# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:25 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 3RAJ |
| Title | : | Crystal structure of human CD38 in complex with the Fab fragment of antibody HB7 |
| Authors | : | Zhang, H.; Lee, H.C.; Hao, Q. |
| Deposited on | : | 2011-03-28 |
| Resolution | : | 3.04 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

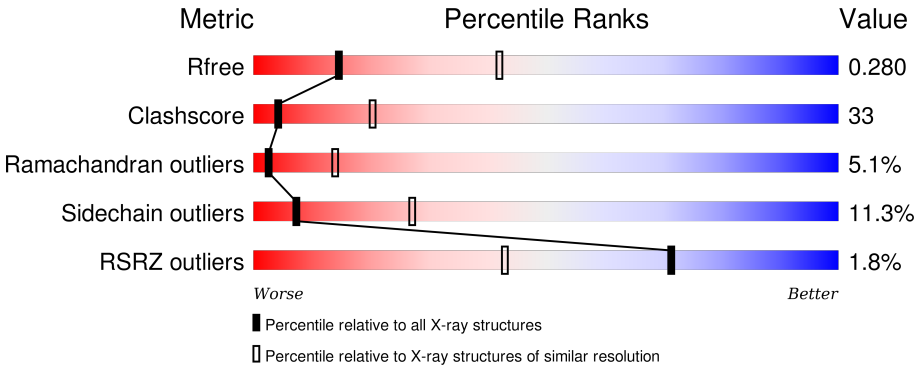
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 1995 (3.08-3.00) |
| Clashscore | 102246 | 2351 (3.08-3.00) |
| Ramachandran outliers | 100387 | 2272 (3.08-3.00) |
| Sidechain outliers | 100360 | 2275 (3.08-3.00) |
| RSRZ outliers | 91569 | 2013 (3.08-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 257 | 43% 37% 9% • 11% |
| 2 | H | 220 | 3% 37% 50% 10% • |
| 3 | L | 211 | 2% 44% 48% 7% • |

# 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5034 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ADP-ribosyl cyclase 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 230 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1851 | 1168 | 318 | 351 | 14 | | | |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 44 | GLU | - | EXPRESSION TAG | UNP P28907 |
| A | 45 | PHE | - | EXPRESSION TAG | UNP P28907 |
| A | 49 | THR | GLN | ENGINEERED MUTATION | UNP P28907 |
| A | 100 | ASP | ASN | ENGINEERED MUTATION | UNP P28907 |
| A | 164 | ASP | ASN | ENGINEERED MUTATION | UNP P28907 |
| A | 209 | ASP | ASN | ENGINEERED MUTATION | UNP P28907 |
| A | 219 | ASP | ASN | ENGINEERED MUTATION | UNP P28907 |

- Molecule 2 is a protein called heavy chain of the Fab fragment of antibody HB7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | H | 215 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1584 | 1012 | 256 | 309 | 7 | | | |

- Molecule 3 is a protein called light chain of the Fab fragment of antibody HB7.

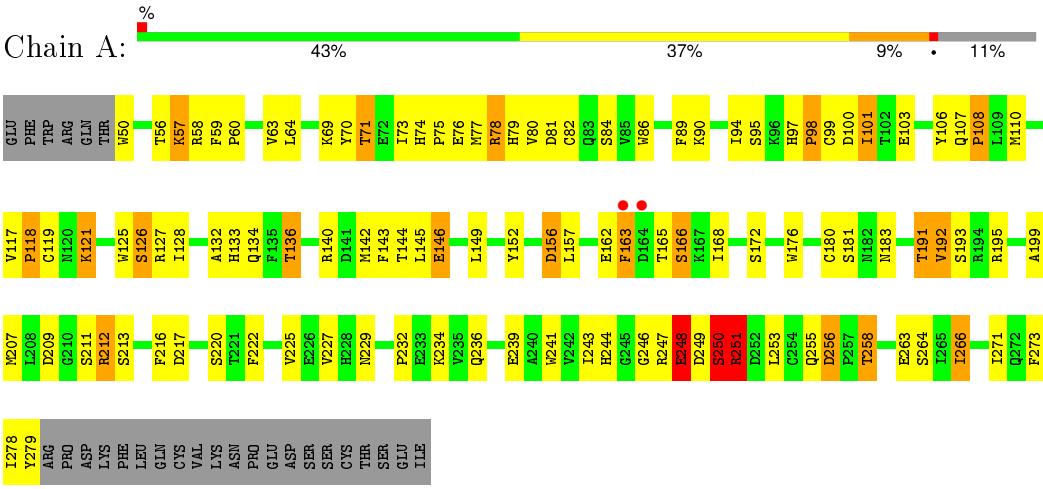
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | L | 208 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1599 | 996 | 265 | 332 | 6 | | | |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

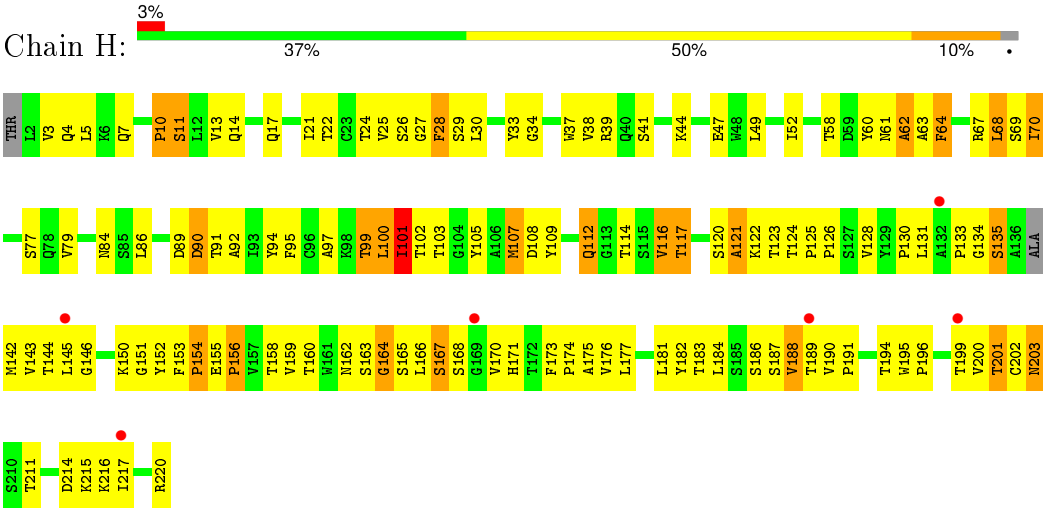
- Molecule 1: ADP-ribosyl cyclase 1

Chain A:



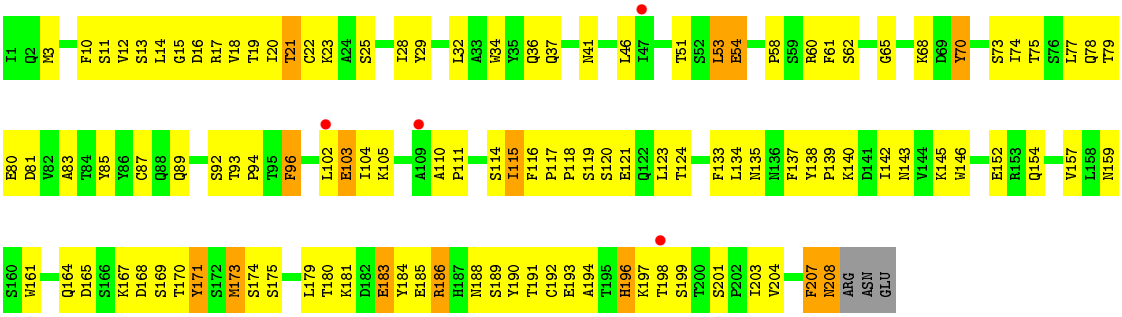

- Molecule 2: heavy chain of the Fab fragment of antibody HB7

Chain H:




- Molecule 3: light chain of the Fab fragment of antibody HB7

Chain L:


I1 Q2 M3 F10 S11 V12 S13 L14 G15 D16 R17 V18 T19 I20 T21 C22 K23 A24 S25 I28 Y29 L32 A33 W34 Y35 Q36 Q37 N41 L46 I47 T51 S52 L53 E54 P58 S59 R60 F61 S62 G65 K68 D69 Y70 S73 I74 T75 S76 L77 Q78 T79
E80 D81 Y82 A83 T84 Y85 Y86 C87 Q88 Q89 S92 T93 P94 T95 F96 L102 E103 I104 K105 A109 A110 P111 S114 I115 F116 P117 P118 S119 S120 E121 Q122 L123 T124 F133 L134 N135 N136 F137 Y138 P139 K140 D141 I142 N143 V144 K145 W146 E152 R153 Q154 V157 L158 N159
S160 W161 Q164 D165 S166 K167 D168 S169 T170 Y171 S172 M173 S174 S175 L179 T180 K181 D182 E183 Y184 E185 R186 H187 N188 S189 Y190 T191 C192 E193 A194 T195 H196 K197 T198 S199 T200 S201 P202 I203 V204 F207 N208 ARG ASN GLU

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 59.66Å 271.52Å 136.66Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 48.16 – 3.04<br>49.81 – 3.04 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 90.5 (48.16-3.04)<br>90.6 (49.81-3.04) | Depositor<br>EDS |
| $R_{merge}$ | 0.09 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.47 (at 3.07Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: dev_378) | Depositor |
| R, $R_{free}$ | 0.205 , 0.275<br>0.202 , 0.280 | Depositor<br>DCC |
| $R_{free}$ test set | 1003 reflections (5.34%) | DCC |
| Wilson B-factor (Å$^2$) | 83.3 | Xtriage |
| Anisotropy | 0.472 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 88.4 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Outliers | 0 of 19860 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 5034 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 98.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

# 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 | 0.63 | 0/1896 | 0.77 | 1/2570 (0.0%) |
| 2 | H | 0.46 | 0/1625 | 0.66 | 2/2224 (0.1%) |
| 3 | L | 0.47 | 0/1634 | 0.63 | 0/2221 |
| All | All | 0.53 | 0/5155 | 0.69 | 3/7015 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 3 | L | 0 | 1 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | H | 100 | LEU | CA-CB-CG | 6.72 | 130.75 | 115.30 |
| 1 | A | 192 | VAL | CB-CA-C | -5.18 | 101.56 | 111.40 |
| 2 | H | 3 | VAL | CB-CA-C | -5.04 | 101.83 | 111.40 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | L | 70 | TYR | Peptide |

## 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 | 1851 | 0 | 1777 | 108 | 0 |
| 2 | H | 1584 | 0 | 1518 | 130 | 0 |
| 3 | L | 1599 | 0 | 1530 | 100 | 0 |
| All | All | 5034 | 0 | 4825 | 329 | 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 33.

