



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2017 – 02:48 PM EST

PDB ID : 4MTK
Title : Crystal structure of PA0091 VgrG1, the central spike of the Type VI Secretion System
Authors : Sycheva, L.V.; Shneider, M.M.; Leiman, P.G.
Deposited on : unknown
Resolution : 3.32 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

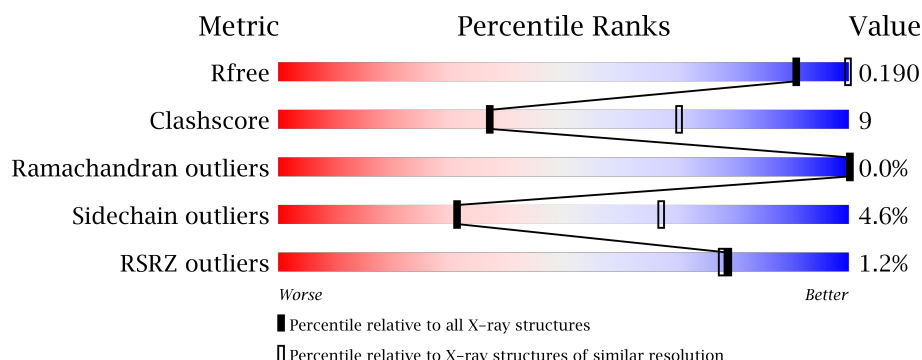
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.32 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} | 100719 | 1002 (3.38-3.26) |
| Clashscore | 112137 | 1066 (3.38-3.26) |
| Ramachandran outliers | 110173 | 1048 (3.38-3.26) |
| Sidechain outliers | 110143 | 1047 (3.38-3.26) |
| RSRZ outliers | 101464 | 1007 (3.38-3.26) |

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 $\leq 5\%$. 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 | 643 |  67% 27% .. |
| 1 | B | 643 |  74% 21% .. |
| 1 | C | 643 |  76% 21% .. |
| 1 | D | 643 |  78% 19% .. |
| 1 | E | 643 |  76% 20% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | F | 643 |  |

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 | SO4 | A | 703 | - | - | - | X |
| 2 | SO4 | A | 705 | - | - | - | X |
| 2 | SO4 | A | 727 | - | - | - | X |
| 2 | SO4 | A | 731 | - | - | - | X |
| 2 | SO4 | A | 745 | - | - | - | X |
| 2 | SO4 | A | 747 | - | - | - | X |
| 2 | SO4 | B | 714 | - | - | - | X |
| 2 | SO4 | B | 718 | - | - | - | X |
| 2 | SO4 | B | 719 | - | - | X | - |
| 2 | SO4 | B | 720 | - | - | - | X |
| 2 | SO4 | B | 732 | - | - | X | - |
| 2 | SO4 | B | 735 | - | - | X | - |
| 2 | SO4 | B | 736 | - | - | - | X |
| 2 | SO4 | B | 739 | - | - | X | - |
| 2 | SO4 | B | 746 | - | - | - | X |
| 2 | SO4 | B | 749 | - | - | - | X |
| 2 | SO4 | B | 750 | - | - | - | X |
| 2 | SO4 | C | 726 | - | - | - | X |
| 2 | SO4 | C | 731 | - | - | X | - |
| 2 | SO4 | C | 732 | - | - | - | X |
| 2 | SO4 | C | 733 | - | - | - | X |
| 2 | SO4 | C | 734 | - | - | - | X |
| 2 | SO4 | C | 739 | - | - | X | - |
| 2 | SO4 | C | 741 | - | - | - | X |
| 2 | SO4 | D | 706 | - | - | - | X |
| 2 | SO4 | D | 726 | - | - | - | X |
| 2 | SO4 | D | 730 | - | - | - | X |
| 2 | SO4 | E | 701 | - | - | - | X |
| 2 | SO4 | E | 720 | - | - | - | X |
| 2 | SO4 | E | 725 | - | - | - | X |
| 2 | SO4 | E | 728 | - | - | - | X |
| 2 | SO4 | E | 734 | - | - | - | X |
| 2 | SO4 | F | 704 | - | - | - | X |
| 2 | SO4 | F | 709 | - | - | - | X |
| 2 | SO4 | F | 712 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2 | SO4 | F | 714 | - | - | - | X |
| 2 | SO4 | F | 729 | - | - | - | X |
| 2 | SO4 | F | 736 | - | - | - | X |
| 2 | SO4 | F | 737 | - | - | - | X |
| 2 | SO4 | F | 739 | - | - | - | X |
| 2 | SO4 | F | 742 | - | - | - | X |
| 3 | TAM | A | 749 | - | - | - | X |
| 3 | TAM | D | 735 | - | - | - | X |

2 Entry composition [i](#)

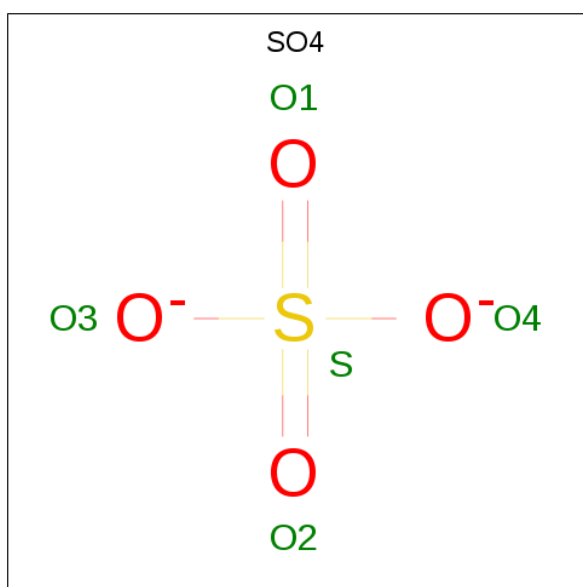
There are 4 unique types of molecules in this entry. The entry contains 31170 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 VgrG1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 627 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4977 | 3113 | 910 | 939 | 15 | | | |
| 1 | B | 627 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4977 | 3113 | 910 | 939 | 15 | | | |
| 1 | C | 627 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4977 | 3113 | 910 | 939 | 15 | | | |
| 1 | D | 627 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4977 | 3113 | 910 | 939 | 15 | | | |
| 1 | E | 627 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4977 | 3113 | 910 | 939 | 15 | | | |
| 1 | F | 627 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4977 | 3113 | 910 | 939 | 15 | | | |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



[illegible]

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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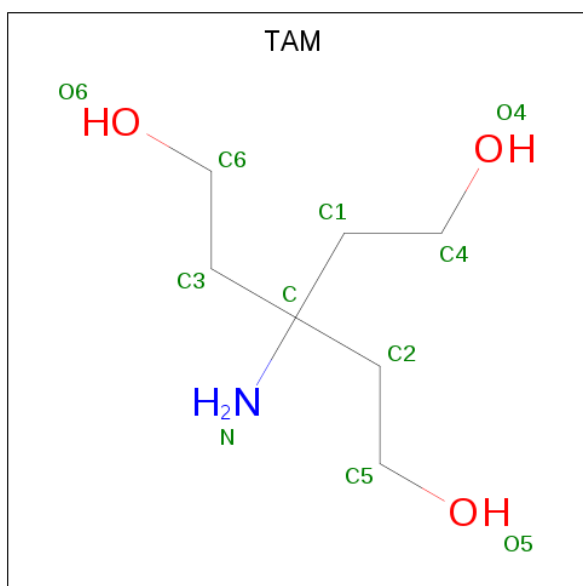
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 2 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C₇H₁₇NO₃).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 11 | 7 | 1 | 3 | | |
| 3 | D | 1 | Total | C | N | O | 0 | 0 |
| | | | 11 | 7 | 1 | 3 | | |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4 | A | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | B | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | C | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | D | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

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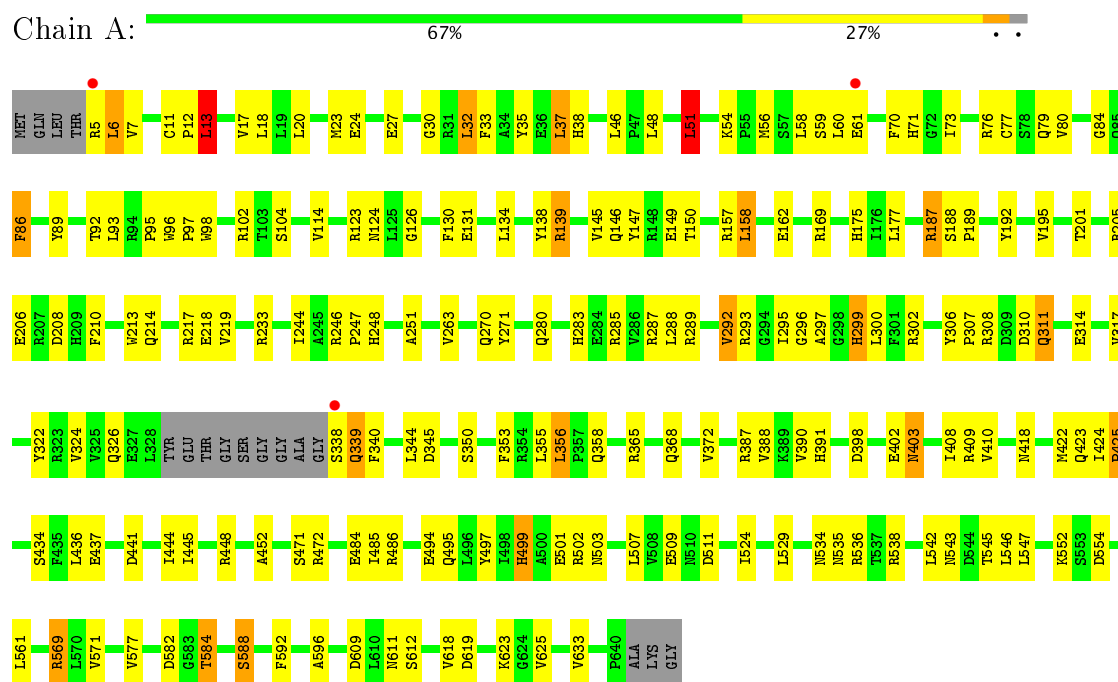
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4 | E | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | F | 1 | Total | O | 0 | 0 |
| | | | 1 | 1 | | |

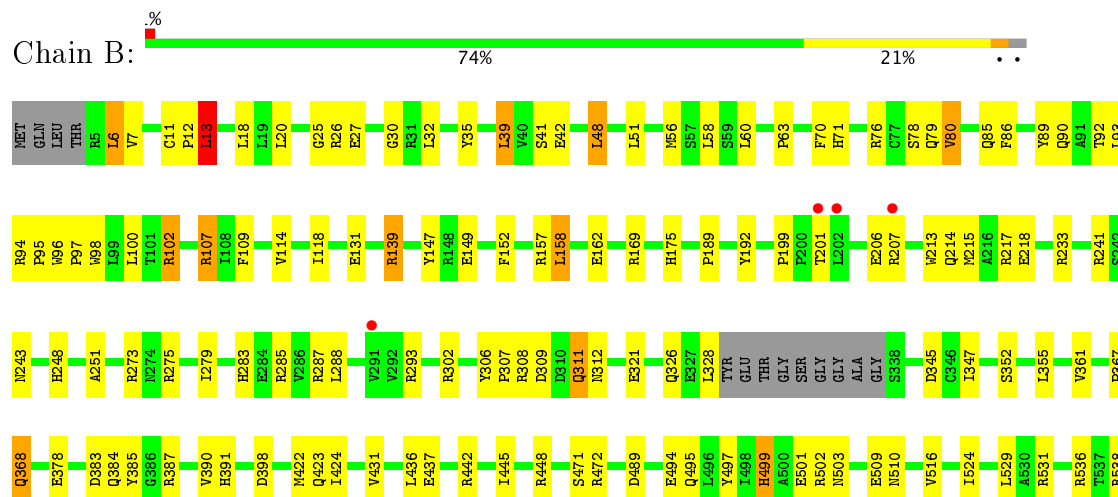
3 Residue-property plots

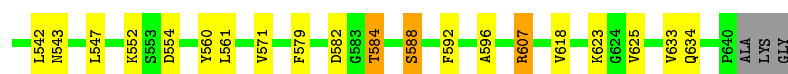
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: VgrG1

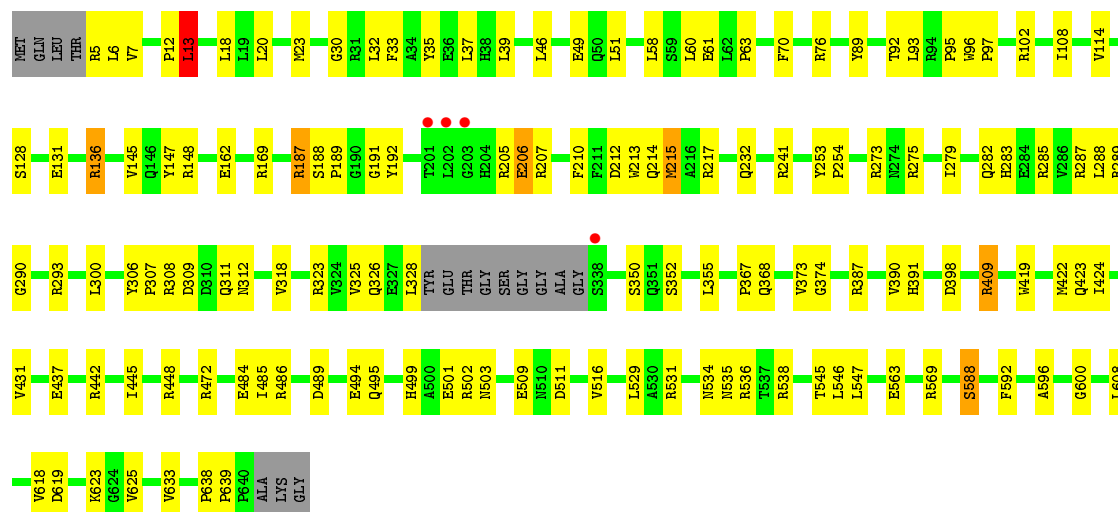
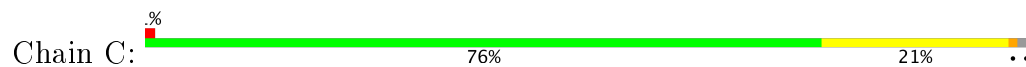


• Molecule 1: VgrG1

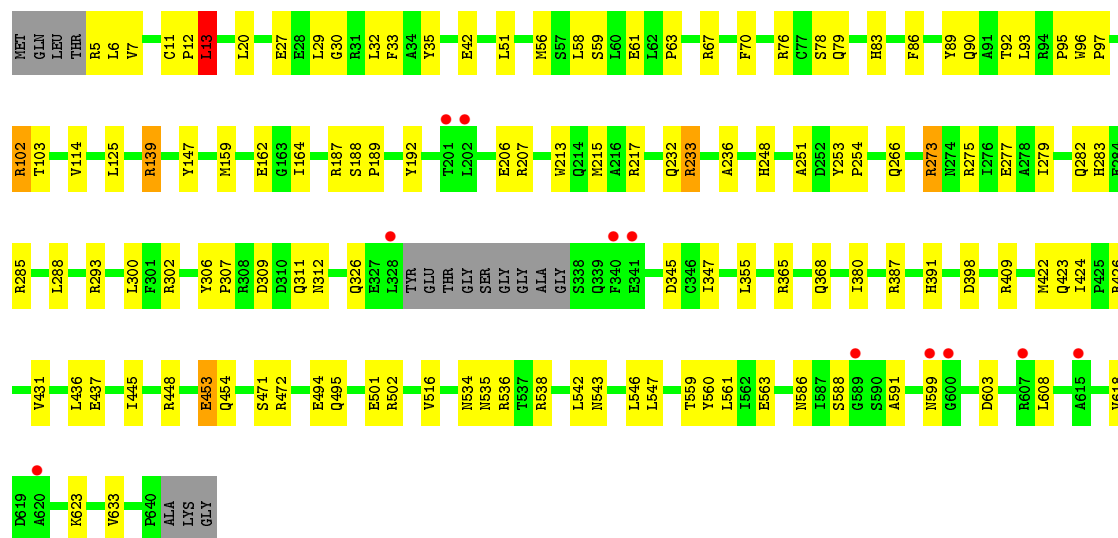
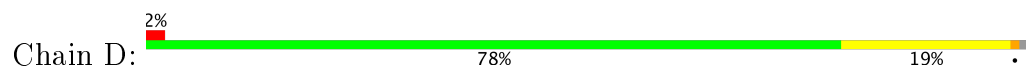




