# Full wwPDB EM Validation Report

Jun 28, 2022 – 01:38 pm BST

| | | |
|---|---|---|
| PDB ID | : | 7PL9 |
| EMDB ID | : | EMD-13485 |
| Title | : | Cryo-EM structure of Bestrhodopsin (rhodopsin-rhodopsin-bestrophin) complex |
| Authors | : | Matzov, D.; Kaczmarczyk, I.; Shalev-Benami, M. |
| Deposited on | : | 2021-08-29 |
| Resolution | : | 3.21 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:

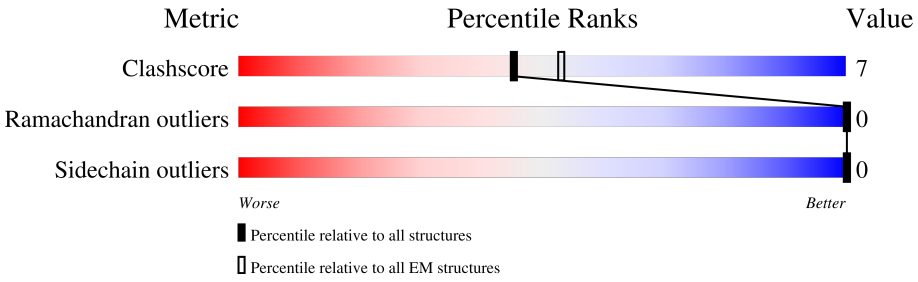
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev8 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.29 |

# 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 3.21 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 | 1187 | 48% 71% 13% 16% |
| 1 | B | 1187 | 48% 71% 12% 16% |
| 1 | C | 1187 | 48% 71% 12% 16% |
| 1 | D | 1187 | 48% 71% 12% 16% |
| 1 | E | 1187 | 48% 72% 12% 16% |

## 2 Entry composition

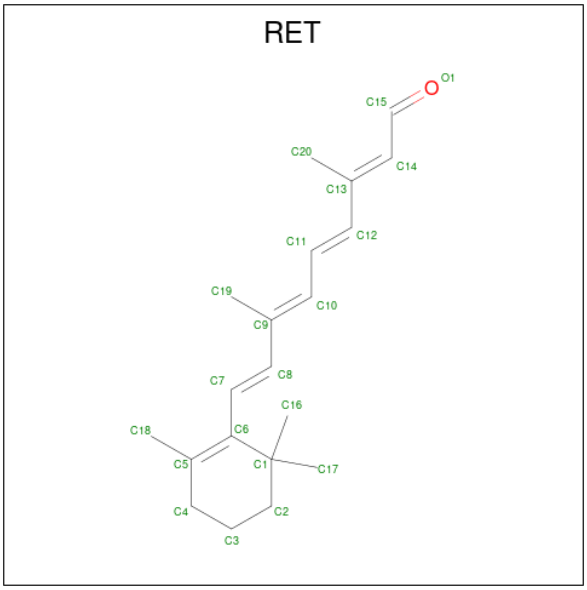
There are 2 unique types of molecules in this entry. The entry contains 37945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rhodopsin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 994 | Total | C | N | O | S | 0 | 0 |
| | | | 7569 | 4978 | 1261 | 1283 | 47 | | |
| 1 | B | 994 | Total | C | N | O | S | 0 | 0 |
| | | | 7569 | 4978 | 1261 | 1283 | 47 | | |
| 1 | C | 994 | Total | C | N | O | S | 0 | 0 |
| | | | 7569 | 4978 | 1261 | 1283 | 47 | | |
| 1 | D | 994 | Total | C | N | O | S | 0 | 0 |
| | | | 7569 | 4978 | 1261 | 1283 | 47 | | |
| 1 | E | 994 | Total | C | N | O | S | 0 | 0 |
| | | | 7569 | 4978 | 1261 | 1283 | 47 | | |

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | 0 |
| | | | 20 | 20 | |

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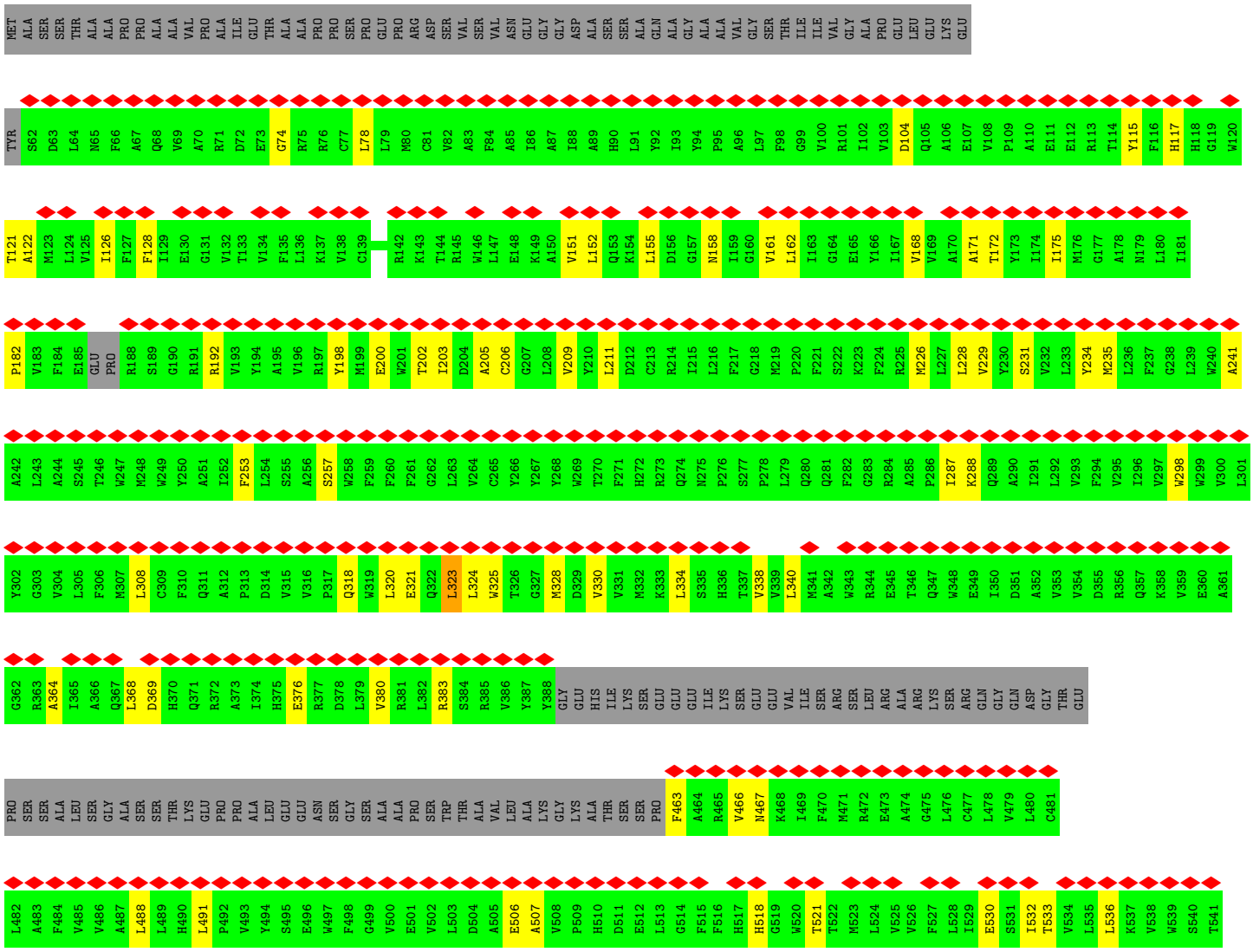
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 2 | B | 1 | Total C<br>20 20 | 0 |
| 2 | C | 1 | Total C<br>20 20 | 0 |
| 2 | D | 1 | Total C<br>20 20 | 0 |
| 2 | E | 1 | Total C<br>20 20 | 0 |

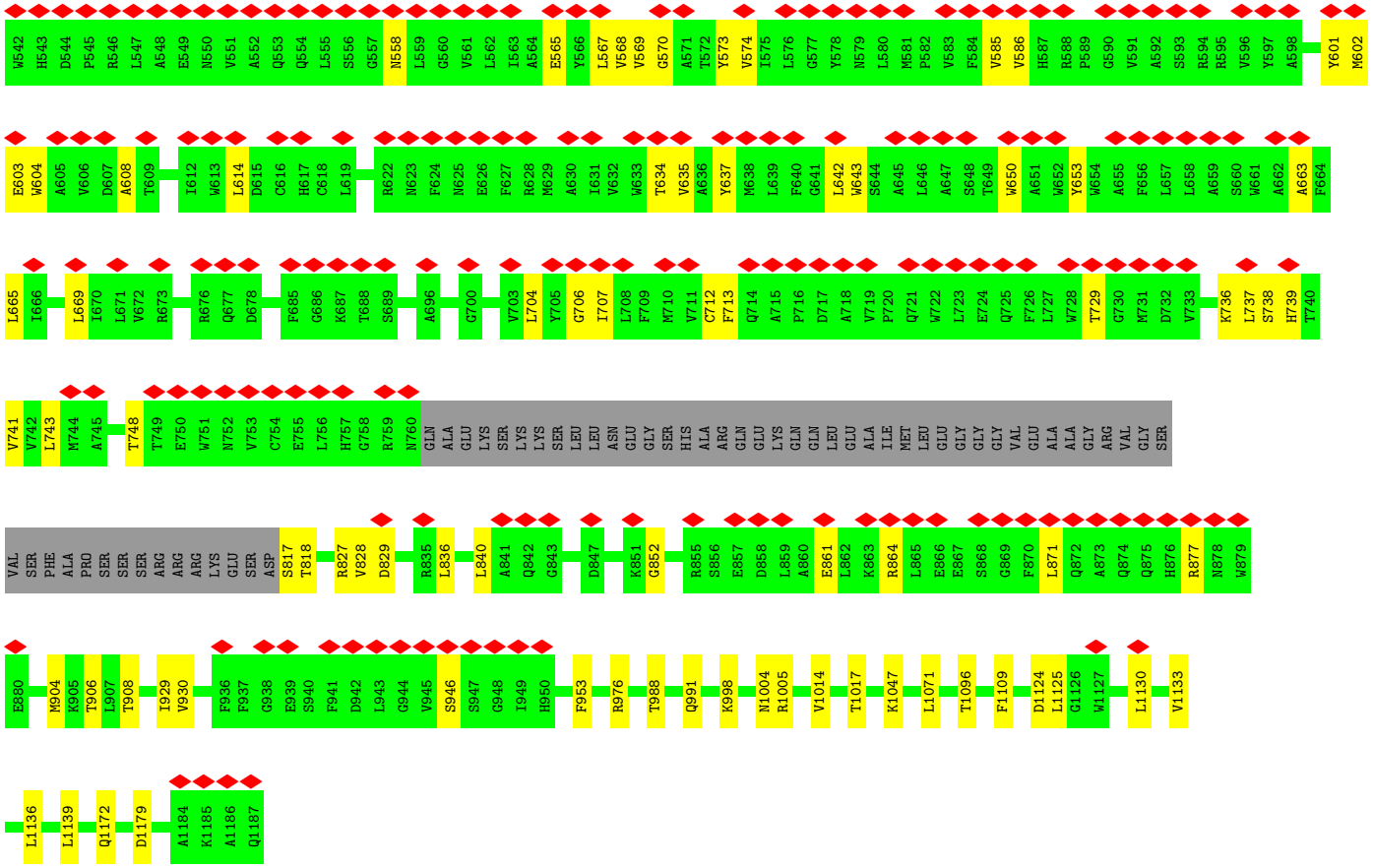
# 3 Residue-property plots (i)

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: Rhodopsin

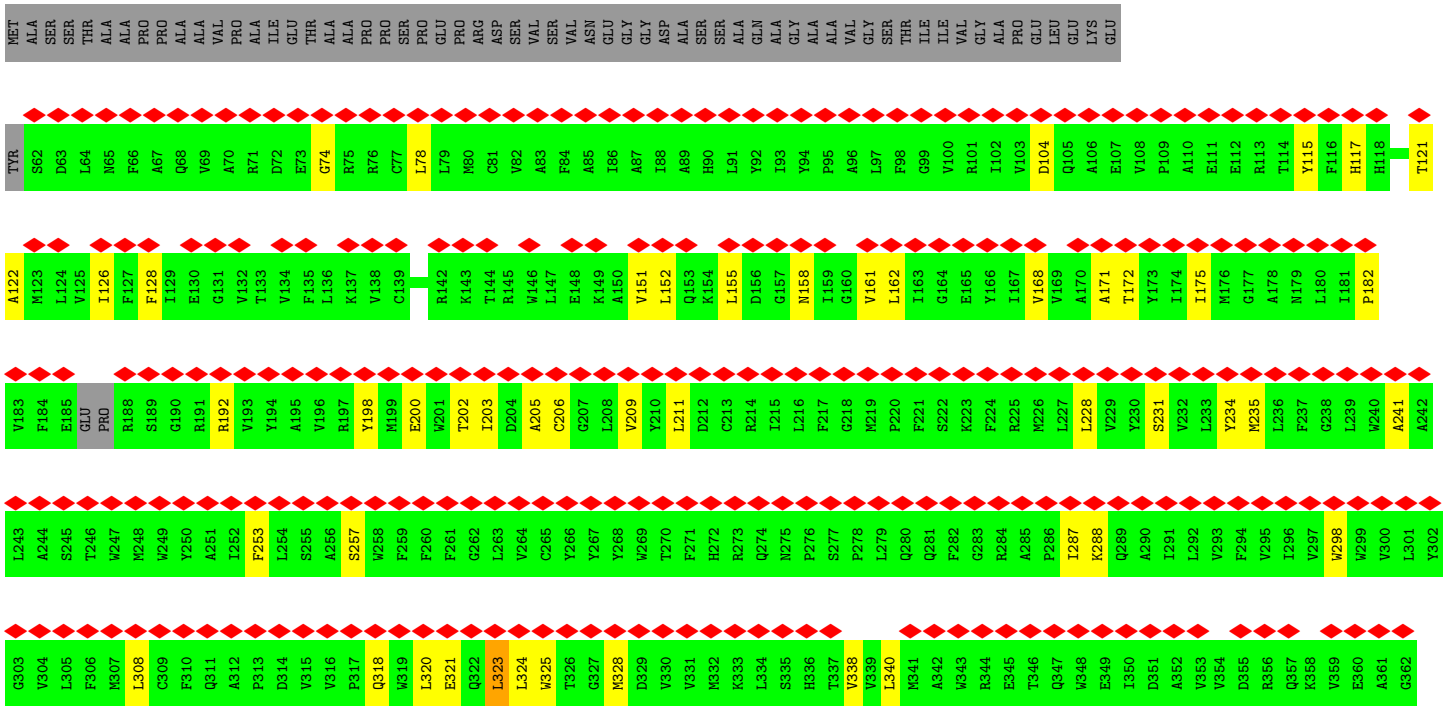
Chain A:

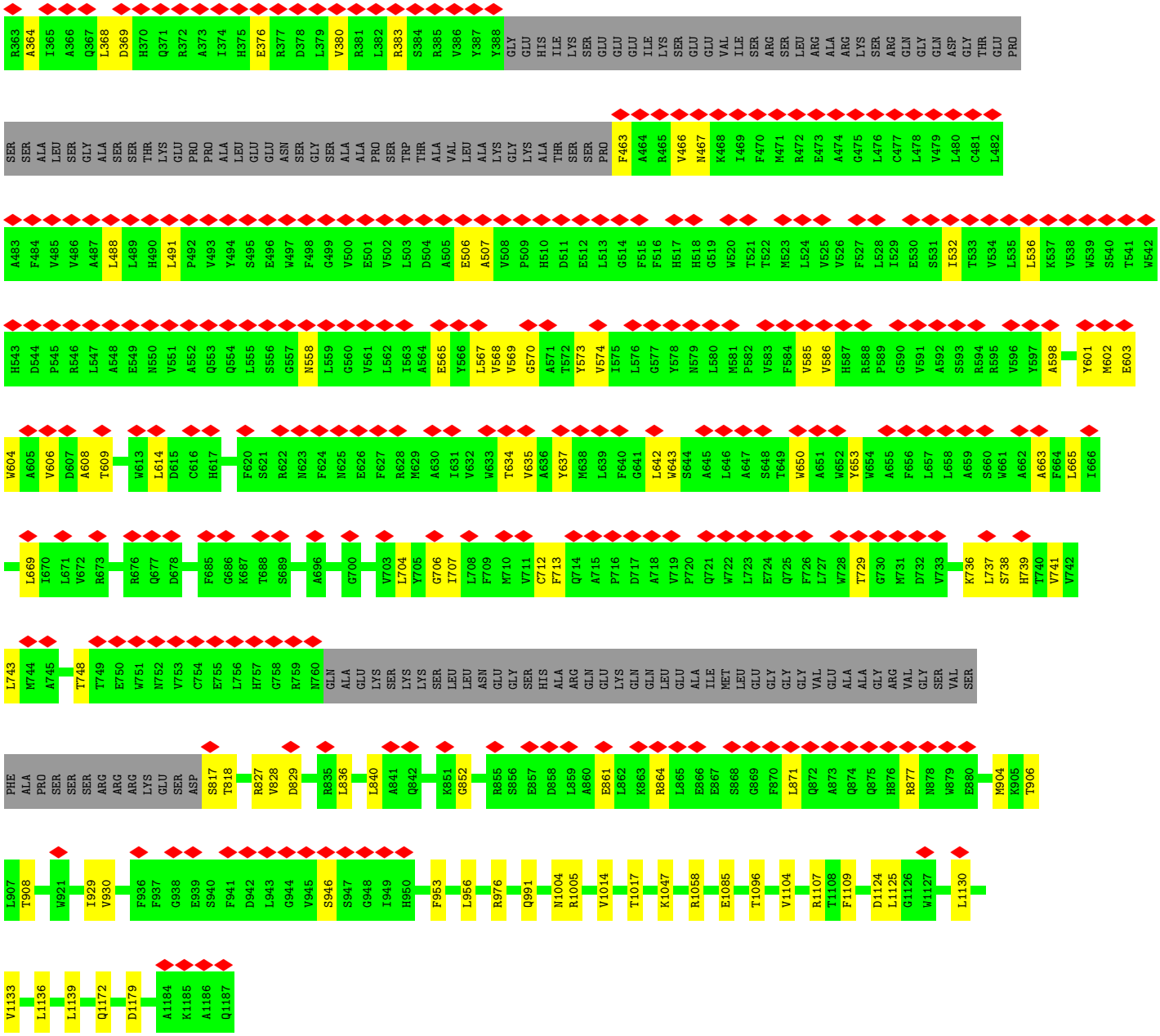





• Molecule 1: Rhodopsin

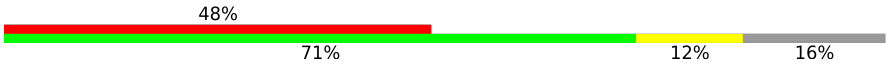
Chain B:

