



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 5, 2018 – 09:17 PM EST

PDB ID : 4RVY
Title : Serial Time resolved crystallography of Photosystem II using a femtosecond X-ray laser. The S state after two flashes (S3)
Authors : Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.-H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.
Deposited on : 2014-11-29
Resolution : 5.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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-20030736

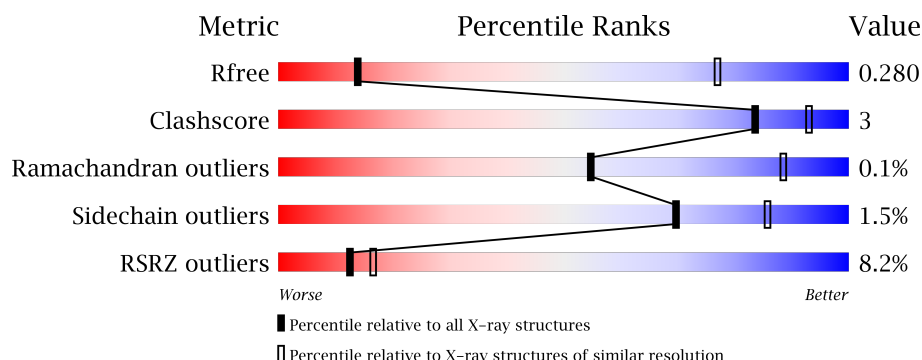
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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 | 1052 (7.20-3.70) |
| Clashscore | 112137 | 1021 (7.20-3.76) |
| Ramachandran outliers | 110173 | 1082 (7.20-3.70) |
| Sidechain outliers | 110143 | 1055 (7.20-3.70) |
| RSRZ outliers | 101464 | 1061 (7.20-3.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 | 334 | <div> <div>6%</div> <div>94%</div> <div>6%</div> </div> |
| 1 | a | 334 | <div> <div>8%</div> <div>100%</div> </div> |

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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-20030736

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | B | 504 | |
| 2 | b | 504 | |
| 3 | C | 461 | |
| 3 | c | 461 | |
| 4 | D | 342 | |
| 4 | d | 342 | |
| 5 | E | 81 | |
| 5 | e | 81 | |
| 6 | F | 34 | |
| 6 | f | 34 | |
| 7 | H | 65 | |
| 7 | h | 65 | |
| 8 | I | 38 | |
| 8 | i | 38 | |
| 9 | J | 40 | |
| 9 | j | 40 | |
| 10 | K | 37 | |
| 10 | k | 37 | |
| 11 | L | 37 | |
| 11 | l | 37 | |
| 12 | M | 34 | |
| 12 | m | 34 | |
| 13 | O | 243 | |
| 13 | o | 243 | |
| 14 | T | 30 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 14 | t | 30 | |
| 15 | U | 97 | |
| 15 | u | 97 | |
| 16 | V | 137 | |
| 16 | v | 137 | |
| 17 | X | 39 | |
| 17 | x | 39 | |
| 18 | Y | 29 | |
| 18 | y | 29 | |
| 19 | Z | 62 | |
| 19 | z | 62 | |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 20 | OEX | a | 601 | - | - | - | X |
| 22 | CLA | A | 603 | X | - | - | X |
| 22 | CLA | A | 604 | X | - | - | X |
| 22 | CLA | A | 607 | X | - | - | X |
| 22 | CLA | B | 602 | X | - | - | X |
| 22 | CLA | B | 603 | X | - | - | X |
| 22 | CLA | B | 604 | X | - | - | X |
| 22 | CLA | B | 605 | X | - | - | X |
| 22 | CLA | B | 606 | X | - | - | X |
| 22 | CLA | B | 607 | X | - | - | X |
| 22 | CLA | B | 608 | X | - | - | X |
| 22 | CLA | B | 609 | X | - | - | X |
| 22 | CLA | B | 610 | X | - | - | X |
| 22 | CLA | B | 611 | X | - | - | X |
| 22 | CLA | B | 612 | X | - | - | X |
| 22 | CLA | B | 613 | X | - | - | X |
| 22 | CLA | B | 614 | X | - | - | - |
| 22 | CLA | B | 615 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | B | 616 | X | - | - | X |
| 22 | CLA | B | 617 | X | - | - | X |
| 22 | CLA | C | 501 | X | - | - | X |
| 22 | CLA | C | 502 | X | - | - | X |
| 22 | CLA | C | 503 | X | - | - | X |
| 22 | CLA | C | 504 | X | - | - | X |
| 22 | CLA | C | 505 | X | - | - | X |
| 22 | CLA | C | 506 | X | - | - | X |
| 22 | CLA | C | 507 | X | - | - | X |
| 22 | CLA | C | 508 | X | - | - | X |
| 22 | CLA | C | 509 | X | - | - | X |
| 22 | CLA | C | 510 | X | - | - | X |
| 22 | CLA | C | 511 | X | - | - | X |
| 22 | CLA | C | 512 | X | - | - | X |
| 22 | CLA | C | 513 | X | - | - | X |
| 22 | CLA | D | 401 | X | - | - | X |
| 22 | CLA | D | 402 | X | - | - | X |
| 22 | CLA | D | 403 | X | - | - | X |
| 22 | CLA | a | 603 | X | - | - | X |
| 22 | CLA | a | 604 | X | - | - | X |
| 22 | CLA | a | 607 | X | - | - | X |
| 22 | CLA | b | 602 | X | - | - | X |
| 22 | CLA | b | 603 | X | - | - | X |
| 22 | CLA | b | 604 | X | - | - | X |
| 22 | CLA | b | 605 | X | - | - | X |
| 22 | CLA | b | 606 | X | - | - | X |
| 22 | CLA | b | 607 | X | - | - | X |
| 22 | CLA | b | 608 | X | - | - | X |
| 22 | CLA | b | 609 | X | - | - | X |
| 22 | CLA | b | 610 | X | - | - | X |
| 22 | CLA | b | 611 | X | - | - | X |
| 22 | CLA | b | 612 | X | - | - | X |
| 22 | CLA | b | 613 | X | - | - | X |
| 22 | CLA | b | 614 | X | - | - | X |
| 22 | CLA | b | 615 | X | - | - | X |
| 22 | CLA | b | 616 | X | - | - | X |
| 22 | CLA | b | 617 | X | - | - | X |
| 22 | CLA | c | 501 | X | - | - | X |
| 22 | CLA | c | 502 | X | - | - | X |
| 22 | CLA | c | 503 | X | - | - | X |
| 22 | CLA | c | 504 | X | - | - | X |
| 22 | CLA | c | 505 | X | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 22 | CLA | c | 506 | X | - | - | X |
| 22 | CLA | c | 507 | X | - | - | X |
| 22 | CLA | c | 508 | X | - | - | X |
| 22 | CLA | c | 509 | X | - | - | X |
| 22 | CLA | c | 510 | X | - | - | X |
| 22 | CLA | c | 511 | X | - | - | X |
| 22 | CLA | c | 512 | X | - | - | X |
| 22 | CLA | c | 513 | X | - | - | X |
| 22 | CLA | d | 401 | X | - | - | X |
| 22 | CLA | d | 402 | X | - | - | X |
| 22 | CLA | d | 403 | X | - | - | X |
| 23 | PHO | A | 605 | - | - | - | X |
| 23 | PHO | A | 606 | - | - | - | X |
| 23 | PHO | a | 605 | - | - | - | X |
| 23 | PHO | a | 606 | - | - | - | X |
| 24 | BCR | A | 608 | - | - | - | X |
| 24 | BCR | B | 622 | - | - | - | X |
| 24 | BCR | C | 514 | - | - | - | X |
| 24 | BCR | C | 515 | - | - | - | X |
| 24 | BCR | D | 404 | - | - | - | X |
| 24 | BCR | H | 101 | - | - | - | X |
| 24 | BCR | K | 101 | - | - | - | X |
| 24 | BCR | K | 102 | - | - | - | X |
| 24 | BCR | T | 102 | - | - | - | X |
| 24 | BCR | a | 608 | - | - | - | X |
| 24 | BCR | b | 618 | - | - | - | X |
| 24 | BCR | b | 622 | - | - | - | X |
| 24 | BCR | c | 514 | - | - | - | X |
| 24 | BCR | c | 515 | - | - | - | X |
| 24 | BCR | d | 404 | - | - | - | X |
| 24 | BCR | h | 101 | - | - | - | X |
| 24 | BCR | k | 101 | - | - | - | X |
| 24 | BCR | k | 102 | - | - | - | X |
| 24 | BCR | t | 101 | - | - | - | X |
| 25 | SQD | A | 609 | - | - | - | X |
| 25 | SQD | D | 411 | - | - | - | X |
| 25 | SQD | L | 101 | - | - | - | X |
| 25 | SQD | a | 609 | - | - | - | X |
| 25 | SQD | b | 601 | - | - | - | X |
| 25 | SQD | b | 621 | - | - | - | X |
| 25 | SQD | d | 411 | - | - | - | X |
| 26 | CL | A | 610 | - | - | - | X |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 26 | CL | a | 610 | - | - | - | X |
| 27 | BCT | A | 612 | - | - | - | X |
| 27 | BCT | a | 612 | - | - | - | X |
| 28 | PL9 | A | 613 | - | - | - | X |
| 28 | PL9 | D | 408 | - | - | - | X |
| 28 | PL9 | a | 613 | - | - | - | X |
| 29 | LMG | A | 614 | - | - | - | X |
| 29 | LMG | C | 519 | - | - | - | X |
| 29 | LMG | C | 520 | - | - | - | X |
| 29 | LMG | D | 406 | - | - | - | X |
| 29 | LMG | Z | 101 | - | - | - | X |
| 29 | LMG | a | 614 | - | - | - | X |
| 29 | LMG | c | 519 | - | - | - | X |
| 29 | LMG | c | 520 | - | - | - | X |
| 29 | LMG | d | 406 | - | - | - | X |
| 29 | LMG | z | 101 | - | - | - | X |
| 31 | DGD | C | 516 | - | - | - | X |
| 31 | DGD | C | 517 | - | - | - | X |
| 31 | DGD | C | 518 | - | - | - | X |
| 31 | DGD | D | 410 | - | - | - | X |
| 31 | DGD | H | 102 | - | - | - | X |
| 31 | DGD | c | 516 | - | - | - | X |
| 31 | DGD | c | 518 | - | - | - | X |
| 31 | DGD | d | 410 | - | - | - | X |
| 31 | DGD | h | 102 | - | - | - | X |
| 32 | LHG | D | 407 | - | - | - | X |
| 32 | LHG | D | 409 | - | - | - | X |
| 32 | LHG | E | 101 | - | - | - | X |
| 32 | LHG | d | 405 | - | - | - | X |
| 32 | LHG | d | 409 | - | - | - | X |
| 32 | LHG | e | 101 | - | - | - | X |
| 33 | HEM | F | 101 | - | - | - | X |
| 33 | HEM | V | 201 | - | - | - | X |
| 33 | HEM | f | 101 | - | - | - | X |
| 33 | HEM | v | 201 | - | - | - | X |

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 49594 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 Photosystem II protein D1 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2620 | 1716 | 431 | 458 | 15 | | | |
| 1 | a | 334 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2620 | 1716 | 431 | 458 | 15 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| A | 286 | ALA | THR | CONFLICT | UNP P0A444 |
| a | 286 | ALA | THR | CONFLICT | UNP P0A444 |

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | B | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3969 | 2605 | 661 | 690 | 13 | | | |
| 2 | b | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3969 | 2605 | 661 | 690 | 13 | | | |

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | C | 451 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3486 | 2281 | 584 | 608 | 13 | | | |
| 3 | c | 451 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3486 | 2281 | 584 | 608 | 13 | | | |

- Molecule 4 is a protein called Photosystem II D2 protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | D | 342 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2726 | 1805 | 445 | 464 | 12 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | d | 342 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2726 | 1805 | 445 | 464 | 12 | | | |

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 5 | E | 81 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 662 | 432 | 107 | 123 | | | | |
| 5 | e | 81 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 662 | 432 | 107 | 123 | | | | |

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6 | F | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 187 | 45 | 42 | 1 | | | |
| 6 | f | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 187 | 45 | 42 | 1 | | | |

- Molecule 7 is a protein called Photosystem II reaction center protein H.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | H | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 511 | 341 | 82 | 86 | 2 | | | |
| 7 | h | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 511 | 341 | 82 | 86 | 2 | | | |

- Molecule 8 is a protein called Photosystem II reaction center protein I.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | I | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 312 | 210 | 48 | 53 | 1 | | | |
| 8 | i | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 312 | 210 | 48 | 53 | 1 | | | |

- Molecule 9 is a protein called Photosystem II reaction center protein J.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | J | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 272 | 182 | 42 | 47 | 1 | | | |
| 9 | j | 38 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 272 | 182 | 42 | 47 | 1 | | | |

- Molecule 10 is a protein called Photosystem II reaction center protein K.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10 | K | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 43 | 46 | | | |
| 10 | k | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 43 | 46 | | | |

- Molecule 11 is a protein called Photosystem II reaction center protein L.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 11 | L | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 304 | 202 | 48 | 53 | 1 | | | |
| 11 | l | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 304 | 202 | 48 | 53 | 1 | | | |

- Molecule 12 is a protein called Photosystem II reaction center protein M.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | M | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 267 | 178 | 40 | 48 | 1 | | | |
| 12 | m | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 267 | 178 | 40 | 48 | 1 | | | |

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13 | O | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1865 | 1165 | 315 | 381 | 4 | | | |
| 13 | o | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1865 | 1165 | 315 | 381 | 4 | | | |

- Molecule 14 is a protein called Photosystem II reaction center protein T.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14 | T | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 256 | 180 | 36 | 38 | 2 | | | |
| 14 | t | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 256 | 180 | 36 | 38 | 2 | | | |

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 15 | U | 97 | Total | C | N | O | 0 | 0 | 0 |
| | | | 774 | 491 | 129 | 154 | | | |
| 15 | u | 97 | Total | C | N | O | 0 | 0 | 0 |
| | | | 774 | 491 | 129 | 154 | | | |

- Molecule 16 is a protein called Cytochrome c-550.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16 | V | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1064 | 675 | 177 | 208 | 4 | | | |
| 16 | v | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1064 | 675 | 177 | 208 | 4 | | | |

- Molecule 17 is a protein called Photosystem II reaction center X protein.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 17 | X | 39 | Total | C | N | O | 0 | 0 | 0 |
| | | | 287 | 191 | 46 | 50 | | | |
| 17 | x | 39 | Total | C | N | O | 0 | 0 | 0 |
| | | | 287 | 191 | 46 | 50 | | | |

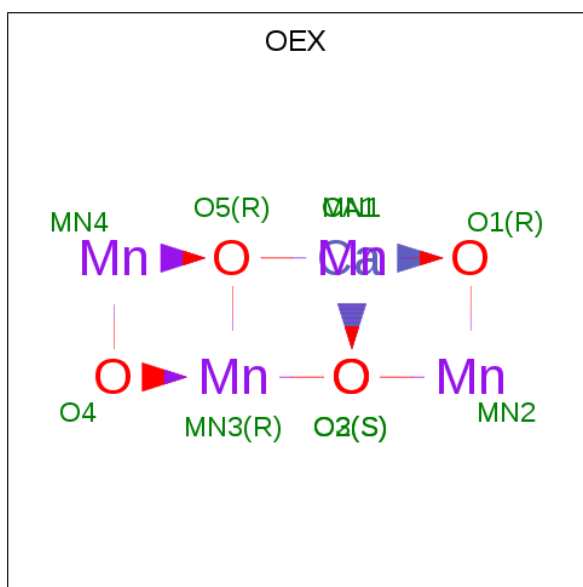
- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 18 | Y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |
| 18 | y | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 215 | 142 | 37 | 33 | 3 | | | |

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 19 | Z | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 479 | 328 | 72 | 77 | 2 | | | |
| 19 | z | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 479 | 328 | 72 | 77 | 2 | | | |

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).

