



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 AM GMT

PDB ID : 3KGV
Title : Crystal Structure of Human DNA-dependent Protein Kinase Catalytic Subunit (DNA-PKcs)
Authors : Sibanda, B.L.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2009-10-29
Resolution : 6.60 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 ⓘ](#)) 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

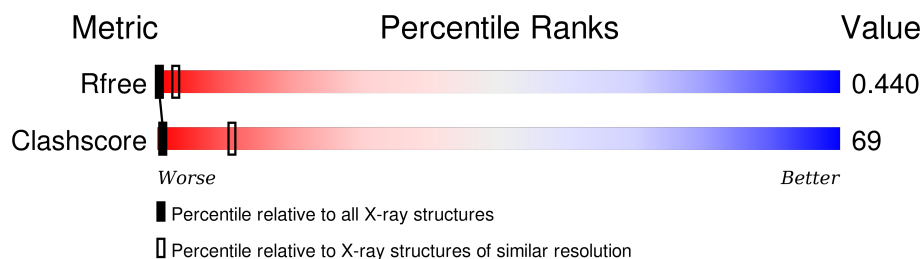
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.60 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 | 1014 (9.50-3.66) |
| Clashscore | 102246 | 1062 (9.50-3.70) |

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 $\leq 5\%$. 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 | 4128 | 91% |
| 1 | B | 4128 | 93% |
| 1 | C | 4128 | 90% |
| 1 | D | 4128 | 96% |
| 1 | E | 4128 | 98% |
| 1 | F | 4128 | 87% |
| 1 | O | 4128 | 91% |
| 1 | P | 4128 | 93% |
| 1 | Q | 4128 | 90% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | R | 4128 |  96% |
| 1 | S | 4128 |  98% |
| 1 | T | 4128 |  87% |
| 1 | X | 4128 |  95% |
| 1 | Y | 4128 |  95% |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20320 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.

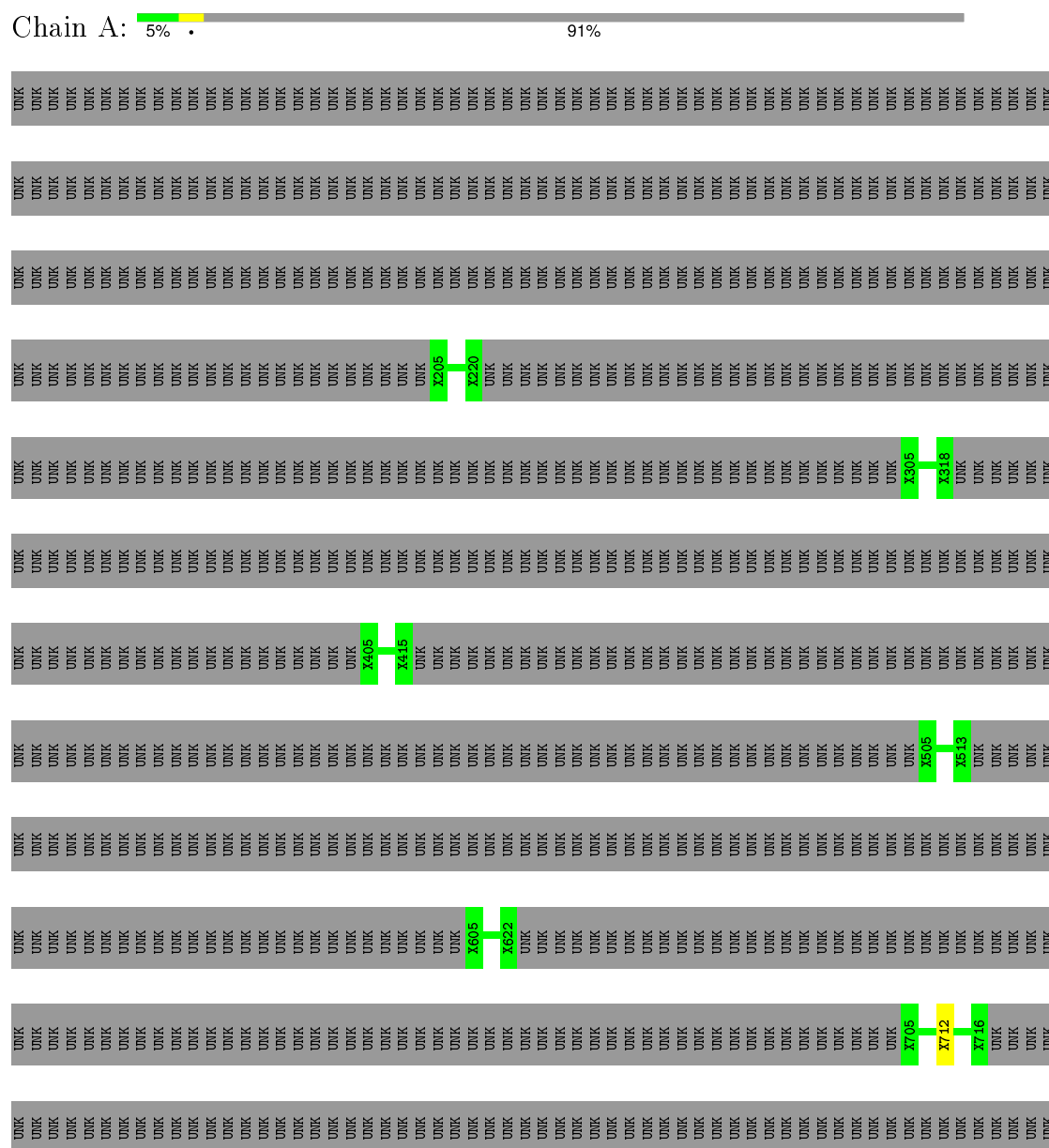
- Molecule 1 is a protein called DNA-dependent Protein Kinase Catalytic Subunit.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|
| 1 | A | 354 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1770 | 1062 | 354 | 354 | | | |
| 1 | B | 283 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1415 | 849 | 283 | 283 | | | |
| 1 | C | 406 | Total | C | N | O | 0 | 0 | 0 |
| | | | 2030 | 1218 | 406 | 406 | | | |
| 1 | D | 182 | Total | C | N | O | 0 | 0 | 0 |
| | | | 910 | 546 | 182 | 182 | | | |
| 1 | E | 65 | Total | C | N | O | 0 | 0 | 0 |
| | | | 325 | 195 | 65 | 65 | | | |
| 1 | F | 531 | Total | C | N | O | 0 | 0 | 0 |
| | | | 2655 | 1593 | 531 | 531 | | | |
| 1 | X | 211 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1055 | 633 | 211 | 211 | | | |
| 1 | O | 354 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1770 | 1062 | 354 | 354 | | | |
| 1 | P | 283 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1415 | 849 | 283 | 283 | | | |
| 1 | Q | 406 | Total | C | N | O | 0 | 0 | 0 |
| | | | 2030 | 1218 | 406 | 406 | | | |
| 1 | R | 182 | Total | C | N | O | 0 | 0 | 0 |
| | | | 910 | 546 | 182 | 182 | | | |
| 1 | S | 65 | Total | C | N | O | 0 | 0 | 0 |
| | | | 325 | 195 | 65 | 65 | | | |
| 1 | T | 531 | Total | C | N | O | 0 | 0 | 0 |
| | | | 2655 | 1593 | 531 | 531 | | | |
| 1 | Y | 211 | Total | C | N | O | 0 | 0 | 0 |
| | | | 1055 | 633 | 211 | 211 | | | |

3 Residue-property plots

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.

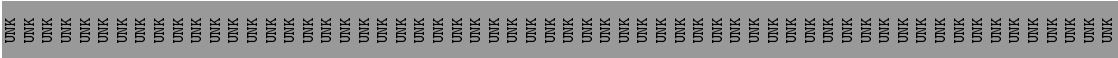
• Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit



[illegible]

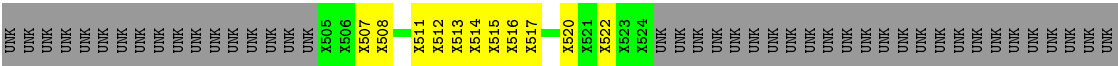
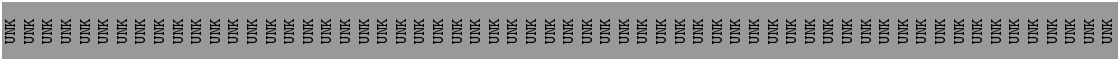
[illegible]

[illegible]



● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain B: . . 93%



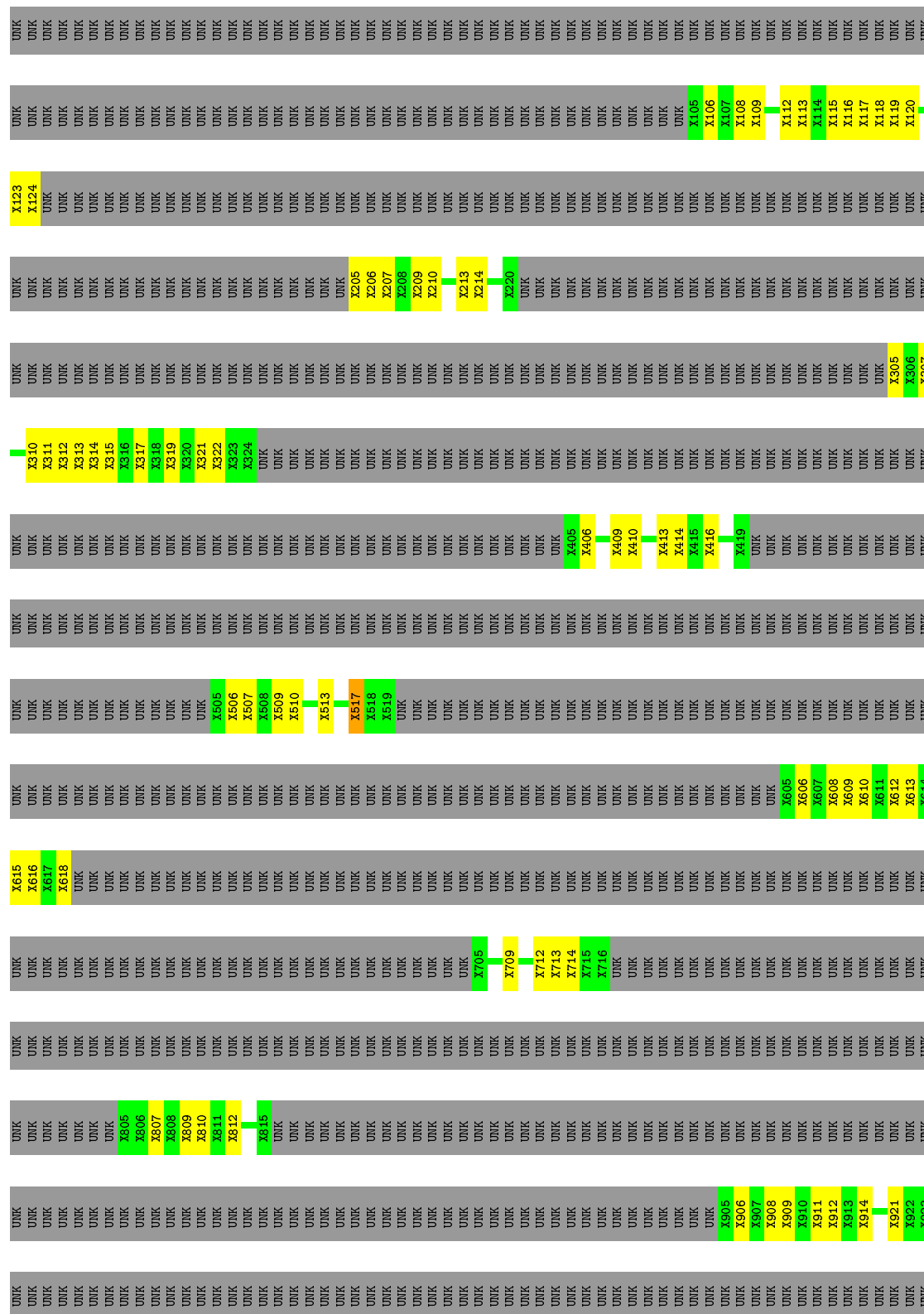
WORLDWIDE
PDB
PROTEIN DATA BANK

[illegible]

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● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain C:  90%



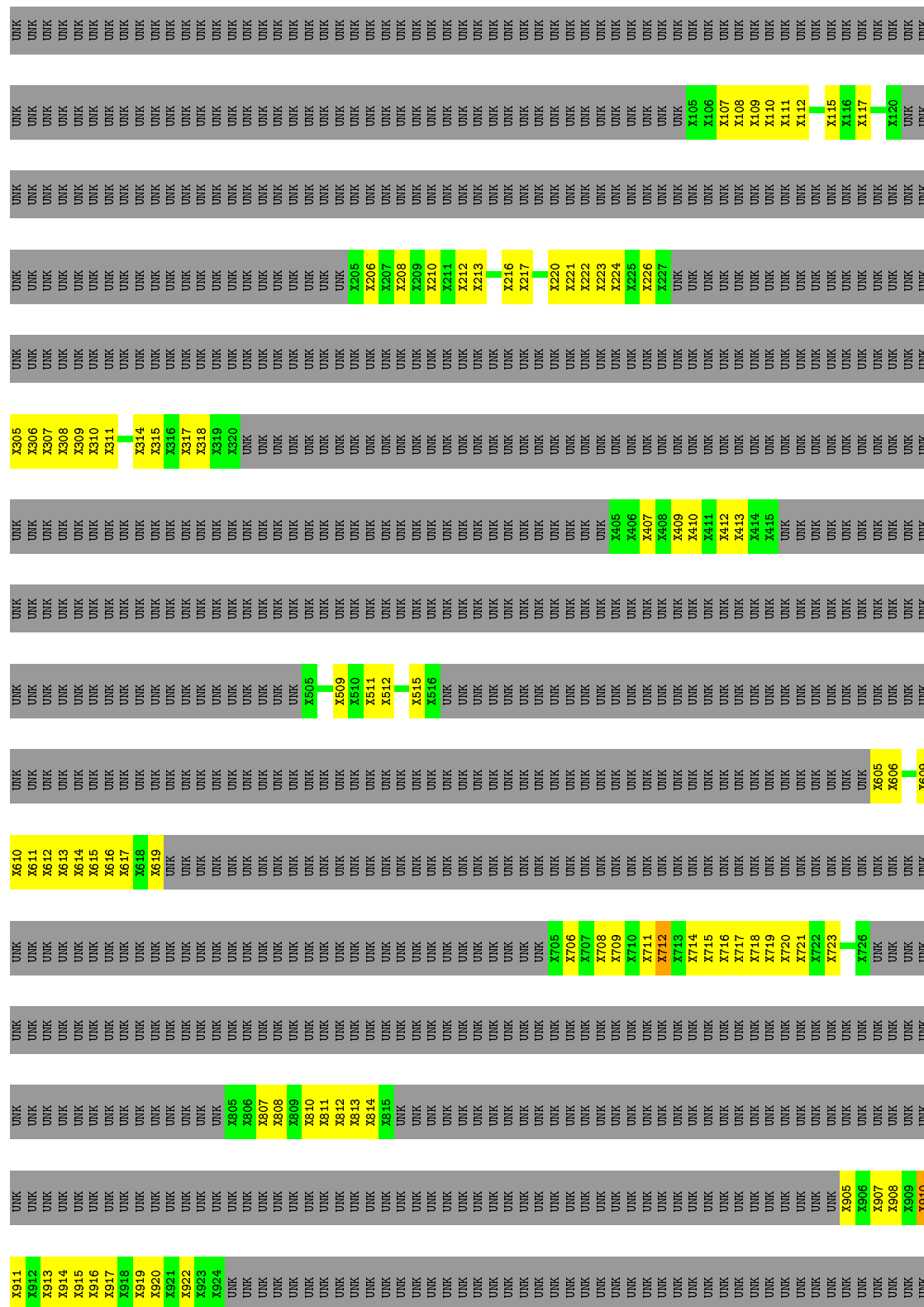
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[illegible]

● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain D: . . 96%



[illegible]

[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain E:  98%

[illegible]



[illegible]

[illegible]

[illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

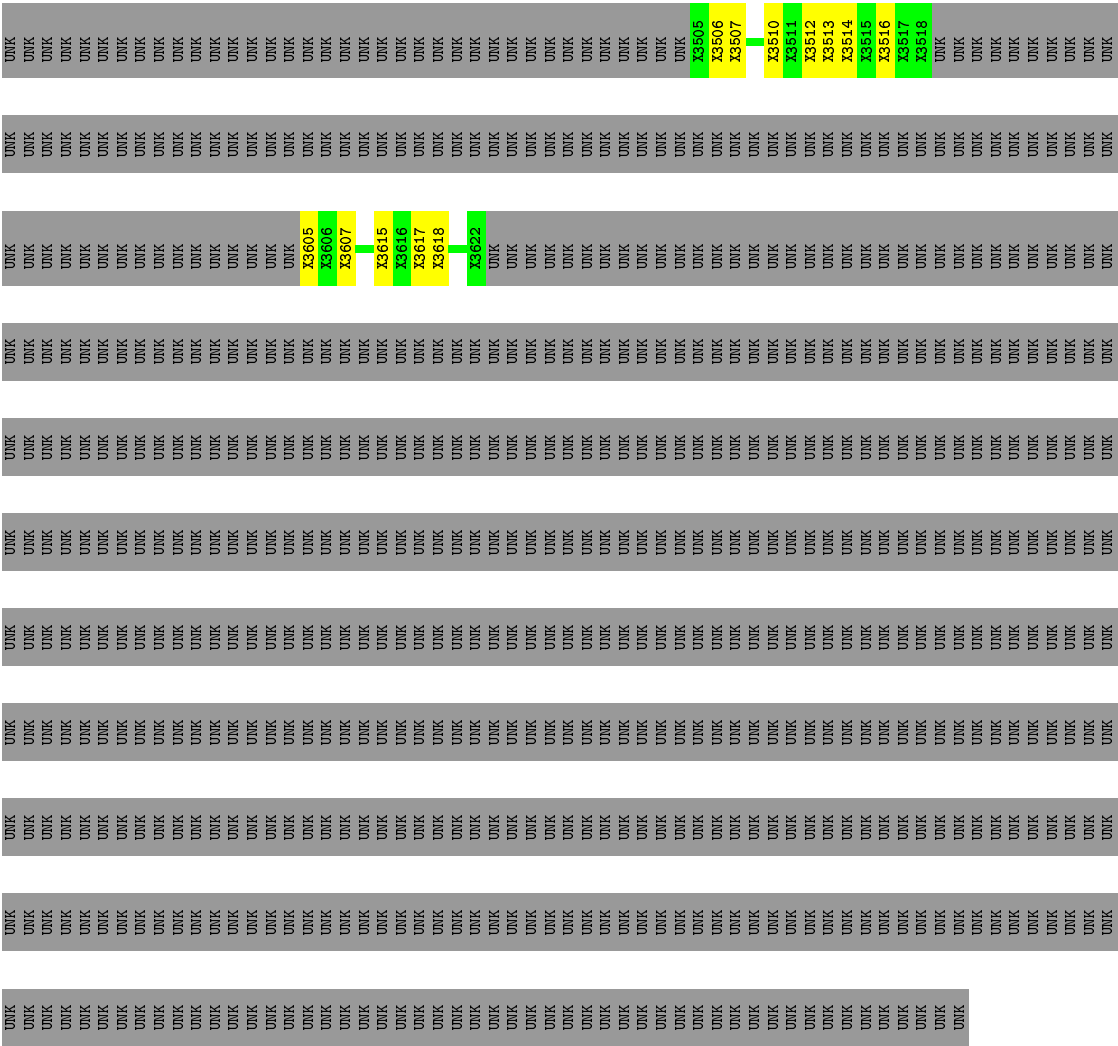
Chain F:  7% 6% 87%

[illegible]

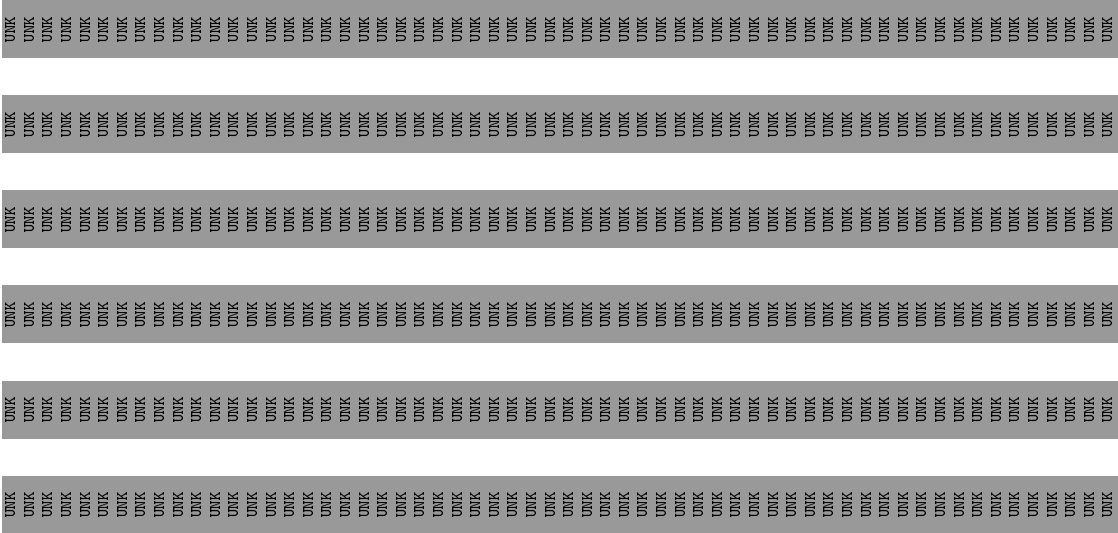
[illegible]

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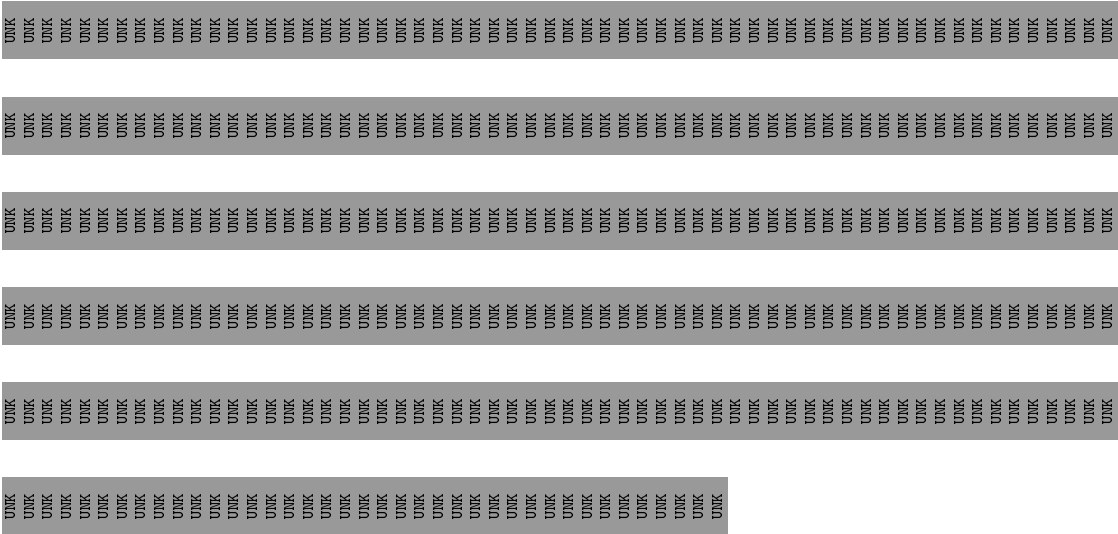
● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit



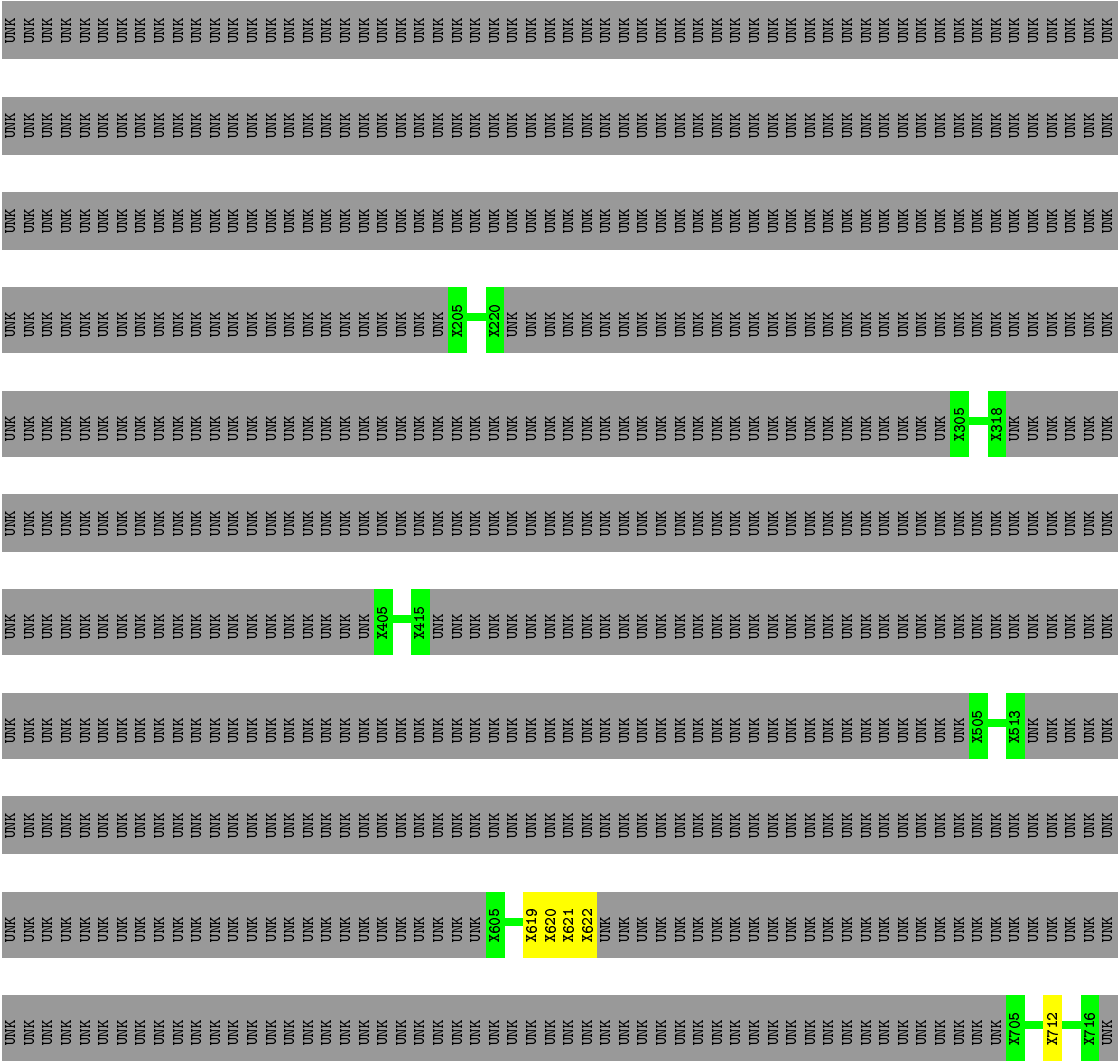
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● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit



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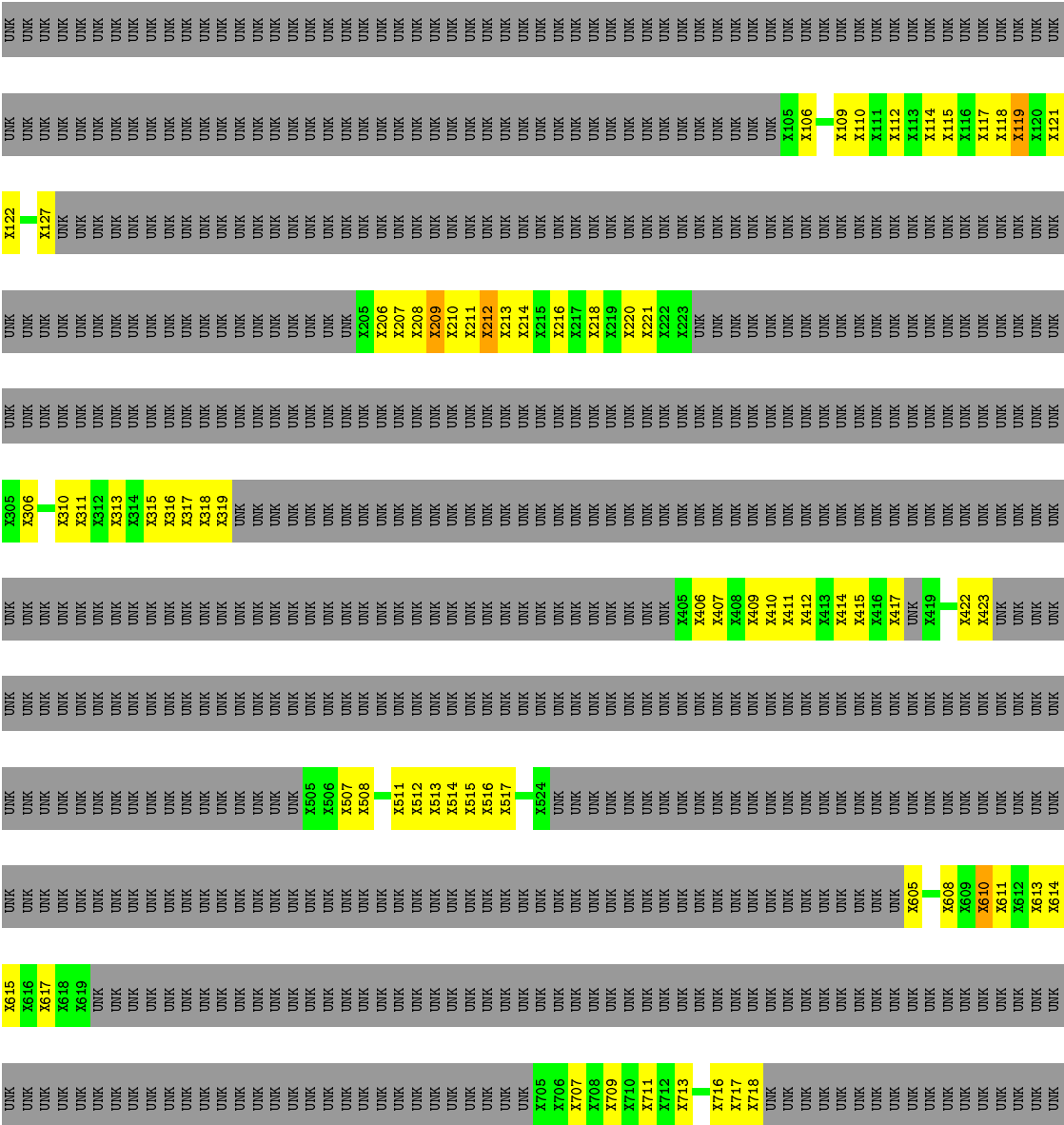
[illegible]

[illegible]



● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain P:  93%



[illegible]

[illegible]

[illegible]

[illegible][illegible]

- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain Q:  5% 5% 90%

[illegible][illegible][illegible][illegible][illegible][illegible][illegible][illegible][illegible][illegible][illegible][illegible][illegible][illegible]



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- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain R: 96%

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- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain S:

98%

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- Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

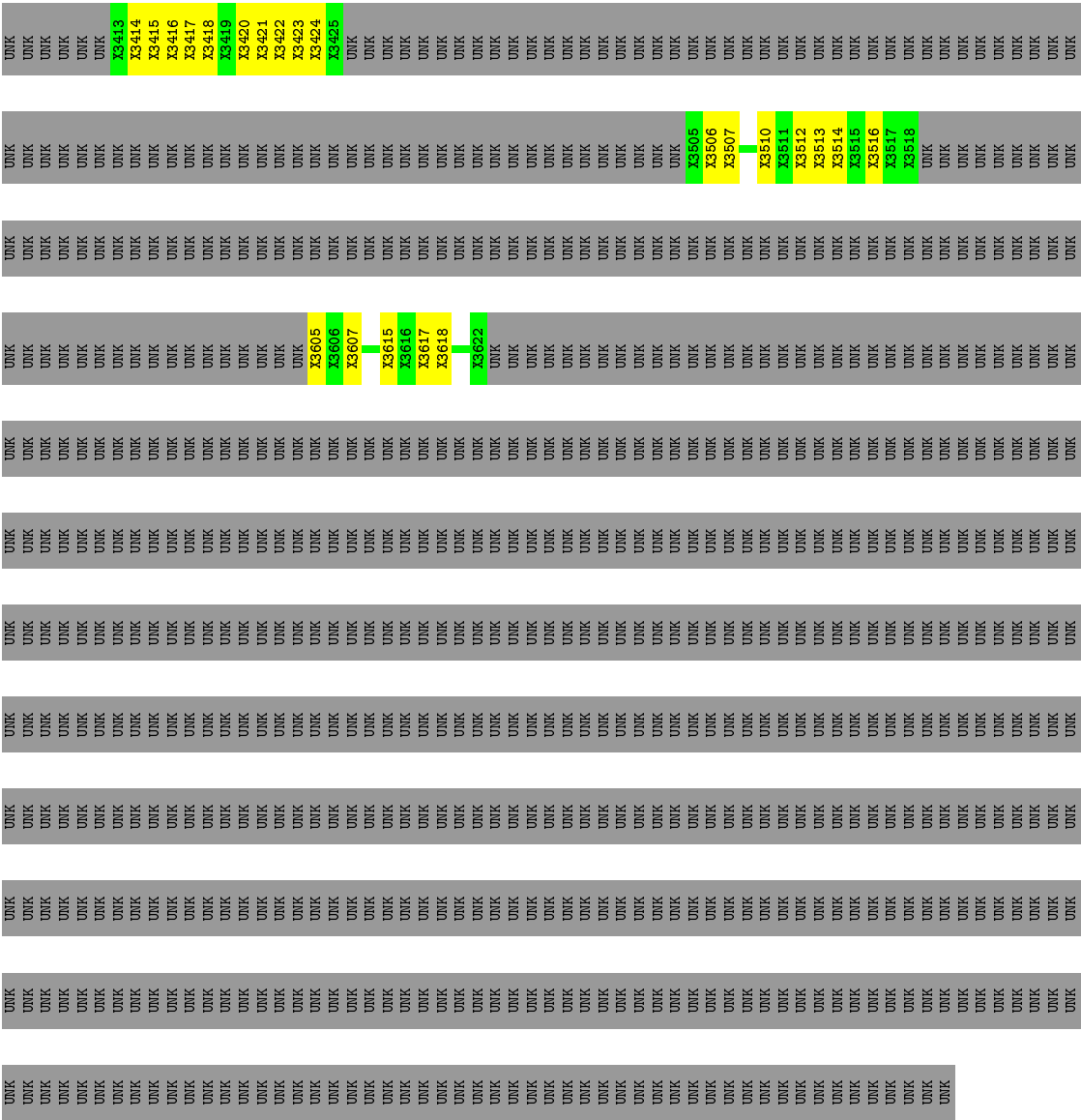
Chain T: 7% 6% 87%

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| X106 | X107 | X108 | X109 | X110 | X111 | X112 | X113 | X114 | X115 | X116 | X117 | X118 | X119 | X120 | X121 | X122 | X123 | X124 | X125 |
| X126 | X127 | X128 | X129 | X130 | X131 | X132 | X133 | X134 | X135 | X136 | X137 | X138 | X139 | X140 | X141 | X142 | X143 | X144 | X145 |
| X146 | X147 | X148 | X149 | X150 | X151 | X152 | X153 | X154 | X155 | X156 | X157 | X158 | X159 | X160 | X161 | X162 | X163 | X164 | X165 |
| X166 | X167 | X168 | X169 | X170 | X171 | X172 | X173 | X174 | X175 | X176 | X177 | X178 | X179 | X180 | X181 | X182 | X183 | X184 | X185 |
| X186 | X187 | X188 | X189 | X190 | X191 | X192 | X193 | X194 | X195 | X196 | X197 | X198 | X199 | X200 | X201 | X202 | X203 | X204 | X205 |
| X206 | X207 | X208 | X209 | X210 | X211 | X212 | X213 | X214 | X215 | X216 | X217 | X218 | X219 | X220 | X221 | X222 | X223 | X224 | X225 |
| X226 | X227 | X228 | X229 | X230 | X231 | X232 | X233 | X234 | X235 | X236 | X237 | X238 | X239 | X240 | X241 | X242 | X243 | X244 | X245 |
| X246 | X247 | X248 | X249 | X250 | X251 | X252 | X253 | X254 | X255 | X256 | X257 | X258 | X259 | X260 | X261 | X262 | X263 | X264 | X265 |
| X266 | X267 | X268 | X269 | X270 | X271 | X272 | X273 | X274 | X275 | X276 | X277 | X278 | X279 | X280 | X281 | X282 | X283 | X284 | X285 |
| X286 | X287 | X288 | X289 | X290 | X291 | X292 | X293 | X294 | X295 | X296 | X297 | X298 | X299 | X300 | X301 | X302 | X303 | X304 | X305 |
| X306 | X307 | X308 | X309 | X310 | X311 | X312 | X313 | X314 | X315 | X316 | X317 | X318 | X319 | X320 | X321 | X322 | X323 | X324 | X325 |
| X326 | X327 | X328 | X329 | X330 | X331 | X332 | X333 | X334 | X335 | X336 | X337 | X338 | X339 | X340 | X341 | X342 | X343 | X344 | X345 |
| X346 | X347 | X348 | X349 | X350 | X351 | X352 | X353 | X354 | X355 | X356 | X357 | X358 | X359 | X360 | X361 | X362 | X363 | X364 | X365 |
| X366 | X367 | X368 | X369 | X370 | X371 | X372 | X373 | X374 | X375 | X376 | X377 | X378 | X379 | X380 | X381 | X382 | X383 | X384 | X385 |
| X386 | X387 | X388 | X389 | X390 | X391 | X392 | X393 | X394 | X395 | X396 | X397 | X398 | X399 | X400 | X401 | X402 | X403 | X404 | X405 |
| X406 | X407 | X408 | X409 | X410 | X411 | X412 | X413 | X414 | X415 | X416 | X417 | X418 | X419 | X420 | X421 | X422 | X423 | X424 | X425 |
| X426 | X427 | X428 | X429 | X430 | X431 | X432 | X433 | X434 | X435 | X436 | X437 | X438 | X439 | X440 | X441 | X442 | X443 | X444 | X445 |
| X446 | X447 | X448 | X449 | X450 | X451 | X452 | X453 | X454 | X455 | X456 | X457 | X458 | X459 | X460 | X461 | X462 | X463 | X464 | X465 |
| X466 | X467 | X468 | X469 | X470 | X471 | X472 | X473 | X474 | X475 | X476 | X477 | X478 | X479 | X480 | X481 | X482 | X483 | X484 | X485 |
| X486 | X487 | X488 | X489 | X490 | X491 | X492 | X493 | X494 | X495 | X496 | X497 | X498 | X499 | X500 | X501 | X502 | X503 | X504 | X505 |
| X506 | X507 | X508 | X509 | X510 | X511 | X512 | X513 | X514 | X515 | X516 | X517 | X518 | X519 | X520 | X521 | X522 | X523 | X524 | X525 |
| X526 | X527 | X528 | X529 | X530 | X531 | X532 | X533 | X534 | X535 | X536 | X537 | X538 | X539 | X540 | X541 | X542 | X543 | X544 | X545 |
| X546 | X547 | X548 | X549 | X550 | X551 | X552 | X553 | X554 | X555 | X556 | X557 | X558 | X559 | X560 | X561 | X562 | X563 | X564 | X565 |
| X566 | X567 | X568 | X569 | X570 | X571 | X572 | X573 | X574 | X575 | X576 | X577 | X578 | X579 | X580 | X581 | X582 | X583 | X584 | X585 |
| X586 | X587 | X588 | X589 | X590 | X591 | X592 | X593 | X594 | X595 | X596 | X597 | X598 | X599 | X600 | X601 | X602 | X603 | X604 | X60 |

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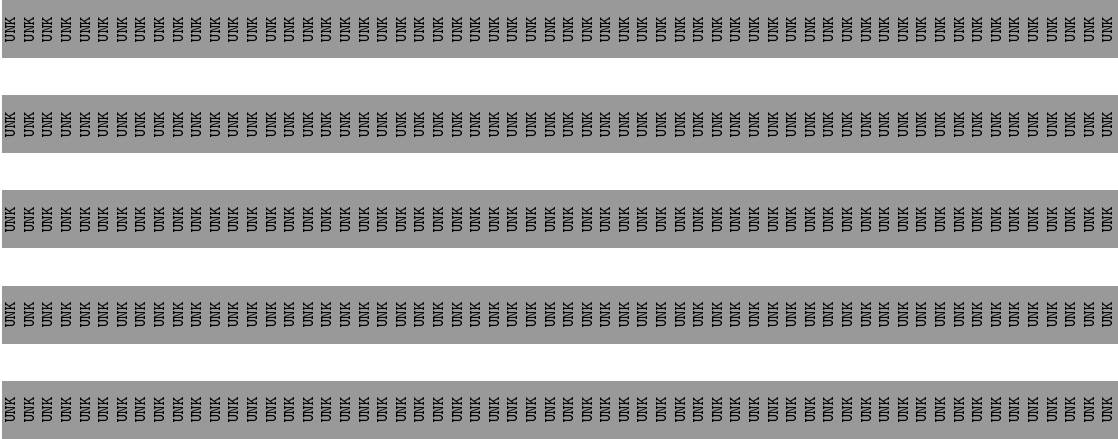
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● Molecule 1: DNA-dependent Protein Kinase Catalytic Subunit

Chain Y: 95%



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| | ١ | ٢ | ٣ | ٤ | ٥ | ٦ | ٧ | ٨ | ٩ | ١٠ | ١١ | ١٢ | ١٣ | ١٤ | ١٥ | ١٦ | ١٧ | ١٨ | ١٩ | ٢٠ | ٢١ | ٢٢ | ٢٣ | ٢٤ | ٢٥ | ٢٦ | ٢٧ | ٢٨ | ٢٩ | ٣٠ | ٣١ | ٣٢ | ٣٣ | ٣٤ | ٣٥ | ٣٦ | ٣٧ | ٣٨ | ٣٩ | ٤٠ | ٤١ | ٤٢ | ٤٣ | ٤٤ | ٤٥ | ٤٦ | ٤٧ | ٤٨ | ٤٩ | ٥٠ | ٥١ | ٥٢ | ٥٣ | ٥٤ | ٥٥ | ٥٦ | ٥٧ | ٥٨ | ٥٩ | ٦٠ | ٦١ | ٦٢ | ٦٣ | ٦٤ | ٦٥ | ٦٦ | ٦٧ | ٦٨ | ٦٩ | ٧٠ | ٧١ | ٧٢ | ٧٣ | ٧٤ | ٧٥ | ٧٦ | ٧٧ | ٧٨ | ٧٩ | ٨٠ | ٨١ | ٨٢ | ٨٣ | ٨٤ | ٨٥ | ٨٦ | ٨٧ | ٨٨ | ٨٩ | ٩٠ | ٩١ | ٩٢ | ٩٣ | ٩٤ | ٩٥ | ٩٦ | ٩٧ | ٩٨ | ٩٩ | ١٠٠ |
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4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 168.60Å 132.99Å 297.00Å 90.00° 105.58° 90.00° | Depositor |
| Resolution (Å) | 100.00 – 6.60 91.97 – 6.58 | Depositor EDS |
| % Data completeness (in resolution range) | 97.6 (100.00-6.60) 97.6 (91.97-6.58) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | 0.08 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 12.86 (at 6.72Å) | Xtriage |
| Refinement program | REFMAC 5.5.0102 | Depositor |
| R, R_{free} | 0.442 , 0.441 0.441 , 0.440 | Depositor DCC |
| R_{free} test set | 1214 reflections (5.41%) | DCC |
| Wilson B-factor (Å ²) | 269.3 | Xtriage |
| Anisotropy | 0.049 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.23 , 633.9 | EDS |
| Estimated twinning fraction | 0.010 for h,-k,-h-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Outliers | 0 of 23876 reflections | Xtriage |
| F_o, F_c correlation | 0.63 | EDS |
| Total number of atoms | 20320 | wwPDB-VP |
| Average B, all atoms (Å ²) | 80.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 1 | B | 0 | 18 |
| 1 | C | 0 | 8 |
| 1 | D | 0 | 8 |
| 1 | E | 0 | 3 |
| 1 | F | 0 | 6 |
| 1 | O | 0 | 2 |
| 1 | P | 0 | 18 |
| 1 | Q | 0 | 8 |
| 1 | R | 0 | 8 |
| 1 | S | 0 | 3 |
| 1 | T | 0 | 6 |
| 1 | X | 0 | 7 |
| 1 | Y | 0 | 7 |
| All | All | 0 | 104 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (104) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | A | 1214 | UNK | Peptide |
| 1 | A | 2306 | UNK | Peptide |
| 1 | B | 1109 | UNK | Peptide |
| 1 | B | 119 | UNK | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | B | 122 | UNK | Peptide |
| 1 | B | 1309 | UNK | Peptide |
| 1 | B | 1406 | UNK | Peptide |
| 1 | B | 1408 | UNK | Peptide |
| 1 | B | 1411 | UNK | Peptide |
| 1 | B | 1413 | UNK | Peptide |
| 1 | B | 1415 | UNK | Peptide |
| 1 | B | 1417 | UNK | Peptide |
| 1 | B | 1419 | UNK | Peptide |
| 1 | B | 1617 | UNK | Peptide |
| 1 | B | 1618 | UNK | Peptide |
| 1 | B | 1619 | UNK | Peptide |
| 1 | B | 209 | UNK | Peptide |
| 1 | B | 212 | UNK | Peptide |
| 1 | B | 406 | UNK | Peptide |
| 1 | B | 610 | UNK | Peptide |
| 1 | C | 1016 | UNK | Peptide |
| 1 | C | 1812 | UNK | Peptide |
| 1 | C | 2507 | UNK | Peptide |
| 1 | C | 2616 | UNK | Peptide |
| 1 | C | 517 | UNK | Peptide |
| 1 | C | 608 | UNK | Peptide |
| 1 | C | 609 | UNK | Peptide |
| 1 | C | 921 | UNK | Peptide |
| 1 | D | 1013 | UNK | Peptide |
| 1 | D | 1015 | UNK | Peptide |
| 1 | D | 1108 | UNK | Peptide |
| 1 | D | 1111 | UNK | Peptide |
| 1 | D | 1210 | UNK | Peptide |
| 1 | D | 712 | UNK | Peptide |
| 1 | D | 910 | UNK | Peptide |
| 1 | D | 920 | UNK | Peptide |
| 1 | E | 114 | UNK | Peptide |
| 1 | E | 120 | UNK | Peptide |
| 1 | E | 306 | UNK | Peptide |
| 1 | F | 1008 | UNK | Peptide |
| 1 | F | 1509 | UNK | Peptide |
| 1 | F | 222 | UNK | Peptide |
| 1 | F | 2625 | UNK | Peptide |
| 1 | F | 2908 | UNK | Peptide |
| 1 | F | 3212 | UNK | Peptide |
| 1 | O | 1214 | UNK | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | O | 2306 | UNK | Peptide |
| 1 | P | 1109 | UNK | Peptide |
| 1 | P | 119 | UNK | Peptide |
| 1 | P | 122 | UNK | Peptide |
| 1 | P | 1309 | UNK | Peptide |
| 1 | P | 1406 | UNK | Peptide |
| 1 | P | 1408 | UNK | Peptide |
| 1 | P | 1411 | UNK | Peptide |
| 1 | P | 1413 | UNK | Peptide |
| 1 | P | 1415 | UNK | Peptide |
| 1 | P | 1417 | UNK | Peptide |
| 1 | P | 1419 | UNK | Peptide |
| 1 | P | 1617 | UNK | Peptide |
| 1 | P | 1618 | UNK | Peptide |
| 1 | P | 1619 | UNK | Peptide |
| 1 | P | 209 | UNK | Peptide |
| 1 | P | 212 | UNK | Peptide |
| 1 | P | 406 | UNK | Peptide |
| 1 | P | 610 | UNK | Peptide |
| 1 | Q | 1016 | UNK | Peptide |
| 1 | Q | 1812 | UNK | Peptide |
| 1 | Q | 2507 | UNK | Peptide |
| 1 | Q | 2616 | UNK | Peptide |
| 1 | Q | 517 | UNK | Peptide |
| 1 | Q | 608 | UNK | Peptide |
| 1 | Q | 609 | UNK | Peptide |
| 1 | Q | 921 | UNK | Peptide |
| 1 | R | 1013 | UNK | Peptide |
| 1 | R | 1015 | UNK | Peptide |
| 1 | R | 1108 | UNK | Peptide |
| 1 | R | 1111 | UNK | Peptide |
| 1 | R | 1210 | UNK | Peptide |
| 1 | R | 712 | UNK | Peptide |
| 1 | R | 910 | UNK | Peptide |
| 1 | R | 920 | UNK | Peptide |
| 1 | S | 114 | UNK | Peptide |
| 1 | S | 120 | UNK | Peptide |
| 1 | S | 306 | UNK | Peptide |
| 1 | T | 1008 | UNK | Peptide |
| 1 | T | 1509 | UNK | Peptide |
| 1 | T | 222 | UNK | Peptide |
| 1 | T | 2625 | UNK | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | T | 2908 | UNK | Peptide |
| 1 | T | 3212 | UNK | Peptide |
| 1 | X | 1042 | UNK | Peptide |
| 1 | X | 865 | UNK | Peptide |
| 1 | X | 876 | UNK | Peptide |
| 1 | X | 885 | UNK | Peptide |
| 1 | X | 910 | UNK | Peptide |
| 1 | X | 924 | UNK | Peptide |
| 1 | X | 990 | UNK | Peptide |
| 1 | Y | 1042 | UNK | Peptide |
| 1 | Y | 865 | UNK | Peptide |
| 1 | Y | 876 | UNK | Peptide |
| 1 | Y | 885 | UNK | Peptide |
| 1 | Y | 910 | UNK | Peptide |
| 1 | Y | 924 | UNK | Peptide |
| 1 | Y | 990 | UNK | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1770 | 0 | 429 | 123 | 0 |
| 1 | B | 1415 | 0 | 356 | 149 | 0 |
| 1 | C | 2030 | 0 | 489 | 178 | 0 |
| 1 | D | 910 | 0 | 239 | 117 | 0 |
| 1 | E | 325 | 0 | 78 | 20 | 0 |
| 1 | F | 2655 | 0 | 648 | 203 | 0 |
| 1 | O | 1770 | 0 | 429 | 123 | 48 |
| 1 | P | 1415 | 0 | 358 | 153 | 0 |
| 1 | Q | 2030 | 0 | 489 | 180 | 0 |
| 1 | R | 910 | 0 | 239 | 119 | 0 |
| 1 | S | 325 | 0 | 78 | 19 | 0 |
| 1 | T | 2655 | 0 | 648 | 208 | 48 |
| 1 | X | 1055 | 0 | 263 | 74 | 0 |
| 1 | Y | 1055 | 0 | 264 | 75 | 0 |
| All | All | 20320 | 0 | 5007 | 1740 | 48 |

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 69.