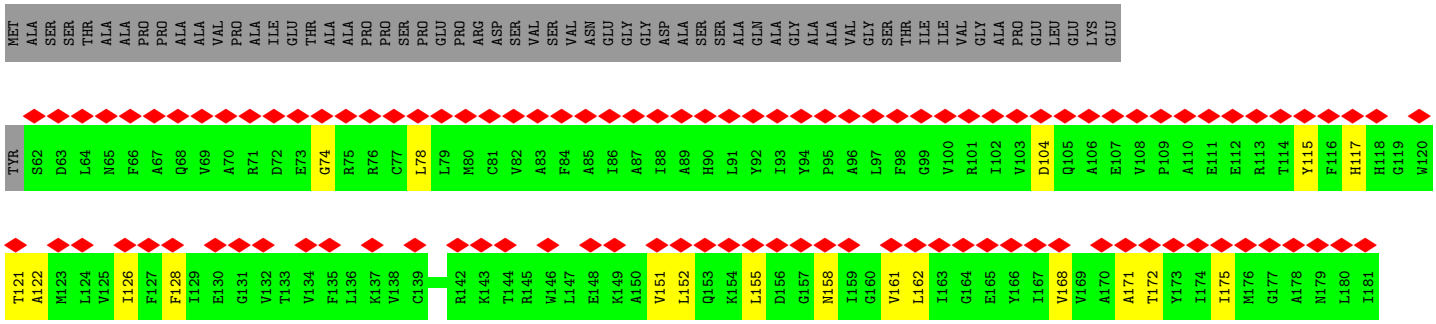



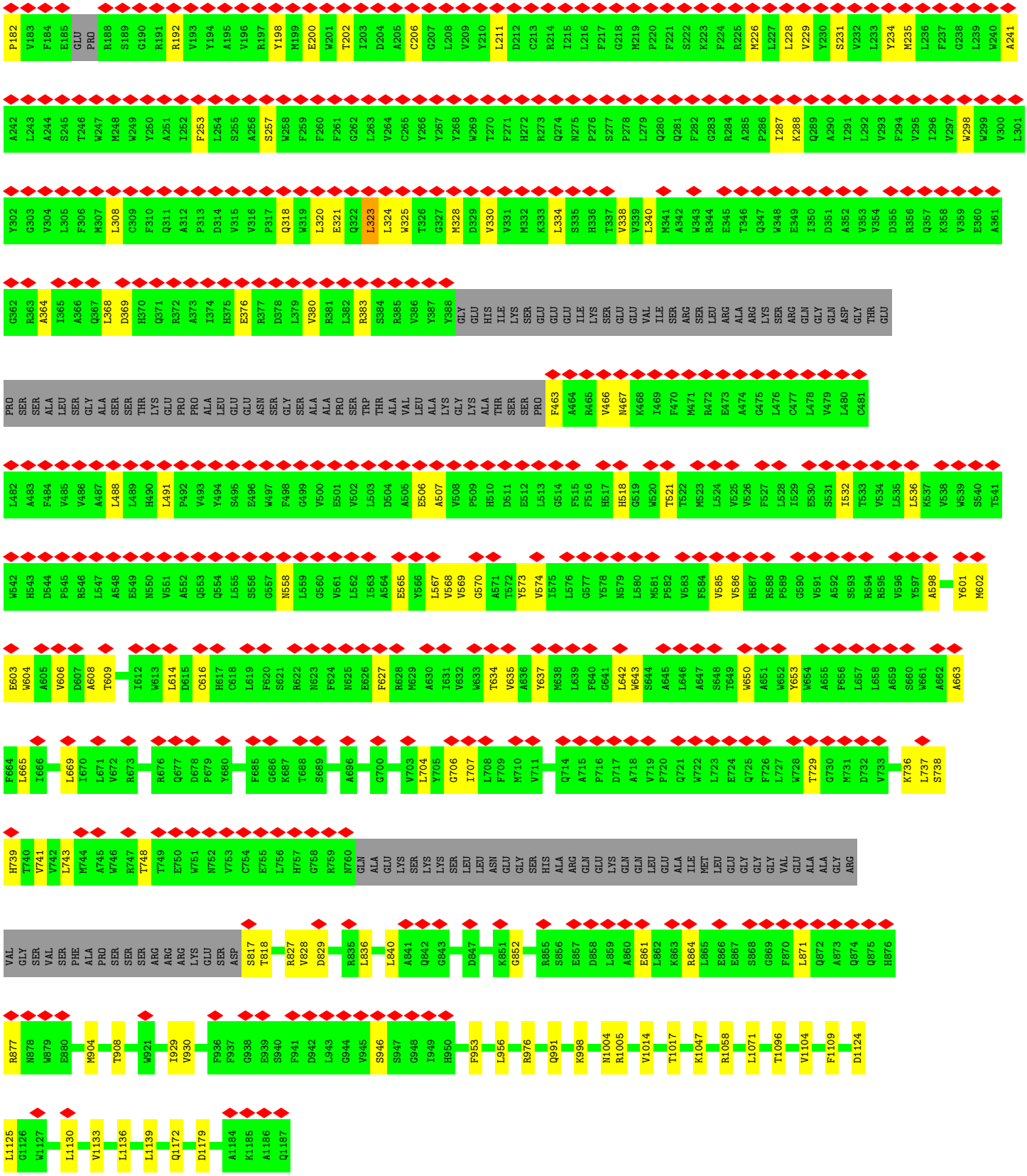



- Molecule 1: Rhodopsin

Chain C:



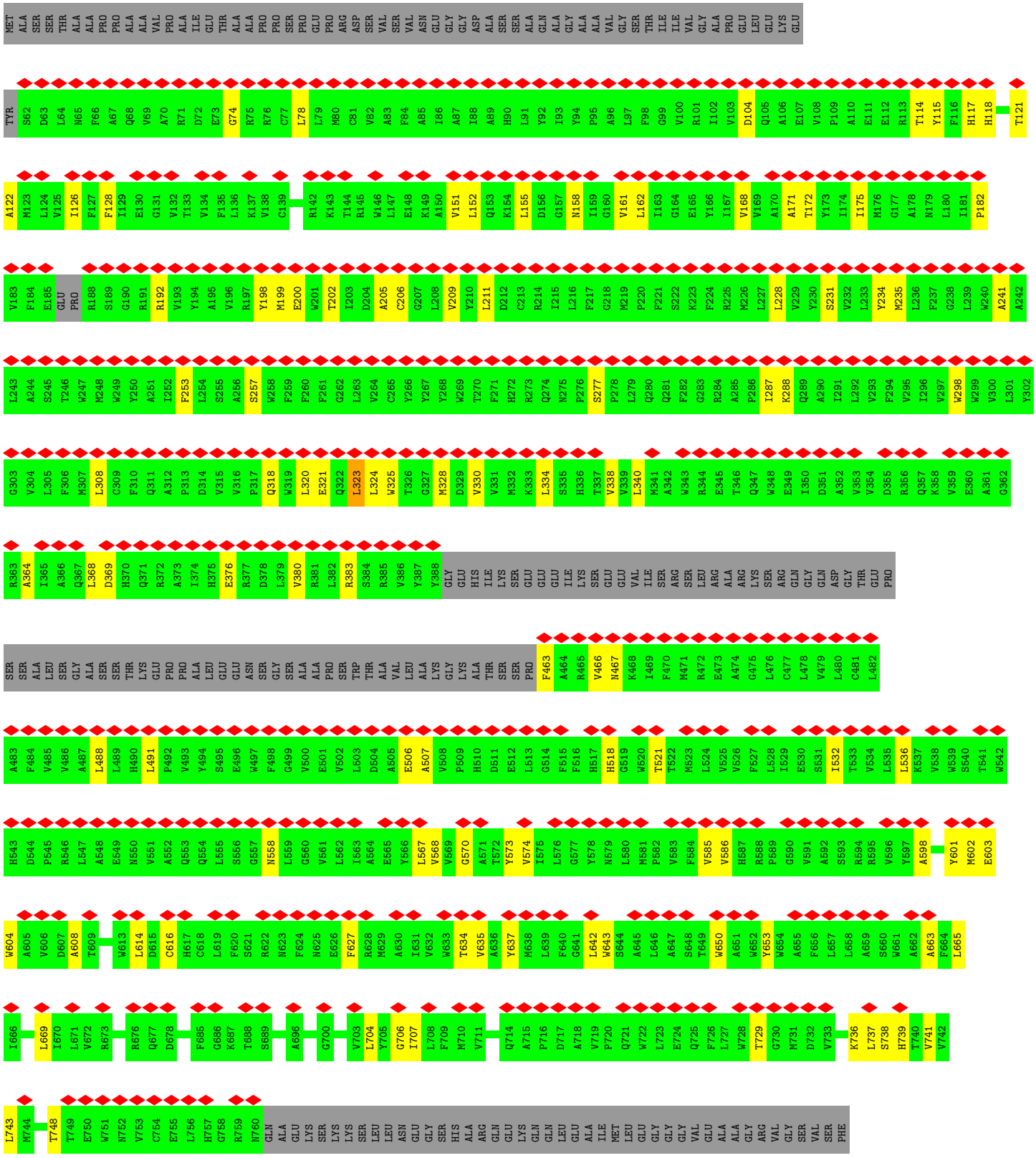



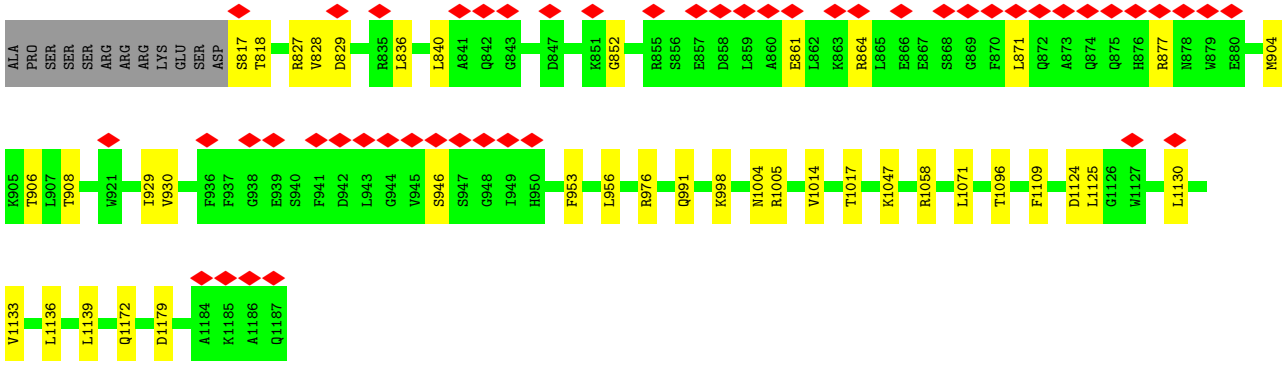



• Molecule 1: Rhodopsin

Chain D:

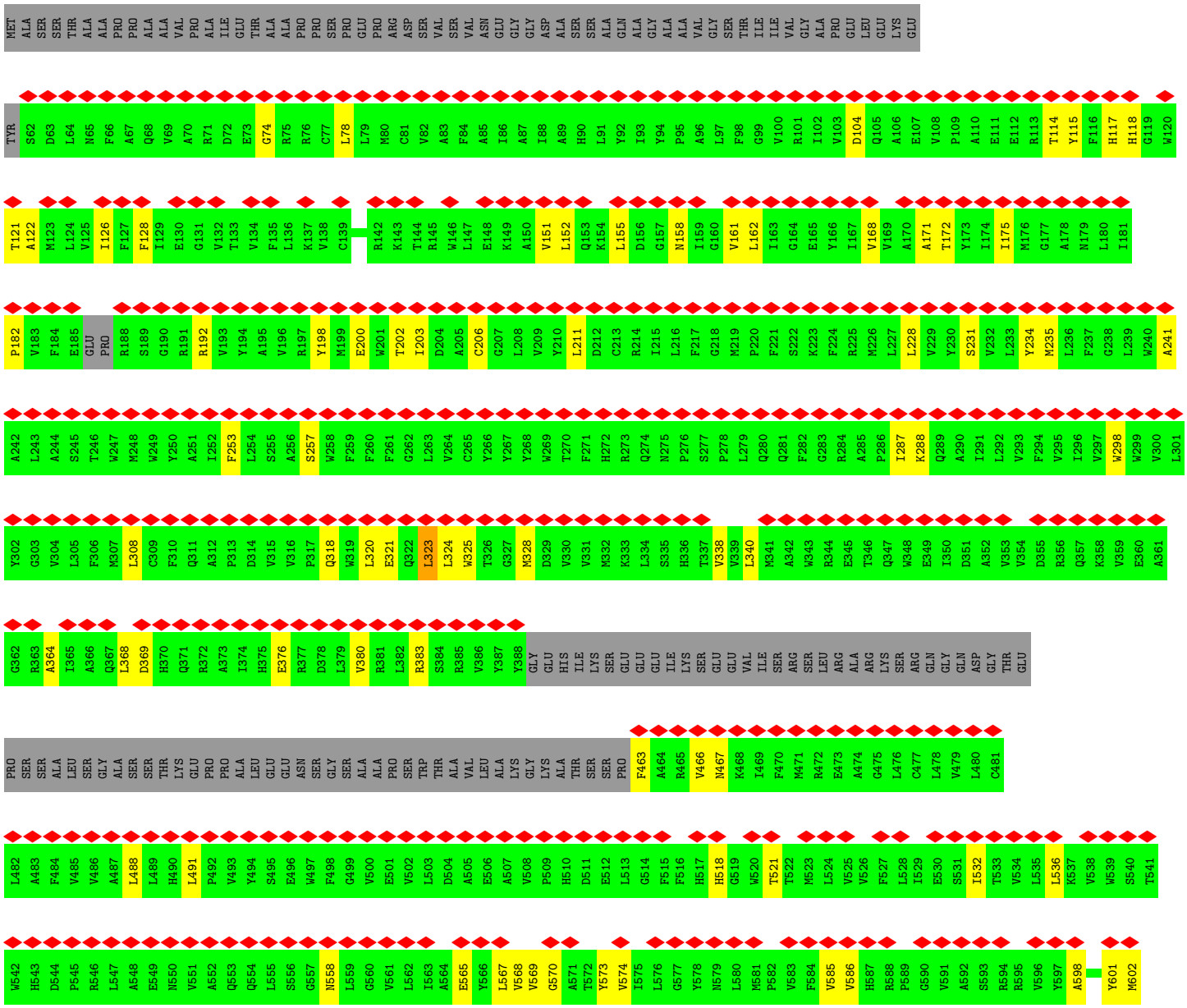

48%
71%
12%
16%

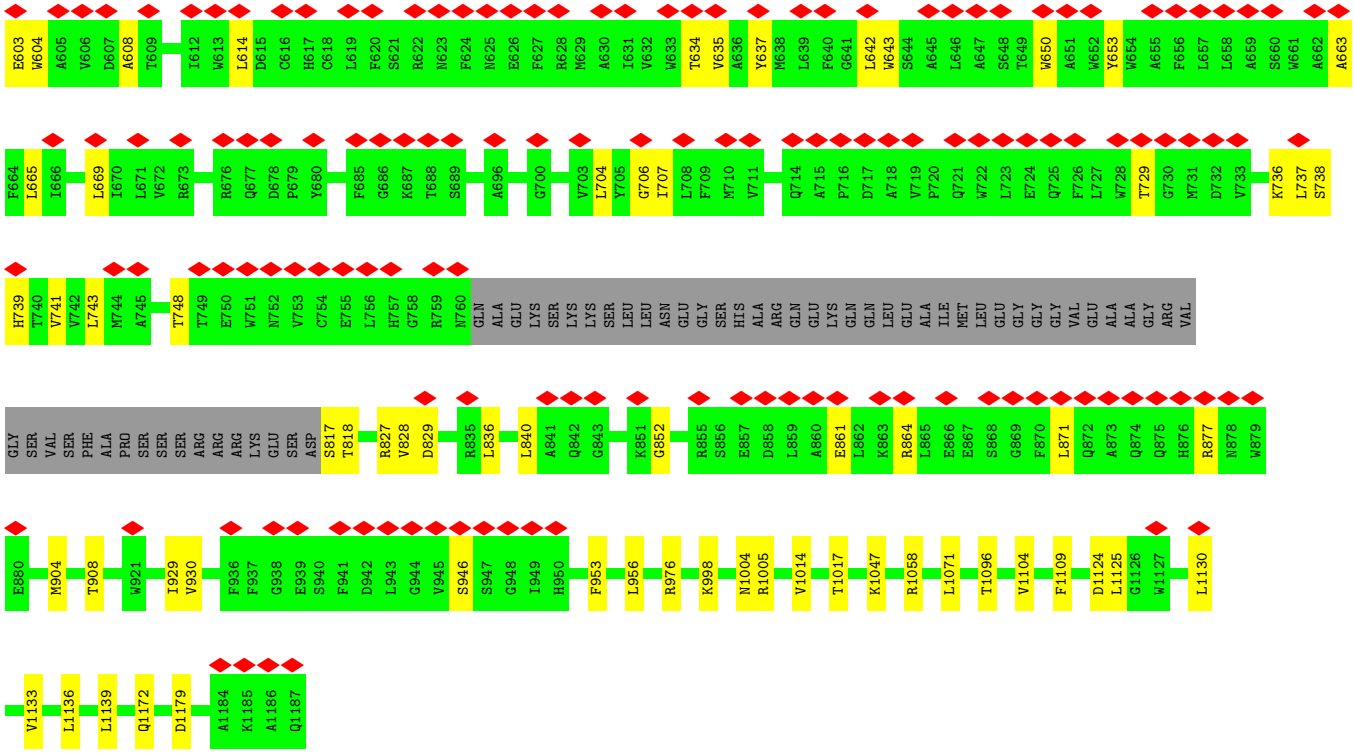

MET ALA SER SER THR ALA ALA PRO PRO ALA ALA VAL PRO ALA ILE GLU THR ALA ALA PRO PRO SER PRO GLU PRO ARG ASP SER VAL SER VAL ASN GLU GLY GLY ASP ALA SER SER ALA GLN ALA GLY ALA ALA VAL GLY SER THR ILE ILE VAL GLY ALA PRO GLU LEU GLU LYS GLU
TYR S62 D63 L64 M65 F66 A67 Q68 V69 A70 R71 D72 E73 G74 R75 R76 C77 L78 L79 M80 C81 V82 A83 F84 A85 I86 A87 I88 A89 H90 L91 Y92 I93 Y94 P95 A96 L97 F98 G99 V100 R101 I102 V103 D104 Q105 A106 E107 V108 P109 A110 E111 E112 R113 T114 Y115 F116 H117 H118 T121
A122 M123 L124 V125 I126 F127 F128 I129 E130 G131 V132 T133 V134 F135 L136 K137 V138 C139 R142 K143 T144 R145 W146 L147 E148 K149 A150 V151 L152 Q153 K154 L155 D156 G157 N158 I159 G160 V161 L162 I163 G164 E165 Y166 I167 V168 V169 A170 A171 T172 Y173 I174 I175 M176 G177 A178 N179 L180 I181 P182
V183 F184 E185 GLU PRO R188 S189 G190 R191 R192 V193 Y194 A195 V196 R197 Y198 M199 E200 W201 T202 I203 D204 A205 C206 G207 L208 V209 Y210 L211 D212 C213 R214 I215 L216 F217 G218 M219 P220 F221 S222 K223 F224 R225 M226 L227 L228 V229 Y230 S231 V232 L233 Y234 M235 L236 F237 G238 L239 W240 A241 A242
L243 A244 S245 T246 W247 M248 W249 Y250 A251 I252 F253 L254 S255 A256 S257 W258 F259 F260 F261 G262 L263 V264 C265 Y266 Y267 Y268 W269 T270 F271 H272 R273 Q274 N275 P276 S277 P278 L279 Q280 Q281 F282 G283 R284 A285 P286 I287 K288 Q289 A290 I291 L292 V293 F294 V295 I296 V297 W298 W299 V300 L301 Y302
G303 V304 L305 F306 M307 L308 C309 F310 Q311 A312 P313 D314 V315 V316 P317 Q318 W319 L320 E321 Q322 L323 L324 W325 T326 G327 M328 D329 V330 V331 M332 K333 L334 S335 H336 T337 V338 V339 L340 M341 A342 W343 R344 E345 T346 Q347 W348 E349 I350 D351 A352 V353 V354 D355 R356 Q357 K358 V359 E360 A361 G362
R363 A364 I365 A366 Q367 L368 D369 H370 Q371 R372 A373 I374 H375 E376 R377 D378 L379 V380 R381 L382 R383 S384 R385 V386 Y387 Y388 GLY GLU HIS ILE LYS SER GLU GLU GLU ILE LYS SER GLU GLU VAL ILE SER ARG SER LEU ARG ALA ARG LYS SER ARG GLN GLY GLN ASP GLY THR GLU PRO
SER SER ALA LEU SER GLY ALA SER SER THR LYS GLU PRO PRO ALA LEU GLU GLU ASN SER GLY SER ALA ALA PRO SER TRP THR ALA VAL LEU ALA LYS GLY LYS ALA THR SER SER PRO F463 A464 R465 V466 N467 K468 I469 F470 M471 R472 E473 A474 G475 L476 C477 L478 V479 L480 C481 L482
A483 F484 V485 V486 A487 L488 L489 H490 L491 P492 V493 Y494 S495 E496 W497 F498 G499 V500 E501 V502 L503 D504 A505 E506 A507 V508 P509 H510 D511 E512 L513 G514 F515 F516 H517 H518 G519 W520 T521 T522 M523 L524 V525 V526 F527 L528 I529 E530 S531 I532 T533 V534 L535 L536 K537 V538 W539 S540 T541 W542
H543 D544 P545 R546 L547 A548 E549 N550 V551 A552 Q553 Q554 L555 S556 G557 N558 L559 G560 V561 L562 I563 A564 E565 Y566 L567 V568 V569 G570 A571 T572 Y573 V574 I575 L576 G577 Y578 N579 L580 M581 P582 V583 F584 V585 V586 H587 R588 P589 G590 V591 A592 S593 R594 R595 V596 Y597 A598 Y601 M602 E603
W604 A605 V606 D607 A608 T609 W613 L614 D615 C616 H617 C618 L619 F620 S621 R622 N623 F624 M625 E626 F627 R628 M629 A630 I631 V632 W633 T634 V635 A636 Y637 M638 L639 F640 G641 L642 W643 S644 A645 L646 A647 S648 T649 W650 A651 W652 Y653 W654 A655 F656 L657 L658 A659 S660 W661 A662 A663 F664 L665
I666 L669 I670 L671 V672 R673 R676 Q677 D678 F685 G686 K687 T688 S689 A696 G700 V703 L704 Y705 G706 I707 L708 F709 M710 V711 Q714 A715 P716 D717 A718 V719 P720 Q721 W722 L723 E724 Q725 F726 L727 W728 T729 G730 M731 D732 V733 K736 L737 S738 H739 T740 V741 V742
L743 M744 T748 T749 E750 W751 N752 V753 C754 E755 L756 H757 G758 R759 N760 GLN ALA GLU LYS SER LYS LYS SER LEU LEU ASN GLU GLY SER HIS ALA ARG GLN GLU LYS GLN GLN LEU GLU ALA ILE MET LEU GLU GLY GLY GLY VAL GLU ALA ALA GLY ARG VAL GLY SER VAL SER PHE




- Molecule 1: Rhodopsin

Chain E:


E603 W604 A605 V606 D607 A608 T609 I612 W613 L614 D615 C616 H617 C618 L619 F620 S621 R622 N623 F624 N625 E626 F627 R628 M629 A630 I631 V632 W633 T634 V635 A636 Y637 M638 L639 F640 G641 L642 W643 S644 A645 L646 A647 S648 T649 W650 A651 W652 Y653 W654 A655 F656 L657 L658 A659 S660 W661 A662 A663
F664 L665 I666 L669 I670 L671 V672 R673 R676 Q677 D678 P679 Y680 F685 G686 K687 T688 S689 A696 G700 V703 L704 Y705 G706 I707 L708 F709 M710 V711 Q714 A715 P716 D717 A718 V719 P720 Q721 W722 L723 E724 Q725 F726 L727 W728 T729 G730 M731 D732 V733 K736 L737 S738
H739 T740 V741 V742 L743 M744 A745 T748 T749 E750 W751 N752 V753 C754 E755 L756 H757 G758 R759 N760 GLN ALA GLU LYS SER LYS LYS SER LEU LEU ASN GLU GLY SER HIS ALA ARG GLN GLU LYS GLN GLN LEU GLU ALA ILE MET LEU GLU GLY GLY GLY VAL GLU ALA ALA GLY ARG VAL
GLY SER VAL SER PHE ALA PRO SER SER SER ARG ARG ARG LYS GLU SER ASP S817 T818 R827 V828 D829 R835 L836 L840 A841 Q842 G843 K851 G852 R855 S856 E857 D858 L859 A860 E861 L862 K863 R864 L865 E866 E867 S868 G869 F870 L871 Q872 A873 Q874 Q875 H876 R877 N878 W879
E880 M904 T908 W921 I929 V930 F936 F937 G938 E939 S940 F941 D942 L943 G944 V945 S946 S947 G948 I949 H950 F953 L956 R976 K998 N1004 R1005 V1014 T1017 K1047 R1058 L1071 T1096 V1104 F1109 D1124 L1125 G1126 W1127 L1130
V1133 L1136 L1139 Q1172 D1179 A1184 K1185 A1186 Q1187

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 27749 | 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 ($e^-/Å^2$) | 0.86 | 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 | 0.067 | Depositor |
| Minimum map value | -0.029 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.002 | Depositor |
| Recommended contour level | 0.013 | Depositor |
| Map size (Å) | 344.0, 344.0, 344.0 | wwPDB |
| Map dimensions | 400, 400, 400 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.86, 0.86, 0.86 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.33 | 0/7779 | 0.45 | 4/10645 (0.0%) |
| 1 | B | 0.33 | 0/7779 | 0.45 | 4/10645 (0.0%) |
| 1 | C | 0.33 | 0/7779 | 0.45 | 4/10645 (0.0%) |
| 1 | D | 0.33 | 0/7779 | 0.45 | 4/10645 (0.0%) |
| 1 | E | 0.33 | 0/7779 | 0.45 | 4/10645 (0.0%) |
| All | All | 0.33 | 0/38895 | 0.45 | 20/53225 (0.0%) |

There are no bond length outliers.

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 871 | LEU | CB-CG-CD2 | 6.06 | 121.30 | 111.00 |
| 1 | B | 871 | LEU | CB-CG-CD2 | 6.05 | 121.29 | 111.00 |
| 1 | C | 871 | LEU | CB-CG-CD2 | 6.05 | 121.29 | 111.00 |
| 1 | A | 871 | LEU | CB-CG-CD2 | 6.05 | 121.28 | 111.00 |
| 1 | E | 871 | LEU | CB-CG-CD2 | 6.04 | 121.26 | 111.00 |
| 1 | D | 323 | LEU | CB-CG-CD1 | 5.90 | 121.03 | 111.00 |
| 1 | A | 323 | LEU | CB-CG-CD1 | 5.88 | 121.00 | 111.00 |
| 1 | C | 323 | LEU | CB-CG-CD1 | 5.87 | 120.97 | 111.00 |
| 1 | E | 323 | LEU | CB-CG-CD1 | 5.86 | 120.95 | 111.00 |
| 1 | B | 323 | LEU | CB-CG-CD1 | 5.85 | 120.95 | 111.00 |
| 1 | B | 323 | LEU | CB-CG-CD2 | 5.62 | 120.56 | 111.00 |
| 1 | C | 323 | LEU | CB-CG-CD2 | 5.61 | 120.53 | 111.00 |
| 1 | E | 323 | LEU | CB-CG-CD2 | 5.61 | 120.53 | 111.00 |
| 1 | D | 323 | LEU | CB-CG-CD2 | 5.60 | 120.51 | 111.00 |
| 1 | A | 323 | LEU | CB-CG-CD2 | 5.60 | 120.51 | 111.00 |
| 1 | A | 871 | LEU | CB-CG-CD1 | 5.02 | 119.53 | 111.00 |
| 1 | C | 871 | LEU | CB-CG-CD1 | 5.02 | 119.53 | 111.00 |
| 1 | E | 871 | LEU | CB-CG-CD1 | 5.02 | 119.53 | 111.00 |
| 1 | B | 871 | LEU | CB-CG-CD1 | 5.01 | 119.52 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 871 | LEU | CB-CG-CD1 | 5.00 | 119.51 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 7569 | 0 | 7216 | 112 | 0 |
| 1 | B | 7569 | 0 | 7216 | 110 | 0 |
| 1 | C | 7569 | 0 | 7216 | 109 | 0 |
| 1 | D | 7569 | 0 | 7216 | 109 | 0 |
| 1 | E | 7569 | 0 | 7216 | 106 | 0 |
| 2 | A | 20 | 0 | 27 | 5 | 0 |
| 2 | B | 20 | 0 | 27 | 5 | 0 |
| 2 | C | 20 | 0 | 27 | 5 | 0 |
| 2 | D | 20 | 0 | 27 | 5 | 0 |
| 2 | E | 20 | 0 | 27 | 5 | 0 |
| All | All | 37945 | 0 | 36215 | 499 | 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 7.

