# Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 05:33 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 6ZH4 |
| EMDB ID | : | EMD-11213 |
| Title | : | Cryo-EM structure of DNA-PKcs (State 3) |
| Authors | : | Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L. |
| Deposited on | : | 2020-06-20 |
| Resolution | : | 3.62 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.

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

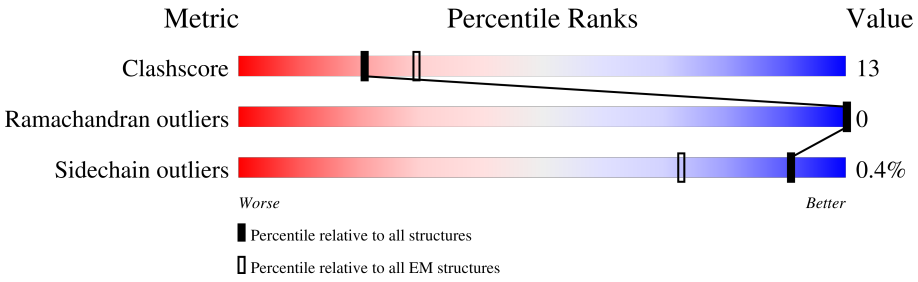
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.31.3 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.62 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 | 4156 | 7% 62% 27% 11% |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 29352 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 DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

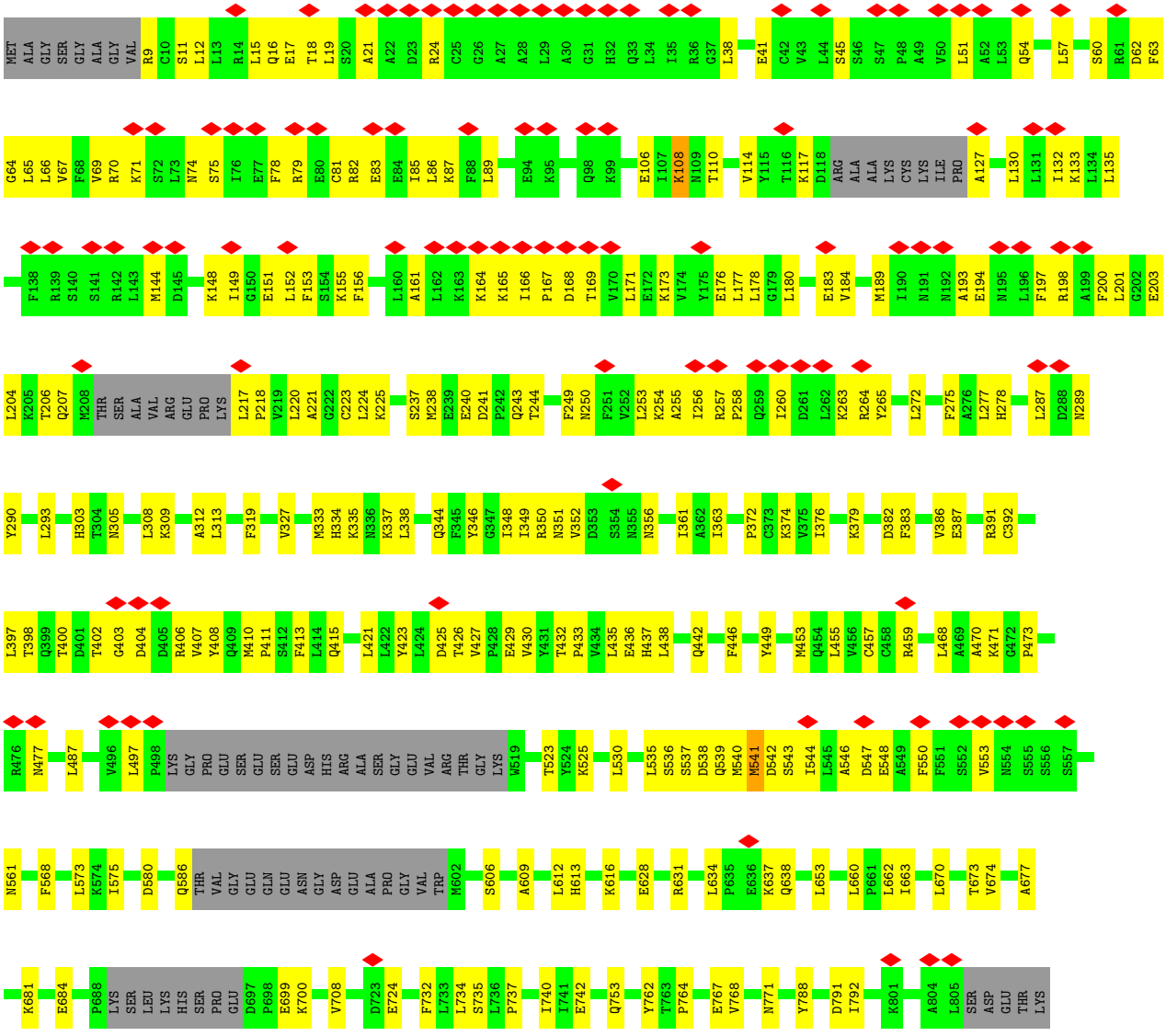
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 3698 | 29352 | 18827 | 4960 | 5372 | 193 | 0 | 0 |

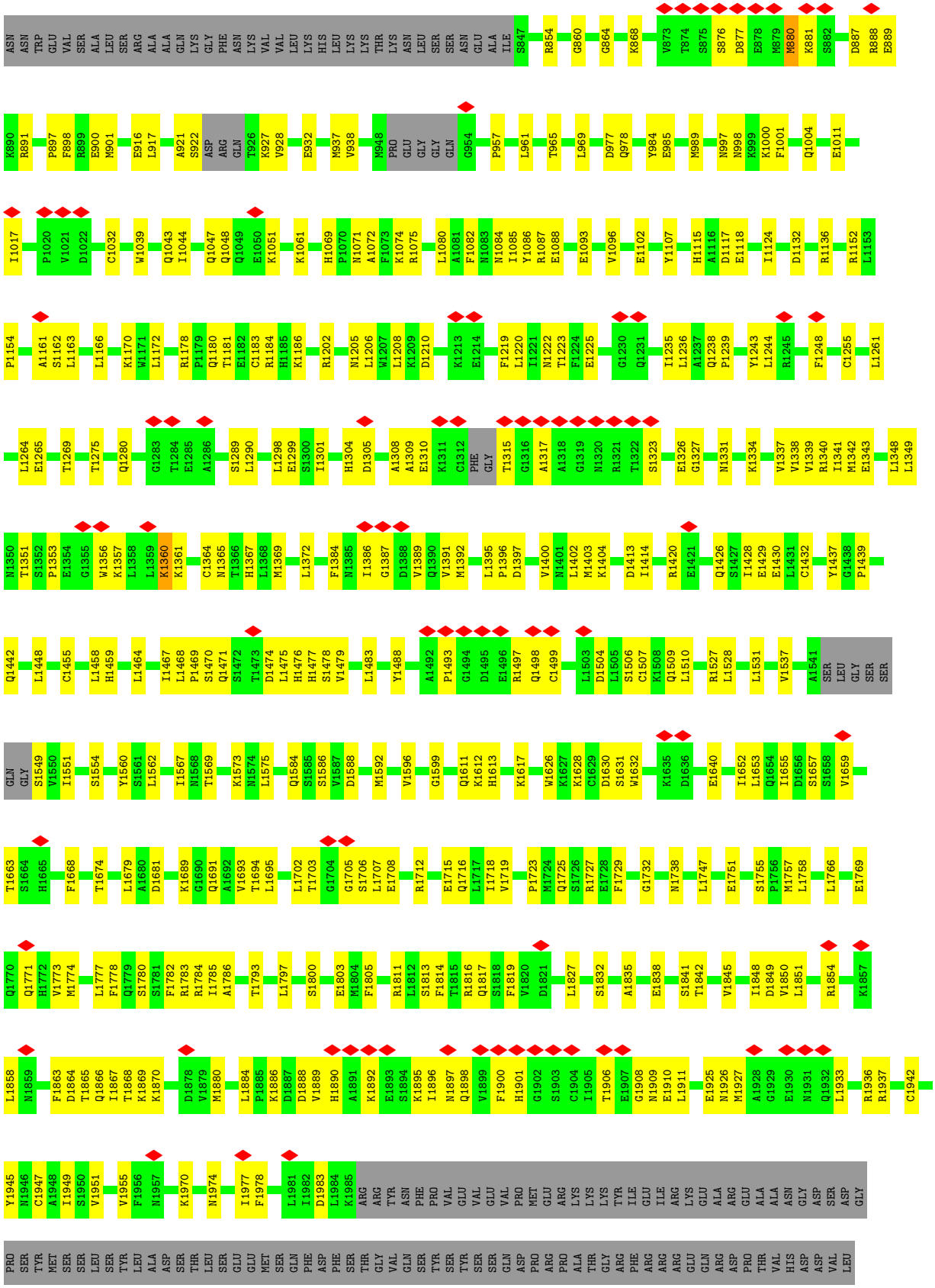
# 3 Residue-property plots (i)

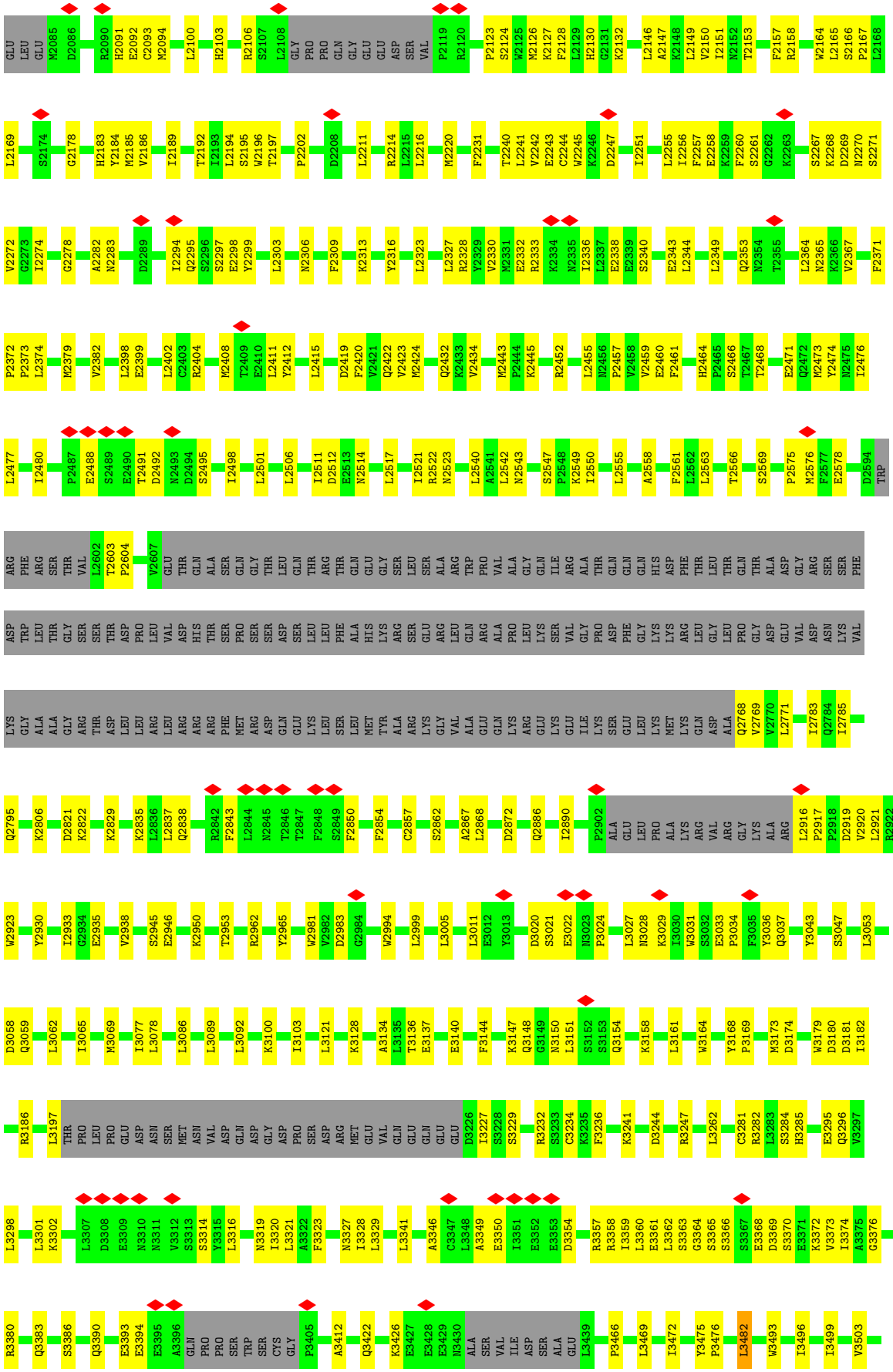
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

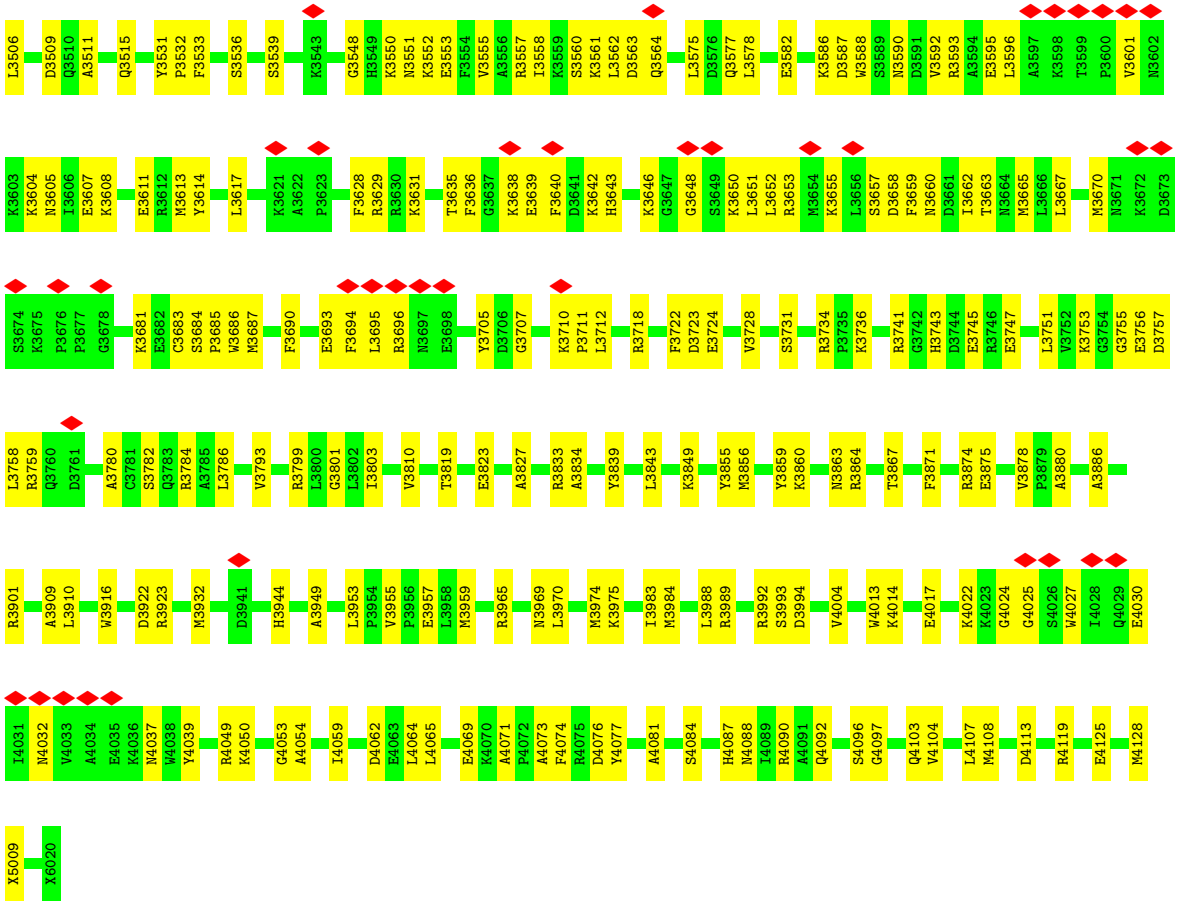
• Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-PKcs

Chain A:






L3506 D3509 Q3510 A3511 Q3515 Y3531 P3532 F3533 S3536 S3539 K3543 G3548 H3549 K3550 N3551 K3552 E3553 F3554 V3555 A3556 R3557 I3558 K3559 S3560 K3561 L3562 D3563 Q3564 L3575 D3576 Q3577 L3578 E3582 K3586 D3587 W3588 S3589 N3590 D3591 V3592 R3593 A3594 E3595 L3596 A3597 K3598 T3599 P3600 V3601 N3602
K3603 K3604 N3605 I3606 E3607 K3608 E3611 R3612 M3613 Y3614 L3617 K3621 A3622 P3623 F3628 R3629 R3630 K3631 T3635 F3636 G3637 K3638 E3639 F3640 D3641 K3642 H3643 K3646 G3647 G3648 S3649 K3650 L3651 L3652 R3653 M3654 K3655 L3656 S3657 D3658 F3659 N3660 D3661 I3662 T3663 N3664 M3665 I3666 L3667 M3670 N3671 K3672 D3673
S3674 K3675 P3676 P3677 G3678 K3681 E3682 C3683 S3684 P3685 W3686 M3687 F3690 E3693 F3694 L3695 R3696 N3697 E3698 Y3705 D3706 G3707 K3710 P3711 L3712 R3718 F3722 D3723 E3724 V3728 S3731 R3734 P3735 K3736 R3741 G3742 H3743 D3744 E3745 R3746 E3747 L3751 V3752 K3753 G3754 G3755 E3756 D3757
L3758 R3759 Q3760 D3761 A3780 C3781 S3782 Q3783 R3784 A3785 L3786 V3793 R3799 L3800 G3801 L3802 I3803 V3810 T3819 E3823 A3827 R3833 A3834 Y3839 L3843 K3849 Y3855 M3856 Y3859 K3860 N3863 R3864 T3867 F3871 R3874 E3875 V3878 P3879 A3880 A3886
R3901 A3909 L3910 W3916 D3922 R3923 M3932 D3941 H3944 A3949 L3953 P3954 V3955 P3956 E3957 L3958 M3959 R3965 N3969 L3970 M3974 K3975 I3983 M3984 L3988 R3989 R3992 S3993 D3994 V4004 W4013 K4014 E4017 K4022 K4023 G4024 G4025 S4026 W4027 I4028 Q4029 E4030
I4031 N4032 V4033 A4034 E4035 K4036 N4037 W4038 Y4039 R4049 K4050 G4053 A4054 I4059 D4062 E4063 L4064 L4065 E4069 K4070 A4071 P4072 A4073 F4074 R4075 D4076 Y4077 A4081 S4084 H4087 N4088 I4089 R4090 A4091 Q4092 S4096 G4097 Q4103 V4104 L4107 M4108 D4113 R4119 E4125 M4128
X5009 X6020

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 47183 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 53.95 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.195 | Depositor |
| Minimum map value | -0.068 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.010 | Depositor |
| Recommended contour level | 0.055 | Depositor |
| Map size (Å) | 280.36002, 280.36002, 280.36002 | wwPDB |
| Map dimensions | 430, 430, 430 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.652, 0.652, 0.652 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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 | 0.31 | 0/29811 | 0.45 | 0/40307 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 29352 | 0 | 29489 | 783 | 0 |
| All | All | 29352 | 0 | 29489 | 783 | 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 13.

