



## Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:57 PM UTC

PDB ID : 6X32 / pdb\_00006x32  
EMDB ID : EMD-22015  
Title : Wt pig RyR1 in complex with apoCaM, EGTA condition (class 1 and 2, closed)  
Authors : Woll, K.W.; Haji-Ghassemi, O.; Van Petegem, F.  
Deposited on : 2020-05-21  
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

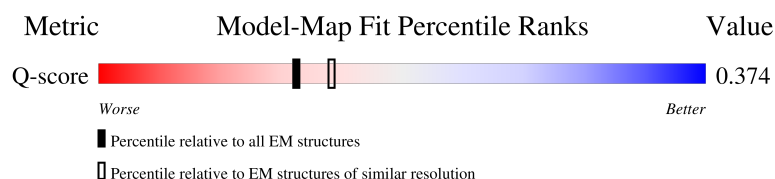
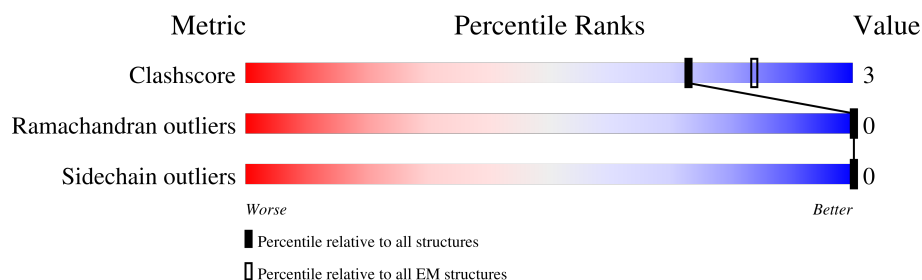
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 1   | A     | 110    | <br>81% 15% . |
| 1   | D     | 110    | <br>78% 18% . |
| 1   | G     | 110    | <br>78% 18% . |
| 1   | J     | 110    | <br>81% 15% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | B     | 3800   |                  |
| 2   | E     | 3800   |                  |
| 2   | H     | 3800   |                  |
| 2   | K     | 3800   |                  |
| 3   | C     | 146    |                  |
| 3   | F     | 146    |                  |
| 3   | I     | 146    |                  |
| 3   | L     | 146    |                  |

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 114280 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 474 | 128 | 136 | 4 |         |       |
| 1   | D     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 474 | 128 | 136 | 4 |         |       |
| 1   | G     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 474 | 128 | 136 | 4 |         |       |
| 1   | J     | 106      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 474 | 128 | 136 | 4 |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -2      | SER      | -      | expression tag | UNP P68106 |
| A     | -1      | ASN      | -      | expression tag | UNP P68106 |
| A     | 0       | ALA      | -      | expression tag | UNP P68106 |
| D     | -2      | SER      | -      | expression tag | UNP P68106 |
| D     | -1      | ASN      | -      | expression tag | UNP P68106 |
| D     | 0       | ALA      | -      | expression tag | UNP P68106 |
| G     | -2      | SER      | -      | expression tag | UNP P68106 |
| G     | -1      | ASN      | -      | expression tag | UNP P68106 |
| G     | 0       | ALA      | -      | expression tag | UNP P68106 |
| J     | -2      | SER      | -      | expression tag | UNP P68106 |
| J     | -1      | ASN      | -      | expression tag | UNP P68106 |
| J     | 0       | ALA      | -      | expression tag | UNP P68106 |

- Molecule 2 is a protein called Ryanodine Receptor.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 2   | B     | 3798     | Total | C     | N    | O    | S   | 6       | 0     |
|     |       |          | 27011 | 17294 | 4767 | 4780 | 170 |         |       |
| 2   | E     | 3798     | Total | C     | N    | O    | S   | 6       | 0     |
|     |       |          | 27011 | 17294 | 4767 | 4780 | 170 |         |       |
| 2   | H     | 3798     | Total | C     | N    | O    | S   | 6       | 0     |
|     |       |          | 27011 | 17294 | 4767 | 4780 | 170 |         |       |

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| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 2   | K     | 3798     | Total | C     | N    | O    | S   | 6       | 0     |
|     |       |          | 27011 | 17294 | 4767 | 4780 | 170 |         |       |

- Molecule 3 is a protein called Calmodulin-1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | C     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 505 | 142 | 165 | 4 |         |       |
| 3   | F     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 505 | 142 | 165 | 4 |         |       |
| 3   | I     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 505 | 142 | 165 | 4 |         |       |
| 3   | L     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 505 | 142 | 165 | 4 |         |       |

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 4   | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 4   | E     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 4   | H     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 4   | K     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

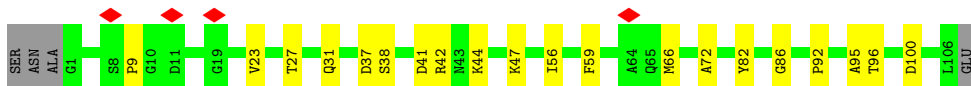
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 



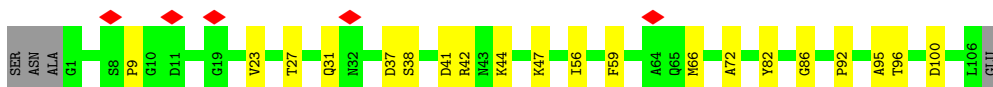
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 

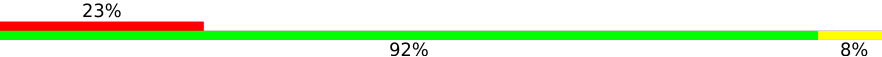


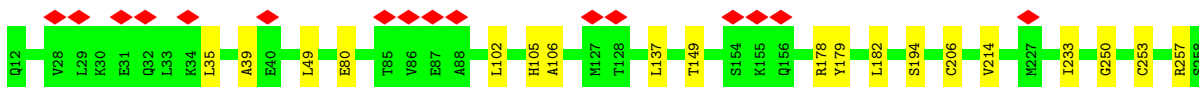
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

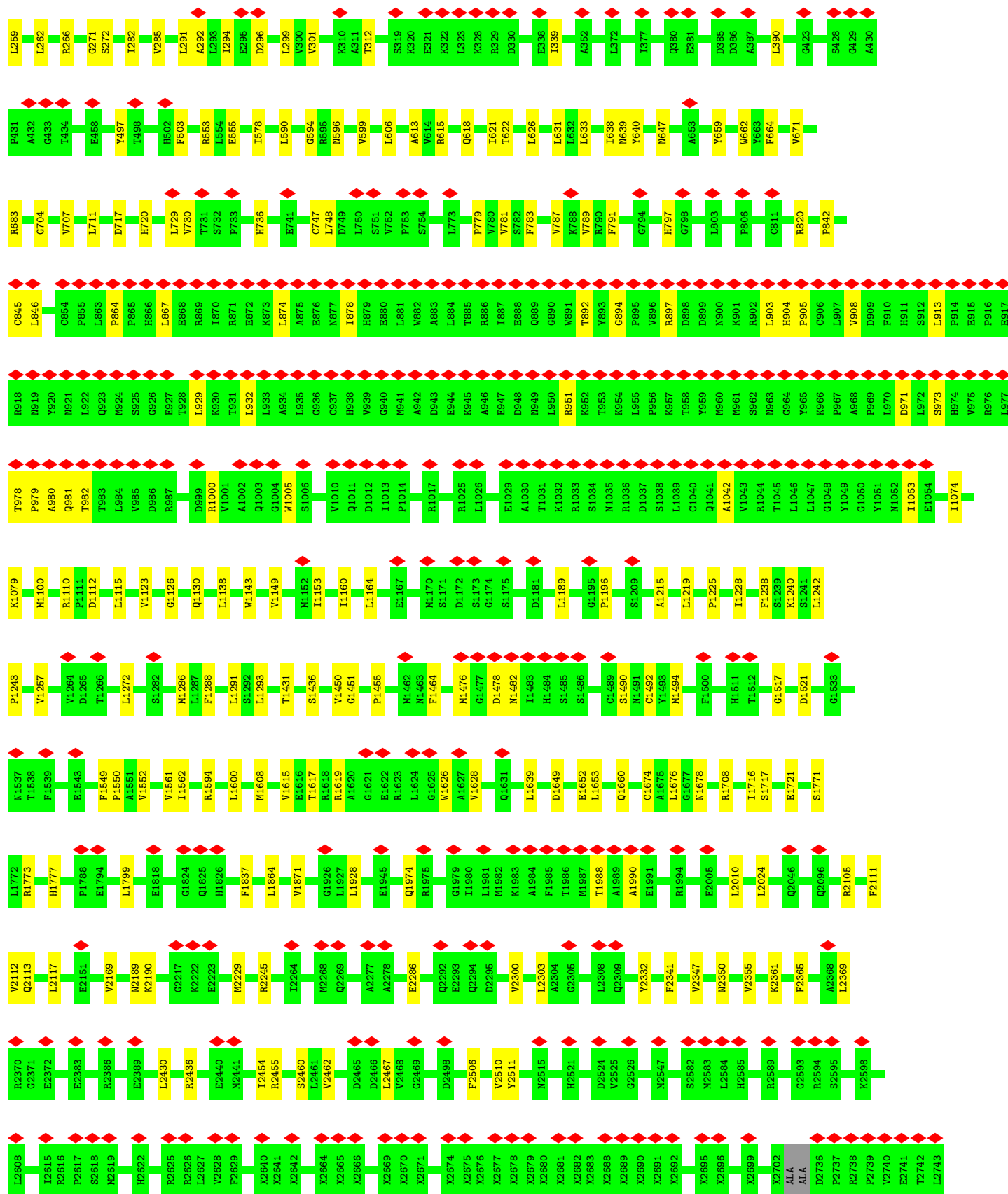
Chain J: 



- Molecule 2: Ryanodine Receptor

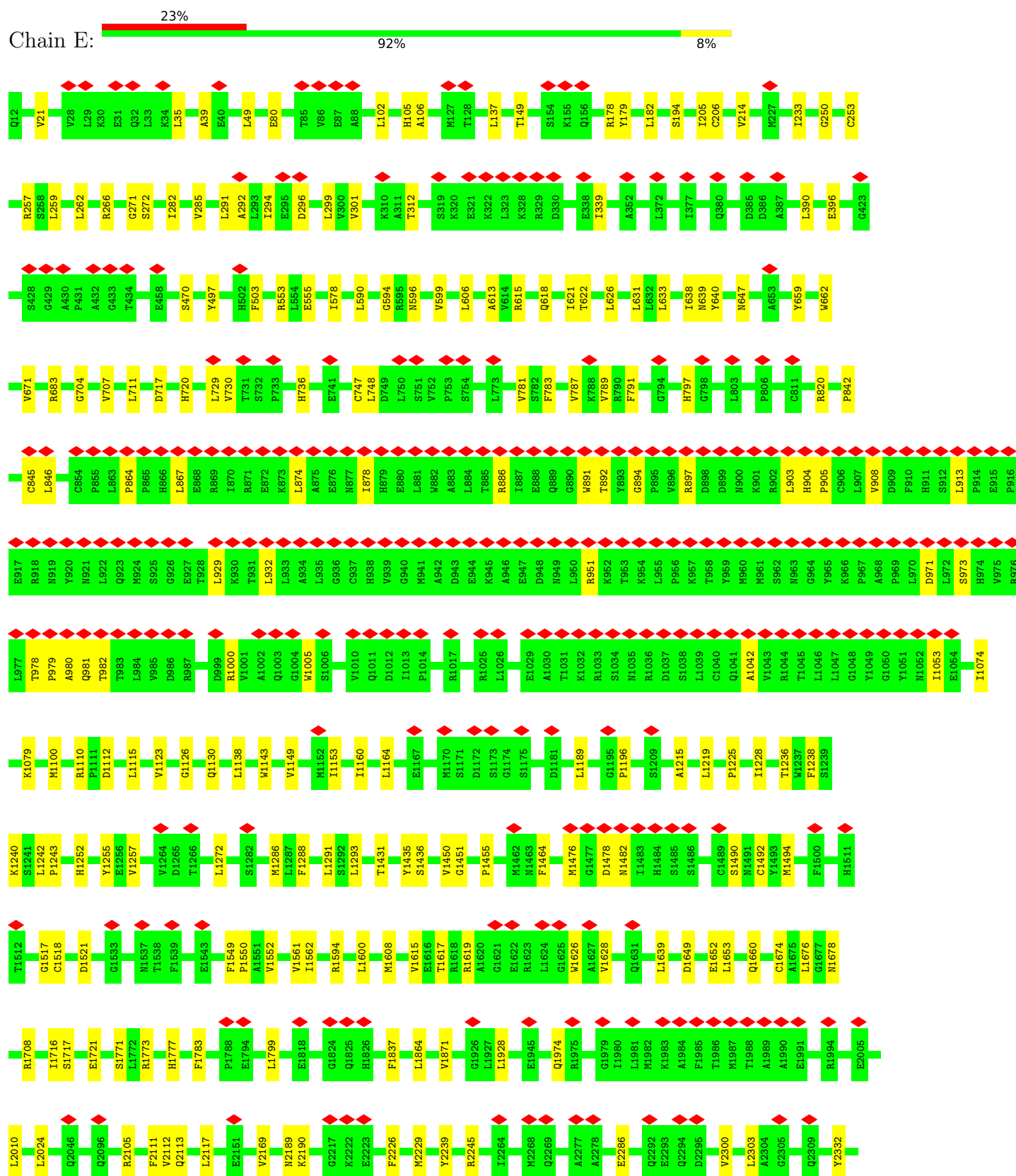
Chain B: 