All (499) 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:D:704:LEU:HD12 | 1:D:707:ILE:HD11 | 1.66 | 0.78 |
| 1:C:704:LEU:HD12 | 1:C:707:ILE:HD11 | 1.66 | 0.77 |
| 1:E:704:LEU:HD12 | 1:E:707:ILE:HD11 | 1.66 | 0.77 |
| 1:B:704:LEU:HD12 | 1:B:707:ILE:HD11 | 1.66 | 0.76 |
| 1:A:704:LEU:HD12 | 1:A:707:ILE:HD11 | 1.66 | 0.76 |
| 1:E:904:MET:O | 1:E:908:THR:HG22 | 1.88 | 0.73 |
| 1:A:904:MET:O | 1:A:908:THR:HG22 | 1.88 | 0.73 |
| 1:D:904:MET:O | 1:D:908:THR:HG22 | 1.88 | 0.73 |
| 1:B:904:MET:O | 1:B:908:THR:HG22 | 1.88 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:904:MET:O | 1:C:908:THR:HG22 | 1.88 | 0.72 |
| 1:A:1125:LEU:HD11 | 1:B:946:SER:OG | 1.89 | 0.71 |
| 1:D:128:PHE:CD2 | 1:D:737:LEU:HD21 | 2.28 | 0.69 |
| 1:A:128:PHE:CD2 | 1:A:737:LEU:HD21 | 2.28 | 0.68 |
| 1:C:128:PHE:CD2 | 1:C:737:LEU:HD21 | 2.28 | 0.68 |
| 1:E:128:PHE:CD2 | 1:E:737:LEU:HD21 | 2.28 | 0.68 |
| 1:B:128:PHE:CD2 | 1:B:737:LEU:HD21 | 2.28 | 0.68 |
| 1:C:241:ALA:HB2 | 1:C:253:PHE:HB2 | 1.75 | 0.68 |
| 1:C:608:ALA:HB2 | 2:C:1201:RET:H202 | 1.76 | 0.68 |
| 1:D:608:ALA:HB2 | 2:D:1201:RET:H202 | 1.76 | 0.68 |
| 1:D:241:ALA:HB2 | 1:D:253:PHE:HB2 | 1.75 | 0.68 |
| 1:A:608:ALA:HB2 | 2:A:1201:RET:H202 | 1.76 | 0.67 |
| 1:B:241:ALA:HB2 | 1:B:253:PHE:HB2 | 1.75 | 0.67 |
| 1:A:241:ALA:HB2 | 1:A:253:PHE:HB2 | 1.75 | 0.67 |
| 1:A:1172:GLN:OE1 | 1:B:1047:LYS:NZ | 2.26 | 0.67 |
| 1:B:608:ALA:HB2 | 2:B:1201:RET:H202 | 1.76 | 0.67 |
| 1:B:155:LEU:O | 1:B:155:LEU:HD12 | 1.95 | 0.67 |
| 1:E:241:ALA:HB2 | 1:E:253:PHE:HB2 | 1.75 | 0.67 |
| 1:A:155:LEU:HD12 | 1:A:155:LEU:O | 1.95 | 0.66 |
| 1:C:155:LEU:HD12 | 1:C:155:LEU:O | 1.95 | 0.66 |
| 1:E:155:LEU:HD12 | 1:E:155:LEU:O | 1.95 | 0.65 |
| 1:E:608:ALA:HB2 | 2:E:1201:RET:H202 | 1.76 | 0.65 |
| 1:D:155:LEU:HD12 | 1:D:155:LEU:O | 1.95 | 0.65 |
| 1:D:338:VAL:HG21 | 1:D:532:ILE:HG13 | 1.79 | 0.65 |
| 1:A:338:VAL:HG21 | 1:A:532:ILE:HG13 | 1.80 | 0.64 |
| 1:D:861:GLU:OE2 | 1:D:864:ARG:NH2 | 2.31 | 0.64 |
| 1:E:861:GLU:OE2 | 1:E:864:ARG:NH2 | 2.31 | 0.64 |
| 1:E:338:VAL:HG21 | 1:E:532:ILE:HG13 | 1.79 | 0.64 |
| 1:A:614:LEU:HD21 | 1:A:743:LEU:HD13 | 1.80 | 0.64 |
| 1:B:861:GLU:OE2 | 1:B:864:ARG:NH2 | 2.31 | 0.64 |
| 1:C:338:VAL:HG21 | 1:C:532:ILE:HG13 | 1.80 | 0.64 |
| 1:D:1125:LEU:HD11 | 1:E:946:SER:OG | 1.98 | 0.64 |
| 1:E:614:LEU:HD21 | 1:E:743:LEU:HD13 | 1.80 | 0.64 |
| 1:C:861:GLU:OE2 | 1:C:864:ARG:NH2 | 2.31 | 0.64 |
| 1:B:338:VAL:HG21 | 1:B:532:ILE:HG13 | 1.80 | 0.64 |
| 1:D:614:LEU:HD21 | 1:D:743:LEU:HD13 | 1.80 | 0.63 |
| 1:C:637:TYR:HE1 | 2:C:1201:RET:H192 | 1.64 | 0.63 |
| 1:C:1125:LEU:HD11 | 1:D:946:SER:OG | 1.98 | 0.63 |
| 1:A:1109:PHE:CG | 1:E:1139:LEU:HD13 | 2.33 | 0.63 |
| 1:B:614:LEU:HD21 | 1:B:743:LEU:HD13 | 1.80 | 0.63 |
| 1:A:861:GLU:OE2 | 1:A:864:ARG:NH2 | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:198:TYR:O | 1:E:202:THR:HG23 | 1.99 | 0.63 |
| 1:B:198:TYR:O | 1:B:202:THR:HG23 | 1.99 | 0.62 |
| 1:D:198:TYR:O | 1:D:202:THR:HG23 | 1.99 | 0.62 |
| 1:A:198:TYR:O | 1:A:202:THR:HG23 | 1.99 | 0.62 |
| 1:A:1096:THR:HG21 | 1:E:976:ARG:HE | 1.64 | 0.62 |
| 1:B:369:ASP:OD1 | 1:B:877:ARG:HG3 | 2.00 | 0.62 |
| 1:B:1125:LEU:HD11 | 1:C:946:SER:OG | 1.98 | 0.62 |
| 1:C:614:LEU:HD21 | 1:C:743:LEU:HD13 | 1.80 | 0.62 |
| 1:D:637:TYR:HE1 | 2:D:1201:RET:H192 | 1.63 | 0.62 |
| 1:C:198:TYR:O | 1:C:202:THR:HG23 | 1.99 | 0.62 |
| 1:C:369:ASP:OD1 | 1:C:877:ARG:HG3 | 2.00 | 0.62 |
| 1:A:369:ASP:OD1 | 1:A:877:ARG:HG3 | 2.00 | 0.62 |
| 1:B:637:TYR:HE1 | 2:B:1201:RET:H192 | 1.64 | 0.62 |
| 1:A:637:TYR:HE1 | 2:A:1201:RET:H192 | 1.64 | 0.61 |
| 1:A:162:LEU:HD11 | 1:A:340:LEU:CD2 | 2.31 | 0.61 |
| 1:C:162:LEU:HD11 | 1:C:340:LEU:CD2 | 2.31 | 0.61 |
| 1:D:162:LEU:HD11 | 1:D:340:LEU:CD2 | 2.31 | 0.61 |
| 1:A:650:TRP:HA | 1:A:653:TYR:HB3 | 1.82 | 0.61 |
| 1:B:162:LEU:HD11 | 1:B:340:LEU:CD2 | 2.31 | 0.61 |
| 1:D:369:ASP:OD1 | 1:D:877:ARG:HG3 | 2.00 | 0.61 |
| 1:E:369:ASP:OD1 | 1:E:877:ARG:HG3 | 2.00 | 0.61 |
| 1:E:637:TYR:HE1 | 2:E:1201:RET:H192 | 1.64 | 0.61 |
| 1:B:650:TRP:HA | 1:B:653:TYR:HB3 | 1.82 | 0.60 |
| 1:C:650:TRP:HA | 1:C:653:TYR:HB3 | 1.82 | 0.60 |
| 1:D:650:TRP:HA | 1:D:653:TYR:HB3 | 1.83 | 0.60 |
| 1:E:162:LEU:HD11 | 1:E:340:LEU:CD2 | 2.31 | 0.60 |
| 1:E:567:LEU:HD12 | 1:E:568:VAL:N | 2.17 | 0.60 |
| 1:D:567:LEU:HD12 | 1:D:568:VAL:N | 2.17 | 0.60 |
| 1:A:1047:LYS:NZ | 1:E:1172:GLN:OE1 | 2.35 | 0.60 |
| 1:A:567:LEU:HD12 | 1:A:568:VAL:N | 2.17 | 0.59 |
| 1:E:463:PHE:O | 1:E:467:ASN:ND2 | 2.36 | 0.59 |
| 1:A:463:PHE:O | 1:A:467:ASN:ND2 | 2.36 | 0.59 |
| 1:A:704:LEU:CD1 | 1:A:707:ILE:HD11 | 2.33 | 0.59 |
| 1:E:650:TRP:HA | 1:E:653:TYR:HB3 | 1.83 | 0.59 |
| 1:A:946:SER:OG | 1:E:1125:LEU:HD11 | 2.03 | 0.59 |
| 1:C:567:LEU:HD12 | 1:C:568:VAL:N | 2.17 | 0.59 |
| 1:D:817:SER:OG | 1:D:818:THR:N | 2.36 | 0.59 |
| 1:B:463:PHE:O | 1:B:467:ASN:ND2 | 2.36 | 0.59 |
| 1:C:704:LEU:CD1 | 1:C:707:ILE:HD11 | 2.33 | 0.59 |
| 1:D:704:LEU:CD1 | 1:D:707:ILE:HD11 | 2.33 | 0.59 |
| 1:B:567:LEU:HD12 | 1:B:568:VAL:N | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:463:PHE:O | 1:D:467:ASN:ND2 | 2.36 | 0.59 |
| 1:C:817:SER:OG | 1:C:818:THR:N | 2.36 | 0.58 |
| 1:B:704:LEU:CD1 | 1:B:707:ILE:HD11 | 2.33 | 0.58 |
| 1:D:168:VAL:O | 1:D:172:THR:HG23 | 2.04 | 0.58 |
| 1:E:817:SER:OG | 1:E:818:THR:N | 2.36 | 0.58 |
| 1:A:953:PHE:HE1 | 1:E:1136:LEU:HD13 | 1.68 | 0.58 |
| 1:B:168:VAL:O | 1:B:172:THR:HG23 | 2.04 | 0.58 |
| 1:C:168:VAL:O | 1:C:172:THR:HG23 | 2.04 | 0.58 |
| 1:C:976:ARG:HE | 1:D:1096:THR:HG21 | 1.69 | 0.58 |
| 1:C:463:PHE:O | 1:C:467:ASN:ND2 | 2.36 | 0.58 |
| 1:E:168:VAL:O | 1:E:172:THR:HG23 | 2.04 | 0.58 |
| 1:D:74:GLY:O | 1:D:78:LEU:HD23 | 2.04 | 0.58 |
| 1:A:168:VAL:O | 1:A:172:THR:HG23 | 2.04 | 0.57 |
| 1:E:74:GLY:O | 1:E:78:LEU:HD23 | 2.04 | 0.57 |
| 1:C:1172:GLN:OE1 | 1:D:1047:LYS:NZ | 2.37 | 0.57 |
| 1:A:74:GLY:O | 1:A:78:LEU:HD23 | 2.04 | 0.57 |
| 1:B:817:SER:OG | 1:B:818:THR:N | 2.36 | 0.57 |
| 1:C:74:GLY:O | 1:C:78:LEU:HD23 | 2.04 | 0.57 |
| 1:B:634:THR:HA | 1:B:637:TYR:CE2 | 2.40 | 0.57 |
| 1:B:74:GLY:O | 1:B:78:LEU:HD23 | 2.04 | 0.56 |
| 1:E:704:LEU:CD1 | 1:E:707:ILE:HD11 | 2.33 | 0.56 |
| 1:A:634:THR:HA | 1:A:637:TYR:CE2 | 2.40 | 0.56 |
| 1:C:634:THR:HA | 1:C:637:TYR:CE2 | 2.40 | 0.56 |
| 1:B:1172:GLN:OE1 | 1:C:1047:LYS:NZ | 2.39 | 0.56 |
| 1:D:1172:GLN:OE1 | 1:E:1047:LYS:NZ | 2.38 | 0.56 |
| 1:A:976:ARG:HE | 1:B:1096:THR:HG21 | 1.70 | 0.56 |
| 1:B:976:ARG:HE | 1:C:1096:THR:HG21 | 1.71 | 0.56 |
| 1:D:634:THR:HA | 1:D:637:TYR:CE2 | 2.40 | 0.55 |
| 1:E:634:THR:HA | 1:E:637:TYR:CE2 | 2.40 | 0.55 |
| 1:D:827:ARG:HB2 | 1:E:1047:LYS:HD2 | 1.88 | 0.55 |
| 1:D:976:ARG:HE | 1:E:1096:THR:HG21 | 1.71 | 0.55 |
| 1:B:706:GLY:HA2 | 2:B:1201:RET:H172 | 1.89 | 0.55 |
| 1:D:532:ILE:O | 1:D:536:LEU:HD23 | 2.07 | 0.55 |
| 1:C:532:ILE:O | 1:C:536:LEU:HD23 | 2.07 | 0.54 |
| 1:A:532:ILE:O | 1:A:536:LEU:HD23 | 2.07 | 0.54 |
| 1:C:1139:LEU:HD13 | 1:D:1109:PHE:CG | 2.42 | 0.54 |
| 1:C:706:GLY:HA2 | 2:C:1201:RET:H172 | 1.89 | 0.54 |
| 1:E:706:GLY:HA2 | 2:E:1201:RET:H172 | 1.89 | 0.54 |
| 1:A:706:GLY:HA2 | 2:A:1201:RET:H172 | 1.89 | 0.54 |
| 1:A:991:GLN:OE1 | 1:B:1058:ARG:NH1 | 2.40 | 0.54 |
| 1:A:1109:PHE:CE2 | 1:E:1139:LEU:HB2 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:827:ARG:HB2 | 1:B:1047:LYS:HD2 | 1.88 | 0.54 |
| 1:E:532:ILE:O | 1:E:536:LEU:HD23 | 2.07 | 0.54 |
| 1:D:706:GLY:HA2 | 2:D:1201:RET:H172 | 1.89 | 0.54 |
| 1:B:532:ILE:O | 1:B:536:LEU:HD23 | 2.07 | 0.53 |
| 1:B:827:ARG:HB2 | 1:C:1047:LYS:HD2 | 1.89 | 0.53 |
| 1:D:172:THR:HG21 | 1:D:200:GLU:HB3 | 1.90 | 0.53 |
| 1:D:162:LEU:HD11 | 1:D:340:LEU:HD21 | 1.91 | 0.53 |
| 1:B:573:TYR:CE2 | 1:B:729:THR:HG23 | 2.44 | 0.53 |
| 1:D:573:TYR:CE2 | 1:D:729:THR:HG23 | 2.44 | 0.53 |
| 1:E:162:LEU:HD11 | 1:E:340:LEU:HD21 | 1.91 | 0.53 |
| 1:A:573:TYR:CE2 | 1:A:729:THR:HG23 | 2.44 | 0.53 |
| 1:C:172:THR:HG21 | 1:C:200:GLU:HB3 | 1.90 | 0.53 |
| 1:C:573:TYR:CE2 | 1:C:729:THR:HG23 | 2.44 | 0.53 |
| 1:C:827:ARG:HB2 | 1:D:1047:LYS:HD2 | 1.90 | 0.53 |
| 1:D:637:TYR:CE1 | 2:D:1201:RET:H192 | 2.44 | 0.53 |
| 1:E:573:TYR:CE2 | 1:E:729:THR:HG23 | 2.44 | 0.53 |
| 1:B:206:CYS:HB2 | 1:B:228:LEU:CD1 | 2.39 | 0.53 |
| 1:C:637:TYR:CE1 | 2:C:1201:RET:H192 | 2.44 | 0.53 |
| 1:A:172:THR:HG21 | 1:A:200:GLU:HB3 | 1.90 | 0.53 |
| 1:B:162:LEU:HD11 | 1:B:340:LEU:HD21 | 1.91 | 0.53 |
| 1:B:172:THR:HG21 | 1:B:200:GLU:HB3 | 1.90 | 0.52 |
| 1:A:206:CYS:HB2 | 1:A:228:LEU:CD1 | 2.39 | 0.52 |
| 1:D:206:CYS:HB2 | 1:D:228:LEU:CD1 | 2.39 | 0.52 |
| 1:E:172:THR:HG21 | 1:E:200:GLU:HB3 | 1.90 | 0.52 |
| 1:A:518:HIS:O | 1:A:521:THR:OG1 | 2.24 | 0.52 |
| 1:C:162:LEU:HD11 | 1:C:340:LEU:HD21 | 1.91 | 0.52 |
| 1:E:206:CYS:HB2 | 1:E:228:LEU:CD1 | 2.39 | 0.52 |
| 1:B:637:TYR:CE1 | 2:B:1201:RET:H192 | 2.44 | 0.52 |
| 1:D:1139:LEU:HD13 | 1:E:1109:PHE:CG | 2.45 | 0.52 |
| 1:E:637:TYR:CE1 | 2:E:1201:RET:H192 | 2.44 | 0.52 |
| 1:A:162:LEU:HD11 | 1:A:340:LEU:HD21 | 1.91 | 0.52 |
| 1:C:206:CYS:HB2 | 1:C:228:LEU:CD1 | 2.39 | 0.52 |
| 1:C:1136:LEU:HD13 | 1:D:953:PHE:HE1 | 1.75 | 0.51 |
| 1:B:1139:LEU:HD13 | 1:C:1109:PHE:CG | 2.45 | 0.51 |
| 1:C:518:HIS:O | 1:C:521:THR:OG1 | 2.24 | 0.51 |
| 1:A:637:TYR:CE1 | 2:A:1201:RET:H192 | 2.44 | 0.51 |
| 1:A:1130:LEU:O | 1:A:1133:VAL:HG12 | 2.11 | 0.51 |
| 1:C:665:LEU:O | 1:C:669:LEU:HD23 | 2.11 | 0.51 |
| 1:E:665:LEU:O | 1:E:669:LEU:HD23 | 2.11 | 0.51 |
| 1:E:1130:LEU:O | 1:E:1133:VAL:HG12 | 2.11 | 0.51 |
| 1:E:287:ILE:O | 1:E:288:LYS:HB3 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1130:LEU:O | 1:B:1133:VAL:HG12 | 2.11 | 0.50 |
| 1:C:1130:LEU:O | 1:C:1133:VAL:HG12 | 2.11 | 0.50 |
| 1:A:491:LEU:HD21 | 1:A:602:MET:SD | 2.52 | 0.50 |
| 1:A:1047:LYS:HD2 | 1:E:827:ARG:HB2 | 1.94 | 0.50 |
| 1:C:929:ILE:HG13 | 1:C:930:VAL:N | 2.27 | 0.50 |
| 1:D:1130:LEU:O | 1:D:1133:VAL:HG12 | 2.11 | 0.50 |
| 1:A:1139:LEU:HD13 | 1:B:1109:PHE:CG | 2.47 | 0.50 |
| 1:B:929:ILE:HG13 | 1:B:930:VAL:N | 2.27 | 0.50 |
| 1:D:665:LEU:O | 1:D:669:LEU:HD23 | 2.11 | 0.50 |
| 1:E:491:LEU:HD21 | 1:E:602:MET:SD | 2.52 | 0.50 |
| 1:A:115:TYR:CD2 | 1:A:323:LEU:HD21 | 2.47 | 0.50 |
| 1:A:665:LEU:O | 1:A:669:LEU:HD23 | 2.11 | 0.50 |
| 1:B:748:THR:HG23 | 1:B:748:THR:O | 2.12 | 0.50 |
| 1:C:491:LEU:HD21 | 1:C:602:MET:SD | 2.52 | 0.50 |
| 1:D:115:TYR:CD2 | 1:D:323:LEU:HD21 | 2.47 | 0.50 |
| 1:D:929:ILE:HG13 | 1:D:930:VAL:N | 2.27 | 0.50 |
| 1:A:712:CYS:HG | 1:A:713:PHE:HD1 | 1.58 | 0.49 |
| 1:A:748:THR:HG23 | 1:A:748:THR:O | 2.12 | 0.49 |
| 1:E:115:TYR:CD2 | 1:E:323:LEU:HD21 | 2.47 | 0.49 |
| 1:E:748:THR:HG23 | 1:E:748:THR:O | 2.12 | 0.49 |
| 1:A:287:ILE:O | 1:A:288:LYS:HB3 | 2.12 | 0.49 |
| 1:A:988:THR:HG22 | 1:B:1085:GLU:OE1 | 2.13 | 0.49 |
| 1:B:115:TYR:CD2 | 1:B:323:LEU:HD21 | 2.47 | 0.49 |
| 1:B:287:ILE:O | 1:B:288:LYS:HB3 | 2.11 | 0.49 |
| 1:C:287:ILE:O | 1:C:288:LYS:HB3 | 2.12 | 0.49 |
| 1:C:558:ASN:HB2 | 1:C:743:LEU:HD21 | 1.95 | 0.49 |
| 1:D:491:LEU:HD21 | 1:D:602:MET:SD | 2.52 | 0.49 |
| 1:B:558:ASN:HB2 | 1:B:743:LEU:HD21 | 1.95 | 0.49 |
| 1:D:287:ILE:O | 1:D:288:LYS:HB3 | 2.12 | 0.49 |
| 1:D:518:HIS:O | 1:D:521:THR:OG1 | 2.24 | 0.49 |
| 1:D:642:LEU:HD23 | 1:D:643:TRP:N | 2.28 | 0.49 |
| 1:B:491:LEU:HD21 | 1:B:602:MET:SD | 2.52 | 0.49 |
| 1:B:665:LEU:O | 1:B:669:LEU:HD23 | 2.11 | 0.49 |
| 1:C:642:LEU:HD23 | 1:C:643:TRP:N | 2.28 | 0.49 |
| 1:A:320:LEU:O | 1:A:324:LEU:HD23 | 2.13 | 0.49 |
| 1:A:558:ASN:HB2 | 1:A:743:LEU:HD21 | 1.95 | 0.49 |
| 1:A:828:VAL:HG12 | 1:A:829:ASP:N | 2.28 | 0.49 |
| 1:C:115:TYR:CD2 | 1:C:323:LEU:HD21 | 2.47 | 0.49 |
| 1:D:320:LEU:O | 1:D:324:LEU:HD23 | 2.13 | 0.49 |
| 1:D:748:THR:O | 1:D:748:THR:HG23 | 2.12 | 0.49 |
| 1:D:1124:ASP:O | 1:D:1125:LEU:HD23 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:320:LEU:O | 1:E:324:LEU:HD23 | 2.13 | 0.49 |
| 1:E:614:LEU:HD22 | 1:E:739:HIS:NE2 | 2.28 | 0.49 |
| 1:B:320:LEU:O | 1:B:324:LEU:HD23 | 2.13 | 0.49 |
| 1:B:642:LEU:HD23 | 1:B:643:TRP:N | 2.28 | 0.49 |
| 1:C:320:LEU:O | 1:C:324:LEU:HD23 | 2.13 | 0.49 |
| 1:E:338:VAL:HG21 | 1:E:532:ILE:CG1 | 2.43 | 0.49 |
| 1:E:558:ASN:HB2 | 1:E:743:LEU:HD21 | 1.95 | 0.49 |
| 1:B:712:CYS:HG | 1:B:713:PHE:HD1 | 1.61 | 0.49 |
| 1:E:642:LEU:HD23 | 1:E:643:TRP:N | 2.28 | 0.49 |
| 1:A:642:LEU:HD23 | 1:A:643:TRP:N | 2.28 | 0.48 |
| 1:C:616:CYS:HG | 1:C:627:PHE:HE1 | 1.61 | 0.48 |
| 1:D:338:VAL:HG21 | 1:D:532:ILE:CG1 | 2.43 | 0.48 |
| 1:D:558:ASN:HB2 | 1:D:743:LEU:HD21 | 1.95 | 0.48 |
| 1:D:828:VAL:HG12 | 1:D:829:ASP:N | 2.28 | 0.48 |
| 1:A:614:LEU:HD22 | 1:A:739:HIS:NE2 | 2.28 | 0.48 |
| 1:A:1109:PHE:CD2 | 1:E:1139:LEU:HD13 | 2.48 | 0.48 |
| 1:E:828:VAL:HG12 | 1:E:829:ASP:N | 2.28 | 0.48 |
| 1:A:231:SER:HA | 1:A:234:TYR:CE2 | 2.48 | 0.48 |
| 1:B:231:SER:HA | 1:B:234:TYR:CE2 | 2.48 | 0.48 |
| 1:B:614:LEU:HD22 | 1:B:739:HIS:NE2 | 2.28 | 0.48 |
| 1:B:1124:ASP:O | 1:B:1125:LEU:HD23 | 2.13 | 0.48 |
| 1:D:614:LEU:HD22 | 1:D:739:HIS:NE2 | 2.28 | 0.48 |
| 1:A:1124:ASP:O | 1:A:1125:LEU:HD23 | 2.13 | 0.48 |
| 1:E:929:ILE:HG13 | 1:E:930:VAL:N | 2.27 | 0.48 |
| 1:A:338:VAL:HG21 | 1:A:532:ILE:CG1 | 2.43 | 0.48 |
| 1:D:1136:LEU:HD13 | 1:E:953:PHE:HE1 | 1.78 | 0.48 |
| 1:A:126:ILE:HD12 | 1:A:126:ILE:H | 1.79 | 0.48 |
| 1:A:1139:LEU:CD2 | 1:B:956:LEU:HD13 | 2.43 | 0.48 |
| 1:B:126:ILE:HD12 | 1:B:126:ILE:H | 1.79 | 0.48 |
| 1:B:1136:LEU:HD13 | 1:C:953:PHE:HE1 | 1.78 | 0.48 |
| 1:C:748:THR:HG23 | 1:C:748:THR:O | 2.12 | 0.48 |
| 1:E:1124:ASP:O | 1:E:1125:LEU:HD23 | 2.13 | 0.48 |
| 1:C:614:LEU:HD22 | 1:C:739:HIS:NE2 | 2.28 | 0.48 |
| 1:C:1124:ASP:O | 1:C:1125:LEU:HD23 | 2.13 | 0.48 |
| 1:A:929:ILE:HG13 | 1:A:930:VAL:N | 2.27 | 0.48 |
| 1:D:231:SER:HA | 1:D:234:TYR:CE2 | 2.48 | 0.48 |
| 1:A:634:THR:HG23 | 1:A:635:VAL:N | 2.29 | 0.47 |
| 1:A:817:SER:OG | 1:A:818:THR:N | 2.36 | 0.47 |
| 1:C:634:THR:HG23 | 1:C:635:VAL:N | 2.29 | 0.47 |
| 1:C:828:VAL:HG12 | 1:C:829:ASP:N | 2.28 | 0.47 |
| 1:A:1136:LEU:HD13 | 1:B:953:PHE:HE1 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:634:THR:HG23 | 1:B:635:VAL:N | 2.29 | 0.47 |
| 1:C:338:VAL:HG21 | 1:C:532:ILE:CG1 | 2.43 | 0.47 |
| 1:E:298:TRP:HZ2 | 1:E:328:MET:HA | 1.79 | 0.47 |
| 1:A:298:TRP:HZ2 | 1:A:328:MET:HA | 1.79 | 0.47 |
| 1:D:634:THR:HG23 | 1:D:635:VAL:N | 2.29 | 0.47 |
| 1:B:828:VAL:HG12 | 1:B:829:ASP:N | 2.28 | 0.47 |
| 1:C:231:SER:HA | 1:C:234:TYR:CE2 | 2.48 | 0.47 |
| 1:D:616:CYS:HG | 1:D:627:PHE:HE1 | 1.61 | 0.47 |
| 1:E:231:SER:HA | 1:E:234:TYR:CE2 | 2.48 | 0.47 |
| 1:B:338:VAL:HG21 | 1:B:532:ILE:CG1 | 2.43 | 0.47 |
| 1:C:126:ILE:HD12 | 1:C:126:ILE:H | 1.79 | 0.47 |
| 1:C:637:TYR:HB3 | 1:C:663:ALA:HB3 | 1.97 | 0.47 |
| 1:D:637:TYR:HB3 | 1:D:663:ALA:HB3 | 1.97 | 0.47 |
| 1:E:634:THR:HG23 | 1:E:635:VAL:N | 2.29 | 0.47 |
| 1:A:211:LEU:HD23 | 1:A:211:LEU:C | 2.35 | 0.47 |
| 1:D:298:TRP:HZ2 | 1:D:328:MET:HA | 1.79 | 0.47 |
| 1:D:601:TYR:O | 1:D:604:TRP:HB2 | 2.15 | 0.47 |
| 1:D:126:ILE:H | 1:D:126:ILE:HD12 | 1.79 | 0.47 |
| 1:E:211:LEU:C | 1:E:211:LEU:HD23 | 2.35 | 0.47 |
| 1:A:601:TYR:O | 1:A:604:TRP:HB2 | 2.15 | 0.47 |
| 1:B:298:TRP:HZ2 | 1:B:328:MET:HA | 1.80 | 0.47 |
| 1:C:298:TRP:HZ2 | 1:C:328:MET:HA | 1.79 | 0.47 |
| 1:E:126:ILE:HD12 | 1:E:126:ILE:H | 1.79 | 0.47 |
| 1:E:518:HIS:O | 1:E:521:THR:OG1 | 2.24 | 0.47 |
| 1:D:117:HIS:O | 1:D:121:THR:HG23 | 2.16 | 0.46 |
| 1:C:601:TYR:O | 1:C:604:TRP:HB2 | 2.15 | 0.46 |
| 1:D:104:ASP:N | 1:D:182:PRO:O | 2.49 | 0.46 |
| 1:B:211:LEU:C | 1:B:211:LEU:HD23 | 2.35 | 0.46 |
| 1:C:1139:LEU:HB2 | 1:D:1109:PHE:CE2 | 2.51 | 0.46 |
| 1:E:637:TYR:HB3 | 1:E:663:ALA:HB3 | 1.97 | 0.46 |
| 1:B:117:HIS:O | 1:B:121:THR:HG23 | 2.16 | 0.46 |
| 1:B:637:TYR:HB3 | 1:B:663:ALA:HB3 | 1.97 | 0.46 |
| 1:B:104:ASP:N | 1:B:182:PRO:O | 2.49 | 0.46 |
| 1:B:601:TYR:O | 1:B:604:TRP:HB2 | 2.15 | 0.46 |
| 2:A:1201:RET:C8 | 2:A:1201:RET:H161 | 2.46 | 0.46 |
| 1:D:211:LEU:HD23 | 1:D:211:LEU:C | 2.35 | 0.46 |
| 1:C:117:HIS:O | 1:C:121:THR:HG23 | 2.16 | 0.46 |
| 1:B:364:ALA:O | 1:B:368:LEU:HD23 | 2.16 | 0.46 |
| 1:E:601:TYR:O | 1:E:604:TRP:HB2 | 2.15 | 0.46 |
| 1:E:104:ASP:N | 1:E:182:PRO:O | 2.49 | 0.45 |
| 1:E:117:HIS:O | 1:E:121:THR:HG23 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:585:VAL:HG12 | 1:E:586:VAL:H | 1.81 | 0.45 |
| 1:C:211:LEU:C | 1:C:211:LEU:HD23 | 2.35 | 0.45 |
| 2:B:1201:RET:C8 | 2:B:1201:RET:H161 | 2.46 | 0.45 |
| 1:C:104:ASP:N | 1:C:182:PRO:O | 2.49 | 0.45 |
| 1:D:585:VAL:HG12 | 1:D:586:VAL:H | 1.81 | 0.45 |
| 1:A:364:ALA:O | 1:A:368:LEU:HD23 | 2.16 | 0.45 |
| 1:A:637:TYR:HB3 | 1:A:663:ALA:HB3 | 1.97 | 0.45 |
| 1:B:991:GLN:OE1 | 1:C:1058:ARG:NH1 | 2.50 | 0.45 |
| 2:C:1201:RET:C8 | 2:C:1201:RET:H161 | 2.46 | 0.45 |
| 1:B:585:VAL:HG12 | 1:B:586:VAL:H | 1.81 | 0.45 |
| 1:B:1014:VAL:O | 1:B:1017:THR:HG22 | 2.17 | 0.45 |
| 2:E:1201:RET:H161 | 2:E:1201:RET:C8 | 2.46 | 0.45 |
| 1:C:121:THR:OG1 | 1:C:122:ALA:N | 2.50 | 0.45 |
| 1:D:121:THR:OG1 | 1:D:122:ALA:N | 2.50 | 0.45 |
| 1:A:104:ASP:N | 1:A:182:PRO:O | 2.49 | 0.45 |
| 1:A:585:VAL:HG12 | 1:A:586:VAL:H | 1.81 | 0.45 |
| 1:C:364:ALA:O | 1:C:368:LEU:HD23 | 2.16 | 0.45 |
| 2:D:1201:RET:H161 | 2:D:1201:RET:C8 | 2.46 | 0.45 |
| 1:E:364:ALA:O | 1:E:368:LEU:HD23 | 2.16 | 0.45 |
| 1:A:117:HIS:O | 1:A:121:THR:HG23 | 2.16 | 0.45 |
| 1:C:585:VAL:HG12 | 1:C:586:VAL:H | 1.81 | 0.45 |
| 1:A:642:LEU:HD23 | 1:A:642:LEU:C | 2.38 | 0.44 |
| 1:D:158:ASN:O | 1:D:161:VAL:HG22 | 2.18 | 0.44 |
| 1:D:199:MET:O | 1:D:202:THR:OG1 | 2.28 | 0.44 |
| 1:D:642:LEU:HD23 | 1:D:642:LEU:C | 2.38 | 0.44 |
| 1:A:1014:VAL:O | 1:A:1017:THR:HG22 | 2.17 | 0.44 |
| 1:D:364:ALA:O | 1:D:368:LEU:HD23 | 2.16 | 0.44 |
| 1:D:1014:VAL:O | 1:D:1017:THR:HG22 | 2.17 | 0.44 |
| 1:A:121:THR:OG1 | 1:A:122:ALA:N | 2.50 | 0.44 |
| 1:B:121:THR:OG1 | 1:B:122:ALA:N | 2.50 | 0.44 |
| 1:C:642:LEU:HD23 | 1:C:642:LEU:C | 2.38 | 0.44 |
| 1:E:642:LEU:HD23 | 1:E:642:LEU:C | 2.38 | 0.44 |
| 1:B:202:THR:HG22 | 1:B:235:MET:HG2 | 2.00 | 0.44 |
| 1:C:158:ASN:O | 1:C:161:VAL:HG22 | 2.18 | 0.44 |
| 1:C:598:ALA:O | 1:C:602:MET:HE2 | 2.17 | 0.44 |
| 1:D:376:GLU:O | 1:D:380:VAL:HG12 | 2.18 | 0.44 |
| 1:D:836:LEU:HD11 | 1:D:840:LEU:HD11 | 2.00 | 0.44 |
| 1:E:376:GLU:O | 1:E:380:VAL:HG12 | 2.17 | 0.44 |
| 1:A:836:LEU:HD11 | 1:A:840:LEU:HD11 | 2.00 | 0.44 |
| 1:C:1014:VAL:O | 1:C:1017:THR:HG22 | 2.17 | 0.44 |
| 1:B:642:LEU:HD23 | 1:B:642:LEU:C | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:376:GLU:O | 1:A:380:VAL:HG12 | 2.18 | 0.43 |
| 1:B:158:ASN:O | 1:B:161:VAL:HG22 | 2.18 | 0.43 |
| 1:B:1139:LEU:HB2 | 1:C:1109:PHE:CE2 | 2.53 | 0.43 |
| 1:C:202:THR:HG22 | 1:C:235:MET:HG2 | 1.99 | 0.43 |
| 1:D:1139:LEU:HB2 | 1:E:1109:PHE:CE2 | 2.53 | 0.43 |
| 1:E:202:THR:HG22 | 1:E:235:MET:HG2 | 2.00 | 0.43 |
| 1:A:158:ASN:O | 1:A:161:VAL:HG22 | 2.18 | 0.43 |
| 1:C:376:GLU:O | 1:C:380:VAL:HG12 | 2.18 | 0.43 |
| 1:C:603:GLU:OE2 | 1:C:604:TRP:CD1 | 2.71 | 0.43 |
| 1:E:1014:VAL:O | 1:E:1017:THR:HG22 | 2.17 | 0.43 |
| 1:B:603:GLU:OE2 | 1:B:604:TRP:CD1 | 2.71 | 0.43 |
| 1:D:603:GLU:OE2 | 1:D:604:TRP:CD1 | 2.71 | 0.43 |
| 1:A:151:VAL:HG23 | 1:A:152:LEU:N | 2.34 | 0.43 |
| 1:A:202:THR:HG22 | 1:A:235:MET:HG2 | 1.99 | 0.43 |
| 1:B:376:GLU:O | 1:B:380:VAL:HG12 | 2.18 | 0.43 |
| 1:A:234:TYR:HB2 | 1:A:257:SER:HA | 2.01 | 0.43 |
| 1:A:383:ARG:HD3 | 1:A:1179:ASP:OD1 | 2.19 | 0.43 |
| 1:A:603:GLU:OE2 | 1:A:604:TRP:CD1 | 2.71 | 0.43 |
| 1:C:192:ARG:NH1 | 1:C:318:GLN:O | 2.52 | 0.43 |
| 1:A:603:GLU:O | 1:A:604:TRP:C | 2.57 | 0.43 |
| 1:B:906:THR:O | 1:C:1104:VAL:HG13 | 2.19 | 0.43 |
| 1:D:192:ARG:NH1 | 1:D:318:GLN:O | 2.52 | 0.43 |
| 1:E:383:ARG:HD3 | 1:E:1179:ASP:OD1 | 2.19 | 0.43 |
| 1:E:603:GLU:OE2 | 1:E:604:TRP:CD1 | 2.71 | 0.43 |
| 1:D:383:ARG:HD3 | 1:D:1179:ASP:OD1 | 2.19 | 0.43 |
| 1:E:192:ARG:NH1 | 1:E:318:GLN:O | 2.52 | 0.43 |
| 1:A:570:GLY:O | 1:A:574:VAL:HG23 | 2.19 | 0.43 |
| 1:B:234:TYR:HB2 | 1:B:257:SER:HA | 2.01 | 0.43 |
| 1:C:991:GLN:OE1 | 1:D:1058:ARG:NH1 | 2.51 | 0.43 |
| 1:E:603:GLU:O | 1:E:604:TRP:C | 2.57 | 0.43 |
| 1:E:836:LEU:HD11 | 1:E:840:LEU:HD11 | 2.00 | 0.43 |
| 1:B:383:ARG:HD3 | 1:B:1179:ASP:OD1 | 2.19 | 0.43 |
| 1:B:570:GLY:O | 1:B:574:VAL:HG23 | 2.19 | 0.42 |
| 1:C:383:ARG:HD3 | 1:C:1179:ASP:OD1 | 2.19 | 0.42 |
| 1:C:570:GLY:O | 1:C:574:VAL:HG23 | 2.19 | 0.42 |
| 1:E:151:VAL:HG23 | 1:E:152:LEU:N | 2.34 | 0.42 |
| 1:E:570:GLY:O | 1:E:574:VAL:HG23 | 2.19 | 0.42 |
| 1:C:736:LYS:N | 1:C:736:LYS:CD | 2.82 | 0.42 |
| 1:E:121:THR:OG1 | 1:E:122:ALA:N | 2.50 | 0.42 |
| 1:A:202:THR:HG22 | 1:A:235:MET:CG | 2.50 | 0.42 |
| 1:B:192:ARG:NH1 | 1:B:318:GLN:O | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:488:LEU:HA | 1:D:491:LEU:HD12 | 2.01 | 0.42 |
| 1:D:736:LYS:N | 1:D:736:LYS:CD | 2.82 | 0.42 |
| 1:E:158:ASN:O | 1:E:161:VAL:HG22 | 2.18 | 0.42 |
| 1:E:827:ARG:NH1 | 1:E:852:GLY:O | 2.53 | 0.42 |
| 1:B:151:VAL:HG23 | 1:B:152:LEU:N | 2.34 | 0.42 |
| 1:B:827:ARG:NH1 | 1:B:852:GLY:O | 2.53 | 0.42 |
| 1:D:202:THR:HG22 | 1:D:235:MET:HG2 | 1.99 | 0.42 |
| 1:D:570:GLY:O | 1:D:574:VAL:HG23 | 2.19 | 0.42 |
| 1:D:991:GLN:OE1 | 1:E:1058:ARG:NH1 | 2.50 | 0.42 |
| 1:D:1139:LEU:CD2 | 1:E:956:LEU:HD13 | 2.49 | 0.42 |
| 1:E:234:TYR:HB2 | 1:E:257:SER:HA | 2.01 | 0.42 |
| 1:A:192:ARG:NH1 | 1:A:318:GLN:O | 2.52 | 0.42 |
| 1:B:598:ALA:O | 1:B:602:MET:HE2 | 2.19 | 0.42 |
| 1:B:603:GLU:O | 1:B:604:TRP:C | 2.57 | 0.42 |
| 1:B:836:LEU:HD11 | 1:B:840:LEU:HD11 | 2.00 | 0.42 |
| 1:C:151:VAL:HG23 | 1:C:152:LEU:N | 2.34 | 0.42 |
| 1:C:488:LEU:HA | 1:C:491:LEU:HD12 | 2.01 | 0.42 |
| 1:D:151:VAL:HG23 | 1:D:152:LEU:N | 2.34 | 0.42 |
| 1:D:466:VAL:HG13 | 1:D:467:ASN:N | 2.35 | 0.42 |
| 1:D:827:ARG:NH1 | 1:D:852:GLY:O | 2.53 | 0.42 |
| 1:B:202:THR:HG22 | 1:B:235:MET:CG | 2.50 | 0.42 |
| 1:B:736:LYS:N | 1:B:736:LYS:CD | 2.82 | 0.42 |
| 1:C:836:LEU:HD11 | 1:C:840:LEU:HD11 | 2.00 | 0.42 |
| 1:E:488:LEU:HA | 1:E:491:LEU:HD12 | 2.01 | 0.42 |
| 1:A:1004:ASN:O | 1:A:1005:ARG:C | 2.58 | 0.42 |
| 1:B:606:VAL:O | 1:B:609:THR:OG1 | 2.30 | 0.42 |
| 1:B:1004:ASN:O | 1:B:1005:ARG:C | 2.58 | 0.42 |
| 1:C:466:VAL:HG13 | 1:C:467:ASN:N | 2.35 | 0.42 |
| 1:A:308:LEU:HD23 | 1:A:308:LEU:O | 2.20 | 0.42 |
| 1:A:321:GLU:CG | 1:A:325:TRP:HZ3 | 2.33 | 0.42 |
| 1:A:585:VAL:HG12 | 1:A:586:VAL:N | 2.35 | 0.42 |
| 1:A:736:LYS:N | 1:A:736:LYS:CD | 2.82 | 0.42 |
| 1:C:234:TYR:HB2 | 1:C:257:SER:HA | 2.01 | 0.42 |
| 1:D:234:TYR:HB2 | 1:D:257:SER:HA | 2.01 | 0.42 |
| 1:D:321:GLU:CG | 1:D:325:TRP:HZ3 | 2.33 | 0.42 |
| 1:D:585:VAL:HG12 | 1:D:586:VAL:N | 2.35 | 0.42 |
| 1:E:736:LYS:N | 1:E:736:LYS:CD | 2.82 | 0.42 |
| 1:A:466:VAL:HG13 | 1:A:467:ASN:N | 2.35 | 0.42 |
| 1:C:321:GLU:CG | 1:C:325:TRP:HZ3 | 2.33 | 0.42 |
| 1:C:738:SER:O | 1:C:741:VAL:HG12 | 2.20 | 0.42 |
| 1:E:321:GLU:CG | 1:E:325:TRP:HZ3 | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:906:THR:O | 1:B:1104:VAL:HG13 | 2.20 | 0.41 |
| 1:D:308:LEU:HD23 | 1:D:308:LEU:O | 2.20 | 0.41 |
| 1:E:1004:ASN:O | 1:E:1005:ARG:C | 2.58 | 0.41 |
| 1:C:338:VAL:HG21 | 1:C:532:ILE:CD1 | 2.51 | 0.41 |
| 1:C:827:ARG:NH1 | 1:C:852:GLY:O | 2.53 | 0.41 |
| 1:E:585:VAL:HG12 | 1:E:586:VAL:N | 2.35 | 0.41 |
| 1:A:488:LEU:HA | 1:A:491:LEU:HD12 | 2.01 | 0.41 |
| 1:A:1139:LEU:HB2 | 1:B:1109:PHE:CE2 | 2.55 | 0.41 |
| 1:B:488:LEU:HA | 1:B:491:LEU:HD12 | 2.01 | 0.41 |
| 1:C:585:VAL:HG12 | 1:C:586:VAL:N | 2.35 | 0.41 |
| 1:D:202:THR:HG22 | 1:D:235:MET:CG | 2.50 | 0.41 |
| 1:D:598:ALA:O | 1:D:602:MET:HE2 | 2.20 | 0.41 |
| 1:E:466:VAL:HG13 | 1:E:467:ASN:N | 2.35 | 0.41 |
| 1:A:530:GLU:O | 1:A:533:THR:OG1 | 2.36 | 0.41 |
| 1:B:171:ALA:O | 1:B:175:ILE:HG12 | 2.21 | 0.41 |
| 1:B:338:VAL:HG21 | 1:B:532:ILE:CD1 | 2.51 | 0.41 |
| 1:C:202:THR:HG22 | 1:C:235:MET:CG | 2.50 | 0.41 |
| 1:C:565:GLU:OE2 | 1:C:569:VAL:HG21 | 2.21 | 0.41 |
| 1:C:1139:LEU:HD13 | 1:D:1109:PHE:CD2 | 2.55 | 0.41 |
| 1:D:338:VAL:HG21 | 1:D:532:ILE:CD1 | 2.51 | 0.41 |
| 1:D:506:GLU:O | 1:D:507:ALA:C | 2.59 | 0.41 |
| 1:D:906:THR:O | 1:E:1104:VAL:HG13 | 2.20 | 0.41 |
| 1:E:338:VAL:HG21 | 1:E:532:ILE:CD1 | 2.50 | 0.41 |
| 1:B:321:GLU:CG | 1:B:325:TRP:HZ3 | 2.33 | 0.41 |
| 1:B:738:SER:O | 1:B:741:VAL:HG12 | 2.20 | 0.41 |
| 1:C:308:LEU:HD23 | 1:C:308:LEU:O | 2.20 | 0.41 |
| 1:D:114:THR:O | 1:D:118:HIS:ND1 | 2.52 | 0.41 |
| 1:D:171:ALA:O | 1:D:175:ILE:HG12 | 2.21 | 0.41 |
| 1:B:506:GLU:O | 1:B:507:ALA:C | 2.59 | 0.41 |
| 1:C:828:VAL:HG12 | 1:C:829:ASP:H | 1.85 | 0.41 |
| 1:D:277:SER:O | 1:D:288:LYS:NZ | 2.41 | 0.41 |
| 1:D:330:VAL:O | 1:D:334:LEU:HD23 | 2.21 | 0.41 |
| 1:E:598:ALA:O | 1:E:602:MET:HE2 | 2.21 | 0.41 |
| 1:B:466:VAL:HG13 | 1:B:467:ASN:N | 2.35 | 0.41 |
| 1:C:603:GLU:O | 1:C:604:TRP:C | 2.57 | 0.41 |
| 1:A:205:ALA:O | 1:A:209:VAL:HG23 | 2.21 | 0.41 |
| 1:A:738:SER:O | 1:A:741:VAL:HG12 | 2.20 | 0.41 |
| 1:A:827:ARG:NH1 | 1:A:852:GLY:O | 2.53 | 0.41 |
| 1:B:203:ILE:HA | 1:B:206:CYS:SG | 2.61 | 0.41 |
| 1:B:308:LEU:HD23 | 1:B:308:LEU:O | 2.20 | 0.41 |
| 1:B:1139:LEU:CD2 | 1:C:956:LEU:HD13 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:506:GLU:O | 1:C:507:ALA:C | 2.59 | 0.41 |
| 1:C:1004:ASN:O | 1:C:1005:ARG:C | 2.58 | 0.41 |
| 1:D:998:LYS:HE2 | 1:D:1071:LEU:HD21 | 2.03 | 0.41 |
| 1:A:953:PHE:CE1 | 1:E:1136:LEU:HD13 | 2.50 | 0.41 |
| 1:B:585:VAL:HG12 | 1:B:586:VAL:N | 2.35 | 0.41 |
| 1:C:1139:LEU:CD2 | 1:D:956:LEU:HD13 | 2.51 | 0.41 |
| 1:E:202:THR:HG22 | 1:E:235:MET:CG | 2.50 | 0.41 |
| 1:E:998:LYS:HE2 | 1:E:1071:LEU:HD21 | 2.03 | 0.41 |
| 1:A:115:TYR:CG | 1:A:323:LEU:HD21 | 2.56 | 0.41 |
| 1:A:338:VAL:HG21 | 1:A:532:ILE:CD1 | 2.51 | 0.41 |
| 1:B:205:ALA:O | 1:B:209:VAL:HG23 | 2.21 | 0.41 |
| 1:B:828:VAL:HG12 | 1:B:829:ASP:H | 1.86 | 0.41 |
| 1:E:114:THR:O | 1:E:118:HIS:ND1 | 2.52 | 0.41 |
| 1:E:203:ILE:HA | 1:E:206:CYS:SG | 2.61 | 0.41 |
| 1:E:738:SER:O | 1:E:741:VAL:HG12 | 2.20 | 0.41 |
| 1:A:506:GLU:O | 1:A:507:ALA:C | 2.59 | 0.40 |
| 1:C:171:ALA:O | 1:C:175:ILE:HG12 | 2.21 | 0.40 |
| 1:C:330:VAL:O | 1:C:334:LEU:HD23 | 2.21 | 0.40 |
| 1:E:827:ARG:HE | 1:E:827:ARG:HA | 1.87 | 0.40 |
| 1:A:998:LYS:HE2 | 1:A:1071:LEU:HD21 | 2.03 | 0.40 |
| 1:B:565:GLU:OE2 | 1:B:569:VAL:HG21 | 2.21 | 0.40 |
| 1:D:738:SER:O | 1:D:741:VAL:HG12 | 2.20 | 0.40 |
| 1:E:565:GLU:OE2 | 1:E:569:VAL:HG21 | 2.21 | 0.40 |
| 1:A:330:VAL:O | 1:A:334:LEU:HD23 | 2.21 | 0.40 |
| 1:A:1139:LEU:HD21 | 1:B:956:LEU:HD13 | 2.03 | 0.40 |
| 1:D:827:ARG:HE | 1:D:827:ARG:HA | 1.87 | 0.40 |
| 1:E:115:TYR:CG | 1:E:323:LEU:HD21 | 2.56 | 0.40 |
| 1:E:171:ALA:O | 1:E:175:ILE:HG12 | 2.21 | 0.40 |
| 1:E:308:LEU:O | 1:E:308:LEU:HD23 | 2.20 | 0.40 |
| 1:A:226:MET:O | 1:A:229:VAL:HG22 | 2.22 | 0.40 |
| 1:A:565:GLU:OE2 | 1:A:569:VAL:HG21 | 2.21 | 0.40 |
| 1:A:906:THR:HG21 | 1:B:1107:ARG:NH1 | 2.36 | 0.40 |
| 1:C:226:MET:O | 1:C:229:VAL:HG22 | 2.22 | 0.40 |
| 1:C:606:VAL:O | 1:C:609:THR:OG1 | 2.31 | 0.40 |
| 1:D:205:ALA:O | 1:D:209:VAL:HG23 | 2.21 | 0.40 |
| 1:A:171:ALA:O | 1:A:175:ILE:HG12 | 2.21 | 0.40 |
| 1:A:203:ILE:HA | 1:A:206:CYS:SG | 2.61 | 0.40 |
| 1:C:998:LYS:HE2 | 1:C:1071:LEU:HD21 | 2.03 | 0.40 |
| 1:D:1004:ASN:O | 1:D:1005:ARG:C | 2.58 | 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 | 986/1187 (83%) | 934 (95%) | 52 (5%) | 0 | 100 | 100 |
| 1 | B | 986/1187 (83%) | 933 (95%) | 53 (5%) | 0 | 100 | 100 |
| 1 | C | 986/1187 (83%) | 933 (95%) | 53 (5%) | 0 | 100 | 100 |
| 1 | D | 986/1187 (83%) | 934 (95%) | 52 (5%) | 0 | 100 | 100 |
| 1 | E | 986/1187 (83%) | 933 (95%) | 53 (5%) | 0 | 100 | 100 |
| All | All | 4930/5935 (83%) | 4667 (95%) | 263 (5%) | 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 | 726/999 (73%) | 726 (100%) | 0 | 100 | 100 |
| 1 | B | 726/999 (73%) | 726 (100%) | 0 | 100 | 100 |
| 1 | C | 726/999 (73%) | 726 (100%) | 0 | 100 | 100 |
| 1 | D | 726/999 (73%) | 726 (100%) | 0 | 100 | 100 |
| 1 | E | 726/999 (73%) | 726 (100%) | 0 | 100 | 100 |
| All | All | 3630/4995 (73%) | 3630 (100%) | 0 | 100 | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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)