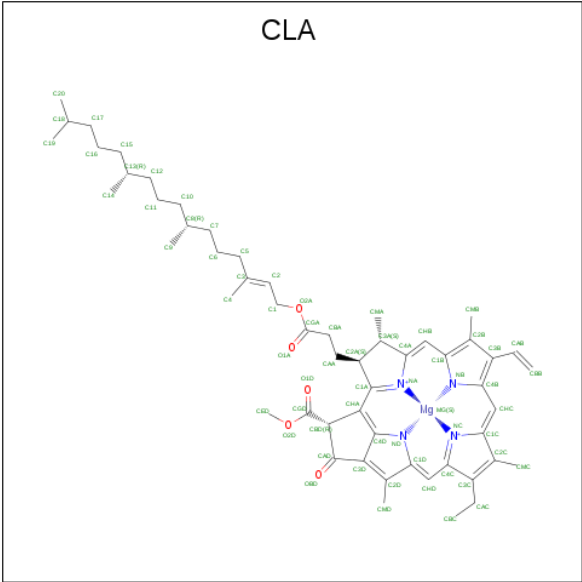


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 20 | A | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |
| 20 | a | 1 | Total | Ca | Mn | O | 0 | 0 |
| | | | 10 | 1 | 4 | 5 | | |

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21 | A | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |
| 21 | a | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 22 | A | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | A | 1 | Total | C | Mg | N | O | | |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | A | 1 | Total | C | Mg | N | O | | |
| 22 | a | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | a | 1 | Total | C | Mg | N | O | | |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | a | 1 | Total | C | Mg | N | O | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | B | 1 | Total | C | Mg | N | O | | |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | B | 1 | Total | C | Mg | N | O | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | B | 1 | Total | C | Mg | N | O | | |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | B | 1 | Total | C | Mg | N | O | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | B | 1 | Total | C | Mg | N | O | | |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | B | 1 | Total | C | Mg | N | O | | |
| 22 | B | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | B | 1 | Total | C | Mg | N | O | | |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| | B | 1 | Total | C | Mg | N | O | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | B | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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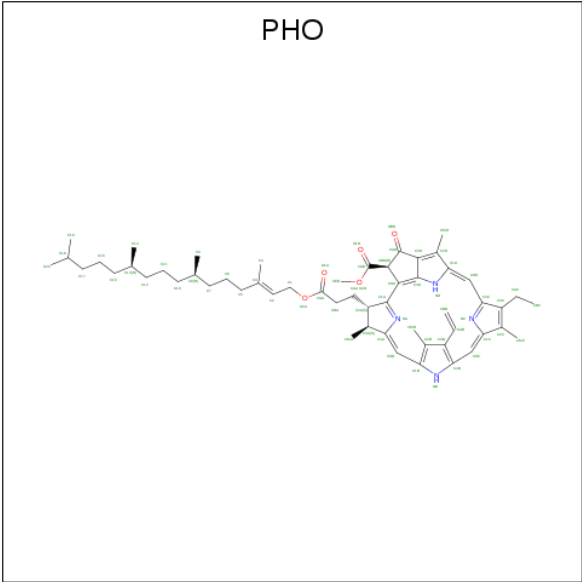
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | b | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | C | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

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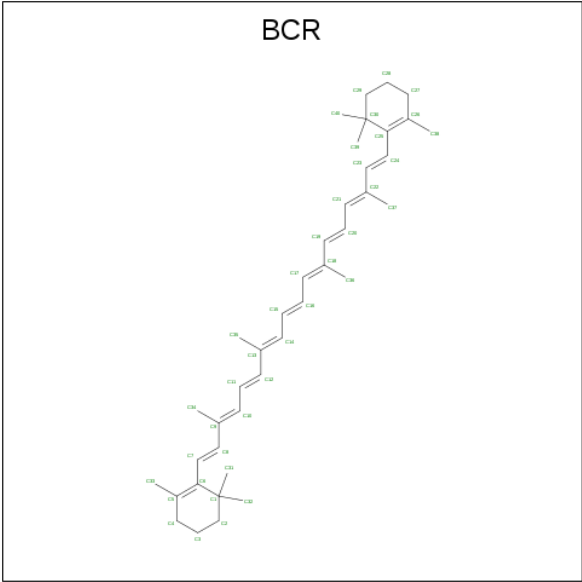
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | c | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | D | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | D | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | D | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | d | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | d | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | d | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



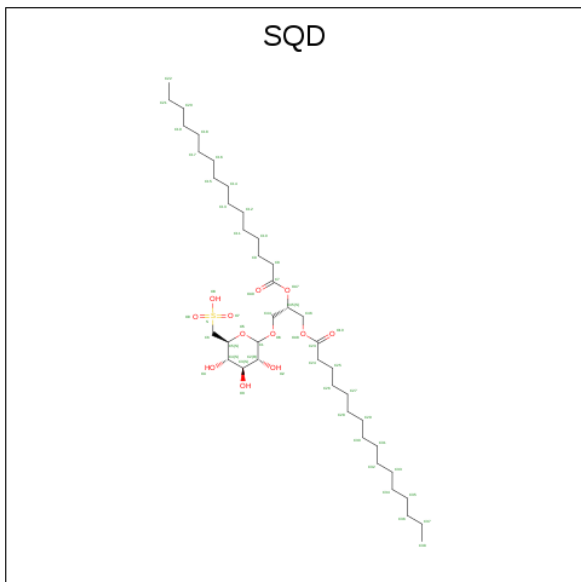
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 23 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | a | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 24 | A | 1 | Total C 40 40 | 0 | 0 |
| 24 | a | 1 | Total C 40 40 | 0 | 0 |
| 24 | B | 1 | Total C 40 40 | 0 | 0 |
| 24 | B | 1 | Total C 40 40 | 0 | 0 |
| 24 | B | 1 | Total C 40 40 | 0 | 0 |
| 24 | b | 1 | Total C 40 40 | 0 | 0 |
| 24 | b | 1 | Total C 40 40 | 0 | 0 |
| 24 | C | 1 | Total C 40 40 | 0 | 0 |
| 24 | C | 1 | Total C 40 40 | 0 | 0 |
| 24 | c | 1 | Total C 40 40 | 0 | 0 |
| 24 | c | 1 | Total C 40 40 | 0 | 0 |
| 24 | D | 1 | Total C 40 40 | 0 | 0 |
| 24 | d | 1 | Total C 40 40 | 0 | 0 |
| 24 | H | 1 | Total C 40 40 | 0 | 0 |
| 24 | h | 1 | Total C 40 40 | 0 | 0 |
| 24 | K | 1 | Total C 40 40 | 0 | 0 |
| 24 | K | 1 | Total C 40 40 | 0 | 0 |
| 24 | k | 1 | Total C 40 40 | 0 | 0 |
| 24 | k | 1 | Total C 40 40 | 0 | 0 |
| 24 | T | 1 | Total C 40 40 | 0 | 0 |
| 24 | T | 1 | Total C 40 40 | 0 | 0 |
| 24 | t | 1 | Total C 40 40 | 0 | 0 |

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

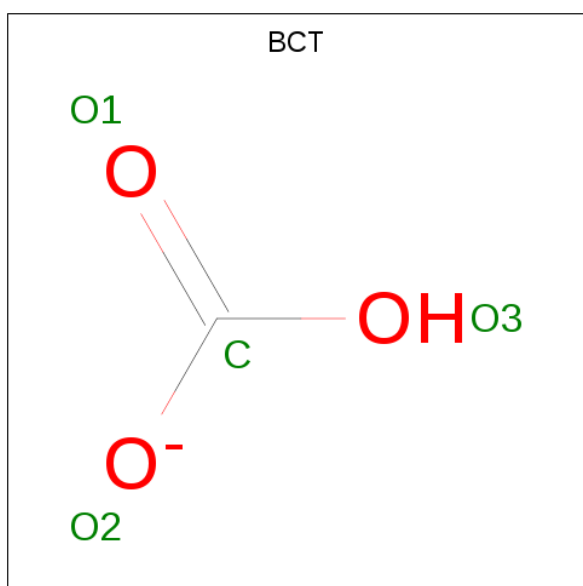


| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 25 | A | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | a | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | B | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | b | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | D | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 25 | d | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 25 | L | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | l | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 25 | l | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

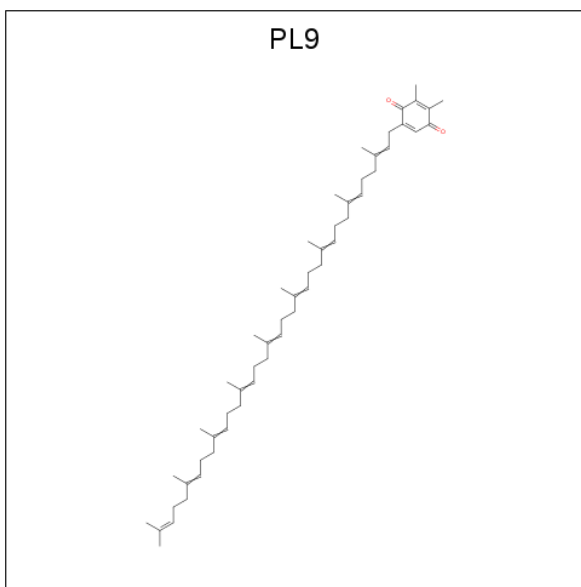
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 26 | A | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 26 | u | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 26 | a | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |
| 26 | U | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 27 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



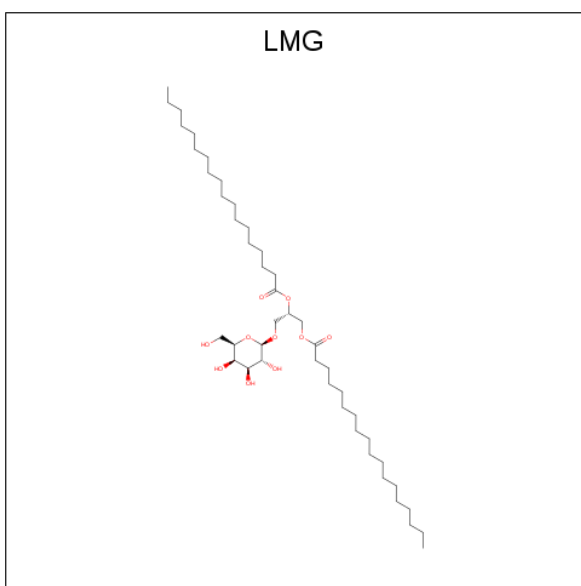
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 27 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 27 | a | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 28 | A | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 28 | a | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 28 | D | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 28 | d | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

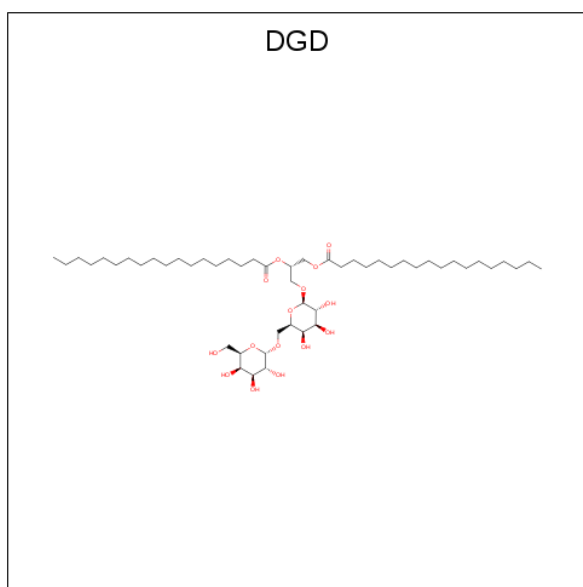


| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 29 | A | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | a | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | B | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | b | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | C | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | C | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | c | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | c | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | D | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | d | 1 | Total C O 51 41 10 | 0 | 0 |
| 29 | Z | 1 | Total C O 37 27 10 | 0 | 0 |
| 29 | z | 1 | Total C O 37 27 10 | 0 | 0 |

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

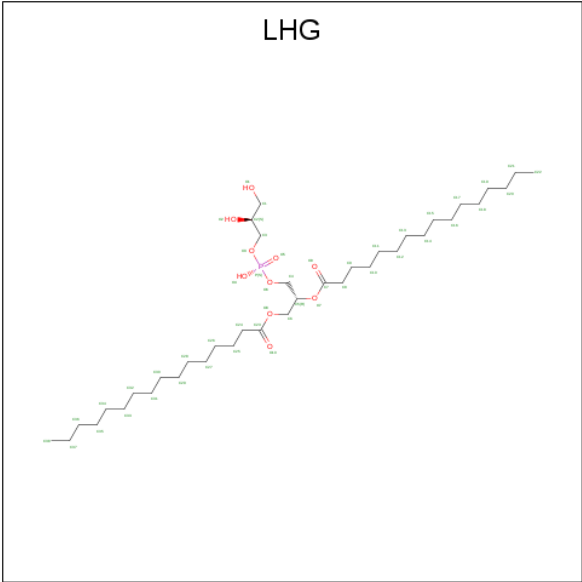
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 30 | B | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | F | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | o | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | O | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | b | 1 | Total Ca 1 1 | 0 | 0 |
| 30 | f | 1 | Total Ca 1 1 | 0 | 0 |

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



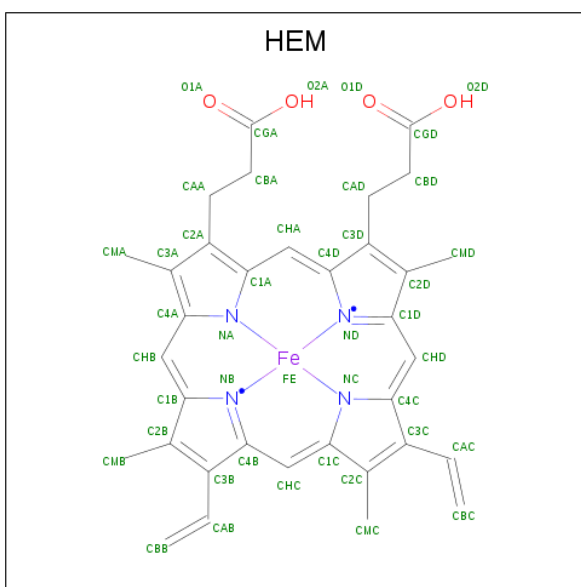
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 31 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | C | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | c | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | D | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | d | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | H | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 31 | h | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |

- Molecule 32 is 1,3-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 32 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | D | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | d | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | E | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |
| 32 | e | 1 | Total | C | O | P | 0 | 0 |
| | | | 42 | 31 | 10 | 1 | | |
| 32 | L | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |
| 32 | l | 1 | Total | C | O | P | 0 | 0 |
| | | | 49 | 38 | 10 | 1 | | |

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 33 | F | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 33 | f | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 33 | V | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 33 | v | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

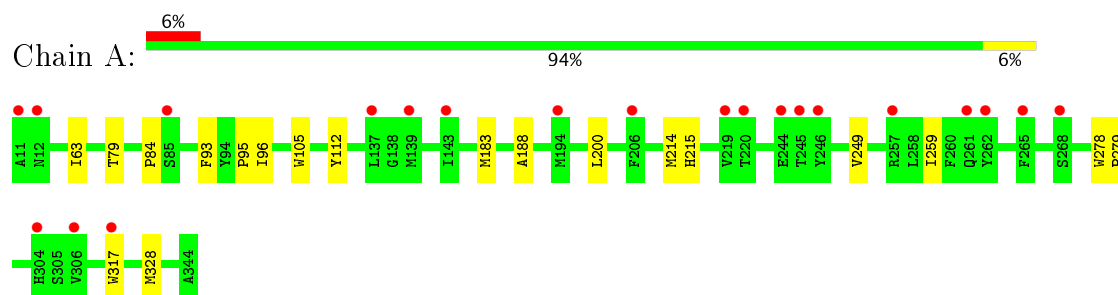
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 34 | J | 1 | Total Mg 1 1 | 0 | 0 |
| 34 | j | 1 | Total Mg 1 1 | 0 | 0 |

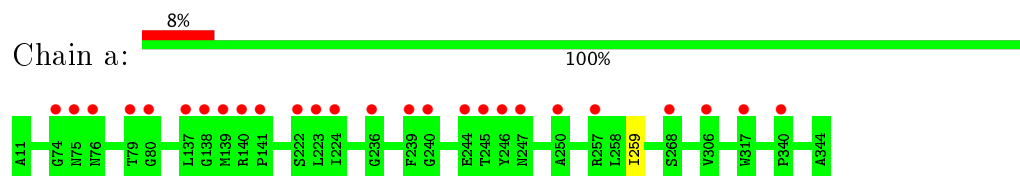
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

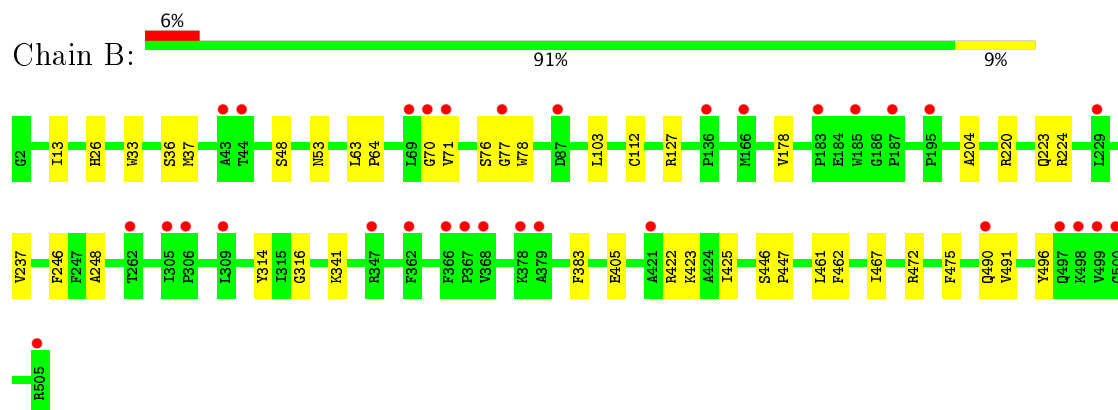
- Molecule 1: Photosystem II protein D1 1



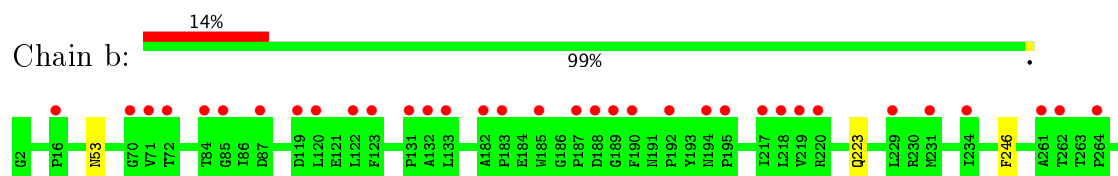
- Molecule 1: Photosystem II protein D1 1