All (1740) 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:B:1412:UNK:CA | 1:B:1412:UNK:C | 1.75 | 1.64 |
| 1:P:1412:UNK:C | 1:P:1412:UNK:CA | 1.74 | 1.58 |
| 1:P:1412:UNK:HA | 1:P:1415:UNK:CB | 1.69 | 1.22 |
| 1:B:1412:UNK:HA | 1:B:1415:UNK:CB | 1.69 | 1.20 |
| 1:E:116:UNK:O | 1:E:118:UNK:N | 1.76 | 1.17 |
| 1:S:116:UNK:O | 1:S:118:UNK:N | 1.76 | 1.16 |
| 1:B:214:UNK:O | 1:B:216:UNK:N | 1.82 | 1.13 |
| 1:P:1412:UNK:C | 1:P:1414:UNK:H | 1.59 | 1.12 |
| 1:P:214:UNK:O | 1:P:216:UNK:N | 1.82 | 1.12 |
| 1:C:906:UNK:O | 1:C:908:UNK:N | 1.81 | 1.11 |
| 1:Q:906:UNK:O | 1:Q:908:UNK:N | 1.82 | 1.11 |
| 1:B:1412:UNK:C | 1:B:1414:UNK:H | 1.59 | 1.09 |
| 1:R:1109:UNK:O | 1:R:1111:UNK:N | 1.86 | 1.08 |
| 1:O:2606:UNK:O | 1:O:2608:UNK:N | 1.87 | 1.08 |
| 1:A:2606:UNK:O | 1:A:2608:UNK:N | 1.87 | 1.08 |
| 1:P:1018:UNK:O | 1:P:1020:UNK:N | 1.87 | 1.08 |
| 1:B:1018:UNK:O | 1:B:1020:UNK:N | 1.87 | 1.07 |
| 1:Q:2509:UNK:O | 1:Q:2511:UNK:N | 1.88 | 1.06 |
| 1:D:1109:UNK:O | 1:D:1111:UNK:N | 1.86 | 1.06 |
| 1:C:2509:UNK:O | 1:C:2511:UNK:N | 1.88 | 1.06 |
| 1:Y:838:UNK:O | 1:Y:841:UNK:N | 1.89 | 1.06 |
| 1:Y:838:UNK:O | 1:Y:840:UNK:N | 1.88 | 1.05 |
| 1:X:838:UNK:O | 1:X:841:UNK:N | 1.89 | 1.05 |
| 1:X:838:UNK:O | 1:X:840:UNK:N | 1.88 | 1.04 |
| 1:A:1514:UNK:O | 1:A:1516:UNK:N | 1.91 | 1.04 |
| 1:C:315:UNK:O | 1:C:317:UNK:N | 1.91 | 1.02 |
| 1:Q:315:UNK:O | 1:Q:317:UNK:N | 1.92 | 1.02 |
| 1:B:1711:UNK:O | 1:B:1715:UNK:CB | 2.07 | 1.02 |
| 1:P:1711:UNK:O | 1:P:1715:UNK:CB | 2.07 | 1.02 |
| 1:O:1514:UNK:O | 1:O:1516:UNK:N | 1.91 | 1.02 |
| 1:D:1012:UNK:O | 1:D:1015:UNK:N | 1.92 | 1.02 |
| 1:R:1012:UNK:O | 1:R:1015:UNK:N | 1.92 | 1.01 |
| 1:O:2507:UNK:HA | 1:O:2510:UNK:CB | 1.89 | 1.01 |
| 1:A:2507:UNK:HA | 1:A:2510:UNK:CB | 1.89 | 1.01 |
| 1:O:1212:UNK:O | 1:O:1215:UNK:N | 1.95 | 0.99 |
| 1:C:2513:UNK:O | 1:C:2515:UNK:N | 1.96 | 0.99 |
| 1:F:2219:UNK:O | 1:F:2221:UNK:N | 1.96 | 0.98 |
| 1:F:420:UNK:CB | 1:F:508:UNK:HA | 1.92 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:1212:UNK:O | 1:A:1215:UNK:N | 1.95 | 0.98 |
| 1:R:221:UNK:O | 1:R:223:UNK:N | 1.96 | 0.98 |
| 1:Q:2513:UNK:O | 1:Q:2515:UNK:N | 1.96 | 0.98 |
| 1:T:420:UNK:CB | 1:T:508:UNK:HA | 1.92 | 0.98 |
| 1:D:221:UNK:O | 1:D:223:UNK:N | 1.96 | 0.98 |
| 1:C:1209:UNK:C | 1:C:1211:UNK:H | 1.77 | 0.98 |
| 1:C:2010:UNK:O | 1:C:2012:UNK:N | 1.98 | 0.97 |
| 1:F:2215:UNK:O | 1:F:2218:UNK:N | 1.98 | 0.97 |
| 1:D:407:UNK:O | 1:D:409:UNK:N | 1.98 | 0.97 |
| 1:T:2219:UNK:O | 1:T:2221:UNK:N | 1.96 | 0.97 |
| 1:D:305:UNK:O | 1:D:307:UNK:N | 1.98 | 0.97 |
| 1:T:2215:UNK:O | 1:T:2218:UNK:N | 1.98 | 0.96 |
| 1:Y:1034:UNK:HA | 1:Y:1038:UNK:CB | 1.95 | 0.96 |
| 1:D:509:UNK:C | 1:D:511:UNK:H | 1.77 | 0.96 |
| 1:R:305:UNK:O | 1:R:307:UNK:N | 1.98 | 0.96 |
| 1:R:407:UNK:O | 1:R:409:UNK:N | 1.98 | 0.96 |
| 1:Q:2010:UNK:O | 1:Q:2012:UNK:N | 1.97 | 0.95 |
| 1:Q:1209:UNK:C | 1:Q:1211:UNK:H | 1.77 | 0.95 |
| 1:X:1034:UNK:HA | 1:X:1038:UNK:CB | 1.95 | 0.95 |
| 1:D:1012:UNK:O | 1:D:1014:UNK:N | 2.00 | 0.95 |
| 1:P:1412:UNK:O | 1:P:1414:UNK:N | 1.97 | 0.95 |
| 1:R:1012:UNK:O | 1:R:1014:UNK:N | 2.00 | 0.95 |
| 1:R:509:UNK:C | 1:R:511:UNK:H | 1.77 | 0.94 |
| 1:Y:1070:UNK:O | 1:Y:1073:UNK:N | 2.00 | 0.94 |
| 1:Q:615:UNK:HA | 1:Q:618:UNK:CB | 1.97 | 0.94 |
| 1:R:109:UNK:HA | 1:R:112:UNK:CB | 1.98 | 0.94 |
| 1:X:1070:UNK:O | 1:X:1073:UNK:N | 2.00 | 0.94 |
| 1:O:913:UNK:CB | 1:O:1009:UNK:CB | 2.46 | 0.94 |
| 1:T:317:UNK:C | 1:T:319:UNK:H | 1.82 | 0.93 |
| 1:C:615:UNK:HA | 1:C:618:UNK:CB | 1.97 | 0.93 |
| 1:A:913:UNK:CB | 1:A:1009:UNK:CB | 2.46 | 0.93 |
| 1:B:1412:UNK:O | 1:B:1414:UNK:N | 1.97 | 0.93 |
| 1:D:109:UNK:HA | 1:D:112:UNK:CB | 1.98 | 0.92 |
| 1:Q:809:UNK:HA | 1:Q:812:UNK:CB | 1.99 | 0.92 |
| 1:C:809:UNK:HA | 1:C:812:UNK:CB | 1.99 | 0.92 |
| 1:A:1608:UNK:HA | 1:A:1611:UNK:CB | 2.00 | 0.91 |
| 1:F:317:UNK:C | 1:F:319:UNK:H | 1.82 | 0.91 |
| 1:C:1607:UNK:C | 1:C:1609:UNK:H | 1.81 | 0.91 |
| 1:O:1514:UNK:C | 1:O:1516:UNK:N | 2.33 | 0.91 |
| 1:P:1309:UNK:CB | 1:P:1405:UNK:O | 2.19 | 0.91 |
| 1:Y:873:UNK:O | 1:Y:876:UNK:CB | 2.18 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Y:838:UNK:C | 1:Y:840:UNK:H | 1.84 | 0.91 |
| 1:Q:1209:UNK:O | 1:Q:1211:UNK:N | 2.04 | 0.90 |
| 1:B:1309:UNK:CB | 1:B:1405:UNK:O | 2.19 | 0.90 |
| 1:O:1608:UNK:HA | 1:O:1611:UNK:CB | 2.00 | 0.90 |
| 1:X:873:UNK:O | 1:X:876:UNK:CB | 2.18 | 0.90 |
| 1:X:838:UNK:C | 1:X:840:UNK:H | 1.84 | 0.90 |
| 1:C:1412:UNK:C | 1:C:1414:UNK:H | 1.83 | 0.90 |
| 1:A:1514:UNK:C | 1:A:1516:UNK:N | 2.33 | 0.90 |
| 1:F:415:UNK:O | 1:F:418:UNK:N | 2.05 | 0.89 |
| 1:Q:1607:UNK:C | 1:Q:1609:UNK:H | 1.81 | 0.89 |
| 1:T:415:UNK:O | 1:T:418:UNK:N | 2.05 | 0.89 |
| 1:C:1209:UNK:O | 1:C:1211:UNK:N | 2.04 | 0.89 |
| 1:Q:1412:UNK:C | 1:Q:1414:UNK:H | 1.83 | 0.89 |
| 1:D:1012:UNK:C | 1:D:1014:UNK:H | 1.84 | 0.89 |
| 1:P:1507:UNK:HA | 1:P:1510:UNK:CB | 2.04 | 0.88 |
| 1:Q:2112:UNK:O | 1:Q:2114:UNK:N | 2.07 | 0.88 |
| 1:E:313:UNK:C | 1:E:315:UNK:H | 1.86 | 0.87 |
| 1:F:1312:UNK:C | 1:F:1314:UNK:H | 1.87 | 0.87 |
| 1:Q:414:UNK:O | 1:Q:416:UNK:N | 2.08 | 0.86 |
| 1:B:1507:UNK:HA | 1:B:1510:UNK:CB | 2.03 | 0.86 |
| 1:C:2112:UNK:O | 1:C:2114:UNK:N | 2.07 | 0.86 |
| 1:T:1312:UNK:C | 1:T:1314:UNK:H | 1.87 | 0.86 |
| 1:C:312:UNK:O | 1:C:314:UNK:N | 2.09 | 0.86 |
| 1:S:313:UNK:C | 1:S:315:UNK:H | 1.87 | 0.86 |
| 1:P:1107:UNK:O | 1:P:1109:UNK:N | 2.09 | 0.86 |
| 1:R:1012:UNK:C | 1:R:1014:UNK:H | 1.84 | 0.85 |
| 1:P:1515:UNK:O | 1:P:1517:UNK:N | 2.09 | 0.85 |
| 1:Q:312:UNK:O | 1:Q:314:UNK:N | 2.09 | 0.85 |
| 1:C:113:UNK:O | 1:C:115:UNK:N | 2.09 | 0.85 |
| 1:C:1308:UNK:HA | 1:C:1311:UNK:CB | 2.06 | 0.85 |
| 1:C:414:UNK:O | 1:C:416:UNK:N | 2.08 | 0.85 |
| 1:B:1515:UNK:O | 1:B:1517:UNK:N | 2.09 | 0.85 |
| 1:T:407:UNK:O | 1:T:411:UNK:N | 2.10 | 0.85 |
| 1:B:1107:UNK:O | 1:B:1109:UNK:N | 2.09 | 0.85 |
| 1:S:207:UNK:O | 1:S:209:UNK:N | 2.10 | 0.85 |
| 1:B:615:UNK:O | 1:B:617:UNK:N | 2.10 | 0.85 |
| 1:F:407:UNK:O | 1:F:411:UNK:N | 2.10 | 0.84 |
| 1:Q:113:UNK:O | 1:Q:115:UNK:N | 2.09 | 0.84 |
| 1:E:207:UNK:O | 1:E:209:UNK:N | 2.10 | 0.84 |
| 1:Q:1308:UNK:HA | 1:Q:1311:UNK:CB | 2.06 | 0.84 |
| 1:B:415:UNK:O | 1:B:417:UNK:N | 2.10 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:P:415:UNK:O | 1:P:417:UNK:N | 2.10 | 0.84 |
| 1:P:615:UNK:O | 1:P:617:UNK:N | 2.11 | 0.83 |
| 1:F:1010:UNK:HA | 1:F:1013:UNK:CB | 2.09 | 0.83 |
| 1:Q:1313:UNK:O | 1:Q:1316:UNK:N | 2.12 | 0.83 |
| 1:R:605:UNK:O | 1:R:606:UNK:O | 1.96 | 0.83 |
| 1:A:1312:UNK:O | 1:A:1316:UNK:N | 2.11 | 0.83 |
| 1:C:1408:UNK:C | 1:C:1410:UNK:H | 1.90 | 0.83 |
| 1:C:1313:UNK:O | 1:C:1316:UNK:N | 2.12 | 0.83 |
| 1:Q:1408:UNK:C | 1:Q:1410:UNK:H | 1.90 | 0.82 |
| 1:T:1010:UNK:HA | 1:T:1013:UNK:CB | 2.09 | 0.82 |
| 1:T:310:UNK:O | 1:T:312:UNK:N | 2.12 | 0.82 |
| 1:F:310:UNK:O | 1:F:312:UNK:N | 2.12 | 0.82 |
| 1:X:922:UNK:C | 1:X:924:UNK:H | 1.92 | 0.82 |
| 1:P:813:UNK:O | 1:P:817:UNK:N | 2.13 | 0.82 |
| 1:O:1312:UNK:O | 1:O:1316:UNK:N | 2.11 | 0.82 |
| 1:Q:807:UNK:O | 1:Q:809:UNK:N | 2.13 | 0.82 |
| 1:A:1517:UNK:C | 1:A:1519:UNK:H | 1.93 | 0.82 |
| 1:F:3414:UNK:C | 1:F:3416:UNK:N | 2.38 | 0.82 |
| 1:T:3414:UNK:C | 1:T:3416:UNK:N | 2.38 | 0.82 |
| 1:B:813:UNK:O | 1:B:817:UNK:N | 2.13 | 0.82 |
| 1:D:605:UNK:O | 1:D:606:UNK:O | 1.96 | 0.82 |
| 1:Y:922:UNK:C | 1:Y:924:UNK:H | 1.92 | 0.82 |
| 1:C:807:UNK:O | 1:C:809:UNK:N | 2.13 | 0.82 |
| 1:F:2113:UNK:O | 1:F:2115:UNK:O | 1.99 | 0.81 |
| 1:P:214:UNK:C | 1:P:216:UNK:N | 2.43 | 0.81 |
| 1:C:1313:UNK:O | 1:C:1315:UNK:N | 2.13 | 0.81 |
| 1:Q:1408:UNK:O | 1:Q:1410:UNK:N | 2.14 | 0.81 |
| 1:T:1309:UNK:O | 1:T:1311:UNK:N | 2.14 | 0.81 |
| 1:C:1408:UNK:O | 1:C:1410:UNK:N | 2.13 | 0.81 |
| 1:O:1517:UNK:C | 1:O:1519:UNK:H | 1.93 | 0.81 |
| 1:F:1309:UNK:O | 1:F:1311:UNK:N | 2.14 | 0.81 |
| 1:T:913:UNK:O | 1:T:917:UNK:N | 2.15 | 0.80 |
| 1:Q:1313:UNK:O | 1:Q:1315:UNK:N | 2.13 | 0.80 |
| 1:A:1509:UNK:C | 1:A:1511:UNK:H | 1.94 | 0.80 |
| 1:T:2616:UNK:C | 1:T:2618:UNK:H | 1.95 | 0.80 |
| 1:B:422:UNK:O | 1:B:423:UNK:O | 1.99 | 0.80 |
| 1:P:422:UNK:O | 1:P:423:UNK:O | 1.99 | 0.80 |
| 1:F:2616:UNK:C | 1:F:2618:UNK:H | 1.95 | 0.80 |
| 1:R:1205:UNK:O | 1:R:1207:UNK:N | 2.14 | 0.80 |
| 1:T:2113:UNK:O | 1:T:2115:UNK:O | 1.98 | 0.80 |
| 1:Q:1209:UNK:C | 1:Q:1211:UNK:N | 2.41 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:1205:UNK:O | 1:D:1207:UNK:N | 2.14 | 0.80 |
| 1:F:913:UNK:O | 1:F:917:UNK:N | 2.15 | 0.80 |
| 1:Q:305:UNK:O | 1:Q:307:UNK:N | 2.15 | 0.80 |
| 1:C:305:UNK:O | 1:C:307:UNK:N | 2.15 | 0.80 |
| 1:S:116:UNK:C | 1:S:118:UNK:N | 2.45 | 0.79 |
| 1:B:1412:UNK:C | 1:B:1412:UNK:HA | 2.09 | 0.79 |
| 1:C:613:UNK:C | 1:C:615:UNK:N | 2.42 | 0.79 |
| 1:P:1110:UNK:O | 1:P:1112:UNK:N | 2.15 | 0.79 |
| 1:C:1209:UNK:C | 1:C:1211:UNK:N | 2.41 | 0.79 |
| 1:B:1110:UNK:O | 1:B:1112:UNK:N | 2.15 | 0.79 |
| 1:Q:906:UNK:O | 1:Q:909:UNK:N | 2.15 | 0.79 |
| 1:Q:2509:UNK:C | 1:Q:2511:UNK:N | 2.46 | 0.79 |
| 1:O:1509:UNK:C | 1:O:1511:UNK:H | 1.94 | 0.79 |
| 1:E:116:UNK:C | 1:E:118:UNK:N | 2.45 | 0.79 |
| 1:R:1109:UNK:C | 1:R:1111:UNK:H | 1.96 | 0.79 |
| 1:B:214:UNK:C | 1:B:216:UNK:N | 2.43 | 0.78 |
| 1:Q:613:UNK:C | 1:Q:615:UNK:N | 2.42 | 0.78 |
| 1:T:516:UNK:O | 1:T:605:UNK:N | 2.16 | 0.78 |
| 1:F:418:UNK:C | 1:F:420:UNK:H | 1.96 | 0.78 |
| 1:Q:206:UNK:O | 1:Q:210:UNK:CB | 2.32 | 0.78 |
| 1:C:406:UNK:HA | 1:C:409:UNK:CB | 2.13 | 0.78 |
| 1:T:810:UNK:O | 1:T:812:UNK:N | 2.16 | 0.78 |
| 1:Q:406:UNK:HA | 1:Q:409:UNK:CB | 2.13 | 0.78 |
| 1:P:1412:UNK:HA | 1:P:1412:UNK:C | 2.09 | 0.78 |
| 1:C:206:UNK:O | 1:C:210:UNK:CB | 2.32 | 0.78 |
| 1:F:810:UNK:O | 1:F:812:UNK:N | 2.16 | 0.78 |
| 1:D:1109:UNK:C | 1:D:1111:UNK:H | 1.96 | 0.77 |
| 1:T:418:UNK:C | 1:T:420:UNK:H | 1.96 | 0.77 |
| 1:P:608:UNK:C | 1:P:610:UNK:H | 1.97 | 0.77 |
| 1:Q:1919:UNK:O | 1:Q:1921:UNK:N | 2.18 | 0.77 |
| 1:F:516:UNK:O | 1:F:605:UNK:N | 2.17 | 0.77 |
| 1:P:1420:UNK:O | 1:P:1421:UNK:C | 2.32 | 0.77 |
| 1:C:906:UNK:O | 1:C:909:UNK:N | 2.15 | 0.77 |
| 1:C:1919:UNK:O | 1:C:1921:UNK:N | 2.18 | 0.77 |
| 1:O:1421:UNK:C | 1:O:1423:UNK:H | 1.98 | 0.77 |
| 1:Q:1415:UNK:O | 1:Q:1418:UNK:N | 2.17 | 0.77 |
| 1:P:1507:UNK:C | 1:P:1509:UNK:H | 1.97 | 0.77 |
| 1:C:307:UNK:O | 1:C:311:UNK:CB | 2.32 | 0.77 |
| 1:A:2113:UNK:O | 1:A:2116:UNK:N | 2.18 | 0.77 |
| 1:Q:307:UNK:O | 1:Q:311:UNK:CB | 2.32 | 0.77 |
| 1:B:608:UNK:C | 1:B:610:UNK:H | 1.97 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:O:2113:UNK:O | 1:O:2116:UNK:N | 2.18 | 0.77 |
| 1:C:1415:UNK:O | 1:C:1418:UNK:N | 2.17 | 0.77 |
| 1:F:105:UNK:O | 1:F:109:UNK:N | 2.18 | 0.76 |
| 1:C:2509:UNK:C | 1:C:2511:UNK:N | 2.46 | 0.76 |
| 1:C:2010:UNK:C | 1:C:2012:UNK:H | 1.98 | 0.76 |
| 1:A:1310:UNK:C | 1:A:1312:UNK:N | 2.45 | 0.76 |
| 1:A:1421:UNK:C | 1:A:1423:UNK:H | 1.98 | 0.76 |
| 1:B:1507:UNK:C | 1:B:1509:UNK:H | 1.97 | 0.76 |
| 1:B:1420:UNK:O | 1:B:1421:UNK:C | 2.32 | 0.76 |
| 1:C:1010:UNK:O | 1:C:1012:UNK:N | 2.19 | 0.76 |
| 1:T:2814:UNK:O | 1:T:2816:UNK:N | 2.18 | 0.76 |
| 1:F:505:UNK:O | 1:F:507:UNK:N | 2.19 | 0.76 |
| 1:D:908:UNK:O | 1:D:910:UNK:N | 2.19 | 0.76 |
| 1:B:207:UNK:HA | 1:B:210:UNK:CB | 2.17 | 0.76 |
| 1:T:105:UNK:O | 1:T:109:UNK:N | 2.18 | 0.75 |
| 1:R:107:UNK:O | 1:R:111:UNK:N | 2.19 | 0.75 |
| 1:P:207:UNK:HA | 1:P:210:UNK:CB | 2.16 | 0.75 |
| 1:D:107:UNK:O | 1:D:111:UNK:N | 2.19 | 0.75 |
| 1:Q:2010:UNK:C | 1:Q:2012:UNK:H | 1.98 | 0.75 |
| 1:Q:1010:UNK:O | 1:Q:1012:UNK:N | 2.19 | 0.75 |
| 1:Q:906:UNK:C | 1:Q:908:UNK:N | 2.50 | 0.75 |
| 1:B:1613:UNK:O | 1:B:1615:UNK:N | 2.20 | 0.75 |
| 1:O:2109:UNK:HA | 1:O:2112:UNK:CB | 2.16 | 0.75 |
| 1:F:2814:UNK:O | 1:F:2816:UNK:N | 2.18 | 0.75 |
| 1:T:3420:UNK:O | 1:T:3423:UNK:O | 2.05 | 0.75 |
| 1:P:1613:UNK:O | 1:P:1615:UNK:N | 2.20 | 0.75 |
| 1:T:505:UNK:O | 1:T:507:UNK:N | 2.19 | 0.75 |
| 1:C:2207:UNK:O | 1:C:2210:UNK:N | 2.20 | 0.75 |
| 1:A:2109:UNK:HA | 1:A:2112:UNK:CB | 2.16 | 0.74 |
| 1:F:3420:UNK:O | 1:F:3423:UNK:O | 2.05 | 0.74 |
| 1:Q:1320:UNK:O | 1:Q:1322:UNK:N | 2.21 | 0.74 |
| 1:B:1110:UNK:O | 1:B:1113:UNK:N | 2.21 | 0.74 |
| 1:O:2106:UNK:C | 1:O:2108:UNK:H | 2.00 | 0.74 |
| 1:R:908:UNK:O | 1:R:910:UNK:N | 2.19 | 0.74 |
| 1:F:2515:UNK:C | 1:F:2517:UNK:N | 2.48 | 0.74 |
| 1:A:2106:UNK:C | 1:A:2108:UNK:H | 2.00 | 0.73 |
| 1:Q:2207:UNK:O | 1:Q:2210:UNK:N | 2.20 | 0.73 |
| 1:C:1320:UNK:O | 1:C:1322:UNK:N | 2.21 | 0.73 |
| 1:D:610:UNK:O | 1:D:612:UNK:N | 2.21 | 0.73 |
| 1:C:906:UNK:C | 1:C:908:UNK:N | 2.50 | 0.73 |
| 1:P:1614:UNK:HA | 1:P:1617:UNK:CB | 2.19 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:1014:UNK:C | 1:F:1016:UNK:N | 2.49 | 0.73 |
| 1:R:610:UNK:O | 1:R:612:UNK:N | 2.21 | 0.73 |
| 1:P:1110:UNK:O | 1:P:1113:UNK:N | 2.21 | 0.73 |
| 1:T:1309:UNK:C | 1:T:1311:UNK:N | 2.52 | 0.73 |
| 1:D:716:UNK:O | 1:D:720:UNK:N | 2.22 | 0.73 |
| 1:C:106:UNK:O | 1:C:109:UNK:N | 2.21 | 0.73 |
| 1:Q:106:UNK:O | 1:Q:109:UNK:N | 2.21 | 0.73 |
| 1:F:1309:UNK:C | 1:F:1311:UNK:N | 2.52 | 0.73 |
| 1:Q:2216:UNK:C | 1:Q:2218:UNK:H | 2.01 | 0.73 |
| 1:O:2209:UNK:O | 1:O:2213:UNK:CB | 2.36 | 0.73 |
| 1:O:1310:UNK:C | 1:O:1312:UNK:N | 2.45 | 0.73 |
| 1:D:914:UNK:HA | 1:D:917:UNK:CB | 2.19 | 0.73 |
| 1:R:716:UNK:O | 1:R:720:UNK:N | 2.22 | 0.73 |
| 1:R:1214:UNK:C | 1:R:1216:UNK:N | 2.50 | 0.73 |
| 1:T:2515:UNK:C | 1:T:2517:UNK:N | 2.48 | 0.73 |
| 1:B:112:UNK:O | 1:B:115:UNK:N | 2.22 | 0.73 |
| 1:T:123:UNK:C | 1:T:125:UNK:H | 2.01 | 0.73 |
| 1:T:3208:UNK:C | 1:T:3210:UNK:N | 2.51 | 0.73 |
| 1:B:1614:UNK:HA | 1:B:1617:UNK:CB | 2.19 | 0.73 |
| 1:S:225:UNK:O | 1:S:227:UNK:N | 2.22 | 0.72 |
| 1:R:1005:UNK:O | 1:R:1007:UNK:N | 2.22 | 0.72 |
| 1:F:1211:UNK:O | 1:F:1212:UNK:C | 2.38 | 0.72 |
| 1:F:1014:UNK:O | 1:F:1017:UNK:N | 2.22 | 0.72 |
| 1:T:715:UNK:C | 1:T:717:UNK:H | 2.01 | 0.72 |
| 1:F:123:UNK:C | 1:F:125:UNK:H | 2.01 | 0.72 |
| 1:R:307:UNK:O | 1:R:308:UNK:C | 2.37 | 0.72 |
| 1:F:715:UNK:C | 1:F:717:UNK:H | 2.01 | 0.72 |
| 1:T:1014:UNK:C | 1:T:1016:UNK:N | 2.49 | 0.72 |
| 1:A:2209:UNK:O | 1:A:2213:UNK:CB | 2.36 | 0.72 |
| 1:E:225:UNK:O | 1:E:227:UNK:N | 2.22 | 0.72 |
| 1:C:2216:UNK:C | 1:C:2218:UNK:H | 2.01 | 0.72 |
| 1:D:1005:UNK:O | 1:D:1007:UNK:N | 2.22 | 0.72 |
| 1:P:1311:UNK:O | 1:P:1315:UNK:N | 2.22 | 0.72 |
| 1:R:914:UNK:HA | 1:R:917:UNK:CB | 2.19 | 0.72 |
| 1:F:2005:UNK:C | 1:F:2007:UNK:N | 2.51 | 0.72 |
| 1:X:1030:UNK:O | 1:X:1031:UNK:C | 2.38 | 0.72 |
| 1:A:1114:UNK:O | 1:A:1117:UNK:N | 2.23 | 0.72 |
| 1:C:1906:UNK:O | 1:C:1909:UNK:N | 2.23 | 0.72 |
| 1:F:913:UNK:C | 1:F:915:UNK:N | 2.52 | 0.72 |
| 1:T:1014:UNK:O | 1:T:1017:UNK:N | 2.22 | 0.72 |
| 1:B:1412:UNK:CA | 1:B:1415:UNK:CB | 2.62 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:T:913:UNK:C | 1:T:915:UNK:N | 2.52 | 0.71 |
| 1:P:407:UNK:O | 1:P:410:UNK:N | 2.23 | 0.71 |
| 1:X:1029:UNK:O | 1:X:1030:UNK:C | 2.38 | 0.71 |
| 1:Q:1906:UNK:O | 1:Q:1909:UNK:N | 2.23 | 0.71 |
| 1:B:1311:UNK:O | 1:B:1315:UNK:N | 2.22 | 0.71 |
| 1:B:407:UNK:O | 1:B:410:UNK:N | 2.23 | 0.71 |
| 1:P:112:UNK:O | 1:P:115:UNK:N | 2.22 | 0.71 |
| 1:F:120:UNK:O | 1:F:122:UNK:N | 2.23 | 0.71 |
| 1:D:307:UNK:O | 1:D:308:UNK:C | 2.37 | 0.71 |
| 1:T:3207:UNK:O | 1:T:3211:UNK:CB | 2.39 | 0.71 |
| 1:X:847:UNK:C | 1:X:849:UNK:H | 2.03 | 0.71 |
| 1:O:1114:UNK:O | 1:O:1117:UNK:N | 2.23 | 0.71 |
| 1:A:1810:UNK:O | 1:A:1814:UNK:N | 2.23 | 0.71 |
| 1:F:3414:UNK:O | 1:F:3416:UNK:N | 2.24 | 0.71 |
| 1:T:3414:UNK:O | 1:T:3416:UNK:N | 2.24 | 0.71 |
| 1:F:3207:UNK:O | 1:F:3211:UNK:CB | 2.39 | 0.71 |
| 1:O:2115:UNK:O | 1:O:2118:UNK:CB | 2.39 | 0.71 |
| 1:R:221:UNK:C | 1:R:223:UNK:N | 2.53 | 0.71 |
| 1:Y:804:UNK:C | 1:Y:806:UNK:N | 2.51 | 0.71 |
| 1:A:2115:UNK:O | 1:A:2118:UNK:CB | 2.39 | 0.71 |
| 1:D:609:UNK:O | 1:D:610:UNK:O | 2.08 | 0.71 |
| 1:T:120:UNK:O | 1:T:122:UNK:N | 2.23 | 0.71 |
| 1:O:1810:UNK:O | 1:O:1814:UNK:N | 2.23 | 0.71 |
| 1:Y:1029:UNK:O | 1:Y:1030:UNK:C | 2.38 | 0.71 |
| 1:F:1312:UNK:HA | 1:F:1315:UNK:CB | 2.21 | 0.70 |
| 1:S:309:UNK:O | 1:S:311:UNK:N | 2.24 | 0.70 |
| 1:D:221:UNK:C | 1:D:223:UNK:N | 2.53 | 0.70 |
| 1:T:1312:UNK:HA | 1:T:1315:UNK:CB | 2.21 | 0.70 |
| 1:P:118:UNK:O | 1:P:121:UNK:CB | 2.40 | 0.70 |
| 1:X:804:UNK:C | 1:X:806:UNK:N | 2.51 | 0.70 |
| 1:F:3208:UNK:C | 1:F:3210:UNK:N | 2.51 | 0.70 |
| 1:T:2005:UNK:C | 1:T:2007:UNK:N | 2.51 | 0.70 |
| 1:Q:2207:UNK:O | 1:Q:2208:UNK:C | 2.39 | 0.70 |
| 1:T:2620:UNK:O | 1:T:2623:UNK:N | 2.25 | 0.70 |
| 1:E:309:UNK:O | 1:E:311:UNK:N | 2.24 | 0.70 |
| 1:X:1048:UNK:O | 1:X:1050:UNK:N | 2.25 | 0.70 |
| 1:Y:1048:UNK:O | 1:Y:1050:UNK:N | 2.25 | 0.70 |
| 1:T:120:UNK:C | 1:T:122:UNK:N | 2.55 | 0.69 |
| 1:P:605:UNK:CB | 1:P:905:UNK:H | 2.05 | 0.69 |
| 1:C:2211:UNK:C | 1:C:2213:UNK:H | 2.06 | 0.69 |
| 1:P:1107:UNK:O | 1:P:1110:UNK:N | 2.26 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:120:UNK:C | 1:F:122:UNK:N | 2.55 | 0.69 |
| 1:Y:847:UNK:C | 1:Y:849:UNK:H | 2.03 | 0.69 |
| 1:F:2620:UNK:O | 1:F:2623:UNK:N | 2.25 | 0.69 |
| 1:T:1211:UNK:O | 1:T:1212:UNK:C | 2.38 | 0.69 |
| 1:Q:709:UNK:O | 1:Q:713:UNK:N | 2.25 | 0.69 |
| 1:C:2207:UNK:O | 1:C:2208:UNK:C | 2.39 | 0.69 |
| 1:R:609:UNK:O | 1:R:610:UNK:O | 2.08 | 0.69 |
| 1:D:1214:UNK:C | 1:D:1216:UNK:N | 2.50 | 0.69 |
| 1:C:709:UNK:O | 1:C:713:UNK:N | 2.25 | 0.69 |
| 1:Q:1209:UNK:O | 1:Q:1212:UNK:N | 2.26 | 0.69 |
| 1:Y:1030:UNK:O | 1:Y:1031:UNK:C | 2.38 | 0.69 |
| 1:T:1908:UNK:C | 1:T:1910:UNK:N | 2.52 | 0.69 |
| 1:C:1209:UNK:O | 1:C:1212:UNK:N | 2.26 | 0.69 |
| 1:B:1210:UNK:O | 1:B:1211:UNK:C | 2.41 | 0.69 |
| 1:B:1608:UNK:HA | 1:B:1611:UNK:CB | 2.23 | 0.69 |
| 1:Y:873:UNK:O | 1:Y:874:UNK:C | 2.41 | 0.69 |
| 1:B:1107:UNK:O | 1:B:1110:UNK:N | 2.26 | 0.69 |
| 1:C:2208:UNK:C | 1:C:2210:UNK:H | 2.06 | 0.69 |
| 1:B:118:UNK:O | 1:B:121:UNK:CB | 2.40 | 0.69 |
| 1:F:1908:UNK:C | 1:F:1910:UNK:N | 2.52 | 0.69 |
| 1:F:1417:UNK:O | 1:F:1418:UNK:C | 2.41 | 0.69 |
| 1:D:115:UNK:C | 1:D:117:UNK:N | 2.54 | 0.68 |
