



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 08:05 PM EDT

PDB ID : 5TAP
EMDB ID: : EMD-8381
Title : Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 4.40 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

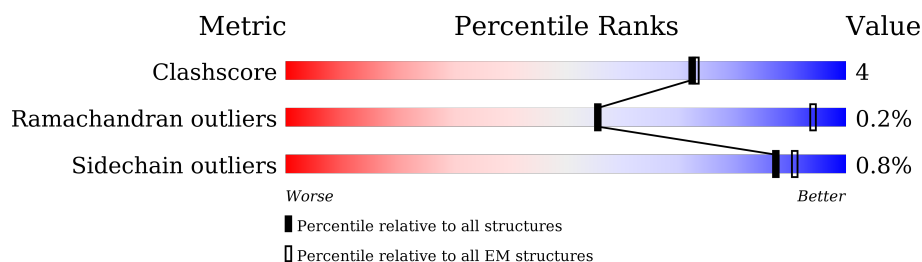
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 108 | 85% 14% . |
| 1 | F | 108 | 85% 14% . |
| 1 | H | 108 | 83% 16% . |
| 1 | J | 108 | 84% 15% . |
| 2 | B | 4416 | 85% 9% 5% |
| 2 | E | 4416 | 85% 9% 5% |
| 2 | G | 4416 | 86% 9% 5% |
| 2 | I | 4416 | 86% 9% 5% |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

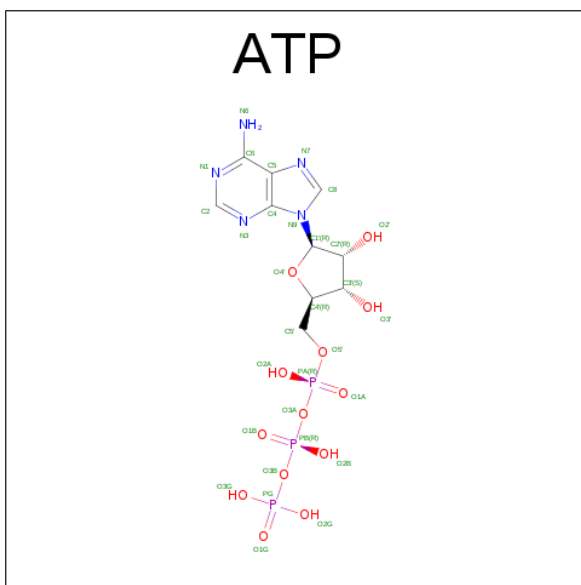
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1 | F | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 516 | 144 | 154 | 4 | | |
| 1 | A | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 516 | 144 | 154 | 4 | | |
| 1 | H | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 516 | 144 | 154 | 4 | | |
| 1 | J | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 516 | 144 | 154 | 4 | | |

- Molecule 2 is a protein called Ryanodine receptor 1.

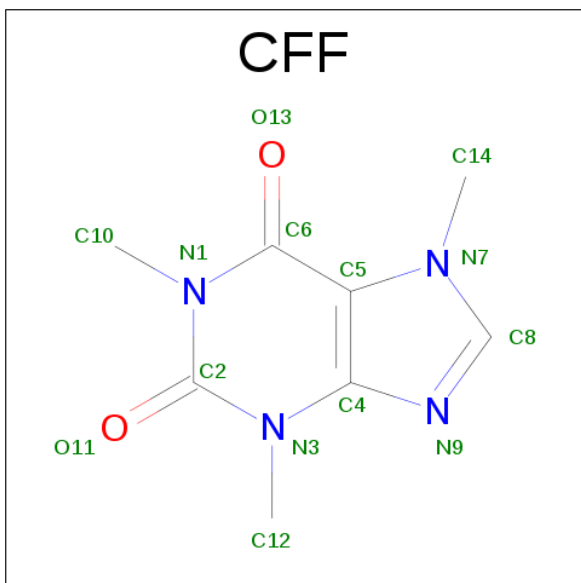
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 2 | B | 4194 | Total | C | N | O | S | 0 | 0 |
| | | | 29499 | 18686 | 5228 | 5428 | 157 | | |
| 2 | E | 4194 | Total | C | N | O | S | 0 | 0 |
| | | | 29499 | 18686 | 5228 | 5428 | 157 | | |
| 2 | I | 4194 | Total | C | N | O | S | 0 | 0 |
| | | | 29499 | 18686 | 5228 | 5428 | 157 | | |
| 2 | G | 4194 | Total | C | N | O | S | 0 | 0 |
| | | | 29499 | 18686 | 5228 | 5428 | 157 | | |