All (783) 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:3628:PHE:H | 1:A:3684:SER:HB3 | 1.42 | 0.85 |
| 1:A:1712:ARG:HH12 | 1:A:1716:GLN:HB2 | 1.44 | 0.82 |
| 1:A:3282:ARG:HE | 1:A:3329:LEU:HD21 | 1.46 | 0.80 |
| 1:A:1351:THR:HG22 | 1:A:1353:PRO:HD2 | 1.61 | 0.80 |
| 1:A:3482:LEU:HD12 | 1:A:3482:LEU:O | 1.81 | 0.80 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3683:CYS:SG | 1:A:3684:SER:N | 2.55 | 0.79 |
| 1:A:3653:ARG:HH22 | 1:A:3659:PHE:HB2 | 1.46 | 0.79 |
| 1:A:1626:TRP:HE1 | 1:A:1674:THR:HG21 | 1.48 | 0.78 |
| 1:A:2768:GLN:HG3 | 1:A:2769:VAL:HG23 | 1.66 | 0.77 |
| 1:A:2837:LEU:HD21 | 1:A:2872:ASP:H | 1.48 | 0.77 |
| 1:A:3027:LEU:HB2 | 1:A:3031:TRP:HB2 | 1.67 | 0.76 |
| 1:A:2103:HIS:HA | 1:A:2106:ARG:HH11 | 1.51 | 0.75 |
| 1:A:442:GLN:NE2 | 1:A:457:CYS:SG | 2.58 | 0.75 |
| 1:A:3357:ARG:O | 1:A:3360:LEU:HB3 | 1.88 | 0.74 |
| 1:A:3586:LYS:O | 1:A:3590:ASN:ND2 | 2.21 | 0.73 |
| 1:A:3648:GLY:H | 1:A:3651:LEU:HD22 | 1.53 | 0.73 |
| 1:A:1889:VAL:O | 1:A:1909:ASN:ND2 | 2.21 | 0.73 |
| 1:A:2295:GLN:HG3 | 1:A:2297:SER:H | 1.53 | 0.73 |
| 1:A:3469:LEU:HD13 | 1:A:3472:ILE:HD11 | 1.68 | 0.73 |
| 1:A:3320:ILE:HG12 | 1:A:3321:LEU:HG | 1.69 | 0.73 |
| 1:A:4013:TRP:NE1 | 1:A:4017:GLU:OE1 | 2.22 | 0.73 |
| 1:A:1933:LEU:O | 1:A:1937:ARG:NE | 2.22 | 0.73 |
| 1:A:860:GLY:HA3 | 1:A:3136:THR:HG21 | 1.71 | 0.72 |
| 1:A:1439:PRO:O | 1:A:1442:GLN:NE2 | 2.23 | 0.72 |
| 1:A:2443:MET:HE3 | 1:A:2476:ILE:HG23 | 1.72 | 0.71 |
| 1:A:86:LEU:HD13 | 1:A:89:LEU:HD12 | 1.73 | 0.70 |
| 1:A:1017:ILE:HD11 | 1:A:1074:LYS:HE2 | 1.73 | 0.69 |
| 1:A:3731:SER:H | 1:A:3734:ARG:HH21 | 1.40 | 0.69 |
| 1:A:2091:HIS:NE2 | 1:A:2093:CYS:SG | 2.65 | 0.69 |
| 1:A:4064:LEU:HD13 | 1:A:4077:TYR:HB3 | 1.74 | 0.69 |
| 1:A:2412:TYR:HA | 1:A:2415:LEU:HB2 | 1.75 | 0.69 |
| 1:A:3611:GLU:N | 1:A:3611:GLU:OE1 | 2.24 | 0.69 |
| 1:A:2365:ASN:ND2 | 1:A:2399:GLU:OE2 | 2.21 | 0.69 |
| 1:A:2332:GLU:O | 1:A:2333:ARG:NH2 | 2.24 | 0.69 |
| 1:A:15:LEU:HA | 1:A:18:THR:HG22 | 1.74 | 0.68 |
| 1:A:1715:GLU:HA | 1:A:1718:ILE:HG12 | 1.76 | 0.68 |
| 1:A:4074:PHE:HA | 1:A:4077:TYR:HD2 | 1.58 | 0.68 |
| 1:A:881:LYS:NZ | 1:A:916:GLU:OE2 | 2.26 | 0.68 |
| 1:A:3613:MET:O | 1:A:3617:LEU:N | 2.26 | 0.67 |
| 1:A:9:ARG:NH2 | 1:A:11:SER:OG | 2.27 | 0.67 |
| 1:A:3244:ASP:OD1 | 1:A:3247:ARG:NH1 | 2.27 | 0.67 |
| 1:A:3354:ASP:OD1 | 1:A:3358:ARG:NH2 | 2.27 | 0.67 |
| 1:A:2332:GLU:HG3 | 1:A:2333:ARG:HG2 | 1.77 | 0.67 |
| 1:A:349:ILE:HD11 | 1:A:391:ARG:HG3 | 1.76 | 0.66 |
| 1:A:3859:TYR:HE1 | 1:A:4119:ARG:HB2 | 1.59 | 0.66 |
| 1:A:275:PHE:HE2 | 1:A:319:PHE:HB2 | 1.59 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:4049:ARG:NH2 | 1:A:4062:ASP:OD2 | 2.28 | 0.66 |
| 1:A:1896:ILE:HD12 | 1:A:1898:GLN:HB2 | 1.76 | 0.66 |
| 1:A:2540:LEU:O | 1:A:2835:LYS:NZ | 2.29 | 0.66 |
| 1:A:4030:GLU:OE1 | 1:A:4032:ASN:ND2 | 2.29 | 0.66 |
| 1:A:152:LEU:O | 1:A:155:LYS:NZ | 2.29 | 0.66 |
| 1:A:2195:SER:O | 1:A:5009:UNK:N | 2.28 | 0.66 |
| 1:A:3058:ASP:O | 1:A:3059:GLN:NE2 | 2.30 | 0.65 |
| 1:A:3323:PHE:O | 1:A:3327:ASN:ND2 | 2.28 | 0.65 |
| 1:A:1712:ARG:NH1 | 1:A:1715:GLU:OE2 | 2.30 | 0.65 |
| 1:A:2946:GLU:OE2 | 1:A:3975:LYS:NZ | 2.26 | 0.65 |
| 1:A:3693:GLU:OE2 | 1:A:3696:ARG:NH2 | 2.30 | 0.64 |
| 1:A:402:THR:OG1 | 1:A:406:ARG:NH2 | 2.29 | 0.64 |
| 1:A:2126:MET:O | 1:A:2130:HIS:N | 2.26 | 0.64 |
| 1:A:3506:LEU:HD23 | 1:A:3555:VAL:HG12 | 1.80 | 0.64 |
| 1:A:132:ILE:HA | 1:A:135:LEU:HD12 | 1.79 | 0.63 |
| 1:A:3169:PRO:HG2 | 1:A:3179:TRP:CE2 | 2.33 | 0.63 |
| 1:A:3639:GLU:O | 1:A:3643:HIS:N | 2.21 | 0.63 |
| 1:A:541:MET:HA | 1:A:544:ILE:HG12 | 1.80 | 0.63 |
| 1:A:86:LEU:HD12 | 1:A:133:LYS:HE2 | 1.81 | 0.63 |
| 1:A:3863:ASN:OD1 | 1:A:3864:ARG:N | 2.31 | 0.63 |
| 1:A:1854:ARG:HH11 | 1:A:1870:LYS:HE2 | 1.62 | 0.63 |
| 1:A:200:PHE:HZ | 1:A:224:LEU:HA | 1.63 | 0.62 |
| 1:A:1075:ARG:NH1 | 1:A:1117:ASP:OD2 | 2.32 | 0.62 |
| 1:A:1455:CYS:HA | 1:A:1458:LEU:HD12 | 1.79 | 0.62 |
| 1:A:3922:ASP:O | 1:A:3923:ARG:NE | 2.31 | 0.62 |
| 1:A:1702:LEU:HD21 | 1:A:1706:SER:HB3 | 1.79 | 0.62 |
| 1:A:135:LEU:HD11 | 1:A:173:LYS:HG2 | 1.79 | 0.62 |
| 1:A:4050:LYS:HE3 | 1:A:4059:ILE:HG21 | 1.82 | 0.62 |
| 1:A:333:MET:HG2 | 1:A:334:HIS:ND1 | 2.15 | 0.62 |
| 1:A:3020:ASP:OD1 | 1:A:3021:SER:N | 2.33 | 0.61 |
| 1:A:3144:PHE:O | 1:A:3150:ASN:ND2 | 2.32 | 0.61 |
| 1:A:997:ASN:OD1 | 1:A:998:ASN:N | 2.32 | 0.61 |
| 1:A:1248:PHE:H | 1:A:1317:ALA:HB3 | 1.65 | 0.61 |
| 1:A:1712:ARG:NH1 | 1:A:1716:GLN:HB2 | 2.14 | 0.61 |
| 1:A:3365:SER:HB3 | 1:A:3376:GLY:HA3 | 1.83 | 0.61 |
| 1:A:3780:ALA:O | 1:A:3784:ARG:NH1 | 2.32 | 0.61 |
| 1:A:335:LYS:HE3 | 1:A:376:ILE:HD11 | 1.80 | 0.61 |
| 1:A:1337:VAL:O | 1:A:1341:ILE:HD12 | 2.01 | 0.61 |
| 1:A:1653:LEU:HD12 | 1:A:1695:LEU:HD12 | 1.81 | 0.61 |
| 1:A:407:VAL:HA | 1:A:410:MET:HG2 | 1.83 | 0.61 |
| 1:A:459:ARG:HD3 | 1:A:544:ILE:HD11 | 1.82 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3100:LYS:O | 1:A:3103:ILE:HG22 | 2.01 | 0.61 |
| 1:A:161:ALA:O | 1:A:164:LYS:NZ | 2.35 | 0.60 |
| 1:A:1244:LEU:HD21 | 1:A:1310:GLU:HB2 | 1.84 | 0.60 |
| 1:A:397:LEU:HD11 | 1:A:437:HIS:HB3 | 1.84 | 0.60 |
| 1:A:1132:ASP:OD1 | 1:A:1136:ARG:NH2 | 2.34 | 0.60 |
| 1:A:4090:ARG:NH2 | 1:A:4113:ASP:OD2 | 2.34 | 0.60 |
| 1:A:425:ASP:OD1 | 1:A:426:THR:N | 2.35 | 0.60 |
| 1:A:1348:LEU:HB3 | 1:A:1360:LYS:NZ | 2.16 | 0.60 |
| 1:A:2575:PRO:O | 1:A:2576:MET:HG2 | 2.02 | 0.60 |
| 1:A:3154:GLN:HE22 | 1:A:3158:LYS:HE3 | 1.66 | 0.59 |
| 1:A:21:ALA:HA | 1:A:24:ARG:HD2 | 1.84 | 0.59 |
| 1:A:166:ILE:HG13 | 1:A:167:PRO:HD3 | 1.83 | 0.59 |
| 1:A:3370:SER:O | 1:A:3373:VAL:N | 2.35 | 0.59 |
| 1:A:3058:ASP:OD1 | 1:A:3059:GLN:N | 2.36 | 0.59 |
| 1:A:535:LEU:HB3 | 1:A:637:LYS:HE2 | 1.85 | 0.59 |
| 1:A:2522:ARG:HG2 | 1:A:2561:PHE:HE1 | 1.67 | 0.59 |
| 1:A:3358:ARG:NE | 1:A:3361:GLU:OE2 | 2.34 | 0.59 |
| 1:A:1301:ILE:HG23 | 1:A:1334:LYS:HD2 | 1.84 | 0.59 |
| 1:A:1814:PHE:O | 1:A:1817:GLN:NE2 | 2.34 | 0.59 |
| 1:A:3655:LYS:HE3 | 1:A:3657:SER:HB3 | 1.85 | 0.59 |
| 1:A:180:LEU:HD12 | 1:A:183:GLU:HB3 | 1.85 | 0.58 |
| 1:A:3180:ASP:OD1 | 1:A:3181:ASP:N | 2.35 | 0.58 |
| 1:A:70:ARG:O | 1:A:74:ASN:ND2 | 2.36 | 0.58 |
| 1:A:1813:SER:HB3 | 1:A:1865:THR:HG22 | 1.85 | 0.58 |
| 1:A:194:GLU:O | 1:A:198:ARG:HG3 | 2.03 | 0.58 |
| 1:A:887:ASP:OD1 | 1:A:888:ARG:N | 2.36 | 0.58 |
| 1:A:3646:LYS:H | 1:A:3650:LYS:HB2 | 1.67 | 0.58 |
| 1:A:3992:ARG:HH12 | 1:A:4053:GLY:HA2 | 1.67 | 0.58 |
| 1:A:4088:ASN:ND2 | 1:A:4113:ASP:OD2 | 2.37 | 0.58 |
| 1:A:2923:TRP:CE2 | 1:A:2946:GLU:HG3 | 2.39 | 0.58 |
| 1:A:1892:LYS:HD2 | 1:A:1908:GLY:H | 1.69 | 0.58 |
| 1:A:3137:GLU:OE2 | 1:A:3186:ARG:NE | 2.33 | 0.57 |
| 1:A:193:ALA:HA | 1:A:197:PHE:HE2 | 1.69 | 0.57 |
| 1:A:1448:LEU:HD23 | 1:A:1510:LEU:HD21 | 1.87 | 0.57 |
| 1:A:3653:ARG:NH2 | 1:A:3658:ASP:OD1 | 2.37 | 0.57 |
| 1:A:3363:SER:O | 1:A:3380:ARG:NH2 | 2.37 | 0.57 |
| 1:A:3285:HIS:HD2 | 1:A:3298:LEU:HD11 | 1.70 | 0.57 |
| 1:A:3466:PRO:HB2 | 1:A:4004:VAL:HG11 | 1.87 | 0.57 |
| 1:A:3875:GLU:O | 1:A:3965:ARG:NH1 | 2.38 | 0.57 |
| 1:A:2150:VAL:HG13 | 1:A:2157:PHE:HD2 | 1.70 | 0.57 |
| 1:A:16:GLN:HG3 | 1:A:17:GLU:HG2 | 1.87 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1584:GLN:OE1 | 1:A:1628:LYS:NZ | 2.31 | 0.57 |
| 1:A:1848:ILE:HA | 1:A:1851:LEU:HB2 | 1.85 | 0.56 |
| 1:A:864:GLY:O | 1:A:868:LYS:NZ | 2.34 | 0.56 |
| 1:A:2313:LYS:HA | 1:A:2316:TYR:CE1 | 2.40 | 0.56 |
| 1:A:3379:GLN:HG3 | 1:A:3383:GLN:HE22 | 1.69 | 0.56 |
| 1:A:3786:LEU:HB3 | 1:A:3910:LEU:HD22 | 1.87 | 0.56 |
| 1:A:1000:LYS:HE2 | 1:A:1004:GLN:HE21 | 1.70 | 0.56 |
| 1:A:1702:LEU:HD22 | 1:A:1707:LEU:HB3 | 1.88 | 0.56 |
| 1:A:2260:PHE:HA | 1:A:2270:ASN:HA | 1.87 | 0.56 |
| 1:A:1208:LEU:HD21 | 1:A:1220:LEU:HD11 | 1.86 | 0.56 |
| 1:A:1047:GLN:O | 1:A:1051:LYS:NZ | 2.38 | 0.56 |
| 1:A:1298:LEU:HD12 | 1:A:1364:CYS:HB3 | 1.88 | 0.56 |
| 1:A:1426:GLN:O | 1:A:1430:GLU:HG2 | 2.04 | 0.56 |
| 1:A:1727:ARG:NH2 | 1:A:1771:GLN:O | 2.39 | 0.56 |
| 1:A:2492:ASP:OD1 | 1:A:2495:SER:N | 2.35 | 0.56 |
| 1:A:724:GLU:HG2 | 1:A:2604:PRO:HA | 1.86 | 0.56 |
| 1:A:2192:THR:O | 1:A:2195:SER:OG | 2.20 | 0.56 |
| 1:A:3723:ASP:OD1 | 1:A:3724:GLU:N | 2.34 | 0.56 |
| 1:A:303:HIS:CE1 | 1:A:305:ASN:HB2 | 2.41 | 0.56 |
| 1:A:374:LYS:HD2 | 1:A:423:TYR:HB3 | 1.87 | 0.56 |
| 1:A:2945:SER:HB3 | 1:A:3975:LYS:HZ1 | 1.70 | 0.56 |
| 1:A:1391:VAL:HG23 | 1:A:1392:MET:SD | 2.46 | 0.55 |
| 1:A:4092:GLN:N | 1:A:4092:GLN:OE1 | 2.39 | 0.55 |
| 1:A:240:GLU:OE1 | 1:A:240:GLU:N | 2.40 | 0.55 |
| 1:A:900:GLU:N | 1:A:900:GLU:OE1 | 2.39 | 0.55 |
| 1:A:1926:ASN:ND2 | 1:A:1974:ASN:OD1 | 2.39 | 0.55 |
| 1:A:1301:ILE:HD12 | 1:A:1334:LYS:HG3 | 1.88 | 0.55 |
| 1:A:168:ASP:HB3 | 1:A:171:LEU:HB2 | 1.87 | 0.55 |
| 1:A:1867:ILE:HA | 1:A:1870:LYS:HE3 | 1.88 | 0.55 |
| 1:A:3151:LEU:HD22 | 1:A:3197:LEU:HD13 | 1.88 | 0.55 |
| 1:A:114:VAL:HG13 | 1:A:130:LEU:HD21 | 1.87 | 0.55 |
| 1:A:2202:PRO:HG3 | 1:A:2245:TRP:CE2 | 2.41 | 0.55 |
| 1:A:3284:SER:HB3 | 1:A:3301:LEU:HD12 | 1.88 | 0.55 |
| 1:A:1071:ASN:OD1 | 1:A:1072:ALA:N | 2.39 | 0.55 |
| 1:A:3655:LYS:HG3 | 1:A:3657:SER:H | 1.71 | 0.55 |
| 1:A:449:TYR:HB3 | 1:A:453:MET:HB3 | 1.87 | 0.55 |
| 1:A:2965:TYR:HB2 | 1:A:3005:LEU:HD21 | 1.88 | 0.55 |
| 1:A:1001:PHE:HZ | 1:A:1044:ILE:HG12 | 1.72 | 0.55 |
| 1:A:1178:ARG:O | 1:A:1184:ARG:NH2 | 2.40 | 0.55 |
| 1:A:1372:LEU:HD11 | 1:A:1403:MET:HE3 | 1.89 | 0.55 |
| 1:A:2563:LEU:HD23 | 1:A:2795:GLN:HB2 | 1.88 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1238:GLN:HA | 1:A:1243:TYR:HE2 | 1.72 | 0.54 |
| 1:A:1898:GLN:HB3 | 1:A:1900:PHE:CD1 | 2.42 | 0.54 |
| 1:A:2278:GLY:O | 1:A:2282:ALA:N | 2.40 | 0.54 |
| 1:A:3475:TYR:N | 1:A:3476:PRO:HD3 | 2.21 | 0.54 |
| 1:A:3596:LEU:HD13 | 1:A:3601:VAL:HA | 1.89 | 0.54 |
| 1:A:108:LYS:HE2 | 1:A:151:GLU:HG3 | 1.88 | 0.54 |
| 1:A:535:LEU:O | 1:A:561:ASN:ND2 | 2.40 | 0.54 |
| 1:A:2543:ASN:HB2 | 1:A:2835:LYS:HD2 | 1.90 | 0.54 |
| 1:A:1689:LYS:O | 1:A:1693:VAL:HG13 | 2.08 | 0.54 |
| 1:A:3536:SER:O | 1:A:3539:SER:OG | 2.25 | 0.54 |
| 1:A:734:LEU:HD12 | 1:A:768:VAL:HG12 | 1.90 | 0.54 |
| 1:A:1817:GLN:HB3 | 1:A:1868:THR:HG23 | 1.90 | 0.54 |
| 1:A:2298:GLU:OE1 | 1:A:2298:GLU:N | 2.37 | 0.54 |
| 1:A:2566:THR:O | 1:A:2569:SER:OG | 2.21 | 0.54 |
| 1:A:3150:ASN:OD1 | 1:A:3151:LEU:N | 2.40 | 0.54 |
| 1:A:110:THR:O | 1:A:114:VAL:HG12 | 2.07 | 0.54 |
| 1:A:3588:TRP:CD1 | 1:A:3613:MET:HE1 | 2.42 | 0.54 |
| 1:A:12:LEU:HA | 1:A:15:LEU:HG | 1.90 | 0.54 |
| 1:A:1470:SER:HA | 1:A:1477:HIS:CD2 | 2.43 | 0.54 |
| 1:A:3867:THR:HG21 | 1:A:4119:ARG:HE | 1.73 | 0.54 |
| 1:A:1264:LEU:HD22 | 1:A:1290:LEU:HD11 | 1.90 | 0.53 |
| 1:A:1309:ALA:HB1 | 1:A:1315:THR:HG23 | 1.90 | 0.53 |
| 1:A:2843:PHE:HZ | 1:A:2850:PHE:HA | 1.74 | 0.53 |
| 1:A:542:ASP:OD1 | 1:A:543:SER:N | 2.41 | 0.53 |
| 1:A:2147:ALA:O | 1:A:2151:ILE:HG12 | 2.08 | 0.53 |
| 1:A:1679:LEU:O | 1:A:1689:LYS:NZ | 2.26 | 0.53 |
