# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:11 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 3WCH |
| Title | : | The complex structure of HsSQS wtih ligand BPH1237 |
| Authors | : | Shang, N.; Li, Q.; Ko, T.P.; Chan, H.C.; Huang, C.H.; Ren, F.; Zheng, Y.; Zhu, Z.; Chen, C.C.; Guo, R.T. |
| Deposited on | : | 2013-05-27 |
| Resolution | : | 2.50 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:

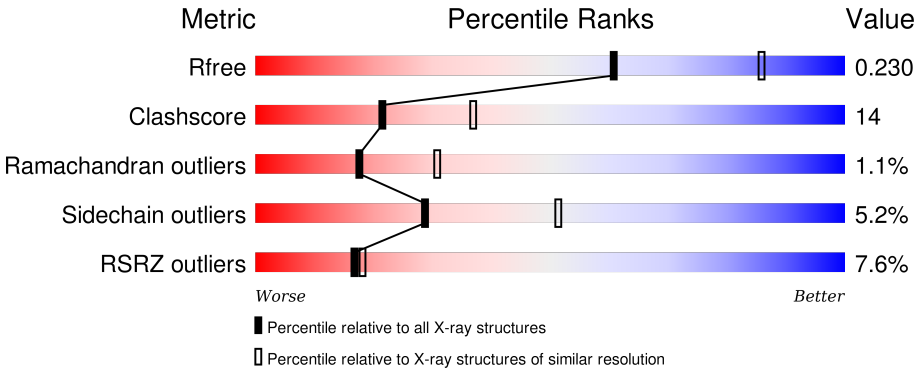
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| 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 2.50 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 | 3553 (2.50-2.50) |
| Clashscore | 102246 | 4242 (2.50-2.50) |
| Ramachandran outliers | 100387 | 4156 (2.50-2.50) |
| Sidechain outliers | 100360 | 4158 (2.50-2.50) |
| RSRZ outliers | 91569 | 3562 (2.50-2.50) |

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 | 360 | 5% 68% 23% • 7% |
| 1 | B | 360 | 8% 65% 26% • 7% |
| 1 | C | 360 | 4% 68% 23% • 7% |
| 1 | D | 360 | 9% 61% 28% • 7% |
| 1 | E | 360 | 7% 69% 21% • 7% |

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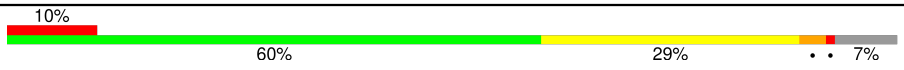
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 360 |   |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 2 | 8PH | A | 401 | - | - | - | X |
| 2 | 8PH | A | 402 | - | - | - | X |
| 2 | 8PH | C | 401 | - | - | - | X |
| 2 | 8PH | D | 401 | - | - | - | X |
| 2 | 8PH | E | 401 | - | - | - | X |

# 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16820 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 Squalene synthase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2696 | 1717 | 458 | 503 | 18 | | | |
| 1 | B | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2696 | 1717 | 458 | 503 | 18 | | | |
| 1 | C | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2696 | 1717 | 458 | 503 | 18 | | | |
| 1 | D | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2696 | 1717 | 458 | 503 | 18 | | | |
| 1 | E | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2696 | 1717 | 458 | 503 | 18 | | | |
| 1 | F | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2696 | 1717 | 458 | 503 | 18 | | | |

There are 144 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 11 | MET | - | EXPRESSION TAG | UNP P37268 |
| A | 12 | GLY | - | EXPRESSION TAG | UNP P37268 |
| A | 13 | SER | - | EXPRESSION TAG | UNP P37268 |
| A | 14 | SER | - | EXPRESSION TAG | UNP P37268 |
| A | 15 | HIS | - | EXPRESSION TAG | UNP P37268 |
| A | 16 | HIS | - | EXPRESSION TAG | UNP P37268 |
| A | 17 | HIS | - | EXPRESSION TAG | UNP P37268 |
| A | 18 | HIS | - | EXPRESSION TAG | UNP P37268 |
| A | 19 | HIS | - | EXPRESSION TAG | UNP P37268 |
| A | 20 | HIS | - | EXPRESSION TAG | UNP P37268 |
| A | 21 | SER | - | EXPRESSION TAG | UNP P37268 |
| A | 22 | SER | - | EXPRESSION TAG | UNP P37268 |
| A | 23 | GLY | - | EXPRESSION TAG | UNP P37268 |
| A | 24 | LEU | - | EXPRESSION TAG | UNP P37268 |
| A | 25 | VAL | - | EXPRESSION TAG | UNP P37268 |
| A | 26 | PRO | - | EXPRESSION TAG | UNP P37268 |
| A | 27 | ARG | - | EXPRESSION TAG | UNP P37268 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 28 | GLY | - | EXPRESSION TAG | UNP P37268 |
| A | 29 | SER | - | EXPRESSION TAG | UNP P37268 |
| A | 30 | HIS | - | EXPRESSION TAG | UNP P37268 |
| A | 248 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| A | 315 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| A | 318 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| A | 353 | ASN | ASP | SEE REMARK 999 | UNP P37268 |
| B | 11 | MET | - | EXPRESSION TAG | UNP P37268 |
| B | 12 | GLY | - | EXPRESSION TAG | UNP P37268 |
| B | 13 | SER | - | EXPRESSION TAG | UNP P37268 |
| B | 14 | SER | - | EXPRESSION TAG | UNP P37268 |
| B | 15 | HIS | - | EXPRESSION TAG | UNP P37268 |
| B | 16 | HIS | - | EXPRESSION TAG | UNP P37268 |
| B | 17 | HIS | - | EXPRESSION TAG | UNP P37268 |
| B | 18 | HIS | - | EXPRESSION TAG | UNP P37268 |
| B | 19 | HIS | - | EXPRESSION TAG | UNP P37268 |
| B | 20 | HIS | - | EXPRESSION TAG | UNP P37268 |
| B | 21 | SER | - | EXPRESSION TAG | UNP P37268 |
| B | 22 | SER | - | EXPRESSION TAG | UNP P37268 |
| B | 23 | GLY | - | EXPRESSION TAG | UNP P37268 |
| B | 24 | LEU | - | EXPRESSION TAG | UNP P37268 |
| B | 25 | VAL | - | EXPRESSION TAG | UNP P37268 |
| B | 26 | PRO | - | EXPRESSION TAG | UNP P37268 |
| B | 27 | ARG | - | EXPRESSION TAG | UNP P37268 |
| B | 28 | GLY | - | EXPRESSION TAG | UNP P37268 |
| B | 29 | SER | - | EXPRESSION TAG | UNP P37268 |
| B | 30 | HIS | - | EXPRESSION TAG | UNP P37268 |
| B | 248 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| B | 315 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| B | 318 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| B | 353 | ASN | ASP | SEE REMARK 999 | UNP P37268 |
| C | 11 | MET | - | EXPRESSION TAG | UNP P37268 |
| C | 12 | GLY | - | EXPRESSION TAG | UNP P37268 |
| C | 13 | SER | - | EXPRESSION TAG | UNP P37268 |
| C | 14 | SER | - | EXPRESSION TAG | UNP P37268 |
| C | 15 | HIS | - | EXPRESSION TAG | UNP P37268 |
| C | 16 | HIS | - | EXPRESSION TAG | UNP P37268 |
| C | 17 | HIS | - | EXPRESSION TAG | UNP P37268 |
| C | 18 | HIS | - | EXPRESSION TAG | UNP P37268 |
| C | 19 | HIS | - | EXPRESSION TAG | UNP P37268 |
| C | 20 | HIS | - | EXPRESSION TAG | UNP P37268 |
| C | 21 | SER | - | EXPRESSION TAG | UNP P37268 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | 22 | SER | - | EXPRESSION TAG | UNP P37268 |
| C | 23 | GLY | - | EXPRESSION TAG | UNP P37268 |
| C | 24 | LEU | - | EXPRESSION TAG | UNP P37268 |
| C | 25 | VAL | - | EXPRESSION TAG | UNP P37268 |
| C | 26 | PRO | - | EXPRESSION TAG | UNP P37268 |
| C | 27 | ARG | - | EXPRESSION TAG | UNP P37268 |
| C | 28 | GLY | - | EXPRESSION TAG | UNP P37268 |
| C | 29 | SER | - | EXPRESSION TAG | UNP P37268 |
| C | 30 | HIS | - | EXPRESSION TAG | UNP P37268 |
| C | 248 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| C | 315 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| C | 318 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| C | 353 | ASN | ASP | SEE REMARK 999 | UNP P37268 |
| D | 11 | MET | - | EXPRESSION TAG | UNP P37268 |
| D | 12 | GLY | - | EXPRESSION TAG | UNP P37268 |
| D | 13 | SER | - | EXPRESSION TAG | UNP P37268 |
| D | 14 | SER | - | EXPRESSION TAG | UNP P37268 |
| D | 15 | HIS | - | EXPRESSION TAG | UNP P37268 |
| D | 16 | HIS | - | EXPRESSION TAG | UNP P37268 |
| D | 17 | HIS | - | EXPRESSION TAG | UNP P37268 |
| D | 18 | HIS | - | EXPRESSION TAG | UNP P37268 |
| D | 19 | HIS | - | EXPRESSION TAG | UNP P37268 |
| D | 20 | HIS | - | EXPRESSION TAG | UNP P37268 |
| D | 21 | SER | - | EXPRESSION TAG | UNP P37268 |
| D | 22 | SER | - | EXPRESSION TAG | UNP P37268 |
| D | 23 | GLY | - | EXPRESSION TAG | UNP P37268 |
| D | 24 | LEU | - | EXPRESSION TAG | UNP P37268 |
| D | 25 | VAL | - | EXPRESSION TAG | UNP P37268 |
| D | 26 | PRO | - | EXPRESSION TAG | UNP P37268 |
| D | 27 | ARG | - | EXPRESSION TAG | UNP P37268 |
| D | 28 | GLY | - | EXPRESSION TAG | UNP P37268 |
| D | 29 | SER | - | EXPRESSION TAG | UNP P37268 |
| D | 30 | HIS | - | EXPRESSION TAG | UNP P37268 |
| D | 248 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| D | 315 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| D | 318 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| D | 353 | ASN | ASP | SEE REMARK 999 | UNP P37268 |
| E | 11 | MET | - | EXPRESSION TAG | UNP P37268 |
| E | 12 | GLY | - | EXPRESSION TAG | UNP P37268 |
| E | 13 | SER | - | EXPRESSION TAG | UNP P37268 |
| E | 14 | SER | - | EXPRESSION TAG | UNP P37268 |
| E | 15 | HIS | - | EXPRESSION TAG | UNP P37268 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 16 | HIS | - | EXPRESSION TAG | UNP P37268 |
| E | 17 | HIS | - | EXPRESSION TAG | UNP P37268 |
| E | 18 | HIS | - | EXPRESSION TAG | UNP P37268 |
| E | 19 | HIS | - | EXPRESSION TAG | UNP P37268 |
| E | 20 | HIS | - | EXPRESSION TAG | UNP P37268 |
| E | 21 | SER | - | EXPRESSION TAG | UNP P37268 |
| E | 22 | SER | - | EXPRESSION TAG | UNP P37268 |
| E | 23 | GLY | - | EXPRESSION TAG | UNP P37268 |
| E | 24 | LEU | - | EXPRESSION TAG | UNP P37268 |
| E | 25 | VAL | - | EXPRESSION TAG | UNP P37268 |
| E | 26 | PRO | - | EXPRESSION TAG | UNP P37268 |
| E | 27 | ARG | - | EXPRESSION TAG | UNP P37268 |
| E | 28 | GLY | - | EXPRESSION TAG | UNP P37268 |
| E | 29 | SER | - | EXPRESSION TAG | UNP P37268 |
| E | 30 | HIS | - | EXPRESSION TAG | UNP P37268 |
| E | 248 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| E | 315 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| E | 318 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| E | 353 | ASN | ASP | SEE REMARK 999 | UNP P37268 |
| F | 11 | MET | - | EXPRESSION TAG | UNP P37268 |
| F | 12 | GLY | - | EXPRESSION TAG | UNP P37268 |
| F | 13 | SER | - | EXPRESSION TAG | UNP P37268 |
| F | 14 | SER | - | EXPRESSION TAG | UNP P37268 |
| F | 15 | HIS | - | EXPRESSION TAG | UNP P37268 |
| F | 16 | HIS | - | EXPRESSION TAG | UNP P37268 |
| F | 17 | HIS | - | EXPRESSION TAG | UNP P37268 |
| F | 18 | HIS | - | EXPRESSION TAG | UNP P37268 |
| F | 19 | HIS | - | EXPRESSION TAG | UNP P37268 |
| F | 20 | HIS | - | EXPRESSION TAG | UNP P37268 |
| F | 21 | SER | - | EXPRESSION TAG | UNP P37268 |
| F | 22 | SER | - | EXPRESSION TAG | UNP P37268 |
| F | 23 | GLY | - | EXPRESSION TAG | UNP P37268 |
| F | 24 | LEU | - | EXPRESSION TAG | UNP P37268 |
| F | 25 | VAL | - | EXPRESSION TAG | UNP P37268 |
| F | 26 | PRO | - | EXPRESSION TAG | UNP P37268 |
| F | 27 | ARG | - | EXPRESSION TAG | UNP P37268 |
| F | 28 | GLY | - | EXPRESSION TAG | UNP P37268 |
| F | 29 | SER | - | EXPRESSION TAG | UNP P37268 |
| F | 30 | HIS | - | EXPRESSION TAG | UNP P37268 |
| F | 248 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| F | 315 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |
| F | 318 | LEU | LYS | ENGINEERED MUTATION | UNP P37268 |

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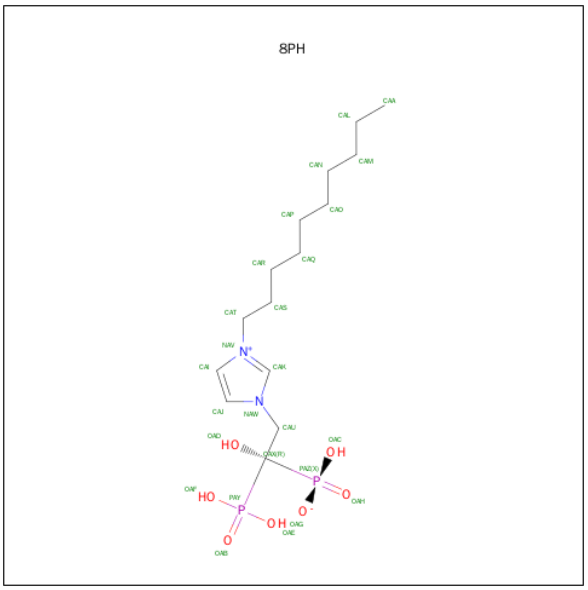
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| F | 353 | ASN | ASP | SEE REMARK 999 | UNP P37268 |

- Molecule 2 is HYDROGEN [(1R)-2-(3-DECYL-1H-IMIDAZOL-3-IUM-1-YL)-1-HYDROXY-1-PHOSPHONOETHYL]PHOSPHONATE (three-letter code: 8PH) (formula: $C_{15}H_{30}N_2O_7P_2$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | A | 1 | Total C N O P<br>26 15 2 7 2 | 0 | 0 |
| 2 | A | 1 | Total C<br>8 8 | 0 | 0 |
| 2 | A | 1 | Total C N O P<br>18 7 2 7 2 | 0 | 0 |
| 2 | B | 1 | Total C N O P<br>26 15 2 7 2 | 0 | 0 |
| 2 | B | 1 | Total C<br>9 9 | 0 | 0 |
| 2 | C | 1 | Total C N O P<br>26 15 2 7 2 | 0 | 0 |
| 2 | D | 1 | Total C N O P<br>26 15 2 7 2 | 0 | 0 |
| 2 | E | 1 | Total C N O P<br>26 15 2 7 2 | 0 | 0 |
| 2 | F | 1 | Total C N O P<br>26 15 2 7 2 | 0 | 0 |
| 2 | F | 1 | Total C N O P<br>26 15 2 7 2 | 0 | 0 |

- Molecule 3 is water.