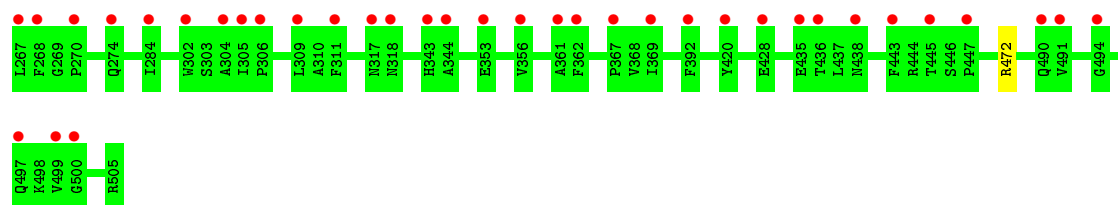


- Molecule 2: Photosystem II CP47 reaction center protein

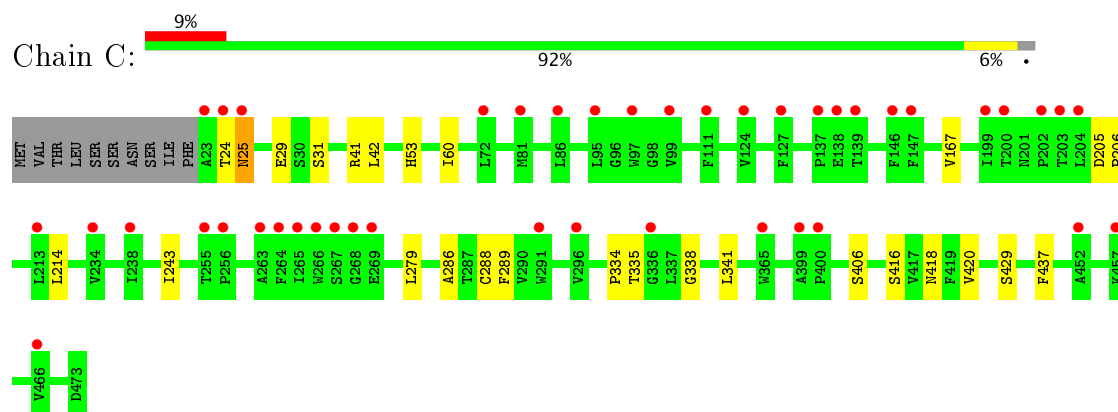


- Molecule 2: Photosystem II CP47 reaction center protein

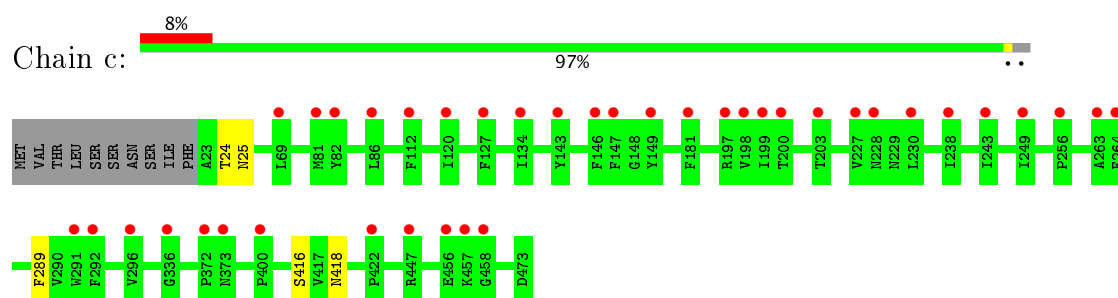




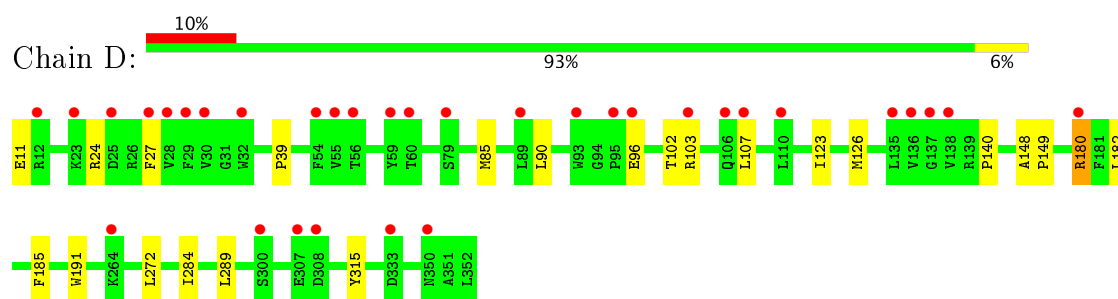
- Molecule 3: Photosystem II CP43 reaction center protein



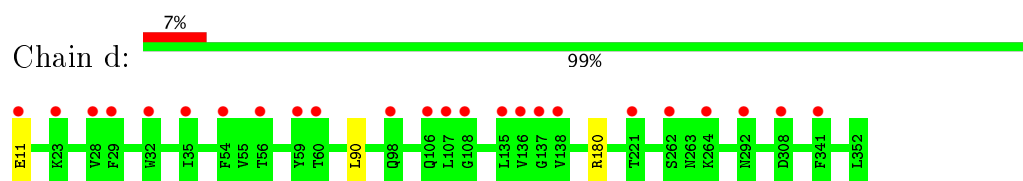
- Molecule 3: Photosystem II CP43 reaction center protein



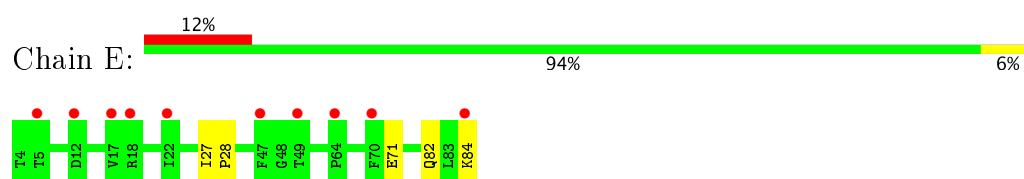
- Molecule 4: Photosystem II D2 protein



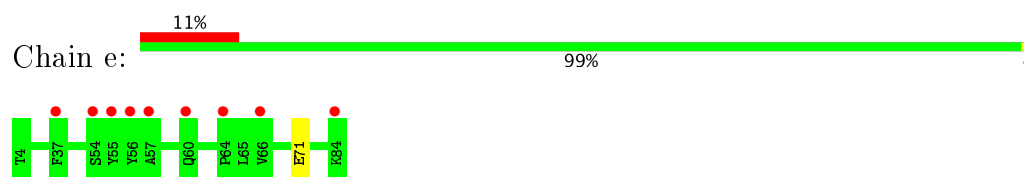
- Molecule 4: Photosystem II D2 protein



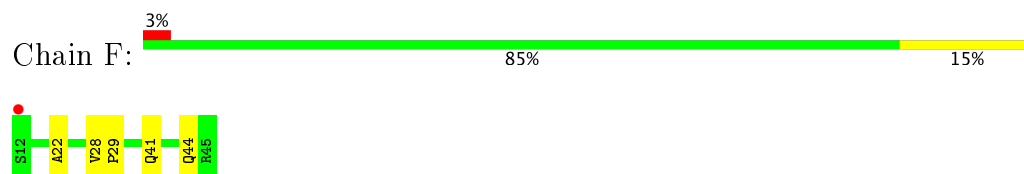
- Molecule 5: Cytochrome b559 subunit alpha



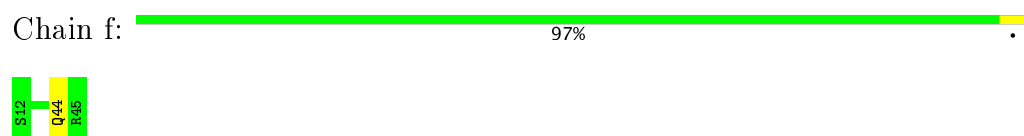
- Molecule 5: Cytochrome b559 subunit alpha



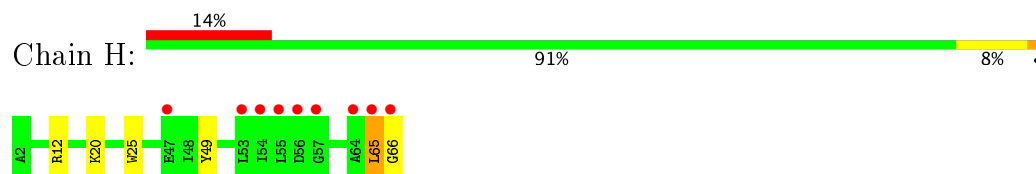
- Molecule 6: Cytochrome b559 subunit beta



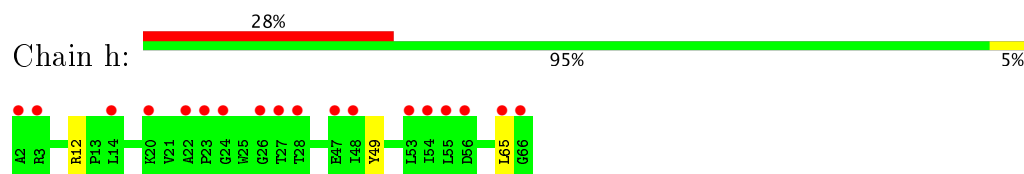
- Molecule 6: Cytochrome b559 subunit beta



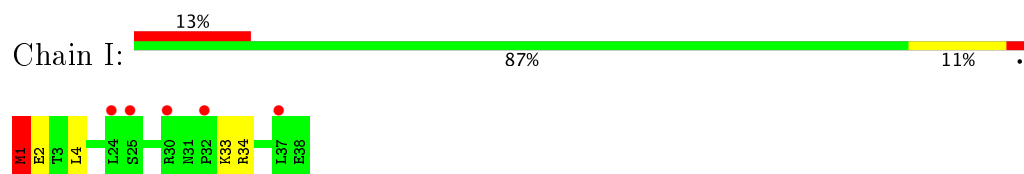
- Molecule 7: Photosystem II reaction center protein H



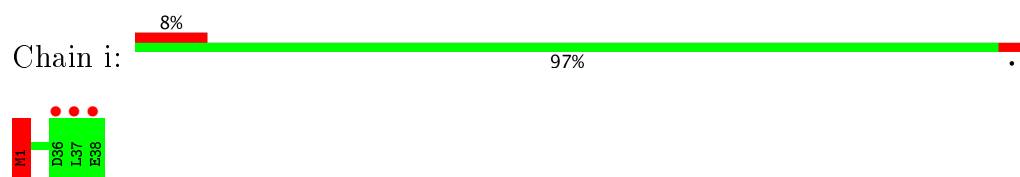
- Molecule 7: Photosystem II reaction center protein H



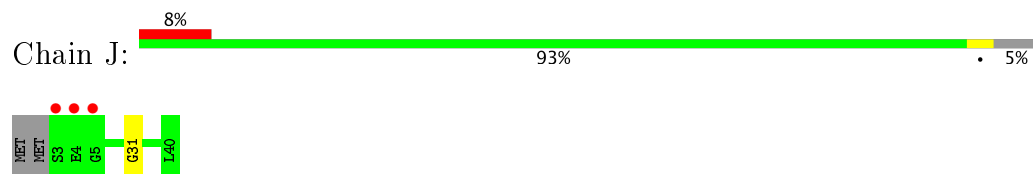
- Molecule 8: Photosystem II reaction center protein I



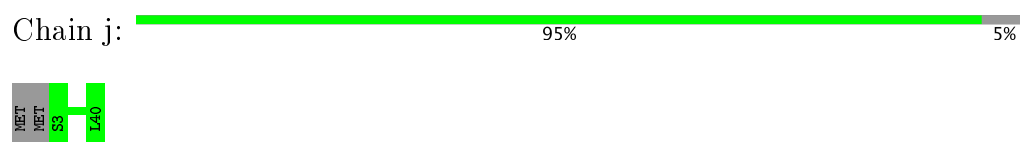
- Molecule 8: Photosystem II reaction center protein I



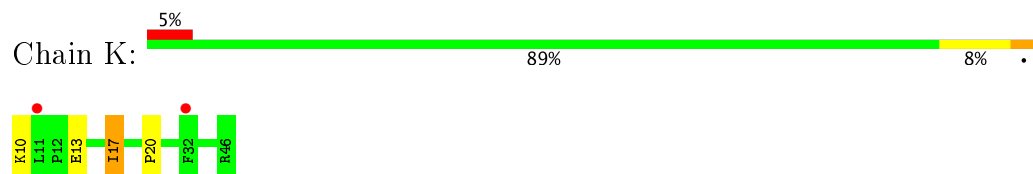
- Molecule 9: Photosystem II reaction center protein J



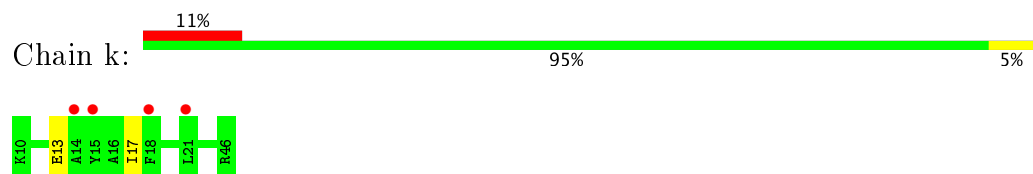
- Molecule 9: Photosystem II reaction center protein J



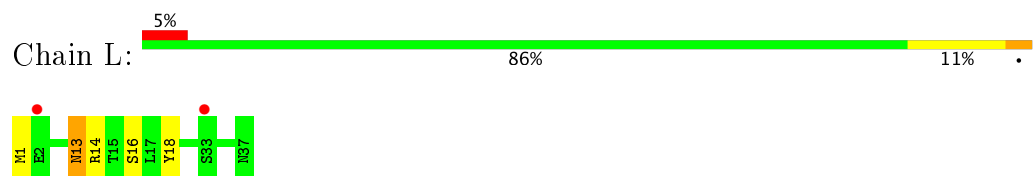
- Molecule 10: Photosystem II reaction center protein K



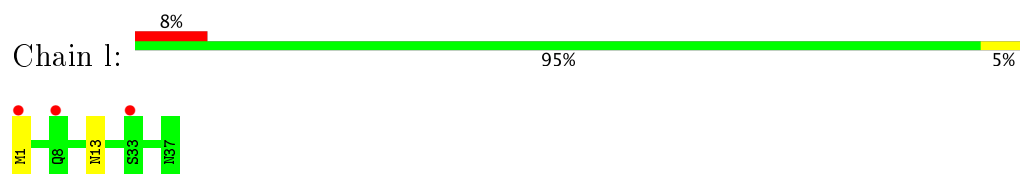
- Molecule 10: Photosystem II reaction center protein K



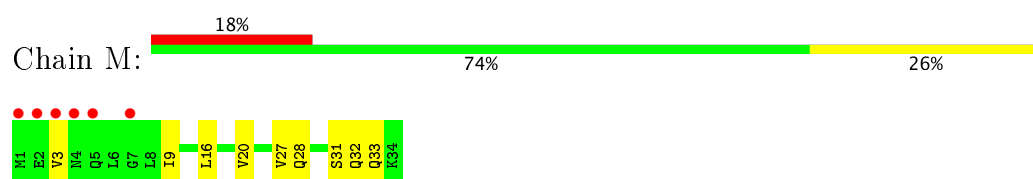
- Molecule 11: Photosystem II reaction center protein L



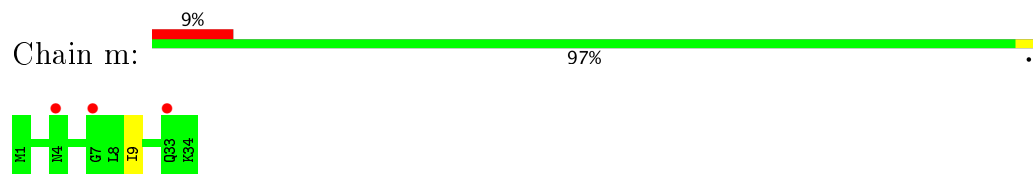
- Molecule 11: Photosystem II reaction center protein L



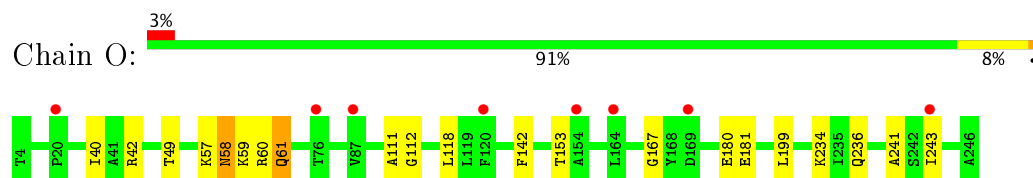
- Molecule 12: Photosystem II reaction center protein M



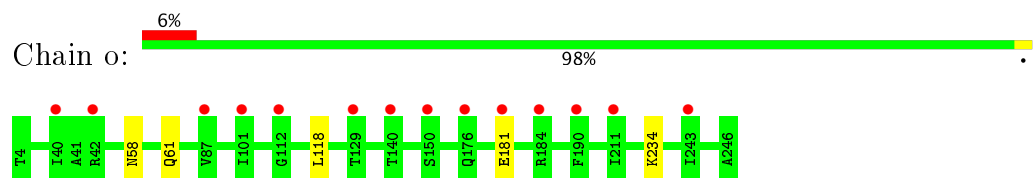
- Molecule 12: Photosystem II reaction center protein M



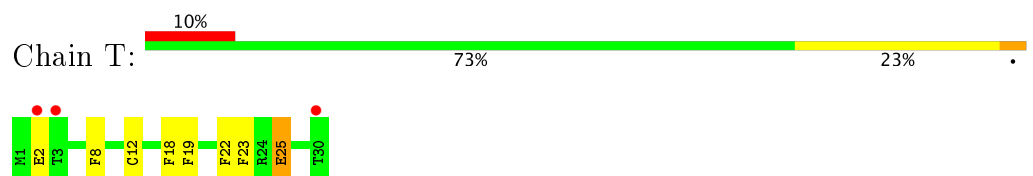
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



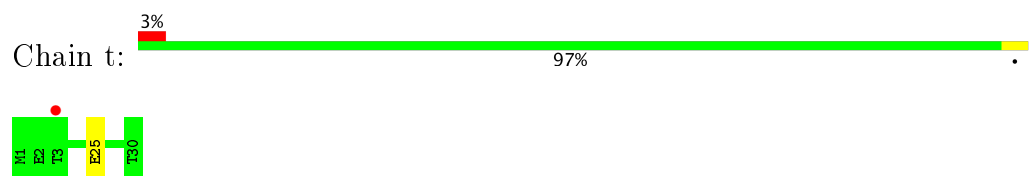
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



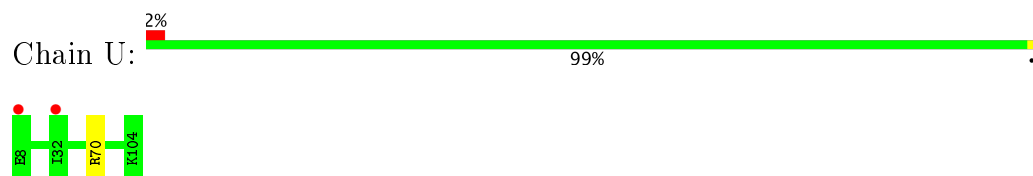
- Molecule 14: Photosystem II reaction center protein T