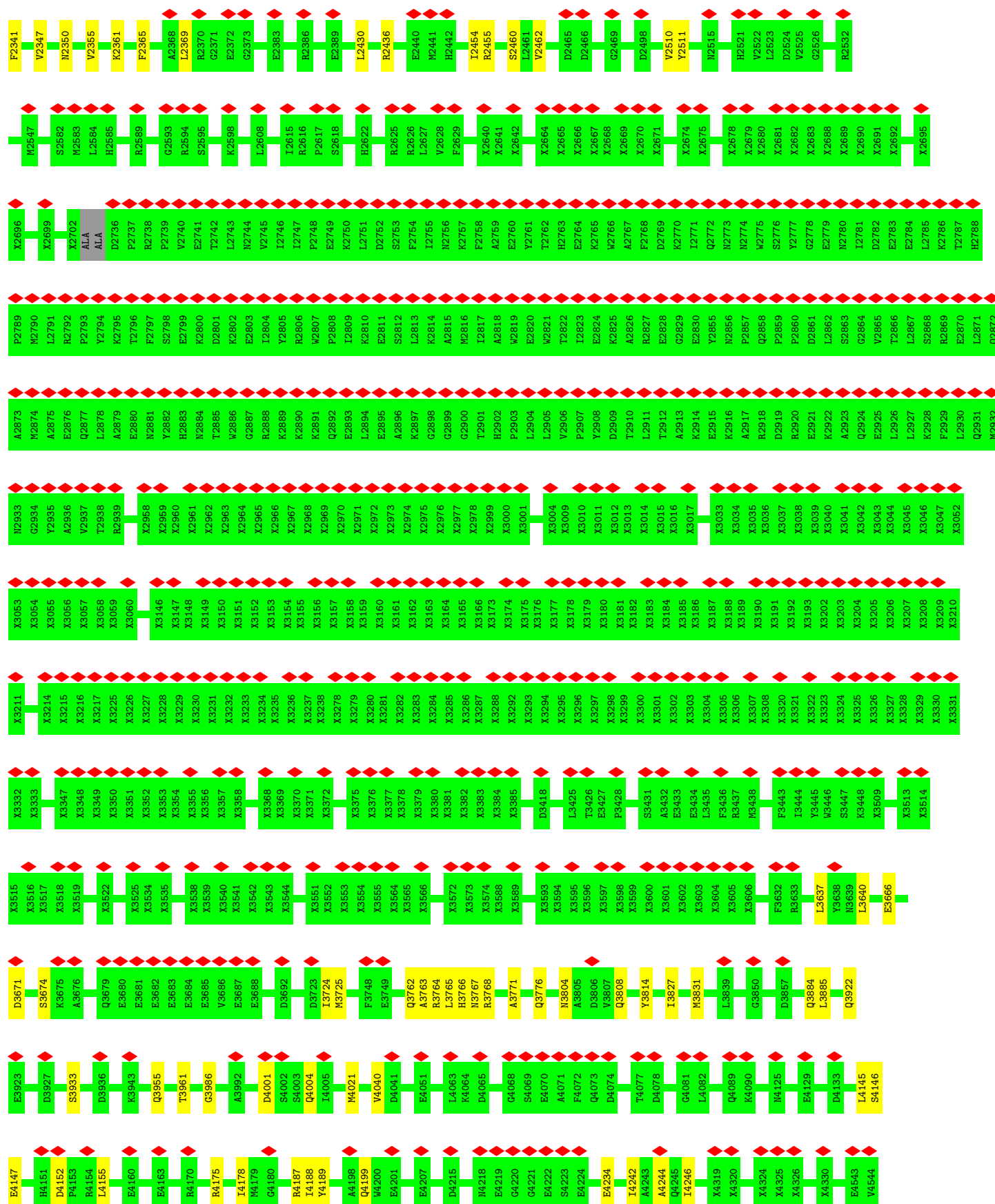


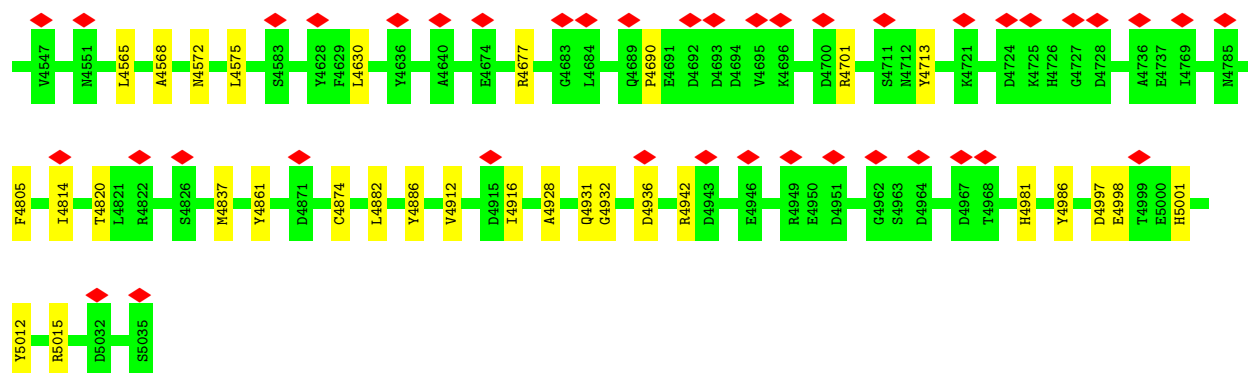


|       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| V4912 | A4640 | M4179 | D4001 | X3869 | X3236 | X3153 | X2965 | R2888 | Y2804 | M2744 |
| D4915 | L4641 | G4180 | S4002 | X3370 | X3237 | X3154 | X2966 | K2889 | V2745 | V2745 |
| I4916 | E4674 | R4187 | S4003 | X3371 | X3238 | X3155 | X2967 | K2890 | I2746 | I2746 |
| Q4931 | E4677 | I4188 | Q4004 | X3372 | X3278 | X3156 | X2968 | K2891 | I2747 | I2747 |
| D4936 | R4677 | Y4189 | I4005 | X3375 | X3279 | X3157 | X2969 | K2892 | P2748 | P2748 |
| R4942 | A4198 | A4198 | M4021 | X3376 | X3280 | X3158 | X2970 | E2893 | E2749 | E2749 |
| R4942 | W4200 | W4200 | V4040 | X3377 | X3281 | X3159 | X2971 | L2894 | K2750 | K2750 |
| D4943 | E4201 | E4201 | M4042 | X3378 | X3282 | X3160 | X2972 | E2895 | L2751 | L2751 |
| E4946 | M4202 | M4202 | M4042 | X3379 | X3283 | X3161 | X2973 | K2896 | D2752 | D2752 |
| R4949 | E4207 | E4207 | E4051 | X3380 | X3284 | X3162 | X2974 | K2897 | S2753 | S2753 |
| E4950 | D4215 | D4215 | L4063 | X3381 | X3285 | X3163 | X2975 | G2898 | F2754 | F2754 |
| D4951 | M4218 | M4218 | K4064 | X3382 | X3286 | X3164 | X2976 | G2899 | I2755 | I2755 |
| K4695 | E4219 | E4219 | D4065 | X3383 | X3287 | X3165 | X2977 | G2900 | M2756 | M2756 |
| K4696 | G4220 | G4220 | G4068 | X3384 | X3288 | X3166 | X2978 | T2901 | K2757 | K2757 |
| D4700 | G4221 | G4221 | S4069 | X3385 | X3292 | X3174 | X2999 | H2902 | F2758 | F2758 |
| R4701 | E4222 | E4222 | A4070 | D3418 | X3293 | X3175 | X3000 | P2903 | A2759 | A2759 |
| S4711 | S4223 | S4223 | F4072 | X3294 | X3294 | X3176 | X3001 | L2904 | E2760 | E2760 |
| M4712 | E4224 | E4224 | Q4073 | X3295 | X3295 | X3177 | X3004 | L2905 | V2761 | V2761 |
| Y4713 | E4234 | E4234 | D4074 | L3425 | X3296 | X3178 | X3009 | V2906 | T2762 | T2762 |
| K4721 | I4242 | I4242 | T4077 | T3426 | X3297 | X3179 | X3010 | P2907 | H2763 | H2763 |
| D4724 | A4243 | A4243 | D4078 | E4427 | X3298 | X3180 | X3011 | D2908 | E2764 | E2764 |
| K4725 | Q4244 | Q4244 | G4081 | P3428 | X3299 | X3181 | X3012 | T2910 | K2765 | K2765 |
| H4726 | Q4245 | Q4245 | L4082 | S3431 | X3300 | X3182 | X3013 | T2911 | K2766 | K2766 |
| G4727 | I4246 | I4246 | L4082 | E4432 | X3301 | X3183 | X3014 | L2912 | A2767 | A2767 |
| D4728 | X4317 | X4317 | Q4089 | E4433 | X3302 | X3184 | X3015 | T2912 | F2768 | F2768 |
| A4736 | X4318 | X4318 | K4090 | E4434 | X3303 | X3185 | X3016 | G2829 | D2769 | D2769 |
| E4737 | X4319 | X4319 | M4125 | L3435 | X3304 | X3188 | X3017 | E2830 | K2770 | K2770 |
| I4769 | X4320 | X4320 | E4129 | F3436 | X3305 | X3189 | X3033 | E2915 | I2771 | I2771 |
| N4785 | X4324 | X4324 | E4129 | M3438 | X3306 | X3190 | X3034 | A2916 | Q2772 | Q2772 |
| I4814 | X4325 | X4325 | D4133 | E4438 | X3307 | X3191 | X3035 | A2917 | Q2773 | Q2773 |
| T4820 | X4326 | X4326 | L4145 | M3438 | X3308 | X3192 | X3036 | R2918 | I2774 | I2774 |
| L4821 | E4543 | E4543 | L4146 | I3444 | X3309 | X3193 | X3037 | D2919 | W2775 | W2775 |
| R4822 | V4544 | V4544 | E4147 | W3446 | X3321 | X3202 | X3038 | E2920 | S2776 | S2776 |
| S4826 | L4565 | L4565 | H4151 | S3447 | X3322 | X3203 | X3039 | E2921 | G2778 | G2778 |
| M4837 | A4568 | A4568 | D4152 | K3448 | X3323 | X3204 | X3040 | L2922 | E2779 | E2779 |
| Y4861 | N4572 | N4572 | F4153 | X3509 | X3324 | X3205 | X3041 | Q2924 | I2780 | I2780 |
| Y4861 | F4573 | F4573 | R4154 | X3513 | X3325 | X3206 | X3042 | E2925 | I2781 | I2781 |
| D4871 | I4574 | I4574 | L4155 | X3514 | X3326 | X3207 | X3043 | E2926 | D2782 | D2782 |
| C4874 | D4582 | D4582 | E4160 | X3515 | X3327 | X3208 | X3044 | L2927 | E2783 | E2783 |
| L4882 | S4583 | S4583 | E4163 | X3516 | X3331 | X3209 | X3045 | K2928 | E2784 | E2784 |
| Y4886 | L4630 | L4630 | R4170 | X3517 | X3332 | X3210 | X3046 | P2929 | L2785 | L2785 |
|       | Y4636 | Y4636 | R4175 | X3518 | X3333 | X3211 | X3052 | E2870 | K2786 | K2786 |
|       |       |       | I4178 | X3519 | X3334 | X3212 | X3053 | L2871 | T2787 | T2787 |
|       |       |       |       | X3522 | X3347 | X3215 | X3054 | Q2872 | H2788 | H2788 |
|       |       |       |       | X3525 | X3348 | X3216 | X3055 | A2873 | P2789 | P2789 |
|       |       |       |       | X3534 | X3349 | X3217 | X3056 | M2874 | K2790 | K2790 |
|       |       |       |       | X3535 | X3350 | X3225 | X3057 | L2791 | L2791 | L2791 |
|       |       |       |       | X3538 | X3351 | X3226 | X3060 | E2876 | D2792 | D2792 |
|       |       |       |       | X3539 | X3352 | X3228 | X3060 | Q2877 | P2793 | P2793 |
|       |       |       |       | X3540 | X3353 | X3229 | X3146 | L2794 | Y2794 | Y2794 |
|       |       |       |       | X3541 | X3354 | X3230 | X3147 | K2795 | T2796 | T2796 |
|       |       |       |       | X3542 | X3355 | X3231 | X3148 | E2880 | T2796 | T2796 |
|       |       |       |       |       | X3357 | X3232 | X3149 | Y2881 | S2798 | S2798 |
|       |       |       |       |       | X3358 | X3233 | X3150 | H2883 | E2799 | E2799 |
|       |       |       |       |       |       | X3234 | X3151 | N2884 | K2800 | K2800 |
|       |       |       |       |       |       | X3235 | X3152 | W2885 | D2801 | D2801 |
|       |       |       |       |       |       |       |       | X2963 | K2802 | K2802 |
|       |       |       |       |       |       |       |       | X2964 | E2803 | E2803 |

