141:SER:N | 1.99 | 0.78 |
| 1:A:723:PHE:CZ | 3:B:53:PRO:HD2 | 2.19 | 0.78 |
| 2:E:147:LEU:O | 2:E:148:PRO:C | 2.22 | 0.77 |
| 1:A:164:ASN:HD22 | 1:A:164:ASN:H | 1.33 | 0.77 |
| 1:A:114:THR:HG22 | 1:A:115:ASN:H | 1.50 | 0.76 |
| 2:E:660:VAL:HG11 | 2:E:741:GLU:HB3 | 1.68 | 0.76 |
| 2:E:296:TYR:O | 2:E:624:ARG:NH1 | 2.19 | 0.75 |
| 2:E:567:ARG:HH21 | 2:E:599:ASN:HD22 | 1.36 | 0.74 |
| 1:A:512:LEU:HD13 | 1:A:516:THR:HG21 | 1.70 | 0.74 |
| 2:E:709:MET:HE1 | 2:E:712:LEU:HD23 | 1.68 | 0.73 |
| 1:A:176:ILE:HD11 | 2:E:413:ILE:CG1 | 2.18 | 0.73 |
| 2:E:142:ASP:CG | 2:E:700:PRO:HB3 | 2.08 | 0.73 |
| 3:B:140:VAL:HG12 | 3:B:141:SER:H | 1.52 | 0.73 |
| 1:A:674:ARG:HA | 1:A:679:GLN:NE2 | 2.04 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:226:GLY:O | 2:E:293:PRO:HG3 | 1.90 | 0.72 |
| 2:E:557:VAL:HG13 | 2:E:582:LEU:HD11 | 1.70 | 0.71 |
| 1:A:722:ARG:NH1 | 5:B:201:GNP:O2A | 2.24 | 0.71 |
| 2:E:493:VAL:HG23 | 2:E:495:ILE:HG13 | 1.73 | 0.71 |
| 1:A:430:ASN:HD22 | 1:A:430:ASN:H | 1.39 | 0.71 |
| 1:A:616:GLU:CG | 1:A:620:ASN:HB2 | 2.21 | 0.71 |
| 1:A:176:ILE:HD12 | 2:E:413:ILE:HG12 | 1.73 | 0.70 |
| 2:E:142:ASP:O | 2:E:146:GLU:HG2 | 1.91 | 0.70 |
| 2:E:225:ASP:OD2 | 2:E:227:LEU:HB3 | 1.90 | 0.70 |
| 2:E:768:LEU:HG | 2:E:769:PRO:HD2 | 1.74 | 0.70 |
| 2:E:279:ASP:HA | 2:E:284:LYS:HE3 | 1.73 | 0.70 |
| 2:E:696:ALA:HB2 | 2:E:702:ARG:HH21 | 1.57 | 0.69 |
| 1:A:347:ALA:HB2 | 1:A:353:ILE:HD13 | 1.73 | 0.69 |
| 2:E:459:ARG:HG2 | 2:E:459:ARG:NH1 | 2.07 | 0.69 |
| 1:A:114:THR:HG22 | 1:A:115:ASN:N | 2.07 | 0.69 |
| 3:B:36:LYS:HG2 | 3:B:97:LEU:HD13 | 1.75 | 0.68 |
| 1:A:399:ALA:HB3 | 1:A:450:LEU:HD13 | 1.74 | 0.68 |
| 2:E:699:ALA:HB1 | 2:E:921:LYS:NZ | 2.08 | 0.68 |
| 2:E:801:LEU:HD11 | 2:E:808:LEU:HD22 | 1.74 | 0.68 |
| 2:E:154:LEU:HG | 2:E:709:MET:HE2 | 1.75 | 0.68 |
| 2:E:766:ALA:O | 2:E:768:LEU:N | 2.26 | 0.67 |
| 1:A:96:LEU:CG | 1:A:97:SER:H | 2.07 | 0.67 |
| 1:A:651:ASN:H | 1:A:651:ASN:ND2 | 1.85 | 0.67 |
| 2:E:764:ASP:HA | 2:E:851:ARG:HH22 | 1.60 | 0.67 |
| 2:E:362:ASP:OD1 | 2:E:401:GLN:HB2 | 1.95 | 0.67 |
| 2:E:312:VAL:HG11 | 2:E:414:PHE:CD1 | 2.30 | 0.66 |
| 3:B:61:GLU:OE1 | 3:B:68:LYS:HE2 | 1.95 | 0.66 |
| 2:E:303:PRO:HG3 | 2:E:342:ARG:CZ | 2.25 | 0.66 |
| 2:E:312:VAL:HG11 | 2:E:414:PHE:CG | 2.31 | 0.66 |
| 3:B:130:LEU:HD22 | 3:B:171:CYS:SG | 2.35 | 0.66 |
| 1:A:634:MET:HE1 | 1:A:686:ASP:O | 1.96 | 0.65 |
| 2:E:812:MET:SD | 2:E:820:LEU:HD22 | 2.35 | 0.65 |
| 2:E:149:PRO:O | 2:E:151:ILE:HG12 | 1.97 | 0.65 |
| 2:E:750:LYS:HE3 | 2:E:805:GLY:HA2 | 1.77 | 0.65 |
| 2:E:399:CYS:O | 2:E:403:ILE:HG13 | 1.97 | 0.65 |
| 1:A:177:ASP:OD1 | 1:A:237:LYS:HE3 | 1.96 | 0.65 |
| 2:E:297:THR:HG22 | 2:E:624:ARG:HD3 | 1.79 | 0.65 |
| 1:A:323:LYS:O | 1:A:327:LYS:HG2 | 1.97 | 0.65 |
| 1:A:719:SER:OG | 3:B:33:ASN:HB2 | 1.96 | 0.65 |
| 2:E:422:PHE:H | 2:E:451:ASN:HB3 | 1.61 | 0.65 |
| 2:E:672:ARG:HH11 | 2:E:725:SER:HB3 | 1.62 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:856:ILE:HD13 | 2:E:871:LEU:HD22 | 1.79 | 0.65 |
| 1:A:757:THR:O | 1:A:761:GLN:HG3 | 1.97 | 0.64 |
| 2:E:525:PHE:CE2 | 2:E:527:PRO:HG3 | 2.33 | 0.64 |
| 2:E:920:MET:HE3 | 2:E:920:MET:HA | 1.78 | 0.64 |
| 1:A:164:ASN:H | 1:A:164:ASN:ND2 | 1.94 | 0.64 |
| 1:A:432:ILE:HD13 | 1:A:442:THR:HA | 1.78 | 0.64 |
| 2:E:817:VAL:C | 2:E:819:ALA:H | 2.01 | 0.64 |
| 2:E:750:LYS:HD2 | 2:E:803:ASP:OD2 | 1.98 | 0.64 |
| 2:E:914:ARG:O | 2:E:918:GLN:HG2 | 1.98 | 0.63 |
| 2:E:789:ALA:O | 2:E:904:GLU:HB2 | 1.98 | 0.63 |
| 2:E:147:LEU:HD13 | 2:E:914:ARG:HH12 | 1.61 | 0.63 |
| 3:B:164:ARG:HG2 | 3:B:166:VAL:HG23 | 1.80 | 0.63 |
| 2:E:255:PHE:CZ | 2:E:612:GLN:HB2 | 2.33 | 0.63 |
| 2:E:312:VAL:HG12 | 2:E:312:VAL:O | 1.99 | 0.63 |