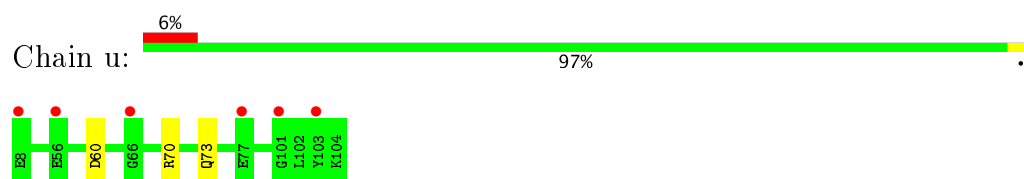
- Molecule 14: Photosystem II reaction center protein T



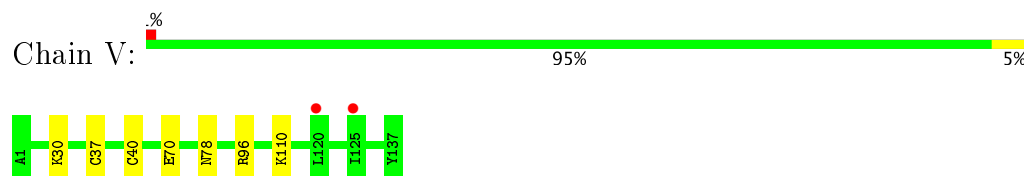
- Molecule 15: Photosystem II 12 kDa extrinsic protein



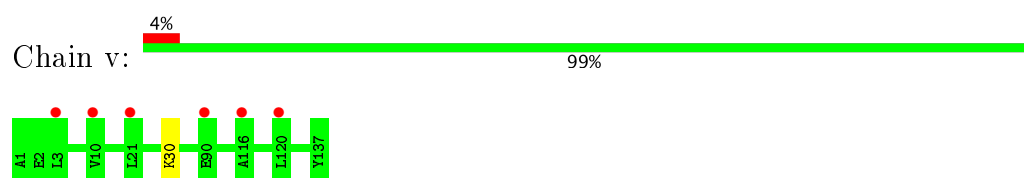
- Molecule 15: Photosystem II 12 kDa extrinsic protein



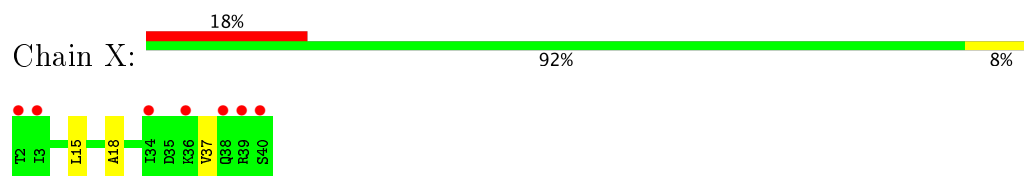
- Molecule 16: Cytochrome c-550



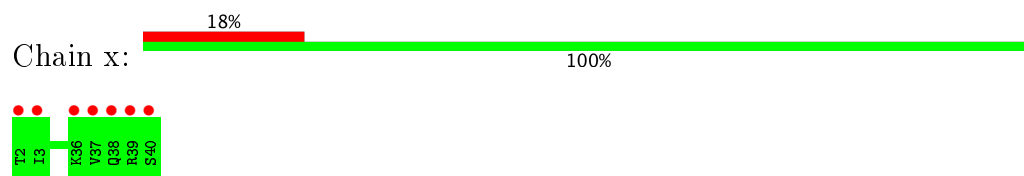
- Molecule 16: Cytochrome c-550



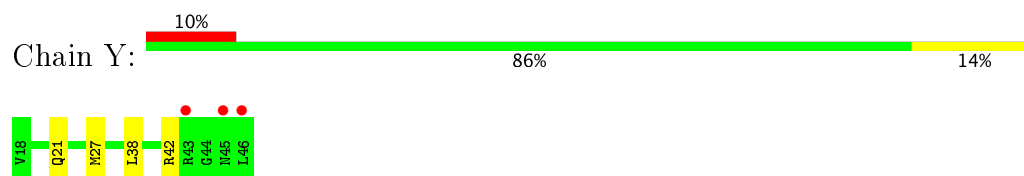
- Molecule 17: Photosystem II reaction center X protein



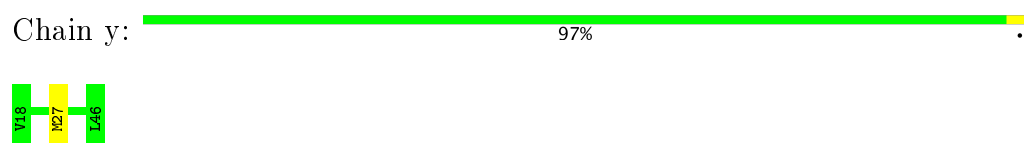
- Molecule 17: Photosystem II reaction center X protein



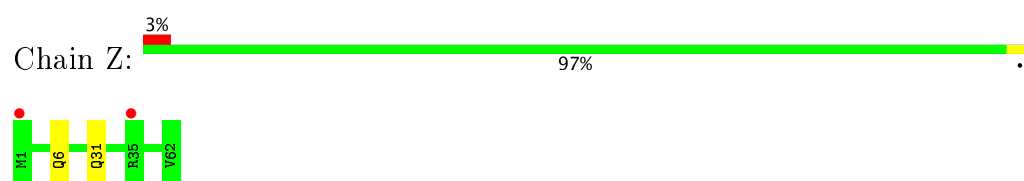
- Molecule 18: Photosystem II reaction center protein Ycf12



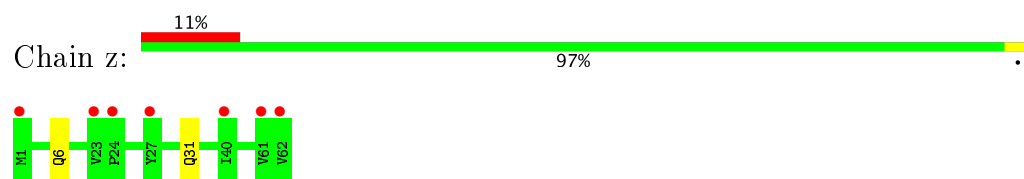
- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 136.61Å 228.09Å 308.68Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 102.30 – 5.50 102.29 – 5.50 | Depositor EDS |
| % Data completeness (in resolution range) | 99.9 (102.30-5.50) 100.0 (102.29-5.50) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.75 (at 5.42Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8.2_1336) | Depositor |
| R, R_{free} | 0.281 , 0.291 0.272 , 0.280 | Depositor DCC |
| R_{free} test set | 1625 reflections (5.07%) | DCC |
| Wilson B-factor (Å ²) | 357.8 | Xtriage |
| Anisotropy | 0.241 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.33 , 62.0 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.87 | EDS |
| Total number of atoms | 49594 | wwPDB-VP |
| Average B, all atoms (Å ²) | 32.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, MG, OEX, PHO, DGD, CL, CA, CLA, PL9, FE2, BCT, HEM, SQD, BCR, LMG

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 | 0.53 | 0/2705 | 0.55 | 0/3689 |
| 1 | a | 0.53 | 0/2705 | 0.55 | 0/3689 |
| 2 | B | 0.50 | 0/4109 | 0.54 | 0/5600 |
| 2 | b | 0.50 | 0/4109 | 0.54 | 0/5600 |
| 3 | C | 0.46 | 0/3599 | 0.51 | 0/4900 |
| 3 | c | 0.46 | 0/3599 | 0.51 | 0/4900 |
| 4 | D | 0.53 | 0/2821 | 0.55 | 0/3844 |
| 4 | d | 0.53 | 0/2821 | 0.55 | 0/3844 |
| 5 | E | 0.43 | 0/681 | 0.51 | 0/928 |
| 5 | e | 0.43 | 0/681 | 0.51 | 0/928 |
| 6 | F | 0.49 | 0/284 | 0.45 | 0/387 |
| 6 | f | 0.49 | 0/284 | 0.45 | 0/387 |
| 7 | H | 0.47 | 0/524 | 0.50 | 0/713 |
| 7 | h | 0.47 | 0/524 | 0.50 | 0/713 |
| 8 | I | 2.22 | 2/319 (0.6%) | 1.25 | 4/429 (0.9%) |
| 8 | i | 2.22 | 2/319 (0.6%) | 1.25 | 4/429 (0.9%) |
| 9 | J | 0.46 | 0/278 | 0.43 | 0/376 |
| 9 | j | 0.46 | 0/278 | 0.43 | 0/376 |
| 10 | K | 0.42 | 0/303 | 0.50 | 0/416 |
| 10 | k | 0.43 | 0/303 | 0.50 | 0/416 |
| 11 | L | 0.55 | 0/311 | 0.51 | 0/422 |
| 11 | l | 0.55 | 0/311 | 0.51 | 0/422 |
| 12 | M | 0.47 | 0/270 | 0.59 | 0/367 |
| 12 | m | 0.47 | 0/270 | 0.59 | 0/367 |
| 13 | O | 0.45 | 0/1896 | 0.58 | 0/2571 |
| 13 | o | 0.45 | 0/1896 | 0.58 | 0/2571 |
| 14 | T | 0.53 | 0/265 | 0.54 | 0/359 |
| 14 | t | 0.53 | 0/265 | 0.54 | 0/359 |
| 15 | U | 0.46 | 0/785 | 0.55 | 0/1064 |
| 15 | u | 0.46 | 0/785 | 0.55 | 0/1064 |
| 16 | V | 0.47 | 0/1085 | 0.53 | 0/1473 |
| 16 | v | 0.47 | 0/1085 | 0.53 | 0/1473 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | X | 0.43 | 0/290 | 0.47 | 0/392 |
| 17 | x | 0.43 | 0/290 | 0.47 | 0/392 |
| 18 | Y | 0.41 | 0/216 | 0.45 | 0/289 |
| 18 | y | 0.41 | 0/216 | 0.45 | 0/289 |
| 19 | Z | 0.41 | 0/490 | 0.45 | 0/669 |
| 19 | z | 0.41 | 0/490 | 0.45 | 0/669 |
| All | All | 0.55 | 4/42462 (0.0%) | 0.55 | 8/57776 (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 |
|-----|-------|---------------------|---------------------|
| 8 | I | 1 | 1 |
| 8 | i | 1 | 1 |
| All | All | 2 | 2 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8 | i | 1 | MET | N-CA | 36.97 | 2.20 | 1.46 |
| 8 | I | 1 | MET | N-CA | 36.95 | 2.20 | 1.46 |
| 8 | I | 1 | MET | CA-C | 12.27 | 1.84 | 1.52 |
| 8 | i | 1 | MET | CA-C | 12.26 | 1.84 | 1.52 |

The worst 5 of 8 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 8 | i | 1 | MET | N-CA-CB | -17.88 | 78.41 | 110.60 |
| 8 | I | 1 | MET | N-CA-CB | -17.86 | 78.45 | 110.60 |
| 8 | I | 1 | MET | N-CA-C | -12.99 | 75.92 | 111.00 |
| 8 | i | 1 | MET | N-CA-C | -12.98 | 75.94 | 111.00 |
| 8 | I | 1 | MET | CA-C-N | -6.32 | 103.29 | 117.20 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 8 | I | 1 | MET | CA |
| 8 | i | 1 | MET | CA |

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 8 | I | 1 | MET | Mainchain |
| 8 | i | 1 | MET | Mainchain |

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 | 2620 | 0 | 2517 | 16 | 0 |
| 1 | a | 2620 | 0 | 2517 | 0 | 0 |
| 2 | B | 3969 | 0 | 3828 | 47 | 0 |
| 2 | b | 3969 | 0 | 3828 | 0 | 0 |
| 3 | C | 3486 | 0 | 3407 | 20 | 0 |
| 3 | c | 3486 | 0 | 3407 | 0 | 0 |
| 4 | D | 2726 | 0 | 2627 | 21 | 0 |
| 4 | d | 2726 | 0 | 2627 | 0 | 0 |
| 5 | E | 662 | 0 | 648 | 3 | 0 |
| 5 | e | 662 | 0 | 648 | 0 | 0 |
| 6 | F | 275 | 0 | 282 | 3 | 0 |
| 6 | f | 275 | 0 | 282 | 0 | 0 |
| 7 | H | 511 | 0 | 532 | 4 | 0 |
| 7 | h | 511 | 0 | 532 | 0 | 0 |
| 8 | I | 312 | 0 | 329 | 16 | 0 |
| 8 | i | 312 | 0 | 329 | 0 | 0 |
| 9 | J | 272 | 0 | 279 | 1 | 0 |
| 9 | j | 272 | 0 | 279 | 0 | 0 |
| 10 | K | 293 | 0 | 305 | 5 | 0 |
| 10 | k | 293 | 0 | 305 | 0 | 0 |
| 11 | L | 304 | 0 | 316 | 6 | 0 |
| 11 | l | 304 | 0 | 316 | 0 | 0 |
| 12 | M | 267 | 0 | 288 | 21 | 0 |
| 12 | m | 267 | 0 | 287 | 0 | 0 |
| 13 | O | 1865 | 0 | 1838 | 21 | 0 |
| 13 | o | 1865 | 0 | 1838 | 0 | 0 |
| 14 | T | 256 | 0 | 262 | 12 | 0 |
| 14 | t | 256 | 0 | 262 | 0 | 0 |
| 15 | U | 774 | 0 | 773 | 0 | 0 |
| 15 | u | 774 | 0 | 773 | 0 | 7 |
| 16 | V | 1064 | 0 | 1073 | 10 | 7 |
| 16 | v | 1064 | 0 | 1073 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17 | X | 287 | 0 | 317 | 3 | 0 |
| 17 | x | 287 | 0 | 317 | 0 | 0 |
| 18 | Y | 215 | 0 | 246 | 2 | 0 |
| 18 | y | 215 | 0 | 246 | 0 | 0 |
| 19 | Z | 479 | 0 | 516 | 0 | 0 |
| 19 | z | 479 | 0 | 516 | 0 | 0 |
| 20 | A | 10 | 0 | 0 | 0 | 0 |
| 20 | a | 10 | 0 | 0 | 0 | 0 |
| 21 | A | 1 | 0 | 0 | 0 | 0 |
| 21 | a | 1 | 0 | 0 | 0 | 0 |
| 22 | A | 195 | 0 | 216 | 10 | 0 |
| 22 | B | 1040 | 0 | 1152 | 32 | 0 |
| 22 | C | 845 | 0 | 936 | 29 | 0 |
| 22 | D | 195 | 0 | 216 | 8 | 0 |
| 22 | a | 195 | 0 | 216 | 0 | 0 |
| 22 | b | 1040 | 0 | 1152 | 0 | 0 |
| 22 | c | 845 | 0 | 936 | 0 | 0 |
| 22 | d | 195 | 0 | 216 | 0 | 0 |
| 23 | A | 128 | 0 | 148 | 6 | 0 |
| 23 | a | 128 | 0 | 148 | 0 | 0 |
| 24 | A | 40 | 0 | 48 | 1 | 0 |
| 24 | B | 120 | 0 | 140 | 8 | 0 |
| 24 | C | 80 | 0 | 93 | 0 | 0 |
| 24 | D | 40 | 0 | 48 | 3 | 0 |
| 24 | H | 40 | 0 | 46 | 1 | 0 |
| 24 | K | 80 | 0 | 93 | 1 | 0 |
| 24 | T | 80 | 0 | 95 | 9 | 0 |
| 24 | a | 40 | 0 | 48 | 0 | 0 |
| 24 | b | 80 | 0 | 92 | 0 | 0 |
| 24 | c | 80 | 0 | 93 | 0 | 0 |
| 24 | d | 40 | 0 | 48 | 0 | 0 |
| 24 | h | 40 | 0 | 46 | 0 | 0 |
| 24 | k | 80 | 0 | 93 | 0 | 0 |
| 24 | t | 40 | 0 | 47 | 0 | 0 |
| 25 | A | 54 | 0 | 78 | 2 | 0 |
| 25 | B | 54 | 0 | 78 | 4 | 0 |
| 25 | D | 43 | 0 | 53 | 0 | 0 |
| 25 | L | 54 | 0 | 34 | 5 | 0 |
| 25 | a | 54 | 0 | 78 | 0 | 0 |
| 25 | b | 108 | 0 | 112 | 0 | 0 |
| 25 | d | 43 | 0 | 53 | 0 | 0 |
| 25 | l | 108 | 0 | 59 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 26 | A | 2 | 0 | 0 | 0 | 0 |
| 26 | U | 1 | 0 | 0 | 0 | 0 |
| 26 | a | 2 | 0 | 0 | 0 | 0 |
| 26 | u | 1 | 0 | 0 | 0 | 0 |
| 27 | A | 4 | 0 | 0 | 0 | 0 |
| 27 | a | 4 | 0 | 0 | 0 | 0 |
| 28 | A | 55 | 0 | 80 | 8 | 0 |
| 28 | D | 55 | 0 | 80 | 0 | 0 |
| 28 | a | 55 | 0 | 80 | 0 | 0 |
| 28 | d | 55 | 0 | 80 | 0 | 0 |
| 29 | A | 51 | 0 | 72 | 3 | 0 |
| 29 | B | 51 | 0 | 72 | 3 | 0 |
| 29 | C | 102 | 0 | 144 | 1 | 0 |
| 29 | D | 51 | 0 | 72 | 2 | 0 |
| 29 | Z | 37 | 0 | 44 | 1 | 0 |
| 29 | a | 51 | 0 | 72 | 0 | 0 |
| 29 | b | 51 | 0 | 72 | 0 | 0 |
| 29 | c | 102 | 0 | 144 | 0 | 0 |
| 29 | d | 51 | 0 | 72 | 0 | 0 |
| 29 | z | 37 | 0 | 44 | 0 | 0 |
| 30 | B | 1 | 0 | 0 | 0 | 0 |
| 30 | F | 1 | 0 | 0 | 0 | 0 |
| 30 | O | 1 | 0 | 0 | 0 | 0 |
| 30 | b | 1 | 0 | 0 | 0 | 0 |
| 30 | f | 1 | 0 | 0 | 0 | 0 |
| 30 | o | 1 | 0 | 0 | 0 | 0 |
| 31 | C | 186 | 0 | 246 | 5 | 0 |
| 31 | D | 62 | 0 | 82 | 3 | 0 |
| 31 | H | 62 | 0 | 82 | 1 | 0 |
| 31 | c | 186 | 0 | 246 | 0 | 0 |
| 31 | d | 62 | 0 | 82 | 0 | 0 |
| 31 | h | 62 | 0 | 82 | 0 | 0 |
| 32 | D | 147 | 0 | 222 | 13 | 0 |
| 32 | E | 42 | 0 | 57 | 2 | 0 |
| 32 | L | 49 | 0 | 74 | 1 | 0 |
| 32 | d | 147 | 0 | 222 | 0 | 0 |
| 32 | e | 42 | 0 | 57 | 0 | 0 |
| 32 | l | 49 | 0 | 74 | 0 | 0 |
| 33 | F | 43 | 0 | 30 | 1 | 0 |
| 33 | V | 43 | 0 | 30 | 9 | 0 |
| 33 | f | 43 | 0 | 30 | 0 | 0 |
| 33 | v | 43 | 0 | 30 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 34 | J | 1 | 0 | 0 | 0 | 0 |
| 34 | j | 1 | 0 | 0 | 0 | 0 |
| All | All | 49594 | 0 | 50450 | 263 | 7 |

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 3.