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:162:ASN:HA | 2:H:201:THR:HG23 | 1.42 | 1.01 |
| 2:H:171:HIS:HB2 | 3:L:135:ASN:HD21 | 1.23 | 1.01 |
| 2:H:128:VAL:HG21 | 2:H:204:VAL:HG21 | 1.47 | 0.94 |
| 1:A:71:THR:HG22 | 1:A:78:ARG:H | 1.35 | 0.92 |
| 2:H:135:SER:HB2 | 2:H:220:ARG:HB2 | 1.53 | 0.91 |
| 2:H:131:LEU:HB3 | 3:L:116:PHE:CD2 | 2.08 | 0.89 |
| 3:L:117:PRO:HB3 | 3:L:207:PHE:HE1 | 1.34 | 0.88 |
| 2:H:209:SER:O | 2:H:211:THR:HG23 | 1.75 | 0.86 |
| 2:H:100:LEU:O | 2:H:101:ILE:HG12 | 1.76 | 0.85 |
| 2:H:60:TYR:HE1 | 2:H:70:ILE:HG13 | 1.37 | 0.85 |
| 1:A:250:SER:O | 1:A:251:ARG:CB | 2.24 | 0.84 |
| 3:L:36:GLN:HB2 | 3:L:46:LEU:HD11 | 1.57 | 0.84 |
| 1:A:128:ILE:O | 1:A:128:ILE:HG23 | 1.75 | 0.83 |
| 3:L:77:LEU:HD12 | 3:L:78:GLN:H | 1.46 | 0.80 |
| 2:H:195:TRP:CG | 2:H:196:PRO:HA | 2.17 | 0.80 |
| 2:H:131:LEU:HB3 | 3:L:116:PHE:HD2 | 1.45 | 0.79 |
| 3:L:117:PRO:HB3 | 3:L:207:PHE:CE1 | 2.17 | 0.79 |
| 2:H:170:VAL:HG13 | 2:H:187:SER:O | 1.82 | 0.79 |
| 1:A:103:GLU:HG2 | 1:A:191:THR:OG1 | 1.81 | 0.79 |
| 3:L:13:SER:O | 3:L:16:ASP:HB2 | 1.83 | 0.79 |
| 1:A:248:GLU:HG2 | 1:A:249:ASP:N | 1.97 | 0.79 |
| 3:L:77:LEU:HD12 | 3:L:78:GLN:N | 1.98 | 0.79 |
| 1:A:60:PRO:HB3 | 1:A:86:TRP:CZ2 | 2.20 | 0.77 |
| 3:L:140:LYS:HB3 | 3:L:171:TYR:CE1 | 2.21 | 0.76 |
| 2:H:123:THR:HG23 | 2:H:153:PHE:O | 1.86 | 0.75 |
| 3:L:37:GLN:O | 3:L:83:ALA:HB1 | 1.85 | 0.75 |
| 2:H:144:THR:HG22 | 2:H:189:THR:HG23 | 1.67 | 0.75 |
| 1:A:132:ALA:C | 1:A:134:GLN:H | 1.91 | 0.75 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:160:THR:OG1 | 2:H:203:ASN:HB2 | 1.87 | 0.74 |
| 2:H:143:VAL:HG13 | 2:H:190:VAL:HG23 | 1.68 | 0.74 |
| 3:L:53:LEU:O | 3:L:54:GLU:HB2 | 1.86 | 0.74 |
| 1:A:250:SER:O | 1:A:251:ARG:HB2 | 1.88 | 0.73 |
| 3:L:14:LEU:HD23 | 3:L:15:GLY:N | 2.03 | 0.73 |
| 3:L:22:CYS:HB2 | 3:L:34:TRP:CH2 | 2.24 | 0.73 |
| 1:A:94:ILE:HD12 | 1:A:94:ILE:O | 1.87 | 0.72 |
| 1:A:207:MET:HE2 | 1:A:241:TRP:HE3 | 1.53 | 0.72 |
| 1:A:90:LYS:O | 1:A:94:ILE:HG13 | 1.88 | 0.72 |
| 2:H:162:ASN:HB2 | 2:H:165:SER:HB2 | 1.72 | 0.71 |
| 3:L:119:SER:O | 3:L:123:LEU:HD12 | 1.90 | 0.71 |
| 1:A:50:TRP:HB2 | 1:A:172:SER:HB2 | 1.72 | 0.71 |
| 2:H:38:VAL:HG13 | 2:H:47:GLU:O | 1.91 | 0.71 |
| 2:H:120:SER:O | 2:H:121:ALA:HB2 | 1.89 | 0.70 |
| 3:L:123:LEU:HB3 | 3:L:181:LYS:HD3 | 1.74 | 0.70 |
| 2:H:200:VAL:H | 2:H:216:LYS:HE3 | 1.57 | 0.69 |
| 3:L:11:SER:HA | 3:L:103:GLU:O | 1.92 | 0.69 |
| 3:L:142:ILE:HG12 | 3:L:143:ASN:H | 1.57 | 0.69 |
| 3:L:145:LYS:HB3 | 3:L:193:GLU:HG3 | 1.73 | 0.69 |
| 2:H:171:HIS:HB2 | 3:L:135:ASN:ND2 | 2.02 | 0.69 |
| 3:L:133:PHE:O | 3:L:134:LEU:HD12 | 1.92 | 0.69 |
| 2:H:145:LEU:HD13 | 2:H:217:ILE:HG21 | 1.74 | 0.68 |
| 2:H:7:GLN:HE22 | 2:H:95:PHE:HA | 1.58 | 0.67 |
| 3:L:181:LYS:O | 3:L:184:TYR:HB3 | 1.95 | 0.67 |
| 3:L:190:TYR:HB2 | 3:L:207:PHE:CE2 | 2.29 | 0.67 |
| 3:L:115:ILE:O | 3:L:115:ILE:HG12 | 1.94 | 0.67 |
| 1:A:69:LYS:HG3 | 1:A:73:ILE:HD11 | 1.77 | 0.67 |
| 2:H:195:TRP:CD1 | 2:H:196:PRO:HA | 2.29 | 0.67 |
| 2:H:170:VAL:HG22 | 2:H:188:VAL:HA | 1.77 | 0.66 |
| 3:L:190:TYR:HB2 | 3:L:207:PHE:HE2 | 1.59 | 0.66 |
| 1:A:50:TRP:HB2 | 1:A:172:SER:CB | 2.26 | 0.66 |
| 2:H:68:LEU:HD12 | 2:H:69:SER:H | 1.61 | 0.65 |
| 2:H:190:VAL:HB | 2:H:191:PRO:HD2 | 1.77 | 0.65 |
| 3:L:179:LEU:HD22 | 3:L:183:GLU:HG3 | 1.79 | 0.64 |
| 1:A:263:GLU:HG3 | 1:A:273:PHE:CD2 | 2.32 | 0.64 |
| 1:A:253:LEU:C | 1:A:255:GLN:H | 2.00 | 0.64 |
| 1:A:250:SER:O | 1:A:251:ARG:HB3 | 1.97 | 0.64 |
| 2:H:64:PHE:CD2 | 2:H:64:PHE:N | 2.64 | 0.64 |
| 3:L:117:PRO:CB | 3:L:207:PHE:HE1 | 2.09 | 0.64 |
| 2:H:135:SER:H | 2:H:220:ARG:HD3 | 1.63 | 0.63 |
| 2:H:60:TYR:CE1 | 2:H:70:ILE:HG13 | 2.28 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:244:HIS:CD2 | 1:A:253:LEU:HD12 | 2.33 | 0.63 |
