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

Feb 1, 2016 – 06:07 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 2VZV |
| Title | : | SUBSTRATE COMPLEX OF AMYCOLATOPSIS ORIENTALIS EXO-CHITOSANASE CSXA E541A WITH CHITOSAN |
| Authors | : | Lammerts Van Bueren, A.; Ghinet, M.G.; Gregg, K.; Fleury, A.; Brzezinski, R.; Boraston, A.B. |
| Deposited on | : | 2008-08-05 |
| Resolution | : | 2.70 Å(reported) |

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

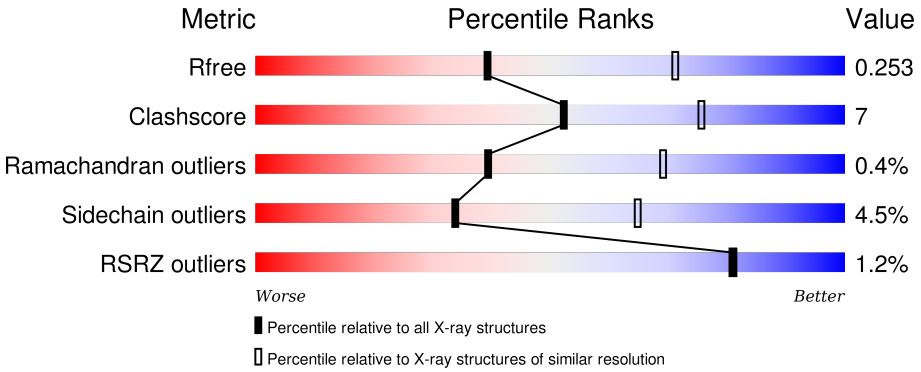
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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 | 2103 (2.70-2.70) |
| Clashscore | 102246 | 2422 (2.70-2.70) |
| Ramachandran outliers | 100387 | 2382 (2.70-2.70) |
| Sidechain outliers | 100360 | 2382 (2.70-2.70) |
| RSRZ outliers | 91569 | 2107 (2.70-2.70) |

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 <=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 | 1032 | % 70% 13% • 17% |
| 1 | B | 1032 | % 69% 12% • 17% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 2 | GCS | A | 1900 | - | - | - | X |
| 2 | GCS | B | 1900 | - | - | - | X |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13565 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 EXO-BETA-D-GLUCOSAMINIDASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 858 | Total | C | N | O | S | 4 | 0 | 1 |
| | | | 6548 | 4113 | 1133 | 1285 | 17 | | | |
| 1 | B | 858 | Total | C | N | O | S | 4 | 0 | 1 |
| | | | 6548 | 4113 | 1133 | 1285 | 17 | | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 541 | ALA | GLU | ENGINEERED MUTATION | UNP Q56F26 |
| A | 750 | ASN | TRP | CONFLICT | UNP Q56F26 |
| B | 541 | ALA | GLU | ENGINEERED MUTATION | UNP Q56F26 |
| B | 750 | ASN | TRP | CONFLICT | UNP Q56F26 |

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 2 | Total | C | N | O | 0 | 0 |
| | | | 23 | 12 | 2 | 9 | | |
| 2 | B | 2 | Total | C | N | O | 0 | 0 |
| | | | 23 | 12 | 2 | 9 | | |

- Molecule 3 is water.