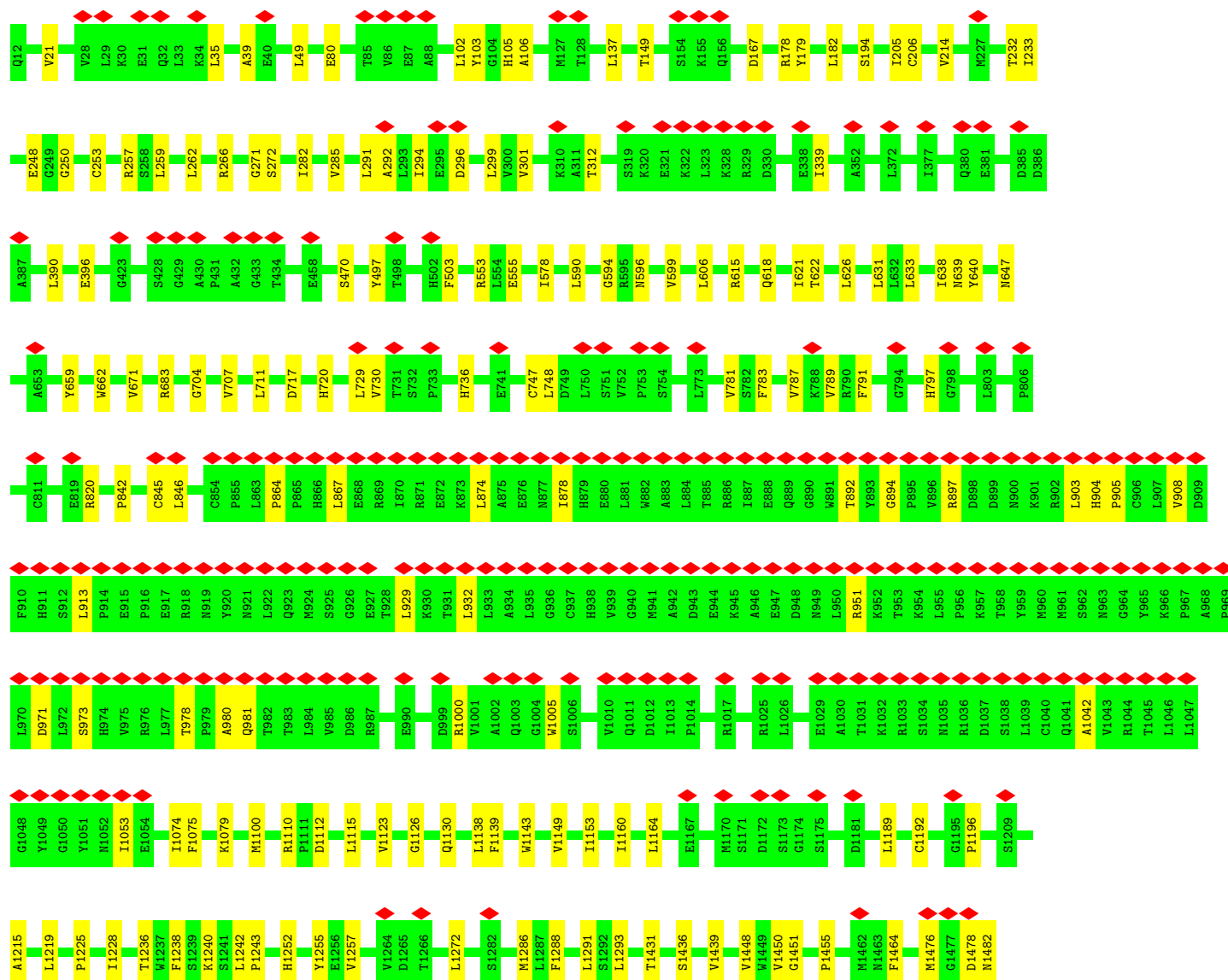
• Molecule 2: Ryanodine Receptor



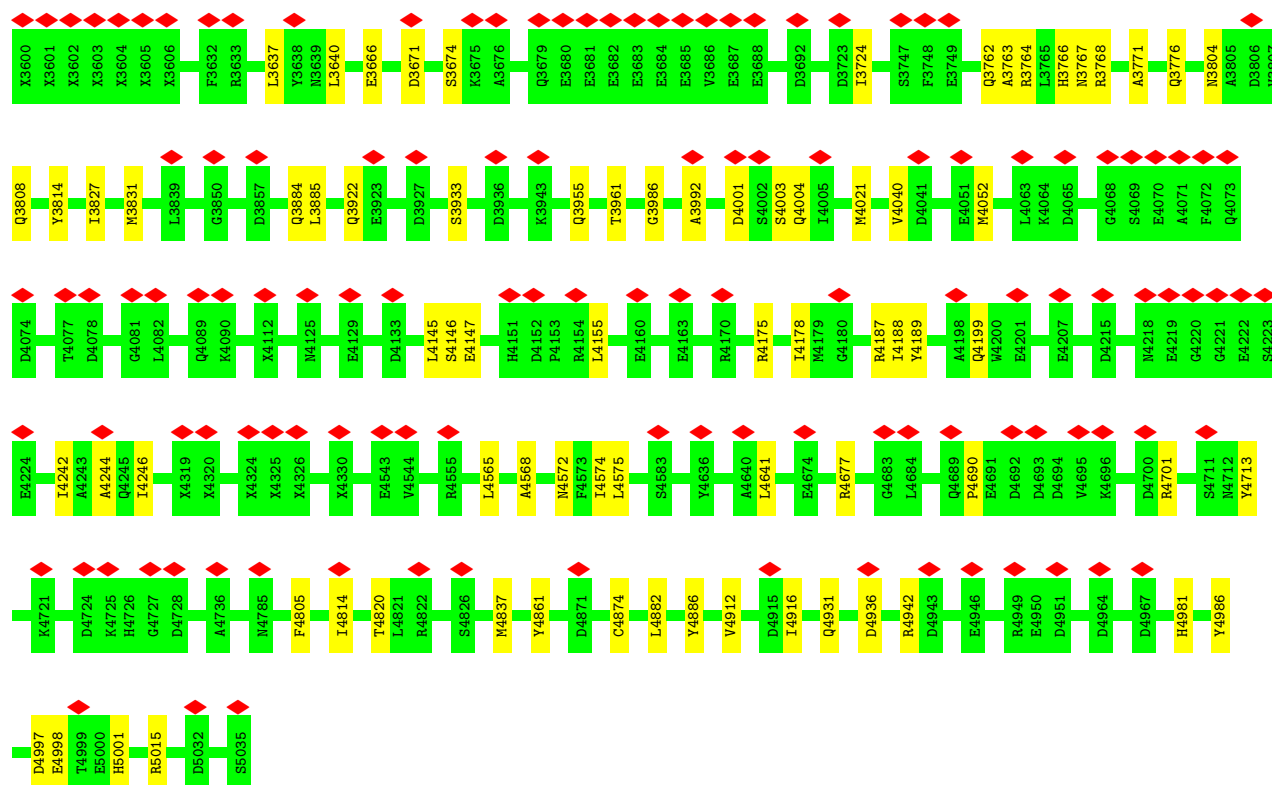




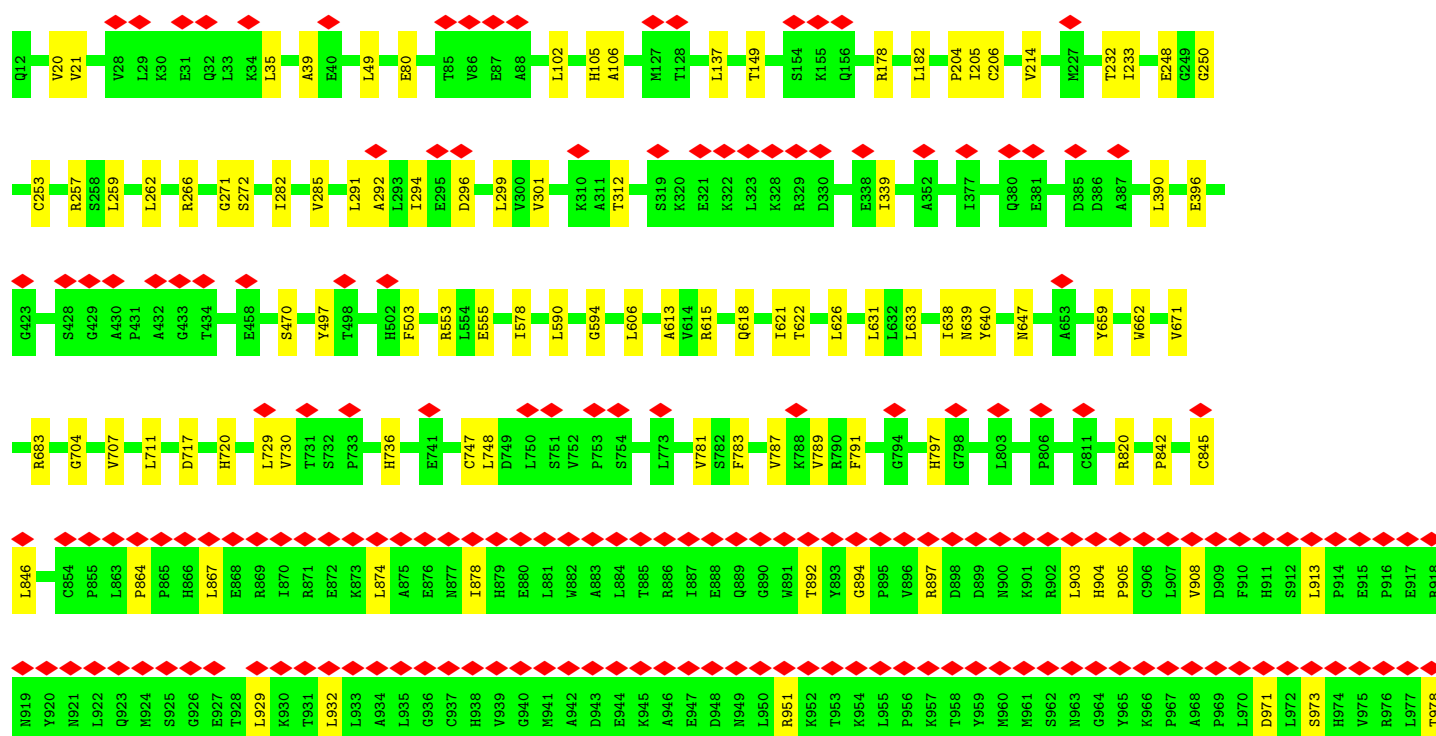
• Molecule 2: Ryanodine Receptor

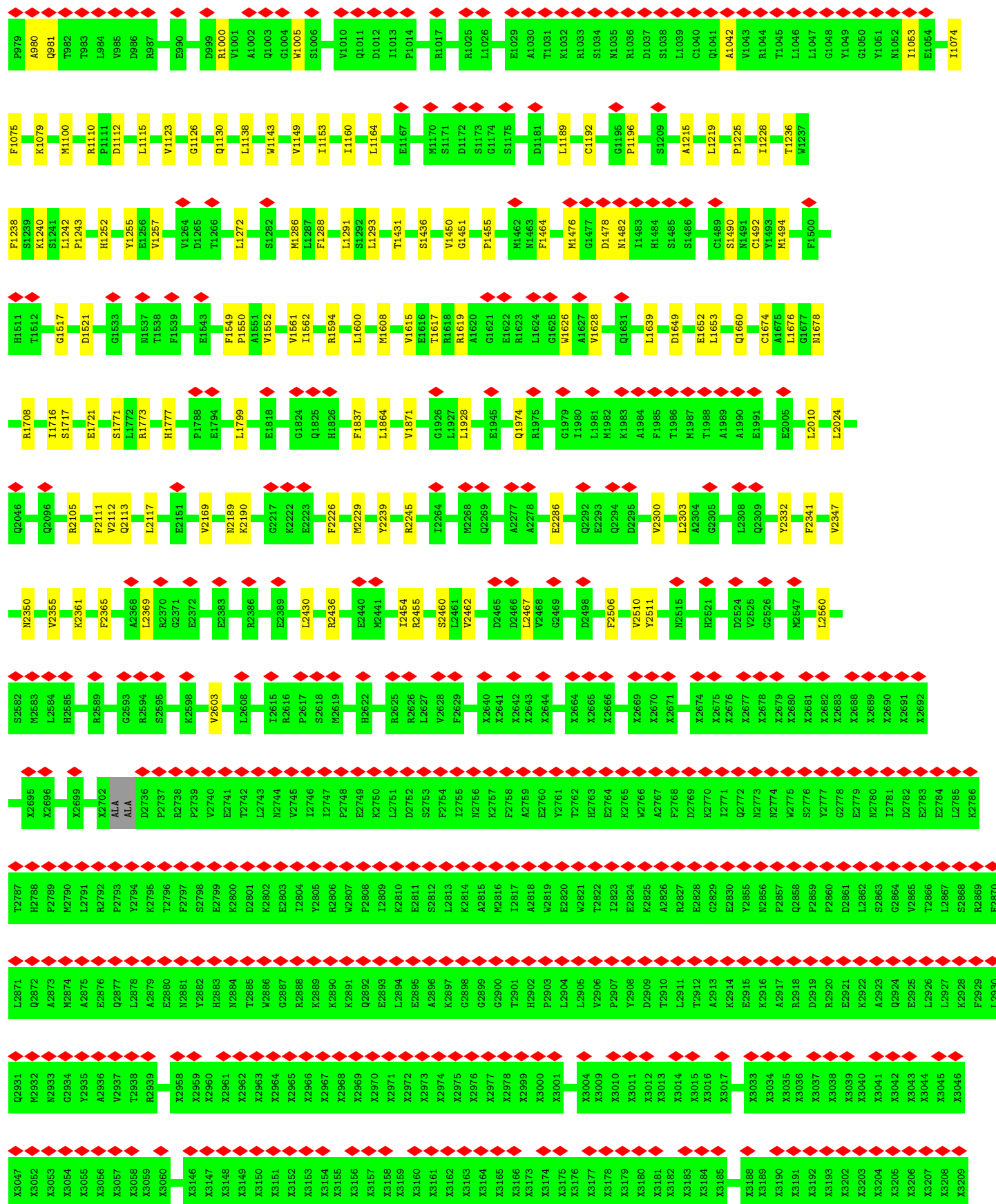




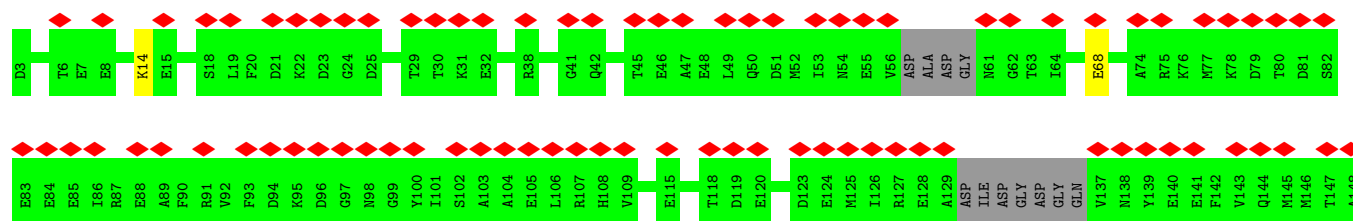


• Molecule 2: Ryanodine Receptor

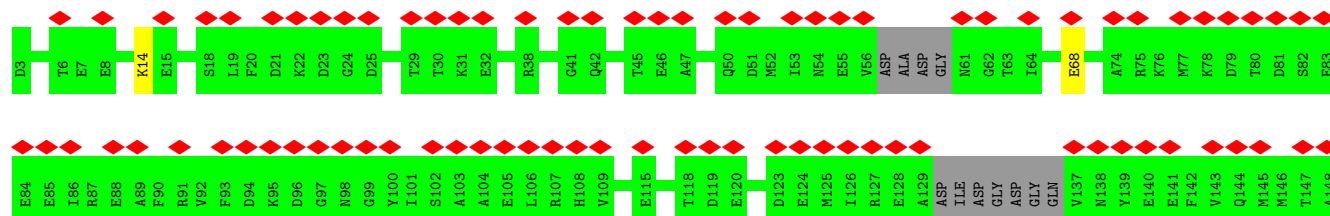




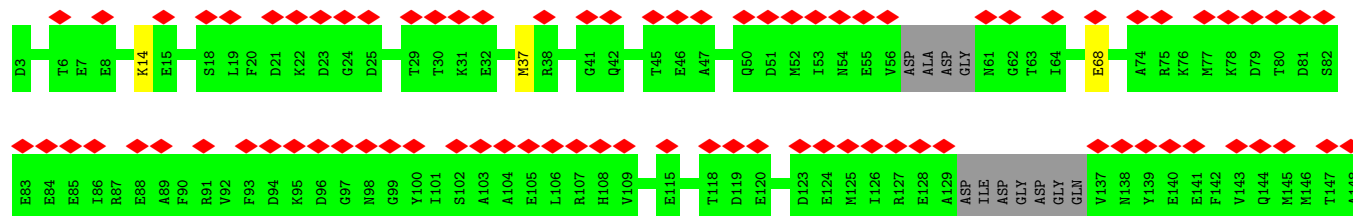
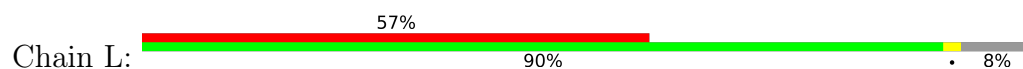




• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



## 4 Experimental information

| Property                             | Value                    | Source    |
|--------------------------------------|--------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE          | Depositor |
| Imposed symmetry                     | POINT, C4                | Depositor |
| Number of particles used             | 44957                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF        | Depositor |
| CTF correction method                | NONE                     | Depositor |
| Microscope                           | FEI TITAN KRIOS          | Depositor |
| Voltage (kV)                         | 300                      | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                       | Depositor |
| Minimum defocus (nm)                 | Not provided             |           |
| Maximum defocus (nm)                 | Not provided             |           |
| Magnification                        | Not provided             |           |
| Image detector                       | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value                    | 0.243                    | Depositor |
| Minimum map value                    | -0.195                   | Depositor |
| Average map value                    | -0.000                   | Depositor |
| Map value standard deviation         | 0.005                    | Depositor |
| Recommended contour level            | 0.022                    | Depositor |
| Map size ( $\text{\AA}$ )            | 523.2, 523.2, 523.2      | wwPDB     |
| Map dimensions                       | 480, 480, 480            | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0         | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.09, 1.09, 1.09         | Depositor |

