Jun 2, 2020 – 03:04 pm BST

PDB ID : 5YQ7
EMDB ID : EMD-6828
Title : Cryo-EM structure of the RC-LH core complex from Roseiflexus castenholzii
Authors : Shi, Y.; Xin, Y.Y.; Niu, T.X.; Wang, Q.Q.; Niu, W.Q.; Huang, X.J.; Ding, W.; Blankenship, R.E.; Xu, X.L.; Sun, F.
Deposited on : 2017-11-05
Resolution : 4.10 Å (reported)

This is a Full wwPDB EM Map/Model Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
with specific help available everywhere you see the symbol.

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

- EMDB validation analysis : 0.0.0.dev33
  - Mogul : 1.8.5 (274361), CSD as541be (2020)
  - MolProbity : 4.02b-467
  - buster-report : 1.1.7 (2018)
- Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
- Ideal geometry (proteins) : Engh & Huber (2001)
- Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
- Validation Pipeline (wwPDB-VP) : 2.11
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 4.10 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.

<table>
<thead>
<tr>
<th>Metric</th>
<th>Whole archive (#Entries)</th>
<th>EM structures (#Entries)</th>
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The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. 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 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 EM map (all atom inclusion < 40%). The numeric value is given above the bar.

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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:

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<th>Mol</th>
<th>Type</th>
<th>Chain</th>
<th>Res</th>
<th>Chirality</th>
<th>Geometry</th>
<th>Clashes</th>
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<td>-</td>
<td>-</td>
<td>X</td>
<td>-</td>
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</tbody>
</table>
2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 20009 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 Beta subunit of light-harvesting 1.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>AltConf</th>
<th>Trace</th>
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<td>Total 325</td>
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<td>N 55</td>
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<td>C 223</td>
<td>N 55</td>
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<td>Total 325</td>
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<td>N 54</td>
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</tbody>
</table>

- Molecule 2 is a protein called Precursor for L subunits of photosynthetic reaction center.
• Molecule 3 is a protein called Cytochrome subunit of photosynthetic reaction center.

• Molecule 4 is a protein called Alpha subunit of light-harvesting 1.

• Molecule 5 is a protein called Peptide from Precursor for L and M subunits of photosynthetic
reaction center.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
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- Molecule 6 is a protein called Subunit X.

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</table>

- Molecule 7 is a protein called Precursor for M subunits of photosynthetic reaction center.

<table>
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<th>Chain</th>
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<th>Atoms</th>
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</table>

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C_{55}H_{74}MgN_{4}O_{6}).
Continued from previous page...

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<th>Atoms</th>
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</table>

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C_{55}H_{76}N_{4}O_{6}).

![BPH](image)

<table>
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<tr>
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<td></td>
<td>130 110 8 12</td>
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- Molecule 10 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaen-1-yl]naphtalene-1,4-dione (three-letter code: MQE) (formula: C_{66}H_{96}O_{2}).
Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C_{34}H_{32}FeN_{4}O_{4}).
Molecule 13 is beta,psi-caroten-4-one (three-letter code: KGD) (formula: C\(_{40}\)H\(_{54}\)O).
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<th>AltConf</th>
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</table>
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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all atom inclusion < 40%). 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: Beta subunit of light-harvesting 1

  Chain E:

  ![Chain E Residue-property plot]

- Molecule 1: Beta subunit of light-harvesting 1

  Chain B:

  ![Chain B Residue-property plot]

- Molecule 1: Beta subunit of light-harvesting 1

  Chain 0:

  ![Chain 0 Residue-property plot]

- Molecule 1: Beta subunit of light-harvesting 1

  Chain 8:

  ![Chain 8 Residue-property plot]

- Molecule 1: Beta subunit of light-harvesting 1

  Chain 6:

  ![Chain 6 Residue-property plot]
Chain 4:

- Molecule 1: Beta subunit of light-harvesting 1

Chain 2:

- Molecule 1: Beta subunit of light-harvesting 1

Chain K:

- Molecule 1: Beta subunit of light-harvesting 1

Chain I:

- Molecule 1: Beta subunit of light-harvesting 1

Chain G:

- Molecule 1: Beta subunit of light-harvesting 1

Chain W:

- Molecule 1: Beta subunit of light-harvesting 1

Chain U:

- Molecule 1: Beta subunit of light-harvesting 1
- **Molecule 1:** Beta subunit of light-harvesting 1

  **Chain S:**

  - MET
  - THR
  - ASP
  - LYS
  - PRO
  - GLN
  - ASN
  - ASP
  - LEU
  - VAL
  - P11
  - W14
  - D27
  - ♦
  - I28
  - ♦
  - V29
  - ♦
  - I33
  - ♦
  - L37
  - ♦
  - I38
  - ♦
  - ♦
  - W50
  - ♦
  - T51
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦

- **Molecule 1:** Beta subunit of light-harvesting 1

  **Chain Q:**

  - MET
  - THR
  - ASP
  - LYS
  - PRO
  - GLN
  - ASN
  - ASP
  - LEU
  - VAL
  - P11
  - W14
  - K15
  - P16
  - ♦
  - L17
  - ♦
  - ♦
  - H26
  - ♦
  - D27
  - ♦
  - I28
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦

- **Molecule 1:** Beta subunit of light-harvesting 1

  **Chain O:**

  - MET
  - THR
  - ASP
  - LYS
  - PRO
  - GLN
  - ASN
  - ASP
  - LEU
  - VAL
  - P11
  - W14
  - L24
  - ♦
  - V25
  - ♦
  - ♦
  - H26
  - ♦
  - D27
  - ♦
  - I28
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦

- **Molecule 2:** Precursor for L subunits of photosynthetic reaction center

  **Chain L:**

  - MET
  - S2
  - A3
  - V4
  - P5
  - R6
  - A7
  - L8
  - P9
  - ♦
  - L10
  - P11
  - S12
  - ♦
  - G13
  - E14
  - ♦
  - T15
  - ♦
  - L16
  - P17
  - A18
  - E19
  - ♦
  - ♦
  - ♦
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  - ♦
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  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦

- **Molecule 3:** Cytochrome subunit of photosynthetic reaction center

  **Chain C:**

  - MET
  - ILE
  - GLN
  - GLN
  - PRO
  - PRO
  - THR
  - LEU
  - PHE
  - PRO
  - GLU
  - ILE
  - THR
  - ASN
  - THR
  - VAL
  - R17
  - ♦
  - G18
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
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  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
  - ♦
- Molecule 4: Alpha subunit of light-harvesting 1

Chain T: [Diagram]

- Molecule 4: Alpha subunit of light-harvesting 1

Chain V: [Diagram]

- Molecule 4: Alpha subunit of light-harvesting 1

Chain R: [Diagram]

- Molecule 4: Alpha subunit of light-harvesting 1

Chain P: [Diagram]

- Molecule 4: Alpha subunit of light-harvesting 1

Chain N: [Diagram]

- Molecule 4: Alpha subunit of light-harvesting 1

Chain J: [Diagram]
• Molecule 4: Alpha subunit of light-harvesting 1

Chain H:

• Molecule 4: Alpha subunit of light-harvesting 1

Chain F:

• Molecule 4: Alpha subunit of light-harvesting 1

Chain D:

• Molecule 4: Alpha subunit of light-harvesting 1

Chain A:

• Molecule 4: Alpha subunit of light-harvesting 1

Chain 9:

• Molecule 4: Alpha subunit of light-harvesting 1

Chain 7:
Chain 5:

- Molecule 4: Alpha subunit of light-harvesting 1

Chain 3:

- Molecule 4: Alpha subunit of light-harvesting 1

Chain 1:

- Molecule 5: Peptide from Precursor for L and M subunits of photosynthetic reaction center

Chain Y:

- Molecule 6: Subunit X

Chain X:

- Molecule 7: Precursor for M subunits of photosynthetic reaction center
4 Experimental information

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## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, MQE, BPH, FE, HEM, KGD

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).