| 2:E:818:PRO:C | 2:E:820:LEU:H | 2.00 | 0.63 |
| 2:E:680:GLN:CG | 2:E:920:MET:HE1 | 2.29 | 0.63 |
| 1:A:170:ASP:C | 1:A:171:LEU:HD12 | 2.20 | 0.63 |
| 2:E:808:LEU:O | 2:E:871:LEU:HD12 | 1.98 | 0.62 |
| 2:E:424:LEU:HG | 2:E:428:LEU:HD22 | 1.81 | 0.62 |
| 2:E:449:LEU:HD12 | 2:E:450:PRO:HD2 | 1.82 | 0.62 |
| 2:E:352:ASN:HD22 | 2:E:353:ALA:H | 1.47 | 0.62 |
| 1:A:96:LEU:HD21 | 1:A:101:MET:SD | 2.39 | 0.62 |
| 1:A:136:ASN:HD21 | 1:A:374:ALA:HB1 | 1.65 | 0.62 |
| 1:A:176:ILE:CD1 | 2:E:413:ILE:CG1 | 2.70 | 0.62 |
| 2:E:539:LYS:HA | 2:E:868:TYR:CD2 | 2.34 | 0.62 |
| 1:A:219:VAL:HG22 | 1:A:225:ASN:ND2 | 2.14 | 0.62 |
| 3:B:154:THR:HB | 3:B:166:VAL:O | 2.00 | 0.62 |
| 1:A:19:PHE:HB2 | 1:A:511:LEU:HD23 | 1.80 | 0.61 |
| 1:A:183:ARG:NH1 | 2:E:383:GLU:HB2 | 2.15 | 0.61 |
| 2:E:135:MET:HE2 | 2:E:641:GLU:OE1 | 2.00 | 0.61 |
| 1:A:634:MET:HA | 1:A:634:MET:HE3 | 1.81 | 0.61 |
| 3:B:140:VAL:CG1 | 3:B:141:SER:H | 2.12 | 0.61 |
| 2:E:205:LEU:HD13 | 2:E:611:VAL:HG11 | 1.83 | 0.61 |
| 1:A:723:PHE:CE2 | 3:B:53:PRO:HD2 | 2.36 | 0.60 |
| 2:E:270:ASP:HB2 | 2:E:273:ASP:HB3 | 1.83 | 0.60 |
| 1:A:651:ASN:HD22 | 1:A:651:ASN:N | 1.81 | 0.60 |
| 2:E:699:ALA:HB1 | 2:E:921:LYS:HZ1 | 1.67 | 0.60 |
| 3:B:23:HIS:CD2 | 3:B:67:ILE:HA | 2.36 | 0.60 |
| 2:E:524:HIS:CE1 | 2:E:866:ILE:HD11 | 2.37 | 0.60 |
| 1:A:618:THR:O | 1:A:622:LEU:HG | 2.01 | 0.60 |
| 2:E:375:MET:CE | 2:E:413:ILE:HG21 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:681:ASP:HB2 | 1:A:682:PRO:HD2 | 1.84 | 0.59 |
| 2:E:764:ASP:HA | 2:E:851:ARG:NH2 | 2.17 | 0.59 |
| 2:E:687:LYS:NZ | 2:E:925:SER:HA | 2.15 | 0.59 |
| 1:A:722:ARG:CD | 5:B:201:GNP:H5'1 | 2.32 | 0.59 |
| 2:E:333:LEU:HB2 | 2:E:400:ARG:CZ | 2.32 | 0.59 |
| 2:E:539:LYS:HE3 | 2:E:543:GLU:OE2 | 2.02 | 0.59 |
| 1:A:723:PHE:CE1 | 3:B:52:GLN:HB2 | 2.38 | 0.59 |
| 2:E:209:PRO:HG3 | 2:E:558:MET:CE | 2.32 | 0.59 |
| 3:B:140:VAL:CG1 | 3:B:141:SER:N | 2.65 | 0.59 |
| 2:E:668:LEU:HG | 2:E:672:ARG:HH21 | 1.67 | 0.59 |
| 2:E:729:PRO:HB2 | 2:E:732:HIS:HD2 | 1.68 | 0.59 |
| 1:A:511:LEU:O | 1:A:512:LEU:HD23 | 2.03 | 0.59 |
| 2:E:138:LEU:HD22 | 2:E:704:CYS:HB3 | 1.85 | 0.58 |
| 1:A:10:ASN:O | 1:A:12:VAL:HG23 | 2.03 | 0.58 |
| 2:E:915:GLU:O | 2:E:919:ILE:HG13 | 2.02 | 0.58 |
| 2:E:209:PRO:HG3 | 2:E:558:MET:HE1 | 1.85 | 0.58 |
| 2:E:378:ILE:HD11 | 2:E:387:PRO:HG3 | 1.86 | 0.58 |
| 2:E:728:VAL:HG21 | 2:E:733:ARG:NH2 | 2.18 | 0.58 |
| 2:E:228:ILE:HD13 | 2:E:290:TYR:CD2 | 2.38 | 0.58 |
| 2:E:667:SER:HB3 | 2:E:670:ASP:HB2 | 1.85 | 0.58 |
| 1:A:44:ASP:O | 1:A:45:GLU:HG3 | 2.04 | 0.58 |
| 2:E:133:ARG:NH2 | 2:E:635:THR:O | 2.36 | 0.58 |
| 3:B:140:VAL:CG1 | 3:B:144:GLU:HB2 | 2.34 | 0.58 |
| 3:B:141:SER:OG | 3:B:144:GLU:HG3 | 2.03 | 0.58 |
| 1:A:234:VAL:HG12 | 1:A:234:VAL:O | 2.04 | 0.57 |
| 2:E:849:ASN:OD1 | 2:E:853:ARG:HD3 | 2.04 | 0.57 |
| 3:B:83:LEU:O | 3:B:86:ASP:HB2 | 2.04 | 0.57 |
| 2:E:672:ARG:NH1 | 2:E:725:SER:HB3 | 2.19 | 0.57 |
| 2:E:872:TYR:CE2 | 2:E:897:TRP:HZ3 | 2.23 | 0.57 |
| 3:B:23:HIS:HD2 | 3:B:67:ILE:HA | 1.70 | 0.57 |
| 2:E:563:SER:HB3 | 2:E:610:TYR:H | 1.68 | 0.57 |
| 1:A:450:LEU:N | 1:A:450:LEU:HD12 | 2.19 | 0.57 |
| 2:E:272:ASN:O | 2:E:274:PRO:HD3 | 2.03 | 0.57 |
| 2:E:352:ASN:ND2 | 2:E:353:ALA:N | 2.49 | 0.57 |
| 2:E:593:SER:HB2 | 2:E:744:PRO:HA | 1.86 | 0.57 |
| 2:E:802:ILE:O | 2:E:808:LEU:HD23 | 2.05 | 0.57 |
| 2:E:147:LEU:HD13 | 2:E:914:ARG:CZ | 2.34 | 0.56 |
| 1:A:102:PRO:HD2 | 1:A:105:LEU:HD12 | 1.87 | 0.56 |
| 2:E:303:PRO:HG3 | 2:E:342:ARG:NH1 | 2.19 | 0.56 |
| 1:A:373:ASP:OD1 | 3:B:55:TRP:NE1 | 2.37 | 0.56 |
| 3:B:122:LEU:O | 3:B:164:ARG:NH2 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:696:ALA:CB | 2:E:702:ARG:HH21 | 2.18 | 0.56 |