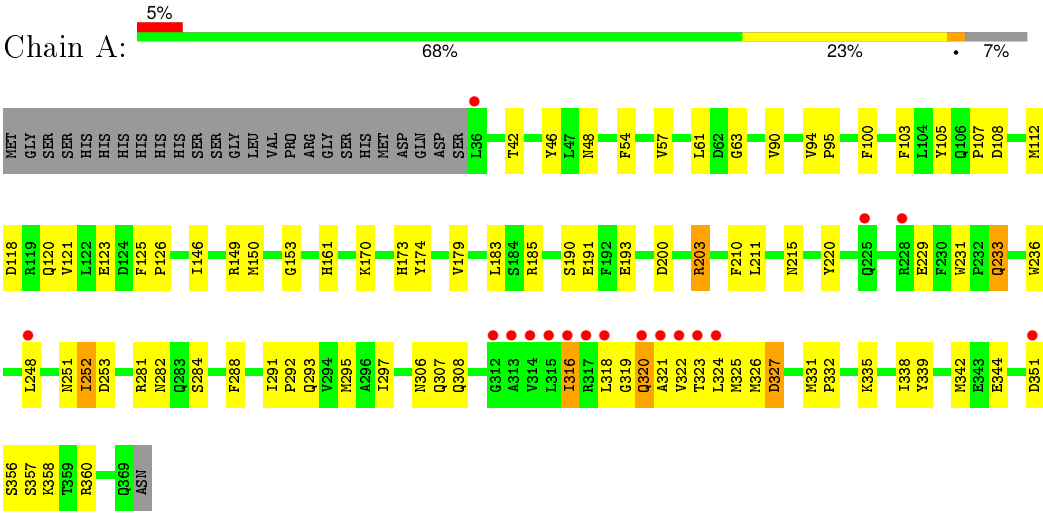
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 99 | Total O<br>99 99 | 0 | 0 |
| 3 | B | 89 | Total O<br>89 89 | 0 | 0 |
| 3 | C | 86 | Total O<br>86 86 | 0 | 0 |
| 3 | D | 62 | Total O<br>62 62 | 0 | 0 |
| 3 | E | 50 | Total O<br>50 50 | 0 | 0 |
| 3 | F | 41 | Total O<br>41 41 | 0 | 0 |

# 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.

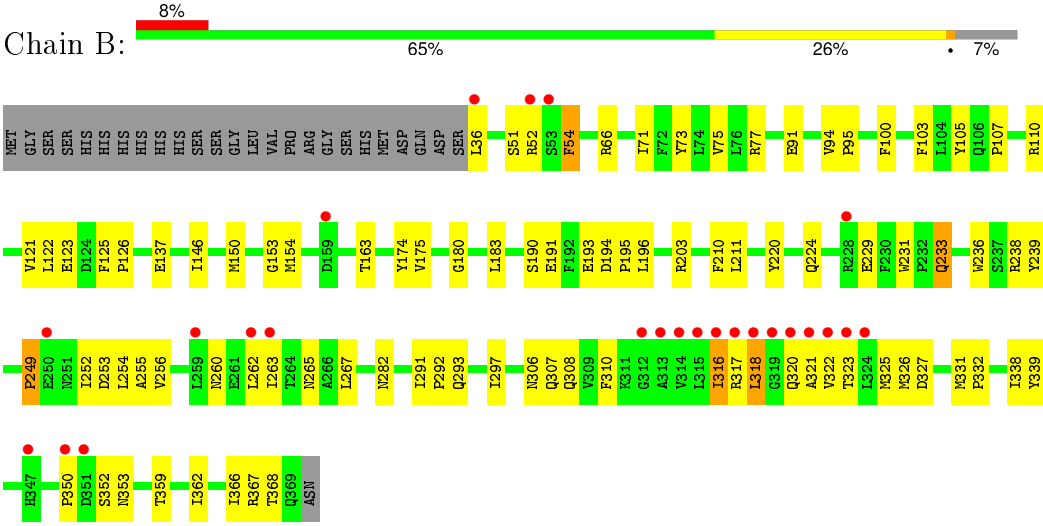
- Molecule 1: Squalene synthase

Chain A:



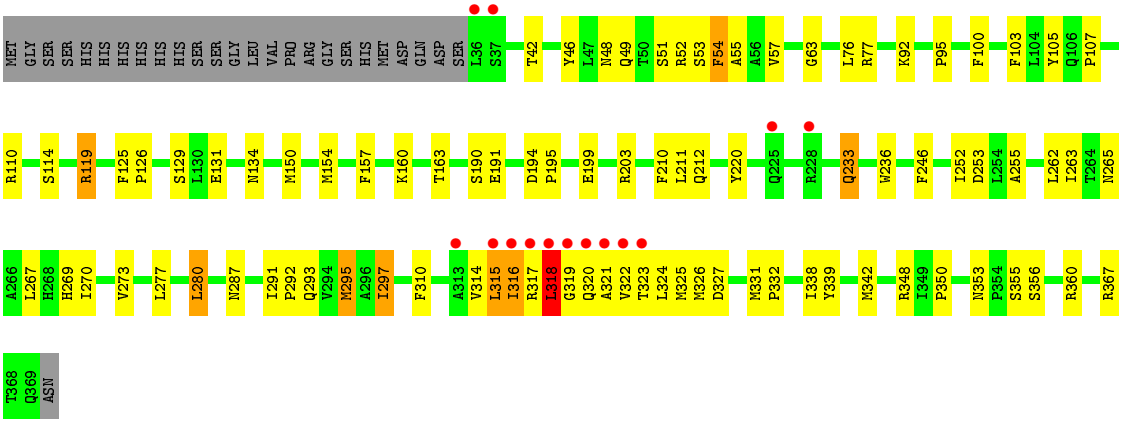

- Molecule 1: Squalene synthase

Chain B:



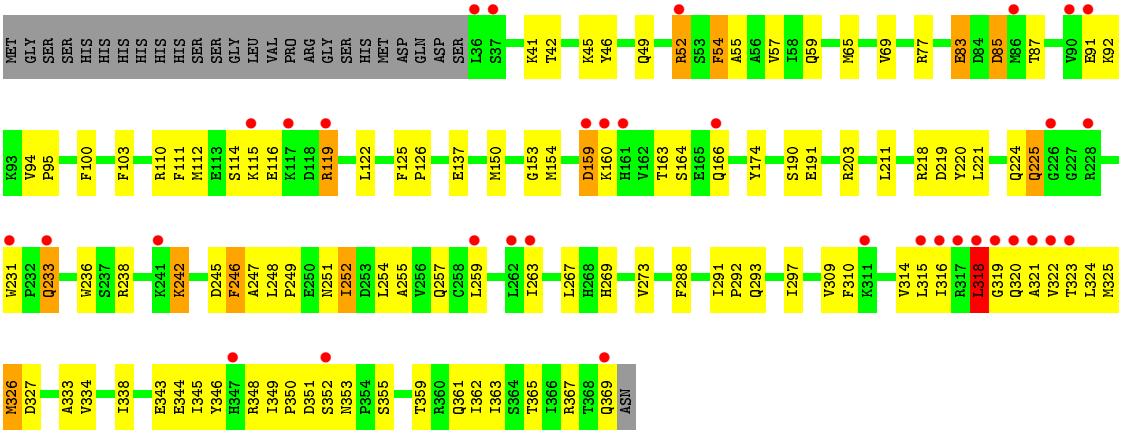

- Molecule 1: Squalene synthase

Chain C:



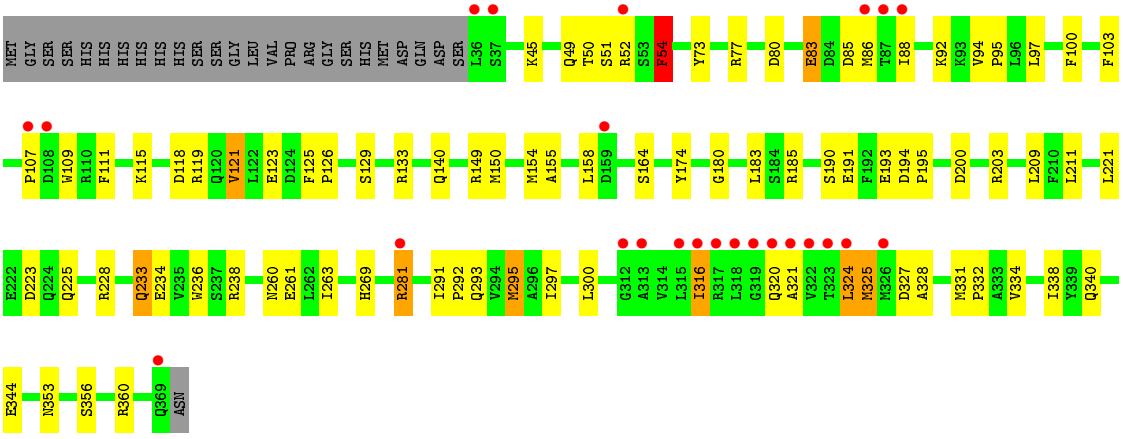
• Molecule 1: Squalene synthase

Chain D:

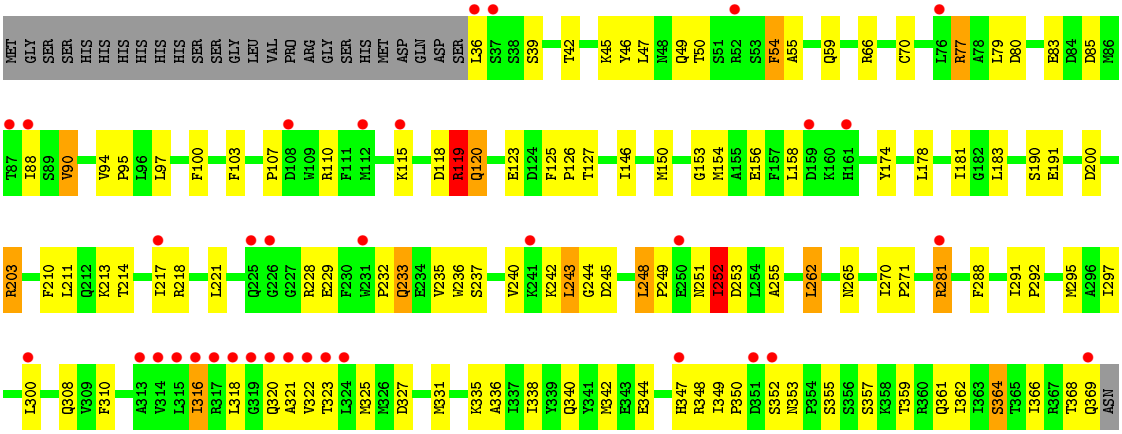
• Molecule 1: Squalene synthase

Chain E:

• Molecule 1: Squalene synthase

Chain F:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ASP GLN ASP SER L36 S37 S38 S39 T42 K45 Y46 L47 W48 Q49 T50 S51 R52 S53 F54 A55 Q59 R66 C70 L76 R77 A78 L79 D80 E83 D84 D85 M86
T87 I88 S89 V90 V94 P95 L96 L97 F100 F103 P107 D108 W109 R110 F111 M112 K115 D118 R119 Q120 E123 D124 F125 P126 T127 I146 M150 G153 M154 A155 E156 F157 L158 D159 K160 H161 Y174 L178 I181 G182 L183 S190 E191 D200
R203 F210 L211 Q212 K213 T214 I217 R218 L221 Q225 G226 G227 R228 E229 F230 W231 P232 Q233 E234 V235 W236 S237 V240 K241 K242 L243 G244 D245 L248 P249 E250 N251 I252 D253 L254 A255 L262 N265 I270 P271 R281 F288 I291 P292 M295 A296 I297
L300 Q308 V309 F310 A313 V314 L315 I316 R317 L318 G319 Q320 A321 V322 T323 L324 M325 M326 D327 M331 K335 A336 I337 I338 Y339 Q340 Y341 M342 E343 E344 H347 R348 I349 P350 D351 S352 N353 P354 S355 S356 S357 K358 T359 R360 Q361 I362 I363 S364 T365 I366 R367 T368 Q369 ASN