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<th>Bond angles</th>
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<td>0/272</td>
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</table>
### Bond lengths

| Mol | Chain | Bond lengths RMSZ | #Z > 5 | Bond angles RMSZ | #|Z| > 5 |
|-----|-------|------------------|--------|-----------------|------|
| 7   | M     | 0.35             | 0/2478 | 0.48            | 0/3417 |
| All | All   | 0.32             | 0/16024| 0.52            | 2/22106 (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.

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<th>#Planarity outliers</th>
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<tr>
<td>4</td>
<td>5</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>7</td>
<td>M</td>
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<tr>
<td>All</td>
<td>All</td>
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There are no bond length outliers.

All (2) bond angle outliers are listed below:

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<th>Type</th>
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<td>127.19</td>
<td>115.30</td>
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There are no chirality outliers.

All (5) planarity outliers are listed below:

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<tr>
<th>Mol</th>
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#### 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.
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<thead>
<tr>
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<th>H(added)</th>
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Continued on next page...
Continued from previous page...

| Mol | 8 | 9 | A | B | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W |
| Chain | 8 | 9 | A | B | D | E | F | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W |
| H(model) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| H(added) | 148 | 74 | 74 | 148 | 74 | 148 | 74 | 148 | 74 | 148 | 74 | 148 | 74 | 148 | 74 | 148 | 74 | 148 | 74 | 148 | 74 | 148 | 74 | 148 |
| Clashes | 16 | 2 | 6 | 31 | 2 | 10 | 4 | 14 | 8 | 19 | 4 | 20 | 4 | 5 | 4 | 12 | 2 | 14 | 8 | 11 | 3 | 14 | 5 |
| Symm-Clashes | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 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 15.

All (582) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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<tr>
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<th>Atom-2</th>
<th>Interatomic distance (Å)</th>
<th>Clash overlap (Å)</th>
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### Interatomic Distance (Å) and Clash Overlap (Å)

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<tr>
<td>7:M:498:PRO:HG3</td>
<td>7:M:508:TRP:CD2</td>
<td>2.56</td>
<td>0.40</td>
</tr>
</tbody>
</table>

*Continued on next page...*
Continued from previous page...

<table>
<thead>
<tr>
<th>Atom-1</th>
<th>Atom-2</th>
<th>Interatomic distance (Å)</th>
<th>Clash overlap (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:P:101:BCL:H2C</td>
<td>8:P:101:BCL:HBC2</td>
<td>1.82</td>
<td>0.40</td>
</tr>
<tr>
<td>2:L:89:TYR:HD1</td>
<td>4:P:28:PHE:HE1</td>
<td>1.68</td>
<td>0.40</td>
</tr>
<tr>
<td>4:P:31:LEU:HD23</td>
<td>4:P:38:TRP:CZ3</td>
<td>2.57</td>
<td>0.40</td>
</tr>
<tr>
<td>1:Q:29:VAL:HG22</td>
<td>8:Q:102:BCL:CED</td>
<td>2.51</td>
<td>0.40</td>
</tr>
<tr>
<td>1:E:41:VAL:O</td>
<td>1:E:45:VAL:HG23</td>
<td>2.21</td>
<td>0.40</td>
</tr>
<tr>
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<td>8:R:102:BCL:HBB3</td>
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</tr>
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<td>3:C:235:SER:OG</td>
<td>3:C:236:MET:N</td>
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<td>0.40</td>
</tr>
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<td>2:L:93:VAL:HG21</td>
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<td>0.40</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Favoured</th>
<th>Allowed</th>
<th>Outliers</th>
<th>Percentiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>42/55 (76%)</td>
<td>38 (90%)</td>
<td>4 (10%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>42/55 (76%)</td>
<td>36 (86%)</td>
<td>6 (14%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>42/55 (76%)</td>
<td>40 (95%)</td>
<td>2 (5%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>42/55 (76%)</td>
<td>38 (90%)</td>
<td>4 (10%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>8</td>
<td>42/55 (76%)</td>
<td>34 (81%)</td>
<td>8 (19%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>42/55 (76%)</td>
<td>39 (93%)</td>
<td>3 (7%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>E</td>
<td>42/55 (76%)</td>
<td>39 (93%)</td>
<td>3 (7%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>G</td>
<td>42/55 (76%)</td>
<td>38 (90%)</td>
<td>4 (10%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>I</td>
<td>42/55 (76%)</td>
<td>35 (83%)</td>
<td>7 (17%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>K</td>
<td>42/55 (76%)</td>
<td>38 (90%)</td>
<td>4 (10%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>O</td>
<td>42/55 (76%)</td>
<td>37 (88%)</td>
<td>5 (12%)</td>
<td>0</td>
<td>100 100</td>
</tr>
</tbody>
</table>

