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

Jun 11, 2024 – 08:35 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 6N4X |
| Title | : | Metabotropic Glutamate Receptor 5 Apo Form Ligand Binding Domain |
| Authors | : | Koehl, A.; Hu, H.; Feng, D.; Sun, B.; Weis, W.I.; Skiniotis, G.S.; Mathiesen, J.M.; Kobilka, B.K. |
| Deposited on | : | 2018-11-20 |
| Resolution | : | 4.00 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.

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

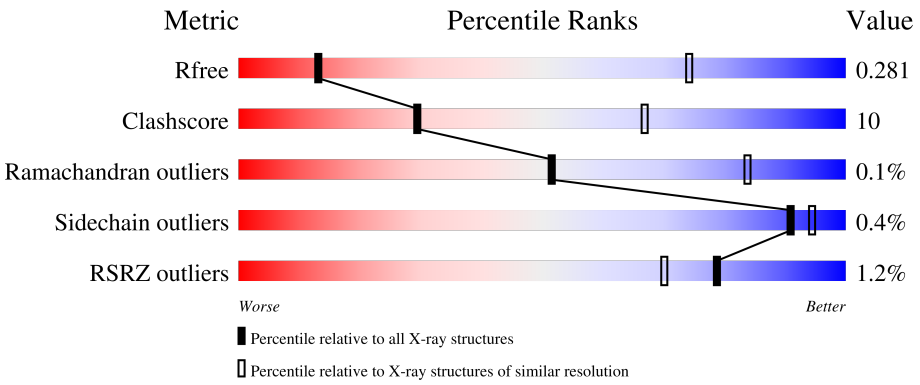
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36.2 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 1087 (4.30-3.70) |
| Clashscore | 141614 | 1148 (4.30-3.70) |
| Ramachandran outliers | 138981 | 1108 (4.30-3.70) |
| Sidechain outliers | 138945 | 1099 (4.30-3.70) |
| RSRZ outliers | 127900 | 1028 (4.34-3.66) |

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 | 877 | % 45% 13% 42% |
| 1 | B | 877 | % 43% 13% 44% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7736 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 Metabotropic glutamate receptor 5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 506 | 3897 | 2456 | 666 | 739 | 36 | 0 | 0 | 0 |
| 1 | B | 487 | 3754 | 2362 | 646 | 712 | 34 | 0 | 0 | 0 |

There are 62 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -5 | MET | - | initiating methionine | UNP P41594 |
| A | -4 | LYS | - | expression tag | UNP P41594 |
| A | -3 | THR | - | expression tag | UNP P41594 |
| A | -2 | ILE | - | expression tag | UNP P41594 |
| A | -1 | ILE | - | expression tag | UNP P41594 |
| A | 0 | ALA | - | expression tag | UNP P41594 |
| A | 1 | LEU | - | expression tag | UNP P41594 |
| A | 2 | SER | - | expression tag | UNP P41594 |
| A | 3 | TYR | - | expression tag | UNP P41594 |
| A | 4 | ILE | - | expression tag | UNP P41594 |
| A | 5 | PHE | - | expression tag | UNP P41594 |
| A | 6 | CYS | - | expression tag | UNP P41594 |
| A | 7 | LEU | - | expression tag | UNP P41594 |
| A | 8 | VAL | - | expression tag | UNP P41594 |
| A | 9 | PHE | - | expression tag | UNP P41594 |
| A | 10 | ALA | - | expression tag | UNP P41594 |
| A | 11 | ASP | - | expression tag | UNP P41594 |
| A | 12 | TYR | - | expression tag | UNP P41594 |
| A | 13 | LYS | - | expression tag | UNP P41594 |
| A | 14 | ASP | - | expression tag | UNP P41594 |
| A | 15 | ASP | - | expression tag | UNP P41594 |
| A | 16 | ASP | - | expression tag | UNP P41594 |
| A | 17 | ASP | - | expression tag | UNP P41594 |
| A | 18 | ALA | - | expression tag | UNP P41594 |
| A | 19 | ALA | - | expression tag | UNP P41594 |

