



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 04:24 PM BST

PDB ID : 6WGK
Title : Fab portion of dupilumab with Crystal Kappa design and intrachain disulfide
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Deposited on : 2020-04-05
Resolution : 1.62 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

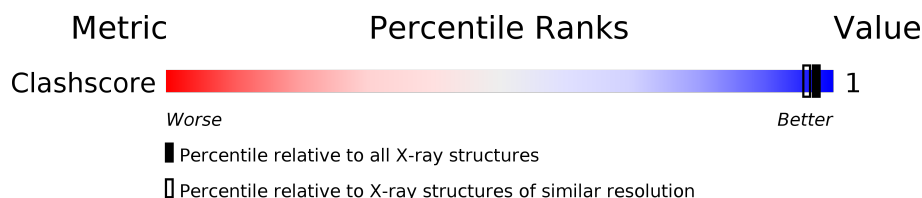
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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)) |
|------------|-----------------------------|---|
| Clashscore | 141614 | 5002 (1.64-1.60) |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 235 |  89% • 7% |
| 1 | C | 235 |  91% • 8% |
| 1 | E | 235 |  92% • 7% |
| 1 | G | 235 |  89% • 9% |
| 2 | B | 217 |  96% •• |
| 2 | D | 217 |  97% •• |
| 2 | F | 217 |  96% •• |
| 2 | H | 217 |  96% •• |

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13743 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dupilumab Fab heavy chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 218 | Total | C | N | O | S | 0 | 4 | 0 |
| | | | 1636 | 1027 | 275 | 327 | 7 | | | |
| 1 | C | 217 | Total | C | N | O | S | 0 | 3 | 0 |
| | | | 1624 | 1019 | 274 | 324 | 7 | | | |
| 1 | E | 219 | Total | C | N | O | S | 0 | 1 | 0 |
| | | | 1629 | 1022 | 275 | 324 | 8 | | | |
| 1 | G | 214 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 1535 | 968 | 257 | 303 | 7 | | | |

- Molecule 2 is a protein called Dupilumab Fab light chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 215 | Total | C | N | O | S | 0 | 10 | 0 |
| | | | 1681 | 1058 | 274 | 342 | 7 | | | |
| 2 | D | 214 | Total | C | N | O | S | 0 | 6 | 0 |
| | | | 1648 | 1039 | 266 | 336 | 7 | | | |
| 2 | F | 214 | Total | C | N | O | S | 0 | 11 | 0 |
| | | | 1636 | 1030 | 266 | 333 | 7 | | | |
| 2 | H | 212 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 1563 | 986 | 257 | 313 | 7 | | | |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3 | A | 140 | Total | O | 0 | 0 |
| | | | 140 | 140 | | |
| 3 | B | 113 | Total | O | 0 | 0 |
| | | | 113 | 113 | | |
| 3 | C | 114 | Total | O | 0 | 0 |
| | | | 114 | 114 | | |
| 3 | D | 72 | Total | O | 0 | 0 |
| | | | 72 | 72 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3 | E | 89 | Total 89 | O 89 | 0 | 0 |
| 3 | F | 94 | Total 94 | O 94 | 0 | 0 |
| 3 | G | 77 | Total 77 | O 77 | 0 | 0 |
| 3 | H | 92 | Total 92 | O 92 | 0 | 0 |

Chain D:  97% ..



- Molecule 2: Dupilumab Fab light chain

Chain F:  96% ..



- Molecule 2: Dupilumab Fab light chain

Chain H:  96% ..



