



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:51 AM GMT

PDB ID : 3JWD
Title : Structure of HIV-1 gp120 with gp41-Interactive Region: Layered Architecture and Basis of Conformational Mobility
Authors : Pancera, M.; Majeed, S.; Ban, Y.A.; Chen, L.; Huang, C.C.; Kong, L.; Kwon, Y.D.; Stuckey, J.; Zhou, T.; Robinson, J.E.; Schief, W.R.; Sodroski, J.; Wyatt, R.; Kwong, P.D.
Deposited on : 2009-09-18
Resolution : 2.61 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

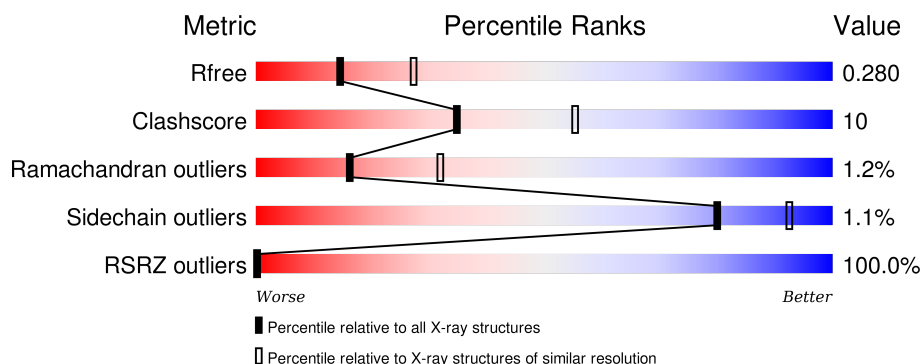
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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} | 91344 | 2700 (2.64-2.60) |
| Clashscore | 102246 | 3065 (2.64-2.60) |
| Ramachandran outliers | 100387 | 3015 (2.64-2.60) |
| Sidechain outliers | 100360 | 3015 (2.64-2.60) |
| RSRZ outliers | 91569 | 2706 (2.64-2.60) |

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 379 | <div> <div>95%</div> <div>69% 25% 5%</div> </div> |
| 1 | B | 379 | <div> <div>93%</div> <div>69% 24% 7%</div> </div> |
| 2 | C | 184 | <div> <div>100%</div> <div>74% 24%</div> </div> |
| 2 | D | 184 | <div> <div>99%</div> <div>79% 20%</div> </div> |
| 3 | L | 213 | <div> <div>100%</div> <div>77% 23%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | O | 213 | |
| 4 | H | 220 | |
| 4 | P | 220 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | NAG | A | 734 | X | - | - | X |
| 5 | NAG | A | 762 | - | - | - | X |
| 5 | NAG | A | 776 | - | - | - | X |
| 5 | NAG | A | 789 | - | - | - | X |
| 5 | NAG | A | 886 | - | - | - | X |
| 5 | NAG | A | 897 | - | - | - | X |
| 5 | NAG | A | 948 | X | - | - | X |
| 5 | NAG | B | 588 | X | - | - | - |
| 5 | NAG | B | 734 | - | - | - | X |
| 5 | NAG | B | 762 | - | - | - | X |
| 5 | NAG | B | 776 | - | - | - | X |
| 5 | NAG | B | 789 | - | - | - | X |
| 6 | GOL | B | 1 | - | - | - | X |
| 6 | GOL | P | 215 | - | - | - | X |

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15697 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 HIV-1 GP120 ENVELOPE GLYCOPROTEIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 360 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2800 | 1769 | 480 | 531 | 20 | | | |
| 1 | B | 354 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2756 | 1744 | 472 | 520 | 20 | | | |

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | C | 184 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1432 | 896 | 250 | 281 | 5 | | | |
| 2 | D | 183 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1424 | 891 | 249 | 280 | 4 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| C | 1000 | MET | - | INITIATING METHIONINE | UNP P01730 |
| D | 1000 | MET | - | INITIATING METHIONINE | UNP P01730 |

- Molecule 3 is a protein called FAB 48D LIGHT CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | L | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1635 | 1022 | 274 | 333 | 6 | | | |
| 3 | O | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1624 | 1017 | 272 | 330 | 5 | | | |

- Molecule 4 is a protein called FAB 48D HEAVY CHAIN.

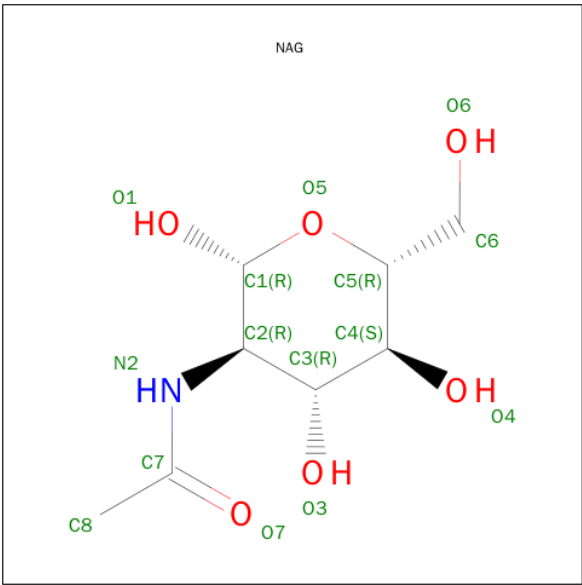
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | H | 220 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1654 | 1048 | 267 | 332 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | P | 219 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1644 | 1042 | 265 | 330 | 7 | | | |