## 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: ZN

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     | 0.07         | 0/758       | 0.22        | 0/1033      |
| 1   | D     | 0.07         | 0/758       | 0.22        | 0/1033      |
| 1   | G     | 0.07         | 0/758       | 0.22        | 0/1033      |
| 1   | J     | 0.07         | 0/758       | 0.22        | 0/1033      |
| 2   | B     | 0.07         | 0/25809     | 0.21        | 0/35154     |
| 2   | E     | 0.07         | 0/25809     | 0.21        | 0/35154     |
| 2   | H     | 0.07         | 0/25809     | 0.21        | 0/35154     |
| 2   | K     | 0.07         | 0/25809     | 0.21        | 0/35154     |
| 3   | C     | 0.06         | 0/820       | 0.18        | 0/1120      |
| 3   | F     | 0.06         | 0/820       | 0.18        | 0/1120      |
| 3   | I     | 0.06         | 0/820       | 0.18        | 0/1120      |
| 3   | L     | 0.06         | 0/820       | 0.18        | 0/1120      |
| All | All   | 0.07         | 0/109548    | 0.21        | 0/149228    |

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     | 742   | 0        | 702      | 9       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | D     | 742    | 0        | 702      | 11      | 0            |
| 1   | G     | 742    | 0        | 702      | 11      | 0            |
| 1   | J     | 742    | 0        | 702      | 9       | 0            |
| 2   | B     | 27011  | 0        | 23901    | 173     | 0            |
| 2   | E     | 27011  | 0        | 23901    | 179     | 0            |
| 2   | H     | 27011  | 0        | 23901    | 181     | 0            |
| 2   | K     | 27011  | 0        | 23901    | 176     | 0            |
| 3   | C     | 816    | 0        | 573      | 1       | 0            |
| 3   | F     | 816    | 0        | 573      | 2       | 0            |
| 3   | I     | 816    | 0        | 573      | 2       | 0            |
| 3   | L     | 816    | 0        | 573      | 3       | 0            |
| 4   | B     | 1      | 0        | 0        | 0       | 0            |
| 4   | E     | 1      | 0        | 0        | 0       | 0            |
| 4   | H     | 1      | 0        | 0        | 0       | 0            |
| 4   | K     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 114280 | 0        | 100704   | 716     | 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 3.