| 3:L:207:PHE:HD2 | 3:L:207:PHE:H | 1.47 | 0.63 |
| 2:H:72:LYS:HB3 | 2:H:79:VAL:HG22 | 1.80 | 0.62 |
| 3:L:137:PHE:O | 3:L:170:THR:HB | 2.00 | 0.62 |
| 3:L:173:MET:HG3 | 3:L:174:SER:N | 2.15 | 0.62 |
| 2:H:174:PRO:HG2 | 3:L:161:TRP:O | 1.99 | 0.62 |
| 1:A:77:MET:O | 1:A:79:HIS:N | 2.26 | 0.62 |
| 2:H:99:THR:HG23 | 2:H:101:ILE:O | 1.99 | 0.62 |
| 1:A:162:GLU:HG3 | 1:A:165:THR:OG1 | 1.99 | 0.62 |
| 3:L:62:SER:HB2 | 3:L:73:SER:HB2 | 1.82 | 0.61 |
| 3:L:120:SER:O | 3:L:124:THR:HG23 | 2.01 | 0.61 |
| 3:L:60:ARG:NH2 | 3:L:81:ASP:OD1 | 2.29 | 0.61 |
| 3:L:146:TRP:HE1 | 3:L:175:SER:HB3 | 1.65 | 0.61 |
| 2:H:25:VAL:CG2 | 2:H:77:SER:HB3 | 2.31 | 0.61 |
| 2:H:200:VAL:O | 2:H:200:VAL:HG22 | 2.00 | 0.60 |
| 3:L:118:PRO:HB2 | 3:L:123:LEU:HD11 | 1.82 | 0.60 |
| 1:A:128:ILE:O | 1:A:128:ILE:CG2 | 2.49 | 0.60 |
| 2:H:64:PHE:HD2 | 2:H:64:PHE:H | 1.50 | 0.60 |
| 3:L:193:GLU:HB3 | 3:L:204:VAL:HG22 | 1.83 | 0.60 |
| 3:L:3:MET:HB2 | 3:L:96:PHE:O | 2.02 | 0.59 |
| 2:H:159:VAL:HG22 | 2:H:204:VAL:HG12 | 1.84 | 0.59 |
| 1:A:247:ARG:O | 1:A:248:GLU:CB | 2.51 | 0.59 |
| 1:A:145:LEU:HD21 | 1:A:192:VAL:HG23 | 1.84 | 0.59 |
| 1:A:163:PHE:CD2 | 1:A:163:PHE:N | 2.72 | 0.58 |
| 1:A:126:SER:O | 1:A:127:ARG:C | 2.42 | 0.58 |
| 2:H:89:ASP:C | 2:H:91:THR:H | 2.06 | 0.58 |
| 1:A:71:THR:HG22 | 1:A:78:ARG:N | 2.12 | 0.58 |
| 1:A:207:MET:HE2 | 1:A:241:TRP:CE3 | 2.36 | 0.58 |
| 3:L:22:CYS:HB2 | 3:L:34:TRP:HH2 | 1.66 | 0.58 |
| 1:A:101:ILE:N | 1:A:101:ILE:CD1 | 2.66 | 0.58 |
| 3:L:184:TYR:CE1 | 3:L:190:TYR:CE2 | 2.92 | 0.58 |
| 2:H:190:VAL:HB | 2:H:194:THR:CG2 | 2.34 | 0.57 |
| 1:A:132:ALA:O | 1:A:134:GLN:N | 2.38 | 0.57 |
| 2:H:91:THR:HG23 | 2:H:117:THR:HA | 1.86 | 0.57 |
| 1:A:244:HIS:CD2 | 1:A:253:LEU:CD1 | 2.87 | 0.57 |
| 2:H:5:LEU:HD13 | 2:H:109:TYR:O | 2.05 | 0.57 |
| 2:H:142:MET:HB3 | 2:H:190:VAL:O | 2.05 | 0.56 |
| 2:H:10:PRO:O | 2:H:11:SER:CB | 2.53 | 0.56 |
| 2:H:202:CYS:O | 2:H:214:ASP:HA | 2.06 | 0.56 |
| 2:H:166:LEU:HD12 | 2:H:167:SER:H | 1.70 | 0.56 |
| 2:H:22:THR:O | 2:H:22:THR:HG22 | 2.06 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:162:ASN:C | 2:H:164:GLY:H | 2.08 | 0.56 |
| 3:L:96:PHE:CD2 | 3:L:96:PHE:N | 2.74 | 0.56 |
| 2:H:27:GLY:O | 2:H:28:PHE:HB3 | 2.06 | 0.56 |
| 3:L:168:ASP:O | 3:L:170:THR:HG23 | 2.06 | 0.56 |
| 2:H:162:ASN:HA | 2:H:201:THR:CG2 | 2.28 | 0.55 |
| 2:H:162:ASN:HB2 | 2:H:165:SER:CB | 2.36 | 0.55 |
| 2:H:37:TRP:CD1 | 2:H:70:ILE:HD13 | 2.41 | 0.55 |
| 3:L:171:TYR:CD2 | 3:L:171:TYR:N | 2.73 | 0.55 |
| 2:H:146:GLY:HA3 | 2:H:186:SER:O | 2.06 | 0.55 |
| 1:A:247:ARG:O | 1:A:248:GLU:HB3 | 2.05 | 0.55 |
| 2:H:166:LEU:HD11 | 2:H:168:SER:OG | 2.07 | 0.55 |
| 3:L:138:TYR:CD1 | 3:L:139:PRO:HA | 2.42 | 0.55 |
| 2:H:99:THR:CG2 | 2:H:101:ILE:O | 2.55 | 0.55 |
| 1:A:192:VAL:HG23 | 1:A:193:SER:N | 2.21 | 0.55 |
| 2:H:176:VAL:O | 2:H:182:TYR:HA | 2.06 | 0.55 |
| 3:L:10:PHE:O | 3:L:103:GLU:HG3 | 2.06 | 0.55 |
| 2:H:28:PHE:CD1 | 2:H:29:SER:N | 2.75 | 0.55 |
| 2:H:158:THR:OG1 | 2:H:205:ALA:HB3 | 2.08 | 0.54 |
| 3:L:184:TYR:O | 3:L:190:TYR:OH | 2.24 | 0.54 |
| 3:L:65:GLY:HA3 | 3:L:70:TYR:HA | 1.90 | 0.54 |
| 2:H:10:PRO:O | 2:H:11:SER:HB2 | 2.07 | 0.54 |
| 1:A:132:ALA:C | 1:A:134:GLN:N | 2.55 | 0.54 |
| 2:H:150:LYS:HA | 2:H:183:THR:HG23 | 1.90 | 0.54 |
| 2:H:130:PRO:O | 2:H:131:LEU:HD23 | 2.09 | 0.53 |
| 2:H:120:SER:O | 2:H:121:ALA:CB | 2.54 | 0.53 |
| 1:A:101:ILE:N | 1:A:101:ILE:HD12 | 2.23 | 0.53 |
| 3:L:114:SER:O | 3:L:115:ILE:HB | 2.09 | 0.53 |
| 2:H:199:THR:HA | 2:H:216:LYS:NZ | 2.23 | 0.53 |
| 2:H:152:TYR:CE1 | 2:H:182:TYR:HB2 | 2.45 | 0.52 |
| 1:A:98:PRO:O | 1:A:183:ASN:HA | 2.08 | 0.52 |
| 3:L:110:ALA:HB2 | 3:L:198:THR:HG21 | 1.91 | 0.52 |
| 2:H:34:GLY:O | 2:H:99:THR:HB | 2.08 | 0.52 |