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 109.16 Å 79.27 Å 109.56 Å 90.00° 91.87° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 1.62 | Depositor |
| % Data completeness (in resolution range) | 95.2 (30.00-1.62) | Depositor |
| R_{merge} | 0.05 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.42 (at 1.62 Å) | Xtriage |
| Refinement program | REFMAC 5.8.0103 | Depositor |
| R, R_{free} | 0.210 , 0.236 | Depositor |
| Wilson B-factor (Å ²) | 24.8 | Xtriage |
| Anisotropy | 0.017 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.000 for l,k,-h 0.012 for h,-k,-l 0.007 for l,-k,h | Xtriage |
| Total number of atoms | 13743 | wwPDB-VP |
| Average B, all atoms (Å ²) | 28.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1219e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.30 | 0/1684 | 0.63 | 0/2293 |
| 1 | C | 0.29 | 0/1669 | 0.62 | 0/2273 |
| 1 | E | 0.29 | 0/1668 | 0.61 | 0/2273 |
| 1 | G | 0.30 | 0/1575 | 0.62 | 0/2152 |
| 2 | B | 0.29 | 0/1743 | 0.62 | 0/2370 |
| 2 | D | 0.28 | 0/1701 | 0.61 | 0/2316 |
| 2 | F | 0.29 | 0/1698 | 0.61 | 0/2316 |
| 2 | H | 0.28 | 0/1604 | 0.61 | 0/2190 |
| All | All | 0.29 | 0/13342 | 0.62 | 0/18183 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | C | 0 | 1 |
| 2 | B | 0 | 3 |
| 2 | D | 0 | 2 |
| All | All | 0 | 7 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|--------|------|-----------|
| 1 | A | 30 | ARG | Sidechain |
| 2 | B | 147[A] | ARG | Sidechain |
| 2 | B | 24 | ARG | Sidechain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | B | 59 | ARG | Sidechain |
| 1 | C | 108 | ARG | Sidechain |
| 2 | D | 147 | ARG | Sidechain |
| 2 | D | 59 | ARG | Sidechain |

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1636 | 0 | 1589 | 4 | 0 |
| 1 | C | 1624 | 0 | 1570 | 1 | 0 |
| 1 | E | 1629 | 0 | 1576 | 1 | 0 |
| 1 | G | 1535 | 0 | 1435 | 3 | 0 |
| 2 | B | 1681 | 0 | 1635 | 5 | 0 |
| 2 | D | 1648 | 0 | 1593 | 1 | 0 |
| 2 | F | 1636 | 0 | 1545 | 3 | 0 |
| 2 | H | 1563 | 0 | 1447 | 2 | 0 |
| 3 | A | 140 | 0 | 0 | 0 | 0 |
| 3 | B | 113 | 0 | 0 | 0 | 0 |
| 3 | C | 114 | 0 | 0 | 0 | 0 |
| 3 | D | 72 | 0 | 0 | 0 | 0 |
| 3 | E | 89 | 0 | 0 | 0 | 0 |
| 3 | F | 94 | 0 | 0 | 0 | 0 |
| 3 | G | 77 | 0 | 0 | 0 | 0 |
| 3 | H | 92 | 0 | 0 | 0 | 0 |
| All | All | 13743 | 0 | 12390 | 20 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:B:147[B]:ARG:HD2 | 2:B:147[B]:ARG:O | 1.66 | 0.93 |
| 2:B:147[B]:ARG:HD2 | 2:B:147[B]:ARG:C | 2.02 | 0.75 |
| 2:D:88:VAL:HG21 | 2:D:171:GLN:HB3 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:H:12:PRO:HB2 | 2:H:112:LYS:HE3 | 1.91 | 0.53 |
| 1:G:135:PRO:HD3 | 1:G:221:LYS:HE2 | 1.93 | 0.49 |
| 2:F:42:LEU:HD21 | 2:F:44:LYS:HE3 | 1.95 | 0.47 |
| 1:A:2:VAL:HG13 | 1:A:27:PHE:CD1 | 2.52 | 0.45 |
| 1:A:11:LEU:HB2 | 1:A:159:PRO:HG3 | 1.99 | 0.44 |
| 1:A:34:MET:HB3 | 1:A:79:LEU:HD22 | 2.00 | 0.44 |
| 2:B:171:GLN:HG3 | 2:B:178:TYR:CZ | 2.54 | 0.43 |
| 1:C:154:VAL:HG11 | 1:C:162:VAL:HG11 | 2.00 | 0.42 |
| 2:H:191:TYR:HA | 2:H:197:TYR:OH | 2.20 | 0.42 |
| 2:F:191:TYR:HA | 2:F:197:TYR:OH | 2.20 | 0.41 |
| 2:B:88[B]:VAL:HG21 | 2:B:171:GLN:HB2 | 2.01 | 0.41 |
| 2:B:88[A]:VAL:HG21 | 2:B:171:GLN:HB2 | 2.02 | 0.41 |
| 1:E:2:VAL:HG13 | 1:E:27:PHE:CD1 | 2.56 | 0.41 |
| 2:F:42:LEU:HB2 | 2:F:52:LEU:HD11 | 2.03 | 0.41 |
| 1:G:34:MET:HB3 | 1:G:79:LEU:HD22 | 2.04 | 0.40 |
| 1:A:2:VAL:HG12 | 1:A:114:VAL:HG11 | 2.04 | 0.40 |
| 1:G:2:VAL:HG13 | 1:G:27:PHE:CD1 | 2.57 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.