# Full wwPDB X-ray Structure Validation Report (i)

Jun 7, 2025 – 01:26 pm BST

| | | |
|---|---|---|
| PDB ID | : | 9FLI / pdb_00009fli |
| Title | : | The structure of GanA, the extracellular galactanase of G.proteiniphilus T-6 |
| Authors | : | Hadad, N.; Lavid, N.; Shulami, S.; Dessau, M.; Shoham, Y.; Shoham, G. |
| Deposited on | : | 2024-06-05 |
| Resolution | : | 3.20 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

| | | |
|---|---|---|
| MolProbity | : | 4-5-2 with Phenix2.0rc1 |
| Xtriage (Phenix) | : | 2.0rc1 |
| EDS | : | 3.0 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4 | : | 9.0.003 (Gargrove) |
| Density-Fitness | : | 1.0.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.43.1 |

# 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 3.20 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.
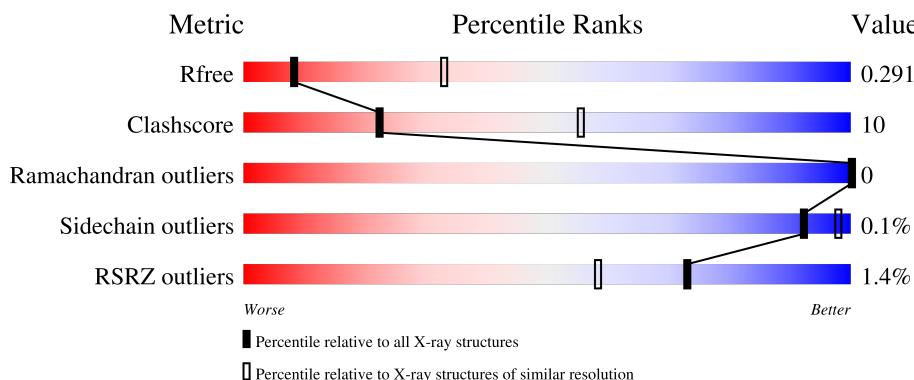


| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 164625 | 1370 (3.20-3.20) |
| Clashscore | 180529 | 1497 (3.20-3.20) |
| Ramachandran outliers | 177936 | 1479 (3.20-3.20) |
| Sidechain outliers | 177891 | 1478 (3.20-3.20) |
| RSRZ outliers | 164620 | 1371 (3.20-3.20) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 814 | 37% 10% 53% |
| 1 | B | 814 | .% 35% 12% 53% |
| 1 | C | 814 | 38% 9% 53% |
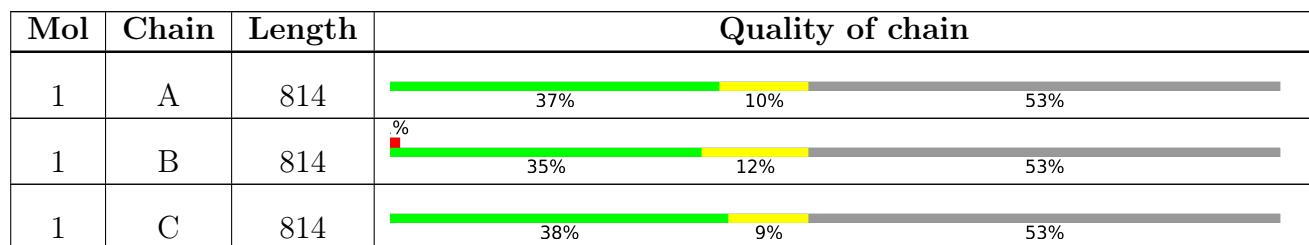
# 2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9069 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 Arabinogalactan endo-beta-1,4-galactanase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 384 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3010 | 1935 | 507 | 562 | 6 | | | |
| 1 | B | 384 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3010 | 1935 | 507 | 562 | 6 | | | |
| 1 | C | 384 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3010 | 1935 | 507 | 562 | 6 | | | |

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | A | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | B | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | C | 1 | Total | Ca | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | A | 9 | Total | O | 0 | 0 |
| | | | 9 | 9 | | |
| 3 | B | 16 | Total | O | 0 | 0 |
| | | | 16 | 16 | | |
| 3 | C | 11 | Total | O | 0 | 0 |
| | | | 11 | 11 | | |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Arabinogalactan endo-beta-1,4-galactanase

Chain A:

• Molecule 1: Arabinogalactan endo-beta-1,4-galactanase

Chain B:

ASP LEU GLN ARG PHE SER TYR ILE SER ASN ASP ALA TRP ILE VAL PRO ASN GLU GLY ASP ALA SER ALA PHE LYS TYR TRP ILE ARG ASP ILE ALA ASN GLY ASN GLN THR PHE THR LEU LYS GLN THR ILE GLY LEU LEU PRO PRO GLY SER TYR GLU LEU SER VAL GLN SER MET GLY GLY ALA