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



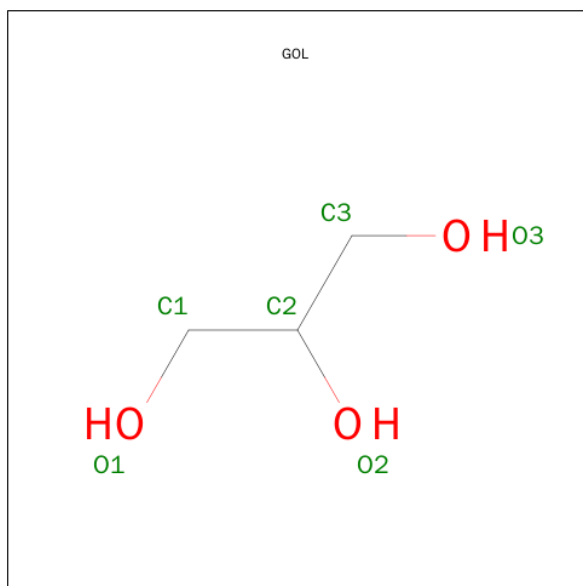
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6 | B | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |
| 6 | P | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 3 | 3 | | |

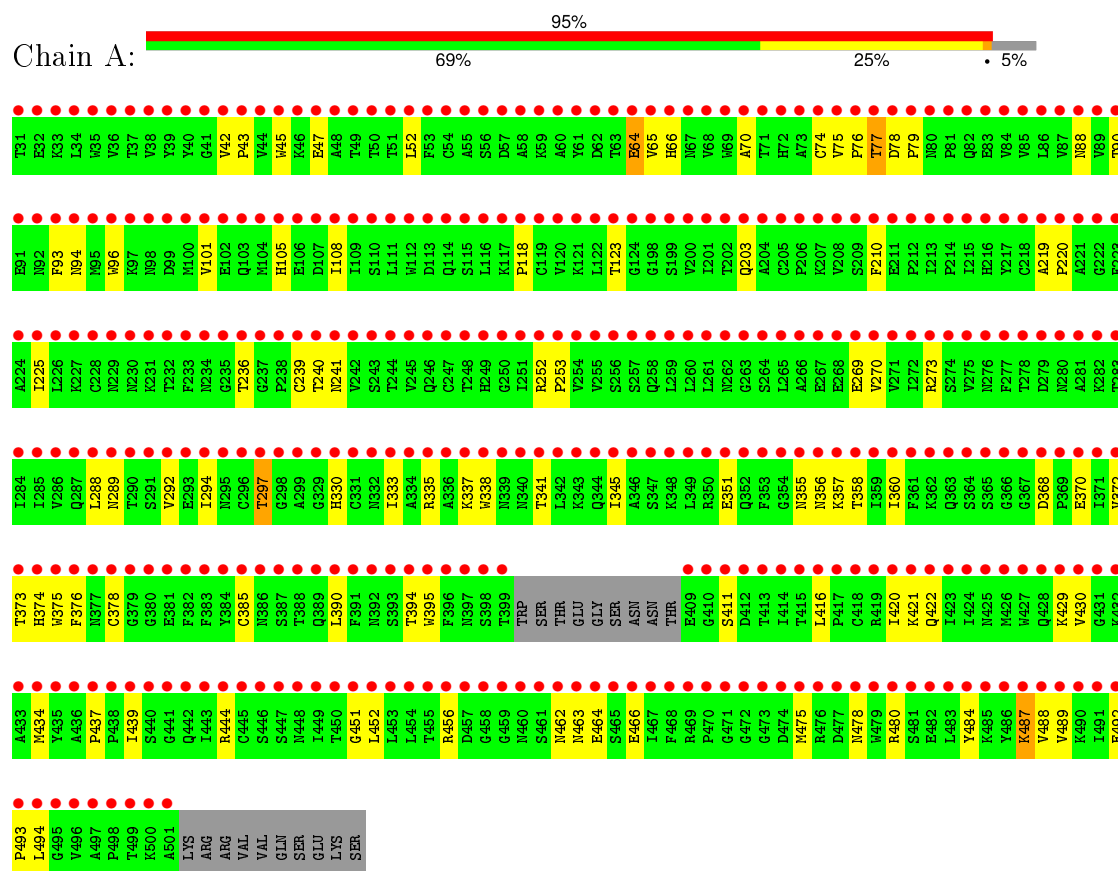
- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7 | A | 135 | Total 135 | O 135 | 0 | 0 |
| 7 | C | 50 | Total 50 | O 50 | 0 | 0 |
| 7 | L | 54 | Total 54 | O 54 | 0 | 0 |
| 7 | H | 47 | Total 47 | O 47 | 0 | 0 |
| 7 | B | 68 | Total 68 | O 68 | 0 | 0 |
| 7 | D | 34 | Total 34 | O 34 | 0 | 0 |
| 7 | O | 23 | Total 23 | O 23 | 0 | 0 |
| 7 | P | 39 | Total 39 | O 39 | 0 | 0 |