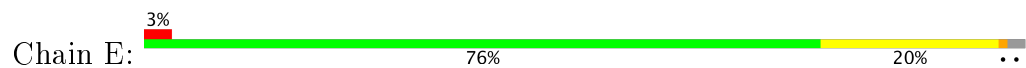
• Molecule 1: VgrG1

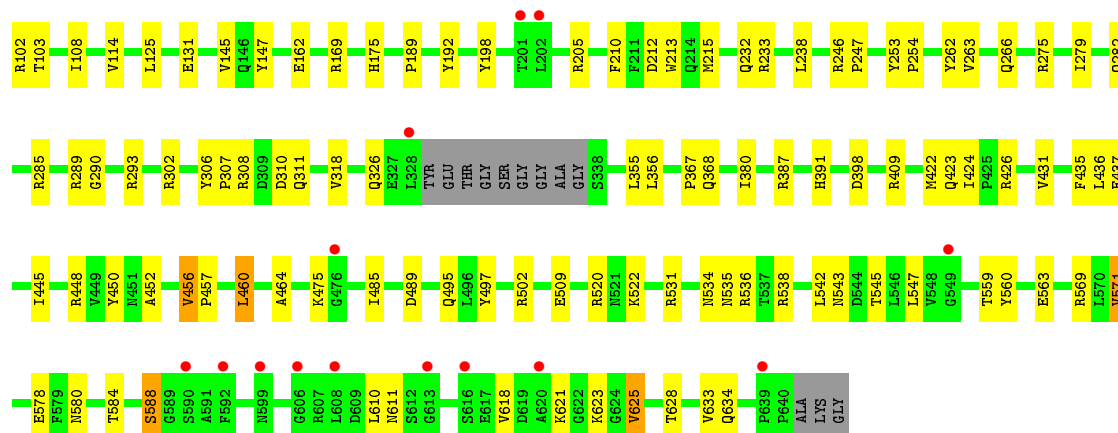


• Molecule 1: VgrG1

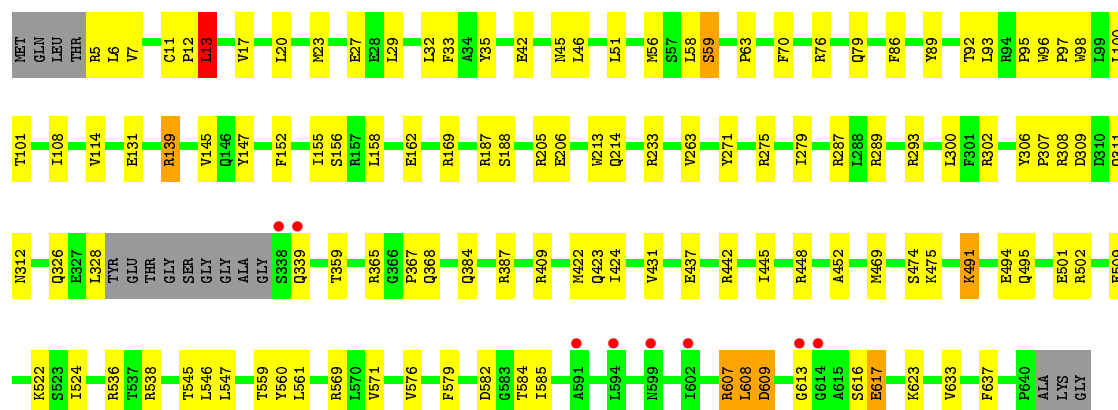
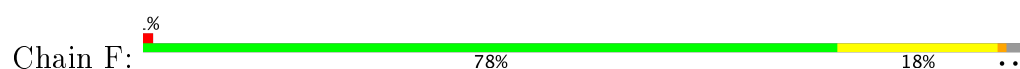


• Molecule 1: VgrG1





• Molecule 1: VgrG1



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 61 | Depositor |
| Cell constants a, b, c, α , β , γ | 168.28Å 168.28Å 652.85Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 49.14 – 3.32 49.14 – 3.32 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (49.14-3.32) 99.8 (49.14-3.32) | Depositor EDS |
| R_{merge} | 0.17 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.04 (at 3.33Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.2_1309) | Depositor |
| R, R_{free} | 0.170 , 0.195 0.164 , 0.190 | Depositor DCC |
| R_{free} test set | 3052 reflections (2.00%) | DCC |
| Wilson B-factor (Å ²) | 70.2 | Xtriage |
| Anisotropy | 0.090 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 70.1 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtriage |
| Estimated twinning fraction | 0.049 for h,-h-k,-l | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 31170 | wwPDB-VP |
| Average B, all atoms (Å ²) | 106.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TAM, SO4

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 | 0.28 | 0/5095 | 0.70 | 4/6905 (0.1%) |
| 1 | B | 0.23 | 0/5095 | 0.48 | 1/6905 (0.0%) |
| 1 | C | 0.23 | 0/5095 | 0.49 | 1/6905 (0.0%) |
| 1 | D | 0.22 | 0/5095 | 0.46 | 1/6905 (0.0%) |
| 1 | E | 0.22 | 0/5095 | 0.44 | 0/6905 |
| 1 | F | 0.22 | 0/5095 | 0.46 | 1/6905 (0.0%) |
| All | All | 0.24 | 0/30570 | 0.51 | 8/41430 (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 |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1 | A | 84 | GLY | N-CA-C | 8.04 | 133.21 | 113.10 |
| 1 | A | 13 | LEU | CA-CB-CG | 6.46 | 130.15 | 115.30 |
| 1 | A | 51 | LEU | CA-CB-CG | 5.97 | 129.03 | 115.30 |
| 1 | F | 13 | LEU | CA-CB-CG | 5.63 | 128.26 | 115.30 |
| 1 | D | 13 | LEU | CA-CB-CG | 5.39 | 127.70 | 115.30 |
| 1 | C | 13 | LEU | CA-CB-CG | 5.21 | 127.29 | 115.30 |
| 1 | B | 13 | LEU | CA-CB-CG | 5.14 | 127.13 | 115.30 |
| 1 | A | 37 | LEU | CA-CB-CG | 5.04 | 126.90 | 115.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 339 | GLN | 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 | 4977 | 0 | 4794 | 144 | 1 |
| 1 | B | 4977 | 0 | 4794 | 117 | 0 |
| 1 | C | 4977 | 0 | 4794 | 100 | 0 |
| 1 | D | 4977 | 0 | 4794 | 79 | 0 |
| 1 | E | 4977 | 0 | 4794 | 86 | 0 |
| 1 | F | 4977 | 0 | 4794 | 79 | 0 |
| 2 | A | 245 | 0 | 0 | 6 | 0 |
| 2 | B | 250 | 0 | 0 | 16 | 0 |
| 2 | C | 220 | 0 | 0 | 13 | 0 |
| 2 | D | 175 | 0 | 0 | 10 | 0 |
| 2 | E | 170 | 0 | 0 | 1 | 0 |
| 2 | F | 220 | 0 | 0 | 5 | 0 |
| 3 | A | 11 | 0 | 17 | 2 | 0 |
| 3 | D | 11 | 0 | 17 | 2 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | E | 1 | 0 | 0 | 0 | 0 |
| 4 | F | 1 | 0 | 0 | 0 | 0 |
| All | All | 31170 | 0 | 28798 | 535 | 1 |

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 9.