| 1:B:605:UNK:CB | 1:B:905:UNK:H | 2.05 | 0.68 |
| 1:Q:2208:UNK:C | 1:Q:2210:UNK:H | 2.06 | 0.68 |
| 1:P:1608:UNK:C | 1:P:1610:UNK:H | 2.05 | 0.68 |
| 1:T:3308:UNK:C | 1:T:3310:UNK:N | 2.56 | 0.68 |
| 1:X:873:UNK:O | 1:X:874:UNK:C | 2.41 | 0.68 |
| 1:P:1608:UNK:HA | 1:P:1611:UNK:CB | 2.23 | 0.68 |
| 1:Q:2211:UNK:C | 1:Q:2213:UNK:H | 2.06 | 0.68 |
| 1:B:611:UNK:O | 1:B:613:UNK:N | 2.26 | 0.68 |
| 1:A:2110:UNK:O | 1:A:2114:UNK:N | 2.27 | 0.68 |
| 1:O:2110:UNK:O | 1:O:2114:UNK:N | 2.27 | 0.68 |
| 1:A:2606:UNK:O | 1:A:2609:UNK:N | 2.27 | 0.68 |
| 1:A:1212:UNK:O | 1:A:1214:UNK:N | 2.27 | 0.68 |
| 1:P:1412:UNK:CA | 1:P:1415:UNK:CB | 2.62 | 0.68 |
| 1:O:1212:UNK:O | 1:O:1214:UNK:N | 2.27 | 0.68 |
| 1:O:2606:UNK:O | 1:O:2609:UNK:N | 2.27 | 0.68 |
| 1:R:509:UNK:O | 1:R:512:UNK:N | 2.27 | 0.68 |
| 1:P:1511:UNK:C | 1:P:1513:UNK:N | 2.55 | 0.68 |
| 1:X:922:UNK:C | 1:X:924:UNK:N | 2.56 | 0.68 |
| 1:P:1210:UNK:O | 1:P:1211:UNK:C | 2.41 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:709:UNK:C | 1:D:711:UNK:H | 2.08 | 0.68 |
| 1:C:315:UNK:C | 1:C:317:UNK:N | 2.56 | 0.67 |
| 1:D:509:UNK:O | 1:D:512:UNK:N | 2.27 | 0.67 |
| 1:F:3308:UNK:C | 1:F:3310:UNK:N | 2.56 | 0.67 |
| 1:P:611:UNK:O | 1:P:613:UNK:N | 2.26 | 0.67 |
| 1:F:2817:UNK:O | 1:F:2820:UNK:CB | 2.43 | 0.67 |
| 1:F:418:UNK:O | 1:F:421:UNK:N | 2.28 | 0.67 |
| 1:Q:315:UNK:C | 1:Q:317:UNK:N | 2.56 | 0.67 |
| 1:T:2817:UNK:O | 1:T:2820:UNK:CB | 2.43 | 0.67 |
| 1:D:911:UNK:O | 1:D:913:UNK:N | 2.28 | 0.67 |
| 1:B:1010:UNK:O | 1:B:1011:UNK:C | 2.43 | 0.67 |
| 1:O:2111:UNK:HA | 1:O:2114:UNK:CB | 2.24 | 0.67 |
| 1:D:224:UNK:O | 1:D:226:UNK:N | 2.24 | 0.67 |
| 1:T:2319:UNK:O | 1:T:2321:UNK:N | 2.28 | 0.67 |
| 1:T:418:UNK:O | 1:T:421:UNK:N | 2.28 | 0.67 |
| 1:R:115:UNK:C | 1:R:117:UNK:N | 2.54 | 0.67 |
| 1:A:2111:UNK:HA | 1:A:2114:UNK:CB | 2.24 | 0.67 |
| 1:R:212:UNK:O | 1:R:213:UNK:C | 2.43 | 0.67 |
| 1:R:224:UNK:C | 1:R:226:UNK:H | 2.08 | 0.67 |
| 1:F:2219:UNK:C | 1:F:2221:UNK:N | 2.58 | 0.66 |
| 1:A:1820:UNK:CB | 1:A:2012:UNK:CB | 2.73 | 0.66 |
| 1:F:2319:UNK:O | 1:F:2321:UNK:N | 2.28 | 0.66 |
| 1:T:1417:UNK:O | 1:T:1418:UNK:C | 2.41 | 0.66 |
| 1:D:315:UNK:HA | 1:D:318:UNK:CB | 2.25 | 0.66 |
| 1:D:315:UNK:HA | 1:D:318:UNK:CA | 2.25 | 0.66 |
| 1:R:709:UNK:C | 1:R:711:UNK:H | 2.08 | 0.66 |
| 1:T:3206:UNK:O | 1:T:3210:UNK:CB | 2.44 | 0.66 |
| 1:D:224:UNK:C | 1:D:226:UNK:H | 2.08 | 0.66 |
| 1:F:1521:UNK:O | 1:F:1523:UNK:N | 2.28 | 0.66 |
| 1:P:1010:UNK:O | 1:P:1011:UNK:C | 2.43 | 0.66 |
| 1:C:2112:UNK:C | 1:C:2114:UNK:N | 2.59 | 0.66 |
| 1:C:117:UNK:C | 1:C:119:UNK:N | 2.58 | 0.66 |
| 1:R:911:UNK:O | 1:R:913:UNK:N | 2.28 | 0.66 |
| 1:Q:2305:UNK:O | 1:Q:2307:UNK:N | 2.29 | 0.66 |
| 1:Y:917:UNK:C | 1:Y:919:UNK:H | 2.09 | 0.66 |
| 1:C:2305:UNK:O | 1:C:2307:UNK:N | 2.28 | 0.66 |
| 1:O:1820:UNK:CB | 1:O:2012:UNK:CB | 2.73 | 0.66 |
| 1:T:1521:UNK:O | 1:T:1523:UNK:N | 2.28 | 0.66 |
| 1:R:208:UNK:C | 1:R:210:UNK:N | 2.55 | 0.66 |
| 1:O:1317:UNK:O | 1:O:1318:UNK:C | 2.44 | 0.66 |
| 1:P:1213:UNK:C | 1:P:1215:UNK:H | 2.08 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:315:UNK:HA | 1:R:318:UNK:CB | 2.25 | 0.66 |
| 1:P:711:UNK:C | 1:P:713:UNK:H | 2.09 | 0.66 |
| 1:T:2219:UNK:C | 1:T:2221:UNK:N | 2.58 | 0.66 |
| 1:A:2121:UNK:C | 1:A:2123:UNK:H | 2.09 | 0.66 |
| 1:Q:117:UNK:C | 1:Q:119:UNK:N | 2.57 | 0.65 |
| 1:F:3206:UNK:O | 1:F:3210:UNK:CB | 2.44 | 0.65 |
| 1:R:315:UNK:HA | 1:R:318:UNK:CA | 2.25 | 0.65 |
| 1:A:1418:UNK:O | 1:A:1420:UNK:N | 2.29 | 0.65 |
| 1:O:1114:UNK:C | 1:O:1116:UNK:N | 2.56 | 0.65 |
| 1:O:2121:UNK:C | 1:O:2123:UNK:H | 2.09 | 0.65 |
| 1:B:707:UNK:C | 1:B:709:UNK:N | 2.58 | 0.65 |
| 1:C:2112:UNK:O | 1:C:2115:UNK:N | 2.29 | 0.65 |
| 1:A:2415:UNK:O | 1:A:2417:UNK:N | 2.30 | 0.65 |
| 1:Q:2112:UNK:O | 1:Q:2115:UNK:N | 2.30 | 0.65 |
| 1:B:1511:UNK:C | 1:B:1513:UNK:N | 2.55 | 0.65 |
| 1:C:613:UNK:O | 1:C:615:UNK:N | 2.30 | 0.65 |
| 1:O:1418:UNK:O | 1:O:1420:UNK:N | 2.30 | 0.65 |
| 1:C:1320:UNK:O | 1:C:1321:UNK:C | 2.45 | 0.65 |
| 1:O:2415:UNK:O | 1:O:2417:UNK:N | 2.30 | 0.65 |
| 1:F:3305:UNK:O | 1:F:3307:UNK:N | 2.30 | 0.65 |
| 1:T:3305:UNK:O | 1:T:3307:UNK:N | 2.29 | 0.65 |
| 1:Q:1320:UNK:O | 1:Q:1321:UNK:C | 2.45 | 0.65 |
| 1:T:2006:UNK:O | 1:T:2007:UNK:C | 2.45 | 0.65 |
| 1:B:1213:UNK:C | 1:B:1215:UNK:H | 2.09 | 0.65 |
| 1:E:112:UNK:C | 1:E:114:UNK:H | 2.10 | 0.65 |
| 1:F:2215:UNK:O | 1:F:2216:UNK:C | 2.45 | 0.65 |
| 1:A:1317:UNK:O | 1:A:1318:UNK:C | 2.44 | 0.65 |
| 1:X:917:UNK:C | 1:X:919:UNK:H | 2.09 | 0.65 |
| 1:D:208:UNK:C | 1:D:210:UNK:N | 2.55 | 0.65 |
| 1:T:2215:UNK:O | 1:T:2216:UNK:C | 2.45 | 0.65 |
| 1:P:615:UNK:C | 1:P:617:UNK:H | 2.07 | 0.65 |
| 1:T:1208:UNK:O | 1:T:1210:UNK:N | 2.30 | 0.65 |
| 1:D:212:UNK:O | 1:D:213:UNK:C | 2.43 | 0.65 |
| 1:Q:1005:UNK:HA | 1:Q:1120:UNK:CB | 2.26 | 0.65 |
| 1:A:1114:UNK:C | 1:A:1116:UNK:N | 2.56 | 0.65 |
| 1:C:2408:UNK:O | 1:C:2409:UNK:C | 2.45 | 0.65 |
| 1:T:316:UNK:O | 1:T:320:UNK:N | 2.30 | 0.65 |
| 1:F:316:UNK:O | 1:F:320:UNK:N | 2.30 | 0.65 |
| 1:C:113:UNK:C | 1:C:115:UNK:N | 2.60 | 0.65 |
| 1:F:2006:UNK:O | 1:F:2007:UNK:C | 2.45 | 0.65 |
| 1:Q:513:UNK:O | 1:Q:517:UNK:N | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:308:UNK:O | 1:R:310:UNK:N | 2.30 | 0.64 |
| 1:C:117:UNK:O | 1:C:119:UNK:N | 2.29 | 0.64 |
| 1:Y:922:UNK:C | 1:Y:924:UNK:N | 2.56 | 0.64 |
| 1:F:1208:UNK:O | 1:F:1210:UNK:N | 2.30 | 0.64 |
| 1:C:1005:UNK:HA | 1:C:1120:UNK:CB | 2.26 | 0.64 |
| 1:C:513:UNK:O | 1:C:517:UNK:N | 2.31 | 0.64 |
| 1:O:1209:UNK:HA | 1:O:1212:UNK:CB | 2.28 | 0.64 |
| 1:Q:117:UNK:O | 1:Q:119:UNK:N | 2.29 | 0.64 |
| 1:B:711:UNK:C | 1:B:713:UNK:H | 2.09 | 0.64 |
| 1:Y:1048:UNK:C | 1:Y:1050:UNK:N | 2.60 | 0.64 |
| 1:D:808:UNK:O | 1:D:812:UNK:N | 2.31 | 0.64 |
| 1:Q:912:UNK:O | 1:Q:914:UNK:N | 2.30 | 0.64 |
| 1:A:1209:UNK:HA | 1:A:1212:UNK:CB | 2.28 | 0.64 |
| 1:R:808:UNK:O | 1:R:812:UNK:N | 2.31 | 0.64 |
| 1:P:1015:UNK:O | 1:P:1017:UNK:N | 2.31 | 0.64 |
| 1:F:415:UNK:O | 1:F:417:UNK:N | 2.31 | 0.64 |
| 1:B:615:UNK:C | 1:B:617:UNK:H | 2.07 | 0.64 |
| 1:C:912:UNK:O | 1:C:914:UNK:N | 2.30 | 0.64 |
| 1:F:2814:UNK:O | 1:F:2817:UNK:N | 2.31 | 0.64 |
| 1:C:1806:UNK:C | 1:C:1808:UNK:N | 2.61 | 0.64 |
| 1:P:818:UNK:C | 1:P:820:UNK:N | 2.59 | 0.64 |
| 1:R:1009:UNK:O | 1:R:1013:UNK:N | 2.31 | 0.64 |
| 1:D:308:UNK:O | 1:D:310:UNK:N | 2.31 | 0.64 |
| 1:Q:613:UNK:O | 1:Q:615:UNK:N | 2.30 | 0.64 |
| 1:B:818:UNK:C | 1:B:820:UNK:N | 2.59 | 0.64 |
| 1:Q:2112:UNK:C | 1:Q:2114:UNK:N | 2.59 | 0.64 |
| 1:A:2108:UNK:O | 1:A:2112:UNK:N | 2.31 | 0.64 |
| 1:P:306:UNK:O | 1:P:310:UNK:N | 2.31 | 0.64 |
| 1:A:2406:UNK:O | 1:A:2407:UNK:O | 2.16 | 0.64 |
| 1:C:807:UNK:C | 1:C:809:UNK:N | 2.61 | 0.63 |
| 1:C:2409:UNK:O | 1:C:2410:UNK:O | 2.16 | 0.63 |
| 1:B:1015:UNK:O | 1:B:1017:UNK:N | 2.31 | 0.63 |
| 1:A:1221:UNK:O | 1:A:1307:UNK:HA | 1.99 | 0.63 |
| 1:S:112:UNK:C | 1:S:114:UNK:H | 2.10 | 0.63 |
| 1:P:211:UNK:HA | 1:P:214:UNK:CB | 2.27 | 0.63 |
| 1:D:1009:UNK:O | 1:D:1013:UNK:N | 2.31 | 0.63 |
| 1:T:415:UNK:O | 1:T:417:UNK:N | 2.31 | 0.63 |
| 1:B:306:UNK:O | 1:B:310:UNK:N | 2.31 | 0.63 |
| 1:Q:2121:UNK:O | 1:Q:2125:UNK:N | 2.31 | 0.63 |
| 1:Q:2409:UNK:O | 1:Q:2410:UNK:O | 2.16 | 0.63 |
| 1:C:2121:UNK:O | 1:C:2125:UNK:N | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Q:2408:UNK:O | 1:Q:2409:UNK:C | 2.45 | 0.63 |
| 1:F:3007:UNK:C | 1:F:3009:UNK:N | 2.60 | 0.63 |
| 1:O:2406:UNK:O | 1:O:2407:UNK:O | 2.16 | 0.63 |
| 1:T:2006:UNK:O | 1:T:2010:UNK:N | 2.32 | 0.63 |
| 1:P:707:UNK:C | 1:P:709:UNK:N | 2.58 | 0.63 |
| 1:C:2305:UNK:C | 1:C:2307:UNK:N | 2.61 | 0.63 |
| 1:Q:1818:UNK:O | 1:Q:1820:UNK:N | 2.32 | 0.63 |
| 1:P:716:UNK:O | 1:P:718:UNK:N | 2.32 | 0.63 |
| 1:B:211:UNK:HA | 1:B:214:UNK:CB | 2.27 | 0.63 |
| 1:A:2406:UNK:O | 1:A:2407:UNK:C | 2.47 | 0.63 |
| 1:B:716:UNK:O | 1:B:718:UNK:N | 2.32 | 0.63 |
| 1:Q:113:UNK:C | 1:Q:115:UNK:N | 2.60 | 0.63 |
| 1:T:3414:UNK:O | 1:T:3417:UNK:N | 2.32 | 0.63 |
| 1:Y:924:UNK:O | 1:Y:928:UNK:N | 2.32 | 0.63 |
| 1:F:2109:UNK:C | 1:F:2111:UNK:N | 2.60 | 0.63 |
| 1:P:210:UNK:C | 1:P:212:UNK:H | 2.11 | 0.63 |
| 1:P:1313:UNK:O | 1:P:1317:UNK:N | 2.32 | 0.63 |
| 1:X:1048:UNK:C | 1:X:1050:UNK:N | 2.60 | 0.63 |
| 1:A:2411:UNK:C | 1:A:2413:UNK:N | 2.60 | 0.63 |
| 1:O:1008:UNK:C | 1:O:1010:UNK:N | 2.60 | 0.63 |
| 1:Q:807:UNK:C | 1:Q:809:UNK:N | 2.61 | 0.62 |
| 1:Q:1411:UNK:O | 1:Q:1415:UNK:N | 2.32 | 0.62 |
| 1:O:2406:UNK:O | 1:O:2407:UNK:C | 2.47 | 0.62 |
| 1:Q:1415:UNK:C | 1:Q:1417:UNK:N | 2.61 | 0.62 |
| 1:C:1305:UNK:O | 1:C:1307:UNK:N | 2.32 | 0.62 |
| 1:F:3414:UNK:O | 1:F:3417:UNK:N | 2.32 | 0.62 |
| 1:C:1013:UNK:O | 1:C:1015:UNK:N | 2.32 | 0.62 |
| 1:O:2307:UNK:O | 1:O:2310:UNK:N | 2.32 | 0.62 |
| 1:R:509:UNK:C | 1:R:511:UNK:N | 2.52 | 0.62 |
| 1:X:924:UNK:O | 1:X:928:UNK:N | 2.32 | 0.62 |
| 1:F:512:UNK:C | 1:F:514:UNK:N | 2.61 | 0.62 |
| 1:A:1418:UNK:O | 1:A:1421:UNK:N | 2.32 | 0.62 |
| 1:O:2108:UNK:O | 1:O:2112:UNK:N | 2.31 | 0.62 |
| 1:F:2817:UNK:O | 1:F:2820:UNK:N | 2.32 | 0.62 |
| 1:D:714:UNK:O | 1:D:716:UNK:N | 2.33 | 0.62 |
| 1:B:1313:UNK:O | 1:B:1317:UNK:N | 2.32 | 0.62 |
| 1:O:1221:UNK:O | 1:O:1307:UNK:HA | 1.98 | 0.62 |
| 1:F:512:UNK:O | 1:F:514:UNK:N | 2.33 | 0.62 |
| 1:D:919:UNK:HA | 1:D:922:UNK:CB | 2.30 | 0.62 |
| 1:Y:1025:UNK:HA | 1:Y:1028:UNK:CB | 2.30 | 0.62 |
| 1:T:2109:UNK:C | 1:T:2111:UNK:N | 2.60 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:1418:UNK:C | 1:A:1420:UNK:N | 2.62 | 0.62 |
| 1:Y:1066:UNK:HA | 1:Y:1069:UNK:CB | 2.30 | 0.62 |
| 1:D:706:UNK:O | 1:D:708:UNK:N | 2.33 | 0.62 |
| 1:C:1415:UNK:C | 1:C:1417:UNK:N | 2.61 | 0.62 |
| 1:Q:1412:UNK:O | 1:Q:1414:UNK:N | 2.31 | 0.62 |
| 1:T:512:UNK:O | 1:T:514:UNK:N | 2.33 | 0.62 |
| 1:R:919:UNK:HA | 1:R:922:UNK:CB | 2.30 | 0.62 |
| 1:O:2411:UNK:C | 1:O:2413:UNK:N | 2.61 | 0.62 |
| 1:C:1411:UNK:O | 1:C:1415:UNK:N | 2.32 | 0.62 |
| 1:Q:506:UNK:HA | 1:Q:509:UNK:CB | 2.30 | 0.62 |
| 1:Q:1806:UNK:C | 1:Q:1808:UNK:N | 2.61 | 0.62 |
| 1:T:317:UNK:O | 1:T:321:UNK:N | 2.33 | 0.62 |
| 1:O:1418:UNK:O | 1:O:1421:UNK:N | 2.32 | 0.62 |
| 1:T:2814:UNK:O | 1:T:2817:UNK:N | 2.31 | 0.62 |
| 1:A:1008:UNK:C | 1:A:1010:UNK:N | 2.60 | 0.62 |
| 1:B:1310:UNK:O | 1:B:1314:UNK:N | 2.33 | 0.62 |
| 1:T:1517:UNK:O | 1:T:1521:UNK:N | 2.33 | 0.62 |
| 1:B:1015:UNK:C | 1:B:1017:UNK:N | 2.60 | 0.62 |
| 1:F:2207:UNK:O | 1:F:2210:UNK:N | 2.33 | 0.62 |
| 1:R:706:UNK:O | 1:R:708:UNK:N | 2.33 | 0.62 |
| 1:P:1015:UNK:C | 1:P:1017:UNK:N | 2.61 | 0.62 |
| 1:B:911:UNK:C | 1:B:913:UNK:N | 2.61 | 0.62 |
| 1:F:220:UNK:C | 1:F:222:UNK:N | 2.60 | 0.62 |
| 1:C:1818:UNK:O | 1:C:1820:UNK:N | 2.32 | 0.62 |
| 1:R:719:UNK:C | 1:R:721:UNK:N | 2.61 | 0.61 |
| 1:P:1310:UNK:O | 1:P:1314:UNK:N | 2.33 | 0.61 |
| 1:A:1712:UNK:O | 1:A:1715:UNK:N | 2.33 | 0.61 |
| 1:C:1919:UNK:C | 1:C:1921:UNK:N | 2.63 | 0.61 |
| 1:F:1517:UNK:O | 1:F:1521:UNK:N | 2.33 | 0.61 |
| 1:F:708:UNK:O | 1:F:710:UNK:N | 2.33 | 0.61 |
| 1:T:220:UNK:C | 1:T:222:UNK:N | 2.60 | 0.61 |
| 1:X:855:UNK:O | 1:X:858:UNK:C | 2.48 | 0.61 |
| 1:A:2307:UNK:O | 1:A:2310:UNK:N | 2.32 | 0.61 |
| 1:P:1708:UNK:O | 1:P:1709:UNK:C | 2.48 | 0.61 |
| 1:Q:1305:UNK:O | 1:Q:1307:UNK:N | 2.32 | 0.61 |
| 1:Q:1919:UNK:C | 1:Q:1921:UNK:N | 2.63 | 0.61 |
| 1:D:717:UNK:HA | 1:D:720:UNK:CB | 2.30 | 0.61 |
| 1:C:506:UNK:HA | 1:C:509:UNK:CB | 2.30 | 0.61 |
| 1:X:1025:UNK:HA | 1:X:1028:UNK:CB | 2.30 | 0.61 |
| 1:T:2207:UNK:O | 1:T:2210:UNK:N | 2.33 | 0.61 |
| 1:R:717:UNK:HA | 1:R:720:UNK:CB | 2.30 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:2006:UNK:O | 1:F:2010:UNK:N | 2.32 | 0.61 |
| 1:C:1507:UNK:O | 1:C:1510:UNK:N | 2.33 | 0.61 |
| 1:D:509:UNK:C | 1:D:511:UNK:N | 2.52 | 0.61 |
| 1:T:2817:UNK:O | 1:T:2820:UNK:N | 2.32 | 0.61 |
| 1:Q:1814:UNK:O | 1:Q:1815:UNK:C | 2.49 | 0.61 |
| 1:O:1712:UNK:O | 1:O:1715:UNK:N | 2.33 | 0.61 |
| 1:F:1514:UNK:O | 1:F:1518:UNK:N | 2.33 | 0.61 |
| 1:F:418:UNK:C | 1:F:420:UNK:N | 2.60 | 0.61 |
| 1:Q:2010:UNK:C | 1:Q:2012:UNK:N | 2.60 | 0.61 |
| 1:O:1418:UNK:C | 1:O:1420:UNK:N | 2.62 | 0.61 |
| 1:D:709:UNK:O | 1:D:711:UNK:N | 2.33 | 0.61 |
| 1:R:224:UNK:O | 1:R:226:UNK:N | 2.24 | 0.61 |
| 1:C:1505:UNK:O | 1:C:1507:UNK:N | 2.33 | 0.61 |
| 1:C:2513:UNK:C | 1:C:2515:UNK:N | 2.64 | 0.61 |
| 1:P:1515:UNK:C | 1:P:1517:UNK:N | 2.63 | 0.61 |
| 1:C:1309:UNK:O | 1:C:1312:UNK:N | 2.34 | 0.61 |
| 1:P:615:UNK:C | 1:P:617:UNK:N | 2.64 | 0.61 |
| 1:R:714:UNK:O | 1:R:716:UNK:N | 2.33 | 0.61 |
| 1:T:119:UNK:HA | 1:T:122:UNK:CB | 2.31 | 0.61 |
| 1:Q:1505:UNK:O | 1:Q:1507:UNK:N | 2.33 | 0.61 |
| 1:B:1708:UNK:O | 1:B:1709:UNK:C | 2.48 | 0.61 |
| 1:B:210:UNK:C | 1:B:212:UNK:H | 2.11 | 0.61 |
| 1:T:1514:UNK:O | 1:T:1518:UNK:N | 2.34 | 0.61 |
| 1:X:1066:UNK:HA | 1:X:1069:UNK:CB | 2.30 | 0.61 |
| 1:A:1406:UNK:C | 1:A:1408:UNK:H | 2.14 | 0.61 |
| 1:F:317:UNK:O | 1:F:321:UNK:N | 2.33 | 0.60 |
| 1:B:210:UNK:O | 1:B:213:UNK:N | 2.34 | 0.60 |
| 1:R:709:UNK:O | 1:R:711:UNK:N | 2.33 | 0.60 |
| 1:A:2406:UNK:O | 1:A:2410:UNK:N | 2.34 | 0.60 |
| 1:P:911:UNK:C | 1:P:913:UNK:N | 2.61 | 0.60 |
| 1:Y:806:UNK:C | 1:Y:808:UNK:H | 2.14 | 0.60 |
| 1:Y:855:UNK:O | 1:Y:858:UNK:C | 2.48 | 0.60 |
| 1:C:1814:UNK:O | 1:C:1815:UNK:C | 2.49 | 0.60 |
| 1:R:610:UNK:O | 1:R:611:UNK:C | 2.49 | 0.60 |
| 1:Q:1507:UNK:O | 1:Q:1510:UNK:N | 2.33 | 0.60 |
| 1:A:1206:UNK:C | 1:A:1208:UNK:N | 2.64 | 0.60 |
| 1:C:2010:UNK:C | 1:C:2012:UNK:N | 2.60 | 0.60 |
| 1:P:1307:UNK:O | 1:P:1309:UNK:N | 2.35 | 0.60 |
| 1:B:615:UNK:C | 1:B:617:UNK:N | 2.64 | 0.60 |
| 1:D:905:UNK:C | 1:D:907:UNK:N | 2.62 | 0.60 |
| 1:F:2814:UNK:C | 1:F:2816:UNK:N | 2.63 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Q:2305:UNK:C | 1:Q:2307:UNK:N | 2.61 | 0.60 |
| 1:R:1211:UNK:O | 1:R:1213:UNK:N | 2.35 | 0.60 |
| 1:C:2309:UNK:C | 1:C:2311:UNK:N | 2.64 | 0.60 |
| 1:T:310:UNK:C | 1:T:312:UNK:N | 2.63 | 0.60 |
| 1:P:210:UNK:O | 1:P:213:UNK:N | 2.34 | 0.60 |
| 1:D:719:UNK:C | 1:D:721:UNK:N | 2.62 | 0.60 |
| 1:X:834:UNK:O | 1:X:835:UNK:CB | 2.49 | 0.60 |
| 1:T:418:UNK:C | 1:T:420:UNK:N | 2.60 | 0.60 |
| 1:D:407:UNK:C | 1:D:409:UNK:N | 2.64 | 0.60 |
| 1:R:407:UNK:C | 1:R:409:UNK:N | 2.65 | 0.60 |
| 1:Q:1309:UNK:O | 1:Q:1312:UNK:N | 2.34 | 0.60 |
| 1:Y:920:UNK:O | 1:Y:923:UNK:N | 2.35 | 0.60 |
| 1:C:2216:UNK:C | 1:C:2218:UNK:N | 2.64 | 0.60 |
| 1:Q:2211:UNK:C | 1:Q:2213:UNK:N | 2.62 | 0.60 |
| 1:D:1211:UNK:O | 1:D:1213:UNK:N | 2.34 | 0.60 |
| 1:D:107:UNK:HA | 1:D:110:UNK:CB | 2.32 | 0.60 |
| 1:B:1307:UNK:O | 1:B:1309:UNK:N | 2.35 | 0.60 |
| 1:T:512:UNK:C | 1:T:514:UNK:N | 2.61 | 0.60 |
| 1:T:1417:UNK:O | 1:T:1420:UNK:N | 2.35 | 0.60 |
| 1:D:610:UNK:O | 1:D:611:UNK:C | 2.49 | 0.60 |
| 1:Y:843:UNK:O | 1:Y:846:UNK:N | 2.35 | 0.60 |
| 1:F:119:UNK:HA | 1:F:122:UNK:CB | 2.31 | 0.59 |
| 1:T:1906:UNK:O | 1:T:1910:UNK:N | 2.35 | 0.59 |
| 1:Q:2309:UNK:C | 1:Q:2311:UNK:N | 2.64 | 0.59 |
| 1:D:1112:UNK:O | 1:D:1114:UNK:N | 2.35 | 0.59 |
| 1:R:1112:UNK:O | 1:R:1114:UNK:N | 2.35 | 0.59 |
| 1:R:107:UNK:HA | 1:R:110:UNK:CB | 2.32 | 0.59 |
| 1:R:721:UNK:C | 1:R:723:UNK:N | 2.65 | 0.59 |
| 1:O:2406:UNK:O | 1:O:2410:UNK:N | 2.34 | 0.59 |
| 1:T:3007:UNK:C | 1:T:3009:UNK:N | 2.60 | 0.59 |
| 1:T:708:UNK:O | 1:T:710:UNK:N | 2.33 | 0.59 |
| 1:T:2616:UNK:C | 1:T:2618:UNK:N | 2.59 | 0.59 |
| 1:O:1206:UNK:C | 1:O:1208:UNK:N | 2.65 | 0.59 |
| 1:O:1406:UNK:C | 1:O:1408:UNK:H | 2.13 | 0.59 |
| 1:A:2005:UNK:C | 1:A:2007:UNK:N | 2.63 | 0.59 |
| 1:T:3305:UNK:C | 1:T:3307:UNK:N | 2.64 | 0.59 |
| 1:O:2305:UNK:O | 1:O:2308:UNK:CB | 2.50 | 0.59 |
| 1:P:508:UNK:O | 1:P:511:UNK:N | 2.35 | 0.59 |
| 1:C:911:UNK:O | 1:C:914:UNK:CB | 2.51 | 0.59 |
| 1:O:2507:UNK:CA | 1:O:2510:UNK:CB | 2.75 | 0.59 |
| 1:Q:117:UNK:O | 1:Q:120:UNK:N | 2.36 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:T:709:UNK:HA | 1:T:712:UNK:CB | 2.33 | 0.59 |
| 1:X:920:UNK:O | 1:X:923:UNK:N | 2.35 | 0.59 |
| 1:T:3308:UNK:O | 1:T:3310:UNK:N | 2.36 | 0.59 |
| 1:F:3308:UNK:O | 1:F:3310:UNK:N | 2.36 | 0.59 |
| 1:Q:2118:UNK:O | 1:Q:2122:UNK:N | 2.36 | 0.59 |
| 1:B:508:UNK:O | 1:B:511:UNK:N | 2.35 | 0.59 |
| 1:A:712:UNK:CB | 1:A:905:UNK:CB | 2.81 | 0.59 |
| 1:C:1313:UNK:C | 1:C:1315:UNK:N | 2.64 | 0.59 |
| 1:T:2814:UNK:C | 1:T:2816:UNK:N | 2.63 | 0.59 |
| 1:X:803:UNK:HA | 1:X:810:UNK:O | 2.03 | 0.59 |
| 1:F:3308:UNK:O | 1:F:3311:UNK:N | 2.36 | 0.59 |
| 1:O:2005:UNK:C | 1:O:2007:UNK:N | 2.63 | 0.59 |
| 1:B:1515:UNK:C | 1:B:1517:UNK:N | 2.63 | 0.59 |
| 1:X:1050:UNK:O | 1:X:1053:UNK:CB | 2.51 | 0.59 |
| 1:F:3305:UNK:C | 1:F:3307:UNK:N | 2.64 | 0.59 |
| 1:Y:834:UNK:O | 1:Y:835:UNK:CB | 2.50 | 0.59 |
| 1:F:2616:UNK:C | 1:F:2618:UNK:N | 2.59 | 0.59 |
| 1:C:1013:UNK:C | 1:C:1015:UNK:H | 2.16 | 0.59 |
| 1:A:2305:UNK:O | 1:A:2308:UNK:CB | 2.50 | 0.59 |
| 1:X:843:UNK:O | 1:X:846:UNK:N | 2.35 | 0.59 |
| 1:C:2118:UNK:O | 1:C:2122:UNK:N | 2.36 | 0.59 |
| 1:C:117:UNK:O | 1:C:120:UNK:N | 2.36 | 0.59 |
| 1:F:3421:UNK:C | 1:F:3423:UNK:N | 2.61 | 0.59 |
| 1:F:1417:UNK:O | 1:F:1420:UNK:N | 2.35 | 0.59 |
| 1:T:3308:UNK:O | 1:T:3311:UNK:N | 2.36 | 0.59 |
| 1:T:1309:UNK:O | 1:T:1313:UNK:N | 2.36 | 0.58 |
| 1:X:880:UNK:O | 1:X:881:UNK:C | 2.50 | 0.58 |
| 1:D:908:UNK:O | 1:D:911:UNK:N | 2.37 | 0.58 |
| 1:Q:911:UNK:O | 1:Q:914:UNK:CB | 2.51 | 0.58 |
| 1:Y:803:UNK:HA | 1:Y:810:UNK:O | 2.03 | 0.58 |
| 1:Y:1050:UNK:O | 1:Y:1053:UNK:CB | 2.51 | 0.58 |
| 1:O:712:UNK:CB | 1:O:905:UNK:CB | 2.81 | 0.58 |
| 1:F:310:UNK:C | 1:F:312:UNK:N | 2.64 | 0.58 |
| 1:D:907:UNK:O | 1:D:908:UNK:C | 2.51 | 0.58 |
| 1:A:2106:UNK:C | 1:A:2108:UNK:N | 2.64 | 0.58 |
| 1:Q:2513:UNK:C | 1:Q:2515:UNK:N | 2.64 | 0.58 |
| 1:D:221:UNK:O | 1:D:222:UNK:C | 2.52 | 0.58 |
| 1:F:1005:UNK:C | 1:F:1007:UNK:N | 2.62 | 0.58 |
| 1:Q:109:UNK:O | 1:Q:112:UNK:N | 2.37 | 0.58 |
| 1:Y:880:UNK:O | 1:Y:881:UNK:C | 2.50 | 0.58 |
| 1:Q:2512:UNK:O | 1:Q:2513:UNK:O | 2.22 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Y:874:UNK:O | 1:Y:875:UNK:C | 2.50 | 0.58 |