The worst 5 of 263 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) |
|----------------|------------------|--------------------------|-------------------|
| 16:V:37:CYS:SG | 33:V:201:HEM:HAB | 1.52 | 1.48 |
| 16:V:37:CYS:SG | 33:V:201:HEM:CAB | 2.02 | 1.47 |
| 16:V:40:CYS:SG | 33:V:201:HEM:CAC | 2.04 | 1.46 |
| 16:V:40:CYS:SG | 33:V:201:HEM:HAC | 1.57 | 1.44 |
| 8:I:1:MET:CA | 8:I:1:MET:C | 1.84 | 1.44 |

The worst 5 of 7 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) |
|-----------------|------------------------|--------------------------|-------------------|
| 15:u:73:GLN:OE1 | 16:V:70:GLU:CD[3_544] | 0.80 | 1.40 |
| 15:u:73:GLN:OE1 | 16:V:70:GLU:OE1[3_544] | 1.22 | 0.98 |
| 15:u:73:GLN:OE1 | 16:V:70:GLU:OE2[3_544] | 1.45 | 0.75 |
| 15:u:73:GLN:CD | 16:V:70:GLU:OE1[3_544] | 1.79 | 0.41 |
| 15:u:73:GLN:CD | 16:V:70:GLU:CD[3_544] | 1.89 | 0.31 |

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 | 332/334 (99%) | 328 (99%) | 3 (1%) | 1 (0%) | 44 81 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | a | 332/334 (99%) | 328 (99%) | 3 (1%) | 1 (0%) | 44 | 81 |
| 2 | B | 502/504 (100%) | 497 (99%) | 5 (1%) | 0 | 100 | 100 |
| 2 | b | 502/504 (100%) | 496 (99%) | 6 (1%) | 0 | 100 | 100 |
| 3 | C | 449/461 (97%) | 440 (98%) | 8 (2%) | 1 (0%) | 51 | 84 |
| 3 | c | 449/461 (97%) | 440 (98%) | 8 (2%) | 1 (0%) | 51 | 84 |
| 4 | D | 340/342 (99%) | 332 (98%) | 8 (2%) | 0 | 100 | 100 |
| 4 | d | 340/342 (99%) | 332 (98%) | 8 (2%) | 0 | 100 | 100 |
| 5 | E | 79/81 (98%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 5 | e | 79/81 (98%) | 78 (99%) | 1 (1%) | 0 | 100 | 100 |
| 6 | F | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 6 | f | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 7 | H | 63/65 (97%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 7 | h | 63/65 (97%) | 58 (92%) | 5 (8%) | 0 | 100 | 100 |
| 8 | I | 36/38 (95%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |
| 8 | i | 36/38 (95%) | 34 (94%) | 2 (6%) | 0 | 100 | 100 |
| 9 | J | 36/40 (90%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 9 | j | 36/40 (90%) | 36 (100%) | 0 | 0 | 100 | 100 |
| 10 | K | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 10 | k | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | L | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 11 | l | 35/37 (95%) | 35 (100%) | 0 | 0 | 100 | 100 |
| 12 | M | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 12 | m | 32/34 (94%) | 32 (100%) | 0 | 0 | 100 | 100 |
| 13 | O | 241/243 (99%) | 233 (97%) | 7 (3%) | 1 (0%) | 38 | 77 |
| 13 | o | 241/243 (99%) | 233 (97%) | 7 (3%) | 1 (0%) | 38 | 77 |
| 14 | T | 28/30 (93%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 14 | t | 28/30 (93%) | 27 (96%) | 1 (4%) | 0 | 100 | 100 |
| 15 | U | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 15 | u | 95/97 (98%) | 93 (98%) | 2 (2%) | 0 | 100 | 100 |
| 16 | V | 135/137 (98%) | 132 (98%) | 3 (2%) | 0 | 100 | 100 |
| 16 | v | 135/137 (98%) | 132 (98%) | 3 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 17 | X | 37/39 (95%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 17 | x | 37/39 (95%) | 36 (97%) | 1 (3%) | 0 | 100 | 100 |
| 18 | Y | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 18 | y | 27/29 (93%) | 27 (100%) | 0 | 0 | 100 | 100 |
| 19 | Z | 60/62 (97%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| 19 | z | 60/62 (97%) | 58 (97%) | 2 (3%) | 0 | 100 | 100 |
| All | All | 5188/5288 (98%) | 5085 (98%) | 97 (2%) | 6 (0%) | 55 | 88 |

5 of 6 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | O | 58 | ASN |
| 13 | o | 58 | ASN |
| 3 | C | 416 | SER |
| 3 | c | 416 | SER |
| 1 | A | 259 | ILE |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 269/269 (100%) | 269 (100%) | 0 | 100 | 100 |
| 1 | a | 269/269 (100%) | 269 (100%) | 0 | 100 | 100 |
| 2 | B | 402/402 (100%) | 398 (99%) | 4 (1%) | 80 | 90 |
| 2 | b | 402/402 (100%) | 398 (99%) | 4 (1%) | 80 | 90 |
| 3 | C | 352/362 (97%) | 348 (99%) | 4 (1%) | 78 | 89 |
| 3 | c | 352/362 (97%) | 348 (99%) | 4 (1%) | 78 | 89 |
| 4 | D | 277/277 (100%) | 274 (99%) | 3 (1%) | 78 | 89 |
| 4 | d | 277/277 (100%) | 274 (99%) | 3 (1%) | 78 | 89 |
| 5 | E | 72/72 (100%) | 71 (99%) | 1 (1%) | 71 | 86 |
| 5 | e | 72/72 (100%) | 71 (99%) | 1 (1%) | 71 | 86 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 6 | F | 28/28 (100%) | 27 (96%) | 1 (4%) | 40 | 69 |
| 6 | f | 28/28 (100%) | 27 (96%) | 1 (4%) | 40 | 69 |
| 7 | H | 54/54 (100%) | 51 (94%) | 3 (6%) | 25 | 57 |
| 7 | h | 54/54 (100%) | 51 (94%) | 3 (6%) | 25 | 57 |
| 8 | I | 35/35 (100%) | 34 (97%) | 1 (3%) | 48 | 73 |
| 8 | i | 35/35 (100%) | 34 (97%) | 1 (3%) | 48 | 73 |
| 9 | J | 26/28 (93%) | 26 (100%) | 0 | 100 | 100 |
| 9 | j | 26/28 (93%) | 26 (100%) | 0 | 100 | 100 |
| 10 | K | 30/30 (100%) | 28 (93%) | 2 (7%) | 19 | 52 |
| 10 | k | 30/30 (100%) | 28 (93%) | 2 (7%) | 19 | 52 |
| 11 | L | 35/35 (100%) | 33 (94%) | 2 (6%) | 24 | 57 |
| 11 | l | 35/35 (100%) | 33 (94%) | 2 (6%) | 24 | 57 |
| 12 | M | 31/31 (100%) | 30 (97%) | 1 (3%) | 44 | 71 |
| 12 | m | 31/31 (100%) | 30 (97%) | 1 (3%) | 44 | 71 |
| 13 | O | 206/206 (100%) | 202 (98%) | 4 (2%) | 62 | 82 |
| 13 | o | 206/206 (100%) | 202 (98%) | 4 (2%) | 62 | 82 |
| 14 | T | 27/27 (100%) | 26 (96%) | 1 (4%) | 39 | 68 |
| 14 | t | 27/27 (100%) | 26 (96%) | 1 (4%) | 39 | 68 |
| 15 | U | 84/84 (100%) | 83 (99%) | 1 (1%) | 75 | 88 |
| 15 | u | 84/84 (100%) | 83 (99%) | 1 (1%) | 75 | 88 |
| 16 | V | 117/117 (100%) | 116 (99%) | 1 (1%) | 82 | 91 |
| 16 | v | 117/117 (100%) | 116 (99%) | 1 (1%) | 82 | 91 |
| 17 | X | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 17 | x | 32/32 (100%) | 32 (100%) | 0 | 100 | 100 |
| 18 | Y | 22/22 (100%) | 21 (96%) | 1 (4%) | 32 | 63 |
| 18 | y | 22/22 (100%) | 21 (96%) | 1 (4%) | 32 | 63 |
| 19 | Z | 52/52 (100%) | 50 (96%) | 2 (4%) | 38 | 67 |
| 19 | z | 52/52 (100%) | 50 (96%) | 2 (4%) | 38 | 67 |
| All | All | 4302/4326 (99%) | 4238 (98%) | 64 (2%) | 70 | 86 |

5 of 64 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7 | H | 65 | LEU |
| 10 | K | 17 | ILE |
| 18 | y | 27 | MET |
| 7 | h | 12 | ARG |
| 8 | I | 1 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | D | 83 | ASN |
| 6 | F | 44 | GLN |
| 16 | v | 34 | GLN |
| 4 | d | 83 | ASN |
| 6 | f | 44 | 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](#)