All (535) 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:588:SER:HB3 | 1:A:618:VAL:HG12 | 1.55 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:35:TYR:HB2 | 1:A:93:LEU:HB2 | 1.56 | 0.86 |
| 1:C:588:SER:HB2 | 1:C:618:VAL:HG12 | 1.61 | 0.83 |
| 1:A:208:ASP:HB3 | 1:A:292:VAL:HA | 1.60 | 0.83 |
| 1:B:588:SER:HB2 | 1:B:618:VAL:HG12 | 1.61 | 0.82 |
| 1:D:368:GLN:NE2 | 1:F:437:GLU:OE1 | 2.14 | 0.80 |
| 1:A:285:ARG:NH1 | 1:A:345:ASP:OD2 | 2.17 | 0.77 |
| 1:C:35:TYR:HB2 | 1:C:93:LEU:HB2 | 1.66 | 0.77 |
| 1:F:5:ARG:HG3 | 1:F:6:LEU:HD12 | 1.65 | 0.77 |
| 1:C:273:ARG:NH1 | 2:C:731:SO4:S | 2.60 | 0.75 |
| 1:A:295:ILE:HG21 | 1:A:344:LEU:HD21 | 1.68 | 0.75 |
| 1:F:131:GLU:OE1 | 1:F:169:ARG:NH2 | 2.19 | 0.74 |
| 1:A:60:LEU:HD21 | 1:A:293:ARG:HD2 | 1.68 | 0.74 |
| 1:E:569:ARG:HG2 | 1:E:578:GLU:HG2 | 1.69 | 0.73 |
| 1:A:95:PRO:HB2 | 1:A:97:PRO:HD2 | 1.69 | 0.73 |
| 1:F:35:TYR:HB2 | 1:F:93:LEU:HB2 | 1.70 | 0.73 |
| 1:A:356:LEU:HB3 | 1:A:358:GLN:HG3 | 1.71 | 0.73 |
| 1:D:561:LEU:HD12 | 1:F:569:ARG:HH21 | 1.53 | 0.72 |
| 1:A:147:TYR:OH | 1:C:437:GLU:OE1 | 2.07 | 0.72 |
| 1:A:437:GLU:OE2 | 1:B:147:TYR:OH | 2.08 | 0.72 |
| 1:F:7:VAL:HG21 | 1:F:20:LEU:HD23 | 1.70 | 0.72 |
| 1:A:214:GLN:HG2 | 1:B:80:VAL:HA | 1.72 | 0.71 |
| 1:E:423:GLN:O | 1:E:448:ARG:NH2 | 2.23 | 0.71 |
| 1:E:22:ARG:NH2 | 1:E:24:GLU:OE2 | 2.23 | 0.71 |
| 1:D:285:ARG:NH1 | 1:D:345:ASP:OD2 | 2.24 | 0.70 |
| 1:D:35:TYR:HB2 | 1:D:93:LEU:HB2 | 1.73 | 0.70 |
| 1:B:437:GLU:OE1 | 1:C:147:TYR:OH | 2.10 | 0.70 |
| 1:A:7:VAL:HG21 | 1:A:20:LEU:HD23 | 1.73 | 0.69 |
| 1:D:147:TYR:OH | 1:F:437:GLU:OE1 | 2.11 | 0.69 |
| 1:F:98:TRP:O | 1:F:101:THR:OG1 | 2.09 | 0.69 |
| 1:A:423:GLN:O | 1:A:448:ARG:NH2 | 2.25 | 0.69 |
| 1:F:423:GLN:O | 1:F:448:ARG:NH2 | 2.26 | 0.68 |
| 1:B:241:ARG:NH2 | 2:B:739:SO4:O1 | 2.26 | 0.68 |
| 1:D:437:GLU:OE2 | 1:E:147:TYR:OH | 2.11 | 0.68 |
| 1:B:149:GLU:OE2 | 1:B:157:ARG:NH2 | 2.27 | 0.68 |
| 1:C:423:GLN:O | 1:C:448:ARG:NH2 | 2.25 | 0.68 |
| 1:E:437:GLU:OE1 | 1:F:147:TYR:OH | 2.12 | 0.68 |
| 1:A:11:CYS:HB2 | 1:A:12:PRO:HD2 | 1.76 | 0.68 |
| 1:E:588:SER:HB2 | 1:E:618:VAL:HG12 | 1.74 | 0.68 |
| 1:F:95:PRO:HB2 | 1:F:97:PRO:HD2 | 1.77 | 0.67 |
| 1:A:296:GLY:O | 1:A:299:HIS:HB2 | 1.95 | 0.67 |
| 1:E:456:VAL:HG21 | 1:E:460:LEU:HD22 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:205:ARG:NH1 | 1:A:206:GLU:OE1 | 2.28 | 0.67 |
| 1:D:423:GLN:O | 1:D:448:ARG:NH2 | 2.28 | 0.67 |
| 1:C:531:ARG:NH2 | 2:C:705:SO4:O2 | 2.28 | 0.66 |
| 1:D:233:ARG:HG2 | 1:D:236:ALA:HB2 | 1.77 | 0.66 |
| 1:A:218:GLU:HG3 | 1:B:76:ARG:HB3 | 1.77 | 0.66 |
| 1:E:35:TYR:HB2 | 1:E:93:LEU:HB2 | 1.77 | 0.66 |
| 1:B:423:GLN:O | 1:B:448:ARG:NH2 | 2.29 | 0.65 |
| 1:E:58:LEU:HB2 | 1:E:70:PHE:HB2 | 1.78 | 0.65 |
| 1:A:486:ARG:NH2 | 2:A:739:SO4:O1 | 2.30 | 0.65 |
| 1:B:60:LEU:HD21 | 1:B:293:ARG:HD2 | 1.79 | 0.64 |
| 1:A:189:PRO:HG2 | 1:A:192:TYR:HB2 | 1.79 | 0.64 |
| 1:A:23:MET:HG3 | 1:A:37:LEU:HD12 | 1.79 | 0.64 |
| 1:A:365:ARG:NH2 | 2:A:715:SO4:O1 | 2.31 | 0.64 |
| 1:C:95:PRO:HB2 | 1:C:97:PRO:HD2 | 1.79 | 0.64 |
| 1:A:471:SER:OG | 1:A:472:ARG:N | 2.30 | 0.64 |
| 1:A:437:GLU:OE2 | 1:B:368:GLN:NE2 | 2.30 | 0.64 |
| 1:B:206:GLU:HG2 | 1:B:207:ARG:HG3 | 1.79 | 0.64 |
| 1:A:35:TYR:CZ | 1:A:70:PHE:HD2 | 2.16 | 0.64 |
| 1:C:282:GLN:HA | 1:C:285:ARG:HH11 | 1.63 | 0.64 |
| 1:D:502:ARG:NH1 | 2:D:710:SO4:O3 | 2.32 | 0.63 |
| 1:E:103:THR:HG21 | 1:E:125:LEU:HD21 | 1.81 | 0.63 |
| 1:F:609:ASP:N | 1:F:609:ASP:OD1 | 2.31 | 0.63 |
| 1:B:471:SER:OG | 1:B:472:ARG:N | 2.30 | 0.63 |
| 1:A:391:HIS:ND1 | 1:A:398:ASP:OD2 | 2.32 | 0.63 |
| 1:C:387:ARG:HG2 | 1:C:409:ARG:HA | 1.80 | 0.63 |
| 1:E:95:PRO:HB2 | 1:E:97:PRO:HD2 | 1.79 | 0.63 |
| 1:E:387:ARG:HG2 | 1:E:409:ARG:HA | 1.81 | 0.62 |
| 1:B:35:TYR:HB2 | 1:B:93:LEU:HB2 | 1.80 | 0.62 |
| 1:A:388:VAL:HG11 | 1:A:425:PRO:HB2 | 1.81 | 0.62 |
| 2:A:708:SO4:O3 | 1:C:308:ARG:NH2 | 2.30 | 0.62 |
| 1:A:422:MET:HE2 | 1:A:424:ILE:HG12 | 1.82 | 0.62 |
| 1:A:502:ARG:HB3 | 1:B:494:GLU:O | 1.99 | 0.62 |
| 1:D:5:ARG:N | 1:D:61:GLU:OE1 | 2.32 | 0.62 |
| 1:A:494:GLU:O | 1:C:502:ARG:HB3 | 2.00 | 0.62 |
| 1:B:502:ARG:HB3 | 1:C:494:GLU:O | 2.00 | 0.62 |
| 1:C:486:ARG:NH2 | 2:C:712:SO4:O4 | 2.31 | 0.62 |
| 1:A:538:ARG:HH21 | 1:B:536:ARG:HD2 | 1.66 | 0.61 |
| 1:B:95:PRO:HB2 | 1:B:97:PRO:HD2 | 1.83 | 0.61 |
| 1:F:20:LEU:HD21 | 1:F:23:MET:HB2 | 1.82 | 0.61 |
| 1:E:20:LEU:HD11 | 1:E:23:MET:HB2 | 1.83 | 0.60 |
| 1:C:187:ARG:NH2 | 2:C:717:SO4:O2 | 2.33 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:323:ARG:NH2 | 2:C:739:SO4:S | 2.74 | 0.60 |
| 1:B:20:LEU:O | 1:B:326:GLN:NE2 | 2.35 | 0.60 |
| 1:C:422:MET:HE2 | 1:C:424:ILE:HG12 | 1.84 | 0.60 |
| 1:E:282:GLN:HA | 1:E:285:ARG:HH11 | 1.66 | 0.60 |
| 1:B:422:MET:HE2 | 1:B:424:ILE:HG12 | 1.83 | 0.60 |
| 1:D:471:SER:OG | 1:D:472:ARG:N | 2.33 | 0.59 |
| 1:A:145:VAL:N | 1:A:441:ASP:OD1 | 2.33 | 0.59 |
| 1:D:623:LYS:NZ | 2:D:723:SO4:O1 | 2.33 | 0.59 |
| 1:A:561:LEU:HD11 | 1:C:623:LYS:HG3 | 1.84 | 0.59 |
| 1:D:58:LEU:HB2 | 1:D:70:PHE:HB2 | 1.85 | 0.59 |
| 1:C:131:GLU:OE1 | 1:C:169:ARG:NH1 | 2.36 | 0.59 |
| 1:B:502:ARG:HG2 | 1:B:503:ASN:H | 1.67 | 0.59 |
| 1:A:71:HIS:HB3 | 1:A:175:HIS:HB3 | 1.85 | 0.58 |
| 1:A:30:GLY:HA3 | 1:A:355:LEU:HD11 | 1.85 | 0.58 |
| 1:F:387:ARG:HG2 | 1:F:409:ARG:HA | 1.85 | 0.58 |
| 1:A:79:GLN:HG2 | 1:A:89:TYR:CE1 | 2.39 | 0.58 |
| 1:D:95:PRO:HB2 | 1:D:97:PRO:HD2 | 1.86 | 0.58 |
| 1:F:205:ARG:NH1 | 1:F:206:GLU:OE1 | 2.37 | 0.58 |
| 1:C:232:GLN:NE2 | 2:C:719:SO4:O1 | 2.37 | 0.58 |
| 1:A:293:ARG:HG2 | 1:A:340:PHE:CD1 | 2.39 | 0.58 |
| 1:C:241:ARG:NH2 | 2:C:710:SO4:O3 | 2.37 | 0.58 |
| 1:A:547:LEU:HB3 | 1:A:633:VAL:HG22 | 1.86 | 0.57 |
| 1:C:5:ARG:N | 1:C:61:GLU:OE1 | 2.37 | 0.57 |
| 1:F:139:ARG:NH2 | 1:F:271:TYR:OH | 2.37 | 0.57 |
| 1:A:302:ARG:NH1 | 1:A:314:GLU:HB2 | 2.19 | 0.57 |
| 1:C:20:LEU:HD21 | 1:C:23:MET:HB2 | 1.86 | 0.57 |
| 1:C:569:ARG:NH2 | 1:C:619:ASP:O | 2.36 | 0.57 |
| 1:E:131:GLU:OE1 | 1:E:169:ARG:NH1 | 2.37 | 0.57 |
| 1:A:471:SER:OG | 1:B:489:ASP:OD1 | 2.21 | 0.57 |
| 1:A:536:ARG:HD2 | 1:C:538:ARG:HH21 | 1.69 | 0.57 |
| 1:A:502:ARG:HG2 | 1:A:503:ASN:H | 1.70 | 0.57 |
| 1:E:27:GLU:OE2 | 1:E:35:TYR:OH | 2.23 | 0.57 |
| 1:A:233:ARG:NH2 | 1:A:263:VAL:O | 2.38 | 0.57 |
| 1:B:552:LYS:NZ | 1:B:554:ASP:OD1 | 2.37 | 0.57 |
| 1:E:502:ARG:HB3 | 1:F:494:GLU:O | 2.05 | 0.57 |
| 1:B:385:TYR:HB2 | 1:B:387:ARG:HD2 | 1.87 | 0.57 |
| 1:F:365:ARG:NH2 | 2:F:727:SO4:S | 2.78 | 0.56 |
| 1:C:285:ARG:NH2 | 1:C:318:VAL:HG11 | 2.20 | 0.56 |
| 1:A:27:GLU:OE2 | 1:A:35:TYR:OH | 2.22 | 0.56 |
| 1:A:96:TRP:HD1 | 1:A:175:HIS:CE1 | 2.24 | 0.56 |
| 1:D:79:GLN:HG2 | 1:D:89:TYR:CE1 | 2.41 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:273:ARG:NH2 | 2:B:735:SO4:S | 2.78 | 0.56 |
| 1:A:76:ARG:HG2 | 1:A:92:THR:HB | 1.87 | 0.56 |
| 1:C:32:LEU:HD22 | 1:C:95:PRO:HG2 | 1.88 | 0.56 |
| 1:E:308:ARG:HH11 | 1:E:311:GLN:NE2 | 2.03 | 0.56 |
| 1:B:114:VAL:O | 1:B:118:ILE:HG12 | 2.06 | 0.55 |
| 1:F:58:LEU:HB2 | 1:F:70:PHE:HB2 | 1.87 | 0.55 |
| 1:C:547:LEU:HB3 | 1:C:633:VAL:HG22 | 1.88 | 0.55 |
| 1:A:497:TYR:HH | 1:A:499:HIS:CE1 | 2.23 | 0.55 |
| 1:E:625:VAL:HG22 | 1:E:628:THR:H | 1.72 | 0.55 |
| 1:F:32:LEU:HD22 | 1:F:95:PRO:HG2 | 1.87 | 0.55 |
| 1:C:502:ARG:HG2 | 1:C:503:ASN:H | 1.71 | 0.55 |
| 1:D:30:GLY:HA3 | 1:D:355:LEU:HD11 | 1.88 | 0.55 |
| 1:D:187:ARG:NH2 | 2:D:705:SO4:O4 | 2.37 | 0.55 |
| 1:E:531:ARG:HB3 | 1:F:637:PHE:HE1 | 1.71 | 0.55 |
| 1:F:42:GLU:HG2 | 1:F:86:PHE:HE1 | 1.72 | 0.55 |
| 1:B:391:HIS:ND1 | 1:B:398:ASP:OD2 | 2.35 | 0.55 |
| 1:B:42:GLU:HG2 | 1:B:86:PHE:HE1 | 1.72 | 0.55 |
| 1:E:285:ARG:NH2 | 1:E:318:VAL:HG11 | 2.22 | 0.54 |
| 1:A:157:ARG:HG3 | 1:A:158:LEU:HD13 | 1.89 | 0.54 |
| 1:A:205:ARG:NH2 | 1:A:206:GLU:OE2 | 2.39 | 0.54 |
| 1:A:195:VAL:HG21 | 1:A:210:PHE:CE2 | 2.42 | 0.54 |
| 1:D:102:ARG:HD2 | 1:D:102:ARG:N | 2.22 | 0.54 |
| 1:F:502:ARG:NH1 | 2:F:703:SO4:O2 | 2.32 | 0.54 |
| 1:E:547:LEU:HB3 | 1:E:633:VAL:HG22 | 1.89 | 0.54 |
| 1:B:189:PRO:HG2 | 1:B:192:TYR:HB2 | 1.90 | 0.54 |
| 1:A:324:VAL:HG22 | 1:A:340:PHE:HD2 | 1.73 | 0.54 |
| 1:A:131:GLU:OE1 | 1:A:169:ARG:NH2 | 2.39 | 0.54 |
| 1:C:323:ARG:NH2 | 2:C:739:SO4:O3 | 2.30 | 0.54 |
| 1:F:571:VAL:HG13 | 1:F:576:VAL:HG22 | 1.90 | 0.54 |
| 1:A:214:GLN:CD | 1:A:287:ARG:HH21 | 2.11 | 0.54 |
| 1:A:310:ASP:OD1 | 1:A:311:GLN:N | 2.40 | 0.54 |
| 1:A:596:ALA:HB2 | 1:B:592:PHE:HD2 | 1.73 | 0.54 |
| 1:B:63:PRO:HD3 | 1:B:293:ARG:HH21 | 1.73 | 0.54 |
| 1:F:214:GLN:OE1 | 1:F:287:ARG:NH2 | 2.38 | 0.54 |
| 1:A:104:SER:HB3 | 1:A:150:THR:HG22 | 1.89 | 0.53 |
| 1:B:596:ALA:HB2 | 1:C:592:PHE:HD1 | 1.74 | 0.53 |
| 1:B:78:SER:HB2 | 1:B:90:GLN:HG3 | 1.90 | 0.53 |
| 1:B:39:LEU:HD12 | 1:B:89:TYR:HB2 | 1.90 | 0.53 |
| 1:D:78:SER:OG | 1:D:90:GLN:HG3 | 2.08 | 0.53 |
| 1:E:7:VAL:HG22 | 1:E:326:GLN:OE1 | 2.08 | 0.53 |
| 1:D:536:ARG:HD2 | 1:F:538:ARG:HH21 | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:509:GLU:HB2 | 1:C:501:GLU:O | 2.08 | 0.53 |
| 1:C:273:ARG:NH1 | 2:C:731:SO4:O3 | 2.41 | 0.53 |
| 1:B:11:CYS:HB3 | 1:B:56:MET:HG3 | 1.91 | 0.53 |
| 1:D:547:LEU:HB3 | 1:D:633:VAL:HG22 | 1.91 | 0.53 |
| 1:B:497:TYR:OH | 1:B:499:HIS:ND1 | 2.41 | 0.53 |
| 1:C:502:ARG:NH2 | 2:C:701:SO4:O2 | 2.42 | 0.53 |
| 1:D:391:HIS:ND1 | 1:D:398:ASP:OD2 | 2.37 | 0.53 |
| 1:F:114:VAL:HG21 | 1:F:162:GLU:HG3 | 1.91 | 0.53 |
| 1:F:63:PRO:HD3 | 1:F:293:ARG:HH21 | 1.72 | 0.53 |
| 1:B:79:GLN:HG2 | 1:B:89:TYR:CE1 | 2.44 | 0.53 |
| 1:C:212:ASP:HB3 | 1:C:289:ARG:HG3 | 1.89 | 0.53 |
| 1:D:273:ARG:NH2 | 2:D:722:SO4:O1 | 2.41 | 0.53 |