| 1:A:115:GLN:HG2 | 1:A:116:THR:H | 1.73 | 0.52 |
| 1:A:106:TYR:O | 1:A:110:MET:HG2 | 2.08 | 0.52 |
| 2:H:25:VAL:HG22 | 2:H:77:SER:HB3 | 1.90 | 0.52 |
| 2:H:130:PRO:HD3 | 3:L:121:GLU:OE1 | 2.09 | 0.52 |
| 3:L:104:ILE:CG2 | 3:L:105:LYS:N | 2.73 | 0.52 |
| 3:L:189:SER:HA | 3:L:207:PHE:O | 2.09 | 0.52 |
| 1:A:103:GLU:HG2 | 1:A:191:THR:HG1 | 1.74 | 0.52 |
| 3:L:134:LEU:HD21 | 3:L:194:ALA:HB2 | 1.92 | 0.52 |
| 2:H:67:ARG:NH1 | 2:H:90:ASP:OD2 | 2.43 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:131:LEU:HB2 | 2:H:146:GLY:O | 2.10 | 0.52 |
| 1:A:275:CYS:O | 1:A:276:LYS:HG3 | 2.10 | 0.52 |
| 3:L:207:PHE:N | 3:L:207:PHE:HD2 | 2.07 | 0.51 |
| 2:H:144:THR:HG22 | 2:H:189:THR:CG2 | 2.39 | 0.51 |
| 1:A:94:ILE:O | 1:A:95:SER:CB | 2.57 | 0.51 |
| 2:H:91:THR:HG23 | 2:H:116:VAL:O | 2.09 | 0.51 |
| 1:A:216:PHE:O | 1:A:258:THR:HG22 | 2.10 | 0.51 |
| 2:H:133:PRO:O | 2:H:220:ARG:HD2 | 2.11 | 0.51 |
| 2:H:144:THR:O | 2:H:145:LEU:HD23 | 2.11 | 0.51 |
| 1:A:207:MET:CE | 1:A:241:TRP:HE3 | 2.21 | 0.51 |
| 3:L:203:ILE:HD12 | 3:L:204:VAL:H | 1.76 | 0.51 |
| 2:H:103:THR:HG22 | 2:H:103:THR:O | 2.10 | 0.51 |
| 1:A:107:GLN:HB3 | 1:A:108:PRO:HD2 | 1.93 | 0.51 |
| 2:H:39:ARG:HG2 | 2:H:49:LEU:HD21 | 1.91 | 0.51 |
| 2:H:34:GLY:H | 2:H:99:THR:HG21 | 1.76 | 0.51 |
| 1:A:253:LEU:C | 1:A:255:GLN:N | 2.65 | 0.51 |
| 1:A:278:ILE:HG13 | 1:A:279:TYR:H | 1.75 | 0.51 |
| 2:H:52:ILE:HG12 | 2:H:72:LYS:HG2 | 1.92 | 0.51 |
| 2:H:72:LYS:HD2 | 2:H:74:ASN:OD1 | 2.10 | 0.51 |
| 1:A:165:THR:OG1 | 1:A:166:SER:N | 2.44 | 0.51 |
| 1:A:136:THR:O | 1:A:140:ARG:HB3 | 2.11 | 0.51 |
| 3:L:142:ILE:HG23 | 3:L:143:ASN:N | 2.26 | 0.50 |
| 1:A:239:GLU:HA | 1:A:274:SER:O | 2.12 | 0.50 |
| 1:A:107:GLN:OE1 | 1:A:107:GLN:HA | 2.12 | 0.50 |
| 1:A:145:LEU:HD21 | 1:A:192:VAL:CG2 | 2.42 | 0.50 |
| 2:H:175:ALA:HA | 2:H:184:LEU:HB3 | 1.93 | 0.50 |
| 3:L:207:PHE:CD2 | 3:L:207:PHE:N | 2.77 | 0.50 |
| 3:L:20:ILE:HG22 | 3:L:21:THR:N | 2.26 | 0.50 |
| 1:A:249:ASP:C | 1:A:250:SER:O | 2.46 | 0.50 |
| 1:A:274:SER:HB2 | 2:H:101:ILE:HB | 1.94 | 0.50 |
| 1:A:100:ASP:CG | 1:A:100:ASP:O | 2.51 | 0.49 |
| 1:A:202:ASP:HA | 1:A:236:GLN:HG2 | 1.93 | 0.49 |
| 3:L:114:SER:OG | 3:L:116:PHE:CE1 | 2.65 | 0.49 |
| 3:L:186:ARG:HG3 | 3:L:186:ARG:O | 2.11 | 0.49 |
| 1:A:207:MET:CE | 1:A:241:TRP:CE3 | 2.94 | 0.49 |
| 2:H:52:ILE:HD12 | 2:H:58:THR:CG2 | 2.42 | 0.49 |
| 3:L:159:ASN:HA | 3:L:174:SER:O | 2.12 | 0.49 |
| 1:A:209:ASP:HB3 | 1:A:212:ARG:HG3 | 1.95 | 0.49 |
| 3:L:171:TYR:N | 3:L:171:TYR:HD2 | 2.11 | 0.48 |
| 1:A:81:ASP:O | 1:A:84:SER:N | 2.46 | 0.48 |
| 2:H:190:VAL:HB | 2:H:191:PRO:CD | 2.43 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:44:LYS:NZ | 2:H:89:ASP:HB2 | 2.27 | 0.48 |
| 2:H:17:GLN:HA | 2:H:17:GLN:OE1 | 2.14 | 0.48 |
| 1:A:256:ASP:OD2 | 1:A:256:ASP:C | 2.51 | 0.48 |
| 1:A:279:TYR:CD2 | 1:A:279:TYR:N | 2.81 | 0.48 |
| 2:H:14:GLN:OE1 | 2:H:120:SER:HA | 2.13 | 0.48 |
| 2:H:61:ASN:O | 2:H:63:ALA:N | 2.47 | 0.48 |
| 1:A:222:PHE:O | 1:A:227:VAL:HG23 | 2.13 | 0.48 |
| 3:L:104:ILE:HB | 3:L:164:GLN:NE2 | 2.28 | 0.48 |
| 2:H:126:PRO:HB3 | 2:H:152:TYR:CD2 | 2.49 | 0.48 |
| 1:A:211:SER:O | 1:A:212:ARG:C | 2.52 | 0.48 |
| 1:A:81:ASP:HB3 | 1:A:84:SER:HB2 | 1.96 | 0.48 |
| 3:L:104:ILE:HB | 3:L:164:GLN:HE22 | 1.79 | 0.47 |
| 2:H:128:VAL:CG2 | 2:H:204:VAL:HG21 | 2.33 | 0.47 |
| 2:H:63:ALA:HB3 | 2:H:64:PHE:CD2 | 2.50 | 0.47 |
| 1:A:57:LYS:HD2 | 1:A:57:LYS:H | 1.79 | 0.47 |
| 1:A:70:TYR:O | 1:A:74:HIS:HB2 | 2.14 | 0.47 |
| 2:H:97:ALA:HB1 | 2:H:107:MET:HB2 | 1.96 | 0.47 |
| 3:L:53:LEU:O | 3:L:54:GLU:CB | 2.57 | 0.47 |
| 2:H:14:GLN:O | 2:H:17:GLN:HG2 | 2.14 | 0.47 |
| 1:A:278:ILE:CG1 | 1:A:279:TYR:N | 2.78 | 0.47 |
| 1:A:225:VAL:O | 1:A:229:ASN:ND2 | 2.40 | 0.47 |