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 20 | OEX | A | 601 | 1,3 | 0,15,15 | 0.00 | - | 0,32,32 | 0.00 | - |
| 22 | CLA | A | 603 | - | 56,73,73 | 1.82 | 10 (17%) | 65,113,113 | 2.01 | 15 (23%) |
| 22 | CLA | A | 604 | - | 56,73,73 | 1.74 | 10 (17%) | 65,113,113 | 2.29 | 18 (27%) |
| 23 | PHO | A | 605 | - | 67,69,69 | 1.89 | 13 (19%) | 87,99,99 | 1.91 | 19 (21%) |
| 23 | PHO | A | 606 | - | 67,69,69 | 2.00 | 15 (22%) | 87,99,99 | 1.93 | 21 (24%) |
| 22 | CLA | A | 607 | - | 56,73,73 | 1.85 | 10 (17%) | 65,113,113 | 2.06 | 18 (27%) |
| 24 | BCR | A | 608 | - | 41,41,41 | 3.70 | 14 (34%) | 56,56,56 | 7.71 | 37 (66%) |
| 25 | SQD | A | 609 | - | 53,54,54 | 0.96 | 3 (5%) | 63,65,65 | 1.69 | 12 (19%) |
| 27 | BCT | A | 612 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 28 | PL9 | A | 613 | - | 55,55,55 | 0.69 | 2 (3%) | 69,69,69 | 1.52 | 13 (18%) |
| 29 | LMG | A | 614 | - | 51,51,55 | 0.93 | 2 (3%) | 59,59,63 | 0.98 | 3 (5%) |
| 25 | SQD | B | 601 | - | 53,54,54 | 1.02 | 3 (5%) | 63,65,65 | 1.37 | 8 (12%) |
| 22 | CLA | B | 602 | - | 56,73,73 | 1.92 | 11 (19%) | 65,113,113 | 1.94 | 14 (21%) |
| 22 | CLA | B | 603 | - | 56,73,73 | 1.90 | 11 (19%) | 65,113,113 | 1.85 | 15 (23%) |
| 22 | CLA | B | 604 | - | 56,73,73 | 1.85 | 11 (19%) | 65,113,113 | 2.18 | 17 (26%) |
| 22 | CLA | B | 605 | - | 56,73,73 | 1.73 | 12 (21%) | 65,113,113 | 2.27 | 15 (23%) |
| 22 | CLA | B | 606 | - | 56,73,73 | 1.79 | 10 (17%) | 65,113,113 | 2.04 | 14 (21%) |
| 22 | CLA | B | 607 | - | 56,73,73 | 1.86 | 11 (19%) | 65,113,113 | 2.04 | 16 (24%) |
| 22 | CLA | B | 608 | - | 56,73,73 | 1.80 | 11 (19%) | 65,113,113 | 2.01 | 16 (24%) |
| 22 | CLA | B | 609 | - | 56,73,73 | 1.77 | 10 (17%) | 65,113,113 | 2.25 | 17 (26%) |
| 22 | CLA | B | 610 | - | 56,73,73 | 1.80 | 9 (16%) | 65,113,113 | 2.08 | 15 (23%) |
| 22 | CLA | B | 611 | - | 56,73,73 | 1.83 | 11 (19%) | 65,113,113 | 1.94 | 15 (23%) |
| 22 | CLA | B | 612 | - | 56,73,73 | 1.68 | 9 (16%) | 65,113,113 | 2.17 | 15 (23%) |
| 22 | CLA | B | 613 | - | 56,73,73 | 1.81 | 11 (19%) | 65,113,113 | 2.05 | 17 (26%) |
| 22 | CLA | B | 614 | - | 56,73,73 | 1.81 | 11 (19%) | 65,113,113 | 1.98 | 18 (27%) |
| 22 | CLA | B | 615 | - | 56,73,73 | 1.78 | 12 (21%) | 65,113,113 | 2.08 | 19 (29%) |
| 22 | CLA | B | 616 | - | 56,73,73 | 1.84 | 11 (19%) | 65,113,113 | 1.94 | 14 (21%) |
| 22 | CLA | B | 617 | - | 56,73,73 | 1.86 | 10 (17%) | 65,113,113 | 2.06 | 19 (29%) |
| 24 | BCR | B | 618 | - | 41,41,41 | 3.65 | 14 (34%) | 56,56,56 | 7.46 | 38 (67%) |
| 24 | BCR | B | 619 | - | 41,41,41 | 3.64 | 14 (34%) | 56,56,56 | 7.69 | 41 (73%) |
| 29 | LMG | B | 620 | - | 51,51,55 | 0.92 | 2 (3%) | 59,59,63 | 1.03 | 3 (5%) |
| 24 | BCR | B | 622 | - | 41,41,41 | 3.79 | 14 (34%) | 56,56,56 | 6.99 | 38 (67%) |
| 22 | CLA | C | 501 | - | 56,73,73 | 1.86 | 11 (19%) | 65,113,113 | 2.05 | 16 (24%) |
| 22 | CLA | C | 502 | - | 56,73,73 | 1.81 | 10 (17%) | 65,113,113 | 1.97 | 15 (23%) |
| 22 | CLA | C | 503 | - | 56,73,73 | 1.88 | 11 (19%) | 65,113,113 | 1.87 | 12 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | C | 504 | - | 56,73,73 | 1.86 | 10 (17%) | 65,113,113 | 2.01 | 14 (21%) |
| 22 | CLA | C | 505 | - | 56,73,73 | 1.86 | 12 (21%) | 65,113,113 | 1.96 | 16 (24%) |
| 22 | CLA | C | 506 | - | 56,73,73 | 1.89 | 11 (19%) | 65,113,113 | 2.05 | 15 (23%) |
| 22 | CLA | C | 507 | - | 56,73,73 | 1.95 | 11 (19%) | 65,113,113 | 1.98 | 16 (24%) |
| 22 | CLA | C | 508 | - | 56,73,73 | 1.92 | 12 (21%) | 65,113,113 | 1.94 | 15 (23%) |
| 22 | CLA | C | 509 | - | 56,73,73 | 1.86 | 12 (21%) | 65,113,113 | 2.08 | 17 (26%) |
| 22 | CLA | C | 510 | - | 56,73,73 | 1.84 | 11 (19%) | 65,113,113 | 2.03 | 15 (23%) |
| 22 | CLA | C | 511 | 3 | 56,73,73 | 1.89 | 11 (19%) | 65,113,113 | 1.99 | 14 (21%) |
| 22 | CLA | C | 512 | - | 56,73,73 | 1.91 | 12 (21%) | 65,113,113 | 1.93 | 18 (27%) |
| 22 | CLA | C | 513 | - | 56,73,73 | 1.97 | 11 (19%) | 65,113,113 | 1.82 | 14 (21%) |
| 24 | BCR | C | 514 | - | 41,41,41 | 3.85 | 14 (34%) | 56,56,56 | 8.33 | 35 (62%) |
| 24 | BCR | C | 515 | - | 41,41,41 | 3.81 | 14 (34%) | 56,56,56 | 8.14 | 39 (69%) |
| 31 | DGD | C | 516 | - | 63,63,67 | 0.86 | 2 (3%) | 77,77,81 | 1.01 | 3 (3%) |
| 31 | DGD | C | 517 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 0.88 | 4 (5%) |
| 31 | DGD | C | 518 | - | 63,63,67 | 0.78 | 3 (4%) | 77,77,81 | 0.92 | 3 (3%) |
| 29 | LMG | C | 519 | - | 51,51,55 | 0.92 | 2 (3%) | 59,59,63 | 1.05 | 4 (6%) |
| 29 | LMG | C | 520 | - | 51,51,55 | 0.99 | 3 (5%) | 59,59,63 | 1.01 | 2 (3%) |
| 22 | CLA | D | 401 | - | 56,73,73 | 1.83 | 12 (21%) | 65,113,113 | 2.14 | 18 (27%) |
| 22 | CLA | D | 402 | - | 56,73,73 | 1.77 | 11 (19%) | 65,113,113 | 2.34 | 15 (23%) |
| 22 | CLA | D | 403 | - | 56,73,73 | 1.88 | 12 (21%) | 65,113,113 | 1.90 | 16 (24%) |
| 24 | BCR | D | 404 | - | 41,41,41 | 3.80 | 14 (34%) | 56,56,56 | 7.70 | 40 (71%) |
| 32 | LHG | D | 405 | - | 48,48,48 | 0.85 | 2 (4%) | 49,54,54 | 1.04 | 4 (8%) |
| 29 | LMG | D | 406 | 34 | 51,51,55 | 0.86 | 2 (3%) | 59,59,63 | 0.81 | 3 (5%) |
| 32 | LHG | D | 407 | - | 48,48,48 | 0.88 | 2 (4%) | 49,54,54 | 0.87 | 2 (4%) |
| 28 | PL9 | D | 408 | - | 55,55,55 | 0.78 | 1 (1%) | 69,69,69 | 1.31 | 8 (11%) |
| 32 | LHG | D | 409 | - | 48,48,48 | 0.93 | 2 (4%) | 49,54,54 | 0.92 | 3 (6%) |
| 31 | DGD | D | 410 | - | 63,63,67 | 0.98 | 4 (6%) | 77,77,81 | 1.06 | 6 (7%) |
| 25 | SQD | D | 411 | - | 42,43,54 | 1.19 | 3 (7%) | 52,54,65 | 1.63 | 8 (15%) |
| 32 | LHG | E | 101 | - | 41,41,48 | 1.04 | 2 (4%) | 42,47,54 | 1.13 | 3 (7%) |
| 33 | HEM | F | 101 | 5,6 | 28,50,50 | 2.15 | 6 (21%) | 17,82,82 | 2.01 | 4 (23%) |
| 24 | BCR | H | 101 | - | 41,41,41 | 3.78 | 14 (34%) | 56,56,56 | 8.18 | 41 (73%) |
| 31 | DGD | H | 102 | - | 63,63,67 | 0.91 | 3 (4%) | 77,77,81 | 0.96 | 5 (6%) |
| 24 | BCR | K | 101 | - | 41,41,41 | 3.82 | 14 (34%) | 56,56,56 | 7.97 | 36 (64%) |
| 24 | BCR | K | 102 | - | 41,41,41 | 3.75 | 14 (34%) | 56,56,56 | 7.71 | 41 (73%) |
| 25 | SQD | L | 101 | - | 53,54,54 | 1.02 | 4 (7%) | 63,65,65 | 1.50 | 8 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 32 | LHG | L | 102 | - | 48,48,48 | 0.88 | 2 (4%) | 49,54,54 | 1.01 | 3 (6%) |
| 24 | BCR | T | 101 | - | 41,41,41 | 3.65 | 14 (34%) | 56,56,56 | 7.46 | 38 (67%) |
| 24 | BCR | T | 102 | - | 41,41,41 | 3.71 | 14 (34%) | 56,56,56 | 8.36 | 41 (73%) |
| 33 | HEM | V | 201 | 16 | 28,50,50 | 2.17 | 6 (21%) | 17,82,82 | 1.86 | 4 (23%) |
| 29 | LMG | Z | 101 | - | 37,37,55 | 1.00 | 3 (8%) | 45,45,63 | 1.31 | 4 (8%) |
| 20 | OEX | a | 601 | 1,3 | 0,15,15 | 0.00 | - | 0,32,32 | 0.00 | - |
| 22 | CLA | a | 603 | - | 56,73,73 | 1.82 | 10 (17%) | 65,113,113 | 2.01 | 15 (23%) |
| 22 | CLA | a | 604 | - | 56,73,73 | 1.74 | 10 (17%) | 65,113,113 | 2.29 | 18 (27%) |
| 23 | PHO | a | 605 | - | 67,69,69 | 1.90 | 13 (19%) | 87,99,99 | 1.92 | 19 (21%) |
| 23 | PHO | a | 606 | - | 67,69,69 | 2.00 | 15 (22%) | 87,99,99 | 1.93 | 21 (24%) |
| 22 | CLA | a | 607 | - | 56,73,73 | 1.85 | 10 (17%) | 65,113,113 | 2.06 | 18 (27%) |
| 24 | BCR | a | 608 | - | 41,41,41 | 3.70 | 14 (34%) | 56,56,56 | 7.70 | 37 (66%) |
| 25 | SQD | a | 609 | - | 53,54,54 | 0.96 | 3 (5%) | 63,65,65 | 1.70 | 12 (19%) |
| 27 | BCT | a | 612 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 28 | PL9 | a | 613 | - | 55,55,55 | 0.69 | 2 (3%) | 69,69,69 | 1.53 | 13 (18%) |
| 29 | LMG | a | 614 | - | 51,51,55 | 0.93 | 2 (3%) | 59,59,63 | 0.98 | 3 (5%) |
| 25 | SQD | b | 601 | - | 53,54,54 | 1.02 | 3 (5%) | 63,65,65 | 1.37 | 8 (12%) |
| 22 | CLA | b | 602 | - | 56,73,73 | 1.92 | 11 (19%) | 65,113,113 | 1.95 | 14 (21%) |
| 22 | CLA | b | 603 | - | 56,73,73 | 1.90 | 11 (19%) | 65,113,113 | 1.85 | 16 (24%) |
| 22 | CLA | b | 604 | - | 56,73,73 | 1.85 | 11 (19%) | 65,113,113 | 2.20 | 17 (26%) |
| 22 | CLA | b | 605 | - | 56,73,73 | 1.74 | 12 (21%) | 65,113,113 | 2.25 | 15 (23%) |
| 22 | CLA | b | 606 | - | 56,73,73 | 1.79 | 10 (17%) | 65,113,113 | 2.03 | 14 (21%) |
| 22 | CLA | b | 607 | - | 56,73,73 | 1.86 | 11 (19%) | 65,113,113 | 2.04 | 16 (24%) |
| 22 | CLA | b | 608 | - | 56,73,73 | 1.80 | 10 (17%) | 65,113,113 | 2.00 | 16 (24%) |
| 22 | CLA | b | 609 | - | 56,73,73 | 1.78 | 10 (17%) | 65,113,113 | 2.25 | 19 (29%) |
| 22 | CLA | b | 610 | - | 56,73,73 | 1.80 | 9 (16%) | 65,113,113 | 2.06 | 15 (23%) |
| 22 | CLA | b | 611 | - | 56,73,73 | 1.83 | 10 (17%) | 65,113,113 | 1.94 | 15 (23%) |
| 22 | CLA | b | 612 | - | 56,73,73 | 1.68 | 9 (16%) | 65,113,113 | 2.17 | 15 (23%) |
| 22 | CLA | b | 613 | - | 56,73,73 | 1.81 | 11 (19%) | 65,113,113 | 2.06 | 17 (26%) |
| 22 | CLA | b | 614 | - | 56,73,73 | 1.81 | 11 (19%) | 65,113,113 | 1.99 | 18 (27%) |
| 22 | CLA | b | 615 | - | 56,73,73 | 1.77 | 12 (21%) | 65,113,113 | 2.09 | 19 (29%) |
| 22 | CLA | b | 616 | - | 56,73,73 | 1.84 | 11 (19%) | 65,113,113 | 1.93 | 14 (21%) |
| 22 | CLA | b | 617 | - | 56,73,73 | 1.87 | 10 (17%) | 65,113,113 | 2.07 | 19 (29%) |
| 24 | BCR | b | 618 | - | 41,41,41 | 3.64 | 14 (34%) | 56,56,56 | 7.69 | 41 (73%) |
| 29 | LMG | b | 619 | - | 51,51,55 | 0.93 | 2 (3%) | 59,59,63 | 1.03 | 3 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 25 | SQD | b | 621 | - | 53,54,54 | 1.06 | 4 (7%) | 63,65,65 | 1.58 | 10 (15%) |
| 24 | BCR | b | 622 | - | 41,41,41 | 3.79 | 14 (34%) | 56,56,56 | 6.99 | 38 (67%) |
| 22 | CLA | c | 501 | - | 56,73,73 | 1.86 | 11 (19%) | 65,113,113 | 2.05 | 16 (24%) |
| 22 | CLA | c | 502 | - | 56,73,73 | 1.81 | 10 (17%) | 65,113,113 | 1.97 | 15 (23%) |
| 22 | CLA | c | 503 | - | 56,73,73 | 1.88 | 11 (19%) | 65,113,113 | 1.86 | 12 (18%) |
| 22 | CLA | c | 504 | - | 56,73,73 | 1.85 | 10 (17%) | 65,113,113 | 2.01 | 14 (21%) |
| 22 | CLA | c | 505 | - | 56,73,73 | 1.87 | 12 (21%) | 65,113,113 | 1.96 | 17 (26%) |
| 22 | CLA | c | 506 | - | 56,73,73 | 1.89 | 11 (19%) | 65,113,113 | 2.04 | 15 (23%) |
| 22 | CLA | c | 507 | - | 56,73,73 | 1.95 | 11 (19%) | 65,113,113 | 1.97 | 16 (24%) |
| 22 | CLA | c | 508 | - | 56,73,73 | 1.93 | 12 (21%) | 65,113,113 | 1.94 | 15 (23%) |
| 22 | CLA | c | 509 | - | 56,73,73 | 1.87 | 12 (21%) | 65,113,113 | 2.09 | 17 (26%) |
| 22 | CLA | c | 510 | - | 56,73,73 | 1.84 | 11 (19%) | 65,113,113 | 2.03 | 15 (23%) |
| 22 | CLA | c | 511 | 3 | 56,73,73 | 1.88 | 11 (19%) | 65,113,113 | 1.99 | 14 (21%) |
| 22 | CLA | c | 512 | - | 56,73,73 | 1.91 | 12 (21%) | 65,113,113 | 1.93 | 18 (27%) |
| 22 | CLA | c | 513 | - | 56,73,73 | 1.98 | 11 (19%) | 65,113,113 | 1.81 | 14 (21%) |
| 24 | BCR | c | 514 | - | 41,41,41 | 3.85 | 14 (34%) | 56,56,56 | 8.33 | 36 (64%) |
| 24 | BCR | c | 515 | - | 41,41,41 | 3.81 | 14 (34%) | 56,56,56 | 8.13 | 38 (67%) |
| 31 | DGD | c | 516 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 1.01 | 3 (3%) |
| 31 | DGD | c | 517 | - | 63,63,67 | 0.87 | 2 (3%) | 77,77,81 | 0.88 | 4 (5%) |
| 31 | DGD | c | 518 | - | 63,63,67 | 0.78 | 2 (3%) | 77,77,81 | 0.92 | 3 (3%) |
| 29 | LMG | c | 519 | - | 51,51,55 | 0.93 | 2 (3%) | 59,59,63 | 1.05 | 5 (8%) |
| 29 | LMG | c | 520 | - | 51,51,55 | 0.99 | 3 (5%) | 59,59,63 | 1.00 | 2 (3%) |
| 22 | CLA | d | 401 | - | 56,73,73 | 1.82 | 13 (23%) | 65,113,113 | 2.15 | 17 (26%) |
| 22 | CLA | d | 402 | - | 56,73,73 | 1.77 | 11 (19%) | 65,113,113 | 2.33 | 15 (23%) |
| 22 | CLA | d | 403 | - | 56,73,73 | 1.88 | 12 (21%) | 65,113,113 | 1.91 | 15 (23%) |
| 24 | BCR | d | 404 | - | 41,41,41 | 3.80 | 14 (34%) | 56,56,56 | 7.70 | 40 (71%) |
| 32 | LHG | d | 405 | - | 48,48,48 | 0.85 | 2 (4%) | 49,54,54 | 1.03 | 4 (8%) |
| 29 | LMG | d | 406 | 34 | 51,51,55 | 0.86 | 2 (3%) | 59,59,63 | 0.81 | 3 (5%) |
| 32 | LHG | d | 407 | - | 48,48,48 | 0.88 | 2 (4%) | 49,54,54 | 0.87 | 2 (4%) |
| 28 | PL9 | d | 408 | - | 55,55,55 | 0.77 | 1 (1%) | 69,69,69 | 1.31 | 8 (11%) |
| 32 | LHG | d | 409 | - | 48,48,48 | 0.92 | 2 (4%) | 49,54,54 | 0.92 | 3 (6%) |
| 31 | DGD | d | 410 | - | 63,63,67 | 0.98 | 4 (6%) | 77,77,81 | 1.05 | 6 (7%) |
| 25 | SQD | d | 411 | - | 42,43,54 | 1.18 | 3 (7%) | 52,54,65 | 1.63 | 8 (15%) |
| 32 | LHG | e | 101 | - | 41,41,48 | 1.04 | 2 (4%) | 42,47,54 | 1.12 | 3 (7%) |
| 33 | HEM | f | 101 | 5,6 | 28,50,50 | 2.16 | 6 (21%) | 17,82,82 | 2.00 | 4 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 24 | BCR | h | 101 | - | 41,41,41 | 3.78 | 14 (34%) | 56,56,56 | 8.18 | 40 (71%) |
| 31 | DGD | h | 102 | - | 63,63,67 | 0.91 | 3 (4%) | 77,77,81 | 0.96 | 5 (6%) |
| 24 | BCR | k | 101 | - | 41,41,41 | 3.82 | 14 (34%) | 56,56,56 | 7.97 | 36 (64%) |
| 24 | BCR | k | 102 | - | 41,41,41 | 3.75 | 14 (34%) | 56,56,56 | 7.70 | 41 (73%) |
| 25 | SQD | l | 101 | - | 53,54,54 | 1.02 | 4 (7%) | 63,65,65 | 1.49 | 7 (11%) |
| 25 | SQD | l | 102 | - | 53,54,54 | 1.06 | 4 (7%) | 63,65,65 | 1.57 | 10 (15%) |
| 32 | LHG | l | 103 | - | 48,48,48 | 0.88 | 2 (4%) | 49,54,54 | 1.01 | 3 (6%) |
| 24 | BCR | t | 101 | - | 41,41,41 | 3.71 | 14 (34%) | 56,56,56 | 8.36 | 42 (75%) |
| 33 | HEM | v | 201 | 16 | 28,50,50 | 2.17 | 7 (25%) | 17,82,82 | 1.87 | 4 (23%) |
| 29 | LMG | z | 101 | - | 37,37,55 | 1.00 | 3 (8%) | 45,45,63 | 1.31 | 4 (8%) |