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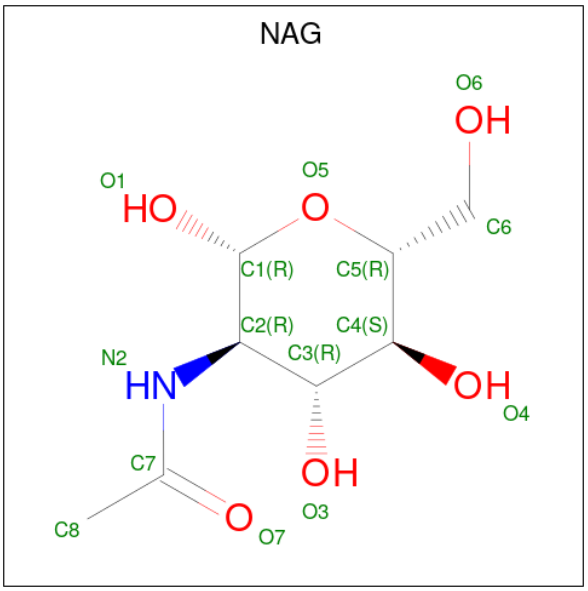
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 866 | HIS | - | expression tag | UNP P41594 |
| A | 867 | HIS | - | expression tag | UNP P41594 |
| A | 868 | HIS | - | expression tag | UNP P41594 |
| A | 869 | HIS | - | expression tag | UNP P41594 |
| A | 870 | HIS | - | expression tag | UNP P41594 |
| A | 871 | HIS | - | expression tag | UNP P41594 |
| B | -5 | MET | - | initiating methionine | UNP P41594 |
| B | -4 | LYS | - | expression tag | UNP P41594 |
| B | -3 | THR | - | expression tag | UNP P41594 |
| B | -2 | ILE | - | expression tag | UNP P41594 |
| B | -1 | ILE | - | expression tag | UNP P41594 |
| B | 0 | ALA | - | expression tag | UNP P41594 |
| B | 1 | LEU | - | expression tag | UNP P41594 |
| B | 2 | SER | - | expression tag | UNP P41594 |
| B | 3 | TYR | - | expression tag | UNP P41594 |
| B | 4 | ILE | - | expression tag | UNP P41594 |
| B | 5 | PHE | - | expression tag | UNP P41594 |
| B | 6 | CYS | - | expression tag | UNP P41594 |
| B | 7 | LEU | - | expression tag | UNP P41594 |
| B | 8 | VAL | - | expression tag | UNP P41594 |
| B | 9 | PHE | - | expression tag | UNP P41594 |
| B | 10 | ALA | - | expression tag | UNP P41594 |
| B | 11 | ASP | - | expression tag | UNP P41594 |
| B | 12 | TYR | - | expression tag | UNP P41594 |
| B | 13 | LYS | - | expression tag | UNP P41594 |
| B | 14 | ASP | - | expression tag | UNP P41594 |
| B | 15 | ASP | - | expression tag | UNP P41594 |
| B | 16 | ASP | - | expression tag | UNP P41594 |
| B | 17 | ASP | - | expression tag | UNP P41594 |
| B | 18 | ALA | - | expression tag | UNP P41594 |
| B | 19 | ALA | - | expression tag | UNP P41594 |
| B | 866 | HIS | - | expression tag | UNP P41594 |
| B | 867 | HIS | - | expression tag | UNP P41594 |
| B | 868 | HIS | - | expression tag | UNP P41594 |
| B | 869 | HIS | - | expression tag | UNP P41594 |
| B | 870 | HIS | - | expression tag | UNP P41594 |
| B | 871 | HIS | - | expression tag | UNP P41594 |

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 2 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 2 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 2 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 2 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 2 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

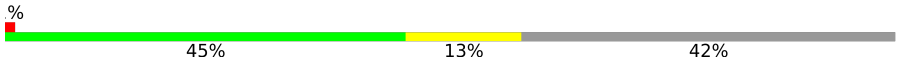
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | B | 1 | Total | Mg | 0 | 0 |
| | | | 1 | 1 | | |

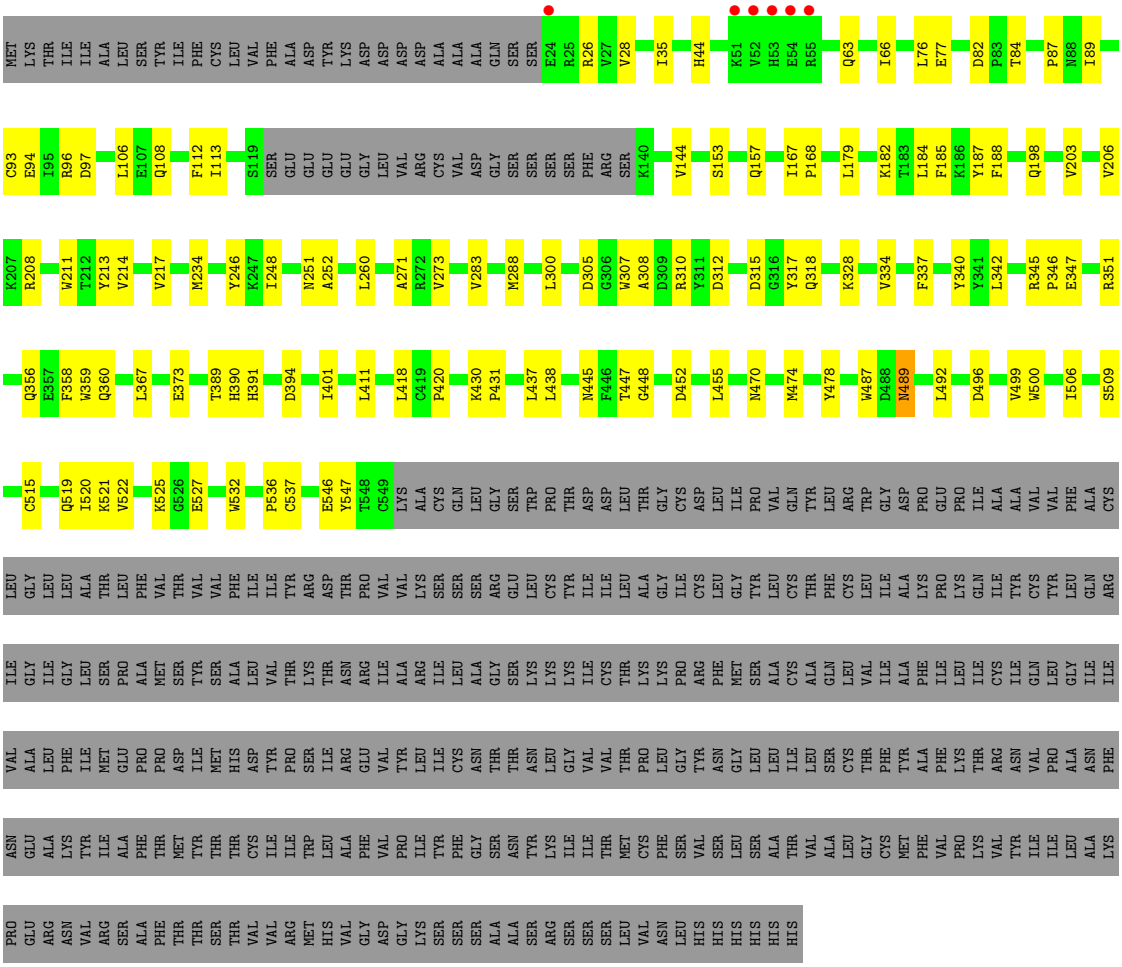
# 3 Residue-property plots (i)