| 1:A:1849:ASP:OD1 | 1:A:1850:VAL:N | 2.40 | 0.53 |
| 1:A:3575:LEU:HD23 | 1:A:3687:MET:HE1 | 1.91 | 0.53 |
| 1:A:3577:GLN:HA | 1:A:3629:ARG:HH21 | 1.73 | 0.53 |
| 1:A:86:LEU:HB3 | 1:A:133:LYS:HD3 | 1.89 | 0.53 |
| 1:A:922:SER:HB3 | 1:A:927:LYS:HA | 1.91 | 0.53 |
| 1:A:1080:LEU:O | 1:A:1084:ASN:ND2 | 2.42 | 0.53 |
| 1:A:1082:PHE:HA | 1:A:1085:ILE:HG12 | 1.91 | 0.53 |
| 1:A:1575:LEU:HD11 | 1:A:1617:LYS:HG3 | 1.90 | 0.53 |
| 1:A:2091:HIS:HD2 | 1:A:2094:MET:HB2 | 1.73 | 0.53 |
| 1:A:3953:LEU:HD23 | 1:A:4027:TRP:HD1 | 1.74 | 0.53 |
| 1:A:327:VAL:HG11 | 1:A:338:LEU:HD13 | 1.91 | 0.53 |
| 1:A:3169:PRO:HD3 | 1:A:3182:ILE:HD11 | 1.91 | 0.53 |
| 1:A:3593:ARG:HD3 | 1:A:3660:ASN:HD21 | 1.74 | 0.53 |
| 1:A:240:GLU:HB2 | 1:A:243:GLN:HE22 | 1.73 | 0.53 |
| 1:A:1349:LEU:HD13 | 1:A:1357:LYS:HE3 | 1.89 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:708:VAL:HG22 | 1:A:740:ILE:HG23 | 1.91 | 0.52 |
| 1:A:2402:LEU:HD22 | 1:A:2434:VAL:HG23 | 1.91 | 0.52 |
| 1:A:3349:ALA:HB3 | 1:A:3357:ARG:NE | 2.24 | 0.52 |
| 1:A:1864:ASP:HA | 1:A:1867:ILE:HG12 | 1.91 | 0.52 |
| 1:A:1933:LEU:HD13 | 1:A:1936:ARG:HB2 | 1.92 | 0.52 |
| 1:A:1949:ILE:HD12 | 1:A:2100:LEU:HD22 | 1.90 | 0.52 |
| 1:A:2216:LEU:O | 1:A:2220:MET:HG2 | 2.09 | 0.52 |
| 1:A:586:GLN:HB2 | 1:A:613:HIS:HD2 | 1.75 | 0.52 |
| 1:A:1586:SER:O | 1:A:1632:TRP:NE1 | 2.37 | 0.52 |
| 1:A:1069:HIS:CE1 | 1:A:1074:LYS:HD2 | 2.45 | 0.52 |
| 1:A:1886:LYS:O | 1:A:1890:HIS:N | 2.42 | 0.52 |
| 1:A:2183:HIS:CE1 | 1:A:2186:VAL:HG23 | 2.44 | 0.52 |
| 1:A:2424:MET:O | 1:A:2432:GLN:NE2 | 2.29 | 0.52 |
| 1:A:3319:ASN:HA | 1:A:3323:PHE:HB3 | 1.91 | 0.52 |
| 1:A:1239:PRO:HB3 | 1:A:1289:SER:HB2 | 1.92 | 0.52 |
| 1:A:2372:PRO:O | 1:A:2374:LEU:N | 2.35 | 0.52 |
| 1:A:1900:PHE:CG | 1:A:1901:HIS:N | 2.78 | 0.52 |
| 1:A:4104:VAL:O | 1:A:4108:MET:HG2 | 2.10 | 0.52 |
| 1:A:1372:LEU:HD13 | 1:A:1402:LEU:HD23 | 1.92 | 0.52 |
| 1:A:1528:LEU:HD21 | 1:A:1567:ILE:HG23 | 1.90 | 0.52 |
| 1:A:2542:LEU:HD21 | 1:A:2558:ALA:HA | 1.92 | 0.52 |
| 1:A:3370:SER:O | 1:A:3374:ILE:HD12 | 2.10 | 0.52 |
| 1:A:3386:SER:O | 1:A:3390:GLN:HG3 | 2.08 | 0.52 |
| 1:A:1166:LEU:HG | 1:A:1170:LYS:HE2 | 1.92 | 0.51 |
| 1:A:2422:GLN:OE1 | 1:A:2422:GLN:N | 2.41 | 0.51 |
| 1:A:2999:LEU:HD13 | 1:A:3043:TYR:HD2 | 1.74 | 0.51 |
| 1:A:144:MET:SD | 1:A:144:MET:N | 2.83 | 0.51 |
| 1:A:206:THR:HG23 | 1:A:207:GLN:HG3 | 1.92 | 0.51 |
| 1:A:1304:HIS:CE1 | 1:A:1308:ALA:HA | 2.45 | 0.51 |
| 1:A:1681:ASP:O | 1:A:1689:LYS:NZ | 2.27 | 0.51 |
| 1:A:1476:HIS:CE1 | 1:A:1478:SER:HB3 | 2.44 | 0.51 |
| 1:A:3319:ASN:OD1 | 1:A:3320:ILE:N | 2.43 | 0.51 |
| 1:A:2349:LEU:O | 1:A:2353:GLN:HB2 | 2.11 | 0.51 |
| 1:A:2890:ILE:HG12 | 1:A:2930:TYR:CE1 | 2.45 | 0.51 |
| 1:A:977:ASP:OD1 | 1:A:978:GLN:N | 2.44 | 0.51 |
| 1:A:1255:CYS:HB3 | 1:A:3695:LEU:HD12 | 1.93 | 0.51 |
| 1:A:2443:MET:O | 1:A:2445:LYS:N | 2.44 | 0.51 |
| 1:A:880:MET:O | 1:A:880:MET:HG2 | 2.11 | 0.51 |
| 1:A:1420:ARG:HH21 | 1:A:1467:ILE:HA | 1.75 | 0.51 |
| 1:A:1945:TYR:O | 1:A:1949:ILE:HG12 | 2.11 | 0.51 |
| 1:A:1011:GLU:OE1 | 1:A:1032:CYS:HB3 | 2.10 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:225:LYS:HE2 | 1:A:253:LEU:HD13 | 1.93 | 0.51 |
| 1:A:1471:GLN:HG2 | 1:A:1477:HIS:CG | 2.46 | 0.51 |
| 1:A:3236:PHE:CE1 | 1:A:3262:LEU:HD21 | 2.46 | 0.51 |
| 1:A:3856:MET:HE2 | 1:A:4071:ALA:HB1 | 1.93 | 0.51 |
| 1:A:1970:LYS:O | 1:A:1974:ASN:ND2 | 2.43 | 0.51 |
| 1:A:3077:ILE:HG13 | 1:A:3078:LEU:N | 2.26 | 0.51 |
| 1:A:487:LEU:HD23 | 1:A:575:ILE:HD12 | 1.93 | 0.50 |
| 1:A:2399:GLU:HA | 1:A:2402:LEU:HB3 | 1.92 | 0.50 |
| 1:A:2412:TYR:H | 1:A:2415:LEU:HD13 | 1.76 | 0.50 |
| 1:A:2522:ARG:NH1 | 1:A:2523:ASN:OD1 | 2.43 | 0.50 |
| 1:A:3758:LEU:HD12 | 1:A:3801:GLY:HA3 | 1.92 | 0.50 |
| 1:A:69:VAL:HG23 | 1:A:70:ARG:HD3 | 1.91 | 0.50 |
| 1:A:2150:VAL:HG22 | 1:A:2157:PHE:HE2 | 1.75 | 0.50 |
| 1:A:2169:LEU:HB3 | 1:A:2211:LEU:HD13 | 1.92 | 0.50 |
| 1:A:169:THR:HA | 1:A:220:LEU:HD21 | 1.93 | 0.50 |
| 1:A:660:LEU:HB3 | 1:A:663:ILE:HD13 | 1.93 | 0.50 |
| 1:A:1586:SER:OG | 1:A:1632:TRP:NE1 | 2.44 | 0.50 |
| 1:A:1751:GLU:OE2 | 1:A:1784:ARG:NE | 2.43 | 0.50 |
| 1:A:1800:SER:O | 1:A:1803:GLU:HG3 | 2.12 | 0.50 |
| 1:A:2257:PHE:HA | 1:A:2260:PHE:CZ | 2.46 | 0.50 |
| 1:A:2408:MET:HG3 | 1:A:2411:LEU:HD13 | 1.93 | 0.50 |
| 1:A:455:LEU:O | 1:A:459:ARG:HG3 | 2.12 | 0.50 |
| 1:A:2512:ASP:OD1 | 1:A:2512:ASP:N | 2.44 | 0.50 |
| 1:A:2919:ASP:OD1 | 1:A:2920:VAL:N | 2.45 | 0.50 |
| 1:A:313:LEU:HD22 | 1:A:361:ILE:HD11 | 1.94 | 0.50 |
| 1:A:998:ASN:OD1 | 1:A:1048:GLN:NE2 | 2.34 | 0.50 |
| 1:A:1537:VAL:HA | 1:A:1554:SER:HA | 1.94 | 0.50 |
| 1:A:3823:GLU:OE1 | 1:A:3823:GLU:N | 2.39 | 0.50 |
| 1:A:277:LEU:O | 1:A:278:HIS:ND1 | 2.44 | 0.50 |
| 1:A:3718:ARG:H | 1:A:3743:HIS:CD2 | 2.29 | 0.50 |
| 1:A:411:PRO:O | 1:A:415:GLN:N | 2.37 | 0.50 |
| 1:A:771:ASN:OD1 | 1:A:854:ARG:NH2 | 2.40 | 0.50 |
| 1:A:3028:ASN:OD1 | 1:A:3029:LYS:N | 2.44 | 0.50 |
| 1:A:106:GLU:OE1 | 1:A:106:GLU:N | 2.42 | 0.49 |
| 1:A:204:LEU:HB3 | 1:A:249:PHE:CZ | 2.46 | 0.49 |
| 1:A:1280:GLN:N | 1:A:1280:GLN:OE1 | 2.45 | 0.49 |
| 1:A:2194:LEU:HD23 | 1:A:2240:THR:HG22 | 1.94 | 0.49 |
| 1:A:2933:ILE:HD11 | 1:A:3121:LEU:HD22 | 1.92 | 0.49 |
| 1:A:3944:HIS:HB3 | 1:A:3949:ALA:HB2 | 1.93 | 0.49 |
| 1:A:165:LYS:HB2 | 1:A:167:PRO:HD2 | 1.95 | 0.49 |
| 1:A:2511:ILE:HD13 | 1:A:2550:ILE:HA | 1.93 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:197:PHE:O | 1:A:201:LEU:HG | 2.11 | 0.49 |
| 1:A:289:ASN:O | 1:A:293:LEU:N | 2.31 | 0.49 |
| 1:A:699:GLU:OE1 | 1:A:699:GLU:N | 2.37 | 0.49 |
| 1:A:1900:PHE:O | 1:A:1901:HIS:ND1 | 2.46 | 0.49 |
| 1:A:3511:ALA:O | 1:A:3515:GLN:HG3 | 2.12 | 0.49 |
| 1:A:539:GLN:HG3 | 1:A:540:MET:H | 1.77 | 0.49 |
| 1:A:742:GLU:OE1 | 1:A:742:GLU:N | 2.45 | 0.49 |
| 1:A:1479:VAL:O | 1:A:1483:LEU:N | 2.39 | 0.49 |
| 1:A:1896:ILE:HD13 | 1:A:1911:LEU:HB3 | 1.95 | 0.49 |
| 1:A:1898:GLN:HB3 | 1:A:1900:PHE:HD1 | 1.77 | 0.49 |
| 1:A:3493:TRP:CE2 | 1:A:3711:PRO:HD3 | 2.47 | 0.49 |
| 1:A:9:ARG:HH22 | 1:A:12:LEU:H | 1.61 | 0.49 |
| 1:A:580:ASP:OD2 | 1:A:616:LYS:NZ | 2.45 | 0.49 |
| 1:A:961:LEU:O | 1:A:965:THR:OG1 | 2.25 | 0.49 |
| 1:A:1488:TYR:CZ | 1:A:1531:LEU:HD11 | 2.47 | 0.49 |
| 1:A:3728:VAL:HG22 | 1:A:3736:LYS:HG3 | 1.95 | 0.49 |
| 1:A:3359:ILE:HA | 1:A:3362:LEU:HB2 | 1.95 | 0.49 |
| 1:A:397:LEU:HD21 | 1:A:438:LEU:HD22 | 1.94 | 0.49 |
| 1:A:1892:LYS:NZ | 1:A:1906:THR:O | 2.36 | 0.49 |
| 1:A:2306:ASN:HA | 1:A:2309:PHE:CE2 | 2.48 | 0.49 |
| 1:A:3582:GLU:OE1 | 1:A:3582:GLU:N | 2.31 | 0.49 |
| 1:A:3663:THR:O | 1:A:3667:LEU:HG | 2.12 | 0.49 |
| 1:A:204:LEU:HB3 | 1:A:249:PHE:CE2 | 2.48 | 0.49 |
| 1:A:1835:ALA:HA | 1:A:1838:GLU:HG2 | 1.93 | 0.49 |
| 1:A:2166:SER:OG | 1:A:2167:PRO:HD3 | 2.13 | 0.49 |
| 1:A:1244:LEU:H | 1:A:1244:LEU:HD23 | 1.76 | 0.48 |
| 1:A:1850:VAL:HG21 | 1:A:1869:LYS:HZ2 | 1.78 | 0.48 |
| 1:A:2443:MET:C | 1:A:2445:LYS:H | 2.16 | 0.48 |
| 1:A:75:SER:H | 1:A:78:PHE:HB3 | 1.77 | 0.48 |
| 1:A:1652:ILE:O | 1:A:1655:ILE:HG22 | 2.13 | 0.48 |
| 1:A:1071:ASN:ND2 | 1:A:3745:GLU:HB2 | 2.28 | 0.48 |
| 1:A:2336:ILE:N | 1:A:2338:GLU:OE2 | 2.42 | 0.48 |
| 1:A:628:GLU:OE1 | 1:A:631:ARG:NH2 | 2.28 | 0.48 |
| 1:A:889:GLU:OE1 | 1:A:891:ARG:NE | 2.35 | 0.48 |
| 1:A:57:LEU:O | 1:A:60:SER:OG | 2.20 | 0.48 |
| 1:A:3140:GLU:OE2 | 1:A:3164:TRP:NE1 | 2.35 | 0.48 |
| 1:A:4054:ALA:H | 1:A:4103:GLN:NE2 | 2.12 | 0.48 |
| 1:A:86:LEU:O | 1:A:133:LYS:NZ | 2.32 | 0.48 |
| 1:A:1353:PRO:HB3 | 1:A:1356:TRP:CD1 | 2.49 | 0.48 |
| 1:A:2783:ILE:O | 1:A:2785:ILE:N | 2.47 | 0.48 |
| 1:A:3564:GLN:OE1 | 1:A:3564:GLN:N | 2.46 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3974:MET:SD | 1:A:3974:MET:N | 2.86 | 0.48 |
| 1:A:74:ASN:HA | 1:A:78:PHE:HD2 | 1.77 | 0.48 |
| 1:A:430:VAL:HG11 | 1:A:1640:GLU:HB2 | 1.95 | 0.48 |
| 1:A:762:TYR:CD1 | 1:A:764:PRO:HD2 | 2.49 | 0.48 |
| 1:A:2202:PRO:HG3 | 1:A:2245:TRP:CD2 | 2.48 | 0.48 |
| 1:A:1334:LYS:O | 1:A:1338:VAL:HG23 | 2.13 | 0.48 |
| 1:A:1339:VAL:HA | 1:A:1342:MET:HE3 | 1.95 | 0.48 |
| 1:A:2340:SER:O | 1:A:2344:LEU:HG | 2.14 | 0.48 |
| 1:A:3605:ASN:HA | 1:A:3608:LYS:HD3 | 1.96 | 0.48 |
| 1:A:4125:GLU:OE2 | 1:A:4128:MET:HG2 | 2.14 | 0.48 |
| 1:A:473:PRO:O | 1:A:477:ASN:ND2 | 2.45 | 0.48 |
| 1:A:2327:LEU:HA | 1:A:2330:VAL:HG22 | 1.96 | 0.48 |
| 1:A:149:ILE:HD12 | 1:A:149:ILE:H | 1.79 | 0.48 |
| 1:A:788:TYR:O | 1:A:792:ILE:HG13 | 2.14 | 0.48 |
| 1:A:3033:GLU:HB3 | 1:A:3034:PRO:HD3 | 1.94 | 0.48 |
| 1:A:3482:LEU:HD12 | 1:A:3482:LEU:C | 2.34 | 0.48 |
| 1:A:3607:GLU:OE1 | 1:A:3607:GLU:N | 2.47 | 0.48 |
| 1:A:3658:ASP:OD1 | 1:A:3659:PHE:N | 2.46 | 0.48 |
| 1:A:153:PHE:HA | 1:A:156:PHE:CE2 | 2.49 | 0.47 |
| 1:A:290:TYR:CZ | 1:A:337:LYS:HG2 | 2.49 | 0.47 |
| 1:A:917:LEU:HD12 | 1:A:921:ALA:HB3 | 1.95 | 0.47 |
| 1:A:1384:PHE:O | 1:A:1386:ILE:HD12 | 2.14 | 0.47 |
| 1:A:1851:LEU:HD23 | 1:A:1870:LYS:HG2 | 1.94 | 0.47 |
| 1:A:2862:SER:OG | 1:A:2868:LEU:O | 2.32 | 0.47 |
| 1:A:204:LEU:HD23 | 1:A:224:LEU:HD13 | 1.95 | 0.47 |
| 1:A:1888:ASP:OD1 | 1:A:1889:VAL:HG13 | 2.13 | 0.47 |
| 1:A:2183:HIS:CE1 | 1:A:2185:MET:HB2 | 2.49 | 0.47 |
| 1:A:3065:ILE:O | 1:A:3069:MET:HG2 | 2.14 | 0.47 |
| 1:A:3078:LEU:HD23 | 1:A:3086:LEU:HD11 | 1.96 | 0.47 |
| 1:A:3705:TYR:HD1 | 1:A:3712:LEU:HG | 1.79 | 0.47 |
| 1:A:4081:ALA:O | 1:A:4090:ARG:NH1 | 2.47 | 0.47 |
| 1:A:189:MET:HA | 1:A:193:ALA:HB2 | 1.96 | 0.47 |
| 1:A:243:GLN:OE1 | 1:A:243:GLN:N | 2.42 | 0.47 |
| 1:A:253:LEU:HD12 | 1:A:254:LYS:N | 2.29 | 0.47 |
| 1:A:937:MET:HE2 | 1:A:937:MET:HA | 1.96 | 0.47 |
| 1:A:1428:ILE:HG13 | 1:A:1429:GLU:N | 2.29 | 0.47 |
| 1:A:1942:CYS:SG | 1:A:2092:GLU:HB2 | 2.54 | 0.47 |
| 1:A:3718:ARG:HG3 | 1:A:3743:HIS:CD2 | 2.49 | 0.47 |
| 1:A:1755:SER:HB3 | 1:A:1758:LEU:HB2 | 1.96 | 0.47 |
| 1:A:3747:GLU:N | 1:A:3747:GLU:OE1 | 2.47 | 0.47 |
| 1:A:203:GLU:O | 1:A:206:THR:HG22 | 2.14 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:290:TYR:HA | 1:A:293:LEU:HB3 | 1.97 | 0.47 |
| 1:A:546:ALA:HA | 1:A:550:PHE:CD1 | 2.49 | 0.47 |
| 1:A:1475:LEU:HD11 | 1:A:1527:ARG:CZ | 2.45 | 0.47 |
| 1:A:1202:ARG:NH2 | 1:A:1210:ASP:OD2 | 2.47 | 0.47 |
| 1:A:2243:GLU:HB3 | 1:A:2283:ASN:ND2 | 2.30 | 0.47 |
| 1:A:2420:PHE:O | 1:A:2423:VAL:HG22 | 2.15 | 0.47 |
| 1:A:2917:PRO:HB2 | 1:A:2919:ASP:OD1 | 2.15 | 0.47 |
| 1:A:237:SER:OG | 1:A:238:MET:N | 2.48 | 0.47 |
| 1:A:891:ARG:NH2 | 1:A:957:PRO:HD2 | 2.29 | 0.47 |
| 1:A:1506:SER:HA | 1:A:1509:GLN:HB3 | 1.97 | 0.47 |
| 1:A:2123:PRO:HD2 | 1:A:2126:MET:HE1 | 1.96 | 0.47 |
| 1:A:2461:PHE:O | 1:A:2464:HIS:HB3 | 2.15 | 0.47 |
| 1:A:2935:GLU:HG2 | 1:A:2938:VAL:HG12 | 1.95 | 0.47 |
| 1:A:660:LEU:HA | 1:A:660:LEU:HD23 | 1.81 | 0.47 |
| 1:A:264:ARG:HE | 1:A:265:TYR:H | 1.63 | 0.47 |
| 1:A:2916:LEU:HD21 | 1:A:2921:LEU:HB2 | 1.96 | 0.47 |
| 1:A:1323:SER:O | 1:A:1326:GLU:HG3 | 2.16 | 0.47 |
| 1:A:1592:MET:HB2 | 1:A:1592:MET:HE2 | 1.87 | 0.47 |