| 1:C:312:UNK:O | 1:C:313:UNK:C | 2.51 | 0.58 |
| 1:F:1309:UNK:O | 1:F:1313:UNK:N | 2.36 | 0.58 |
| 1:C:2505:UNK:HA | 1:C:2508:UNK:CB | 2.33 | 0.58 |
| 1:Q:1010:UNK:O | 1:Q:1013:UNK:N | 2.37 | 0.58 |
| 1:T:3421:UNK:C | 1:T:3423:UNK:N | 2.61 | 0.58 |
| 1:D:721:UNK:C | 1:D:723:UNK:N | 2.65 | 0.58 |
| 1:R:108:UNK:O | 1:R:112:UNK:N | 2.37 | 0.58 |
| 1:X:1067:UNK:O | 1:X:1071:UNK:N | 2.37 | 0.58 |
| 1:F:1906:UNK:O | 1:F:1910:UNK:N | 2.35 | 0.58 |
| 1:P:507:UNK:O | 1:P:511:UNK:N | 2.37 | 0.58 |
| 1:R:1205:UNK:C | 1:R:1207:UNK:N | 2.67 | 0.58 |
| 1:Q:2505:UNK:HA | 1:Q:2508:UNK:CB | 2.33 | 0.58 |
| 1:O:2207:UNK:O | 1:O:2210:UNK:N | 2.37 | 0.58 |
| 1:D:1205:UNK:C | 1:D:1207:UNK:N | 2.67 | 0.58 |
| 1:F:1420:UNK:O | 1:F:1423:UNK:N | 2.37 | 0.58 |
| 1:F:2212:UNK:C | 1:F:2214:UNK:N | 2.67 | 0.58 |
| 1:D:108:UNK:O | 1:D:112:UNK:N | 2.37 | 0.57 |
| 1:F:2113:UNK:C | 1:F:2115:UNK:N | 2.66 | 0.57 |
| 1:B:1614:UNK:HA | 1:B:1617:UNK:CA | 2.34 | 0.57 |
| 1:Y:1067:UNK:O | 1:Y:1071:UNK:N | 2.37 | 0.57 |
| 1:E:225:UNK:C | 1:E:227:UNK:N | 2.67 | 0.57 |
| 1:S:225:UNK:C | 1:S:227:UNK:N | 2.67 | 0.57 |
| 1:A:1008:UNK:O | 1:A:1011:UNK:N | 2.38 | 0.57 |
| 1:C:2612:UNK:HA | 1:C:2615:UNK:CB | 2.34 | 0.57 |
| 1:C:2512:UNK:O | 1:C:2513:UNK:O | 2.22 | 0.57 |
| 1:R:221:UNK:O | 1:R:222:UNK:C | 2.52 | 0.57 |
| 1:A:1509:UNK:O | 1:A:1513:UNK:N | 2.37 | 0.57 |
| 1:Q:1013:UNK:O | 1:Q:1015:UNK:N | 2.32 | 0.57 |
| 1:R:905:UNK:C | 1:R:907:UNK:N | 2.62 | 0.57 |
| 1:C:109:UNK:O | 1:C:112:UNK:N | 2.37 | 0.57 |
| 1:Q:2612:UNK:HA | 1:Q:2615:UNK:CB | 2.34 | 0.57 |
| 1:Q:312:UNK:O | 1:Q:313:UNK:C | 2.51 | 0.57 |
| 1:O:1509:UNK:O | 1:O:1513:UNK:N | 2.37 | 0.57 |
| 1:C:1010:UNK:O | 1:C:1013:UNK:N | 2.37 | 0.57 |
| 1:Q:1013:UNK:C | 1:Q:1015:UNK:H | 2.16 | 0.57 |
| 1:R:907:UNK:O | 1:R:908:UNK:C | 2.52 | 0.57 |
| 1:P:1311:UNK:C | 1:P:1313:UNK:N | 2.67 | 0.57 |
| 1:Y:843:UNK:O | 1:Y:844:UNK:C | 2.53 | 0.57 |
| 1:F:3510:UNK:O | 1:F:3512:UNK:N | 2.38 | 0.57 |
| 1:A:2207:UNK:O | 1:A:2210:UNK:N | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:224:UNK:C | 1:R:226:UNK:N | 2.68 | 0.57 |
| 1:B:1711:UNK:HA | 1:B:1714:UNK:CB | 2.35 | 0.57 |
| 1:B:507:UNK:O | 1:B:511:UNK:N | 2.37 | 0.57 |
| 1:F:709:UNK:HA | 1:F:712:UNK:CB | 2.33 | 0.57 |
| 1:D:605:UNK:O | 1:D:606:UNK:C | 2.53 | 0.57 |
| 1:T:2512:UNK:O | 1:T:2515:UNK:N | 2.37 | 0.57 |
| 1:T:1420:UNK:O | 1:T:1423:UNK:N | 2.37 | 0.57 |
| 1:Q:1313:UNK:C | 1:Q:1315:UNK:N | 2.65 | 0.57 |
| 1:F:2512:UNK:O | 1:F:2515:UNK:N | 2.37 | 0.57 |
| 1:P:1614:UNK:HA | 1:P:1617:UNK:CA | 2.34 | 0.57 |
| 1:B:513:UNK:O | 1:B:517:UNK:N | 2.37 | 0.57 |
| 1:C:912:UNK:C | 1:C:914:UNK:N | 2.67 | 0.57 |
| 1:R:908:UNK:O | 1:R:911:UNK:N | 2.37 | 0.57 |
| 1:C:1412:UNK:O | 1:C:1414:UNK:N | 2.31 | 0.56 |
| 1:T:2113:UNK:C | 1:T:2115:UNK:N | 2.66 | 0.56 |
| 1:T:2005:UNK:O | 1:T:2006:UNK:C | 2.53 | 0.56 |
| 1:T:512:UNK:O | 1:T:515:UNK:N | 2.38 | 0.56 |
| 1:P:1613:UNK:O | 1:P:1616:UNK:N | 2.38 | 0.56 |
| 1:R:611:UNK:CB | 1:R:813:UNK:CB | 2.83 | 0.56 |
| 1:A:1713:UNK:C | 1:A:1715:UNK:N | 2.67 | 0.56 |
| 1:Q:1412:UNK:O | 1:Q:1415:UNK:N | 2.39 | 0.56 |
| 1:D:611:UNK:CB | 1:D:813:UNK:CB | 2.83 | 0.56 |
| 1:P:115:UNK:C | 1:P:117:UNK:N | 2.68 | 0.56 |
| 1:O:1008:UNK:O | 1:O:1011:UNK:N | 2.38 | 0.56 |
| 1:T:3510:UNK:O | 1:T:3512:UNK:N | 2.38 | 0.56 |
| 1:E:214:UNK:O | 1:E:215:UNK:C | 2.53 | 0.56 |
| 1:P:513:UNK:O | 1:P:517:UNK:N | 2.37 | 0.56 |
| 1:C:2119:UNK:O | 1:C:2123:UNK:N | 2.38 | 0.56 |
| 1:C:1412:UNK:O | 1:C:1415:UNK:N | 2.39 | 0.56 |
| 1:R:605:UNK:O | 1:R:606:UNK:C | 2.53 | 0.56 |
| 1:A:1305:UNK:O | 1:A:1308:UNK:N | 2.39 | 0.56 |
| 1:Q:2119:UNK:O | 1:Q:2123:UNK:N | 2.38 | 0.56 |
| 1:Y:908:UNK:O | 1:Y:910:UNK:N | 2.39 | 0.56 |
| 1:P:1711:UNK:HA | 1:P:1714:UNK:CB | 2.35 | 0.56 |
| 1:D:1006:UNK:O | 1:D:1007:UNK:C | 2.52 | 0.56 |
| 1:X:908:UNK:O | 1:X:909:UNK:C | 2.53 | 0.56 |
| 1:X:908:UNK:O | 1:X:910:UNK:N | 2.39 | 0.56 |
| 1:F:2316:UNK:O | 1:F:2320:UNK:N | 2.38 | 0.56 |
| 1:X:874:UNK:O | 1:X:875:UNK:C | 2.50 | 0.56 |
| 1:F:512:UNK:O | 1:F:515:UNK:N | 2.38 | 0.56 |
| 1:O:1908:UNK:C | 1:O:1910:UNK:N | 2.65 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Q:319:UNK:O | 1:Q:322:UNK:N | 2.39 | 0.56 |
| 1:T:2316:UNK:O | 1:T:2320:UNK:N | 2.38 | 0.56 |
| 1:O:2307:UNK:O | 1:O:2311:UNK:N | 2.39 | 0.56 |
| 1:X:843:UNK:O | 1:X:844:UNK:C | 2.53 | 0.56 |
| 1:S:214:UNK:O | 1:S:215:UNK:C | 2.53 | 0.56 |
| 1:F:1517:UNK:O | 1:F:1520:UNK:N | 2.39 | 0.56 |
| 1:Y:908:UNK:O | 1:Y:909:UNK:C | 2.53 | 0.56 |
| 1:T:1913:UNK:O | 1:T:1917:UNK:N | 2.39 | 0.56 |
| 1:T:3510:UNK:C | 1:T:3512:UNK:N | 2.68 | 0.56 |
| 1:B:1713:UNK:C | 1:B:1715:UNK:N | 2.64 | 0.55 |
| 1:Q:1010:UNK:C | 1:Q:1012:UNK:N | 2.69 | 0.55 |
| 1:C:319:UNK:O | 1:C:322:UNK:N | 2.39 | 0.55 |
| 1:B:1709:UNK:O | 1:B:1712:UNK:CB | 2.54 | 0.55 |
| 1:Q:912:UNK:C | 1:Q:914:UNK:N | 2.67 | 0.55 |
| 1:P:1709:UNK:O | 1:P:1712:UNK:CB | 2.54 | 0.55 |
| 1:Y:1070:UNK:O | 1:Y:1071:UNK:C | 2.54 | 0.55 |
| 1:B:1613:UNK:O | 1:B:1616:UNK:N | 2.38 | 0.55 |
| 1:R:1006:UNK:O | 1:R:1007:UNK:C | 2.52 | 0.55 |
| 1:Y:1068:UNK:HA | 1:Y:1071:UNK:CB | 2.37 | 0.55 |
| 1:T:1005:UNK:C | 1:T:1007:UNK:N | 2.62 | 0.55 |
| 1:C:2313:UNK:C | 1:C:2315:UNK:N | 2.69 | 0.55 |
| 1:Y:838:UNK:C | 1:Y:840:UNK:N | 2.52 | 0.55 |
| 1:X:1068:UNK:HA | 1:X:1071:UNK:CB | 2.37 | 0.55 |
| 1:O:1517:UNK:O | 1:O:1519:UNK:N | 2.40 | 0.55 |
| 1:T:3208:UNK:O | 1:T:3211:UNK:N | 2.39 | 0.55 |
| 1:O:1713:UNK:C | 1:O:1715:UNK:N | 2.67 | 0.55 |
| 1:Q:2313:UNK:C | 1:Q:2315:UNK:N | 2.69 | 0.55 |
| 1:B:1311:UNK:C | 1:B:1313:UNK:N | 2.67 | 0.55 |
| 1:O:1305:UNK:O | 1:O:1308:UNK:N | 2.39 | 0.55 |
| 1:P:1013:UNK:O | 1:P:1014:UNK:C | 2.55 | 0.55 |
| 1:A:2008:UNK:O | 1:A:2010:UNK:N | 2.40 | 0.55 |
| 1:E:118:UNK:O | 1:E:121:UNK:N | 2.40 | 0.55 |
| 1:C:1607:UNK:HA | 1:C:1610:UNK:CB | 2.36 | 0.55 |
| 1:T:2109:UNK:O | 1:T:2112:UNK:N | 2.39 | 0.55 |
| 1:T:1517:UNK:O | 1:T:1520:UNK:N | 2.39 | 0.55 |
| 1:F:1913:UNK:O | 1:F:1917:UNK:N | 2.39 | 0.55 |
| 1:B:1713:UNK:O | 1:B:1714:UNK:C | 2.53 | 0.55 |
| 1:C:2211:UNK:C | 1:C:2213:UNK:N | 2.62 | 0.55 |
| 1:F:3510:UNK:C | 1:F:3512:UNK:N | 2.68 | 0.55 |
| 1:F:205:UNK:O | 1:F:207:UNK:N | 2.40 | 0.55 |
| 1:Q:1607:UNK:HA | 1:Q:1610:UNK:CB | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:B:1107:UNK:C | 1:B:1109:UNK:N | 2.69 | 0.55 |
| 1:F:2109:UNK:O | 1:F:2112:UNK:N | 2.39 | 0.55 |
| 1:F:3208:UNK:O | 1:F:3211:UNK:N | 2.39 | 0.55 |
| 1:Y:1024:UNK:O | 1:Y:1026:UNK:N | 2.39 | 0.55 |
| 1:S:118:UNK:O | 1:S:121:UNK:N | 2.40 | 0.55 |
| 1:R:220:UNK:HA | 1:R:223:UNK:CB | 2.37 | 0.55 |
| 1:Q:2216:UNK:C | 1:Q:2218:UNK:N | 2.64 | 0.55 |
| 1:D:315:UNK:HA | 1:D:318:UNK:N | 2.22 | 0.55 |
| 1:Y:906:UNK:C | 1:Y:908:UNK:N | 2.70 | 0.55 |
| 1:Q:2313:UNK:O | 1:Q:2315:UNK:N | 2.40 | 0.55 |
| 1:T:2415:UNK:O | 1:T:2419:UNK:CB | 2.55 | 0.55 |
| 1:Q:1922:UNK:C | 1:Q:1924:UNK:N | 2.69 | 0.55 |
| 1:P:818:UNK:O | 1:P:820:UNK:N | 2.40 | 0.54 |
| 1:B:818:UNK:O | 1:B:820:UNK:N | 2.40 | 0.54 |
| 1:A:2307:UNK:O | 1:A:2311:UNK:N | 2.39 | 0.54 |
| 1:C:2313:UNK:O | 1:C:2315:UNK:N | 2.40 | 0.54 |
| 1:B:1013:UNK:O | 1:B:1014:UNK:C | 2.55 | 0.54 |
| 1:C:410:UNK:O | 1:C:413:UNK:CB | 2.55 | 0.54 |
| 1:X:1024:UNK:O | 1:X:1026:UNK:N | 2.39 | 0.54 |
| 1:T:2212:UNK:C | 1:T:2214:UNK:N | 2.67 | 0.54 |
| 1:X:1070:UNK:O | 1:X:1071:UNK:C | 2.54 | 0.54 |
| 1:F:3007:UNK:O | 1:F:3009:UNK:N | 2.40 | 0.54 |
| 1:B:316:UNK:O | 1:B:317:UNK:C | 2.55 | 0.54 |
| 1:Q:410:UNK:O | 1:Q:413:UNK:CB | 2.55 | 0.54 |
| 1:B:210:UNK:O | 1:B:213:UNK:CB | 2.56 | 0.54 |
| 1:A:1908:UNK:C | 1:A:1910:UNK:N | 2.65 | 0.54 |
| 1:X:838:UNK:C | 1:X:840:UNK:N | 2.52 | 0.54 |
| 1:R:107:UNK:O | 1:R:108:UNK:C | 2.55 | 0.54 |
| 1:P:1110:UNK:C | 1:P:1112:UNK:N | 2.70 | 0.54 |
| 1:A:1517:UNK:O | 1:A:1519:UNK:N | 2.40 | 0.54 |
| 1:S:225:UNK:O | 1:S:228:UNK:N | 2.41 | 0.54 |
| 1:O:2008:UNK:O | 1:O:2010:UNK:N | 2.40 | 0.54 |
| 1:B:605:UNK:CB | 1:B:905:UNK:N | 2.71 | 0.54 |
| 1:F:1208:UNK:O | 1:F:1209:UNK:C | 2.55 | 0.54 |
| 1:E:225:UNK:O | 1:E:228:UNK:N | 2.41 | 0.54 |
| 1:R:811:UNK:O | 1:R:814:UNK:N | 2.41 | 0.54 |
| 1:X:906:UNK:C | 1:X:908:UNK:N | 2.70 | 0.54 |
| 1:F:3418:UNK:O | 1:F:3422:UNK:CB | 2.55 | 0.54 |
| 1:C:1922:UNK:C | 1:C:1924:UNK:N | 2.69 | 0.54 |
| 1:D:1005:UNK:C | 1:D:1007:UNK:N | 2.71 | 0.54 |
| 1:F:2112:UNK:O | 1:F:2115:UNK:C | 2.56 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:P:605:UNK:CB | 1:P:905:UNK:N | 2.71 | 0.54 |
| 1:B:115:UNK:C | 1:B:117:UNK:N | 2.68 | 0.54 |
| 1:F:2005:UNK:O | 1:F:2006:UNK:C | 2.53 | 0.54 |
| 1:D:811:UNK:O | 1:D:814:UNK:N | 2.41 | 0.54 |
| 1:X:911:UNK:O | 1:X:915:UNK:O | 2.26 | 0.54 |
| 1:T:2112:UNK:O | 1:T:2115:UNK:C | 2.56 | 0.54 |
| 1:T:3007:UNK:O | 1:T:3009:UNK:N | 2.40 | 0.54 |
| 1:O:1707:UNK:C | 1:O:1709:UNK:N | 2.68 | 0.54 |
| 1:A:2110:UNK:O | 1:A:2113:UNK:N | 2.41 | 0.54 |
| 1:S:308:UNK:HA | 1:S:311:UNK:CB | 2.38 | 0.54 |
| 1:R:315:UNK:HA | 1:R:318:UNK:N | 2.22 | 0.54 |
| 1:A:1707:UNK:C | 1:A:1709:UNK:N | 2.68 | 0.54 |
| 1:F:2415:UNK:O | 1:F:2419:UNK:CB | 2.55 | 0.54 |
| 1:R:1005:UNK:C | 1:R:1007:UNK:N | 2.71 | 0.54 |
| 1:B:1110:UNK:C | 1:B:1112:UNK:N | 2.70 | 0.54 |
| 1:P:210:UNK:O | 1:P:213:UNK:CB | 2.56 | 0.54 |
| 1:Y:804:UNK:O | 1:Y:806:UNK:N | 2.41 | 0.54 |
| 1:A:1305:UNK:O | 1:A:1309:UNK:N | 2.41 | 0.54 |
| 1:Q:1813:UNK:O | 1:Q:1817:UNK:CB | 2.56 | 0.54 |
| 1:D:220:UNK:HA | 1:D:223:UNK:CB | 2.37 | 0.54 |
| 1:F:810:UNK:O | 1:F:811:UNK:C | 2.55 | 0.54 |
| 1:O:2110:UNK:O | 1:O:2113:UNK:N | 2.41 | 0.54 |
| 1:R:915:UNK:C | 1:R:917:UNK:N | 2.71 | 0.54 |
| 1:X:804:UNK:O | 1:X:806:UNK:N | 2.41 | 0.54 |
| 1:Q:911:UNK:O | 1:Q:912:UNK:C | 2.57 | 0.53 |
| 1:F:418:UNK:O | 1:F:420:UNK:N | 2.25 | 0.53 |
| 1:F:1413:UNK:O | 1:F:1417:UNK:CB | 2.56 | 0.53 |
| 1:A:2407:UNK:O | 1:A:2408:UNK:C | 2.56 | 0.53 |
| 1:O:2407:UNK:O | 1:O:2408:UNK:C | 2.56 | 0.53 |
| 1:T:3418:UNK:O | 1:T:3422:UNK:CB | 2.55 | 0.53 |
| 1:O:1812:UNK:O | 1:O:1816:UNK:N | 2.41 | 0.53 |
| 1:D:107:UNK:O | 1:D:108:UNK:C | 2.55 | 0.53 |
| 1:T:218:UNK:C | 1:T:220:UNK:N | 2.70 | 0.53 |
| 1:X:813:UNK:O | 1:X:814:UNK:C | 2.56 | 0.53 |
| 1:T:205:UNK:O | 1:T:207:UNK:N | 2.40 | 0.53 |
| 1:A:1812:UNK:O | 1:A:1816:UNK:N | 2.41 | 0.53 |
| 1:T:1208:UNK:O | 1:T:1209:UNK:C | 2.55 | 0.53 |
| 1:O:1305:UNK:O | 1:O:1309:UNK:N | 2.41 | 0.53 |
| 1:Y:911:UNK:O | 1:Y:915:UNK:O | 2.26 | 0.53 |
| 1:P:611:UNK:O | 1:P:614:UNK:N | 2.42 | 0.53 |
| 1:D:224:UNK:C | 1:D:226:UNK:N | 2.68 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:O:2011:UNK:O | 1:O:2015:UNK:N | 2.41 | 0.53 |
| 1:A:2005:UNK:O | 1:A:2007:UNK:N | 2.42 | 0.53 |
| 1:A:2011:UNK:O | 1:A:2015:UNK:N | 2.42 | 0.53 |
| 1:P:716:UNK:O | 1:P:717:UNK:C | 2.56 | 0.53 |
| 1:O:2005:UNK:O | 1:O:2007:UNK:N | 2.42 | 0.53 |
| 1:T:3109:UNK:C | 1:T:3111:UNK:N | 2.69 | 0.53 |
| 1:C:911:UNK:O | 1:C:912:UNK:C | 2.56 | 0.53 |
| 1:P:1713:UNK:O | 1:P:1714:UNK:C | 2.53 | 0.53 |
| 1:B:611:UNK:O | 1:B:614:UNK:N | 2.42 | 0.53 |
| 1:B:407:UNK:O | 1:B:409:UNK:N | 2.42 | 0.53 |
| 1:C:1813:UNK:O | 1:C:1817:UNK:CB | 2.56 | 0.53 |
| 1:Y:813:UNK:O | 1:Y:814:UNK:C | 2.56 | 0.53 |
| 1:A:2609:UNK:O | 1:A:2611:UNK:N | 2.42 | 0.53 |
| 1:D:915:UNK:O | 1:D:916:UNK:C | 2.56 | 0.53 |
| 1:D:715:UNK:HA | 1:D:718:UNK:CB | 2.39 | 0.53 |
| 1:B:508:UNK:O | 1:B:512:UNK:N | 2.42 | 0.53 |
| 1:Q:2313:UNK:O | 1:Q:2315:UNK:O | 2.27 | 0.53 |
| 1:F:3109:UNK:C | 1:F:3111:UNK:N | 2.69 | 0.53 |
| 1:T:3506:UNK:O | 1:T:3507:UNK:C | 2.57 | 0.53 |
| 1:F:2414:UNK:HA | 1:F:2417:UNK:CB | 2.39 | 0.53 |
| 1:C:2515:UNK:C | 1:C:2517:UNK:N | 2.72 | 0.53 |
| 1:P:1107:UNK:C | 1:P:1109:UNK:N | 2.69 | 0.53 |
| 1:Q:1919:UNK:O | 1:Q:1920:UNK:C | 2.57 | 0.53 |
| 1:R:915:UNK:O | 1:R:916:UNK:C | 2.56 | 0.53 |
| 1:T:3210:UNK:CB | 1:T:3316:UNK:CB | 2.87 | 0.53 |
| 1:P:1313:UNK:C | 1:P:1315:UNK:N | 2.72 | 0.53 |
| 1:T:1413:UNK:O | 1:T:1417:UNK:CB | 2.56 | 0.53 |
| 1:P:316:UNK:O | 1:P:317:UNK:C | 2.55 | 0.53 |
| 1:Q:1511:UNK:C | 1:Q:1513:UNK:N | 2.70 | 0.53 |
| 1:P:1713:UNK:C | 1:P:1715:UNK:N | 2.64 | 0.53 |
| 1:A:2507:UNK:CA | 1:A:2510:UNK:CB | 2.75 | 0.53 |
| 1:T:512:UNK:HA | 1:T:515:UNK:CB | 2.39 | 0.53 |
| 1:A:1114:UNK:O | 1:A:1116:UNK:N | 2.42 | 0.53 |
| 1:C:1511:UNK:C | 1:C:1513:UNK:N | 2.70 | 0.53 |
| 1:R:305:UNK:C | 1:R:307:UNK:N | 2.72 | 0.53 |
| 1:O:1114:UNK:O | 1:O:1116:UNK:N | 2.42 | 0.53 |
| 1:E:308:UNK:HA | 1:E:311:UNK:CB | 2.38 | 0.53 |
| 1:F:2207:UNK:O | 1:F:2208:UNK:C | 2.57 | 0.53 |
| 1:P:608:UNK:C | 1:P:610:UNK:N | 2.67 | 0.52 |
| 1:T:3421:UNK:HA | 1:T:3424:UNK:CB | 2.39 | 0.52 |
| 1:D:609:UNK:O | 1:D:610:UNK:C | 2.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:R:614:UNK:O | 1:R:617:UNK:CB | 2.57 | 0.52 |
| 1:P:112:UNK:C | 1:P:114:UNK:N | 2.72 | 0.52 |
| 1:T:2714:UNK:C | 1:T:2716:UNK:H | 2.22 | 0.52 |
| 1:F:3615:UNK:C | 1:F:3617:UNK:N | 2.70 | 0.52 |
| 1:T:2414:UNK:HA | 1:T:2417:UNK:CB | 2.39 | 0.52 |
| 1:P:1507:UNK:O | 1:P:1511:UNK:N | 2.43 | 0.52 |
| 1:T:2111:UNK:O | 1:T:2115:UNK:CB | 2.57 | 0.52 |
| 1:A:2110:UNK:O | 1:A:2113:UNK:CB | 2.57 | 0.52 |
| 1:R:715:UNK:HA | 1:R:718:UNK:CB | 2.39 | 0.52 |
| 1:C:319:UNK:C | 1:C:321:UNK:N | 2.72 | 0.52 |
| 1:T:407:UNK:C | 1:T:409:UNK:H | 2.22 | 0.52 |
| 1:T:810:UNK:O | 1:T:811:UNK:C | 2.56 | 0.52 |
| 1:R:807:UNK:O | 1:R:808:UNK:C | 2.57 | 0.52 |
| 1:C:2313:UNK:O | 1:C:2315:UNK:O | 2.27 | 0.52 |
| 1:F:213:UNK:HA | 1:F:216:UNK:CB | 2.39 | 0.52 |
| 1:F:2111:UNK:O | 1:F:2115:UNK:CB | 2.57 | 0.52 |
| 1:O:2110:UNK:O | 1:O:2113:UNK:CB | 2.57 | 0.52 |
| 1:B:407:UNK:C | 1:B:409:UNK:N | 2.72 | 0.52 |
| 1:O:2416:UNK:O | 1:O:2417:UNK:C | 2.57 | 0.52 |
| 1:B:716:UNK:O | 1:B:717:UNK:C | 2.56 | 0.52 |
| 1:P:216:UNK:O | 1:P:218:UNK:N | 2.42 | 0.52 |
| 1:C:1919:UNK:O | 1:C:1920:UNK:C | 2.57 | 0.52 |
| 1:F:3210:UNK:CB | 1:F:3316:UNK:CB | 2.87 | 0.52 |
| 1:F:108:UNK:C | 1:F:110:UNK:N | 2.68 | 0.52 |
| 1:O:2609:UNK:O | 1:O:2611:UNK:N | 2.42 | 0.52 |
| 1:Q:2515:UNK:C | 1:Q:2517:UNK:N | 2.72 | 0.52 |
| 1:D:111:UNK:O | 1:D:115:UNK:CB | 2.58 | 0.52 |
| 1:T:607:UNK:C | 1:T:609:UNK:N | 2.71 | 0.52 |
| 1:F:2714:UNK:C | 1:F:2716:UNK:H | 2.22 | 0.52 |
| 1:C:809:UNK:CA | 1:C:812:UNK:CB | 2.83 | 0.52 |
| 1:C:1010:UNK:C | 1:C:1012:UNK:N | 2.69 | 0.52 |
| 1:D:614:UNK:O | 1:D:617:UNK:CB | 2.57 | 0.52 |
| 1:F:2006:UNK:O | 1:F:2007:UNK:O | 2.28 | 0.52 |
| 1:Y:880:UNK:O | 1:Y:881:UNK:O | 2.27 | 0.52 |
| 1:F:407:UNK:C | 1:F:409:UNK:H | 2.22 | 0.52 |
| 1:F:1017:UNK:HA | 1:F:1020:UNK:CB | 2.40 | 0.52 |
| 1:R:609:UNK:O | 1:R:610:UNK:C | 2.57 | 0.52 |
| 1:P:407:UNK:O | 1:P:409:UNK:N | 2.42 | 0.52 |
| 1:P:407:UNK:C | 1:P:409:UNK:N | 2.72 | 0.52 |
| 1:T:2006:UNK:O | 1:T:2007:UNK:O | 2.28 | 0.52 |
| 1:A:2416:UNK:O | 1:A:2417:UNK:C | 2.57 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:F:305:UNK:O | 1:F:306:UNK:C | 2.57 | 0.52 |
| 1:T:305:UNK:O | 1:T:306:UNK:C | 2.57 | 0.52 |
| 1:T:213:UNK:HA | 1:T:216:UNK:CB | 2.39 | 0.52 |
| 1:B:1506:UNK:O | 1:B:1510:UNK:N | 2.43 | 0.52 |
| 1:F:3421:UNK:HA | 1:F:3424:UNK:CB | 2.39 | 0.52 |
| 1:O:1817:UNK:O | 1:O:1819:UNK:N | 2.43 | 0.52 |
| 1:O:2008:UNK:C | 1:O:2010:UNK:N | 2.72 | 0.52 |
| 1:B:1507:UNK:O | 1:B:1511:UNK:N | 2.43 | 0.51 |
| 1:B:1313:UNK:C | 1:B:1315:UNK:N | 2.72 | 0.51 |
| 1:P:508:UNK:O | 1:P:512:UNK:N | 2.42 | 0.51 |
| 1:A:2008:UNK:C | 1:A:2010:UNK:N | 2.72 | 0.51 |
| 1:A:1908:UNK:O | 1:A:1909:UNK:C | 2.58 | 0.51 |
| 1:F:607:UNK:C | 1:F:609:UNK:N | 2.71 | 0.51 |
| 1:C:1214:UNK:C | 1:C:1216:UNK:N | 2.73 | 0.51 |
| 1:B:1307:UNK:O | 1:B:1308:UNK:C | 2.58 | 0.51 |
| 1:P:1506:UNK:O | 1:P:1510:UNK:N | 2.43 | 0.51 |
| 1:R:721:UNK:O | 1:R:723:UNK:N | 2.43 | 0.51 |
| 1:T:1017:UNK:HA | 1:T:1020:UNK:CB | 2.40 | 0.51 |
| 1:F:3210:UNK:C | 1:F:3212:UNK:N | 2.71 | 0.51 |
| 1:B:216:UNK:O | 1:B:218:UNK:N | 2.42 | 0.51 |
| 1:P:1307:UNK:O | 1:P:1308:UNK:C | 2.58 | 0.51 |
| 1:F:310:UNK:O | 1:F:313:UNK:N | 2.44 | 0.51 |
| 1:F:512:UNK:HA | 1:F:515:UNK:CB | 2.39 | 0.51 |
| 1:F:3506:UNK:O | 1:F:3507:UNK:C | 2.57 | 0.51 |
| 1:R:306:UNK:O | 1:R:309:UNK:N | 2.44 | 0.51 |
| 1:O:1416:UNK:O | 1:O:1420:UNK:CB | 2.59 | 0.51 |
| 1:Q:1708:UNK:O | 1:Q:1712:UNK:N | 2.43 | 0.51 |
| 1:F:1012:UNK:HA | 1:F:1015:UNK:CB | 2.41 | 0.51 |
| 1:B:1018:UNK:C | 1:B:1020:UNK:N | 2.70 | 0.51 |
| 1:P:415:UNK:C | 1:P:417:UNK:N | 2.74 | 0.51 |
| 1:R:709:UNK:O | 1:R:712:UNK:N | 2.44 | 0.51 |
| 1:Q:319:UNK:C | 1:Q:321:UNK:N | 2.72 | 0.51 |
| 1:B:220:UNK:O | 1:B:221:UNK:C | 2.59 | 0.51 |
| 1:A:1811:UNK:O | 1:A:1815:UNK:CB | 2.59 | 0.51 |
| 1:B:1620:UNK:O | 1:B:1621:UNK:CB | 2.58 | 0.51 |
| 1:T:1012:UNK:HA | 1:T:1015:UNK:CB | 2.41 | 0.51 |
| 1:D:305:UNK:C | 1:D:307:UNK:N | 2.72 | 0.51 |
| 1:B:415:UNK:C | 1:B:417:UNK:N | 2.73 | 0.51 |
| 1:A:1315:UNK:O | 1:A:1318:UNK:N | 2.43 | 0.51 |
| 1:D:807:UNK:O | 1:D:808:UNK:C | 2.57 | 0.51 |
| 1:Y:1078:UNK:O | 1:Y:1079:UNK:CB | 2.59 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:T:3615:UNK:C | 1:T:3617:UNK:N | 2.70 | 0.51 |
| 1:D:306:UNK:O | 1:D:309:UNK:N | 2.44 | 0.51 |
| 1:T:2714:UNK:C | 1:T:2716:UNK:N | 2.74 | 0.51 |
| 1:Q:809:UNK:CA | 1:Q:812:UNK:CB | 2.83 | 0.51 |
| 1:O:1421:UNK:O | 1:O:1423:UNK:N | 2.35 | 0.51 |
| 1:D:721:UNK:O | 1:D:723:UNK:N | 2.43 | 0.51 |
| 1:T:2207:UNK:O | 1:T:2208:UNK:C | 2.57 | 0.51 |
| 1:F:2714:UNK:C | 1:F:2716:UNK:N | 2.74 | 0.51 |
| 1:A:1416:UNK:O | 1:A:1420:UNK:CB | 2.59 | 0.51 |
| 1:R:610:UNK:C | 1:R:612:UNK:N | 2.74 | 0.51 |
| 1:A:2312:UNK:O | 1:A:2314:UNK:N | 2.44 | 0.51 |
| 1:R:111:UNK:O | 1:R:115:UNK:CB | 2.58 | 0.51 |
| 1:F:2109:UNK:O | 1:F:2111:UNK:N | 2.44 | 0.51 |
| 1:B:206:UNK:O | 1:B:207:UNK:C | 2.59 | 0.51 |
| 1:P:206:UNK:O | 1:P:207:UNK:C | 2.59 | 0.51 |
| 1:A:1809:UNK:O | 1:A:1810:UNK:C | 2.57 | 0.51 |
| 1:O:1206:UNK:O | 1:O:1208:UNK:N | 2.44 | 0.51 |
| 1:C:1708:UNK:O | 1:C:1712:UNK:N | 2.43 | 0.51 |
| 1:O:1811:UNK:O | 1:O:1815:UNK:CB | 2.59 | 0.51 |
| 1:T:310:UNK:O | 1:T:313:UNK:N | 2.44 | 0.50 |
| 1:O:1315:UNK:O | 1:O:1318:UNK:N | 2.43 | 0.50 |
