# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 11:41 am BST

| | | |
|---|---|---|
| PDB ID | : | 6TJP |
| Title | : | Crystal structure of T7 bacteriophage portal protein, 13mer, closed valve - P212121 |
| Authors | : | Fabrega-Ferrer, M.; Cuervo, A.; Fernandez, F.J.; Machon, C.; Perez-Luque, R.; Pous, J.; Vega, M.C.; Carrascosa, J.L.; Coll, M. |
| Deposited on | : | 2019-11-26 |
| Resolution | : | 3.74 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

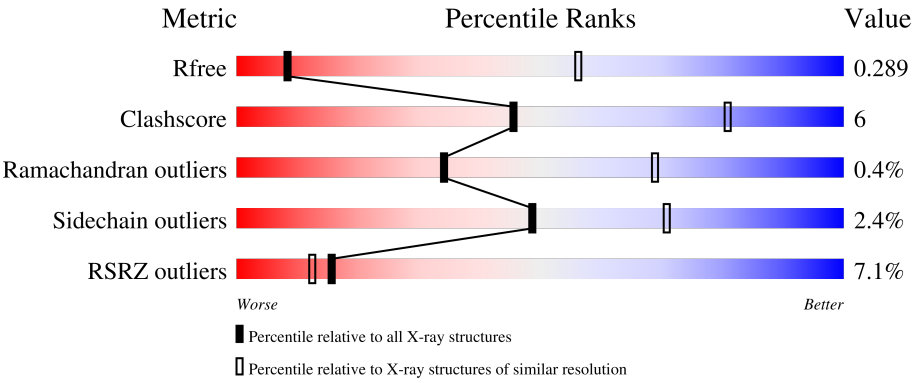
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36.2 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 3.74 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)) |
|---|---|---|
| $R_{free}$ | 130704 | 1001 (3.90-3.58) |
| Clashscore | 141614 | 1063 (3.90-3.58) |
| Ramachandran outliers | 138981 | 1027 (3.90-3.58) |
| Sidechain outliers | 138945 | 1023 (3.90-3.58) |
| RSRZ outliers | 127900 | 1006 (3.92-3.56) |

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 536 | 6% 75% 12% • 12% |
| 1 | B | 536 | 5% 74% 14% 12% |
| 1 | C | 536 | 9% 72% 16% • 12% |
| 1 | D | 536 | 7% 73% 15% 12% |
| 1 | E | 536 | 9% 73% 15% • 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 536 | 6% 70% 18% 12% |
| 1 | G | 536 | 5% 72% 16% 12% |
| 1 | H | 536 | 4% 71% 17% 12% |
| 1 | I | 536 | 5% 71% 17% 12% |
| 1 | J | 536 | 8% 70% 18% 12% |
| 1 | K | 536 | 6% 75% 13% 12% |
| 1 | L | 536 | 6% 73% 15% 12% |
| 1 | M | 536 | 5% 73% 15% 12% |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 48126 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 Portal protein.

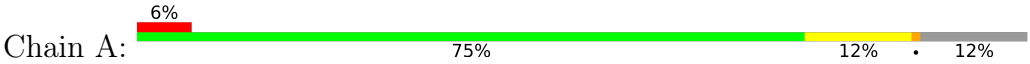
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 473 | Total | C | N | O | S | 2 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | B | 473 | Total | C | N | O | S | 1 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | C | 473 | Total | C | N | O | S | 2 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | D | 473 | Total | C | N | O | S | 2 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | E | 473 | Total | C | N | O | S | 2 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | F | 473 | Total | C | N | O | S | 1 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | G | 473 | Total | C | N | O | S | 2 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | H | 473 | Total | C | N | O | S | 3 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | I | 473 | Total | C | N | O | S | 1 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | J | 473 | Total | C | N | O | S | 3 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | K | 473 | Total | C | N | O | S | 1 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | L | 473 | Total | C | N | O | S | 2 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |
| 1 | M | 473 | Total | C | N | O | S | 2 | 0 | 0 |
| | | | 3702 | 2331 | 627 | 727 | 17 | | | |

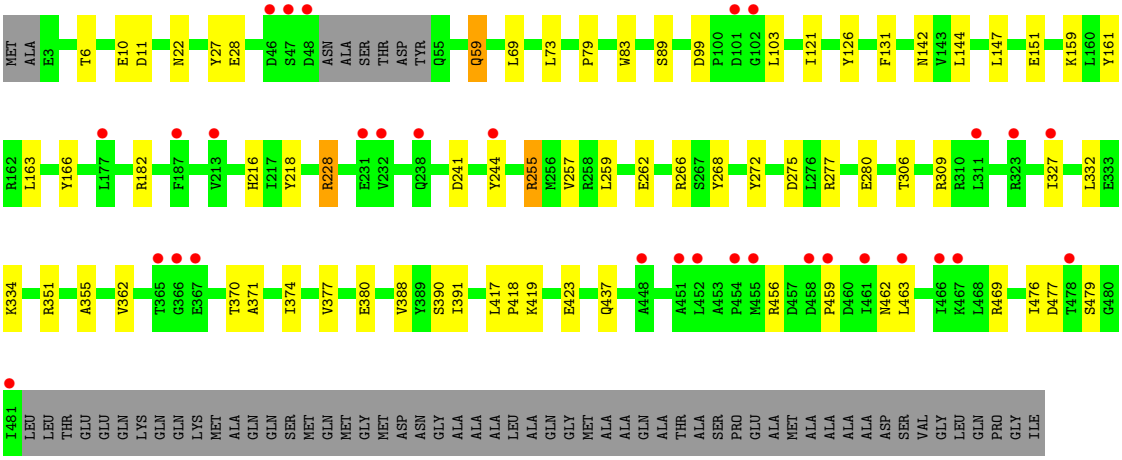
# 3 Residue-property plots (i)

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

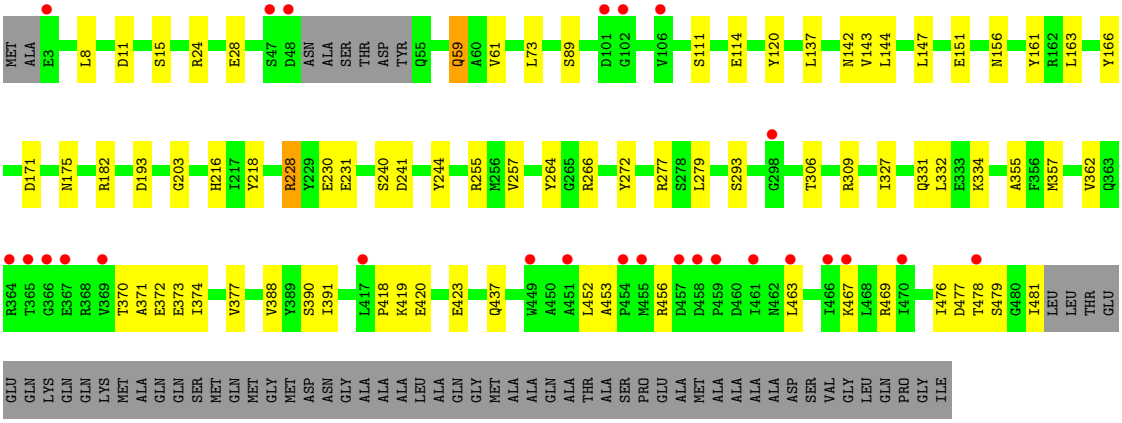
Chain A:



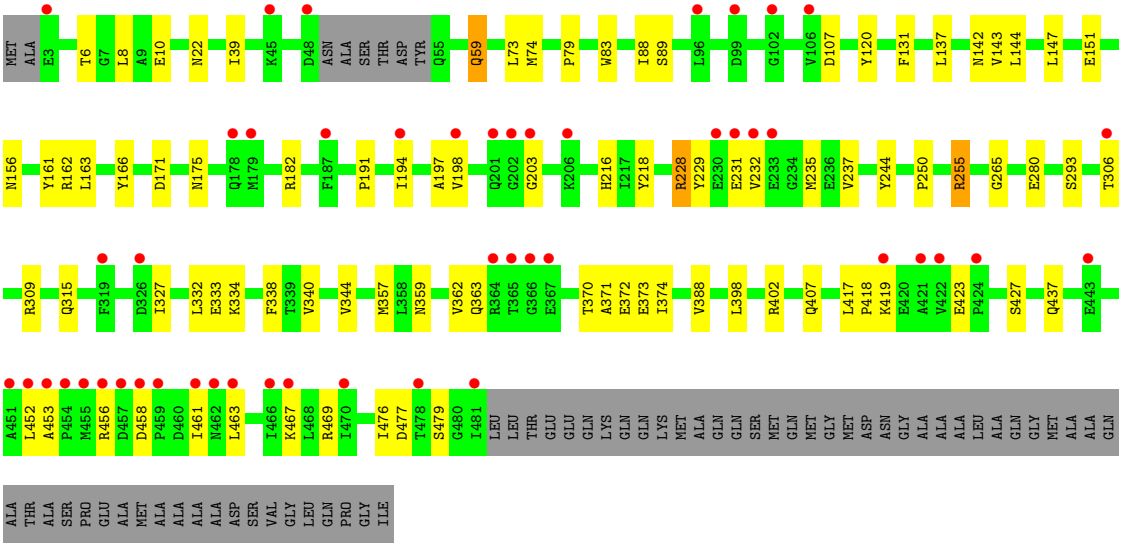
• Molecule 1: Portal protein

Chain B:

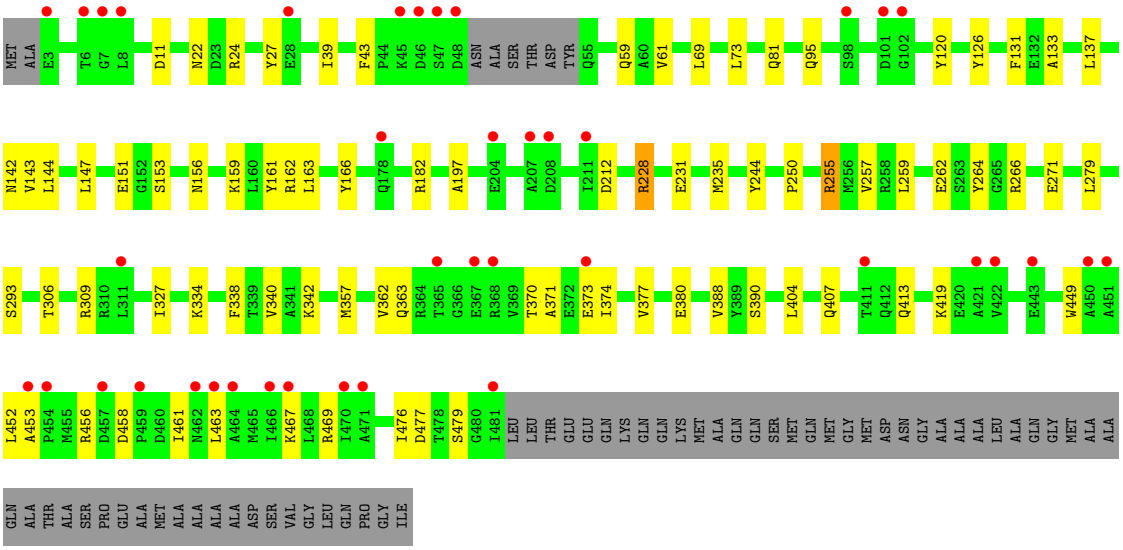
• Molecule 1: Portal protein

Chain C:



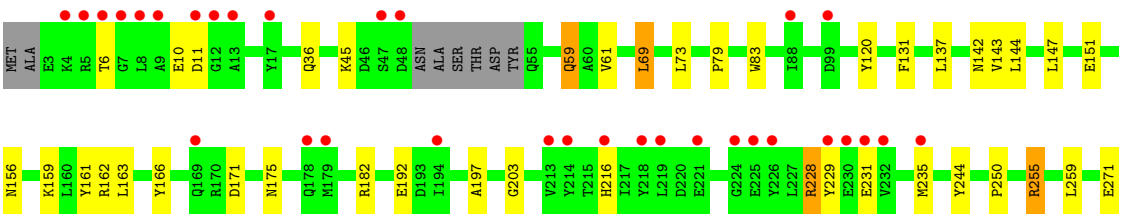
• Molecule 1: Portal protein

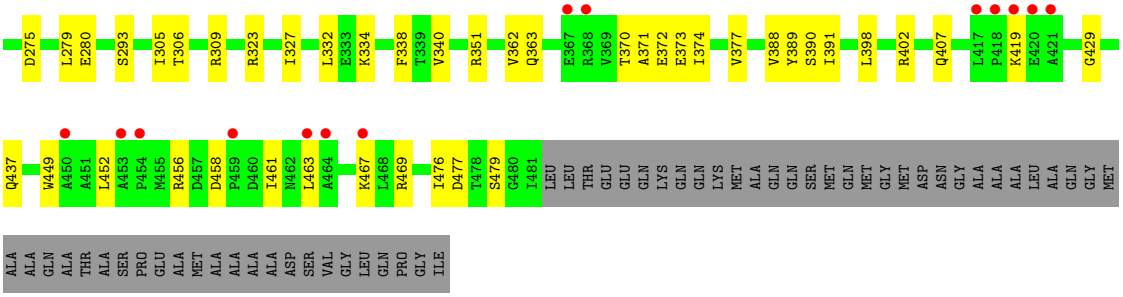
Chain D:

• Molecule 1: Portal protein

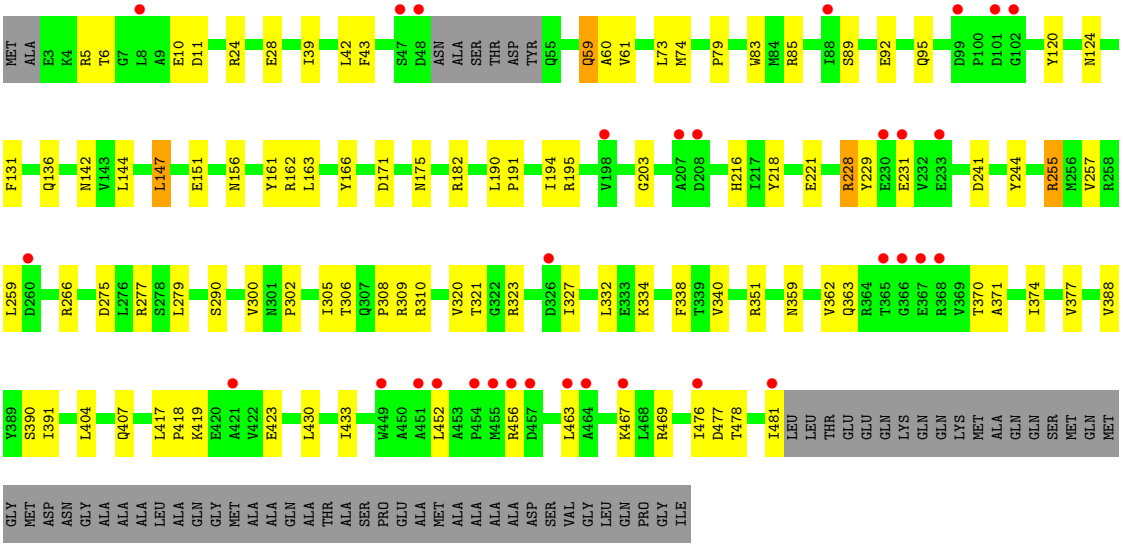
Chain E:



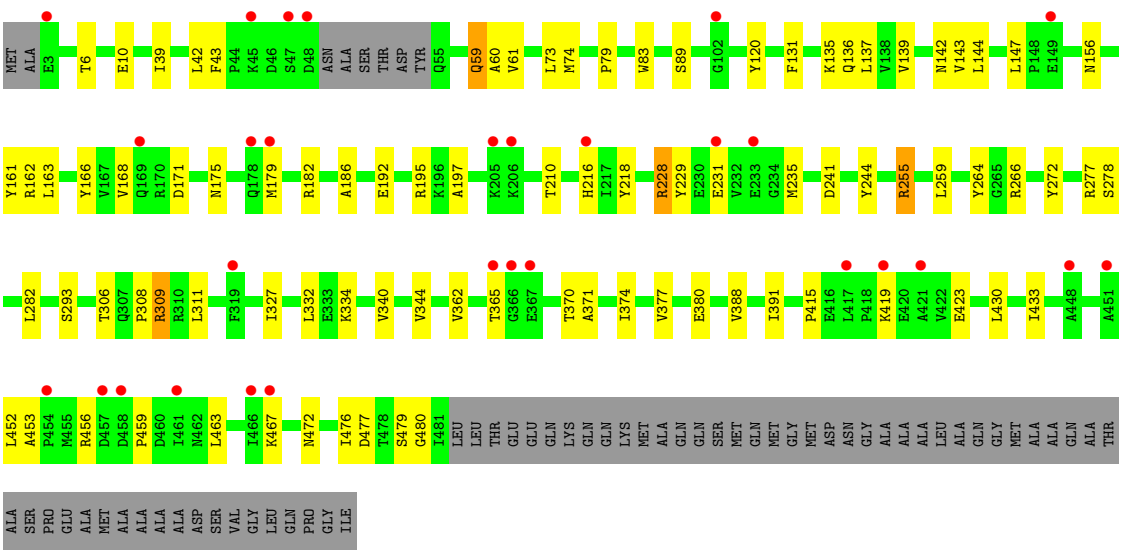
• Molecule 1: Portal protein

Chain F:

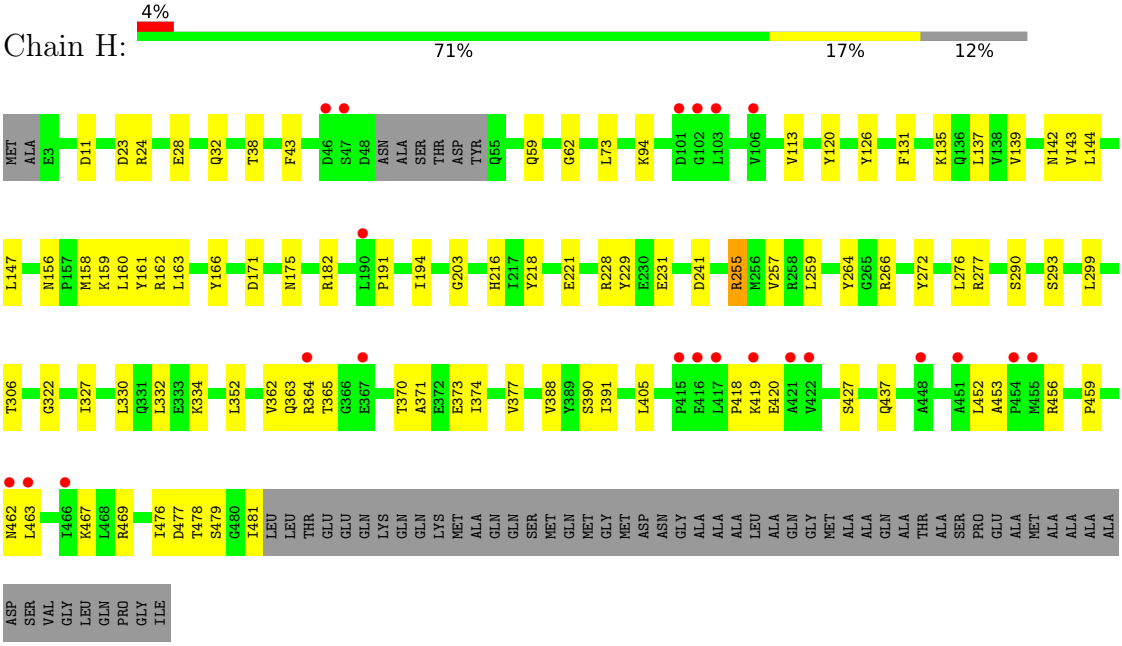
• Molecule 1: Portal protein

Chain G:

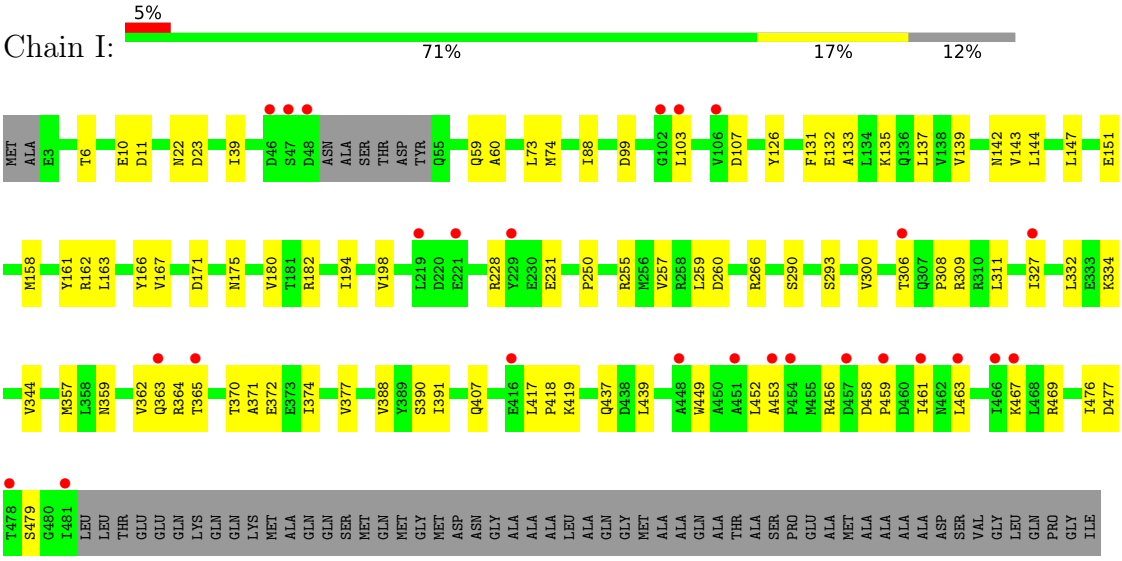
• Molecule 1: Portal protein

Chain H:



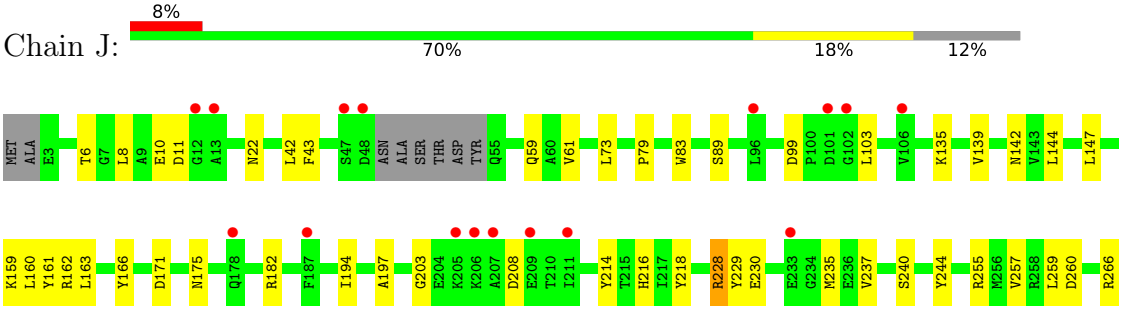

• Molecule 1: Portal protein

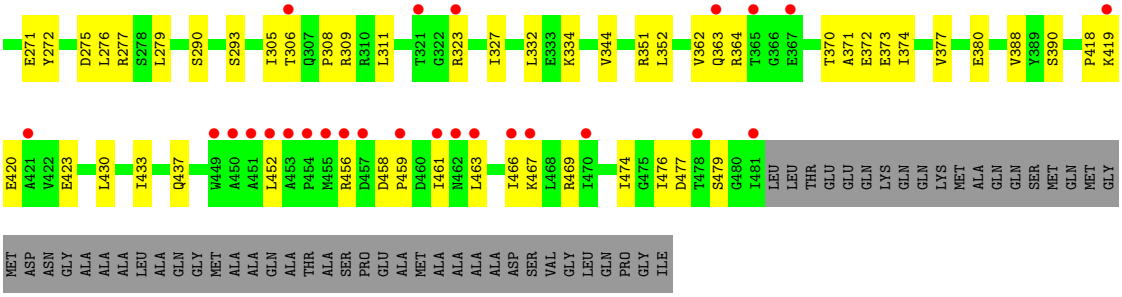
Chain I:




• Molecule 1: Portal protein

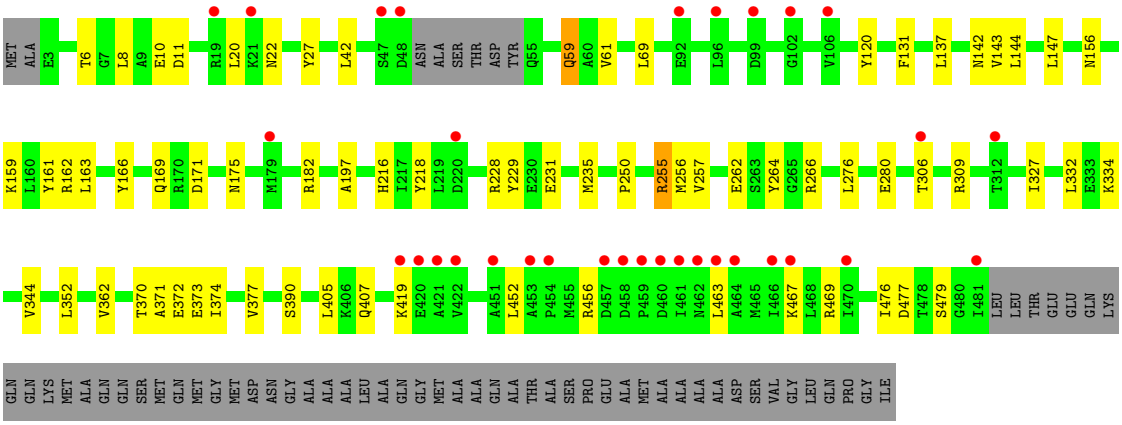
Chain J:





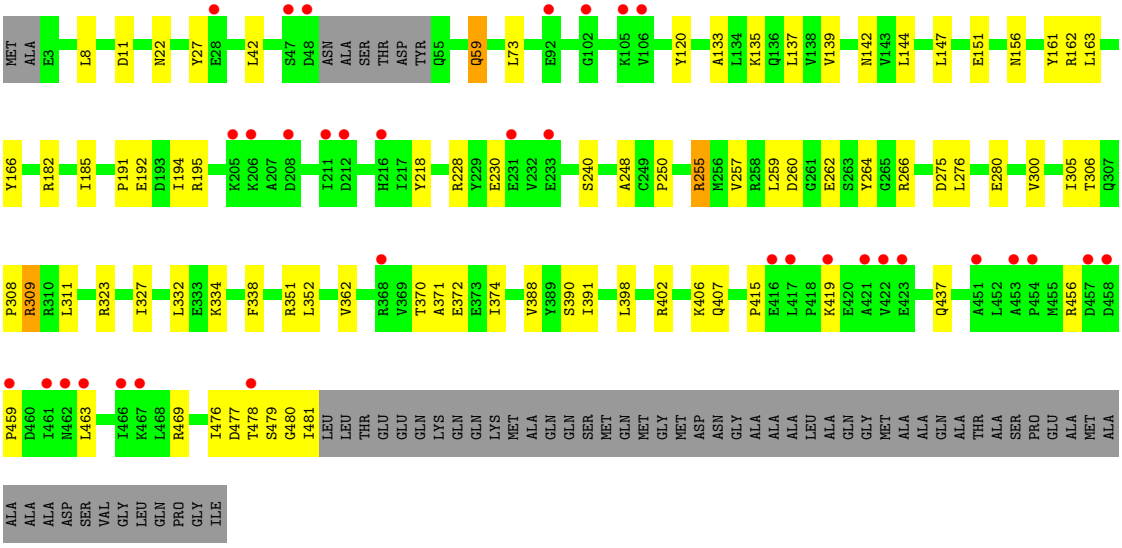
• Molecule 1: Portal protein

Chain K:

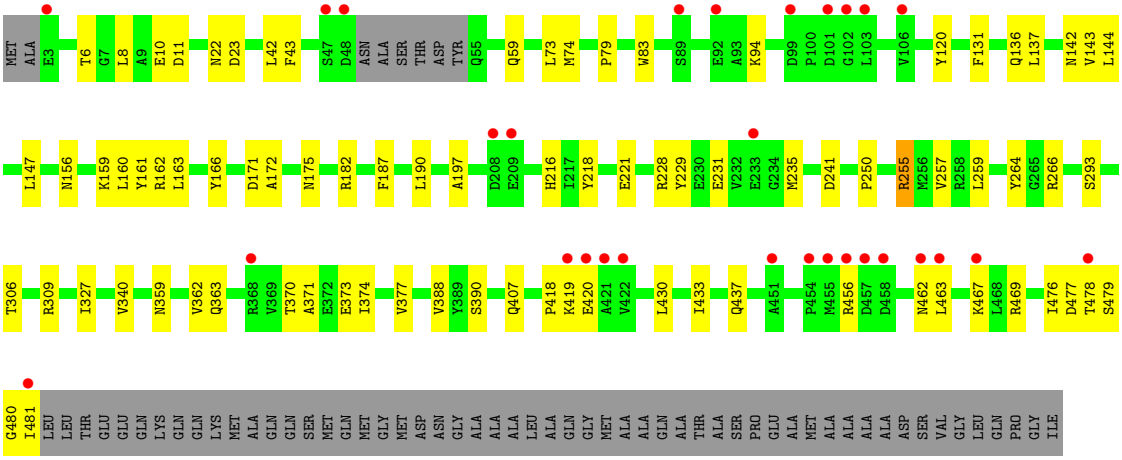
• Molecule 1: Portal protein

Chain L:

• Molecule 1: Portal protein

Chain M:


MET ALA E3 T6 G7 L8 A9 E10 D11 N22 D23 L42 F43 S47 D48 ASN ALA SER THR ASP TYR Q55 Q59 L73 M74 P79 W83 S89 E92 A93 K94 D99 P100 D101 G102 L103 V106 Y120 F131 Q136 L137 N142 V143 L144
L147 N156 K159 L160 Y161 R162 L163 Y166 D171 A172 N175 R182 F187 L190 A197 D208 E209 H216 I217 Y218 E221 R228 Y229 E230 E231 V232 E233 G234 M235 D241 P250 R255 M256 V257 R258 L259 Y264 G265 R266 S293
T306 R309 I327 V340 N359 V362 Q363 R368 V369 T370 A371 E372 E373 I374 V377 V388 Y389 S390 Q407 P418 K419 E420 A421 V422 L430 I433 Q437 A451 P454 M455 R456 D457 D458 N462 L463 K467 L468 R469 I476 D477 T478 S479
G480 I481 LEU LEU THR GLU GLU GLN LYS GLN GLN LYS MET ALA GLN GLN SER MET GLN MET GLY MET ASP ASN GLY ALA ALA ALA LEU ALA GLN GLY MET ALA ALA GLN ALA THR ALA SER PRO GLU ALA MET ALA ALA ALA ALA ASP SER VAL GLY LEU GLN PRO GLY ILE

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 119.85Å 238.57Å 265.61Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.47 – 3.74<br>49.47 – 3.74 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.5 (49.47-3.74)<br>98.5 (49.47-3.74) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.58 (at 3.77Å) | Xtriage |
| Refinement program | REFMAC 5.5, PHENIX 1.17.1_3660 | Depositor |
| R, $R_{free}$ | 0.244 , 0.286<br>0.257 , 0.289 | Depositor<br>DCC |
| $R_{free}$ test set | 3918 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 130.3 | Xtriage |
| Anisotropy | 0.431 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 108.9 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.42$, $< L^2 > = 0.25$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 48126 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 151.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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, 0.333 respectively for untwinned datasets, and 0.375, 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 | 0.26 | 0/3760 | 0.46 | 0/5089 |
| 1 | B | 0.26 | 0/3760 | 0.46 | 0/5089 |
| 1 | C | 0.26 | 0/3760 | 0.47 | 0/5089 |
| 1 | D | 0.26 | 0/3760 | 0.46 | 0/5089 |
| 1 | E | 0.26 | 0/3760 | 0.47 | 0/5089 |
| 1 | F | 0.27 | 0/3760 | 0.47 | 0/5089 |
| 1 | G | 0.27 | 0/3760 | 0.47 | 0/5089 |
| 1 | H | 0.26 | 0/3760 | 0.46 | 0/5089 |
| 1 | I | 0.26 | 0/3760 | 0.47 | 0/5089 |
| 1 | J | 0.27 | 0/3760 | 0.47 | 0/5089 |
| 1 | K | 0.27 | 0/3760 | 0.47 | 0/5089 |
| 1 | L | 0.26 | 0/3760 | 0.47 | 0/5089 |
| 1 | M | 0.26 | 0/3760 | 0.47 | 0/5089 |
| All | All | 0.26 | 0/48880 | 0.47 | 0/66157 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 3702 | 0 | 3710 | 44 | 0 |
| 1 | B | 3702 | 0 | 3710 | 48 | 2 |
| 1 | C | 3702 | 0 | 3710 | 50 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | D | 3702 | 0 | 3710 | 52 | 1 |
| 1 | E | 3702 | 0 | 3710 | 54 | 0 |
| 1 | F | 3702 | 0 | 3710 | 67 | 0 |
| 1 | G | 3702 | 0 | 3710 | 63 | 0 |
| 1 | H | 3702 | 0 | 3710 | 61 | 0 |
| 1 | I | 3702 | 0 | 3710 | 60 | 0 |
| 1 | J | 3702 | 0 | 3710 | 60 | 0 |
| 1 | K | 3702 | 0 | 3710 | 55 | 0 |
| 1 | L | 3702 | 0 | 3710 | 53 | 0 |
| 1 | M | 3702 | 0 | 3710 | 55 | 1 |
| All | All | 48126 | 0 | 48230 | 620 | 2 |

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 6.