| 1:A:1780:SER:HA | 1:A:1783:ARG:HD3 | 1.97 | 0.47 |
| 1:A:3365:SER:OG | 1:A:3366:SER:N | 2.47 | 0.47 |
| 1:A:3722:PHE:O | 1:A:3741:ARG:NH1 | 2.48 | 0.47 |
| 1:A:356:ASN:ND2 | 1:A:404:ASP:HB3 | 2.30 | 0.46 |
| 1:A:446:PHE:CE2 | 1:A:530:LEU:HB2 | 2.50 | 0.46 |
| 1:A:1327:GLY:O | 1:A:1331:ASN:ND2 | 2.47 | 0.46 |
| 1:A:3819:THR:HG21 | 1:A:3886:ALA:HB2 | 1.97 | 0.46 |
| 1:A:60:SER:HA | 1:A:63:PHE:CG | 2.50 | 0.46 |
| 1:A:553:VAL:HA | 1:A:1549:SER:HA | 1.97 | 0.46 |
| 1:A:3168:TYR:CE2 | 1:A:3241:LYS:HG2 | 2.50 | 0.46 |
| 1:A:3349:ALA:H | 1:A:3357:ARG:HH11 | 1.62 | 0.46 |
| 1:A:3681:LYS:HB3 | 1:A:3724:GLU:HA | 1.97 | 0.46 |
| 1:A:3878:VAL:HG13 | 1:A:3965:ARG:HH22 | 1.80 | 0.46 |
| 1:A:3878:VAL:HG13 | 1:A:3965:ARG:NH2 | 2.30 | 0.46 |
| 1:A:898:PHE:HB2 | 1:A:901:MET:O | 2.14 | 0.46 |
| 1:A:3020:ASP:OD1 | 1:A:3022:GLU:N | 2.38 | 0.46 |
| 1:A:351:ASN:OD1 | 1:A:352:VAL:N | 2.49 | 0.46 |
| 1:A:523:THR:HG23 | 1:A:525:LYS:H | 1.80 | 0.46 |
| 1:A:1115:HIS:CE1 | 1:A:1180:GLN:HA | 2.50 | 0.46 |
| 1:A:2330:VAL:HB | 1:A:2338:GLU:OE1 | 2.16 | 0.46 |
| 1:A:3393:GLU:HG2 | 1:A:3394:GLU:HG3 | 1.97 | 0.46 |
| 1:A:4024:GLY:HA3 | 1:A:4025:GLY:HA2 | 1.58 | 0.46 |
| 1:A:51:LEU:O | 1:A:54:GLN:NE2 | 2.49 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1298:LEU:HD23 | 1:A:1298:LEU:HA | 1.67 | 0.46 |
| 1:A:3174:ASP:OD1 | 1:A:3174:ASP:N | 2.48 | 0.46 |
| 1:A:41:GLU:O | 1:A:45:SER:OG | 2.33 | 0.46 |
| 1:A:250:ASN:HA | 1:A:253:LEU:HG | 1.97 | 0.46 |
| 1:A:547:ASP:OD1 | 1:A:548:GLU:N | 2.44 | 0.46 |
| 1:A:938:VAL:HB | 1:A:984:TYR:OH | 2.16 | 0.46 |
| 1:A:1071:ASN:HB3 | 1:A:1074:LYS:HB2 | 1.98 | 0.46 |
| 1:A:1118:GLU:N | 1:A:1118:GLU:OE1 | 2.46 | 0.46 |
| 1:A:2242:VAL:HG23 | 1:A:2283:ASN:ND2 | 2.30 | 0.46 |
| 1:A:2999:LEU:HD23 | 1:A:2999:LEU:HA | 1.73 | 0.46 |
| 1:A:3173:MET:SD | 1:A:3782:SER:OG | 2.69 | 0.46 |
| 1:A:3227:ILE:HD12 | 1:A:3227:ILE:H | 1.81 | 0.46 |
| 1:A:74:ASN:HA | 1:A:78:PHE:CD2 | 2.51 | 0.46 |
| 1:A:3710:LYS:HB2 | 1:A:3711:PRO:HD2 | 1.97 | 0.46 |
| 1:A:356:ASN:HD22 | 1:A:404:ASP:HB3 | 1.81 | 0.46 |
| 1:A:1222:ASN:HA | 1:A:1236:LEU:HD11 | 1.96 | 0.46 |
| 1:A:1474:ASP:OD1 | 1:A:1474:ASP:N | 2.48 | 0.46 |
| 1:A:2151:ILE:HD11 | 1:A:2189:ILE:HG22 | 1.98 | 0.46 |
| 1:A:2247:ASP:N | 1:A:2247:ASP:OD1 | 2.46 | 0.46 |
| 1:A:221:ALA:HB1 | 1:A:225:LYS:NZ | 2.30 | 0.46 |
| 1:A:1475:LEU:HD21 | 1:A:1527:ARG:HH22 | 1.81 | 0.46 |
| 1:A:3134:ALA:HB2 | 1:A:3182:ILE:HG22 | 1.98 | 0.46 |
| 1:A:1663:THR:HA | 1:A:1668:PHE:CD2 | 2.51 | 0.46 |
| 1:A:2829:LYS:HE3 | 1:A:2867:ALA:HB3 | 1.98 | 0.46 |
| 1:A:470:ALA:C | 1:A:471:LYS:HD2 | 2.37 | 0.45 |
| 1:A:1086:TYR:O | 1:A:1087:ARG:HB2 | 2.16 | 0.45 |
| 1:A:2294:ILE:HG22 | 1:A:2299:TYR:CZ | 2.50 | 0.45 |
| 1:A:3509:ASP:OD1 | 1:A:3509:ASP:N | 2.47 | 0.45 |
| 1:A:3531:TYR:HB2 | 1:A:3532:PRO:HD3 | 1.98 | 0.45 |
| 1:A:3653:ARG:HH12 | 1:A:3659:PHE:HD1 | 1.64 | 0.45 |
| 1:A:383:PHE:O | 1:A:387:GLU:HG2 | 2.16 | 0.45 |
| 1:A:398:THR:O | 1:A:400:THR:OG1 | 2.34 | 0.45 |
| 1:A:1178:ARG:HD3 | 1:A:1183:CYS:SG | 2.57 | 0.45 |
| 1:A:1219:PHE:O | 1:A:1223:THR:HG23 | 2.16 | 0.45 |
| 1:A:1353:PRO:HB3 | 1:A:1356:TRP:HD1 | 1.81 | 0.45 |
| 1:A:1933:LEU:H | 1:A:1937:ARG:HH11 | 1.63 | 0.45 |
| 1:A:3810:VAL:HG22 | 1:A:3932:MET:SD | 2.56 | 0.45 |
| 1:A:3916:TRP:CE3 | 1:A:4107:LEU:HD11 | 2.51 | 0.45 |
| 1:A:3993:SER:OG | 1:A:3994:ASP:N | 2.49 | 0.45 |
| 1:A:432:THR:O | 1:A:435:LEU:N | 2.49 | 0.45 |
| 1:A:609:ALA:HB2 | 1:A:662:LEU:HD22 | 1.97 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:637:LYS:HG3 | 1:A:638:GLN:HG2 | 1.99 | 0.45 |
| 1:A:1786:ALA:HB2 | 1:A:1827:LEU:HD23 | 1.97 | 0.45 |
| 1:A:2835:LYS:O | 1:A:2838:GLN:HG2 | 2.16 | 0.45 |
| 1:A:4084:SER:HB3 | 1:A:4087:HIS:HB2 | 1.98 | 0.45 |
| 1:A:79:ARG:NH1 | 1:A:117:LYS:O | 2.50 | 0.45 |
| 1:A:2303:LEU:HA | 1:A:2306:ASN:HD22 | 1.81 | 0.45 |
| 1:A:2371:PHE:CZ | 1:A:2373:PRO:HG2 | 2.50 | 0.45 |
| 1:A:2886:GLN:O | 1:A:2890:ILE:HD12 | 2.17 | 0.45 |
| 1:A:3349:ALA:HB3 | 1:A:3357:ARG:HE | 1.81 | 0.45 |
| 1:A:3592:VAL:O | 1:A:3595:GLU:HG3 | 2.16 | 0.45 |
| 1:A:305:ASN:HB3 | 1:A:308:LEU:HB2 | 1.97 | 0.45 |
| 1:A:568:PHE:HE2 | 1:A:634:LEU:HD21 | 1.82 | 0.45 |
| 1:A:2340:SER:O | 1:A:2343:GLU:HG2 | 2.17 | 0.45 |
| 1:A:3229:SER:HA | 1:A:3232:ARG:HG3 | 1.98 | 0.45 |
| 1:A:3354:ASP:O | 1:A:3358:ARG:HG2 | 2.16 | 0.45 |
| 1:A:3550:LYS:O | 1:A:3553:GLU:HG3 | 2.17 | 0.45 |
| 1:A:609:ALA:HA | 1:A:612:LEU:HD12 | 1.99 | 0.45 |
| 1:A:1181:THR:HG22 | 1:A:1184:ARG:HH12 | 1.82 | 0.45 |
| 1:A:2128:PHE:O | 1:A:2132:LYS:HG2 | 2.17 | 0.45 |
| 1:A:2578:GLU:O | 1:A:2578:GLU:HG2 | 2.17 | 0.45 |
| 1:A:3631:LYS:O | 1:A:3635:THR:HG22 | 2.17 | 0.45 |
| 1:A:928:VAL:O | 1:A:928:VAL:HG12 | 2.17 | 0.45 |
| 1:A:1205:ASN:HB3 | 1:A:1275:THR:HA | 1.97 | 0.45 |
| 1:A:1338:VAL:HG12 | 1:A:1342:MET:CE | 2.47 | 0.45 |
| 1:A:1459:HIS:HB2 | 1:A:1464:LEU:HD22 | 1.99 | 0.45 |
| 1:A:2443:MET:CE | 1:A:2476:ILE:HG23 | 2.46 | 0.45 |
| 1:A:3036:TYR:CG | 1:A:3037:GLN:N | 2.84 | 0.45 |
| 1:A:4065:LEU:O | 1:A:4069:GLU:HB2 | 2.16 | 0.45 |
| 1:A:732:PHE:O | 1:A:735:SER:OG | 2.34 | 0.45 |
| 1:A:1493:PRO:HD2 | 1:A:1498:GLN:HB2 | 1.98 | 0.45 |
| 1:A:3328:ILE:HD11 | 1:A:3412:ALA:HB2 | 1.98 | 0.45 |
| 1:A:4107:LEU:HD23 | 1:A:4107:LEU:HA | 1.80 | 0.45 |
| 1:A:3314:SER:C | 1:A:3316:LEU:H | 2.20 | 0.45 |
| 1:A:177:LEU:HD12 | 1:A:178:LEU:N | 2.32 | 0.45 |
| 1:A:1299:GLU:OE2 | 1:A:1367:HIS:ND1 | 2.50 | 0.45 |
| 1:A:1471:GLN:H | 1:A:1477:HIS:CD2 | 2.35 | 0.45 |
| 1:A:1611:GLN:HA | 1:A:1613:HIS:CE1 | 2.51 | 0.45 |
| 1:A:1947:CYS:O | 1:A:1951:VAL:HG22 | 2.16 | 0.45 |
| 1:A:86:LEU:HB3 | 1:A:133:LYS:CD | 2.47 | 0.44 |
| 1:A:114:VAL:HG13 | 1:A:130:LEU:CD2 | 2.48 | 0.44 |
| 1:A:699:GLU:HG2 | 1:A:700:LYS:N | 2.33 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1161:ALA:O | 1:A:1162:SER:OG | 2.31 | 0.44 |
| 1:A:1413:ASP:OD1 | 1:A:1413:ASP:N | 2.50 | 0.44 |
| 1:A:1850:VAL:HG21 | 1:A:1869:LYS:NZ | 2.32 | 0.44 |
| 1:A:2455:LEU:HD12 | 1:A:2455:LEU:HA | 1.78 | 0.44 |
| 1:A:2477:LEU:HD23 | 1:A:2480:ILE:HD12 | 1.99 | 0.44 |
| 1:A:3350:GLU:OE2 | 1:A:3357:ARG:NH1 | 2.50 | 0.44 |
| 1:A:3839:TYR:O | 1:A:3843:LEU:HG | 2.17 | 0.44 |
| 1:A:753:GLN:NE2 | 1:A:791:ASP:O | 2.49 | 0.44 |
| 1:A:1727:ARG:HE | 1:A:1773:VAL:HG13 | 1.81 | 0.44 |
| 1:A:1848:ILE:HD11 | 1:A:1898:GLN:NE2 | 2.32 | 0.44 |
| 1:A:3587:ASP:OD1 | 1:A:4022:LYS:HE3 | 2.17 | 0.44 |
| 1:A:392:CYS:SG | 1:A:413:PHE:HB3 | 2.58 | 0.44 |
| 1:A:1977:ILE:HG13 | 1:A:1978:PHE:H | 1.82 | 0.44 |
| 1:A:2267:SER:OG | 1:A:2269:ASP:OD1 | 2.29 | 0.44 |
| 1:A:2917:PRO:O | 1:A:2920:VAL:HG12 | 2.17 | 0.44 |
| 1:A:3557:ARG:O | 1:A:3561:LYS:HG3 | 2.17 | 0.44 |
| 1:A:255:ALA:O | 1:A:258:PRO:HD3 | 2.18 | 0.44 |
| 1:A:670:LEU:O | 1:A:673:THR:HB | 2.17 | 0.44 |
| 1:A:1309:ALA:O | 1:A:1310:GLU:HG3 | 2.18 | 0.44 |
| 1:A:1338:VAL:HA | 1:A:1341:ILE:HD13 | 1.98 | 0.44 |
| 1:A:1588:ASP:N | 1:A:1588:ASP:OD1 | 2.50 | 0.44 |
| 1:A:1718:ILE:HG13 | 1:A:1719:VAL:N | 2.33 | 0.44 |
| 1:A:2379:MET:HA | 1:A:2382:VAL:HG12 | 1.99 | 0.44 |
| 1:A:3281:CYS:HA | 1:A:3301:LEU:HD11 | 1.99 | 0.44 |
| 1:A:3833:ARG:HD2 | 1:A:3833:ARG:HA | 1.77 | 0.44 |
| 1:A:3860:LYS:HA | 1:A:4076:ASP:OD2 | 2.18 | 0.44 |
| 1:A:553:VAL:HG11 | 1:A:1551:ILE:HD11 | 1.99 | 0.44 |
| 1:A:1039:TRP:HZ3 | 1:A:1043:GLN:HE21 | 1.65 | 0.44 |
| 1:A:1504:ASP:HB3 | 1:A:1507:CYS:H | 1.81 | 0.44 |
| 1:A:1951:VAL:O | 1:A:1955:VAL:HG12 | 2.18 | 0.44 |
| 1:A:3053:LEU:HD23 | 1:A:3092:LEU:HD21 | 1.99 | 0.44 |
| 1:A:3341:LEU:HD23 | 1:A:3341:LEU:HA | 1.84 | 0.44 |
| 1:A:3636:PHE:CD2 | 1:A:3670:MET:HG2 | 2.52 | 0.44 |
| 1:A:4037:ASN:HB2 | 1:A:4039:TYR:CE2 | 2.53 | 0.44 |
| 1:A:81:CYS:O | 1:A:85:ILE:HG12 | 2.17 | 0.44 |
| 1:A:1172:LEU:HD23 | 1:A:1172:LEU:HA | 1.84 | 0.44 |
| 1:A:1757:MET:SD | 1:A:1758:LEU:N | 2.90 | 0.44 |
| 1:A:2251:ILE:HD12 | 1:A:2251:ILE:H | 1.81 | 0.44 |
| 1:A:2930:TYR:HA | 1:A:2933:ILE:HG22 | 1.99 | 0.44 |
| 1:A:3369:ASP:O | 1:A:3373:VAL:HG23 | 2.17 | 0.44 |
| 1:A:3855:TYR:HB2 | 1:A:3955:VAL:HG22 | 1.99 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:83:GLU:HG3 | 1:A:127:ALA:HB1 | 1.99 | 0.44 |
| 1:A:217:LEU:HB2 | 1:A:218:PRO:HD3 | 1.99 | 0.44 |
| 1:A:429:GLU:O | 1:A:432:THR:HG22 | 2.18 | 0.44 |
| 1:A:767:GLU:OE2 | 1:A:771:ASN:ND2 | 2.51 | 0.44 |
| 1:A:771:ASN:CG | 1:A:854:ARG:HH22 | 2.21 | 0.44 |
| 1:A:876:SER:OG | 1:A:877:ASP:N | 2.51 | 0.44 |
| 1:A:1082:PHE:HB2 | 1:A:1107:TYR:OH | 2.18 | 0.44 |
| 1:A:1102:GLU:HA | 1:A:1154:PRO:HB3 | 1.99 | 0.44 |
| 1:A:3422:GLN:O | 1:A:3426:LYS:HG2 | 2.17 | 0.44 |
| 1:A:3548:GLY:HA2 | 1:A:3551:ASN:ND2 | 2.33 | 0.44 |
| 1:A:674:VAL:O | 1:A:677:ALA:HB3 | 2.18 | 0.44 |
| 1:A:897:PRO:O | 1:A:2566:THR:OG1 | 2.35 | 0.44 |
| 1:A:3011:LEU:HD23 | 1:A:3047:SER:HB3 | 2.00 | 0.44 |
| 1:A:19:LEU:HD13 | 1:A:38:LEU:HD21 | 2.00 | 0.44 |
| 1:A:225:LYS:H | 1:A:225:LYS:HD2 | 1.83 | 0.44 |
| 1:A:932:GLU:OE2 | 1:A:2771:LEU:HD13 | 2.17 | 0.44 |
| 1:A:1703:THR:HA | 1:A:1707:LEU:HD22 | 2.00 | 0.44 |
| 1:A:60:SER:HA | 1:A:63:PHE:CD2 | 2.53 | 0.43 |
| 1:A:1705:GLY:O | 1:A:1708:GLU:HG3 | 2.18 | 0.43 |
| 1:A:2547:SER:O | 1:A:2549:LYS:N | 2.50 | 0.43 |
| 1:A:3496:ILE:HA | 1:A:3499:ILE:HG12 | 1.99 | 0.43 |
| 1:A:3558:ILE:O | 1:A:3562:LEU:HG | 2.18 | 0.43 |
| 1:A:538:ASP:N | 1:A:561:ASN:OD1 | 2.49 | 0.43 |
| 1:A:87:LYS:HE3 | 1:A:87:LYS:HB3 | 1.92 | 0.43 |
| 1:A:1890:HIS:HA | 1:A:1909:ASN:HD22 | 1.83 | 0.43 |
| 1:A:2983:ASP:OD1 | 1:A:2983:ASP:N | 2.51 | 0.43 |
| 1:A:3686:TRP:HZ3 | 1:A:3690:PHE:HD1 | 1.65 | 0.43 |
| 1:A:66:LEU:O | 1:A:70:ARG:HG2 | 2.17 | 0.43 |
| 1:A:79:ARG:HD2 | 1:A:127:ALA:HA | 2.00 | 0.43 |
| 1:A:344:GLN:O | 1:A:348:ILE:HG12 | 2.19 | 0.43 |
| 1:A:1093:GLU:HA | 1:A:1096:VAL:HG22 | 1.99 | 0.43 |
| 1:A:2165:LEU:HD23 | 1:A:2165:LEU:HA | 1.85 | 0.43 |
| 1:A:3364:GLY:O | 1:A:3380:ARG:NH1 | 2.51 | 0.43 |
| 1:A:3757:ASP:OD1 | 1:A:3759:ARG:NE | 2.51 | 0.43 |
| 1:A:1426:GLN:HA | 1:A:1429:GLU:HG2 | 2.01 | 0.43 |
| 1:A:1845:VAL:HB | 1:A:1897:ASN:O | 2.18 | 0.43 |
| 1:A:3588:TRP:O | 1:A:3592:VAL:HG22 | 2.17 | 0.43 |
| 1:A:3642:LYS:O | 1:A:3646:LYS:HB2 | 2.18 | 0.43 |
| 1:A:85:ILE:HG13 | 1:A:86:LEU:HD22 | 2.00 | 0.43 |
| 1:A:497:LEU:HD13 | 1:A:2603:THR:HG21 | 1.99 | 0.43 |
| 1:A:1569:THR:HG22 | 1:A:1573:LYS:HZ1 | 1.84 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2340:SER:HA | 1:A:2343:GLU:OE1 | 2.19 | 0.43 |
| 1:A:3147:LYS:HE3 | 1:A:3150:ASN:HB3 | 1.99 | 0.43 |
| 1:A:3475:TYR:N | 1:A:3476:PRO:CD | 2.82 | 0.43 |
| 1:A:3988:LEU:HA | 1:A:3988:LEU:HD12 | 1.82 | 0.43 |
| 1:A:303:HIS:O | 1:A:309:LYS:HE2 | 2.18 | 0.43 |
| 1:A:468:LEU:HA | 1:A:468:LEU:HD23 | 1.79 | 0.43 |
| 1:A:537:SER:OG | 1:A:561:ASN:OD1 | 2.21 | 0.43 |
| 1:A:681:LYS:O | 1:A:684:GLU:HG3 | 2.19 | 0.43 |
| 1:A:1562:LEU:HD23 | 1:A:1562:LEU:HA | 1.88 | 0.43 |
| 1:A:1715:GLU:O | 1:A:1719:VAL:HG12 | 2.18 | 0.43 |
| 1:A:1816:ARG:O | 1:A:1819:PHE:HB2 | 2.18 | 0.43 |