| 1:A:255:GLN:O | 1:A:256:ASP:C | 2.52 | 0.47 |
| 2:H:91:THR:O | 2:H:92:ALA:HB2 | 2.14 | 0.47 |
| 1:A:97:HIS:CE1 | 1:A:99:CYS:HB2 | 2.50 | 0.47 |
| 2:H:13:VAL:HG11 | 2:H:86:LEU:CD1 | 2.45 | 0.47 |
| 1:A:114:THR:HA | 1:A:195:ARG:HH12 | 1.80 | 0.47 |
| 2:H:124:THR:HG22 | 2:H:125:PRO:O | 2.14 | 0.47 |
| 2:H:99:THR:HG22 | 2:H:99:THR:O | 2.14 | 0.46 |
| 1:A:57:LYS:N | 1:A:57:LYS:HD2 | 2.29 | 0.46 |
| 2:H:61:ASN:O | 2:H:62:ALA:C | 2.54 | 0.46 |
| 2:H:67:ARG:HB2 | 2:H:84:ASN:H | 1.80 | 0.46 |
| 1:A:94:ILE:O | 1:A:95:SER:HB2 | 2.15 | 0.46 |
| 2:H:146:GLY:CA | 2:H:186:SER:O | 2.63 | 0.46 |
| 2:H:162:ASN:HD22 | 2:H:165:SER:HB2 | 1.81 | 0.46 |
| 1:A:192:VAL:CG2 | 1:A:193:SER:N | 2.79 | 0.46 |
| 1:A:75:PRO:HD2 | 1:A:76:GLU:H | 1.81 | 0.46 |
| 1:A:113:GLY:O | 1:A:114:THR:C | 2.54 | 0.46 |
| 3:L:167:LYS:C | 3:L:169:SER:H | 2.19 | 0.46 |
| 3:L:199:SER:C | 3:L:201:SER:H | 2.18 | 0.46 |
| 2:H:216:LYS:HG2 | 2:H:217:ILE:N | 2.31 | 0.46 |
| 3:L:110:ALA:HB1 | 3:L:111:PRO:HD2 | 1.98 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:70:TYR:CD2 | 1:A:149:LEU:HD13 | 2.51 | 0.46 |
| 3:L:196:HIS:CG | 3:L:197:LYS:H | 2.34 | 0.46 |
| 3:L:23:LYS:HA | 3:L:68:LYS:O | 2.16 | 0.45 |
| 3:L:154:GLN:N | 3:L:154:GLN:OE1 | 2.49 | 0.45 |
| 2:H:72:LYS:NZ | 2:H:74:ASN:HD21 | 2.14 | 0.45 |
| 2:H:4:GLN:HB2 | 2:H:26:SER:OG | 2.17 | 0.45 |
| 1:A:117:VAL:HG12 | 1:A:143:PHE:CE2 | 2.51 | 0.45 |
| 3:L:89:GLN:O | 3:L:94:PRO:HA | 2.16 | 0.45 |
| 3:L:179:LEU:HD22 | 3:L:183:GLU:CG | 2.46 | 0.45 |
| 2:H:200:VAL:N | 2:H:216:LYS:HE3 | 2.28 | 0.45 |
| 1:A:57:LYS:O | 1:A:58:ARG:C | 2.55 | 0.45 |
| 1:A:75:PRO:C | 1:A:77:MET:H | 2.20 | 0.45 |
| 3:L:165:ASP:O | 3:L:169:SER:HA | 2.17 | 0.45 |
| 1:A:232:PRO:C | 1:A:234:LYS:H | 2.20 | 0.45 |
| 2:H:30:LEU:HB2 | 2:H:74:ASN:OD1 | 2.17 | 0.45 |
| 1:A:216:PHE:O | 1:A:258:THR:CG2 | 2.65 | 0.45 |
| 1:A:125:TRP:HZ3 | 1:A:146:GLU:OE1 | 2.00 | 0.45 |
| 1:A:100:ASP:C | 1:A:101:ILE:HD12 | 2.37 | 0.45 |
| 2:H:105:TYR:O | 2:H:107:MET:HG2 | 2.17 | 0.45 |
| 3:L:115:ILE:O | 3:L:115:ILE:CG1 | 2.65 | 0.44 |
| 3:L:168:ASP:N | 3:L:168:ASP:OD1 | 2.50 | 0.44 |
| 2:H:144:THR:CG2 | 2:H:189:THR:HG23 | 2.43 | 0.44 |
| 2:H:126:PRO:CA | 2:H:152:TYR:HB3 | 2.47 | 0.44 |
| 1:A:115:GLN:CG | 1:A:116:THR:H | 2.30 | 0.44 |
| 3:L:58:PRO:HG2 | 3:L:61:PHE:CD1 | 2.51 | 0.44 |
| 2:H:153:PHE:HA | 2:H:154:PRO:HA | 1.66 | 0.44 |
| 1:A:50:TRP:HB2 | 1:A:172:SER:OG | 2.16 | 0.44 |
| 2:H:39:ARG:HD3 | 2:H:94:TYR:CZ | 2.53 | 0.44 |
| 2:H:215:LYS:HE2 | 2:H:215:LYS:HB2 | 1.87 | 0.44 |
| 1:A:246:GLY:C | 1:A:247:ARG:O | 2.51 | 0.44 |
| 1:A:119:CYS:HB2 | 1:A:199:ALA:O | 2.18 | 0.44 |
| 1:A:73:ILE:H | 1:A:73:ILE:HG13 | 1.51 | 0.44 |
| 3:L:28:ILE:O | 3:L:29:TYR:C | 2.55 | 0.44 |
| 2:H:134:GLY:O | 2:H:135:SER:C | 2.57 | 0.44 |
| 2:H:199:THR:HA | 2:H:216:LYS:HE3 | 1.99 | 0.44 |
| 1:A:207:MET:SD | 1:A:243:ILE:HD11 | 2.58 | 0.44 |
| 3:L:18:VAL:HG12 | 3:L:19:THR:N | 2.33 | 0.44 |
| 2:H:145:LEU:HD13 | 2:H:217:ILE:CG2 | 2.46 | 0.44 |
| 2:H:155:GLU:OE2 | 2:H:156:PRO:HA | 2.18 | 0.44 |
| 1:A:69:LYS:O | 1:A:73:ILE:HG13 | 2.17 | 0.43 |
| 2:H:142:MET:SD | 2:H:191:PRO:HA | 2.59 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:149:LEU:O | 1:A:152:TYR:HB3 | 2.18 | 0.43 |
| 2:H:13:VAL:HG11 | 2:H:86:LEU:HD11 | 2.01 | 0.43 |
| 1:A:118:PRO:HB2 | 1:A:121:LYS:HB2 | 1.99 | 0.43 |
| 1:A:217:ASP:O | 1:A:220:SER:OG | 2.29 | 0.43 |
| 1:A:56:THR:O | 1:A:59:PHE:HB2 | 2.18 | 0.43 |
| 3:L:146:TRP:NE1 | 3:L:175:SER:HB3 | 2.33 | 0.43 |
| 3:L:14:LEU:CD1 | 3:L:79:THR:HG22 | 2.49 | 0.43 |
| 2:H:41:SER:OG | 2:H:44:LYS:HE3 | 2.18 | 0.43 |
| 2:H:151:GLY:C | 2:H:181:LEU:HD22 | 2.39 | 0.43 |
| 1:A:266:ILE:HG22 | 1:A:271:ILE:O | 2.18 | 0.43 |
| 2:H:89:ASP:C | 2:H:91:THR:N | 2.71 | 0.43 |