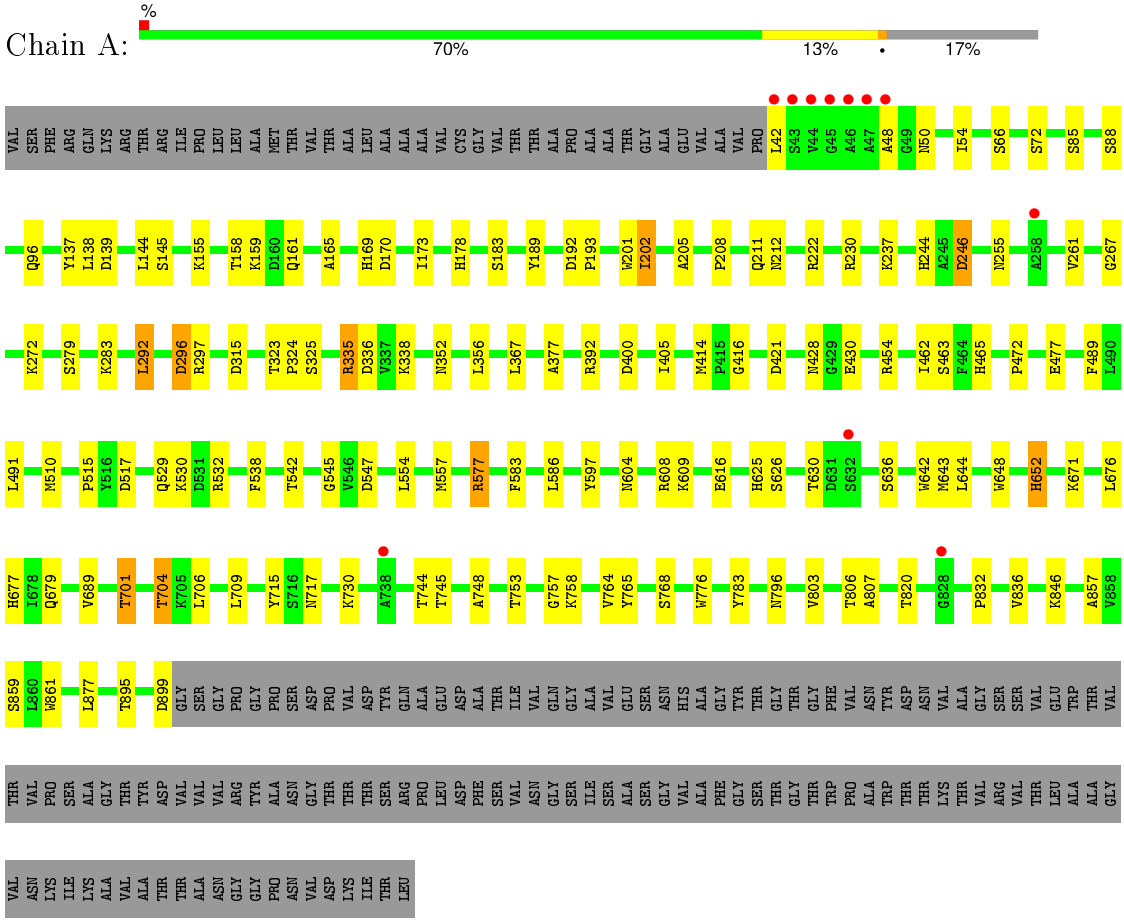
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | A | 212 | Total | O | 0 | 0 |
| | | | 212 | 212 | | |
| 3 | B | 211 | Total | O | 0 | 0 |
| | | | 211 | 211 | | |

# 3 Residue-property plots (i)

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

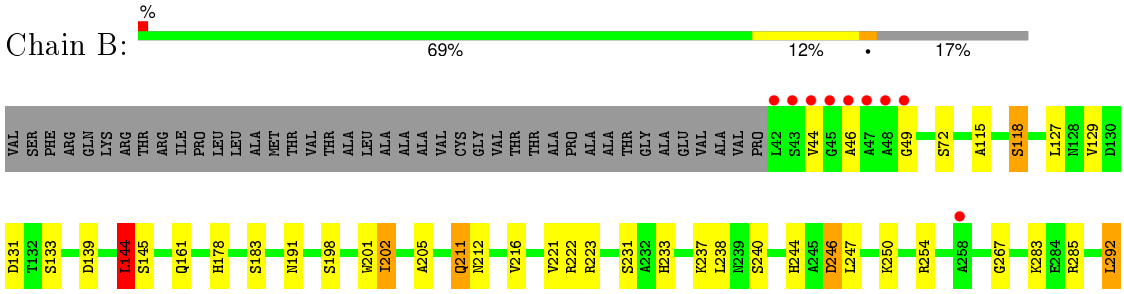
- Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