All (716) 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:E:647:ASN:ND2  | 2:E:820:ARG:O    | 2.27                     | 0.67              |
| 2:K:647:ASN:ND2  | 2:K:820:ARG:O    | 2.27                     | 0.67              |
| 2:B:647:ASN:ND2  | 2:B:820:ARG:O    | 2.27                     | 0.67              |
| 2:H:647:ASN:ND2  | 2:H:820:ARG:O    | 2.27                     | 0.66              |
| 2:E:1215:ALA:HA  | 2:E:1219:LEU:HB2 | 1.81                     | 0.63              |
| 2:H:1000:ARG:HB3 | 2:H:1005:TRP:HB2 | 1.81                     | 0.62              |
| 2:H:1215:ALA:HA  | 2:H:1219:LEU:HB2 | 1.81                     | 0.62              |
| 2:K:1000:ARG:HB3 | 2:K:1005:TRP:HB2 | 1.81                     | 0.62              |
| 2:E:2190:LYS:HG2 | 3:F:14:LYS:HG2   | 1.81                     | 0.62              |
| 2:B:2190:LYS:HG2 | 3:C:14:LYS:HG2   | 1.81                     | 0.61              |
| 2:B:1215:ALA:HA  | 2:B:1219:LEU:HB2 | 1.81                     | 0.61              |
| 2:K:2190:LYS:HG2 | 3:L:14:LYS:HG2   | 1.81                     | 0.61              |
| 2:B:1000:ARG:HB3 | 2:B:1005:TRP:HB2 | 1.81                     | 0.61              |
| 2:E:1000:ARG:HB3 | 2:E:1005:TRP:HB2 | 1.81                     | 0.61              |
| 2:K:1649:ASP:HB3 | 2:K:1652:GLU:HG3 | 1.83                     | 0.61              |
| 2:E:638:ILE:HG12 | 2:E:704:GLY:H    | 1.66                     | 0.61              |
| 1:J:23:VAL:HG22  | 1:J:47:LYS:HG2   | 1.83                     | 0.61              |
| 2:K:1215:ALA:HA  | 2:K:1219:LEU:HB2 | 1.81                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:23:VAL:HG22  | 1:A:47:LYS:HG2    | 1.83                     | 0.61              |
| 2:H:638:ILE:HG12 | 2:H:704:GLY:H     | 1.66                     | 0.61              |
| 2:H:1649:ASP:HB3 | 2:H:1652:GLU:HG3  | 1.83                     | 0.61              |
| 2:K:638:ILE:HG12 | 2:K:704:GLY:H     | 1.66                     | 0.60              |
| 2:B:638:ILE:HG12 | 2:B:704:GLY:H     | 1.66                     | 0.60              |
| 2:H:951:ARG:HH12 | 2:H:973:SER:HB3   | 1.66                     | 0.60              |
| 2:H:2190:LYS:HG2 | 3:I:14:LYS:HG2    | 1.81                     | 0.60              |
| 2:E:951:ARG:HH12 | 2:E:973:SER:HB3   | 1.66                     | 0.60              |
| 2:B:1649:ASP:HB3 | 2:B:1652:GLU:HG3  | 1.83                     | 0.60              |
| 1:D:23:VAL:HG22  | 1:D:47:LYS:HG2    | 1.83                     | 0.60              |
| 1:G:23:VAL:HG22  | 1:G:47:LYS:HG2    | 1.83                     | 0.60              |
| 2:K:951:ARG:HH12 | 2:K:973:SER:HB3   | 1.66                     | 0.60              |
| 2:E:1649:ASP:HB3 | 2:E:1652:GLU:HG3  | 1.83                     | 0.59              |
| 2:B:49:LEU:HD11  | 2:B:182:LEU:HD11  | 1.85                     | 0.59              |
| 2:B:951:ARG:HH12 | 2:B:973:SER:HB3   | 1.66                     | 0.59              |
| 2:E:49:LEU:HD11  | 2:E:182:LEU:HD11  | 1.85                     | 0.59              |
| 2:B:4147:GLU:OE2 | 2:B:4187:ARG:NH1  | 2.36                     | 0.59              |
| 2:K:206:CYS:HB2  | 2:K:271:GLY:HA3   | 1.85                     | 0.59              |
| 2:H:4931:GLN:NE2 | 2:K:4931:GLN:OE1  | 2.36                     | 0.58              |
| 2:B:590:LEU:HD22 | 2:B:631:LEU:HD23  | 1.86                     | 0.58              |
| 2:H:49:LEU:HD11  | 2:H:182:LEU:HD11  | 1.85                     | 0.58              |
| 2:K:49:LEU:HD11  | 2:K:182:LEU:HD11  | 1.85                     | 0.58              |
| 2:B:294:ILE:HG12 | 2:B:296:ASP:H     | 1.69                     | 0.58              |
| 2:E:206:CYS:HB2  | 2:E:271:GLY:HA3   | 1.85                     | 0.58              |
| 2:E:294:ILE:HG12 | 2:E:296:ASP:H     | 1.69                     | 0.58              |
| 2:K:4147:GLU:OE2 | 2:K:4187:ARG:NH1  | 2.36                     | 0.58              |
| 2:B:1240:LYS:HG2 | 2:B:1242:LEU:H    | 1.69                     | 0.58              |
| 2:E:4147:GLU:OE2 | 2:E:4187:ARG:NH1  | 2.36                     | 0.58              |
| 2:E:4931:GLN:NE2 | 2:H:4931:GLN:OE1  | 2.36                     | 0.58              |
| 2:K:294:ILE:HG12 | 2:K:296:ASP:H     | 1.69                     | 0.58              |
| 2:K:1240:LYS:HG2 | 2:K:1242:LEU:H    | 1.69                     | 0.58              |
| 2:B:206:CYS:HB2  | 2:B:271:GLY:HA3   | 1.85                     | 0.58              |
| 2:H:294:ILE:HG12 | 2:H:296:ASP:H     | 1.69                     | 0.58              |
| 2:E:4942:ARG:NH1 | 2:H:4936:ASP:OD1  | 2.37                     | 0.57              |
| 2:B:1115:LEU:HB3 | 2:B:1123:VAL:HG11 | 1.86                     | 0.57              |
| 2:B:4936:ASP:OD1 | 2:K:4942:ARG:NH1  | 2.37                     | 0.57              |
| 2:B:4942:ARG:NH1 | 2:E:4936:ASP:OD1  | 2.37                     | 0.57              |
| 2:E:590:LEU:HD22 | 2:E:631:LEU:HD23  | 1.86                     | 0.57              |
| 2:H:4147:GLU:OE2 | 2:H:4187:ARG:NH1  | 2.36                     | 0.57              |
| 2:H:1240:LYS:HG2 | 2:H:1242:LEU:H    | 1.69                     | 0.57              |
| 2:H:206:CYS:HB2  | 2:H:271:GLY:HA3   | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1115:LEU:HB3  | 2:H:1123:VAL:HG11 | 1.86                     | 0.57              |
| 2:B:4931:GLN:OE1  | 2:K:4931:GLN:NE2  | 2.36                     | 0.57              |
| 2:E:1115:LEU:HB3  | 2:E:1123:VAL:HG11 | 1.86                     | 0.57              |
| 2:H:590:LEU:HD22  | 2:H:631:LEU:HD23  | 1.86                     | 0.57              |
| 2:H:4942:ARG:NH1  | 2:K:4936:ASP:OD1  | 2.37                     | 0.57              |
| 2:B:4146:SER:HA   | 2:B:4155:LEU:HD21 | 1.87                     | 0.57              |
| 2:E:1240:LYS:HG2  | 2:E:1242:LEU:H    | 1.69                     | 0.57              |
| 2:E:4146:SER:HA   | 2:E:4155:LEU:HD21 | 1.87                     | 0.56              |
| 2:K:791:PHE:HB2   | 2:K:1626:TRP:HB2  | 1.87                     | 0.56              |
| 2:K:1115:LEU:HB3  | 2:K:1123:VAL:HG11 | 1.86                     | 0.56              |
| 2:B:4001:ASP:HB3  | 2:B:4004:GLN:HG2  | 1.88                     | 0.56              |
| 2:B:4568:ALA:O    | 2:B:4572:ASN:ND2  | 2.39                     | 0.56              |
| 2:E:291:LEU:HD12  | 2:E:299:LEU:HD11  | 1.88                     | 0.56              |
| 2:K:590:LEU:HD22  | 2:K:631:LEU:HD23  | 1.86                     | 0.56              |
| 2:H:4146:SER:HA   | 2:H:4155:LEU:HD21 | 1.87                     | 0.56              |
| 2:B:3671:ASP:OD1  | 2:B:3764:ARG:NH1  | 2.39                     | 0.56              |
| 2:H:791:PHE:HB2   | 2:H:1626:TRP:HB2  | 1.87                     | 0.56              |
| 2:H:1617:THR:HG22 | 2:H:1628:VAL:HG22 | 1.88                     | 0.56              |
| 2:B:291:LEU:HD12  | 2:B:299:LEU:HD11  | 1.88                     | 0.56              |
| 2:E:1291:LEU:HB2  | 2:E:1550:PRO:HG2  | 1.88                     | 0.56              |
| 2:K:3671:ASP:OD1  | 2:K:3764:ARG:NH1  | 2.39                     | 0.56              |
| 2:K:4146:SER:HA   | 2:K:4155:LEU:HD21 | 1.87                     | 0.56              |
| 2:B:4931:GLN:NE2  | 2:E:4931:GLN:OE1  | 2.36                     | 0.56              |
| 2:E:291:LEU:HA    | 2:E:301:VAL:HA    | 1.88                     | 0.55              |
| 2:E:4001:ASP:HB3  | 2:E:4004:GLN:HG2  | 1.88                     | 0.55              |
| 2:B:1617:THR:HG22 | 2:B:1628:VAL:HG22 | 1.88                     | 0.55              |
| 2:E:4568:ALA:O    | 2:E:4572:ASN:ND2  | 2.39                     | 0.55              |
| 2:H:3671:ASP:OD1  | 2:H:3764:ARG:NH1  | 2.39                     | 0.55              |
| 2:B:291:LEU:HA    | 2:B:301:VAL:HA    | 1.88                     | 0.55              |
| 2:H:4677:ARG:NH1  | 2:H:4713:TYR:OH   | 2.38                     | 0.55              |
| 2:E:3671:ASP:OD1  | 2:E:3764:ARG:NH1  | 2.39                     | 0.55              |
| 2:K:4001:ASP:HB3  | 2:K:4004:GLN:HG2  | 1.88                     | 0.55              |
| 2:K:4568:ALA:O    | 2:K:4572:ASN:ND2  | 2.39                     | 0.55              |
| 2:B:4677:ARG:NH1  | 2:B:4713:TYR:OH   | 2.38                     | 0.55              |
| 2:H:291:LEU:HA    | 2:H:301:VAL:HA    | 1.88                     | 0.55              |
| 2:H:1928:LEU:O    | 2:H:2105:ARG:NH2  | 2.40                     | 0.55              |
| 2:H:4568:ALA:O    | 2:H:4572:ASN:ND2  | 2.39                     | 0.55              |
| 2:K:291:LEU:HD12  | 2:K:299:LEU:HD11  | 1.88                     | 0.55              |
| 2:K:291:LEU:HA    | 2:K:301:VAL:HA    | 1.88                     | 0.55              |
| 2:E:4677:ARG:NH1  | 2:E:4713:TYR:OH   | 2.38                     | 0.55              |
| 2:H:1291:LEU:HB2  | 2:H:1550:PRO:HG2  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:K:1492:CYS:HB3  | 2:K:1494:MET:HE2  | 1.89                     | 0.55              |
| 2:B:178:ARG:NH1   | 2:K:2460:SER:OG   | 2.40                     | 0.55              |
| 2:B:1928:LEU:O    | 2:B:2105:ARG:NH2  | 2.40                     | 0.55              |
| 2:E:1436:SER:HA   | 2:E:1517:GLY:HA2  | 1.89                     | 0.55              |
| 2:K:1617:THR:HG22 | 2:K:1628:VAL:HG22 | 1.88                     | 0.55              |
| 2:E:791:PHE:HB2   | 2:E:1626:TRP:HB2  | 1.87                     | 0.55              |
| 2:E:1450:VAL:HA   | 2:E:1552:VAL:HG22 | 1.89                     | 0.55              |
| 2:H:1450:VAL:HA   | 2:H:1552:VAL:HG22 | 1.89                     | 0.55              |
| 2:H:1492:CYS:HB3  | 2:H:1494:MET:HE2  | 1.89                     | 0.55              |
| 2:B:791:PHE:HB2   | 2:B:1626:TRP:HB2  | 1.87                     | 0.55              |
| 2:H:4199:GLN:HE22 | 2:H:4244:ALA:HB2  | 1.72                     | 0.55              |
| 2:B:1291:LEU:HB2  | 2:B:1550:PRO:HG2  | 1.88                     | 0.55              |
| 2:B:1492:CYS:HB3  | 2:B:1494:MET:HE2  | 1.89                     | 0.55              |