GLY ASP GLU ALA GLY TYR ILE LEU GLN LEU PHE ALA GLY ASP LYS MET ASP ALA VAL VAL THR LYS GLY TYR ASN SER TRP GLU THR VAL LYS LEU GLU GLU THR PHE THR LEU GLU GLU GLU ALA ASN PHE GLU VAL GLY VAL ALA ILE VAL THR GLY GLU GLU PRO PRO ASN ALA TRP GLY TYR MET ASP

HIS PHE GLN LEU VAL SER LEU ASN SER ALA GLY GLY ARG GLU MET PRO LYS PRO VAL PRO ALA D202 I203 K206 L211 I216 V219 D220 I224 I225 F234 K240 A251 Y255 V256 R257 N262 D266 G269 H270 L279 E280 I283 E284 K287

L297 V298 D299 Y302 A307 D308 P309 A310 K311 Q312 R313 P314 W318 F323 E324 K327 L330 S337 L338 K339 A340 M341 V351 Q352 I353 A360 E364 E372 S385 I388 L389 V390 F394 P397 E398 T399 S422 F427 W428 H429 N434

V438 L439 K440 A443 N444 V450 M451 E454 Y457 P458 G464 D465 N469 T470 A471 P472 S475 G476 Q477 T478 I483 T484 V485 I492 V495 I496 V502 P505 G506 I507 G508 W512 E513 P514 A515 W516 I517 P518 P521 Q524 E529 W532

E533 K534 Y535 W539 F543 A544 A545 A552 M553 W554 A559 N562 P574 K580 G585 ALA VAL ALA PRO LEU LYS ILE ASP GLU ILE LYS ASP ILE TYR ILE ARG ALA ALA PHE GLY GLN VAL LEU VAL LEU PRO THR VAL THR ALA THR TYR ASN ASP GLY SER

LYS HIS LEU VAL SER VAL LYS TRP ASP GLN ALA ALA LEU GLU GLN ALA LEU ARG THR GLY VAL THR TYR VAL ILE GLN GLY VAL VAL GLU THR VAL LYS ALA HIS LEU GLU GLU ILE THR PRO LYS ASN TYR VAL ASN PRO SER PHE GLU ASP GLN ASP ARG THR MET

TRP ASN ILE ILE TYR ARG ASN GLY THR SER PRO HIS THR ASP TYR LEU GLU LYS ALA THR ASP ALA LYS GLY TYR ARG ILE ALA VAL ASP PHE GLN VAL GLU GLN THR ILE THR GLY LEU LEU LYS PRO GLY TYR TYR ASN LEU SER MET PHE LEU GLN

ALA GLY ASP ALA PRO ASN ALA GLU ILE GLU ILE TYR LEU TYR LYS THR GLY ASP ALA LYS GLU GLY THR TYR ARG ALA ALA ALA SER VAL ASN GLY TRP LEU ASN TRP SER ASP GLU TRP PRO GLU ILE HIS ASP ILE TYR ILE LYS ILE ALA ASP GLY THR VAL THR ILE GLY LYS PRO GLY TYR TYR ASN LEU SER MET PHE LEU GLN

GLY THR LEU ASP ASP PHE GLN LEU TYR GLN THR LYS

**• Molecule 1: Arabinogalactan endo-beta-1,4-galactanase**

Chain C: 

38%      9%      53%

MET GLY LYS GLN PHE LEU PHE VAL LEU VAL ALA MET VAL MET MET SER PHE SER SER ASN HIS ILE HIS LYS ALA ALA ALA ASP SER TYR ASN TYR LEU ILE ASN GLY GLY PHE GLU SER ASP PHE TRP ALA ASP SER TRP THR VAL THR THR GLN ASP SER SER VAL

ASP LEU GLN ARG PHE SER TYR ILE SER ASN ASP ALA TRP ILE VAL PRO ASN GLU GLY ASP ALA SER ALA PHE LYS TYR TRP ILE ARG ASP ILE ALA ASN GLY ASN GLN THR PHE THR LEU LYS GLN THR ILE GLY LEU LEU PRO PRO GLY SER TYR GLU LEU SER VAL GLN SER MET GLY GLY ALA

GLY ASP GLU ALA GLY TYR ILE LEU GLN LEU PHE ALA GLY ASP LYS MET ASP ALA VAL VAL THR LYS GLY TYR ASN SER TRP GLU THR VAL LYS LEU GLU GLU THR PHE THR LEU GLU GLU GLU ALA ASN PHE GLU VAL GLY VAL ALA ILE VAL THR GLY GLU GLU PRO PRO ASN ALA TRP GLY TYR MET ASP