| 1:O:1813:UNK:O | 1:O:1817:UNK:N | 2.44 | 0.50 |
| 1:O:1221:UNK:HA | 1:O:1306:UNK:O | 2.11 | 0.50 |
| 1:X:1078:UNK:O | 1:X:1079:UNK:CB | 2.59 | 0.50 |
| 1:X:940:UNK:O | 1:X:1054:UNK:CB | 2.59 | 0.50 |
| 1:P:310:UNK:O | 1:P:311:UNK:C | 2.59 | 0.50 |
| 1:X:812:UNK:C | 1:X:814:UNK:H2 | 2.22 | 0.50 |
| 1:T:3605:UNK:O | 1:T:3607:UNK:N | 2.45 | 0.50 |
| 1:Q:911:UNK:O | 1:Q:914:UNK:N | 2.44 | 0.50 |
| 1:O:2106:UNK:C | 1:O:2108:UNK:N | 2.64 | 0.50 |
| 1:D:610:UNK:C | 1:D:612:UNK:N | 2.74 | 0.50 |
| 1:O:1809:UNK:O | 1:O:1810:UNK:C | 2.57 | 0.50 |
| 1:X:880:UNK:O | 1:X:881:UNK:O | 2.27 | 0.50 |
| 1:B:516:UNK:O | 1:B:517:UNK:C | 2.59 | 0.50 |
| 1:Y:940:UNK:O | 1:Y:1054:UNK:CB | 2.59 | 0.50 |
| 1:D:509:UNK:HA | 1:D:512:UNK:CB | 2.41 | 0.50 |
| 1:B:1113:UNK:O | 1:B:1114:UNK:C | 2.59 | 0.50 |
| 1:Q:115:UNK:O | 1:Q:119:UNK:N | 2.45 | 0.50 |
| 1:F:2411:UNK:O | 1:F:2414:UNK:N | 2.45 | 0.50 |
| 1:E:205:UNK:O | 1:E:206:UNK:O | 2.30 | 0.50 |
| 1:F:1009:UNK:O | 1:F:1013:UNK:N | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:T:3210:UNK:C | 1:T:3212:UNK:N | 2.71 | 0.50 |
| 1:P:1210:UNK:O | 1:P:1213:UNK:N | 2.44 | 0.50 |
| 1:Q:2309:UNK:O | 1:Q:2311:UNK:N | 2.45 | 0.50 |
| 1:F:3605:UNK:O | 1:F:3607:UNK:N | 2.45 | 0.50 |
| 1:A:1012:UNK:O | 1:A:1015:UNK:N | 2.45 | 0.50 |
| 1:O:2312:UNK:O | 1:O:2314:UNK:N | 2.44 | 0.50 |
| 1:R:1008:UNK:O | 1:R:1011:UNK:N | 2.45 | 0.50 |
| 1:Q:312:UNK:C | 1:Q:314:UNK:N | 2.75 | 0.50 |
| 1:T:1009:UNK:O | 1:T:1013:UNK:N | 2.44 | 0.50 |
| 1:A:1817:UNK:O | 1:A:1819:UNK:N | 2.44 | 0.50 |
| 1:T:1908:UNK:N | 1:T:1911:UNK:N | 2.60 | 0.50 |
| 1:A:2121:UNK:C | 1:A:2123:UNK:N | 2.72 | 0.50 |
| 1:B:310:UNK:O | 1:B:311:UNK:C | 2.59 | 0.50 |
| 1:T:319:UNK:O | 1:T:322:UNK:N | 2.45 | 0.50 |
| 1:Q:1607:UNK:C | 1:Q:1609:UNK:N | 2.59 | 0.50 |
| 1:C:312:UNK:C | 1:C:314:UNK:N | 2.75 | 0.50 |
| 1:P:1113:UNK:O | 1:P:1114:UNK:C | 2.59 | 0.50 |
| 1:C:115:UNK:O | 1:C:119:UNK:N | 2.45 | 0.50 |
| 1:D:709:UNK:O | 1:D:712:UNK:N | 2.44 | 0.50 |
| 1:C:1818:UNK:C | 1:C:1820:UNK:N | 2.74 | 0.50 |
| 1:A:1206:UNK:O | 1:A:1208:UNK:N | 2.44 | 0.50 |
| 1:P:516:UNK:O | 1:P:517:UNK:C | 2.59 | 0.50 |
| 1:A:1906:UNK:C | 1:A:1908:UNK:N | 2.74 | 0.50 |
| 1:Q:1910:UNK:O | 1:Q:1913:UNK:N | 2.45 | 0.50 |
| 1:S:205:UNK:O | 1:S:206:UNK:O | 2.30 | 0.50 |
| 1:B:1712:UNK:O | 1:B:1716:UNK:N | 2.45 | 0.50 |
| 1:B:1210:UNK:O | 1:B:1213:UNK:N | 2.44 | 0.50 |
| 1:F:1908:UNK:N | 1:F:1911:UNK:N | 2.60 | 0.50 |
| 1:P:711:UNK:C | 1:P:713:UNK:N | 2.75 | 0.50 |
| 1:O:1008:UNK:O | 1:O:1010:UNK:N | 2.45 | 0.50 |
| 1:C:2309:UNK:O | 1:C:2311:UNK:N | 2.45 | 0.50 |
| 1:B:507:UNK:O | 1:B:511:UNK:CB | 2.60 | 0.50 |
| 1:P:1620:UNK:O | 1:P:1621:UNK:CB | 2.58 | 0.50 |
| 1:C:911:UNK:O | 1:C:914:UNK:N | 2.44 | 0.50 |
| 1:Q:1214:UNK:C | 1:Q:1216:UNK:N | 2.73 | 0.50 |
| 1:A:1813:UNK:O | 1:A:1817:UNK:N | 2.44 | 0.50 |
| 1:D:1211:UNK:C | 1:D:1213:UNK:N | 2.75 | 0.50 |
| 1:O:1906:UNK:C | 1:O:1908:UNK:N | 2.74 | 0.50 |
| 1:O:2506:UNK:O | 1:O:2510:UNK:N | 2.45 | 0.49 |
| 1:A:2506:UNK:O | 1:A:2510:UNK:N | 2.45 | 0.49 |
| 1:R:509:UNK:HA | 1:R:512:UNK:CB | 2.41 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Y:1073:UNK:O | 1:Y:1076:UNK:N | 2.45 | 0.49 |
| 1:F:319:UNK:O | 1:F:322:UNK:N | 2.45 | 0.49 |
| 1:X:924:UNK:HA | 1:X:927:UNK:CB | 2.42 | 0.49 |
| 1:F:1911:UNK:O | 1:F:1912:UNK:C | 2.59 | 0.49 |
| 1:C:1910:UNK:O | 1:C:1913:UNK:N | 2.45 | 0.49 |
| 1:P:220:UNK:O | 1:P:221:UNK:C | 2.59 | 0.49 |
| 1:X:1073:UNK:O | 1:X:1076:UNK:N | 2.45 | 0.49 |
| 1:Y:920:UNK:C | 1:Y:922:UNK:N | 2.74 | 0.49 |
| 1:A:1221:UNK:HA | 1:A:1306:UNK:O | 2.11 | 0.49 |
| 1:F:3615:UNK:O | 1:F:3618:UNK:N | 2.46 | 0.49 |
| 1:Q:1706:UNK:C | 1:Q:1708:UNK:N | 2.74 | 0.49 |
| 1:O:1212:UNK:C | 1:O:1214:UNK:N | 2.75 | 0.49 |
| 1:R:913:UNK:C | 1:R:915:UNK:N | 2.75 | 0.49 |
| 1:T:123:UNK:O | 1:T:126:UNK:N | 2.46 | 0.49 |
| 1:F:1915:UNK:O | 1:F:1918:UNK:CB | 2.61 | 0.49 |
| 1:T:1915:UNK:O | 1:T:1918:UNK:CB | 2.61 | 0.49 |
| 1:O:1012:UNK:O | 1:O:1015:UNK:N | 2.45 | 0.49 |
| 1:A:1611:UNK:O | 1:A:1615:UNK:N | 2.45 | 0.49 |
| 1:F:407:UNK:O | 1:F:410:UNK:N | 2.46 | 0.49 |
| 1:T:2109:UNK:O | 1:T:2111:UNK:N | 2.44 | 0.49 |
| 1:D:915:UNK:C | 1:D:917:UNK:N | 2.71 | 0.49 |
| 1:Q:1818:UNK:C | 1:Q:1820:UNK:N | 2.74 | 0.49 |
| 1:O:1908:UNK:O | 1:O:1909:UNK:C | 2.58 | 0.49 |
| 1:Y:924:UNK:HA | 1:Y:927:UNK:CB | 2.42 | 0.49 |
| 1:F:218:UNK:C | 1:F:220:UNK:N | 2.70 | 0.49 |
| 1:T:2411:UNK:O | 1:T:2414:UNK:N | 2.45 | 0.49 |
| 1:T:412:UNK:O | 1:T:416:UNK:N | 2.46 | 0.49 |
| 1:C:1508:UNK:O | 1:C:1512:UNK:CB | 2.60 | 0.49 |
| 1:Q:1508:UNK:O | 1:Q:1512:UNK:CB | 2.60 | 0.49 |
| 1:O:1514:UNK:O | 1:O:1515:UNK:C | 2.59 | 0.49 |
| 1:Y:873:UNK:O | 1:Y:874:UNK:O | 2.30 | 0.49 |
| 1:C:1305:UNK:O | 1:C:1309:UNK:N | 2.46 | 0.49 |
| 1:T:511:UNK:O | 1:T:512:UNK:C | 2.60 | 0.49 |
| 1:P:507:UNK:O | 1:P:511:UNK:CB | 2.60 | 0.49 |
| 1:Y:812:UNK:C | 1:Y:814:UNK:H2 | 2.22 | 0.49 |
| 1:R:1012:UNK:O | 1:R:1014:UNK:C | 2.58 | 0.49 |
| 1:O:1611:UNK:O | 1:O:1615:UNK:N | 2.45 | 0.49 |
| 1:Q:310:UNK:HA | 1:Q:313:UNK:CB | 2.43 | 0.49 |
| 1:T:3615:UNK:O | 1:T:3618:UNK:N | 2.46 | 0.49 |
| 1:B:1417:UNK:C | 1:B:1419:UNK:H | 2.26 | 0.49 |
| 1:X:873:UNK:O | 1:X:874:UNK:O | 2.30 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Q:1305:UNK:O | 1:Q:1309:UNK:N | 2.46 | 0.49 |
| 1:F:511:UNK:O | 1:F:512:UNK:C | 2.60 | 0.49 |
| 1:A:2113:UNK:HA | 1:A:2116:UNK:CB | 2.43 | 0.49 |
| 1:O:2113:UNK:HA | 1:O:2116:UNK:CB | 2.43 | 0.49 |
| 1:P:206:UNK:O | 1:P:210:UNK:N | 2.46 | 0.49 |
| 1:Q:610:UNK:C | 1:Q:612:UNK:N | 2.75 | 0.49 |
| 1:P:1712:UNK:O | 1:P:1716:UNK:N | 2.45 | 0.49 |
| 1:B:206:UNK:O | 1:B:210:UNK:N | 2.46 | 0.49 |
| 1:D:720:UNK:HA | 1:D:723:UNK:CB | 2.43 | 0.49 |
| 1:F:123:UNK:O | 1:F:126:UNK:N | 2.46 | 0.49 |
| 1:T:1208:UNK:O | 1:T:1211:UNK:N | 2.46 | 0.49 |
| 1:B:1007:UNK:C | 1:B:1009:UNK:N | 2.74 | 0.49 |
| 1:Q:2305:UNK:O | 1:Q:2308:UNK:N | 2.46 | 0.49 |
| 1:R:1211:UNK:C | 1:R:1213:UNK:N | 2.75 | 0.49 |
| 1:X:1014:UNK:CB | 1:X:1065:UNK:CB | 2.91 | 0.49 |
| 1:D:1008:UNK:O | 1:D:1011:UNK:N | 2.45 | 0.49 |
| 1:A:1212:UNK:C | 1:A:1214:UNK:N | 2.75 | 0.49 |
| 1:C:310:UNK:HA | 1:C:313:UNK:CB | 2.43 | 0.49 |
| 1:R:720:UNK:HA | 1:R:723:UNK:CB | 2.43 | 0.49 |
| 1:C:2305:UNK:O | 1:C:2308:UNK:N | 2.46 | 0.49 |
| 1:X:917:UNK:C | 1:X:919:UNK:N | 2.69 | 0.49 |
| 1:A:2012:UNK:O | 1:A:2013:UNK:CB | 2.61 | 0.48 |
| 1:C:712:UNK:C | 1:C:714:UNK:H | 2.26 | 0.48 |
| 1:T:407:UNK:O | 1:T:410:UNK:N | 2.46 | 0.48 |
| 1:F:1007:UNK:O | 1:F:1009:UNK:N | 2.47 | 0.48 |
| 1:A:2411:UNK:O | 1:A:2413:UNK:N | 2.46 | 0.48 |
| 1:A:1406:UNK:HA | 1:A:1409:UNK:CB | 2.43 | 0.48 |
| 1:D:310:UNK:O | 1:D:314:UNK:N | 2.47 | 0.48 |
| 1:A:1607:UNK:O | 1:A:1611:UNK:N | 2.47 | 0.48 |
| 1:O:2012:UNK:O | 1:O:2013:UNK:CB | 2.61 | 0.48 |
| 1:A:1008:UNK:O | 1:A:1010:UNK:N | 2.45 | 0.48 |
| 1:F:2627:UNK:C | 1:F:2629:UNK:N | 2.75 | 0.48 |
| 1:T:418:UNK:O | 1:T:420:UNK:N | 2.25 | 0.48 |
| 1:B:112:UNK:C | 1:B:114:UNK:N | 2.72 | 0.48 |
| 1:F:1208:UNK:O | 1:F:1211:UNK:N | 2.46 | 0.48 |
| 1:F:412:UNK:O | 1:F:416:UNK:N | 2.46 | 0.48 |
| 1:F:1305:UNK:O | 1:F:1306:UNK:C | 2.62 | 0.48 |
| 1:Y:1073:UNK:O | 1:Y:1074:UNK:C | 2.61 | 0.48 |
| 1:X:1073:UNK:O | 1:X:1074:UNK:C | 2.61 | 0.48 |
| 1:T:319:UNK:O | 1:T:320:UNK:C | 2.61 | 0.48 |
| 1:F:319:UNK:O | 1:F:320:UNK:C | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:T:1007:UNK:O | 1:T:1009:UNK:N | 2.46 | 0.48 |
| 1:D:913:UNK:C | 1:D:915:UNK:N | 2.75 | 0.48 |
| 1:Y:808:UNK:O | 1:Y:809:UNK:C | 2.62 | 0.48 |
| 1:T:1911:UNK:O | 1:T:1912:UNK:C | 2.59 | 0.48 |
| 1:O:1107:UNK:O | 1:O:1110:UNK:CB | 2.61 | 0.48 |
| 1:X:920:UNK:C | 1:X:922:UNK:N | 2.74 | 0.48 |
| 1:P:1417:UNK:C | 1:P:1419:UNK:H | 2.26 | 0.48 |
| 1:C:1212:UNK:O | 1:C:1216:UNK:N | 2.46 | 0.48 |
| 1:O:1607:UNK:O | 1:O:1611:UNK:N | 2.47 | 0.48 |
| 1:D:807:UNK:O | 1:D:811:UNK:N | 2.46 | 0.48 |
| 1:Q:2411:UNK:C | 1:Q:2413:UNK:N | 2.76 | 0.48 |
| 1:R:1006:UNK:C | 1:R:1008:UNK:N | 2.75 | 0.48 |
| 1:F:1014:UNK:O | 1:F:1016:UNK:N | 2.46 | 0.48 |
| 1:D:719:UNK:O | 1:D:721:UNK:N | 2.47 | 0.48 |
| 1:F:205:UNK:O | 1:F:208:UNK:N | 2.47 | 0.48 |
| 1:T:613:UNK:O | 1:T:615:UNK:N | 2.47 | 0.48 |
| 1:A:1107:UNK:O | 1:A:1110:UNK:CB | 2.61 | 0.48 |
| 1:Q:414:UNK:C | 1:Q:416:UNK:H | 2.21 | 0.48 |
| 1:C:1305:UNK:O | 1:C:1306:UNK:C | 2.62 | 0.48 |
| 1:O:2411:UNK:O | 1:O:2413:UNK:N | 2.46 | 0.48 |
| 1:C:2610:UNK:C | 1:C:2612:UNK:N | 2.77 | 0.48 |
| 1:C:2411:UNK:C | 1:C:2413:UNK:N | 2.76 | 0.48 |
| 1:X:1033:UNK:C | 1:X:1035:UNK:H | 2.26 | 0.48 |
| 1:D:1012:UNK:O | 1:D:1014:UNK:C | 2.58 | 0.48 |
| 1:A:1214:UNK:HA | 1:A:1217:UNK:CB | 2.44 | 0.48 |
| 1:Q:1212:UNK:O | 1:Q:1216:UNK:N | 2.46 | 0.48 |
| 1:O:1414:UNK:O | 1:O:1417:UNK:N | 2.47 | 0.48 |
| 1:F:2512:UNK:C | 1:F:2514:UNK:N | 2.77 | 0.48 |
| 1:P:1007:UNK:C | 1:P:1009:UNK:N | 2.74 | 0.48 |
| 1:Q:2610:UNK:C | 1:Q:2612:UNK:N | 2.77 | 0.48 |
| 1:T:205:UNK:O | 1:T:208:UNK:N | 2.47 | 0.48 |
| 1:Y:1014:UNK:CB | 1:Y:1065:UNK:CB | 2.91 | 0.48 |
| 1:T:108:UNK:C | 1:T:110:UNK:N | 2.68 | 0.48 |
| 1:Y:1033:UNK:C | 1:Y:1035:UNK:H | 2.26 | 0.48 |
| 1:D:1008:UNK:O | 1:D:1009:UNK:C | 2.62 | 0.47 |
| 1:C:414:UNK:C | 1:C:416:UNK:H | 2.21 | 0.47 |
| 1:Y:917:UNK:C | 1:Y:919:UNK:N | 2.69 | 0.47 |
| 1:Q:1808:UNK:O | 1:Q:1809:UNK:C | 2.60 | 0.47 |
| 1:C:610:UNK:C | 1:C:612:UNK:N | 2.75 | 0.47 |
| 1:B:1511:UNK:O | 1:B:1515:UNK:N | 2.47 | 0.47 |
| 1:B:608:UNK:C | 1:B:610:UNK:N | 2.67 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:1808:UNK:O | 1:C:1809:UNK:C | 2.60 | 0.47 |
| 1:O:1406:UNK:HA | 1:O:1409:UNK:CB | 2.43 | 0.47 |
| 1:B:1107:UNK:O | 1:B:1108:UNK:C | 2.62 | 0.47 |
| 1:T:1014:UNK:O | 1:T:1016:UNK:N | 2.46 | 0.47 |
| 1:F:2007:UNK:O | 1:F:2008:UNK:C | 2.62 | 0.47 |
| 1:R:807:UNK:O | 1:R:810:UNK:N | 2.47 | 0.47 |
| 1:Q:712:UNK:C | 1:Q:714:UNK:H | 2.26 | 0.47 |
| 1:R:1008:UNK:O | 1:R:1009:UNK:C | 2.62 | 0.47 |
| 1:S:207:UNK:C | 1:S:209:UNK:N | 2.76 | 0.47 |
| 1:Q:1309:UNK:C | 1:Q:1311:UNK:N | 2.76 | 0.47 |
| 1:R:719:UNK:O | 1:R:721:UNK:N | 2.47 | 0.47 |
| 1:R:310:UNK:O | 1:R:314:UNK:N | 2.47 | 0.47 |
| 1:O:2121:UNK:C | 1:O:2123:UNK:N | 2.72 | 0.47 |
| 1:R:807:UNK:O | 1:R:811:UNK:N | 2.46 | 0.47 |
| 1:P:718:UNK:CB | 1:P:1019:UNK:O | 2.62 | 0.47 |
| 1:C:1706:UNK:C | 1:C:1708:UNK:N | 2.74 | 0.47 |
| 1:T:1424:UNK:C | 1:T:1426:UNK:H | 2.27 | 0.47 |
| 1:F:1424:UNK:C | 1:F:1426:UNK:H | 2.27 | 0.47 |
| 1:T:1312:UNK:C | 1:T:1314:UNK:N | 2.63 | 0.47 |
| 1:A:1414:UNK:O | 1:A:1417:UNK:N | 2.47 | 0.47 |
| 1:C:1320:UNK:C | 1:C:1322:UNK:N | 2.78 | 0.47 |
| 1:X:808:UNK:O | 1:X:809:UNK:C | 2.62 | 0.47 |
| 1:T:1305:UNK:O | 1:T:1306:UNK:C | 2.62 | 0.47 |
| 1:F:317:UNK:O | 1:F:320:UNK:N | 2.47 | 0.47 |
| 1:E:207:UNK:C | 1:E:209:UNK:N | 2.76 | 0.47 |
| 1:P:613:UNK:O | 1:P:617:UNK:CB | 2.63 | 0.47 |
| 1:T:2512:UNK:C | 1:T:2514:UNK:N | 2.77 | 0.47 |
| 1:B:317:UNK:O | 1:B:319:UNK:N | 2.48 | 0.47 |
| 1:P:317:UNK:O | 1:P:319:UNK:N | 2.48 | 0.47 |
| 1:F:607:UNK:O | 1:F:609:UNK:N | 2.48 | 0.47 |
| 1:Q:1910:UNK:C | 1:Q:1912:UNK:N | 2.78 | 0.47 |
| 1:C:1910:UNK:C | 1:C:1912:UNK:N | 2.78 | 0.47 |
| 1:F:613:UNK:O | 1:F:615:UNK:N | 2.47 | 0.47 |
| 1:T:2627:UNK:C | 1:T:2629:UNK:N | 2.75 | 0.47 |
| 1:P:106:UNK:O | 1:P:110:UNK:N | 2.48 | 0.47 |
| 1:F:3106:UNK:C | 1:F:3108:UNK:N | 2.76 | 0.47 |
| 1:T:317:UNK:O | 1:T:320:UNK:N | 2.47 | 0.47 |
| 1:P:1511:UNK:O | 1:P:1515:UNK:N | 2.47 | 0.47 |
| 1:P:310:UNK:O | 1:P:313:UNK:N | 2.48 | 0.47 |
| 1:B:310:UNK:O | 1:B:313:UNK:N | 2.48 | 0.47 |
| 1:T:3106:UNK:C | 1:T:3108:UNK:N | 2.76 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:213:UNK:O | 1:C:214:UNK:C | 2.62 | 0.47 |
| 1:C:1309:UNK:C | 1:C:1311:UNK:N | 2.76 | 0.47 |
| 1:D:807:UNK:O | 1:D:810:UNK:N | 2.47 | 0.47 |
| 1:B:718:UNK:CB | 1:B:1019:UNK:O | 2.62 | 0.47 |
| 1:Y:851:UNK:O | 1:Y:855:UNK:CB | 2.63 | 0.47 |
| 1:B:106:UNK:O | 1:B:110:UNK:N | 2.48 | 0.47 |
| 1:B:613:UNK:O | 1:B:617:UNK:CB | 2.63 | 0.47 |
| 1:C:1115:UNK:C | 1:C:1117:UNK:N | 2.76 | 0.47 |
| 1:O:1605:UNK:O | 1:O:1609:UNK:CB | 2.63 | 0.47 |
| 1:T:2609:UNK:C | 1:T:2611:UNK:N | 2.78 | 0.47 |
| 1:P:1613:UNK:C | 1:P:1615:UNK:N | 2.78 | 0.46 |
| 1:D:717:UNK:O | 1:D:721:UNK:N | 2.48 | 0.46 |
| 1:T:3208:UNK:O | 1:T:3212:UNK:N | 2.48 | 0.46 |
| 1:T:2007:UNK:O | 1:T:2008:UNK:C | 2.62 | 0.46 |
| 1:T:2319:UNK:C | 1:T:2321:UNK:N | 2.78 | 0.46 |
| 1:A:2013:UNK:O | 1:A:2014:UNK:C | 2.61 | 0.46 |
| 1:F:2319:UNK:C | 1:F:2321:UNK:N | 2.78 | 0.46 |
| 1:O:1214:UNK:HA | 1:O:1217:UNK:CB | 2.44 | 0.46 |
| 1:P:1107:UNK:O | 1:P:1108:UNK:C | 2.62 | 0.46 |
| 1:B:611:UNK:C | 1:B:613:UNK:N | 2.79 | 0.46 |
| 1:R:610:UNK:O | 1:R:613:UNK:N | 2.48 | 0.46 |
| 1:B:106:UNK:O | 1:B:109:UNK:N | 2.48 | 0.46 |
| 1:Q:1115:UNK:C | 1:Q:1117:UNK:N | 2.76 | 0.46 |
| 1:P:115:UNK:O | 1:P:119:UNK:N | 2.48 | 0.46 |
| 1:F:3208:UNK:O | 1:F:3212:UNK:N | 2.48 | 0.46 |
| 1:C:1817:UNK:O | 1:C:1820:UNK:CB | 2.64 | 0.46 |
| 1:P:106:UNK:O | 1:P:109:UNK:N | 2.48 | 0.46 |
| 1:T:2814:UNK:O | 1:T:2815:UNK:C | 2.64 | 0.46 |
| 1:B:127:UNK:CB | 1:B:1019:UNK:CB | 2.93 | 0.46 |
| 1:P:411:UNK:O | 1:P:412:UNK:C | 2.63 | 0.46 |
| 1:R:512:UNK:O | 1:R:515:UNK:CB | 2.64 | 0.46 |
| 1:Q:1320:UNK:C | 1:Q:1322:UNK:N | 2.78 | 0.46 |
| 1:D:615:UNK:C | 1:D:617:UNK:N | 2.76 | 0.46 |
| 1:R:717:UNK:O | 1:R:721:UNK:N | 2.48 | 0.46 |
| 1:B:1608:UNK:C | 1:B:1610:UNK:N | 2.79 | 0.46 |
| 1:P:127:UNK:CB | 1:P:1019:UNK:CB | 2.93 | 0.46 |
| 1:P:1018:UNK:C | 1:P:1020:UNK:N | 2.71 | 0.46 |
| 1:B:1708:UNK:O | 1:B:1711:UNK:N | 2.48 | 0.46 |
| 1:B:605:UNK:HA | 1:B:608:UNK:CB | 2.46 | 0.46 |
| 1:X:806:UNK:O | 1:X:808:UNK:N | 2.48 | 0.46 |
| 1:X:851:UNK:O | 1:X:855:UNK:CB | 2.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:2411:UNK:O | 1:C:2414:UNK:N | 2.49 | 0.46 |
| 1:A:1605:UNK:O | 1:A:1609:UNK:CB | 2.63 | 0.46 |
| 1:B:411:UNK:O | 1:B:412:UNK:C | 2.63 | 0.46 |
| 1:X:838:UNK:CB | 1:X:871:UNK:HA | 2.46 | 0.46 |
| 1:P:1708:UNK:O | 1:P:1711:UNK:N | 2.48 | 0.46 |
| 1:T:2620:UNK:O | 1:T:2623:UNK:CA | 2.63 | 0.46 |
| 1:T:2620:UNK:O | 1:T:2623:UNK:CB | 2.64 | 0.46 |
| 1:D:610:UNK:O | 1:D:613:UNK:N | 2.49 | 0.46 |
| 1:D:611:UNK:O | 1:D:615:UNK:CB | 2.64 | 0.46 |
| 1:T:607:UNK:O | 1:T:609:UNK:N | 2.48 | 0.46 |
| 1:S:106:UNK:O | 1:S:108:UNK:N | 2.49 | 0.46 |
| 1:R:107:UNK:O | 1:R:108:UNK:O | 2.34 | 0.46 |
| 1:P:611:UNK:C | 1:P:613:UNK:N | 2.79 | 0.46 |
| 1:P:605:UNK:HA | 1:P:608:UNK:CB | 2.46 | 0.46 |
| 1:R:611:UNK:O | 1:R:615:UNK:CB | 2.64 | 0.46 |
| 1:T:1908:UNK:O | 1:T:1912:UNK:N | 2.49 | 0.46 |
| 1:R:315:UNK:C | 1:R:317:UNK:N | 2.78 | 0.46 |
| 1:Q:2411:UNK:O | 1:Q:2414:UNK:N | 2.49 | 0.46 |
| 1:D:512:UNK:O | 1:D:515:UNK:CB | 2.64 | 0.46 |
| 1:Y:920:UNK:O | 1:Y:923:UNK:CB | 2.64 | 0.46 |
| 1:F:2620:UNK:O | 1:F:2623:UNK:CA | 2.63 | 0.46 |
| 1:B:1613:UNK:C | 1:B:1615:UNK:N | 2.78 | 0.46 |
| 1:B:115:UNK:O | 1:B:119:UNK:N | 2.48 | 0.46 |
| 1:X:847:UNK:C | 1:X:849:UNK:N | 2.75 | 0.46 |
| 1:F:2814:UNK:O | 1:F:2815:UNK:C | 2.64 | 0.45 |
| 1:D:1216:UNK:C | 1:D:1218:UNK:H | 2.27 | 0.45 |
| 1:F:1908:UNK:O | 1:F:1912:UNK:N | 2.49 | 0.45 |
| 1:P:311:UNK:O | 1:P:315:UNK:N | 2.49 | 0.45 |
| 1:Q:1214:UNK:O | 1:Q:1217:UNK:N | 2.49 | 0.45 |
| 1:D:107:UNK:O | 1:D:108:UNK:O | 2.34 | 0.45 |
| 1:F:913:UNK:O | 1:F:916:UNK:N | 2.50 | 0.45 |
| 1:R:615:UNK:C | 1:R:617:UNK:N | 2.76 | 0.45 |
| 1:Q:606:UNK:O | 1:Q:610:UNK:N | 2.49 | 0.45 |
| 1:Y:838:UNK:CB | 1:Y:871:UNK:HA | 2.46 | 0.45 |
| 1:B:414:UNK:O | 1:B:415:UNK:C | 2.64 | 0.45 |
| 1:A:1814:UNK:HA | 1:A:1817:UNK:CB | 2.46 | 0.45 |
| 1:Q:1817:UNK:O | 1:Q:1820:UNK:CB | 2.64 | 0.45 |
| 1:C:606:UNK:O | 1:C:610:UNK:N | 2.49 | 0.45 |
| 1:C:205:UNK:C | 1:C:207:UNK:N | 2.78 | 0.45 |
| 1:Q:213:UNK:O | 1:Q:214:UNK:C | 2.62 | 0.45 |
| 1:P:216:UNK:C | 1:P:218:UNK:N | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:1514:UNK:O | 1:A:1515:UNK:C | 2.59 | 0.45 |
| 1:Q:1417:UNK:C | 1:Q:1419:UNK:H | 2.30 | 0.45 |
| 1:X:920:UNK:O | 1:X:923:UNK:CB | 2.64 | 0.45 |
| 1:F:3414:UNK:O | 1:F:3415:UNK:C | 2.64 | 0.45 |
| 1:P:115:UNK:O | 1:P:118:UNK:N | 2.50 | 0.45 |
| 1:F:3510:UNK:O | 1:F:3513:UNK:N | 2.50 | 0.45 |
| 1:F:2609:UNK:C | 1:F:2611:UNK:N | 2.78 | 0.45 |
| 1:A:2609:UNK:C | 1:A:2611:UNK:N | 2.80 | 0.45 |
| 1:C:1214:UNK:O | 1:C:1217:UNK:N | 2.49 | 0.45 |
| 1:D:308:UNK:O | 1:D:311:UNK:N | 2.49 | 0.45 |
| 1:T:2213:UNK:HA | 1:T:2216:UNK:CB | 2.47 | 0.45 |
| 1:R:308:UNK:O | 1:R:311:UNK:N | 2.49 | 0.45 |
| 1:Q:1305:UNK:O | 1:Q:1306:UNK:C | 2.62 | 0.45 |
| 1:R:1216:UNK:C | 1:R:1218:UNK:H | 2.27 | 0.45 |
| 1:O:1814:UNK:HA | 1:O:1817:UNK:CB | 2.46 | 0.45 |
| 1:F:209:UNK:O | 1:F:210:UNK:C | 2.65 | 0.45 |
| 1:S:307:UNK:O | 1:S:310:UNK:N | 2.50 | 0.45 |
| 1:C:116:UNK:HA | 1:C:119:UNK:CB | 2.47 | 0.45 |
| 1:P:414:UNK:O | 1:P:415:UNK:C | 2.64 | 0.45 |
| 1:F:1007:UNK:O | 1:F:1008:UNK:C | 2.65 | 0.45 |
| 1:X:811:UNK:N | 1:X:832:UNK:O | 2.50 | 0.45 |
| 1:T:2605:UNK:O | 1:T:2607:UNK:N | 2.50 | 0.45 |
| 1:B:1612:UNK:O | 1:B:1613:UNK:C | 2.62 | 0.45 |
| 1:T:1417:UNK:C | 1:T:1419:UNK:N | 2.79 | 0.45 |
| 1:E:313:UNK:C | 1:E:315:UNK:N | 2.65 | 0.45 |
| 1:C:1408:UNK:C | 1:C:1410:UNK:N | 2.64 | 0.45 |
| 1:T:1007:UNK:O | 1:T:1008:UNK:C | 2.65 | 0.45 |
| 1:F:2620:UNK:O | 1:F:2623:UNK:CB | 2.64 | 0.45 |
| 1:T:913:UNK:O | 1:T:916:UNK:N | 2.50 | 0.45 |
| 1:T:515:UNK:O | 1:T:605:UNK:N | 2.50 | 0.45 |
| 1:B:1608:UNK:O | 1:B:1610:UNK:N | 2.50 | 0.45 |
| 1:T:3510:UNK:O | 1:T:3513:UNK:N | 2.50 | 0.45 |
| 1:Y:811:UNK:N | 1:Y:832:UNK:O | 2.50 | 0.45 |
| 1:P:1708:UNK:C | 1:P:1710:UNK:N | 2.80 | 0.45 |
| 1:X:872:UNK:CB | 1:X:876:UNK:O | 2.65 | 0.45 |
| 1:C:1417:UNK:C | 1:C:1419:UNK:H | 2.29 | 0.45 |
| 1:C:1907:UNK:C | 1:C:1909:UNK:N | 2.77 | 0.45 |
| 1:Q:1007:UNK:C | 1:Q:1009:UNK:N | 2.80 | 0.45 |
| 1:T:209:UNK:O | 1:T:210:UNK:C | 2.65 | 0.45 |
| 1:B:311:UNK:O | 1:B:315:UNK:N | 2.49 | 0.44 |
| 1:A:2307:UNK:O | 1:A:2309:UNK:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Q:2520:UNK:O | 1:Q:2521:UNK:O | 2.35 | 0.44 |