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

• Molecule 1: Metabotropic glutamate receptor 5

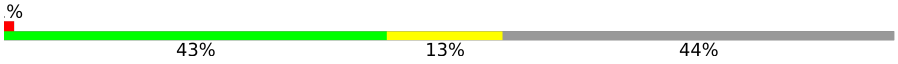
Chain A:

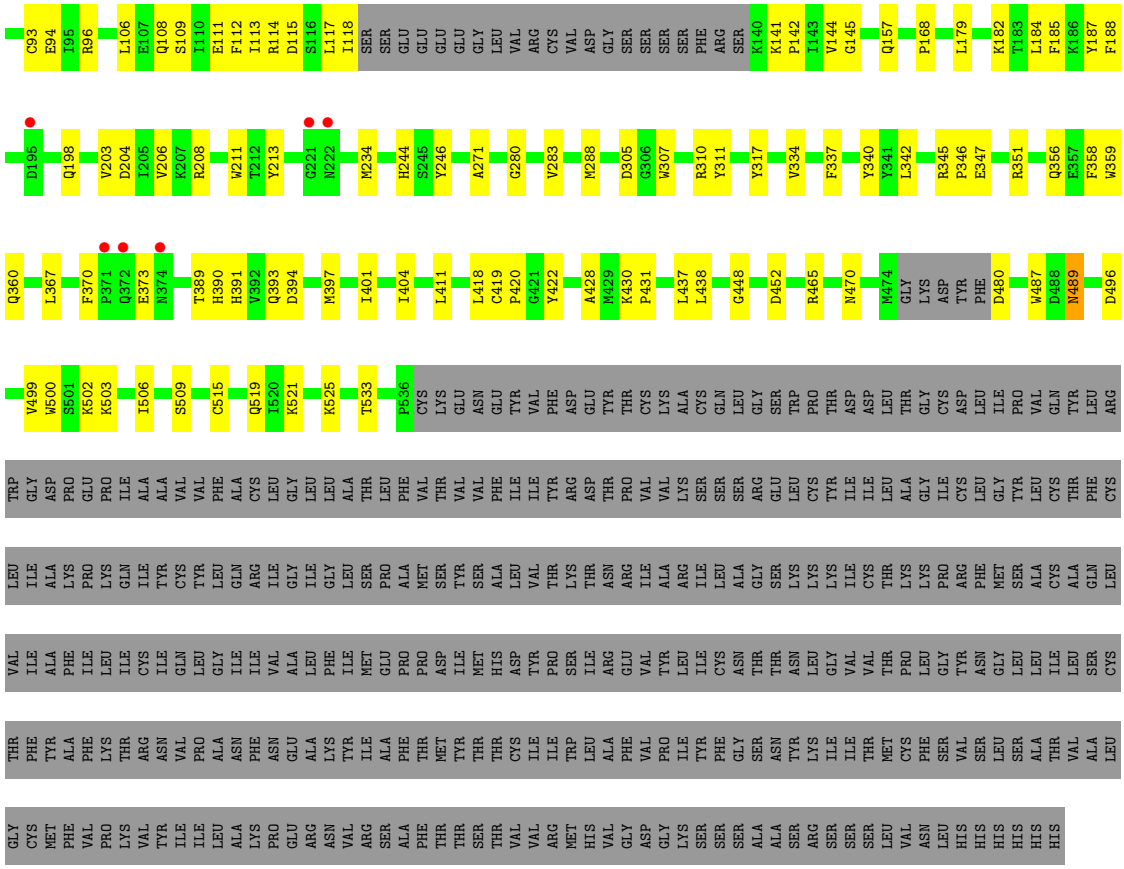



• Molecule 1: Metabotropic glutamate receptor 5

Chain B:




C93 E94 I95 R96 L106 E107 Q108 S109 I110 E111 F112 I113 R114 D115 S116 L117 I118 SER SER GLU GLU GLU GLU GLY LEU VAL ARG CYS VAL ASP GLY SER SER SER SER PHE ARG SER K140 K141 P142 I143 V144 G145 Q157 P168 L179 K182 T183 L184 F185 K186 Y187 F188
D195 Q198 V203 D204 I205 V206 K207 R208 W211 T212 Y213 G221 N222 M234 H244 S245 Y246 A271 G280 V283 M288 D305 G306 W307 R310 Y311 Y317 V334 F337 Y340 Y341 L342 R345 P346 E347 R351 Q356 E357 F358 W359
Q360 L367 F370 P371 Q372 E373 N374 T389 H390 H391 V392 Q393 D394 M397 I401 I404 L411 L418 C419 P420 G421 Y422 A428 M429 K430 P431 L437 L438 G448 D452 R465 N470 M474 GLY LYS ASP TYR PHE D480 W487 D488 N489 D496
V499 W500 S501 K502 K503 I506 S509 C515 Q519 I520 K521 K525 T533 P536 CYS LYS GLU ASN GLU TYR VAL PHE ASP GLU TYR THR CYS LYS ALA CYS GLN LEU GLY SER TRP PRO THR ASP ASP LEU THR GLY CYS ASP LEU ILE PRO VAL GLN TYR LEU ARG
TRP GLY ASP PRO GLU PRO ILE ALA ALA VAL VAL PHE ALA CYS LEU GLY LEU LEU ALA THR LEU PHE VAL THR VAL VAL PHE ILE ILE TYR ARG ASP THR PRO VAL VAL LYS SER SER SER ARG GLU LEU CYS TYR ILE ILE LEU ALA GLY ILE CYS LEU GLY TYR LEU CYS THR CYS
LEU ILE ALA LYS PRO LYS GLN ILE TYR CYS TYR LEU GLN ARG ILE GLY ILE GLY LEU SER PRO ALA MET SER TYR SER ALA LEU VAL THR LYS THR ASN ARG ILE ALA ARG ILE LEU ALA SER LYS LYS LYS ILE CYS THR LYS LYS PRO ARG PHE MET SER ALA CYS ALA GLN LEU
VAL ILE ALA PHE ILE LEU ILE CYS ILE GLN LEU GLY ILE ILE VAL ALA LEU PHE ILE MET GLU PRO PRO ASP ILE MET HIS ASP TYR PRO SER ILE ARG GLU VAL TYR LEU ILE CYS ASN THR THR ASN LEU GLY VAL VAL THR PRO LEU GLY TYR ASN GLY LEU LEU ILE LEU SER ALA CYS
THR PHE TYR ALA PHE LYS THR ARG ASN VAL PRO ALA ASN PHE ASN GLU ALA LYS TYR ILE ALA PHE THR MET TYR THR THR CYS ILE ILE TRP LEU ALA PHE VAL PRO ILE TYR PHE GLY SER ASN TYR LYS ILE ILE THR MET CYS PHE SER VAL SER LEU SER ALA THR VAL ALA LEU
GLY CYS MET PHE VAL PRO LYS VAL TYR ILE ILE LEU ALA LYS PRO GLU ARG ASN VAL ARG SER ALA PHE THR THR SER THR VAL VAL ARG MET HIS VAL GLY ASP GLY LYS SER SER SER ALA ALA SER ARG SER SER SER LEU VAL ASN LEU HIS HIS HIS HIS HIS HIS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 119.08Å 174.10Å 180.90Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.57 – 4.00<br>49.57 – 4.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 93.2 (49.57-4.00)<br>83.5 (49.57-4.00) | Depositor<br>EDS |
| $R_{merge}$ | 0.14 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.85 (at 4.00Å) | Xtriage |
| Refinement program | PHENIX 1.14_3211 | Depositor |
| R, $R_{free}$ | 0.270 , 0.282<br>0.268 , 0.281 | Depositor<br>DCC |
| $R_{free}$ test set | 1540 reflections (5.08%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 172.6 | Xtriage |
| Anisotropy | 0.246 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 160.1 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.42$, $< L^2 > = 0.25$ | Xtriage |
| Estimated twinning fraction | 0.064 for -h,l,k | Xtriage |
| $F_o$,$F_c$ correlation | 0.82 | EDS |
| Total number of atoms | 7736 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 184.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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 (i)

