# wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:15 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 4KXF |
| Title | : | Crystal structure of NLRC4 reveals its autoinhibition mechanism |
| Authors | : | Chai, J.; Hu, Z. |
| Deposited on | : | 2013-05-25 |
| Resolution | : | 3.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

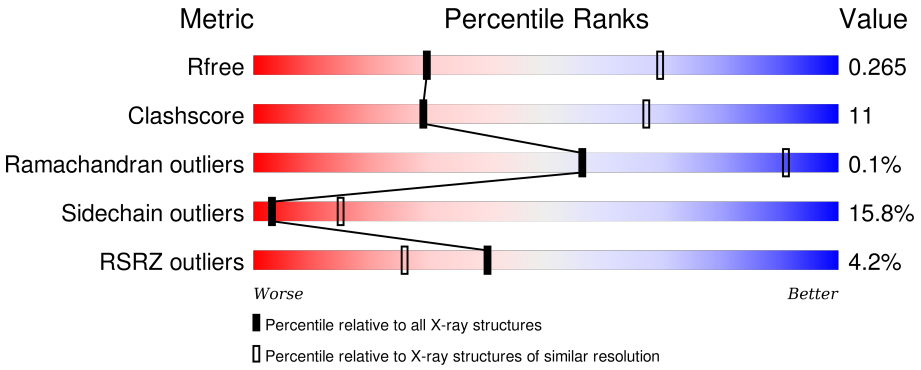
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| 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 (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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 | 1124 (3.24-3.16) |
| Clashscore | 102246 | 1024 (3.22-3.18) |
| Ramachandran outliers | 100387 | 1004 (3.22-3.18) |
| Sidechain outliers | 100360 | 1003 (3.22-3.18) |
| RSRZ outliers | 91569 | 1129 (3.24-3.16) |

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 <=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 | B | 1024 | 2% 57% 26% 5% 12% |
| 1 | D | 1024 | 3% 59% 26% • 12% |
| 1 | F | 1024 | 3% 58% 25% • 12% |
| 1 | H | 1024 | 3% 57% 27% • 12% |
| 1 | K | 1024 | 2% 56% 28% • 12% |

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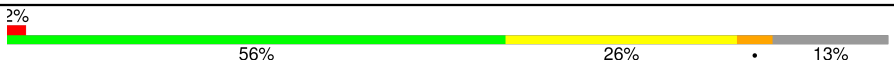
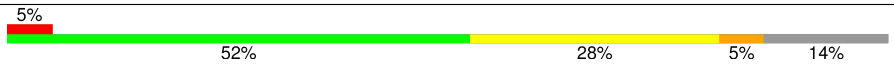
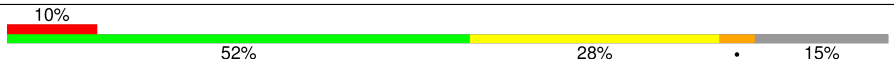
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | L | 1024 |   |
| 1 | N | 1024 |   |
| 1 | P | 1024 |   |

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 |
|---|---|---|---|---|---|---|---|
| 3 | SO4 | B | 1102 | - | - | - | X |

## 2 Entry composition (i)

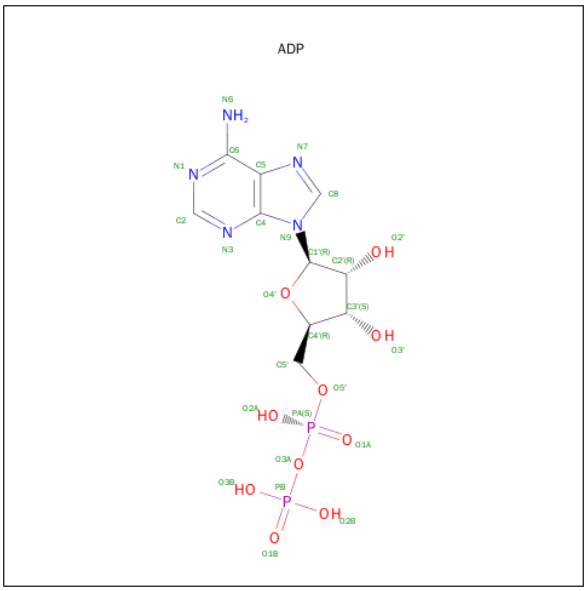
There are 3 unique types of molecules in this entry. The entry contains 57081 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NLR family CARD domain-containing protein 4.

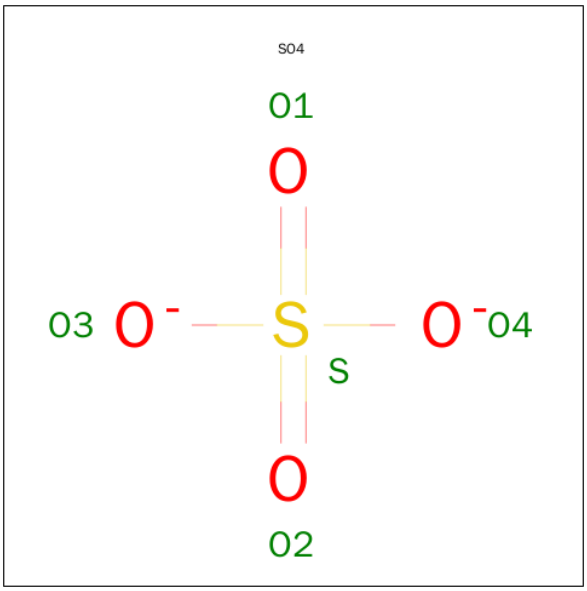
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | K | 904 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7208 | 4600 | 1215 | 1352 | 1 | 40 | | | |
| 1 | B | 903 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7204 | 4599 | 1222 | 1342 | 1 | 40 | | | |
| 1 | D | 900 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7177 | 4581 | 1208 | 1347 | 1 | 40 | | | |
| 1 | F | 899 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7172 | 4577 | 1208 | 1346 | 1 | 40 | | | |
| 1 | H | 898 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7135 | 4553 | 1201 | 1340 | 1 | 40 | | | |
| 1 | L | 893 | Total | C | N | O | P | S | 0 | 0 | 0 |
| | | | 7107 | 4540 | 1199 | 1327 | 1 | 40 | | | |
| 1 | N | 882 | Total | C | N | O | S | | 0 | 0 | 0 |
| | | | 6996 | 4468 | 1181 | 1307 | 40 | | | | |
| 1 | P | 866 | Total | C | N | O | S | | 0 | 0 | 0 |
| | | | 6856 | 4377 | 1157 | 1282 | 40 | | | | |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | K | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | L | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | N | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 2 | P | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: $O_4S$).