| 1:A:145:ILE:HA | 1:A:148:LEU:HD12 | 1.88 | 0.56 |
| 1:A:635:GLU:H | 1:A:635:GLU:CD | 2.08 | 0.56 |
| 2:E:488:ILE:HD11 | 2:E:578:ARG:HH22 | 1.71 | 0.56 |
| 1:A:679:GLN:HG3 | 1:A:687:PHE:CE2 | 2.41 | 0.55 |
| 1:A:68:TYR:O | 1:A:81:PRO:HG3 | 2.07 | 0.55 |
| 1:A:219:VAL:HG22 | 1:A:225:ASN:HD22 | 1.71 | 0.55 |
| 1:A:46:LEU:HD12 | 1:A:47:ASN:H | 1.71 | 0.55 |
| 3:B:137:PRO:HG2 | 3:B:138:ASN:H | 1.71 | 0.55 |
| 1:A:65:LEU:HD11 | 1:A:105:LEU:HD21 | 1.88 | 0.55 |
| 1:A:455:SER:O | 1:A:534:ARG:NH2 | 2.40 | 0.55 |
| 2:E:809:PHE:CD2 | 2:E:898:ALA:HB2 | 2.42 | 0.55 |
| 1:A:77:SER:HA | 1:A:89:LEU:HB2 | 1.88 | 0.55 |
| 1:A:634:MET:HA | 1:A:634:MET:CE | 2.36 | 0.55 |
| 3:B:57:PRO:HB3 | 3:B:74:LEU:HD13 | 1.89 | 0.55 |
| 3:B:102:ASP:N | 3:B:103:PRO:HD3 | 2.22 | 0.55 |
| 2:E:677:LYS:HG2 | 2:E:681:ASP:OD2 | 2.06 | 0.54 |
| 2:E:822:PHE:N | 2:E:822:PHE:CD1 | 2.74 | 0.54 |
| 1:A:564:ALA:HB2 | 1:A:576:LEU:HD13 | 1.89 | 0.54 |
| 1:A:566:TYR:CG | 1:A:764:VAL:HG12 | 2.42 | 0.54 |
| 1:A:679:GLN:HG2 | 1:A:691:LEU:CD1 | 2.38 | 0.54 |
| 1:A:583:TYR:HB3 | 1:A:584:PRO:HD3 | 1.88 | 0.54 |
| 1:A:411:ASP:OD1 | 1:A:411:ASP:N | 2.33 | 0.54 |
| 1:A:761:GLN:O | 1:A:765:SER:HB2 | 2.07 | 0.54 |
| 2:E:410:ILE:HB | 2:E:411:PRO:HD3 | 1.89 | 0.54 |
| 2:E:496:THR:HA | 2:E:519:THR:HB | 1.89 | 0.54 |
| 2:E:146:GLU:O | 2:E:147:LEU:O | 2.26 | 0.54 |
| 2:E:216:ASP:O | 2:E:219:PRO:HD3 | 2.07 | 0.54 |
| 2:E:277:ARG:O | 2:E:279:ASP:N | 2.41 | 0.54 |
| 1:A:644:ASP:OD1 | 1:A:645:SER:N | 2.41 | 0.54 |
| 2:E:142:ASP:OD2 | 2:E:700:PRO:HB3 | 2.08 | 0.54 |
| 2:E:429:LYS:HD2 | 2:E:454:ILE:CD1 | 2.38 | 0.54 |
| 1:A:114:THR:HG22 | 1:A:116:LYS:H | 1.72 | 0.54 |
| 2:E:801:LEU:HD12 | 2:E:809:PHE:O | 2.07 | 0.54 |
| 1:A:722:ARG:HD3 | 5:B:201:GNP:C5' | 2.34 | 0.53 |
| 2:E:361:LEU:HD22 | 2:E:398:ALA:HB1 | 1.90 | 0.53 |
| 1:A:96:LEU:HD11 | 1:A:102:PRO:HD3 | 1.90 | 0.53 |
| 2:E:191:LYS:HE3 | 2:E:604:ILE:O | 2.08 | 0.53 |
| 2:E:147:LEU:CB | 2:E:148:PRO:CD | 2.74 | 0.53 |
| 2:E:699:ALA:N | 2:E:700:PRO:HD3 | 2.24 | 0.53 |
| 1:A:171:LEU:HD22 | 1:A:234:VAL:HG11 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:162:VAL:O | 2:E:634:PRO:HG3 | 2.08 | 0.53 |
| 2:E:601:ASP:OD1 | 2:E:602:GLU:N | 2.41 | 0.53 |
| 2:E:819:ALA:HA | 2:E:822:PHE:CE1 | 2.44 | 0.53 |
| 3:B:82:ARG:O | 3:B:85:LYS:HE2 | 2.09 | 0.53 |
| 3:B:50:THR:O | 3:B:50:THR:HG23 | 2.07 | 0.53 |
| 2:E:346:SER:OG | 2:E:393:VAL:HG22 | 2.09 | 0.52 |
| 3:B:155:THR:CG2 | 3:B:166:VAL:H | 2.22 | 0.52 |
| 1:A:723:PHE:O | 1:A:727:LYS:HG2 | 2.09 | 0.52 |
| 2:E:352:ASN:HA | 2:E:452:LEU:HD23 | 1.90 | 0.52 |
| 2:E:754:PRO:HG3 | 2:E:901:THR:O | 2.09 | 0.52 |
| 2:E:250:ARG:HB3 | 2:E:260:ASN:O | 2.09 | 0.52 |
| 3:B:128:VAL:HG23 | 3:B:186:LEU:HD13 | 1.91 | 0.52 |
| 2:E:303:PRO:HG3 | 2:E:342:ARG:NH2 | 2.24 | 0.52 |
| 2:E:822:PHE:N | 2:E:822:PHE:HD1 | 2.08 | 0.52 |
| 3:B:32:ASP:OD1 | 3:B:77:HIS:HA | 2.10 | 0.52 |
| 2:E:498:ASP:C | 2:E:499:LEU:HD12 | 2.29 | 0.52 |
| 1:A:365:THR:HB | 1:A:448:ALA:HB3 | 1.92 | 0.52 |
| 1:A:682:PRO:C | 1:A:684:TYR:H | 2.13 | 0.52 |
| 2:E:519:THR:O | 2:E:520:ALA:HB3 | 2.10 | 0.52 |
| 2:E:533:ASN:HB3 | 2:E:536:ASP:OD2 | 2.10 | 0.52 |
| 2:E:162:VAL:O | 2:E:163:ILE:HD13 | 2.10 | 0.52 |
| 3:B:136:ALA:HB1 | 3:B:137:PRO:HD2 | 1.92 | 0.52 |
| 2:E:704:CYS:SG | 2:E:707:LEU:HD12 | 2.50 | 0.52 |
| 3:B:155:THR:HG23 | 3:B:156:GLY:N | 2.25 | 0.52 |
| 2:E:817:VAL:O | 2:E:819:ALA:N | 2.42 | 0.51 |
| 2:E:420:THR:HG22 | 2:E:420:THR:O | 2.10 | 0.51 |
| 3:B:155:THR:HG22 | 3:B:166:VAL:H | 1.75 | 0.51 |
| 2:E:715:HIS:HB2 | 2:E:916:PHE:CE2 | 2.45 | 0.51 |
| 1:A:682:PRO:O | 1:A:683:GLN:HB3 | 2.10 | 0.51 |
| 2:E:406:LEU:O | 2:E:410:ILE:HG13 | 2.10 | 0.51 |
| 1:A:176:ILE:CG1 | 2:E:413:ILE:HG12 | 2.41 | 0.51 |