All (620) 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:F:144:LEU:HB3 | 1:F:161:TYR:HB2 | 1.60 | 0.83 |
| 1:C:306:THR:HG21 | 1:C:327:ILE:HD11 | 1.66 | 0.78 |
| 1:C:479:SER:O | 1:D:469:ARG:NH2 | 2.16 | 0.78 |
| 1:I:162:ARG:HH22 | 1:J:259:LEU:HD22 | 1.50 | 0.77 |
| 1:K:456:ARG:HA | 1:K:463:LEU:HD11 | 1.66 | 0.76 |
| 1:M:306:THR:HG21 | 1:M:327:ILE:HD11 | 1.67 | 0.75 |
| 1:L:195:ARG:NH2 | 1:M:221:GLU:OE2 | 2.17 | 0.75 |
| 1:B:144:LEU:HB3 | 1:B:161:TYR:HB2 | 1.69 | 0.74 |
| 1:B:230:GLU:H | 1:B:240:SER:HB2 | 1.52 | 0.74 |
| 1:J:456:ARG:HA | 1:J:463:LEU:HD11 | 1.68 | 0.74 |
| 1:B:306:THR:HG21 | 1:B:327:ILE:HD11 | 1.70 | 0.73 |
| 1:D:479:SER:O | 1:E:469:ARG:NH2 | 2.21 | 0.73 |
| 1:K:306:THR:HG21 | 1:K:327:ILE:HD11 | 1.70 | 0.73 |
| 1:D:306:THR:HG21 | 1:D:327:ILE:HD11 | 1.69 | 0.73 |
| 1:H:306:THR:HG21 | 1:H:327:ILE:HD11 | 1.71 | 0.73 |
| 1:G:306:THR:HG21 | 1:G:327:ILE:HD11 | 1.69 | 0.73 |
| 1:E:144:LEU:HB3 | 1:E:161:TYR:HB2 | 1.70 | 0.72 |
| 1:K:42:LEU:O | 1:K:162:ARG:NH1 | 2.23 | 0.71 |
| 1:D:24:ARG:NH1 | 1:D:166:TYR:O | 2.23 | 0.71 |
| 1:I:476:ILE:HG22 | 1:I:477:ASP:H | 1.55 | 0.71 |
| 1:E:306:THR:HG21 | 1:E:327:ILE:HD11 | 1.72 | 0.71 |
| 1:B:293:SER:O | 1:C:334:LYS:NZ | 2.24 | 0.70 |
| 1:B:479:SER:O | 1:C:469:ARG:NH2 | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:162:ARG:HH22 | 1:F:259:LEU:HD22 | 1.57 | 0.70 |
| 1:G:144:LEU:HB3 | 1:G:161:TYR:HB2 | 1.74 | 0.70 |
| 1:L:306:THR:HG21 | 1:L:327:ILE:HD11 | 1.72 | 0.70 |
| 1:I:306:THR:HG21 | 1:I:327:ILE:HD11 | 1.74 | 0.70 |
| 1:J:476:ILE:HG22 | 1:J:477:ASP:H | 1.57 | 0.70 |
| 1:B:476:ILE:HG22 | 1:B:477:ASP:H | 1.57 | 0.69 |
| 1:C:362:VAL:HG11 | 1:C:374:ILE:HG12 | 1.74 | 0.69 |
| 1:I:456:ARG:HA | 1:I:463:LEU:HD11 | 1.73 | 0.69 |
| 1:K:476:ILE:HG22 | 1:K:477:ASP:H | 1.58 | 0.69 |
| 1:D:144:LEU:HB3 | 1:D:161:TYR:HB2 | 1.73 | 0.69 |
| 1:D:476:ILE:HG22 | 1:D:477:ASP:H | 1.59 | 0.68 |
| 1:E:476:ILE:HG22 | 1:E:477:ASP:H | 1.57 | 0.68 |
| 1:A:476:ILE:HG22 | 1:A:477:ASP:H | 1.59 | 0.67 |
| 1:L:476:ILE:HG22 | 1:L:477:ASP:H | 1.57 | 0.67 |
| 1:G:476:ILE:HG22 | 1:G:477:ASP:H | 1.58 | 0.67 |
| 1:H:476:ILE:HG22 | 1:H:477:ASP:H | 1.59 | 0.67 |
| 1:A:144:LEU:HB3 | 1:A:161:TYR:HB2 | 1.77 | 0.67 |
| 1:L:162:ARG:HH22 | 1:M:259:LEU:HD22 | 1.59 | 0.67 |
| 1:L:456:ARG:HA | 1:L:463:LEU:HD11 | 1.78 | 0.66 |
| 1:J:306:THR:HG21 | 1:J:327:ILE:HD11 | 1.77 | 0.66 |
| 1:E:456:ARG:HA | 1:E:463:LEU:HD11 | 1.77 | 0.66 |
| 1:C:476:ILE:HG22 | 1:C:477:ASP:H | 1.60 | 0.65 |
| 1:F:476:ILE:HG22 | 1:F:477:ASP:H | 1.61 | 0.65 |
| 1:F:306:THR:HG21 | 1:F:327:ILE:HD11 | 1.78 | 0.65 |
| 1:I:479:SER:O | 1:J:469:ARG:NH2 | 2.30 | 0.65 |
| 1:E:36:GLN:HB2 | 1:E:45:LYS:HD2 | 1.77 | 0.64 |
| 1:I:257:VAL:HB | 1:I:266:ARG:HB2 | 1.78 | 0.64 |
| 1:I:144:LEU:HB3 | 1:I:161:TYR:HB2 | 1.78 | 0.64 |
| 1:L:362:VAL:HG11 | 1:L:374:ILE:HG12 | 1.80 | 0.64 |
| 1:D:362:VAL:HG11 | 1:D:374:ILE:HG12 | 1.79 | 0.64 |
| 1:A:456:ARG:HA | 1:A:463:LEU:HD11 | 1.80 | 0.63 |
| 1:D:456:ARG:HA | 1:D:463:LEU:HD11 | 1.80 | 0.63 |
| 1:A:306:THR:HG21 | 1:A:327:ILE:HD11 | 1.81 | 0.63 |
| 1:M:476:ILE:HG22 | 1:M:477:ASP:H | 1.62 | 0.62 |
| 1:G:137:LEU:HD13 | 1:G:143:VAL:HG23 | 1.80 | 0.62 |
| 1:I:362:VAL:HG11 | 1:I:374:ILE:HG12 | 1.79 | 0.62 |
| 1:E:362:VAL:HG11 | 1:E:374:ILE:HG12 | 1.82 | 0.62 |
| 1:K:137:LEU:HD13 | 1:K:143:VAL:HG23 | 1.82 | 0.62 |
| 1:F:456:ARG:HA | 1:F:463:LEU:HD11 | 1.80 | 0.62 |
| 1:H:144:LEU:HB3 | 1:H:161:TYR:HB2 | 1.82 | 0.62 |
| 1:C:137:LEU:HD13 | 1:C:143:VAL:HG23 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:480:GLY:O | 1:H:462:ASN:ND2 | 2.33 | 0.61 |
| 1:J:362:VAL:HG11 | 1:J:374:ILE:HG12 | 1.82 | 0.61 |
| 1:C:456:ARG:HA | 1:C:463:LEU:HD11 | 1.81 | 0.61 |
| 1:C:197:ALA:HB1 | 1:C:235:MET:HE3 | 1.82 | 0.61 |
| 1:G:456:ARG:HA | 1:G:463:LEU:HD11 | 1.83 | 0.61 |
| 1:B:456:ARG:HA | 1:B:463:LEU:HD11 | 1.83 | 0.61 |
| 1:F:300:VAL:HG21 | 1:F:308:PRO:HD3 | 1.83 | 0.60 |
| 1:L:275:ASP:OD2 | 1:L:351:ARG:NH1 | 2.33 | 0.60 |
| 1:I:73:LEU:HD21 | 1:I:388:VAL:HG23 | 1.83 | 0.60 |
| 1:L:120:TYR:OH | 1:L:156:ASN:ND2 | 2.27 | 0.60 |
| 1:H:479:SER:O | 1:I:469:ARG:NH2 | 2.35 | 0.59 |
| 1:K:144:LEU:HB3 | 1:K:161:TYR:HB2 | 1.84 | 0.59 |
| 1:A:6:THR:HA | 1:A:10:GLU:HA | 1.83 | 0.59 |
| 1:M:362:VAL:HG11 | 1:M:374:ILE:HG12 | 1.84 | 0.59 |
| 1:H:362:VAL:HG11 | 1:H:374:ILE:HG12 | 1.84 | 0.59 |
| 1:H:456:ARG:HA | 1:H:463:LEU:HD11 | 1.83 | 0.59 |
| 1:B:142:ASN:HD21 | 1:B:264:TYR:HB3 | 1.67 | 0.59 |
| 1:K:216:HIS:HE1 | 1:K:218:TYR:HB3 | 1.67 | 0.59 |
| 1:F:162:ARG:HH22 | 1:G:259:LEU:HD22 | 1.66 | 0.59 |
| 1:J:144:LEU:HB3 | 1:J:161:TYR:HB2 | 1.84 | 0.59 |
| 1:K:452:LEU:HD11 | 1:K:467:LYS:HE3 | 1.85 | 0.58 |
| 1:F:142:ASN:HD22 | 1:F:163:LEU:HD12 | 1.68 | 0.58 |
| 1:K:11:ASP:OD1 | 1:K:11:ASP:N | 2.35 | 0.58 |
| 1:M:43:PHE:HD2 | 1:M:136:GLN:HE22 | 1.51 | 0.58 |
| 1:I:293:SER:O | 1:J:334:LYS:NZ | 2.35 | 0.58 |
| 1:K:362:VAL:HG11 | 1:K:374:ILE:HG12 | 1.85 | 0.58 |
| 1:J:479:SER:O | 1:K:469:ARG:NH2 | 2.35 | 0.58 |
| 1:E:142:ASN:HD22 | 1:E:163:LEU:HD12 | 1.68 | 0.58 |
| 1:M:144:LEU:HB3 | 1:M:161:TYR:HB2 | 1.86 | 0.57 |
| 1:B:362:VAL:HG11 | 1:B:374:ILE:HG12 | 1.86 | 0.57 |
| 1:A:11:ASP:OD1 | 1:A:11:ASP:N | 2.37 | 0.57 |
| 1:A:259:LEU:HD22 | 1:M:162:ARG:HH22 | 1.69 | 0.57 |
| 1:M:120:TYR:OH | 1:M:156:ASN:ND2 | 2.37 | 0.57 |
| 1:C:171:ASP:OD1 | 1:C:175:ASN:N | 2.36 | 0.57 |
| 1:F:24:ARG:NH1 | 1:F:166:TYR:O | 2.34 | 0.57 |
| 1:I:11:ASP:OD1 | 1:I:11:ASP:N | 2.35 | 0.57 |
| 1:B:171:ASP:OD1 | 1:B:175:ASN:N | 2.37 | 0.57 |
| 1:K:162:ARG:HH22 | 1:L:259:LEU:HD22 | 1.69 | 0.57 |
| 1:C:120:TYR:OH | 1:C:156:ASN:ND2 | 2.37 | 0.56 |
| 1:E:338:PHE:CD2 | 1:F:340:VAL:HG13 | 2.40 | 0.56 |
| 1:D:452:LEU:HD11 | 1:D:467:LYS:HE3 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:11:ASP:OD1 | 1:H:11:ASP:N | 2.39 | 0.56 |
| 1:M:478:THR:HA | 1:M:481:ILE:HD12 | 1.87 | 0.56 |
| 1:A:257:VAL:HB | 1:A:266:ARG:HB2 | 1.87 | 0.56 |
| 1:I:371:ALA:HB2 | 1:J:372:GLU:HG3 | 1.88 | 0.56 |
| 1:J:437:GLN:OE1 | 1:J:437:GLN:N | 2.37 | 0.56 |
| 1:M:456:ARG:HA | 1:M:463:LEU:HD11 | 1.88 | 0.56 |
| 1:L:185:ILE:HD11 | 1:M:172:ALA:HB2 | 1.86 | 0.56 |
| 1:C:6:THR:HA | 1:C:10:GLU:HA | 1.88 | 0.55 |
| 1:K:257:VAL:HB | 1:K:266:ARG:HB2 | 1.87 | 0.55 |
| 1:L:480:GLY:O | 1:M:462:ASN:ND2 | 2.35 | 0.55 |
| 1:F:467:LYS:HZ3 | 1:G:459:PRO:HG2 | 1.71 | 0.55 |
| 1:K:27:TYR:OH | 1:K:262:GLU:HG2 | 2.07 | 0.55 |
| 1:A:459:PRO:HG2 | 1:M:467:LYS:NZ | 2.20 | 0.55 |
| 1:L:73:LEU:HD21 | 1:L:388:VAL:HG23 | 1.89 | 0.55 |
| 1:D:11:ASP:OD1 | 1:D:11:ASP:N | 2.39 | 0.55 |
| 1:A:362:VAL:HG22 | 1:A:377:VAL:HG23 | 1.89 | 0.54 |
| 1:G:309:ARG:HB2 | 1:G:309:ARG:HH11 | 1.72 | 0.54 |
| 1:B:216:HIS:HE1 | 1:B:218:TYR:HB3 | 1.72 | 0.54 |
| 1:C:162:ARG:HH22 | 1:D:259:LEU:HD22 | 1.72 | 0.54 |
| 1:I:452:LEU:HD11 | 1:I:467:LYS:HE3 | 1.89 | 0.54 |
| 1:A:362:VAL:HG11 | 1:A:374:ILE:HG12 | 1.90 | 0.54 |
| 1:F:305:ILE:HG12 | 1:F:323:ARG:HH21 | 1.72 | 0.54 |
| 1:B:142:ASN:HD22 | 1:B:163:LEU:HD12 | 1.71 | 0.54 |
| 1:J:452:LEU:HD11 | 1:J:467:LYS:HE3 | 1.89 | 0.54 |
| 1:F:6:THR:HA | 1:F:10:GLU:HA | 1.90 | 0.54 |
| 1:F:362:VAL:HG11 | 1:F:374:ILE:HG12 | 1.89 | 0.54 |
| 1:H:142:ASN:HD22 | 1:H:163:LEU:HD12 | 1.73 | 0.54 |
| 1:J:11:ASP:OD1 | 1:J:11:ASP:N | 2.38 | 0.54 |
| 1:J:293:SER:O | 1:K:334:LYS:NZ | 2.40 | 0.54 |
| 1:B:61:VAL:HG21 | 1:B:279:LEU:HD21 | 1.90 | 0.54 |
| 1:J:305:ILE:HG12 | 1:J:323:ARG:HH21 | 1.72 | 0.54 |
| 1:L:11:ASP:OD1 | 1:L:11:ASP:N | 2.41 | 0.54 |
| 1:A:459:PRO:HG2 | 1:M:467:LYS:HZ3 | 1.73 | 0.53 |
| 1:K:276:LEU:HD12 | 1:K:352:LEU:HD13 | 1.91 | 0.53 |
| 1:K:6:THR:HA | 1:K:10:GLU:HA | 1.90 | 0.53 |
| 1:M:250:PRO:HB3 | 1:M:407:GLN:HE21 | 1.73 | 0.53 |
| 1:A:275:ASP:OD2 | 1:A:351:ARG:HD2 | 2.08 | 0.53 |
| 1:K:131:PHE:CG | 1:L:391:ILE:HD11 | 2.44 | 0.53 |
| 1:E:6:THR:HA | 1:E:10:GLU:HA | 1.90 | 0.53 |
| 1:I:142:ASN:HD22 | 1:I:163:LEU:HD12 | 1.74 | 0.53 |
| 1:B:257:VAL:HB | 1:B:266:ARG:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:137:LEU:HD13 | 1:I:143:VAL:HG23 | 1.91 | 0.53 |
| 1:A:462:ASN:ND2 | 1:M:480:GLY:O | 2.41 | 0.53 |
| 1:H:162:ARG:HH22 | 1:I:259:LEU:HD22 | 1.74 | 0.53 |
| 1:L:144:LEU:HB3 | 1:L:161:TYR:HB2 | 1.91 | 0.53 |
| 1:A:142:ASN:OD1 | 1:A:255:ARG:HG3 | 2.09 | 0.52 |
| 1:A:334:LYS:NZ | 1:M:293:SER:O | 2.42 | 0.52 |
| 1:E:73:LEU:HD21 | 1:E:388:VAL:HG23 | 1.91 | 0.52 |
| 1:M:42:LEU:O | 1:M:162:ARG:NH1 | 2.42 | 0.52 |
| 1:E:437:GLN:OE1 | 1:E:437:GLN:N | 2.36 | 0.52 |
| 1:F:11:ASP:OD1 | 1:F:11:ASP:N | 2.43 | 0.52 |
| 1:G:162:ARG:HH22 | 1:H:259:LEU:HD22 | 1.75 | 0.52 |
| 1:H:171:ASP:OD1 | 1:H:175:ASN:N | 2.43 | 0.52 |
| 1:I:171:ASP:OD1 | 1:I:175:ASN:N | 2.42 | 0.52 |
| 1:J:171:ASP:OD1 | 1:J:175:ASN:N | 2.42 | 0.52 |
| 1:J:332:LEU:HD13 | 1:J:334:LYS:H | 1.74 | 0.52 |
| 1:D:228:ARG:NH1 | 1:D:244:TYR:OH | 2.43 | 0.52 |
| 1:E:11:ASP:OD1 | 1:E:11:ASP:N | 2.40 | 0.52 |
| 1:E:293:SER:O | 1:F:334:LYS:NZ | 2.42 | 0.52 |
| 1:C:79:PRO:HD2 | 1:C:83:TRP:CD1 | 2.44 | 0.52 |
| 1:E:59:GLN:OE1 | 1:E:61:VAL:N | 2.42 | 0.52 |
| 1:C:73:LEU:HD21 | 1:C:388:VAL:HG23 | 1.91 | 0.52 |
| 1:L:305:ILE:HG12 | 1:L:323:ARG:HH21 | 1.75 | 0.52 |
| 1:K:216:HIS:CE1 | 1:K:218:TYR:HB3 | 2.44 | 0.52 |
| 1:G:192:GLU:HB2 | 1:H:221:GLU:HG2 | 1.92 | 0.52 |
| 1:K:142:ASN:OD1 | 1:K:255:ARG:HG3 | 2.10 | 0.52 |
| 1:M:79:PRO:HD2 | 1:M:83:TRP:CD1 | 2.45 | 0.52 |
| 1:C:437:GLN:OE1 | 1:C:437:GLN:N | 2.36 | 0.52 |
| 1:H:142:ASN:HD21 | 1:H:264:TYR:HB3 | 1.75 | 0.52 |
| 1:D:228:ARG:HG2 | 1:D:244:TYR:CE2 | 2.45 | 0.52 |
| 1:E:479:SER:HB3 | 1:F:469:ARG:HH22 | 1.75 | 0.52 |
| 1:F:257:VAL:HB | 1:F:266:ARG:HB2 | 1.92 | 0.52 |
| 1:J:308:PRO:HA | 1:J:311:LEU:HD12 | 1.92 | 0.52 |
| 1:D:159:LYS:HE3 | 1:D:161:TYR:CZ | 2.44 | 0.51 |
| 1:E:192:GLU:HB2 | 1:F:221:GLU:HG2 | 1.91 | 0.51 |
| 1:G:171:ASP:OD1 | 1:G:175:ASN:N | 2.43 | 0.51 |
| 1:C:144:LEU:HB3 | 1:C:161:TYR:HB2 | 1.90 | 0.51 |
| 1:B:120:TYR:OH | 1:B:156:ASN:ND2 | 2.31 | 0.51 |
| 1:D:142:ASN:HD22 | 1:D:163:LEU:HD12 | 1.76 | 0.51 |
| 1:H:453:ALA:HA | 1:H:456:ARG:HG3 | 1.93 | 0.51 |
| 1:B:142:ASN:ND2 | 1:B:264:TYR:HB3 | 2.26 | 0.51 |
| 1:I:362:VAL:HG22 | 1:I:377:VAL:HG23 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:59:GLN:OE1 | 1:F:61:VAL:N | 2.43 | 0.51 |
| 1:F:430:LEU:HD12 | 1:F:433:ILE:HD12 | 1.92 | 0.51 |
| 1:K:120:TYR:OH | 1:K:156:ASN:ND2 | 2.36 | 0.51 |
| 1:M:6:THR:HA | 1:M:10:GLU:HA | 1.92 | 0.51 |
| 1:G:142:ASN:HD22 | 1:G:163:LEU:HD12 | 1.75 | 0.51 |
| 1:A:469:ARG:HH22 | 1:M:479:SER:HB3 | 1.76 | 0.51 |
| 1:C:74:MET:SD | 1:C:131:PHE:HB2 | 2.51 | 0.51 |
| 1:E:250:PRO:HB3 | 1:E:407:GLN:HE21 | 1.75 | 0.51 |
| 1:F:478:THR:HA | 1:F:481:ILE:HD12 | 1.92 | 0.51 |
| 1:G:42:LEU:O | 1:G:162:ARG:NH1 | 2.44 | 0.51 |
| 1:J:163:LEU:HA | 1:J:166:TYR:CE2 | 2.46 | 0.51 |
| 1:B:8:LEU:HD22 | 1:B:218:TYR:HB2 | 1.93 | 0.51 |
| 1:J:197:ALA:HB1 | 1:J:235:MET:HE3 | 1.93 | 0.51 |
| 1:I:371:ALA:CB | 1:J:372:GLU:HG3 | 2.41 | 0.50 |
| 1:L:332:LEU:HD13 | 1:L:334:LYS:HB2 | 1.92 | 0.50 |
| 1:B:332:LEU:HD13 | 1:B:334:LYS:HB2 | 1.93 | 0.50 |
| 1:G:467:LYS:NZ | 1:H:459:PRO:HG2 | 2.26 | 0.50 |
| 1:K:362:VAL:HG22 | 1:K:377:VAL:HG23 | 1.93 | 0.50 |
| 1:C:88:ILE:HD11 | 1:C:107:ASP:HB2 | 1.93 | 0.50 |
| 1:M:73:LEU:HD21 | 1:M:388:VAL:HG23 | 1.93 | 0.50 |
| 1:K:59:GLN:OE1 | 1:K:61:VAL:N | 2.44 | 0.50 |
| 1:F:241:ASP:OD1 | 1:F:241:ASP:N | 2.44 | 0.50 |
| 1:I:439:LEU:HD22 | 1:J:474:ILE:HG12 | 1.93 | 0.50 |
| 1:M:257:VAL:HB | 1:M:266:ARG:HB2 | 1.94 | 0.50 |
| 1:I:365:THR:HG22 | 1:J:364:ARG:HH11 | 1.76 | 0.50 |
| 1:J:135:LYS:O | 1:J:139:VAL:HG12 | 2.11 | 0.50 |
| 1:J:230:GLU:H | 1:J:240:SER:HB2 | 1.77 | 0.50 |
| 1:J:309:ARG:HH11 | 1:J:309:ARG:HB2 | 1.77 | 0.50 |
| 1:F:359:ASN:HB2 | 1:G:380:GLU:HB2 | 1.93 | 0.50 |
| 1:H:467:LYS:NZ | 1:I:459:PRO:HG2 | 2.26 | 0.50 |
| 1:B:111:SER:HA | 1:B:114:GLU:HB2 | 1.94 | 0.49 |
| 1:F:452:LEU:HD11 | 1:F:467:LYS:HE3 | 1.94 | 0.49 |
| 1:L:250:PRO:HB3 | 1:L:407:GLN:HE21 | 1.77 | 0.49 |
| 1:B:163:LEU:HA | 1:B:166:TYR:CE2 | 2.48 | 0.49 |
| 1:D:142:ASN:OD1 | 1:D:255:ARG:HG3 | 2.13 | 0.49 |
| 1:H:191:PRO:HD2 | 1:H:194:ILE:HD12 | 1.94 | 0.49 |
| 1:M:216:HIS:HE1 | 1:M:218:TYR:HB3 | 1.78 | 0.49 |
| 1:C:338:PHE:CD2 | 1:D:340:VAL:HG13 | 2.46 | 0.49 |
| 1:F:92:GLU:HA | 1:F:95:GLN:HG3 | 1.94 | 0.49 |
| 1:G:79:PRO:HD2 | 1:G:83:TRP:CD1 | 2.47 | 0.49 |
| 1:H:478:THR:HA | 1:H:481:ILE:HD12 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:458:ASP:HB2 | 1:D:461:ILE:HB | 1.94 | 0.49 |
| 1:H:365:THR:HG22 | 1:I:364:ARG:HH11 | 1.76 | 0.49 |
| 1:I:308:PRO:HA | 1:I:311:LEU:HD12 | 1.94 | 0.49 |
| 1:M:137:LEU:HD13 | 1:M:143:VAL:HG23 | 1.93 | 0.49 |
| 1:B:216:HIS:CE1 | 1:B:218:TYR:HB3 | 2.47 | 0.49 |
| 1:E:120:TYR:OH | 1:E:156:ASN:ND2 | 2.40 | 0.49 |
| 1:C:163:LEU:HA | 1:C:166:TYR:CE2 | 2.48 | 0.49 |
| 1:J:79:PRO:HD2 | 1:J:83:TRP:CD1 | 2.48 | 0.49 |
| 1:L:308:PRO:HA | 1:L:311:LEU:HD12 | 1.95 | 0.49 |
| 1:F:5:ARG:NH1 | 1:F:218:TYR:OH | 2.46 | 0.49 |
| 1:F:467:LYS:NZ | 1:G:459:PRO:HG2 | 2.27 | 0.49 |
| 1:H:137:LEU:HD13 | 1:H:143:VAL:HG23 | 1.95 | 0.49 |
| 1:B:28:GLU:HB3 | 1:B:163:LEU:HD22 | 1.95 | 0.48 |
| 1:A:437:GLN:OE1 | 1:A:437:GLN:N | 2.41 | 0.48 |
| 1:G:43:PHE:HD2 | 1:G:136:GLN:HE22 | 1.61 | 0.48 |
| 1:I:370:THR:OG1 | 1:I:371:ALA:N | 2.46 | 0.48 |
| 1:J:290:SER:HB3 | 1:K:344:VAL:HG21 | 1.94 | 0.48 |
| 1:K:250:PRO:HB3 | 1:K:407:GLN:HE21 | 1.78 | 0.48 |
| 1:D:163:LEU:HA | 1:D:166:TYR:CE2 | 2.48 | 0.48 |
| 1:J:275:ASP:OD2 | 1:J:351:ARG:HD2 | 2.13 | 0.48 |
| 1:M:11:ASP:OD1 | 1:M:11:ASP:N | 2.40 | 0.48 |
| 1:A:391:ILE:HD11 | 1:M:131:PHE:CG | 2.48 | 0.48 |
| 1:D:338:PHE:CD2 | 1:E:340:VAL:HG13 | 2.48 | 0.48 |
| 1:G:163:LEU:HA | 1:G:166:TYR:CE2 | 2.48 | 0.48 |
| 1:J:89:SER:HB3 | 1:J:423:GLU:O | 2.14 | 0.48 |
| 1:F:300:VAL:HG12 | 1:F:327:ILE:HG12 | 1.95 | 0.48 |
| 1:I:60:ALA:HB1 | 1:J:272:TYR:HD1 | 1.77 | 0.48 |
| 1:K:332:LEU:CD1 | 1:K:334:LYS:HB2 | 2.44 | 0.48 |
| 1:G:73:LEU:HD21 | 1:G:388:VAL:HG23 | 1.96 | 0.48 |
| 1:L:59:GLN:HG3 | 1:L:280:GLU:OE1 | 2.13 | 0.48 |
| 1:L:248:ALA:HB2 | 1:L:406:LYS:HD3 | 1.95 | 0.48 |
| 1:G:89:SER:HB3 | 1:G:423:GLU:O | 2.14 | 0.48 |
| 1:I:162:ARG:NH2 | 1:J:259:LEU:HD22 | 2.26 | 0.48 |
| 1:I:290:SER:HB3 | 1:J:344:VAL:HG21 | 1.95 | 0.48 |
| 1:C:142:ASN:OD1 | 1:C:255:ARG:HG3 | 2.14 | 0.48 |
| 1:D:293:SER:O | 1:E:334:LYS:NZ | 2.47 | 0.48 |
| 1:L:8:LEU:HD22 | 1:L:218:TYR:HB2 | 1.96 | 0.48 |
| 1:D:137:LEU:HD13 | 1:D:143:VAL:HG23 | 1.96 | 0.48 |
| 1:I:250:PRO:HB3 | 1:I:407:GLN:HE21 | 1.78 | 0.48 |
| 1:I:359:ASN:HB2 | 1:J:380:GLU:HB2 | 1.95 | 0.48 |
| 1:D:453:ALA:HA | 1:D:456:ARG:HG3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:228:ARG:HG2 | 1:G:244:TYR:CE2 | 2.49 | 0.47 |
| 1:H:371:ALA:HB2 | 1:I:372:GLU:HG3 | 1.94 | 0.47 |
| 1:A:479:SER:O | 1:B:469:ARG:NH2 | 2.48 | 0.47 |
| 1:F:190:LEU:O | 1:F:195:ARG:NH1 | 2.47 | 0.47 |
| 1:L:42:LEU:O | 1:L:162:ARG:NH1 | 2.47 | 0.47 |
| 1:B:59:GLN:OE1 | 1:B:61:VAL:N | 2.47 | 0.47 |
| 1:M:430:LEU:HD12 | 1:M:433:ILE:HD12 | 1.96 | 0.47 |
| 1:E:131:PHE:CG | 1:F:391:ILE:HD11 | 2.50 | 0.47 |
| 1:F:332:LEU:HD13 | 1:F:334:LYS:HB2 | 1.96 | 0.47 |
| 1:G:308:PRO:HA | 1:G:311:LEU:HD12 | 1.95 | 0.47 |
| 1:G:452:LEU:HD11 | 1:G:467:LYS:HE3 | 1.97 | 0.47 |
| 1:K:216:HIS:HB3 | 1:K:229:TYR:CE2 | 2.49 | 0.47 |
| 1:A:272:TYR:CE2 | 1:A:355:ALA:HB1 | 2.50 | 0.47 |
| 1:D:133:ALA:O | 1:D:137:LEU:N | 2.40 | 0.47 |
| 1:B:452:LEU:HD11 | 1:B:467:LYS:HE3 | 1.96 | 0.47 |
| 1:E:79:PRO:HD2 | 1:E:83:TRP:CD1 | 2.50 | 0.47 |
| 1:G:120:TYR:OH | 1:G:156:ASN:ND2 | 2.34 | 0.47 |
| 1:H:142:ASN:ND2 | 1:H:264:TYR:HB3 | 2.30 | 0.47 |
| 1:J:73:LEU:HD21 | 1:J:388:VAL:HG23 | 1.95 | 0.47 |
| 1:J:430:LEU:HD12 | 1:J:433:ILE:HD12 | 1.95 | 0.47 |
| 1:A:73:LEU:HD21 | 1:A:388:VAL:HG23 | 1.96 | 0.47 |
| 1:B:241:ASP:OD1 | 1:B:241:ASP:N | 2.46 | 0.47 |
| 1:I:163:LEU:HA | 1:I:166:TYR:CE2 | 2.50 | 0.47 |
| 1:K:163:LEU:HA | 1:K:166:TYR:CE2 | 2.49 | 0.47 |
| 1:F:216:HIS:HB3 | 1:F:229:TYR:CE2 | 2.50 | 0.47 |
| 1:F:310:ARG:HD3 | 1:F:320:VAL:HG13 | 1.97 | 0.47 |
| 1:L:133:ALA:O | 1:L:137:LEU:N | 2.36 | 0.47 |
| 1:M:142:ASN:ND2 | 1:M:264:TYR:HB3 | 2.30 | 0.47 |
| 1:C:309:ARG:HH11 | 1:C:309:ARG:HB2 | 1.80 | 0.47 |
| 1:B:357:MET:N | 1:B:357:MET:SD | 2.88 | 0.47 |
| 1:B:478:THR:HA | 1:B:481:ILE:HD12 | 1.98 | 0.47 |
| 1:F:290:SER:HB3 | 1:G:344:VAL:HG21 | 1.95 | 0.47 |
| 1:L:192:GLU:HB2 | 1:M:221:GLU:OE2 | 2.15 | 0.47 |
| 1:I:437:GLN:OE1 | 1:I:437:GLN:N | 2.40 | 0.46 |
| 1:E:137:LEU:HD13 | 1:E:143:VAL:HG23 | 1.97 | 0.46 |
| 1:G:365:THR:HG22 | 1:H:364:ARG:HH11 | 1.79 | 0.46 |
| 1:L:162:ARG:NH2 | 1:M:259:LEU:HD22 | 2.27 | 0.46 |
| 1:A:370:THR:OG1 | 1:A:371:ALA:N | 2.48 | 0.46 |
| 1:D:120:TYR:OH | 1:D:156:ASN:OD1 | 2.32 | 0.46 |
| 1:F:60:ALA:HB1 | 1:G:272:TYR:HD1 | 1.78 | 0.46 |
| 1:F:79:PRO:HD2 | 1:F:83:TRP:CD1 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:131:PHE:CG | 1:G:391:ILE:HD11 | 2.50 | 0.46 |