| 1:A:2157:PHE:HB3 | 1:A:2164:TRP:CD1 | 2.53 | 0.43 |
| 1:A:3161:LEU:HD22 | 1:A:3234:CYS:SG | 2.59 | 0.43 |
| 1:A:3493:TRP:CZ2 | 1:A:3711:PRO:HD3 | 2.54 | 0.43 |
| 1:A:3614:TYR:HA | 1:A:3617:LEU:O | 2.18 | 0.43 |
| 1:A:3639:GLU:HG2 | 1:A:3640:PHE:N | 2.34 | 0.43 |
| 1:A:1429:GLU:HA | 1:A:1432:CYS:SG | 2.59 | 0.43 |
| 1:A:1691:GLN:O | 1:A:1694:THR:HG22 | 2.18 | 0.43 |
| 1:A:372:PRO:O | 1:A:376:ILE:HG22 | 2.19 | 0.43 |
| 1:A:2150:VAL:HG13 | 1:A:2157:PHE:CD2 | 2.52 | 0.43 |
| 1:A:3638:LYS:O | 1:A:3642:LYS:NZ | 2.52 | 0.43 |
| 1:A:257:ARG:HA | 1:A:260:ILE:HG12 | 2.01 | 0.43 |
| 1:A:397:LEU:HD13 | 1:A:397:LEU:HA | 1.87 | 0.43 |
| 1:A:1004:GLN:OE1 | 1:A:1004:GLN:N | 2.41 | 0.43 |
| 1:A:2150:VAL:HG22 | 1:A:2157:PHE:CE2 | 2.53 | 0.43 |
| 1:A:3563:ASP:OD1 | 1:A:3563:ASP:N | 2.49 | 0.43 |
| 1:A:3653:ARG:HH21 | 1:A:3655:LYS:HB3 | 1.84 | 0.43 |
| 1:A:1437:TYR:HB2 | 1:A:1499:CYS:SG | 2.58 | 0.42 |
| 1:A:1758:LEU:HD23 | 1:A:1758:LEU:HA | 1.90 | 0.42 |
| 1:A:1811:ARG:HG2 | 1:A:1816:ARG:HH11 | 1.84 | 0.42 |
| 1:A:2124:SER:HA | 1:A:2127:LYS:HG2 | 2.01 | 0.42 |
| 1:A:2506:LEU:HD23 | 1:A:2506:LEU:HA | 1.76 | 0.42 |
| 1:A:2164:TRP:O | 1:A:2167:PRO:HD2 | 2.19 | 0.42 |
| 1:A:2197:THR:HG21 | 1:A:2244:CYS:HB3 | 2.01 | 0.42 |
| 1:A:2419:ASP:O | 1:A:2423:VAL:HG13 | 2.19 | 0.42 |
| 1:A:2514:ASN:HD22 | 1:A:2517:LEU:HD13 | 1.84 | 0.42 |
| 1:A:3681:LYS:HZ3 | 1:A:3685:PRO:HG2 | 1.83 | 0.42 |
| 1:A:180:LEU:O | 1:A:184:VAL:HG23 | 2.19 | 0.42 |
| 1:A:1186:LYS:HD3 | 1:A:1186:LYS:HA | 1.90 | 0.42 |
| 1:A:1202:ARG:NH1 | 1:A:1206:LEU:HB3 | 2.33 | 0.42 |
| 1:A:1301:ILE:HG21 | 1:A:1338:VAL:HG21 | 2.02 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1397:ASP:N | 1:A:1397:ASP:OD1 | 2.52 | 0.42 |
| 1:A:1560:TYR:OH | 1:A:1599:GLY:HA3 | 2.19 | 0.42 |
| 1:A:1723:PRO:HG3 | 1:A:1729:PHE:CZ | 2.54 | 0.42 |
| 1:A:2459:VAL:HG11 | 1:A:2501:LEU:HD21 | 1.99 | 0.42 |
| 1:A:2953:THR:HB | 1:A:2994:TRP:HE1 | 1.84 | 0.42 |
| 1:A:2962:ARG:HG2 | 1:A:3989:ARG:NH2 | 2.33 | 0.42 |
| 1:A:3022:GLU:HG3 | 1:A:3024:PRO:HD2 | 2.01 | 0.42 |
| 1:A:272:LEU:HD23 | 1:A:312:ALA:HA | 2.01 | 0.42 |
| 1:A:1468:LEU:HA | 1:A:1469:PRO:HD3 | 1.89 | 0.42 |
| 1:A:1774:MET:HE2 | 1:A:1777:LEU:HB2 | 2.01 | 0.42 |
| 1:A:2092:GLU:H | 1:A:2092:GLU:CD | 2.21 | 0.42 |
| 1:A:3662:ILE:HA | 1:A:3665:MET:HG3 | 2.01 | 0.42 |
| 1:A:433:PRO:HA | 1:A:436:GLU:OE1 | 2.19 | 0.42 |
| 1:A:1630:ASP:OD1 | 1:A:1631:SER:N | 2.52 | 0.42 |
| 1:A:1896:ILE:HD13 | 1:A:1911:LEU:HD23 | 2.01 | 0.42 |
| 1:A:2158:ARG:HG3 | 1:A:2196:TRP:HE1 | 1.84 | 0.42 |
| 1:A:1702:LEU:HD23 | 1:A:1703:THR:N | 2.35 | 0.42 |
| 1:A:1725:GLN:HA | 1:A:1769:GLU:HG3 | 2.02 | 0.42 |
| 1:A:1880:MET:O | 1:A:1884:LEU:HD23 | 2.19 | 0.42 |
| 1:A:1983:ASP:HA | 1:A:2184:TYR:OH | 2.19 | 0.42 |
| 1:A:2404:ARG:HD2 | 1:A:2404:ARG:HA | 1.76 | 0.42 |
| 1:A:3880:ALA:HB1 | 1:A:3969:ASN:ND2 | 2.35 | 0.42 |
| 1:A:1766:LEU:HD13 | 1:A:1778:PHE:CD2 | 2.55 | 0.42 |
| 1:A:1858:LEU:HA | 1:A:1863:PHE:CE1 | 2.54 | 0.42 |
| 1:A:3499:ILE:HD13 | 1:A:3499:ILE:HA | 1.90 | 0.42 |
| 1:A:3557:ARG:O | 1:A:3560:SER:OG | 2.32 | 0.42 |
| 1:A:3684:SER:H | 1:A:3685:PRO:HD3 | 1.83 | 0.42 |
| 1:A:3755:GLY:HA2 | 1:A:3799:ARG:O | 2.19 | 0.42 |
| 1:A:653:LEU:HD23 | 1:A:653:LEU:HA | 1.83 | 0.42 |
| 1:A:1365:ASN:O | 1:A:1369:MET:HG2 | 2.20 | 0.42 |
| 1:A:1657:SER:HB2 | 1:A:1659:VAL:HG12 | 2.02 | 0.42 |
| 1:A:1890:HIS:CG | 1:A:1955:VAL:HG23 | 2.54 | 0.42 |
| 1:A:1983:ASP:CG | 1:A:2185:MET:HG2 | 2.40 | 0.42 |
| 1:A:3503:VAL:HG11 | 1:A:3533:PHE:HA | 2.01 | 0.42 |
| 1:A:240:GLU:HB2 | 1:A:243:GLN:NE2 | 2.33 | 0.42 |
| 1:A:1497:ARG:HD3 | 1:A:1499:CYS:O | 2.20 | 0.42 |
| 1:A:1504:ASP:C | 1:A:1506:SER:H | 2.22 | 0.42 |
| 1:A:2466:SER:C | 1:A:2468:THR:H | 2.23 | 0.42 |
| 1:A:2821:ASP:OD1 | 1:A:2822:LYS:N | 2.53 | 0.42 |
| 1:A:3604:LYS:HZ2 | 1:A:3652:LEU:HD13 | 1.84 | 0.42 |
| 1:A:3793:VAL:HG13 | 1:A:3803:ILE:HG22 | 2.01 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1163:LEU:HD23 | 1:A:1163:LEU:HA | 1.74 | 0.42 |
| 1:A:1805:PHE:O | 1:A:1816:ARG:HD3 | 2.20 | 0.42 |
| 1:A:2457:PRO:HA | 1:A:2460:GLU:CD | 2.40 | 0.42 |
| 1:A:3148:GLN:N | 1:A:3148:GLN:OE1 | 2.52 | 0.42 |
| 1:A:64:GLY:HA2 | 1:A:67:VAL:HG22 | 2.01 | 0.41 |
| 1:A:176:GLU:HG2 | 1:A:223:CYS:HB2 | 2.02 | 0.41 |
| 1:A:200:PHE:CZ | 1:A:224:LEU:HA | 2.50 | 0.41 |
| 1:A:1225:GLU:HB2 | 1:A:1235:ILE:HG12 | 2.02 | 0.41 |
| 1:A:1305:ASP:N | 1:A:1305:ASP:OD1 | 2.52 | 0.41 |
| 1:A:2178:GLY:O | 1:A:2183:HIS:NE2 | 2.52 | 0.41 |
| 1:A:3346:ALA:C | 1:A:3357:ARG:HH12 | 2.23 | 0.41 |
| 1:A:3578:LEU:HD11 | 1:A:3681:LYS:HE2 | 2.02 | 0.41 |
| 1:A:3756:GLU:OE1 | 1:A:3756:GLU:N | 2.42 | 0.41 |
| 1:A:3959:MET:SD | 1:A:3959:MET:N | 2.92 | 0.41 |
| 1:A:82:ARG:HA | 1:A:85:ILE:HG12 | 2.02 | 0.41 |
| 1:A:148:LYS:HE2 | 1:A:153:PHE:CE2 | 2.55 | 0.41 |
| 1:A:241:ASP:O | 1:A:244:THR:HG22 | 2.19 | 0.41 |
| 1:A:2474:TYR:HB3 | 1:A:2521:ILE:HD11 | 2.02 | 0.41 |
| 1:A:2575:PRO:HB3 | 1:A:2785:ILE:O | 2.20 | 0.41 |
| 1:A:3368:GLU:HG3 | 1:A:3372:LYS:HZ3 | 1.85 | 0.41 |
| 1:A:1261:LEU:CD1 | 1:A:1340:ARG:HG3 | 2.50 | 0.41 |
| 1:A:2398:LEU:HA | 1:A:2398:LEU:HD23 | 1.86 | 0.41 |
| 1:A:2488:GLU:O | 1:A:2491:THR:OG1 | 2.33 | 0.41 |
| 1:A:4014:LYS:HA | 1:A:4017:GLU:HG3 | 2.02 | 0.41 |
| 1:A:406:ARG:HB3 | 1:A:408:TYR:HD1 | 1.85 | 0.41 |
| 1:A:455:LEU:HD12 | 1:A:459:ARG:NH2 | 2.36 | 0.41 |
| 1:A:1560:TYR:CE2 | 1:A:1596:VAL:HG22 | 2.55 | 0.41 |
| 1:A:1747:LEU:HD21 | 1:A:1778:PHE:CE1 | 2.56 | 0.41 |
| 1:A:3640:PHE:HA | 1:A:3643:HIS:HB3 | 2.02 | 0.41 |
| 1:A:256:ILE:HD12 | 1:A:256:ILE:HA | 1.88 | 0.41 |
| 1:A:2806:LYS:HB2 | 1:A:2857:CYS:HB2 | 2.02 | 0.41 |
| 1:A:3496:ILE:HB | 1:A:3707:GLY:HA2 | 2.02 | 0.41 |
| 1:A:3604:LYS:HZ2 | 1:A:3652:LEU:HD22 | 1.85 | 0.41 |
| 1:A:3901:ARG:HG3 | 1:A:3970:LEU:HD11 | 2.03 | 0.41 |
| 1:A:363:ILE:HD13 | 1:A:363:ILE:HA | 1.89 | 0.41 |
| 1:A:397:LEU:HD11 | 1:A:437:HIS:CB | 2.48 | 0.41 |
| 1:A:1061:LYS:NZ | 1:A:1152:ARG:HH22 | 2.19 | 0.41 |
| 1:A:1838:GLU:O | 1:A:1841:SER:OG | 2.34 | 0.41 |
| 1:A:1854:ARG:CZ | 1:A:1866:GLN:HB3 | 2.50 | 0.41 |
| 1:A:2443:MET:HE2 | 1:A:2476:ILE:HD12 | 2.03 | 0.41 |
| 1:A:2471:GLU:HB2 | 1:A:2517:LEU:HD11 | 2.01 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2555:LEU:HD11 | 1:A:2854:PHE:HA | 2.03 | 0.41 |
| 1:A:3957:GLU:HG2 | 1:A:3959:MET:SD | 2.60 | 0.41 |
| 1:A:1848:ILE:HD11 | 1:A:1898:GLN:HE21 | 1.85 | 0.41 |
| 1:A:2211:LEU:HA | 1:A:2214:ARG:HG2 | 2.03 | 0.41 |
| 1:A:2268:LYS:O | 1:A:2271:SER:HB3 | 2.21 | 0.41 |
| 1:A:2461:PHE:HB2 | 1:A:2473:MET:HE3 | 2.03 | 0.41 |
| 1:A:62:ASP:HA | 1:A:65:LEU:HG | 2.02 | 0.41 |
| 1:A:421:LEU:HD12 | 1:A:421:LEU:HA | 1.88 | 0.41 |
| 1:A:1369:MET:HG3 | 1:A:1414:ILE:HG22 | 2.02 | 0.41 |
| 1:A:1832:SER:O | 1:A:1832:SER:OG | 2.31 | 0.41 |
| 1:A:1838:GLU:O | 1:A:1842:THR:HG23 | 2.20 | 0.41 |
| 1:A:2364:LEU:HA | 1:A:2367:VAL:HG12 | 2.03 | 0.41 |
| 1:A:3856:MET:CE | 1:A:4073:ALA:H | 2.34 | 0.41 |
| 1:A:4096:SER:OG | 1:A:4097:GLY:N | 2.53 | 0.41 |
| 1:A:221:ALA:HA | 1:A:224:LEU:CD1 | 2.51 | 0.41 |
| 1:A:606:SER:HB3 | 1:A:1080:LEU:HD22 | 2.03 | 0.41 |
| 1:A:969:LEU:HD23 | 1:A:969:LEU:HA | 1.87 | 0.41 |
| 1:A:985:GLU:O | 1:A:989:MET:HG2 | 2.21 | 0.41 |
| 1:A:1361:LYS:HZ3 | 1:A:1364:CYS:H | 1.67 | 0.41 |
| 1:A:1396:PRO:O | 1:A:1400:VAL:HG13 | 2.21 | 0.41 |
| 1:A:2146:LEU:O | 1:A:2150:VAL:HG23 | 2.20 | 0.41 |
| 1:A:2257:PHE:O | 1:A:2261:SER:N | 2.54 | 0.41 |
| 1:A:2333:ARG:CZ | 1:A:2333:ARG:HA | 2.51 | 0.41 |
| 1:A:3128:LYS:HD3 | 1:A:3128:LYS:HA | 1.85 | 0.41 |
| 1:A:3694:PHE:O | 1:A:3695:LEU:HB2 | 2.20 | 0.41 |
| 1:A:3856:MET:CE | 1:A:4071:ALA:HB1 | 2.50 | 0.41 |
| 1:A:3909:ALA:HB1 | 1:A:3984:MET:HG3 | 2.03 | 0.41 |
| 1:A:225:LYS:HE3 | 1:A:253:LEU:HD22 | 2.03 | 0.41 |
| 1:A:346:TYR:HB3 | 1:A:350:ARG:NH1 | 2.36 | 0.41 |
| 1:A:403:GLY:O | 1:A:406:ARG:NE | 2.54 | 0.41 |
| 1:A:573:LEU:HD23 | 1:A:573:LEU:HA | 1.83 | 0.41 |
| 1:A:1124:ILE:H | 1:A:1124:ILE:HD12 | 1.86 | 0.41 |
| 1:A:1827:LEU:HD23 | 1:A:1827:LEU:HA | 1.90 | 0.41 |
| 1:A:1896:ILE:HD11 | 1:A:1910:GLU:OE2 | 2.21 | 0.41 |
| 1:A:2185:MET:O | 1:A:2189:ILE:HG12 | 2.21 | 0.41 |
| 1:A:2186:VAL:HA | 1:A:2189:ILE:HG12 | 2.03 | 0.41 |
| 1:A:2256:ILE:HD12 | 1:A:2256:ILE:H | 1.86 | 0.41 |
| 1:A:2271:SER:HA | 1:A:2274:ILE:HD12 | 2.03 | 0.41 |
| 1:A:2323:LEU:O | 1:A:2327:LEU:HG | 2.21 | 0.41 |
| 1:A:2835:LYS:HA | 1:A:2838:GLN:HG2 | 2.03 | 0.41 |
| 1:A:3295:GLU:HG2 | 1:A:3296:GLN:N | 2.36 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3827:ALA:O | 1:A:3834:ALA:HB2 | 2.21 | 0.41 |
| 1:A:3871:PHE:HA | 1:A:3874:ARG:NH1 | 2.36 | 0.41 |
| 1:A:3983:ILE:HD13 | 1:A:3983:ILE:HA | 1.92 | 0.41 |
| 1:A:263:LYS:HA | 1:A:263:LYS:HD2 | 1.88 | 0.40 |
| 1:A:382:ASP:O | 1:A:386:VAL:HG23 | 2.21 | 0.40 |
| 1:A:536:SER:HB3 | 1:A:637:LYS:NZ | 2.36 | 0.40 |
| 1:A:1086:TYR:C | 1:A:1088:GLU:H | 2.24 | 0.40 |
| 1:A:1395:LEU:HB3 | 1:A:1396:PRO:HD3 | 2.02 | 0.40 |
| 1:A:1925:GLU:OE1 | 1:A:1927:MET:N | 2.54 | 0.40 |
| 1:A:2216:LEU:HD13 | 1:A:2241:LEU:HD23 | 2.03 | 0.40 |
| 1:A:2950:LYS:HG2 | 1:A:2981:TRP:CZ3 | 2.55 | 0.40 |
| 1:A:737:PRO:HD2 | 1:A:740:ILE:HD12 | 2.03 | 0.40 |
| 1:A:1069:HIS:CE1 | 1:A:3741:ARG:HD2 | 2.56 | 0.40 |
| 1:A:1265:GLU:O | 1:A:1269:THR:HG22 | 2.22 | 0.40 |
| 1:A:1404:LYS:HB2 | 1:A:1404:LYS:HE2 | 1.71 | 0.40 |
| 1:A:3753:LYS:HB3 | 1:A:3756:GLU:OE2 | 2.22 | 0.40 |
| 1:A:75:SER:O | 1:A:79:ARG:HG2 | 2.20 | 0.40 |
| 1:A:287:LEU:HA | 1:A:337:LYS:NZ | 2.35 | 0.40 |
| 1:A:404:ASP:HB2 | 1:A:1732:GLY:O | 2.21 | 0.40 |
| 1:A:1782:PHE:O | 1:A:1785:ILE:HG22 | 2.20 | 0.40 |
| 1:A:2149:LEU:O | 1:A:2153:THR:OG1 | 2.26 | 0.40 |
| 1:A:3751:LEU:HD23 | 1:A:3803:ILE:HD11 | 2.03 | 0.40 |
| 1:A:3753:LYS:HD3 | 1:A:3803:ILE:HD11 | 2.02 | 0.40 |
| 1:A:363:ILE:HG13 | 1:A:413:PHE:CE2 | 2.56 | 0.40 |
| 1:A:410:MET:HB3 | 1:A:442:GLN:OE1 | 2.21 | 0.40 |
| 1:A:637:LYS:HG3 | 1:A:638:GLN:N | 2.36 | 0.40 |
| 1:A:1387:GLY:O | 1:A:1389:VAL:HG13 | 2.21 | 0.40 |
| 1:A:1397:ASP:HA | 1:A:1400:VAL:HG22 | 2.04 | 0.40 |
| 1:A:1793:THR:O | 1:A:1797:LEU:HG | 2.21 | 0.40 |
| 1:A:2132:LYS:HD2 | 1:A:2132:LYS:HA | 1.79 | 0.40 |
| 1:A:2269:ASP:OD1 | 1:A:2269:ASP:N | 2.52 | 0.40 |
| 1:A:2461:PHE:HB2 | 1:A:2473:MET:CE | 2.52 | 0.40 |
| 1:A:3062:LEU:HB3 | 1:A:3089:LEU:HD11 | 2.03 | 0.40 |
| 1:A:3859:TYR:CE1 | 1:A:4119:ARG:HB2 | 2.48 | 0.40 |
| 1:A:421:LEU:HD11 | 1:A:427:VAL:HG22 | 2.03 | 0.40 |
| 1:A:1340:ARG:HD3 | 1:A:1343:GLU:OE2 | 2.22 | 0.40 |
| 1:A:2231:PHE:CZ | 1:A:2272:VAL:HG12 | 2.57 | 0.40 |
| 1:A:2255:LEU:HA | 1:A:2258:GLU:OE1 | 2.21 | 0.40 |
| 1:A:2452:ARG:HB2 | 1:A:2498:ILE:HD11 | 2.04 | 0.40 |
| 1:A:3358:ARG:NE | 1:A:3358:ARG:HA | 2.36 | 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 | 3632/4156 (87%) | 3357 (92%) | 275 (8%) | 0 | 100 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 3229/3671 (88%) | 3215 (100%) | 14 (0%) | 91 96 |