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 3 | B | 1 | Total 31 | C 10 | N 5 | O 13 | P 3 | 0 |
| 3 | E | 1 | Total 31 | C 10 | N 5 | O 13 | P 3 | 0 |
| 3 | I | 1 | Total 31 | C 10 | N 5 | O 13 | P 3 | 0 |
| 3 | G | 1 | Total 31 | C 10 | N 5 | O 13 | P 3 | 0 |

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 4 | B | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 4 | 2 | |
| 4 | E | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 4 | 2 | |
| 4 | I | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 4 | 2 | |
| 4 | G | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 4 | 2 | |


- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

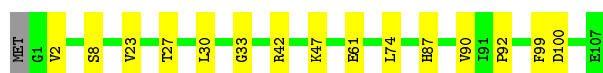
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 5 | G | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 5 | B | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 5 | I | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 5 | E | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

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. 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. 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.

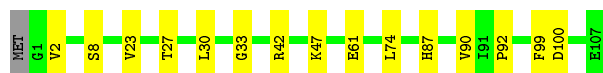
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




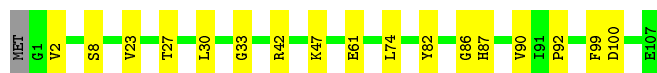
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




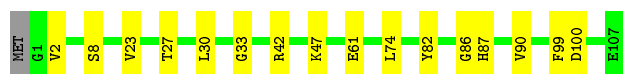
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




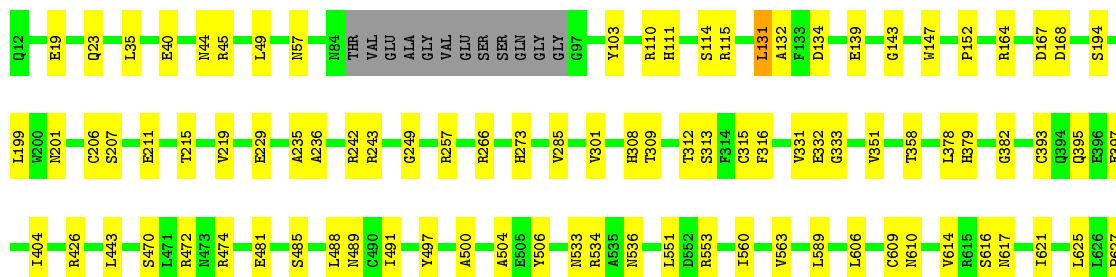
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryanodine receptor 1

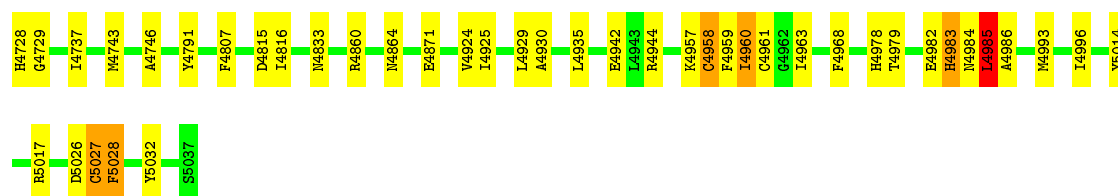
Chain B: 