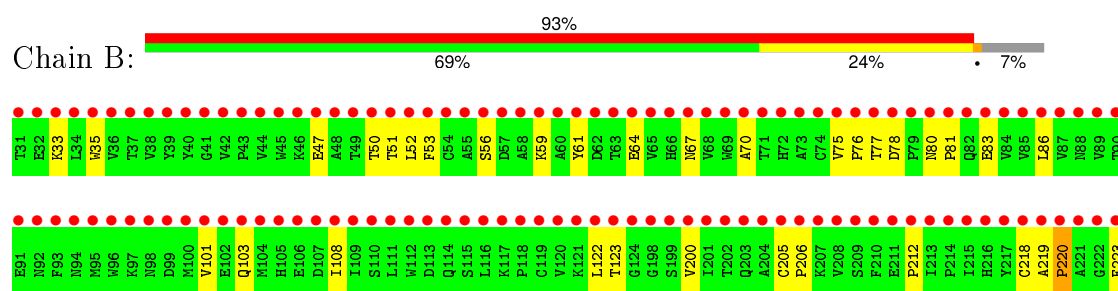
3 Residue-property plots

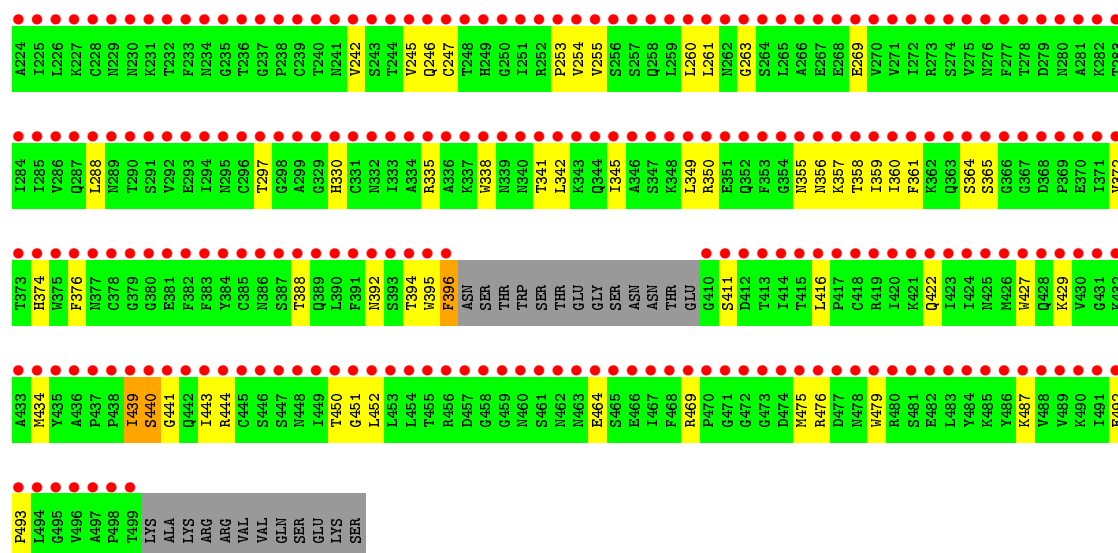
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: HIV-1 GP120 ENVELOPE GLYCOPROTEIN

