



wwPDB X-ray Structure Validation Summary Report i

Jun 17, 2014 – 04:54 AM BST

PDB ID : 4V62
Title : Crystal Structure of cyanobacterial Photosystem II
Authors : Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.
Deposited on : 2008-01-17
Resolution : 2.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

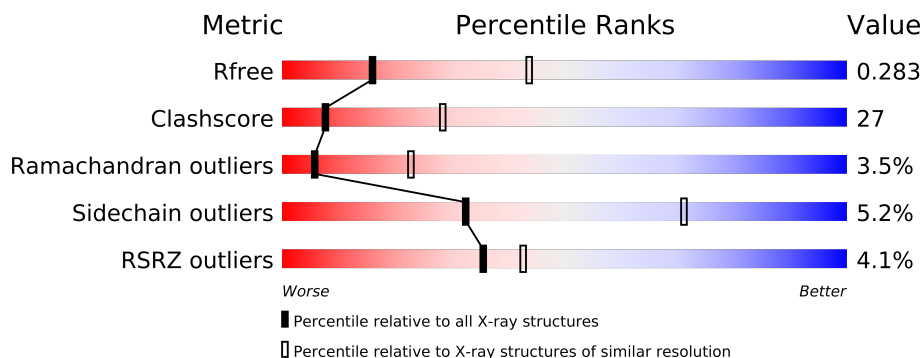
The following versions of software and data (see [references](#)) were used in the production of this report:

| | | |
|--------------------------------|---|--------------------------|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.16 November 2013 |
| Xtriage (Phenix) | : | dev-1323 |
| EDS | : | stable23397 |
| Percentile statistics | : | 21963 |
| Refmac | : | 5.8.0049 |
| CCP4 | : | 6.3.0 (Settle) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | stable23397 |

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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} | 66092 | 1053 (2.90-2.90) |
| Clashscore | 79885 | 1326 (2.90-2.90) |
| Ramachandran outliers | 78287 | 1290 (2.90-2.90) |
| Sidechain outliers | 78261 | 1292 (2.90-2.90) |
| RSRZ outliers | 66119 | 1054 (2.90-2.90) |

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AA | 344 | |
| 1 | BA | 344 | |
| 2 | AB | 510 | |
| 2 | BB | 510 | |
| 3 | AC | 473 | |
| 3 | BC | 473 | |
| 4 | AD | 352 | |
| 4 | BD | 352 | |
| 5 | AE | 84 | |
| 5 | BE | 84 | |
| 6 | AF | 45 | |
| 6 | BF | 45 | |
| 7 | AH | 66 | |
| 7 | BH | 66 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 8 | AI | 38 | |
| 8 | BI | 38 | |
| 9 | AJ | 40 | |
| 9 | BJ | 40 | |
| 10 | AK | 37 | |
| 10 | BK | 37 | |
| 11 | AL | 37 | |
| 11 | BL | 37 | |
| 12 | AM | 36 | |
| 12 | BM | 36 | |
| 13 | AO | 247 | |
| 13 | BO | 247 | |
| 14 | AT | 32 | |
| 14 | BT | 32 | |
| 15 | AU | 104 | |
| 15 | BU | 104 | |
| 16 | AV | 137 | |
| 16 | BV | 137 | |
| 17 | Ay | 46 | |
| 17 | By | 46 | |
| 18 | AX | 50 | |
| 18 | BX | 50 | |
| 19 | AY | 28 | |
| 19 | BY | 28 | |
| 20 | AZ | 62 | |
| 20 | BZ | 62 | |

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 22 | CLA | AA | 406 | - | X |
| 22 | CLA | AB | 601 | - | X |
| 22 | CLA | AB | 604 | - | X |
| 22 | CLA | AB | 614 | - | X |
| 22 | CLA | AC | 504 | - | X |
| 22 | CLA | AC | 507 | - | X |
| 22 | CLA | AC | 512 | - | X |
| 22 | CLA | AC | 513 | - | X |
| 22 | CLA | AD | 404 | - | X |
| 22 | CLA | BA | 405 | - | X |
| 22 | CLA | BA | 407 | - | X |

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| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 22 | CLA | BB | 612 | - | X |
| 22 | CLA | BC | 513 | - | X |
| 23 | PHO | BD | 403 | - | X |
| 24 | PL9 | AA | 407 | - | X |
| 24 | PL9 | AJ | 101 | - | X |
| 24 | PL9 | BA | 408 | - | X |
| 24 | PL9 | BJ | 101 | - | X |
| 26 | BCR | AH | 101 | - | X |
| 26 | BCR | AJ | 102 | - | X |
| 26 | BCR | AK | 102 | - | X |
| 26 | BCR | AZ | 101 | - | X |
| 26 | BCR | BB | 622 | - | X |
| 26 | BCR | BC | 514 | - | X |
| 26 | BCR | BJ | 102 | - | X |
| 26 | BCR | BK | 102 | - | X |
| 26 | BCR | BZ | 101 | - | X |
| 27 | DGD | AB | 626 | - | X |
| 27 | DGD | AD | 410 | - | X |
| 27 | DGD | BA | 411 | - | X |
| 27 | DGD | BB | 602 | - | X |
| 27 | DGD | BD | 410 | - | X |
| 28 | LHG | AC | 521 | - | X |
| 28 | LHG | BC | 521 | - | X |
| 29 | SQD | AA | 415 | - | X |
| 29 | SQD | AF | 101 | - | X |
| 29 | SQD | BA | 401 | - | X |
| 29 | SQD | BF | 101 | - | X |
| 30 | LMG | AA | 416 | - | X |
| 30 | LMG | AB | 623 | - | X |
| 30 | LMG | AC | 520 | - | X |
| 30 | LMG | AD | 408 | - | X |
| 30 | LMG | AI | 101 | - | X |
| 30 | LMG | BB | 623 | - | X |
| 30 | LMG | BC | 519 | - | X |
| 30 | LMG | BC | 520 | - | X |
| 30 | LMG | BD | 407 | - | X |
| 30 | LMG | BD | 408 | - | X |
| 30 | LMG | BE | 102 | - | X |
| 30 | LMG | BI | 101 | - | X |
| 31 | CL | AA | 414 | - | X |
| 31 | CL | BA | 415 | - | X |
| 32 | LMT | AB | 624 | - | X |

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| Mol | Type | Chain | Res | Geometry | Electron density |
|-----|------|-------|-----|----------|------------------|
| 32 | LMT | AB | 625 | - | X |
| 32 | LMT | AB | 627 | - | X |
| 32 | LMT | AD | 411 | - | X |
| 32 | LMT | AI | 102 | - | X |
| 32 | LMT | AT | 101 | - | X |
| 32 | LMT | BB | 625 | - | X |
| 32 | LMT | BB | 626 | - | X |
| 32 | LMT | BD | 411 | - | X |
| 32 | LMT | BI | 102 | - | X |
| 32 | LMT | BT | 101 | - | X |
| 33 | BCT | AD | 401 | - | X |
| 35 | CA | BO | 301 | - | X |

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50234 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Q(B) protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | AA | 335 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2628 | 1720 | 432 | 461 | 15 | | | |
| 1 | BA | 335 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2628 | 1720 | 432 | 461 | 15 | | | |

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2 | AB | 490 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3850 | 2528 | 641 | 668 | 13 | | | |
| 2 | BB | 490 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3850 | 2528 | 641 | 668 | 13 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3 | AC | 447 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3444 | 2256 | 576 | 599 | 13 | | | |
| 3 | BC | 447 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3444 | 2256 | 576 | 599 | 13 | | | |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| AC | 2 | LYS | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 3 | THR | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 4 | LEU | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 5 | SER | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 6 | SER | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 7 | GLN | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 8 | LYS | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 9 | ARG | - | SEE REMARK 999 | UNP Q8DIF8 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| AC | 10 | TYR | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 11 | SER | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 12 | PRO | - | SEE REMARK 999 | UNP Q8DIF8 |
| AC | 13 | VAL | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 2 | LYS | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 3 | THR | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 4 | LEU | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 5 | SER | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 6 | SER | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 7 | GLN | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 8 | LYS | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 9 | ARG | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 10 | TYR | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 11 | SER | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 12 | PRO | - | SEE REMARK 999 | UNP Q8DIF8 |
| BC | 13 | VAL | - | SEE REMARK 999 | UNP Q8DIF8 |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4 | AD | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2706 | 1794 | 440 | 460 | 12 | | | |
| 4 | BD | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2706 | 1794 | 440 | 460 | 12 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 5 | AE | 82 | Total | C | N | O | 0 | 0 | 0 |
| | | | 666 | 434 | 108 | 124 | | | |
| 5 | BE | 82 | Total | C | N | O | 0 | 0 | 0 |
| | | | 666 | 434 | 108 | 124 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 6 | AF | 35 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 282 | 192 | 46 | 43 | 1 | | | |
| 6 | BF | 35 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 282 | 192 | 46 | 43 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | AH | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 507 | 338 | 81 | 86 | 2 | | | |
| 7 | BH | 65 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 507 | 338 | 81 | 86 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | AI | 35 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 286 | 195 | 45 | 45 | 1 | | | |
| 8 | BI | 35 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 286 | 195 | 45 | 45 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9 | AJ | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 249 | 170 | 38 | 40 | 1 | | | |
| 9 | BJ | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 249 | 170 | 38 | 40 | 1 | | | |

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

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 10 | AK | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 293 | 204 | 43 | 46 | | | |
| 10 | BK | 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 | AL | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 304 | 202 | 48 | 53 | 1 | | | |
| 11 | BL | 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 | AM | 34 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 267 | 178 | 40 | 48 | 1 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 12 | BM | 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 | AO | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1845 | 1154 | 308 | 379 | 4 | | | |
| 13 | BO | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1845 | 1154 | 308 | 379 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 14 | AT | 32 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 192 | 40 | 41 | 2 | | | |
| 14 | BT | 32 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 275 | 192 | 40 | 41 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|---------|-------|
| 15 | AU | 97 | Total | C | N | O | | 0 | 0 | 0 |
| | | | 774 | 491 | 129 | 154 | | | | |
| 15 | BU | 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 | AV | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1060 | 673 | 177 | 206 | 4 | | | |
| 16 | BV | 137 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1060 | 673 | 177 | 206 | 4 | | | |

- Molecule 17 is a protein called Protein ycf12.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 17 | Ay | 28 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 201 | 134 | 33 | 31 | 3 | | | |
| 17 | By | 28 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 201 | 134 | 33 | 31 | 3 | | | |

- Molecule 18 is a protein called Photosystem II PsbX protein.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18 | AX | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 270 | 182 | 41 | 47 | | | |
| 18 | BX | 37 | Total | C | N | O | 0 | 0 | 0 |
| | | | 270 | 182 | 41 | 47 | | | |

- Molecule 19 is a protein called Photosystem II protein Y.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 19 | AY | 28 | Total | C | N | O | 0 | 0 | 0 |
| | | | 140 | 84 | 28 | 28 | | | |
| 19 | BY | 28 | Total | C | N | O | 0 | 0 | 0 |
| | | | 140 | 84 | 28 | 28 | | | |

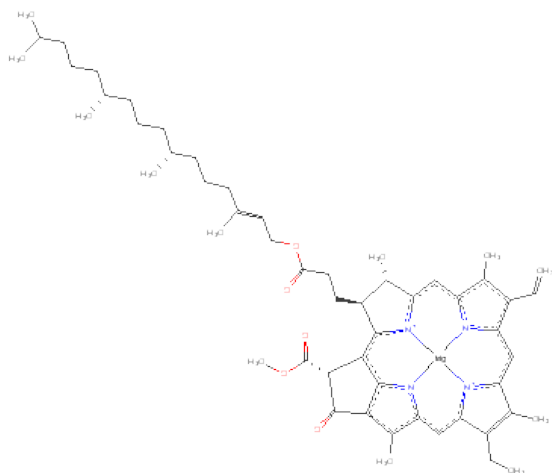
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 20 | AZ | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 479 | 328 | 72 | 77 | 2 | | | |
| 20 | BZ | 62 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 479 | 328 | 72 | 77 | 2 | | | |

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

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 21 | AA | 1 | Total | Fe | 0 | 0 |
| | | | 1 | 1 | | |
| 21 | BA | 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 | AA | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AA | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AA | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AA | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |
| 22 | AB | 1 | Total | C | Mg | N | O | 0 | 0 |
| | | | 65 | 55 | 1 | 4 | 5 | | |

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

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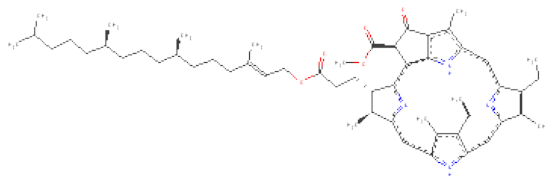
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22 | BA | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | BA | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | BA | 1 | Total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

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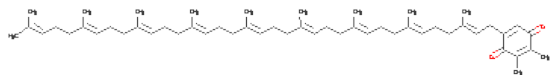
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 22 | BC | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | BC | 1 | Total 65 | C 55 | Mg 1 | N 4 | O 5 | 0 | 0 |
| 22 | BC | 1 | Total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

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



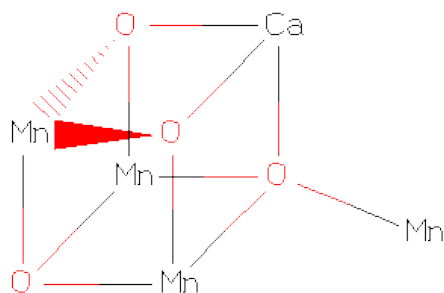
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 23 | AA | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | AD | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | BA | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |
| 23 | BD | 1 | Total | C | N | O | 0 | 0 |
| | | | 64 | 55 | 4 | 5 | | |

- Molecule 24 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: C₅₃H₈₀O₂).



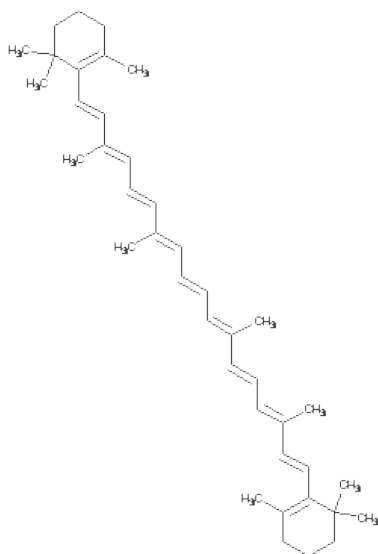
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 24 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 45 | 43 | 2 | | |
| 24 | AD | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 24 | AJ | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 33 | 2 | | |
| 24 | BA | 1 | Total | C | O | 0 | 0 |
| | | | 45 | 43 | 2 | | |
| 24 | BD | 1 | Total | C | O | 0 | 0 |
| | | | 55 | 53 | 2 | | |
| 24 | BJ | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 33 | 2 | | |

- Molecule 25 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 25 | AA | 1 | Total | Ca | Mn | 0 | 0 |
| | | | 5 | 1 | 4 | | |
| 25 | BA | 1 | Total | Ca | Mn | 0 | 0 |
| | | | 5 | 1 | 4 | | |

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 26 | AA | 1 | Total | C | 0 | 0 |
| | | | 40 | 40 | | |
| 26 | AB | 1 | Total | C | 0 | 0 |
| | | | 40 | 40 | | |

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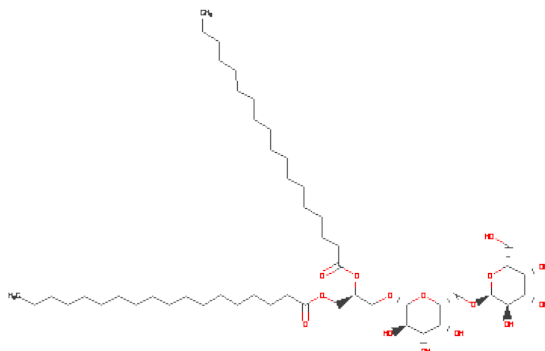
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 26 | AB | 1 | Total C 40 40 | 0 | 0 |
| 26 | AB | 1 | Total C 40 40 | 0 | 0 |
| 26 | AB | 1 | Total C 40 40 | 0 | 0 |
| 26 | AC | 1 | Total C 40 40 | 0 | 0 |
| 26 | AC | 1 | Total C 40 40 | 0 | 0 |
| 26 | AD | 1 | Total C 40 40 | 0 | 0 |
| 26 | AH | 1 | Total C 40 40 | 0 | 0 |
| 26 | AJ | 1 | Total C 40 40 | 0 | 0 |
| 26 | AK | 1 | Total C 40 40 | 0 | 0 |
| 26 | AT | 1 | Total C 40 40 | 0 | 0 |
| 26 | AZ | 1 | Total C 40 40 | 0 | 0 |
| 26 | BA | 1 | Total C 40 40 | 0 | 0 |
| 26 | BB | 1 | Total C 40 40 | 0 | 0 |
| 26 | BB | 1 | Total C 40 40 | 0 | 0 |
| 26 | BB | 1 | Total C 40 40 | 0 | 0 |
| 26 | BC | 1 | Total C 40 40 | 0 | 0 |
| 26 | BC | 1 | Total C 40 40 | 0 | 0 |
| 26 | BD | 1 | Total C 40 40 | 0 | 0 |
| 26 | BJ | 1 | Total C 40 40 | 0 | 0 |
| 26 | BK | 1 | Total C 40 40 | 0 | 0 |
| 26 | BX | 1 | Total C 40 40 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 26 | BZ | 1 | Total C 40 40 | 0 | 0 |