All (14) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 71 | LYS |
| 1 | A | 108 | LYS |
| 1 | A | 379 | LYS |
| 1 | A | 541 | MET |
| 1 | A | 880 | MET |
| 1 | A | 1360 | LYS |
| 1 | A | 1612 | LYS |
| 1 | A | 1738 | ASN |
| 1 | A | 1895 | LYS |
| 1 | A | 2328 | ARG |
| 1 | A | 3302 | LYS |
| 1 | A | 3482 | LEU |
| 1 | A | 3552 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3849 | LYS |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 16 | GLN |
| 1 | A | 303 | HIS |
| 1 | A | 3154 | GLN |

#### 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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 1 | A | 2 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | A | 4128:MET | C | 5009:UNK | N | 96.48 |
| 1 | A | 5016:UNK | C | 6001:UNK | N | 49.88 |

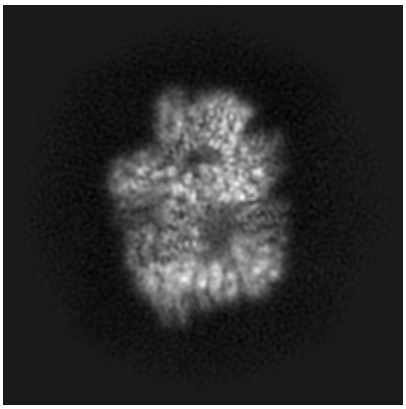
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11213. These allow visual inspection of the internal detail of the map and identification of artifacts.