| 1:M:250:PRO:HB3 | 1:M:407:GLN:NE2 | 2.29 | 0.46 |
| 1:E:61:VAL:HG21 | 1:E:279:LEU:HD21 | 1.96 | 0.46 |
| 1:L:27:TYR:OH | 1:L:262:GLU:HG2 | 2.16 | 0.46 |
| 1:E:452:LEU:HD11 | 1:E:467:LYS:HE3 | 1.98 | 0.46 |
| 1:H:452:LEU:HD11 | 1:H:467:LYS:HE3 | 1.98 | 0.46 |
| 1:C:191:PRO:HD2 | 1:C:194:ILE:HD12 | 1.97 | 0.46 |
| 1:F:124:ASN:OD1 | 1:F:156:ASN:N | 2.44 | 0.46 |
| 1:K:159:LYS:HE3 | 1:K:161:TYR:CZ | 2.51 | 0.46 |
| 1:H:38:THR:HG22 | 1:H:62:GLY:HA3 | 1.97 | 0.46 |
| 1:I:332:LEU:HD13 | 1:I:334:LYS:HB2 | 1.97 | 0.46 |
| 1:J:194:ILE:HG12 | 1:J:237:VAL:HG13 | 1.97 | 0.46 |
| 1:J:228:ARG:HG2 | 1:J:244:TYR:CE2 | 2.51 | 0.46 |
| 1:K:142:ASN:HD22 | 1:K:163:LEU:HD12 | 1.81 | 0.46 |
| 1:K:332:LEU:HD13 | 1:K:334:LYS:HB2 | 1.98 | 0.46 |
| 1:D:73:LEU:HD21 | 1:D:388:VAL:HG23 | 1.97 | 0.46 |
| 1:D:27:TYR:OH | 1:D:262:GLU:HG2 | 2.16 | 0.46 |
| 1:F:73:LEU:HD21 | 1:F:388:VAL:HG23 | 1.97 | 0.46 |
| 1:F:370:THR:OG1 | 1:F:371:ALA:N | 2.47 | 0.46 |
| 1:G:309:ARG:HB2 | 1:G:309:ARG:NH1 | 2.30 | 0.46 |
| 1:M:216:HIS:CE1 | 1:M:218:TYR:HB3 | 2.51 | 0.46 |
| 1:A:241:ASP:OD1 | 1:A:241:ASP:N | 2.43 | 0.45 |
| 1:A:380:GLU:HB2 | 1:M:359:ASN:HB2 | 1.97 | 0.45 |
| 1:I:88:ILE:HD11 | 1:I:107:ASP:HB2 | 1.97 | 0.45 |
| 1:I:458:ASP:HB2 | 1:I:461:ILE:HB | 1.97 | 0.45 |
| 1:D:309:ARG:HH11 | 1:D:309:ARG:HB2 | 1.81 | 0.45 |
| 1:G:362:VAL:HG11 | 1:G:374:ILE:HG12 | 1.98 | 0.45 |
| 1:J:61:VAL:HG21 | 1:J:279:LEU:HD21 | 1.98 | 0.45 |
| 1:C:194:ILE:O | 1:C:198:VAL:HG23 | 2.16 | 0.45 |
| 1:C:453:ALA:HA | 1:C:456:ARG:HG3 | 1.99 | 0.45 |
| 1:J:370:THR:OG1 | 1:J:371:ALA:N | 2.49 | 0.45 |
| 1:E:216:HIS:HB3 | 1:E:229:TYR:CE2 | 2.51 | 0.45 |
| 1:F:85:ARG:NH2 | 1:G:472:ASN:O | 2.50 | 0.45 |
| 1:J:42:LEU:O | 1:J:162:ARG:NH1 | 2.49 | 0.45 |
| 1:M:163:LEU:HA | 1:M:166:TYR:CE2 | 2.52 | 0.45 |
| 1:B:437:GLN:OE1 | 1:B:437:GLN:N | 2.41 | 0.45 |
| 1:A:131:PHE:CD1 | 1:B:391:ILE:HD11 | 2.51 | 0.45 |
| 1:A:309:ARG:HH11 | 1:A:309:ARG:HB2 | 1.82 | 0.45 |
| 1:C:39:ILE:HG21 | 1:D:271:GLU:HG2 | 1.99 | 0.45 |
| 1:E:305:ILE:HG12 | 1:E:323:ARG:HH21 | 1.82 | 0.45 |
| 1:F:228:ARG:HG2 | 1:F:244:TYR:CE2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:479:SER:HB3 | 1:K:469:ARG:HH22 | 1.82 | 0.45 |
| 1:L:479:SER:HB3 | 1:M:469:ARG:HH22 | 1.82 | 0.45 |
| 1:A:121:ILE:HG23 | 1:A:126:TYR:HB2 | 1.98 | 0.45 |
| 1:A:163:LEU:HA | 1:A:166:TYR:CE2 | 2.51 | 0.45 |
| 1:B:370:THR:OG1 | 1:B:371:ALA:N | 2.50 | 0.45 |
| 1:C:293:SER:O | 1:D:334:LYS:NZ | 2.50 | 0.45 |
| 1:E:305:ILE:HG21 | 1:F:302:PRO:HG3 | 1.99 | 0.45 |
| 1:I:309:ARG:HH11 | 1:I:309:ARG:HB2 | 1.82 | 0.45 |
| 1:I:467:LYS:NZ | 1:J:459:PRO:HG2 | 2.32 | 0.45 |
| 1:G:362:VAL:HG22 | 1:G:377:VAL:HG23 | 1.99 | 0.45 |
| 1:L:27:TYR:CD2 | 1:L:264:TYR:HB2 | 2.52 | 0.45 |
| 1:M:437:GLN:OE1 | 1:M:437:GLN:N | 2.44 | 0.45 |
| 1:F:171:ASP:OD1 | 1:F:175:ASN:N | 2.50 | 0.45 |
| 1:K:142:ASN:ND2 | 1:K:264:TYR:HB3 | 2.32 | 0.45 |
| 1:L:191:PRO:HD2 | 1:L:194:ILE:HD12 | 1.98 | 0.45 |
| 1:J:142:ASN:OD1 | 1:J:255:ARG:HG3 | 2.17 | 0.45 |
| 1:L:142:ASN:ND2 | 1:L:264:TYR:HB3 | 2.32 | 0.45 |
| 1:L:309:ARG:HH11 | 1:L:309:ARG:HB2 | 1.82 | 0.45 |
| 1:B:142:ASN:HD22 | 1:B:163:LEU:CD1 | 2.29 | 0.44 |
| 1:F:120:TYR:OH | 1:F:156:ASN:OD1 | 2.32 | 0.44 |
| 1:F:163:LEU:HA | 1:F:166:TYR:CE2 | 2.53 | 0.44 |
| 1:G:192:GLU:HG3 | 1:G:195:ARG:NH2 | 2.32 | 0.44 |
| 1:G:370:THR:OG1 | 1:G:371:ALA:N | 2.51 | 0.44 |
| 1:G:453:ALA:HA | 1:G:456:ARG:HG3 | 1.99 | 0.44 |
| 1:M:142:ASN:HD21 | 1:M:264:TYR:HB3 | 1.82 | 0.44 |
| 1:A:27:TYR:OH | 1:A:262:GLU:HG2 | 2.17 | 0.44 |
| 1:J:6:THR:HA | 1:J:10:GLU:HA | 1.99 | 0.44 |
| 1:J:8:LEU:HD22 | 1:J:218:TYR:HB2 | 1.99 | 0.44 |
| 1:J:373:GLU:O | 1:J:377:VAL:HG22 | 2.17 | 0.44 |
| 1:L:362:VAL:CG1 | 1:L:374:ILE:HG12 | 2.46 | 0.44 |
| 1:C:8:LEU:HD22 | 1:C:218:TYR:HB2 | 1.98 | 0.44 |
| 1:H:24:ARG:NH1 | 1:H:166:TYR:O | 2.40 | 0.44 |
| 1:H:142:ASN:OD1 | 1:H:255:ARG:HG3 | 2.18 | 0.44 |
| 1:I:135:LYS:O | 1:I:139:VAL:HG12 | 2.18 | 0.44 |
| 1:J:276:LEU:HD12 | 1:J:352:LEU:HD13 | 1.99 | 0.44 |
| 1:M:418:PRO:O | 1:M:420:GLU:N | 2.50 | 0.44 |
| 1:A:69:LEU:HD11 | 1:A:268:TYR:CE2 | 2.53 | 0.44 |
| 1:C:194:ILE:CG2 | 1:C:232:VAL:HG21 | 2.47 | 0.44 |
| 1:D:370:THR:OG1 | 1:D:371:ALA:N | 2.51 | 0.44 |
| 1:G:142:ASN:HD21 | 1:G:264:TYR:HB3 | 1.83 | 0.44 |
| 1:H:266:ARG:HA | 1:H:266:ARG:HD2 | 1.88 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:159:LYS:HE3 | 1:A:161:TYR:CZ | 2.52 | 0.44 |
| 1:B:228:ARG:NH1 | 1:B:244:TYR:OH | 2.51 | 0.44 |
| 1:C:370:THR:OG1 | 1:C:371:ALA:N | 2.51 | 0.44 |
| 1:D:197:ALA:O | 1:D:235:MET:HE1 | 2.18 | 0.44 |
| 1:H:257:VAL:HB | 1:H:266:ARG:HB2 | 1.99 | 0.44 |
| 1:J:309:ARG:HB2 | 1:J:309:ARG:NH1 | 2.31 | 0.44 |
| 1:M:197:ALA:HB1 | 1:M:235:MET:HE3 | 1.99 | 0.44 |
| 1:B:453:ALA:HA | 1:B:456:ARG:HG3 | 1.99 | 0.44 |
| 1:F:74:MET:SD | 1:F:131:PHE:HB2 | 2.57 | 0.44 |
| 1:G:59:GLN:OE1 | 1:G:61:VAL:N | 2.51 | 0.44 |
| 1:H:216:HIS:HB3 | 1:H:229:TYR:CE2 | 2.53 | 0.44 |
| 1:A:391:ILE:HD11 | 1:M:131:PHE:CD1 | 2.53 | 0.44 |
| 1:E:163:LEU:HA | 1:E:166:TYR:CE2 | 2.53 | 0.44 |
| 1:E:449:TRP:CD1 | 1:E:467:LYS:HG2 | 2.52 | 0.44 |
| 1:H:370:THR:OG1 | 1:H:371:ALA:N | 2.50 | 0.44 |
| 1:K:370:THR:OG1 | 1:K:371:ALA:N | 2.50 | 0.44 |
| 1:L:135:LYS:O | 1:L:139:VAL:HG12 | 2.17 | 0.44 |
| 1:L:163:LEU:HA | 1:L:166:TYR:CE2 | 2.52 | 0.44 |
| 1:L:230:GLU:H | 1:L:240:SER:HB2 | 1.82 | 0.44 |
| 1:D:162:ARG:HH22 | 1:E:259:LEU:HD22 | 1.82 | 0.44 |
| 1:E:59:GLN:HG3 | 1:E:280:GLU:OE1 | 2.18 | 0.44 |
| 1:E:69:LEU:HA | 1:E:69:LEU:HD23 | 1.75 | 0.44 |
| 1:G:74:MET:SD | 1:G:131:PHE:HB2 | 2.58 | 0.44 |
| 1:K:362:VAL:CG1 | 1:K:374:ILE:HG12 | 2.47 | 0.44 |
| 1:L:370:THR:OG1 | 1:L:371:ALA:N | 2.51 | 0.44 |
| 1:M:8:LEU:HD22 | 1:M:218:TYR:HB2 | 1.99 | 0.44 |
| 1:M:142:ASN:HD22 | 1:M:163:LEU:HD12 | 1.83 | 0.44 |
| 1:A:228:ARG:HG2 | 1:A:244:TYR:CE2 | 2.53 | 0.43 |
| 1:A:89:SER:HB3 | 1:A:423:GLU:O | 2.18 | 0.43 |
| 1:F:142:ASN:OD1 | 1:F:255:ARG:HG3 | 2.19 | 0.43 |
| 1:G:131:PHE:CD1 | 1:H:391:ILE:HD11 | 2.53 | 0.43 |
| 1:I:74:MET:SD | 1:I:131:PHE:HB2 | 2.57 | 0.43 |
| 1:I:194:ILE:O | 1:I:198:VAL:HG23 | 2.19 | 0.43 |
| 1:L:398:LEU:HD12 | 1:L:402:ARG:NH2 | 2.32 | 0.43 |
| 1:M:171:ASP:OD1 | 1:M:175:ASN:N | 2.49 | 0.43 |
| 1:E:171:ASP:OD1 | 1:E:175:ASN:N | 2.49 | 0.43 |
| 1:I:300:VAL:HG12 | 1:I:327:ILE:HG12 | 1.99 | 0.43 |
| 1:B:373:GLU:O | 1:B:377:VAL:HG22 | 2.18 | 0.43 |
| 1:D:131:PHE:CG | 1:E:391:ILE:HD11 | 2.54 | 0.43 |
| 1:D:371:ALA:HB2 | 1:E:372:GLU:HG3 | 1.99 | 0.43 |
| 1:E:250:PRO:HB3 | 1:E:407:GLN:NE2 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:191:PRO:HD2 | 1:F:194:ILE:HD12 | 2.00 | 0.43 |
| 1:I:103:LEU:HD23 | 1:I:103:LEU:HA | 1.86 | 0.43 |
| 1:K:8:LEU:HD22 | 1:K:218:TYR:HB2 | 2.00 | 0.43 |
| 1:A:131:PHE:CG | 1:B:391:ILE:HD11 | 2.54 | 0.43 |
| 1:C:309:ARG:HB2 | 1:C:309:ARG:NH1 | 2.34 | 0.43 |
| 1:H:159:LYS:HG3 | 1:H:160:LEU:N | 2.33 | 0.43 |
| 1:K:405:LEU:HD23 | 1:K:405:LEU:HA | 1.91 | 0.43 |
| 1:L:338:PHE:CD2 | 1:M:340:VAL:HG13 | 2.53 | 0.43 |
| 1:D:357:MET:SD | 1:D:357:MET:N | 2.91 | 0.43 |
| 1:E:142:ASN:OD1 | 1:E:255:ARG:HG3 | 2.18 | 0.43 |
| 1:E:275:ASP:OD2 | 1:E:351:ARG:HD2 | 2.18 | 0.43 |
| 1:E:309:ARG:HH11 | 1:E:309:ARG:HB2 | 1.83 | 0.43 |
| 1:E:398:LEU:HB3 | 1:E:402:ARG:HH22 | 1.83 | 0.43 |
| 1:G:6:THR:HA | 1:G:10:GLU:HA | 2.01 | 0.43 |
| 1:C:452:LEU:HD11 | 1:C:467:LYS:HE3 | 2.01 | 0.43 |
| 1:D:212:ASP:OD1 | 1:D:212:ASP:N | 2.52 | 0.43 |
| 1:D:373:GLU:O | 1:D:377:VAL:HG22 | 2.19 | 0.43 |
| 1:E:373:GLU:O | 1:E:377:VAL:HG22 | 2.19 | 0.43 |
| 1:F:43:PHE:HD2 | 1:F:136:GLN:HE22 | 1.67 | 0.43 |
| 1:G:415:PRO:HB2 | 1:H:94:LYS:NZ | 2.34 | 0.43 |
| 1:G:467:LYS:HZ3 | 1:H:459:PRO:HG2 | 1.82 | 0.43 |
| 1:G:479:SER:O | 1:H:469:ARG:NH2 | 2.52 | 0.43 |
| 1:J:159:LYS:HG3 | 1:J:160:LEU:N | 2.32 | 0.43 |
| 1:C:250:PRO:HB3 | 1:C:407:GLN:HE21 | 1.84 | 0.43 |
| 1:D:257:VAL:HB | 1:D:266:ARG:HB2 | 2.01 | 0.43 |
| 1:H:163:LEU:HA | 1:H:166:TYR:CE2 | 2.54 | 0.43 |
| 1:C:194:ILE:HG12 | 1:C:237:VAL:HG13 | 2.01 | 0.43 |
| 1:C:370:THR:HG23 | 1:C:373:GLU:H | 1.83 | 0.43 |
| 1:D:126:TYR:HE2 | 1:D:404:LEU:HD11 | 1.83 | 0.43 |
| 1:F:309:ARG:HH11 | 1:F:309:ARG:HB2 | 1.84 | 0.43 |
| 1:I:6:THR:HA | 1:I:10:GLU:HA | 2.00 | 0.43 |
| 1:I:453:ALA:HA | 1:I:456:ARG:HG3 | 2.01 | 0.43 |
| 1:K:20:LEU:HD21 | 1:K:169:GLN:NE2 | 2.34 | 0.43 |
| 1:H:276:LEU:HD12 | 1:H:352:LEU:HD13 | 2.00 | 0.42 |
| 1:H:290:SER:HB3 | 1:I:344:VAL:HG21 | 2.01 | 0.42 |
| 1:H:418:PRO:O | 1:H:420:GLU:N | 2.51 | 0.42 |
| 1:I:357:MET:SD | 1:I:357:MET:N | 2.92 | 0.42 |
| 1:L:276:LEU:HD12 | 1:L:352:LEU:HD13 | 2.01 | 0.42 |
| 1:I:452:LEU:CD1 | 1:I:467:LYS:HE3 | 2.49 | 0.42 |
| 1:K:309:ARG:HH11 | 1:K:309:ARG:HB2 | 1.85 | 0.42 |
| 1:K:371:ALA:CB | 1:L:372:GLU:HG3 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:99:ASP:O | 1:A:103:LEU:HB2 | 2.19 | 0.42 |
| 1:B:272:TYR:CE2 | 1:B:355:ALA:HB1 | 2.54 | 0.42 |
| 1:C:142:ASN:OD1 | 1:C:265:GLY:N | 2.48 | 0.42 |
| 1:C:359:ASN:HB2 | 1:D:380:GLU:HB2 | 2.01 | 0.42 |
| 1:F:275:ASP:OD2 | 1:F:351:ARG:NH1 | 2.48 | 0.42 |
| 1:G:168:VAL:HG22 | 1:G:179:MET:HG2 | 2.02 | 0.42 |
| 1:G:186:ALA:HA | 1:G:210:THR:HA | 2.00 | 0.42 |
| 1:H:241:ASP:OD1 | 1:H:241:ASP:N | 2.46 | 0.42 |
| 1:I:99:ASP:O | 1:I:103:LEU:HB2 | 2.19 | 0.42 |
| 1:C:216:HIS:HB3 | 1:C:229:TYR:CE2 | 2.54 | 0.42 |
| 1:C:228:ARG:HG2 | 1:C:244:TYR:CE2 | 2.55 | 0.42 |
| 1:F:310:ARG:NH1 | 1:F:321:THR:OG1 | 2.53 | 0.42 |
| 1:H:73:LEU:HD21 | 1:H:388:VAL:HG23 | 2.02 | 0.42 |
| 1:L:437:GLN:OE1 | 1:L:437:GLN:N | 2.46 | 0.42 |
| 1:B:11:ASP:OD1 | 1:B:11:ASP:N | 2.42 | 0.42 |
| 1:H:365:THR:HG22 | 1:I:364:ARG:NH1 | 2.35 | 0.42 |
| 1:L:300:VAL:HG12 | 1:L:327:ILE:HG12 | 2.02 | 0.42 |
| 1:M:74:MET:SD | 1:M:131:PHE:HB2 | 2.60 | 0.42 |
| 1:M:241:ASP:OD1 | 1:M:241:ASP:N | 2.47 | 0.42 |
| 1:M:370:THR:OG1 | 1:M:371:ALA:N | 2.52 | 0.42 |
| 1:E:228:ARG:HG2 | 1:E:244:TYR:CE2 | 2.55 | 0.42 |
| 1:G:293:SER:O | 1:H:334:LYS:NZ | 2.53 | 0.42 |
| 1:H:28:GLU:HB3 | 1:H:163:LEU:HD22 | 2.02 | 0.42 |
| 1:I:39:ILE:HG21 | 1:J:271:GLU:HG2 | 2.02 | 0.42 |
| 1:M:142:ASN:OD1 | 1:M:255:ARG:HG3 | 2.19 | 0.42 |
| 1:B:137:LEU:HD13 | 1:B:143:VAL:HG23 | 2.02 | 0.42 |
| 1:C:340:VAL:O | 1:C:344:VAL:HG23 | 2.20 | 0.42 |
| 1:C:357:MET:SD | 1:C:357:MET:N | 2.93 | 0.42 |
| 1:F:309:ARG:HB2 | 1:F:309:ARG:NH1 | 2.34 | 0.42 |
| 1:G:39:ILE:HB | 1:G:42:LEU:HG | 2.01 | 0.42 |
| 1:G:241:ASP:OD1 | 1:G:241:ASP:N | 2.42 | 0.42 |
| 1:I:126:TYR:CE1 | 1:I:158:MET:HB2 | 2.55 | 0.42 |
| 1:D:81:GLN:HG2 | 1:E:437:GLN:HG3 | 2.01 | 0.42 |
| 1:E:389:TYR:OH | 1:E:429:GLY:HA2 | 2.19 | 0.42 |
| 1:F:28:GLU:HB3 | 1:F:163:LEU:HD22 | 2.02 | 0.42 |
| 1:K:467:LYS:HZ3 | 1:L:459:PRO:HG2 | 1.85 | 0.42 |
| 1:F:42:LEU:O | 1:F:162:ARG:NH1 | 2.53 | 0.42 |
| 1:F:61:VAL:HG21 | 1:F:279:LEU:HD21 | 2.02 | 0.42 |
| 1:H:216:HIS:HE1 | 1:H:218:TYR:HB3 | 1.83 | 0.42 |
| 1:I:167:VAL:HG12 | 1:I:180:VAL:O | 2.20 | 0.42 |
| 1:A:371:ALA:CB | 1:B:372:GLU:HG3 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:309:ARG:HB2 | 1:B:309:ARG:HH11 | 1.85 | 0.41 |
| 1:B:418:PRO:O | 1:B:420:GLU:N | 2.53 | 0.41 |
| 1:E:370:THR:OG1 | 1:E:371:ALA:N | 2.53 | 0.41 |
| 1:F:362:VAL:HG22 | 1:F:377:VAL:HG23 | 2.01 | 0.41 |
| 1:G:131:PHE:CG | 1:H:391:ILE:HD11 | 2.55 | 0.41 |
| 1:J:257:VAL:HB | 1:J:266:ARG:HB2 | 2.01 | 0.41 |
| 1:K:332:LEU:HD13 | 1:K:334:LYS:H | 1.85 | 0.41 |
| 1:C:417:LEU:HB3 | 1:C:418:PRO:HD2 | 2.02 | 0.41 |
| 1:D:142:ASN:HD21 | 1:D:264:TYR:HB3 | 1.84 | 0.41 |
| 1:D:338:PHE:CZ | 1:D:342:LYS:HD2 | 2.55 | 0.41 |
| 1:F:89:SER:HB3 | 1:F:423:GLU:O | 2.20 | 0.41 |
| 1:G:197:ALA:HB1 | 1:G:235:MET:HE3 | 2.01 | 0.41 |
| 1:H:32:GLN:HG3 | 1:H:43:PHE:CD1 | 2.56 | 0.41 |
| 1:A:28:GLU:HB3 | 1:A:163:LEU:HD22 | 2.02 | 0.41 |
| 1:I:133:ALA:O | 1:I:137:LEU:N | 2.45 | 0.41 |
| 1:K:59:GLN:HG3 | 1:K:280:GLU:OE1 | 2.19 | 0.41 |
| 1:K:371:ALA:HB2 | 1:L:372:GLU:HG3 | 2.01 | 0.41 |
| 1:M:373:GLU:O | 1:M:377:VAL:HG22 | 2.21 | 0.41 |
| 1:C:458:ASP:HB2 | 1:C:461:ILE:HB | 2.02 | 0.41 |
| 1:I:417:LEU:HB3 | 1:I:418:PRO:HD2 | 2.02 | 0.41 |
| 1:J:216:HIS:HB3 | 1:J:229:TYR:CE2 | 2.56 | 0.41 |
| 1:J:452:LEU:CD1 | 1:J:467:LYS:HE3 | 2.49 | 0.41 |
| 1:L:257:VAL:HB | 1:L:266:ARG:HB2 | 2.02 | 0.41 |
| 1:F:338:PHE:CD2 | 1:G:340:VAL:HG13 | 2.55 | 0.41 |
| 1:G:266:ARG:HA | 1:G:266:ARG:HD2 | 1.86 | 0.41 |
| 1:H:299:LEU:HD11 | 1:H:330:LEU:HD23 | 2.02 | 0.41 |
| 1:H:373:GLU:O | 1:H:377:VAL:HG22 | 2.21 | 0.41 |
| 1:M:159:LYS:HG3 | 1:M:160:LEU:N | 2.34 | 0.41 |
| 1:B:89:SER:HB3 | 1:B:423:GLU:O | 2.20 | 0.41 |
| 1:C:332:LEU:HD13 | 1:C:334:LYS:HB2 | 2.02 | 0.41 |
| 1:I:142:ASN:HD22 | 1:I:163:LEU:CD1 | 2.32 | 0.41 |
| 1:L:142:ASN:OD1 | 1:L:255:ARG:HG3 | 2.20 | 0.41 |
| 1:A:79:PRO:HD2 | 1:A:83:TRP:CD1 | 2.55 | 0.41 |
| 1:H:437:GLN:OE1 | 1:H:437:GLN:N | 2.42 | 0.41 |
| 1:J:214:TYR:N | 1:J:214:TYR:CD1 | 2.89 | 0.41 |
| 1:A:59:GLN:HG3 | 1:A:280:GLU:OE1 | 2.20 | 0.41 |
| 1:B:362:VAL:CG1 | 1:B:374:ILE:HG12 | 2.50 | 0.41 |
| 1:C:398:LEU:HB3 | 1:C:402:ARG:HH22 | 1.86 | 0.41 |
| 1:D:452:LEU:CD1 | 1:D:467:LYS:HE3 | 2.51 | 0.41 |
| 1:G:135:LYS:O | 1:G:139:VAL:HG12 | 2.21 | 0.41 |
| 1:G:142:ASN:OD1 | 1:G:255:ARG:HG3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:131:PHE:CD1 | 1:I:391:ILE:HD11 | 2.55 | 0.41 |
| 1:H:332:LEU:HD13 | 1:H:334:LYS:HB2 | 2.02 | 0.41 |
| 1:B:331:GLN:NE2 | 1:C:333:GLU:O | 2.54 | 0.41 |
| 1:C:89:SER:HB3 | 1:C:423:GLU:O | 2.21 | 0.41 |
| 1:D:309:ARG:HB2 | 1:D:309:ARG:NH1 | 2.36 | 0.41 |
| 1:E:197:ALA:O | 1:E:235:MET:HE1 | 2.21 | 0.41 |
| 1:F:39:ILE:HB | 1:F:42:LEU:HG | 2.02 | 0.41 |
| 1:F:266:ARG:HA | 1:F:266:ARG:HD2 | 1.86 | 0.41 |
| 1:G:60:ALA:HB1 | 1:H:272:TYR:HD1 | 1.85 | 0.41 |
| 1:G:332:LEU:HD13 | 1:G:334:LYS:HB2 | 2.01 | 0.41 |
| 1:H:142:ASN:HD22 | 1:H:163:LEU:CD1 | 2.33 | 0.41 |
| 1:I:309:ARG:HB2 | 1:I:309:ARG:NH1 | 2.36 | 0.41 |
| 1:I:449:TRP:HZ3 | 1:J:466:ILE:HD13 | 1.86 | 0.41 |
| 1:K:479:SER:HB3 | 1:L:469:ARG:HH22 | 1.85 | 0.41 |
| 1:L:250:PRO:HB3 | 1:L:407:GLN:NE2 | 2.34 | 0.41 |
| 1:C:59:GLN:HG3 | 1:C:280:GLU:OE1 | 2.21 | 0.41 |
| 1:D:142:ASN:ND2 | 1:D:264:TYR:HB3 | 2.36 | 0.41 |
| 1:D:153:SER:HB3 | 1:D:413:GLN:NE2 | 2.36 | 0.41 |
| 1:E:332:LEU:HD13 | 1:E:334:LYS:HB2 | 2.02 | 0.41 |
| 1:E:458:ASP:HB2 | 1:E:461:ILE:HB | 2.02 | 0.41 |
| 1:K:142:ASN:HD21 | 1:K:264:TYR:HB3 | 1.85 | 0.41 |
| 1:L:478:THR:HA | 1:L:481:ILE:HD12 | 2.03 | 0.41 |
| 1:A:332:LEU:HD13 | 1:A:334:LYS:HB2 | 2.03 | 0.40 |
| 1:B:24:ARG:NH1 | 1:B:166:TYR:O | 2.45 | 0.40 |
| 1:D:39:ILE:HG21 | 1:E:271:GLU:HG2 | 2.03 | 0.40 |
| 1:G:216:HIS:HB3 | 1:G:229:TYR:CE2 | 2.56 | 0.40 |
| 1:G:430:LEU:HD12 | 1:G:433:ILE:HD12 | 2.01 | 0.40 |
| 1:H:113:VAL:HG11 | 1:H:405:LEU:HD21 | 2.02 | 0.40 |
| 1:H:126:TYR:CE1 | 1:H:158:MET:HB2 | 2.56 | 0.40 |
| 1:H:306:THR:HG23 | 1:H:322:GLY:HA3 | 2.04 | 0.40 |
| 1:K:162:ARG:NH2 | 1:L:259:LEU:HD22 | 2.34 | 0.40 |
| 1:K:250:PRO:HB3 | 1:K:407:GLN:NE2 | 2.36 | 0.40 |
| 1:A:216:HIS:HE1 | 1:A:218:TYR:HB3 | 1.86 | 0.40 |
| 1:D:250:PRO:HB3 | 1:D:407:GLN:HE21 | 1.86 | 0.40 |
| 1:E:159:LYS:HE3 | 1:E:161:TYR:CZ | 2.56 | 0.40 |
| 1:F:404:LEU:HD23 | 1:F:404:LEU:HA | 1.88 | 0.40 |
| 1:F:417:LEU:HB3 | 1:F:418:PRO:HD2 | 2.02 | 0.40 |
| 1:F:452:LEU:CD1 | 1:F:467:LYS:HE3 | 2.51 | 0.40 |
| 1:H:135:LYS:O | 1:H:139:VAL:HG12 | 2.21 | 0.40 |
| 1:J:371:ALA:HB2 | 1:K:372:GLU:HG3 | 2.04 | 0.40 |
| 1:J:418:PRO:O | 1:J:420:GLU:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:452:LEU:CD1 | 1:K:467:LYS:HE3 | 2.51 | 0.40 |
| 1:M:216:HIS:HB3 | 1:M:229:TYR:CE2 | 2.57 | 0.40 |
| 1:A:417:LEU:HB3 | 1:A:418:PRO:HD2 | 2.03 | 0.40 |
| 1:B:371:ALA:HB2 | 1:C:372:GLU:HG3 | 2.03 | 0.40 |
| 1:D:61:VAL:HG21 | 1:D:279:LEU:HD21 | 2.03 | 0.40 |
| 1:D:449:TRP:CD1 | 1:D:467:LYS:HG2 | 2.56 | 0.40 |
| 1:E:362:VAL:HG22 | 1:E:377:VAL:HG23 | 2.02 | 0.40 |
| 1:H:120:TYR:OH | 1:H:156:ASN:ND2 | 2.45 | 0.40 |
| 1:K:256:MET:HB3 | 1:K:266:ARG:O | 2.22 | 0.40 |
| 1:M:187:PHE:HA | 1:M:190:LEU:HD12 | 2.03 | 0.40 |
| 1:B:73:LEU:HD21 | 1:B:388:VAL:HG23 | 2.03 | 0.40 |
| 1:F:147:LEU:O | 1:F:407:GLN:NE2 | 2.48 | 0.40 |
| 1:G:216:HIS:HE1 | 1:G:218:TYR:HB3 | 1.87 | 0.40 |
| 1:G:278:SER:O | 1:G:282:LEU:HB2 | 2.21 | 0.40 |
| 1:K:171:ASP:OD1 | 1:K:175:ASN:N | 2.53 | 0.40 |
| 1:K:197:ALA:O | 1:K:235:MET:HE1 | 2.21 | 0.40 |
| 1:K:266:ARG:HA | 1:K:266:ARG:HD2 | 1.84 | 0.40 |
| 1:K:373:GLU:O | 1:K:377:VAL:HG22 | 2.21 | 0.40 |
| 1:L:415:PRO:HB2 | 1:M:94:LYS:NZ | 2.36 | 0.40 |
| 1:G:362:VAL:CG1 | 1:G:374:ILE:HG12 | 2.51 | 0.40 |
| 1:J:99:ASP:O | 1:J:103:LEU:HB2 | 2.21 | 0.40 |
| 1:J:458:ASP:HB2 | 1:J:461:ILE:HB | 2.02 | 0.40 |
| 1:L:266:ARG:HA | 1:L:266:ARG:HD2 | 1.87 | 0.40 |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:15:SER:OG | 1:D:95:GLN:OE1[4_555] | 2.15 | 0.05 |
| 1:B:193:ASP:OD2 | 1:M:309:ARG:NH1[4_455] | 2.17 | 0.03 |