| 2:B:2245:ARG:NH2  | 2:B:2286:GLU:OE1  | 2.40                     | 0.54              |
| 2:B:4882:LEU:HD11 | 2:E:4912:VAL:HG11 | 1.89                     | 0.54              |
| 2:E:4199:GLN:HE22 | 2:E:4244:ALA:HB2  | 1.72                     | 0.54              |
| 2:E:4882:LEU:HD11 | 2:H:4912:VAL:HG11 | 1.90                     | 0.54              |
| 2:H:3808:GLN:NE2  | 2:H:3885:LEU:O    | 2.40                     | 0.54              |
| 2:E:1928:LEU:O    | 2:E:2105:ARG:NH2  | 2.40                     | 0.54              |
| 2:K:4677:ARG:NH1  | 2:K:4713:TYR:OH   | 2.38                     | 0.54              |
| 2:B:3808:GLN:NE2  | 2:B:3885:LEU:O    | 2.40                     | 0.54              |
| 2:H:291:LEU:HD12  | 2:H:299:LEU:HD11  | 1.88                     | 0.54              |
| 2:H:1436:SER:HA   | 2:H:1517:GLY:HA2  | 1.89                     | 0.54              |
| 2:H:2460:SER:OG   | 2:K:178:ARG:NH1   | 2.40                     | 0.54              |
| 2:K:1674:CYS:HA   | 2:K:1678:ASN:HB3  | 1.90                     | 0.54              |
| 2:K:1771:SER:OG   | 2:K:1773:ARG:NH1  | 2.40                     | 0.54              |
| 2:K:2245:ARG:NH2  | 2:K:2286:GLU:OE1  | 2.40                     | 0.54              |
| 2:K:3808:GLN:NE2  | 2:K:3885:LEU:O    | 2.40                     | 0.54              |
| 2:B:1238:PHE:HB3  | 2:B:1608:MET:HE3  | 1.90                     | 0.54              |
| 2:B:1771:SER:OG   | 2:B:1773:ARG:NH1  | 2.40                     | 0.54              |
| 2:E:1617:THR:HG22 | 2:E:1628:VAL:HG22 | 1.88                     | 0.54              |
| 2:E:1674:CYS:HA   | 2:E:1678:ASN:HB3  | 1.90                     | 0.54              |
| 2:H:4001:ASP:HB3  | 2:H:4004:GLN:HG2  | 1.88                     | 0.54              |
| 2:K:233:ILE:O     | 2:K:257:ARG:NH1   | 2.41                     | 0.54              |
| 2:K:1291:LEU:HB2  | 2:K:1550:PRO:HG2  | 1.88                     | 0.54              |
| 2:K:1436:SER:HA   | 2:K:1517:GLY:HA2  | 1.89                     | 0.54              |
| 2:K:1928:LEU:O    | 2:K:2105:ARG:NH2  | 2.40                     | 0.54              |
| 2:E:1771:SER:OG   | 2:E:1773:ARG:NH1  | 2.40                     | 0.54              |
| 2:E:2245:ARG:NH2  | 2:E:2286:GLU:OE1  | 2.40                     | 0.54              |
| 2:B:4912:VAL:HG11 | 2:K:4882:LEU:HD11 | 1.90                     | 0.54              |
| 2:E:3808:GLN:NE2  | 2:E:3885:LEU:O    | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1238:PHE:HB3  | 2:H:1608:MET:HE3  | 1.90                     | 0.54              |
| 2:H:1674:CYS:HA   | 2:H:1678:ASN:HB3  | 1.90                     | 0.54              |
| 2:H:1771:SER:OG   | 2:H:1773:ARG:NH1  | 2.40                     | 0.54              |
| 2:H:2245:ARG:NH2  | 2:H:2286:GLU:OE1  | 2.40                     | 0.54              |
| 2:B:233:ILE:O     | 2:B:257:ARG:NH1   | 2.41                     | 0.54              |
| 2:E:1238:PHE:HB3  | 2:E:1608:MET:HE3  | 1.90                     | 0.54              |
| 2:B:2460:SER:OG   | 2:E:178:ARG:NH1   | 2.40                     | 0.54              |
| 2:E:2460:SER:OG   | 2:H:178:ARG:NH1   | 2.40                     | 0.54              |
| 2:K:1450:VAL:HA   | 2:K:1552:VAL:HG22 | 1.89                     | 0.54              |
| 2:B:1450:VAL:HA   | 2:B:1552:VAL:HG22 | 1.89                     | 0.54              |
| 2:B:1674:CYS:HA   | 2:B:1678:ASN:HB3  | 1.90                     | 0.54              |
| 2:E:2347:VAL:HG12 | 2:E:2350:ASN:H    | 1.73                     | 0.54              |
| 2:B:1436:SER:HA   | 2:B:1517:GLY:HA2  | 1.89                     | 0.53              |
| 2:B:2347:VAL:HG12 | 2:B:2350:ASN:H    | 1.73                     | 0.53              |
| 2:B:4886:TYR:HA   | 2:E:4916:ILE:HD11 | 1.90                     | 0.53              |
| 2:H:4882:LEU:HD11 | 2:K:4912:VAL:HG11 | 1.89                     | 0.53              |
| 2:K:1238:PHE:HB3  | 2:K:1608:MET:HE3  | 1.90                     | 0.53              |
| 2:K:4199:GLN:HE22 | 2:K:4244:ALA:HB2  | 1.72                     | 0.53              |
| 2:K:878:ILE:HD11  | 2:K:1042:ALA:HB2  | 1.90                     | 0.53              |
| 2:B:878:ILE:HD11  | 2:B:1042:ALA:HB2  | 1.90                     | 0.53              |
| 2:E:1492:CYS:HB3  | 2:E:1494:MET:HE2  | 1.89                     | 0.53              |
| 2:E:4175:ARG:NH1  | 2:E:4189:TYR:OH   | 2.42                     | 0.53              |
| 2:B:3666:GLU:HA   | 2:B:3724:ILE:HG23 | 1.91                     | 0.53              |
| 2:E:2111:PHE:HD2  | 2:E:2113:GLN:HG2  | 1.74                     | 0.53              |
| 2:K:2111:PHE:HD2  | 2:K:2113:GLN:HG2  | 1.74                     | 0.53              |
| 2:E:3666:GLU:HA   | 2:E:3724:ILE:HG23 | 1.91                     | 0.53              |
| 2:H:2347:VAL:HG12 | 2:H:2350:ASN:H    | 1.73                     | 0.53              |
| 2:H:4175:ARG:NH1  | 2:H:4189:TYR:OH   | 2.42                     | 0.53              |
| 2:B:4199:GLN:HE22 | 2:B:4244:ALA:HB2  | 1.72                     | 0.53              |
| 2:E:3762:GLN:OE1  | 2:E:3804:ASN:ND2  | 2.40                     | 0.53              |
| 2:H:233:ILE:O     | 2:H:257:ARG:NH1   | 2.41                     | 0.53              |
| 2:H:2111:PHE:HD2  | 2:H:2113:GLN:HG2  | 1.74                     | 0.53              |
| 2:K:1293:LEU:HD11 | 2:K:1594:ARG:HG2  | 1.90                     | 0.53              |
| 2:H:1293:LEU:HD11 | 2:H:1594:ARG:HG2  | 1.90                     | 0.52              |
| 2:H:4886:TYR:HA   | 2:K:4916:ILE:HD11 | 1.90                     | 0.52              |
| 2:K:2347:VAL:HG12 | 2:K:2350:ASN:H    | 1.73                     | 0.52              |
| 2:B:259:LEU:HB2   | 2:B:285:VAL:HG21  | 1.91                     | 0.52              |
| 2:B:4175:ARG:NH1  | 2:B:4189:TYR:OH   | 2.42                     | 0.52              |
| 2:B:4916:ILE:HD11 | 2:K:4886:TYR:HA   | 1.90                     | 0.52              |
| 2:B:4997:ASP:OD1  | 2:B:4997:ASP:N    | 2.42                     | 0.52              |
| 2:E:4886:TYR:HA   | 2:H:4916:ILE:HD11 | 1.90                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:1149:VAL:HG22 | 2:H:1164:LEU:HD13 | 1.92                     | 0.52              |
| 2:K:259:LEU:HB2   | 2:K:285:VAL:HG21  | 1.91                     | 0.52              |
| 2:K:4175:ARG:NH1  | 2:K:4189:TYR:OH   | 2.42                     | 0.52              |
| 2:E:233:ILE:O     | 2:E:257:ARG:NH1   | 2.41                     | 0.52              |
| 2:E:878:ILE:HD11  | 2:E:1042:ALA:HB2  | 1.90                     | 0.52              |
| 1:D:82:TYR:HB3    | 1:D:86:GLY:HA2    | 1.92                     | 0.52              |
| 2:E:633:LEU:HD13  | 2:E:1639:LEU:HD21 | 1.91                     | 0.52              |
| 2:E:1293:LEU:HD11 | 2:E:1594:ARG:HG2  | 1.90                     | 0.52              |
| 2:H:633:LEU:HD13  | 2:H:1639:LEU:HD21 | 1.91                     | 0.52              |
| 2:H:878:ILE:HD11  | 2:H:1042:ALA:HB2  | 1.90                     | 0.52              |
| 2:H:897:ARG:HE    | 2:H:905:PRO:HD2   | 1.75                     | 0.52              |
| 2:H:951:ARG:NH2   | 2:H:971:ASP:O     | 2.43                     | 0.52              |
| 2:B:1293:LEU:HD11 | 2:B:1594:ARG:HG2  | 1.90                     | 0.52              |
| 2:E:1130:GLN:HG2  | 2:E:1138:LEU:HA   | 1.92                     | 0.52              |
| 2:E:1149:VAL:HG22 | 2:E:1164:LEU:HD13 | 1.92                     | 0.52              |
| 2:H:259:LEU:HB2   | 2:H:285:VAL:HG21  | 1.91                     | 0.52              |
| 2:B:106:ALA:HA    | 2:B:149:THR:HA    | 1.92                     | 0.52              |
| 2:E:747:CYS:SG    | 2:E:748:LEU:N     | 2.83                     | 0.52              |
| 2:H:1777:HIS:HB3  | 2:H:1799:LEU:HD13 | 1.92                     | 0.52              |
| 2:K:3666:GLU:HA   | 2:K:3724:ILE:HG23 | 1.91                     | 0.52              |
| 2:H:3666:GLU:HA   | 2:H:3724:ILE:HG23 | 1.91                     | 0.51              |
| 2:K:633:LEU:HD13  | 2:K:1639:LEU:HD21 | 1.91                     | 0.51              |
| 2:B:633:LEU:HD13  | 2:B:1639:LEU:HD21 | 1.91                     | 0.51              |
| 2:B:2111:PHE:HD2  | 2:B:2113:GLN:HG2  | 1.74                     | 0.51              |
| 1:G:82:TYR:HB3    | 1:G:86:GLY:HA2    | 1.92                     | 0.51              |
| 2:K:897:ARG:HE    | 2:K:905:PRO:HD2   | 1.75                     | 0.51              |
| 2:K:1149:VAL:HG22 | 2:K:1164:LEU:HD13 | 1.92                     | 0.51              |
| 2:K:1777:HIS:HB3  | 2:K:1799:LEU:HD13 | 1.92                     | 0.51              |
| 2:E:4997:ASP:N    | 2:E:4997:ASP:OD1  | 2.42                     | 0.51              |
| 2:K:618:GLN:OE1   | 2:K:1678:ASN:ND2  | 2.39                     | 0.51              |
| 2:B:951:ARG:NH2   | 2:B:971:ASP:O     | 2.43                     | 0.51              |
| 2:E:259:LEU:HB2   | 2:E:285:VAL:HG21  | 1.91                     | 0.51              |
| 2:H:747:CYS:SG    | 2:H:748:LEU:N     | 2.83                     | 0.51              |
| 2:H:4242:ILE:O    | 2:H:4246:ILE:N    | 2.44                     | 0.51              |
| 2:E:951:ARG:NH2   | 2:E:971:ASP:O     | 2.43                     | 0.51              |
| 2:E:3766:HIS:HB2  | 2:E:3771:ALA:HB2  | 1.93                     | 0.51              |
| 2:K:747:CYS:SG    | 2:K:748:LEU:N     | 2.83                     | 0.51              |
| 2:K:951:ARG:NH2   | 2:K:971:ASP:O     | 2.43                     | 0.51              |
| 2:B:864:PRO:HD2   | 2:B:867:LEU:HD12  | 1.93                     | 0.51              |
| 2:K:266:ARG:NH1   | 2:K:272:SER:OG    | 2.44                     | 0.51              |
| 2:B:4242:ILE:O    | 2:B:4246:ILE:N    | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1777:HIS:HB3  | 2:E:1799:LEU:HD13 | 1.92                     | 0.51              |
| 2:H:3766:HIS:HB2  | 2:H:3771:ALA:HB2  | 1.93                     | 0.51              |