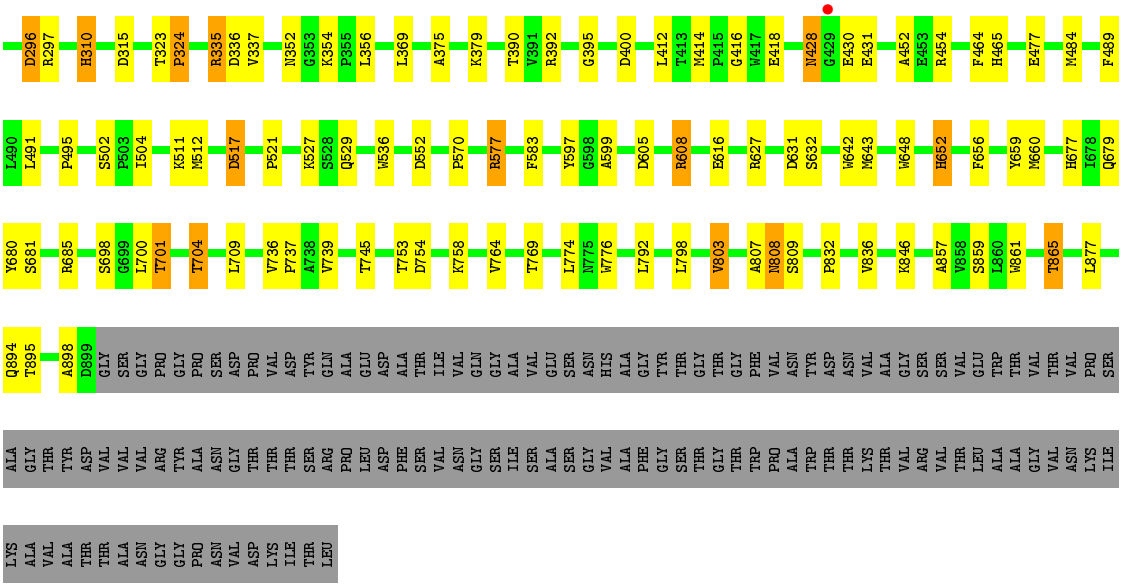
Chain A:




- Molecule 1: EXO-BETA-D-GLUCOSAMINIDASE

Chain B:




D296 R297 H310 D315 T323 P324 R335 D336 V337 N352 G353 K354 P355 L356 L369 A375 K379 T390 V391 R392 G395 D400 L412 T413 N414 P415 G416 W417 E418 N428 G429 E430 E431 A452 E453 R454 F464 H465 E477 M484 F489
L490 L491 P495 S502 P503 I504 K511 M512 D517 P521 K527 S528 Q529 W536 D552 P570 R577 F583 Y597 G598 A599 D605 R608 E616 R627 D631 S632 W642 M643 W648 H652 F656 Y659 M660 H677 I678 Q679
Y680 S681 R685 S698 G699 L700 T701 T704 L709 V736 P737 A738 V739 T745 T753 D754 K758 V764 T769 L774 N775 W776 L792 L798 V803 A807 N808 S809 P832 V836 K846 A857 V858 S859 L860 W861 T865 L877
Q894 T895 A898 D899 GLY SER GLY PRO GLY PRO SER ASP PRO VAL ASP TYR GLN ALA GLU ASP ALA THR ILE VAL GLN GLY ALA VAL GLU SER ASN HIS ALA GLY TYR THR GLY THR GLY PHE VAL ASN TYR ASP ASN VAL ALA GLY SER SER VAL GLU TRP THR VAL THR VAL PRO SER
ALA GLY THR TYR ASP VAL VAL VAL ARG TYR ALA ASN GLY THR THR THR SER ARG PRO LEU ASP PHE SER VAL ASN GLY SER ILE SER ALA SER GLY VAL ALA PHE GLY SER THR GLY THR TRP PRO ALA TRP THR THR LYS THR VAL ARG VAL THR LEU GLU ALA ALA GLY VAL ASN LYS ILE
LYS ALA VAL ALA THR THR ALA ASN GLY GLY PRO ASN VAL ASP LYS ILE THR LEU