HIS PHE GLN LEU VAL SER LEU ASN SER ALA GLY GLY ARG GLU MET PRO LYS PRO VAL PRO ALA D202 I203 F204 V205 K206 D209 I216 K217 G218 V219 I224 L227 V232 K240 F245 K249 E250 A251 Y255 V256 R257 V258 E280 K281 A282 A289 S292

G293 M294 L297 V298 D299 Q312 W318 L338 M350 V351 Q352 I353 A360 S385 I388 L389 V390 V391 E398 T399 V419 L439 K440 V450 M451 E454 G464 N469 T470 A471 P472 K473 Q477 Q486 I492 V495 V502 I507 G508

Y511 W512 E513 P514 A515 W516 I517 P518 V519 G520 N528 K534 S537 G538 A545 A552 G557 S558 A559 N562 P574 S575 V578 F579 K580 D583 T584 G585 ALA VAL ALA PRO LEU LYS ILE ASP GLU ILE LYS ASP ILE TYR ILE ARG ALA ALA ALA PHE GLY GLU

GLN VAL VAL LEU PRO THR THR VAL THR ALA THR TYR ASN ASP GLY SER LYS HIS LEU VAL SER VAL LYS TRP ASP GLN ALA ALA LEU GLU GLN ALA LEU ARG THR GLY VAL GLY THR TYR VAL ILE GLN GLY VAL VAL GLU GLY GLU THR VAL LYS ALA HIS LEU GLU ILE THR PRO

LYS ASN TYR VAL VAL ASN PRO SER PHE GLU ASP GLN ASP ARG THR MET TRP ASN ILE ILE TYR ARG ASN GLY THR SER PRO HIS THR ASP TYR LEU GLU LYS ALA THR ASP ALA LYS SER GLY ASN TYR SER LEU HIS PHE TYR SER ASN GLU ALA VAL ASP PHE GLN VAL GLU GLN THR

ILE THR GLY LEU LYS PRO GLY TYR TYR ASN LEU SER MET PHE LEU GLN ALA GLY ASP ALA PRO ASN ALA GLU ILE TYR LEU TYR ALA LYS THR GLY ASP LYS GLU TYR ARG ALA ALA ALA SER VAL ASN GLY TRP LEU ASN TRP SER SER PRO GLU ILE HIS ASP ILE TYR ILE ALA ASP

GLY THR VAL THR ILE GLY ALA SER ILE LYS ALA ASN GLY GLY ALA TRP GLY THR LEU ASP ASP PHE GLN LEU TYR GLN THR LYS

# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | P 41 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 160.34Å    160.34Å    155.72Å<br>90.00°    90.00°    90.00° | Depositor |
| Resolution (Å) | 70.04  –  3.20<br>70.04  –  3.20 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.7 (70.04-3.20)<br>99.6 (70.04-3.20) | Depositor<br>EDS |
| $R_{merge}$ | 0.43 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.88 (at 3.19Å) | Xtriage |
| Refinement program | PHENIX 1.17.1_3660, PHENIX 1.17.1_3660 | Depositor |
| R, $R_{free}$ | 0.253  ,   0.289<br>0.254  ,   0.291 | Depositor<br>DCC |
| $R_{free}$ test set | 1657 reflections (4.86%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 33.8 | Xtriage |
| Anisotropy | 0.188 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 37.4 | EDS |
| L-test for twinning[2] | $< |L| > = 0.54, < L^2 > = 0.38$ | Xtriage |
| Estimated twinning fraction | 0.000 for -h,-l,-k<br>0.000 for l,-k,h | Xtriage |
| $F_o,F_c$ correlation | 0.87 | EDS |
| Total number of atoms | 9069 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 23.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

---

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

## 5   Model quality ⓘ

### 5.1   Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|------|----------|------|----------|
| | | RMSZ | #$|Z|$ >5 | RMSZ | #$|Z|$ >5 |
| 1 | A | 0.54 | 1/3091 (0.0%) | 0.77 | 0/4194 |
| 1 | B | 0.51 | 0/3091 | 0.76 | 0/4194 |
| 1 | C | 0.49 | 0/3091 | 0.75 | 0/4194 |
| All | All | 0.51 | 1/9273 (0.0%) | 0.76 | 0/12582 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | A | 513 | GLU | C-O | 9.49 | 1.28 | 1.23 |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2   Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3010 | 0 | 2950 | 72 | 0 |
| 1 | B | 3010 | 0 | 2949 | 67 | 0 |
| 1 | C | 3010 | 0 | 2949 | 47 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 9 | 0 | 0 | 0 | 0 |