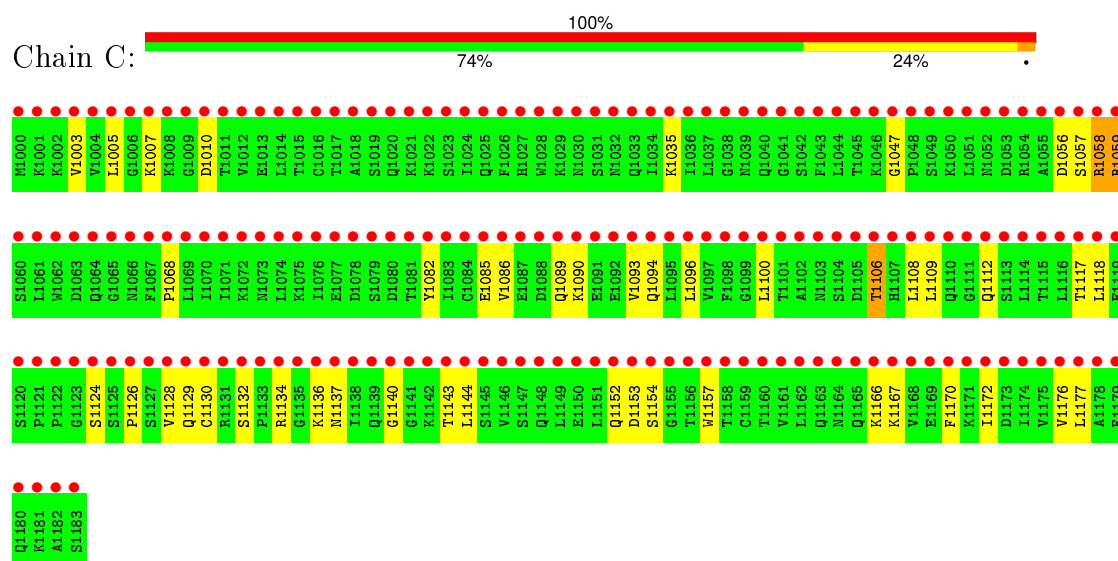


• Molecule 1: HIV-1 GP120 ENVELOPE GLYCOPROTEIN

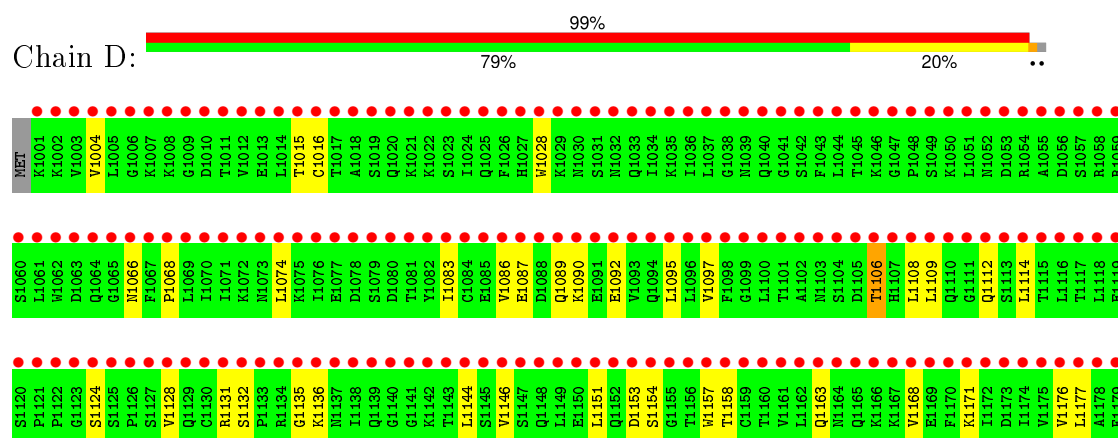




• Molecule 2: T-cell surface glycoprotein CD4



• Molecule 2: T-cell surface glycoprotein CD4



Q1180
K1181
A1182
S1183

• Molecule 3: FAB 48D LIGHT CHAIN

Chain L:  100% 77% 23%

D1 I2 Q3 M4 T5 Q6 S7 P8 S9 S10 S11 V11 S12 S13 A13 S14 V15 G16 D17 R18 R19 T20 T21 T22 T23 C23 R24 A25 S26 Q27 Q28 Q29 Q30 S30 T31 T32 L33 A34 W35 Y36 Q37 Q38 Q39 P40 G41 T42 K42 A43 P44 K45 L46 L47 L48 Y49 V10 A50 A51 S52 T53 L54 Q55 S56 G57 V58 P59 S60

R61 F62 S63 G64 S65 S66 S67 G68 T69 D70 F71 V72 S73 L73 T74 T75 W76 S77 L78 Q79 P80 E81 D82 F83 A84 T85 Y86 Y87 Y88 F98 G99 G100 G101 T102 K103 K104 A105 E106 K107 R108 T109 V110 A111 A112 P113 S114 V115 F116 I117 F118 P119 P120 S121

D122 E123 Q124 L125 K126 S127 G128 T129 R130 D131 V132 C133 A134 L135 V136 M137 N138 F139 G140 P141 P142 E143 F144 K145 T146 Q147 W148 F149 D150 V151 D152 A153 L154 S155 S156 G157 M158 S159 Q160 E161 S162 V163 T164 E165 Q166 D167 S168 K169 D170 S171 T172 V173 S174 L175 S176 S177 T178 L179 T180 L181

S182 K183 A184 D185 Y186 E187 K188 H189 K190 L191 Y192 A193 C194 E195 T196 T197 H198 Q199 G200 L201 S202 S203 F204 V205 T206 K207 S208 F209 N210 R211 G212 E213 C214

• Molecule 3: FAB 48D LIGHT CHAIN

Chain O:  100% 83% 16%

D1 I2 Q3 M4 T5 Q6 S7 P8 S9 S10 S11 V11 S12 S13 A13 S14 V15 G16 D17 R18 R19 T20 T21 T22 T23 C23 R24 A25 S26 Q27 Q28 Q29 Q30 S30 T31 T32 L33 A34 W35 Y36 Q37 Q38 Q39 P40 G41 T42 K42 A43 P44 K45 L46 L47 L48 Y49 V10 A50 A51 S52 T53 L54 Q55 S56 G57 V58 P59 S60