| 1:B:216:UNK:C | 1:B:218:UNK:N | 2.79 | 0.44 |
| 1:T:415:UNK:C | 1:T:417:UNK:N | 2.80 | 0.44 |
| 1:F:2213:UNK:HA | 1:F:2216:UNK:CB | 2.46 | 0.44 |
| 1:P:1612:UNK:O | 1:P:1613:UNK:C | 2.62 | 0.44 |
| 1:P:1213:UNK:C | 1:P:1215:UNK:N | 2.78 | 0.44 |
| 1:C:507:UNK:C | 1:C:509:UNK:N | 2.80 | 0.44 |
| 1:Q:1708:UNK:O | 1:Q:1709:UNK:C | 2.65 | 0.44 |
| 1:C:123:UNK:O | 1:C:124:UNK:C | 2.66 | 0.44 |
| 1:E:106:UNK:O | 1:E:108:UNK:N | 2.49 | 0.44 |
| 1:O:2606:UNK:C | 1:O:2608:UNK:N | 2.67 | 0.44 |
| 1:B:1708:UNK:C | 1:B:1710:UNK:N | 2.80 | 0.44 |
| 1:T:3207:UNK:HA | 1:T:3316:UNK:CB | 2.47 | 0.44 |
| 1:S:112:UNK:C | 1:S:114:UNK:N | 2.76 | 0.44 |
| 1:X:829:UNK:O | 1:X:880:UNK:HA | 2.17 | 0.44 |
| 1:Q:1910:UNK:O | 1:Q:1914:UNK:N | 2.51 | 0.44 |
| 1:F:2605:UNK:O | 1:F:2607:UNK:N | 2.50 | 0.44 |
| 1:C:1007:UNK:C | 1:C:1009:UNK:N | 2.80 | 0.44 |
| 1:Q:116:UNK:HA | 1:Q:119:UNK:CB | 2.47 | 0.44 |
| 1:O:2307:UNK:O | 1:O:2309:UNK:N | 2.51 | 0.44 |
| 1:E:307:UNK:O | 1:E:310:UNK:N | 2.50 | 0.44 |
| 1:O:2315:UNK:C | 1:O:2317:UNK:N | 2.79 | 0.44 |
| 1:O:2013:UNK:O | 1:O:2014:UNK:C | 2.61 | 0.44 |
| 1:O:1305:UNK:C | 1:O:1307:UNK:N | 2.80 | 0.44 |
| 1:X:1014:UNK:HA | 1:X:1017:UNK:CB | 2.48 | 0.44 |
| 1:F:2609:UNK:O | 1:F:2612:UNK:N | 2.51 | 0.44 |
| 1:T:910:UNK:C | 1:T:912:UNK:N | 2.79 | 0.44 |
| 1:F:415:UNK:C | 1:F:417:UNK:N | 2.80 | 0.44 |
| 1:F:320:UNK:O | 1:F:323:UNK:N | 2.51 | 0.44 |
| 1:Y:872:UNK:CB | 1:Y:876:UNK:O | 2.66 | 0.44 |
| 1:P:1113:UNK:O | 1:P:1116:UNK:N | 2.51 | 0.44 |
| 1:A:1315:UNK:O | 1:A:1318:UNK:CB | 2.66 | 0.44 |
| 1:B:115:UNK:O | 1:B:118:UNK:N | 2.50 | 0.44 |
| 1:O:2115:UNK:O | 1:O:2118:UNK:N | 2.51 | 0.44 |
| 1:P:1608:UNK:O | 1:P:1610:UNK:N | 2.50 | 0.44 |
| 1:D:206:UNK:O | 1:D:208:UNK:N | 2.51 | 0.44 |
| 1:T:2609:UNK:O | 1:T:2612:UNK:N | 2.51 | 0.44 |
| 1:B:206:UNK:O | 1:B:209:UNK:N | 2.51 | 0.44 |
| 1:F:3207:UNK:HA | 1:F:3316:UNK:CB | 2.47 | 0.44 |
| 1:E:309:UNK:C | 1:E:311:UNK:N | 2.81 | 0.44 |
| 1:C:1708:UNK:O | 1:C:1709:UNK:C | 2.65 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:1910:UNK:O | 1:C:1914:UNK:N | 2.51 | 0.44 |
| 1:D:306:UNK:O | 1:D:309:UNK:CB | 2.66 | 0.44 |
| 1:X:922:UNK:O | 1:X:926:UNK:N | 2.51 | 0.44 |
| 1:F:515:UNK:O | 1:F:605:UNK:N | 2.50 | 0.44 |
| 1:Q:1907:UNK:C | 1:Q:1909:UNK:N | 2.77 | 0.44 |
| 1:T:1521:UNK:C | 1:T:1523:UNK:N | 2.81 | 0.44 |
| 1:R:206:UNK:O | 1:R:208:UNK:N | 2.51 | 0.44 |
| 1:Q:1505:UNK:C | 1:Q:1507:UNK:N | 2.81 | 0.44 |
| 1:Y:1014:UNK:HA | 1:Y:1017:UNK:CB | 2.48 | 0.44 |
| 1:Q:1115:UNK:O | 1:Q:1118:UNK:N | 2.51 | 0.44 |
| 1:F:910:UNK:C | 1:F:912:UNK:N | 2.79 | 0.44 |
| 1:F:2810:UNK:C | 1:F:2812:UNK:H | 2.31 | 0.44 |
| 1:O:2609:UNK:C | 1:O:2611:UNK:N | 2.80 | 0.44 |
| 1:A:2115:UNK:O | 1:A:2118:UNK:N | 2.51 | 0.44 |
| 1:O:2013:UNK:N | 1:O:2015:UNK:O | 2.51 | 0.44 |
| 1:B:818:UNK:O | 1:B:821:UNK:N | 2.51 | 0.44 |
| 1:Q:507:UNK:C | 1:Q:509:UNK:N | 2.80 | 0.44 |
| 1:C:1505:UNK:C | 1:C:1507:UNK:N | 2.81 | 0.44 |
| 1:Q:1922:UNK:O | 1:Q:1924:UNK:N | 2.51 | 0.44 |
| 1:Y:802:UNK:O | 1:Y:811:UNK:HA | 2.18 | 0.44 |
| 1:O:1315:UNK:O | 1:O:1318:UNK:CB | 2.66 | 0.43 |
| 1:B:813:UNK:HA | 1:B:816:UNK:CB | 2.48 | 0.43 |
| 1:D:917:UNK:C | 1:D:919:UNK:H | 2.31 | 0.43 |
| 1:C:509:UNK:O | 1:C:510:UNK:C | 2.66 | 0.43 |
| 1:Y:829:UNK:O | 1:Y:880:UNK:HA | 2.17 | 0.43 |
| 1:X:802:UNK:O | 1:X:812:UNK:N | 2.51 | 0.43 |
| 1:C:2520:UNK:O | 1:C:2521:UNK:O | 2.36 | 0.43 |
| 1:Y:1043:UNK:O | 1:Y:1044:UNK:CB | 2.65 | 0.43 |
| 1:D:616:UNK:O | 1:D:619:UNK:C | 2.66 | 0.43 |
| 1:O:1421:UNK:C | 1:O:1423:UNK:N | 2.68 | 0.43 |
| 1:T:507:UNK:HA | 1:T:510:UNK:CB | 2.48 | 0.43 |
| 1:T:1208:UNK:C | 1:T:1210:UNK:N | 2.81 | 0.43 |
| 1:Q:2410:UNK:C | 1:Q:2412:UNK:N | 2.81 | 0.43 |
| 1:Y:856:UNK:C | 1:Y:858:UNK:H | 2.31 | 0.43 |
| 1:X:1043:UNK:O | 1:X:1044:UNK:CB | 2.65 | 0.43 |
| 1:C:117:UNK:O | 1:C:118:UNK:C | 2.67 | 0.43 |
| 1:B:1113:UNK:O | 1:B:1116:UNK:N | 2.51 | 0.43 |
| 1:Q:117:UNK:O | 1:Q:118:UNK:C | 2.67 | 0.43 |
| 1:Y:922:UNK:O | 1:Y:926:UNK:N | 2.51 | 0.43 |
| 1:P:206:UNK:O | 1:P:209:UNK:N | 2.51 | 0.43 |
| 1:F:1521:UNK:C | 1:F:1523:UNK:N | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:P:818:UNK:O | 1:P:821:UNK:N | 2.51 | 0.43 |
| 1:X:856:UNK:C | 1:X:858:UNK:H | 2.31 | 0.43 |
| 1:D:308:UNK:C | 1:D:310:UNK:N | 2.81 | 0.43 |
| 1:R:306:UNK:O | 1:R:309:UNK:CB | 2.66 | 0.43 |
| 1:B:1307:UNK:C | 1:B:1309:UNK:N | 2.82 | 0.43 |
| 1:O:2110:UNK:O | 1:O:2113:UNK:CA | 2.67 | 0.43 |
| 1:A:2013:UNK:N | 1:A:2015:UNK:O | 2.51 | 0.43 |
| 1:X:802:UNK:O | 1:X:811:UNK:HA | 2.18 | 0.43 |
| 1:O:2313:UNK:CB | 1:T:1414:UNK:CB | 2.97 | 0.43 |
| 1:O:2612:UNK:O | 1:O:2614:UNK:N | 2.51 | 0.43 |
| 1:T:320:UNK:O | 1:T:323:UNK:N | 2.51 | 0.43 |
| 1:R:715:UNK:C | 1:R:718:UNK:N | 2.82 | 0.43 |
| 1:D:315:UNK:C | 1:D:317:UNK:N | 2.78 | 0.43 |
| 1:C:2410:UNK:C | 1:C:2412:UNK:N | 2.81 | 0.43 |
| 1:Q:509:UNK:O | 1:Q:510:UNK:C | 2.66 | 0.43 |
| 1:R:616:UNK:O | 1:R:619:UNK:C | 2.66 | 0.43 |
| 1:O:1209:UNK:C | 1:O:1211:UNK:N | 2.80 | 0.43 |
| 1:Q:1305:UNK:C | 1:Q:1307:UNK:N | 2.81 | 0.43 |
| 1:Q:1305:UNK:O | 1:Q:1308:UNK:N | 2.52 | 0.43 |
| 1:C:1922:UNK:O | 1:C:1924:UNK:N | 2.51 | 0.43 |
| 1:Y:802:UNK:O | 1:Y:812:UNK:N | 2.51 | 0.43 |
| 1:B:1619:UNK:C | 1:B:1621:UNK:H | 2.31 | 0.43 |
| 1:C:1206:UNK:C | 1:C:1208:UNK:N | 2.81 | 0.43 |
| 1:P:1117:UNK:C | 1:P:1118:UNK:O | 2.67 | 0.43 |
| 1:Q:909:UNK:C | 1:Q:911:UNK:N | 2.82 | 0.43 |
| 1:R:509:UNK:O | 1:R:511:UNK:N | 2.30 | 0.43 |
| 1:O:1414:UNK:C | 1:O:1416:UNK:N | 2.82 | 0.43 |
| 1:P:207:UNK:O | 1:P:208:UNK:C | 2.67 | 0.43 |
| 1:B:1007:UNK:O | 1:B:1010:UNK:N | 2.52 | 0.43 |
| 1:C:1115:UNK:O | 1:C:1118:UNK:N | 2.51 | 0.43 |
| 1:Q:123:UNK:O | 1:Q:124:UNK:C | 2.66 | 0.43 |
| 1:O:1616:UNK:O | 1:O:1617:UNK:C | 2.67 | 0.43 |
| 1:A:2612:UNK:O | 1:A:2614:UNK:N | 2.51 | 0.43 |
| 1:P:218:UNK:C | 1:P:220:UNK:N | 2.78 | 0.43 |
| 1:F:507:UNK:HA | 1:F:510:UNK:CB | 2.48 | 0.43 |
| 1:F:1208:UNK:C | 1:F:1210:UNK:N | 2.81 | 0.43 |
| 1:C:1511:UNK:O | 1:C:1514:UNK:N | 2.52 | 0.43 |
| 1:F:3514:UNK:O | 1:F:3516:UNK:N | 2.51 | 0.43 |
| 1:T:2106:UNK:O | 1:T:2107:UNK:CB | 2.66 | 0.43 |
| 1:B:1117:UNK:C | 1:B:1118:UNK:O | 2.67 | 0.43 |
| 1:F:2221:UNK:C | 1:F:2223:UNK:N | 2.80 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:D:718:UNK:O | 1:D:721:UNK:CB | 2.67 | 0.43 |
| 1:R:719:UNK:O | 1:R:723:UNK:N | 2.52 | 0.43 |
| 1:B:711:UNK:C | 1:B:713:UNK:N | 2.75 | 0.43 |
| 1:P:1619:UNK:C | 1:P:1621:UNK:H | 2.31 | 0.43 |
| 1:Q:1206:UNK:C | 1:Q:1208:UNK:N | 2.81 | 0.43 |
| 1:Y:838:UNK:CB | 1:Y:871:UNK:CA | 2.97 | 0.43 |
| 1:T:418:UNK:HA | 1:T:421:UNK:CB | 2.49 | 0.43 |
| 1:F:317:UNK:C | 1:F:319:UNK:N | 2.66 | 0.43 |
| 1:C:1305:UNK:C | 1:C:1307:UNK:N | 2.81 | 0.43 |
| 1:R:605:UNK:C | 1:R:606:UNK:O | 2.66 | 0.43 |
| 1:D:715:UNK:C | 1:D:718:UNK:N | 2.82 | 0.43 |
| 1:X:1030:UNK:O | 1:X:1032:UNK:N | 2.52 | 0.43 |
| 1:F:117:UNK:HA | 1:F:120:UNK:CB | 2.49 | 0.43 |
| 1:Y:804:UNK:N | 1:Y:810:UNK:O | 2.52 | 0.43 |
| 1:C:205:UNK:O | 1:C:209:UNK:N | 2.52 | 0.43 |
| 1:T:2810:UNK:C | 1:T:2812:UNK:H | 2.31 | 0.43 |
| 1:B:207:UNK:O | 1:B:208:UNK:C | 2.67 | 0.42 |
| 1:P:1315:UNK:C | 1:P:1317:UNK:N | 2.82 | 0.42 |
| 1:R:216:UNK:O | 1:R:217:UNK:C | 2.67 | 0.42 |
| 1:C:909:UNK:C | 1:C:911:UNK:N | 2.82 | 0.42 |
| 1:P:1307:UNK:C | 1:P:1309:UNK:N | 2.82 | 0.42 |
| 1:P:1515:UNK:O | 1:P:1517:UNK:C | 2.67 | 0.42 |
| 1:Q:1309:UNK:O | 1:Q:1312:UNK:CB | 2.67 | 0.42 |
| 1:P:813:UNK:HA | 1:P:816:UNK:CB | 2.49 | 0.42 |
| 1:C:106:UNK:O | 1:C:108:UNK:N | 2.53 | 0.42 |
| 1:R:718:UNK:O | 1:R:721:UNK:CB | 2.67 | 0.42 |
| 1:S:309:UNK:C | 1:S:311:UNK:N | 2.81 | 0.42 |
| 1:X:804:UNK:N | 1:X:810:UNK:O | 2.52 | 0.42 |
| 1:B:1406:UNK:O | 1:B:1407:UNK:CB | 2.67 | 0.42 |
| 1:T:3514:UNK:O | 1:T:3516:UNK:N | 2.51 | 0.42 |
| 1:F:1405:UNK:C | 1:F:1407:UNK:H | 2.32 | 0.42 |
| 1:P:214:UNK:O | 1:P:216:UNK:C | 2.68 | 0.42 |
| 1:D:1006:UNK:C | 1:D:1008:UNK:N | 2.75 | 0.42 |
| 1:C:807:UNK:O | 1:C:810:UNK:N | 2.52 | 0.42 |
| 1:C:1412:UNK:C | 1:C:1414:UNK:N | 2.62 | 0.42 |
| 1:O:1414:UNK:O | 1:O:1416:UNK:N | 2.52 | 0.42 |
| 1:T:125:UNK:C | 1:T:127:UNK:N | 2.82 | 0.42 |
| 1:P:1007:UNK:O | 1:P:1010:UNK:N | 2.52 | 0.42 |
| 1:F:613:UNK:C | 1:F:615:UNK:N | 2.83 | 0.42 |
| 1:D:216:UNK:O | 1:D:217:UNK:C | 2.67 | 0.42 |
| 1:Q:205:UNK:C | 1:Q:207:UNK:N | 2.78 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:P:1406:UNK:O | 1:P:1407:UNK:CB | 2.67 | 0.42 |
| 1:F:418:UNK:HA | 1:F:421:UNK:CB | 2.49 | 0.42 |
| 1:C:1309:UNK:O | 1:C:1312:UNK:CB | 2.67 | 0.42 |
| 1:A:2110:UNK:O | 1:A:2113:UNK:CA | 2.67 | 0.42 |
| 1:A:1414:UNK:O | 1:A:1416:UNK:N | 2.52 | 0.42 |
| 1:Q:2205:UNK:C | 1:Q:2207:UNK:N | 2.83 | 0.42 |
| 1:D:811:UNK:O | 1:D:812:UNK:C | 2.68 | 0.42 |
| 1:F:2106:UNK:O | 1:F:2107:UNK:CB | 2.66 | 0.42 |
| 1:R:308:UNK:C | 1:R:310:UNK:N | 2.81 | 0.42 |
| 1:Q:106:UNK:O | 1:Q:108:UNK:N | 2.52 | 0.42 |
| 1:Q:109:UNK:O | 1:Q:112:UNK:CB | 2.67 | 0.42 |
| 1:P:1317:UNK:O | 1:P:1318:UNK:C | 2.68 | 0.42 |
| 1:A:2306:UNK:O | 1:A:2307:UNK:C | 2.62 | 0.42 |
| 1:A:1005:UNK:C | 1:A:1007:UNK:N | 2.83 | 0.42 |
| 1:Q:909:UNK:O | 1:Q:911:UNK:N | 2.53 | 0.42 |
| 1:O:2506:UNK:C | 1:O:2508:UNK:N | 2.82 | 0.42 |
| 1:A:2506:UNK:C | 1:A:2508:UNK:N | 2.82 | 0.42 |
| 1:B:1515:UNK:O | 1:B:1517:UNK:C | 2.67 | 0.42 |
| 1:T:812:UNK:HA | 1:T:815:UNK:CB | 2.50 | 0.42 |
| 1:F:1521:UNK:O | 1:F:1524:UNK:N | 2.53 | 0.42 |
| 1:T:1521:UNK:O | 1:T:1524:UNK:N | 2.53 | 0.42 |
| 1:Q:1511:UNK:O | 1:Q:1514:UNK:N | 2.52 | 0.42 |
| 1:Q:205:UNK:O | 1:Q:209:UNK:N | 2.52 | 0.42 |
| 1:T:1430:UNK:O | 1:T:1431:UNK:C | 2.67 | 0.42 |
| 1:O:1005:UNK:O | 1:O:1007:UNK:N | 2.53 | 0.42 |
| 1:B:214:UNK:O | 1:B:216:UNK:C | 2.68 | 0.42 |
| 1:T:317:UNK:C | 1:T:319:UNK:N | 2.66 | 0.42 |
| 1:F:812:UNK:HA | 1:F:815:UNK:CB | 2.50 | 0.42 |
| 1:F:810:UNK:C | 1:F:812:UNK:N | 2.82 | 0.42 |
| 1:R:917:UNK:C | 1:R:919:UNK:H | 2.31 | 0.42 |
| 1:C:109:UNK:O | 1:C:112:UNK:CB | 2.67 | 0.42 |
| 1:T:117:UNK:HA | 1:T:120:UNK:CB | 2.49 | 0.42 |
| 1:B:317:UNK:O | 1:B:318:UNK:C | 2.68 | 0.42 |
| 1:Y:811:UNK:O | 1:Y:813:UNK:N | 2.53 | 0.42 |
| 1:F:1430:UNK:O | 1:F:1431:UNK:C | 2.67 | 0.42 |
| 1:A:1616:UNK:O | 1:A:1617:UNK:C | 2.67 | 0.42 |
| 1:D:410:UNK:O | 1:D:413:UNK:N | 2.53 | 0.42 |
| 1:D:412:UNK:O | 1:D:413:UNK:C | 2.67 | 0.42 |
| 1:R:410:UNK:O | 1:R:413:UNK:N | 2.53 | 0.42 |
| 1:P:1715:UNK:O | 1:P:1716:UNK:O | 2.38 | 0.42 |
| 1:A:1209:UNK:C | 1:A:1211:UNK:N | 2.80 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:C:1305:UNK:O | 1:C:1308:UNK:N | 2.52 | 0.42 |
| 1:R:908:UNK:C | 1:R:910:UNK:N | 2.82 | 0.42 |
| 1:P:1311:UNK:HA | 1:P:1314:UNK:CB | 2.50 | 0.42 |
| 1:Y:917:UNK:O | 1:Y:918:UNK:C | 2.67 | 0.42 |
| 1:T:1517:UNK:O | 1:T:1518:UNK:C | 2.68 | 0.42 |
| 1:A:1005:UNK:O | 1:A:1007:UNK:N | 2.53 | 0.42 |
| 1:R:412:UNK:O | 1:R:413:UNK:C | 2.67 | 0.42 |
| 1:F:2507:UNK:O | 1:F:2511:UNK:CB | 2.68 | 0.42 |
| 1:X:838:UNK:CB | 1:X:871:UNK:CA | 2.97 | 0.42 |
| 1:C:613:UNK:O | 1:C:616:UNK:N | 2.53 | 0.42 |
| 1:Q:1415:UNK:O | 1:Q:1418:UNK:CB | 2.68 | 0.42 |
| 1:A:1415:UNK:HA | 1:A:1418:UNK:CB | 2.49 | 0.42 |
| 1:D:719:UNK:O | 1:D:723:UNK:N | 2.52 | 0.42 |
| 1:B:1315:UNK:C | 1:B:1317:UNK:N | 2.82 | 0.42 |
| 1:Y:1030:UNK:O | 1:Y:1032:UNK:N | 2.52 | 0.42 |
| 1:P:514:UNK:O | 1:P:515:UNK:C | 2.68 | 0.42 |
| 1:X:811:UNK:O | 1:X:813:UNK:N | 2.53 | 0.42 |
| 1:T:613:UNK:C | 1:T:615:UNK:N | 2.83 | 0.42 |
| 1:Y:1013:UNK:O | 1:Y:1017:UNK:CB | 2.68 | 0.42 |
| 1:T:1405:UNK:C | 1:T:1407:UNK:H | 2.33 | 0.42 |
| 1:T:410:UNK:O | 1:T:413:UNK:N | 2.53 | 0.42 |
| 1:P:811:UNK:C | 1:P:813:UNK:N | 2.82 | 0.42 |
| 1:D:908:UNK:C | 1:D:910:UNK:N | 2.82 | 0.42 |
| 1:B:1311:UNK:HA | 1:B:1314:UNK:CB | 2.50 | 0.42 |
| 1:B:1317:UNK:O | 1:B:1318:UNK:C | 2.68 | 0.42 |
| 1:T:1507:UNK:O | 1:T:1511:UNK:N | 2.53 | 0.42 |
| 1:F:1507:UNK:O | 1:F:1511:UNK:N | 2.53 | 0.42 |
| 1:A:1108:UNK:O | 1:A:1109:UNK:C | 2.66 | 0.42 |
| 1:B:1712:UNK:O | 1:B:1715:UNK:CB | 2.68 | 0.41 |
| 1:Q:1412:UNK:C | 1:Q:1414:UNK:N | 2.62 | 0.41 |
| 1:A:1414:UNK:C | 1:A:1416:UNK:N | 2.82 | 0.41 |
| 1:F:125:UNK:C | 1:F:127:UNK:N | 2.82 | 0.41 |
| 1:R:706:UNK:C | 1:R:708:UNK:N | 2.83 | 0.41 |
| 1:A:1521:UNK:C | 1:A:1523:UNK:N | 2.83 | 0.41 |
| 1:F:2809:UNK:O | 1:F:2813:UNK:N | 2.53 | 0.41 |
| 1:Q:613:UNK:O | 1:Q:616:UNK:N | 2.53 | 0.41 |
| 1:O:1005:UNK:C | 1:O:1007:UNK:N | 2.83 | 0.41 |
| 1:F:817:UNK:O | 1:F:818:UNK:C | 2.68 | 0.41 |
| 1:B:520:UNK:C | 1:B:522:UNK:N | 2.83 | 0.41 |
| 1:P:1412:UNK:HA | 1:P:1415:UNK:CA | 2.44 | 0.41 |
| 1:P:1712:UNK:O | 1:P:1715:UNK:CB | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:Q:1214:UNK:O | 1:Q:1216:UNK:N | 2.53 | 0.41 |
| 1:Q:807:UNK:O | 1:Q:810:UNK:N | 2.52 | 0.41 |
| 1:C:1415:UNK:O | 1:C:1418:UNK:CB | 2.68 | 0.41 |
| 1:O:1415:UNK:HA | 1:O:1418:UNK:CB | 2.49 | 0.41 |
| 1:B:514:UNK:O | 1:B:515:UNK:C | 2.68 | 0.41 |
| 1:B:514:UNK:O | 1:B:517:UNK:CB | 2.69 | 0.41 |
| 1:X:1013:UNK:O | 1:X:1017:UNK:CB | 2.68 | 0.41 |
| 1:T:2809:UNK:O | 1:T:2813:UNK:N | 2.53 | 0.41 |
| 1:R:1109:UNK:C | 1:R:1111:UNK:N | 2.67 | 0.41 |
| 1:A:1312:UNK:O | 1:A:1315:UNK:N | 2.54 | 0.41 |
| 1:T:2618:UNK:C | 1:T:2620:UNK:N | 2.83 | 0.41 |
| 1:T:1911:UNK:C | 1:T:1913:UNK:N | 2.83 | 0.41 |
| 1:F:1417:UNK:C | 1:F:1419:UNK:N | 2.79 | 0.41 |
| 1:R:811:UNK:O | 1:R:812:UNK:C | 2.68 | 0.41 |
| 1:A:1305:UNK:C | 1:A:1307:UNK:N | 2.80 | 0.41 |
| 1:C:507:UNK:O | 1:C:509:UNK:N | 2.54 | 0.41 |
| 1:Y:908:UNK:C | 1:Y:910:UNK:N | 2.83 | 0.41 |
| 1:Y:1033:UNK:O | 1:Y:1037:UNK:N | 2.54 | 0.41 |
| 1:Q:1115:UNK:O | 1:Q:1117:UNK:N | 2.54 | 0.41 |
| 1:T:209:UNK:O | 1:T:211:UNK:N | 2.54 | 0.41 |
| 1:T:2507:UNK:O | 1:T:2511:UNK:CB | 2.68 | 0.41 |
| 1:T:2221:UNK:C | 1:T:2223:UNK:N | 2.80 | 0.41 |
| 1:P:1113:UNK:C | 1:P:1115:UNK:N | 2.84 | 0.41 |
| 1:P:514:UNK:O | 1:P:517:UNK:CB | 2.68 | 0.41 |
| 1:X:908:UNK:C | 1:X:910:UNK:N | 2.83 | 0.41 |
| 1:P:317:UNK:O | 1:P:318:UNK:C | 2.68 | 0.41 |
| 1:P:1412:UNK:HA | 1:P:1415:UNK:N | 2.36 | 0.41 |
| 1:C:909:UNK:O | 1:C:911:UNK:N | 2.53 | 0.41 |
| 1:S:313:UNK:O | 1:S:315:UNK:N | 2.54 | 0.41 |
| 1:T:3414:UNK:O | 1:T:3415:UNK:C | 2.64 | 0.41 |
| 1:T:1518:UNK:O | 1:T:1522:UNK:N | 2.54 | 0.41 |
| 1:D:706:UNK:C | 1:D:708:UNK:N | 2.83 | 0.41 |
| 1:T:817:UNK:O | 1:T:818:UNK:C | 2.68 | 0.41 |
| 1:X:1062:UNK:C | 1:X:1064:UNK:N | 2.82 | 0.41 |
| 1:C:1214:UNK:O | 1:C:1216:UNK:N | 2.53 | 0.41 |
| 1:R:307:UNK:C | 1:R:309:UNK:N | 2.81 | 0.41 |
| 1:C:113:UNK:O | 1:C:116:UNK:N | 2.54 | 0.41 |
| 1:C:1309:UNK:O | 1:C:1311:UNK:N | 2.54 | 0.41 |
| 1:A:1310:UNK:O | 1:A:1312:UNK:N | 2.53 | 0.41 |
| 1:Q:2208:UNK:O | 1:Q:2210:UNK:N | 2.42 | 0.41 |
| 1:T:2319:UNK:O | 1:T:2321:UNK:C | 2.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:D:315:UNK:C | 1:D:318:UNK:N | 2.84 | 0.41 |
| 1:F:1412:UNK:O | 1:F:1415:UNK:N | 2.54 | 0.41 |
| 1:B:909:UNK:O | 1:B:910:UNK:C | 2.66 | 0.41 |
| 1:F:2319:UNK:O | 1:F:2321:UNK:C | 2.69 | 0.41 |
| 1:F:1517:UNK:O | 1:F:1518:UNK:C | 2.68 | 0.41 |
| 1:F:1518:UNK:O | 1:F:1522:UNK:N | 2.54 | 0.41 |
| 1:P:1015:UNK:O | 1:P:1016:UNK:C | 2.68 | 0.41 |
| 1:P:909:UNK:O | 1:P:910:UNK:C | 2.66 | 0.41 |
| 1:T:1412:UNK:O | 1:T:1415:UNK:N | 2.54 | 0.41 |
| 1:B:1412:UNK:HA | 1:B:1415:UNK:N | 2.36 | 0.41 |
| 1:D:307:UNK:C | 1:D:309:UNK:N | 2.80 | 0.41 |
| 1:T:410:UNK:HA | 1:T:413:UNK:CB | 2.51 | 0.41 |
| 1:F:410:UNK:HA | 1:F:413:UNK:CB | 2.51 | 0.41 |
| 1:F:410:UNK:O | 1:F:413:UNK:N | 2.53 | 0.41 |
| 1:Q:113:UNK:O | 1:Q:116:UNK:N | 2.54 | 0.41 |
| 1:Q:1309:UNK:O | 1:Q:1311:UNK:N | 2.54 | 0.41 |
| 1:Q:507:UNK:O | 1:Q:509:UNK:N | 2.54 | 0.41 |
| 1:B:911:UNK:O | 1:B:913:UNK:N | 2.54 | 0.41 |
| 1:C:1115:UNK:O | 1:C:1117:UNK:N | 2.54 | 0.41 |
| 1:F:209:UNK:O | 1:F:211:UNK:N | 2.54 | 0.41 |
| 1:T:705:UNK:C | 1:T:707:UNK:N | 2.84 | 0.41 |
| 1:B:1715:UNK:O | 1:B:1716:UNK:O | 2.38 | 0.41 |
| 1:E:313:UNK:O | 1:E:315:UNK:N | 2.54 | 0.41 |
| 1:O:1312:UNK:O | 1:O:1315:UNK:N | 2.54 | 0.41 |
| 1:R:210:UNK:O | 1:R:211:UNK:C | 2.69 | 0.41 |
| 1:R:1112:UNK:C | 1:R:1114:UNK:N | 2.84 | 0.41 |
| 1:Q:1819:UNK:HA | 1:Q:1822:UNK:CB | 2.51 | 0.41 |
| 1:F:1018:UNK:C | 1:F:1020:UNK:N | 2.84 | 0.40 |
| 1:T:1417:UNK:O | 1:T:1419:UNK:N | 2.54 | 0.40 |
| 1:D:1112:UNK:C | 1:D:1114:UNK:N | 2.84 | 0.40 |
| 1:T:305:UNK:O | 1:T:306:UNK:O | 2.40 | 0.40 |
| 1:D:605:UNK:C | 1:D:606:UNK:O | 2.66 | 0.40 |
| 1:R:315:UNK:C | 1:R:318:UNK:N | 2.84 | 0.40 |
| 1:A:2307:UNK:O | 1:A:2308:UNK:C | 2.69 | 0.40 |
| 1:P:911:UNK:O | 1:P:913:UNK:N | 2.54 | 0.40 |
| 1:X:1033:UNK:O | 1:X:1037:UNK:N | 2.54 | 0.40 |
| 1:Y:1062:UNK:C | 1:Y:1064:UNK:N | 2.82 | 0.40 |
| 1:C:1407:UNK:O | 1:C:1411:UNK:N | 2.55 | 0.40 |
| 1:B:811:UNK:C | 1:B:813:UNK:N | 2.82 | 0.40 |
| 1:A:1509:UNK:C | 1:A:1511:UNK:N | 2.71 | 0.40 |
| 1:T:810:UNK:C | 1:T:812:UNK:N | 2.82 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:D:715:UNK:O | 1:D:718:UNK:N | 2.55 | 0.40 |
| 1:T:1018:UNK:C | 1:T:1020:UNK:N | 2.84 | 0.40 |
| 1:C:2216:UNK:O | 1:C:2218:UNK:N | 2.35 | 0.40 |
| 1:E:112:UNK:C | 1:E:114:UNK:N | 2.76 | 0.40 |
| 1:D:212:UNK:O | 1:D:213:UNK:O | 2.38 | 0.40 |
| 1:O:1521:UNK:C | 1:O:1523:UNK:N | 2.83 | 0.40 |
| 1:D:1008:UNK:O | 1:D:1012:UNK:N | 2.54 | 0.40 |
| 1:Q:1407:UNK:O | 1:Q:1408:UNK:C | 2.68 | 0.40 |
| 1:O:1312:UNK:O | 1:O:1313:UNK:C | 2.70 | 0.40 |
| 1:F:3420:UNK:O | 1:F:3423:UNK:C | 2.70 | 0.40 |
| 1:R:715:UNK:O | 1:R:718:UNK:N | 2.55 | 0.40 |
| 1:O:2307:UNK:O | 1:O:2308:UNK:C | 2.69 | 0.40 |
| 1:Q:1814:UNK:O | 1:Q:1815:UNK:O | 2.39 | 0.40 |
| 1:C:2612:UNK:C | 1:C:2614:UNK:N | 2.83 | 0.40 |
| 1:Y:906:UNK:O | 1:Y:908:UNK:N | 2.54 | 0.40 |
| 1:C:1511:UNK:O | 1:C:1513:UNK:N | 2.55 | 0.40 |
| 1:R:1008:UNK:O | 1:R:1012:UNK:N | 2.54 | 0.40 |
| 1:Q:1511:UNK:O | 1:Q:1513:UNK:N | 2.55 | 0.40 |
| 1:A:1811:UNK:O | 1:A:1815:UNK:N | 2.55 | 0.40 |
| 1:F:2107:UNK:O | 1:F:2108:UNK:C | 2.69 | 0.40 |
| 1:A:2315:UNK:C | 1:A:2317:UNK:N | 2.79 | 0.40 |