Continued on next page...
Continued from previous page...

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Favoured</th>
<th>Allowed</th>
<th>Outliers</th>
<th>Percentiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Q</td>
<td>42/55 (76%)</td>
<td>38 (90%)</td>
<td>4 (10%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>1</td>
<td>S</td>
<td>42/55 (76%)</td>
<td>38 (90%)</td>
<td>4 (10%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>1</td>
<td>U</td>
<td>42/55 (76%)</td>
<td>36 (86%)</td>
<td>6 (14%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>1</td>
<td>W</td>
<td>42/55 (76%)</td>
<td>38 (90%)</td>
<td>4 (10%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>2</td>
<td>L</td>
<td>307/310 (99%)</td>
<td>253 (82%)</td>
<td>53 (17%)</td>
<td>1 (0%)</td>
<td>41</td>
</tr>
<tr>
<td>3</td>
<td>C</td>
<td>291/320 (91%)</td>
<td>213 (73%)</td>
<td>76 (26%)</td>
<td>2 (1%)</td>
<td>22</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>34/42 (81%)</td>
<td>30 (88%)</td>
<td>4 (12%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>34/42 (81%)</td>
<td>28 (82%)</td>
<td>6 (18%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>34/42 (81%)</td>
<td>33 (97%)</td>
<td>1 (3%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>7</td>
<td>34/42 (81%)</td>
<td>26 (76%)</td>
<td>8 (24%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>9</td>
<td>34/42 (81%)</td>
<td>32 (94%)</td>
<td>2 (6%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>A</td>
<td>34/42 (81%)</td>
<td>27 (79%)</td>
<td>7 (21%)</td>
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<td>100</td>
</tr>
<tr>
<td>4</td>
<td>D</td>
<td>34/42 (81%)</td>
<td>31 (91%)</td>
<td>3 (9%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>F</td>
<td>34/42 (81%)</td>
<td>30 (88%)</td>
<td>4 (12%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>H</td>
<td>34/42 (81%)</td>
<td>31 (91%)</td>
<td>3 (9%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>J</td>
<td>34/42 (81%)</td>
<td>32 (94%)</td>
<td>2 (6%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>N</td>
<td>34/42 (81%)</td>
<td>32 (94%)</td>
<td>2 (6%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>P</td>
<td>34/42 (81%)</td>
<td>30 (88%)</td>
<td>4 (12%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>R</td>
<td>34/42 (81%)</td>
<td>30 (88%)</td>
<td>4 (12%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>T</td>
<td>34/42 (81%)</td>
<td>33 (97%)</td>
<td>1 (3%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>4</td>
<td>V</td>
<td>34/42 (81%)</td>
<td>32 (94%)</td>
<td>2 (6%)</td>
<td>0</td>
<td>100</td>
</tr>
<tr>
<td>7</td>
<td>M</td>
<td>303/306 (99%)</td>
<td>253 (84%)</td>
<td>49 (16%)</td>
<td>1 (0%)</td>
<td>41</td>
</tr>
<tr>
<td>All</td>
<td>All</td>
<td>2041/2391 (85%)</td>
<td>1738 (85%)</td>
<td>299 (15%)</td>
<td>4 (0%)</td>
<td>50</td>
</tr>
</tbody>
</table>