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



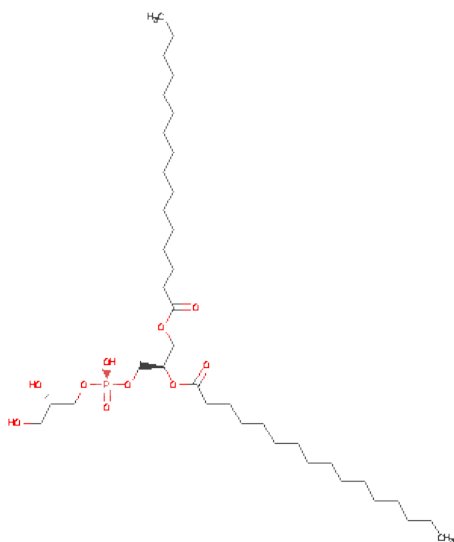
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------------|---------|---------|
| 27 | AA | 1 | Total C O 56 41 15 | 0 | 0 |
| 27 | AB | 1 | Total C O 52 37 15 | 0 | 0 |
| 27 | AC | 1 | Total C O 53 38 15 | 0 | 0 |
| 27 | AC | 1 | Total C O 62 47 15 | 0 | 0 |
| 27 | AC | 1 | Total C O 66 51 15 | 0 | 0 |
| 27 | AD | 1 | Total C O 63 48 15 | 0 | 0 |
| 27 | AH | 1 | Total C O 58 43 15 | 0 | 0 |
| 27 | BA | 1 | Total C O 56 41 15 | 0 | 0 |
| 27 | BB | 1 | Total C O 52 37 15 | 0 | 0 |
| 27 | BC | 1 | Total C O 53 38 15 | 0 | 0 |

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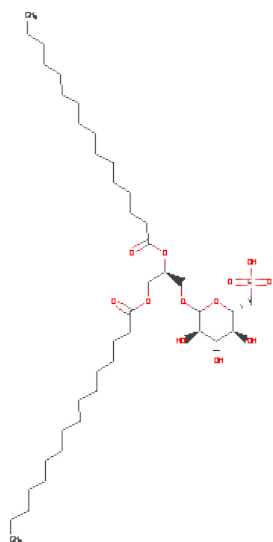
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 27 | BC | 1 | Total | C | O | 0 | 0 |
| | | | 62 | 47 | 15 | | |
| 27 | BC | 1 | Total | C | O | 0 | 0 |
| | | | 66 | 51 | 15 | | |
| 27 | BD | 1 | Total | C | O | 0 | 0 |
| | | | 63 | 48 | 15 | | |
| 27 | BH | 1 | Total | C | O | 0 | 0 |
| | | | 58 | 43 | 15 | | |

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



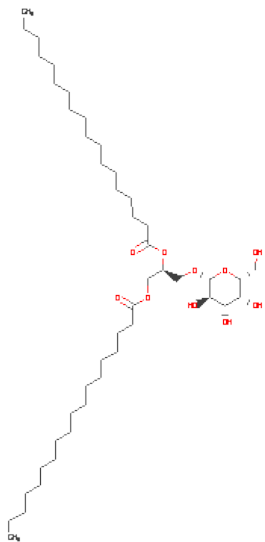
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 28 | AA | 1 | Total | C | O | P | 0 | 0 |
| | | | 39 | 28 | 10 | 1 | | |
| 28 | AC | 1 | Total | C | O | P | 0 | 0 |
| | | | 37 | 26 | 10 | 1 | | |
| 28 | BA | 1 | Total | C | O | P | 0 | 0 |
| | | | 39 | 28 | 10 | 1 | | |
| 28 | BC | 1 | Total | C | O | P | 0 | 0 |
| | | | 37 | 26 | 10 | 1 | | |

- Molecule 29 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 |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 29 | AA | 1 | Total | C | O | S | 0 | 0 |
| | | | 51 | 38 | 12 | 1 | | |
| 29 | AA | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 29 | AD | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 29 | AF | 1 | Total | C | O | S | 0 | 0 |
| | | | 45 | 32 | 12 | 1 | | |
| 29 | BA | 1 | Total | C | O | S | 0 | 0 |
| | | | 54 | 41 | 12 | 1 | | |
| 29 | BA | 1 | Total | C | O | S | 0 | 0 |
| | | | 51 | 38 | 12 | 1 | | |
| 29 | BB | 1 | Total | C | O | S | 0 | 0 |
| | | | 47 | 34 | 12 | 1 | | |
| 29 | BD | 1 | Total | C | O | S | 0 | 0 |
| | | | 43 | 30 | 12 | 1 | | |
| 29 | BF | 1 | Total | C | O | S | 0 | 0 |
| | | | 45 | 32 | 12 | 1 | | |
| 29 | BL | 1 | Total | C | O | S | 0 | 0 |
| | | | 47 | 34 | 12 | 1 | | |

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 30 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 30 | AA | 1 | Total | C | O | 0 | 0 |
| | | | 42 | 32 | 10 | | |
| 30 | AB | 1 | Total | C | O | 0 | 0 |
| | | | 49 | 39 | 10 | | |
| 30 | AB | 1 | Total | C | O | 0 | 0 |
| | | | 49 | 39 | 10 | | |
| 30 | AB | 1 | Total | C | O | 0 | 0 |
| | | | 42 | 32 | 10 | | |
| 30 | AC | 1 | Total | C | O | 0 | 0 |
| | | | 48 | 38 | 10 | | |
| 30 | AC | 1 | Total | C | O | 0 | 0 |
| | | | 45 | 35 | 10 | | |
| 30 | AD | 1 | Total | C | O | 0 | 0 |
| | | | 46 | 36 | 10 | | |
| 30 | AD | 1 | Total | C | O | 0 | 0 |
| | | | 48 | 38 | 10 | | |
| 30 | AE | 1 | Total | C | O | 0 | 0 |
| | | | 44 | 34 | 10 | | |
| 30 | AI | 1 | Total | C | O | 0 | 0 |
| | | | 43 | 33 | 10 | | |
| 30 | AM | 1 | Total | C | O | 0 | 0 |
| | | | 42 | 32 | 10 | | |
| 30 | BA | 1 | Total | C | O | 0 | 0 |
| | | | 51 | 41 | 10 | | |
| 30 | BB | 1 | Total | C | O | 0 | 0 |
| | | | 49 | 39 | 10 | | |

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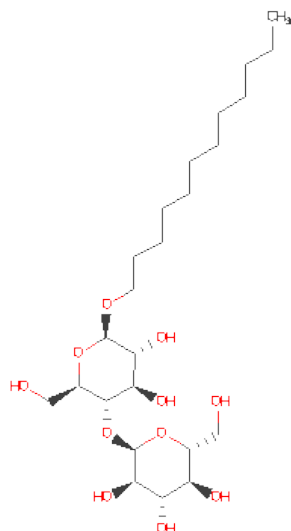
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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 30 | BB | 1 | Total | C | O | 0 | 0 |
| | | | 49 | 39 | 10 | | |
| 30 | BC | 1 | Total | C | O | 0 | 0 |
| | | | 48 | 38 | 10 | | |
| 30 | BC | 1 | Total | C | O | 0 | 0 |
| | | | 45 | 35 | 10 | | |
| 30 | BD | 1 | Total | C | O | 0 | 0 |
| | | | 46 | 36 | 10 | | |
| 30 | BD | 1 | Total | C | O | 0 | 0 |
| | | | 48 | 38 | 10 | | |
| 30 | BE | 1 | Total | C | O | 0 | 0 |
| | | | 44 | 34 | 10 | | |
| 30 | BI | 1 | Total | C | O | 0 | 0 |
| | | | 43 | 33 | 10 | | |
| 30 | BM | 1 | Total | C | O | 0 | 0 |
| | | | 42 | 32 | 10 | | |

- Molecule 31 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

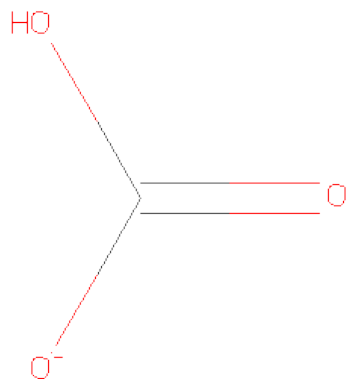
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 31 | AA | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 31 | BA | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



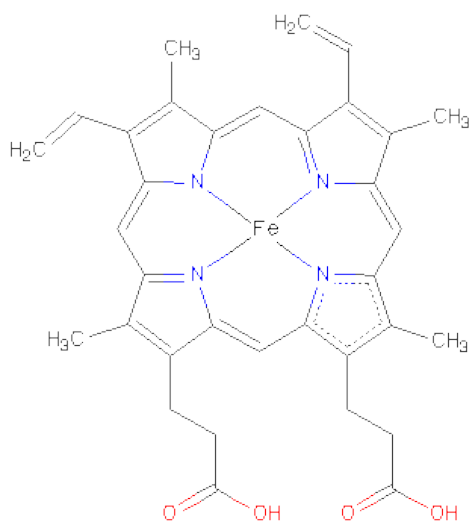
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 32 | AB | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | AB | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | AB | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | AD | 1 | Total | C | O | 0 | 0 |
| | | | 31 | 20 | 11 | | |
| 32 | AI | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | AM | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | AT | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | BB | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | BB | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | BB | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | BD | 1 | Total | C | O | 0 | 0 |
| | | | 31 | 20 | 11 | | |
| 32 | BI | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | BM | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |
| 32 | BT | 1 | Total | C | O | 0 | 0 |
| | | | 35 | 24 | 11 | | |

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 33 | AD | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 33 | BD | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 34 | AE | 1 | Total | C | Fe | N | O | 0 | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 34 | AV | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 34 | BE | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |
| 34 | BV | 1 | Total 43 | C 34 | Fe 1 | N 4 | O 4 | 0 | 0 |

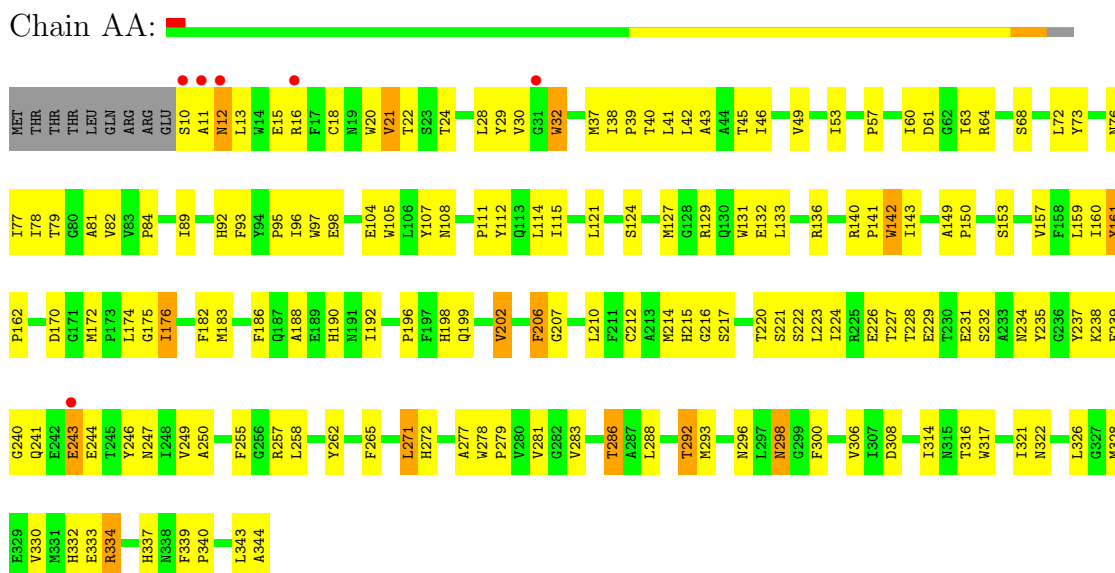
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 35 | AO | 1 | Total 1 | Ca 1 | 0 | 0 |
| 35 | BO | 1 | Total 1 | Ca 1 | 0 | 0 |
| 35 | AK | 1 | Total 1 | Ca 1 | 0 | 0 |
| 35 | BK | 1 | Total 1 | Ca 1 | 0 | 0 |

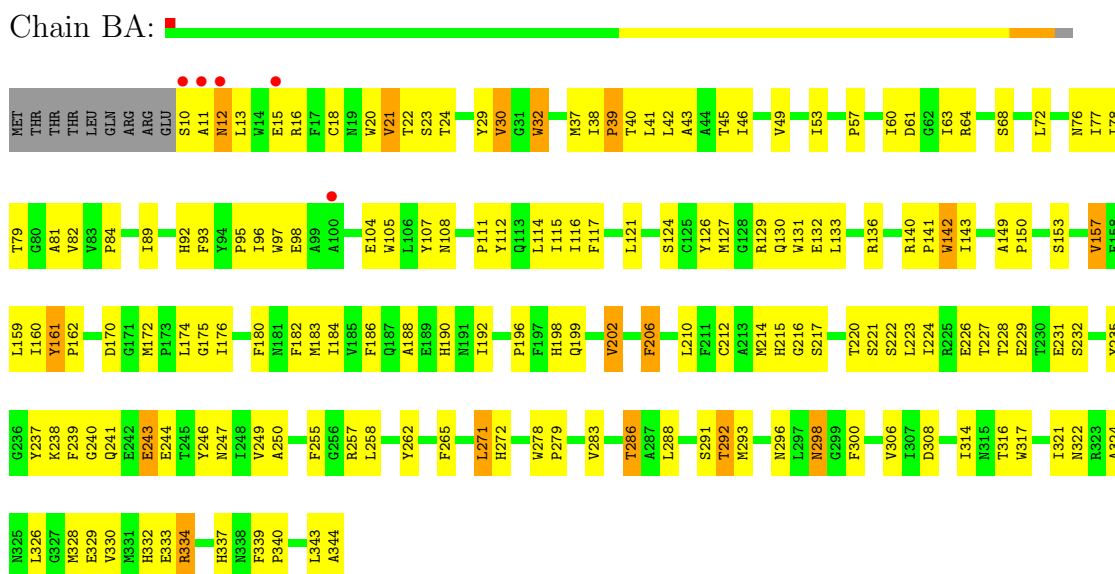
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 Q(B) protein



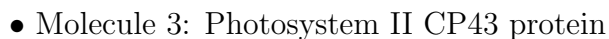
- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II core light harvesting protein

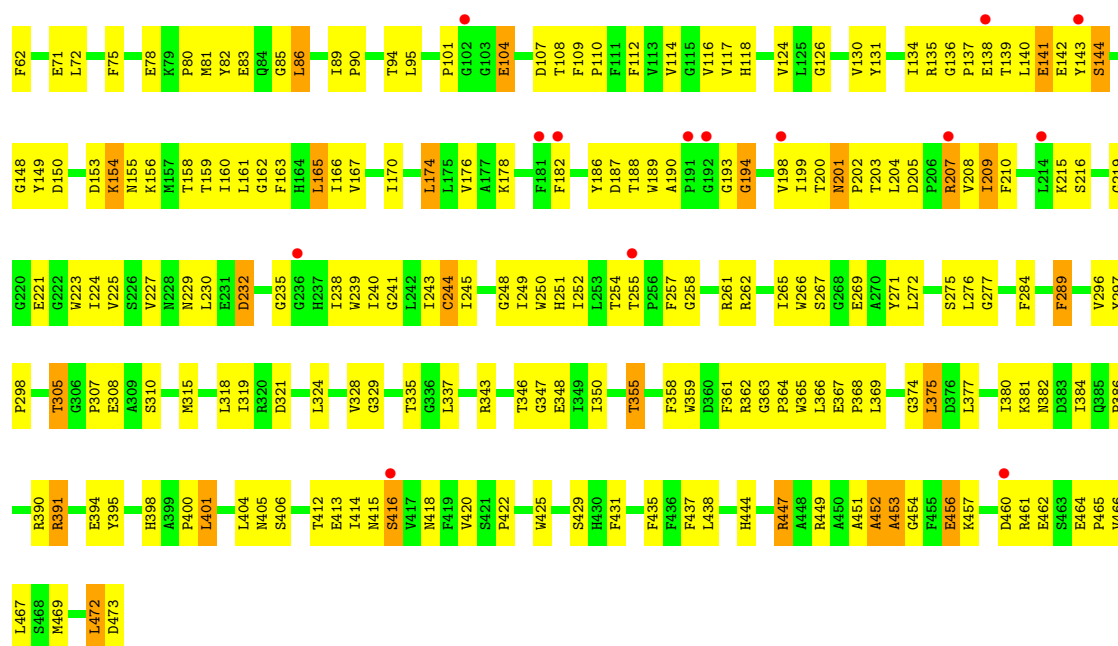


| Age Group | Percentage |
|-----------|------------|
| 18-29 | 90% |
| 30-49 | 85% |
| 50-64 | 75% |
| 65-74 | 65% |
| 75+ | 55% |



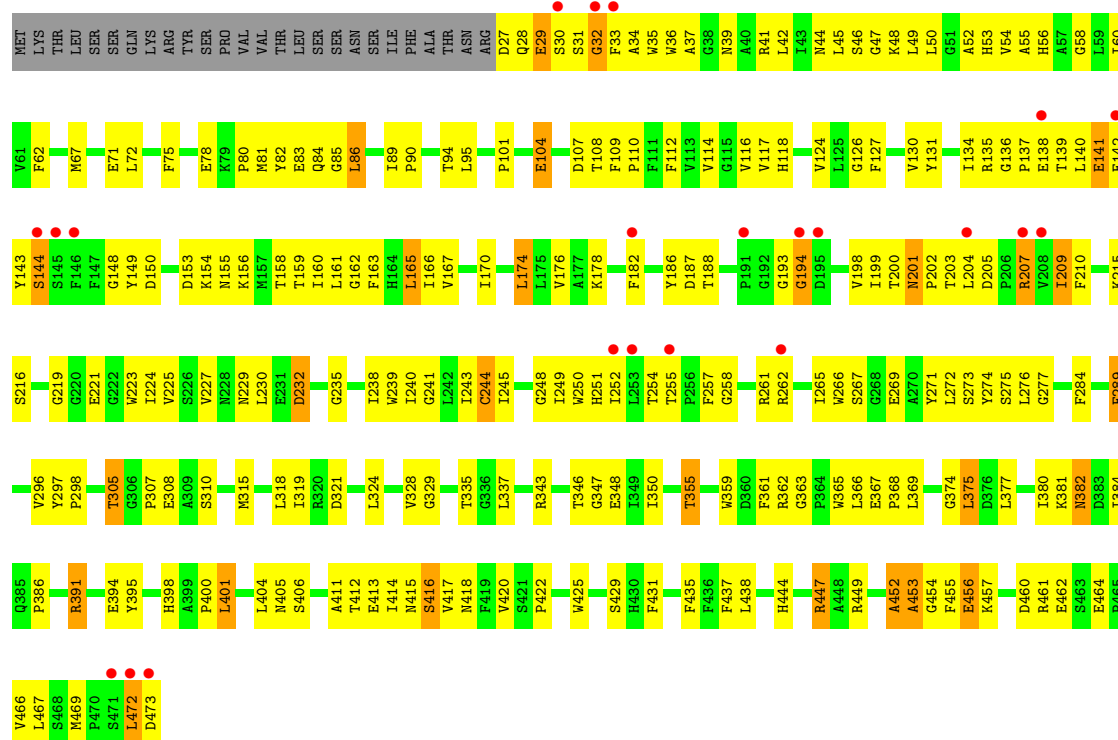
| Age Group | Percentage |
|-----------|------------|
| 18-29 | 90% |
| 30-49 | 83% |
| 50-64 | 70% |
| 65+ | 55% |