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 |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 20 | OEX | A | 601 | 1,3 | - | 0/0/68/68 | 0/0/6/6 |
| 22 | CLA | A | 603 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | A | 604 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 23 | PHO | A | 605 | - | - | 0/53/103/103 | 0/1/6/6 |
| 23 | PHO | A | 606 | - | - | 0/53/103/103 | 0/1/6/6 |
| 22 | CLA | A | 607 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | A | 608 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | SQD | A | 609 | - | - | 0/49/69/69 | 0/1/1/1 |
| 27 | BCT | A | 612 | 21 | - | 0/0/0/0 | 0/0/0/0 |
| 28 | PL9 | A | 613 | - | - | 0/53/73/73 | 0/1/1/1 |
| 29 | LMG | A | 614 | - | - | 0/46/66/70 | 0/1/1/1 |
| 25 | SQD | B | 601 | - | - | 0/49/69/69 | 0/1/1/1 |
| 22 | CLA | B | 602 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 603 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 604 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 605 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 606 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 607 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 608 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 609 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 610 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 22 | CLA | B | 611 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 612 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 613 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 614 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 615 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 616 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | B | 617 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | B | 618 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | B | 619 | - | - | 0/29/63/63 | 0/2/2/2 |
| 29 | LMG | B | 620 | - | - | 0/46/66/70 | 0/1/1/1 |
| 24 | BCR | B | 622 | - | - | 0/29/63/63 | 0/2/2/2 |
| 22 | CLA | C | 501 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 502 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 503 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 504 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 505 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 506 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 507 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 508 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 509 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 510 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 511 | 3 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 512 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | C | 513 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | C | 514 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | C | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | DGD | C | 516 | - | - | 0/51/91/95 | 0/2/2/2 |
| 31 | DGD | C | 517 | - | - | 0/51/91/95 | 0/2/2/2 |
| 31 | DGD | C | 518 | - | - | 0/51/91/95 | 0/2/2/2 |
| 29 | LMG | C | 519 | - | - | 0/46/66/70 | 0/1/1/1 |
| 29 | LMG | C | 520 | - | - | 0/46/66/70 | 0/1/1/1 |
| 22 | CLA | D | 401 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | D | 402 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | D | 403 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | D | 404 | - | - | 0/29/63/63 | 0/2/2/2 |
| 32 | LHG | D | 405 | - | - | 0/53/53/53 | 0/0/0/0 |
| 29 | LMG | D | 406 | 34 | - | 0/46/66/70 | 0/1/1/1 |
| 32 | LHG | D | 407 | - | - | 0/53/53/53 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 28 | PL9 | D | 408 | - | - | 0/53/73/73 | 0/1/1/1 |
| 32 | LHG | D | 409 | - | - | 0/53/53/53 | 0/0/0/0 |
| 31 | DGD | D | 410 | - | - | 0/51/91/95 | 0/2/2/2 |
| 25 | SQD | D | 411 | - | - | 0/38/58/69 | 0/1/1/1 |
| 32 | LHG | E | 101 | - | - | 0/46/46/53 | 0/0/0/0 |
| 33 | HEM | F | 101 | 5,6 | - | 0/6/54/54 | 0/0/8/8 |
| 24 | BCR | H | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | DGD | H | 102 | - | - | 0/51/91/95 | 0/2/2/2 |
| 24 | BCR | K | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | K | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | SQD | L | 101 | - | - | 0/49/69/69 | 0/1/1/1 |
| 32 | LHG | L | 102 | - | - | 0/53/53/53 | 0/0/0/0 |
| 24 | BCR | T | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | T | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 33 | HEM | V | 201 | 16 | - | 0/6/54/54 | 0/0/8/8 |
| 29 | LMG | Z | 101 | - | - | 1/31/51/70 | 0/1/1/1 |
| 20 | OEX | a | 601 | 1,3 | - | 0/0/68/68 | 0/0/6/6 |
| 22 | CLA | a | 603 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | a | 604 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 23 | PHO | a | 605 | - | - | 0/53/103/103 | 0/1/6/6 |
| 23 | PHO | a | 606 | - | - | 0/53/103/103 | 0/1/6/6 |
| 22 | CLA | a | 607 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | a | 608 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | SQD | a | 609 | - | - | 0/49/69/69 | 0/1/1/1 |
| 27 | BCT | a | 612 | 21 | - | 0/0/0/0 | 0/0/0/0 |
| 28 | PL9 | a | 613 | - | - | 0/53/73/73 | 0/1/1/1 |
| 29 | LMG | a | 614 | - | - | 0/46/66/70 | 0/1/1/1 |
| 25 | SQD | b | 601 | - | - | 0/49/69/69 | 0/1/1/1 |
| 22 | CLA | b | 602 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 603 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 604 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 605 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 606 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 607 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 608 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 609 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 610 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 611 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 612 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 22 | CLA | b | 613 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 614 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 615 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 616 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | b | 617 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | b | 618 | - | - | 0/29/63/63 | 0/2/2/2 |
| 29 | LMG | b | 619 | - | - | 0/46/66/70 | 0/1/1/1 |
| 25 | SQD | b | 621 | - | - | 0/49/69/69 | 0/1/1/1 |
| 24 | BCR | b | 622 | - | - | 0/29/63/63 | 0/2/2/2 |
| 22 | CLA | c | 501 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 502 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 503 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 504 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 505 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 506 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 507 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 508 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 509 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 510 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 511 | 3 | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 512 | - | 3/3/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | c | 513 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | c | 514 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | c | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | DGD | c | 516 | - | - | 0/51/91/95 | 0/2/2/2 |
| 31 | DGD | c | 517 | - | - | 0/51/91/95 | 0/2/2/2 |
| 31 | DGD | c | 518 | - | - | 0/51/91/95 | 0/2/2/2 |
| 29 | LMG | c | 519 | - | - | 0/46/66/70 | 0/1/1/1 |
| 29 | LMG | c | 520 | - | - | 0/46/66/70 | 0/1/1/1 |
| 22 | CLA | d | 401 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | d | 402 | - | 1/1/20/25 | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | d | 403 | - | 2/2/20/25 | 0/37/135/135 | 0/0/9/9 |
| 24 | BCR | d | 404 | - | - | 0/29/63/63 | 0/2/2/2 |
| 32 | LHG | d | 405 | - | - | 0/53/53/53 | 0/0/0/0 |
| 29 | LMG | d | 406 | 34 | - | 0/46/66/70 | 0/1/1/1 |
| 32 | LHG | d | 407 | - | - | 0/53/53/53 | 0/0/0/0 |
| 28 | PL9 | d | 408 | - | - | 0/53/73/73 | 0/1/1/1 |
| 32 | LHG | d | 409 | - | - | 0/53/53/53 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 31 | DGD | d | 410 | - | - | 0/51/91/95 | 0/2/2/2 |
| 25 | SQD | d | 411 | - | - | 0/38/58/69 | 0/1/1/1 |
| 32 | LHG | e | 101 | - | - | 0/46/46/53 | 0/0/0/0 |
| 33 | HEM | f | 101 | 5,6 | - | 0/6/54/54 | 0/0/8/8 |
| 24 | BCR | h | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 31 | DGD | h | 102 | - | - | 0/51/91/95 | 0/2/2/2 |
| 24 | BCR | k | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 24 | BCR | k | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 25 | SQD | l | 101 | - | - | 0/49/69/69 | 0/1/1/1 |
| 25 | SQD | l | 102 | - | - | 0/49/69/69 | 0/1/1/1 |
| 32 | LHG | l | 103 | - | - | 0/53/53/53 | 0/0/0/0 |
| 24 | BCR | t | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 33 | HEM | v | 201 | 16 | - | 0/6/54/54 | 0/0/8/8 |
| 29 | LMG | z | 101 | - | - | 1/31/51/70 | 0/1/1/1 |

The worst 5 of 1265 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24 | C | 514 | BCR | C8-C9 | -8.70 | 1.27 | 1.45 |
| 24 | c | 514 | BCR | C8-C9 | -8.66 | 1.27 | 1.45 |
| 24 | d | 404 | BCR | C8-C9 | -8.63 | 1.27 | 1.45 |
| 24 | C | 514 | BCR | C12-C13 | -8.62 | 1.27 | 1.45 |
| 24 | K | 102 | BCR | C8-C9 | -8.61 | 1.27 | 1.45 |

The worst 5 of 2302 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 24 | T | 102 | BCR | C36-C18-C17 | -10.60 | 108.08 | 122.92 |
| 24 | t | 101 | BCR | C36-C18-C17 | -10.59 | 108.09 | 122.92 |
| 24 | a | 608 | BCR | C37-C22-C21 | -9.76 | 109.26 | 122.92 |
| 24 | A | 608 | BCR | C37-C22-C21 | -9.72 | 109.31 | 122.92 |
| 24 | D | 404 | BCR | C30-C25-C26 | -9.10 | 109.80 | 122.59 |

5 of 166 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 22 | B | 617 | CLA | NC |
| 22 | B | 617 | CLA | ND |
| 22 | B | 617 | CLA | NA |
| 22 | c | 513 | CLA | NC |
| 22 | c | 513 | CLA | NA |

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 29 | z | 101 | LMG | C7-O1-C1-O6 |
| 29 | Z | 101 | LMG | C7-O1-C1-O6 |

There are no ring outliers.

62 monomers are involved in 148 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | A | 603 | CLA | 5 | 0 |
| 22 | A | 604 | CLA | 3 | 0 |
| 23 | A | 605 | PHO | 2 | 0 |
| 23 | A | 606 | PHO | 4 | 0 |
| 22 | A | 607 | CLA | 2 | 0 |
| 24 | A | 608 | BCR | 1 | 0 |
| 25 | A | 609 | SQD | 2 | 0 |
| 28 | A | 613 | PL9 | 8 | 0 |
| 29 | A | 614 | LMG | 3 | 0 |
| 25 | B | 601 | SQD | 4 | 0 |
| 22 | B | 603 | CLA | 1 | 0 |
| 22 | B | 604 | CLA | 2 | 0 |
| 22 | B | 605 | CLA | 2 | 0 |
| 22 | B | 606 | CLA | 5 | 0 |
| 22 | B | 607 | CLA | 2 | 0 |
| 22 | B | 609 | CLA | 2 | 0 |
| 22 | B | 611 | CLA | 4 | 0 |
| 22 | B | 612 | CLA | 2 | 0 |
| 22 | B | 613 | CLA | 3 | 0 |
| 22 | B | 614 | CLA | 5 | 0 |
| 22 | B | 615 | CLA | 3 | 0 |
| 22 | B | 616 | CLA | 2 | 0 |
| 22 | B | 617 | CLA | 4 | 0 |
| 24 | B | 618 | BCR | 3 | 0 |
| 24 | B | 619 | BCR | 1 | 0 |
| 29 | B | 620 | LMG | 3 | 0 |
| 24 | B | 622 | BCR | 4 | 0 |
| 22 | C | 501 | CLA | 2 | 0 |
| 22 | C | 502 | CLA | 3 | 0 |
| 22 | C | 503 | CLA | 3 | 0 |
| 22 | C | 504 | CLA | 1 | 0 |
| 22 | C | 505 | CLA | 2 | 0 |
| 22 | C | 506 | CLA | 4 | 0 |
| 22 | C | 507 | CLA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22 | C | 508 | CLA | 3 | 0 |
| 22 | C | 509 | CLA | 2 | 0 |
| 22 | C | 510 | CLA | 6 | 0 |
| 22 | C | 511 | CLA | 2 | 0 |
| 22 | C | 512 | CLA | 3 | 0 |
| 22 | C | 513 | CLA | 1 | 0 |
| 31 | C | 516 | DGD | 2 | 0 |
| 31 | C | 517 | DGD | 2 | 0 |
| 31 | C | 518 | DGD | 1 | 0 |
| 29 | C | 519 | LMG | 1 | 0 |
| 22 | D | 401 | CLA | 1 | 0 |
| 22 | D | 402 | CLA | 4 | 0 |
| 22 | D | 403 | CLA | 3 | 0 |
| 24 | D | 404 | BCR | 3 | 0 |
| 29 | D | 406 | LMG | 2 | 0 |
| 32 | D | 409 | LHG | 13 | 0 |
| 31 | D | 410 | DGD | 3 | 0 |
| 32 | E | 101 | LHG | 2 | 0 |
| 33 | F | 101 | HEM | 1 | 0 |
| 24 | H | 101 | BCR | 1 | 0 |
| 31 | H | 102 | DGD | 1 | 0 |
| 24 | K | 102 | BCR | 1 | 0 |
| 25 | L | 101 | SQD | 5 | 0 |
| 32 | L | 102 | LHG | 1 | 0 |
| 24 | T | 101 | BCR | 7 | 0 |
| 24 | T | 102 | BCR | 2 | 0 |
| 33 | V | 201 | HEM | 9 | 0 |
| 29 | Z | 101 | LMG | 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 | 334/334 (100%) | 0.59 | 21 (6%) 21 22 | 16, 22, 43, 53 | 0 |
| 1 | a | 334/334 (100%) | 0.60 | 26 (7%) 14 17 | 16, 22, 43, 53 | 0 |
| 2 | B | 504/504 (100%) | 0.47 | 32 (6%) 21 22 | 18, 27, 49, 70 | 0 |
| 2 | b | 504/504 (100%) | 0.76 | 70 (13%) 3 8 | 18, 27, 49, 70 | 0 |
| 3 | C | 451/461 (97%) | 0.64 | 43 (9%) 9 13 | 21, 31, 44, 56 | 0 |
| 3 | c | 451/461 (97%) | 0.52 | 39 (8%) 11 15 | 21, 31, 44, 56 | 0 |
| 4 | D | 342/342 (100%) | 0.78 | 33 (9%) 9 13 | 17, 23, 39, 61 | 0 |
| 4 | d | 342/342 (100%) | 0.70 | 24 (7%) 17 20 | 17, 23, 39, 61 | 0 |
| 5 | E | 81/81 (100%) | 0.82 | 10 (12%) 5 10 | 27, 40, 57, 63 | 0 |
| 5 | e | 81/81 (100%) | 0.42 | 9 (11%) 6 10 | 27, 40, 57, 63 | 0 |
| 6 | F | 34/34 (100%) | 0.36 | 1 (2%) 52 48 | 28, 33, 58, 61 | 0 |
| 6 | f | 34/34 (100%) | -0.00 | 0 100 100 | 28, 33, 58, 61 | 0 |
| 7 | H | 65/65 (100%) | 0.65 | 9 (13%) 3 8 | 23, 34, 40, 58 | 0 |
| 7 | h | 65/65 (100%) | 1.42 | 18 (27%) 1 5 | 23, 34, 40, 58 | 0 |
| 8 | I | 38/38 (100%) | 0.54 | 5 (13%) 4 8 | 30, 34, 65, 68 | 0 |
| 8 | i | 38/38 (100%) | 0.08 | 3 (7%) 13 17 | 30, 34, 65, 68 | 0 |
| 9 | J | 38/40 (95%) | 0.56 | 3 (7%) 13 17 | 26, 37, 68, 72 | 0 |
| 9 | j | 38/40 (95%) | -0.14 | 0 100 100 | 26, 37, 68, 72 | 0 |
| 10 | K | 37/37 (100%) | 0.52 | 2 (5%) 26 28 | 33, 38, 45, 47 | 0 |
| 10 | k | 37/37 (100%) | 0.60 | 4 (10%) 6 11 | 33, 38, 45, 47 | 0 |
| 11 | L | 37/37 (100%) | 0.60 | 2 (5%) 26 28 | 17, 22, 50, 59 | 0 |
| 11 | l | 37/37 (100%) | 0.59 | 3 (8%) 13 17 | 17, 22, 50, 59 | 0 |
| 12 | M | 34/34 (100%) | 1.02 | 6 (17%) 2 6 | 21, 23, 36, 52 | 0 |
| 12 | m | 34/34 (100%) | 0.74 | 3 (8%) 11 15 | 21, 23, 36, 52 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | O | 243/243 (100%) | 0.38 | 8 (3%) 47 43 | 18, 32, 55, 71 | 0 |
| 13 | o | 243/243 (100%) | 0.56 | 14 (5%) 24 25 | 18, 32, 55, 71 | 0 |
| 14 | T | 30/30 (100%) | 0.87 | 3 (10%) 8 12 | 19, 23, 44, 52 | 0 |
| 14 | t | 30/30 (100%) | 0.85 | 1 (3%) 47 43 | 19, 23, 44, 52 | 0 |
| 15 | U | 97/97 (100%) | 0.30 | 2 (2%) 64 59 | 23, 30, 48, 50 | 0 |
| 15 | u | 97/97 (100%) | 0.55 | 6 (6%) 21 23 | 23, 30, 48, 50 | 0 |
| 16 | V | 137/137 (100%) | 0.22 | 2 (1%) 74 68 | 23, 28, 39, 48 | 0 |
| 16 | v | 137/137 (100%) | 0.38 | 6 (4%) 35 33 | 23, 28, 39, 48 | 0 |
| 17 | X | 39/39 (100%) | 0.99 | 7 (17%) 2 6 | 33, 40, 66, 68 | 0 |
| 17 | x | 39/39 (100%) | 1.00 | 7 (17%) 2 6 | 33, 40, 66, 68 | 0 |
| 18 | Y | 29/29 (100%) | 0.69 | 3 (10%) 7 11 | 42, 48, 75, 77 | 0 |
| 18 | y | 29/29 (100%) | 0.29 | 0 100 100 | 42, 48, 75, 77 | 0 |
| 19 | Z | 62/62 (100%) | 0.48 | 2 (3%) 48 44 | 39, 48, 68, 72 | 0 |
| 19 | z | 62/62 (100%) | 0.69 | 7 (11%) 6 10 | 39, 48, 68, 72 | 0 |
| All | All | 5264/5288 (99%) | 0.59 | 434 (8%) 12 16 | 16, 29, 51, 77 | 0 |