5 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | RET | C | 1201 | 1 | 20,20,21 | 0.69 | 1 (5%) | 27,27,28 | 0.38 | 0 |
| 2 | RET | B | 1201 | 1 | 20,20,21 | 0.69 | 1 (5%) | 27,27,28 | 0.38 | 0 |
| 2 | RET | A | 1201 | 1 | 20,20,21 | 0.68 | 1 (5%) | 27,27,28 | 0.38 | 0 |
| 2 | RET | D | 1201 | 1 | 20,20,21 | 0.67 | 1 (5%) | 27,27,28 | 0.38 | 0 |
| 2 | RET | E | 1201 | 1 | 20,20,21 | 0.69 | 1 (5%) | 27,27,28 | 0.39 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | RET | C | 1201 | 1 | - | 7/13/30/31 | 0/1/1/1 |
| 2 | RET | B | 1201 | 1 | - | 7/13/30/31 | 0/1/1/1 |
| 2 | RET | A | 1201 | 1 | - | 7/13/30/31 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | RET | D | 1201 | 1 | - | 7/13/30/31 | 0/1/1/1 |
| 2 | RET | E | 1201 | 1 | - | 7/13/30/31 | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 1201 | RET | C14-C13 | 2.66 | 1.35 | 1.33 |
| 2 | E | 1201 | RET | C14-C13 | 2.65 | 1.35 | 1.33 |
| 2 | C | 1201 | RET | C14-C13 | 2.63 | 1.35 | 1.33 |
| 2 | A | 1201 | RET | C14-C13 | 2.61 | 1.35 | 1.33 |
| 2 | D | 1201 | RET | C14-C13 | 2.57 | 1.35 | 1.33 |