• Molecule 3: Photosystem II CP43 protein

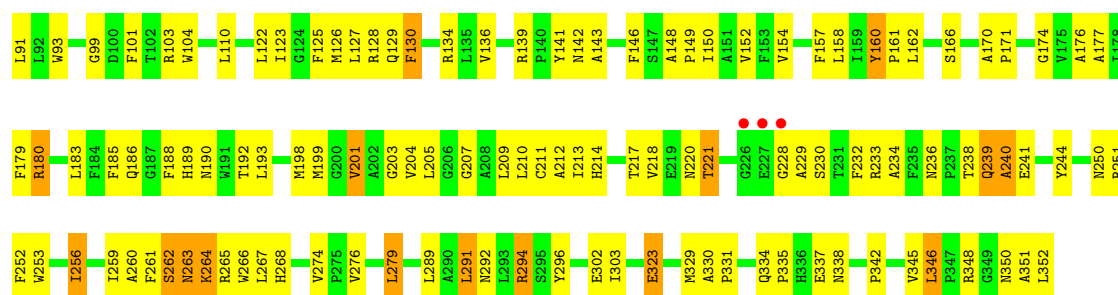
Chain BC:



• Molecule 4: Photosystem II reaction center D2 protein

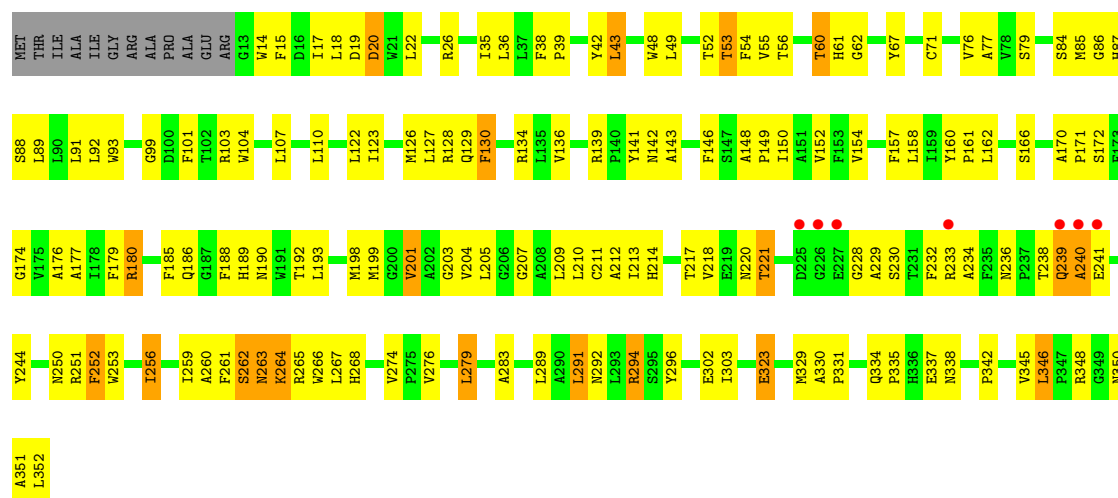
Chain AD:





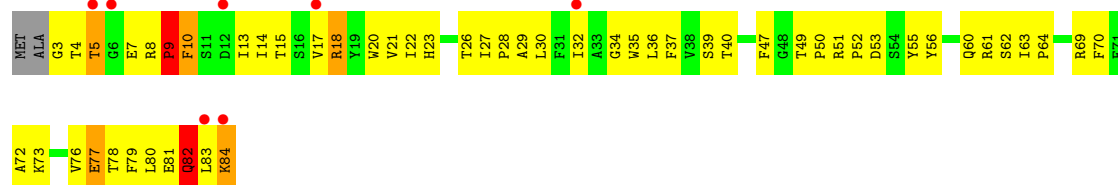
• Molecule 4: Photosystem II reaction center D2 protein

Chain BD:



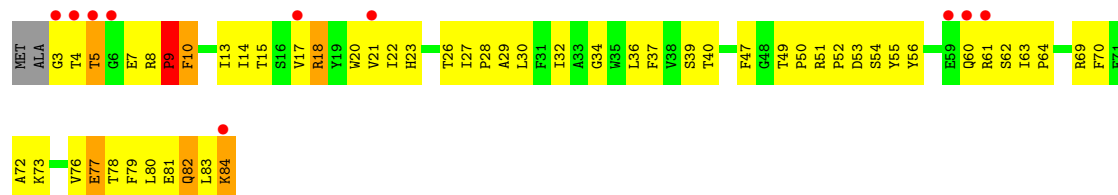
• Molecule 5: Cytochrome b559 subunit alpha

Chain AE:



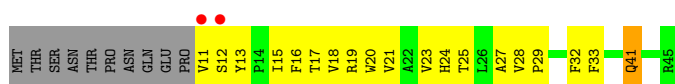
• Molecule 5: Cytochrome b559 subunit alpha

Chain BE:



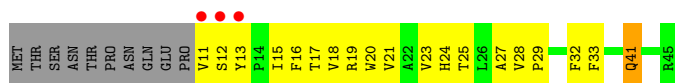
• Molecule 6: Cytochrome b559 subunit beta

Chain AF:



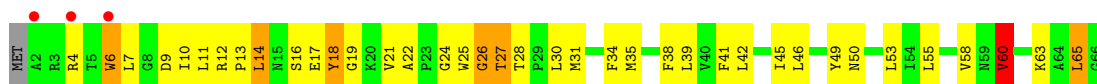
- Molecule 6: Cytochrome b559 subunit beta

Chain BF:



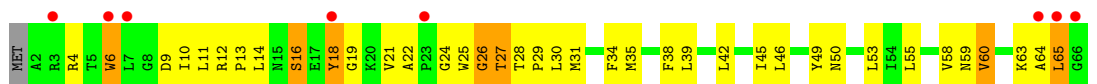
- Molecule 7: Photosystem II reaction center protein H

Chain AH:



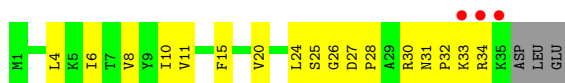
- Molecule 7: Photosystem II reaction center protein H

Chain BH:



- Molecule 8: Photosystem II reaction center protein I

Chain AI:



- Molecule 8: Photosystem II reaction center protein I

Chain BI:



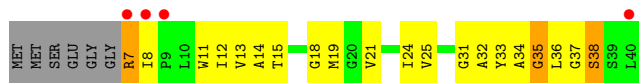
- Molecule 9: Photosystem II reaction center protein J

Chain AJ:



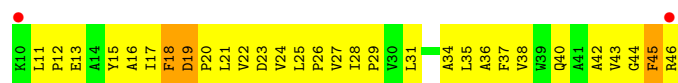
- Molecule 9: Photosystem II reaction center protein J

Chain BJ:



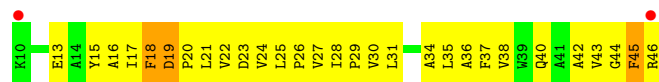
- Molecule 10: Photosystem II reaction center protein K

Chain AK: 



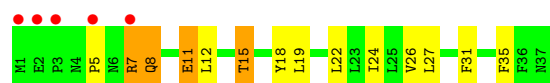
- Molecule 10: Photosystem II reaction center protein K

Chain BK: 



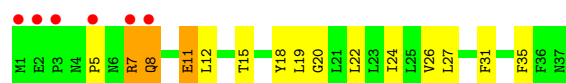
- Molecule 11: Photosystem II reaction center protein L

Chain AL: 



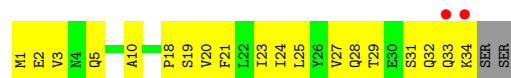
- Molecule 11: Photosystem II reaction center protein L

Chain BL: 



- Molecule 12: Photosystem II reaction center protein M

Chain AM: 



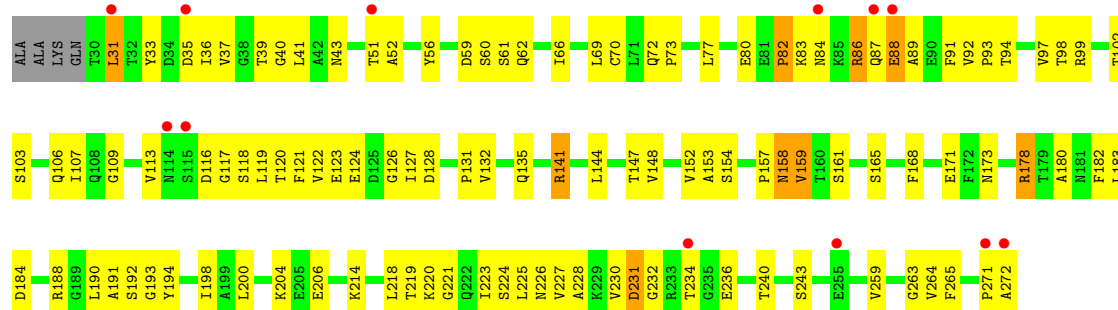
- Molecule 12: Photosystem II reaction center protein M

Chain BM: 

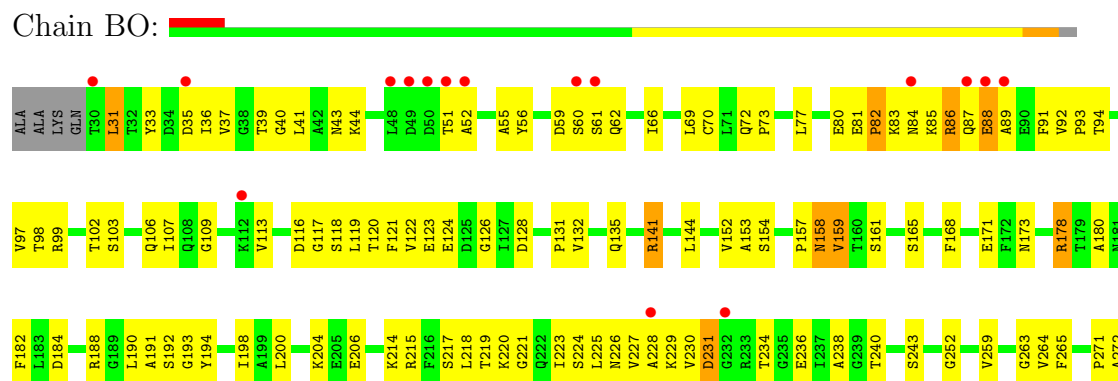


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain AO: 



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



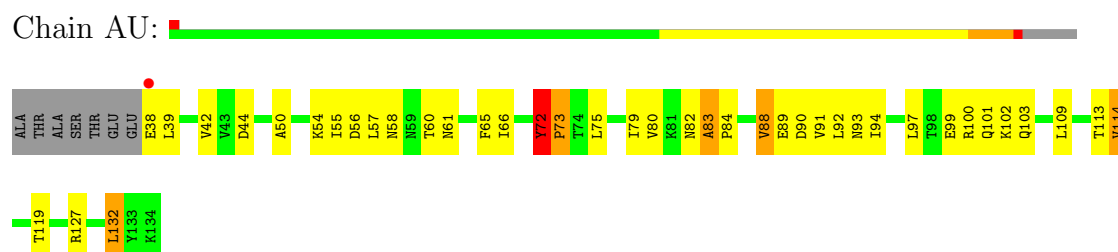
- Molecule 14: Photosystem II reaction center protein T



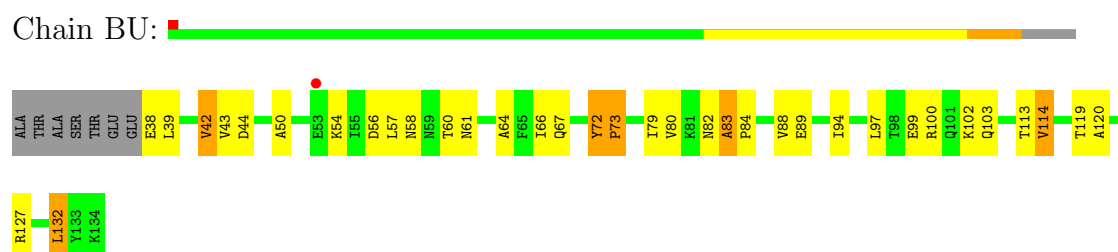
- Molecule 14: Photosystem II reaction center protein T



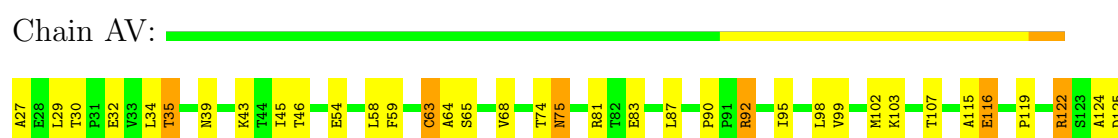
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550





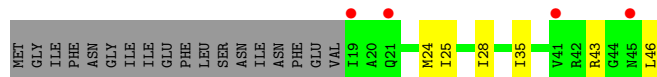
• Molecule 16: Cytochrome c-550

Chain BV:



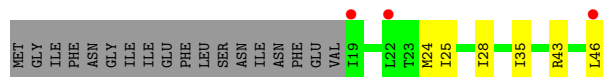
• Molecule 17: Protein ycf12

Chain Ay:



• Molecule 17: Protein ycf12

Chain By:



• Molecule 18: Photosystem II PsbX protein

Chain AX:



• Molecule 18: Photosystem II PsbX protein

Chain BX:



• Molecule 19: Photosystem II protein Y

Chain AY:



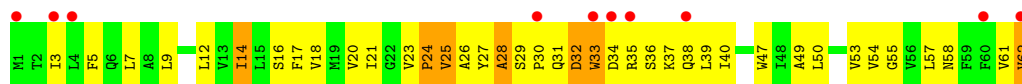
• Molecule 19: Photosystem II protein Y

Chain BY:



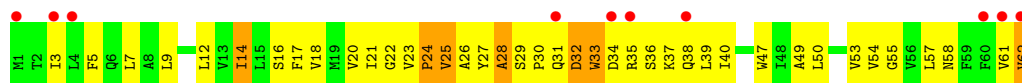
- Molecule 20: Photosystem II reaction center protein Z

Chain AZ:



- Molecule 20: Photosystem II reaction center protein Z

Chain BZ:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 10.00 – 2.90 20.00 – 2.90 | Depositor EDS |
| % Data completeness (in resolution range) | 97.7 (10.00-2.90) 99.3 (20.00-2.90) | Depositor EDS |
| R_{merge} | 0.09 | Depositor |
| R_{sym} | 0.10 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.81 (at 2.88Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.249 , 0.292 0.250 , 0.283 | Depositor DCC |
| R_{free} test set | 3869 reflections (2.04%) | DCC |
| Wilson B-factor (Å ²) | 78.2 | Xtriage |
| Anisotropy | 0.357 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.30 , 46.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 1 of 193457 reflections (0.001%) | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 50234 | wwPDB-VP |
| Average B, all atoms (Å ²) | 73.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, 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 | AA | 0.44 | 0/2713 | 0.66 | 0/3700 |
| 1 | BA | 0.43 | 0/2713 | 0.65 | 0/3700 |
| 2 | AB | 0.44 | 0/3986 | 0.67 | 3/5433 (0.1%) |
| 2 | BB | 0.43 | 0/3986 | 0.66 | 3/5433 (0.1%) |
| 3 | AC | 0.41 | 0/3556 | 0.64 | 1/4842 (0.0%) |
| 3 | BC | 0.39 | 0/3556 | 0.63 | 1/4842 (0.0%) |
| 4 | AD | 0.47 | 0/2801 | 0.65 | 0/3818 |
| 4 | BD | 0.45 | 0/2801 | 0.65 | 0/3818 |
| 5 | AE | 0.45 | 0/685 | 0.71 | 0/933 |
| 5 | BE | 0.45 | 0/685 | 0.70 | 0/933 |
| 6 | AF | 0.45 | 0/291 | 0.59 | 0/397 |
| 6 | BF | 0.47 | 0/291 | 0.57 | 0/397 |
| 7 | AH | 0.42 | 0/520 | 0.73 | 1/709 (0.1%) |
| 7 | BH | 0.40 | 0/520 | 0.72 | 1/709 (0.1%) |
| 8 | AI | 0.51 | 0/293 | 0.68 | 0/395 |
| 8 | BI | 0.50 | 0/293 | 0.67 | 0/395 |
| 9 | AJ | 0.43 | 0/255 | 0.69 | 0/346 |
| 9 | BJ | 0.45 | 0/255 | 0.66 | 0/346 |
| 10 | AK | 0.43 | 0/303 | 0.63 | 0/416 |
| 10 | BK | 0.44 | 0/303 | 0.61 | 0/416 |
| 11 | AL | 0.39 | 0/311 | 0.65 | 0/422 |
| 11 | BL | 0.41 | 0/311 | 0.65 | 0/422 |
| 12 | AM | 0.44 | 0/270 | 0.70 | 0/367 |
| 12 | BM | 0.45 | 0/270 | 0.67 | 0/367 |
| 13 | AO | 0.44 | 0/1876 | 0.70 | 0/2548 |
| 13 | BO | 0.43 | 0/1876 | 0.70 | 0/2548 |
| 14 | AT | 0.50 | 0/284 | 0.62 | 0/381 |
| 14 | BT | 0.48 | 0/284 | 0.62 | 0/381 |
| 15 | AU | 0.42 | 0/785 | 0.73 | 1/1064 (0.1%) |
| 15 | BU | 0.40 | 0/785 | 0.73 | 0/1064 |
| 16 | AV | 0.38 | 0/1081 | 0.65 | 0/1468 |
| 16 | BV | 0.37 | 0/1081 | 0.64 | 0/1468 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 17 | Ay | 0.46 | 0/202 | 0.73 | 0/272 |
| 17 | By | 0.41 | 0/202 | 0.74 | 0/272 |
| 18 | AX | 0.43 | 0/273 | 0.63 | 0/370 |
| 18 | BX | 0.41 | 0/273 | 0.63 | 0/370 |
| 20 | AZ | 0.45 | 0/490 | 0.69 | 0/669 |
| 20 | BZ | 0.47 | 0/490 | 0.70 | 0/669 |
| All | All | 0.43 | 0/41950 | 0.66 | 11/57100 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AA | 0 | 1 |
| 1 | BA | 0 | 1 |
| All | All | 0 | 2 |