## 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 | 469/536 (88%) | 423 (90%) | 45 (10%) | 1 (0%) | 47 | 78 |
| 1 | B | 469/536 (88%) | 424 (90%) | 43 (9%) | 2 (0%) | 34 | 69 |
| 1 | C | 469/536 (88%) | 420 (90%) | 46 (10%) | 3 (1%) | 25 | 61 |
| 1 | D | 469/536 (88%) | 420 (90%) | 47 (10%) | 2 (0%) | 34 | 69 |
| 1 | E | 469/536 (88%) | 421 (90%) | 45 (10%) | 3 (1%) | 25 | 61 |
| 1 | F | 469/536 (88%) | 421 (90%) | 45 (10%) | 3 (1%) | 25 | 61 |
| 1 | G | 469/536 (88%) | 420 (90%) | 48 (10%) | 1 (0%) | 47 | 78 |
| 1 | H | 469/536 (88%) | 421 (90%) | 45 (10%) | 3 (1%) | 25 | 61 |
| 1 | I | 469/536 (88%) | 421 (90%) | 46 (10%) | 2 (0%) | 34 | 69 |
| 1 | J | 469/536 (88%) | 421 (90%) | 45 (10%) | 3 (1%) | 25 | 61 |
| 1 | K | 469/536 (88%) | 422 (90%) | 46 (10%) | 1 (0%) | 47 | 78 |
| 1 | L | 469/536 (88%) | 420 (90%) | 48 (10%) | 1 (0%) | 47 | 78 |
| 1 | M | 469/536 (88%) | 423 (90%) | 44 (9%) | 2 (0%) | 34 | 69 |
| All | All | 6097/6968 (88%) | 5477 (90%) | 593 (10%) | 27 (0%) | 34 | 69 |