| 2:H:97:ALA:HB1 | 2:H:107:MET:CB | 2.49 | 0.43 |
| 1:A:248:GLU:HG2 | 1:A:249:ASP:H | 1.79 | 0.43 |
| 1:A:263:GLU:HG3 | 1:A:273:PHE:HD2 | 1.82 | 0.43 |
| 2:H:173:PHE:HE1 | 3:L:173:MET:CA | 2.32 | 0.43 |
| 1:A:63:VAL:HG12 | 1:A:63:VAL:O | 2.19 | 0.43 |
| 3:L:188:ASN:O | 3:L:208:ASN:HB3 | 2.19 | 0.43 |
| 3:L:17:ARG:HG2 | 3:L:74:ILE:O | 2.18 | 0.43 |
| 3:L:164:GLN:HB2 | 3:L:171:TYR:CZ | 2.53 | 0.42 |
| 3:L:37:GLN:C | 3:L:83:ALA:HB1 | 2.39 | 0.42 |
| 1:A:59:PHE:HB3 | 1:A:60:PRO:HD3 | 2.01 | 0.42 |
| 1:A:78:ARG:C | 1:A:80:VAL:H | 2.23 | 0.42 |
| 2:H:152:TYR:OH | 2:H:184:LEU:HD23 | 2.20 | 0.42 |
| 2:H:199:THR:HA | 2:H:216:LYS:CE | 2.50 | 0.42 |
| 2:H:7:GLN:HB2 | 2:H:112:GLN:HE21 | 1.83 | 0.42 |
| 3:L:80:GLU:H | 3:L:80:GLU:CD | 2.22 | 0.42 |
| 1:A:191:THR:HG22 | 1:A:192:VAL:N | 2.34 | 0.42 |
| 1:A:273:PHE:O | 2:H:102:THR:HB | 2.19 | 0.42 |
| 3:L:96:PHE:N | 3:L:96:PHE:HD2 | 2.18 | 0.42 |
| 1:A:156:ASP:C | 1:A:157:LEU:HD23 | 2.40 | 0.42 |
| 3:L:145:LYS:HE3 | 3:L:152:GLU:OE2 | 2.20 | 0.41 |
| 1:A:163:PHE:N | 1:A:163:PHE:HD2 | 2.16 | 0.41 |
| 3:L:21:THR:HB | 3:L:23:LYS:NZ | 2.36 | 0.41 |
| 2:H:37:TRP:HE1 | 2:H:79:VAL:HG11 | 1.85 | 0.41 |
| 2:H:11:SER:O | 2:H:116:VAL:HA | 2.20 | 0.41 |
| 2:H:68:LEU:HD12 | 2:H:69:SER:N | 2.31 | 0.41 |
| 3:L:54:GLU:HA | 3:L:54:GLU:OE1 | 2.21 | 0.41 |
| 1:A:216:PHE:H | 1:A:258:THR:HB | 1.85 | 0.41 |
| 3:L:22:CYS:C | 3:L:23:LYS:HG3 | 2.40 | 0.41 |
| 1:A:244:HIS:CD2 | 1:A:253:LEU:HD11 | 2.56 | 0.41 |
| 3:L:165:ASP:C | 3:L:167:LYS:H | 2.23 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:L:17:ARG:HD3 | 3:L:17:ARG:O | 2.21 | 0.41 |
| 3:L:92:SER:OG | 3:L:93:THR:N | 2.54 | 0.41 |
| 3:L:123:LEU:H | 3:L:123:LEU:HD12 | 1.85 | 0.41 |
| 2:H:191:PRO:HD2 | 2:H:194:THR:CG2 | 2.51 | 0.41 |
| 3:L:142:ILE:HG12 | 3:L:143:ASN:N | 2.32 | 0.41 |
| 2:H:33:TYR:HB3 | 2:H:99:THR:HG22 | 2.03 | 0.40 |
| 1:A:278:ILE:CG1 | 1:A:279:TYR:H | 2.34 | 0.40 |
| 3:L:21:THR:HB | 3:L:23:LYS:HZ1 | 1.86 | 0.40 |
| 1:A:75:PRO:C | 1:A:77:MET:N | 2.75 | 0.40 |
| 3:L:3:MET:HB2 | 3:L:96:PHE:C | 2.41 | 0.40 |
| 1:A:266:ILE:HD13 | 1:A:266:ILE:HA | 1.66 | 0.40 |
| 3:L:36:GLN:HG3 | 3:L:85:TYR:CZ | 2.56 | 0.40 |
| 2:H:143:VAL:CG1 | 2:H:190:VAL:HG23 | 2.44 | 0.40 |
| 2:H:52:ILE:HG23 | 2:H:52:ILE:O | 2.21 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 228/257 (89%) | 184 (81%) | 30 (13%) | 14 (6%) | 2 10 |
| 2 | H | 211/220 (96%) | 169 (80%) | 28 (13%) | 14 (7%) | 1 8 |
| 3 | L | 206/211 (98%) | 163 (79%) | 38 (18%) | 5 (2%) | 7 33 |
| All | All | 645/688 (94%) | 516 (80%) | 96 (15%) | 33 (5%) | 2 14 |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 166 | SER |
| 1 | A | 251 | ARG |
| 2 | H | 10 | PRO |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 11 | SER |
| 2 | H | 101 | ILE |
| 2 | H | 121 | ALA |
| 3 | L | 75 | THR |
| 3 | L | 115 | ILE |
| 1 | A | 248 | GLU |
| 2 | H | 62 | ALA |
| 2 | H | 164 | GLY |
| 3 | L | 53 | LEU |
| 3 | L | 54 | GLU |
| 1 | A | 78 | ARG |
| 1 | A | 82 | CYS |
| 2 | H | 90 | ASP |
| 2 | H | 122 | LYS |
| 1 | A | 114 | THR |
| 1 | A | 133 | HIS |
| 1 | A | 212 | ARG |
| 2 | H | 135 | SER |
| 2 | H | 167 | SER |
| 1 | A | 98 | PRO |
| 1 | A | 250 | SER |
| 1 | A | 108 | PRO |
| 1 | A | 180 | CYS |
| 2 | H | 163 | SER |
| 3 | L | 183 | GLU |
| 1 | A | 168 | ILE |
| 1 | A | 118 | PRO |
| 2 | H | 188 | VAL |
| 2 | H | 154 | PRO |
| 2 | H | 156 | PRO |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 208/238 (87%) | 182 (88%) | 26 (12%) | 6 23 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | H | 174/191 (91%) | 157 (90%) | 17 (10%) | 10 34 |
| 3 | L | 183/187 (98%) | 162 (88%) | 21 (12%) | 7 26 |
| All | All | 565/616 (92%) | 501 (89%) | 64 (11%) | 7 27 |