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | BB | 486 | LEU | CA-CB-CG | 7.12 | 131.67 | 115.30 |
| 2 | AB | 486 | LEU | CA-CB-CG | 6.99 | 131.39 | 115.30 |
| 2 | AB | 488 | PRO | N-CA-C | 5.86 | 127.33 | 112.10 |
| 2 | AB | 489 | GLU | N-CA-C | 5.76 | 126.56 | 111.00 |
| 7 | AH | 65 | LEU | CA-CB-CG | 5.72 | 128.45 | 115.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | AA | 161 | TYR | Sidechain |
| 1 | BA | 161 | TYR | Sidechain |

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 2628 | 0 | 2524 | 179 | 0 |
| 1 | BA | 2628 | 0 | 2524 | 179 | 0 |
| 2 | AB | 3850 | 0 | 3718 | 224 | 0 |
| 2 | BB | 3850 | 0 | 3718 | 227 | 0 |
| 3 | AC | 3444 | 0 | 3365 | 258 | 0 |
| 3 | BC | 3444 | 0 | 3365 | 263 | 0 |
| 4 | AD | 2706 | 0 | 2608 | 177 | 0 |
| 4 | BD | 2706 | 0 | 2608 | 184 | 0 |
| 5 | AE | 666 | 0 | 651 | 71 | 0 |
| 5 | BE | 666 | 0 | 651 | 74 | 0 |
| 6 | AF | 282 | 0 | 291 | 28 | 0 |
| 6 | BF | 282 | 0 | 291 | 29 | 0 |
| 7 | AH | 507 | 0 | 521 | 52 | 0 |
| 7 | BH | 507 | 0 | 521 | 50 | 0 |
| 8 | AI | 286 | 0 | 308 | 15 | 0 |
| 8 | BI | 286 | 0 | 308 | 18 | 0 |
| 9 | AJ | 249 | 0 | 262 | 28 | 0 |
| 9 | BJ | 249 | 0 | 262 | 26 | 0 |
| 10 | AK | 293 | 0 | 305 | 42 | 0 |
| 10 | BK | 293 | 0 | 305 | 44 | 0 |
| 11 | AL | 304 | 0 | 316 | 15 | 0 |
| 11 | BL | 304 | 0 | 316 | 17 | 0 |
| 12 | AM | 267 | 0 | 289 | 27 | 0 |
| 12 | BM | 267 | 0 | 289 | 26 | 0 |
| 13 | AO | 1845 | 0 | 1801 | 115 | 0 |
| 13 | BO | 1845 | 0 | 1801 | 118 | 0 |
| 14 | AT | 275 | 0 | 288 | 21 | 0 |
| 14 | BT | 275 | 0 | 288 | 20 | 0 |
| 15 | AU | 774 | 0 | 773 | 46 | 0 |
| 15 | BU | 774 | 0 | 773 | 42 | 0 |
| 16 | AV | 1060 | 0 | 1068 | 42 | 0 |
| 16 | BV | 1060 | 0 | 1068 | 39 | 0 |
| 17 | Ay | 201 | 0 | 226 | 0 | 0 |
| 17 | By | 201 | 0 | 226 | 0 | 0 |
| 18 | AX | 270 | 0 | 299 | 27 | 0 |
| 18 | BX | 270 | 0 | 299 | 25 | 0 |
| 19 | AY | 140 | 0 | 32 | 4 | 0 |
| 19 | BY | 140 | 0 | 32 | 6 | 0 |
| 20 | AZ | 479 | 0 | 516 | 54 | 0 |
| 20 | BZ | 479 | 0 | 516 | 55 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 21 | AA | 1 | 0 | 0 | 0 | 0 |
| 21 | BA | 1 | 0 | 0 | 0 | 0 |
| 22 | AA | 260 | 0 | 288 | 18 | 0 |
| 22 | AB | 1040 | 0 | 1152 | 77 | 0 |
| 22 | AC | 845 | 0 | 936 | 61 | 0 |
| 22 | AD | 130 | 0 | 144 | 11 | 0 |
| 22 | BA | 260 | 0 | 288 | 18 | 0 |
| 22 | BB | 1040 | 0 | 1152 | 83 | 0 |
| 22 | BC | 845 | 0 | 936 | 62 | 0 |
| 22 | BD | 130 | 0 | 144 | 12 | 0 |
| 23 | AA | 64 | 0 | 74 | 5 | 0 |
| 23 | AD | 64 | 0 | 74 | 2 | 0 |
| 23 | BA | 64 | 0 | 74 | 5 | 0 |
| 23 | BD | 64 | 0 | 74 | 5 | 0 |
| 24 | AA | 45 | 0 | 61 | 5 | 0 |
| 24 | AD | 55 | 0 | 80 | 9 | 0 |
| 24 | AJ | 35 | 0 | 45 | 0 | 0 |
| 24 | BA | 45 | 0 | 61 | 6 | 0 |
| 24 | BD | 55 | 0 | 80 | 8 | 0 |
| 24 | BJ | 35 | 0 | 45 | 0 | 0 |
| 25 | AA | 5 | 0 | 0 | 0 | 0 |
| 25 | BA | 5 | 0 | 0 | 0 | 0 |
| 26 | AA | 40 | 0 | 56 | 6 | 0 |
| 26 | AB | 160 | 0 | 224 | 10 | 0 |
| 26 | AC | 80 | 0 | 112 | 15 | 0 |
| 26 | AD | 40 | 0 | 56 | 3 | 0 |
| 26 | AH | 40 | 0 | 56 | 5 | 0 |
| 26 | AJ | 40 | 0 | 56 | 5 | 0 |
| 26 | AK | 40 | 0 | 56 | 13 | 0 |
| 26 | AT | 40 | 0 | 56 | 8 | 0 |
| 26 | AZ | 40 | 0 | 56 | 5 | 0 |
| 26 | BA | 40 | 0 | 56 | 3 | 0 |
| 26 | BB | 120 | 0 | 168 | 5 | 0 |
| 26 | BC | 80 | 0 | 112 | 17 | 0 |
| 26 | BD | 40 | 0 | 56 | 3 | 0 |
| 26 | BJ | 40 | 0 | 56 | 5 | 0 |
| 26 | BK | 40 | 0 | 56 | 13 | 0 |
| 26 | BX | 40 | 0 | 56 | 6 | 0 |
| 26 | BZ | 40 | 0 | 56 | 5 | 0 |
| 27 | AA | 56 | 0 | 70 | 0 | 0 |
| 27 | AB | 52 | 0 | 62 | 3 | 0 |
| 27 | AC | 181 | 0 | 245 | 19 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 27 | AD | 63 | 0 | 87 | 0 | 0 |
| 27 | AH | 58 | 0 | 74 | 1 | 0 |
| 27 | BA | 56 | 0 | 70 | 0 | 0 |
| 27 | BB | 52 | 0 | 62 | 3 | 0 |
| 27 | BC | 181 | 0 | 245 | 21 | 0 |
| 27 | BD | 63 | 0 | 87 | 0 | 0 |
| 27 | BH | 58 | 0 | 74 | 1 | 0 |
| 28 | AA | 39 | 0 | 51 | 3 | 0 |
| 28 | AC | 37 | 0 | 44 | 5 | 0 |
| 28 | BA | 39 | 0 | 51 | 4 | 0 |
| 28 | BC | 37 | 0 | 44 | 4 | 0 |
| 29 | AA | 105 | 0 | 145 | 10 | 0 |
| 29 | AD | 43 | 0 | 49 | 2 | 0 |
| 29 | AF | 45 | 0 | 53 | 2 | 0 |
| 29 | BA | 105 | 0 | 145 | 6 | 0 |
| 29 | BB | 47 | 0 | 60 | 2 | 0 |
| 29 | BD | 43 | 0 | 49 | 2 | 0 |
| 29 | BF | 45 | 0 | 53 | 1 | 0 |
| 29 | BL | 47 | 0 | 60 | 2 | 0 |
| 30 | AA | 93 | 0 | 126 | 5 | 0 |
| 30 | AB | 140 | 0 | 190 | 4 | 0 |
| 30 | AC | 93 | 0 | 126 | 6 | 0 |
| 30 | AD | 94 | 0 | 128 | 9 | 0 |
| 30 | AE | 44 | 0 | 58 | 4 | 0 |
| 30 | AI | 43 | 0 | 56 | 3 | 0 |
| 30 | AM | 42 | 0 | 54 | 4 | 0 |
| 30 | BA | 51 | 0 | 72 | 2 | 0 |
| 30 | BB | 98 | 0 | 136 | 2 | 0 |
| 30 | BC | 93 | 0 | 126 | 8 | 0 |
| 30 | BD | 94 | 0 | 128 | 10 | 0 |
| 30 | BE | 44 | 0 | 58 | 4 | 0 |
| 30 | BI | 43 | 0 | 56 | 3 | 0 |
| 30 | BM | 42 | 0 | 54 | 4 | 0 |
| 31 | AA | 1 | 0 | 0 | 0 | 0 |
| 31 | BA | 1 | 0 | 0 | 0 | 0 |
| 32 | AB | 105 | 0 | 138 | 6 | 0 |
| 32 | AD | 31 | 0 | 35 | 2 | 0 |
| 32 | AI | 35 | 0 | 46 | 4 | 0 |
| 32 | AM | 35 | 0 | 46 | 1 | 0 |
| 32 | AT | 35 | 0 | 46 | 3 | 0 |
| 32 | BB | 105 | 0 | 138 | 5 | 0 |
| 32 | BD | 31 | 0 | 35 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 32 | BI | 35 | 0 | 46 | 3 | 0 |
| 32 | BM | 35 | 0 | 46 | 1 | 0 |
| 32 | BT | 35 | 0 | 46 | 3 | 0 |
| 33 | AD | 4 | 0 | 0 | 1 | 0 |
| 33 | BD | 4 | 0 | 0 | 1 | 0 |
| 34 | AE | 43 | 0 | 30 | 5 | 0 |
| 34 | AV | 43 | 0 | 30 | 3 | 0 |
| 34 | BE | 43 | 0 | 30 | 6 | 0 |
| 34 | BV | 43 | 0 | 30 | 3 | 0 |
| 35 | AK | 1 | 0 | 0 | 0 | 0 |
| 35 | AO | 1 | 0 | 0 | 0 | 0 |
| 35 | BK | 1 | 0 | 0 | 0 | 0 |
| 35 | BO | 1 | 0 | 0 | 0 | 0 |
| All | All | 50234 | 0 | 51364 | 2715 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

The worst 5 of 2715 close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 16:AV:63:CYS:SG | 34:AV:201:HEM:HAB | 1.85 | 1.16 |
| 15:BU:83:ALA:HB1 | 15:BU:84:PRO:HD2 | 1.23 | 1.16 |
| 9:AJ:15:THR:HG21 | 10:AK:38:VAL:HG13 | 1.23 | 1.16 |
| 16:BV:63:CYS:SG | 34:BV:201:HEM:HAB | 1.85 | 1.15 |
| 9:BJ:15:THR:HG21 | 10:BK:38:VAL:HG13 | 1.24 | 1.13 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | AA | 333/344 (97%) | 285 (86%) | 41 (12%) | 7 (2%) | 11 39 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | BA | 333/344 (97%) | 285 (86%) | 41 (12%) | 7 (2%) | 11 | 39 |
| 2 | AB | 488/510 (96%) | 417 (86%) | 57 (12%) | 14 (3%) | 7 | 28 |
| 2 | BB | 488/510 (96%) | 422 (86%) | 52 (11%) | 14 (3%) | 7 | 28 |
| 3 | AC | 445/473 (94%) | 371 (83%) | 58 (13%) | 16 (4%) | 5 | 22 |
| 3 | BC | 445/473 (94%) | 372 (84%) | 56 (13%) | 17 (4%) | 5 | 19 |
| 4 | AD | 338/352 (96%) | 286 (85%) | 43 (13%) | 9 (3%) | 8 | 30 |
| 4 | BD | 338/352 (96%) | 288 (85%) | 42 (12%) | 8 (2%) | 9 | 35 |
| 5 | AE | 80/84 (95%) | 71 (89%) | 5 (6%) | 4 (5%) | 3 | 11 |
| 5 | BE | 80/84 (95%) | 70 (88%) | 6 (8%) | 4 (5%) | 3 | 11 |
| 6 | AF | 33/45 (73%) | 24 (73%) | 8 (24%) | 1 (3%) | 7 | 27 |
| 6 | BF | 33/45 (73%) | 24 (73%) | 8 (24%) | 1 (3%) | 7 | 27 |
| 7 | AH | 63/66 (96%) | 47 (75%) | 10 (16%) | 6 (10%) | 1 | 2 |
| 7 | BH | 63/66 (96%) | 48 (76%) | 11 (18%) | 4 (6%) | 2 | 6 |
| 8 | AI | 33/38 (87%) | 20 (61%) | 11 (33%) | 2 (6%) | 2 | 7 |
| 8 | BI | 33/38 (87%) | 21 (64%) | 10 (30%) | 2 (6%) | 2 | 7 |
| 9 | AJ | 32/40 (80%) | 26 (81%) | 4 (12%) | 2 (6%) | 2 | 6 |
| 9 | BJ | 32/40 (80%) | 26 (81%) | 4 (12%) | 2 (6%) | 2 | 6 |
| 10 | AK | 35/37 (95%) | 28 (80%) | 5 (14%) | 2 (6%) | 3 | 8 |
| 10 | BK | 35/37 (95%) | 28 (80%) | 5 (14%) | 2 (6%) | 3 | 8 |
| 11 | AL | 35/37 (95%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 11 | BL | 35/37 (95%) | 33 (94%) | 2 (6%) | 0 | 100 | 100 |
| 12 | AM | 32/36 (89%) | 23 (72%) | 9 (28%) | 0 | 100 | 100 |
| 12 | BM | 32/36 (89%) | 24 (75%) | 8 (25%) | 0 | 100 | 100 |
| 13 | AO | 241/247 (98%) | 199 (83%) | 30 (12%) | 12 (5%) | 3 | 11 |
| 13 | BO | 241/247 (98%) | 199 (83%) | 31 (13%) | 11 (5%) | 4 | 14 |
| 14 | AT | 30/32 (94%) | 25 (83%) | 4 (13%) | 1 (3%) | 6 | 24 |
| 14 | BT | 30/32 (94%) | 25 (83%) | 4 (13%) | 1 (3%) | 6 | 24 |
| 15 | AU | 95/104 (91%) | 79 (83%) | 12 (13%) | 4 (4%) | 4 | 16 |
| 15 | BU | 95/104 (91%) | 79 (83%) | 12 (13%) | 4 (4%) | 4 | 16 |
| 16 | AV | 135/137 (98%) | 111 (82%) | 23 (17%) | 1 (1%) | 30 | 72 |
| 16 | BV | 135/137 (98%) | 112 (83%) | 22 (16%) | 1 (1%) | 30 | 72 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 17 | Ay | 26/46 (56%) | 14 (54%) | 8 (31%) | 4 (15%) | 0 | 1 |
| 17 | By | 26/46 (56%) | 14 (54%) | 8 (31%) | 4 (15%) | 0 | 1 |
| 18 | AX | 35/50 (70%) | 26 (74%) | 5 (14%) | 4 (11%) | 1 | 1 |
| 18 | BX | 35/50 (70%) | 27 (77%) | 4 (11%) | 4 (11%) | 1 | 1 |
| 20 | AZ | 60/62 (97%) | 48 (80%) | 9 (15%) | 3 (5%) | 3 | 11 |
| 20 | BZ | 60/62 (97%) | 48 (80%) | 9 (15%) | 3 (5%) | 3 | 11 |
| All | All | 5138/5480 (94%) | 4278 (83%) | 679 (13%) | 181 (4%) | 6 | 23 |