R61 F62 S63 G64 S65 S66 S67 G68 T69 D70 F71 V72 S73 L73 T74 T75 W76 S77 L78 Q79 P80 E81 D82 F83 A84 T85 Y86 Y87 Y88 F98 G99 G100 G101 T102 K103 K104 A105 E106 K107 R108 T109 V110 A111 A112 P113 S114 V115 F116 I117 F118 P119 P120 S121

D122 E123 Q124 L125 K126 S127 G128 T129 R130 D131 V132 C133 A134 L135 V136 M137 N138 F139 G140 P141 P142 E143 F144 K145 T146 Q147 W148 F149 D150 V151 D152 A153 L154 S155 S156 G157 M158 S159 Q160 E161 S162 V163 T164 E165 Q166 D167 S168 K169 D170 S171 T172 V173 S174 L175 S176 S177 T178 L179 T180 L181

S182 K183 A184 D185 Y186 E187 K188 H189 K190 L191 Y192 A193 C194 E195 T196 T197 H198 Q199 G200 L201 S202 S203 F204 V205 T206 K207 S208 F209 N210 R211 G212 E213 YCM

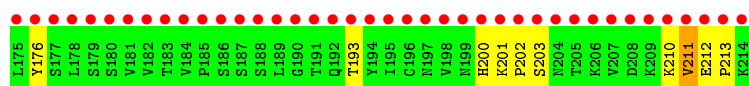
• Molecule 4: FAB 48D HEAVY CHAIN

Chain H:  100% 78% 21%

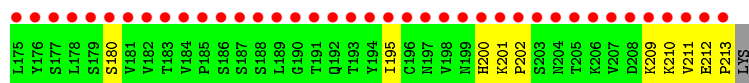
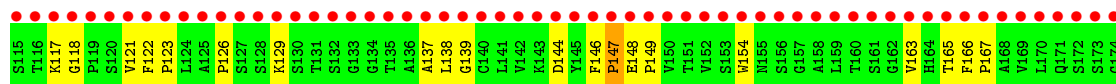
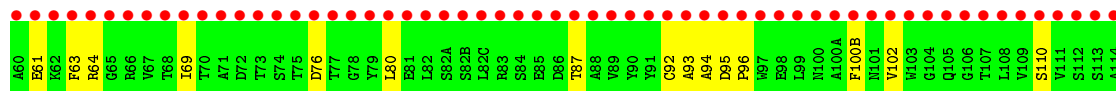
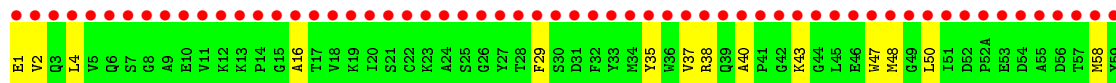
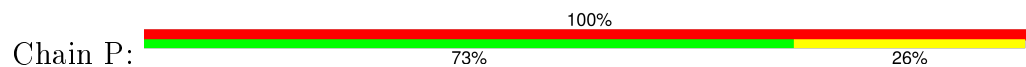
E1 V2 R3 L4 V5 Q6 S7 G8 A9 P10 V11 K12 K13 P14 G15 A16 T17 T18 K19 L20 S21 C22 R23 A24 S25 G26 T27 S28 F29 S30 S31 D31 F32 T33 Y34 Y35 R36 V37 R38 Q39 P41 P42 K43 G44 L45 E46 W47 M48 G49 L50 L51 D52 P52A E53 D54 A55 D56 T57 S58 Y59

A60 E61 K62 G63 F64 R65 S66 R67 T68 T69 I69 T70 A71 D72 T73 T74 G15 S130 T75 D76 T77 G78 L90 E81 L82 L83 S82A S82B L82C R83 S84 T88 E85 K86 D86 T87 T88 A88 V89 Y90 P149 Y91 C92 C93 A94 D95 P96 W97 G98 L99 N100 A100A F100B M101 S161 G162 V102 V103 G104 Q105 G106 T107 L108 V109 S110 V110 V111 S112 S113 A114

S115 T116 K117 G118 P119 S120 V121 F122 T123 L124 A125 P126 S127 S128 K129 S130 T131 S132 G133 T134 T135 A136 A137 L138 G139 C140 L141 T142 S143 K144 D145 T146 F147 V148 P149 Y150 C150 C151 A152 S153 M155 S156 G157 L158 L159 T160 S161 G162 V163 G164 T165 F166 P167 A168 V169 L170 Q171 S172 S173 G174



● Molecule 4: FAB 48D HEAVY CHAIN



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 83.11Å 172.95Å 193.14Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 43.86 – 2.61 43.86 – 2.61 | Depositor EDS |
| % Data completeness (in resolution range) | 63.8 (43.86-2.61) 63.9 (43.86-2.61) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | 0.08 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.04 (at 2.61Å) | Xtriage |
| Refinement program | PHENIX (CCI APPS 2007_04_06_1210) | Depositor |
| R, R_{free} | 0.201 , 0.275 0.198 , 0.280 | Depositor DCC |
| R_{free} test set | 5577 reflections (10.14%) | DCC |
| Wilson B-factor (Å ²) | -10.7 | Xtriage |
| Anisotropy | -7.799 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.27 , 62.7 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Outliers | 23 of 59587 reflections (0.039%) | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 15697 | wwPDB-VP |
| Average B, all atoms (Å ²) | 114.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, YCM