*Continued on next page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | B | 16 | 0 | 0 | 0 | 0 |
| 3 | C | 11 | 0 | 0 | 1 | 0 |
| All | All | 9069 | 0 | 8848 | 185 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (185) 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:A:382:ARG:NH1 | 1:A:390:VAL:HG21 | 1.39 | 1.35 |
| 1:A:382:ARG:NH1 | 1:A:390:VAL:CG2 | 2.02 | 1.21 |
| 1:A:382:ARG:NH1 | 1:A:390:VAL:CB | 2.29 | 0.96 |
| 1:A:382:ARG:HH11 | 1:A:390:VAL:HG21 | 1.07 | 0.89 |
| 1:A:203:ILE:HD12 | 1:A:574:PRO:HB2 | 1.54 | 0.89 |
| 1:B:299:ASP:OD1 | 1:B:352:GLN:NE2 | 2.08 | 0.87 |
| 1:C:297:LEU:HG | 1:C:350:MET:HB2 | 1.59 | 0.82 |
| 1:B:203:ILE:HD12 | 1:B:574:PRO:HB2 | 1.61 | 0.81 |
| 1:A:382:ARG:HH12 | 1:A:390:VAL:CB | 1.92 | 0.79 |
| 1:A:382:ARG:NH1 | 1:A:390:VAL:HB | 1.99 | 0.75 |
| 1:A:382:ARG:CZ | 1:A:390:VAL:CG2 | 2.66 | 0.73 |
| 1:C:292:SER:HB2 | 1:C:294:MET:HE2 | 1.70 | 0.72 |
| 1:B:216:ILE:HG23 | 1:B:255:TYR:CD2 | 2.27 | 0.69 |
| 1:C:203:ILE:HD12 | 1:C:574:PRO:HB2 | 1.74 | 0.69 |
| 1:A:382:ARG:HH12 | 1:A:390:VAL:HB | 1.55 | 0.69 |
| 1:C:219:VAL:HB | 1:C:514:PRO:HG3 | 1.74 | 0.68 |
| 1:B:219:VAL:HB | 1:B:514:PRO:HG3 | 1.77 | 0.66 |
| 1:A:297:LEU:HG | 1:A:350:MET:HB3 | 1.78 | 0.66 |
| 1:A:216:ILE:HB | 1:A:508:GLY:HA3 | 1.76 | 0.65 |
| 1:A:257:ARG:NH2 | 1:A:454:GLU:OE2 | 2.29 | 0.65 |
| 1:A:338:LEU:HD21 | 1:A:351:VAL:HG21 | 1.80 | 0.64 |
| 1:A:443:ALA:HB2 | 1:A:450:VAL:HG13 | 1.80 | 0.63 |
| 1:C:232:VAL:HG13 | 1:C:517:ILE:HD11 | 1.83 | 0.61 |
| 1:A:230:SER:OG | 1:A:537:SER:OG | 2.15 | 0.61 |
| 1:C:299:ASP:HA | 1:C:352:GLN:HB2 | 1.82 | 0.61 |
| 1:A:265:TYR:HD1 | 1:A:271:GLY:HA2 | 1.66 | 0.61 |
| 1:A:382:ARG:NH2 | 1:A:418:ASP:OD1 | 2.33 | 0.61 |
| 1:C:353:ILE:HD13 | 1:C:390:VAL:HG13 | 1.84 | 0.60 |
| 1:B:216:ILE:HB | 1:B:508:GLY:HA3 | 1.83 | 0.59 |
| 1:C:297:LEU:HD21 | 1:C:352:GLN:HG3 | 1.84 | 0.59 |
| 1:C:203:ILE:HG12 | 1:C:486:GLN:HG2 | 1.85 | 0.59 |