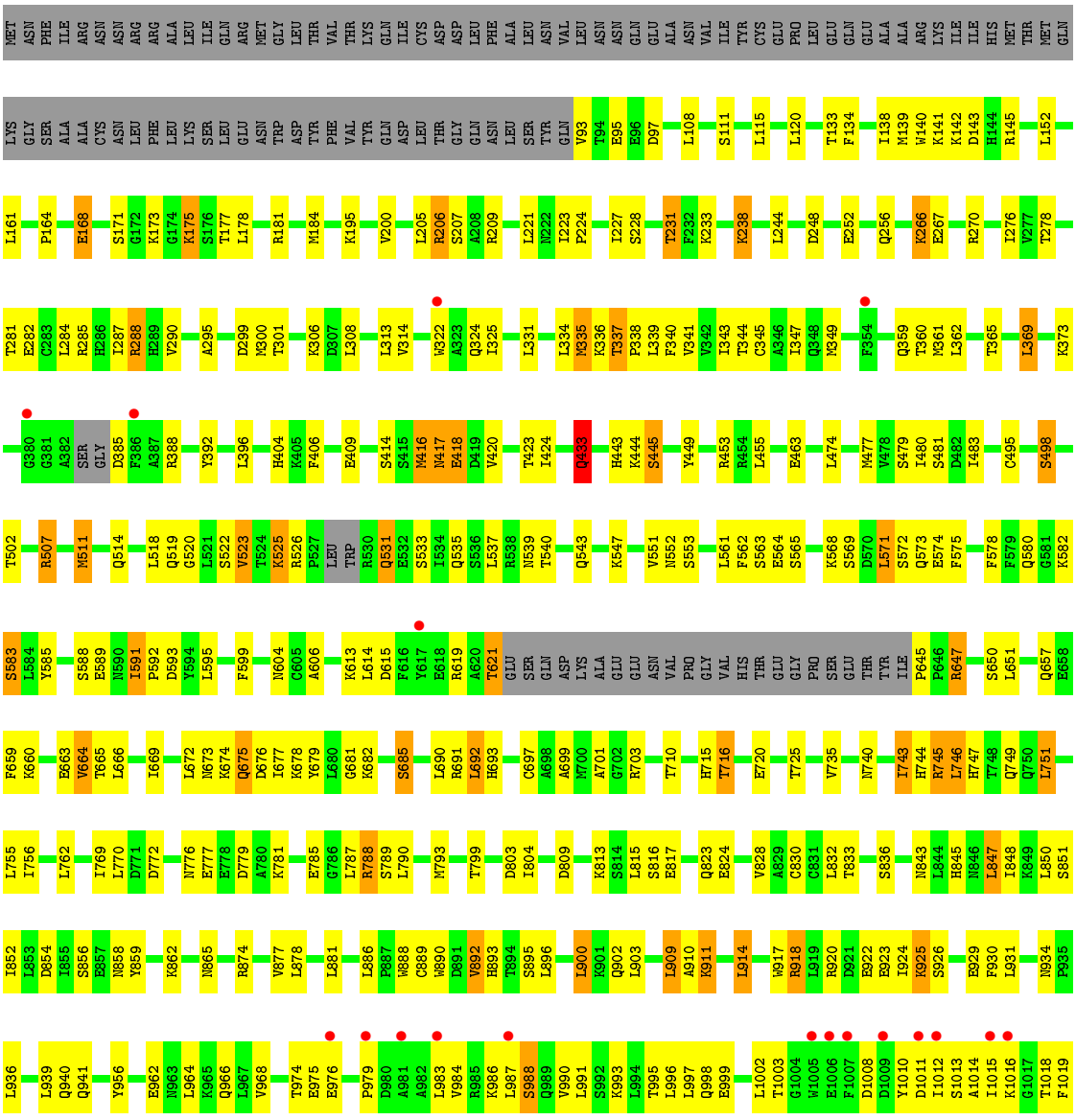

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | B | 1 | Total O S<br>5 4 1 | 0 | 0 |
| 3 | N | 1 | Total O S<br>5 4 1 | 0 | 0 |

# 3 Residue-property plots (i)

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

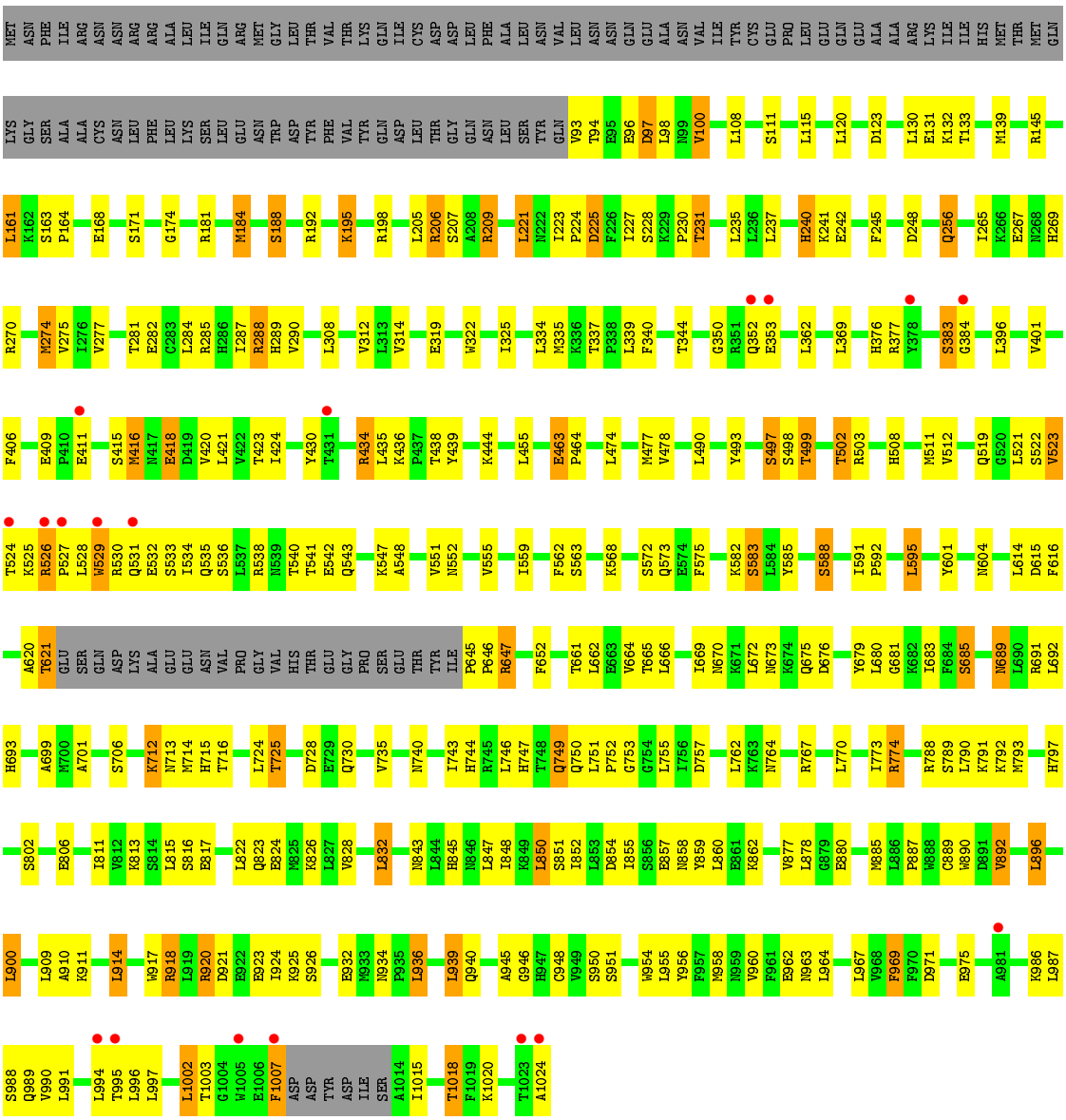
- Molecule 1: NLR family CARD domain-containing protein 4

Chain K:



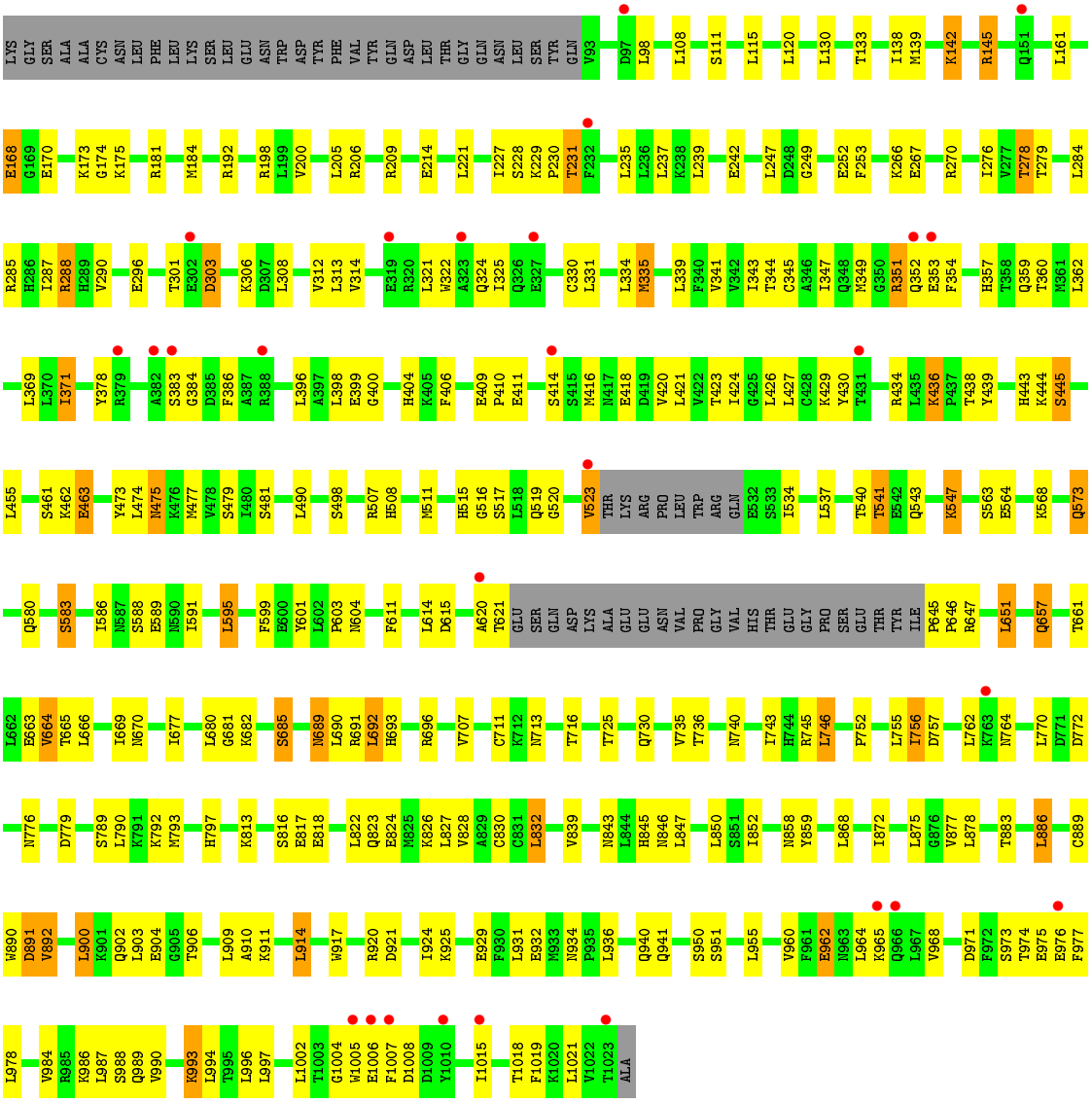
• Molecule 1: NLR family CARD domain-containing protein 4

Chain B:



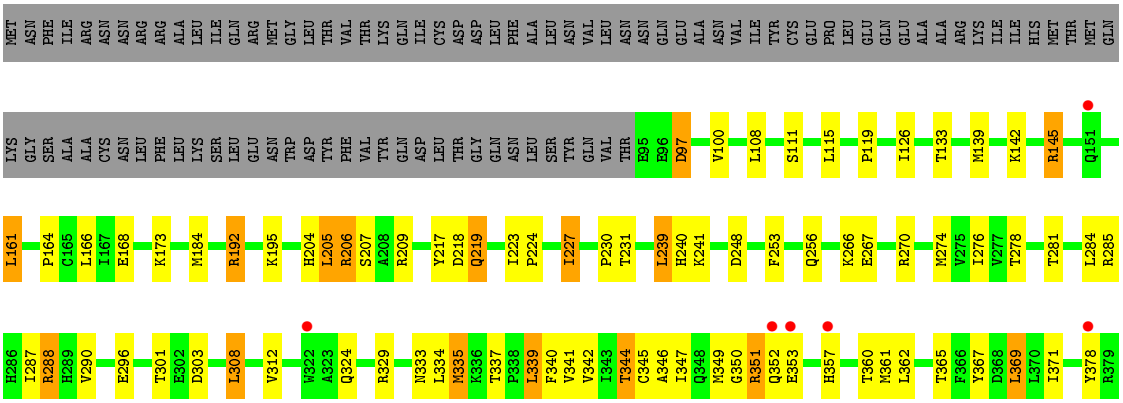
• Molecule 1: NLR family CARD domain-containing protein 4

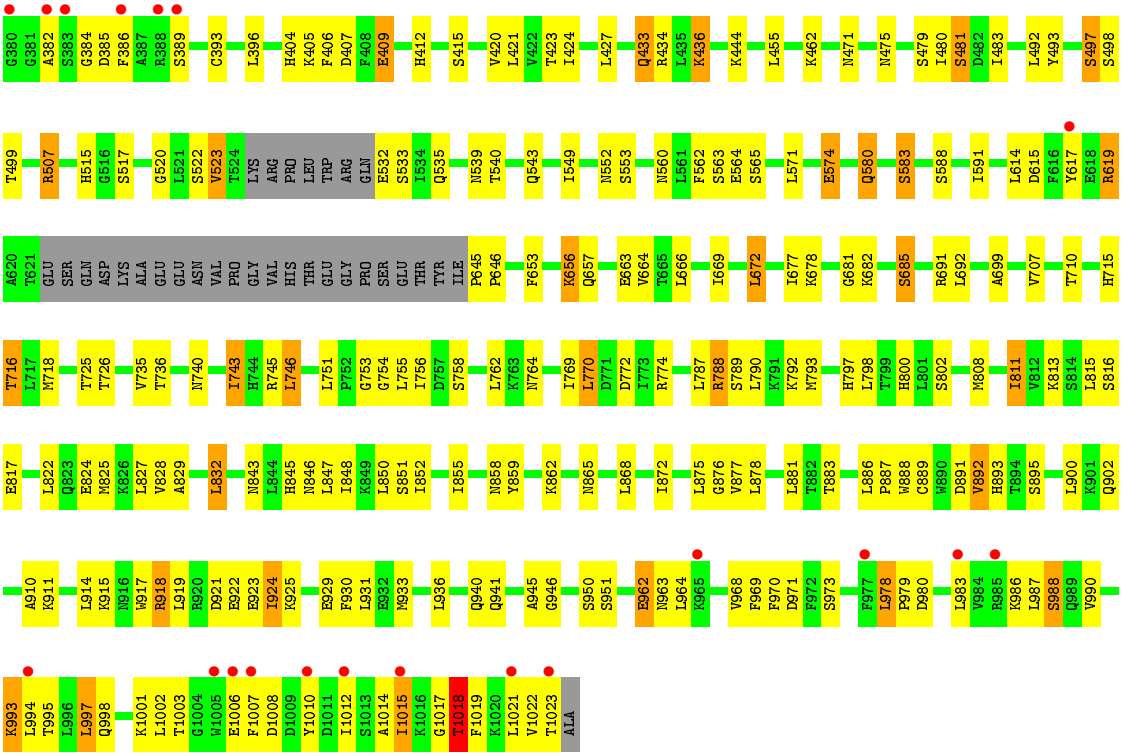
Chain D:



• Molecule 1: NLR family CARD domain-containing protein 4

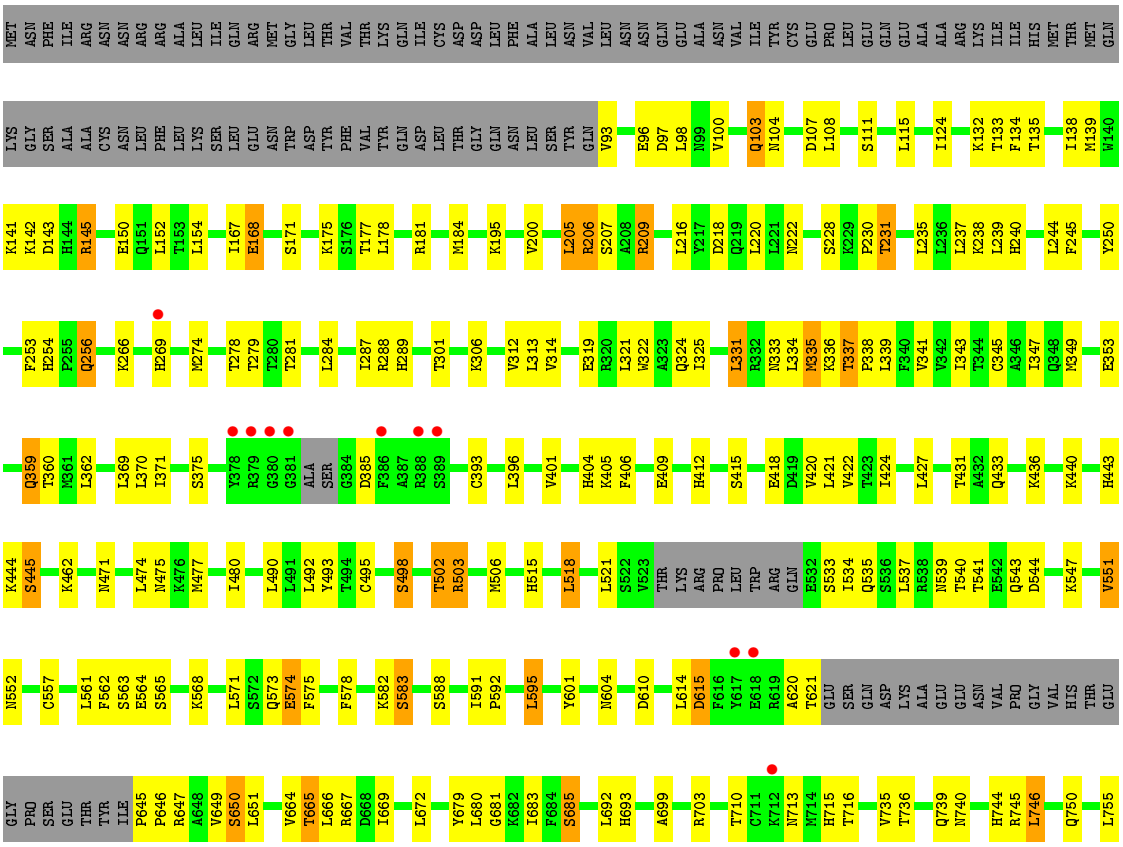
Chain F:

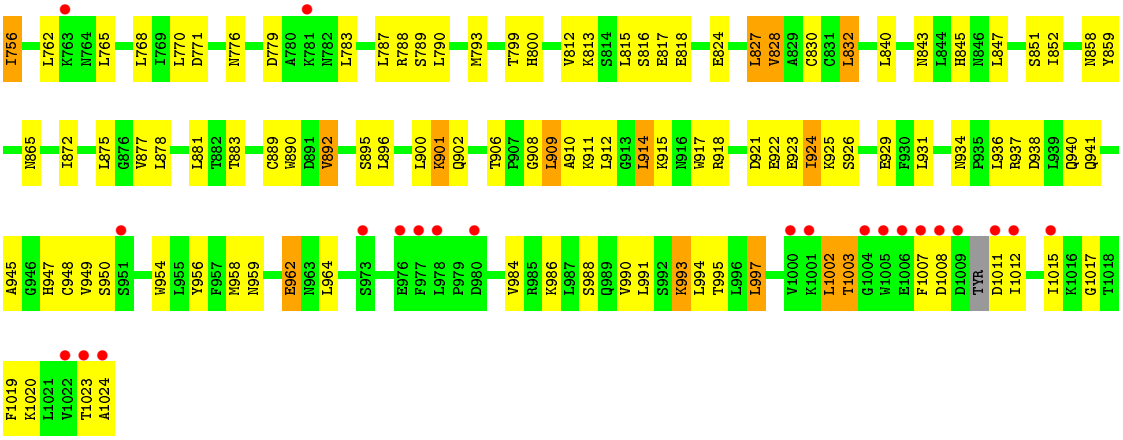




• Molecule 1: NLR family CARD domain-containing protein 4

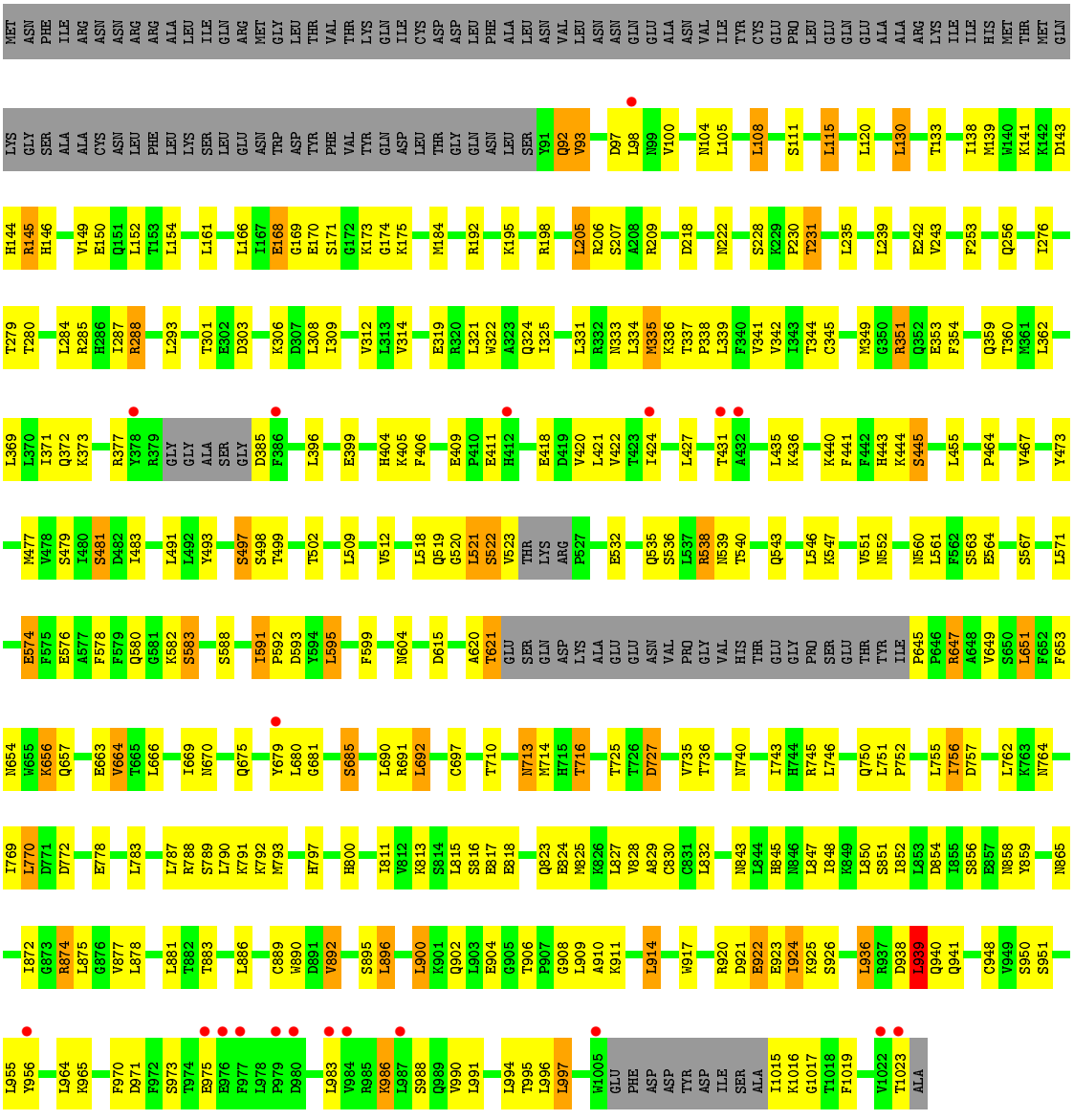
Chain H:





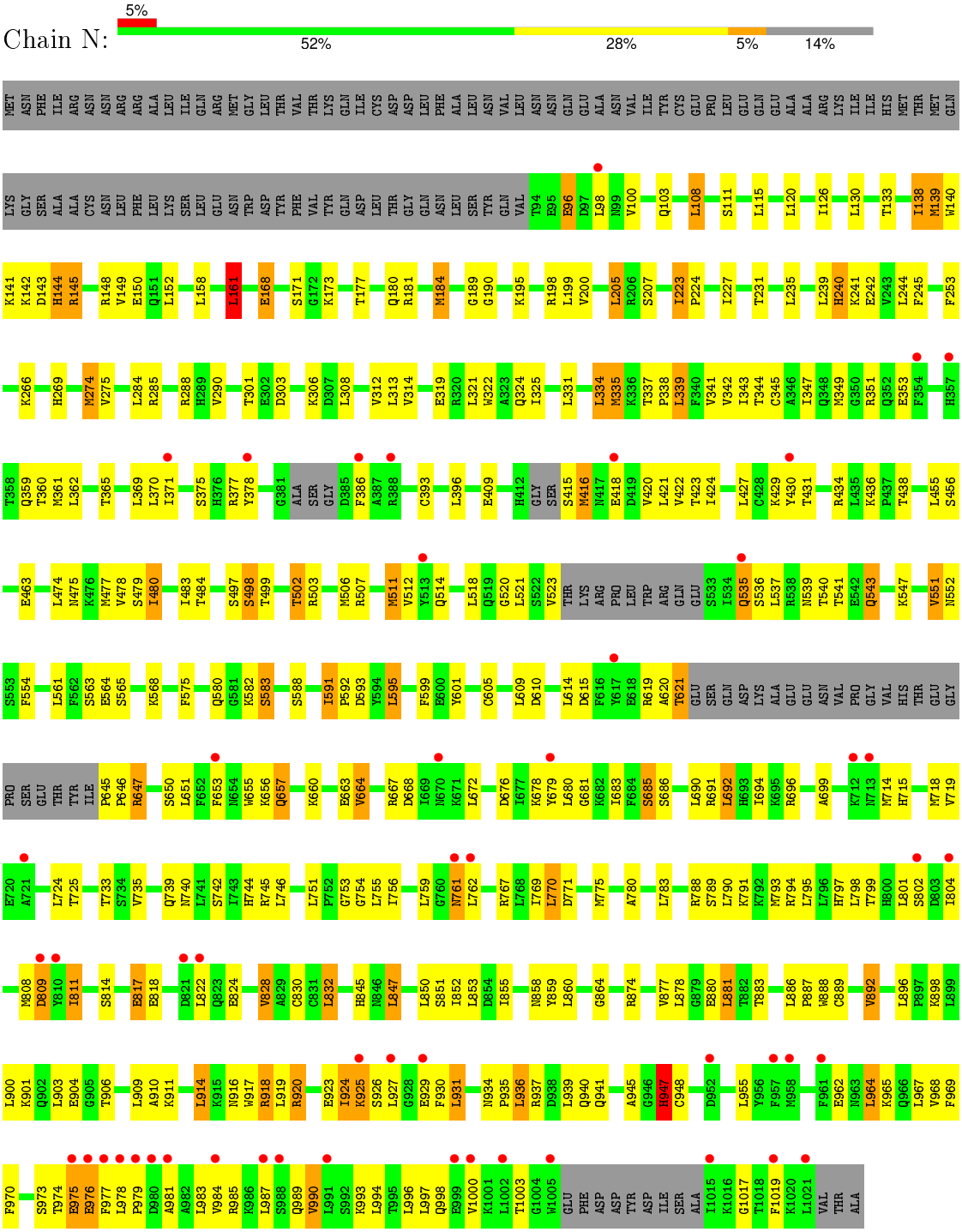
• Molecule 1: NLR family CARD domain-containing protein 4

Chain L:



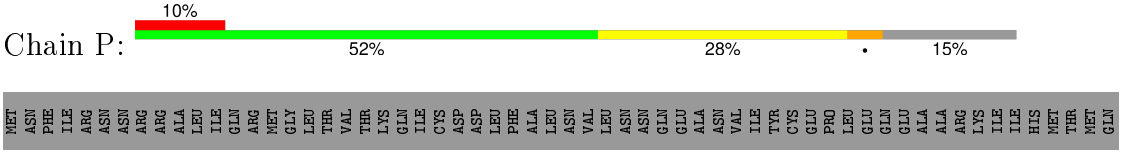
• Molecule 1: NLR family CARD domain-containing protein 4