## 5.1 Standard geometry (i)

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

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 | 0.25 | 0/3985 | 0.45 | 0/5407 |
| 1 | B | 0.24 | 0/3836 | 0.45 | 0/5200 |
| All | All | 0.25 | 0/7821 | 0.45 | 0/10607 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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 | 3897 | 0 | 3649 | 73 | 0 |
| 1 | B | 3754 | 0 | 3546 | 71 | 0 |
| 2 | A | 56 | 0 | 52 | 0 | 0 |
| 2 | B | 28 | 0 | 26 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| All | All | 7736 | 0 | 7273 | 143 | 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 (143) 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:520:ILE:HD13 | 1:A:546:GLU:C | 1.90 | 0.90 |
| 1:A:77:GLU:OE2 | 1:A:351:ARG:NH1 | 2.18 | 0.76 |
| 1:B:77:GLU:OE2 | 1:B:351:ARG:NH1 | 2.19 | 0.74 |
| 1:B:360:GLN:HE22 | 1:B:373:GLU:HA | 1.52 | 0.74 |
| 1:A:360:GLN:HE22 | 1:A:373:GLU:HA | 1.53 | 0.73 |
| 1:A:522:VAL:HG22 | 1:A:547:TYR:HA | 1.72 | 0.70 |
| 1:B:419:CYS:HB3 | 1:B:422:TYR:HB2 | 1.74 | 0.69 |
| 1:B:198:GLN:HE22 | 1:B:305:ASP:H | 1.40 | 0.69 |
| 1:A:182:LYS:NZ | 1:A:188:PHE:O | 2.27 | 0.67 |
| 1:A:198:GLN:HE22 | 1:A:305:ASP:H | 1.42 | 0.66 |
| 1:B:182:LYS:NZ | 1:B:188:PHE:O | 2.29 | 0.65 |
| 1:A:82:ASP:OD2 | 1:A:84:THR:OG1 | 2.11 | 0.64 |
| 1:A:94:GLU:OE2 | 1:A:96:ARG:NH2 | 2.32 | 0.63 |
| 1:A:447:THR:HG21 | 1:B:428:ALA:HB2 | 1.80 | 0.63 |
| 1:B:213:TYR:O | 1:B:509:SER:OG | 2.16 | 0.63 |
| 1:B:106:LEU:HD21 | 1:B:157:GLN:HB3 | 1.81 | 0.61 |
| 1:A:198:GLN:NE2 | 1:A:305:ASP:H | 1.97 | 0.61 |
| 1:B:525:LYS:HG2 | 1:B:533:THR:HG23 | 1.82 | 0.61 |
| 1:A:345:ARG:HD3 | 1:A:346:PRO:HD2 | 1.83 | 0.60 |
| 1:A:106:LEU:HD21 | 1:A:157:GLN:HB3 | 1.83 | 0.60 |
| 1:B:311:TYR:OH | 1:B:480:ASP:OD1 | 2.16 | 0.60 |
| 1:B:109:SER:HA | 1:B:112:PHE:HD2 | 1.65 | 0.60 |
| 1:A:520:ILE:HD13 | 1:A:546:GLU:O | 2.02 | 0.60 |
| 1:B:345:ARG:HD3 | 1:B:346:PRO:HD2 | 1.84 | 0.59 |
| 1:A:35:ILE:HG23 | 1:A:144:VAL:HG21 | 1.83 | 0.59 |
| 1:A:310:ARG:HG2 | 1:A:312:ASP:OD1 | 2.03 | 0.59 |
| 1:B:208:ARG:NH1 | 1:B:496:ASP:OD1 | 2.31 | 0.58 |
| 1:B:342:LEU:HD21 | 1:B:391:HIS:CG | 2.39 | 0.57 |
| 1:B:35:ILE:HG23 | 1:B:144:VAL:HG21 | 1.86 | 0.57 |
| 1:A:487:TRP:HD1 | 1:A:492:LEU:HD13 | 1.71 | 0.56 |
| 1:A:213:TYR:O | 1:A:509:SER:OG | 2.22 | 0.56 |
| 1:A:342:LEU:HD21 | 1:A:391:HIS:CG | 2.41 | 0.55 |
| 1:A:525:LYS:HG3 | 1:A:527:GLU:H | 1.71 | 0.55 |
| 1:A:26:ARG:HD2 | 1:A:108:GLN:NE2 | 2.21 | 0.55 |
| 1:A:168:PRO:HG2 | 1:A:437:LEU:HD23 | 1.88 | 0.55 |
| 1:A:203:VAL:HG21 | 1:A:234:MET:HB2 | 1.89 | 0.54 |
| 1:A:208:ARG:NH1 | 1:A:496:ASP:OD1 | 2.27 | 0.54 |
| 1:A:28:VAL:HG11 | 1:A:94:GLU:HG3 | 1.88 | 0.54 |
| 1:A:340:TYR:OH | 1:A:351:ARG:NH2 | 2.33 | 0.54 |
| 1:A:519:GLN:HB3 | 1:A:536:PRO:HA | 1.89 | 0.54 |
| 1:B:198:GLN:NE2 | 1:B:305:ASP:H | 2.04 | 0.54 |
| 1:B:206:VAL:HG13 | 1:B:211:TRP:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:94:GLU:OE2 | 1:B:96:ARG:NH2 | 2.41 | 0.53 |
| 1:A:520:ILE:HG13 | 1:A:521:LYS:H | 1.74 | 0.53 |
| 1:B:203:VAL:HG21 | 1:B:234:MET:HB2 | 1.90 | 0.53 |