| 1:B:302:ARG:NH2 | 2:B:732:SO4:S | 2.81 | 0.53 |
| 1:A:114:VAL:HG21 | 1:A:162:GLU:HG3 | 1.91 | 0.52 |
| 1:A:7:VAL:HG22 | 1:A:326:GLN:OE1 | 2.09 | 0.52 |
| 1:F:547:LEU:HB3 | 1:F:633:VAL:HG22 | 1.90 | 0.52 |
| 1:E:302:ARG:NH1 | 2:E:716:SO4:O4 | 2.31 | 0.52 |
| 1:F:7:VAL:HG22 | 1:F:326:GLN:OE1 | 2.09 | 0.52 |
| 1:B:32:LEU:HD22 | 1:B:95:PRO:HG2 | 1.91 | 0.52 |
| 1:E:422:MET:HE2 | 1:E:424:ILE:HG12 | 1.91 | 0.52 |
| 1:F:302:ARG:NH1 | 2:F:714:SO4:O4 | 2.42 | 0.52 |
| 1:C:60:LEU:HD21 | 1:C:293:ARG:HD2 | 1.92 | 0.52 |
| 1:D:453:GLU:HG3 | 1:D:454:GLN:H | 1.75 | 0.52 |
| 1:A:509:GLU:HB2 | 1:B:501:GLU:O | 2.10 | 0.52 |
| 1:A:7:VAL:HG22 | 1:A:326:GLN:CD | 2.30 | 0.52 |
| 1:B:547:LEU:HB3 | 1:B:633:VAL:HG22 | 1.91 | 0.52 |
| 1:A:80:VAL:HA | 1:C:214:GLN:HG3 | 1.91 | 0.52 |
| 1:A:192:TYR:CE2 | 1:A:292:VAL:HG23 | 2.46 | 0.51 |
| 1:C:188:SER:OG | 1:C:300:LEU:O | 2.20 | 0.51 |
| 1:C:63:PRO:HD3 | 1:C:293:ARG:HH21 | 1.75 | 0.51 |
| 1:B:384:GLN:N | 2:B:740:SO4:O4 | 2.43 | 0.51 |
| 1:B:102:ARG:N | 1:B:102:ARG:HD2 | 2.25 | 0.51 |
| 1:A:213:TRP:NE1 | 1:A:311:GLN:HG2 | 2.25 | 0.51 |
| 1:A:623:LYS:HG3 | 1:B:561:LEU:HD11 | 1.92 | 0.51 |
| 1:B:241:ARG:NH2 | 2:B:739:SO4:S | 2.83 | 0.51 |
| 1:D:586:ASN:HB3 | 1:D:618:VAL:HG21 | 1.91 | 0.51 |
| 1:A:48:LEU:HB3 | 1:A:77:CYS:SG | 2.50 | 0.51 |
| 1:D:437:GLU:OE2 | 1:E:368:GLN:NE2 | 2.44 | 0.51 |
| 1:B:114:VAL:HG13 | 1:B:158:LEU:HB3 | 1.93 | 0.51 |
| 1:B:131:GLU:OE1 | 1:B:169:ARG:NH1 | 2.43 | 0.51 |
| 1:E:308:ARG:HH11 | 1:E:311:GLN:HE22 | 1.57 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:387:ARG:HG2 | 1:D:409:ARG:HA | 1.93 | 0.51 |
| 1:F:27:GLU:OE2 | 1:F:35:TYR:OH | 2.29 | 0.51 |
| 1:E:63:PRO:HD3 | 1:E:293:ARG:HH21 | 1.76 | 0.51 |
| 1:A:5:ARG:HB2 | 1:A:6:LEU:HG | 1.92 | 0.50 |
| 1:C:37:LEU:HB3 | 1:C:39:LEU:HD11 | 1.91 | 0.50 |
| 1:E:210:PHE:HD1 | 1:E:290:GLY:HA3 | 1.76 | 0.50 |
| 1:D:538:ARG:HH21 | 1:E:536:ARG:HD2 | 1.75 | 0.50 |
| 1:B:431:VAL:HG21 | 1:B:445:ILE:HD13 | 1.93 | 0.50 |
| 1:B:502:ARG:NH2 | 2:B:701:SO4:O4 | 2.44 | 0.50 |
| 1:D:63:PRO:HD3 | 1:D:293:ARG:NH2 | 2.26 | 0.50 |
| 1:B:241:ARG:HH11 | 1:B:243:ASN:HD21 | 1.60 | 0.50 |
| 1:E:37:LEU:HB3 | 1:E:39:LEU:HD11 | 1.93 | 0.50 |
| 1:A:139:ARG:NH1 | 1:A:271:TYR:OH | 2.44 | 0.50 |
| 1:B:214:GLN:OE1 | 1:B:287:ARG:NH2 | 2.45 | 0.50 |
| 1:D:266:GLN:N | 1:D:266:GLN:OE1 | 2.38 | 0.50 |
| 1:E:32:LEU:HD22 | 1:E:95:PRO:HG2 | 1.92 | 0.50 |
| 2:D:736:SO4:O2 | 1:F:538:ARG:NH1 | 2.45 | 0.50 |
| 1:C:373:VAL:HG22 | 1:C:374:GLY:H | 1.76 | 0.50 |
| 1:D:591:ALA:O | 1:E:584:THR:HA | 2.12 | 0.50 |
| 1:D:285:ARG:HD3 | 1:D:347:ILE:HG22 | 1.93 | 0.50 |
| 1:E:308:ARG:HG2 | 1:E:310:ASP:OD1 | 2.11 | 0.50 |
| 1:B:18:LEU:HD22 | 1:B:39:LEU:HD13 | 1.93 | 0.49 |
| 1:B:302:ARG:NH2 | 2:B:732:SO4:O2 | 2.45 | 0.49 |
| 1:B:538:ARG:NH1 | 2:B:750:SO4:O4 | 2.45 | 0.49 |
| 1:D:114:VAL:HG21 | 1:D:162:GLU:HG3 | 1.92 | 0.49 |
| 1:C:529:LEU:HD21 | 1:C:531:ARG:HH11 | 1.78 | 0.49 |
| 1:D:42:GLU:HG2 | 1:D:86:PHE:HE1 | 1.77 | 0.49 |
| 1:A:503:ASN:ND2 | 1:C:511:ASP:HB2 | 2.28 | 0.49 |
| 1:B:27:GLU:OE2 | 1:B:35:TYR:OH | 2.31 | 0.49 |
| 1:A:501:GLU:O | 1:C:509:GLU:HB2 | 2.13 | 0.49 |
| 1:A:17:VAL:HG12 | 1:A:46:LEU:HD11 | 1.93 | 0.49 |
| 1:A:507:LEU:HD23 | 1:B:499:HIS:CE1 | 2.48 | 0.49 |
| 1:E:114:VAL:HG21 | 1:E:162:GLU:HG3 | 1.94 | 0.49 |
| 1:B:285:ARG:HD3 | 1:B:347:ILE:HG22 | 1.95 | 0.49 |
| 1:F:17:VAL:HG12 | 1:F:46:LEU:HD11 | 1.95 | 0.49 |
| 1:B:12:PRO:O | 1:B:13:LEU:HB3 | 2.12 | 0.49 |
| 1:C:60:LEU:HD21 | 1:C:293:ARG:HB3 | 1.95 | 0.49 |
| 1:B:582:ASP:OD1 | 1:B:584:THR:OG1 | 2.24 | 0.48 |
| 1:A:11:CYS:SG | 1:A:18:LEU:HD12 | 2.53 | 0.48 |
| 1:C:419:TRP:NE1 | 2:C:741:SO4:O2 | 2.36 | 0.48 |
| 1:A:11:CYS:HB3 | 1:A:56:MET:HG3 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:187:ARG:NH1 | 2:A:702:SO4:O2 | 2.43 | 0.48 |
| 1:E:108:ILE:HG12 | 1:E:145:VAL:HG22 | 1.95 | 0.48 |
| 1:F:582:ASP:OD1 | 1:F:584:THR:OG1 | 2.26 | 0.48 |
| 1:F:79:GLN:HG2 | 1:F:89:TYR:CE1 | 2.48 | 0.48 |
| 1:C:308:ARG:NH1 | 1:C:311:GLN:OE1 | 2.40 | 0.48 |
| 1:E:380:ILE:HG12 | 1:E:426:ARG:HG2 | 1.96 | 0.48 |
| 1:F:11:CYS:HB3 | 1:F:56:MET:HG3 | 1.94 | 0.48 |
| 1:B:233:ARG:NH2 | 2:B:717:SO4:O1 | 2.44 | 0.48 |
| 1:C:7:VAL:HG22 | 1:C:326:GLN:OE1 | 2.12 | 0.48 |
| 1:D:213:TRP:HD1 | 1:D:288:LEU:HD21 | 1.78 | 0.48 |
| 1:D:27:GLU:OE2 | 1:D:35:TYR:OH | 2.30 | 0.48 |
| 1:E:578:GLU:OE2 | 1:E:621:LYS:NZ | 2.46 | 0.48 |
| 1:A:96:TRP:CG | 1:A:97:PRO:HD3 | 2.49 | 0.48 |
| 1:C:484:GLU:HG2 | 1:C:485:ILE:N | 2.29 | 0.48 |
| 1:F:289:ARG:NH2 | 2:F:707:SO4:O3 | 2.44 | 0.48 |
| 1:C:58:LEU:HB2 | 1:C:70:PHE:HB2 | 1.94 | 0.48 |
| 1:A:248:HIS:CE1 | 1:A:251:ALA:HB2 | 2.48 | 0.47 |
| 1:C:7:VAL:HG21 | 1:C:20:LEU:HD23 | 1.97 | 0.47 |
| 1:D:365:ARG:NH2 | 2:D:734:SO4:O2 | 2.47 | 0.47 |
| 1:E:238:LEU:O | 1:E:262:TYR:OH | 2.25 | 0.47 |
| 1:F:309:ASP:HA | 1:F:312:ASN:HD22 | 1.79 | 0.47 |
| 1:A:410:VAL:HA | 1:A:445:ILE:HB | 1.95 | 0.47 |
| 1:A:502:ARG:NH2 | 2:A:701:SO4:O4 | 2.27 | 0.47 |
| 1:B:241:ARG:NH1 | 1:B:243:ASN:HD21 | 2.12 | 0.47 |
| 2:D:708:SO4:O2 | 1:F:308:ARG:NH2 | 2.47 | 0.47 |
| 1:B:18:LEU:HD23 | 1:B:41:SER:HB2 | 1.95 | 0.47 |
| 1:D:422:MET:HE2 | 1:D:424:ILE:HG12 | 1.95 | 0.47 |
| 1:D:275:ARG:O | 1:D:279:ILE:HG13 | 2.14 | 0.47 |
| 1:E:5:ARG:HB3 | 1:E:6:LEU:HD12 | 1.97 | 0.47 |
| 1:E:30:GLY:HA3 | 1:E:355:LEU:HD11 | 1.96 | 0.47 |
| 1:C:431:VAL:HG21 | 1:C:445:ILE:HD13 | 1.95 | 0.47 |
| 1:A:592:PHE:HD2 | 1:C:596:ALA:HB2 | 1.80 | 0.47 |
| 1:A:390:VAL:HG22 | 1:A:408:ILE:HD12 | 1.97 | 0.47 |
| 3:A:749:TAM:H41 | 3:A:749:TAM:H21 | 1.58 | 0.47 |
| 1:B:42:GLU:HG2 | 1:B:86:PHE:CE1 | 2.48 | 0.47 |
| 1:A:484:GLU:HG2 | 1:A:485:ILE:N | 2.30 | 0.47 |
| 1:B:217:ARG:HA | 1:B:283:HIS:O | 2.14 | 0.47 |
| 1:C:30:GLY:HA3 | 1:C:355:LEU:HD11 | 1.97 | 0.47 |
| 1:F:233:ARG:NH2 | 1:F:263:VAL:O | 2.48 | 0.47 |
| 1:E:308:ARG:NE | 1:F:45:ASN:OD1 | 2.38 | 0.47 |
| 1:B:538:ARG:HH21 | 1:C:536:ARG:HD2 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:273:ARG:NH1 | 2:C:731:SO4:O2 | 2.48 | 0.47 |
| 1:D:380:ILE:HG21 | 1:E:464:ALA:HB1 | 1.97 | 0.47 |
| 1:A:213:TRP:HD1 | 1:A:288:LEU:HD21 | 1.80 | 0.47 |
| 1:C:391:HIS:ND1 | 1:C:398:ASP:OD2 | 2.44 | 0.47 |
| 1:D:309:ASP:HA | 1:D:312:ASN:HD22 | 1.80 | 0.47 |
| 1:E:198:TYR:CD2 | 1:E:205:ARG:HG2 | 2.50 | 0.47 |
| 1:E:96:TRP:CG | 1:E:97:PRO:HD3 | 2.50 | 0.47 |
| 1:B:213:TRP:HD1 | 1:B:288:LEU:HD21 | 1.79 | 0.46 |
| 1:B:623:LYS:HD2 | 1:C:563:GLU:OE2 | 2.15 | 0.46 |
| 1:B:94:ARG:NH2 | 2:B:710:SO4:O1 | 2.47 | 0.46 |
| 1:C:12:PRO:O | 1:C:13:LEU:HB3 | 2.14 | 0.46 |
| 1:B:471:SER:OG | 1:C:489:ASP:OD2 | 2.28 | 0.46 |
| 1:B:30:GLY:HA3 | 1:B:355:LEU:HD11 | 1.96 | 0.46 |
| 1:D:453:GLU:HG3 | 1:D:454:GLN:N | 2.30 | 0.46 |
| 1:C:114:VAL:HG21 | 1:C:162:GLU:HG3 | 1.96 | 0.46 |
| 1:F:96:TRP:CG | 1:F:97:PRO:HD3 | 2.51 | 0.46 |
| 1:B:436:LEU:HA | 1:C:367:PRO:O | 2.16 | 0.46 |
| 1:B:502:ARG:HB2 | 1:C:494:GLU:HB2 | 1.97 | 0.46 |
| 1:E:475:LYS:O | 1:F:491:LYS:HG3 | 2.15 | 0.46 |
| 1:A:210:PHE:HD1 | 1:A:289:ARG:O | 1.97 | 0.46 |
| 1:A:353:PHE:HZ | 1:A:355:LEU:HD23 | 1.79 | 0.46 |
| 1:A:511:ASP:HB2 | 1:B:503:ASN:ND2 | 2.31 | 0.46 |
| 1:C:217:ARG:HA | 1:C:283:HIS:O | 2.15 | 0.46 |
| 1:D:309:ASP:OD1 | 1:D:309:ASP:N | 2.49 | 0.46 |
| 1:D:471:SER:OG | 1:E:489:ASP:OD1 | 2.28 | 0.46 |
| 1:A:12:PRO:HG3 | 1:A:54:LYS:HB3 | 1.98 | 0.46 |
| 1:A:582:ASP:OD1 | 1:A:584:THR:OG1 | 2.30 | 0.46 |
| 1:D:139:ARG:NH2 | 2:D:724:SO4:S | 2.89 | 0.46 |
| 1:F:213:TRP:CE2 | 1:F:311:GLN:HG2 | 2.51 | 0.46 |
| 1:F:431:VAL:HG21 | 1:F:445:ILE:HD13 | 1.97 | 0.46 |
| 1:A:162:GLU:OE2 | 1:A:271:TYR:OH | 2.32 | 0.46 |
| 1:A:306:TYR:HA | 1:A:307:PRO:HD2 | 1.67 | 0.46 |
| 1:E:210:PHE:CD1 | 1:E:290:GLY:HA3 | 2.51 | 0.46 |
| 1:F:384:GLN:N | 2:F:715:SO4:O4 | 2.49 | 0.46 |
| 1:A:436:LEU:HA | 1:B:367:PRO:O | 2.16 | 0.46 |
| 3:A:749:TAM:H61 | 3:A:749:TAM:H11 | 1.72 | 0.46 |
| 1:B:273:ARG:NH2 | 2:B:735:SO4:O1 | 2.49 | 0.46 |
| 1:C:147:TYR:CE2 | 1:C:148:ARG:HG3 | 2.51 | 0.46 |
| 1:D:7:VAL:N | 1:D:326:GLN:OE1 | 2.46 | 0.46 |
| 1:E:520:ARG:HH21 | 1:E:522:LYS:HD3 | 1.79 | 0.46 |
| 1:F:63:PRO:HD3 | 1:F:293:ARG:NH2 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:452:ALA:HB2 | 1:C:232:GLN:HA | 1.97 | 0.46 |
| 1:B:139:ARG:NH1 | 2:B:719:SO4:S | 2.89 | 0.46 |
| 1:B:531:ARG:NH2 | 2:B:726:SO4:O2 | 2.45 | 0.46 |
| 1:D:12:PRO:O | 1:D:13:LEU:HB3 | 2.15 | 0.46 |
| 1:F:108:ILE:HG12 | 1:F:145:VAL:HG22 | 1.97 | 0.45 |
| 1:B:100:LEU:HB2 | 1:B:152:PHE:HB2 | 1.97 | 0.45 |
| 1:B:542:LEU:HB3 | 1:B:543:ASN:H | 1.57 | 0.45 |
| 1:E:12:PRO:O | 1:E:13:LEU:HB3 | 2.15 | 0.45 |
| 1:F:12:PRO:O | 1:F:13:LEU:HB3 | 2.16 | 0.45 |
| 1:F:275:ARG:O | 1:F:279:ILE:HG13 | 2.16 | 0.45 |
| 1:D:253:TYR:HA | 1:D:254:PRO:HD3 | 1.87 | 0.45 |
| 1:D:96:TRP:CG | 1:D:97:PRO:HD3 | 2.51 | 0.45 |
| 1:E:71:HIS:HB3 | 1:E:175:HIS:HB3 | 1.99 | 0.45 |
| 1:E:538:ARG:HH21 | 1:F:536:ARG:HD2 | 1.82 | 0.45 |
| 1:E:11:CYS:HB3 | 1:E:56:MET:HG3 | 1.99 | 0.45 |
| 1:B:218:GLU:HG3 | 1:C:76:ARG:HB3 | 1.99 | 0.45 |
| 1:D:67:ARG:N | 2:D:731:SO4:O4 | 2.48 | 0.45 |
| 1:E:275:ARG:O | 1:E:279:ILE:HG13 | 2.16 | 0.45 |
| 1:A:76:ARG:HA | 1:C:217:ARG:O | 2.17 | 0.45 |
| 1:A:73:ILE:O | 1:A:93:LEU:HA | 2.17 | 0.45 |
| 1:F:33:PHE:CE2 | 1:F:95:PRO:HB3 | 2.51 | 0.45 |
| 1:B:309:ASP:HA | 1:B:312:ASN:HD22 | 1.81 | 0.45 |
| 1:B:139:ARG:NH1 | 2:B:719:SO4:O3 | 2.49 | 0.45 |
| 1:A:79:GLN:HG2 | 1:A:89:TYR:CD1 | 2.52 | 0.45 |
| 1:B:25:GLY:O | 1:B:26:ARG:HD3 | 2.16 | 0.45 |
| 1:A:145:VAL:HG12 | 1:A:147:TYR:HB2 | 1.99 | 0.45 |
| 1:A:217:ARG:HA | 1:A:283:HIS:O | 2.15 | 0.45 |
| 1:A:219:VAL:HB | 1:B:98:TRP:CH2 | 2.51 | 0.45 |