| 2:E:906:LYS:O | 2:E:907:ILE:HD13 | 2.11 | 0.51 |
| 2:E:860:ARG:HG2 | 2:E:869:GLN:HB2 | 1.93 | 0.51 |
| 2:E:516:SER:HB2 | 2:E:521:GLY:C | 2.31 | 0.50 |
| 1:A:430:ASN:H | 1:A:430:ASN:ND2 | 2.06 | 0.50 |
| 1:A:171:LEU:HD12 | 1:A:171:LEU:N | 2.26 | 0.50 |
| 2:E:372:GLN:HG2 | 2:E:373:ILE:N | 2.26 | 0.50 |
| 2:E:516:SER:HB2 | 2:E:522:GLN:N | 2.26 | 0.50 |
| 2:E:710:PHE:HB3 | 2:E:711:PRO:HD3 | 1.93 | 0.50 |
| 2:E:715:HIS:CE1 | 2:E:719:LYS:HE3 | 2.46 | 0.50 |
| 2:E:817:VAL:C | 2:E:819:ALA:N | 2.64 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:907:ILE:HG22 | 2:E:908:LEU:N | 2.27 | 0.50 |
| 2:E:279:ASP:CA | 2:E:284:LYS:HE3 | 2.39 | 0.50 |
| 3:B:107:ASP:O | 3:B:111:VAL:HG23 | 2.11 | 0.50 |
| 2:E:722:ALA:HB1 | 2:E:737:LEU:CD2 | 2.41 | 0.50 |
| 2:E:768:LEU:CG | 2:E:769:PRO:HD2 | 2.41 | 0.50 |
| 1:A:144:ILE:O | 1:A:148:LEU:HG | 2.11 | 0.50 |
| 1:A:645:SER:HA | 1:A:728:LEU:HD13 | 1.94 | 0.50 |
| 1:A:739:ARG:HG3 | 1:A:739:ARG:HH11 | 1.76 | 0.50 |
| 2:E:911:GLU:HG3 | 2:E:919:ILE:HD11 | 1.94 | 0.50 |
| 2:E:680:GLN:CB | 2:E:920:MET:HE1 | 2.42 | 0.49 |
| 2:E:703:LEU:HG | 2:E:704:CYS:H | 1.77 | 0.49 |
| 2:E:722:ALA:HB1 | 2:E:737:LEU:HD23 | 1.92 | 0.49 |
| 2:E:764:ASP:CA | 2:E:851:ARG:HH22 | 2.24 | 0.49 |
| 3:B:176:ARG:HA | 3:B:179:TYR:HE2 | 1.77 | 0.49 |
| 1:A:644:ASP:OD2 | 1:A:731:SER:HB3 | 2.12 | 0.49 |
| 2:E:417:ASN:OD1 | 2:E:419:ILE:N | 2.42 | 0.49 |
| 2:E:448:THR:HG22 | 2:E:449:LEU:O | 2.11 | 0.49 |
| 2:E:589:PRO:O | 2:E:590:ARG:HD3 | 2.13 | 0.49 |
| 3:B:172:SER:OG | 3:B:175:MET:HG2 | 2.12 | 0.49 |
| 2:E:504:GLU:OE2 | 2:E:530:SER:HB3 | 2.12 | 0.49 |
| 1:A:147:SER:HB3 | 1:A:384:TYR:CE2 | 2.48 | 0.49 |
| 1:A:179:CYS:O | 2:E:377:ASP:HB2 | 2.13 | 0.49 |
| 1:A:395:TYR:CD1 | 1:A:497:SER:HA | 2.48 | 0.49 |
| 2:E:215:ASP:O | 2:E:219:PRO:HG3 | 2.13 | 0.49 |
| 1:A:183:ARG:HH12 | 2:E:383:GLU:HB2 | 1.78 | 0.49 |
| 3:B:140:VAL:HG13 | 3:B:144:GLU:CD | 2.33 | 0.49 |
| 1:A:66:ASN:HD22 | 1:A:68:TYR:H | 1.60 | 0.49 |
| 3:B:88:PHE:N | 3:B:89:PRO:CD | 2.76 | 0.49 |
| 2:E:338:ASN:OD1 | 2:E:341:GLU:HA | 2.13 | 0.48 |
| 2:E:855:ILE:O | 2:E:858:GLN:HB3 | 2.12 | 0.48 |
| 2:E:192:ASN:HA | 2:E:603:SER:HA | 1.96 | 0.48 |
| 2:E:423:ALA:HA | 2:E:452:LEU:O | 2.13 | 0.48 |
| 2:E:499:LEU:HD12 | 2:E:499:LEU:N | 2.27 | 0.48 |
| 2:E:795:GLU:C | 2:E:797:TYR:H | 2.16 | 0.48 |
| 1:A:96:LEU:CG | 1:A:97:SER:N | 2.76 | 0.48 |
| 1:A:171:LEU:CD2 | 1:A:234:VAL:HG11 | 2.43 | 0.48 |
| 1:A:390:LYS:HD2 | 1:A:390:LYS:N | 2.28 | 0.48 |
| 1:A:96:LEU:HG | 1:A:97:SER:N | 2.18 | 0.48 |
| 2:E:312:VAL:O | 2:E:312:VAL:CG1 | 2.61 | 0.48 |
| 2:E:667:SER:HB3 | 2:E:670:ASP:CB | 2.44 | 0.48 |
| 2:E:795:GLU:HB3 | 2:E:797:TYR:CE2 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:687:LYS:HZ1 | 2:E:925:SER:HA | 1.77 | 0.48 |
| 3:B:176:ARG:HA | 3:B:179:TYR:CE2 | 2.48 | 0.48 |
| 2:E:356:TYR:OH | 2:E:430:SER:HB3 | 2.13 | 0.48 |
| 3:B:85:LYS:HA | 3:B:88:PHE:CD2 | 2.48 | 0.48 |
| 2:E:250:ARG:HA | 2:E:262:VAL:HG23 | 1.94 | 0.48 |
| 1:A:739:ARG:HG2 | 1:A:744:ILE:HD11 | 1.96 | 0.48 |
| 2:E:177:ALA:HB1 | 2:E:182:ILE:HG22 | 1.96 | 0.48 |
| 3:B:99:ASP:OD1 | 3:B:133:LYS:HD2 | 2.14 | 0.48 |
| 2:E:715:HIS:NE2 | 2:E:719:LYS:HE3 | 2.29 | 0.47 |
| 3:B:23:HIS:HD2 | 3:B:68:LYS:H | 1.62 | 0.47 |
| 2:E:133:ARG:NE | 2:E:135:MET:SD | 2.87 | 0.47 |
| 2:E:230:ARG:HD3 | 2:E:237:TYR:CD2 | 2.49 | 0.47 |
| 2:E:488:ILE:HD11 | 2:E:578:ARG:NH2 | 2.28 | 0.47 |
| 2:E:277:ARG:C | 2:E:279:ASP:H | 2.18 | 0.47 |
| 2:E:352:ASN:HD22 | 2:E:352:ASN:C | 2.12 | 0.47 |
| 2:E:534:PRO:O | 2:E:538:VAL:HG23 | 2.13 | 0.47 |
| 2:E:794:PHE:HA | 2:E:800:TYR:CZ | 2.48 | 0.47 |
| 3:B:103:PRO:HG3 | 3:B:140:VAL:HG21 | 1.96 | 0.47 |