| 1:B:82:ASP:OD2 | 1:B:84:THR:OG1 | 2.13 | 0.53 |
| 1:A:345:ARG:HG3 | 1:A:347:GLU:H | 1.74 | 0.53 |
| 1:B:109:SER:O | 1:B:113:ILE:HG12 | 2.09 | 0.53 |
| 1:A:182:LYS:HZ3 | 1:A:188:PHE:HB3 | 1.73 | 0.52 |
| 1:B:288:MET:HG2 | 1:B:317:TYR:CZ | 2.45 | 0.52 |
| 1:B:345:ARG:HG3 | 1:B:347:GLU:H | 1.74 | 0.52 |
| 1:A:44:HIS:ND1 | 1:A:97:ASP:OD2 | 2.42 | 0.51 |
| 1:A:500:TRP:CD1 | 1:A:506:ILE:HG12 | 2.46 | 0.51 |
| 1:A:273:VAL:HG22 | 1:A:300:LEU:HD23 | 1.93 | 0.51 |
| 1:A:519:GLN:HB3 | 1:A:537:CYS:H | 1.76 | 0.51 |
| 1:A:334:VAL:HG21 | 1:A:401:ILE:HD12 | 1.94 | 0.50 |
| 1:B:179:LEU:HD13 | 1:B:188:PHE:CZ | 2.47 | 0.50 |
| 1:B:418:LEU:O | 1:B:420:PRO:HD3 | 2.11 | 0.50 |
| 1:B:26:ARG:HD2 | 1:B:108:GLN:NE2 | 2.27 | 0.49 |
| 1:B:499:VAL:HG13 | 1:B:500:TRP:CD1 | 2.47 | 0.49 |
| 1:B:61:ARG:HG2 | 1:B:64:TYR:HB2 | 1.93 | 0.49 |
| 1:A:520:ILE:CD1 | 1:A:546:GLU:C | 2.75 | 0.49 |
| 1:A:499:VAL:HG13 | 1:A:500:TRP:CD1 | 2.47 | 0.49 |
| 1:B:36:ILE:HD12 | 1:B:141:LYS:HB3 | 1.94 | 0.49 |
| 1:A:448:GLY:N | 1:A:452:ASP:O | 2.31 | 0.49 |
| 1:B:28:VAL:HG11 | 1:B:94:GLU:HG3 | 1.93 | 0.49 |
| 1:B:76:LEU:CD1 | 1:B:93:CYS:HB3 | 2.43 | 0.48 |
| 1:B:334:VAL:HG21 | 1:B:401:ILE:HD12 | 1.94 | 0.48 |
| 1:A:515:CYS:SG | 1:A:532:TRP:NE1 | 2.85 | 0.48 |
| 1:A:248:ILE:HB | 1:A:260:LEU:HD13 | 1.94 | 0.48 |
| 1:A:474:MET:O | 1:A:478:TYR:HB3 | 2.12 | 0.48 |
| 1:A:418:LEU:O | 1:A:420:PRO:HD3 | 2.13 | 0.48 |
| 1:A:179:LEU:HD13 | 1:A:188:PHE:CZ | 2.49 | 0.47 |
| 1:A:288:MET:HG2 | 1:A:317:TYR:CZ | 2.49 | 0.47 |
| 1:A:445:ASN:HB2 | 1:A:455:LEU:HD12 | 1.95 | 0.47 |
| 1:A:206:VAL:HG13 | 1:A:211:TRP:HB2 | 1.96 | 0.47 |
| 1:A:144:VAL:HG11 | 1:A:411:LEU:HD21 | 1.96 | 0.47 |
| 1:B:76:LEU:HD11 | 1:B:93:CYS:HB3 | 1.96 | 0.47 |
| 1:B:168:PRO:HG2 | 1:B:437:LEU:HD23 | 1.97 | 0.47 |
| 1:A:76:LEU:CD1 | 1:A:93:CYS:HB3 | 2.45 | 0.47 |
| 1:B:28:VAL:HG22 | 1:B:96:ARG:HG2 | 1.97 | 0.47 |
| 1:B:489:ASN:C | 1:B:489:ASN:HD22 | 2.18 | 0.47 |
| 1:B:470:ASN:ND2 | 1:B:499:VAL:HG23 | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:187:TYR:CD1 | 1:B:438:LEU:HD22 | 2.50 | 0.46 |
| 1:A:489:ASN:C | 1:A:489:ASN:HD22 | 2.19 | 0.46 |
| 1:B:87:PRO:O | 1:B:89:ILE:HD12 | 2.16 | 0.45 |
| 1:B:117:LEU:HD13 | 1:B:117:LEU:O | 2.15 | 0.45 |
| 1:A:521:LYS:HD3 | 1:A:537:CYS:HA | 1.99 | 0.45 |
| 1:A:187:TYR:CD1 | 1:A:438:LEU:HD22 | 2.51 | 0.45 |
| 1:B:502:LYS:HG2 | 1:B:503:LYS:N | 2.32 | 0.45 |
| 1:A:28:VAL:HG22 | 1:A:96:ARG:HG2 | 1.97 | 0.45 |
| 1:A:96:ARG:HD3 | 1:A:108:GLN:HB3 | 1.98 | 0.45 |
| 1:A:470:ASN:ND2 | 1:A:499:VAL:HG23 | 2.31 | 0.45 |
| 1:B:283:VAL:HG11 | 1:B:307:TRP:CE3 | 2.52 | 0.45 |
| 1:B:367:LEU:HB3 | 1:B:370:PHE:CD2 | 2.51 | 0.44 |
| 1:B:244:HIS:CE1 | 1:B:246:TYR:CZ | 3.05 | 0.44 |
| 1:B:448:GLY:N | 1:B:452:ASP:O | 2.37 | 0.44 |
| 1:A:389:THR:HG22 | 1:A:390:HIS:ND1 | 2.33 | 0.44 |
| 1:B:114:ARG:O | 1:B:117:LEU:HB2 | 2.18 | 0.44 |
| 1:B:184:LEU:HD22 | 1:B:185:PHE:CZ | 2.53 | 0.44 |
| 1:B:356:GLN:O | 1:B:360:GLN:HG3 | 2.18 | 0.44 |
| 1:A:251:ASN:OD1 | 1:A:252:ALA:N | 2.51 | 0.44 |
| 1:B:389:THR:HG22 | 1:B:390:HIS:ND1 | 2.32 | 0.44 |