5 of 181 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | AA | 12 | ASN |
| 1 | AA | 141 | PRO |
| 1 | AA | 142 | TRP |
| 2 | AB | 176 | GLY |
| 2 | AB | 230 | ARG |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | AA | 271/280 (97%) | 258 (95%) | 13 (5%) | 35 | 74 |
| 1 | BA | 271/280 (97%) | 259 (96%) | 12 (4%) | 39 | 77 |
| 2 | AB | 390/407 (96%) | 374 (96%) | 16 (4%) | 41 | 80 |
| 2 | BB | 390/407 (96%) | 373 (96%) | 17 (4%) | 39 | 77 |
| 3 | AC | 347/374 (93%) | 329 (95%) | 18 (5%) | 32 | 71 |
| 3 | BC | 347/374 (93%) | 329 (95%) | 18 (5%) | 32 | 71 |
| 4 | AD | 275/283 (97%) | 256 (93%) | 19 (7%) | 22 | 54 |
| 4 | BD | 275/283 (97%) | 256 (93%) | 19 (7%) | 22 | 54 |
| 5 | AE | 72/73 (99%) | 66 (92%) | 6 (8%) | 16 | 43 |
| 5 | BE | 72/73 (99%) | 66 (92%) | 6 (8%) | 16 | 43 |
| 6 | AF | 29/39 (74%) | 29 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 6 | BF | 29/39 (74%) | 29 (100%) | 0 | 100 | 100 |
| 7 | AH | 53/55 (96%) | 50 (94%) | 3 (6%) | 29 | 66 |
| 7 | BH | 53/55 (96%) | 50 (94%) | 3 (6%) | 29 | 66 |
| 8 | AI | 32/35 (91%) | 31 (97%) | 1 (3%) | 52 | 88 |
| 8 | BI | 32/35 (91%) | 31 (97%) | 1 (3%) | 52 | 88 |
| 9 | AJ | 24/28 (86%) | 23 (96%) | 1 (4%) | 40 | 79 |
| 9 | BJ | 24/28 (86%) | 23 (96%) | 1 (4%) | 40 | 79 |
| 10 | AK | 30/30 (100%) | 28 (93%) | 2 (7%) | 23 | 56 |
| 10 | BK | 30/30 (100%) | 28 (93%) | 2 (7%) | 23 | 56 |
| 11 | AL | 35/35 (100%) | 31 (89%) | 4 (11%) | 8 | 24 |
| 11 | BL | 35/35 (100%) | 32 (91%) | 3 (9%) | 15 | 41 |
| 12 | AM | 31/33 (94%) | 31 (100%) | 0 | 100 | 100 |
| 12 | BM | 31/33 (94%) | 31 (100%) | 0 | 100 | 100 |
| 13 | AO | 202/208 (97%) | 195 (96%) | 7 (4%) | 48 | 85 |
| 13 | BO | 202/208 (97%) | 194 (96%) | 8 (4%) | 42 | 81 |
| 14 | AT | 29/29 (100%) | 28 (97%) | 1 (3%) | 49 | 86 |
| 14 | BT | 29/29 (100%) | 28 (97%) | 1 (3%) | 49 | 86 |
| 15 | AU | 84/89 (94%) | 80 (95%) | 4 (5%) | 35 | 74 |
| 15 | BU | 84/89 (94%) | 80 (95%) | 4 (5%) | 35 | 74 |
| 16 | AV | 116/117 (99%) | 111 (96%) | 5 (4%) | 40 | 78 |
| 16 | BV | 116/117 (99%) | 111 (96%) | 5 (4%) | 40 | 78 |
| 17 | Ay | 20/37 (54%) | 18 (90%) | 2 (10%) | 11 | 32 |
| 17 | By | 20/37 (54%) | 18 (90%) | 2 (10%) | 11 | 32 |
| 18 | AX | 30/42 (71%) | 26 (87%) | 4 (13%) | 6 | 16 |
| 18 | BX | 30/42 (71%) | 26 (87%) | 4 (13%) | 6 | 16 |
| 20 | AZ | 52/52 (100%) | 47 (90%) | 5 (10%) | 12 | 35 |
| 20 | BZ | 52/52 (100%) | 47 (90%) | 5 (10%) | 12 | 35 |
| All | All | 4244/4492 (94%) | 4022 (95%) | 222 (5%) | 32 | 71 |

5 of 222 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17 | Ay | 28 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | BB | 18 | ARG |
| 15 | BU | 132 | LEU |
| 18 | AX | 12 | ILE |
| 1 | BA | 32 | TRP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15 | AU | 93 | ASN |
| 1 | BA | 241 | GLN |
| 13 | BO | 222 | GLN |
| 17 | Ay | 21 | GLN |
| 1 | BA | 12 | ASN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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 |
| 22 | CLA | AA | 402 | 1 | 73,73,73 | 1.53 | 10 (13%) | 96,113,113 | 1.60 | 19 (19%) |
| 22 | CLA | AA | 403 | - | 73,73,73 | 1.55 | 10 (13%) | 96,113,113 | 1.72 | 17 (17%) |
| 22 | CLA | AA | 404 | - | 73,73,73 | 1.45 | 8 (10%) | 96,113,113 | 1.51 | 17 (17%) |
| 23 | PHO | AA | 405 | - | 69,69,69 | 1.86 | 3 (4%) | 92,99,99 | 1.56 | 17 (18%) |
| 22 | CLA | AA | 406 | 1 | 73,73,73 | 1.45 | 8 (10%) | 96,113,113 | 1.52 | 18 (18%) |
| 24 | PL9 | AA | 407 | - | 45,45,55 | 1.00 | 2 (4%) | 55,57,69 | 1.87 | 15 (27%) |
| 25 | OEC | AA | 408 | 1,3 | 0,0,13 | 0.00 | - | 0,0,27 | 0.00 | - |
| 26 | BCR | AA | 409 | - | 41,41,41 | 1.61 | 7 (17%) | 56,56,56 | 2.07 | 20 (35%) |
| 27 | DGD | AA | 410 | - | 57,57,67 | 2.09 | 14 (24%) | 71,71,81 | 1.47 | 9 (12%) |
| 28 | LHG | AA | 411 | - | 38,38,48 | 1.96 | 6 (15%) | 44,44,54 | 1.31 | 4 (9%) |
| 29 | SQD | AA | 412 | - | 51,51,54 | 6.74 | 27 (52%) | 62,62,65 | 3.25 | 21 (33%) |
| 30 | LMG | AA | 413 | - | 51,51,55 | 1.42 | 4 (7%) | 59,59,63 | 1.01 | 4 (6%) |
| 29 | SQD | AA | 415 | - | 54,54,54 | 2.79 | 29 (53%) | 65,65,65 | 2.96 | 19 (29%) |
| 30 | LMG | AA | 416 | - | 42,42,55 | 2.22 | 10 (23%) | 50,50,63 | 1.01 | 3 (6%) |
| 22 | CLA | AB | 601 | - | 73,73,73 | 1.74 | 11 (15%) | 96,113,113 | 1.53 | 19 (19%) |
| 22 | CLA | AB | 602 | 2 | 73,73,73 | 1.52 | 11 (15%) | 96,113,113 | 1.52 | 18 (18%) |
| 22 | CLA | AB | 603 | 2 | 73,73,73 | 1.52 | 8 (10%) | 96,113,113 | 1.58 | 17 (17%) |
| 22 | CLA | AB | 604 | 2 | 73,73,73 | 1.64 | 9 (12%) | 96,113,113 | 1.52 | 19 (19%) |
| 22 | CLA | AB | 605 | - | 73,73,73 | 1.61 | 11 (15%) | 96,113,113 | 1.53 | 17 (17%) |
| 22 | CLA | AB | 606 | 2 | 73,73,73 | 1.54 | 10 (13%) | 96,113,113 | 1.51 | 18 (18%) |
| 22 | CLA | AB | 607 | - | 73,73,73 | 1.58 | 12 (16%) | 96,113,113 | 1.58 | 17 (17%) |
| 22 | CLA | AB | 608 | 2 | 73,73,73 | 1.55 | 9 (12%) | 96,113,113 | 1.58 | 19 (19%) |
| 22 | CLA | AB | 609 | 2 | 73,73,73 | 1.70 | 13 (17%) | 96,113,113 | 1.53 | 19 (19%) |
| 22 | CLA | AB | 610 | - | 73,73,73 | 1.52 | 9 (12%) | 96,113,113 | 1.57 | 23 (23%) |
| 22 | CLA | AB | 611 | 2 | 73,73,73 | 1.50 | 7 (9%) | 96,113,113 | 1.53 | 17 (17%) |
| 22 | CLA | AB | 612 | - | 73,73,73 | 1.55 | 9 (12%) | 96,113,113 | 1.56 | 20 (20%) |
| 22 | CLA | AB | 613 | - | 73,73,73 | 1.48 | 7 (9%) | 96,113,113 | 1.53 | 20 (20%) |
| 22 | CLA | AB | 614 | 2 | 73,73,73 | 1.62 | 11 (15%) | 96,113,113 | 1.61 | 24 (25%) |
| 22 | CLA | AB | 615 | - | 73,73,73 | 1.66 | 13 (17%) | 96,113,113 | 1.59 | 20 (20%) |
| 22 | CLA | AB | 616 | - | 73,73,73 | 1.59 | 10 (13%) | 96,113,113 | 1.61 | 21 (21%) |
| 26 | BCR | AB | 617 | - | 41,41,41 | 1.68 | 7 (17%) | 56,56,56 | 1.96 | 14 (25%) |
| 26 | BCR | AB | 618 | - | 41,41,41 | 1.68 | 6 (14%) | 56,56,56 | 2.18 | 27 (48%) |
| 26 | BCR | AB | 619 | - | 41,41,41 | 1.91 | 8 (19%) | 56,56,56 | 2.06 | 15 (26%) |
| 26 | BCR | AB | 620 | - | 41,41,41 | 1.83 | 7 (17%) | 56,56,56 | 2.03 | 17 (30%) |
| 30 | LMG | AB | 621 | - | 49,49,55 | 1.53 | 7 (14%) | 57,57,63 | 1.05 | 4 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 30 | LMG | AB | 622 | - | 49,49,55 | 1.82 | 6 (12%) | 57,57,63 | 1.06 | 4 (7%) |
| 30 | LMG | AB | 623 | - | 42,42,55 | 2.12 | 9 (21%) | 50,50,63 | 1.03 | 3 (6%) |
| 32 | LMT | AB | 624 | - | 36,36,36 | 1.42 | 5 (13%) | 47,47,47 | 1.20 | 3 (6%) |
| 32 | LMT | AB | 625 | - | 36,36,36 | 1.36 | 7 (19%) | 47,47,47 | 0.96 | 3 (6%) |
| 27 | DGD | AB | 626 | - | 53,53,67 | 2.59 | 18 (33%) | 67,67,81 | 1.66 | 8 (11%) |
| 32 | LMT | AB | 627 | - | 36,36,36 | 1.44 | 5 (13%) | 47,47,47 | 1.03 | 3 (6%) |
| 22 | CLA | AC | 501 | 3 | 73,73,73 | 1.52 | 6 (8%) | 96,113,113 | 1.54 | 19 (19%) |
| 22 | CLA | AC | 502 | 3 | 73,73,73 | 1.56 | 11 (15%) | 96,113,113 | 1.51 | 17 (17%) |
| 22 | CLA | AC | 503 | 3 | 73,73,73 | 1.70 | 11 (15%) | 96,113,113 | 1.52 | 17 (17%) |
| 22 | CLA | AC | 504 | - | 73,73,73 | 1.62 | 9 (12%) | 96,113,113 | 1.57 | 17 (17%) |
| 22 | CLA | AC | 505 | 3 | 73,73,73 | 1.68 | 10 (13%) | 96,113,113 | 1.60 | 19 (19%) |
| 22 | CLA | AC | 506 | 3 | 73,73,73 | 1.54 | 10 (13%) | 96,113,113 | 1.55 | 18 (18%) |
| 22 | CLA | AC | 507 | - | 73,73,73 | 1.43 | 10 (13%) | 96,113,113 | 1.56 | 21 (21%) |
| 22 | CLA | AC | 508 | 3 | 73,73,73 | 1.62 | 12 (16%) | 96,113,113 | 1.58 | 20 (20%) |
| 22 | CLA | AC | 509 | - | 73,73,73 | 1.61 | 10 (13%) | 96,113,113 | 1.59 | 19 (19%) |
| 22 | CLA | AC | 510 | - | 73,73,73 | 1.61 | 11 (15%) | 96,113,113 | 1.55 | 19 (19%) |
| 22 | CLA | AC | 511 | 3 | 73,73,73 | 1.71 | 10 (13%) | 96,113,113 | 1.55 | 18 (18%) |
| 22 | CLA | AC | 512 | - | 73,73,73 | 1.73 | 13 (17%) | 96,113,113 | 1.61 | 21 (21%) |
| 22 | CLA | AC | 513 | 3 | 73,73,73 | 1.68 | 10 (13%) | 96,113,113 | 1.53 | 19 (19%) |
| 26 | BCR | AC | 514 | - | 41,41,41 | 1.74 | 6 (14%) | 56,56,56 | 2.11 | 22 (39%) |
| 26 | BCR | AC | 515 | - | 41,41,41 | 1.66 | 6 (14%) | 56,56,56 | 2.14 | 18 (32%) |
| 27 | DGD | AC | 516 | - | 54,54,67 | 1.58 | 10 (18%) | 68,68,81 | 1.60 | 8 (11%) |
| 27 | DGD | AC | 517 | - | 63,63,67 | 1.29 | 6 (9%) | 77,77,81 | 1.64 | 8 (10%) |
| 27 | DGD | AC | 518 | - | 67,67,67 | 1.02 | 6 (8%) | 81,81,81 | 1.27 | 4 (4%) |
| 30 | LMG | AC | 519 | - | 48,48,55 | 1.90 | 7 (14%) | 56,56,63 | 0.88 | 3 (5%) |
| 30 | LMG | AC | 520 | - | 45,45,55 | 2.01 | 10 (22%) | 53,53,63 | 1.04 | 4 (7%) |
| 28 | LHG | AC | 521 | - | 36,36,48 | 1.73 | 4 (11%) | 42,42,54 | 1.10 | 3 (7%) |
| 33 | BCT | AD | 401 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 22 | CLA | AD | 402 | 4 | 73,73,73 | 1.65 | 11 (15%) | 96,113,113 | 1.55 | 19 (19%) |
| 23 | PHO | AD | 403 | - | 69,69,69 | 1.96 | 4 (5%) | 92,99,99 | 1.59 | 16 (17%) |
| 22 | CLA | AD | 404 | - | 73,73,73 | 1.67 | 10 (13%) | 96,113,113 | 1.54 | 18 (18%) |
| 24 | PL9 | AD | 405 | - | 55,55,55 | 0.54 | 0 | 69,69,69 | 1.87 | 18 (26%) |
| 26 | BCR | AD | 406 | - | 41,41,41 | 1.82 | 7 (17%) | 56,56,56 | 2.27 | 18 (32%) |
| 30 | LMG | AD | 407 | - | 46,46,55 | 2.08 | 6 (13%) | 54,54,63 | 0.93 | 2 (3%) |
| 30 | LMG | AD | 408 | - | 48,48,55 | 1.68 | 5 (10%) | 56,56,63 | 1.04 | 3 (5%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|-------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 29 | SQD | AD | 409 | - | 43,43,54 | 7.74 | 23 (53%) | 54,54,65 | 3.66 | 18 (33%) |
| 27 | DGD | AD | 410 | - | 64,64,67 | 1.91 | 18 (28%) | 78,78,81 | 1.43 | 7 (8%) |
| 32 | LMT | AD | 411 | - | 32,32,36 | 1.72 | 5 (15%) | 43,43,47 | 1.01 | 2 (4%) |
| 34 | HEM | AE | 101 | 5,6 | 50,50,50 | 2.54 | 26 (52%) | 46,82,82 | 2.51 | 11 (23%) |
| 30 | LMG | AE | 102 | - | 44,44,55 | 1.89 | 7 (15%) | 52,52,63 | 1.12 | 6 (11%) |
| 29 | SQD | AF | 101 | - | 45,45,54 | 10.21 | 25 (55%) | 56,56,65 | 3.43 | 20 (35%) |
| 26 | BCR | AH | 101 | - | 41,41,41 | 1.85 | 8 (19%) | 56,56,56 | 2.23 | 21 (37%) |
| 27 | DGD | AH | 102 | - | 59,59,67 | 2.11 | 10 (16%) | 73,73,81 | 1.47 | 7 (9%) |
| 30 | LMG | AI | 101 | - | 43,43,55 | 2.18 | 10 (23%) | 51,51,63 | 1.09 | 4 (7%) |
| 32 | LMT | AI | 102 | - | 36,36,36 | 1.40 | 4 (11%) | 47,47,47 | 0.95 | 1 (2%) |
| 24 | PL9 | AJ | 101 | - | 35,35,55 | 1.40 | 5 (14%) | 43,45,69 | 1.95 | 13 (30%) |
| 26 | BCR | AJ | 102 | - | 41,41,41 | 2.04 | 8 (19%) | 56,56,56 | 3.25 | 22 (39%) |
| 26 | BCR | AK | 102 | - | 41,41,41 | 1.83 | 7 (17%) | 56,56,56 | 2.50 | 24 (42%) |
| 30 | LMG | AM | 101 | - | 42,42,55 | 2.34 | 8 (19%) | 50,50,63 | 1.22 | 5 (10%) |
| 32 | LMT | AM | 102 | - | 36,36,36 | 1.17 | 2 (5%) | 47,47,47 | 0.94 | 2 (4%) |
| 32 | LMT | AT | 101 | - | 36,36,36 | 1.35 | 5 (13%) | 47,47,47 | 1.09 | 4 (8%) |
| 26 | BCR | AT | 102 | - | 41,41,41 | 1.60 | 6 (14%) | 56,56,56 | 2.18 | 24 (42%) |
| 34 | HEM | AV | 201 | 16 | 50,50,50 | 2.57 | 23 (46%) | 46,82,82 | 2.39 | 13 (28%) |
| 26 | BCR | AZ | 101 | - | 41,41,41 | 1.81 | 7 (17%) | 56,56,56 | 2.06 | 18 (32%) |
| 29 | SQD | BA | 401 | - | 54,54,54 | 2.85 | 30 (55%) | 65,65,65 | 3.00 | 21 (32%) |
| 22 | CLA | BA | 403 | 1 | 73,73,73 | 1.54 | 11 (15%) | 96,113,113 | 1.57 | 16 (16%) |
| 22 | CLA | BA | 404 | - | 73,73,73 | 1.54 | 8 (10%) | 96,113,113 | 1.75 | 20 (20%) |
| 22 | CLA | BA | 405 | - | 73,73,73 | 1.49 | 9 (12%) | 96,113,113 | 1.52 | 17 (17%) |
| 23 | PHO | BA | 406 | - | 69,69,69 | 1.97 | 6 (8%) | 92,99,99 | 1.55 | 18 (19%) |
| 22 | CLA | BA | 407 | 1 | 73,73,73 | 1.46 | 10 (13%) | 96,113,113 | 1.53 | 18 (18%) |
| 24 | PL9 | BA | 408 | - | 45,45,55 | 1.06 | 3 (6%) | 55,57,69 | 1.80 | 15 (27%) |
| 25 | OEC | BA | 409 | 1,3 | 0,0,13 | 0.00 | - | 0,0,27 | 0.00 | - |
| 26 | BCR | BA | 410 | - | 41,41,41 | 1.68 | 7 (17%) | 56,56,56 | 2.06 | 21 (37%) |
| 27 | DGD | BA | 411 | - | 57,57,67 | 2.18 | 14 (24%) | 71,71,81 | 1.47 | 8 (11%) |
| 28 | LHG | BA | 412 | - | 38,38,48 | 1.87 | 7 (18%) | 44,44,54 | 1.29 | 4 (9%) |
| 29 | SQD | BA | 413 | - | 51,51,54 | 6.87 | 26 (50%) | 62,62,65 | 3.19 | 22 (35%) |
| 30 | LMG | BA | 414 | - | 51,51,55 | 1.32 | 5 (9%) | 59,59,63 | 1.03 | 4 (6%) |
| 29 | SQD | BB | 601 | - | 47,47,54 | 3.19 | 24 (51%) | 58,58,65 | 3.31 | 16 (27%) |
| 27 | DGD | BB | 602 | - | 53,53,67 | 2.50 | 19 (35%) | 67,67,81 | 1.64 | 8 (11%) |
| 32 | LMT | BB | 603 | - | 36,36,36 | 1.42 | 7 (19%) | 47,47,47 | 1.05 | 3 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | BB | 604 | - | 73,73,73 | 1.77 | 11 (15%) | 96,113,113 | 1.54 | 19 (19%) |
| 22 | CLA | BB | 605 | 2 | 73,73,73 | 1.50 | 11 (15%) | 96,113,113 | 1.54 | 17 (17%) |
| 22 | CLA | BB | 606 | 2 | 73,73,73 | 1.49 | 9 (12%) | 96,113,113 | 1.59 | 18 (18%) |
| 22 | CLA | BB | 607 | 2 | 73,73,73 | 1.68 | 11 (15%) | 96,113,113 | 1.52 | 18 (18%) |
| 22 | CLA | BB | 608 | 2 | 73,73,73 | 1.54 | 9 (12%) | 96,113,113 | 1.52 | 16 (16%) |
| 22 | CLA | BB | 609 | 2 | 73,73,73 | 1.58 | 6 (8%) | 96,113,113 | 1.52 | 18 (18%) |
| 22 | CLA | BB | 610 | - | 73,73,73 | 1.60 | 12 (16%) | 96,113,113 | 1.58 | 18 (18%) |
| 22 | CLA | BB | 611 | 2 | 73,73,73 | 1.59 | 12 (16%) | 96,113,113 | 1.57 | 19 (19%) |
| 22 | CLA | BB | 612 | 2 | 73,73,73 | 1.65 | 12 (16%) | 96,113,113 | 1.53 | 17 (17%) |
| 22 | CLA | BB | 613 | - | 73,73,73 | 1.55 | 11 (15%) | 96,113,113 | 1.56 | 23 (23%) |
| 22 | CLA | BB | 614 | 2 | 73,73,73 | 1.41 | 8 (10%) | 96,113,113 | 1.52 | 17 (17%) |
| 22 | CLA | BB | 615 | - | 73,73,73 | 1.57 | 11 (15%) | 96,113,113 | 1.55 | 18 (18%) |
| 22 | CLA | BB | 616 | - | 73,73,73 | 1.40 | 6 (8%) | 96,113,113 | 1.54 | 20 (20%) |
| 22 | CLA | BB | 617 | 2 | 73,73,73 | 1.59 | 10 (13%) | 96,113,113 | 1.60 | 23 (23%) |
| 22 | CLA | BB | 618 | - | 73,73,73 | 1.61 | 10 (13%) | 96,113,113 | 1.56 | 19 (19%) |
| 22 | CLA | BB | 619 | - | 73,73,73 | 1.59 | 11 (15%) | 96,113,113 | 1.63 | 21 (21%) |
| 26 | BCR | BB | 620 | - | 41,41,41 | 1.55 | 8 (19%) | 56,56,56 | 1.97 | 14 (25%) |
| 26 | BCR | BB | 621 | - | 41,41,41 | 1.84 | 7 (17%) | 56,56,56 | 2.10 | 16 (28%) |
| 26 | BCR | BB | 622 | - | 41,41,41 | 1.79 | 7 (17%) | 56,56,56 | 2.03 | 18 (32%) |
| 30 | LMG | BB | 623 | - | 49,49,55 | 1.50 | 7 (14%) | 57,57,63 | 1.07 | 4 (7%) |
| 30 | LMG | BB | 624 | - | 49,49,55 | 1.80 | 6 (12%) | 57,57,63 | 1.04 | 3 (5%) |
| 32 | LMT | BB | 625 | - | 36,36,36 | 1.53 | 8 (22%) | 47,47,47 | 1.23 | 3 (6%) |
| 32 | LMT | BB | 626 | - | 36,36,36 | 1.34 | 5 (13%) | 47,47,47 | 0.94 | 2 (4%) |
| 22 | CLA | BC | 501 | 3 | 73,73,73 | 1.55 | 8 (10%) | 96,113,113 | 1.54 | 17 (17%) |
| 22 | CLA | BC | 502 | 3 | 73,73,73 | 1.55 | 11 (15%) | 96,113,113 | 1.53 | 16 (16%) |
| 22 | CLA | BC | 503 | 3 | 73,73,73 | 1.72 | 11 (15%) | 96,113,113 | 1.51 | 20 (20%) |
| 22 | CLA | BC | 504 | - | 73,73,73 | 1.66 | 10 (13%) | 96,113,113 | 1.58 | 16 (16%) |
| 22 | CLA | BC | 505 | 3 | 73,73,73 | 1.74 | 10 (13%) | 96,113,113 | 1.60 | 19 (19%) |
| 22 | CLA | BC | 506 | 3 | 73,73,73 | 1.49 | 8 (10%) | 96,113,113 | 1.52 | 18 (18%) |
| 22 | CLA | BC | 507 | - | 73,73,73 | 1.45 | 8 (10%) | 96,113,113 | 1.57 | 20 (20%) |
| 22 | CLA | BC | 508 | 3 | 73,73,73 | 1.66 | 12 (16%) | 96,113,113 | 1.57 | 20 (20%) |
| 22 | CLA | BC | 509 | - | 73,73,73 | 1.67 | 13 (17%) | 96,113,113 | 1.60 | 19 (19%) |
| 22 | CLA | BC | 510 | - | 73,73,73 | 1.54 | 10 (13%) | 96,113,113 | 1.56 | 18 (18%) |
| 22 | CLA | BC | 511 | 3 | 73,73,73 | 1.72 | 9 (12%) | 96,113,113 | 1.55 | 20 (20%) |
| 22 | CLA | BC | 512 | - | 73,73,73 | 1.73 | 11 (15%) | 96,113,113 | 1.60 | 22 (22%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|-------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 22 | CLA | BC | 513 | 3 | 73,73,73 | 1.65 | 11 (15%) | 96,113,113 | 1.53 | 18 (18%) |
| 26 | BCR | BC | 514 | - | 41,41,41 | 1.87 | 7 (17%) | 56,56,56 | 2.10 | 20 (35%) |
| 26 | BCR | BC | 515 | - | 41,41,41 | 1.79 | 7 (17%) | 56,56,56 | 2.12 | 19 (33%) |
| 27 | DGD | BC | 516 | - | 54,54,67 | 1.63 | 11 (20%) | 68,68,81 | 1.56 | 8 (11%) |
| 27 | DGD | BC | 517 | - | 63,63,67 | 1.24 | 7 (11%) | 77,77,81 | 1.64 | 8 (10%) |
| 27 | DGD | BC | 518 | - | 67,67,67 | 1.14 | 6 (8%) | 81,81,81 | 1.27 | 4 (4%) |
| 30 | LMG | BC | 519 | - | 48,48,55 | 2.02 | 8 (16%) | 56,56,63 | 0.88 | 3 (5%) |
| 30 | LMG | BC | 520 | - | 45,45,55 | 2.14 | 12 (26%) | 53,53,63 | 1.06 | 4 (7%) |
| 28 | LHG | BC | 521 | - | 36,36,48 | 1.71 | 4 (11%) | 42,42,54 | 1.10 | 3 (7%) |
| 33 | BCT | BD | 401 | 21 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 22 | CLA | BD | 402 | 4 | 73,73,73 | 1.66 | 9 (12%) | 96,113,113 | 1.54 | 20 (20%) |
| 23 | PHO | BD | 403 | - | 69,69,69 | 1.94 | 4 (5%) | 92,99,99 | 1.60 | 18 (19%) |
| 22 | CLA | BD | 404 | - | 73,73,73 | 1.71 | 12 (16%) | 96,113,113 | 1.50 | 15 (15%) |
| 24 | PL9 | BD | 405 | - | 55,55,55 | 0.51 | 0 | 69,69,69 | 1.89 | 18 (26%) |
| 26 | BCR | BD | 406 | - | 41,41,41 | 1.90 | 8 (19%) | 56,56,56 | 2.26 | 20 (35%) |
| 30 | LMG | BD | 407 | - | 46,46,55 | 1.65 | 6 (13%) | 54,54,63 | 0.95 | 2 (3%) |
| 30 | LMG | BD | 408 | - | 48,48,55 | 1.61 | 4 (8%) | 56,56,63 | 1.03 | 3 (5%) |
| 29 | SQD | BD | 409 | - | 43,43,54 | 7.63 | 23 (53%) | 54,54,65 | 3.63 | 19 (35%) |
| 27 | DGD | BD | 410 | - | 64,64,67 | 1.82 | 18 (28%) | 78,78,81 | 1.43 | 7 (8%) |
| 32 | LMT | BD | 411 | - | 32,32,36 | 1.62 | 5 (15%) | 43,43,47 | 0.96 | 2 (4%) |
| 34 | HEM | BE | 101 | 5,6 | 50,50,50 | 2.60 | 26 (52%) | 46,82,82 | 2.56 | 14 (30%) |
| 30 | LMG | BE | 102 | - | 44,44,55 | 1.97 | 8 (18%) | 52,52,63 | 1.12 | 5 (9%) |
| 29 | SQD | BF | 101 | - | 45,45,54 | 10.47 | 25 (55%) | 56,56,65 | 3.41 | 19 (33%) |
| 27 | DGD | BH | 101 | - | 59,59,67 | 1.89 | 11 (18%) | 73,73,81 | 1.47 | 7 (9%) |
| 30 | LMG | BI | 101 | - | 43,43,55 | 2.18 | 10 (23%) | 51,51,63 | 1.12 | 4 (7%) |
| 32 | LMT | BI | 102 | - | 36,36,36 | 1.49 | 4 (11%) | 47,47,47 | 0.97 | 2 (4%) |
| 24 | PL9 | BJ | 101 | - | 35,35,55 | 1.44 | 6 (17%) | 43,45,69 | 1.88 | 13 (30%) |
| 26 | BCR | BJ | 102 | - | 41,41,41 | 2.15 | 8 (19%) | 56,56,56 | 3.25 | 24 (42%) |
| 26 | BCR | BK | 102 | - | 41,41,41 | 1.84 | 7 (17%) | 56,56,56 | 2.50 | 26 (46%) |
| 29 | SQD | BL | 101 | - | 47,47,54 | 3.30 | 23 (48%) | 58,58,65 | 3.33 | 16 (27%) |
| 32 | LMT | BM | 101 | - | 36,36,36 | 1.17 | 3 (8%) | 47,47,47 | 0.96 | 2 (4%) |
| 30 | LMG | BM | 102 | - | 42,42,55 | 2.45 | 10 (23%) | 50,50,63 | 1.16 | 5 (10%) |
| 32 | LMT | BT | 101 | - | 36,36,36 | 1.29 | 4 (11%) | 47,47,47 | 1.05 | 4 (8%) |
| 34 | HEM | BV | 201 | 16 | 50,50,50 | 2.55 | 23 (46%) | 46,82,82 | 2.39 | 13 (28%) |
| 26 | BCR | BX | 101 | - | 41,41,41 | 1.83 | 8 (19%) | 56,56,56 | 2.24 | 22 (39%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 26 | BCR | BZ | 101 | - | 41,41,41 | 1.92 | 9 (21%) | 56,56,56 | 2.05 | 19 (33%) |