All (64) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 57 | LYS |
| 1 | A | 64 | LEU |
| 1 | A | 71 | THR |
| 1 | A | 89 | PHE |
| 1 | A | 101 | ILE |
| 1 | A | 116 | THR |
| 1 | A | 121 | LYS |
| 1 | A | 126 | SER |
| 1 | A | 136 | THR |
| 1 | A | 142 | MET |
| 1 | A | 144 | THR |
| 1 | A | 146 | GLU |
| 1 | A | 156 | ASP |
| 1 | A | 163 | PHE |
| 1 | A | 176 | TRP |
| 1 | A | 181 | SER |
| 1 | A | 191 | THR |
| 1 | A | 206 | VAL |
| 1 | A | 213 | SER |
| 1 | A | 248 | GLU |
| 1 | A | 250 | SER |
| 1 | A | 251 | ARG |
| 1 | A | 256 | ASP |
| 1 | A | 258 | THR |
| 1 | A | 264 | SER |
| 1 | A | 266 | ILE |
| 2 | H | 21 | ILE |
| 2 | H | 24 | THR |
| 2 | H | 28 | PHE |
| 2 | H | 64 | PHE |
| 2 | H | 68 | LEU |
| 2 | H | 70 | ILE |
| 2 | H | 99 | THR |
| 2 | H | 101 | ILE |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 107 | MET |
| 2 | H | 108 | ASP |
| 2 | H | 112 | GLN |
| 2 | H | 114 | THR |
| 2 | H | 116 | VAL |
| 2 | H | 117 | THR |
| 2 | H | 177 | LEU |
| 2 | H | 201 | THR |
| 2 | H | 203 | ASN |
| 3 | L | 12 | VAL |
| 3 | L | 21 | THR |
| 3 | L | 25 | SER |
| 3 | L | 32 | LEU |
| 3 | L | 41 | ASN |
| 3 | L | 51 | THR |
| 3 | L | 87 | CYS |
| 3 | L | 96 | PHE |
| 3 | L | 102 | LEU |
| 3 | L | 103 | GLU |
| 3 | L | 157 | VAL |
| 3 | L | 171 | TYR |
| 3 | L | 173 | MET |
| 3 | L | 180 | THR |
| 3 | L | 185 | GLU |
| 3 | L | 186 | ARG |
| 3 | L | 191 | THR |
| 3 | L | 192 | CYS |
| 3 | L | 196 | HIS |
| 3 | L | 207 | PHE |
| 3 | L | 208 | ASN |

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

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 230/257 (89%) | -0.09 | 2 (0%) | 85 | 64 | 47, 74, 112, 139 | 0 |
| 2 | H | 215/220 (97%) | -0.02 | 6 (2%) | 56 | 27 | 58, 102, 182, 204 | 0 |
| 3 | L | 208/211 (98%) | 0.06 | 4 (1%) | 70 | 41 | 70, 112, 150, 160 | 0 |
| All | All | 653/688 (94%) | -0.02 | 12 (1%) | 71 | 43 | 47, 94, 159, 204 | 0 |

All (12) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | H | 217 | ILE | 3.9 |
| 3 | L | 102 | LEU | 2.9 |
| 2 | H | 189 | THR | 2.9 |
| 3 | L | 109 | ALA | 2.8 |
| 2 | H | 132 | ALA | 2.7 |
| 2 | H | 199 | THR | 2.5 |
| 3 | L | 198 | THR | 2.4 |
| 1 | A | 164 | ASP | 2.2 |
| 3 | L | 47 | ILE | 2.2 |
| 2 | H | 145 | LEU | 2.1 |
| 1 | A | 163 | PHE | 2.0 |
| 2 | H | 169 | GLY | 2.0 |

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.