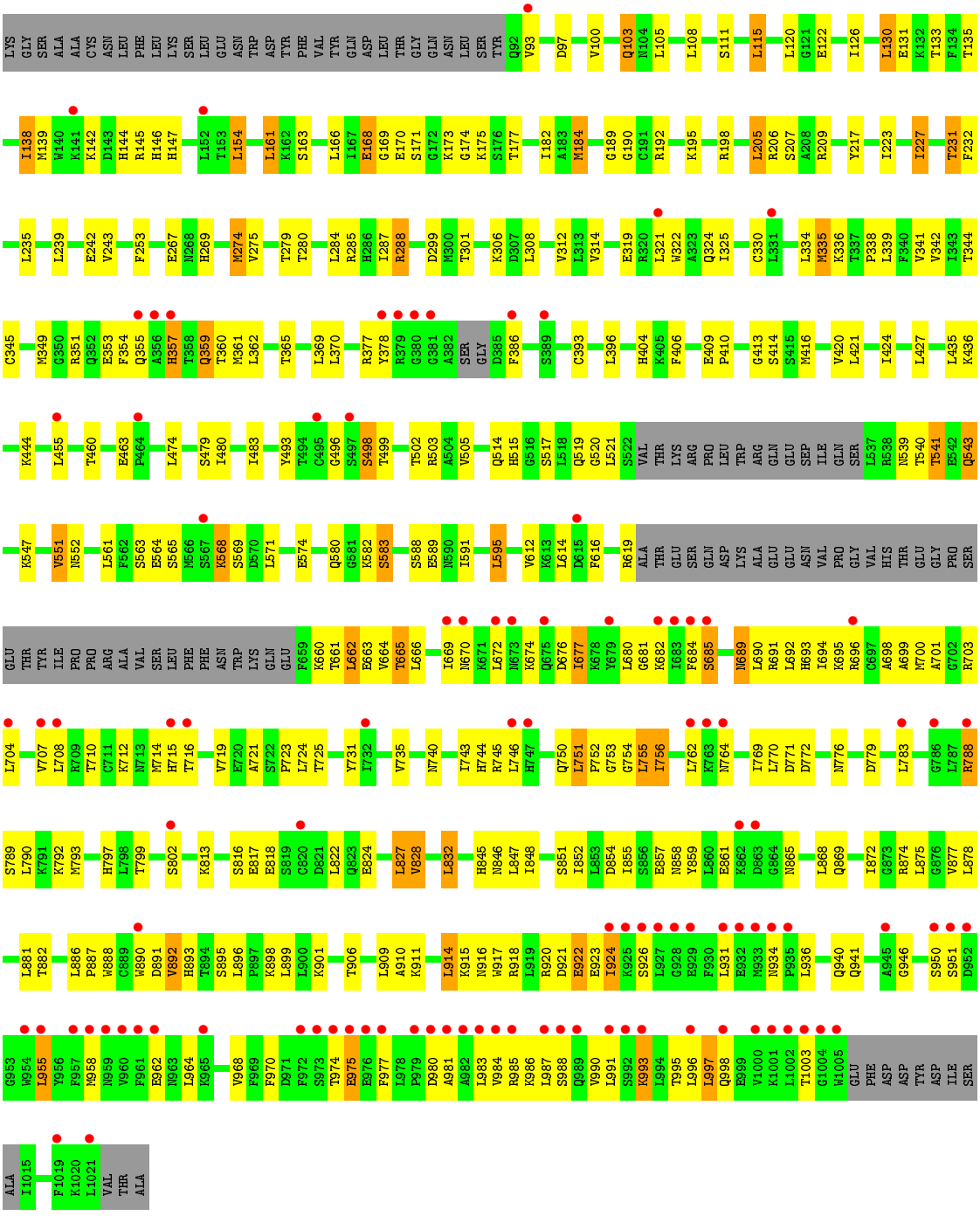
Chain N:




• Molecule 1: NLR family CARD domain-containing protein 4

Chain P:




LYS GLY SER ALA ALA CYS ASN LEU PHE LEU LYS SER LEU GLU ASN TRP ASP TYR PHE VAL TYR GLN ASP LEU THR GLY GLN ASN LEU SER TYR Q92 V93 D97 V100 Q103 N104 L105 L108 S111 L115 L120 G121 E122 I126 L130 E131 K132 T133 F134 T135
I138 M139 W140 K141 K142 D143 H144 R145 H146 H147 L152 T153 L154 L161 K162 S163 L166 I167 E168 G169 E170 S171 G172 K173 G174 K175 S176 T177 I182 A183 M184 G189 G190 C191 R192 K195 R198 L205 R206 S207 A208 R209 Y217 I223 I227 T231 F232
L235 L239 E242 V243 F253 E267 N268 H269 M274 V275 T279 T280 L284 R285 H286 I287 R288 D299 M300 T301 K306 D307 L308 V312 L313 V314 E319 R320 L321 W322 A323 Q324 I325 C330 L331 L334 M335 K336 T337 P338 L339 F340 V341 V342 I343 T344
C345 M349 G350 R351 Q352 E353 F354 Q355 A356 H357 T358 Q359 T360 M361 L362 T365 L369 L370 R377 Y378 R379 G380 G381 A382 SER GLY D385 F386 S389 C393 L396 H404 K405 F406 E409 P410 G413 S414 S415 N416 V420 L421 I424 L427 L435 K436
K444 L455 T460 E463 P464 L474 S479 I480 I483 Y493 T494 C495 G496 S497 S498 T499 T502 R503 A504 V505 Q514 H515 G516 S517 L518 Q519 G520 L521 S522 VAL THR LYS ARG PRO LEU TRP ARG GLN GLU SEP ILE GLN SER L537 R538 N539 T540 T541 E542 Q543
K547 V551 N552 L561 F562 S563 E564 S565 M566 S567 K568 S569 D570 L571 E574 Q580 G581 K582 S583 S588 E589 N590 I591 L595 V612 K613 L614 D615 F616 R619 ALA THR GLU SER GLN ASP LYS ALA GLU GLU ASN VAL PRO GLY VAL HIS THR GLU GLY PRO SER
GLU THR TYR ILE PRO PRO ARG ALA VAL SER LEU PHE PHE ASN TRP LYS GLN GLU F659 K660 T661 L662 E663 V664 T665 L666 I669 N670 K671 L672 N673 K674 Q675 D676 I677 K678 Y679 L680 G681 K682 I683 F684 S685 N689 L690 R691 L692 H693 I694 K695 R696 C697 A698 A699 M700 A701 G702 R703
L704 V707 L708 R709 T710 C711 K712 N713 M714 H715 T716 V719 E720 A721 S722 P723 L724 T725 Y731 I732 V735 N740 I743 H744 R745 L746 H747 Q750 L751 P752 G753 G754 L755 I756 L762 K763 N764 I769 L770 D771 D772 N776 D779 L783 G786 L787 R788
S789 L790 K791 K792 M793 H797 L798 T799 S802 K813 S816 E817 E818 S819 C820 D821 L822 Q823 E824 L827 V828 L832 H845 N846 L847 I848 S851 I852 L853 D854 I855 S856 E857 N858 Y859 L860 E861 K862 D863 G864 N865 L868 Q869 I872 G873 R874 L875 G876 V877 L878
L881 T882 L886 P887 W888 C889 W890 D891 V892 H893 T894 S895 L896 P897 K898 L899 L900 K901 T906 L909 A910 K911 L914 K915 N916 W917 R918 L919 R920 D921 E922 E923 I924 K925 S926 L927 G928 E929 F930 L931 E932 M933 N934 P935 L936 Q940 Q941 A945 G946 S950 S951 D952
G953 W954 L955 Y956 R957 M958 N959 V960 F961 E962 N963 L964 K965 V968 F969 F970 D971 F972 S973 T974 E975 E976 F977 L978 P979 D980 A981 A982 L983 V984 R985 K986 L987 S988 Q989 V990 L991 S992 K993 L994 T995 L996 I997 Q998 E999 Y1000 K1001 L1002 T1003 G1004 W1005 GLU PHE ASP ASP TYR ASP ILE SER
ALA I1015 F1019 K1020 L1021 VAL THR ALA

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 41 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 334.05Å 334.05Å 177.57Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 39.33 – 3.20<br>39.33 – 3.18 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 90.9 (39.33-3.20)<br>89.8 (39.33-3.18) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.11 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.84 (at 3.18Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.8_1069) | Depositor |
| R, $R_{free}$ | 0.226 , 0.266<br>0.226 , 0.265 | Depositor<br>DCC |
| $R_{free}$ test set | 7523 reflections (5.04%) | DCC |
| Wilson B-factor (Å$^2$) | 78.8 | Xtriage |
| Anisotropy | 0.007 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.29 , 19.3 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.31$ | Xtriage |
| Outliers | 2 of 150157 reflections (0.001%) | Xtriage |
| $F_o$,$F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 57081 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 31.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