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 |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 22 | CLA | AA | 402 | 1 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AA | 403 | - | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | AA | 404 | - | - | 0/37/135/135 | 0/0/9/9 |
| 23 | PHO | AA | 405 | - | 3/3/17/22 | 1/49/103/103 | 0/1/6/6 |
| 22 | CLA | AA | 406 | 1 | - | 0/37/135/135 | 0/0/9/9 |
| 24 | PL9 | AA | 407 | - | - | 0/41/61/73 | 0/1/1/1 |
| 25 | OEC | AA | 408 | 1,3 | - | 0/0/0/54 | 0/0/0/5 |
| 26 | BCR | AA | 409 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | DGD | AA | 410 | - | 3/3/13/13 | 0/45/85/95 | 0/2/2/2 |
| 28 | LHG | AA | 411 | - | - | 0/43/43/53 | 0/0/0/0 |
| 29 | SQD | AA | 412 | - | - | 0/46/66/69 | 0/1/1/1 |
| 30 | LMG | AA | 413 | - | 2/2/8/8 | 0/46/66/70 | 0/1/1/1 |
| 29 | SQD | AA | 415 | - | - | 0/49/69/69 | 0/1/1/1 |
| 30 | LMG | AA | 416 | - | 2/2/8/8 | 0/37/57/70 | 0/1/1/1 |
| 22 | CLA | AB | 601 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 602 | 2 | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 603 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 604 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 605 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 606 | 2 | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 607 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 608 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 609 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 610 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 611 | 2 | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 612 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 613 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 614 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 615 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AB | 616 | - | - | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | AB | 617 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | AB | 618 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | AB | 619 | - | - | 0/29/63/63 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 26 | BCR | AB | 620 | - | - | 0/29/63/63 | 0/2/2/2 |
| 30 | LMG | AB | 621 | - | 2/2/8/8 | 0/44/64/70 | 0/1/1/1 |
| 30 | LMG | AB | 622 | - | 2/2/8/8 | 0/44/64/70 | 0/1/1/1 |
| 30 | LMG | AB | 623 | - | 2/2/8/8 | 0/37/57/70 | 0/1/1/1 |
| 32 | LMT | AB | 624 | - | - | 0/21/61/61 | 0/2/2/2 |
| 32 | LMT | AB | 625 | - | - | 0/21/61/61 | 0/2/2/2 |
| 27 | DGD | AB | 626 | - | 3/3/13/13 | 0/41/81/95 | 0/2/2/2 |
| 32 | LMT | AB | 627 | - | - | 0/21/61/61 | 0/2/2/2 |
| 22 | CLA | AC | 501 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 502 | 3 | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 503 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 504 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 505 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 506 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 507 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 508 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 509 | - | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 510 | - | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 511 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 512 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | AC | 513 | 3 | - | 1/37/135/135 | 0/0/9/9 |
| 26 | BCR | AC | 514 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | AC | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | DGD | AC | 516 | - | 3/3/13/13 | 0/42/82/95 | 0/2/2/2 |
| 27 | DGD | AC | 517 | - | 3/3/13/13 | 0/51/91/95 | 0/2/2/2 |
| 27 | DGD | AC | 518 | - | 3/3/13/13 | 0/55/95/95 | 0/2/2/2 |
| 30 | LMG | AC | 519 | - | 2/2/8/8 | 0/43/63/70 | 0/1/1/1 |
| 30 | LMG | AC | 520 | - | 2/2/8/8 | 0/40/60/70 | 0/1/1/1 |
| 28 | LHG | AC | 521 | - | - | 0/41/41/53 | 0/0/0/0 |
| 33 | BCT | AD | 401 | 21 | - | 0/0/0/0 | 0/0/0/0 |
| 22 | CLA | AD | 402 | 4 | - | 0/37/135/135 | 0/0/9/9 |
| 23 | PHO | AD | 403 | - | 3/3/17/22 | 0/49/103/103 | 0/1/6/6 |
| 22 | CLA | AD | 404 | - | - | 0/37/135/135 | 0/0/9/9 |
| 24 | PL9 | AD | 405 | - | - | 0/53/73/73 | 0/1/1/1 |
| 26 | BCR | AD | 406 | - | - | 0/29/63/63 | 0/2/2/2 |
| 30 | LMG | AD | 407 | - | 2/2/8/8 | 0/41/61/70 | 0/1/1/1 |
| 30 | LMG | AD | 408 | - | 2/2/8/8 | 1/43/63/70 | 0/1/1/1 |
| 29 | SQD | AD | 409 | - | - | 2/38/58/69 | 0/1/1/1 |
| 27 | DGD | AD | 410 | - | 3/3/13/13 | 0/52/92/95 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 32 | LMT | AD | 411 | - | - | 0/17/57/61 | 0/2/2/2 |
| 34 | HEM | AE | 101 | 5,6 | - | 0/14/114/114 | 0/0/8/8 |
| 30 | LMG | AE | 102 | - | 2/2/8/8 | 0/39/59/70 | 0/1/1/1 |
| 29 | SQD | AF | 101 | - | - | 0/40/60/69 | 0/1/1/1 |
| 26 | BCR | AH | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | DGD | AH | 102 | - | 3/3/13/13 | 0/47/87/95 | 0/2/2/2 |
| 30 | LMG | AI | 101 | - | 2/2/8/8 | 0/38/58/70 | 0/1/1/1 |
| 32 | LMT | AI | 102 | - | - | 0/21/61/61 | 0/2/2/2 |
| 24 | PL9 | AJ | 101 | - | - | 0/29/49/73 | 0/1/1/1 |
| 26 | BCR | AJ | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | AK | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 30 | LMG | AM | 101 | - | 2/2/8/8 | 1/37/57/70 | 0/1/1/1 |
| 32 | LMT | AM | 102 | - | - | 0/21/61/61 | 0/2/2/2 |
| 32 | LMT | AT | 101 | - | - | 0/21/61/61 | 0/2/2/2 |
| 26 | BCR | AT | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 34 | HEM | AV | 201 | 16 | - | 0/14/114/114 | 0/0/8/8 |
| 26 | BCR | AZ | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 29 | SQD | BA | 401 | - | - | 0/49/69/69 | 0/1/1/1 |
| 22 | CLA | BA | 403 | 1 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BA | 404 | - | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | BA | 405 | - | - | 0/37/135/135 | 0/0/9/9 |
| 23 | PHO | BA | 406 | - | 3/3/17/22 | 1/49/103/103 | 0/1/6/6 |
| 22 | CLA | BA | 407 | 1 | - | 0/37/135/135 | 0/0/9/9 |
| 24 | PL9 | BA | 408 | - | - | 0/41/61/73 | 0/1/1/1 |
| 25 | OEC | BA | 409 | 1,3 | - | 0/0/0/54 | 0/0/0/5 |
| 26 | BCR | BA | 410 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | DGD | BA | 411 | - | 3/3/13/13 | 0/45/85/95 | 0/2/2/2 |
| 28 | LHG | BA | 412 | - | - | 0/43/43/53 | 0/0/0/0 |
| 29 | SQD | BA | 413 | - | - | 0/46/66/69 | 0/1/1/1 |
| 30 | LMG | BA | 414 | - | 2/2/8/8 | 0/46/66/70 | 0/1/1/1 |
| 29 | SQD | BB | 601 | - | - | 0/42/62/69 | 0/1/1/1 |
| 27 | DGD | BB | 602 | - | 3/3/13/13 | 0/41/81/95 | 0/2/2/2 |
| 32 | LMT | BB | 603 | - | - | 0/21/61/61 | 0/2/2/2 |
| 22 | CLA | BB | 604 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 605 | 2 | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 606 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 607 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 608 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 609 | 2 | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 610 | - | - | 0/37/135/135 | 0/0/9/9 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 22 | CLA | BB | 611 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 612 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 613 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 614 | 2 | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 615 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 616 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 617 | 2 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 618 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BB | 619 | - | - | 0/37/135/135 | 0/0/9/9 |
| 26 | BCR | BB | 620 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | BB | 621 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | BB | 622 | - | - | 0/29/63/63 | 0/2/2/2 |
| 30 | LMG | BB | 623 | - | 2/2/8/8 | 0/44/64/70 | 0/1/1/1 |
| 30 | LMG | BB | 624 | - | 2/2/8/8 | 0/44/64/70 | 0/1/1/1 |
| 32 | LMT | BB | 625 | - | - | 0/21/61/61 | 0/2/2/2 |
| 32 | LMT | BB | 626 | - | - | 0/21/61/61 | 0/2/2/2 |
| 22 | CLA | BC | 501 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 502 | 3 | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 503 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 504 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 505 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 506 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 507 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 508 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 509 | - | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 510 | - | - | 1/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 511 | 3 | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 512 | - | - | 0/37/135/135 | 0/0/9/9 |
| 22 | CLA | BC | 513 | 3 | - | 1/37/135/135 | 0/0/9/9 |
| 26 | BCR | BC | 514 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | BC | 515 | - | - | 0/29/63/63 | 0/2/2/2 |
| 27 | DGD | BC | 516 | - | 3/3/13/13 | 0/42/82/95 | 0/2/2/2 |
| 27 | DGD | BC | 517 | - | 3/3/13/13 | 0/51/91/95 | 0/2/2/2 |
| 27 | DGD | BC | 518 | - | 3/3/13/13 | 0/55/95/95 | 0/2/2/2 |
| 30 | LMG | BC | 519 | - | 2/2/8/8 | 0/43/63/70 | 0/1/1/1 |
| 30 | LMG | BC | 520 | - | 2/2/8/8 | 0/40/60/70 | 0/1/1/1 |
| 28 | LHG | BC | 521 | - | - | 0/41/41/53 | 0/0/0/0 |
| 33 | BCT | BD | 401 | 21 | - | 0/0/0/0 | 0/0/0/0 |
| 22 | CLA | BD | 402 | 4 | - | 0/37/135/135 | 0/0/9/9 |
| 23 | PHO | BD | 403 | - | 3/3/17/22 | 0/49/103/103 | 0/1/6/6 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|--------------|---------|
| 22 | CLA | BD | 404 | - | - | 0/37/135/135 | 0/0/9/9 |
| 24 | PL9 | BD | 405 | - | - | 0/53/73/73 | 0/1/1/1 |
| 26 | BCR | BD | 406 | - | - | 0/29/63/63 | 0/2/2/2 |
| 30 | LMG | BD | 407 | - | 2/2/8/8 | 0/41/61/70 | 0/1/1/1 |
| 30 | LMG | BD | 408 | - | 2/2/8/8 | 1/43/63/70 | 0/1/1/1 |
| 29 | SQD | BD | 409 | - | - | 2/38/58/69 | 0/1/1/1 |
| 27 | DGD | BD | 410 | - | 3/3/13/13 | 0/52/92/95 | 0/2/2/2 |
| 32 | LMT | BD | 411 | - | - | 0/17/57/61 | 0/2/2/2 |
| 34 | HEM | BE | 101 | 5,6 | - | 0/14/114/114 | 0/0/8/8 |
| 30 | LMG | BE | 102 | - | 2/2/8/8 | 0/39/59/70 | 0/1/1/1 |
| 29 | SQD | BF | 101 | - | - | 0/40/60/69 | 0/1/1/1 |
| 27 | DGD | BH | 101 | - | 3/3/13/13 | 0/47/87/95 | 0/2/2/2 |
| 30 | LMG | BI | 101 | - | 2/2/8/8 | 0/38/58/70 | 0/1/1/1 |
| 32 | LMT | BI | 102 | - | - | 0/21/61/61 | 0/2/2/2 |
| 24 | PL9 | BJ | 101 | - | - | 0/29/49/73 | 0/1/1/1 |
| 26 | BCR | BJ | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | BK | 102 | - | - | 0/29/63/63 | 0/2/2/2 |
| 29 | SQD | BL | 101 | - | - | 0/42/62/69 | 0/1/1/1 |
| 32 | LMT | BM | 101 | - | - | 0/21/61/61 | 0/2/2/2 |
| 30 | LMG | BM | 102 | - | 2/2/8/8 | 1/37/57/70 | 0/1/1/1 |
| 32 | LMT | BT | 101 | - | - | 0/21/61/61 | 0/2/2/2 |
| 34 | HEM | BV | 201 | 16 | - | 0/14/114/114 | 0/0/8/8 |
| 26 | BCR | BX | 101 | - | - | 0/29/63/63 | 0/2/2/2 |
| 26 | BCR | BZ | 101 | - | - | 0/29/63/63 | 0/2/2/2 |