| 3:B:134:ILE:HG12 | 3:B:172:SER:HB2 | 1.96 | 0.47 |
| 2:E:150:PRO:HG2 | 2:E:708:ARG:HH11 | 1.77 | 0.47 |
| 2:E:796:ARG:NH1 | 2:E:815:ASP:OD2 | 2.47 | 0.47 |
| 1:A:114:THR:CG2 | 1:A:115:ASN:N | 2.76 | 0.47 |
| 1:A:451:SER:C | 1:A:453:TYR:H | 2.17 | 0.47 |
| 2:E:388:ARG:HB2 | 2:E:389:PRO:HD2 | 1.97 | 0.47 |
| 2:E:818:PRO:C | 2:E:820:LEU:N | 2.66 | 0.47 |
| 1:A:679:GLN:HG3 | 1:A:687:PHE:HE2 | 1.79 | 0.47 |
| 1:A:42:GLU:OE2 | 1:A:397:LYS:HE2 | 2.14 | 0.47 |
| 1:A:616:GLU:CG | 1:A:620:ASN:CB | 2.91 | 0.47 |
| 2:E:230:ARG:HD2 | 2:E:235:ARG:O | 2.15 | 0.47 |
| 2:E:302:PRO:HA | 2:E:303:PRO:HD3 | 1.73 | 0.47 |
| 2:E:580:SER:O | 2:E:581:ASP:HB2 | 2.14 | 0.47 |
| 1:A:17:ASN:HB2 | 1:A:522:SER:HB2 | 1.96 | 0.47 |
| 2:E:149:PRO:O | 2:E:150:PRO:C | 2.53 | 0.47 |
| 2:E:352:ASN:HD22 | 2:E:352:ASN:N | 2.11 | 0.47 |
| 1:A:114:THR:CG2 | 1:A:115:ASN:H | 2.23 | 0.47 |
| 1:A:164:ASN:HD22 | 1:A:165:VAL:H | 1.63 | 0.47 |
| 3:B:32:ASP:HB3 | 3:B:77:HIS:N | 2.29 | 0.47 |
| 1:A:343:VAL:O | 1:A:362:THR:HG22 | 2.16 | 0.46 |
| 2:E:325:THR:OG1 | 2:E:445:VAL:HG11 | 2.15 | 0.46 |
| 2:E:848:PHE:O | 2:E:851:ARG:HB2 | 2.15 | 0.46 |
| 2:E:352:ASN:ND2 | 2:E:352:ASN:C | 2.67 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:66:ASN:HD21 | 1:A:68:TYR:HB2 | 1.80 | 0.46 |
| 2:E:761:ASP:O | 2:E:762:MET:O | 2.33 | 0.46 |
| 2:E:920:MET:HE3 | 2:E:920:MET:CA | 2.44 | 0.46 |
| 3:B:137:PRO:C | 3:B:139:ALA:H | 2.18 | 0.46 |
| 1:A:485:ALA:HB2 | 1:A:511:LEU:HD11 | 1.97 | 0.46 |
| 1:A:561:GLN:HG2 | 1:A:763:ALA:HA | 1.96 | 0.46 |
| 2:E:378:ILE:CD1 | 2:E:387:PRO:HG3 | 2.45 | 0.46 |
| 3:B:62:LEU:HD12 | 3:B:71:THR:HG21 | 1.97 | 0.46 |
| 1:A:687:PHE:CE2 | 1:A:691:LEU:HD11 | 2.51 | 0.46 |
| 2:E:205:LEU:CD1 | 2:E:611:VAL:HG11 | 2.44 | 0.46 |
| 2:E:170:VAL:HG12 | 2:E:170:VAL:O | 2.16 | 0.46 |
| 2:E:249:ARG:O | 2:E:250:ARG:HG2 | 2.15 | 0.46 |
| 2:E:314:GLN:CG | 2:E:318:LYS:HE3 | 2.46 | 0.46 |
| 2:E:378:ILE:HD13 | 2:E:385:PHE:CZ | 2.51 | 0.46 |
| 1:A:594:GLN:HE21 | 1:A:601:ASN:HD21 | 1.63 | 0.46 |
| 2:E:224:GLU:HA | 2:E:291:MET:HG3 | 1.96 | 0.46 |
| 3:B:32:ASP:O | 3:B:105:ARG:NH2 | 2.49 | 0.46 |
| 2:E:144:LEU:HD22 | 2:E:918:GLN:NE2 | 2.31 | 0.46 |
| 2:E:600:VAL:HG13 | 2:E:604:ILE:HD11 | 1.96 | 0.46 |
| 2:E:133:ARG:HG3 | 2:E:135:MET:HG2 | 1.97 | 0.45 |
| 2:E:279:ASP:C | 2:E:284:LYS:HE3 | 2.36 | 0.45 |
| 2:E:417:ASN:HD21 | 2:E:419:ILE:HD12 | 1.81 | 0.45 |
| 3:B:97:LEU:HD12 | 3:B:97:LEU:N | 2.31 | 0.45 |
| 1:A:642:LEU:O | 1:A:644:ASP:N | 2.48 | 0.45 |
| 2:E:557:VAL:CG1 | 2:E:582:LEU:HD11 | 2.44 | 0.45 |
| 1:A:551:TRP:CE3 | 1:A:552:LEU:HD13 | 2.50 | 0.45 |
| 2:E:212:HIS:O | 2:E:590:ARG:HB3 | 2.16 | 0.45 |
| 1:A:556:LEU:HD22 | 1:A:587:THR:HG21 | 1.98 | 0.45 |
| 2:E:668:LEU:HD21 | 2:E:733:ARG:NH1 | 2.31 | 0.45 |
| 2:E:750:LYS:HE3 | 2:E:805:GLY:CA | 2.46 | 0.45 |
| 1:A:96:LEU:HD11 | 1:A:101:MET:HA | 1.97 | 0.45 |
| 2:E:506:TYR:CE2 | 2:E:508:ASP:HB2 | 2.52 | 0.45 |
| 3:B:31:LEU:HD22 | 3:B:81:ARG:NH2 | 2.31 | 0.45 |
| 1:A:19:PHE:HB2 | 1:A:511:LEU:CD2 | 2.44 | 0.45 |
| 1:A:464:ASN:ND2 | 1:A:465:THR:H | 2.15 | 0.45 |
| 2:E:150:PRO:HG2 | 2:E:708:ARG:HD3 | 1.97 | 0.45 |
| 3:B:110:ARG:HH11 | 3:B:110:ARG:HG3 | 1.82 | 0.45 |
| 1:A:187:GLU:HB2 | 1:A:296:PRO:HG3 | 1.99 | 0.45 |
| 1:A:371:LEU:HG | 3:B:55:TRP:CH2 | 2.52 | 0.45 |
| 2:E:313:SER:O | 2:E:317:ILE:HG12 | 2.16 | 0.45 |
| 2:E:795:GLU:O | 2:E:797:TYR:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:37:THR:HG22 | 3:B:51:LEU:HD13 | 1.99 | 0.45 |
| 1:A:15:THR:HG22 | 1:A:528:ALA:HA | 1.99 | 0.45 |
| 1:A:661:PHE:HA | 1:A:709:PRO:HB2 | 1.97 | 0.45 |
| 1:A:734:TYR:HA | 1:A:744:ILE:HG21 | 1.98 | 0.45 |
| 2:E:419:ILE:HG22 | 2:E:421:ASN:H | 1.82 | 0.45 |
| 2:E:900:SER:HA | 2:E:907:ILE:HG21 | 1.98 | 0.45 |