All (27) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 419 | LYS |
| 1 | A | 419 | LYS |
| 1 | B | 419 | LYS |
| 1 | C | 419 | LYS |
| 1 | D | 419 | LYS |
| 1 | E | 419 | LYS |
| 1 | F | 419 | LYS |
| 1 | G | 419 | LYS |
| 1 | H | 419 | LYS |
| 1 | I | 419 | LYS |
| 1 | J | 419 | LYS |
| 1 | K | 419 | LYS |
| 1 | L | 419 | LYS |
| 1 | C | 363 | GLN |
| 1 | M | 363 | GLN |
| 1 | D | 363 | GLN |
| 1 | E | 363 | GLN |
| 1 | F | 363 | GLN |
| 1 | I | 363 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 363 | GLN |
| 1 | H | 363 | GLN |
| 1 | J | 203 | GLY |
| 1 | B | 203 | GLY |
| 1 | E | 203 | GLY |
| 1 | H | 203 | GLY |
| 1 | C | 203 | GLY |
| 1 | F | 203 | 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 | 400/442 (90%) | 391 (98%) | 9 (2%) | 50 | 71 |
| 1 | B | 400/442 (90%) | 391 (98%) | 9 (2%) | 50 | 71 |
| 1 | C | 400/442 (90%) | 390 (98%) | 10 (2%) | 47 | 70 |
| 1 | D | 400/442 (90%) | 389 (97%) | 11 (3%) | 43 | 67 |
| 1 | E | 400/442 (90%) | 391 (98%) | 9 (2%) | 50 | 71 |
| 1 | F | 400/442 (90%) | 391 (98%) | 9 (2%) | 50 | 71 |
| 1 | G | 400/442 (90%) | 392 (98%) | 8 (2%) | 55 | 75 |
| 1 | H | 400/442 (90%) | 389 (97%) | 11 (3%) | 43 | 67 |
| 1 | I | 400/442 (90%) | 388 (97%) | 12 (3%) | 41 | 65 |
| 1 | J | 400/442 (90%) | 390 (98%) | 10 (2%) | 47 | 70 |
| 1 | K | 400/442 (90%) | 391 (98%) | 9 (2%) | 50 | 71 |
| 1 | L | 400/442 (90%) | 390 (98%) | 10 (2%) | 47 | 70 |
| 1 | M | 400/442 (90%) | 391 (98%) | 9 (2%) | 50 | 71 |
| All | All | 5200/5746 (90%) | 5074 (98%) | 126 (2%) | 49 | 71 |