All (4) Ramachandran outliers are listed below:

<table>
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<tr>
<th>Mol</th>
<th>Chain</th>
<th>Res</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>L</td>
<td>206</td>
<td>PHE</td>
</tr>
<tr>
<td>3</td>
<td>C</td>
<td>118</td>
<td>CYS</td>
</tr>
<tr>
<td>3</td>
<td>C</td>
<td>124</td>
<td>ILE</td>
</tr>
<tr>
<td>7</td>
<td>M</td>
<td>349</td>
<td>GLY</td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Rotameric</th>
<th>Outliers</th>
<th>Percentiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>27/49 (55%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>26/49 (53%)</td>
<td>26 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>24/49 (49%)</td>
<td>24 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>6</td>
<td>27/49 (55%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>8</td>
<td>27/49 (55%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>B</td>
<td>26/49 (53%)</td>
<td>26 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>E</td>
<td>26/49 (53%)</td>
<td>26 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>G</td>
<td>27/49 (55%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>I</td>
<td>27/49 (55%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>K</td>
<td>26/49 (53%)</td>
<td>26 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>O</td>
<td>26/49 (53%)</td>
<td>26 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>Q</td>
<td>25/49 (51%)</td>
<td>25 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>S</td>
<td>26/49 (53%)</td>
<td>26 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>U</td>
<td>27/49 (55%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>1</td>
<td>W</td>
<td>23/49 (47%)</td>
<td>23 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>2</td>
<td>L</td>
<td>214/251 (85%)</td>
<td>214 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>3</td>
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<td>183/262 (70%)</td>
<td>183 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>24/37 (65%)</td>
<td>24 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>27/37 (73%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>5</td>
<td>28/37 (76%)</td>
<td>28 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>7</td>
<td>28/37 (76%)</td>
<td>28 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>9</td>
<td>28/37 (76%)</td>
<td>28 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>A</td>
<td>28/37 (76%)</td>
<td>27 (96%)</td>
<td>1 (4%)</td>
<td>35 60</td>
</tr>
<tr>
<td>4</td>
<td>D</td>
<td>28/37 (76%)</td>
<td>28 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>F</td>
<td>28/37 (76%)</td>
<td>28 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>H</td>
<td>27/37 (73%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
</tbody>
</table>
Continued from previous page...

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Analysed</th>
<th>Rotameric</th>
<th>Outliers</th>
<th>Percentiles</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>J</td>
<td>27/37 (73%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>N</td>
<td>28/37 (76%)</td>
<td>28 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>P</td>
<td>28/37 (76%)</td>
<td>28 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>R</td>
<td>26/37 (70%)</td>
<td>26 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>T</td>
<td>28/37 (76%)</td>
<td>28 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>4</td>
<td>V</td>
<td>27/37 (73%)</td>
<td>27 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
<td>7</td>
<td>M</td>
<td>216/244 (88%)</td>
<td>216 (100%)</td>
<td>0</td>
<td>100 100</td>
</tr>
<tr>
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<td>All</td>
<td>1413/2047 (69%)</td>
<td>1412 (100%)</td>
<td>1 (0%)</td>
<td>93 97</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
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<th>Chain</th>
<th>Res</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
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<td>A</td>
<td>27</td>
<td>HIS</td>
</tr>
</tbody>
</table>

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Res</th>
<th>Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>B</td>
<td>44</td>
<td>HIS</td>
</tr>
<tr>
<td>2</td>
<td>L</td>
<td>183</td>
<td>HIS</td>
</tr>
<tr>
<td>2</td>
<td>L</td>
<td>252</td>
<td>ASN</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>44</td>
<td>HIS</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>44</td>
<td>HIS</td>
</tr>
<tr>
<td>3</td>
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<td>GLN</td>
</tr>
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<td>176</td>
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<td>C</td>
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<td>ASN</td>
</tr>
<tr>
<td>3</td>
<td>C</td>
<td>301</td>
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</tr>
<tr>
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<td>G</td>
<td>44</td>
<td>HIS</td>
</tr>
<tr>
<td>1</td>
<td>Q</td>
<td>44</td>
<td>HIS</td>
</tr>
<tr>
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<td>R</td>
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<td>HIS</td>
</tr>
<tr>
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<td>HIS</td>
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<td>515</td>
<td>HIS</td>
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<td>7</td>
<td>M</td>
<td>637</td>
<td>GLN</td>
</tr>
</tbody>
</table>

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 carbohydrates in this entry.