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 86.86Å 121.41Å 184.71Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 185.70 – 2.70<br>19.97 – 2.70 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 91.3 (185.70-2.70)<br>91.6 (19.97-2.70) | Depositor<br>EDS |
| $R_{merge}$ | 0.12 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 4.33 (at 2.71Å) | Xtriage |
| Refinement program | REFMAC 5.2.0019 | Depositor |
| R, $R_{free}$ | 0.182 , 0.255<br>0.184 , 0.253 | Depositor<br>DCC |
| $R_{free}$ test set | 2545 reflections (5.40%) | DCC |
| Wilson B-factor (Å$^2$) | 20.5 | Xtriage |
| Anisotropy | 0.152 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.35 , 24.8 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.45$, $< L^2 > = 0.28$ | Xtriage |
| Outliers | 0 of 49770 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 13565 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 15.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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

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 | 3/6711 (0.0%) | 0.66 | 5/9158 (0.1%) |
| 1 | B | 0.52 | 3/6711 (0.0%) | 0.66 | 8/9158 (0.1%) |
| All | All | 0.53 | 6/13422 (0.0%) | 0.66 | 13/18316 (0.1%) |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 430 | GLU | CB-CG | 16.66 | 1.83 | 1.52 |
| 1 | B | 430 | GLU | CB-CG | 10.96 | 1.73 | 1.52 |
| 1 | B | 246 | ASP | CB-CG | 7.18 | 1.66 | 1.51 |
| 1 | B | 296 | ASP | CB-CG | 6.59 | 1.65 | 1.51 |
| 1 | A | 246 | ASP | CB-CG | 6.17 | 1.64 | 1.51 |

The worst 5 of 13 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 246 | ASP | CB-CG-OD1 | 15.77 | 132.49 | 118.30 |
| 1 | B | 246 | ASP | CB-CG-OD1 | 15.13 | 131.92 | 118.30 |
| 1 | B | 296 | ASP | CB-CG-OD1 | 14.89 | 131.71 | 118.30 |
| 1 | A | 296 | ASP | CB-CG-OD2 | 11.98 | 129.08 | 118.30 |
| 1 | A | 430 | GLU | CA-CB-CG | -11.08 | 89.02 | 113.40 |

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 | 6548 | 0 | 6327 | 81 | 9 |
| 1 | B | 6548 | 0 | 6327 | 92 | 9 |
| 2 | A | 23 | 0 | 23 | 0 | 0 |
| 2 | B | 23 | 0 | 23 | 2 | 0 |
| 3 | A | 212 | 0 | 0 | 9 | 0 |
| 3 | B | 211 | 0 | 0 | 17 | 0 |
| All | All | 13565 | 0 | 12700 | 173 | 9 |

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 7.

The worst 5 of 173 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:201:TRP:HE1 | 1:B:212:ASN:HD21 | 1.00 | 0.93 |
| 1:B:310:HIS:CE1 | 3:B:2079:HOH:O | 2.23 | 0.90 |
| 1:B:577:ARG:HG2 | 1:B:583:PHE:O | 1.75 | 0.85 |
| 1:B:244:HIS:HE2 | 1:B:246:ASP:CG | 1.82 | 0.80 |
| 1:B:115:ALA:O | 1:B:118:SER:HB2 | 1.82 | 0.79 |

The worst 5 of 9 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:A:246:ASP:OD2 | 1:B:296:ASP:OD1[3_554] | 1.58 | 0.62 |
| 1:A:296:ASP:OD2 | 1:B:246:ASP:OD1[3_554] | 1.61 | 0.59 |
| 1:A:296:ASP:OD2 | 1:B:246:ASP:OD2[3_554] | 1.61 | 0.59 |
| 1:A:246:ASP:OD1 | 1:B:296:ASP:OD1[3_554] | 1.75 | 0.45 |
| 1:A:246:ASP:OD2 | 1:B:296:ASP:CG[3_554] | 1.82 | 0.38 |

## 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 | 856/1032 (83%) | 811 (95%) | 42 (5%) | 3 (0%) | 39 69 |
| 1 | B | 856/1032 (83%) | 810 (95%) | 42 (5%) | 4 (0%) | 34 63 |
| All | All | 1712/2064 (83%) | 1621 (95%) | 84 (5%) | 7 (0%) | 39 69 |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 758 | LYS |
| 1 | B | 202 | ILE |
| 1 | A | 202 | ILE |
| 1 | A | 205 | ALA |
| 1 | B | 205 | ALA |