| 1:C:189:PRO:HG2 | 1:C:192:TYR:HB2 | 1.99 | 0.45 |
| 1:F:188:SER:OG | 1:F:300:LEU:O | 2.21 | 0.45 |
| 1:A:33:PHE:CE2 | 1:A:95:PRO:HB3 | 2.52 | 0.44 |
| 1:D:436:LEU:HA | 1:E:367:PRO:O | 2.17 | 0.44 |
| 1:A:195:VAL:HG21 | 1:A:210:PHE:HE2 | 1.83 | 0.44 |
| 1:A:37:LEU:HD21 | 1:A:58:LEU:HD11 | 1.98 | 0.44 |
| 1:B:199:PRO:HB2 | 1:B:201:THR:HG22 | 1.99 | 0.44 |
| 1:C:136:ARG:HG3 | 1:C:136:ARG:H | 1.49 | 0.44 |
| 1:C:253:TYR:HA | 1:C:254:PRO:HD3 | 1.85 | 0.44 |
| 1:D:431:VAL:HG21 | 1:D:445:ILE:HD13 | 2.00 | 0.44 |
| 1:D:11:CYS:HB3 | 1:D:56:MET:HG3 | 1.98 | 0.44 |
| 1:A:296:GLY:HA2 | 1:A:322:TYR:OH | 2.18 | 0.44 |
| 1:B:32:LEU:HD21 | 1:B:97:PRO:HB2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:58:LEU:HB2 | 1:B:70:PHE:HB2 | 1.98 | 0.44 |
| 1:B:96:TRP:CG | 1:B:97:PRO:HD3 | 2.52 | 0.44 |
| 1:F:607:ARG:HD2 | 1:F:607:ARG:H | 1.82 | 0.44 |
| 1:A:104:SER:HA | 1:A:150:THR:HA | 1.99 | 0.44 |
| 1:A:308:ARG:HH11 | 1:A:311:GLN:NE2 | 2.16 | 0.44 |
| 1:B:26:ARG:HD2 | 1:B:321:GLU:HG2 | 1.99 | 0.44 |
| 1:D:217:ARG:HA | 1:D:283:HIS:O | 2.17 | 0.44 |
| 1:D:494:GLU:O | 1:F:502:ARG:HB3 | 2.17 | 0.44 |
| 1:B:157:ARG:HD3 | 1:B:361:VAL:HA | 1.98 | 0.44 |
| 1:B:308:ARG:NH2 | 2:B:711:SO4:O1 | 2.47 | 0.44 |
| 1:B:76:ARG:HG2 | 1:B:92:THR:HB | 2.00 | 0.44 |
| 1:D:302:ARG:NH1 | 2:D:716:SO4:O2 | 2.50 | 0.44 |
| 1:E:542:LEU:HB3 | 1:E:543:ASN:H | 1.50 | 0.44 |
| 1:E:623:LYS:HG3 | 1:F:561:LEU:HD11 | 1.98 | 0.44 |
| 1:A:524:ILE:HG13 | 1:B:516:VAL:HB | 2.00 | 0.44 |
| 1:C:205:ARG:NH1 | 1:C:206:GLU:OE1 | 2.51 | 0.44 |
| 1:F:100:LEU:HB2 | 1:F:152:PHE:HB2 | 1.99 | 0.44 |
| 1:C:275:ARG:O | 1:C:279:ILE:HG12 | 2.18 | 0.44 |
| 1:C:76:ARG:HG2 | 1:C:92:THR:HB | 1.99 | 0.44 |
| 1:B:107:ARG:HD3 | 1:B:109:PHE:CZ | 2.53 | 0.44 |
| 1:A:502:ARG:HB2 | 1:B:494:GLU:HB2 | 2.00 | 0.44 |
| 1:C:96:TRP:CG | 1:C:97:PRO:HD3 | 2.52 | 0.44 |
| 1:D:306:TYR:CD1 | 1:D:307:PRO:HD2 | 2.53 | 0.44 |
| 1:E:212:ASP:HB3 | 1:E:289:ARG:HB2 | 1.99 | 0.44 |
| 1:F:522:LYS:HE3 | 1:F:524:ILE:HD13 | 1.98 | 0.44 |
| 1:A:402:GLU:HG2 | 1:A:403:ASN:OD1 | 2.16 | 0.43 |
| 1:B:524:ILE:HG13 | 1:C:516:VAL:HB | 2.00 | 0.43 |
| 1:D:603:ASP:OD1 | 1:F:613:GLY:N | 2.37 | 0.43 |
| 1:C:63:PRO:HD3 | 1:C:293:ARG:NH2 | 2.33 | 0.43 |
| 1:C:472:ARG:HA | 1:C:472:ARG:HD3 | 1.85 | 0.43 |
| 3:D:735:TAM:H61 | 3:D:735:TAM:H12 | 1.59 | 0.43 |
| 1:F:162:GLU:OE2 | 1:F:271:TYR:OH | 2.33 | 0.43 |
| 1:C:46:LEU:HB2 | 1:C:89:TYR:CE2 | 2.53 | 0.43 |
| 1:C:6:LEU:HB3 | 1:C:326:GLN:OE1 | 2.18 | 0.43 |
| 1:A:219:VAL:HB | 1:B:98:TRP:HH2 | 1.83 | 0.43 |
| 1:E:189:PRO:HG2 | 1:E:192:TYR:HB2 | 2.00 | 0.43 |
| 1:B:285:ARG:NH1 | 1:B:345:ASP:OD2 | 2.51 | 0.43 |
| 1:E:233:ARG:NH2 | 1:E:263:VAL:O | 2.52 | 0.43 |
| 1:A:134:LEU:HD13 | 1:A:138:TYR:CE1 | 2.53 | 0.43 |
| 1:A:326:GLN:HG2 | 1:A:338:SER:HA | 2.01 | 0.43 |
| 1:A:609:ASP:HB3 | 1:A:612:SER:HB3 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:123:ARG:NH2 | 2:A:730:SO4:O4 | 2.52 | 0.43 |
| 1:E:391:HIS:ND1 | 1:E:398:ASP:OD2 | 2.45 | 0.43 |
| 1:E:580:ASN:HB2 | 1:E:584:THR:HG22 | 2.00 | 0.43 |
| 1:F:7:VAL:HA | 1:F:59:SER:O | 2.19 | 0.43 |
| 1:A:577:VAL:HG21 | 1:B:579:PHE:CZ | 2.53 | 0.43 |
| 1:B:306:TYR:CD1 | 1:B:307:PRO:HD2 | 2.53 | 0.43 |
| 1:B:510:ASN:ND2 | 1:C:503:ASN:OD1 | 2.36 | 0.43 |
| 1:C:213:TRP:HD1 | 1:C:288:LEU:HD21 | 1.83 | 0.43 |
| 1:C:309:ASP:HA | 1:C:312:ASN:HD22 | 1.84 | 0.43 |
| 1:C:306:TYR:CD1 | 1:C:307:PRO:HD2 | 2.54 | 0.43 |
| 1:D:248:HIS:CE1 | 1:D:251:ALA:HB2 | 2.54 | 0.43 |
| 1:D:623:LYS:HD2 | 1:E:563:GLU:OE2 | 2.19 | 0.43 |
| 1:A:246:ARG:HA | 1:A:247:PRO:HD3 | 1.86 | 0.43 |
| 1:A:542:LEU:HB3 | 1:A:543:ASN:H | 1.59 | 0.43 |
| 1:B:378:GLU:N | 1:B:378:GLU:OE1 | 2.52 | 0.43 |
| 1:D:380:ILE:HG12 | 1:D:426:ARG:HD3 | 2.01 | 0.43 |
| 1:E:266:GLN:N | 1:E:266:GLN:OE1 | 2.39 | 0.43 |
| 1:E:306:TYR:CD1 | 1:E:307:PRO:HD2 | 2.54 | 0.43 |
| 1:E:485:ILE:HA | 1:E:497:TYR:O | 2.19 | 0.43 |
| 1:A:503:ASN:CG | 1:C:511:ASP:HB2 | 2.38 | 0.42 |
| 1:B:71:HIS:HB3 | 1:B:175:HIS:HB3 | 2.01 | 0.42 |
| 1:E:450:TYR:CZ | 1:E:457:PRO:HD3 | 2.54 | 0.42 |
| 1:A:502:ARG:HG2 | 1:A:503:ASN:N | 2.34 | 0.42 |
| 1:B:114:VAL:HG21 | 1:B:162:GLU:HG3 | 2.00 | 0.42 |
| 1:D:232:GLN:HA | 1:E:452:ALA:HB2 | 2.01 | 0.42 |
| 1:E:509:GLU:HB2 | 1:F:501:GLU:O | 2.19 | 0.42 |
| 1:E:431:VAL:HG21 | 1:E:445:ILE:HD13 | 2.00 | 0.42 |
| 1:D:501:GLU:O | 1:F:509:GLU:HB2 | 2.19 | 0.42 |
| 1:B:63:PRO:HD3 | 1:B:293:ARG:NH2 | 2.32 | 0.42 |
| 1:C:33:PHE:CE2 | 1:C:95:PRO:HB3 | 2.53 | 0.42 |
| 1:D:189:PRO:HG2 | 1:D:192:TYR:HB2 | 2.00 | 0.42 |
| 1:F:306:TYR:CD1 | 1:F:307:PRO:HD2 | 2.54 | 0.42 |
| 1:E:308:ARG:NH1 | 1:E:311:GLN:HE22 | 2.16 | 0.42 |
| 1:E:571:VAL:HG21 | 1:E:623:LYS:HB2 | 2.02 | 0.42 |
| 1:A:356:LEU:HD12 | 1:A:356:LEU:HA | 1.85 | 0.42 |
| 1:A:372:VAL:HA | 1:A:390:VAL:HA | 2.00 | 0.42 |
| 1:A:569:ARG:NH2 | 1:A:619:ASP:O | 2.51 | 0.42 |
| 1:B:502:ARG:HG2 | 1:B:503:ASN:N | 2.32 | 0.42 |
| 1:C:534:ASN:HB3 | 1:C:535:ASN:H | 1.66 | 0.42 |
| 1:D:542:LEU:HB3 | 1:D:543:ASN:H | 1.60 | 0.42 |
| 1:A:32:LEU:HD22 | 1:A:98:TRP:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:213:TRP:NE1 | 1:B:311:GLN:HG2 | 2.35 | 0.42 |
| 1:D:188:SER:OG | 1:D:300:LEU:O | 2.22 | 0.42 |
| 3:D:735:TAM:H22 | 1:F:469:MET:HE3 | 2.02 | 0.42 |
| 1:F:213:TRP:NE1 | 1:F:311:GLN:HG2 | 2.34 | 0.42 |
| 1:A:23:MET:HG2 | 1:A:24:GLU:N | 2.34 | 0.42 |
| 1:A:353:PHE:CZ | 1:A:355:LEU:HD23 | 2.55 | 0.42 |
| 1:A:51:LEU:O | 1:A:54:LYS:HB2 | 2.19 | 0.42 |
| 1:D:103:THR:HG21 | 1:D:125:LEU:HD21 | 2.02 | 0.42 |
| 1:D:534:ASN:HB3 | 1:D:535:ASN:H | 1.66 | 0.42 |
| 1:E:611:ASN:OD1 | 1:F:608:LEU:HD21 | 2.19 | 0.42 |
| 1:F:616:SER:OG | 1:F:617:GLU:N | 2.53 | 0.42 |
| 1:C:210:PHE:HD1 | 1:C:290:GLY:HA3 | 1.84 | 0.42 |
| 1:A:297:ALA:HA | 1:A:317:VAL:HB | 2.02 | 0.42 |
| 1:A:324:VAL:HG22 | 1:A:340:PHE:CD2 | 2.54 | 0.42 |
| 1:A:408:ILE:HG22 | 1:A:444:ILE:HA | 2.01 | 0.42 |
| 1:A:86:PHE:HD1 | 1:A:86:PHE:HA | 1.74 | 0.42 |
| 1:B:248:HIS:CE1 | 1:B:251:ALA:HB2 | 2.55 | 0.42 |
| 1:E:63:PRO:HD3 | 1:E:293:ARG:NH2 | 2.34 | 0.42 |
| 1:A:146:GLN:HG3 | 1:A:149:GLU:HG3 | 2.02 | 0.41 |
| 1:B:328:LEU:HD12 | 1:B:328:LEU:HA | 1.88 | 0.41 |
| 1:C:210:PHE:CD1 | 1:C:290:GLY:HA3 | 2.55 | 0.41 |
| 1:C:484:GLU:CG | 1:C:485:ILE:N | 2.83 | 0.41 |
| 1:E:213:TRP:CE2 | 1:E:311:GLN:HG2 | 2.56 | 0.41 |
| 1:A:188:SER:OG | 1:A:300:LEU:O | 2.19 | 0.41 |
| 1:A:410:VAL:HG22 | 1:A:445:ILE:HD12 | 2.01 | 0.41 |
| 1:A:511:ASP:HB2 | 1:B:503:ASN:CG | 2.40 | 0.41 |
| 1:E:37:LEU:HD21 | 1:E:58:LEU:HD11 | 2.01 | 0.41 |
| 1:E:534:ASN:HB3 | 1:E:535:ASN:H | 1.66 | 0.41 |
| 1:B:383:ASP:OD2 | 1:B:387:ARG:HD3 | 2.21 | 0.41 |
| 1:C:287:ARG:NH1 | 1:C:289:ARG:HE | 2.19 | 0.41 |
| 1:B:217:ARG:NH1 | 1:C:49:GLU:OE2 | 2.53 | 0.41 |
| 1:D:206:GLU:HG2 | 1:D:207:ARG:N | 2.36 | 0.41 |
| 1:E:253:TYR:HA | 1:E:254:PRO:HD3 | 1.86 | 0.41 |
| 1:E:436:LEU:HA | 1:F:367:PRO:O | 2.20 | 0.41 |
| 1:E:33:PHE:CE2 | 1:E:95:PRO:HB3 | 2.56 | 0.41 |
| 1:A:552:LYS:NZ | 1:A:554:ASP:OD1 | 2.52 | 0.41 |
| 1:C:213:TRP:CZ2 | 1:C:215:MET:HB2 | 2.55 | 0.41 |
| 1:E:368:GLN:HG2 | 1:E:435:PHE:HE1 | 1.85 | 0.41 |
| 1:C:108:ILE:HG12 | 1:C:145:VAL:HG22 | 2.03 | 0.41 |
| 1:F:29:LEU:HD12 | 1:F:29:LEU:HA | 1.91 | 0.41 |
| 1:F:579:PHE:HE1 | 1:F:585:ILE:HG23 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:244:ILE:HG13 | 1:A:280:GLN:HG3 | 2.02 | 0.41 |
| 1:A:387:ARG:HG2 | 1:A:409:ARG:HA | 2.02 | 0.41 |
| 1:B:6:LEU:HB2 | 1:B:326:GLN:OE1 | 2.20 | 0.41 |
| 1:D:563:GLU:OE2 | 1:F:623:LYS:HD2 | 2.20 | 0.41 |
| 1:A:147:TYR:OH | 1:A:368:GLN:NE2 | 2.53 | 0.41 |
| 1:A:96:TRP:CD2 | 1:A:97:PRO:HD3 | 2.56 | 0.41 |
| 1:B:48:LEU:HD12 | 1:B:48:LEU:HA | 1.84 | 0.41 |
| 1:D:33:PHE:CE2 | 1:D:95:PRO:HB3 | 2.56 | 0.41 |
| 1:D:608:LEU:HA | 1:D:608:LEU:HD23 | 1.96 | 0.41 |
| 1:A:124:ASN:C | 1:A:126:GLY:H | 2.23 | 0.41 |
| 1:A:130:PHE:HA | 1:A:177:LEU:O | 2.21 | 0.41 |
| 1:B:607:ARG:H | 1:B:607:ARG:HG3 | 1.58 | 0.41 |
| 1:D:516:VAL:HB | 1:F:524:ILE:HG13 | 2.03 | 0.41 |
| 1:A:246:ARG:NH2 | 1:A:280:GLN:OE1 | 2.49 | 0.41 |
| 1:A:295:ILE:CG2 | 1:A:344:LEU:HD21 | 2.44 | 0.41 |
| 1:D:273:ARG:NE | 1:D:277:GLU:OE2 | 2.54 | 0.41 |
| 1:E:102:ARG:HH11 | 1:E:102:ARG:HA | 1.86 | 0.41 |
| 1:F:422:MET:HE2 | 1:F:424:ILE:HG12 | 2.03 | 0.41 |
| 1:E:246:ARG:HA | 1:E:247:PRO:HD3 | 1.91 | 0.41 |
| 1:F:155:ILE:HG13 | 1:F:156:SER:N | 2.36 | 0.41 |
| 1:A:145:VAL:CG1 | 1:A:147:TYR:HB2 | 2.52 | 0.40 |
| 1:E:86:PHE:HA | 1:E:86:PHE:HD1 | 1.80 | 0.40 |
| 1:A:20:LEU:HD12 | 1:A:38:HIS:O | 2.22 | 0.40 |
| 1:A:592:PHE:CE2 | 1:C:600:GLY:HA3 | 2.55 | 0.40 |
| 1:C:213:TRP:CE2 | 1:C:311:GLN:HG2 | 2.57 | 0.40 |
| 1:C:20:LEU:O | 1:C:326:GLN:NE2 | 2.53 | 0.40 |
| 1:D:76:ARG:HG2 | 1:D:92:THR:HB | 2.03 | 0.40 |
| 1:F:76:ARG:HG2 | 1:F:92:THR:HB | 2.03 | 0.40 |
| 1:B:241:ARG:NH2 | 2:B:739:SO4:O4 | 2.55 | 0.40 |
| 1:C:285:ARG:HH21 | 1:C:318:VAL:HG11 | 1.87 | 0.40 |
| 1:C:638:PRO:HA | 1:C:639:PRO:HD3 | 1.93 | 0.40 |
| 1:D:20:LEU:O | 1:D:326:GLN:NE2 | 2.53 | 0.40 |
| 1:F:474:SER:HA | 1:F:475:LYS:HA | 1.85 | 0.40 |
| 1:A:534:ASN:HB3 | 1:A:535:ASN:H | 1.67 | 0.40 |
| 1:A:7:VAL:HG22 | 1:A:326:GLN:NE2 | 2.37 | 0.40 |
| 1:D:29:LEU:HA | 1:D:29:LEU:HD12 | 1.89 | 0.40 |
| 1:D:561:LEU:CD2 | 1:D:563:GLU:HG3 | 2.52 | 0.40 |
| 1:E:279:ILE:O | 1:E:282:GLN:HG2 | 2.21 | 0.40 |
| 1:E:232:GLN:HA | 1:F:452:ALA:HB2 | 2.04 | 0.40 |
| 1:B:275:ARG:O | 1:B:279:ILE:HG12 | 2.21 | 0.40 |
| 1:C:191:GLY:N | 2:C:736:SO4:O2 | 2.47 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------|--------------------------|-------------------|
| 1:D:159:MET:HB3 | 1:D:164:ILE:O | 2.22 | 0.40 |