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 85.63Å 153.55Å 90.40Å<br>90.00° 91.18° 90.00° | Depositor |
| Resolution (Å) | 25.00 – 2.50<br>24.92 – 2.49 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | (Not available) (25.00-2.50)<br>96.7 (24.92-2.49) | Depositor<br>EDS |
| $R_{merge}$ | 0.09 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 4.60 (at 2.50Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, $R_{free}$ | 0.192 , 0.250<br>0.202 , 0.230 | Depositor<br>DCC |
| $R_{free}$ test set | 3966 reflections (5.07%) | DCC |
| Wilson B-factor (Å$^2$) | 36.6 | Xtriage |
| Anisotropy | 0.498 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.33 , 49.8 | EDS |
| Estimated twinning fraction | 0.032 for h,-k,-l | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Outliers | 1 of 78898 reflections (0.001%) | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 16820 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 47.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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

Bond lengths and bond angles in the following residue types are not validated in this section: 8PH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.38 | 0/2751 | 0.59 | 0/3724 |
| 1 | B | 0.35 | 0/2751 | 0.58 | 1/3724 (0.0%) |
| 1 | C | 0.36 | 0/2751 | 0.60 | 0/3724 |
| 1 | D | 0.34 | 0/2751 | 0.57 | 1/3724 (0.0%) |
| 1 | E | 0.35 | 0/2751 | 0.58 | 0/3724 |
| 1 | F | 0.33 | 0/2751 | 0.57 | 0/3724 |
| All | All | 0.35 | 0/16506 | 0.58 | 2/22344 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 54 | PHE | N-CA-C | 5.06 | 124.67 | 111.00 |
| 1 | B | 54 | PHE | N-CA-C | 5.04 | 124.62 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2696 | 0 | 2676 | 68 | 0 |
| 1 | B | 2696 | 0 | 2676 | 85 | 0 |
| 1 | C | 2696 | 0 | 2676 | 80 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | D | 2696 | 0 | 2676 | 87 | 0 |
| 1 | E | 2696 | 0 | 2676 | 66 | 0 |
| 1 | F | 2696 | 0 | 2676 | 93 | 0 |
| 2 | A | 52 | 0 | 56 | 3 | 0 |
| 2 | B | 35 | 0 | 47 | 7 | 0 |
| 2 | C | 26 | 0 | 30 | 4 | 0 |
| 2 | D | 26 | 0 | 30 | 2 | 0 |
| 2 | E | 26 | 0 | 30 | 4 | 0 |
| 2 | F | 52 | 0 | 60 | 5 | 0 |
| 3 | A | 99 | 0 | 0 | 5 | 0 |
| 3 | B | 89 | 0 | 0 | 2 | 0 |
| 3 | C | 86 | 0 | 0 | 2 | 0 |
| 3 | D | 62 | 0 | 0 | 3 | 0 |
| 3 | E | 50 | 0 | 0 | 3 | 0 |
| 3 | F | 41 | 0 | 0 | 3 | 0 |
| All | All | 16820 | 0 | 16309 | 460 | 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 14.