The worst 5 of 1683 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 29 | BF | 101 | SQD | C19-C18 | -47.81 | 1.36 | 1.55 |
| 29 | BF | 101 | SQD | C32-C31 | -47.75 | 1.36 | 1.55 |
| 29 | AF | 101 | SQD | C19-C18 | -47.49 | 1.36 | 1.55 |
| 29 | AF | 101 | SQD | C32-C31 | -45.64 | 1.37 | 1.55 |
| 29 | AD | 409 | SQD | C18-C17 | -45.22 | 1.37 | 1.55 |

The worst 5 of 2425 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | AD | 409 | SQD | O7-S-C6 | 12.40 | 117.79 | 106.83 |
| 29 | BD | 409 | SQD | O7-S-C6 | 12.22 | 117.63 | 106.83 |
| 29 | AA | 412 | SQD | O7-S-C6 | 11.43 | 116.93 | 106.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29 | BA | 413 | SQD | O7-S-C6 | 10.83 | 116.40 | 106.83 |
| 29 | BL | 101 | SQD | O7-S-C6 | 10.80 | 116.37 | 106.83 |

5 of 98 chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 30 | AC | 520 | LMG | C2 |
| 30 | AC | 520 | LMG | C5 |
| 27 | AB | 626 | DGD | C2D |
| 27 | AB | 626 | DGD | C5D |
| 27 | AB | 626 | DGD | C5E |

5 of 26 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 29 | AD | 409 | SQD | C45-O47-C7-C8 |
| 29 | BD | 409 | SQD | C45-O47-C7-C8 |
| 29 | AD | 409 | SQD | C45-O47-C7-O49 |
| 29 | BD | 409 | SQD | C45-O47-C7-O49 |
| 30 | BM | 102 | LMG | C8-O7-C10-C11 |

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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 | AA | 335/344 (97%) | -0.43 | 6 (1%) 65 74 | 23, 59, 88, 103 | 0 |
| 1 | BA | 335/344 (97%) | -0.23 | 5 (1%) 70 79 | 47, 70, 89, 103 | 0 |
| 2 | AB | 490/510 (96%) | -0.23 | 6 (1%) 75 83 | 37, 63, 86, 99 | 0 |
| 2 | BB | 490/510 (96%) | -0.23 | 11 (2%) 59 67 | 41, 64, 87, 103 | 0 |
| 3 | AC | 447/473 (94%) | -0.14 | 15 (3%) 43 51 | 43, 72, 87, 102 | 0 |
| 3 | BC | 447/473 (94%) | 0.13 | 22 (4%) 28 34 | 54, 83, 95, 101 | 0 |
| 4 | AD | 340/352 (96%) | -0.39 | 4 (1%) 75 83 | 29, 59, 84, 95 | 0 |
| 4 | BD | 340/352 (96%) | -0.27 | 7 (2%) 60 69 | 40, 69, 91, 101 | 0 |
| 5 | AE | 82/84 (97%) | 0.11 | 7 (8%) 11 13 | 54, 75, 93, 99 | 0 |
| 5 | BE | 82/84 (97%) | 0.50 | 10 (12%) 5 6 | 71, 85, 98, 104 | 0 |
| 6 | AF | 35/45 (77%) | -0.01 | 2 (5%) 23 28 | 56, 73, 94, 97 | 0 |
| 6 | BF | 35/45 (77%) | 0.33 | 3 (8%) 11 13 | 75, 82, 97, 99 | 0 |
| 7 | AH | 65/66 (98%) | 0.14 | 3 (4%) 31 38 | 57, 76, 92, 97 | 0 |
| 7 | BH | 65/66 (98%) | 0.32 | 8 (12%) 5 6 | 62, 80, 91, 103 | 0 |
| 8 | AI | 35/38 (92%) | -0.04 | 3 (8%) 11 13 | 57, 70, 87, 94 | 0 |
| 8 | BI | 35/38 (92%) | 0.04 | 1 (2%) 49 58 | 69, 80, 92, 95 | 0 |
| 9 | AJ | 34/40 (85%) | -0.42 | 1 (2%) 49 58 | 65, 74, 83, 89 | 0 |
| 9 | BJ | 34/40 (85%) | -0.04 | 4 (11%) 5 7 | 73, 81, 93, 98 | 0 |
| 10 | AK | 37/37 (100%) | -0.35 | 2 (5%) 25 30 | 67, 75, 87, 93 | 0 |
| 10 | BK | 37/37 (100%) | -0.00 | 2 (5%) 25 30 | 84, 90, 96, 101 | 0 |
| 11 | AL | 37/37 (100%) | 0.26 | 5 (13%) 4 5 | 45, 60, 98, 107 | 0 |
| 11 | BL | 37/37 (100%) | 0.39 | 6 (16%) 2 3 | 46, 62, 94, 102 | 0 |
| 12 | AM | 34/36 (94%) | -0.03 | 2 (5%) 22 25 | 51, 65, 94, 100 | 0 |
| 12 | BM | 34/36 (94%) | -0.12 | 2 (5%) 22 25 | 55, 61, 76, 91 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | AO | 243/247 (98%) | 0.10 | 12 (4%) 28 34 | 39, 70, 93, 107 | 0 |
| 13 | BO | 243/247 (98%) | 0.18 | 16 (6%) 18 21 | 48, 76, 97, 107 | 0 |
| 14 | AT | 32/32 (100%) | 0.19 | 3 (9%) 9 11 | 53, 63, 102, 104 | 0 |
| 14 | BT | 32/32 (100%) | -0.02 | 2 (6%) 19 23 | 57, 67, 93, 103 | 0 |
| 15 | AU | 97/104 (93%) | -0.06 | 1 (1%) 79 86 | 43, 63, 78, 86 | 0 |
| 15 | BU | 97/104 (93%) | -0.19 | 1 (1%) 79 86 | 55, 67, 77, 87 | 0 |
| 16 | AV | 137/137 (100%) | -0.21 | 0 100 100 | 49, 66, 76, 79 | 0 |
| 16 | BV | 137/137 (100%) | 0.12 | 8 (5%) 22 26 | 64, 79, 95, 102 | 0 |
| 17 | Ay | 28/46 (60%) | 0.30 | 4 (14%) 3 5 | 79, 91, 97, 99 | 0 |
| 17 | By | 28/46 (60%) | 0.34 | 3 (10%) 6 8 | 89, 98, 102, 106 | 0 |
| 18 | AX | 37/50 (74%) | -0.15 | 2 (5%) 25 30 | 70, 79, 93, 95 | 0 |
| 18 | BX | 37/50 (74%) | 0.25 | 5 (13%) 4 5 | 75, 82, 91, 94 | 0 |
| 19 | AY | 0/28 | - | - | - | - |
| 19 | BY | 0/28 | - | - | - | - |
| 20 | AZ | 62/62 (100%) | 0.24 | 10 (16%) 2 3 | 76, 85, 103, 110 | 0 |
| 20 | BZ | 62/62 (100%) | 0.62 | 10 (16%) 2 3 | 86, 96, 105, 110 | 0 |
| All | All | 5214/5536 (94%) | -0.09 | 214 (4%) 35 43 | 23, 71, 94, 110 | 0 |

The worst 5 of 214 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 7 | BH | 65 | LEU | 8.7 |
| 5 | BE | 4 | THR | 7.2 |
| 12 | AM | 33 | GLN | 6.2 |
| 11 | BL | 1 | MET | 6.1 |
| 20 | BZ | 1 | MET | 6.0 |