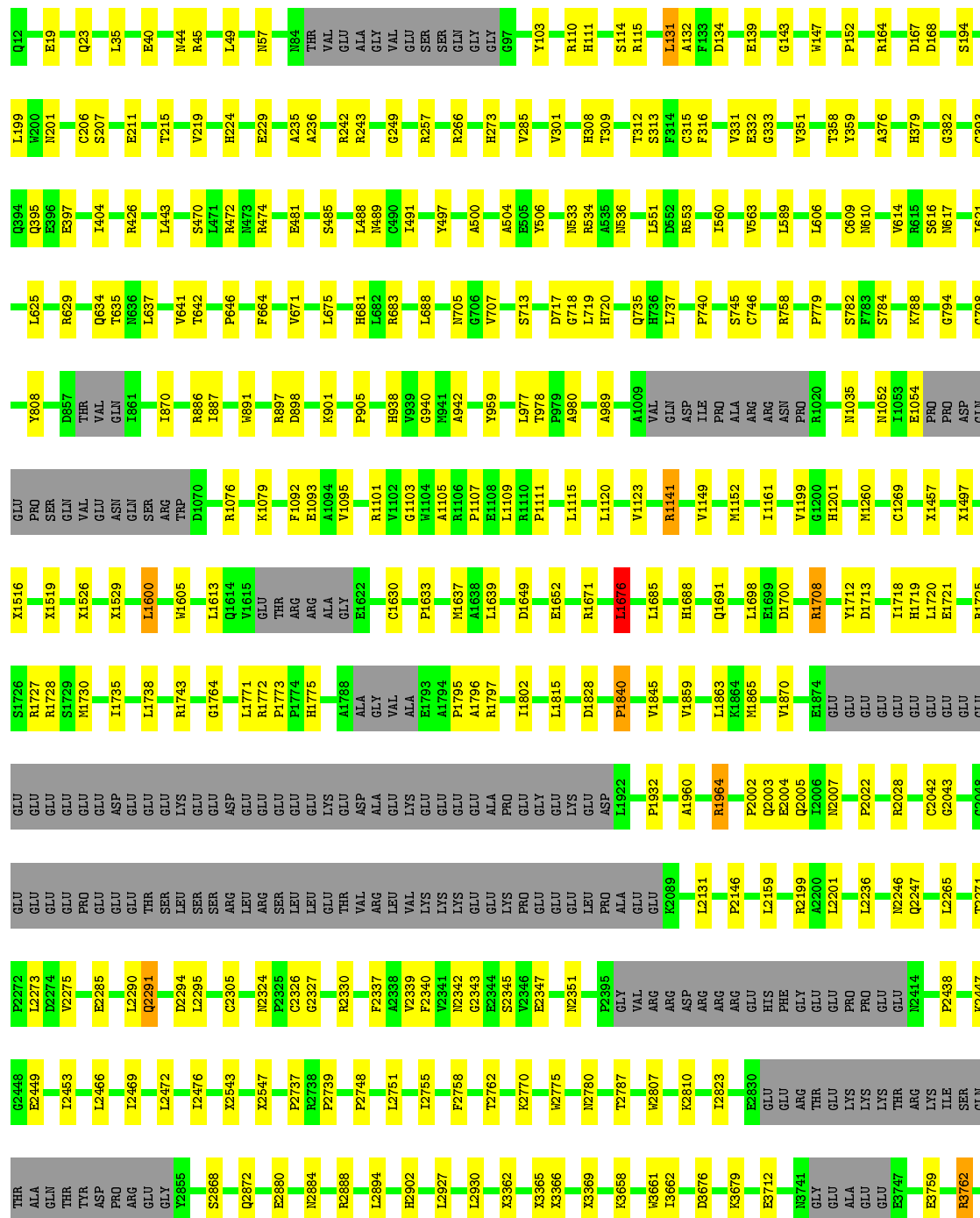






• Molecule 2: Ryanodine receptor 1

Chain I: 86% 9% 5%



| | | | | | |
|-------|-------|-------|-------|-------|-------|
| D4873 | ALA | P4106 | V3779 | SER | GLU |
| V4924 | GLY | M4120 | L3780 | GLN | GLU |
| I4925 | GLU | E4126 | Q3781 | THR | N2414 |
| L4929 | ALA | M4130 | S3784 | GLN | P2438 |
| A4930 | GLY | R4131 | K3787 | TYR | K2447 |
| Q4933 | ASP | D4138 | L3805 | ASP | G2446 |
| G4934 | GLU | M4142 | N3809 | PRO | E2449 |
| L4935 | ASP | V4145 | K3815 | ARG | I2453 |
| E4942 | GLU | L4166 | L3817 | GLY | Y2855 |
| L4945 | N4626 | S4169 | Q3830 | Y2855 | L2466 |
| R4944 | M4639 | R4189 | Q3833 | S2868 | I2469 |
| K4951 | E4640 | I4190 | L3842 | Q2872 | L2472 |
| K4957 | P4641 | K4230 | Q3850 | N2884 | I2476 |
| C4958 | V4666 | L4567 | K3873 | R2888 | P2737 |
| F4959 | E4674 | L4567 | K3873 | L2927 | R2738 |
| I4960 | K4680 | F4571 | N3896 | L2930 | P2739 |
| C4961 | K4686 | F4575 | F3899 | L2930 | T2742 |
| G4962 | Y4687 | V4582 | T3907 | X3362 | P2748 |
| I4963 | I4688 | F4587 | T3910 | X3365 | L2751 |
| F4968 | V4697 | GLY | T3911 | X3366 | I2755 |
| H4978 | K4698 | GLU | L3923 | X3369 | F2758 |
| T4979 | G4699 | GLU | S3929 | K3658 | T2762 |
| E4982 | Q4700 | ASP | Y3937 | W3661 | K2770 |
| H4983 | W4701 | ASP | M3955 | D3676 | W2775 |
| M4984 | Y4715 | GLY | V3961 | K3679 | W2807 |
| A4986 | H4728 | ASP | G3971 | E3712 | K2810 |
| M4993 | G4729 | GLY | L4019 | N3741 | E2811 |
| I4996 | I4737 | LEU | M4034 | GLY | I2823 |
| D5026 | M4743 | ALA | D4063 | GLU | E2830 |
| C5027 | A4746 | ALA | R4085 | GLU | GLU |
| F5028 | Y4791 | ALA | T4104 | GLU | ARG |
| Y5032 | F4807 | GLY | G4105 | THR | THR |
| S5037 | D4815 | GLY | | LYS | LYS |
| | I4816 | SER | | LYS | LYS |
| | M4833 | GLY | | THR | THR |
| | R4860 | GLY | | ARG | ARG |