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 | 0.24 | 0/2865 | 0.42 | 0/3900 |
| 1 | B | 0.22 | 0/2821 | 0.39 | 0/3841 |
| 2 | C | 0.23 | 0/1452 | 0.43 | 0/1955 |
| 2 | D | 0.22 | 0/1444 | 0.38 | 0/1945 |
| 3 | L | 0.23 | 0/1659 | 0.40 | 0/2252 |
| 3 | O | 0.21 | 0/1659 | 0.38 | 0/2252 |
| 4 | H | 0.22 | 0/1695 | 0.42 | 0/2311 |
| 4 | P | 0.21 | 0/1685 | 0.39 | 0/2300 |
| All | All | 0.22 | 0/15280 | 0.40 | 0/20756 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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 | 2800 | 0 | 2724 | 67 | 0 |
| 1 | B | 2756 | 0 | 2683 | 68 | 0 |
| 2 | C | 1432 | 0 | 1460 | 35 | 0 |
| 2 | D | 1424 | 0 | 1451 | 21 | 0 |
| 3 | L | 1635 | 0 | 1582 | 28 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | O | 1624 | 0 | 1574 | 19 | 0 |
| 4 | H | 1654 | 0 | 1613 | 30 | 0 |
| 4 | P | 1644 | 0 | 1600 | 37 | 0 |
| 5 | A | 140 | 0 | 130 | 2 | 0 |
| 5 | B | 126 | 0 | 117 | 2 | 0 |
| 6 | B | 6 | 0 | 8 | 3 | 0 |
| 6 | P | 6 | 0 | 8 | 0 | 0 |
| 7 | A | 135 | 0 | 0 | 1 | 0 |
| 7 | B | 68 | 0 | 0 | 0 | 0 |
| 7 | C | 50 | 0 | 0 | 1 | 0 |
| 7 | D | 34 | 0 | 0 | 0 | 0 |
| 7 | H | 47 | 0 | 0 | 0 | 0 |
| 7 | L | 54 | 0 | 0 | 1 | 0 |
| 7 | O | 23 | 0 | 0 | 0 | 0 |
| 7 | P | 39 | 0 | 0 | 0 | 0 |
| All | All | 15697 | 0 | 14950 | 299 | 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 10.

The worst 5 of 299 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:254:VAL:HB | 6:B:1:GOL:H11 | 1.43 | 1.00 |
| 1:A:492:GLU:HB2 | 1:A:493:PRO:HD2 | 1.55 | 0.88 |
| 4:H:126:PRO:HD3 | 4:H:138:LEU:HD13 | 1.54 | 0.88 |
| 2:C:1085:GLU:HG2 | 2:C:1090:LYS:HG3 | 1.57 | 0.84 |
| 1:B:342:LEU:HB3 | 1:B:395:TRP:HE1 | 1.42 | 0.84 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1 | A | 356/379 (94%) | 311 (87%) | 40 (11%) | 5 (1%) | 14 | 26 |
| 1 | B | 350/379 (92%) | 314 (90%) | 31 (9%) | 5 (1%) | 14 | 26 |
| 2 | C | 182/184 (99%) | 168 (92%) | 13 (7%) | 1 (0%) | 34 | 58 |
| 2 | D | 181/184 (98%) | 159 (88%) | 22 (12%) | 0 | 100 | 100 |
| 3 | L | 211/213 (99%) | 194 (92%) | 14 (7%) | 3 (1%) | 14 | 26 |
| 3 | O | 210/213 (99%) | 181 (86%) | 26 (12%) | 3 (1%) | 14 | 26 |
| 4 | H | 218/220 (99%) | 193 (88%) | 22 (10%) | 3 (1%) | 14 | 26 |
| 4 | P | 217/220 (99%) | 194 (89%) | 20 (9%) | 3 (1%) | 14 | 26 |
| All | All | 1925/1992 (97%) | 1714 (89%) | 188 (10%) | 23 (1%) | 16 | 32 |

5 of 23 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | L | 76 | ASN |
| 3 | L | 138 | ASN |
| 1 | B | 439 | ILE |
| 1 | B | 440 | SER |
| 1 | A | 356 | ASN |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1 | A | 315/333 (95%) | 310 (98%) | 5 (2%) | 70 | 88 |
| 1 | B | 310/333 (93%) | 309 (100%) | 1 (0%) | 94 | 99 |
| 2 | C | 166/166 (100%) | 161 (97%) | 5 (3%) | 48 | 75 |
| 2 | D | 165/166 (99%) | 162 (98%) | 3 (2%) | 66 | 86 |
| 3 | L | 184/184 (100%) | 180 (98%) | 4 (2%) | 60 | 83 |
| 3 | O | 184/184 (100%) | 184 (100%) | 0 | 100 | 100 |
| 4 | H | 185/185 (100%) | 184 (100%) | 1 (0%) | 92 | 98 |
| 4 | P | 184/185 (100%) | 184 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| All | All | 1693/1736 (98%) | 1674 (99%) | 19 (1%) | 80 | 92 |