5.6  **Ligand geometry**

Of 72 ligands modelled in this entry, 1 is monoatomic - leaving 71 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).

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8 | 8 | 102 | BCL | CBD-CGD | -2.01 | 1.46 | 1.52
8 | F | 102 | BCL | C3D-CAD | -2.00 | 1.41 | 1.46
8 | G | 101 | BCL | CBD-CGD | -2.00 | 1.46 | 1.52
8 | Q | 102 | BCL | OBD-CAD | 2.00 | 1.25 | 1.22

All (924) bond angle outliers are listed below:

### Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°)
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8 | U | 101 | BCL | C4-C3-C5 | -27.53 | 68.96 | 115.27
8 | U | 101 | BCL | C5-C3-C2 | 19.65 | 160.88 | 121.12
8 | W | 101 | BCL | C4-C3-C2 | 19.41 | 160.40 | 121.12
13 | N | 102 | KGD | CBM-CBJ-CBH | -14.24 | 106.98 | 127.31
13 | T | 102 | KGD | CBM-CBJ-CBH | -13.10 | 108.61 | 127.31
13 | 5 | 101 | KGD | CBM-CBJ-CBH | -12.77 | 109.08 | 127.31
8 | U | 101 | BCL | C4-C3-C2 | -12.38 | 91.93 | 123.68
8 | W | 101 | BCL | C4-C3-C2 | -12.35 | 91.99 | 123.68
13 | 9 | 102 | KGD | CBG-CBI-CBL | -12.30 | 109.76 | 127.31
13 | J | 101 | KGD | CBG-CBI-CBL | -12.05 | 110.11 | 127.31
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13 | N | 101 | KGD | CBM-CBJ-CBH | -11.47 | 110.95 | 127.31
13 | 5 | 101 | KGD | CBG-CBI-CBL | -11.45 | 110.97 | 127.31
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 8  | 3     | 102 | BCL | C4B-C3B-CAB| -3.95  | 119.51     | 127.13   |
13  | A     | 101 | KGD | CAZ-CAW-CAS|  3.93  | 121.89     | 115.27   |
 8  | 0     | 102 | BCL | C4A-NA-C1A |  3.93  | 108.47     | 106.71   |
13  | A     | 101 | KGD | CBA-CBE-CBF| -3.93  | 110.95     | 123.22   |
 8  | M     | 702 | BCL | C4D-C3D-CAD| -3.92  | 106.28     | 108.47   |
13  | H     | 102 | KGD | CBA-CBE-CBF| -3.91  | 111.02     | 123.22   |
 8  | B     | 102 | BCL | CMB-C2B-C1B| -3.89  | 122.48     | 128.46   |
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13  | 3     | 101 | KGD | CAT-CAX-CAY| -3.87  | 114.52     | 127.75   |
 8  | A     | 102 | BCL | C4B-C3B-CAB| -3.86  | 119.67     | 127.13   |
 8  | T     | 103 | BCL | CMB-C2B-C1B| -3.85  | 122.55     | 128.46   |
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12  | C     | 504 | HEM | CAD-CBD-CGD| -3.84  | 106.22     | 112.67   |
13  | 9     | 102 | KGD | CAP-CAQ-CAR| -3.84  | 115.63     | 126.42   |
 8  | G     | 102 | BCL | C4D-C3D-CAD| -3.83  | 106.33     | 108.47   |
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8 | 9 | 103 | BCL | CHA-C1A-NA | -2.98 | 119.58 | 126.40
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8 | L | 1002 | BCL | C4D-C3D-CAD | -2.97 | 106.81 | 108.47
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8 | 4 | 101 | BCL | CHA-C1A-NA | -2.97 | 119.60 | 126.40
8 | Q | 101 | BCL | C4D-C3D-CAD | -2.96 | 106.82 | 108.47
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8 | 4 | 102 | BCL | C2A-C1A-CHA | 2.96 | 129.04 | 123.86
8 | D | 101 | BCL | C4B-C3B-CAB | -2.96 | 121.41 | 127.13
8 | J | 102 | BCL | CHA-C1A-NA | -2.96 | 119.62 | 126.40
8 | N | 103 | BCL | CMB-C2B-C3B | 2.95 | 130.21 | 124.68
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8 | S | 101 | BCL | C4D-C3D-CAD | -2.95 | 106.83 | 108.47
8 | I | 101 | BCL | C4A-NA-C1A | 2.94 | 108.03 | 106.71
8 | 8 | 101 | BCL | C4D-C3D-CAD | -2.94 | 106.83 | 108.47
13 | N | 102 | KGD | CAZ-CAW-CAS | 2.94 | 120.22 | 115.27
8 | F | 102 | BCL | C16-C15-C13 | 2.94 | 119.70 | 126.40
13 | 9 | 102 | KGD | CAO-CAP-CAQ | -2.94 | 119.70 | 126.40
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8 | 0 | 101 | BCL | CHA-C1A-NA | -2.93 | 119.70 | 126.40
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8 | K | 102 | BCL | C2A-C1A-CHA | 2.92 | 128.96 | 123.86
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10 | L | 1004 | MQE | CBY-CAW-CAG | 2.91 | 120.22 | 115.27
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8 | 6 | 102 | BCL | C2A-C1A-CHA | 2.90 | 128.96 | 123.86
13 | 9 | 101 | KGD | CBA-CBE-CBF | -2.90 | 119.70 | 126.40
8 | 5 | 102 | BCL | CHA-C1A-NA | -2.89 | 119.70 | 126.40
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There are no ring outliers.