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 1201 | RET | C1-C6-C7-C8 |
| 2 | A | 1201 | RET | C5-C6-C7-C8 |
| 2 | A | 1201 | RET | C7-C8-C9-C10 |
| 2 | A | 1201 | RET | C7-C8-C9-C19 |
| 2 | B | 1201 | RET | C1-C6-C7-C8 |
| 2 | B | 1201 | RET | C5-C6-C7-C8 |
| 2 | B | 1201 | RET | C7-C8-C9-C10 |
| 2 | B | 1201 | RET | C7-C8-C9-C19 |
| 2 | C | 1201 | RET | C1-C6-C7-C8 |
| 2 | C | 1201 | RET | C5-C6-C7-C8 |
| 2 | C | 1201 | RET | C7-C8-C9-C10 |
| 2 | C | 1201 | RET | C7-C8-C9-C19 |
| 2 | D | 1201 | RET | C1-C6-C7-C8 |
| 2 | D | 1201 | RET | C5-C6-C7-C8 |
| 2 | D | 1201 | RET | C7-C8-C9-C10 |
| 2 | D | 1201 | RET | C7-C8-C9-C19 |
| 2 | E | 1201 | RET | C1-C6-C7-C8 |
| 2 | E | 1201 | RET | C5-C6-C7-C8 |
| 2 | E | 1201 | RET | C7-C8-C9-C10 |
| 2 | E | 1201 | RET | C7-C8-C9-C19 |
| 2 | A | 1201 | RET | C11-C12-C13-C20 |
| 2 | B | 1201 | RET | C11-C12-C13-C20 |
| 2 | C | 1201 | RET | C11-C12-C13-C20 |
| 2 | D | 1201 | RET | C11-C12-C13-C20 |

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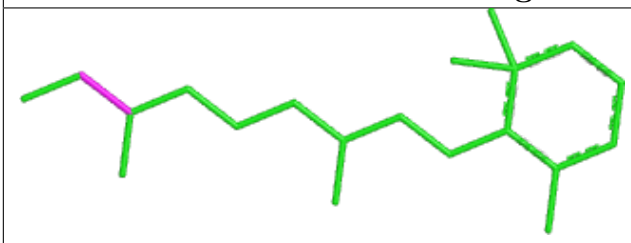
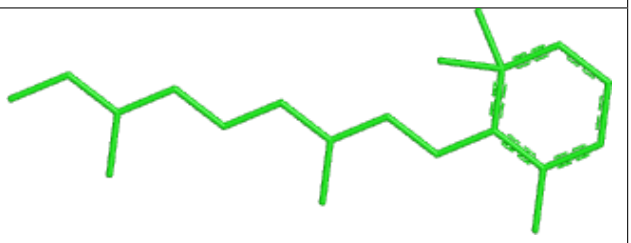
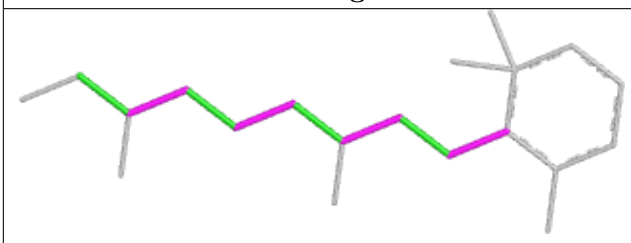
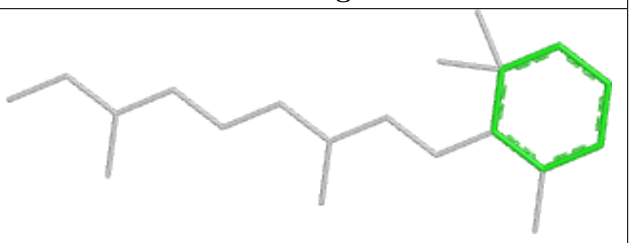
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | E | 1201 | RET | C11-C12-C13-C20 |
| 2 | A | 1201 | RET | C11-C12-C13-C14 |
| 2 | B | 1201 | RET | C11-C12-C13-C14 |
| 2 | C | 1201 | RET | C11-C12-C13-C14 |
| 2 | D | 1201 | RET | C11-C12-C13-C14 |
| 2 | E | 1201 | RET | C11-C12-C13-C14 |
| 2 | A | 1201 | RET | C9-C10-C11-C12 |
| 2 | B | 1201 | RET | C9-C10-C11-C12 |
| 2 | C | 1201 | RET | C9-C10-C11-C12 |
| 2 | D | 1201 | RET | C9-C10-C11-C12 |
| 2 | E | 1201 | RET | C9-C10-C11-C12 |

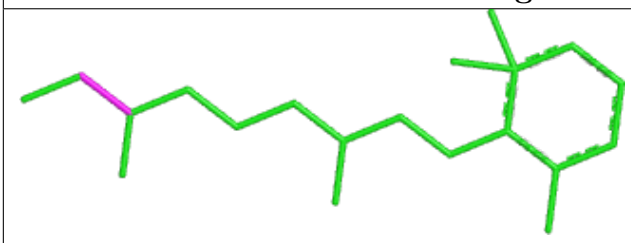
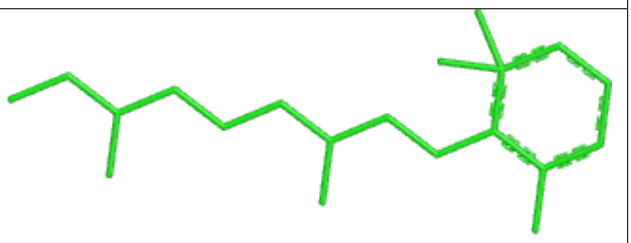
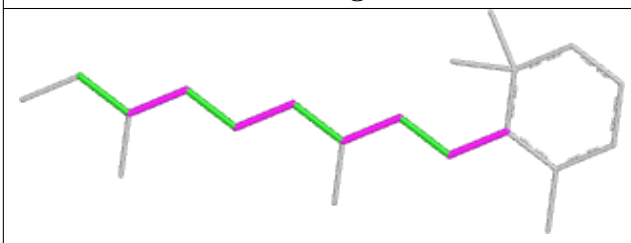
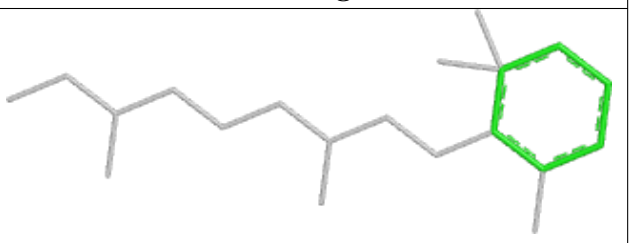
There are no ring outliers.