| | M4864 | SER | | ILE | ILE |
| | K4865 | TRP | | | |
| | E4871 | GLY | | | |
| | P4872 | GLY | | | |

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------|-----------|
| Reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of particles used | 55564 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | Not provided | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, ZN, ATP

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 | $\# Z > 2$ | RMSZ | $\# Z > 2$ |
| 1 | A | 0.32 | 0/834 | 0.51 | 0/1123 |
| 1 | F | 0.32 | 0/834 | 0.51 | 0/1123 |
| 1 | H | 0.32 | 0/834 | 0.51 | 0/1123 |
| 1 | J | 0.32 | 0/834 | 0.51 | 0/1123 |
| 2 | B | 0.31 | 1/25428 (0.0%) | 0.54 | 9/34534 (0.0%) |
| 2 | E | 0.31 | 1/25428 (0.0%) | 0.54 | 9/34534 (0.0%) |
| 2 | G | 0.31 | 1/25428 (0.0%) | 0.54 | 9/34534 (0.0%) |
| 2 | I | 0.31 | 1/25428 (0.0%) | 0.54 | 9/34534 (0.0%) |
| All | All | 0.31 | 4/105048 (0.0%) | 0.54 | 36/142628 (0.0%) |

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 | 1 |
| 1 | F | 0 | 1 |
| 1 | H | 0 | 1 |
| 1 | J | 0 | 1 |
| 2 | B | 0 | 15 |
| 2 | E | 0 | 15 |
| 2 | G | 0 | 15 |
| 2 | I | 0 | 15 |
| All | All | 0 | 64 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | I | 2476 | ILE | C-N | 5.37 | 1.44 | 1.34 |
| 2 | B | 2476 | ILE | C-N | 5.34 | 1.44 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2 | E | 2476 | ILE | C-N | 5.33 | 1.44 | 1.34 |
| 2 | G | 2476 | ILE | C-N | 5.30 | 1.44 | 1.34 |

The worst 5 of 36 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2 | I | 131 | LEU | CA-CB-CG | 8.29 | 134.37 | 115.30 |
| 2 | G | 131 | LEU | CA-CB-CG | 8.28 | 134.35 | 115.30 |
| 2 | B | 131 | LEU | CA-CB-CG | 8.27 | 134.32 | 115.30 |
| 2 | E | 131 | LEU | CA-CB-CG | 8.27 | 134.32 | 115.30 |
| 2 | G | 1600 | LEU | CA-CB-CG | 7.05 | 131.52 | 115.30 |