5 of 19 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | C | 1106 | THR |
| 3 | L | 105 | GLU |
| 1 | B | 396 | PHE |
| 2 | C | 1059 | ARG |
| 2 | D | 1015 | THR |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | O | 27 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 3 | YCM | L | 214 | 3 | 7,10,10 | 1.30 | 2 (28%) | 4,12,12 | 0.82 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3 | YCM | L | 214 | 3 | - | 0/6/10/10 | 0/0/0/0 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | L | 214 | YCM | CB-SG | -2.37 | 1.76 | 1.81 |
| 3 | L | 214 | YCM | CD-SG | -2.27 | 1.76 | 1.81 |

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 5 | NAG | A | 588 | 1 | 14,14,15 | 0.50 | 0 | 15,19,21 | 1.02 | 1 (6%) |
| 5 | NAG | A | 734 | 1 | 14,14,15 | 0.51 | 0 | 15,19,21 | 0.75 | 0 |
| 5 | NAG | A | 741 | 1 | 14,14,15 | 0.46 | 0 | 15,19,21 | 0.98 | 1 (6%) |
| 5 | NAG | A | 762 | 1 | 14,14,15 | 0.50 | 0 | 15,19,21 | 0.90 | 1 (6%) |
| 5 | NAG | A | 776 | 1 | 14,14,15 | 0.47 | 0 | 15,19,21 | 0.92 | 1 (6%) |
| 5 | NAG | A | 789 | 1 | 14,14,15 | 0.55 | 0 | 15,19,21 | 0.72 | 0 |
| 5 | NAG | A | 886 | 1 | 14,14,15 | 0.48 | 0 | 15,19,21 | 0.85 | 1 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | NAG | A | 892 | 1 | 14,14,15 | 0.58 | 0 | 15,19,21 | 1.21 | 1 (6%) |
| 5 | NAG | A | 897 | 1 | 14,14,15 | 0.53 | 0 | 15,19,21 | 0.74 | 0 |
| 5 | NAG | A | 948 | 1 | 14,14,15 | 0.52 | 0 | 15,19,21 | 0.75 | 0 |
| 6 | GOL | B | 1 | - | 5,5,5 | 0.38 | 0 | 5,5,5 | 0.20 | 0 |
| 5 | NAG | B | 588 | 1 | 14,14,15 | 0.48 | 0 | 15,19,21 | 0.80 | 1 (6%) |
| 5 | NAG | B | 734 | 1 | 14,14,15 | 0.48 | 0 | 15,19,21 | 0.75 | 0 |
| 5 | NAG | B | 762 | 1 | 14,14,15 | 0.51 | 0 | 15,19,21 | 0.95 | 1 (6%) |
| 5 | NAG | B | 776 | 1 | 14,14,15 | 0.47 | 0 | 15,19,21 | 0.88 | 1 (6%) |
| 5 | NAG | B | 789 | 1 | 14,14,15 | 0.50 | 0 | 15,19,21 | 0.86 | 1 (6%) |
| 5 | NAG | B | 795 | 1 | 14,14,15 | 0.45 | 0 | 15,19,21 | 0.88 | 1 (6%) |
| 5 | NAG | B | 886 | 1 | 14,14,15 | 0.47 | 0 | 15,19,21 | 0.95 | 1 (6%) |
| 5 | NAG | B | 892 | 1 | 14,14,15 | 0.51 | 0 | 15,19,21 | 0.70 | 0 |
| 5 | NAG | B | 948 | 1 | 14,14,15 | 0.49 | 0 | 15,19,21 | 0.70 | 0 |
| 6 | GOL | P | 215 | - | 5,5,5 | 0.38 | 0 | 5,5,5 | 0.24 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5 | NAG | A | 588 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 734 | 1 | 1/1/5/7 | 1/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 741 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 762 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 776 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 789 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 886 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 892 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 897 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 948 | 1 | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |
| 6 | GOL | B | 1 | - | - | 0/4/4/4 | 0/0/0/0 |
| 5 | NAG | B | 588 | 1 | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 734 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 762 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 776 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 789 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 795 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 886 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 892 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 948 | 1 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|---------|
| 6 | GOL | P | 215 | - | - | 0/4/4/4 | 0/0/0/0 |

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 5 | B | 789 | NAG | C1-O5-C5 | 2.22 | 115.06 | 112.25 |
| 5 | B | 588 | NAG | C1-O5-C5 | 2.27 | 115.13 | 112.25 |
| 5 | B | 776 | NAG | C1-O5-C5 | 2.29 | 115.16 | 112.25 |
| 5 | A | 762 | NAG | C1-O5-C5 | 2.29 | 115.16 | 112.25 |
| 5 | B | 795 | NAG | C1-O5-C5 | 2.34 | 115.21 | 112.25 |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 5 | A | 734 | NAG | C1 |
| 5 | B | 588 | NAG | C1 |
| 5 | A | 948 | NAG | C1 |

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 5 | A | 734 | NAG | O7-C7-N2-C2 |
| 5 | B | 892 | NAG | O7-C7-N2-C2 |
| 5 | A | 789 | NAG | O7-C7-N2-C2 |
| 5 | B | 734 | NAG | O7-C7-N2-C2 |

There are no ring outliers.