The worst 5 of 434 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 17 | X | 2 | THR | 7.2 |
| 4 | D | 59 | TYR | 6.8 |
| 9 | J | 3 | SER | 6.5 |
| 4 | D | 56 | THR | 5.7 |
| 4 | d | 136 | VAL | 5.4 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 24 | BCR | K | 102 | 40/40 | 0.81 | 2.30 | 11.02 | 29,33,37,37 | 0 |
| 28 | PL9 | A | 613 | 55/55 | 0.34 | 1.95 | 7.12 | 52,69,78,78 | 0 |
| 24 | BCR | k | 102 | 40/40 | 0.70 | 2.17 | 6.57 | 29,33,37,37 | 0 |
| 29 | LMG | Z | 101 | 37/55 | 0.33 | 1.65 | 6.14 | 55,84,88,88 | 0 |
| 24 | BCR | D | 404 | 40/40 | 0.40 | 1.52 | 6.09 | 25,30,48,49 | 0 |
| 22 | CLA | c | 501 | 65/65 | 0.72 | 1.66 | 6.07 | 29,32,44,46 | 0 |
| 24 | BCR | c | 514 | 40/40 | 0.72 | 1.69 | 5.47 | 37,43,47,47 | 0 |
| 24 | BCR | C | 515 | 40/40 | 0.73 | 1.99 | 5.43 | 30,37,40,41 | 0 |
| 29 | LMG | c | 520 | 51/55 | 0.21 | 1.84 | 5.31 | 43,76,81,82 | 0 |
| 24 | BCR | K | 101 | 40/40 | 0.61 | 1.39 | 5.10 | 34,38,39,39 | 0 |
| 25 | SQD | D | 411 | 43/54 | 0.66 | 1.27 | 5.06 | 67,74,78,79 | 0 |
| 29 | LMG | C | 519 | 51/55 | 0.42 | 0.86 | 5.03 | 31,57,72,73 | 0 |
| 24 | BCR | c | 515 | 40/40 | 0.79 | 1.59 | 4.80 | 30,37,40,41 | 0 |
| 28 | PL9 | a | 613 | 55/55 | 0.27 | 1.47 | 4.75 | 52,69,78,78 | 0 |
| 24 | BCR | d | 404 | 40/40 | 0.33 | 1.17 | 4.66 | 25,30,48,49 | 0 |
| 24 | BCR | C | 514 | 40/40 | 0.76 | 1.48 | 4.52 | 37,43,47,47 | 0 |
| 22 | CLA | a | 607 | 65/65 | 0.76 | 0.81 | 4.40 | 21,24,71,72 | 0 |
| 23 | PHO | A | 606 | 64/64 | 0.82 | 1.13 | 4.35 | 19,22,28,32 | 0 |
| 22 | CLA | C | 509 | 65/65 | 0.93 | 1.30 | 4.34 | 29,32,46,47 | 0 |
| 22 | CLA | c | 509 | 65/65 | 0.82 | 1.18 | 4.33 | 29,32,46,47 | 0 |
| 24 | BCR | T | 102 | 40/40 | 0.41 | 1.10 | 4.26 | 27,33,39,39 | 0 |
| 22 | CLA | c | 507 | 65/65 | 0.76 | 1.38 | 4.23 | 29,33,52,53 | 0 |
| 22 | CLA | B | 603 | 65/65 | 0.83 | 1.15 | 4.22 | 23,26,32,32 | 0 |
| 31 | DGD | D | 410 | 62/66 | 0.48 | 1.24 | 4.16 | 77,89,103,103 | 0 |
| 22 | CLA | c | 503 | 65/65 | 0.82 | 1.11 | 4.03 | 27,31,35,36 | 0 |
| 22 | CLA | C | 501 | 65/65 | 0.79 | 1.23 | 3.99 | 29,32,44,46 | 0 |
| 22 | CLA | c | 512 | 65/65 | 0.66 | 1.58 | 3.98 | 37,41,62,63 | 0 |
| 29 | LMG | c | 519 | 51/55 | 0.83 | 0.67 | 3.92 | 31,57,72,73 | 0 |
| 22 | CLA | D | 401 | 65/65 | 0.84 | 0.95 | 3.87 | 13,18,34,35 | 0 |
| 24 | BCR | k | 101 | 40/40 | 0.29 | 1.14 | 3.87 | 34,38,39,39 | 0 |
| 22 | CLA | b | 604 | 65/65 | 0.88 | 1.30 | 3.78 | 18,22,31,35 | 0 |
| 25 | SQD | d | 411 | 43/54 | 0.61 | 0.90 | 3.75 | 67,74,78,79 | 0 |
| 29 | LMG | z | 101 | 37/55 | 0.26 | 1.48 | 3.65 | 55,84,88,88 | 0 |
| 31 | DGD | H | 102 | 62/66 | 0.85 | 1.00 | 3.58 | 26,32,38,40 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 22 | CLA | d | 401 | 65/65 | 0.90 | 0.84 | 3.51 | 13,18,34,35 | 0 |
| 22 | CLA | c | 510 | 65/65 | 0.86 | 0.86 | 3.49 | 24,28,35,37 | 0 |
| 22 | CLA | C | 512 | 65/65 | 0.70 | 1.33 | 3.45 | 37,41,62,63 | 0 |
| 22 | CLA | A | 607 | 65/65 | 0.82 | 0.78 | 3.43 | 21,24,71,72 | 0 |
| 22 | CLA | D | 403 | 65/65 | 0.70 | 1.20 | 3.42 | 24,27,65,67 | 0 |
| 29 | LMG | C | 520 | 51/55 | 0.31 | 1.35 | 3.39 | 43,76,81,82 | 0 |
| 22 | CLA | b | 603 | 65/65 | 0.83 | 1.17 | 3.28 | 23,26,32,32 | 0 |
| 33 | HEM | f | 101 | 43/43 | 0.91 | 0.69 | 3.22 | 39,42,45,47 | 0 |
| 22 | CLA | d | 403 | 65/65 | 0.74 | 1.19 | 3.12 | 24,27,65,67 | 0 |
| 29 | LMG | a | 614 | 51/55 | 0.68 | 0.80 | 3.11 | 53,59,64,65 | 0 |
| 22 | CLA | a | 604 | 65/65 | 0.57 | 0.86 | 3.09 | 19,21,63,65 | 0 |
| 32 | LHG | E | 101 | 42/49 | 0.55 | 1.29 | 3.06 | 69,83,86,86 | 0 |
| 24 | BCR | A | 608 | 40/40 | 0.45 | 0.70 | 3.00 | 22,27,32,32 | 0 |
| 22 | CLA | A | 604 | 65/65 | 0.75 | 1.01 | 2.96 | 19,21,63,65 | 0 |
| 22 | CLA | C | 511 | 65/65 | 0.91 | 1.24 | 2.83 | 29,34,37,38 | 0 |
| 22 | CLA | B | 613 | 65/65 | 0.87 | 0.73 | 2.75 | 20,24,30,31 | 0 |
| 22 | CLA | c | 502 | 65/65 | 0.68 | 0.96 | 2.71 | 24,26,39,42 | 0 |
| 29 | LMG | A | 614 | 51/55 | 0.63 | 0.84 | 2.68 | 53,59,64,65 | 0 |
| 23 | PHO | a | 606 | 64/64 | 0.82 | 0.79 | 2.60 | 19,22,28,32 | 0 |
| 32 | LHG | D | 409 | 49/49 | 0.75 | 0.75 | 2.59 | 26,33,62,64 | 0 |
| 22 | CLA | B | 604 | 65/65 | 0.88 | 1.04 | 2.57 | 18,22,31,35 | 0 |
| 25 | SQD | a | 609 | 54/54 | 0.64 | 0.53 | 2.49 | 49,57,66,67 | 0 |
| 29 | LMG | D | 406 | 51/55 | 0.78 | 0.79 | 2.48 | 26,35,65,67 | 0 |
| 22 | CLA | C | 507 | 65/65 | 0.70 | 1.33 | 2.45 | 29,33,52,53 | 0 |
| 22 | CLA | b | 616 | 65/65 | 0.81 | 1.25 | 2.42 | 25,27,45,46 | 0 |
| 31 | DGD | h | 102 | 62/66 | 0.82 | 0.90 | 2.41 | 26,32,38,40 | 0 |
| 22 | CLA | b | 605 | 65/65 | 0.82 | 0.79 | 2.40 | 19,22,50,51 | 0 |
| 24 | BCR | t | 101 | 40/40 | 0.47 | 0.63 | 2.37 | 27,33,39,39 | 0 |
| 22 | CLA | b | 602 | 65/65 | 0.61 | 1.48 | 2.36 | 32,41,66,66 | 0 |
| 22 | CLA | b | 610 | 65/65 | 0.86 | 1.10 | 2.24 | 23,28,31,32 | 0 |
| 22 | CLA | c | 506 | 65/65 | 0.85 | 0.93 | 2.23 | 31,38,74,75 | 0 |
| 22 | CLA | B | 611 | 65/65 | 0.90 | 0.99 | 2.22 | 21,25,32,37 | 0 |
| 22 | CLA | B | 610 | 65/65 | 0.90 | 0.83 | 2.21 | 23,28,31,32 | 0 |
| 22 | CLA | c | 505 | 65/65 | 0.87 | 0.82 | 2.21 | 28,30,44,45 | 0 |
| 27 | BCT | a | 612 | 4/4 | 0.93 | 1.21 | 2.14 | 39,39,40,42 | 0 |
| 22 | CLA | B | 609 | 65/65 | 0.81 | 0.88 | 2.08 | 20,24,31,31 | 0 |
| 22 | CLA | b | 609 | 65/65 | 0.83 | 1.02 | 2.04 | 20,24,31,31 | 0 |
| 33 | HEM | v | 201 | 43/43 | 0.92 | 0.72 | 1.98 | 23,24,27,29 | 0 |
| 22 | CLA | B | 606 | 65/65 | 0.83 | 0.84 | 1.92 | 19,23,34,35 | 0 |
| 22 | CLA | B | 616 | 65/65 | 0.78 | 0.74 | 1.87 | 25,27,45,46 | 0 |
| 22 | CLA | C | 508 | 65/65 | 0.73 | 0.74 | 1.87 | 25,29,54,58 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 22 | CLA | b | 606 | 65/65 | 0.78 | 0.84 | 1.84 | 19,23,34,35 | 0 |
| 22 | CLA | B | 605 | 65/65 | 0.89 | 0.57 | 1.83 | 19,22,50,51 | 0 |
| 24 | BCR | h | 101 | 40/40 | 0.81 | 1.32 | 1.82 | 26,33,42,42 | 0 |
| 22 | CLA | b | 613 | 65/65 | 0.86 | 0.75 | 1.82 | 20,24,30,31 | 0 |
| 22 | CLA | b | 611 | 65/65 | 0.84 | 0.94 | 1.76 | 21,25,32,37 | 0 |
| 22 | CLA | C | 504 | 65/65 | 0.81 | 0.70 | 1.70 | 25,28,54,54 | 0 |
| 22 | CLA | a | 603 | 65/65 | 0.73 | 0.60 | 1.69 | 15,19,25,34 | 0 |
| 22 | CLA | c | 511 | 65/65 | 0.83 | 0.88 | 1.68 | 29,34,37,38 | 0 |
| 26 | CL | a | 610 | 1/1 | 0.57 | 0.55 | 1.68 | 24,24,24,24 | 0 |
| 24 | BCR | H | 101 | 40/40 | 0.67 | 1.32 | 1.66 | 26,33,42,42 | 0 |
| 33 | HEM | V | 201 | 43/43 | 0.91 | 0.69 | 1.65 | 23,24,27,29 | 0 |
| 31 | DGD | d | 410 | 62/66 | 0.53 | 0.76 | 1.65 | 77,89,103,103 | 0 |
| 27 | BCT | A | 612 | 4/4 | 0.88 | 1.02 | 1.63 | 39,39,40,42 | 0 |
| 22 | CLA | c | 508 | 65/65 | 0.87 | 0.60 | 1.60 | 25,29,54,58 | 0 |
| 33 | HEM | F | 101 | 43/43 | 0.89 | 0.79 | 1.56 | 39,42,45,47 | 0 |
| 22 | CLA | C | 510 | 65/65 | 0.83 | 0.81 | 1.55 | 24,28,35,37 | 0 |
| 22 | CLA | C | 513 | 65/65 | 0.66 | 1.10 | 1.52 | 39,45,64,64 | 0 |
| 22 | CLA | c | 513 | 65/65 | 0.68 | 1.02 | 1.49 | 39,45,64,64 | 0 |
| 22 | CLA | C | 502 | 65/65 | 0.86 | 0.79 | 1.47 | 24,26,39,42 | 0 |
| 22 | CLA | b | 617 | 65/65 | 0.67 | 0.91 | 1.45 | 22,29,77,78 | 0 |
| 22 | CLA | C | 505 | 65/65 | 0.90 | 0.90 | 1.44 | 28,30,44,45 | 0 |
| 25 | SQD | A | 609 | 54/54 | 0.65 | 0.63 | 1.42 | 49,57,66,67 | 0 |
| 22 | CLA | A | 603 | 65/65 | 0.77 | 0.67 | 1.41 | 15,19,25,34 | 0 |
| 22 | CLA | B | 602 | 65/65 | 0.62 | 1.02 | 1.37 | 32,41,66,66 | 0 |
| 22 | CLA | b | 607 | 65/65 | 0.51 | 0.88 | 1.34 | 24,28,40,41 | 0 |
| 31 | DGD | C | 518 | 62/66 | 0.75 | 0.64 | 1.25 | 22,31,52,56 | 0 |
| 31 | DGD | C | 516 | 62/66 | 0.85 | 0.58 | 1.25 | 23,33,61,62 | 0 |
| 23 | PHO | A | 605 | 64/64 | 0.77 | 0.59 | 1.22 | 16,21,25,26 | 0 |
| 22 | CLA | C | 506 | 65/65 | 0.76 | 0.97 | 1.21 | 31,38,74,75 | 0 |
| 22 | CLA | C | 503 | 65/65 | 0.90 | 0.80 | 1.13 | 27,31,35,36 | 0 |
| 32 | LHG | d | 409 | 49/49 | 0.77 | 0.71 | 1.09 | 26,33,62,64 | 0 |
| 24 | BCR | a | 608 | 40/40 | 0.39 | 0.47 | 1.07 | 22,27,32,32 | 0 |
| 32 | LHG | e | 101 | 42/49 | 0.52 | 0.61 | 1.06 | 69,83,86,86 | 0 |
| 31 | DGD | c | 518 | 62/66 | 0.81 | 0.53 | 1.02 | 22,31,52,56 | 0 |
| 23 | PHO | a | 605 | 64/64 | 0.81 | 0.52 | 0.99 | 16,21,25,26 | 0 |
| 24 | BCR | b | 618 | 40/40 | 0.75 | 0.41 | 0.98 | 21,28,40,40 | 0 |
| 25 | SQD | b | 601 | 54/54 | 0.73 | 0.49 | 0.84 | 50,63,68,68 | 0 |
| 32 | LHG | D | 407 | 49/49 | 0.81 | 0.49 | 0.82 | 24,28,37,40 | 0 |
| 22 | CLA | B | 617 | 65/65 | 0.69 | 0.51 | 0.78 | 22,29,77,78 | 0 |
| 28 | PL9 | D | 408 | 55/55 | 0.70 | 0.51 | 0.75 | 19,23,29,32 | 0 |
| 29 | LMG | d | 406 | 51/55 | 0.76 | 0.50 | 0.75 | 26,35,65,67 | 0 |
| 22 | CLA | B | 607 | 65/65 | 0.61 | 0.62 | 0.70 | 24,28,40,41 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 22 | CLA | B | 612 | 65/65 | 0.85 | 0.44 | 0.61 | 19,21,32,34 | 0 |
| 31 | DGD | C | 517 | 62/66 | 0.82 | 0.54 | 0.59 | 23,35,62,63 | 0 |
| 31 | DGD | c | 516 | 62/66 | 0.87 | 0.55 | 0.51 | 23,33,61,62 | 0 |
| 22 | CLA | D | 402 | 65/65 | 0.78 | 0.53 | 0.49 | 14,18,29,35 | 0 |
| 22 | CLA | c | 504 | 65/65 | 0.91 | 0.51 | 0.46 | 25,28,54,54 | 0 |
| 22 | CLA | b | 612 | 65/65 | 0.77 | 0.43 | 0.27 | 19,21,32,34 | 0 |
| 20 | OEX | a | 601 | 10/10 | 0.93 | 0.41 | 0.19 | 22,23,26,26 | 0 |
| 22 | CLA | b | 614 | 65/65 | 0.73 | 0.45 | 0.13 | 19,22,45,47 | 0 |
| 24 | BCR | T | 101 | 40/40 | 0.79 | 0.40 | 0.07 | 23,27,28,29 | 0 |
| 24 | BCR | b | 622 | 40/40 | 0.69 | 0.48 | 0.02 | 25,37,44,45 | 0 |
| 31 | DGD | c | 517 | 62/66 | 0.89 | 0.40 | -0.02 | 23,35,62,63 | 0 |
| 25 | SQD | L | 101 | 54/54 | 0.77 | 0.41 | -0.04 | 57,69,84,85 | 0 |
| 22 | CLA | d | 402 | 65/65 | 0.78 | 0.47 | -0.06 | 14,18,29,35 | 0 |
| 22 | CLA | b | 608 | 65/65 | 0.87 | 0.43 | -0.09 | 17,20,32,34 | 0 |
| 25 | SQD | b | 621 | 54/54 | 0.77 | 0.40 | -0.12 | 58,66,80,80 | 0 |
| 32 | LHG | d | 405 | 49/49 | 0.81 | 0.44 | -0.13 | 29,34,41,41 | 0 |
| 26 | CL | a | 611 | 1/1 | 0.91 | 0.37 | -0.22 | 21,21,21,21 | 0 |
| 34 | MG | j | 101 | 1/1 | 0.71 | 0.30 | -0.25 | 27,27,27,27 | 0 |
| 28 | PL9 | d | 408 | 55/55 | 0.78 | 0.40 | -0.38 | 19,23,29,32 | 0 |
| 32 | LHG | d | 407 | 49/49 | 0.80 | 0.37 | -0.39 | 24,28,37,40 | 0 |
| 22 | CLA | b | 615 | 65/65 | 0.67 | 0.44 | -0.40 | 20,24,60,61 | 0 |
| 22 | CLA | B | 608 | 65/65 | 0.91 | 0.41 | -0.51 | 17,20,32,34 | 0 |
| 22 | CLA | B | 614 | 65/65 | 0.91 | 0.38 | -0.52 | 19,22,45,47 | 0 |
| 26 | CL | A | 610 | 1/1 | 0.80 | 0.45 | -0.57 | 24,24,24,24 | 0 |
| 20 | OEX | A | 601 | 10/10 | 0.92 | 0.40 | -0.57 | 22,23,26,26 | 0 |
| 29 | LMG | b | 619 | 51/55 | 0.67 | 0.38 | -0.58 | 29,39,51,54 | 0 |
| 32 | LHG | D | 405 | 49/49 | 0.76 | 0.38 | -0.62 | 29,34,41,41 | 0 |
| 32 | LHG | L | 102 | 49/49 | 0.84 | 0.35 | -0.64 | 23,31,43,44 | 0 |
| 32 | LHG | l | 103 | 49/49 | 0.86 | 0.33 | -0.73 | 23,31,43,44 | 0 |
| 29 | LMG | B | 620 | 51/55 | 0.58 | 0.38 | -0.80 | 29,39,51,54 | 0 |
| 25 | SQD | l | 101 | 54/54 | 0.82 | 0.32 | -0.82 | 57,69,84,85 | 0 |
| 25 | SQD | l | 102 | 54/54 | 0.82 | 0.32 | -0.82 | 58,66,80,80 | 0 |
| 24 | BCR | B | 618 | 40/40 | 0.82 | 0.30 | -0.85 | 23,27,28,29 | 0 |
| 22 | CLA | B | 615 | 65/65 | 0.74 | 0.38 | -0.86 | 20,24,60,61 | 0 |
| 25 | SQD | B | 601 | 54/54 | 0.73 | 0.35 | -0.86 | 50,63,68,68 | 0 |
| 24 | BCR | B | 622 | 40/40 | 0.67 | 0.43 | -0.91 | 25,37,44,45 | 0 |
| 26 | CL | A | 611 | 1/1 | 0.85 | 0.35 | -1.00 | 21,21,21,21 | 0 |
| 34 | MG | J | 101 | 1/1 | 0.87 | 0.11 | -1.31 | 27,27,27,27 | 0 |
| 21 | FE2 | A | 602 | 1/1 | 0.96 | 0.16 | -1.50 | 26,26,26,26 | 0 |
| 30 | CA | o | 301 | 1/1 | 0.95 | 0.28 | -1.83 | 49,49,49,49 | 0 |
| 24 | BCR | B | 619 | 40/40 | 0.73 | 0.31 | -1.99 | 21,28,40,40 | 0 |
| 21 | FE2 | a | 602 | 1/1 | 0.83 | 0.35 | -1.99 | 26,26,26,26 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 30 | CA | O | 301 | 1/1 | 0.93 | 0.14 | -2.63 | 49,49,49,49 | 0 |
| 30 | CA | f | 102 | 1/1 | 0.28 | 0.73 | - | 56,56,56,56 | 0 |
| 26 | CL | U | 201 | 1/1 | 0.02 | 0.17 | - | 50,50,50,50 | 0 |
| 30 | CA | B | 621 | 1/1 | 0.25 | 0.73 | - | 76,76,76,76 | 0 |
| 26 | CL | u | 201 | 1/1 | 0.03 | 0.36 | - | 50,50,50,50 | 0 |
| 30 | CA | F | 102 | 1/1 | 0.70 | 0.50 | - | 56,56,56,56 | 0 |
| 30 | CA | b | 620 | 1/1 | 0.53 | 1.24 | - | 76,76,76,76 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.