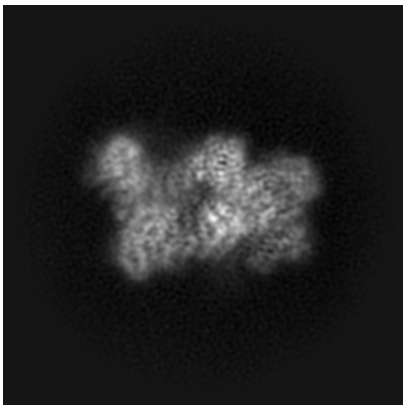
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

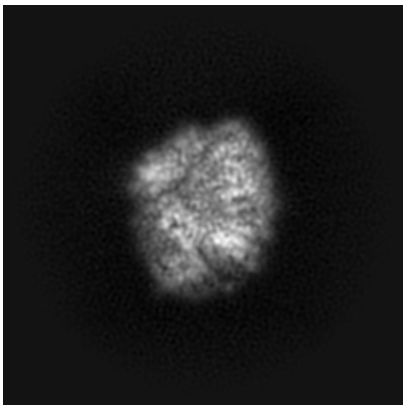
### 6.1.1 Primary map



X

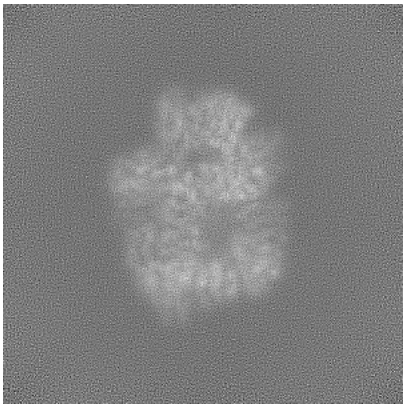


Y

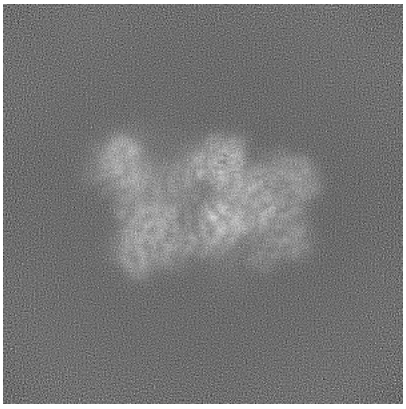


Z

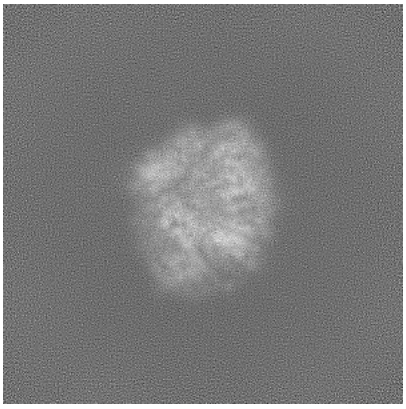
### 6.1.2 Raw map



X



Y

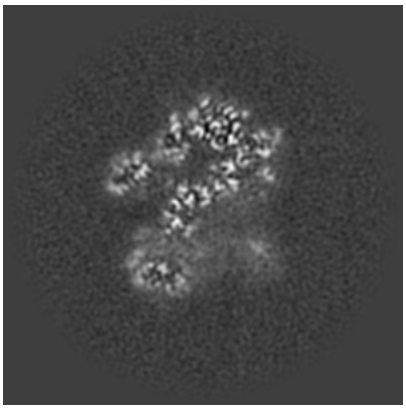


Z

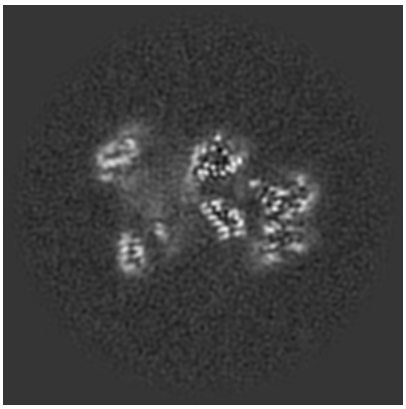
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

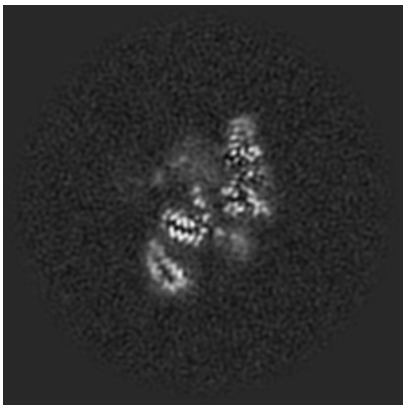
### 6.2.1 Primary map



X Index: 215

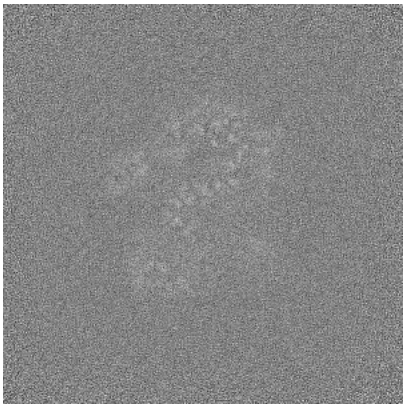


Y Index: 215

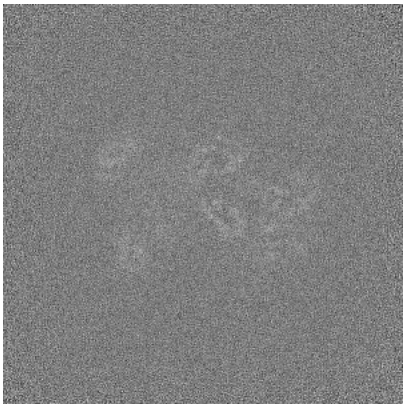


Z Index: 215

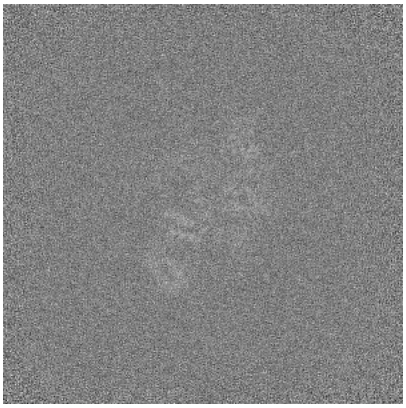
### 6.2.2 Raw map



X Index: 215



Y Index: 215

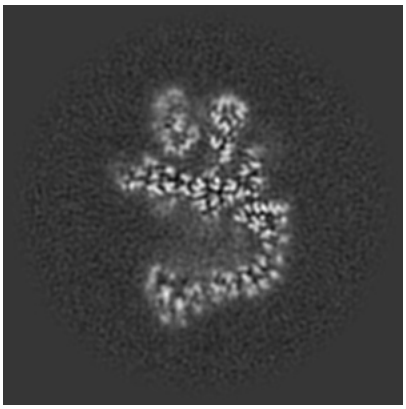


Z Index: 215

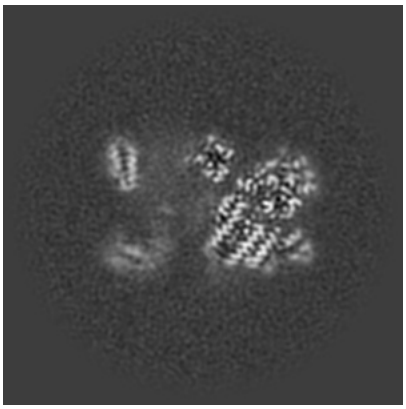
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

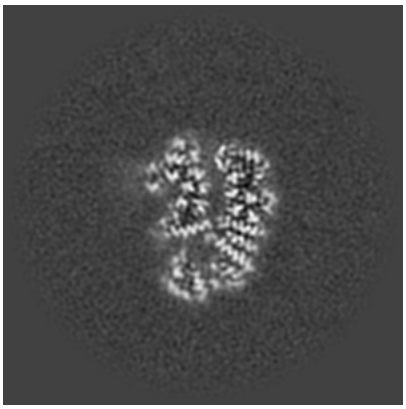
### 6.3.1 Primary map



X Index: 249

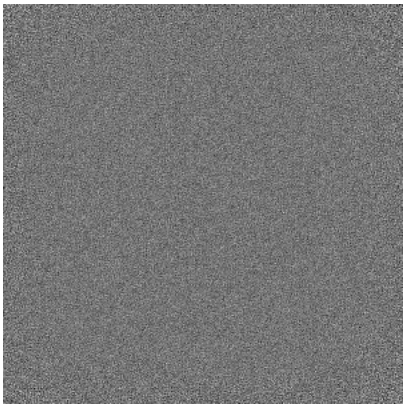


Y Index: 245

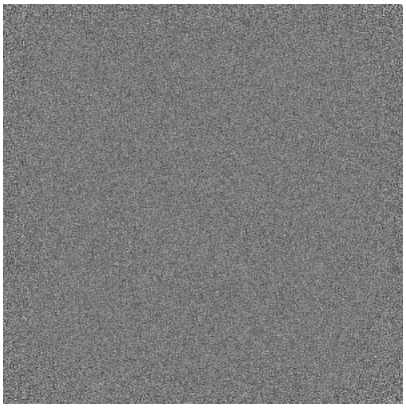


Z Index: 233

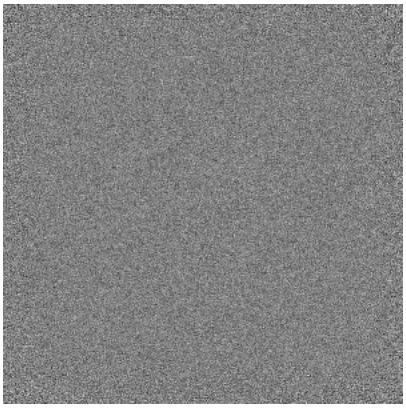
### 6.3.2 Raw map



X Index: 0



Y Index: 0

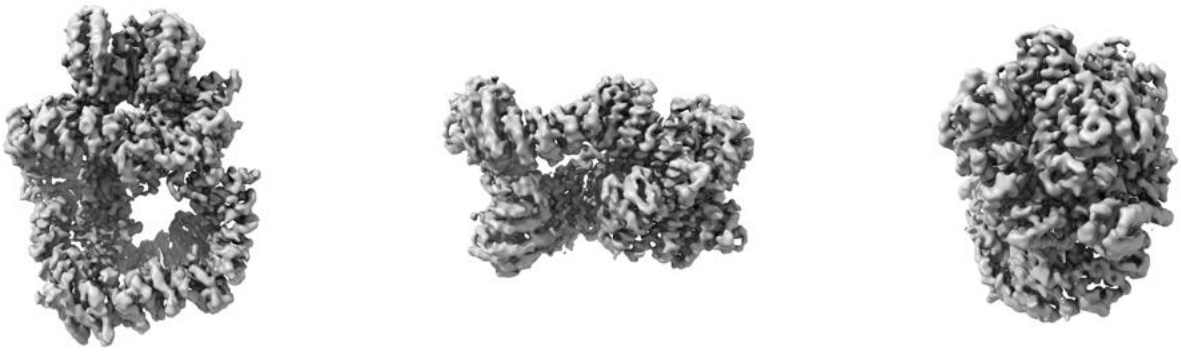


Z Index: 0

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

## 6.4 Orthogonal surface views (i)

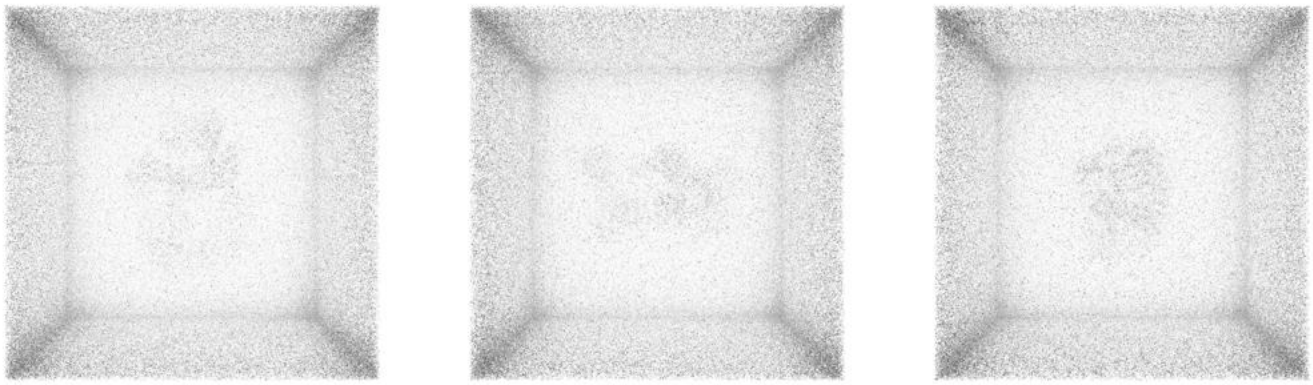
### 6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

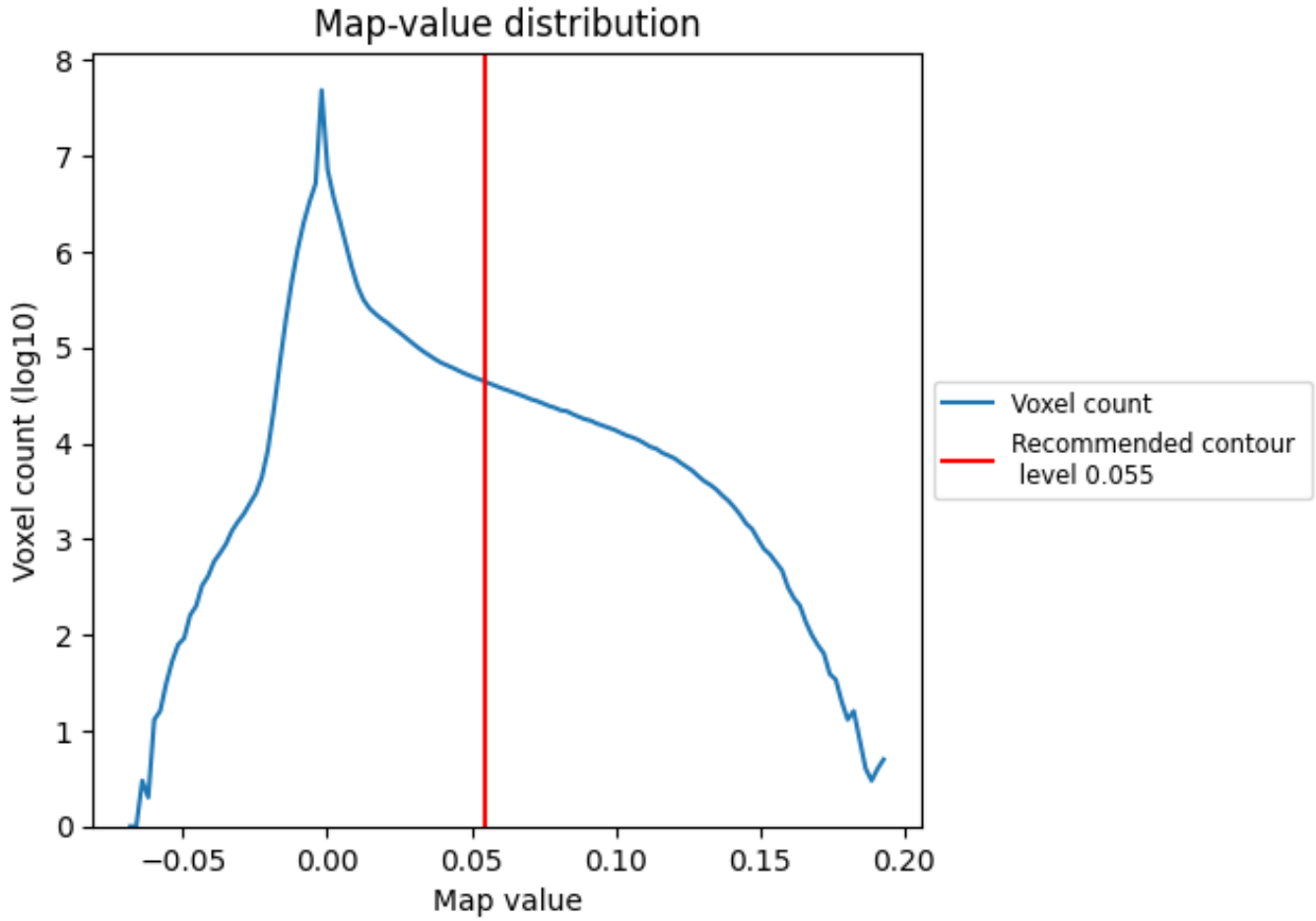
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

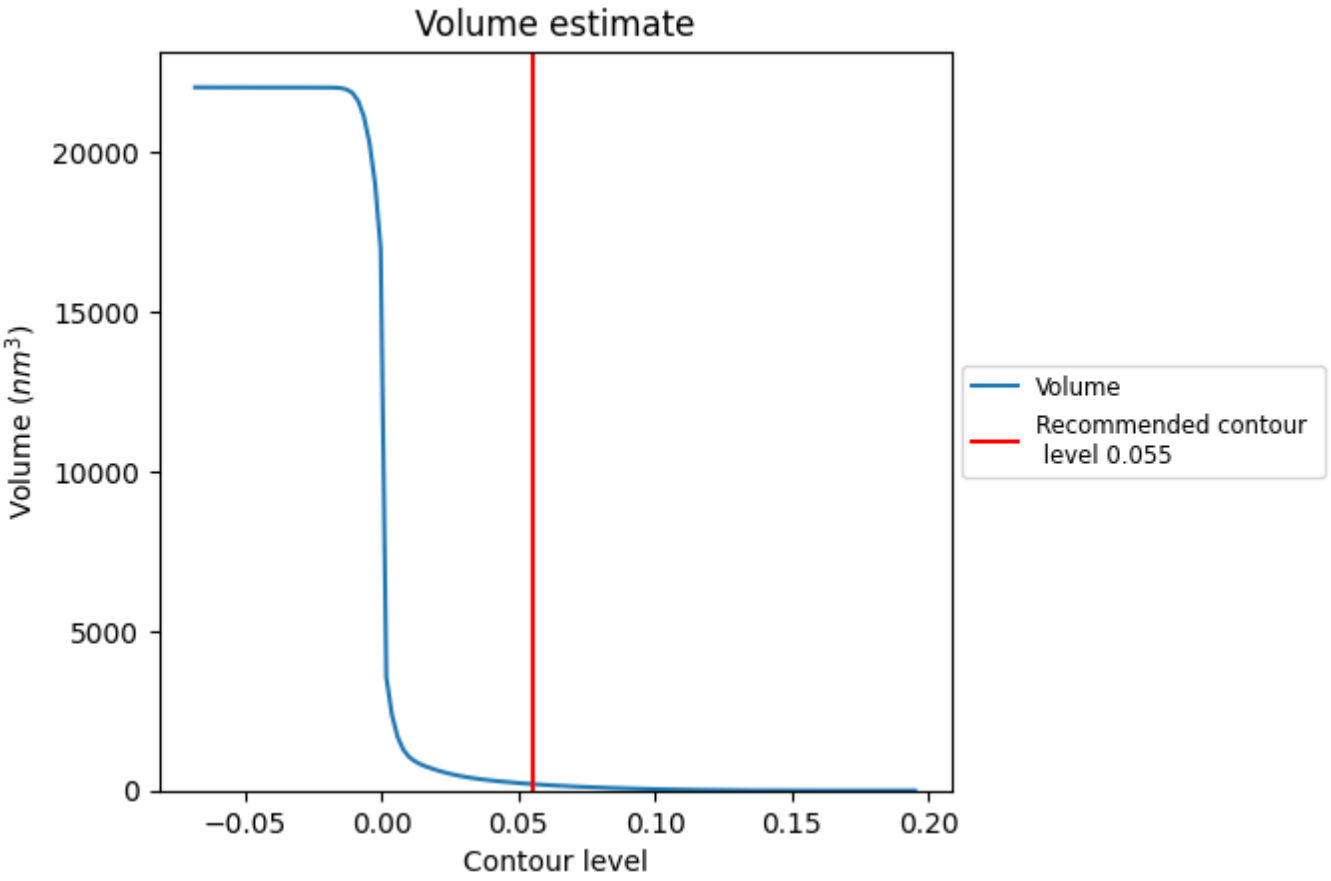
This section contains the results of statistical analysis of the map.