All (126) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 22 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 59 | GLN |
| 1 | A | 147 | LEU |
| 1 | A | 151 | GLU |
| 1 | A | 182 | ARG |
| 1 | A | 228 | ARG |
| 1 | A | 255 | ARG |
| 1 | A | 277 | ARG |
| 1 | A | 390 | SER |
| 1 | B | 59 | GLN |
| 1 | B | 147 | LEU |
| 1 | B | 151 | GLU |
| 1 | B | 182 | ARG |
| 1 | B | 228 | ARG |
| 1 | B | 231 | GLU |
| 1 | B | 255 | ARG |
| 1 | B | 277 | ARG |
| 1 | B | 390 | SER |
| 1 | C | 22 | ASN |
| 1 | C | 59 | GLN |
| 1 | C | 147 | LEU |
| 1 | C | 151 | GLU |
| 1 | C | 182 | ARG |
| 1 | C | 228 | ARG |
| 1 | C | 231 | GLU |
| 1 | C | 255 | ARG |
| 1 | C | 315 | GLN |
| 1 | C | 427 | SER |
| 1 | D | 22 | ASN |
| 1 | D | 43 | PHE |
| 1 | D | 59 | GLN |
| 1 | D | 69 | LEU |
| 1 | D | 147 | LEU |
| 1 | D | 151 | GLU |
| 1 | D | 182 | ARG |
| 1 | D | 228 | ARG |
| 1 | D | 231 | GLU |
| 1 | D | 255 | ARG |
| 1 | D | 390 | SER |
| 1 | E | 59 | GLN |
| 1 | E | 69 | LEU |
| 1 | E | 147 | LEU |
| 1 | E | 151 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 182 | ARG |
| 1 | E | 228 | ARG |
| 1 | E | 231 | GLU |
| 1 | E | 255 | ARG |
| 1 | E | 390 | SER |
| 1 | F | 59 | GLN |
| 1 | F | 147 | LEU |
| 1 | F | 151 | GLU |
| 1 | F | 182 | ARG |
| 1 | F | 228 | ARG |
| 1 | F | 231 | GLU |
| 1 | F | 255 | ARG |
| 1 | F | 277 | ARG |
| 1 | F | 390 | SER |
| 1 | G | 59 | GLN |
| 1 | G | 147 | LEU |
| 1 | G | 182 | ARG |
| 1 | G | 228 | ARG |
| 1 | G | 231 | GLU |
| 1 | G | 255 | ARG |
| 1 | G | 277 | ARG |
| 1 | G | 309 | ARG |
| 1 | H | 23 | ASP |
| 1 | H | 59 | GLN |
| 1 | H | 147 | LEU |
| 1 | H | 182 | ARG |
| 1 | H | 228 | ARG |
| 1 | H | 231 | GLU |
| 1 | H | 255 | ARG |
| 1 | H | 277 | ARG |
| 1 | H | 293 | SER |
| 1 | H | 390 | SER |
| 1 | H | 427 | SER |
| 1 | I | 22 | ASN |
| 1 | I | 23 | ASP |
| 1 | I | 59 | GLN |
| 1 | I | 132 | GLU |
| 1 | I | 147 | LEU |
| 1 | I | 151 | GLU |
| 1 | I | 182 | ARG |
| 1 | I | 228 | ARG |
| 1 | I | 231 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 255 | ARG |
| 1 | I | 260 | ASP |
| 1 | I | 390 | SER |
| 1 | J | 22 | ASN |
| 1 | J | 43 | PHE |
| 1 | J | 59 | GLN |
| 1 | J | 147 | LEU |
| 1 | J | 182 | ARG |
| 1 | J | 208 | ASP |
| 1 | J | 228 | ARG |
| 1 | J | 260 | ASP |
| 1 | J | 277 | ARG |
| 1 | J | 390 | SER |
| 1 | K | 22 | ASN |
| 1 | K | 59 | GLN |
| 1 | K | 69 | LEU |
| 1 | K | 147 | LEU |
| 1 | K | 182 | ARG |
| 1 | K | 228 | ARG |
| 1 | K | 231 | GLU |
| 1 | K | 255 | ARG |
| 1 | K | 390 | SER |
| 1 | L | 22 | ASN |
| 1 | L | 59 | GLN |
| 1 | L | 147 | LEU |
| 1 | L | 151 | GLU |
| 1 | L | 182 | ARG |
| 1 | L | 228 | ARG |
| 1 | L | 255 | ARG |
| 1 | L | 260 | ASP |
| 1 | L | 309 | ARG |
| 1 | L | 390 | SER |
| 1 | M | 22 | ASN |
| 1 | M | 23 | ASP |
| 1 | M | 59 | GLN |
| 1 | M | 147 | LEU |
| 1 | M | 182 | ARG |
| 1 | M | 228 | ARG |
| 1 | M | 231 | GLU |
| 1 | M | 255 | ARG |
| 1 | M | 390 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 184 | GLN |
| 1 | B | 184 | GLN |
| 1 | B | 331 | GLN |
| 1 | C | 156 | ASN |
| 1 | F | 184 | GLN |
| 1 | J | 184 | GLN |
| 1 | J | 216 | HIS |
| 1 | L | 184 | GLN |
| 1 | M | 136 | 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 monosaccharides 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 | 473/536 (88%) | 0.30 | 31 (6%) | 18 | 14 | 68, 139, 224, 386 | 1 (0%) |
| 1 | B | 473/536 (88%) | 0.27 | 26 (5%) | 25 | 21 | 72, 141, 242, 294 | 1 (0%) |
| 1 | C | 473/536 (88%) | 0.40 | 49 (10%) | 6 | 6 | 76, 144, 247, 328 | 1 (0%) |
| 1 | D | 473/536 (88%) | 0.43 | 40 (8%) | 10 | 9 | 90, 160, 263, 353 | 1 (0%) |
| 1 | E | 473/536 (88%) | 0.57 | 46 (9%) | 7 | 7 | 89, 164, 258, 310 | 1 (0%) |
| 1 | F | 473/536 (88%) | 0.32 | 32 (6%) | 17 | 13 | 81, 164, 240, 285 | 1 (0%) |
| 1 | G | 473/536 (88%) | 0.19 | 29 (6%) | 21 | 17 | 78, 149, 242, 341 | 1 (0%) |
| 1 | H | 473/536 (88%) | 0.23 | 22 (4%) | 31 | 27 | 76, 137, 229, 294 | 1 (0%) |
| 1 | I | 473/536 (88%) | 0.19 | 26 (5%) | 25 | 21 | 75, 129, 232, 316 | 1 (0%) |
| 1 | J | 473/536 (88%) | 0.32 | 42 (8%) | 9 | 8 | 67, 128, 233, 363 | 1 (0%) |
| 1 | K | 473/536 (88%) | 0.30 | 32 (6%) | 17 | 13 | 65, 132, 236, 321 | 1 (0%) |
| 1 | L | 473/536 (88%) | 0.33 | 34 (7%) | 15 | 12 | 68, 138, 237, 287 | 1 (0%) |
| 1 | M | 473/536 (88%) | 0.21 | 29 (6%) | 21 | 17 | 66, 141, 231, 329 | 1 (0%) |
| All | All | 6149/6968 (88%) | 0.31 | 438 (7%) | 16 | 12 | 65, 145, 240, 386 | 13 (0%) |