| 1:A:87:PRO:O | 1:A:89:ILE:HD12 | 2.16 | 0.44 |
| 1:B:394:ASP:HB3 | 1:B:397:MET:HB2 | 2.00 | 0.44 |
| 1:B:500:TRP:CD1 | 1:B:506:ILE:HG12 | 2.52 | 0.44 |
| 1:A:315:ASP:HA | 1:A:318:GLN:HE21 | 1.82 | 0.44 |
| 1:B:144:VAL:HG11 | 1:B:411:LEU:HD21 | 2.00 | 0.44 |
| 1:A:94:GLU:HG2 | 1:A:112:PHE:HE1 | 1.83 | 0.44 |
| 1:A:356:GLN:O | 1:A:360:GLN:HG3 | 2.18 | 0.43 |
| 1:B:204:ASP:OD2 | 1:B:487:TRP:HH2 | 2.01 | 0.43 |
| 1:B:346:PRO:HD3 | 1:B:359:TRP:CE3 | 2.53 | 0.43 |
| 1:A:213:TYR:CD2 | 1:A:271:ALA:HB2 | 2.54 | 0.43 |
| 1:A:63:GLN:HG2 | 1:A:394:ASP:HA | 2.00 | 0.43 |
| 1:B:430:LYS:HA | 1:B:431:PRO:HA | 1.86 | 0.43 |
| 1:B:26:ARG:NH2 | 1:B:55:ARG:O | 2.52 | 0.43 |
| 1:B:337:PHE:HD2 | 1:B:393:GLN:HE21 | 1.66 | 0.42 |
| 1:B:38:GLY:N | 1:B:145:GLY:O | 2.52 | 0.42 |
| 1:B:213:TYR:CD2 | 1:B:271:ALA:HB2 | 2.55 | 0.42 |
| 1:A:334:VAL:HG12 | 1:A:337:PHE:H | 1.84 | 0.42 |
| 1:A:346:PRO:HD3 | 1:A:359:TRP:CE3 | 2.54 | 0.42 |
| 1:B:66:ILE:HG13 | 1:B:358:PHE:CG | 2.54 | 0.42 |
| 1:B:334:VAL:HG12 | 1:B:337:PHE:H | 1.85 | 0.42 |
| 1:A:66:ILE:HG13 | 1:A:358:PHE:CG | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:184:LEU:HD22 | 1:A:185:PHE:CZ | 2.55 | 0.42 |
| 1:A:283:VAL:HG11 | 1:A:307:TRP:CE3 | 2.55 | 0.41 |
| 1:A:308:ALA:HB1 | 1:A:328:LYS:HA | 2.01 | 0.41 |
| 1:B:182:LYS:HZ3 | 1:B:188:PHE:HB3 | 1.85 | 0.41 |
| 1:B:280:GLY:HA3 | 1:B:310:ARG:NH1 | 2.34 | 0.41 |
| 1:B:515:CYS:HB3 | 1:B:519:GLN:O | 2.20 | 0.41 |
| 1:B:346:PRO:HG3 | 1:B:359:TRP:CG | 2.55 | 0.41 |
| 1:A:214:VAL:HG12 | 1:A:273:VAL:HB | 2.02 | 0.41 |
| 1:B:359:TRP:CD1 | 1:B:367:LEU:HD21 | 2.56 | 0.41 |
| 1:B:168:PRO:HA | 1:B:187:TYR:HB3 | 2.03 | 0.41 |
| 1:B:118:ILE:HD12 | 1:B:142:PRO:HD3 | 2.03 | 0.41 |
| 1:A:113:ILE:HG22 | 1:A:167:ILE:HD12 | 2.03 | 0.41 |
| 1:A:217:VAL:HG22 | 1:A:246:TYR:HB2 | 2.02 | 0.41 |
| 1:B:72:MET:HA | 1:B:404:ILE:HD13 | 2.03 | 0.41 |
| 1:B:340:TYR:OH | 1:B:351:ARG:NH2 | 2.36 | 0.41 |
| 1:A:153:SER:O | 1:A:157:GLN:NE2 | 2.54 | 0.41 |
| 1:A:359:TRP:CD1 | 1:A:367:LEU:HD21 | 2.55 | 0.41 |
| 1:A:430:LYS:HA | 1:A:431:PRO:HA | 1.84 | 0.40 |
| 1:B:111:GLU:O | 1:B:115:ASP:HB2 | 2.22 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 502/877 (57%) | 471 (94%) | 31 (6%) | 0 | 100 100 |
| 1 | B | 481/877 (55%) | 453 (94%) | 27 (6%) | 1 (0%) | 47 79 |
| All | All | 983/1754 (56%) | 924 (94%) | 58 (6%) | 1 (0%) | 51 84 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 521 | LYS |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 412/763 (54%) | 411 (100%) | 1 (0%) | 93 96 |
| 1 | B | 399/763 (52%) | 397 (100%) | 2 (0%) | 88 93 |
| All | All | 811/1526 (53%) | 808 (100%) | 3 (0%) | 91 94 |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 489 | ASN |
| 1 | B | 465 | ARG |
| 1 | B | 489 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 74 | HIS |
| 1 | A | 157 | GLN |
| 1 | A | 166 | ASN |
| 1 | A | 198 | GLN |
| 1 | A | 364 | GLN |
| 1 | B | 45 | HIS |
| 1 | B | 74 | HIS |
| 1 | B | 157 | GLN |
| 1 | B | 166 | ASN |
| 1 | B | 198 | GLN |
| 1 | B | 218 | HIS |
| 1 | B | 244 | HIS |
| 1 | B | 364 | GLN |