## 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.

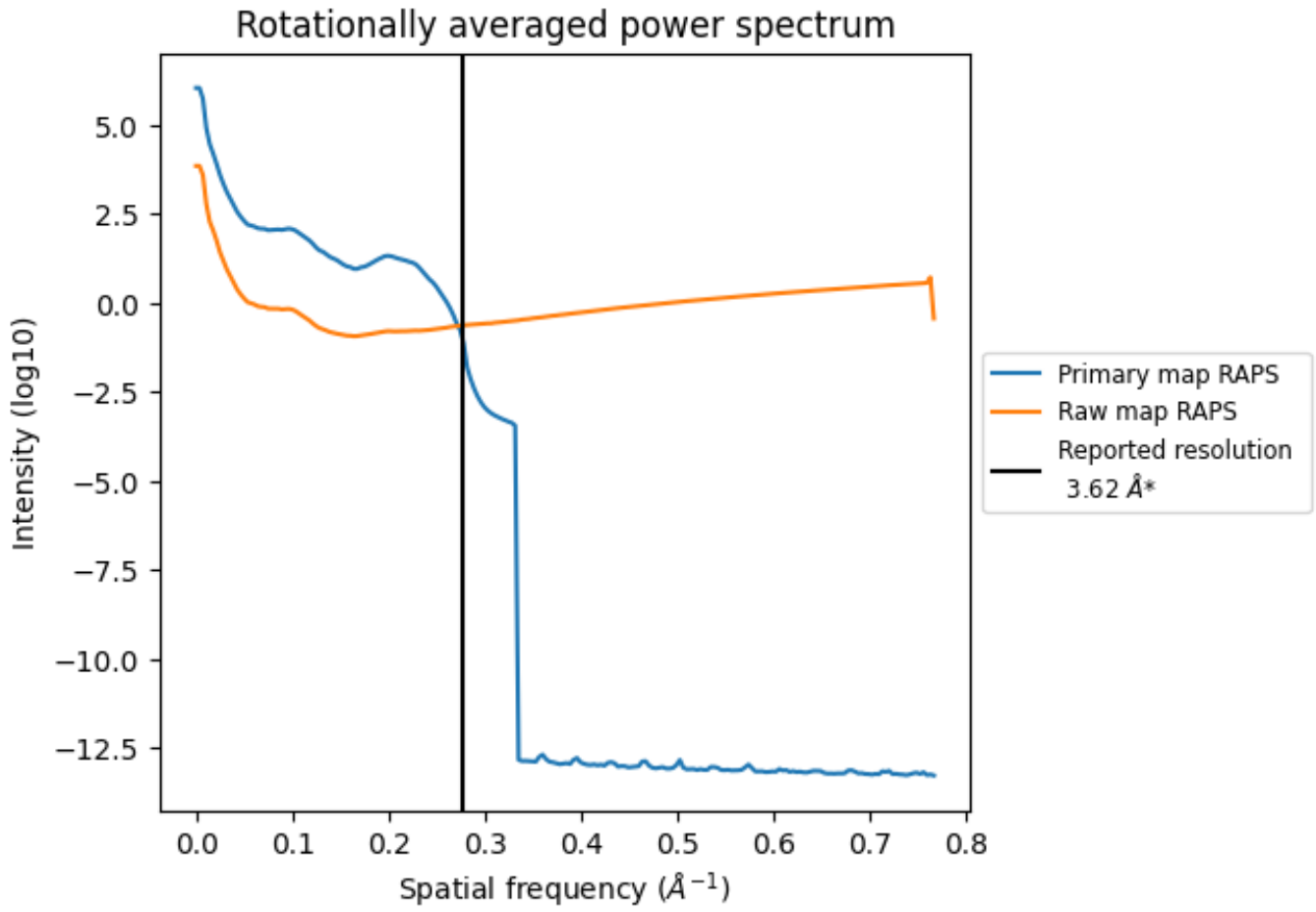
## 7.2 Volume estimate




The volume at the recommended contour level is 203 $nm^3$; this corresponds to an approximate mass of 183 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)

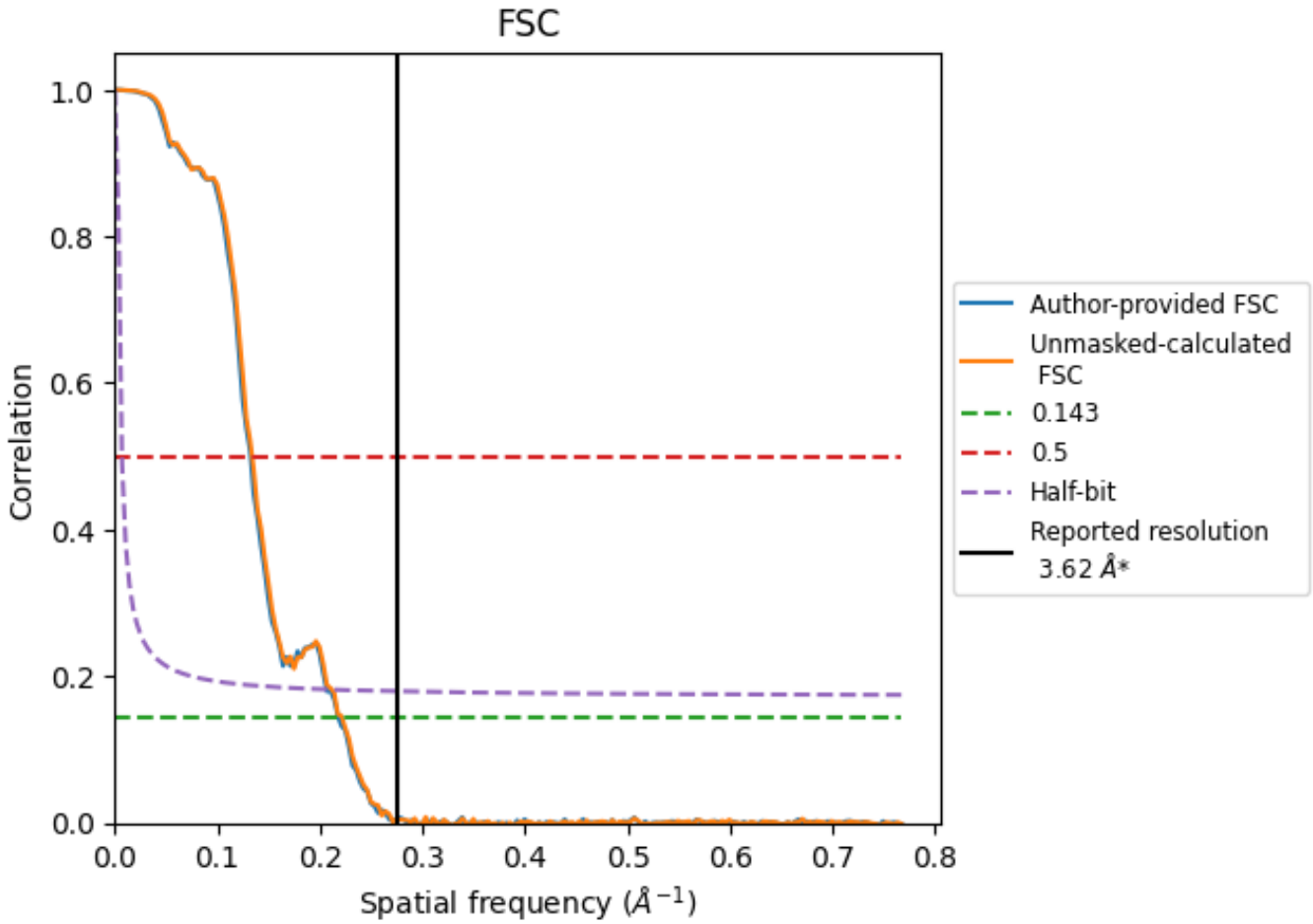



*Reported resolution corresponds to spatial frequency of 0.276 $Å^{-1}$

# 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 0.276 Å$^{-1}$

## 8.2 Resolution estimates (i)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.62 | - | - |
| Author-provided FSC curve | 4.58 | 7.55 | 4.84 |
| Unmasked-calculated* | 4.51 | 7.47 | 4.73 |

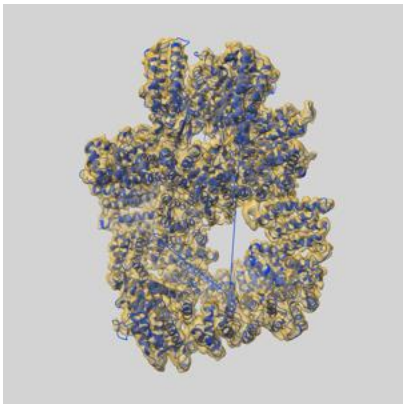
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.58 differs from the reported value 3.62 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.62 by more than 10 %

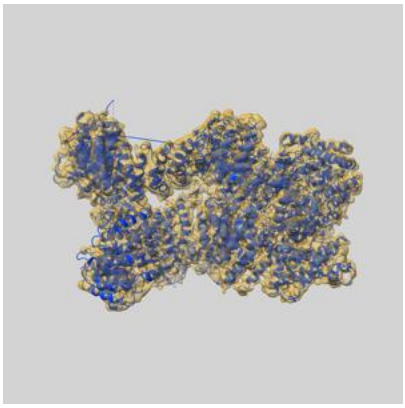
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11213 and PDB model 6ZH4. Per-residue inclusion information can be found in section 3 on page 4.

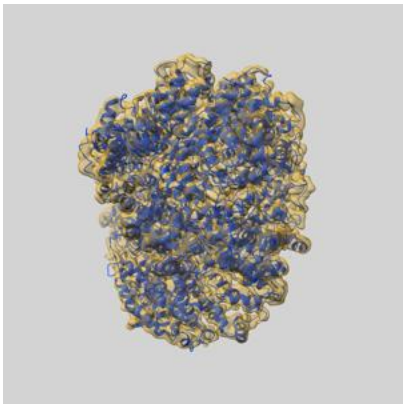
## 9.1 Map-model overlay



X



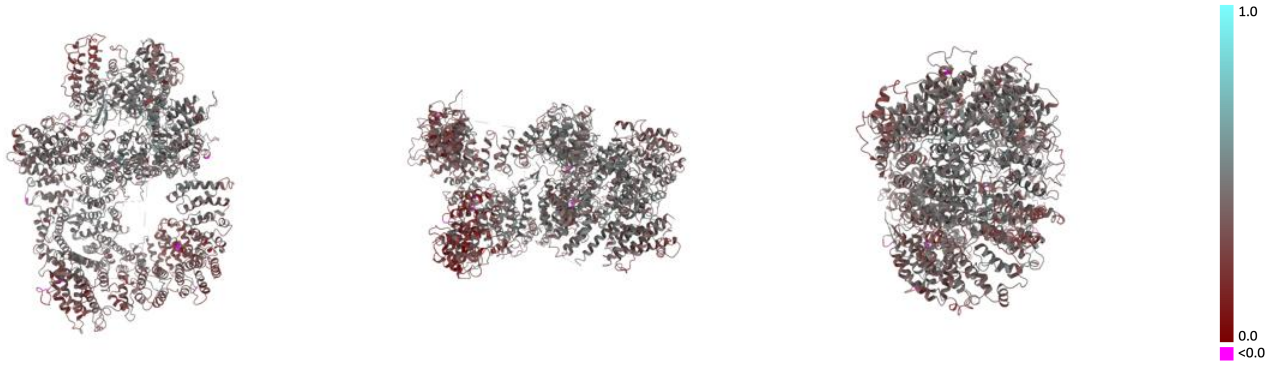
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

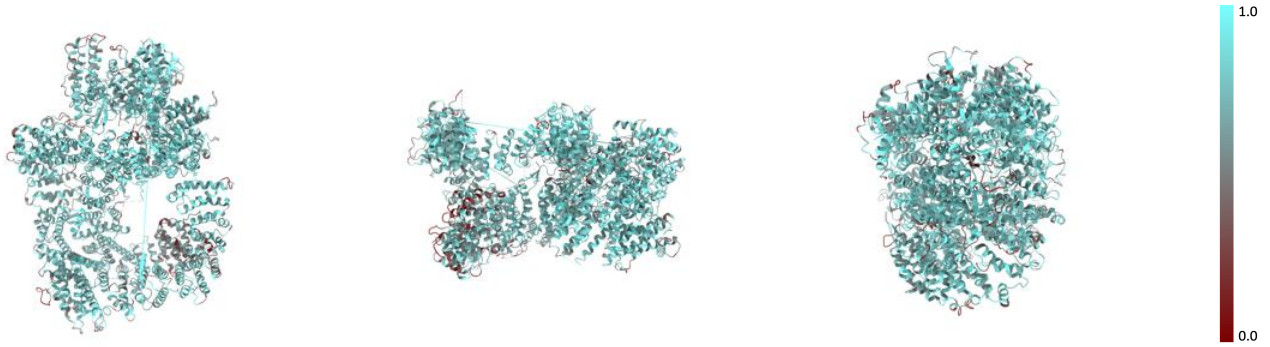
## 9.2 Q-score mapped to coordinate model (i)




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.

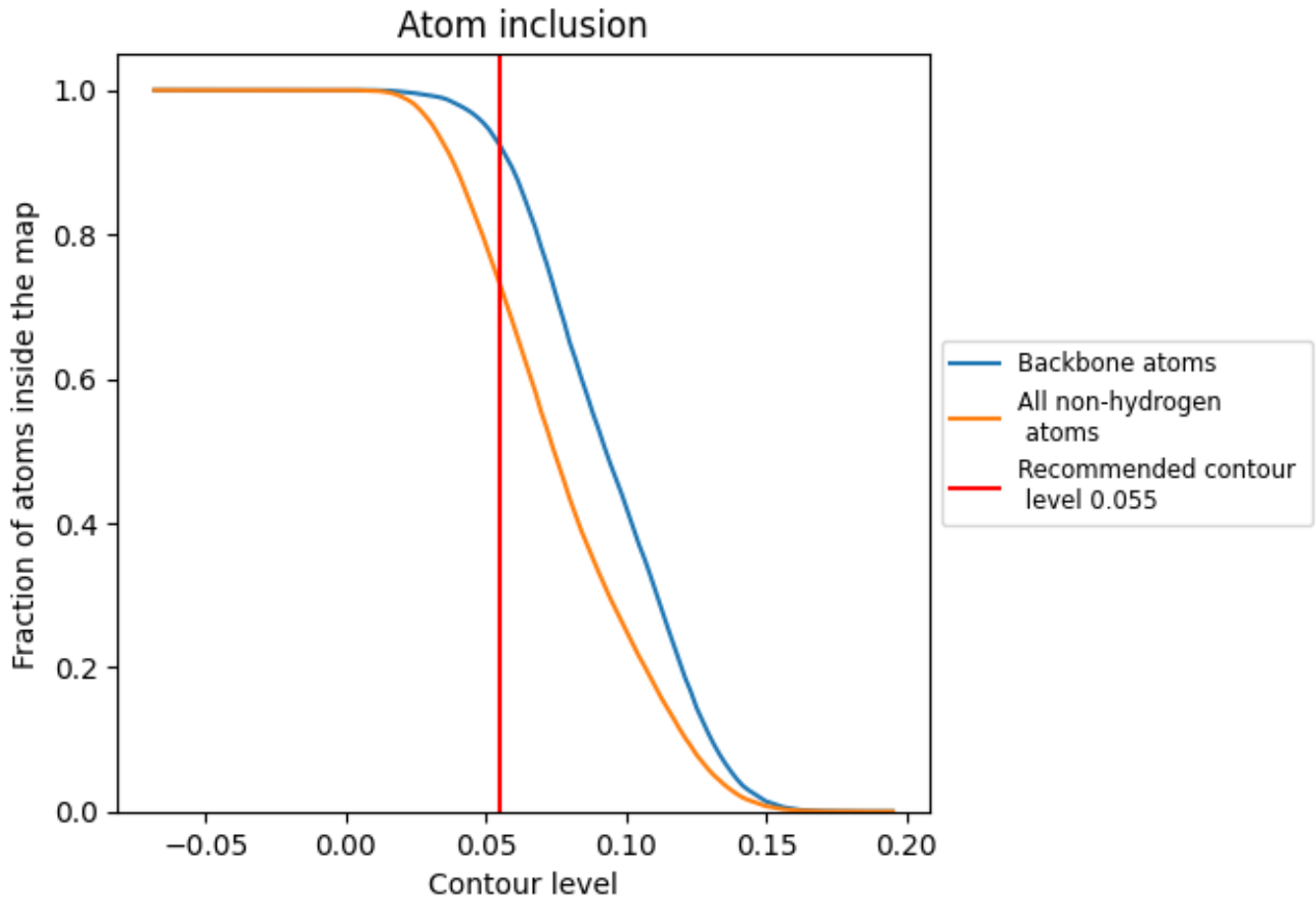
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.055).

## 9.4 Atom inclusion (i)




At the recommended contour level, 92% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7303 | 0.3980 |
| A | 0.7303 | 0.3980 |