All (460) 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:E:164:SER:HA | 1:E:234:GLU:HG3 | 1.22 | 1.08 |
| 1:E:316:ILE:H | 1:E:316:ILE:HD12 | 1.19 | 1.03 |
| 1:D:320:GLN:HG2 | 1:D:321:ALA:H | 1.28 | 0.98 |
| 1:B:316:ILE:H | 1:B:316:ILE:HD12 | 1.29 | 0.96 |
| 1:A:316:ILE:H | 1:A:316:ILE:HD12 | 1.29 | 0.94 |
| 1:B:233:GLN:HA | 1:B:236:TRP:NE1 | 1.82 | 0.94 |
| 1:F:320:GLN:HG2 | 1:F:321:ALA:H | 1.33 | 0.93 |
| 1:A:183:LEU:HD21 | 2:A:402:8PH:H30 | 1.48 | 0.92 |
| 1:B:320:GLN:HG2 | 1:B:321:ALA:H | 1.34 | 0.92 |
| 1:F:235:VAL:HG11 | 1:F:262:LEU:HD21 | 1.51 | 0.91 |
| 1:A:320:GLN:HG2 | 1:A:321:ALA:H | 1.34 | 0.90 |
| 1:F:249:PRO:HA | 1:F:252:ILE:HD13 | 1.55 | 0.88 |
| 1:F:316:ILE:HD12 | 1:F:316:ILE:H | 1.36 | 0.87 |
| 1:E:321:ALA:HA | 1:E:324:LEU:HB2 | 1.54 | 0.87 |
| 1:E:320:GLN:HG2 | 1:E:321:ALA:H | 1.40 | 0.86 |
| 1:E:325:MET:O | 1:F:327:ASP:HB2 | 1.74 | 0.86 |
| 1:B:322:VAL:HG21 | 1:C:53:SER:HB2 | 1.56 | 0.86 |
| 1:A:327:ASP:HB2 | 1:C:325:MET:O | 1.76 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:249:PRO:HA | 1:D:252:ILE:HD13 | 1.59 | 0.85 |
| 1:E:316:ILE:H | 1:E:316:ILE:CD1 | 1.88 | 0.84 |
| 1:C:211:LEU:HD23 | 2:C:401:8PH:H19 | 1.60 | 0.83 |
| 1:B:316:ILE:N | 1:B:316:ILE:HD12 | 1.96 | 0.81 |
| 1:A:320:GLN:HG2 | 1:A:321:ALA:N | 1.95 | 0.80 |
| 1:E:260:ASN:HD22 | 1:E:353:ASN:ND2 | 1.80 | 0.79 |
| 1:B:211:LEU:HD22 | 2:B:401:8PH:H20 | 1.63 | 0.78 |
| 1:F:320:GLN:O | 1:F:323:THR:HG22 | 1.84 | 0.77 |
| 1:C:320:GLN:HG2 | 1:C:321:ALA:H | 1.50 | 0.77 |
| 1:F:150:MET:HG3 | 1:F:174:TYR:O | 1.83 | 0.77 |
| 1:D:116:GLU:O | 1:D:119:ARG:HD3 | 1.86 | 0.76 |
| 1:B:118:ASP:O | 1:B:121:VAL:HG22 | 1.85 | 0.76 |
| 1:B:320:GLN:HG2 | 1:B:321:ALA:N | 2.00 | 0.76 |
| 1:B:320:GLN:O | 1:B:323:THR:HG22 | 1.86 | 0.75 |
| 1:B:325:MET:HG3 | 1:C:291:ILE:HG23 | 1.69 | 0.75 |
| 1:D:211:LEU:HD23 | 2:D:401:8PH:H18 | 1.68 | 0.74 |
| 1:B:325:MET:O | 1:C:327:ASP:HB2 | 1.88 | 0.74 |
| 1:D:321:ALA:HA | 1:D:324:LEU:HG | 1.71 | 0.73 |
| 1:A:325:MET:O | 1:B:327:ASP:HB2 | 1.89 | 0.73 |
| 1:D:353:ASN:ND2 | 1:D:355:SER:H | 1.86 | 0.73 |
| 1:C:316:ILE:HD12 | 1:C:316:ILE:H | 1.54 | 0.73 |
| 1:E:164:SER:CA | 1:E:234:GLU:HG3 | 2.10 | 0.72 |
| 1:C:321:ALA:O | 1:C:325:MET:HG2 | 1.88 | 0.72 |
| 1:E:320:GLN:HG2 | 1:E:321:ALA:N | 2.05 | 0.72 |
| 1:A:211:LEU:HD13 | 1:A:293:GLN:NE2 | 2.04 | 0.71 |
| 1:E:115:LYS:HA | 1:E:115:LYS:HE2 | 1.72 | 0.71 |
| 1:A:320:GLN:CG | 1:A:321:ALA:H | 2.02 | 0.71 |
| 1:D:320:GLN:HG2 | 1:D:321:ALA:N | 2.04 | 0.71 |
| 1:D:319:GLY:HA3 | 1:D:323:THR:HG21 | 1.72 | 0.71 |
| 1:F:320:GLN:HG2 | 1:F:321:ALA:N | 2.06 | 0.70 |
| 1:C:210:PHE:CE2 | 1:C:297:ILE:HD13 | 2.26 | 0.70 |
| 1:E:228:ARG:HG3 | 1:E:228:ARG:HH11 | 1.56 | 0.70 |
| 1:C:320:GLN:O | 1:C:324:LEU:HG | 1.91 | 0.70 |
| 1:D:150:MET:O | 1:D:154:MET:HG3 | 1.92 | 0.70 |
| 1:A:353:ASN:HD22 | 1:A:355:SER:H | 1.37 | 0.70 |
| 2:E:401:8PH:H6 | 3:E:522:HOH:O | 1.92 | 0.70 |
| 1:A:353:ASN:ND2 | 1:A:355:SER:H | 1.89 | 0.69 |
| 1:B:316:ILE:CD1 | 1:B:316:ILE:H | 2.00 | 0.69 |
| 1:E:297:ILE:HD13 | 1:E:338:ILE:HG12 | 1.73 | 0.68 |
| 1:B:183:LEU:HD12 | 2:B:401:8PH:H26 | 1.75 | 0.68 |
| 1:B:343:GLU:OE1 | 1:C:48:ASN:HB3 | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:586:HOH:O | 1:C:325:MET:HE1 | 1.93 | 0.68 |
| 1:B:260:ASN:HD22 | 1:B:353:ASN:ND2 | 1.92 | 0.67 |
| 1:F:297:ILE:HD12 | 1:F:338:ILE:HG12 | 1.75 | 0.67 |
| 1:E:150:MET:O | 1:E:154:MET:HG3 | 1.95 | 0.67 |
| 1:D:325:MET:O | 1:E:327:ASP:HB2 | 1.95 | 0.66 |
| 1:F:255:ALA:HB1 | 1:F:310:PHE:CE2 | 2.30 | 0.66 |
| 1:F:100:PHE:HA | 1:F:103:PHE:CD2 | 2.30 | 0.66 |
| 1:A:306:ASN:OD1 | 1:A:308:GLN:HB3 | 1.96 | 0.66 |
| 1:F:233:GLN:HA | 1:F:236:TRP:NE1 | 2.11 | 0.66 |
| 1:F:350:PRO:HG2 | 1:F:353:ASN:HB2 | 1.77 | 0.66 |
| 1:F:94:VAL:HB | 1:F:95:PRO:HD3 | 1.79 | 0.66 |
| 1:F:235:VAL:HG11 | 1:F:262:LEU:CD2 | 2.24 | 0.65 |
| 1:A:190:SER:O | 1:A:191:GLU:HB2 | 1.95 | 0.65 |
| 1:C:316:ILE:HD12 | 1:C:316:ILE:N | 2.12 | 0.65 |
| 1:B:73:TYR:HD2 | 2:B:402:8PH:H28 | 1.60 | 0.64 |
| 1:E:297:ILE:CD1 | 1:E:338:ILE:HG12 | 2.27 | 0.64 |
| 3:D:518:HOH:O | 1:F:325:MET:HE1 | 1.97 | 0.64 |
| 1:F:353:ASN:ND2 | 1:F:355:SER:H | 1.95 | 0.64 |
| 1:E:51:SER:OG | 1:E:54:PHE:HB2 | 1.97 | 0.64 |
| 1:B:233:GLN:HA | 1:B:236:TRP:CD1 | 2.32 | 0.63 |
| 1:D:87:THR:HG22 | 1:D:87:THR:O | 1.97 | 0.63 |
| 1:F:150:MET:O | 1:F:154:MET:HG3 | 1.99 | 0.63 |
| 1:A:316:ILE:N | 1:A:316:ILE:HD12 | 2.09 | 0.62 |
| 1:B:297:ILE:HD12 | 1:B:338:ILE:HG12 | 1.81 | 0.62 |
| 1:D:320:GLN:O | 1:D:323:THR:HG22 | 2.00 | 0.62 |
| 1:C:320:GLN:HG2 | 1:C:321:ALA:N | 2.15 | 0.62 |
| 1:E:83:GLU:HG3 | 1:E:154:MET:HB3 | 1.82 | 0.62 |
| 1:F:54:PHE:CD2 | 2:F:402:8PH:H17 | 2.34 | 0.62 |
| 1:D:233:GLN:HA | 1:D:236:TRP:NE1 | 2.15 | 0.62 |
| 1:D:85:ASP:OD2 | 1:D:87:THR:HB | 2.00 | 0.61 |
| 1:C:131:GLU:HA | 1:C:134:ASN:ND2 | 2.14 | 0.61 |
| 1:C:317:ARG:HD2 | 1:C:318:LEU:HD12 | 1.82 | 0.61 |
| 1:D:263:ILE:O | 1:D:267:LEU:HG | 2.01 | 0.61 |
| 1:D:211:LEU:HD13 | 1:D:293:GLN:NE2 | 2.15 | 0.61 |
| 1:B:331:MET:HB3 | 1:B:332:PRO:HD3 | 1.82 | 0.61 |
| 1:D:52:ARG:HG3 | 3:D:559:HOH:O | 2.00 | 0.61 |
| 1:A:200:ASP:OD2 | 1:A:203:ARG:HB2 | 2.00 | 0.60 |
| 1:B:368:THR:HG22 | 1:B:368:THR:O | 2.01 | 0.60 |
| 1:C:211:LEU:CD2 | 2:C:401:8PH:H19 | 2.29 | 0.60 |
| 1:B:350:PRO:HG2 | 1:B:353:ASN:HB2 | 1.84 | 0.60 |
| 1:E:50:THR:HG1 | 1:E:73:TYR:HE1 | 1.50 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:119:ARG:O | 1:E:123:GLU:HG3 | 2.02 | 0.60 |
| 1:F:200:ASP:OD2 | 1:F:203:ARG:HB2 | 2.02 | 0.60 |
| 1:D:365:THR:O | 1:D:369:GLN:HG3 | 2.02 | 0.60 |
| 1:A:293:GLN:O | 1:A:297:ILE:HG12 | 2.02 | 0.59 |
| 1:E:260:ASN:HD22 | 1:E:353:ASN:HD21 | 1.46 | 0.59 |
| 1:F:245:ASP:O | 1:F:248:LEU:HG | 2.02 | 0.59 |
| 1:C:211:LEU:HD13 | 1:C:293:GLN:NE2 | 2.16 | 0.59 |
| 1:E:94:VAL:HB | 1:E:95:PRO:HD3 | 1.84 | 0.59 |
| 1:A:211:LEU:HD13 | 1:A:293:GLN:HE22 | 1.67 | 0.59 |
| 1:D:159:ASP:OD1 | 1:D:160:LYS:N | 2.37 | 0.58 |
| 1:A:233:GLN:HA | 1:A:236:TRP:NE1 | 2.18 | 0.58 |
| 1:D:163:THR:OG1 | 1:D:164:SER:N | 2.36 | 0.58 |
| 1:C:353:ASN:ND2 | 1:C:355:SER:H | 2.01 | 0.58 |
| 1:A:319:GLY:O | 1:A:320:GLN:O | 2.20 | 0.58 |
| 1:F:119:ARG:O | 1:F:123:GLU:HG3 | 2.02 | 0.58 |
| 1:C:212:GLN:OE1 | 2:C:401:8PH:H12 | 2.04 | 0.58 |
| 1:C:100:PHE:HA | 1:C:103:PHE:CD2 | 2.38 | 0.58 |
| 1:F:183:LEU:CD1 | 2:F:401:8PH:H26 | 2.33 | 0.58 |
| 1:D:291:ILE:HB | 1:D:292:PRO:HD3 | 1.85 | 0.58 |
| 1:D:322:VAL:HG12 | 1:D:322:VAL:O | 2.04 | 0.58 |
| 1:E:180:GLY:HA2 | 2:E:401:8PH:H27 | 1.86 | 0.57 |
| 1:B:343:GLU:OE1 | 1:B:367:ARG:NH2 | 2.37 | 0.57 |
| 1:D:94:VAL:HB | 1:D:95:PRO:HD3 | 1.86 | 0.57 |
| 1:A:220:TYR:HB2 | 1:A:231:TRP:CZ2 | 2.38 | 0.57 |
| 1:C:348:ARG:O | 1:C:350:PRO:HD3 | 2.05 | 0.57 |
| 1:A:215:ASN:HD21 | 2:A:403:8PH:CAS | 2.16 | 0.57 |
| 1:D:242:LYS:HB2 | 1:D:242:LYS:NZ | 2.19 | 0.57 |
| 1:F:297:ILE:CD1 | 1:F:338:ILE:HG12 | 2.34 | 0.57 |
| 1:D:255:ALA:HB1 | 1:D:310:PHE:CE1 | 2.38 | 0.57 |
| 1:B:66:ARG:HD2 | 3:B:565:HOH:O | 2.03 | 0.57 |
| 1:B:342:MET:CE | 1:B:342:MET:HA | 2.35 | 0.57 |
| 1:D:211:LEU:HD13 | 1:D:293:GLN:HE22 | 1.70 | 0.57 |
| 1:F:79:LEU:O | 1:F:79:LEU:HD12 | 2.05 | 0.56 |
| 1:A:291:ILE:HB | 1:A:292:PRO:HD3 | 1.87 | 0.56 |
| 1:D:346:TYR:HA | 1:D:349:ILE:CD1 | 2.35 | 0.56 |
| 1:A:291:ILE:HD11 | 1:C:326:MET:CE | 2.35 | 0.56 |
| 1:E:238:ARG:HH22 | 1:E:261:GLU:CD | 2.07 | 0.56 |
| 1:B:112:MET:SD | 1:B:123:GLU:HG2 | 2.45 | 0.56 |
| 1:B:326:MET:HE3 | 1:C:291:ILE:HD11 | 1.88 | 0.56 |
| 1:B:190:SER:O | 1:B:191:GLU:HB2 | 2.05 | 0.56 |
| 1:B:320:GLN:CG | 1:B:321:ALA:H | 2.15 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:120:GLN:HE21 | 1:F:120:GLN:HA | 1.70 | 0.56 |
| 1:E:325:MET:C | 1:F:327:ASP:HB2 | 2.26 | 0.56 |
| 1:E:97:LEU:HD12 | 1:E:158:LEU:HD11 | 1.88 | 0.56 |
| 1:E:316:ILE:HD12 | 1:E:316:ILE:N | 2.04 | 0.55 |
| 1:D:220:TYR:HB2 | 1:D:231:TRP:CZ2 | 2.42 | 0.55 |
| 1:A:331:MET:HB3 | 1:A:332:PRO:HD3 | 1.87 | 0.55 |
| 1:E:263:ILE:HG12 | 1:E:300:LEU:HD22 | 1.87 | 0.55 |
| 1:F:291:ILE:HB | 1:F:292:PRO:HD3 | 1.87 | 0.55 |
| 1:A:61:LEU:HA | 1:A:284:SER:HB2 | 1.88 | 0.55 |
| 1:B:94:VAL:HB | 1:B:95:PRO:HD3 | 1.87 | 0.55 |
| 1:C:211:LEU:HD13 | 1:C:293:GLN:HE22 | 1.72 | 0.55 |
| 1:C:277:LEU:HA | 1:C:280:LEU:HD22 | 1.87 | 0.55 |
| 1:C:338:ILE:O | 1:C:342:MET:HG2 | 2.07 | 0.55 |
| 1:B:211:LEU:CD1 | 1:B:293:GLN:NE2 | 2.70 | 0.55 |
| 1:A:291:ILE:HD11 | 1:C:326:MET:HE1 | 1.88 | 0.55 |
| 1:A:316:ILE:H | 1:A:316:ILE:CD1 | 2.09 | 0.55 |
| 1:E:77:ARG:HD3 | 1:E:77:ARG:O | 2.07 | 0.55 |
| 1:F:255:ALA:HB1 | 1:F:310:PHE:CZ | 2.41 | 0.54 |
| 1:A:210:PHE:CZ | 1:A:297:ILE:HD13 | 2.43 | 0.54 |
| 1:A:112:MET:SD | 1:A:123:GLU:HG2 | 2.47 | 0.54 |
| 1:B:362:ILE:O | 1:B:366:ILE:HG13 | 2.07 | 0.54 |
| 1:A:94:VAL:HB | 1:A:95:PRO:HD3 | 1.89 | 0.54 |
| 1:E:320:GLN:CG | 1:E:321:ALA:H | 2.18 | 0.54 |
| 1:F:233:GLN:HA | 1:F:236:TRP:CD1 | 2.43 | 0.54 |
| 1:B:297:ILE:HD13 | 1:B:338:ILE:HG23 | 1.88 | 0.54 |
| 1:E:209:LEU:HD23 | 1:E:269:HIS:CE1 | 2.43 | 0.54 |
| 1:C:321:ALA:HA | 1:C:324:LEU:HG | 1.90 | 0.54 |
| 1:B:338:ILE:O | 1:B:342:MET:HG2 | 2.08 | 0.54 |
| 1:B:36:LEU:HB2 | 1:D:137:GLU:OE1 | 2.08 | 0.54 |
| 1:E:85:ASP:HB3 | 1:E:88:ILE:HD12 | 1.89 | 0.54 |
| 1:C:263:ILE:O | 1:C:267:LEU:HG | 2.08 | 0.54 |
| 1:A:48:ASN:ND2 | 1:C:367:ARG:HD3 | 2.24 | 0.53 |
| 1:F:320:GLN:CG | 1:F:321:ALA:H | 2.14 | 0.53 |
| 1:F:281:ARG:HH21 | 1:F:281:ARG:CG | 2.21 | 0.53 |
| 1:B:229:GLU:HG2 | 1:B:243:LEU:HD23 | 1.91 | 0.53 |
| 1:A:108:ASP:HB2 | 3:A:551:HOH:O | 2.08 | 0.53 |
| 1:E:331:MET:HB3 | 1:E:332:PRO:HD3 | 1.90 | 0.53 |
| 1:B:252:ILE:CG2 | 1:B:253:ASP:N | 2.71 | 0.53 |
| 1:F:336:ALA:O | 1:F:340:GLN:HG2 | 2.09 | 0.53 |
| 1:F:349:ILE:HD13 | 1:F:359:THR:HB | 1.92 | 0.52 |
| 1:B:239:TYR:O | 1:B:254:LEU:HD13 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:317:ARG:HG3 | 1:B:318:LEU:N | 2.22 | 0.52 |
| 1:C:105:TYR:O | 1:C:107:PRO:HD3 | 2.09 | 0.52 |
| 1:F:353:ASN:HD22 | 1:F:355:SER:H | 1.57 | 0.52 |
| 1:F:211:LEU:HD23 | 2:F:401:8PH:H18 | 1.90 | 0.52 |
| 1:D:245:ASP:O | 1:D:247:ALA:N | 2.43 | 0.52 |
| 1:E:211:LEU:HD13 | 1:E:293:GLN:NE2 | 2.25 | 0.52 |
| 1:C:220:TYR:CZ | 1:C:246:PHE:HB2 | 2.43 | 0.52 |
| 1:F:362:ILE:O | 1:F:366:ILE:HG13 | 2.10 | 0.52 |
| 1:F:45:LYS:HG2 | 1:F:49:GLN:HE21 | 1.73 | 0.52 |
| 1:B:175:VAL:O | 2:B:401:8PH:H10 | 2.11 | 0.51 |
| 1:F:344:GLU:O | 1:F:348:ARG:HD3 | 2.10 | 0.51 |
| 1:A:57:VAL:HG11 | 1:A:288:PHE:HA | 1.91 | 0.51 |
| 1:E:321:ALA:CA | 1:E:324:LEU:HB2 | 2.34 | 0.51 |
| 1:A:150:MET:HG3 | 1:A:174:TYR:O | 2.10 | 0.51 |
| 1:D:65:MET:O | 1:D:69:VAL:HG23 | 2.10 | 0.51 |
| 1:C:350:PRO:HG2 | 1:C:353:ASN:HB2 | 1.92 | 0.51 |
| 1:D:159:ASP:CG | 1:D:160:LYS:N | 2.64 | 0.51 |
| 1:E:261:GLU:HG3 | 3:E:543:HOH:O | 2.10 | 0.51 |
| 1:D:55:ALA:O | 1:D:59:GLN:HG3 | 2.10 | 0.51 |
| 1:F:55:ALA:O | 1:F:59:GLN:HG3 | 2.10 | 0.51 |
| 1:F:39:SER:HB2 | 1:F:127:THR:HG23 | 1.93 | 0.51 |
| 1:E:51:SER:HB2 | 1:E:73:TYR:CZ | 2.45 | 0.51 |
| 1:F:271:PRO:HB3 | 1:F:369:GLN:HE22 | 1.76 | 0.51 |
| 1:A:321:ALA:HA | 1:A:324:LEU:CD1 | 2.41 | 0.51 |
| 1:C:255:ALA:HB1 | 1:C:310:PHE:CZ | 2.46 | 0.51 |
| 1:F:77:ARG:HE | 1:F:77:ARG:HA | 1.75 | 0.51 |
| 1:B:193:GLU:OE2 | 1:B:282:ASN:HB3 | 2.11 | 0.51 |
| 1:D:45:LYS:O | 1:D:49:GLN:HG3 | 2.10 | 0.51 |
| 1:B:211:LEU:HD13 | 1:B:293:GLN:HE22 | 1.76 | 0.51 |
| 1:F:353:ASN:ND2 | 1:F:355:SER:HB2 | 2.26 | 0.51 |
| 1:D:91:GLU:HG3 | 1:D:92:LYS:N | 2.25 | 0.51 |
| 1:D:225:GLN:H | 1:D:225:GLN:HE21 | 1.57 | 0.51 |
| 1:A:321:ALA:HA | 1:A:324:LEU:HG | 1.93 | 0.50 |
| 1:C:131:GLU:HA | 1:C:134:ASN:HD22 | 1.73 | 0.50 |
| 1:B:233:GLN:HA | 1:B:236:TRP:HE1 | 1.72 | 0.50 |
| 1:C:291:ILE:HB | 1:C:292:PRO:HD3 | 1.91 | 0.50 |
| 1:D:163:THR:HA | 1:D:233:GLN:HB3 | 1.93 | 0.50 |
| 1:C:339:TYR:O | 1:C:342:MET:HB2 | 2.11 | 0.50 |
| 1:F:357:SER:O | 1:F:361:GLN:HG3 | 2.11 | 0.50 |
| 1:A:327:ASP:HB2 | 1:C:325:MET:C | 2.31 | 0.50 |
| 1:D:85:ASP:OD1 | 1:D:114:SER:HA | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:356:SER:O | 1:E:360:ARG:HG3 | 2.12 | 0.50 |
| 1:B:322:VAL:O | 1:B:322:VAL:HG12 | 2.11 | 0.50 |
| 1:C:293:GLN:O | 1:C:297:ILE:HG12 | 2.11 | 0.50 |
| 1:B:71:ILE:O | 1:B:75:VAL:HG13 | 2.11 | 0.50 |
| 1:E:193:GLU:HA | 1:E:281:ARG:HD3 | 1.93 | 0.50 |
| 1:E:183:LEU:HD12 | 2:E:401:8PH:H26 | 1.92 | 0.50 |
| 1:D:259:LEU:HD21 | 1:D:309:VAL:HG21 | 1.92 | 0.50 |
| 1:B:291:ILE:HB | 1:B:292:PRO:HD3 | 1.94 | 0.50 |
| 1:E:118:ASP:O | 1:E:121:VAL:HG13 | 2.12 | 0.50 |
| 1:E:149:ARG:NH2 | 1:E:185:ARG:HH12 | 2.10 | 0.50 |
| 1:E:321:ALA:HA | 1:E:324:LEU:HD12 | 1.94 | 0.49 |
| 1:B:322:VAL:CG2 | 1:C:53:SER:HB2 | 2.33 | 0.49 |
| 1:F:348:ARG:O | 1:F:350:PRO:HD3 | 2.12 | 0.49 |
| 1:F:281:ARG:HD2 | 3:F:523:HOH:O | 2.12 | 0.49 |
| 1:B:256:VAL:HG21 | 1:B:307:GLN:HG2 | 1.94 | 0.49 |
| 1:B:91:GLU:CD | 1:B:91:GLU:H | 2.15 | 0.49 |