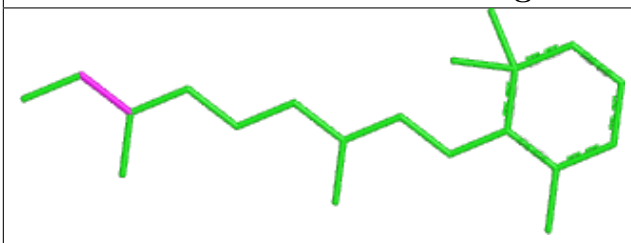
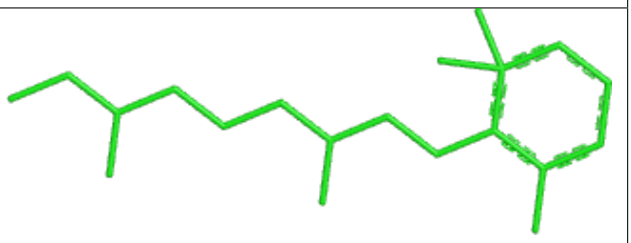
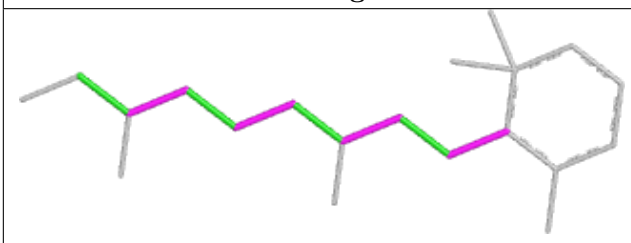
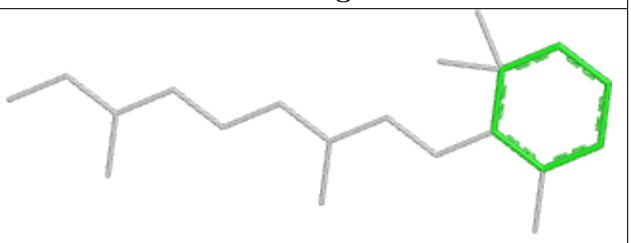
5 monomers are involved in 25 short contacts:

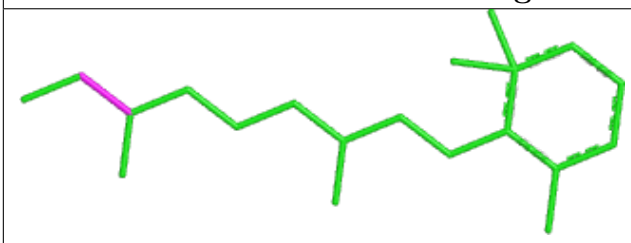
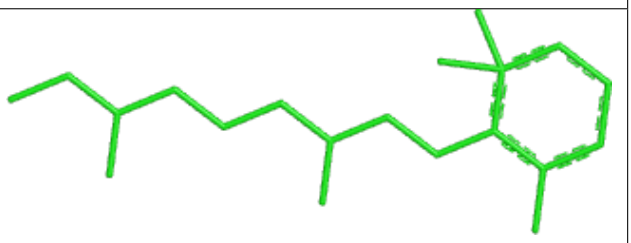
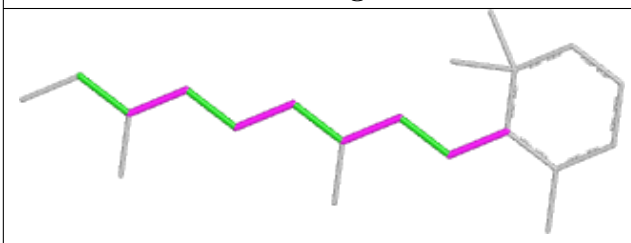
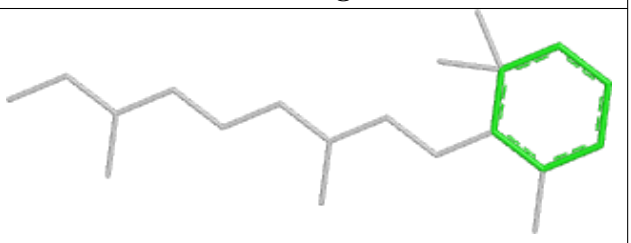
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | C | 1201 | RET | 5 | 0 |
| 2 | B | 1201 | RET | 5 | 0 |
| 2 | A | 1201 | RET | 5 | 0 |
| 2 | D | 1201 | RET | 5 | 0 |
| 2 | E | 1201 | RET | 5 | 0 |

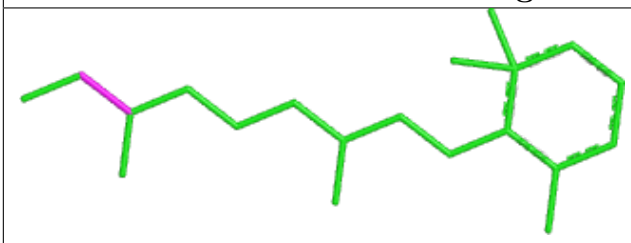
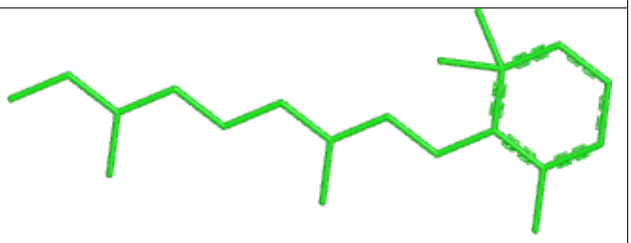
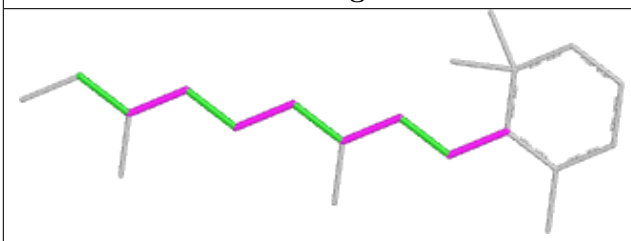
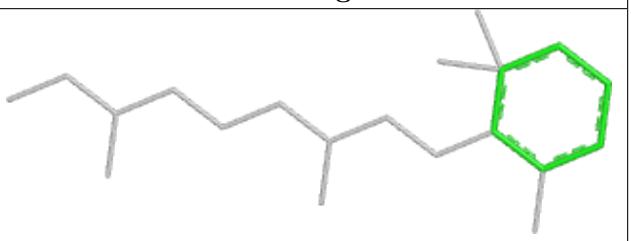
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 RET C 1201 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand RET B 1201 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand RET A 1201 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand RET D 1201 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

| Ligand RET E 1201 | |
|---|---|
|  |  |
| Bond lengths | Bond angles |
|  |  |
| Torsions | Rings |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

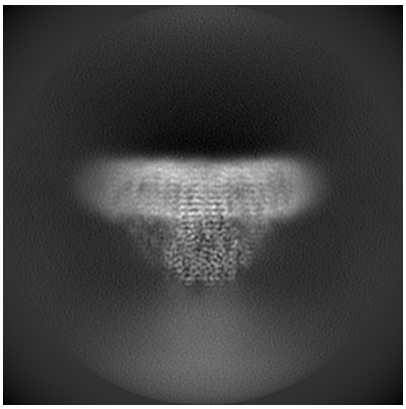
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13485. These allow visual inspection of the internal detail of the map and identification of artifacts.

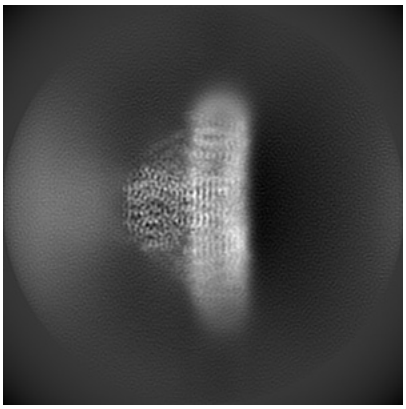
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

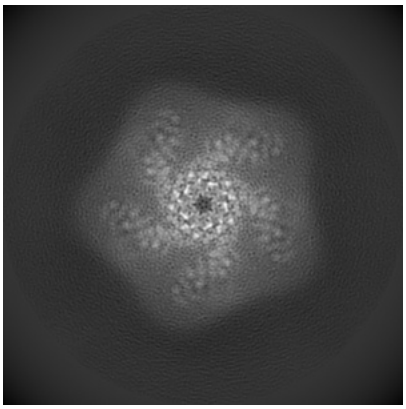
### 6.1.1 Primary map



X

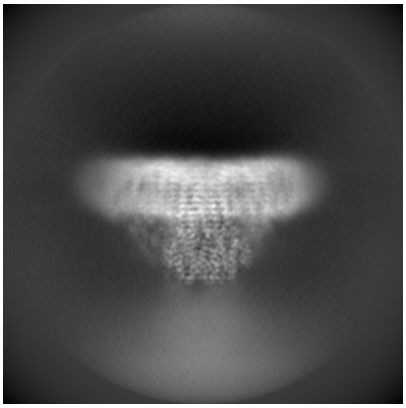


Y

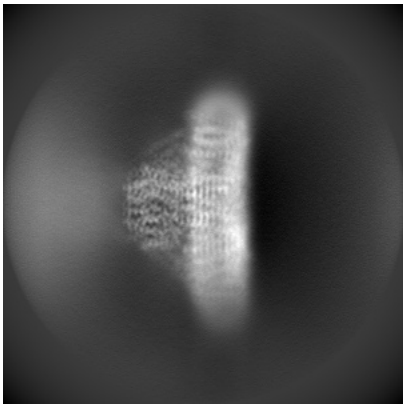


Z

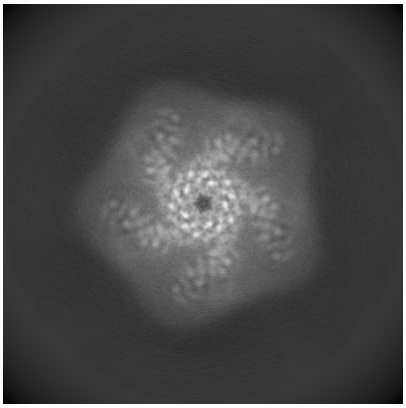
### 6.1.2 Raw map



X



Y

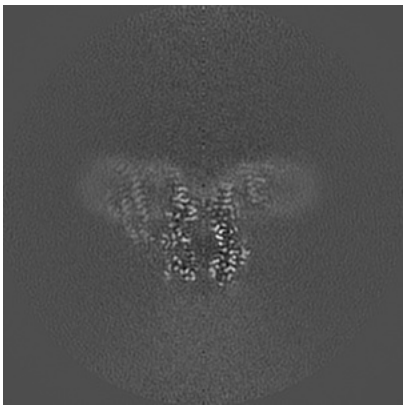


Z

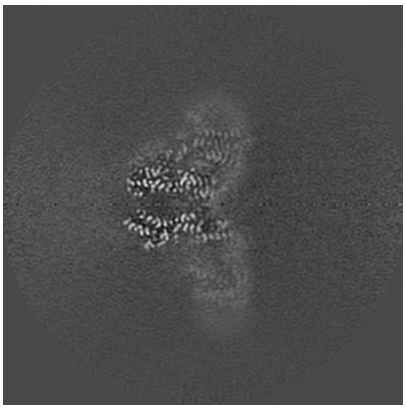
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

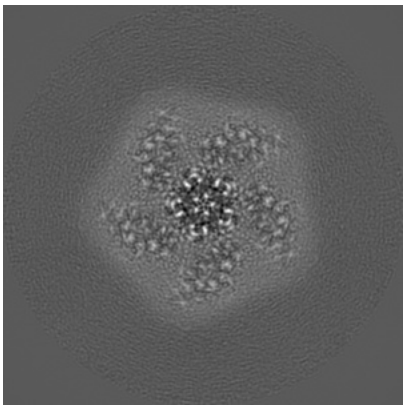
### 6.2.1 Primary map



X Index: 200

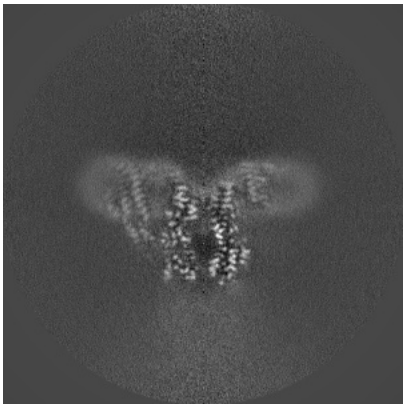


Y Index: 200

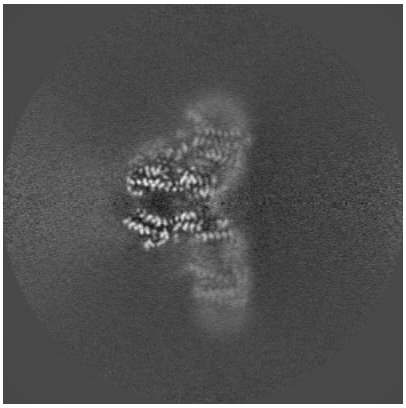


Z Index: 200

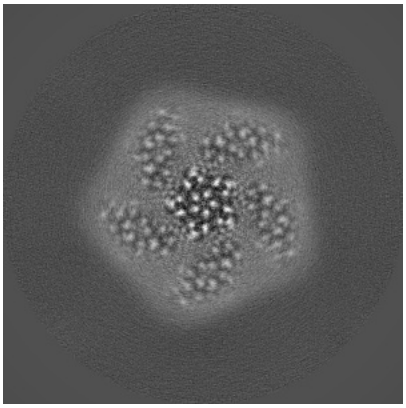
### 6.2.2 Raw map



X Index: 200



Y Index: 200

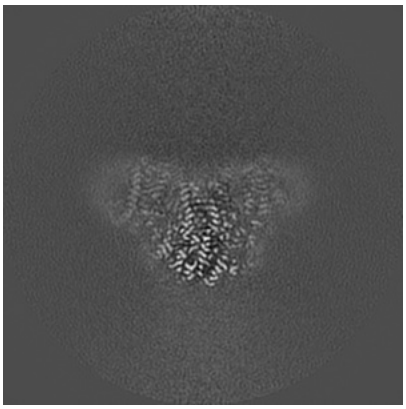


Z Index: 200

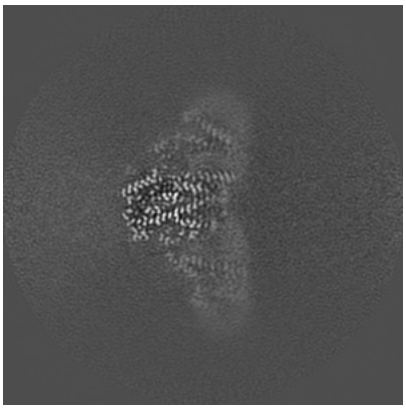
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

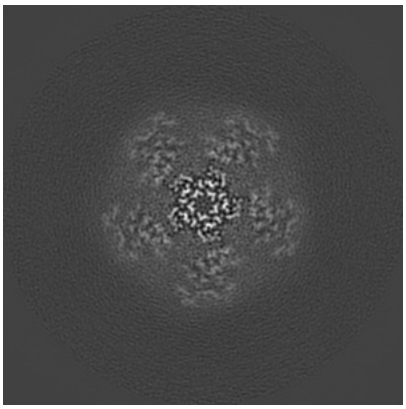
### 6.3.1 Primary map



X Index: 218

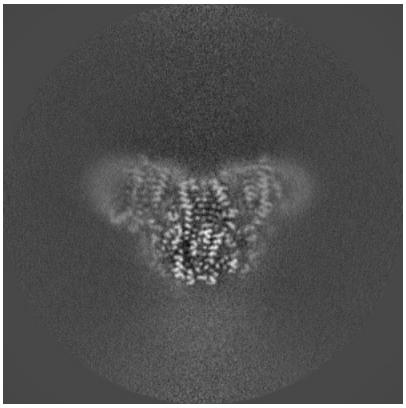


Y Index: 186

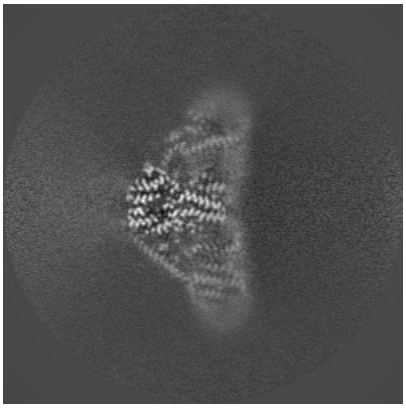


Z Index: 191

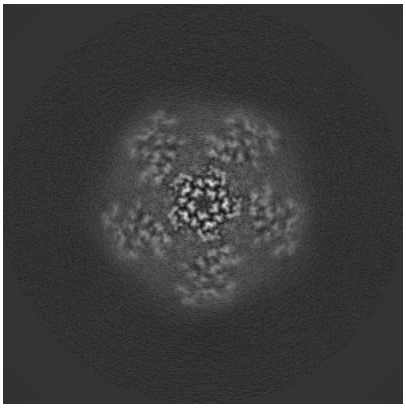
### 6.3.2 Raw map



X Index: 215



Y Index: 178



Z Index: 191

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 0.013. 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.