Full wwPDB X-ray Structure Validation Report

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:382:ARG:NH2 | 1:A:418:ASP:CG | 2.61 | 0.59 |
| 1:A:244:ILE:O | 1:A:248:LEU:HD13 | 2.03 | 0.58 |
| 1:C:385:SER:HB3 | 1:C:388:ILE:HG13 | 1.85 | 0.58 |
| 1:A:299:ASP:HA | 1:A:352:GLN:HB3 | 1.86 | 0.57 |
| 1:A:465:ASP:HB3 | 1:A:518:PRO:HB3 | 1.87 | 0.56 |
| 1:C:519:VAL:HG11 | 1:C:537:SER:HB2 | 1.87 | 0.56 |
| 1:A:297:LEU:HD12 | 1:A:510:PHE:CZ | 2.41 | 0.55 |
| 1:A:382:ARG:HH12 | 1:A:390:VAL:CG1 | 2.20 | 0.55 |
| 1:A:353:ILE:HD13 | 1:A:390:VAL:HG13 | 1.88 | 0.55 |
| 1:B:440:LYS:HE2 | 1:B:444:ASN:HD21 | 1.72 | 0.55 |
| 1:A:270:HIS:HB3 | 1:A:543:PHE:CD2 | 2.42 | 0.54 |
| 1:C:545:ALA:HB1 | 1:C:552:ALA:HB2 | 1.88 | 0.54 |
| 1:B:469:ASN:HB3 | 1:B:559:ALA:O | 2.07 | 0.54 |
| 1:C:440:LYS:HG2 | 1:C:502:VAL:HG13 | 1.89 | 0.54 |
| 1:A:259:ARG:NH2 | 1:A:513:GLU:OE2 | 2.40 | 0.54 |
| 1:B:307:ALA:HA | 1:B:311:LYS:O | 2.08 | 0.54 |
| 1:B:338:LEU:HD21 | 1:B:351:VAL:HG21 | 1.90 | 0.54 |
| 1:B:398:GLU:HG2 | 1:B:399:THR:N | 2.21 | 0.53 |
| 1:A:382:ARG:CZ | 1:A:390:VAL:HB | 2.39 | 0.52 |
| 1:B:206:LYS:HB3 | 1:B:206:LYS:NZ | 2.24 | 0.52 |
| 1:C:217:LYS:NZ | 1:C:583:ASP:OD2 | 2.37 | 0.52 |
| 1:C:216:ILE:HB | 1:C:508:GLY:HA3 | 1.92 | 0.52 |
| 1:A:297:LEU:HD21 | 1:A:352:GLN:HB2 | 1.92 | 0.52 |
| 1:B:279:LEU:HD13 | 1:B:337:SER:HB3 | 1.92 | 0.52 |
| 1:B:327:LYS:NZ | 1:B:372:GLU:OE1 | 2.43 | 0.52 |
| 1:C:398:GLU:HG2 | 1:C:399:THR:N | 2.25 | 0.51 |
| 1:B:313:ARG:HG2 | 1:B:314:PRO:HD2 | 1.91 | 0.51 |
| 1:A:203:ILE:HG12 | 1:A:486:GLN:HG2 | 1.93 | 0.51 |
| 1:B:464:GLY:HA3 | 1:B:518:PRO:HG2 | 1.93 | 0.51 |
| 1:C:575:SER:O | 1:C:578:VAL:HG12 | 2.11 | 0.51 |
| 1:A:270:HIS:HB3 | 1:A:543:PHE:CG | 2.46 | 0.51 |
| 1:B:513:GLU:HG3 | 1:B:516:TRP:CE3 | 2.47 | 0.50 |
| 1:C:245:PHE:HD2 | 1:C:294:MET:HE1 | 1.75 | 0.50 |
| 1:A:382:ARG:NH2 | 1:A:418:ASP:OD2 | 2.45 | 0.50 |
| 1:B:457:TYR:CG | 1:B:458:PRO:HD2 | 2.47 | 0.49 |
| 1:A:215:PHE:CE2 | 1:A:508:GLY:HA2 | 2.48 | 0.49 |
| 1:B:257:ARG:NH1 | 1:B:352:GLN:OE1 | 2.45 | 0.49 |
| 1:A:473:LYS:HA | 1:B:553:MET:HE1 | 1.93 | 0.49 |
| 1:C:492:ILE:O | 1:C:495:VAL:HG12 | 2.13 | 0.49 |
| 1:B:465:ASP:HB2 | 1:B:532:TRP:HZ2 | 1.77 | 0.49 |
| 1:C:520:GLY:HA3 | 1:C:528:ASN:OD1 | 2.12 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:440:LYS:HE2 | 1:B:444:ASN:ND2 | 2.28 | 0.48 |
| 1:A:245:PHE:HD2 | 1:A:294:MET:HE1 | 1.77 | 0.48 |
| 1:C:206:LYS:NZ | 1:C:206:LYS:HB3 | 2.27 | 0.48 |
| 1:B:443:ALA:HB2 | 1:B:450:VAL:HG13 | 1.95 | 0.48 |
| 1:B:353:ILE:HD11 | 1:B:390:VAL:HG13 | 1.95 | 0.48 |
| 1:C:471:ALA:O | 1:C:562:ASN:ND2 | 2.47 | 0.48 |
| 1:C:318:TRP:CD1 | 1:C:318:TRP:N | 2.82 | 0.47 |
| 1:A:382:ARG:HH12 | 1:A:390:VAL:HG11 | 1.78 | 0.47 |
| 1:C:338:LEU:HD21 | 1:C:351:VAL:HG21 | 1.97 | 0.47 |