| 1:A:432:ILE:CD1 | 1:A:442:THR:HA | 2.44 | 0.45 |
| 2:E:919:ILE:HG22 | 2:E:923:ARG:HD2 | 2.00 | 0.45 |
| 1:A:69:CYS:SG | 1:A:81:PRO:HD3 | 2.57 | 0.44 |
| 2:E:309:LEU:C | 2:E:309:LEU:HD12 | 2.38 | 0.44 |
| 1:A:653:ILE:HG13 | 1:A:670:ILE:HD13 | 1.99 | 0.44 |
| 2:E:756:VAL:O | 2:E:786:PRO:HA | 2.17 | 0.44 |
| 1:A:111:GLU:HB2 | 1:A:503:ARG:HD3 | 1.99 | 0.44 |
| 2:E:822:PHE:HD1 | 2:E:822:PHE:H | 1.63 | 0.44 |
| 2:E:908:LEU:C | 2:E:910:ASN:H | 2.21 | 0.44 |
| 3:B:85:LYS:HA | 3:B:88:PHE:CE2 | 2.52 | 0.44 |
| 3:B:134:ILE:CG1 | 3:B:172:SER:HB2 | 2.47 | 0.44 |
| 3:B:155:THR:OG1 | 3:B:156:GLY:N | 2.50 | 0.44 |
| 1:A:550:ARG:O | 1:A:554:ARG:HG3 | 2.18 | 0.44 |
| 2:E:147:LEU:O | 2:E:149:PRO:N | 2.50 | 0.44 |
| 2:E:300:GLN:O | 2:E:301:PRO:C | 2.56 | 0.44 |
| 2:E:791:SER:H | 2:E:905:ASP:CG | 2.20 | 0.44 |
| 1:A:66:ASN:ND2 | 1:A:68:TYR:H | 2.16 | 0.44 |
| 2:E:135:MET:HE1 | 2:E:634:PRO:HB2 | 1.99 | 0.44 |
| 2:E:223:ASN:O | 2:E:291:MET:HG2 | 2.17 | 0.44 |
| 2:E:250:ARG:HD2 | 2:E:260:ASN:O | 2.18 | 0.44 |
| 2:E:344:ARG:HA | 2:E:394:VAL:O | 2.18 | 0.44 |
| 2:E:764:ASP:O | 2:E:851:ARG:NH2 | 2.51 | 0.44 |
| 1:A:588:TYR:O | 1:A:591:ARG:HG2 | 2.18 | 0.44 |
| 2:E:147:LEU:CD1 | 2:E:914:ARG:NH1 | 2.77 | 0.44 |
| 2:E:361:LEU:HD23 | 2:E:399:CYS:SG | 2.58 | 0.44 |
| 1:A:46:LEU:HG | 1:A:47:ASN:N | 2.32 | 0.44 |
| 2:E:253:CYS:SG | 2:E:255:PHE:HB2 | 2.58 | 0.44 |
| 2:E:783:LEU:HA | 2:E:784:PRO:HD3 | 1.81 | 0.44 |
| 3:B:155:THR:HG21 | 3:B:165:PRO:HA | 2.00 | 0.44 |
| 1:A:283:ARG:NE | 1:A:344:ASP:OD2 | 2.51 | 0.44 |
| 1:A:722:ARG:HD3 | 5:B:201:GNP:C3' | 2.47 | 0.44 |
| 2:E:672:ARG:NH1 | 2:E:725:SER:HA | 2.32 | 0.44 |
| 1:A:430:ASN:ND2 | 1:A:430:ASN:N | 2.65 | 0.43 |
| 2:E:571:PHE:HD2 | 2:E:596:PHE:CE1 | 2.36 | 0.43 |
| 1:A:138:ASP:HA | 1:A:141:LYS:HD2 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:561:GLN:CG | 1:A:763:ALA:HA | 2.47 | 0.43 |
| 2:E:209:PRO:CG | 2:E:558:MET:CE | 2.97 | 0.43 |
| 2:E:242:VAL:CG1 | 2:E:251:TRP:HB2 | 2.48 | 0.43 |
| 3:B:40:LEU:HD22 | 3:B:73:ASP:HB2 | 1.99 | 0.43 |
| 2:E:424:LEU:O | 2:E:428:LEU:HB2 | 2.17 | 0.43 |
| 1:A:44:ASP:C | 1:A:45:GLU:HG3 | 2.37 | 0.43 |
| 1:A:90:PRO:HA | 1:A:91:PRO:HD3 | 1.85 | 0.43 |
| 2:E:163:ILE:HD13 | 2:E:634:PRO:HG3 | 2.00 | 0.43 |
| 2:E:789:ALA:HB1 | 2:E:902:LEU:HA | 2.01 | 0.43 |
| 1:A:15:THR:HG23 | 1:A:531:LEU:HD12 | 2.00 | 0.43 |
| 1:A:281:PRO:HB3 | 1:A:400:PHE:HB3 | 2.00 | 0.43 |
| 2:E:546:LYS:NZ | 2:E:862:HIS:O | 2.52 | 0.43 |
| 1:A:52:ASN:HA | 1:A:53:PRO:HD3 | 1.87 | 0.43 |
| 2:E:147:LEU:HD23 | 2:E:147:LEU:HA | 1.74 | 0.43 |
| 2:E:802:ILE:HB | 2:E:809:PHE:HB2 | 2.01 | 0.43 |
| 1:A:430:ASN:HD22 | 1:A:430:ASN:N | 2.03 | 0.43 |
| 2:E:224:GLU:HA | 2:E:291:MET:CG | 2.49 | 0.43 |
| 3:B:32:ASP:HA | 5:B:201:GNP:O3G | 2.19 | 0.43 |
| 2:E:359:ILE:HD11 | 2:E:406:LEU:HD23 | 2.01 | 0.43 |
| 2:E:668:LEU:O | 2:E:671:ALA:HB3 | 2.18 | 0.43 |
| 3:B:181:GLU:CD | 3:B:181:GLU:H | 2.22 | 0.43 |
| 2:E:150:PRO:O | 2:E:151:ILE:HB | 2.18 | 0.42 |
| 2:E:248:GLY:O | 2:E:277:ARG:NH2 | 2.33 | 0.42 |
| 1:A:417:LEU:HD23 | 1:A:417:LEU:C | 2.39 | 0.42 |
| 2:E:253:CYS:O | 2:E:257:ARG:HA | 2.19 | 0.42 |
| 1:A:66:ASN:HB2 | 1:A:67:PRO:CD | 2.50 | 0.42 |
| 2:E:144:LEU:HD22 | 2:E:918:GLN:HE22 | 1.84 | 0.42 |
| 1:A:195:GLU:O | 1:A:199:GLY:N | 2.41 | 0.42 |
| 1:A:411:ASP:HA | 1:A:463:ALA:HB3 | 2.02 | 0.42 |
| 2:E:168:MET:HG2 | 2:E:241:PHE:CE1 | 2.54 | 0.42 |
| 2:E:864:ASP:OD1 | 2:E:864:ASP:N | 2.53 | 0.42 |
| 1:A:561:GLN:HG2 | 1:A:763:ALA:O | 2.20 | 0.42 |
| 2:E:553:CYS:O | 2:E:587:THR:HA | 2.19 | 0.42 |
| 3:B:147:SER:OG | 3:B:152:LEU:HD21 | 2.19 | 0.42 |
| 1:A:574:PHE:CD2 | 1:A:760:GLN:HG2 | 2.55 | 0.42 |
| 2:E:729:PRO:HB2 | 2:E:732:HIS:CD2 | 2.52 | 0.42 |