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

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 | B | 0.28 | 0/7330 | 0.58 | 1/9897 (0.0%) |
| 1 | D | 0.27 | 0/7301 | 0.53 | 0/9857 |
| 1 | F | 0.26 | 0/7296 | 0.52 | 0/9851 |
| 1 | H | 0.26 | 0/7256 | 0.53 | 0/9798 |
| 1 | K | 0.27 | 0/7332 | 0.57 | 2/9900 (0.0%) |
| 1 | L | 0.28 | 0/7230 | 0.54 | 2/9766 (0.0%) |
| 1 | N | 0.30 | 0/7119 | 0.59 | 2/9616 (0.0%) |
| 1 | P | 0.27 | 0/6980 | 0.55 | 1/9426 (0.0%) |
| All | All | 0.27 | 0/57844 | 0.55 | 8/78111 (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 | B | 0 | 1 |
| 1 | F | 0 | 1 |
| 1 | K | 0 | 1 |
| 1 | L | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | K | 433 | GLN | OE1-CD-NE2 | -15.42 | 86.42 | 121.90 |
| 1 | N | 978 | LEU | N-CA-C | -7.16 | 91.66 | 111.00 |
| 1 | N | 161 | LEU | CA-CB-CG | 6.39 | 130.01 | 115.30 |
| 1 | B | 161 | LEU | CA-CB-CG | 6.26 | 129.69 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | P | 161 | LEU | CA-CB-CG | 5.76 | 128.56 | 115.30 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 531 | GLN | Peptide |
| 1 | F | 412 | HIS | Peptide |
| 1 | K | 433 | GLN | Sidechain |
| 1 | L | 92 | GLN | Peptide |

## 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 | B | 7204 | 0 | 7237 | 163 | 0 |
| 1 | D | 7177 | 0 | 7190 | 148 | 0 |
| 1 | F | 7172 | 0 | 7186 | 168 | 0 |
| 1 | H | 7135 | 0 | 7126 | 156 | 0 |
| 1 | K | 7208 | 0 | 7216 | 172 | 2 |
| 1 | L | 7107 | 0 | 7104 | 158 | 0 |
| 1 | N | 6996 | 0 | 6969 | 197 | 0 |
| 1 | P | 6856 | 0 | 6838 | 166 | 0 |
| 2 | B | 27 | 0 | 12 | 1 | 0 |
| 2 | D | 27 | 0 | 12 | 1 | 0 |
| 2 | F | 27 | 0 | 12 | 1 | 0 |
| 2 | H | 27 | 0 | 12 | 0 | 0 |
| 2 | K | 27 | 0 | 12 | 2 | 0 |
| 2 | L | 27 | 0 | 12 | 1 | 0 |
| 2 | N | 27 | 0 | 12 | 0 | 0 |
| 2 | P | 27 | 0 | 12 | 2 | 0 |
| 3 | B | 5 | 0 | 0 | 0 | 0 |
| 3 | N | 5 | 0 | 0 | 0 | 0 |
| All | All | 57081 | 0 | 56962 | 1297 | 2 |

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 11.

The worst 5 of 1297 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:P:983:LEU:HA | 1:P:986:LYS:CB | 1.44 | 1.46 |
| 1:P:983:LEU:O | 1:P:987:LEU:N | 1.59 | 1.32 |
| 1:N:947:HIS:CE1 | 1:N:974:THR:OG1 | 1.92 | 1.22 |
| 1:P:983:LEU:CA | 1:P:986:LYS:CB | 2.32 | 1.06 |
| 1:L:145:ARG:HG2 | 1:L:523:VAL:HG11 | 1.39 | 1.01 |

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:433:GLN:CD | 1:K:433:GLN:NE2[8_555] | 1.34 | 0.86 |
| 1:K:433:GLN:OE1 | 1:K:433:GLN:NE2[8_555] | 1.76 | 0.44 |

## 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 | B | 896/1024 (88%) | 875 (98%) | 21 (2%) | 0 | 100 | 100 |
| 1 | D | 893/1024 (87%) | 864 (97%) | 28 (3%) | 1 (0%) | 56 | 91 |
| 1 | F | 892/1024 (87%) | 868 (97%) | 23 (3%) | 1 (0%) | 56 | 91 |
| 1 | H | 887/1024 (87%) | 862 (97%) | 25 (3%) | 0 | 100 | 100 |
| 1 | K | 895/1024 (87%) | 878 (98%) | 15 (2%) | 2 (0%) | 52 | 88 |
| 1 | L | 882/1024 (86%) | 859 (97%) | 21 (2%) | 2 (0%) | 52 | 88 |
| 1 | N | 870/1024 (85%) | 847 (97%) | 20 (2%) | 3 (0%) | 46 | 85 |
| 1 | P | 856/1024 (84%) | 824 (96%) | 31 (4%) | 1 (0%) | 56 | 91 |
| All | All | 7071/8192 (86%) | 6877 (97%) | 184 (3%) | 10 (0%) | 56 | 91 |

5 of 10 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | L | 93 | VAL |
| 1 | N | 976 | GLU |
| 1 | N | 979 | PRO |
| 1 | K | 568 | LYS |
| 1 | F | 1018 | THR |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | B | 797/912 (87%) | 668 (84%) | 129 (16%) | 3 | 14 |
| 1 | D | 795/912 (87%) | 678 (85%) | 117 (15%) | 4 | 18 |
| 1 | F | 795/912 (87%) | 679 (85%) | 116 (15%) | 4 | 19 |
| 1 | H | 788/912 (86%) | 665 (84%) | 123 (16%) | 3 | 15 |
| 1 | K | 798/912 (88%) | 668 (84%) | 130 (16%) | 3 | 14 |
| 1 | L | 785/912 (86%) | 663 (84%) | 122 (16%) | 3 | 15 |
| 1 | N | 769/912 (84%) | 642 (84%) | 127 (16%) | 3 | 13 |
| 1 | P | 754/912 (83%) | 626 (83%) | 128 (17%) | 2 | 12 |
| All | All | 6281/7296 (86%) | 5289 (84%) | 992 (16%) | 3 | 15 |