| 1:D:87:THR:CG2 | 1:D:87:THR:O | 2.60 | 0.49 |
| 1:D:125:PHE:N | 1:D:126:PRO:CD | 2.76 | 0.49 |
| 1:F:322:VAL:O | 1:F:322:VAL:HG12 | 2.12 | 0.49 |
| 1:A:149:ARG:NH2 | 1:A:185:ARG:HH22 | 2.11 | 0.49 |
| 1:C:314:VAL:CG1 | 1:C:315:LEU:N | 2.74 | 0.49 |
| 1:A:100:PHE:HA | 1:A:103:PHE:CD2 | 2.47 | 0.49 |
| 1:D:343:GLU:CD | 1:D:367:ARG:HH21 | 2.15 | 0.49 |
| 1:F:190:SER:O | 1:F:191:GLU:HB2 | 2.13 | 0.49 |
| 1:C:320:GLN:O | 1:C:323:THR:HG22 | 2.13 | 0.49 |
| 1:C:157:PHE:CE2 | 1:C:160:LYS:HE3 | 2.48 | 0.49 |
| 1:D:254:LEU:HA | 1:D:257:GLN:NE2 | 2.27 | 0.49 |
| 1:D:41:LYS:HD3 | 1:F:364:SER:OG | 2.13 | 0.49 |
| 1:F:240:VAL:HG21 | 1:F:245:ASP:HB2 | 1.95 | 0.49 |
| 1:A:210:PHE:CE2 | 1:A:297:ILE:HD13 | 2.48 | 0.49 |
| 1:C:317:ARG:HD2 | 1:C:318:LEU:CD1 | 2.42 | 0.49 |
| 1:C:195:PRO:O | 1:C:199:GLU:HG3 | 2.12 | 0.49 |
| 1:A:125:PHE:N | 1:A:126:PRO:CD | 2.76 | 0.49 |
| 1:D:110:ARG:HD2 | 1:D:112:MET:SD | 2.53 | 0.49 |
| 1:F:331:MET:O | 1:F:335:LYS:HG3 | 2.13 | 0.49 |
| 1:F:248:LEU:HD12 | 1:F:251:ASN:HD21 | 1.78 | 0.48 |
| 1:F:232:PRO:HD2 | 1:F:262:LEU:HD11 | 1.95 | 0.48 |
| 1:D:246:PHE:CD1 | 1:D:255:ALA:HA | 2.48 | 0.48 |
| 1:D:153:GLY:HA3 | 1:D:174:TYR:CD1 | 2.48 | 0.48 |
| 1:D:345:ILE:O | 1:D:349:ILE:HG13 | 2.12 | 0.48 |
| 1:D:322:VAL:HG22 | 1:E:295:MET:CE | 2.44 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:118:ASP:O | 1:A:121:VAL:HG22 | 2.14 | 0.48 |
| 1:A:327:ASP:OD2 | 1:B:327:ASP:OD2 | 2.32 | 0.48 |
| 1:A:63:GLY:HA3 | 3:A:510:HOH:O | 2.12 | 0.48 |
| 1:B:150:MET:HG3 | 1:B:174:TYR:O | 2.12 | 0.48 |
| 1:F:368:THR:HG22 | 1:F:368:THR:O | 2.12 | 0.48 |
| 1:D:211:LEU:CD2 | 2:D:401:8PH:H18 | 2.42 | 0.48 |
| 1:F:221:LEU:HD13 | 1:F:310:PHE:HA | 1.96 | 0.48 |
| 1:A:90:VAL:O | 1:A:94:VAL:HG23 | 2.14 | 0.48 |
| 1:A:356:SER:O | 1:A:360:ARG:HG3 | 2.13 | 0.48 |
| 1:C:92:LYS:O | 1:C:95:PRO:HG2 | 2.14 | 0.48 |
| 1:C:114:SER:HB3 | 1:C:119:ARG:HB2 | 1.95 | 0.48 |
| 1:E:223:ASP:OD1 | 1:E:228:ARG:NH2 | 2.47 | 0.48 |
| 1:E:228:ARG:NH1 | 1:E:228:ARG:HG3 | 2.26 | 0.48 |
| 1:D:114:SER:O | 1:D:115:LYS:HD2 | 2.14 | 0.47 |
| 1:D:163:THR:HA | 1:D:233:GLN:HE21 | 1.77 | 0.47 |
| 1:C:150:MET:O | 1:C:154:MET:HG3 | 2.14 | 0.47 |
| 1:D:238:ARG:NH1 | 1:D:238:ARG:HB2 | 2.28 | 0.47 |
| 1:A:320:GLN:CG | 1:A:321:ALA:N | 2.63 | 0.47 |
| 1:B:297:ILE:CD1 | 1:B:338:ILE:HG23 | 2.43 | 0.47 |
| 1:D:255:ALA:HB1 | 1:D:310:PHE:CZ | 2.50 | 0.47 |
| 1:C:125:PHE:N | 1:C:126:PRO:CD | 2.78 | 0.47 |
| 1:A:248:LEU:HB2 | 1:A:251:ASN:ND2 | 2.29 | 0.47 |
| 1:D:353:ASN:HD22 | 1:D:355:SER:H | 1.61 | 0.47 |
| 1:D:322:VAL:HG22 | 1:E:295:MET:HE1 | 1.97 | 0.47 |
| 1:C:42:THR:HG22 | 1:C:46:TYR:CE2 | 2.50 | 0.47 |
| 1:F:210:PHE:CZ | 1:F:297:ILE:HG12 | 2.50 | 0.47 |
| 1:E:194:ASP:OD1 | 1:E:195:PRO:HD2 | 2.15 | 0.47 |
| 1:F:36:LEU:N | 3:F:533:HOH:O | 2.48 | 0.47 |
| 1:C:190:SER:O | 1:C:191:GLU:HB2 | 2.14 | 0.47 |
| 1:F:146:ILE:HG22 | 1:F:150:MET:HE3 | 1.97 | 0.47 |
| 1:C:210:PHE:HE2 | 1:C:297:ILE:HD13 | 1.78 | 0.46 |
| 1:F:146:ILE:HG22 | 1:F:150:MET:CE | 2.44 | 0.46 |
| 1:C:270:ILE:HD13 | 1:C:342:MET:SD | 2.55 | 0.46 |
| 1:A:153:GLY:HA3 | 1:A:174:TYR:CG | 2.50 | 0.46 |
| 1:B:326:MET:HE1 | 1:C:287:ASN:HB3 | 1.96 | 0.46 |
| 1:C:322:VAL:O | 1:C:322:VAL:HG12 | 2.15 | 0.46 |
| 1:E:126:PRO:HA | 1:E:129:SER:OG | 2.15 | 0.46 |
| 1:F:47:LEU:HD22 | 1:F:70:CYS:SG | 2.55 | 0.46 |
| 1:E:324:LEU:HD13 | 3:E:517:HOH:O | 2.14 | 0.46 |
| 1:B:100:PHE:HA | 1:B:103:PHE:CD2 | 2.50 | 0.46 |
| 1:C:320:GLN:CG | 1:C:321:ALA:H | 2.25 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:83:GLU:HG3 | 1:D:154:MET:HB3 | 1.98 | 0.46 |
| 1:B:339:TYR:O | 1:B:342:MET:HB2 | 2.16 | 0.46 |
| 1:B:262:LEU:O | 1:B:265:ASN:HB3 | 2.15 | 0.46 |
| 1:A:161:HIS:HD2 | 1:A:229:GLU:HB2 | 1.80 | 0.46 |
| 1:B:252:ILE:HG21 | 1:B:307:GLN:NE2 | 2.31 | 0.46 |
| 1:A:316:ILE:N | 1:A:316:ILE:CD1 | 2.76 | 0.46 |
| 1:E:321:ALA:HA | 1:E:324:LEU:CB | 2.37 | 0.46 |
| 1:F:178:LEU:HD23 | 1:F:181:ILE:HD12 | 1.98 | 0.46 |
| 1:D:359:THR:O | 1:D:362:ILE:HG22 | 2.15 | 0.46 |
| 1:D:318:LEU:HG | 1:D:318:LEU:H | 1.51 | 0.46 |
| 1:F:218:ARG:HG2 | 1:F:218:ARG:O | 2.16 | 0.46 |
| 1:B:125:PHE:N | 1:B:126:PRO:CD | 2.79 | 0.46 |
| 1:C:317:ARG:NH1 | 1:C:348:ARG:NH2 | 2.64 | 0.46 |
| 1:A:338:ILE:O | 1:A:342:MET:HG2 | 2.16 | 0.46 |
| 1:B:105:TYR:O | 1:B:107:PRO:HD3 | 2.16 | 0.46 |
| 1:D:297:ILE:CD1 | 1:D:338:ILE:HG12 | 2.46 | 0.46 |
| 1:A:146:ILE:HG22 | 1:A:150:MET:HE3 | 1.98 | 0.45 |
| 1:F:66:ARG:HB3 | 3:F:532:HOH:O | 2.16 | 0.45 |
| 1:F:85:ASP:HB3 | 1:F:88:ILE:HD12 | 1.98 | 0.45 |
| 1:B:52:ARG:HG3 | 3:B:572:HOH:O | 2.16 | 0.45 |
| 1:A:242:LYS:HB2 | 1:A:242:LYS:NZ | 2.30 | 0.45 |
| 1:D:346:TYR:HA | 1:D:349:ILE:HD11 | 1.97 | 0.45 |
| 1:A:335:LYS:HB3 | 1:A:339:TYR:CE2 | 2.52 | 0.45 |
| 1:D:348:ARG:O | 1:D:350:PRO:HD3 | 2.17 | 0.45 |
| 1:C:220:TYR:OH | 1:C:246:PHE:HB2 | 2.16 | 0.45 |
| 1:B:153:GLY:HA3 | 1:B:174:TYR:CG | 2.52 | 0.45 |
| 1:F:243:LEU:HD12 | 1:F:243:LEU:O | 2.16 | 0.45 |
| 1:F:153:GLY:HA3 | 1:F:174:TYR:CD1 | 2.51 | 0.45 |
| 1:C:316:ILE:CD1 | 1:C:316:ILE:H | 2.13 | 0.45 |
| 1:A:358:LYS:NZ | 3:A:565:HOH:O | 2.49 | 0.45 |
| 1:F:214:THR:HG23 | 1:F:300:LEU:CD2 | 2.46 | 0.45 |
| 1:D:248:LEU:HB2 | 1:D:251:ASN:HD22 | 1.82 | 0.45 |
| 1:B:183:LEU:CD1 | 2:B:401:8PH:H26 | 2.46 | 0.45 |
| 1:D:362:ILE:HG23 | 1:D:363:ILE:N | 2.32 | 0.45 |
| 1:F:42:THR:HG22 | 1:F:46:TYR:CE2 | 2.51 | 0.45 |
| 1:E:45:LYS:HG2 | 1:E:49:GLN:NE2 | 2.32 | 0.45 |
| 1:F:125:PHE:N | 1:F:126:PRO:CD | 2.79 | 0.45 |
| 1:C:321:ALA:O | 1:C:325:MET:CG | 2.60 | 0.44 |
| 1:D:238:ARG:HB2 | 1:D:238:ARG:HH11 | 1.81 | 0.44 |
| 1:A:252:ILE:HD11 | 1:A:307:GLN:HB3 | 1.99 | 0.44 |
| 1:B:51:SER:O | 1:B:52:ARG:C | 2.55 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:248:LEU:HA | 1:F:249:PRO:HD3 | 1.88 | 0.44 |
| 1:F:233:GLN:O | 1:F:237:SER:HB3 | 2.18 | 0.44 |
| 1:E:155:ALA:HA | 1:E:158:LEU:CD1 | 2.48 | 0.44 |
| 1:C:331:MET:HB3 | 1:C:332:PRO:HD3 | 2.00 | 0.44 |
| 1:A:322:VAL:O | 1:A:322:VAL:CG1 | 2.64 | 0.44 |
| 1:D:100:PHE:HA | 1:D:103:PHE:CD2 | 2.53 | 0.44 |
| 1:D:321:ALA:O | 1:D:325:MET:HG2 | 2.17 | 0.44 |
| 1:C:54:PHE:O | 1:C:57:VAL:HG22 | 2.18 | 0.44 |
| 2:C:401:8PH:H27 | 3:C:543:HOH:O | 2.18 | 0.44 |
| 1:D:42:THR:HG22 | 1:D:46:TYR:CE2 | 2.53 | 0.44 |
| 1:B:211:LEU:HD11 | 1:B:293:GLN:NE2 | 2.32 | 0.44 |
| 1:F:156:GLU:O | 1:F:156:GLU:HG2 | 2.18 | 0.44 |
| 1:C:318:LEU:HB2 | 1:C:319:GLY:H | 1.47 | 0.44 |
| 1:B:325:MET:HE2 | 1:C:295:MET:HG3 | 2.00 | 0.43 |
| 1:B:252:ILE:HG23 | 1:B:307:GLN:HE21 | 1.83 | 0.43 |
| 1:E:100:PHE:HA | 1:E:103:PHE:CD2 | 2.53 | 0.43 |
| 1:F:50:THR:HG22 | 1:F:118:ASP:OD1 | 2.18 | 0.43 |
| 1:F:228:ARG:HG3 | 1:F:228:ARG:HH11 | 1.82 | 0.43 |
| 1:D:269:HIS:O | 1:D:273:VAL:HG23 | 2.18 | 0.43 |
| 1:B:211:LEU:CD1 | 1:B:293:GLN:HE22 | 2.31 | 0.43 |
| 1:E:92:LYS:O | 1:E:95:PRO:HD2 | 2.18 | 0.43 |
| 1:D:190:SER:O | 1:D:191:GLU:HB2 | 2.19 | 0.43 |
| 1:D:150:MET:HG3 | 1:D:174:TYR:O | 2.19 | 0.43 |
| 1:A:193:GLU:OE2 | 1:A:282:ASN:HB3 | 2.18 | 0.43 |
| 1:A:291:ILE:HG21 | 1:C:322:VAL:HG13 | 2.01 | 0.43 |
| 1:E:125:PHE:N | 1:E:126:PRO:CD | 2.81 | 0.43 |
| 1:C:51:SER:HB3 | 1:C:55:ALA:HB2 | 2.00 | 0.43 |
| 1:C:163:THR:HA | 1:C:233:GLN:HB3 | 2.00 | 0.43 |
| 1:E:133:ARG:HA | 1:E:140:GLN:NE2 | 2.33 | 0.43 |
| 1:C:324:LEU:HD12 | 3:C:535:HOH:O | 2.18 | 0.43 |
| 1:D:334:VAL:O | 1:D:338:ILE:HG13 | 2.19 | 0.43 |
| 1:F:213:LYS:O | 1:F:217:ILE:HG13 | 2.19 | 0.43 |
| 1:B:359:THR:O | 1:B:362:ILE:HG22 | 2.18 | 0.43 |
| 1:B:150:MET:O | 1:B:154:MET:HG3 | 2.18 | 0.43 |
| 1:B:236:TRP:CZ3 | 1:B:242:LYS:HA | 2.54 | 0.43 |
| 1:D:153:GLY:HA3 | 1:D:174:TYR:CG | 2.53 | 0.43 |
| 1:C:317:ARG:NH1 | 1:C:348:ARG:HH21 | 2.17 | 0.43 |
| 1:F:262:LEU:O | 1:F:265:ASN:HB3 | 2.19 | 0.43 |
| 1:B:194:ASP:OD1 | 1:B:195:PRO:HD2 | 2.18 | 0.43 |
| 1:B:111:PHE:HB3 | 1:B:122:LEU:HB3 | 2.01 | 0.43 |
| 1:B:306:ASN:OD1 | 1:B:306:ASN:C | 2.57 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:401:8PH:H17 | 2:E:401:8PH:H10 | 2.01 | 0.43 |
| 1:F:338:ILE:O | 1:F:342:MET:HG2 | 2.19 | 0.43 |
| 1:D:221:LEU:O | 1:D:224:GLN:N | 2.52 | 0.43 |
| 1:A:238:ARG:HB2 | 1:A:238:ARG:HH11 | 1.84 | 0.43 |
| 1:E:150:MET:HG3 | 1:E:174:TYR:O | 2.19 | 0.42 |
| 1:A:252:ILE:HG23 | 1:A:253:ASP:N | 2.33 | 0.42 |
| 1:F:79:LEU:HB2 | 1:F:100:PHE:CE2 | 2.55 | 0.42 |
| 1:F:281:ARG:NH2 | 1:F:281:ARG:CG | 2.81 | 0.42 |
| 1:E:109:TRP:CH2 | 1:E:111:PHE:HB2 | 2.54 | 0.42 |
| 1:A:238:ARG:NH1 | 1:A:238:ARG:HB2 | 2.35 | 0.42 |
| 1:B:263:ILE:O | 1:B:267:LEU:HG | 2.20 | 0.42 |
| 1:F:233:GLN:HB3 | 1:F:233:GLN:HE21 | 1.51 | 0.42 |
| 1:B:220:TYR:CZ | 1:B:224:GLN:HG3 | 2.54 | 0.42 |
| 1:F:90:VAL:O | 1:F:94:VAL:HG23 | 2.18 | 0.42 |
| 3:A:578:HOH:O | 1:B:66:ARG:HD3 | 2.19 | 0.42 |
| 1:F:45:LYS:HG2 | 1:F:49:GLN:NE2 | 2.35 | 0.42 |
| 1:D:344:GLU:HG2 | 3:D:540:HOH:O | 2.19 | 0.42 |
| 1:F:270:ILE:CD1 | 1:F:342:MET:HE3 | 2.50 | 0.42 |
| 1:A:353:ASN:ND2 | 1:A:355:SER:HB2 | 2.35 | 0.42 |
| 1:B:210:PHE:CZ | 1:B:297:ILE:HG12 | 2.55 | 0.42 |
| 1:F:54:PHE:HE2 | 1:F:288:PHE:CE1 | 2.38 | 0.42 |
| 1:A:170:LYS:O | 1:A:173:HIS:HB3 | 2.20 | 0.42 |
| 1:C:356:SER:O | 1:C:360:ARG:HG3 | 2.20 | 0.42 |
| 1:E:190:SER:O | 1:E:191:GLU:HB2 | 2.20 | 0.42 |
| 1:D:116:GLU:O | 1:D:119:ARG:CD | 2.63 | 0.42 |
| 1:E:334:VAL:O | 1:E:338:ILE:HG13 | 2.20 | 0.42 |
| 1:D:220:TYR:OH | 1:D:246:PHE:HB2 | 2.20 | 0.42 |
| 1:B:252:ILE:CG2 | 1:B:307:GLN:NE2 | 2.82 | 0.42 |
| 1:C:76:LEU:HD22 | 1:C:150:MET:SD | 2.60 | 0.42 |
| 1:B:306:ASN:OD1 | 1:B:308:GLN:N | 2.50 | 0.41 |
| 1:C:269:HIS:O | 1:C:273:VAL:HG23 | 2.20 | 0.41 |
| 1:F:242:LYS:O | 1:F:244:GLY:N | 2.53 | 0.41 |
| 1:E:211:LEU:HD13 | 1:E:293:GLN:HE22 | 1.85 | 0.41 |
| 1:A:179:VAL:HB | 2:A:401:8PH:H19 | 2.02 | 0.41 |
| 2:B:401:8PH:H21 | 2:B:402:8PH:H22 | 2.03 | 0.41 |
| 1:F:100:PHE:HA | 1:F:103:PHE:CE2 | 2.55 | 0.41 |
| 1:E:50:THR:OG1 | 1:E:73:TYR:HE1 | 2.01 | 0.41 |
| 1:D:326:MET:HE1 | 1:D:333:ALA:HA | 2.01 | 0.41 |
| 1:F:229:GLU:HB3 | 1:F:243:LEU:HD23 | 2.03 | 0.41 |
| 1:B:342:MET:HE2 | 1:B:342:MET:HA | 2.00 | 0.41 |
| 1:F:80:ASP:OD1 | 2:F:401:8PH:H7 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:194:ASP:OD2 | 1:C:195:PRO:HD2 | 2.21 | 0.41 |
| 1:E:233:GLN:HA | 1:E:236:TRP:CE2 | 2.56 | 0.41 |
| 1:E:291:ILE:HB | 1:E:292:PRO:HD3 | 2.02 | 0.41 |
| 1:B:255:ALA:HB1 | 1:B:310:PHE:CZ | 2.56 | 0.41 |
| 1:C:252:ILE:HG23 | 1:C:253:ASP:N | 2.36 | 0.41 |
| 1:D:248:LEU:HA | 1:D:249:PRO:HD2 | 1.90 | 0.41 |
| 1:F:153:GLY:HA3 | 1:F:174:TYR:CG | 2.56 | 0.41 |
| 1:D:349:ILE:HA | 1:D:350:PRO:HD3 | 1.91 | 0.41 |
| 1:D:57:VAL:HG11 | 1:D:288:PHE:HA | 2.03 | 0.41 |
| 1:D:159:ASP:CG | 1:D:160:LYS:H | 2.22 | 0.41 |
| 1:D:245:ASP:C | 1:D:247:ALA:N | 2.75 | 0.41 |
| 1:E:149:ARG:HH21 | 1:E:185:ARG:HH12 | 1.69 | 0.41 |
| 1:E:221:LEU:HG | 1:E:225:GLN:OE1 | 2.21 | 0.41 |
| 1:C:77:ARG:HA | 1:C:77:ARG:HD2 | 1.92 | 0.41 |
| 1:F:183:LEU:HD13 | 2:F:401:8PH:H26 | 2.02 | 0.40 |
| 1:C:51:SER:OG | 1:C:54:PHE:HB2 | 2.22 | 0.40 |
| 1:B:220:TYR:HB2 | 1:B:231:TRP:CZ2 | 2.56 | 0.40 |
| 1:D:218:ARG:HG2 | 1:D:218:ARG:O | 2.20 | 0.40 |
| 1:F:252:ILE:HG22 | 1:F:253:ASP:OD2 | 2.21 | 0.40 |
| 1:C:233:GLN:HA | 1:C:236:TRP:NE1 | 2.37 | 0.40 |
| 1:D:77:ARG:HA | 1:D:77:ARG:HD3 | 1.97 | 0.40 |
| 1:D:111:PHE:HB3 | 1:D:122:LEU:HB3 | 2.03 | 0.40 |
| 1:B:163:THR:HA | 1:B:233:GLN:HB3 | 2.04 | 0.40 |
| 1:D:163:THR:CA | 1:D:233:GLN:HE21 | 2.35 | 0.40 |
| 1:A:105:TYR:O | 1:A:107:PRO:HD3 | 2.21 | 0.40 |
| 1:B:180:GLY:HA2 | 2:B:401:8PH:H27 | 2.03 | 0.40 |
| 1:B:146:ILE:HG22 | 1:B:150:MET:HE3 | 2.02 | 0.40 |
| 1:A:251:ASN:O | 1:A:252:ILE:C | 2.60 | 0.40 |
| 1:C:262:LEU:O | 1:C:265:ASN:HB3 | 2.21 | 0.40 |
| 1:F:97:LEU:HD12 | 1:F:158:LEU:HD11 | 2.04 | 0.40 |
| 1:C:353:ASN:HD22 | 1:C:355:SER:H | 1.70 | 0.40 |
| 1:A:42:THR:HG22 | 1:A:46:TYR:CE2 | 2.57 | 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 | 332/360 (92%) | 314 (95%) | 15 (4%) | 3 (1%) | 21 | 37 |
| 1 | B | 332/360 (92%) | 312 (94%) | 18 (5%) | 2 (1%) | 30 | 50 |
| 1 | C | 332/360 (92%) | 317 (96%) | 12 (4%) | 3 (1%) | 21 | 37 |
| 1 | D | 332/360 (92%) | 311 (94%) | 17 (5%) | 4 (1%) | 16 | 29 |
| 1 | E | 332/360 (92%) | 318 (96%) | 10 (3%) | 4 (1%) | 16 | 29 |
| 1 | F | 332/360 (92%) | 305 (92%) | 21 (6%) | 6 (2%) | 11 | 18 |
| All | All | 1992/2160 (92%) | 1877 (94%) | 93 (5%) | 22 (1%) | 17 | 31 |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 318 | LEU |
| 1 | A | 320 | GLN |
| 1 | B | 318 | LEU |
| 1 | C | 318 | LEU |
| 1 | D | 318 | LEU |
| 1 | F | 318 | LEU |
| 1 | D | 85 | ASP |
| 1 | D | 246 | PHE |
| 1 | E | 200 | ASP |
| 1 | F | 243 | LEU |
| 1 | E | 54 | PHE |
| 1 | E | 107 | PRO |
| 1 | E | 328 | ALA |
| 1 | F | 252 | ILE |
| 1 | A | 252 | ILE |
| 1 | B | 249 | PRO |
| 1 | D | 252 | ILE |
| 1 | F | 308 | GLN |
| 1 | C | 54 | PHE |
| 1 | F | 119 | ARG |
| 1 | F | 107 | PRO |
| 1 | C | 63 | GLY |