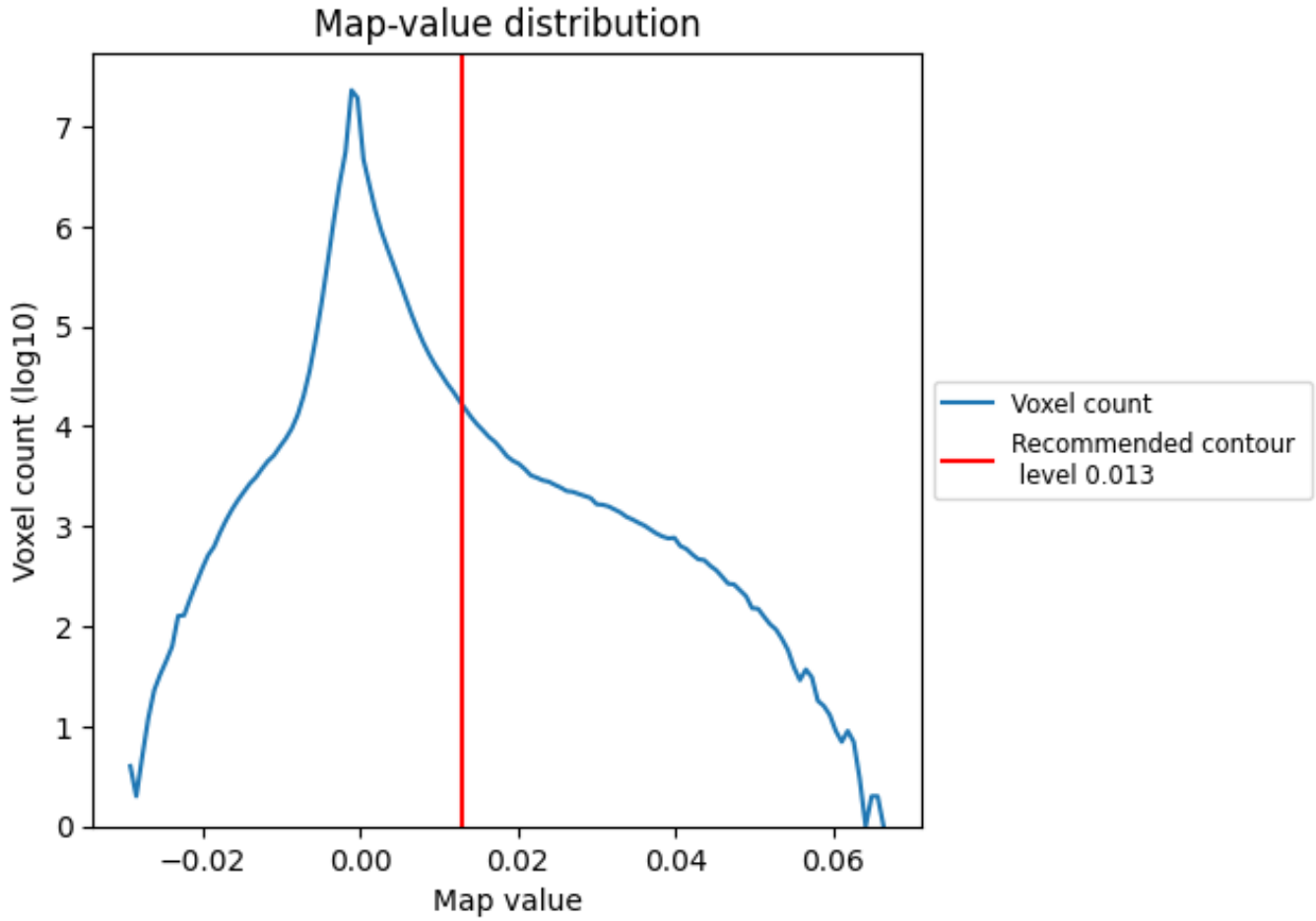
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

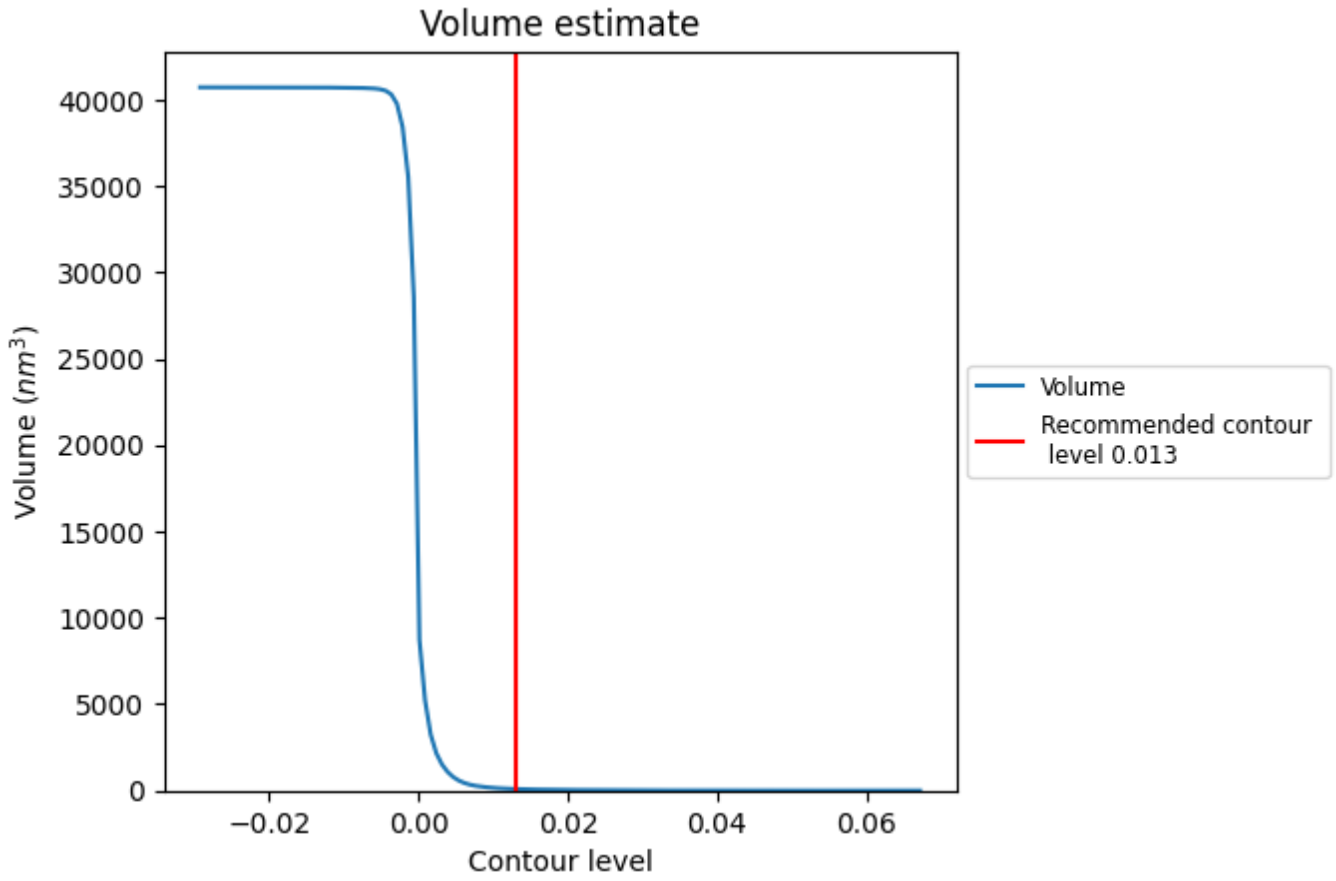
This section contains the results of statistical analysis of the map.

## 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.

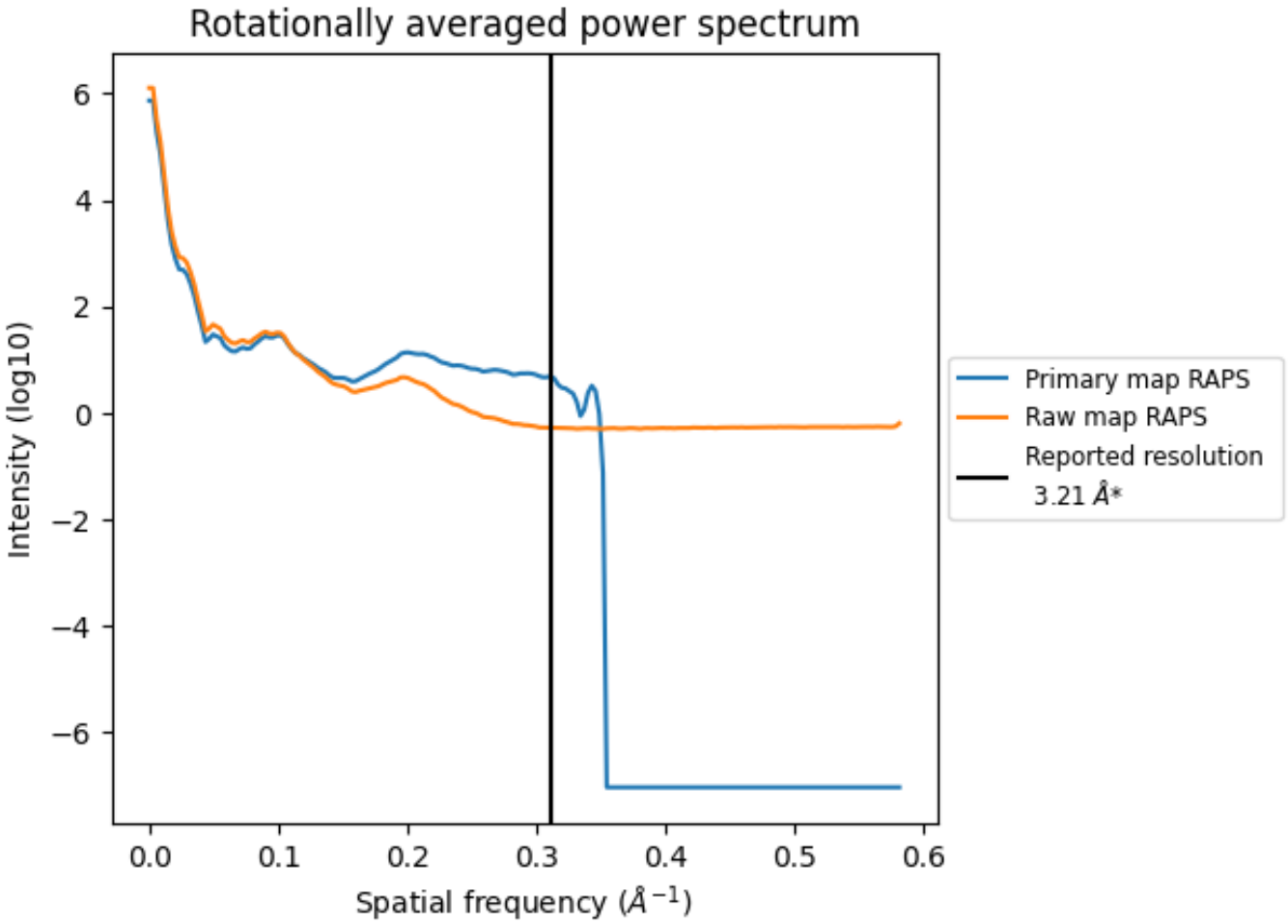
## 7.2 Volume estimate




The volume at the recommended contour level is 90 $nm^3$; this corresponds to an approximate mass of 81 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)

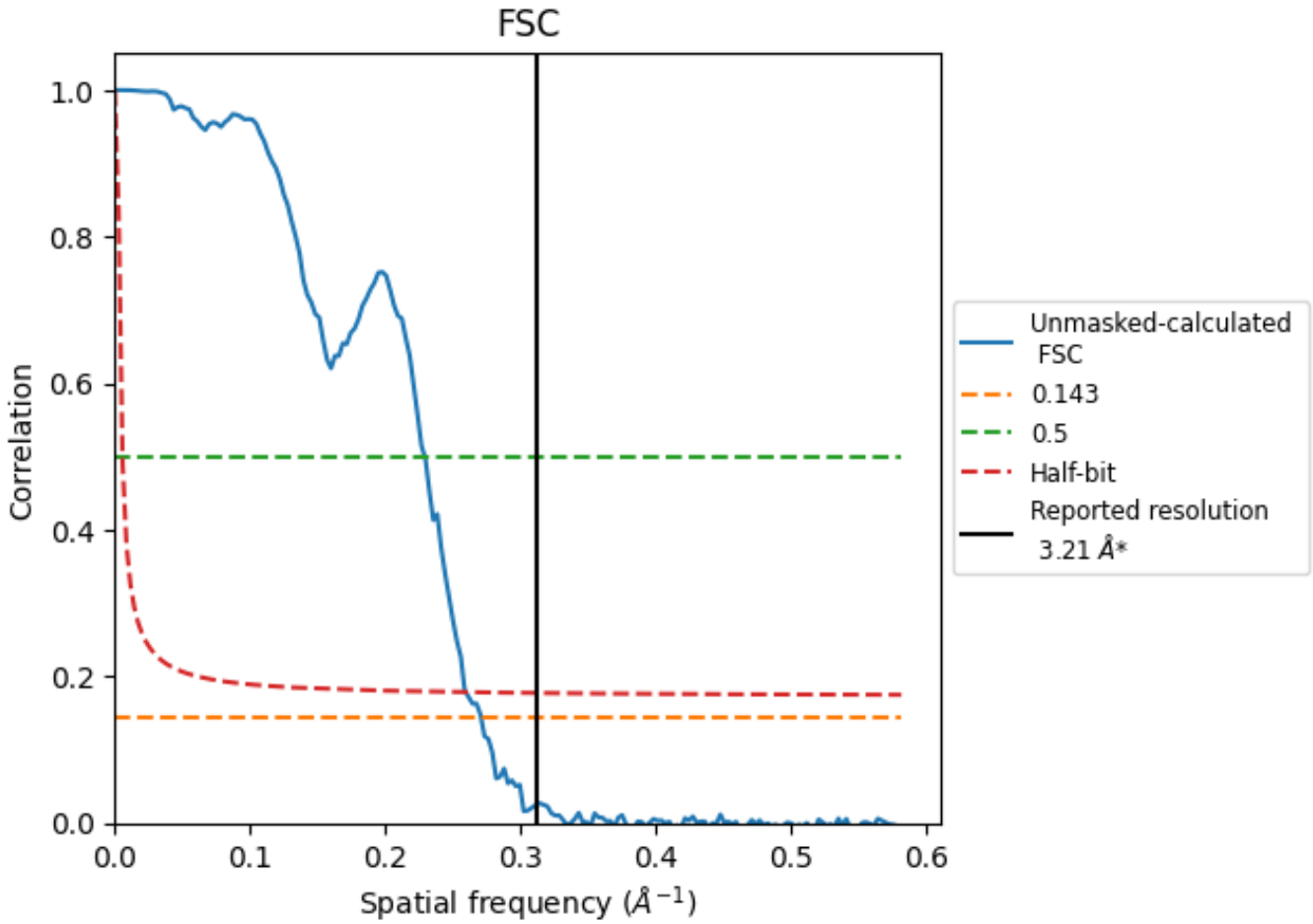



*Reported resolution corresponds to spatial frequency of 0.312 Å$^{-1}$

# 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 0.312 Å$^{-1}$

## 8.2 Resolution estimates (i)

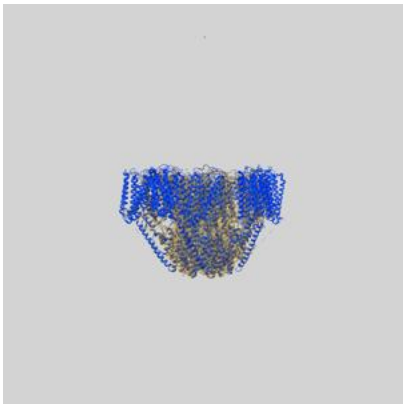
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.21 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 3.69 | 4.36 | 3.86 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.69 differs from the reported value 3.21 by more than 10 %

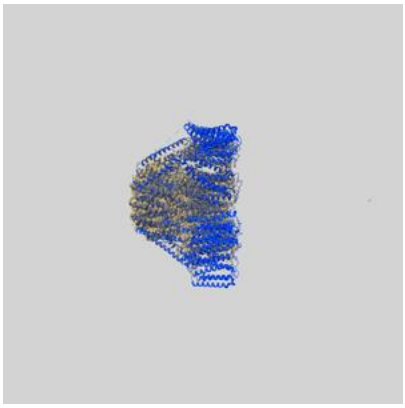
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13485 and PDB model 7PL9. Per-residue inclusion information can be found in section 3 on page 5.

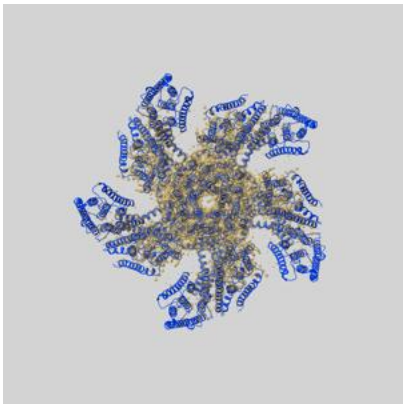
## 9.1 Map-model overlay



X



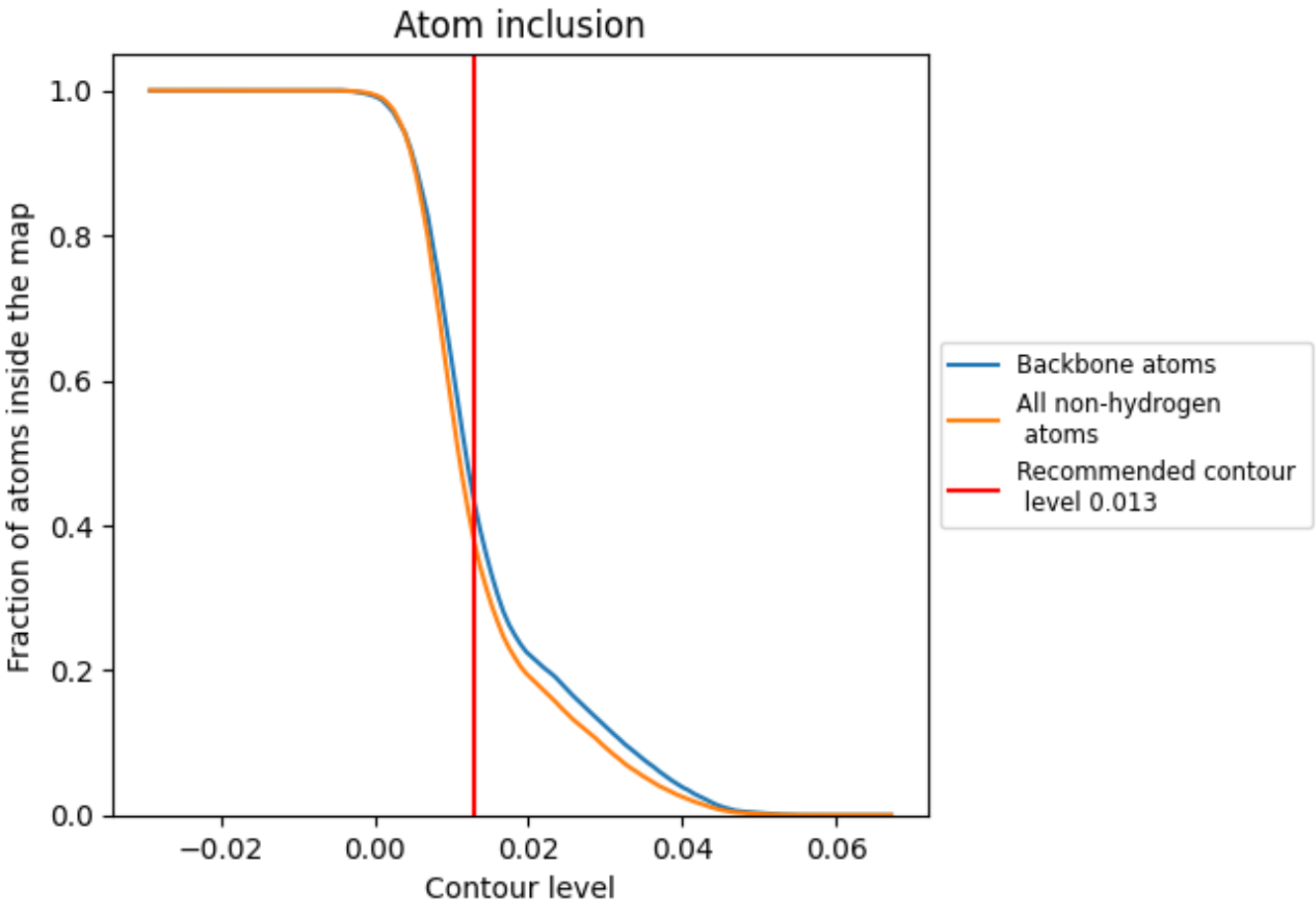
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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 Atom inclusion (i)




At the recommended contour level, 43% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.