All (1) 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:201:THR:O | 1:A:611:ASN:ND2[1_545] | 2.16 | 0.04 |

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 | 623/643 (97%) | 594 (95%) | 28 (4%) | 1 (0%) | 51 | 81 |
| 1 | B | 623/643 (97%) | 601 (96%) | 22 (4%) | 0 | 100 | 100 |
| 1 | C | 623/643 (97%) | 601 (96%) | 22 (4%) | 0 | 100 | 100 |
| 1 | D | 623/643 (97%) | 601 (96%) | 22 (4%) | 0 | 100 | 100 |
| 1 | E | 623/643 (97%) | 603 (97%) | 20 (3%) | 0 | 100 | 100 |
| 1 | F | 623/643 (97%) | 601 (96%) | 22 (4%) | 0 | 100 | 100 |
| All | All | 3738/3858 (97%) | 3601 (96%) | 136 (4%) | 1 (0%) | 100 | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 13 | LEU |

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 | 526/535 (98%) | 494 (94%) | 32 (6%) | 22 | 57 |
| 1 | B | 526/535 (98%) | 498 (95%) | 28 (5%) | 26 | 62 |
| 1 | C | 526/535 (98%) | 501 (95%) | 25 (5%) | 30 | 66 |
| 1 | D | 526/535 (98%) | 506 (96%) | 20 (4%) | 38 | 71 |
| 1 | E | 526/535 (98%) | 508 (97%) | 18 (3%) | 42 | 73 |
| 1 | F | 526/535 (98%) | 505 (96%) | 21 (4%) | 36 | 70 |
| All | All | 3156/3210 (98%) | 3012 (95%) | 144 (5%) | 31 | 67 |