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 8 | SER | Peptide |
| 2 | B | 139 | GLU | Peptide |
| 1 | F | 8 | SER | Peptide |
| 1 | H | 8 | SER | Peptide |
| 1 | J | 8 | SER | 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 | 818 | 0 | 824 | 8 | 0 |
| 1 | F | 818 | 0 | 824 | 8 | 0 |
| 1 | H | 818 | 0 | 824 | 9 | 0 |
| 1 | J | 818 | 0 | 824 | 8 | 0 |
| 2 | B | 29499 | 0 | 24749 | 236 | 0 |
| 2 | E | 29499 | 0 | 24749 | 235 | 0 |
| 2 | G | 29499 | 0 | 24749 | 231 | 0 |
| 2 | I | 29499 | 0 | 24749 | 233 | 0 |
| 3 | B | 31 | 0 | 12 | 2 | 0 |
| 3 | E | 31 | 0 | 12 | 2 | 0 |
| 3 | G | 31 | 0 | 12 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 3 | I | 31 | 0 | 12 | 2 | 0 |
| 4 | B | 14 | 0 | 10 | 0 | 0 |
| 4 | E | 14 | 0 | 10 | 0 | 0 |
| 4 | G | 14 | 0 | 10 | 0 | 0 |
| 4 | I | 14 | 0 | 10 | 0 | 0 |
| 5 | B | 1 | 0 | 0 | 0 | 0 |
| 5 | E | 1 | 0 | 0 | 0 | 0 |
| 5 | G | 1 | 0 | 0 | 0 | 0 |
| 5 | I | 1 | 0 | 0 | 0 | 0 |
| All | All | 121452 | 0 | 102380 | 949 | 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 4.

The worst 5 of 949 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:4230:LYS:HD2 | 2:I:4959:PHE:HE1 | 1.38 | 0.88 |
| 2:E:4230:LYS:HD2 | 2:E:4959:PHE:HE1 | 1.38 | 0.88 |
| 2:B:4230:LYS:HD2 | 2:B:4959:PHE:HE1 | 1.38 | 0.87 |
| 2:G:4230:LYS:HD2 | 2:G:4959:PHE:HE1 | 1.38 | 0.87 |
| 2:B:4983:HIS:H | 2:B:4983:HIS:CD2 | 1.94 | 0.86 |

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 PDB entries followed by that with respect to all EM entries.

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 | 105/108 (97%) | 96 (91%) | 9 (9%) | 0 | 100 | 100 |
| 1 | F | 105/108 (97%) | 96 (91%) | 9 (9%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 1 | H | 105/108 (97%) | 96 (91%) | 9 (9%) | 0 | 100 | 100 |
| 1 | J | 105/108 (97%) | 96 (91%) | 9 (9%) | 0 | 100 | 100 |
| 2 | B | 3235/4416 (73%) | 2906 (90%) | 323 (10%) | 6 (0%) | 52 | 86 |
| 2 | E | 3235/4416 (73%) | 2908 (90%) | 321 (10%) | 6 (0%) | 52 | 86 |
| 2 | G | 3235/4416 (73%) | 2906 (90%) | 323 (10%) | 6 (0%) | 52 | 86 |
| 2 | I | 3235/4416 (73%) | 2906 (90%) | 323 (10%) | 6 (0%) | 52 | 86 |
| All | All | 13360/18096 (74%) | 12010 (90%) | 1326 (10%) | 24 (0%) | 56 | 86 |

5 of 24 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | B | 5028 | PHE |
| 2 | E | 5028 | PHE |
| 2 | I | 5028 | PHE |
| 2 | G | 5028 | PHE |
| 2 | B | 1708 | ARG |

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 PDB entries followed by that with respect to all EM entries.

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 | 88/89 (99%) | 88 (100%) | 0 | 100 | 100 |
| 1 | F | 88/89 (99%) | 88 (100%) | 0 | 100 | 100 |
| 1 | H | 88/89 (99%) | 88 (100%) | 0 | 100 | 100 |
| 1 | J | 88/89 (99%) | 88 (100%) | 0 | 100 | 100 |
| 2 | B | 2493/3022 (82%) | 2472 (99%) | 21 (1%) | 86 | 93 |
| 2 | E | 2493/3022 (82%) | 2472 (99%) | 21 (1%) | 86 | 93 |
| 2 | G | 2493/3022 (82%) | 2472 (99%) | 21 (1%) | 86 | 93 |
| 2 | I | 2493/3022 (82%) | 2472 (99%) | 21 (1%) | 86 | 93 |
| All | All | 10324/12444 (83%) | 10240 (99%) | 84 (1%) | 87 | 93 |