| 1:C:297:LEU:HD11 | 1:C:451:MET:HE1 | 1.96 | 0.47 |
| 1:A:443:ALA:HB2 | 1:A:450:VAL:CG1 | 2.44 | 0.47 |
| 1:B:279:LEU:O | 1:B:283:ILE:HG13 | 2.14 | 0.47 |
| 1:B:397:PRO:HD2 | 1:B:429:HIS:HB3 | 1.95 | 0.47 |
| 1:B:427:PHE:HB2 | 1:B:477:GLN:HB3 | 1.95 | 0.47 |
| 1:B:471:ALA:O | 1:B:562:ASN:ND2 | 2.47 | 0.47 |
| 1:B:297:LEU:HD11 | 1:B:451:MET:HE1 | 1.96 | 0.47 |
| 1:B:529:GLU:HA | 1:B:532:TRP:CE3 | 2.50 | 0.47 |
| 1:C:473:LYS:HB2 | 1:C:477:GLN:NE2 | 2.30 | 0.47 |
| 1:C:391:VAL:HG22 | 1:C:419:VAL:HB | 1.97 | 0.46 |
| 1:C:251:ALA:O | 1:C:580:LYS:HG3 | 2.15 | 0.46 |
| 1:A:219:VAL:HB | 1:A:514:PRO:HG3 | 1.97 | 0.46 |
| 1:A:398:GLU:HG2 | 1:A:399:THR:N | 2.31 | 0.46 |
| 1:B:234:PHE:HE2 | 1:B:515:ALA:HB1 | 1.81 | 0.46 |
| 1:C:439:LEU:O | 1:C:450:VAL:HG11 | 2.16 | 0.46 |
| 1:A:265:TYR:CD1 | 1:A:271:GLY:HA2 | 2.49 | 0.46 |
| 1:B:472:PRO:HG3 | 1:B:483:ILE:HD12 | 1.97 | 0.46 |
| 1:C:204:PHE:O | 1:C:486:GLN:NE2 | 2.48 | 0.46 |
| 1:C:227:LEU:HD11 | 1:C:516:TRP:HA | 1.98 | 0.46 |
| 1:A:514:PRO:O | 1:A:565:LEU:N | 2.47 | 0.45 |
| 1:B:302:TYR:CE1 | 1:B:330:LEU:HG | 2.51 | 0.45 |
| 1:A:360:ALA:HA | 1:A:364:GLU:O | 2.17 | 0.45 |
| 1:B:280:GLU:O | 1:B:284:GLU:HG3 | 2.16 | 0.45 |
| 1:B:308:ASP:OD1 | 1:B:310:ALA:N | 2.49 | 0.45 |
| 1:B:469:ASN:HD22 | 1:B:559:ALA:HA | 1.81 | 0.45 |
| 1:A:261:TRP:HE3 | 1:A:264:PRO:HB3 | 1.81 | 0.45 |
| 1:A:464:GLY:HA3 | 1:A:518:PRO:HG2 | 1.97 | 0.45 |
| 1:A:398:GLU:HA | 1:A:434:ASN:HD22 | 1.81 | 0.45 |
| 1:B:283:ILE:HG12 | 1:B:341:MET:HG2 | 1.98 | 0.45 |
| 1:B:360:ALA:HA | 1:B:364:GLU:O | 2.16 | 0.45 |
| 1:C:469:ASN:HD22 | 1:C:559:ALA:HA | 1.81 | 0.45 |
| 1:A:398:GLU:OE1 | 1:A:429:HIS:HA | 2.16 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:219:VAL:HG12 | 1:C:511:TYR:HB3 | 1.97 | 0.45 |
| 1:A:382:ARG:CZ | 1:A:390:VAL:HG21 | 2.30 | 0.45 |
| 1:C:209:ASP:HB3 | 3:C:1004:HOH:O | 2.17 | 0.45 |
| 1:B:318:TRP:N | 1:B:318:TRP:CD1 | 2.81 | 0.44 |
| 1:C:450:VAL:O | 1:C:507:ILE:HG12 | 2.17 | 0.44 |
| 1:B:220:ASP:HA | 1:B:257:ARG:O | 2.17 | 0.44 |
| 1:A:233:LYS:HD3 | 1:A:241:LYS:HE2 | 1.99 | 0.44 |
| 1:A:279:LEU:O | 1:A:283:ILE:HG13 | 2.17 | 0.44 |
| 1:A:219:VAL:CG1 | 1:A:514:PRO:HG3 | 2.48 | 0.44 |
| 1:B:240:LYS:HE3 | 1:B:240:LYS:HB3 | 1.86 | 0.44 |
| 1:B:394:PHE:O | 1:B:422:SER:HA | 2.18 | 0.44 |
| 1:B:257:ARG:NH2 | 1:B:454:GLU:OE2 | 2.45 | 0.44 |
| 1:B:440:LYS:HG2 | 1:B:502:VAL:HG13 | 1.99 | 0.44 |
| 1:C:513:GLU:HG3 | 1:C:516:TRP:CE3 | 2.52 | 0.44 |
| 1:A:279:LEU:HD13 | 1:A:337:SER:HB3 | 1.99 | 0.44 |
| 1:A:578:VAL:O | 1:A:582:VAL:HG13 | 2.17 | 0.43 |
| 1:A:385:SER:HB3 | 1:A:388:ILE:HG13 | 2.00 | 0.43 |
| 1:B:279:LEU:CD1 | 1:B:337:SER:HB3 | 2.48 | 0.43 |
| 1:A:204:PHE:H | 1:A:486:GLN:NE2 | 2.16 | 0.43 |
| 1:A:575:SER:O | 1:A:578:VAL:HG12 | 2.19 | 0.43 |