| 2:B:1130:GLN:HG2  | 2:B:1138:LEU:HA   | 1.92                     | 0.51              |
| 2:B:1149:VAL:HG22 | 2:B:1164:LEU:HD13 | 1.92                     | 0.51              |
| 2:B:3766:HIS:HB2  | 2:B:3771:ALA:HB2  | 1.93                     | 0.51              |
| 2:E:4242:ILE:O    | 2:E:4246:ILE:N    | 2.44                     | 0.51              |
| 2:E:4861:TYR:HD2  | 2:E:4874:CYS:HB3  | 1.76                     | 0.51              |
| 2:H:266:ARG:NH1   | 2:H:272:SER:OG    | 2.44                     | 0.51              |
| 2:B:266:ARG:NH1   | 2:B:272:SER:OG    | 2.44                     | 0.51              |
| 2:E:266:ARG:NH1   | 2:E:272:SER:OG    | 2.44                     | 0.51              |
| 2:H:106:ALA:HA    | 2:H:149:THR:HA    | 1.92                     | 0.51              |
| 2:H:2341:PHE:HB2  | 2:H:2436:ARG:HD3  | 1.93                     | 0.51              |
| 2:K:106:ALA:HA    | 2:K:149:THR:HA    | 1.92                     | 0.51              |
| 2:B:1777:HIS:HB3  | 2:B:1799:LEU:HD13 | 1.92                     | 0.50              |
| 2:E:864:PRO:HD2   | 2:E:867:LEU:HD12  | 1.93                     | 0.50              |
| 2:H:3762:GLN:OE1  | 2:H:3804:ASN:ND2  | 2.40                     | 0.50              |
| 2:K:3766:HIS:HB2  | 2:K:3771:ALA:HB2  | 1.93                     | 0.50              |
| 2:K:4242:ILE:O    | 2:K:4246:ILE:N    | 2.44                     | 0.50              |
| 1:A:82:TYR:HB3    | 1:A:86:GLY:HA2    | 1.92                     | 0.50              |
| 2:B:683:ARG:HB2   | 2:B:707:VAL:HG21  | 1.94                     | 0.50              |
| 2:B:3762:GLN:OE1  | 2:B:3804:ASN:ND2  | 2.40                     | 0.50              |
| 2:E:106:ALA:HA    | 2:E:149:THR:HA    | 1.92                     | 0.50              |
| 2:H:683:ARG:HB2   | 2:H:707:VAL:HG21  | 1.94                     | 0.50              |
| 2:H:1130:GLN:HG2  | 2:H:1138:LEU:HA   | 1.92                     | 0.50              |
| 2:K:4997:ASP:OD1  | 2:K:4997:ASP:N    | 2.42                     | 0.50              |
| 2:B:747:CYS:SG    | 2:B:748:LEU:N     | 2.83                     | 0.50              |
| 2:K:1130:GLN:HG2  | 2:K:1138:LEU:HA   | 1.92                     | 0.50              |
| 2:E:897:ARG:HE    | 2:E:905:PRO:HD2   | 1.75                     | 0.50              |
| 1:J:82:TYR:HB3    | 1:J:86:GLY:HA2    | 1.92                     | 0.50              |
| 2:E:683:ARG:HB2   | 2:E:707:VAL:HG21  | 1.94                     | 0.50              |
| 2:H:1236:THR:OG1  | 2:H:1608:MET:SD   | 2.67                     | 0.50              |
| 2:K:864:PRO:HD2   | 2:K:867:LEU:HD12  | 1.93                     | 0.50              |
| 2:B:897:ARG:HE    | 2:B:905:PRO:HD2   | 1.75                     | 0.50              |
| 2:E:2341:PHE:HB2  | 2:E:2436:ARG:HD3  | 1.93                     | 0.50              |
| 2:H:892:THR:O     | 2:H:904:HIS:N     | 2.45                     | 0.50              |
| 2:K:4861:TYR:HD2  | 2:K:4874:CYS:HB3  | 1.76                     | 0.50              |
| 2:E:1243:PRO:HB3  | 2:E:1600:LEU:HD21 | 1.94                     | 0.50              |
| 2:H:4861:TYR:HD2  | 2:H:4874:CYS:HB3  | 1.76                     | 0.50              |
| 2:K:683:ARG:HB2   | 2:K:707:VAL:HG21  | 1.94                     | 0.50              |
| 2:B:4861:TYR:HD2  | 2:B:4874:CYS:HB3  | 1.76                     | 0.49              |
| 2:B:2341:PHE:HB2  | 2:B:2436:ARG:HD3  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:H:864:PRO:HD2   | 2:H:867:LEU:HD12  | 1.93                     | 0.49              |
| 2:K:102:LEU:HB2   | 2:K:105:HIS:CD2   | 2.48                     | 0.49              |
| 2:K:1455:PRO:HB3  | 2:K:1549:PHE:HE2  | 1.78                     | 0.49              |
| 2:B:102:LEU:HB2   | 2:B:105:HIS:CD2   | 2.48                     | 0.49              |
| 2:B:1455:PRO:HB3  | 2:B:1549:PHE:HE2  | 1.78                     | 0.49              |
| 2:H:4040:VAL:HG22 | 2:H:4145:LEU:HD21 | 1.95                     | 0.49              |
| 2:E:102:LEU:HB2   | 2:E:105:HIS:CD2   | 2.48                     | 0.49              |
| 2:H:1431:THR:OG1  | 2:H:1521:ASP:OD1  | 2.29                     | 0.49              |
| 2:E:1126:GLY:HA3  | 2:E:1143:TRP:CE2  | 2.48                     | 0.49              |
| 2:H:3763:ALA:O    | 2:H:3767:ASN:ND2  | 2.46                     | 0.49              |
| 2:H:3776:GLN:NE2  | 2:H:3814:TYR:OH   | 2.37                     | 0.49              |
| 2:H:4997:ASP:OD1  | 2:H:4997:ASP:N    | 2.42                     | 0.49              |
| 2:K:892:THR:O     | 2:K:904:HIS:N     | 2.45                     | 0.49              |
| 2:K:3763:ALA:HA   | 2:K:3766:HIS:CE1  | 2.48                     | 0.49              |
| 2:K:3763:ALA:O    | 2:K:3767:ASN:ND2  | 2.46                     | 0.49              |
| 2:E:3776:GLN:NE2  | 2:E:3814:TYR:OH   | 2.37                     | 0.49              |
| 2:K:1243:PRO:HB3  | 2:K:1600:LEU:HD21 | 1.94                     | 0.49              |
| 2:B:2300:VAL:HG12 | 2:B:2361:LYS:HD2  | 1.96                     | 0.48              |
| 2:H:1455:PRO:HB3  | 2:H:1549:PHE:HE2  | 1.78                     | 0.48              |
| 2:H:1561:VAL:HG12 | 2:H:1562:ILE:HG12 | 1.95                     | 0.48              |
| 2:K:1126:GLY:HA3  | 2:K:1143:TRP:CE2  | 2.48                     | 0.48              |
| 2:K:4040:VAL:HG22 | 2:K:4145:LEU:HD21 | 1.95                     | 0.48              |
| 2:H:2300:VAL:HG12 | 2:H:2361:LYS:HD2  | 1.96                     | 0.48              |
| 2:H:3763:ALA:HA   | 2:H:3766:HIS:CE1  | 2.48                     | 0.48              |
| 2:K:2300:VAL:HG12 | 2:K:2361:LYS:HD2  | 1.96                     | 0.48              |
| 2:E:3884:GLN:OE1  | 2:E:3955:GLN:NE2  | 2.47                     | 0.48              |
| 2:H:618:GLN:OE1   | 2:H:1678:ASN:ND2  | 2.39                     | 0.48              |
| 2:H:659:TYR:O     | 2:H:662:TRP:NE1   | 2.47                     | 0.48              |
| 2:B:3763:ALA:HA   | 2:B:3766:HIS:CE1  | 2.48                     | 0.48              |
| 2:B:3884:GLN:OE1  | 2:B:3955:GLN:NE2  | 2.47                     | 0.48              |
| 2:E:671:VAL:HG23  | 2:E:787:VAL:HG22  | 1.96                     | 0.48              |
| 2:E:892:THR:O     | 2:E:904:HIS:N     | 2.45                     | 0.48              |
| 2:E:1561:VAL:HG12 | 2:E:1562:ILE:HG12 | 1.95                     | 0.48              |
| 2:E:3763:ALA:O    | 2:E:3767:ASN:ND2  | 2.46                     | 0.48              |
| 2:B:892:THR:O     | 2:B:904:HIS:N     | 2.45                     | 0.48              |
| 2:E:1455:PRO:HB3  | 2:E:1549:PHE:HE2  | 1.78                     | 0.48              |
| 2:K:2341:PHE:HB2  | 2:K:2436:ARG:HD3  | 1.93                     | 0.48              |
| 1:D:31:GLN:HB2    | 1:D:96:THR:HB     | 1.95                     | 0.48              |
| 2:E:2300:VAL:HG12 | 2:E:2361:LYS:HD2  | 1.96                     | 0.48              |
| 2:K:3762:GLN:OE1  | 2:K:3804:ASN:ND2  | 2.40                     | 0.48              |
| 2:B:618:GLN:OE1   | 2:B:1678:ASN:ND2  | 2.39                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1653:LEU:HD23 | 2:E:1660:GLN:HA   | 1.96                     | 0.48              |
| 2:H:1243:PRO:HB3  | 2:H:1600:LEU:HD21 | 1.94                     | 0.48              |
| 2:K:781:VAL:HG11  | 2:K:789:VAL:HG21  | 1.96                     | 0.48              |
| 2:B:671:VAL:HG23  | 2:B:787:VAL:HG22  | 1.96                     | 0.48              |
| 2:B:1561:VAL:HG12 | 2:B:1562:ILE:HG12 | 1.95                     | 0.48              |
| 2:H:3884:GLN:OE1  | 2:H:3955:GLN:NE2  | 2.47                     | 0.48              |
| 2:K:659:TYR:O     | 2:K:662:TRP:NE1   | 2.47                     | 0.48              |
| 1:A:31:GLN:HB2    | 1:A:96:THR:HB     | 1.95                     | 0.48              |
| 2:B:1243:PRO:HB3  | 2:B:1600:LEU:HD21 | 1.94                     | 0.48              |
| 2:E:4040:VAL:HG22 | 2:E:4145:LEU:HD21 | 1.95                     | 0.48              |
| 2:H:4001:ASP:OD2  | 2:H:4003:SER:OG   | 2.30                     | 0.48              |
| 1:J:31:GLN:HB2    | 1:J:96:THR:HB     | 1.95                     | 0.48              |
| 2:K:1561:VAL:HG12 | 2:K:1562:ILE:HG12 | 1.95                     | 0.48              |
| 2:B:3763:ALA:O    | 2:B:3767:ASN:ND2  | 2.46                     | 0.48              |
| 2:E:3763:ALA:HA   | 2:E:3766:HIS:CE1  | 2.48                     | 0.48              |
| 2:H:1079:LYS:HA   | 2:H:1189:LEU:HD11 | 1.96                     | 0.48              |
| 2:H:1126:GLY:HA3  | 2:H:1143:TRP:CE2  | 2.48                     | 0.48              |
| 2:H:1653:LEU:HD23 | 2:H:1660:GLN:HA   | 1.96                     | 0.48              |
| 2:K:1079:LYS:HA   | 2:K:1189:LEU:HD11 | 1.96                     | 0.48              |
| 2:B:1126:GLY:HA3  | 2:B:1143:TRP:CE2  | 2.48                     | 0.47              |
| 2:H:102:LEU:HB2   | 2:H:105:HIS:CD2   | 2.48                     | 0.47              |
| 2:K:4690:PRO:HB2  | 2:K:4701:ARG:HH11 | 1.79                     | 0.47              |
| 2:B:4040:VAL:HG22 | 2:B:4145:LEU:HD21 | 1.95                     | 0.47              |
| 2:B:4690:PRO:HB2  | 2:B:4701:ARG:HH11 | 1.79                     | 0.47              |
| 2:E:659:TYR:O     | 2:E:662:TRP:NE1   | 2.47                     | 0.47              |
| 2:E:1079:LYS:HA   | 2:E:1189:LEU:HD11 | 1.96                     | 0.47              |
| 2:K:3776:GLN:NE2  | 2:K:3814:TYR:OH   | 2.37                     | 0.47              |
| 2:B:659:TYR:O     | 2:B:662:TRP:NE1   | 2.47                     | 0.47              |
| 1:G:66:MET:HE2    | 1:G:72:ALA:HB3    | 1.97                     | 0.47              |
| 2:K:1431:THR:OG1  | 2:K:1521:ASP:OD1  | 2.29                     | 0.47              |
| 1:J:66:MET:HE2    | 1:J:72:ALA:HB3    | 1.97                     | 0.47              |
| 2:K:2455:ARG:HG3  | 2:K:2510:VAL:HG23 | 1.97                     | 0.47              |
| 2:B:1864:LEU:HB3  | 2:B:1871:VAL:HG11 | 1.97                     | 0.47              |