All (438) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 48 | ASP | 10.9 |
| 1 | A | 48 | ASP | 9.8 |
| 1 | B | 454 | PRO | 9.8 |
| 1 | C | 454 | PRO | 9.3 |
| 1 | B | 463 | LEU | 9.2 |
| 1 | K | 463 | LEU | 9.1 |
| 1 | D | 463 | LEU | 8.8 |
| 1 | D | 454 | PRO | 8.7 |
| 1 | L | 47 | SER | 7.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | M | 102 | GLY | 7.6 |
| 1 | M | 48 | ASP | 7.6 |
| 1 | I | 454 | PRO | 7.5 |
| 1 | K | 467 | LYS | 7.3 |
| 1 | K | 466 | ILE | 7.3 |
| 1 | J | 457 | ASP | 7.2 |
| 1 | K | 459 | PRO | 7.0 |
| 1 | A | 102 | GLY | 7.0 |
| 1 | J | 467 | LYS | 7.0 |
| 1 | C | 463 | LEU | 6.7 |
| 1 | C | 422 | VAL | 6.7 |
| 1 | J | 454 | PRO | 6.6 |
| 1 | L | 454 | PRO | 6.6 |
| 1 | I | 459 | PRO | 6.6 |
| 1 | H | 454 | PRO | 6.5 |
| 1 | L | 48 | ASP | 6.5 |
| 1 | E | 421 | ALA | 6.4 |
| 1 | A | 47 | SER | 6.1 |
| 1 | B | 467 | LYS | 6.1 |
| 1 | I | 451 | ALA | 5.9 |
| 1 | J | 48 | ASP | 5.9 |
| 1 | D | 47 | SER | 5.8 |
| 1 | B | 48 | ASP | 5.8 |
| 1 | K | 454 | PRO | 5.8 |
| 1 | J | 463 | LEU | 5.7 |
| 1 | K | 48 | ASP | 5.6 |
| 1 | A | 451 | ALA | 5.6 |
| 1 | E | 230 | GLU | 5.6 |
| 1 | C | 466 | ILE | 5.5 |
| 1 | C | 461 | ILE | 5.4 |
| 1 | M | 106 | VAL | 5.4 |
| 1 | I | 461 | ILE | 5.4 |
| 1 | A | 454 | PRO | 5.3 |
| 1 | J | 102 | GLY | 5.3 |
| 1 | C | 467 | LYS | 5.3 |
| 1 | F | 454 | PRO | 5.2 |
| 1 | K | 461 | ILE | 5.2 |
| 1 | M | 101 | ASP | 5.1 |
| 1 | J | 459 | PRO | 5.0 |
| 1 | J | 466 | ILE | 5.0 |
| 1 | L | 451 | ALA | 4.9 |
| 1 | L | 467 | LYS | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 3 | GLU | 4.9 |
| 1 | J | 451 | ALA | 4.9 |
| 1 | C | 421 | ALA | 4.9 |
| 1 | K | 451 | ALA | 4.8 |
| 1 | L | 459 | PRO | 4.7 |
| 1 | L | 102 | GLY | 4.7 |
| 1 | J | 101 | ASP | 4.7 |
| 1 | H | 102 | GLY | 4.7 |
| 1 | A | 463 | LEU | 4.7 |
| 1 | J | 461 | ILE | 4.7 |
| 1 | I | 478 | THR | 4.6 |
| 1 | L | 421 | ALA | 4.6 |
| 1 | D | 462 | ASN | 4.6 |
| 1 | J | 205 | LYS | 4.5 |
| 1 | B | 365 | THR | 4.5 |
| 1 | K | 419 | LYS | 4.5 |
| 1 | L | 463 | LEU | 4.4 |
| 1 | E | 419 | LYS | 4.4 |
| 1 | C | 365 | THR | 4.4 |
| 1 | H | 451 | ALA | 4.3 |
| 1 | E | 48 | ASP | 4.2 |
| 1 | B | 366 | GLY | 4.2 |
| 1 | E | 417 | LEU | 4.2 |
| 1 | B | 457 | ASP | 4.2 |
| 1 | B | 47 | SER | 4.1 |
| 1 | D | 467 | LYS | 4.1 |
| 1 | F | 467 | LYS | 4.1 |
| 1 | H | 455 | MET | 4.0 |
| 1 | L | 92 | GLU | 4.0 |
| 1 | M | 92 | GLU | 4.0 |
| 1 | D | 471 | ALA | 4.0 |
| 1 | K | 462 | ASN | 4.0 |
| 1 | K | 421 | ALA | 4.0 |
| 1 | I | 467 | LYS | 4.0 |
| 1 | B | 466 | ILE | 4.0 |
| 1 | E | 216 | HIS | 4.0 |
| 1 | A | 452 | LEU | 4.0 |
| 1 | C | 106 | VAL | 4.0 |
| 1 | I | 102 | GLY | 4.0 |
| 1 | H | 421 | ALA | 3.9 |
| 1 | C | 457 | ASP | 3.9 |
| 1 | D | 457 | ASP | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 178 | GLN | 3.9 |
| 1 | J | 209 | GLU | 3.9 |
| 1 | I | 48 | ASP | 3.9 |
| 1 | M | 419 | LYS | 3.9 |
| 1 | A | 467 | LYS | 3.9 |
| 1 | J | 47 | SER | 3.9 |
| 1 | E | 467 | LYS | 3.8 |
| 1 | M | 103 | LEU | 3.8 |
| 1 | B | 461 | ILE | 3.8 |
| 1 | D | 101 | ASP | 3.8 |
| 1 | G | 48 | ASP | 3.8 |
| 1 | G | 319 | PHE | 3.8 |
| 1 | C | 96 | LEU | 3.8 |
| 1 | M | 455 | MET | 3.8 |
| 1 | A | 455 | MET | 3.7 |
| 1 | D | 450 | ALA | 3.7 |
| 1 | M | 422 | VAL | 3.7 |
| 1 | C | 367 | GLU | 3.7 |
| 1 | A | 461 | ILE | 3.7 |
| 1 | M | 47 | SER | 3.7 |
| 1 | C | 478 | THR | 3.7 |
| 1 | B | 459 | PRO | 3.7 |
| 1 | C | 459 | PRO | 3.7 |
| 1 | A | 478 | THR | 3.7 |
| 1 | G | 102 | GLY | 3.7 |
| 1 | C | 470 | ILE | 3.7 |
| 1 | D | 365 | THR | 3.6 |
| 1 | C | 419 | LYS | 3.6 |
| 1 | J | 453 | ALA | 3.6 |
| 1 | M | 456 | ARG | 3.6 |
| 1 | D | 8 | LEU | 3.6 |
| 1 | E | 8 | LEU | 3.5 |
| 1 | E | 4 | LYS | 3.5 |
| 1 | E | 225 | GLU | 3.5 |
| 1 | K | 422 | VAL | 3.5 |
| 1 | E | 459 | PRO | 3.5 |
| 1 | F | 230 | GLU | 3.5 |
| 1 | D | 102 | GLY | 3.5 |
| 1 | C | 230 | GLU | 3.5 |
| 1 | H | 463 | LEU | 3.5 |
| 1 | M | 368 | ARG | 3.4 |
| 1 | H | 417 | LEU | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | K | 102 | GLY | 3.4 |
| 1 | M | 463 | LEU | 3.4 |
| 1 | J | 96 | LEU | 3.4 |
| 1 | I | 306 | THR | 3.4 |
| 1 | L | 211 | ILE | 3.3 |
| 1 | E | 463 | LEU | 3.3 |
| 1 | B | 417 | LEU | 3.3 |
| 1 | C | 306 | THR | 3.3 |
| 1 | M | 458 | ASP | 3.3 |
| 1 | I | 47 | SER | 3.3 |
| 1 | D | 443 | GLU | 3.3 |
| 1 | D | 98 | SER | 3.3 |
| 1 | F | 366 | GLY | 3.3 |
| 1 | D | 46 | ASP | 3.3 |
| 1 | L | 422 | VAL | 3.3 |
| 1 | G | 367 | GLU | 3.3 |
| 1 | G | 467 | LYS | 3.3 |
| 1 | E | 99 | ASP | 3.2 |
| 1 | G | 457 | ASP | 3.2 |
| 1 | D | 367 | GLU | 3.2 |
| 1 | H | 416 | GLU | 3.2 |
| 1 | F | 102 | GLY | 3.2 |
| 1 | F | 421 | ALA | 3.2 |
| 1 | J | 187 | PHE | 3.2 |
| 1 | I | 221 | GLU | 3.2 |
| 1 | H | 364 | ARG | 3.2 |
| 1 | B | 478 | THR | 3.2 |
| 1 | D | 421 | ALA | 3.2 |
| 1 | G | 169 | GLN | 3.2 |
| 1 | G | 454 | PRO | 3.2 |
| 1 | K | 481 | ILE | 3.2 |
| 1 | J | 323 | ARG | 3.1 |
| 1 | E | 454 | PRO | 3.1 |
| 1 | G | 179 | MET | 3.1 |
| 1 | L | 461 | ILE | 3.1 |
| 1 | E | 169 | GLN | 3.1 |
| 1 | D | 178 | GLN | 3.1 |
| 1 | A | 365 | THR | 3.1 |
| 1 | E | 7 | GLY | 3.1 |
| 1 | J | 106 | VAL | 3.1 |
| 1 | M | 420 | GLU | 3.1 |
| 1 | J | 363 | GLN | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 47 | SER | 3.1 |
| 1 | E | 418 | PRO | 3.0 |
| 1 | I | 416 | GLU | 3.0 |
| 1 | L | 368 | ARG | 3.0 |
| 1 | I | 46 | ASP | 3.0 |
| 1 | K | 457 | ASP | 3.0 |
| 1 | M | 467 | LYS | 3.0 |
| 1 | J | 462 | ASN | 3.0 |
| 1 | L | 106 | VAL | 3.0 |
| 1 | A | 459 | PRO | 3.0 |
| 1 | H | 47 | SER | 3.0 |
| 1 | D | 208 | ASP | 3.0 |
| 1 | L | 208 | ASP | 3.0 |
| 1 | E | 232 | VAL | 3.0 |
| 1 | L | 205 | LYS | 3.0 |
| 1 | D | 466 | ILE | 3.0 |
| 1 | D | 45 | LYS | 3.0 |
| 1 | K | 47 | SER | 3.0 |
| 1 | C | 198 | VAL | 3.0 |
| 1 | K | 21 | LYS | 3.0 |
| 1 | C | 451 | ALA | 2.9 |
| 1 | G | 178 | GLN | 3.0 |
| 1 | I | 453 | ALA | 2.9 |
| 1 | D | 459 | PRO | 2.9 |
| 1 | J | 421 | ALA | 2.9 |
| 1 | M | 421 | ALA | 2.9 |
| 1 | H | 367 | GLU | 2.9 |
| 1 | M | 208 | ASP | 2.9 |
| 1 | J | 481 | ILE | 2.9 |
| 1 | A | 101 | ASP | 2.9 |
| 1 | G | 365 | THR | 2.9 |
| 1 | C | 364 | ARG | 2.9 |
| 1 | K | 470 | ILE | 2.9 |
| 1 | B | 369 | VAL | 2.9 |
| 1 | G | 461 | ILE | 2.9 |
| 1 | F | 367 | GLU | 2.8 |
| 1 | F | 455 | MET | 2.8 |
| 1 | J | 306 | THR | 2.8 |
| 1 | F | 88 | ILE | 2.8 |
| 1 | G | 366 | GLY | 2.8 |
| 1 | G | 458 | ASP | 2.8 |
| 1 | G | 3 | GLU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 102 | GLY | 2.8 |
| 1 | E | 235 | MET | 2.8 |
| 1 | H | 448 | ALA | 2.8 |
| 1 | E | 229 | TYR | 2.8 |
| 1 | G | 417 | LEU | 2.8 |
| 1 | F | 208 | ASP | 2.8 |
| 1 | E | 231 | GLU | 2.8 |
| 1 | L | 462 | ASN | 2.8 |
| 1 | C | 319 | PHE | 2.8 |
| 1 | C | 462 | ASN | 2.8 |
| 1 | F | 101 | ASP | 2.8 |
| 1 | M | 454 | PRO | 2.8 |
| 1 | D | 422 | VAL | 2.8 |
| 1 | B | 106 | VAL | 2.7 |
| 1 | F | 456 | ARG | 2.7 |
| 1 | C | 179 | MET | 2.7 |
| 1 | B | 102 | GLY | 2.7 |
| 1 | A | 231 | GLU | 2.7 |
| 1 | D | 28 | GLU | 2.7 |
| 1 | J | 211 | ILE | 2.7 |
| 1 | C | 231 | GLU | 2.7 |
| 1 | J | 452 | LEU | 2.7 |
| 1 | A | 46 | ASP | 2.7 |
| 1 | A | 311 | LEU | 2.7 |
| 1 | A | 481 | ILE | 2.7 |
| 1 | C | 178 | GLN | 2.7 |
| 1 | J | 367 | GLU | 2.7 |
| 1 | C | 456 | ARG | 2.7 |
| 1 | H | 101 | ASP | 2.7 |
| 1 | H | 103 | LEU | 2.7 |
| 1 | K | 96 | LEU | 2.7 |
| 1 | C | 458 | ASP | 2.7 |
| 1 | D | 451 | ALA | 2.7 |
| 1 | E | 221 | GLU | 2.7 |
| 1 | F | 464 | ALA | 2.7 |
| 1 | L | 466 | ILE | 2.7 |
| 1 | M | 233 | GLU | 2.7 |
| 1 | A | 232 | VAL | 2.7 |
| 1 | D | 464 | ALA | 2.6 |
| 1 | A | 238 | GLN | 2.6 |
| 1 | C | 202 | GLY | 2.6 |
| 1 | B | 455 | MET | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 366 | GLY | 2.6 |
| 1 | E | 12 | GLY | 2.6 |
| 1 | F | 451 | ALA | 2.6 |
| 1 | E | 213 | VAL | 2.6 |
| 1 | M | 478 | THR | 2.6 |
| 1 | J | 419 | LYS | 2.6 |
| 1 | G | 421 | ALA | 2.6 |
| 1 | C | 194 | ILE | 2.6 |
| 1 | I | 457 | ASP | 2.6 |
| 1 | J | 478 | THR | 2.6 |
| 1 | A | 466 | ILE | 2.6 |
| 1 | C | 48 | ASP | 2.6 |
| 1 | C | 453 | ALA | 2.6 |
| 1 | M | 99 | ASP | 2.6 |
| 1 | H | 415 | PRO | 2.6 |
| 1 | M | 457 | ASP | 2.6 |
| 1 | M | 481 | ILE | 2.6 |
| 1 | J | 455 | MET | 2.6 |
| 1 | D | 368 | ARG | 2.6 |
| 1 | K | 99 | ASP | 2.5 |
| 1 | E | 179 | MET | 2.5 |
| 1 | F | 457 | ASP | 2.5 |
| 1 | H | 422 | VAL | 2.5 |
| 1 | L | 458 | ASP | 2.5 |
| 1 | B | 367 | GLU | 2.5 |
| 1 | C | 232 | VAL | 2.5 |
| 1 | I | 363 | GLN | 2.5 |
| 1 | E | 88 | ILE | 2.5 |
| 1 | I | 466 | ILE | 2.5 |
| 1 | L | 416 | GLU | 2.5 |
| 1 | I | 463 | LEU | 2.5 |
| 1 | A | 187 | PHE | 2.5 |
| 1 | B | 101 | ASP | 2.5 |
| 1 | L | 417 | LEU | 2.5 |
| 1 | C | 233 | GLU | 2.5 |
| 1 | K | 106 | VAL | 2.5 |
| 1 | K | 460 | ASP | 2.4 |
| 1 | I | 365 | THR | 2.4 |
| 1 | D | 6 | THR | 2.4 |
| 1 | D | 411 | THR | 2.4 |
| 1 | K | 220 | ASP | 2.4 |
| 1 | E | 367 | GLU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 450 | ALA | 2.4 |
| 1 | G | 47 | SER | 2.4 |
| 1 | L | 478 | THR | 2.4 |
| 1 | D | 470 | ILE | 2.4 |
| 1 | E | 17 | TYR | 2.4 |
| 1 | E | 368 | ARG | 2.4 |
| 1 | F | 463 | LEU | 2.4 |
| 1 | K | 92 | GLU | 2.4 |
| 1 | K | 312 | THR | 2.4 |
| 1 | E | 9 | ALA | 2.4 |
| 1 | L | 216 | HIS | 2.4 |
| 1 | C | 187 | PHE | 2.4 |
| 1 | K | 464 | ALA | 2.4 |
| 1 | K | 453 | ALA | 2.4 |
| 1 | J | 206 | LYS | 2.4 |
| 1 | B | 364 | ARG | 2.4 |
| 1 | B | 451 | ALA | 2.4 |
| 1 | M | 89 | SER | 2.4 |
| 1 | C | 481 | ILE | 2.4 |
| 1 | D | 373 | GLU | 2.4 |
| 1 | G | 466 | ILE | 2.4 |
| 1 | F | 260 | ASP | 2.4 |
| 1 | I | 229 | TYR | 2.4 |
| 1 | K | 458 | ASP | 2.4 |
| 1 | L | 212 | ASP | 2.4 |
| 1 | J | 470 | ILE | 2.3 |
| 1 | H | 46 | ASP | 2.3 |
| 1 | F | 481 | ILE | 2.3 |
| 1 | E | 464 | ALA | 2.3 |
| 1 | H | 106 | VAL | 2.3 |
| 1 | F | 99 | ASP | 2.3 |
| 1 | J | 321 | THR | 2.3 |
| 1 | K | 306 | THR | 2.3 |
| 1 | C | 45 | LYS | 2.3 |
| 1 | J | 178 | GLN | 2.3 |
| 1 | E | 226 | TYR | 2.3 |
| 1 | H | 190 | LEU | 2.3 |
| 1 | L | 457 | ASP | 2.3 |
| 1 | L | 233 | GLU | 2.3 |
| 1 | G | 216 | HIS | 2.3 |
| 1 | J | 13 | ALA | 2.3 |
| 1 | B | 470 | ILE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 194 | ILE | 2.3 |
| 1 | L | 423 | GLU | 2.3 |
| 1 | E | 5 | ARG | 2.3 |
| 1 | I | 448 | ALA | 2.3 |
| 1 | J | 450 | ALA | 2.3 |
| 1 | F | 368 | ARG | 2.3 |
| 1 | J | 12 | GLY | 2.3 |
| 1 | L | 105 | LYS | 2.3 |
| 1 | E | 453 | ALA | 2.3 |
| 1 | H | 419 | LYS | 2.3 |
| 1 | F | 231 | GLU | 2.2 |
| 1 | A | 177 | LEU | 2.2 |
| 1 | D | 481 | ILE | 2.2 |
| 1 | E | 13 | ALA | 2.2 |
| 1 | H | 462 | ASN | 2.2 |
| 1 | D | 453 | ALA | 2.2 |
| 1 | C | 99 | ASP | 2.2 |
| 1 | E | 11 | ASP | 2.2 |
| 1 | C | 3 | GLU | 2.2 |
| 1 | B | 298 | GLY | 2.2 |
| 1 | C | 455 | MET | 2.2 |
| 1 | J | 207 | ALA | 2.2 |
| 1 | F | 449 | TRP | 2.2 |
| 1 | E | 219 | LEU | 2.2 |
| 1 | I | 481 | ILE | 2.2 |
| 1 | G | 206 | LYS | 2.2 |
| 1 | G | 231 | GLU | 2.2 |
| 1 | F | 207 | ALA | 2.2 |
| 1 | L | 206 | LYS | 2.2 |
| 1 | F | 233 | GLU | 2.2 |
| 1 | J | 365 | THR | 2.2 |
| 1 | L | 453 | ALA | 2.2 |
| 1 | G | 233 | GLU | 2.2 |
| 1 | F | 8 | LEU | 2.2 |
| 1 | C | 203 | GLY | 2.2 |
| 1 | K | 19 | ARG | 2.2 |
| 1 | K | 179 | MET | 2.2 |
| 1 | C | 206 | LYS | 2.2 |
| 1 | M | 209 | GLU | 2.2 |
| 1 | G | 45 | LYS | 2.2 |
| 1 | I | 103 | LEU | 2.2 |
| 1 | L | 419 | LYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 7 | GLY | 2.2 |
| 1 | F | 47 | SER | 2.2 |
| 1 | F | 48 | ASP | 2.2 |
| 1 | A | 244 | TYR | 2.2 |
| 1 | L | 231 | GLU | 2.2 |
| 1 | F | 452 | LEU | 2.1 |
| 1 | M | 462 | ASN | 2.1 |
| 1 | G | 205 | LYS | 2.1 |
| 1 | E | 420 | GLU | 2.1 |
| 1 | M | 3 | GLU | 2.1 |
| 1 | A | 448 | ALA | 2.1 |
| 1 | A | 213 | VAL | 2.1 |
| 1 | C | 452 | LEU | 2.1 |
| 1 | E | 218 | TYR | 2.1 |
| 1 | F | 198 | VAL | 2.1 |
| 1 | B | 3 | GLU | 2.1 |
| 1 | L | 28 | GLU | 2.1 |
| 1 | D | 311 | LEU | 2.1 |
| 1 | B | 458 | ASP | 2.1 |
| 1 | D | 211 | ILE | 2.1 |
| 1 | C | 201 | GLN | 2.1 |
| 1 | A | 458 | ASP | 2.1 |
| 1 | E | 214 | TYR | 2.1 |
| 1 | A | 366 | GLY | 2.1 |
| 1 | B | 449 | TRP | 2.1 |
| 1 | C | 424 | PRO | 2.1 |
| 1 | G | 149 | GLU | 2.1 |
| 1 | D | 207 | ALA | 2.1 |
| 1 | F | 476 | ILE | 2.1 |
| 1 | F | 365 | THR | 2.1 |
| 1 | M | 451 | ALA | 2.1 |
| 1 | G | 419 | LYS | 2.1 |
| 1 | A | 367 | GLU | 2.1 |
| 1 | A | 327 | ILE | 2.1 |
| 1 | K | 420 | GLU | 2.1 |
| 1 | I | 219 | LEU | 2.0 |
| 1 | C | 443 | GLU | 2.0 |
| 1 | A | 323 | ARG | 2.0 |
| 1 | H | 466 | ILE | 2.0 |
| 1 | J | 449 | TRP | 2.0 |
| 1 | C | 326 | ASP | 2.0 |
| 1 | E | 6 | THR | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 204 | GLU | 2.0 |
| 1 | I | 106 | VAL | 2.0 |
| 1 | J | 233 | GLU | 2.0 |
| 1 | G | 451 | ALA | 2.0 |
| 1 | I | 327 | ILE | 2.0 |
| 1 | J | 456 | ARG | 2.0 |
| 1 | F | 326 | ASP | 2.0 |
| 1 | G | 448 | ALA | 2.0 |
| 1 | E | 224 | GLY | 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 monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.