65 monomers are involved in 359 short contacts:

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*Continued on next page...*
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
Ligand BCL B 102

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 8 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 702

Bond lengths

Bond angles

Torsions

Rings
Ligand BCL S 102

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 504

Bond lengths

Bond angles

Torsions

Rings
Ligand BCL 6 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL I 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL 9 103

Bond lengths

Bond angles

Torsions

Rings
Ligand BCL S 101

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL I 102

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL U 101

Bond lengths

Bond angles

Torsions

Rings
Ligand BPH M 703

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL W 101

Bond lengths

Bond angles

Torsions

Rings
Ligand BCL O 102

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 503

Bond lengths

Bond angles

Torsions

Rings
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  Map visualisation

This section contains visualisations of the EMDB entry EMD-6828. These are intended to permit visual inspection of the internal detail of the map and identification of artifacts.

6.1 Orthogonal projections

The images above show the map projected in three orthogonal projections, in greyscale.

6.2 Central slices

The images above show central slices of the map in three orthogonal directions, in greyscale.
6.3 Largest variance slices

The images above show the highest variance slices of the map in three orthogonal directions, in greyscale.

6.4 Orthogonal surface views

The images above show the 3D surface view of the map at the recommended contour level 0.03. This in conjunction with the slice images can indicate whether an appropriate contour level has been selected.

6.5 Mask visualisation

This section was not generated. No masks were provided.
7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.
7.2 Volume estimate

The volume at the recommended contour level is 105 nm$^3$; this corresponds to an approximate mass of 95 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.
7.3 Rotationally averaged power spectrum

![Graph showing rotationally averaged power spectrum with reported resolution of 4.10 Å and corresponding spatial frequency of 0.244 Å⁻¹.]

- Intensity (log10) on the y-axis.
- Spatial frequency (Å⁻¹) on the x-axis.
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half maps provided.
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6828 and PDB model 5YQ7. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.
9.2 Atom inclusion

At the recommended contour level, 80% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.