| 1:A:318:TRP:CD1 | 1:A:318:TRP:N | 2.85 | 0.43 |
| 1:A:439:LEU:O | 1:A:450:VAL:HG11 | 2.17 | 0.43 |
| 1:B:545:ALA:HB1 | 1:B:552:ALA:HB2 | 2.01 | 0.43 |
| 1:B:283:ILE:HG22 | 1:B:287:LYS:HD2 | 1.99 | 0.43 |
| 1:B:505:PRO:O | 1:B:507:ILE:HG23 | 2.19 | 0.43 |
| 1:C:224:ILE:HD12 | 1:C:224:ILE:HA | 1.89 | 0.43 |
| 1:A:538:GLY:HA3 | 1:A:557:GLY:HA2 | 2.00 | 0.43 |
| 1:C:289:ALA:HA | 1:C:294:MET:HE3 | 2.00 | 0.43 |
| 1:A:258:VAL:HG11 | 1:A:282:ALA:HB1 | 2.00 | 0.42 |
| 1:A:351:VAL:HG23 | 1:A:388:ILE:HG21 | 2.00 | 0.42 |
| 1:A:396:ASN:HA | 1:A:429:HIS:HD2 | 1.84 | 0.42 |
| 1:B:270:HIS:HB3 | 1:B:543:PHE:CD2 | 2.54 | 0.42 |
| 1:C:258:VAL:HG21 | 1:C:282:ALA:HA | 2.00 | 0.42 |
| 1:C:312:GLN:HG3 | 1:C:360:ALA:HB3 | 2.01 | 0.42 |
| 1:B:353:ILE:CD1 | 1:B:390:VAL:HG13 | 2.49 | 0.42 |
| 1:A:203:ILE:HD11 | 1:A:485:VAL:HB | 2.01 | 0.42 |
| 1:A:283:ILE:HG12 | 1:A:341:MET:HG2 | 2.01 | 0.42 |
| 1:A:532:TRP:HD1 | 1:A:537:SER:HB2 | 1.84 | 0.42 |
| 1:B:224:ILE:HG23 | 1:B:225:ILE:N | 2.35 | 0.42 |
| 1:B:266:ASP:OD1 | 1:B:266:ASP:C | 2.62 | 0.42 |
| 1:C:216:ILE:HG23 | 1:C:255:TYR:CD2 | 2.54 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:485:VAL:HG11 | 1:B:574:PRO:HD2 | 2.00 | 0.42 |
| 1:A:235:TYR:HA | 1:A:241:LYS:HA | 2.02 | 0.42 |
| 1:A:427:PHE:HB2 | 1:A:477:GLN:HB3 | 2.01 | 0.42 |
| 1:A:216:ILE:HG23 | 1:A:255:TYR:CD1 | 2.55 | 0.42 |
| 1:B:234:PHE:CE2 | 1:B:515:ALA:HB1 | 2.55 | 0.42 |
| 1:B:251:ALA:HA | 1:B:580:LYS:HE3 | 2.02 | 0.42 |
| 1:C:464:GLY:HA3 | 1:C:518:PRO:HG2 | 2.02 | 0.42 |
| 1:A:426:PRO:HG2 | 1:A:457:TYR:HD1 | 1.85 | 0.41 |
| 1:B:224:ILE:HA | 1:B:224:ILE:HD12 | 1.82 | 0.41 |
| 1:A:456:SER:HA | 1:A:511:TYR:CE1 | 2.55 | 0.41 |
| 1:A:265:TYR:HD1 | 1:A:271:GLY:CA | 2.32 | 0.41 |
| 1:B:262:ASN:N | 1:B:262:ASN:OD1 | 2.52 | 0.41 |
| 1:A:257:ARG:HG3 | 1:A:297:LEU:HB3 | 2.03 | 0.41 |
| 1:C:249:LYS:HA | 1:C:249:LYS:HD2 | 1.69 | 0.41 |
| 1:B:469:ASN:HA | 1:B:559:ALA:HA | 2.02 | 0.41 |
| 1:B:580:LYS:H | 1:B:580:LYS:HG3 | 1.70 | 0.41 |
| 1:B:385:SER:HB3 | 1:B:388:ILE:HG13 | 2.02 | 0.41 |
| 1:C:240:LYS:HE3 | 1:C:240:LYS:HB3 | 1.75 | 0.41 |
| 1:C:250:GLU:O | 1:C:580:LYS:HE3 | 2.20 | 0.41 |
| 1:B:211:LEU:HA | 1:B:211:LEU:HD12 | 1.83 | 0.41 |
| 1:B:454:GLU:HG2 | 1:B:512:TRP:HB2 | 2.02 | 0.41 |
| 1:B:492:ILE:O | 1:B:496:ILE:HG13 | 2.21 | 0.41 |
| 1:C:257:ARG:NH2 | 1:C:454:GLU:OE2 | 2.51 | 0.41 |
| 1:A:304:ASP:HB2 | 1:A:547:TYR:CZ | 2.56 | 0.40 |
| 1:B:427:PHE:HA | 1:B:478:THR:O | 2.21 | 0.40 |
| 1:B:323:PHE:HZ | 1:B:372:GLU:HB2 | 1.86 | 0.40 |
| 1:B:434:ASN:O | 1:B:438:VAL:HG22 | 2.21 | 0.40 |
| 1:C:538:GLY:HA2 | 1:C:557:GLY:HA2 | 2.03 | 0.40 |
| 1:A:342:LEU:HD23 | 1:A:342:LEU:HA | 1.92 | 0.40 |
| 1:B:492:ILE:O | 1:B:495:VAL:HG12 | 2.22 | 0.40 |
| 1:B:539:TRP:NE1 | 1:B:554:TRP:O | 2.53 | 0.40 |