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 | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|----------------------------|-------|
| 31 | CL | AA | 414 | 1/1 | 0.70 | 26.23 | 73,73,73,73 | 0 |
| 27 | DGD | AD | 410 | 63/66 | 0.51 | 11.93 | 91,97,107,108 | 0 |
| 26 | BCR | BJ | 102 | 40/40 | 0.50 | 8.56 | 93,98,101,102 | 0 |
| 24 | PL9 | AJ | 101 | 35/55 | 0.53 | 7.92 | 93,101,107,109 | 0 |
| 30 | LMG | AA | 416 | 42/55 | 0.36 | 6.71 | 67,92,96,99 | 0 |
| 26 | BCR | AJ | 102 | 40/40 | 0.44 | 6.71 | 85,91,101,102 | 0 |
| 27 | DGD | BD | 410 | 63/66 | 0.50 | 6.43 | 84,100,105,105 | 0 |
| 22 | CLA | AD | 404 | 65/65 | 0.32 | 6.26 | 80,83,102,103 | 0 |
| 24 | PL9 | BA | 408 | 45/55 | 0.34 | 6.24 | 82,88,90,92 | 0 |
| 24 | PL9 | BJ | 101 | 35/55 | 0.41 | 6.18 | 78,99,111,112 | 0 |
| 24 | PL9 | AA | 407 | 45/55 | 0.35 | 5.75 | 83,87,94,95 | 0 |
| 30 | LMG | AB | 623 | 42/55 | 0.38 | 5.75 | 70,89,92,93 | 0 |
| 30 | LMG | AI | 101 | 43/55 | 0.49 | 5.74 | 83,92,97,98 | 0 |
| 30 | LMG | AC | 520 | 45/55 | 0.40 | 5.57 | 75,92,97,98 | 0 |
| 32 | LMT | BI | 102 | 35/35 | 0.55 | 5.57 | 90,104,106,106 | 0 |
| 31 | CL | BA | 415 | 1/1 | 0.37 | 5.53 | 81,81,81,81 | 0 |
| 32 | LMT | AI | 102 | 35/35 | 0.47 | 5.24 | 74,92,95,95 | 0 |
| 22 | CLA | BA | 407 | 65/65 | 0.35 | 5.17 | 72,76,103,104 | 0 |
| 26 | BCR | AK | 102 | 40/40 | 0.34 | 4.99 | 73,77,81,81 | 0 |
| 32 | LMT | AD | 411 | 31/35 | 0.47 | 4.84 | 52,96,104,104 | 0 |
| 28 | LHG | BC | 521 | 37/49 | 0.57 | 4.76 | 90,100,113,114 | 0 |
| 22 | CLA | AB | 601 | 65/65 | 0.37 | 4.71 | 88,97,102,105 | 0 |
| 32 | LMT | AB | 625 | 35/35 | 0.42 | 4.57 | 82,98,100,101 | 0 |
| 32 | LMT | AT | 101 | 35/35 | 0.36 | 4.51 | 72,91,97,98 | 0 |
| 27 | DGD | BB | 602 | 52/66 | 0.30 | 4.33 | 71,85,104,105 | 0 |
| 28 | LHG | AC | 521 | 37/49 | 0.45 | 4.28 | 78,99,109,109 | 0 |
| 32 | LMT | BD | 411 | 31/35 | 0.52 | 4.24 | 67,91,99,100 | 0 |
| 22 | CLA | AA | 406 | 65/65 | 0.30 | 4.22 | 54,60,89,90 | 0 |
| 32 | LMT | AB | 624 | 35/35 | 0.59 | 4.02 | 71,100,106,107 | 0 |
| 27 | DGD | AB | 626 | 52/66 | 0.31 | 3.95 | 79,94,105,107 | 0 |
| 30 | LMG | BC | 520 | 45/55 | 0.44 | 3.94 | 86,93,101,102 | 0 |
| 26 | BCR | BK | 102 | 40/40 | 0.37 | 3.90 | 76,81,85,85 | 0 |
| 29 | SQD | BA | 401 | 54/54 | 0.35 | 3.76 | 82,91,107,108 | 0 |
| 32 | LMT | BB | 625 | 35/35 | 0.49 | 3.74 | 66,103,111,111 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 35 | CA | BO | 301 | 1/1 | 0.32 | 3.74 | 100,100,100,100 | 0 |
| 26 | BCR | AZ | 101 | 40/40 | 0.30 | 3.53 | 75,82,90,91 | 0 |
| 33 | BCT | AD | 401 | 4/4 | 0.24 | 3.48 | 90,91,91,92 | 0 |
| 29 | SQD | AA | 415 | 54/54 | 0.28 | 3.34 | 71,87,105,105 | 0 |
| 30 | LMG | BE | 102 | 44/55 | 0.38 | 3.18 | 75,92,98,99 | 0 |
| 22 | CLA | AB | 604 | 65/65 | 0.24 | 3.13 | 67,73,91,91 | 0 |
| 30 | LMG | BC | 519 | 48/55 | 0.34 | 2.98 | 83,90,94,95 | 0 |
| 30 | LMG | AD | 408 | 48/55 | 0.23 | 2.85 | 63,68,74,80 | 0 |
| 27 | DGD | BA | 411 | 56/66 | 0.35 | 2.84 | 76,85,103,104 | 0 |
| 30 | LMG | BD | 408 | 48/55 | 0.24 | 2.80 | 68,75,85,87 | 0 |
| 22 | CLA | AC | 512 | 65/65 | 0.32 | 2.73 | 91,95,106,106 | 0 |
| 30 | LMG | BI | 101 | 43/55 | 0.35 | 2.70 | 84,90,99,100 | 0 |
| 22 | CLA | BB | 612 | 65/65 | 0.27 | 2.69 | 82,89,92,95 | 0 |
| 26 | BCR | BC | 514 | 40/40 | 0.26 | 2.68 | 81,83,87,87 | 0 |
| 30 | LMG | BD | 407 | 46/55 | 0.24 | 2.68 | 70,80,92,94 | 0 |
| 32 | LMT | AB | 627 | 35/35 | 0.50 | 2.64 | 73,103,106,107 | 0 |
| 26 | BCR | AH | 101 | 40/40 | 0.32 | 2.61 | 76,88,95,95 | 0 |
| 29 | SQD | AF | 101 | 45/54 | 0.35 | 2.47 | 82,97,102,103 | 0 |
| 29 | SQD | BF | 101 | 45/54 | 0.37 | 2.42 | 95,98,103,104 | 0 |
| 22 | CLA | AC | 507 | 65/65 | 0.28 | 2.28 | 83,90,95,97 | 0 |
| 26 | BCR | BB | 622 | 40/40 | 0.27 | 2.24 | 67,71,79,80 | 0 |
| 30 | LMG | BB | 623 | 49/55 | 0.25 | 2.21 | 70,78,88,91 | 0 |
| 22 | CLA | BC | 513 | 65/65 | 0.35 | 2.18 | 96,99,106,107 | 0 |
| 23 | PHO | BD | 403 | 64/64 | 0.22 | 2.17 | 77,88,92,93 | 0 |
| 32 | LMT | BT | 101 | 35/35 | 0.37 | 2.17 | 77,91,94,95 | 0 |
| 22 | CLA | AB | 614 | 65/65 | 0.24 | 2.15 | 78,85,98,99 | 0 |
| 22 | CLA | AC | 513 | 65/65 | 0.37 | 2.14 | 92,98,104,106 | 0 |
| 22 | CLA | AC | 504 | 65/65 | 0.22 | 2.11 | 78,86,107,107 | 0 |
| 26 | BCR | BZ | 101 | 40/40 | 0.29 | 2.08 | 81,90,93,94 | 0 |
| 32 | LMT | BB | 626 | 35/35 | 0.35 | 2.05 | 76,93,101,102 | 0 |
| 22 | CLA | BA | 405 | 65/65 | 0.19 | 2.05 | 72,76,104,105 | 0 |
| 26 | BCR | AC | 514 | 40/40 | 0.21 | 1.92 | 56,66,73,74 | 0 |
| 30 | LMG | AC | 519 | 48/55 | 0.30 | 1.90 | 75,84,89,90 | 0 |
| 22 | CLA | AC | 505 | 65/65 | 0.21 | 1.90 | 69,73,77,79 | 0 |
| 22 | CLA | AB | 609 | 65/65 | 0.23 | 1.85 | 76,87,91,92 | 0 |
| 27 | DGD | AC | 516 | 53/66 | 0.23 | 1.85 | 57,72,91,92 | 0 |
| 27 | DGD | AC | 517 | 62/66 | 0.20 | 1.78 | 70,78,91,92 | 0 |
| 30 | LMG | AB | 621 | 49/55 | 0.23 | 1.74 | 62,75,80,83 | 0 |
| 22 | CLA | AB | 602 | 65/65 | 0.22 | 1.72 | 81,85,88,90 | 0 |
| 24 | PL9 | AD | 405 | 55/55 | 0.21 | 1.71 | 52,67,71,73 | 0 |
| 27 | DGD | BC | 517 | 62/66 | 0.22 | 1.71 | 78,82,100,101 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 24 | PL9 | BD | 405 | 55/55 | 0.21 | 1.70 | 63,70,76,78 | 0 |
| 27 | DGD | AA | 410 | 56/66 | 0.32 | 1.68 | 78,86,91,92 | 0 |
| 22 | CLA | AC | 503 | 65/65 | 0.22 | 1.67 | 78,86,92,95 | 0 |
| 26 | BCR | AB | 620 | 40/40 | 0.26 | 1.64 | 75,77,83,84 | 0 |
| 34 | HEM | AE | 101 | 43/43 | 0.28 | 1.63 | 85,92,103,106 | 0 |
| 32 | LMT | BM | 101 | 35/35 | 0.29 | 1.60 | 70,88,97,101 | 0 |
| 22 | CLA | BB | 609 | 65/65 | 0.25 | 1.57 | 72,80,96,96 | 0 |
| 22 | CLA | AB | 606 | 65/65 | 0.26 | 1.56 | 73,87,96,96 | 0 |
| 29 | SQD | AD | 409 | 43/54 | 0.25 | 1.54 | 68,92,108,111 | 0 |
| 22 | CLA | BD | 404 | 65/65 | 0.25 | 1.53 | 89,92,101,102 | 0 |
| 22 | CLA | BB | 606 | 65/65 | 0.20 | 1.53 | 58,61,74,76 | 0 |
| 22 | CLA | BC | 510 | 65/65 | 0.22 | 1.48 | 79,83,92,92 | 0 |
| 30 | LMG | AA | 413 | 51/55 | 0.22 | 1.42 | 70,74,77,79 | 0 |
| 26 | BCR | AT | 102 | 40/40 | 0.20 | 1.40 | 72,79,91,91 | 0 |
| 27 | DGD | BC | 516 | 53/66 | 0.23 | 1.39 | 69,77,96,97 | 0 |
| 22 | CLA | AD | 402 | 65/65 | 0.20 | 1.37 | 47,58,69,71 | 0 |
| 26 | BCR | BD | 406 | 40/40 | 0.22 | 1.35 | 66,78,92,92 | 0 |
| 28 | LHG | AA | 411 | 39/49 | 0.22 | 1.34 | 63,68,76,78 | 0 |
| 30 | LMG | AE | 102 | 44/55 | 0.30 | 1.33 | 81,91,96,96 | 0 |
| 34 | HEM | BE | 101 | 43/43 | 0.27 | 1.29 | 93,95,104,107 | 0 |
| 30 | LMG | AD | 407 | 46/55 | 0.19 | 1.27 | 63,71,90,92 | 0 |
| 22 | CLA | AB | 616 | 65/65 | 0.29 | 1.26 | 73,85,105,106 | 0 |
| 34 | HEM | AV | 201 | 43/43 | 0.21 | 1.24 | 60,63,66,67 | 0 |
| 26 | BCR | AB | 618 | 40/40 | 0.18 | 1.24 | 75,78,82,83 | 0 |
| 22 | CLA | BB | 608 | 65/65 | 0.19 | 1.23 | 45,53,76,78 | 0 |
| 32 | LMT | BB | 603 | 35/35 | 0.35 | 1.23 | 68,86,95,96 | 0 |
| 22 | CLA | BC | 505 | 65/65 | 0.23 | 1.22 | 88,93,94,95 | 0 |
| 22 | CLA | BC | 512 | 65/65 | 0.32 | 1.21 | 95,99,109,110 | 0 |
| 22 | CLA | AA | 404 | 65/65 | 0.20 | 1.18 | 63,72,97,99 | 0 |
| 22 | CLA | BD | 402 | 65/65 | 0.18 | 1.17 | 50,57,79,83 | 0 |
| 29 | SQD | BB | 601 | 47/54 | 0.28 | 1.16 | 74,87,109,111 | 0 |
| 22 | CLA | AB | 605 | 65/65 | 0.21 | 1.15 | 68,76,84,85 | 0 |
| 22 | CLA | BB | 604 | 65/65 | 0.34 | 1.14 | 86,98,107,109 | 0 |
| 22 | CLA | BB | 613 | 65/65 | 0.21 | 1.13 | 69,77,82,84 | 0 |
| 30 | LMG | AB | 622 | 49/55 | 0.19 | 1.13 | 64,73,80,83 | 0 |
| 29 | SQD | AA | 412 | 51/54 | 0.25 | 1.13 | 73,83,98,99 | 0 |
| 22 | CLA | BB | 617 | 65/65 | 0.23 | 1.12 | 75,79,99,100 | 0 |
| 30 | LMG | BM | 102 | 42/55 | 0.30 | 1.10 | 72,90,95,98 | 0 |
| 27 | DGD | BH | 101 | 58/66 | 0.20 | 1.09 | 66,73,80,81 | 0 |
| 26 | BCR | BC | 515 | 40/40 | 0.29 | 1.09 | 74,80,91,92 | 0 |
| 26 | BCR | AA | 409 | 40/40 | 0.21 | 1.07 | 59,67,70,71 | 0 |
| 26 | BCR | BX | 101 | 40/40 | 0.34 | 1.04 | 76,79,89,90 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 26 | BCR | AB | 619 | 40/40 | 0.18 | 1.04 | 62,70,82,83 | 0 |
| 32 | LMT | AM | 102 | 35/35 | 0.28 | 1.02 | 67,89,93,96 | 0 |
| 27 | DGD | AC | 518 | 66/66 | 0.21 | 1.00 | 62,68,84,86 | 0 |
| 29 | SQD | BL | 101 | 47/54 | 0.29 | 0.99 | 75,91,115,116 | 0 |
| 27 | DGD | BC | 518 | 66/66 | 0.23 | 0.99 | 71,78,89,90 | 0 |
| 22 | CLA | BB | 605 | 65/65 | 0.20 | 0.95 | 77,82,86,89 | 0 |
| 22 | CLA | BB | 619 | 65/65 | 0.29 | 0.92 | 75,81,93,95 | 0 |
| 26 | BCR | BB | 620 | 40/40 | 0.20 | 0.88 | 66,69,72,73 | 0 |
| 22 | CLA | AA | 402 | 65/65 | 0.17 | 0.87 | 51,58,66,69 | 0 |
| 28 | LHG | BA | 412 | 39/49 | 0.24 | 0.86 | 72,77,80,81 | 0 |
| 22 | CLA | AB | 612 | 65/65 | 0.22 | 0.85 | 63,75,81,83 | 0 |
| 22 | CLA | BC | 504 | 65/65 | 0.20 | 0.80 | 87,92,102,102 | 0 |
| 22 | CLA | BB | 615 | 65/65 | 0.18 | 0.80 | 60,72,77,81 | 0 |
| 22 | CLA | AC | 501 | 65/65 | 0.21 | 0.80 | 78,83,85,86 | 0 |
| 22 | CLA | BC | 507 | 65/65 | 0.23 | 0.79 | 84,92,96,97 | 0 |
| 22 | CLA | AA | 403 | 65/65 | 0.16 | 0.78 | 41,48,56,60 | 0 |
| 30 | LMG | BB | 624 | 49/55 | 0.18 | 0.77 | 68,72,78,79 | 0 |
| 23 | PHO | AA | 405 | 64/64 | 0.17 | 0.77 | 40,64,67,69 | 0 |
| 23 | PHO | AD | 403 | 64/64 | 0.17 | 0.76 | 39,56,70,72 | 0 |
| 29 | SQD | BA | 413 | 51/54 | 0.25 | 0.75 | 73,90,103,104 | 0 |
| 22 | CLA | AC | 506 | 65/65 | 0.23 | 0.75 | 83,87,101,102 | 0 |
| 26 | BCR | BA | 410 | 40/40 | 0.20 | 0.71 | 61,74,82,83 | 0 |
| 22 | CLA | AB | 611 | 65/65 | 0.19 | 0.66 | 62,68,71,73 | 0 |
| 22 | CLA | BC | 509 | 65/65 | 0.23 | 0.66 | 73,83,93,94 | 0 |
| 22 | CLA | BC | 508 | 65/65 | 0.23 | 0.62 | 92,97,101,106 | 0 |
| 26 | BCR | AD | 406 | 40/40 | 0.16 | 0.61 | 64,72,85,85 | 0 |
| 27 | DGD | AH | 102 | 58/66 | 0.20 | 0.60 | 57,72,85,86 | 0 |
| 22 | CLA | BB | 607 | 65/65 | 0.19 | 0.59 | 53,64,86,87 | 0 |
| 34 | HEM | BV | 201 | 43/43 | 0.19 | 0.59 | 58,67,76,79 | 0 |
| 30 | LMG | BA | 414 | 51/55 | 0.20 | 0.57 | 62,71,78,80 | 0 |
| 23 | PHO | BA | 406 | 64/64 | 0.17 | 0.57 | 54,61,70,74 | 0 |
| 22 | CLA | AB | 608 | 65/65 | 0.18 | 0.52 | 72,79,87,91 | 0 |
| 29 | SQD | BD | 409 | 43/54 | 0.24 | 0.50 | 73,88,110,111 | 0 |
| 26 | BCR | BB | 621 | 40/40 | 0.18 | 0.48 | 57,69,82,83 | 0 |
| 22 | CLA | AB | 610 | 65/65 | 0.20 | 0.46 | 60,67,79,80 | 0 |
| 22 | CLA | BB | 610 | 65/65 | 0.17 | 0.46 | 60,70,77,81 | 0 |
| 22 | CLA | AB | 613 | 65/65 | 0.17 | 0.46 | 65,69,84,87 | 0 |
| 30 | LMG | AM | 101 | 42/55 | 0.28 | 0.46 | 68,86,93,95 | 0 |
| 22 | CLA | AB | 615 | 65/65 | 0.21 | 0.44 | 83,93,97,99 | 0 |
| 22 | CLA | BC | 502 | 65/65 | 0.22 | 0.43 | 81,85,101,103 | 0 |
| 26 | BCR | AC | 515 | 40/40 | 0.22 | 0.43 | 69,75,80,81 | 0 |
| 22 | CLA | AC | 508 | 65/65 | 0.19 | 0.41 | 80,86,99,101 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|-----------------------------|-------|
| 22 | CLA | AC | 511 | 65/65 | 0.24 | 0.40 | 77,85,89,90 | 0 |
| 22 | CLA | BC | 511 | 65/65 | 0.25 | 0.37 | 91,99,104,105 | 0 |
| 33 | BCT | BD | 401 | 4/4 | 0.17 | 0.37 | 84,86,87,88 | 0 |
| 26 | BCR | AB | 617 | 40/40 | 0.18 | 0.35 | 56,67,75,76 | 0 |
| 22 | CLA | AC | 509 | 65/65 | 0.21 | 0.34 | 59,74,86,89 | 0 |
| 35 | CA | AO | 301 | 1/1 | 0.22 | 0.31 | 87,87,87,87 | 0 |
| 22 | CLA | BB | 618 | 65/65 | 0.21 | 0.29 | 69,84,87,88 | 0 |
| 22 | CLA | BA | 403 | 65/65 | 0.18 | 0.28 | 57,64,71,75 | 0 |
| 22 | CLA | AB | 607 | 65/65 | 0.15 | 0.27 | 50,55,74,74 | 0 |
| 22 | CLA | BC | 506 | 65/65 | 0.23 | 0.24 | 81,85,97,99 | 0 |
| 22 | CLA | AB | 603 | 65/65 | 0.17 | 0.19 | 54,60,72,74 | 0 |
| 22 | CLA | BC | 503 | 65/65 | 0.21 | 0.13 | 82,97,100,101 | 0 |
| 22 | CLA | BC | 501 | 65/65 | 0.19 | 0.02 | 76,80,87,88 | 0 |
| 22 | CLA | BB | 616 | 65/65 | 0.15 | -0.02 | 49,54,79,82 | 0 |
| 22 | CLA | BA | 404 | 65/65 | 0.15 | -0.06 | 55,60,68,70 | 0 |
| 22 | CLA | BB | 614 | 65/65 | 0.16 | -0.13 | 59,68,75,77 | 0 |
| 22 | CLA | BB | 611 | 65/65 | 0.16 | -0.21 | 67,74,81,85 | 0 |
| 25 | OEC | AA | 408 | 5/9 | 0.14 | -0.25 | 56,62,67,75 | 0 |
| 25 | OEC | BA | 409 | 5/9 | 0.15 | -0.27 | 30,74,79,92 | 0 |
| 22 | CLA | AC | 502 | 65/65 | 0.16 | -0.29 | 50,58,81,84 | 0 |
| 35 | CA | BK | 101 | 1/1 | 0.12 | -0.92 | 90,90,90,90 | 0 |
| 22 | CLA | AC | 510 | 65/65 | 0.14 | -1.36 | 48,56,70,72 | 0 |
| 21 | FE2 | AA | 401 | 1/1 | 0.12 | -1.61 | 69,69,69,69 | 0 |
| 35 | CA | AK | 101 | 1/1 | 0.10 | -2.63 | 95,95,95,95 | 0 |
| 21 | FE2 | BA | 402 | 1/1 | 0.11 | -4.20 | 81,81,81,81 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.