### 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 | 297/320 (93%) | 283 (95%) | 14 (5%) | 32 | 56 |
| 1 | B | 297/320 (93%) | 285 (96%) | 12 (4%) | 38 | 64 |
| 1 | C | 297/320 (93%) | 284 (96%) | 13 (4%) | 35 | 60 |
| 1 | D | 297/320 (93%) | 277 (93%) | 20 (7%) | 20 | 37 |
| 1 | E | 297/320 (93%) | 282 (95%) | 15 (5%) | 29 | 52 |
| 1 | F | 297/320 (93%) | 278 (94%) | 19 (6%) | 22 | 39 |
| All | All | 1782/1920 (93%) | 1689 (95%) | 93 (5%) | 29 | 51 |

All (93) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 54 | PHE |
| 1 | A | 115 | LYS |
| 1 | A | 120 | GLN |
| 1 | A | 203 | ARG |
| 1 | A | 233 | GLN |
| 1 | A | 281 | ARG |
| 1 | A | 295 | MET |
| 1 | A | 316 | ILE |
| 1 | A | 323 | THR |
| 1 | A | 326 | MET |
| 1 | A | 327 | ASP |
| 1 | A | 344 | GLU |
| 1 | A | 351 | ASP |
| 1 | A | 357 | SER |
| 1 | B | 54 | PHE |
| 1 | B | 77 | ARG |
| 1 | B | 110 | ARG |
| 1 | B | 137 | GLU |
| 1 | B | 196 | LEU |
| 1 | B | 203 | ARG |
| 1 | B | 233 | GLN |
| 1 | B | 238 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 249 | PRO |
| 1 | B | 316 | ILE |
| 1 | B | 340 | GLN |
| 1 | B | 352 | SER |
| 1 | C | 49 | GLN |
| 1 | C | 52 | ARG |
| 1 | C | 110 | ARG |
| 1 | C | 119 | ARG |
| 1 | C | 129 | SER |
| 1 | C | 203 | ARG |
| 1 | C | 233 | GLN |
| 1 | C | 280 | LEU |
| 1 | C | 295 | MET |
| 1 | C | 297 | ILE |
| 1 | C | 315 | LEU |
| 1 | C | 316 | ILE |
| 1 | C | 318 | LEU |
| 1 | D | 52 | ARG |
| 1 | D | 54 | PHE |
| 1 | D | 83 | GLU |
| 1 | D | 119 | ARG |
| 1 | D | 159 | ASP |
| 1 | D | 166 | GLN |
| 1 | D | 203 | ARG |
| 1 | D | 219 | ASP |
| 1 | D | 225 | GLN |
| 1 | D | 233 | GLN |
| 1 | D | 242 | LYS |
| 1 | D | 314 | VAL |
| 1 | D | 315 | LEU |
| 1 | D | 316 | ILE |
| 1 | D | 318 | LEU |
| 1 | D | 326 | MET |
| 1 | D | 327 | ASP |
| 1 | D | 351 | ASP |
| 1 | D | 352 | SER |
| 1 | D | 361 | GLN |
| 1 | E | 52 | ARG |
| 1 | E | 54 | PHE |
| 1 | E | 80 | ASP |
| 1 | E | 83 | GLU |
| 1 | E | 86 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 121 | VAL |
| 1 | E | 203 | ARG |
| 1 | E | 233 | GLN |
| 1 | E | 281 | ARG |
| 1 | E | 295 | MET |
| 1 | E | 316 | ILE |
| 1 | E | 324 | LEU |
| 1 | E | 325 | MET |
| 1 | E | 340 | GLN |
| 1 | E | 344 | GLU |
| 1 | F | 54 | PHE |
| 1 | F | 77 | ARG |
| 1 | F | 83 | GLU |
| 1 | F | 90 | VAL |
| 1 | F | 110 | ARG |
| 1 | F | 115 | LYS |
| 1 | F | 119 | ARG |
| 1 | F | 120 | GLN |
| 1 | F | 203 | ARG |
| 1 | F | 233 | GLN |
| 1 | F | 248 | LEU |
| 1 | F | 252 | ILE |
| 1 | F | 262 | LEU |
| 1 | F | 281 | ARG |
| 1 | F | 295 | MET |
| 1 | F | 316 | ILE |
| 1 | F | 347 | HIS |
| 1 | F | 352 | SER |
| 1 | F | 364 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 48 | ASN |
| 1 | A | 59 | GLN |
| 1 | A | 161 | HIS |
| 1 | A | 215 | ASN |
| 1 | A | 225 | GLN |
| 1 | A | 233 | GLN |
| 1 | A | 251 | ASN |
| 1 | A | 257 | GLN |
| 1 | A | 293 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 369 | GLN |
| 1 | B | 48 | ASN |
| 1 | B | 59 | GLN |
| 1 | B | 225 | GLN |
| 1 | B | 233 | GLN |
| 1 | B | 251 | ASN |
| 1 | B | 257 | GLN |
| 1 | B | 293 | GLN |
| 1 | B | 307 | GLN |
| 1 | B | 353 | ASN |
| 1 | C | 48 | ASN |
| 1 | C | 59 | GLN |
| 1 | C | 120 | GLN |
| 1 | C | 134 | ASN |
| 1 | C | 225 | GLN |
| 1 | C | 233 | GLN |
| 1 | C | 257 | GLN |
| 1 | C | 293 | GLN |
| 1 | D | 48 | ASN |
| 1 | D | 59 | GLN |
| 1 | D | 101 | HIS |
| 1 | D | 224 | GLN |
| 1 | D | 225 | GLN |
| 1 | D | 233 | GLN |
| 1 | D | 251 | ASN |
| 1 | D | 293 | GLN |
| 1 | D | 353 | ASN |
| 1 | E | 49 | GLN |
| 1 | E | 140 | GLN |
| 1 | E | 215 | ASN |
| 1 | E | 257 | GLN |
| 1 | E | 293 | GLN |
| 1 | E | 353 | ASN |
| 1 | F | 48 | ASN |
| 1 | F | 49 | GLN |
| 1 | F | 59 | GLN |
| 1 | F | 101 | HIS |
| 1 | F | 120 | GLN |
| 1 | F | 225 | GLN |
| 1 | F | 233 | GLN |
| 1 | F | 251 | ASN |
| 1 | F | 257 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 308 | GLN |
| 1 | F | 340 | GLN |
| 1 | F | 369 | GLN |