| 2:E:799:LEU:HD13 | 2:E:812:MET:CE | 2.50 | 0.42 |
| 1:A:66:ASN:ND2 | 1:A:68:TYR:HB2 | 2.35 | 0.42 |
| 1:A:632:PHE:CD1 | 1:A:632:PHE:N | 2.88 | 0.42 |
| 2:E:242:VAL:HG12 | 2:E:243:THR:N | 2.34 | 0.42 |
| 2:E:333:LEU:HD12 | 2:E:400:ARG:NE | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:53:PRO:HG3 | 1:A:112:TYR:CG | 2.55 | 0.42 |
| 1:A:239:ASN:O | 1:A:243:GLU:HB2 | 2.20 | 0.42 |
| 1:A:332:ILE:HG22 | 1:A:361:LEU:HD21 | 2.02 | 0.41 |
| 1:A:360:GLN:HG2 | 1:A:364:SER:OG | 2.19 | 0.41 |
| 1:A:80:CYS:HA | 1:A:81:PRO:HD3 | 1.86 | 0.41 |
| 1:A:420:HIS:CE1 | 1:A:615:ARG:HB2 | 2.55 | 0.41 |
| 2:E:197:LYS:HD2 | 2:E:197:LYS:HA | 1.71 | 0.41 |
| 2:E:301:PRO:HA | 2:E:302:PRO:HD3 | 1.68 | 0.41 |
| 2:E:588:MET:HA | 2:E:589:PRO:HD3 | 1.81 | 0.41 |
| 1:A:83:CYS:O | 1:A:84:ASN:HB2 | 2.21 | 0.41 |
| 1:A:632:PHE:CE2 | 1:A:693:GLU:HG3 | 2.55 | 0.41 |
| 1:A:42:GLU:HG3 | 1:A:452:PRO:HB3 | 2.02 | 0.41 |
| 1:A:171:LEU:HB3 | 1:A:237:LYS:HD3 | 2.03 | 0.41 |
| 2:E:133:ARG:HH21 | 2:E:135:MET:HE2 | 1.86 | 0.41 |
| 2:E:497:VAL:HG12 | 2:E:499:LEU:HD11 | 2.01 | 0.41 |
| 1:A:243:GLU:HA | 1:A:243:GLU:OE1 | 2.20 | 0.41 |
| 1:A:658:THR:O | 1:A:659:PHE:HB3 | 2.20 | 0.41 |
| 1:A:661:PHE:CD1 | 1:A:661:PHE:C | 2.93 | 0.41 |
| 2:E:212:HIS:CD2 | 2:E:217:ILE:HB | 2.55 | 0.41 |
| 2:E:535:ASN:O | 2:E:536:ASP:C | 2.59 | 0.41 |
| 1:A:643:LEU:HD12 | 1:A:728:LEU:HD23 | 2.03 | 0.41 |
| 1:A:677:GLY:O | 1:A:679:GLN:N | 2.52 | 0.41 |
| 2:E:155:THR:O | 2:E:155:THR:HG22 | 2.21 | 0.41 |
| 2:E:496:THR:OG1 | 2:E:587:THR:HG23 | 2.20 | 0.41 |
| 2:E:808:LEU:O | 2:E:872:TYR:N | 2.48 | 0.41 |
| 1:A:20:PRO:HB3 | 1:A:25:ASP:HB2 | 2.02 | 0.41 |
| 1:A:319:ALA:HB1 | 1:A:322:TYR:HB2 | 2.03 | 0.41 |
| 1:A:569:ASP:O | 1:A:571:PRO:HD3 | 2.20 | 0.41 |
| 1:A:723:PHE:CE1 | 3:B:53:PRO:HD2 | 2.56 | 0.41 |
| 2:E:151:ILE:HD13 | 2:E:709:MET:CE | 2.50 | 0.41 |
| 2:E:292:ALA:HA | 2:E:293:PRO:HD3 | 1.83 | 0.41 |
| 2:E:362:ASP:CG | 2:E:401:GLN:HB2 | 2.40 | 0.41 |
| 2:E:560:ALA:HA | 2:E:612:GLN:O | 2.21 | 0.41 |
| 1:A:63:SER:OG | 1:A:82:ILE:HG13 | 2.19 | 0.41 |
| 1:A:67:PRO:HD3 | 1:A:104:GLU:O | 2.21 | 0.41 |
| 1:A:70:VAL:HB | 1:A:79:SER:OG | 2.21 | 0.41 |
| 1:A:164:ASN:HD22 | 1:A:165:VAL:N | 2.19 | 0.41 |
| 1:A:746:LEU:HB3 | 3:B:48:LEU:HD21 | 2.02 | 0.41 |
| 2:E:242:VAL:CG1 | 2:E:243:THR:N | 2.83 | 0.41 |
| 2:E:409:LYS:O | 2:E:412:GLN:N | 2.48 | 0.41 |
| 2:E:781:ILE:HB | 2:E:858:GLN:OE1 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:96:LEU:O | 1:A:97:SER:HB3 | 2.21 | 0.41 |
| 2:E:270:ASP:CB | 2:E:273:ASP:HB3 | 2.50 | 0.41 |
| 2:E:358:LYS:HA | 2:E:391:SER:O | 2.21 | 0.41 |
| 2:E:199:SER:O | 2:E:200:LYS:HB2 | 2.21 | 0.40 |
| 2:E:703:LEU:HD12 | 2:E:703:LEU:HA | 1.96 | 0.40 |
| 2:E:808:LEU:O | 2:E:871:LEU:HA | 2.21 | 0.40 |
| 1:A:41:LYS:O | 1:A:503:ARG:NH2 | 2.53 | 0.40 |
| 1:A:140:LEU:O | 1:A:144:ILE:HG13 | 2.21 | 0.40 |
| 1:A:569:ASP:C | 1:A:571:PRO:HD3 | 2.41 | 0.40 |
| 2:E:217:ILE:C | 2:E:219:PRO:HD3 | 2.41 | 0.40 |
| 1:A:451:SER:C | 1:A:453:TYR:N | 2.75 | 0.40 |
| 1:A:639:GLN:HA | 1:A:640:PRO:HD3 | 1.90 | 0.40 |
| 2:E:187:ASN:O | 2:E:634:PRO:HD2 | 2.20 | 0.40 |
| 2:E:217:ILE:H | 2:E:217:ILE:HG13 | 1.64 | 0.40 |
| 3:B:26:LEU:HB2 | 3:B:71:THR:HG22 | 2.02 | 0.40 |
| 1:A:152:PRO:HA | 1:A:153:PRO:HD3 | 1.93 | 0.40 |
| 1:A:576:LEU:HG | 1:A:580:PHE:HB3 | 2.02 | 0.40 |
| 1:A:702:LEU:O | 1:A:703:VAL:C | 2.59 | 0.40 |
| 2:E:277:ARG:C | 2:E:279:ASP:N | 2.74 | 0.40 |
| 2:E:329:LEU:O | 2:E:333:LEU:HD23 | 2.22 | 0.40 |
| 3:B:138:ASN:O | 3:B:139:ALA:O | 2.40 | 0.40 |
| 1:A:234:VAL:O | 1:A:235:GLU:C | 2.60 | 0.40 |
| 1:A:464:ASN:ND2 | 1:A:465:THR:N | 2.69 | 0.40 |
| 1:A:576:LEU:HG | 1:A:580:PHE:CB | 2.52 | 0.40 |