### 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 | 701/833 (84%) | 672 (96%) | 29 (4%) | 37 69 |
| 1 | B | 701/833 (84%) | 667 (95%) | 34 (5%) | 31 61 |
| All | All | 1402/1666 (84%) | 1339 (96%) | 63 (4%) | 34 65 |

5 of 63 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 895 | THR |
| 1 | B | 237 | LYS |
| 1 | B | 808 | ASN |
| 1 | B | 118 | SER |
| 1 | B | 144 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 796 | ASN |
| 1 | B | 178 | HIS |
| 1 | B | 796 | ASN |
| 1 | B | 128 | ASN |
| 1 | B | 169 | HIS |

#### 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)

4 carbohydrates are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | GCS | A | 1899 | 2 | 11,11,12 | 0.57 | 0 | 13,15,17 | 1.51 | 2 (15%) |
| 2 | GCS | A | 1900 | 2 | 12,12,12 | 1.66 | 4 (33%) | 15,17,17 | 1.39 | 3 (20%) |
| 2 | GCS | B | 1899 | 2 | 11,11,12 | 0.77 | 0 | 13,15,17 | 1.98 | 2 (15%) |
| 2 | GCS | B | 1900 | 2 | 12,12,12 | 1.37 | 1 (8%) | 15,17,17 | 1.50 | 2 (13%) |

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 | GCS | A | 1899 | 2 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | GCS | A | 1900 | 2 | - | 0/2/22/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | GCS | B | 1899 | 2 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | GCS | B | 1900 | 2 | - | 0/2/22/22 | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | A | 1900 | GCS | C6-C5 | 2.08 | 1.59 | 1.51 |
| 2 | A | 1900 | GCS | C4-C5 | 2.12 | 1.57 | 1.53 |
| 2 | A | 1900 | GCS | O5-C5 | 2.25 | 1.50 | 1.44 |
| 2 | B | 1900 | GCS | O4-C4 | 2.71 | 1.49 | 1.43 |
| 2 | A | 1900 | GCS | O4-C4 | 2.72 | 1.49 | 1.43 |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 1899 | GCS | O5-C5-C6 | -2.68 | 101.55 | 107.35 |
| 2 | B | 1899 | GCS | C4-C3-C2 | -2.30 | 108.28 | 111.39 |
| 2 | B | 1900 | GCS | C6-C5-C4 | -2.05 | 107.95 | 113.02 |
| 2 | A | 1900 | GCS | O5-C5-C4 | 2.21 | 113.83 | 109.68 |
| 2 | A | 1900 | GCS | O1-C1-C2 | 2.43 | 114.55 | 109.02 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 1900 | GCS | 2 | 0 |

## 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

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 | 858/1032 (83%) | -0.42 | 11 (1%) | 79 | 79 | 3, 15, 27, 66 | 1 (0%) |
| 1 | B | 858/1032 (83%) | -0.41 | 10 (1%) | 81 | 81 | 3, 15, 25, 68 | 1 (0%) |
| All | All | 1716/2064 (83%) | -0.42 | 21 (1%) | 81 | 81 | 3, 15, 26, 68 | 2 (0%) |

The worst 5 of 21 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 43 | SER | 7.8 |
| 1 | A | 47 | ALA | 6.3 |
| 1 | A | 44 | VAL | 6.0 |
| 1 | A | 45 | GLY | 5.9 |
| 1 | B | 46 | ALA | 5.6 |

## 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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 2 | GCS | B | 1900 | 12/12 | 0.90 | 0.20 | 2.72 | 28,33,34,35 | 0 |
| 2 | GCS | A | 1900 | 12/12 | 0.88 | 0.20 | 2.68 | 26,28,28,29 | 0 |
| 2 | GCS | B | 1899 | 11/12 | 0.94 | 0.15 | 1.56 | 19,22,23,24 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 2 | GCS | A | 1899 | 11/12 | 0.96 | 0.15 | 1.01 | 15,19,21,22 | 0 |

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.