All (144) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 6 | LEU |
| 1 | A | 13 | LEU |
| 1 | A | 32 | LEU |
| 1 | A | 51 | LEU |
| 1 | A | 59 | SER |
| 1 | A | 61 | GLU |
| 1 | A | 86 | PHE |
| 1 | A | 102 | ARG |
| 1 | A | 139 | ARG |
| 1 | A | 158 | LEU |
| 1 | A | 187 | ARG |
| 1 | A | 270 | GLN |
| 1 | A | 292 | VAL |
| 1 | A | 299 | HIS |
| 1 | A | 311 | GLN |
| 1 | A | 339 | GLN |
| 1 | A | 350 | SER |
| 1 | A | 356 | LEU |
| 1 | A | 403 | ASN |
| 1 | A | 418 | ASN |
| 1 | A | 425 | PRO |
| 1 | A | 434 | SER |
| 1 | A | 495 | GLN |
| 1 | A | 499 | HIS |
| 1 | A | 529 | LEU |
| 1 | A | 545 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 546 | LEU |
| 1 | A | 569 | ARG |
| 1 | A | 571 | VAL |
| 1 | A | 584 | THR |
| 1 | A | 588 | SER |
| 1 | A | 625 | VAL |
| 1 | B | 6 | LEU |
| 1 | B | 7 | VAL |
| 1 | B | 13 | LEU |
| 1 | B | 39 | LEU |
| 1 | B | 48 | LEU |
| 1 | B | 51 | LEU |
| 1 | B | 80 | VAL |
| 1 | B | 85 | GLN |
| 1 | B | 102 | ARG |
| 1 | B | 107 | ARG |
| 1 | B | 139 | ARG |
| 1 | B | 158 | LEU |
| 1 | B | 215 | MET |
| 1 | B | 311 | GLN |
| 1 | B | 352 | SER |
| 1 | B | 368 | GLN |
| 1 | B | 390 | VAL |
| 1 | B | 442 | ARG |
| 1 | B | 495 | GLN |
| 1 | B | 499 | HIS |
| 1 | B | 529 | LEU |
| 1 | B | 560 | TYR |
| 1 | B | 571 | VAL |
| 1 | B | 584 | THR |
| 1 | B | 588 | SER |
| 1 | B | 607 | ARG |
| 1 | B | 625 | VAL |
| 1 | B | 634 | GLN |
| 1 | C | 13 | LEU |
| 1 | C | 18 | LEU |
| 1 | C | 51 | LEU |
| 1 | C | 102 | ARG |
| 1 | C | 128 | SER |
| 1 | C | 136 | ARG |
| 1 | C | 187 | ARG |
| 1 | C | 206 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 207 | ARG |
| 1 | C | 215 | MET |
| 1 | C | 325 | VAL |
| 1 | C | 328 | LEU |
| 1 | C | 350 | SER |
| 1 | C | 352 | SER |
| 1 | C | 368 | GLN |
| 1 | C | 390 | VAL |
| 1 | C | 409 | ARG |
| 1 | C | 442 | ARG |
| 1 | C | 495 | GLN |
| 1 | C | 499 | HIS |
| 1 | C | 545 | THR |
| 1 | C | 546 | LEU |
| 1 | C | 588 | SER |
| 1 | C | 608 | LEU |
| 1 | C | 625 | VAL |
| 1 | D | 6 | LEU |
| 1 | D | 13 | LEU |
| 1 | D | 32 | LEU |
| 1 | D | 51 | LEU |
| 1 | D | 59 | SER |
| 1 | D | 83 | HIS |
| 1 | D | 102 | ARG |
| 1 | D | 139 | ARG |
| 1 | D | 215 | MET |
| 1 | D | 233 | ARG |
| 1 | D | 273 | ARG |
| 1 | D | 282 | GLN |
| 1 | D | 311 | GLN |
| 1 | D | 453 | GLU |
| 1 | D | 495 | GLN |
| 1 | D | 546 | LEU |
| 1 | D | 559 | THR |
| 1 | D | 560 | TYR |
| 1 | D | 588 | SER |
| 1 | D | 599 | ASN |
| 1 | E | 13 | LEU |
| 1 | E | 51 | LEU |
| 1 | E | 59 | SER |
| 1 | E | 68 | ARG |
| 1 | E | 78 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 215 | MET |
| 1 | E | 356 | LEU |
| 1 | E | 456 | VAL |
| 1 | E | 460 | LEU |
| 1 | E | 495 | GLN |
| 1 | E | 545 | THR |
| 1 | E | 559 | THR |
| 1 | E | 560 | TYR |
| 1 | E | 571 | VAL |
| 1 | E | 588 | SER |
| 1 | E | 610 | LEU |
| 1 | E | 625 | VAL |
| 1 | E | 634 | GLN |
| 1 | F | 13 | LEU |
| 1 | F | 51 | LEU |
| 1 | F | 59 | SER |
| 1 | F | 139 | ARG |
| 1 | F | 158 | LEU |
| 1 | F | 187 | ARG |
| 1 | F | 328 | LEU |
| 1 | F | 339 | GLN |
| 1 | F | 359 | THR |
| 1 | F | 368 | GLN |
| 1 | F | 442 | ARG |
| 1 | F | 491 | LYS |
| 1 | F | 495 | GLN |
| 1 | F | 545 | THR |
| 1 | F | 546 | LEU |
| 1 | F | 559 | THR |
| 1 | F | 560 | TYR |
| 1 | F | 607 | ARG |
| 1 | F | 608 | LEU |
| 1 | F | 609 | ASP |
| 1 | F | 617 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 270 | 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

258 ligands 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 | SO4 | A | 701 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 702 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 703 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 704 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 705 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 706 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | A | 707 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 708 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.11 | 0 |
| 2 | SO4 | A | 709 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | A | 710 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | A | 711 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 712 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 713 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 714 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 715 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 716 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 717 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 718 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SO4 | A | 719 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 720 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 721 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 722 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 723 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 724 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 725 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 726 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | A | 727 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 728 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 729 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 730 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 731 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | A | 732 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 733 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 734 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.04 | 0 |
| 2 | SO4 | A | 735 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 736 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | A | 737 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 738 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 739 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | A | 740 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 741 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 742 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 743 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | A | 744 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 745 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | A | 746 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 747 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | A | 748 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 3 | TAM | A | 749 | - | 7,10,10 | 0.55 | 0 | 9,12,12 | 0.84 | 0 |
| 2 | SO4 | A | 750 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 701 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | B | 702 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 703 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | B | 704 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 705 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | B | 706 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | B | 707 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 708 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 709 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 710 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 711 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SO4 | B | 712 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 713 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 714 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 715 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | B | 716 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 717 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | B | 718 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | B | 719 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.04 | 0 |
| 2 | SO4 | B | 720 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 721 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 722 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 723 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 724 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 725 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 726 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 727 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 728 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 729 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 730 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | B | 731 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 732 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 733 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 734 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 735 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 736 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 737 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 738 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 739 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 740 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 741 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 742 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 743 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 744 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 745 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 746 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 747 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | B | 748 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 749 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | B | 750 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 701 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 702 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | C | 703 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 704 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SO4 | C | 705 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | C | 706 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 707 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 708 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 709 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 710 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 711 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 712 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.04 | 0 |
| 2 | SO4 | C | 713 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 714 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 715 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 716 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 717 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | C | 718 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 719 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 720 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 721 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 722 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 723 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | C | 724 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 725 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 726 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 727 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 728 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 729 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | C | 730 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 731 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 732 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 733 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 734 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 735 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 736 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 737 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 738 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 739 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 740 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 741 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 742 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 743 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | C | 744 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 701 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | D | 702 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 703 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SO4 | D | 704 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 705 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 706 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 707 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 708 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 709 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 710 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 711 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 712 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | D | 713 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 714 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | D | 715 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 716 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 717 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 718 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 719 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 720 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 721 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 722 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 723 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 724 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 725 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 726 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 727 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 728 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 729 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 730 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | D | 731 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 732 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | D | 733 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | D | 734 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 3 | TAM | D | 735 | - | 7,10,10 | 0.56 | 0 | 9,12,12 | 0.91 | 0 |
| 2 | SO4 | D | 736 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | E | 701 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 702 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 703 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 704 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 705 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 706 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 707 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | E | 708 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 709 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 710 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SO4 | E | 711 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 712 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.04 | 0 |
| 2 | SO4 | E | 713 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 714 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 715 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 716 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 717 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 718 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 719 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | E | 720 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 721 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 722 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 723 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 724 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 725 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | E | 726 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 727 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 728 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 729 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 730 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 731 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | E | 732 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | E | 733 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | E | 734 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 701 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 702 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 703 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | F | 704 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 705 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | F | 706 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | F | 707 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 708 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 709 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 710 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 711 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | F | 712 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | F | 713 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 714 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 715 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 716 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 717 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 718 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 719 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | SO4 | F | 720 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 721 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 722 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 723 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 724 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 725 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 726 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 727 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 728 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | F | 729 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 730 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 731 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 732 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 733 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 734 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | F | 735 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | F | 736 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 737 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 738 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 739 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 740 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 741 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | F | 742 | - | 4,4,4 | 0.13 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | SO4 | F | 743 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.06 | 0 |
| 2 | SO4 | F | 744 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.05 | 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 | SO4 | A | 701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 702 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 703 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 704 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 705 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 706 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 707 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 708 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 709 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 710 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 711 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | SO4 | A | 712 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 713 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 714 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 715 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 716 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 717 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 718 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 719 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 720 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 721 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 722 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 723 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 724 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 725 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 726 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 727 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 728 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 729 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 730 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 731 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 732 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 733 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 734 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 735 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 736 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 737 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 738 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 739 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 740 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 741 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 742 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 743 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 744 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 745 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 746 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 747 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | A | 748 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | TAM | A | 749 | - | - | 0/12/12/12 | 0/0/0/0 |
| 2 | SO4 | A | 750 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 702 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 703 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 2 | SO4 | B | 704 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 705 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 706 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 707 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 708 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 709 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 710 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 711 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 712 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 713 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 714 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 715 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 716 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 717 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 718 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 719 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 720 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 721 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 722 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 723 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 724 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 725 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 726 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 727 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 728 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 729 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 730 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 731 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 732 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 733 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 734 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 735 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 736 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 737 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 738 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 739 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 740 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 741 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 742 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 743 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 744 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 745 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 2 | SO4 | B | 746 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 747 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 748 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 749 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | B | 750 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 702 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 703 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 704 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 705 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 706 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 707 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 708 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 709 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 710 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 711 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 712 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 713 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 714 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 715 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 716 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 717 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 718 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 719 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 720 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 721 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 722 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 723 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 724 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 725 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 726 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 727 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 728 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 729 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 730 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 731 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 732 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 733 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 734 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 735 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 736 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 737 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | SO4 | C | 738 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 739 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 740 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 741 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 742 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 743 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | C | 744 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 702 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 703 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 704 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 705 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 706 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 707 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 708 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 709 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 710 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 711 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 712 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 713 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 714 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 715 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 716 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 717 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 718 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 719 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 720 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 721 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 722 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 723 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 724 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 725 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 726 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 727 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 728 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 729 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 730 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 731 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 732 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 733 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | D | 734 | - | - | 0/0/0/0 | 0/0/0/0 |
| 3 | TAM | D | 735 | - | - | 0/12/12/12 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 2 | SO4 | D | 736 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 702 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 703 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 704 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 705 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 706 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 707 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 708 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 709 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 710 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 711 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 712 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 713 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 714 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 715 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 716 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 717 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 718 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 719 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 720 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 721 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 722 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 723 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 724 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 725 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 726 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 727 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 728 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 729 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 730 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 731 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 732 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 733 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | E | 734 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 701 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 702 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 703 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 704 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 705 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 706 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 707 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 2 | SO4 | F | 708 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 709 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 710 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 711 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 712 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 713 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 714 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 715 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 716 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 717 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 718 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 719 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 720 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 721 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 722 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 723 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 724 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 725 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 726 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 727 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 728 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 729 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 730 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 731 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 732 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 733 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 734 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 735 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 736 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 737 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 738 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 739 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 740 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 741 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 742 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 743 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | SO4 | F | 744 | - | - | 0/0/0/0 | 0/0/0/0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

45 monomers are involved in 55 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | A | 701 | SO4 | 1 | 0 |
| 2 | A | 702 | SO4 | 1 | 0 |
| 2 | A | 708 | SO4 | 1 | 0 |
| 2 | A | 715 | SO4 | 1 | 0 |
| 2 | A | 730 | SO4 | 1 | 0 |
| 2 | A | 739 | SO4 | 1 | 0 |
| 3 | A | 749 | TAM | 2 | 0 |
| 2 | B | 701 | SO4 | 1 | 0 |
| 2 | B | 710 | SO4 | 1 | 0 |
| 2 | B | 711 | SO4 | 1 | 0 |
| 2 | B | 717 | SO4 | 1 | 0 |
| 2 | B | 719 | SO4 | 2 | 0 |
| 2 | B | 726 | SO4 | 1 | 0 |
| 2 | B | 732 | SO4 | 2 | 0 |
| 2 | B | 735 | SO4 | 2 | 0 |
| 2 | B | 739 | SO4 | 3 | 0 |
| 2 | B | 740 | SO4 | 1 | 0 |
| 2 | B | 750 | SO4 | 1 | 0 |
| 2 | C | 701 | SO4 | 1 | 0 |
| 2 | C | 705 | SO4 | 1 | 0 |
| 2 | C | 710 | SO4 | 1 | 0 |
| 2 | C | 712 | SO4 | 1 | 0 |
| 2 | C | 717 | SO4 | 1 | 0 |
| 2 | C | 719 | SO4 | 1 | 0 |
| 2 | C | 731 | SO4 | 3 | 0 |
| 2 | C | 736 | SO4 | 1 | 0 |
| 2 | C | 739 | SO4 | 2 | 0 |
| 2 | C | 741 | SO4 | 1 | 0 |
| 2 | D | 705 | SO4 | 1 | 0 |
| 2 | D | 708 | SO4 | 1 | 0 |
| 2 | D | 710 | SO4 | 1 | 0 |
| 2 | D | 716 | SO4 | 1 | 0 |
| 2 | D | 722 | SO4 | 1 | 0 |
| 2 | D | 723 | SO4 | 1 | 0 |
| 2 | D | 724 | SO4 | 1 | 0 |
| 2 | D | 731 | SO4 | 1 | 0 |
| 2 | D | 734 | SO4 | 1 | 0 |
| 3 | D | 735 | TAM | 2 | 0 |
| 2 | D | 736 | SO4 | 1 | 0 |
| 2 | E | 716 | SO4 | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | F | 703 | SO4 | 1 | 0 |
| 2 | F | 707 | SO4 | 1 | 0 |
| 2 | F | 714 | SO4 | 1 | 0 |
| 2 | F | 715 | SO4 | 1 | 0 |
| 2 | F | 727 | SO4 | 1 | 0 |

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 ⓘ

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, 95th 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 | 627/643 (97%) | -0.25 | 3 (0%) | 90 90 | 53, 88, 124, 190 | 0 |
| 1 | B | 627/643 (97%) | -0.26 | 4 (0%) | 89 89 | 57, 95, 134, 217 | 0 |
| 1 | C | 627/643 (97%) | -0.33 | 4 (0%) | 89 89 | 59, 88, 131, 223 | 0 |
| 1 | D | 627/643 (97%) | 0.03 | 11 (1%) | 69 67 | 73, 112, 189, 244 | 0 |
| 1 | E | 627/643 (97%) | -0.04 | 17 (2%) | 55 53 | 68, 106, 183, 227 | 0 |
| 1 | F | 627/643 (97%) | -0.17 | 8 (1%) | 77 76 | 63, 94, 184, 255 | 0 |
| All | All | 3762/3858 (97%) | -0.17 | 47 (1%) | 79 78 | 53, 97, 171, 255 | 0 |

All (47) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 338 | SER | 3.9 |
| 1 | A | 338 | SER | 3.9 |
| 1 | E | 590 | SER | 3.8 |
| 1 | D | 589 | GLY | 3.6 |
| 1 | E | 82 | GLY | 3.6 |
| 1 | D | 607 | ARG | 3.6 |
| 1 | E | 599 | ASN | 3.6 |
| 1 | F | 613 | GLY | 3.4 |
| 1 | D | 201 | THR | 3.4 |
| 1 | E | 328 | LEU | 3.3 |
| 1 | E | 613 | GLY | 3.2 |
| 1 | E | 201 | THR | 3.0 |
| 1 | E | 549 | GLY | 3.0 |
| 1 | D | 600 | GLY | 2.9 |
| 1 | A | 61 | GLU | 2.9 |
| 1 | E | 83 | HIS | 2.9 |
| 1 | D | 328 | LEU | 2.8 |
| 1 | E | 476 | GLY | 2.8 |
| 1 | F | 602 | ILE | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | C | 202 | LEU | 2.7 |
| 1 | B | 202 | LEU | 2.7 |
| 1 | D | 599 | ASN | 2.7 |
| 1 | E | 620 | ALA | 2.7 |
| 1 | A | 5 | ARG | 2.6 |
| 1 | F | 614 | GLY | 2.5 |
| 1 | F | 338 | SER | 2.5 |
| 1 | D | 202 | LEU | 2.5 |
| 1 | F | 591 | ALA | 2.5 |
| 1 | E | 606 | GLY | 2.4 |
| 1 | F | 599 | ASN | 2.4 |
| 1 | E | 608 | LEU | 2.3 |
| 1 | C | 203 | GLY | 2.3 |
| 1 | B | 291 | VAL | 2.3 |
| 1 | C | 201 | THR | 2.3 |
| 1 | F | 339 | GLN | 2.3 |
| 1 | E | 44 | PRO | 2.3 |
| 1 | E | 202 | LEU | 2.2 |
| 1 | D | 620 | ALA | 2.2 |
| 1 | E | 592 | PHE | 2.2 |
| 1 | D | 615 | ALA | 2.1 |
| 1 | E | 639 | PRO | 2.1 |
| 1 | E | 616 | SER | 2.1 |
| 1 | D | 340 | PHE | 2.1 |
| 1 | D | 341 | GLU | 2.1 |
| 1 | B | 207 | ARG | 2.0 |
| 1 | B | 201 | THR | 2.0 |
| 1 | F | 594 | LEU | 2.0 |