5 of 992 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 725 | THR |
| 1 | H | 595 | LEU |
| 1 | P | 503 | ARG |
| 1 | F | 790 | LEU |
| 1 | H | 171 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 740 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | L | 359 | GLN |
| 1 | P | 941 | GLN |
| 1 | L | 324 | GLN |
| 1 | N | 269 | HIS |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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 | $\#\|Z\| > 2$ |
| 1 | SEP | B | 533 | 1 | 8,9,10 | 1.52 | 1 (12%) | 8,12,14 | 1.64 | 1 (12%) |
| 1 | SEP | D | 533 | 1 | 8,9,10 | 1.49 | 1 (12%) | 8,12,14 | 1.77 | 2 (25%) |
| 1 | SEP | F | 533 | 1 | 8,9,10 | 1.49 | 1 (12%) | 8,12,14 | 1.48 | 2 (25%) |
| 1 | SEP | H | 533 | 1 | 8,9,10 | 1.50 | 1 (12%) | 8,12,14 | 1.16 | 1 (12%) |
| 1 | SEP | K | 533 | 1 | 8,9,10 | 1.50 | 1 (12%) | 8,12,14 | 1.57 | 1 (12%) |
| 1 | SEP | L | 533 | 1 | 8,9,10 | 1.50 | 1 (12%) | 8,12,14 | 1.70 | 2 (25%) |
| 1 | SEP | N | 533 | 1 | 4,5,10 | 0.51 | 0 | 2,5,14 | 1.30 | 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 |
|---|---|---|---|---|---|---|---|
| 1 | SEP | B | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | D | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | F | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | H | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | SEP | K | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | L | 533 | 1 | - | 0/6/8/10 | 0/0/0/0 |
| 1 | SEP | N | 533 | 1 | - | 0/2/4/10 | 0/0/0/0 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | F | 533 | SEP | P-O1P | 3.05 | 1.61 | 1.51 |
| 1 | K | 533 | SEP | P-O1P | 3.05 | 1.61 | 1.51 |
| 1 | D | 533 | SEP | P-O1P | 3.09 | 1.61 | 1.51 |
| 1 | B | 533 | SEP | P-O1P | 3.09 | 1.61 | 1.51 |
| 1 | L | 533 | SEP | P-O1P | 3.12 | 1.61 | 1.51 |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | L | 533 | SEP | O-C-CA | -2.16 | 119.87 | 125.49 |
| 1 | D | 533 | SEP | O-C-CA | -2.04 | 120.17 | 125.49 |
| 1 | F | 533 | SEP | O-C-CA | -2.02 | 120.23 | 125.49 |
| 1 | H | 533 | SEP | OG-CB-CA | 2.02 | 110.00 | 108.27 |
| 1 | F | 533 | SEP | OG-CB-CA | 3.11 | 110.92 | 108.27 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 1 | B | 533 | SEP | 3 | 0 |
| 1 | F | 533 | SEP | 1 | 0 |
| 1 | H | 533 | SEP | 2 | 0 |
| 1 | K | 533 | SEP | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | ADP | B | 1101 | - | 22,29,29 | 0.99 | 1 (4%) | 27,45,45 | 1.88 | 4 (14%) |
| 3 | SO4 | B | 1102 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.08 | 0 |
| 2 | ADP | D | 1101 | - | 22,29,29 | 1.01 | 1 (4%) | 27,45,45 | 1.84 | 5 (18%) |
| 2 | ADP | F | 1101 | - | 22,29,29 | 0.97 | 1 (4%) | 27,45,45 | 1.83 | 4 (14%) |
| 2 | ADP | H | 1101 | - | 22,29,29 | 0.99 | 1 (4%) | 27,45,45 | 1.85 | 4 (14%) |
| 2 | ADP | K | 1101 | - | 22,29,29 | 1.00 | 1 (4%) | 27,45,45 | 1.92 | 4 (14%) |
| 2 | ADP | L | 1101 | - | 22,29,29 | 1.05 | 1 (4%) | 27,45,45 | 1.66 | 4 (14%) |
| 2 | ADP | N | 1101 | - | 22,29,29 | 1.01 | 1 (4%) | 27,45,45 | 1.89 | 4 (14%) |
| 3 | SO4 | N | 1102 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | ADP | P | 1101 | - | 22,29,29 | 1.02 | 1 (4%) | 27,45,45 | 1.73 | 4 (14%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | ADP | B | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 3 | SO4 | B | 1102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | ADP | D | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | F | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | H | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | K | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | L | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | N | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |
| 3 | SO4 | N | 1102 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | ADP | P | 1101 | - | - | 0/12/32/32 | 0/3/3/3 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | F | 1101 | ADP | C5-C4 | 3.05 | 1.47 | 1.40 |
| 2 | K | 1101 | ADP | C5-C4 | 3.10 | 1.47 | 1.40 |
| 2 | H | 1101 | ADP | C5-C4 | 3.12 | 1.47 | 1.40 |
| 2 | B | 1101 | ADP | C5-C4 | 3.13 | 1.47 | 1.40 |
| 2 | D | 1101 | ADP | C5-C4 | 3.17 | 1.47 | 1.40 |

The worst 5 of 33 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | K | 1101 | ADP | N3-C2-N1 | -6.64 | 123.81 | 128.89 |
| 2 | F | 1101 | ADP | N3-C2-N1 | -6.59 | 123.85 | 128.89 |
| 2 | N | 1101 | ADP | N3-C2-N1 | -6.55 | 123.88 | 128.89 |
| 2 | D | 1101 | ADP | N3-C2-N1 | -6.51 | 123.91 | 128.89 |
| 2 | H | 1101 | ADP | N3-C2-N1 | -6.50 | 123.92 | 128.89 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 1101 | ADP | 1 | 0 |
| 2 | D | 1101 | ADP | 1 | 0 |
| 2 | F | 1101 | ADP | 1 | 0 |
| 2 | K | 1101 | ADP | 2 | 0 |
| 2 | L | 1101 | ADP | 1 | 0 |
| 2 | P | 1101 | ADP | 2 | 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

## 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, $95^{th}$ 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 | B | 902/1024 (88%) | -0.02 | 18 (1%) | 68 | 54 | 3, 15, 68, 143 | 0 |
| 1 | D | 899/1024 (87%) | 0.02 | 27 (3%) | 54 | 39 | 3, 22, 71, 148 | 0 |
| 1 | F | 898/1024 (87%) | 0.01 | 26 (2%) | 55 | 41 | 2, 19, 65, 130 | 0 |
| 1 | H | 897/1024 (87%) | 0.09 | 33 (3%) | 45 | 30 | 4, 17, 61, 155 | 0 |
| 1 | K | 903/1024 (88%) | 0.01 | 21 (2%) | 64 | 49 | 4, 19, 66, 152 | 0 |
| 1 | L | 892/1024 (87%) | -0.00 | 20 (2%) | 65 | 50 | 2, 15, 66, 146 | 0 |
| 1 | N | 881/1024 (86%) | 0.33 | 51 (5%) | 26 | 15 | 4, 41, 106, 178 | 0 |
| 1 | P | 866/1024 (84%) | 0.63 | 103 (11%) | 6 | 3 | 5, 53, 156, 254 | 0 |
| All | All | 7138/8192 (87%) | 0.13 | 299 (4%) | 40 | 26 | 2, 23, 92, 254 | 0 |

The worst 5 of 299 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 1007 | PHE | 7.9 |
| 1 | N | 1021 | LEU | 7.8 |
| 1 | N | 961 | PHE | 6.5 |
| 1 | N | 980 | ASP | 6.4 |
| 1 | P | 987 | LEU | 6.3 |

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

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, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | SEP | N | 533 | 6/11 | 0.79 | 0.24 | - | 6,7,16,17 | 0 |
| 1 | SEP | L | 533 | 10/11 | 0.90 | 0.16 | - | 69,69,69,69 | 0 |
| 1 | SEP | B | 533 | 10/11 | 0.83 | 0.22 | - | 54,54,54,54 | 0 |
| 1 | SEP | F | 533 | 10/11 | 0.89 | 0.17 | - | 69,69,69,69 | 0 |
| 1 | SEP | D | 533 | 10/11 | 0.83 | 0.24 | - | 59,59,59,59 | 0 |
| 1 | SEP | K | 533 | 10/11 | 0.92 | 0.15 | - | 67,67,67,68 | 0 |
| 1 | SEP | H | 533 | 10/11 | 0.92 | 0.16 | - | 45,46,46,46 | 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, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 3 | SO4 | B | 1102 | 5/5 | 0.80 | 0.32 | 5.68 | 81,93,103,106 | 0 |
| 2 | ADP | N | 1101 | 27/27 | 0.94 | 0.25 | 0.74 | 9,20,28,39 | 0 |
| 2 | ADP | L | 1101 | 27/27 | 0.94 | 0.25 | 0.65 | 2,4,6,7 | 0 |
| 2 | ADP | B | 1101 | 27/27 | 0.94 | 0.22 | 0.36 | 4,5,7,7 | 0 |
| 2 | ADP | H | 1101 | 27/27 | 0.95 | 0.25 | 0.22 | 4,5,6,8 | 0 |
| 2 | ADP | F | 1101 | 27/27 | 0.95 | 0.21 | 0.00 | 2,2,3,3 | 0 |
| 2 | ADP | K | 1101 | 27/27 | 0.96 | 0.21 | -0.11 | 6,10,15,17 | 0 |
| 2 | ADP | D | 1101 | 27/27 | 0.94 | 0.21 | -0.17 | 3,4,9,10 | 0 |
| 2 | ADP | P | 1101 | 27/27 | 0.95 | 0.23 | -0.25 | 8,18,28,35 | 0 |
| 3 | SO4 | N | 1102 | 5/5 | 0.77 | 0.33 | - | 79,86,87,116 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.