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | NAG | A | 902 | 1 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.59 | 0 |
| 2 | NAG | A | 904 | 1 | 14,14,15 | 0.45 | 0 | 17,19,21 | 0.67 | 1 (5%) |
| 2 | NAG | B | 902 | 1 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.63 | 1 (5%) |
| 2 | NAG | B | 903 | 1 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.56 | 0 |
| 2 | NAG | A | 901 | 1 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.46 | 0 |
| 2 | NAG | A | 903 | 1 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.48 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | NAG | A | 902 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | A | 904 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | B | 902 | 1 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | NAG | B | 903 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | A | 901 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | A | 903 | 1 | - | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 902 | NAG | C1-O5-C5 | 2.22 | 115.20 | 112.19 |
| 2 | A | 904 | NAG | C1-O5-C5 | 2.19 | 115.15 | 112.19 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 901 | NAG | O5-C5-C6-O6 |
| 2 | A | 901 | NAG | C4-C5-C6-O6 |
| 2 | A | 904 | NAG | O5-C5-C6-O6 |
| 2 | A | 904 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

No monomer is involved in short contacts.

## 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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 | 506/877 (57%) | -0.19 | 6 (1%) | 79 | 70 | 127, 180, 254, 270 | 0 |
| 1 | B | 487/877 (55%) | -0.20 | 6 (1%) | 79 | 70 | 114, 183, 252, 292 | 0 |
| All | All | 993/1754 (56%) | -0.19 | 12 (1%) | 79 | 70 | 114, 181, 254, 292 | 0 |

All (12) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 54 | GLU | 4.6 |
| 1 | B | 222 | ASN | 3.8 |
| 1 | A | 51 | LYS | 3.5 |
| 1 | B | 372 | GLN | 3.3 |
| 1 | A | 52 | VAL | 3.2 |
| 1 | B | 371 | PRO | 2.9 |
| 1 | B | 221 | GLY | 2.7 |
| 1 | A | 55 | ARG | 2.7 |
| 1 | A | 24 | GLU | 2.5 |
| 1 | A | 53 | HIS | 2.5 |
| 1 | B | 374 | ASN | 2.4 |
| 1 | B | 195 | ASP | 2.3 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | NAG | A | 903 | 14/15 | 0.59 | 0.26 | 214,233,238,244 | 0 |
| 2 | NAG | A | 901 | 14/15 | 0.62 | 0.28 | 200,209,217,221 | 0 |
| 2 | NAG | B | 902 | 14/15 | 0.64 | 0.27 | 184,210,226,226 | 0 |
| 2 | NAG | A | 902 | 14/15 | 0.72 | 0.24 | 200,219,226,230 | 0 |
| 2 | NAG | A | 904 | 14/15 | 0.84 | 0.16 | 193,206,212,217 | 0 |
| 2 | NAG | B | 903 | 14/15 | 0.84 | 0.24 | 222,240,245,248 | 0 |
| 3 | MG | B | 901 | 1/1 | 0.92 | 0.10 | 165,165,165,165 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.