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 carbohydrates 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. 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, 95th 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 | SO4 | A | 727 | 5/5 | 0.70 | 0.48 | 22.55 | 180,185,189,194 | 0 |
| 2 | SO4 | C | 734 | 5/5 | 0.79 | 0.54 | 20.47 | 187,195,197,201 | 0 |
| 2 | SO4 | C | 741 | 5/5 | 0.80 | 0.59 | 17.19 | 207,208,209,211 | 0 |
| 2 | SO4 | C | 732 | 5/5 | 0.77 | 0.46 | 15.12 | 196,201,206,207 | 0 |
| 2 | SO4 | C | 726 | 5/5 | 0.71 | 0.46 | 14.97 | 170,181,188,197 | 0 |
| 3 | TAM | D | 735 | 11/11 | 0.61 | 0.47 | 14.21 | 135,150,173,175 | 0 |
| 2 | SO4 | F | 709 | 5/5 | 0.89 | 0.34 | 11.58 | 122,144,149,162 | 0 |
| 3 | TAM | A | 749 | 11/11 | 0.82 | 0.46 | 11.22 | 103,136,167,169 | 0 |
| 2 | SO4 | F | 729 | 5/5 | 0.90 | 0.63 | 10.31 | 183,187,189,195 | 0 |
| 2 | SO4 | A | 747 | 5/5 | 0.77 | 0.38 | 9.70 | 197,199,200,204 | 0 |
| 2 | SO4 | D | 726 | 5/5 | 0.75 | 0.44 | 9.20 | 177,177,182,192 | 0 |
| 2 | SO4 | F | 712 | 5/5 | 0.85 | 0.41 | 8.18 | 127,128,147,167 | 0 |
| 2 | SO4 | F | 704 | 5/5 | 0.95 | 0.36 | 8.15 | 182,184,188,188 | 0 |
| 2 | SO4 | B | 746 | 5/5 | 0.72 | 0.49 | 8.07 | 185,200,201,206 | 0 |
| 2 | SO4 | E | 728 | 5/5 | 0.76 | 0.35 | 6.90 | 154,167,175,182 | 0 |
| 2 | SO4 | B | 714 | 5/5 | 0.86 | 0.50 | 5.84 | 157,163,167,172 | 0 |
| 2 | SO4 | D | 706 | 5/5 | 0.82 | 0.30 | 5.78 | 140,149,153,159 | 0 |
| 2 | SO4 | C | 733 | 5/5 | 0.78 | 0.46 | 5.76 | 232,232,235,237 | 0 |
| 2 | SO4 | E | 734 | 5/5 | 0.92 | 0.45 | 5.72 | 155,166,167,172 | 0 |
| 2 | SO4 | F | 739 | 5/5 | 0.85 | 0.33 | 5.39 | 210,213,215,216 | 0 |
| 2 | SO4 | A | 703 | 5/5 | 0.92 | 0.30 | 4.79 | 61,134,142,143 | 0 |
| 2 | SO4 | B | 736 | 5/5 | 0.93 | 0.41 | 4.71 | 175,177,180,181 | 0 |
| 2 | SO4 | B | 749 | 5/5 | 0.76 | 0.54 | 4.34 | 173,182,190,192 | 0 |
| 2 | SO4 | A | 731 | 5/5 | 0.92 | 0.31 | 4.18 | 105,141,156,167 | 0 |
| 2 | SO4 | E | 725 | 5/5 | 0.89 | 0.33 | 4.10 | 113,141,161,162 | 0 |
| 2 | SO4 | F | 737 | 5/5 | 0.87 | 0.50 | 4.07 | 167,177,182,188 | 0 |
| 2 | SO4 | F | 742 | 5/5 | 0.66 | 0.53 | 3.78 | 225,229,229,230 | 0 |
| 2 | SO4 | E | 701 | 5/5 | 0.78 | 0.28 | 3.57 | 176,178,186,188 | 0 |
| 2 | SO4 | B | 750 | 5/5 | 0.98 | 0.22 | 3.36 | 73,92,99,102 | 0 |
| 2 | SO4 | A | 745 | 5/5 | 0.86 | 0.51 | 3.21 | 146,152,162,167 | 0 |
| 2 | SO4 | A | 705 | 5/5 | 0.90 | 0.24 | 3.02 | 86,138,150,150 | 0 |
| 2 | SO4 | F | 714 | 5/5 | 0.94 | 0.20 | 2.97 | 158,164,165,169 | 0 |
| 2 | SO4 | B | 718 | 5/5 | 0.78 | 0.33 | 2.45 | 150,151,166,172 | 0 |
| 2 | SO4 | E | 720 | 5/5 | 0.74 | 0.40 | 2.39 | 168,179,184,185 | 0 |
| 2 | SO4 | B | 720 | 5/5 | 0.75 | 0.28 | 2.30 | 186,188,197,200 | 0 |
| 2 | SO4 | E | 731 | 5/5 | 0.84 | 0.38 | 1.81 | 134,153,160,166 | 0 |
| 2 | SO4 | A | 713 | 5/5 | 0.81 | 0.32 | 1.81 | 149,162,171,177 | 0 |
| 2 | SO4 | B | 706 | 5/5 | 0.93 | 0.24 | 1.81 | 93,105,129,147 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 2 | SO4 | D | 730 | 5/5 | 0.86 | 0.43 | 1.58 | 159,159,166,174 | 0 |
| 2 | SO4 | C | 738 | 5/5 | 0.89 | 0.39 | 1.48 | 153,156,164,177 | 0 |
| 2 | SO4 | A | 733 | 5/5 | 0.95 | 0.20 | 1.38 | 100,112,123,127 | 0 |
| 2 | SO4 | F | 736 | 5/5 | 0.87 | 0.41 | 1.38 | 130,141,152,156 | 0 |
| 2 | SO4 | A | 750 | 5/5 | 0.98 | 0.20 | 1.16 | 84,92,100,101 | 0 |
| 2 | SO4 | C | 744 | 5/5 | 0.94 | 0.21 | 0.99 | 112,118,128,135 | 0 |
| 2 | SO4 | E | 723 | 5/5 | 0.94 | 0.23 | 0.91 | 165,178,181,182 | 0 |
| 2 | SO4 | A | 708 | 5/5 | 0.94 | 0.21 | 0.35 | 70,101,110,118 | 0 |
| 2 | SO4 | C | 725 | 5/5 | 0.95 | 0.20 | 0.21 | 66,108,123,139 | 0 |
| 2 | SO4 | F | 711 | 5/5 | 0.98 | 0.18 | -0.04 | 77,86,97,119 | 0 |
| 2 | SO4 | E | 712 | 5/5 | 0.92 | 0.19 | -0.05 | 81,127,142,146 | 0 |
| 2 | SO4 | D | 713 | 5/5 | 0.86 | 0.22 | -0.17 | 159,168,170,175 | 0 |
| 2 | SO4 | F | 728 | 5/5 | 0.90 | 0.20 | -0.29 | 106,143,151,154 | 0 |
| 2 | SO4 | E | 703 | 5/5 | 0.97 | 0.14 | -0.30 | 139,146,149,154 | 0 |
| 2 | SO4 | E | 721 | 5/5 | 0.96 | 0.16 | -0.34 | 93,121,124,141 | 0 |
| 2 | SO4 | C | 731 | 5/5 | 0.96 | 0.18 | -0.43 | 104,117,126,133 | 0 |
| 2 | SO4 | B | 708 | 5/5 | 0.83 | 0.20 | -0.56 | 139,154,160,166 | 0 |
| 2 | SO4 | D | 708 | 5/5 | 0.97 | 0.16 | -0.71 | 76,91,106,110 | 0 |
| 2 | SO4 | B | 733 | 5/5 | 0.90 | 0.15 | -0.87 | 137,146,159,166 | 0 |
| 2 | SO4 | F | 718 | 5/5 | 0.89 | 0.22 | -0.89 | 137,162,163,170 | 0 |
| 2 | SO4 | C | 736 | 5/5 | 0.98 | 0.10 | -1.04 | 118,130,139,147 | 0 |
| 2 | SO4 | E | 727 | 5/5 | 0.98 | 0.15 | -1.07 | 111,112,119,134 | 0 |
| 2 | SO4 | A | 735 | 5/5 | 0.93 | 0.17 | -1.23 | 106,108,127,148 | 0 |
| 2 | SO4 | C | 711 | 5/5 | 0.98 | 0.15 | -1.28 | 89,92,110,125 | 0 |
| 2 | SO4 | F | 702 | 5/5 | 0.93 | 0.16 | -1.35 | 105,117,131,138 | 0 |
| 2 | SO4 | C | 724 | 5/5 | 0.92 | 0.13 | -1.36 | 110,133,140,151 | 0 |
| 2 | SO4 | D | 736 | 5/5 | 0.93 | 0.14 | -1.42 | 138,150,161,164 | 0 |
| 2 | SO4 | D | 707 | 5/5 | 0.94 | 0.13 | -1.50 | 148,159,164,177 | 0 |
| 2 | SO4 | B | 712 | 5/5 | 0.96 | 0.17 | -1.56 | 75,101,119,123 | 0 |
| 2 | SO4 | D | 711 | 5/5 | 0.98 | 0.17 | -2.00 | 122,124,125,126 | 0 |
| 2 | SO4 | B | 719 | 5/5 | 0.96 | 0.12 | -2.10 | 97,113,130,146 | 0 |
| 2 | SO4 | B | 711 | 5/5 | 0.97 | 0.13 | -2.37 | 95,109,121,132 | 0 |
| 2 | SO4 | F | 713 | 5/5 | 0.98 | 0.11 | -2.48 | 102,116,124,127 | 0 |
| 2 | SO4 | E | 710 | 5/5 | 0.95 | 0.10 | -2.53 | 120,129,133,142 | 0 |
| 2 | SO4 | F | 744 | 5/5 | 0.94 | 0.13 | -2.54 | 136,137,148,165 | 0 |
| 2 | SO4 | F | 734 | 5/5 | 0.95 | 0.10 | -2.65 | 121,134,137,146 | 0 |
| 2 | SO4 | D | 724 | 5/5 | 0.96 | 0.11 | -4.02 | 120,126,129,140 | 0 |
| 2 | SO4 | D | 732 | 5/5 | 0.84 | 0.24 | - | 160,163,173,174 | 0 |
| 2 | SO4 | F | 738 | 5/5 | 0.85 | 0.46 | - | 190,196,205,205 | 0 |
| 2 | SO4 | A | 715 | 5/5 | 0.84 | 0.26 | - | 208,213,215,217 | 0 |
| 2 | SO4 | C | 722 | 5/5 | 0.80 | 0.44 | - | 185,189,190,191 | 0 |
| 2 | SO4 | A | 719 | 5/5 | 0.90 | 0.19 | - | 183,187,189,189 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 2 | SO4 | C | 716 | 5/5 | 0.62 | 0.32 | - | 198,199,205,208 | 0 |
| 2 | SO4 | B | 721 | 5/5 | 0.57 | 0.57 | - | 199,209,211,212 | 0 |
| 2 | SO4 | F | 701 | 5/5 | 0.96 | 0.15 | - | 101,129,134,142 | 0 |
| 2 | SO4 | D | 710 | 5/5 | 0.91 | 0.14 | - | 149,155,163,166 | 0 |
| 2 | SO4 | E | 707 | 5/5 | 0.93 | 0.14 | - | 149,158,163,175 | 0 |
| 2 | SO4 | C | 706 | 5/5 | 0.93 | 0.13 | - | 136,153,156,171 | 0 |
| 2 | SO4 | C | 740 | 5/5 | 0.77 | 0.32 | - | 191,191,196,202 | 0 |
| 2 | SO4 | C | 723 | 5/5 | 0.83 | 0.23 | - | 139,151,156,162 | 0 |
| 2 | SO4 | B | 725 | 5/5 | 0.89 | 0.66 | - | 184,188,192,202 | 0 |
| 2 | SO4 | B | 717 | 5/5 | 0.72 | 0.26 | - | 190,193,197,201 | 0 |
| 2 | SO4 | C | 737 | 5/5 | 0.84 | 0.22 | - | 148,162,164,164 | 0 |
| 2 | SO4 | E | 711 | 5/5 | 0.85 | 0.42 | - | 168,169,175,175 | 0 |
| 2 | SO4 | E | 729 | 5/5 | 0.64 | 0.62 | - | 213,220,223,223 | 0 |
| 2 | SO4 | F | 732 | 5/5 | 0.89 | 0.35 | - | 197,198,202,204 | 0 |
| 2 | SO4 | E | 732 | 5/5 | 0.85 | 0.22 | - | 162,164,171,183 | 0 |
| 2 | SO4 | C | 707 | 5/5 | 0.90 | 0.19 | - | 175,176,179,181 | 0 |
| 2 | SO4 | B | 722 | 5/5 | 0.86 | 0.31 | - | 179,180,185,185 | 0 |
| 2 | SO4 | B | 716 | 5/5 | 0.83 | 0.45 | - | 173,183,191,191 | 0 |
| 2 | SO4 | A | 710 | 5/5 | 0.85 | 0.16 | - | 154,158,169,179 | 0 |
| 2 | SO4 | C | 703 | 5/5 | 0.73 | 0.26 | - | 155,163,182,184 | 0 |
| 2 | SO4 | F | 710 | 5/5 | 0.80 | 0.19 | - | 171,178,179,181 | 0 |
| 2 | SO4 | E | 717 | 5/5 | 0.87 | 0.23 | - | 194,195,198,203 | 0 |
| 2 | SO4 | C | 714 | 5/5 | 0.74 | 0.52 | - | 180,187,188,189 | 0 |
| 2 | SO4 | A | 709 | 5/5 | 0.84 | 0.18 | - | 126,132,158,163 | 0 |
| 2 | SO4 | B | 723 | 5/5 | 0.75 | 0.36 | - | 199,200,202,205 | 0 |
| 2 | SO4 | B | 741 | 5/5 | 0.77 | 0.24 | - | 215,220,223,224 | 0 |
| 2 | SO4 | C | 742 | 5/5 | 0.75 | 0.31 | - | 198,199,207,208 | 0 |
| 2 | SO4 | D | 716 | 5/5 | 0.88 | 0.15 | - | 182,185,186,186 | 0 |
| 2 | SO4 | B | 701 | 5/5 | 0.98 | 0.08 | - | 105,108,120,126 | 0 |
| 2 | SO4 | C | 705 | 5/5 | 0.90 | 0.18 | - | 164,165,169,173 | 0 |
| 2 | SO4 | A | 737 | 5/5 | 0.75 | 0.39 | - | 180,182,192,196 | 0 |
| 2 | SO4 | C | 739 | 5/5 | 0.84 | 0.52 | - | 215,215,218,220 | 0 |
| 2 | SO4 | D | 701 | 5/5 | 0.83 | 0.27 | - | 127,151,156,161 | 0 |
| 2 | SO4 | A | 732 | 5/5 | 0.85 | 0.39 | - | 175,179,181,188 | 0 |
| 2 | SO4 | D | 727 | 5/5 | 0.86 | 0.28 | - | 181,189,190,198 | 0 |
| 2 | SO4 | E | 714 | 5/5 | 0.69 | 0.35 | - | 225,226,228,231 | 0 |
| 2 | SO4 | E | 724 | 5/5 | 0.82 | 0.36 | - | 188,193,196,197 | 0 |
| 2 | SO4 | D | 720 | 5/5 | 0.70 | 0.21 | - | 194,203,204,208 | 0 |
| 2 | SO4 | E | 730 | 5/5 | 0.72 | 0.48 | - | 215,216,219,225 | 0 |
| 2 | SO4 | B | 732 | 5/5 | 0.93 | 0.14 | - | 160,168,174,180 | 0 |
| 2 | SO4 | A | 743 | 5/5 | 0.83 | 0.33 | - | 190,191,196,201 | 0 |
| 2 | SO4 | F | 719 | 5/5 | 0.80 | 0.44 | - | 179,181,185,186 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 2 | SO4 | D | 725 | 5/5 | 0.78 | 0.28 | - | 199,200,202,202 | 0 |
| 2 | SO4 | A | 748 | 5/5 | 0.50 | 0.75 | - | 219,222,226,226 | 0 |
| 2 | SO4 | D | 731 | 5/5 | 0.86 | 0.42 | - | 191,199,202,205 | 0 |
| 2 | SO4 | A | 706 | 5/5 | 0.92 | 0.20 | - | 114,137,140,143 | 0 |
| 2 | SO4 | C | 717 | 5/5 | 0.98 | 0.07 | - | 108,135,145,152 | 0 |
| 2 | SO4 | B | 744 | 5/5 | 0.69 | 0.38 | - | 212,215,218,220 | 0 |
| 2 | SO4 | D | 712 | 5/5 | 0.79 | 0.25 | - | 144,157,162,171 | 0 |
| 2 | SO4 | F | 715 | 5/5 | 0.87 | 0.29 | - | 207,210,212,214 | 0 |
| 2 | SO4 | F | 743 | 5/5 | 0.84 | 0.33 | - | 230,230,233,236 | 0 |
| 2 | SO4 | F | 717 | 5/5 | 0.72 | 0.39 | - | 177,182,190,197 | 0 |
| 2 | SO4 | A | 712 | 5/5 | 0.82 | 0.30 | - | 170,171,173,174 | 0 |
| 2 | SO4 | B | 709 | 5/5 | 0.94 | 0.17 | - | 140,142,145,147 | 0 |
| 2 | SO4 | F | 707 | 5/5 | 0.87 | 0.14 | - | 174,177,182,188 | 0 |
| 2 | SO4 | D | 721 | 5/5 | 0.83 | 0.26 | - | 198,200,200,202 | 0 |
| 2 | SO4 | A | 746 | 5/5 | 0.74 | 0.43 | - | 187,191,195,196 | 0 |
| 2 | SO4 | A | 701 | 5/5 | 0.95 | 0.09 | - | 88,115,123,135 | 0 |
| 2 | SO4 | E | 719 | 5/5 | 0.82 | 0.31 | - | 133,141,159,172 | 0 |
| 2 | SO4 | E | 704 | 5/5 | 0.90 | 0.18 | - | 146,160,168,173 | 0 |
| 2 | SO4 | C | 735 | 5/5 | 0.68 | 0.31 | - | 220,225,227,230 | 0 |
| 2 | SO4 | F | 730 | 5/5 | 0.93 | 0.16 | - | 154,160,163,168 | 0 |
| 2 | SO4 | C | 719 | 5/5 | 0.86 | 0.25 | - | 159,167,172,179 | 0 |
| 2 | SO4 | F | 740 | 5/5 | 0.77 | 0.30 | - | 215,216,217,219 | 0 |
| 2 | SO4 | C | 702 | 5/5 | 0.89 | 0.17 | - | 121,142,146,150 | 0 |
| 2 | SO4 | F | 724 | 5/5 | 0.73 | 0.33 | - | 181,187,189,195 | 0 |
| 2 | SO4 | A | 707 | 5/5 | 0.88 | 0.19 | - | 122,137,139,145 | 0 |
| 2 | SO4 | C | 701 | 5/5 | 0.96 | 0.10 | - | 109,120,128,131 | 0 |
| 2 | SO4 | F | 733 | 5/5 | 0.76 | 0.97 | - | 214,219,221,225 | 0 |
| 2 | SO4 | A | 723 | 5/5 | 0.63 | 0.38 | - | 219,222,224,227 | 0 |
| 2 | SO4 | E | 706 | 5/5 | 0.86 | 0.24 | - | 155,158,163,167 | 0 |
| 2 | SO4 | C | 729 | 5/5 | 0.78 | 0.26 | - | 172,180,190,203 | 0 |
| 2 | SO4 | B | 710 | 5/5 | 0.80 | 0.25 | - | 146,152,154,164 | 0 |
| 2 | SO4 | C | 743 | 5/5 | 0.69 | 0.54 | - | 196,196,203,206 | 0 |
| 2 | SO4 | E | 722 | 5/5 | 0.85 | 0.34 | - | 178,185,187,195 | 0 |
| 2 | SO4 | E | 705 | 5/5 | 0.73 | 0.26 | - | 156,173,175,179 | 0 |
| 2 | SO4 | F | 716 | 5/5 | 0.88 | 0.21 | - | 176,178,180,181 | 0 |
| 2 | SO4 | F | 722 | 5/5 | 0.77 | 0.39 | - | 164,169,176,186 | 0 |
| 2 | SO4 | A | 714 | 5/5 | 0.78 | 0.42 | - | 165,171,178,185 | 0 |
| 2 | SO4 | D | 715 | 5/5 | 0.79 | 0.28 | - | 207,209,211,213 | 0 |
| 2 | SO4 | B | 713 | 5/5 | 0.93 | 0.15 | - | 147,147,157,167 | 0 |
| 2 | SO4 | A | 717 | 5/5 | 0.82 | 0.32 | - | 176,189,190,194 | 0 |
| 2 | SO4 | A | 739 | 5/5 | 0.47 | 0.53 | - | 210,216,220,226 | 0 |
| 2 | SO4 | C | 704 | 5/5 | 0.76 | 0.27 | - | 126,159,168,170 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 2 | SO4 | A | 734 | 5/5 | 0.80 | 0.40 | - | 174,174,188,192 | 0 |
| 2 | SO4 | D | 729 | 5/5 | 0.72 | 0.36 | - | 191,195,198,199 | 0 |
| 2 | SO4 | E | 715 | 5/5 | 0.79 | 0.40 | - | 198,199,202,203 | 0 |
| 2 | SO4 | B | 748 | 5/5 | 0.97 | 0.17 | - | 139,153,155,157 | 0 |
| 2 | SO4 | F | 708 | 5/5 | 0.87 | 0.18 | - | 134,156,161,173 | 0 |
| 2 | SO4 | A | 738 | 5/5 | 0.93 | 0.47 | - | 169,172,178,180 | 0 |
| 2 | SO4 | E | 718 | 5/5 | 0.96 | 0.08 | - | 132,145,148,149 | 0 |
| 2 | SO4 | C | 708 | 5/5 | 0.87 | 0.21 | - | 181,192,193,195 | 0 |
| 2 | SO4 | A | 730 | 5/5 | 0.88 | 0.15 | - | 141,151,158,158 | 0 |
| 2 | SO4 | C | 721 | 5/5 | 0.70 | 0.37 | - | 204,207,211,211 | 0 |
| 2 | SO4 | B | 726 | 5/5 | 0.90 | 0.26 | - | 189,189,191,191 | 0 |
| 2 | SO4 | A | 716 | 5/5 | 0.85 | 0.21 | - | 153,161,165,171 | 0 |
| 2 | SO4 | E | 713 | 5/5 | 0.87 | 0.31 | - | 207,210,212,213 | 0 |
| 2 | SO4 | B | 739 | 5/5 | 0.80 | 0.42 | - | 206,207,212,212 | 0 |
| 2 | SO4 | A | 740 | 5/5 | 0.87 | 0.25 | - | 205,209,211,212 | 0 |
| 2 | SO4 | C | 728 | 5/5 | 0.65 | 0.31 | - | 197,203,204,205 | 0 |
| 2 | SO4 | B | 738 | 5/5 | 0.76 | 0.36 | - | 180,182,187,195 | 0 |
| 2 | SO4 | E | 702 | 5/5 | 0.86 | 0.15 | - | 162,169,177,179 | 0 |
| 2 | SO4 | D | 709 | 5/5 | 0.90 | 0.20 | - | 173,182,183,184 | 0 |
| 2 | SO4 | D | 704 | 5/5 | 0.94 | 0.16 | - | 152,161,164,168 | 0 |
| 2 | SO4 | B | 704 | 5/5 | 0.93 | 0.23 | - | 162,164,171,174 | 0 |
| 2 | SO4 | A | 744 | 5/5 | 0.92 | 0.35 | - | 160,164,174,177 | 0 |
| 2 | SO4 | C | 712 | 5/5 | 0.84 | 0.23 | - | 201,210,212,215 | 0 |
| 2 | SO4 | A | 742 | 5/5 | 0.83 | 0.53 | - | 216,219,221,224 | 0 |
| 2 | SO4 | B | 735 | 5/5 | 0.82 | 0.40 | - | 195,200,200,201 | 0 |
| 2 | SO4 | B | 734 | 5/5 | 0.87 | 0.37 | - | 205,209,211,212 | 0 |
| 2 | SO4 | D | 718 | 5/5 | 0.89 | 0.29 | - | 185,191,193,195 | 0 |
| 2 | SO4 | E | 726 | 5/5 | 0.44 | 0.27 | - | 219,222,224,224 | 0 |
| 2 | SO4 | D | 733 | 5/5 | 0.74 | 0.26 | - | 180,188,190,191 | 0 |
| 2 | SO4 | B | 737 | 5/5 | 0.88 | 0.40 | - | 193,197,199,202 | 0 |
| 2 | SO4 | C | 709 | 5/5 | 0.83 | 0.28 | - | 165,168,177,183 | 0 |
| 2 | SO4 | F | 721 | 5/5 | 0.87 | 0.21 | - | 193,197,201,201 | 0 |
| 2 | SO4 | A | 702 | 5/5 | 0.93 | 0.14 | - | 104,126,131,147 | 0 |
| 2 | SO4 | F | 726 | 5/5 | 0.74 | 0.22 | - | 165,179,184,186 | 0 |
| 2 | SO4 | E | 716 | 5/5 | 0.83 | 0.28 | - | 181,183,187,192 | 0 |
| 2 | SO4 | F | 735 | 5/5 | 0.89 | 0.24 | - | 155,157,170,173 | 0 |
| 2 | SO4 | B | 731 | 5/5 | 0.87 | 0.23 | - | 186,187,191,195 | 0 |
| 2 | SO4 | B | 742 | 5/5 | 0.81 | 0.95 | - | 218,221,224,224 | 0 |
| 2 | SO4 | A | 721 | 5/5 | 0.86 | 0.22 | - | 191,194,201,204 | 0 |
| 2 | SO4 | A | 725 | 5/5 | 0.78 | 0.34 | - | 191,197,199,206 | 0 |
| 2 | SO4 | A | 722 | 5/5 | 0.64 | 0.40 | - | 196,198,200,207 | 0 |
| 2 | SO4 | E | 709 | 5/5 | 0.59 | 0.38 | - | 190,199,199,202 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 2 | SO4 | F | 723 | 5/5 | 0.83 | 0.34 | - | 194,194,199,201 | 0 |
| 2 | SO4 | E | 733 | 5/5 | 0.80 | 0.34 | - | 184,186,189,195 | 0 |
| 2 | SO4 | B | 740 | 5/5 | 0.82 | 0.40 | - | 211,217,219,220 | 0 |
| 2 | SO4 | D | 728 | 5/5 | 0.69 | 0.49 | - | 211,215,216,219 | 0 |
| 2 | SO4 | A | 724 | 5/5 | 0.82 | 0.51 | - | 197,200,204,208 | 0 |
| 2 | SO4 | F | 725 | 5/5 | 0.61 | 0.56 | - | 218,219,223,223 | 0 |
| 2 | SO4 | F | 705 | 5/5 | 0.86 | 0.14 | - | 124,147,160,172 | 0 |
| 2 | SO4 | B | 728 | 5/5 | 0.85 | 0.34 | - | 172,187,193,193 | 0 |
| 2 | SO4 | F | 741 | 5/5 | 0.63 | 0.52 | - | 215,219,221,223 | 0 |
| 2 | SO4 | C | 730 | 5/5 | 0.85 | 0.23 | - | 185,186,191,194 | 0 |
| 2 | SO4 | A | 729 | 5/5 | 0.80 | 0.23 | - | 227,228,228,228 | 0 |
| 2 | SO4 | F | 727 | 5/5 | 0.87 | 0.23 | - | 203,206,208,215 | 0 |
| 2 | SO4 | A | 720 | 5/5 | 0.76 | 0.32 | - | 178,182,186,193 | 0 |
| 2 | SO4 | D | 723 | 5/5 | 0.76 | 0.20 | - | 231,231,232,234 | 0 |
| 2 | SO4 | B | 702 | 5/5 | 0.90 | 0.14 | - | 142,156,162,166 | 0 |
| 2 | SO4 | A | 728 | 5/5 | 0.67 | 0.65 | - | 206,210,213,214 | 0 |
| 2 | SO4 | B | 715 | 5/5 | 0.81 | 0.29 | - | 193,194,197,202 | 0 |
| 2 | SO4 | B | 727 | 5/5 | 0.81 | 0.49 | - | 212,212,217,217 | 0 |
| 2 | SO4 | B | 743 | 5/5 | 0.82 | 0.50 | - | 185,192,193,195 | 0 |
| 2 | SO4 | C | 713 | 5/5 | 0.85 | 0.35 | - | 172,185,186,190 | 0 |
| 2 | SO4 | A | 711 | 5/5 | 0.91 | 0.19 | - | 158,164,167,168 | 0 |
| 2 | SO4 | B | 729 | 5/5 | 0.81 | 0.28 | - | 147,164,172,185 | 0 |
| 2 | SO4 | D | 734 | 5/5 | 0.77 | 0.28 | - | 184,191,202,202 | 0 |
| 2 | SO4 | F | 731 | 5/5 | 0.71 | 0.40 | - | 181,185,187,196 | 0 |
| 2 | SO4 | A | 726 | 5/5 | 0.98 | 0.09 | - | 105,108,123,129 | 0 |
| 2 | SO4 | B | 745 | 5/5 | 0.72 | 0.33 | - | 212,213,215,217 | 0 |
| 2 | SO4 | D | 722 | 5/5 | 0.87 | 0.30 | - | 190,194,195,198 | 0 |
| 2 | SO4 | A | 736 | 5/5 | 0.91 | 0.26 | - | 169,172,175,179 | 0 |
| 2 | SO4 | E | 708 | 5/5 | 0.82 | 0.23 | - | 155,158,161,163 | 0 |
| 2 | SO4 | F | 706 | 5/5 | 0.88 | 0.19 | - | 139,147,152,153 | 0 |
| 2 | SO4 | D | 702 | 5/5 | 0.88 | 0.21 | - | 128,148,152,163 | 0 |
| 2 | SO4 | D | 705 | 5/5 | 0.92 | 0.13 | - | 158,162,165,165 | 0 |
| 2 | SO4 | C | 710 | 5/5 | 0.85 | 0.32 | - | 182,188,189,193 | 0 |
| 2 | SO4 | B | 707 | 5/5 | 0.93 | 0.18 | - | 145,146,149,151 | 0 |
| 2 | SO4 | D | 714 | 5/5 | 0.79 | 0.35 | - | 199,202,204,209 | 0 |
| 2 | SO4 | B | 747 | 5/5 | 0.65 | 0.37 | - | 234,234,235,237 | 0 |
| 2 | SO4 | F | 720 | 5/5 | 0.79 | 0.28 | - | 169,177,181,193 | 0 |
| 2 | SO4 | D | 703 | 5/5 | 0.85 | 0.18 | - | 167,180,183,185 | 0 |
| 2 | SO4 | A | 718 | 5/5 | 0.87 | 0.17 | - | 180,181,183,186 | 0 |
| 2 | SO4 | C | 715 | 5/5 | 0.88 | 0.39 | - | 185,188,198,199 | 0 |
| 2 | SO4 | C | 718 | 5/5 | 0.85 | 0.18 | - | 181,192,195,196 | 0 |
| 2 | SO4 | C | 727 | 5/5 | 0.70 | 0.50 | - | 173,181,183,190 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 2 | SO4 | B | 703 | 5/5 | 0.87 | 0.25 | - | 105,135,151,162 | 0 |
| 2 | SO4 | D | 719 | 5/5 | 0.81 | 0.23 | - | 166,173,181,187 | 0 |
| 2 | SO4 | D | 717 | 5/5 | 0.82 | 0.24 | - | 184,190,191,196 | 0 |
| 2 | SO4 | B | 705 | 5/5 | 0.88 | 0.15 | - | 157,176,179,182 | 0 |
| 2 | SO4 | A | 704 | 5/5 | 0.89 | 0.15 | - | 152,156,158,164 | 0 |
| 2 | SO4 | C | 720 | 5/5 | 0.77 | 0.13 | - | 178,180,182,186 | 0 |
| 2 | SO4 | A | 741 | 5/5 | 0.79 | 0.58 | - | 214,215,219,219 | 0 |
| 2 | SO4 | B | 730 | 5/5 | 0.71 | 0.25 | - | 188,188,196,202 | 0 |
| 2 | SO4 | B | 724 | 5/5 | 0.86 | 0.36 | - | 189,196,200,200 | 0 |
| 2 | SO4 | F | 703 | 5/5 | 0.90 | 0.29 | - | 128,136,151,164 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.