5 of 84 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | E | 4957 | LYS |
| 2 | I | 1600 | LEU |
| 2 | G | 4131 | ARG |
| 2 | E | 4960 | ILE |
| 2 | I | 131 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | E | 3896 | ASN |
| 2 | I | 379 | HIS |
| 2 | G | 3896 | ASN |
| 2 | E | 3946 | GLN |
| 2 | E | 4806 | ASN |

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](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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 |
| 3 | ATP | B | 5101 | - | 26,33,33 | 0.91 | 1 (3%) | 26,52,52 | 1.71 | 3 (11%) |
| 4 | CFF | B | 5102 | - | 8,15,15 | 2.52 | 3 (37%) | 8,23,23 | 1.30 | 1 (12%) |
| 3 | ATP | E | 5101 | - | 26,33,33 | 0.91 | 1 (3%) | 26,52,52 | 1.72 | 3 (11%) |
| 4 | CFF | E | 5102 | - | 8,15,15 | 2.52 | 3 (37%) | 8,23,23 | 1.30 | 1 (12%) |
| 3 | ATP | G | 5101 | - | 26,33,33 | 0.91 | 1 (3%) | 26,52,52 | 1.72 | 3 (11%) |
| 4 | CFF | G | 5102 | - | 8,15,15 | 2.51 | 3 (37%) | 8,23,23 | 1.30 | 1 (12%) |
| 3 | ATP | I | 5101 | - | 26,33,33 | 0.91 | 1 (3%) | 26,52,52 | 1.71 | 3 (11%) |
| 4 | CFF | I | 5102 | - | 8,15,15 | 2.53 | 3 (37%) | 8,23,23 | 1.29 | 1 (12%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 3 | ATP | B | 5101 | - | - | 0/18/38/38 | 0/3/3/3 |
| 4 | CFF | B | 5102 | - | - | 0/0/0/0 | 0/2/2/2 |
| 3 | ATP | E | 5101 | - | - | 0/18/38/38 | 0/3/3/3 |
| 4 | CFF | E | 5102 | - | - | 0/0/0/0 | 0/2/2/2 |
| 3 | ATP | G | 5101 | - | - | 0/18/38/38 | 0/3/3/3 |
| 4 | CFF | G | 5102 | - | - | 0/0/0/0 | 0/2/2/2 |
| 3 | ATP | I | 5101 | - | - | 0/18/38/38 | 0/3/3/3 |
| 4 | CFF | I | 5102 | - | - | 0/0/0/0 | 0/2/2/2 |

The worst 5 of 16 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4 | E | 5102 | CFF | C4-N3 | -4.87 | 1.33 | 1.39 |
| 4 | I | 5102 | CFF | C4-N3 | -4.84 | 1.33 | 1.39 |
| 4 | B | 5102 | CFF | C4-N3 | -4.84 | 1.33 | 1.39 |
| 4 | G | 5102 | CFF | C4-N3 | -4.81 | 1.33 | 1.39 |
| 4 | I | 5102 | CFF | C6-N1 | -4.07 | 1.32 | 1.38 |

The worst 5 of 16 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 3 | G | 5101 | ATP | N3-C2-N1 | -6.72 | 123.60 | 128.87 |
| 3 | E | 5101 | ATP | N3-C2-N1 | -6.68 | 123.62 | 128.87 |
| 3 | B | 5101 | ATP | N3-C2-N1 | -6.65 | 123.64 | 128.87 |
| 3 | I | 5101 | ATP | N3-C2-N1 | -6.60 | 123.69 | 128.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 4 | I | 5102 | CFF | C14-N7-C8 | -2.53 | 112.09 | 125.31 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3 | B | 5101 | ATP | 2 | 0 |
| 3 | E | 5101 | ATP | 2 | 0 |
| 3 | G | 5101 | ATP | 2 | 0 |
| 3 | I | 5101 | ATP | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2 | G | 14 |
| 2 | B | 14 |
| 2 | I | 14 |
| 2 | E | 14 |

The worst 5 of 56 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | B | 4345:UNK | C | 4540:PHE | N | 74.00 |
| 1 | E | 4345:UNK | C | 4540:PHE | N | 74.00 |
| 1 | I | 4345:UNK | C | 4540:PHE | N | 74.00 |
| 1 | G | 4345:UNK | C | 4540:PHE | N | 74.00 |
| 1 | B | 3613:UNK | C | 3639:THR | N | 43.80 |