All (48) 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:O:619:UNK:C | 1:T:2418:UNK:O[1_545] | 0.56 | 1.64 |
| 1:O:620:UNK:C | 1:T:2419:UNK:CA[1_545] | 0.57 | 1.63 |
| 1:O:622:UNK:N | 1:T:2418:UNK:N[1_545] | 0.67 | 1.53 |
| 1:O:622:UNK:C | 1:T:2417:UNK:O[1_545] | 0.68 | 1.52 |
| 1:O:621:UNK:O | 1:T:2417:UNK:CA[1_545] | 0.91 | 1.29 |
| 1:O:621:UNK:O | 1:T:2417:UNK:N[1_545] | 0.91 | 1.29 |
| 1:O:619:UNK:O | 1:T:2418:UNK:O[1_545] | 0.97 | 1.23 |
| 1:O:620:UNK:CA | 1:T:2419:UNK:CA[1_545] | 1.05 | 1.15 |
| 1:O:622:UNK:CA | 1:T:2418:UNK:N[1_545] | 1.06 | 1.14 |
| 1:O:622:UNK:O | 1:T:2417:UNK:O[1_545] | 1.14 | 1.06 |
| 1:O:620:UNK:C | 1:T:2419:UNK:CB[1_545] | 1.18 | 1.02 |
| 1:O:622:UNK:CA | 1:T:2417:UNK:C[1_545] | 1.26 | 0.94 |
| 1:O:619:UNK:O | 1:T:2418:UNK:C[1_545] | 1.28 | 0.92 |
| 1:O:622:UNK:CB | 1:T:2418:UNK:CA[1_545] | 1.33 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:O:621:UNK:N | 1:T:2419:UNK:N[1_545] | 1.34 | 0.86 |
| 1:O:620:UNK:C | 1:T:2419:UNK:N[1_545] | 1.35 | 0.85 |
| 1:O:622:UNK:N | 1:T:2417:UNK:C[1_545] | 1.48 | 0.72 |
| 1:O:620:UNK:O | 1:T:2420:UNK:N[1_545] | 1.48 | 0.72 |
| 1:O:622:UNK:N | 1:T:2418:UNK:CA[1_545] | 1.50 | 0.70 |
| 1:O:620:UNK:O | 1:T:2419:UNK:CA[1_545] | 1.51 | 0.69 |
| 1:O:620:UNK:O | 1:T:2419:UNK:CB[1_545] | 1.52 | 0.68 |
| 1:O:622:UNK:CA | 1:T:2418:UNK:CA[1_545] | 1.54 | 0.66 |
| 1:O:619:UNK:CA | 1:T:2418:UNK:O[1_545] | 1.55 | 0.65 |
| 1:O:622:UNK:CA | 1:T:2417:UNK:O[1_545] | 1.59 | 0.61 |
| 1:O:622:UNK:CB | 1:T:2418:UNK:CB[1_545] | 1.61 | 0.59 |
| 1:O:620:UNK:O | 1:T:2419:UNK:C[1_545] | 1.62 | 0.58 |
| 1:O:621:UNK:O | 1:T:2417:UNK:C[1_545] | 1.63 | 0.57 |
| 1:O:619:UNK:C | 1:T:2418:UNK:C[1_545] | 1.63 | 0.57 |
| 1:O:621:UNK:C | 1:T:2417:UNK:C[1_545] | 1.65 | 0.55 |
| 1:O:622:UNK:C | 1:T:2417:UNK:C[1_545] | 1.67 | 0.53 |
| 1:O:621:UNK:N | 1:T:2419:UNK:CA[1_545] | 1.69 | 0.51 |
| 1:O:621:UNK:C | 1:T:2418:UNK:N[1_545] | 1.74 | 0.46 |
| 1:O:621:UNK:C | 1:T:2417:UNK:CA[1_545] | 1.77 | 0.43 |
| 1:O:620:UNK:N | 1:T:2418:UNK:O[1_545] | 1.81 | 0.39 |
| 1:O:620:UNK:C | 1:T:2419:UNK:C[1_545] | 1.84 | 0.36 |
| 1:O:621:UNK:N | 1:T:2419:UNK:CB[1_545] | 1.86 | 0.34 |
| 1:O:621:UNK:C | 1:T:2417:UNK:N[1_545] | 1.86 | 0.34 |
| 1:O:621:UNK:O | 1:T:2416:UNK:C[1_545] | 1.90 | 0.30 |
| 1:O:620:UNK:CA | 1:T:2419:UNK:C[1_545] | 1.92 | 0.28 |
| 1:O:620:UNK:N | 1:T:2419:UNK:CA[1_545] | 2.01 | 0.19 |
| 1:O:619:UNK:O | 1:T:2419:UNK:O[1_545] | 2.03 | 0.17 |
| 1:O:620:UNK:O | 1:T:2419:UNK:N[1_545] | 2.04 | 0.16 |
| 1:O:620:UNK:CA | 1:T:2419:UNK:CB[1_545] | 2.06 | 0.14 |
| 1:O:622:UNK:CB | 1:T:2418:UNK:N[1_545] | 2.07 | 0.13 |
| 1:O:622:UNK:N | 1:T:2419:UNK:N[1_545] | 2.09 | 0.11 |
| 1:O:622:UNK:N | 1:T:2418:UNK:C[1_545] | 2.10 | 0.10 |
| 1:O:621:UNK:O | 1:T:2417:UNK:CB[1_545] | 2.16 | 0.04 |
| 1:O:619:UNK:O | 1:T:2419:UNK:N[1_545] | 2.17 | 0.03 |

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 95th 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 | 0/4128 | - | - | - | - |
| 1 | B | 0/4128 | - | - | - | - |
| 1 | C | 0/4128 | - | - | - | - |
| 1 | D | 0/4128 | - | - | - | - |
| 1 | E | 0/4128 | - | - | - | - |
| 1 | F | 0/4128 | - | - | - | - |
| 1 | O | 0/4128 | - | - | - | - |
| 1 | P | 0/4128 | - | - | - | - |
| 1 | Q | 0/4128 | - | - | - | - |
| 1 | R | 0/4128 | - | - | - | - |
| 1 | S | 0/4128 | - | - | - | - |
| 1 | T | 0/4128 | - | - | - | - |
| 1 | X | 0/4128 | - | - | - | - |
| 1 | Y | 0/4128 | - | - | - | - |
| All | All | 0/57792 | - | - | - | - |

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.