There are no symmetry-related clashes.

## 3.3 Torsion angles (i)

### 3.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

### 3.3.2 Protein sidechains (i)

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

### 3.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 3.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | GNP | B | 201 | 6 | 29,34,34 | 1.80 | 7 (24%) | 33,54,54 | 2.34 | 6 (18%) |

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 |
|---|---|---|---|---|---|---|---|
| 5 | GNP | B | 201 | 6 | - | 4/14/38/38 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | B | 201 | GNP | C6-N1 | 4.54 | 1.40 | 1.33 |
| 5 | B | 201 | GNP | PB-O2B | -3.49 | 1.47 | 1.56 |
| 5 | B | 201 | GNP | C5-C6 | 3.31 | 1.47 | 1.41 |
| 5 | B | 201 | GNP | PG-O2G | -3.27 | 1.47 | 1.56 |
| 5 | B | 201 | GNP | C2-N1 | 2.78 | 1.40 | 1.35 |
| 5 | B | 201 | GNP | C8-N7 | -2.60 | 1.30 | 1.34 |
| 5 | B | 201 | GNP | PB-O3A | 2.42 | 1.62 | 1.59 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | B | 201 | GNP | C5-C6-N1 | -8.38 | 111.96 | 123.43 |
| 5 | B | 201 | GNP | C2-N1-C6 | 6.24 | 125.84 | 115.93 |
| 5 | B | 201 | GNP | O3G-PG-O1G | -4.29 | 102.66 | 113.45 |
| 5 | B | 201 | GNP | N3-C2-N1 | -3.84 | 122.11 | 127.22 |
| 5 | B | 201 | GNP | O1G-PG-N3B | 2.61 | 115.61 | 111.77 |
| 5 | B | 201 | GNP | C4-C5-C6 | -2.37 | 118.54 | 120.80 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | B | 201 | GNP | PB-N3B-PG-O1G |
| 5 | B | 201 | GNP | PG-N3B-PB-O1B |
| 5 | B | 201 | GNP | PA-O3A-PB-O2B |
| 5 | B | 201 | GNP | PG-N3B-PB-O3A |

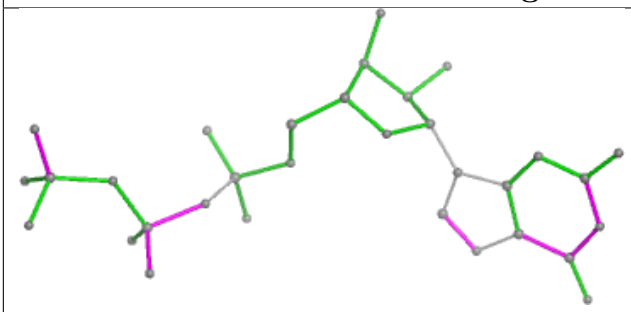
There are no ring outliers.

1 monomer is involved in 6 short contacts:

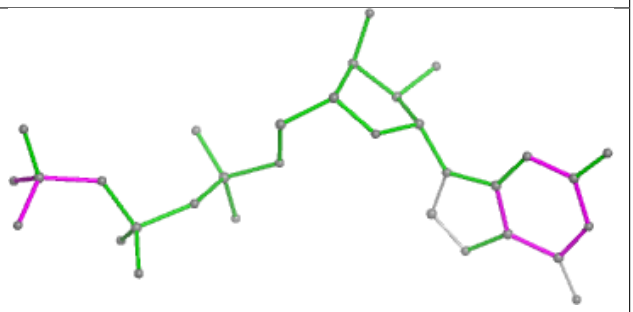
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | B | 201 | GNP | 6 | 0 |

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.

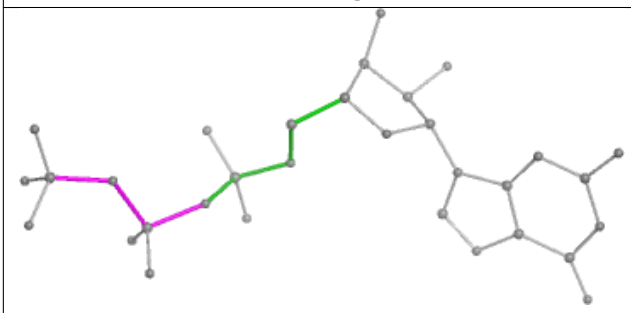
**Ligand GNP B 201**



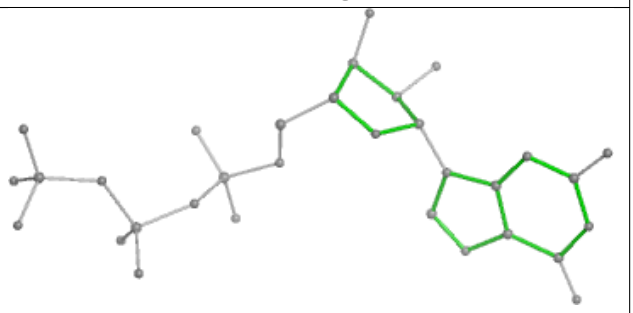
Bond lengths



Bond angles



Torsions



Rings

## 3.7 Other polymers (i)

There are no such residues in this entry.

## 3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 4 Map visualisation

This section contains visualisations of the EMDB entry EMD-0044. 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.

## 4.1 Orthogonal projections

This section was not generated.

## 4.2 Central slices

This section was not generated.

## 4.3 Largest variance slices

This section was not generated.

## 4.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

## 4.5 Orthogonal surface views

This section was not generated.

## 4.6 Mask visualisation

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

# 5 Map analysis

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

## 5.1 Map-value distribution

This section was not generated.

## 5.2 Volume estimate versus contour level

This section was not generated.

## 5.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

# 6 Fourier-Shell correlation

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

# 7 Map-model fit

This section was not generated.