5 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | A | 588 | NAG | 1 | 0 |
| 5 | A | 734 | NAG | 1 | 0 |
| 6 | B | 1 | GOL | 3 | 0 |
| 5 | B | 762 | NAG | 1 | 0 |
| 5 | B | 789 | NAG | 1 | 0 |

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------|-----------------------|-------|
| 1 | A | 360/379 (94%) | 13.52 | 360 (100%) 0 0 | 45, 78, 151, 254 | 0 |
| 1 | B | 354/379 (93%) | 13.23 | 354 (100%) 0 0 | 66, 113, 190, 233 | 0 |
| 2 | C | 184/184 (100%) | 13.79 | 184 (100%) 0 0 | 56, 83, 125, 144 | 0 |
| 2 | D | 183/184 (99%) | 13.38 | 183 (100%) 0 0 | 74, 127, 165, 188 | 0 |
| 3 | L | 212/213 (99%) | 14.03 | 212 (100%) 0 0 | 59, 101, 179, 240 | 0 |
| 3 | O | 212/213 (99%) | 13.07 | 212 (100%) 0 0 | 91, 147, 189, 220 | 0 |
| 4 | H | 220/220 (100%) | 14.19 | 220 (100%) 0 0 | 70, 121, 179, 251 | 0 |
| 4 | P | 219/220 (99%) | 13.71 | 219 (100%) 0 0 | 66, 121, 195, 243 | 0 |
| All | All | 1944/1992 (97%) | 13.58 | 1944 (100%) 0 0 | 45, 110, 180, 254 | 0 |

The worst 5 of 1944 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | O | 41 | GLY | 27.1 |
| 4 | H | 88 | ALA | 24.9 |
| 1 | B | 385 | CYS | 24.6 |
| 4 | P | 26 | GLY | 24.2 |
| 1 | A | 228 | CYS | 23.9 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|-------|------|------|-----------------------------|-------|
| 3 | YCM | L | 214 | 11/11 | -0.30 | 1.01 | - | 180,198,236,238 | 0 |

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|-------|------|-------|-----------------------------|-------|
| 5 | NAG | B | 789 | 14/15 | -0.11 | 1.22 | 1.40 | 139,187,198,202 | 0 |
| 5 | NAG | A | 789 | 14/15 | -0.09 | 1.16 | 0.56 | 86,104,117,128 | 0 |
| 5 | NAG | A | 776 | 14/15 | -0.22 | 1.19 | 0.52 | 80,95,117,119 | 0 |
| 5 | NAG | B | 734 | 14/15 | -0.31 | 1.17 | 0.50 | 167,184,193,194 | 0 |
| 5 | NAG | A | 886 | 14/15 | -0.13 | 1.29 | 0.16 | 70,97,131,139 | 0 |
| 5 | NAG | A | 897 | 14/15 | -0.03 | 1.10 | 0.06 | 124,150,169,175 | 0 |
| 5 | NAG | A | 762 | 14/15 | -0.10 | 1.09 | -0.28 | 70,75,96,97 | 0 |
| 5 | NAG | A | 734 | 14/15 | 0.04 | 1.10 | -0.29 | 113,130,148,153 | 0 |
| 5 | NAG | B | 762 | 14/15 | 0.01 | 1.01 | -0.37 | 102,122,145,155 | 0 |
| 6 | GOL | B | 1 | 6/6 | -0.05 | 0.87 | -0.75 | 127,132,138,143 | 0 |
| 5 | NAG | A | 948 | 14/15 | -0.14 | 1.04 | -0.80 | 143,154,166,166 | 0 |
| 5 | NAG | B | 776 | 14/15 | 0.07 | 1.04 | -1.09 | 118,135,157,161 | 0 |
| 6 | GOL | P | 215 | 6/6 | 0.26 | 0.82 | -2.38 | 134,147,156,162 | 0 |
| 5 | NAG | B | 892 | 14/15 | 0.07 | 1.09 | - | 166,204,227,236 | 0 |
| 5 | NAG | B | 795 | 14/15 | -0.14 | 1.04 | - | 169,190,203,209 | 0 |
| 5 | NAG | A | 892 | 14/15 | -0.01 | 1.13 | - | 117,148,182,193 | 0 |
| 5 | NAG | A | 588 | 14/15 | 0.07 | 1.09 | - | 99,141,159,174 | 0 |
| 5 | NAG | B | 886 | 14/15 | -0.20 | 1.05 | - | 105,122,143,147 | 0 |
| 5 | NAG | B | 948 | 14/15 | -0.20 | 1.11 | - | 147,169,175,179 | 0 |
| 5 | NAG | A | 741 | 14/15 | -0.02 | 1.01 | - | 141,160,164,166 | 0 |
| 5 | NAG | B | 588 | 14/15 | -0.13 | 0.86 | - | 119,161,167,169 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.