### 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

10 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 | 8PH | A | 401 | - | 26,26,26 | 2.20 | 9 (34%) | 31,37,37 | 1.38 | 5 (16%) |
| 2 | 8PH | A | 402 | - | 7,7,26 | 0.34 | 0 | 6,6,37 | 0.72 | 0 |
| 2 | 8PH | A | 403 | - | 18,18,26 | 2.62 | 9 (50%) | 23,29,37 | 1.49 | 5 (21%) |
| 2 | 8PH | B | 401 | - | 26,26,26 | 2.19 | 9 (34%) | 31,37,37 | 1.40 | 5 (16%) |
| 2 | 8PH | B | 402 | - | 8,8,26 | 0.34 | 0 | 7,7,37 | 0.80 | 0 |
| 2 | 8PH | C | 401 | - | 26,26,26 | 2.17 | 9 (34%) | 31,37,37 | 1.38 | 5 (16%) |
| 2 | 8PH | D | 401 | - | 26,26,26 | 2.19 | 9 (34%) | 31,37,37 | 1.31 | 5 (16%) |
| 2 | 8PH | E | 401 | - | 26,26,26 | 2.21 | 9 (34%) | 31,37,37 | 1.32 | 5 (16%) |
| 2 | 8PH | F | 401 | - | 26,26,26 | 2.21 | 9 (34%) | 31,37,37 | 1.36 | 5 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | 8PH | F | 402 | - | 26,26,26 | 2.23 | 9 (34%) | 31,37,37 | 1.40 | 5 (16%) |

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 | 8PH | A | 401 | - | - | 0/33/33/33 | 0/1/1/1 |
| 2 | 8PH | A | 402 | - | - | 0/5/5/33 | 0/0/0/1 |
| 2 | 8PH | A | 403 | - | - | 0/25/25/33 | 0/1/1/1 |
| 2 | 8PH | B | 401 | - | - | 0/33/33/33 | 0/1/1/1 |
| 2 | 8PH | B | 402 | - | - | 0/6/6/33 | 0/0/0/1 |
| 2 | 8PH | C | 401 | - | - | 0/33/33/33 | 0/1/1/1 |
| 2 | 8PH | D | 401 | - | - | 0/33/33/33 | 0/1/1/1 |
| 2 | 8PH | E | 401 | - | - | 0/33/33/33 | 0/1/1/1 |
| 2 | 8PH | F | 401 | - | - | 0/33/33/33 | 0/1/1/1 |
| 2 | 8PH | F | 402 | - | - | 0/33/33/33 | 0/1/1/1 |

All (72) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | F | 402 | 8PH | PAZ-OAC | -3.43 | 1.48 | 1.54 |
| 2 | A | 401 | 8PH | PAZ-OAC | -3.43 | 1.48 | 1.54 |
| 2 | F | 401 | 8PH | PAZ-OAC | -3.40 | 1.48 | 1.54 |
| 2 | A | 403 | 8PH | PAZ-OAC | -3.38 | 1.48 | 1.54 |
| 2 | E | 401 | 8PH | PAZ-OAC | -3.36 | 1.48 | 1.54 |
| 2 | B | 401 | 8PH | PAZ-OAC | -3.36 | 1.48 | 1.54 |
| 2 | D | 401 | 8PH | PAZ-OAC | -3.33 | 1.48 | 1.54 |
| 2 | C | 401 | 8PH | PAZ-OAC | -3.30 | 1.48 | 1.54 |
| 2 | F | 402 | 8PH | CAI-NAV | -2.46 | 1.33 | 1.37 |
| 2 | E | 401 | 8PH | CAJ-NAW | -2.44 | 1.33 | 1.37 |
| 2 | F | 401 | 8PH | CAI-NAV | -2.40 | 1.33 | 1.37 |
| 2 | E | 401 | 8PH | CAI-NAV | -2.38 | 1.33 | 1.37 |
| 2 | B | 401 | 8PH | CAJ-NAW | -2.37 | 1.33 | 1.37 |
| 2 | B | 401 | 8PH | CAI-NAV | -2.32 | 1.33 | 1.37 |
| 2 | F | 401 | 8PH | CAJ-NAW | -2.31 | 1.33 | 1.37 |
| 2 | D | 401 | 8PH | CAI-NAV | -2.30 | 1.33 | 1.37 |
| 2 | D | 401 | 8PH | CAJ-NAW | -2.29 | 1.33 | 1.37 |
| 2 | A | 401 | 8PH | CAJ-NAW | -2.29 | 1.33 | 1.37 |
| 2 | C | 401 | 8PH | CAI-NAV | -2.28 | 1.33 | 1.37 |
| 2 | A | 401 | 8PH | CAI-NAV | -2.25 | 1.33 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | F | 402 | 8PH | CAJ-NAW | -2.24 | 1.33 | 1.37 |
| 2 | A | 403 | 8PH | CAI-NAV | -2.22 | 1.33 | 1.37 |
| 2 | A | 403 | 8PH | CAJ-NAW | -2.21 | 1.33 | 1.37 |
| 2 | C | 401 | 8PH | CAJ-NAW | -2.17 | 1.33 | 1.37 |
| 2 | A | 401 | 8PH | PAY-CAX | 2.52 | 1.86 | 1.85 |
| 2 | C | 401 | 8PH | PAY-CAX | 2.60 | 1.87 | 1.85 |
| 2 | C | 401 | 8PH | PAZ-CAX | 2.67 | 1.87 | 1.85 |
| 2 | F | 401 | 8PH | PAY-CAX | 2.68 | 1.87 | 1.85 |
| 2 | B | 401 | 8PH | PAY-CAX | 2.71 | 1.87 | 1.85 |
| 2 | A | 403 | 8PH | PAZ-CAX | 2.71 | 1.87 | 1.85 |
| 2 | B | 401 | 8PH | PAZ-CAX | 2.74 | 1.87 | 1.85 |
| 2 | D | 401 | 8PH | PAY-CAX | 2.75 | 1.87 | 1.85 |
| 2 | E | 401 | 8PH | PAY-CAX | 2.75 | 1.87 | 1.85 |
| 2 | D | 401 | 8PH | PAZ-CAX | 2.78 | 1.87 | 1.85 |
| 2 | A | 403 | 8PH | PAY-CAX | 2.78 | 1.87 | 1.85 |
| 2 | F | 402 | 8PH | PAY-CAX | 2.89 | 1.87 | 1.85 |
| 2 | E | 401 | 8PH | PAZ-CAX | 2.92 | 1.87 | 1.85 |
| 2 | F | 401 | 8PH | PAZ-CAX | 2.95 | 1.87 | 1.85 |
| 2 | F | 402 | 8PH | PAZ-CAX | 2.99 | 1.87 | 1.85 |
| 2 | A | 401 | 8PH | PAZ-CAX | 3.10 | 1.87 | 1.85 |
| 2 | B | 401 | 8PH | PAY-OAF | 3.44 | 1.61 | 1.54 |
| 2 | A | 401 | 8PH | PAY-OAF | 3.48 | 1.61 | 1.54 |
| 2 | C | 401 | 8PH | PAZ-OAG | 3.48 | 1.61 | 1.54 |
| 2 | B | 401 | 8PH | PAY-OAE | 3.48 | 1.61 | 1.54 |
| 2 | A | 403 | 8PH | PAY-OAE | 3.48 | 1.61 | 1.54 |
| 2 | B | 401 | 8PH | PAZ-OAG | 3.49 | 1.61 | 1.54 |
| 2 | D | 401 | 8PH | PAZ-OAG | 3.49 | 1.61 | 1.54 |
| 2 | F | 402 | 8PH | PAY-OAE | 3.49 | 1.61 | 1.54 |
| 2 | A | 401 | 8PH | PAY-OAE | 3.50 | 1.61 | 1.54 |
| 2 | F | 401 | 8PH | PAZ-OAG | 3.50 | 1.61 | 1.54 |
| 2 | F | 401 | 8PH | PAY-OAE | 3.50 | 1.61 | 1.54 |
| 2 | A | 403 | 8PH | PAY-OAF | 3.51 | 1.61 | 1.54 |
| 2 | C | 401 | 8PH | PAY-OAE | 3.51 | 1.61 | 1.54 |
| 2 | F | 402 | 8PH | PAY-OAF | 3.51 | 1.61 | 1.54 |
| 2 | E | 401 | 8PH | PAZ-OAG | 3.52 | 1.61 | 1.54 |
| 2 | C | 401 | 8PH | PAY-OAF | 3.52 | 1.61 | 1.54 |
| 2 | A | 401 | 8PH | PAZ-OAG | 3.52 | 1.61 | 1.54 |
| 2 | E | 401 | 8PH | PAY-OAF | 3.52 | 1.61 | 1.54 |
| 2 | D | 401 | 8PH | PAY-OAE | 3.52 | 1.61 | 1.54 |
| 2 | F | 401 | 8PH | PAY-OAF | 3.52 | 1.61 | 1.54 |
| 2 | F | 402 | 8PH | PAZ-OAG | 3.52 | 1.61 | 1.54 |
| 2 | E | 401 | 8PH | PAY-OAE | 3.53 | 1.61 | 1.54 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | D | 401 | 8PH | PAY-OAF | 3.54 | 1.61 | 1.54 |
| 2 | A | 403 | 8PH | PAZ-OAG | 3.54 | 1.61 | 1.54 |
| 2 | A | 403 | 8PH | PAZ-OAH | 6.79 | 1.61 | 1.50 |
| 2 | E | 401 | 8PH | PAZ-OAH | 6.81 | 1.61 | 1.50 |
| 2 | D | 401 | 8PH | PAZ-OAH | 6.82 | 1.61 | 1.50 |
| 2 | F | 401 | 8PH | PAZ-OAH | 6.84 | 1.61 | 1.50 |
| 2 | C | 401 | 8PH | PAZ-OAH | 6.85 | 1.61 | 1.50 |
| 2 | A | 401 | 8PH | PAZ-OAH | 6.86 | 1.61 | 1.50 |
| 2 | B | 401 | 8PH | PAZ-OAH | 6.87 | 1.61 | 1.50 |
| 2 | F | 402 | 8PH | PAZ-OAH | 6.91 | 1.61 | 1.50 |