There are no symmetry-related clashes.

## 5.3  Torsion angles ⓘ

### 5.3.1  Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|------|------|
| 1 | A | 382/814 (47%) | 365 (96%) | 17 (4%) | 0 | 100 | 100 |
| 1 | B | 382/814 (47%) | 360 (94%) | 22 (6%) | 0 | 100 | 100 |
| 1 | C | 382/814 (47%) | 368 (96%) | 14 (4%) | 0 | 100 | 100 |
| All | All | 1146/2442 (47%) | 1093 (95%) | 53 (5%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2　Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|------|------|
| 1 | A | 311/662 (47%) | 310 (100%) | 1 (0%) | 91 | 96 |
| 1 | B | 311/662 (47%) | 311 (100%) | 0 | 100 | 100 |
| 1 | C | 311/662 (47%) | 311 (100%) | 0 | 100 | 100 |
| All | All | 933/1986 (47%) | 932 (100%) | 1 (0%) | 92 | 98 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 205 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 467 | HIS |
| 1 | B | 444 | ASN |
| 1 | B | 563 | GLN |
| 1 | C | 277 | ASN |
| 1 | C | 467 | HIS |
| 1 | C | 577 | ASN |

### 5.3.3  RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5  Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6  Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7  Other polymers ⓘ

There are no such residues in this entry.

## 5.8  Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Fit of model and data ⓘ

## 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 384/814 (47%) | 0.08 | 3 (0%) | 82 | 70 | 8, 20, 41, 57 | 0 |
| 1 | B | 384/814 (47%) | 0.15 | 9 (2%) | 61 | 44 | 10, 22, 42, 62 | 0 |
| 1 | C | 384/814 (47%) | 0.12 | 4 (1%) | 79 | 66 | 12, 22, 41, 55 | 0 |
| All | All | 1152/2442 (47%) | 0.12 | 16 (1%) | 73 | 58 | 8, 22, 42, 62 | 0 |

All (16) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 524 | GLN | 2.8 |
| 1 | C | 209 | ASP | 2.6 |
| 1 | C | 203 | ILE | 2.6 |
| 1 | A | 382 | ARG | 2.5 |
| 1 | C | 280 | GLU | 2.5 |
| 1 | A | 347 | GLN | 2.5 |
| 1 | B | 534 | LYS | 2.5 |
| 1 | B | 339 | LYS | 2.4 |
| 1 | B | 585 | GLY | 2.4 |
| 1 | A | 569 | ASN | 2.3 |
| 1 | B | 521 | PRO | 2.3 |
| 1 | B | 324 | GLU | 2.3 |
| 1 | B | 269 | GLY | 2.1 |
| 1 | C | 534 | LYS | 2.1 |
| 1 | B | 535 | TYR | 2.1 |
| 1 | B | 475 | SER | 2.0 |

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors($\text{Å}^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------------------------|-------|
| 2 | CA | B | 901 | 1/1 | 0.98 | 0.04 | 25,25,25,25 | 0 |
| 2 | CA | C | 901 | 1/1 | 0.98 | 0.06 | 30,30,30,30 | 0 |
| 2 | CA | A | 901 | 1/1 | 0.99 | 0.02 | 25,25,25,25 | 0 |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.