All (40) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 401 | 8PH | PAZ-CAX-PAY | -3.27 | 107.84 | 112.84 |
| 2 | A | 401 | 8PH | OAG-PAZ-OAH | -3.00 | 105.92 | 113.04 |
| 2 | F | 402 | 8PH | OAG-PAZ-OAH | -2.97 | 106.00 | 113.04 |
| 2 | D | 401 | 8PH | OAG-PAZ-OAH | -2.95 | 106.05 | 113.04 |
| 2 | A | 403 | 8PH | OAG-PAZ-OAH | -2.93 | 106.11 | 113.04 |
| 2 | B | 401 | 8PH | OAG-PAZ-OAH | -2.89 | 106.20 | 113.04 |
| 2 | E | 401 | 8PH | OAG-PAZ-OAH | -2.87 | 106.24 | 113.04 |
| 2 | C | 401 | 8PH | OAG-PAZ-OAH | -2.86 | 106.26 | 113.04 |
| 2 | F | 401 | 8PH | OAG-PAZ-OAH | -2.86 | 106.26 | 113.04 |
| 2 | F | 401 | 8PH | PAZ-CAX-PAY | -2.78 | 108.59 | 112.84 |
| 2 | C | 401 | 8PH | PAZ-CAX-PAY | -2.76 | 108.62 | 112.84 |
| 2 | B | 401 | 8PH | PAZ-CAX-PAY | -2.67 | 108.77 | 112.84 |
| 2 | F | 402 | 8PH | PAZ-CAX-PAY | -2.51 | 109.00 | 112.84 |
| 2 | E | 401 | 8PH | PAZ-CAX-PAY | -2.40 | 109.17 | 112.84 |
| 2 | D | 401 | 8PH | PAZ-CAX-PAY | -2.37 | 109.22 | 112.84 |
| 2 | A | 403 | 8PH | PAZ-CAX-PAY | -2.24 | 109.42 | 112.84 |
| 2 | E | 401 | 8PH | PAZ-CAX-OAD | 2.48 | 112.45 | 107.60 |
| 2 | D | 401 | 8PH | PAZ-CAX-OAD | 2.71 | 112.91 | 107.60 |
| 2 | E | 401 | 8PH | PAY-CAX-OAD | 2.77 | 113.03 | 107.60 |
| 2 | D | 401 | 8PH | PAY-CAX-OAD | 2.82 | 113.12 | 107.60 |
| 2 | A | 401 | 8PH | PAZ-CAX-OAD | 2.86 | 113.21 | 107.60 |
| 2 | F | 401 | 8PH | OAC-PAZ-CAX | 2.91 | 112.39 | 105.90 |
| 2 | E | 401 | 8PH | OAC-PAZ-CAX | 2.93 | 112.44 | 105.90 |
| 2 | B | 401 | 8PH | PAZ-CAX-OAD | 2.93 | 113.34 | 107.60 |
| 2 | A | 403 | 8PH | PAY-CAX-OAD | 2.95 | 113.37 | 107.60 |
| 2 | A | 403 | 8PH | PAZ-CAX-OAD | 2.96 | 113.39 | 107.60 |
| 2 | F | 401 | 8PH | PAZ-CAX-OAD | 2.96 | 113.39 | 107.60 |
| 2 | A | 401 | 8PH | PAY-CAX-OAD | 2.96 | 113.40 | 107.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 401 | 8PH | PAZ-CAX-OAD | 2.98 | 113.43 | 107.60 |
| 2 | D | 401 | 8PH | OAC-PAZ-CAX | 3.01 | 112.62 | 105.90 |
| 2 | F | 402 | 8PH | PAZ-CAX-OAD | 3.04 | 113.54 | 107.60 |
| 2 | A | 403 | 8PH | OAC-PAZ-CAX | 3.04 | 112.69 | 105.90 |
| 2 | A | 401 | 8PH | OAC-PAZ-CAX | 3.07 | 112.74 | 105.90 |
| 2 | C | 401 | 8PH | PAY-CAX-OAD | 3.07 | 113.62 | 107.60 |
| 2 | C | 401 | 8PH | OAC-PAZ-CAX | 3.07 | 112.76 | 105.90 |
| 2 | B | 401 | 8PH | OAC-PAZ-CAX | 3.09 | 112.78 | 105.90 |
| 2 | B | 401 | 8PH | PAY-CAX-OAD | 3.09 | 113.65 | 107.60 |
| 2 | F | 402 | 8PH | PAY-CAX-OAD | 3.13 | 113.72 | 107.60 |
| 2 | F | 402 | 8PH | OAC-PAZ-CAX | 3.16 | 112.95 | 105.90 |
| 2 | F | 401 | 8PH | PAY-CAX-OAD | 3.22 | 113.90 | 107.60 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 25 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | A | 401 | 8PH | 1 | 0 |
| 2 | A | 402 | 8PH | 1 | 0 |
| 2 | A | 403 | 8PH | 1 | 0 |
| 2 | B | 401 | 8PH | 6 | 0 |
| 2 | B | 402 | 8PH | 2 | 0 |
| 2 | C | 401 | 8PH | 4 | 0 |
| 2 | D | 401 | 8PH | 2 | 0 |
| 2 | E | 401 | 8PH | 4 | 0 |
| 2 | F | 401 | 8PH | 4 | 0 |
| 2 | F | 402 | 8PH | 1 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

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 | 334/360 (92%) | -0.03 | 18 (5%) 29 33 | 17, 32, 68, 114 | 0 |
| 1 | B | 334/360 (92%) | 0.22 | 27 (8%) 15 16 | 20, 36, 74, 119 | 0 |
| 1 | C | 334/360 (92%) | 0.01 | 14 (4%) 40 45 | 19, 35, 63, 107 | 0 |
| 1 | D | 334/360 (92%) | 0.35 | 34 (10%) 9 9 | 22, 48, 86, 123 | 0 |
| 1 | E | 334/360 (92%) | 0.34 | 24 (7%) 18 20 | 28, 48, 85, 123 | 0 |
| 1 | F | 334/360 (92%) | 0.62 | 35 (10%) 8 8 | 28, 56, 95, 137 | 0 |
| All | All | 2004/2160 (92%) | 0.25 | 152 (7%) 17 18 | 17, 41, 86, 137 | 0 |

All (152) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 321 | ALA | 15.3 |
| 1 | F | 320 | GLN | 15.1 |
| 1 | F | 319 | GLY | 10.6 |
| 1 | B | 321 | ALA | 10.0 |
| 1 | D | 319 | GLY | 9.6 |
| 1 | F | 323 | THR | 9.4 |
| 1 | E | 323 | THR | 8.5 |
| 1 | D | 321 | ALA | 8.2 |
| 1 | F | 322 | VAL | 7.9 |
| 1 | E | 320 | GLN | 7.3 |
| 1 | F | 318 | LEU | 7.1 |
| 1 | A | 320 | GLN | 7.1 |
| 1 | B | 317 | ARG | 6.8 |
| 1 | B | 319 | GLY | 6.8 |
| 1 | B | 320 | GLN | 6.6 |
| 1 | F | 315 | LEU | 6.3 |
| 1 | B | 318 | LEU | 6.2 |
| 1 | E | 315 | LEU | 6.1 |
| 1 | C | 321 | ALA | 6.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 317 | ARG | 5.9 |
| 1 | D | 318 | LEU | 5.6 |
| 1 | A | 321 | ALA | 5.5 |
| 1 | E | 36 | LEU | 5.1 |
| 1 | A | 315 | LEU | 5.1 |
| 1 | F | 36 | LEU | 5.1 |
| 1 | D | 323 | THR | 5.1 |
| 1 | E | 319 | GLY | 5.0 |
| 1 | F | 313 | ALA | 4.9 |
| 1 | F | 161 | HIS | 4.8 |
| 1 | D | 317 | ARG | 4.8 |
| 1 | D | 322 | VAL | 4.7 |
| 1 | C | 322 | VAL | 4.6 |
| 1 | B | 322 | VAL | 4.6 |
| 1 | C | 36 | LEU | 4.5 |
| 1 | E | 322 | VAL | 4.5 |
| 1 | F | 316 | ILE | 4.4 |
| 1 | D | 316 | ILE | 4.4 |
| 1 | F | 351 | ASP | 4.3 |
| 1 | B | 316 | ILE | 4.2 |
| 1 | B | 315 | LEU | 4.2 |
| 1 | E | 159 | ASP | 4.2 |
| 1 | E | 318 | LEU | 4.2 |
| 1 | D | 320 | GLN | 4.1 |
| 1 | D | 241 | LYS | 4.1 |
| 1 | D | 160 | LYS | 4.0 |
| 1 | D | 36 | LEU | 4.0 |
| 1 | B | 351 | ASP | 3.9 |
| 1 | F | 37 | SER | 3.9 |
| 1 | E | 321 | ALA | 3.9 |
| 1 | A | 36 | LEU | 3.8 |
| 1 | E | 324 | LEU | 3.8 |
| 1 | A | 322 | VAL | 3.8 |
| 1 | E | 86 | MET | 3.7 |
| 1 | B | 323 | THR | 3.7 |
| 1 | F | 317 | ARG | 3.7 |
| 1 | D | 90 | VAL | 3.6 |
| 1 | B | 36 | LEU | 3.6 |
| 1 | D | 315 | LEU | 3.6 |
| 1 | F | 241 | LYS | 3.6 |
| 1 | F | 352 | SER | 3.5 |
| 1 | C | 313 | ALA | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 347 | HIS | 3.5 |
| 1 | E | 317 | ARG | 3.5 |
| 1 | A | 324 | LEU | 3.5 |
| 1 | C | 320 | GLN | 3.5 |
| 1 | B | 324 | LEU | 3.5 |
| 1 | E | 37 | SER | 3.4 |
| 1 | A | 312 | GLY | 3.4 |
| 1 | C | 316 | ILE | 3.4 |
| 1 | F | 112 | MET | 3.4 |
| 1 | C | 318 | LEU | 3.3 |
| 1 | E | 87 | THR | 3.3 |
| 1 | D | 352 | SER | 3.3 |
| 1 | D | 52 | ARG | 3.2 |
| 1 | D | 159 | ASP | 3.2 |
| 1 | E | 326 | MET | 3.2 |
| 1 | B | 259 | LEU | 3.1 |
| 1 | B | 312 | GLY | 3.1 |
| 1 | B | 313 | ALA | 3.0 |
| 1 | D | 115 | LYS | 3.0 |
| 1 | D | 347 | HIS | 3.0 |
| 1 | E | 52 | ARG | 3.0 |
| 1 | A | 313 | ALA | 2.9 |
| 1 | B | 241 | LYS | 2.9 |
| 1 | D | 166 | GLN | 2.9 |
| 1 | D | 91 | GLU | 2.9 |
| 1 | E | 312 | GLY | 2.9 |
| 1 | F | 369 | GLN | 2.9 |
| 1 | F | 76 | LEU | 2.9 |
| 1 | D | 263 | ILE | 2.8 |
| 1 | F | 225 | GLN | 2.8 |
| 1 | F | 159 | ASP | 2.8 |
| 1 | A | 317 | ARG | 2.8 |
| 1 | A | 318 | LEU | 2.8 |
| 1 | F | 217 | ILE | 2.7 |
| 1 | C | 315 | LEU | 2.7 |
| 1 | B | 350 | PRO | 2.7 |
| 1 | E | 369 | GLN | 2.7 |
| 1 | C | 37 | SER | 2.7 |
| 1 | B | 159 | ASP | 2.7 |
| 1 | D | 262 | LEU | 2.7 |
| 1 | C | 225 | GLN | 2.7 |
| 1 | F | 88 | ILE | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 52 | ARG | 2.7 |
| 1 | A | 323 | THR | 2.7 |
| 1 | B | 314 | VAL | 2.6 |
| 1 | C | 319 | GLY | 2.6 |
| 1 | A | 228 | ARG | 2.6 |
| 1 | F | 52 | ARG | 2.5 |
| 1 | C | 228 | ARG | 2.5 |
| 1 | D | 231 | TRP | 2.5 |
| 1 | E | 313 | ALA | 2.5 |
| 1 | F | 226 | GLY | 2.5 |
| 1 | E | 107 | PRO | 2.5 |
| 1 | B | 250 | GLU | 2.5 |
| 1 | F | 324 | LEU | 2.5 |
| 1 | B | 263 | ILE | 2.5 |
| 1 | D | 119 | ARG | 2.5 |
| 1 | E | 281 | ARG | 2.5 |
| 1 | F | 250 | GLU | 2.4 |
| 1 | B | 228 | ARG | 2.4 |
| 1 | F | 108 | ASP | 2.4 |
| 1 | D | 226 | GLY | 2.4 |
| 1 | A | 351 | ASP | 2.3 |
| 1 | A | 248 | LEU | 2.3 |
| 1 | D | 117 | LYS | 2.3 |
| 1 | A | 314 | VAL | 2.3 |
| 1 | F | 231 | TRP | 2.3 |
| 1 | D | 311 | LYS | 2.2 |
| 1 | B | 262 | LEU | 2.2 |
| 1 | E | 316 | ILE | 2.2 |
| 1 | B | 347 | HIS | 2.2 |
| 1 | F | 87 | THR | 2.2 |
| 1 | F | 281 | ARG | 2.2 |
| 1 | D | 369 | GLN | 2.2 |
| 1 | C | 323 | THR | 2.2 |
| 1 | E | 108 | ASP | 2.2 |
| 1 | D | 37 | SER | 2.1 |
| 1 | D | 259 | LEU | 2.1 |
| 1 | B | 242 | LYS | 2.1 |
| 1 | D | 86 | MET | 2.1 |
| 1 | F | 314 | VAL | 2.1 |
| 1 | E | 88 | ILE | 2.1 |
| 1 | A | 316 | ILE | 2.1 |
| 1 | F | 300 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 228 | ARG | 2.0 |
| 1 | A | 113 | GLU | 2.0 |
| 1 | A | 225 | GLN | 2.0 |
| 1 | D | 233 | GLN | 2.0 |
| 1 | F | 115 | LYS | 2.0 |
| 1 | D | 161 | HIS | 2.0 |
| 1 | B | 53 | SER | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 8PH | A | 402 | 8/26 | 0.92 | 0.30 | 3.94 | 36,38,40,42 | 0 |
| 2 | 8PH | D | 401 | 26/26 | 0.77 | 0.25 | 3.52 | 52,103,114,115 | 0 |
| 2 | 8PH | C | 401 | 26/26 | 0.82 | 0.23 | 2.76 | 33,86,96,97 | 0 |
| 2 | 8PH | E | 401 | 26/26 | 0.64 | 0.33 | 2.74 | 47,93,106,106 | 0 |
| 2 | 8PH | A | 401 | 26/26 | 0.89 | 0.18 | 2.59 | 27,54,69,70 | 0 |
| 2 | 8PH | F | 401 | 26/26 | 0.82 | 0.24 | 1.83 | 50,92,102,102 | 0 |
| 2 | 8PH | A | 403 | 18/26 | 0.80 | 0.19 | 1.00 | 101,106,107,107 | 0 |
| 2 | 8PH | B | 402 | 9/26 | 0.92 | 0.20 | 0.78 | 38,38,40,42 | 0 |
| 2 | 8PH | B | 401 | 26/26 | 0.87 | 0.17 | 0.77 | 31,81,93,94 | 0 |
| 2 | 8PH | F | 402 | 26/26 | 0.74 | 0.33 | 0.70 | 62,101,110,110 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.