| 2:B:1079:LYS:HA   | 2:B:1189:LEU:HD11 | 1.96                     | 0.47              |
| 2:E:781:VAL:HG11  | 2:E:789:VAL:HG21  | 1.96                     | 0.47              |
| 2:H:671:VAL:HG23  | 2:H:787:VAL:HG22  | 1.96                     | 0.47              |
| 2:H:781:VAL:HG11  | 2:H:789:VAL:HG21  | 1.96                     | 0.47              |
| 2:K:1653:LEU:HD23 | 2:K:1660:GLN:HA   | 1.96                     | 0.47              |
| 2:E:1478:ASP:N    | 2:E:1482:ASN:O    | 2.48                     | 0.47              |
| 2:E:2455:ARG:HG3  | 2:E:2510:VAL:HG23 | 1.97                     | 0.47              |
| 2:K:671:VAL:HG23  | 2:K:787:VAL:HG22  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:K:3884:GLN:OE1  | 2:K:3955:GLN:NE2  | 2.47                     | 0.47              |
| 1:A:66:MET:HE2    | 1:A:72:ALA:HB3    | 1.97                     | 0.47              |
| 2:B:781:VAL:HG11  | 2:B:789:VAL:HG21  | 1.96                     | 0.47              |
| 2:B:1653:LEU:HD23 | 2:B:1660:GLN:HA   | 1.96                     | 0.47              |
| 1:D:66:MET:HE2    | 1:D:72:ALA:HB3    | 1.97                     | 0.47              |
| 2:H:4690:PRO:HB2  | 2:H:4701:ARG:HH11 | 1.79                     | 0.47              |
| 2:E:4690:PRO:HB2  | 2:E:4701:ARG:HH11 | 1.79                     | 0.46              |
| 2:E:4981:HIS:HB2  | 2:E:4986:TYR:HE2  | 1.81                     | 0.46              |
| 2:E:2010:LEU:HB3  | 2:E:2024:LEU:HD11 | 1.97                     | 0.46              |
| 1:G:31:GLN:HB2    | 1:G:96:THR:HB     | 1.95                     | 0.46              |
| 2:H:1864:LEU:HB3  | 2:H:1871:VAL:HG11 | 1.97                     | 0.46              |
| 2:H:2010:LEU:HB3  | 2:H:2024:LEU:HD11 | 1.97                     | 0.46              |
| 2:H:4981:HIS:HB2  | 2:H:4986:TYR:HE2  | 1.81                     | 0.46              |
| 2:K:594:GLY:HA2   | 2:K:1594:ARG:HE   | 1.81                     | 0.46              |
| 2:K:908:VAL:HG23  | 2:K:913:LEU:HD23  | 1.98                     | 0.46              |
| 2:B:1717:SER:HA   | 2:B:1721:GLU:HB2  | 1.98                     | 0.46              |
| 2:H:594:GLY:HA2   | 2:H:1594:ARG:HE   | 1.81                     | 0.46              |
| 2:B:2455:ARG:HG3  | 2:B:2510:VAL:HG23 | 1.97                     | 0.46              |
| 2:E:553:ARG:HG3   | 2:E:555:GLU:H     | 1.80                     | 0.46              |
| 2:H:262:LEU:HD23  | 2:H:262:LEU:H     | 1.80                     | 0.46              |
| 2:K:262:LEU:HD23  | 2:K:262:LEU:H     | 1.80                     | 0.46              |
| 2:B:908:VAL:HG23  | 2:B:913:LEU:HD23  | 1.98                     | 0.46              |
| 2:B:1153:ILE:HG13 | 2:B:1160:ILE:HG12 | 1.98                     | 0.46              |
| 2:B:1225:PRO:HD2  | 2:B:1228:ILE:HD12 | 1.97                     | 0.46              |
| 2:B:4981:HIS:HB2  | 2:B:4986:TYR:HE2  | 1.81                     | 0.46              |
| 2:E:594:GLY:HA2   | 2:E:1594:ARG:HE   | 1.81                     | 0.46              |
| 2:K:683:ARG:HG2   | 2:K:717:ASP:HB3   | 1.98                     | 0.46              |
| 2:B:2010:LEU:HB3  | 2:B:2024:LEU:HD11 | 1.97                     | 0.46              |
| 2:B:4565:LEU:HG   | 2:B:4814:ILE:HG22 | 1.98                     | 0.46              |
| 2:E:1717:SER:HA   | 2:E:1721:GLU:HB2  | 1.98                     | 0.46              |
| 2:K:1225:PRO:HD2  | 2:K:1228:ILE:HD12 | 1.97                     | 0.46              |
| 2:K:1864:LEU:HB3  | 2:K:1871:VAL:HG11 | 1.97                     | 0.46              |
| 2:K:4981:HIS:HB2  | 2:K:4986:TYR:HE2  | 1.81                     | 0.46              |
| 2:B:553:ARG:HG3   | 2:B:555:GLU:H     | 1.80                     | 0.46              |
| 2:B:594:GLY:HA2   | 2:B:1594:ARG:HE   | 1.81                     | 0.46              |
| 2:E:4565:LEU:HG   | 2:E:4814:ILE:HG22 | 1.98                     | 0.46              |
| 2:H:908:VAL:HG23  | 2:H:913:LEU:HD23  | 1.98                     | 0.46              |
| 2:B:1478:ASP:N    | 2:B:1482:ASN:O    | 2.48                     | 0.46              |
| 2:E:683:ARG:HG2   | 2:E:717:ASP:HB3   | 1.98                     | 0.46              |
| 2:E:1864:LEU:HB3  | 2:E:1871:VAL:HG11 | 1.97                     | 0.46              |
| 2:H:1225:PRO:HD2  | 2:H:1228:ILE:HD12 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:981:GLN:NE2   | 2:B:1053:ILE:O    | 2.48                     | 0.45              |
| 2:E:711:LEU:HD21  | 2:E:1490:SER:HA   | 1.98                     | 0.45              |
| 2:E:1153:ILE:HG13 | 2:E:1160:ILE:HG12 | 1.98                     | 0.45              |
| 2:H:711:LEU:HD21  | 2:H:1490:SER:HA   | 1.98                     | 0.45              |
| 2:H:553:ARG:HG3   | 2:H:555:GLU:H     | 1.80                     | 0.45              |
| 2:K:2010:LEU:HB3  | 2:K:2024:LEU:HD11 | 1.97                     | 0.45              |
| 2:H:2455:ARG:HG3  | 2:H:2510:VAL:HG23 | 1.97                     | 0.45              |
| 2:H:4820:THR:HB   | 2:K:4837:MET:HG3  | 1.98                     | 0.45              |
| 2:B:262:LEU:H     | 2:B:262:LEU:HD23  | 1.80                     | 0.45              |
| 2:B:3922:GLN:HE21 | 2:B:3986:GLY:HA3  | 1.82                     | 0.45              |
| 2:E:908:VAL:HG23  | 2:E:913:LEU:HD23  | 1.98                     | 0.45              |
| 2:H:1478:ASP:N    | 2:H:1482:ASN:O    | 2.48                     | 0.45              |
| 2:K:553:ARG:HG3   | 2:K:555:GLU:H     | 1.80                     | 0.45              |
| 2:K:981:GLN:NE2   | 2:K:1053:ILE:O    | 2.48                     | 0.45              |
| 2:B:1431:THR:OG1  | 2:B:1521:ASP:OD1  | 2.29                     | 0.45              |
| 2:B:3637:LEU:HD12 | 2:B:3640:LEU:HD12 | 1.99                     | 0.45              |
| 2:E:618:GLN:OE1   | 2:E:1678:ASN:ND2  | 2.39                     | 0.45              |
| 2:H:683:ARG:HG2   | 2:H:717:ASP:HB3   | 1.98                     | 0.45              |
| 2:H:1153:ILE:HG13 | 2:H:1160:ILE:HG12 | 1.98                     | 0.45              |
| 2:K:1717:SER:HA   | 2:K:1721:GLU:HB2  | 1.98                     | 0.45              |
| 2:B:615:ARG:HH21  | 2:B:2169:VAL:HG11 | 1.82                     | 0.45              |
| 1:D:27:THR:HB     | 1:D:100:ASP:HB3   | 1.99                     | 0.45              |
| 2:E:1225:PRO:HD2  | 2:E:1228:ILE:HD12 | 1.97                     | 0.45              |
| 2:H:1717:SER:HA   | 2:H:1721:GLU:HB2  | 1.98                     | 0.45              |
| 1:A:27:THR:HB     | 1:A:100:ASP:HB3   | 1.99                     | 0.45              |
| 2:E:262:LEU:HD23  | 2:E:262:LEU:H     | 1.80                     | 0.45              |
| 2:H:978:THR:HG22  | 2:H:980:ALA:H     | 1.82                     | 0.45              |
| 2:K:622:THR:HG23  | 2:K:626:LEU:HD12  | 1.99                     | 0.45              |
| 2:K:3637:LEU:HD12 | 2:K:3640:LEU:HD12 | 1.99                     | 0.45              |
| 2:B:4820:THR:HB   | 2:E:4837:MET:HG3  | 1.98                     | 0.45              |
| 2:E:1257:VAL:HG12 | 2:E:1272:LEU:HD12 | 1.99                     | 0.45              |
| 2:E:3922:GLN:HE21 | 2:E:3986:GLY:HA3  | 1.82                     | 0.45              |
| 2:H:35:LEU:HD13   | 2:H:49:LEU:HD13   | 1.99                     | 0.45              |
| 2:H:292:ALA:HB2   | 2:H:312:THR:HG22  | 1.99                     | 0.45              |
| 2:H:2239:TYR:OH   | 3:I:68:GLU:OE2    | 2.27                     | 0.45              |
| 1:G:27:THR:HB     | 1:G:100:ASP:HB3   | 1.99                     | 0.45              |
| 2:K:1153:ILE:HG13 | 2:K:1160:ILE:HG12 | 1.98                     | 0.45              |
| 2:B:683:ARG:HG2   | 2:B:717:ASP:HB3   | 1.98                     | 0.44              |
| 2:B:711:LEU:HD21  | 2:B:1490:SER:HA   | 1.98                     | 0.44              |
| 2:H:1257:VAL:HG12 | 2:H:1272:LEU:HD12 | 1.99                     | 0.44              |
| 2:K:3922:GLN:HE21 | 2:K:3986:GLY:HA3  | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:622:THR:HG23  | 2:B:626:LEU:HD12  | 1.99                     | 0.44              |
| 2:E:978:THR:HG22  | 2:E:980:ALA:H     | 1.82                     | 0.44              |
| 2:H:615:ARG:HH21  | 2:H:2169:VAL:HG11 | 1.82                     | 0.44              |
| 2:K:35:LEU:HD13   | 2:K:49:LEU:HD13   | 1.99                     | 0.44              |
| 2:K:978:THR:HG22  | 2:K:980:ALA:H     | 1.82                     | 0.44              |
| 2:K:2462:VAL:O    | 2:K:2511:TYR:OH   | 2.34                     | 0.44              |
| 2:B:497:TYR:HB3   | 2:B:503:PHE:HB3   | 1.99                     | 0.44              |
| 2:E:35:LEU:HD13   | 2:E:49:LEU:HD13   | 1.99                     | 0.44              |
| 2:H:3922:GLN:HE21 | 2:H:3986:GLY:HA3  | 1.82                     | 0.44              |
| 2:K:292:ALA:HB2   | 2:K:312:THR:HG22  | 1.99                     | 0.44              |
| 2:K:711:LEU:HD21  | 2:K:1490:SER:HA   | 1.98                     | 0.44              |
| 2:E:615:ARG:HH21  | 2:E:2169:VAL:HG11 | 1.82                     | 0.44              |
| 2:H:4565:LEU:HG   | 2:H:4814:ILE:HG22 | 1.98                     | 0.44              |
| 2:K:615:ARG:HH21  | 2:K:2169:VAL:HG11 | 1.82                     | 0.44              |
| 2:K:1974:GLN:HE22 | 2:K:3637:LEU:HB3  | 1.83                     | 0.44              |
| 2:K:4565:LEU:HG   | 2:K:4814:ILE:HG22 | 1.98                     | 0.44              |
| 2:B:1974:GLN:HE22 | 2:B:3637:LEU:HB3  | 1.83                     | 0.44              |
| 2:E:622:THR:HG23  | 2:E:626:LEU:HD12  | 1.99                     | 0.44              |
| 2:H:622:THR:HG23  | 2:H:626:LEU:HD12  | 1.99                     | 0.44              |
| 2:B:4837:MET:HG3  | 2:K:4820:THR:HB   | 1.98                     | 0.44              |
| 2:E:497:TYR:HB3   | 2:E:503:PHE:HB3   | 1.99                     | 0.44              |
| 2:E:3637:LEU:HD12 | 2:E:3640:LEU:HD12 | 1.99                     | 0.44              |
| 2:E:4820:THR:HB   | 2:H:4837:MET:HG3  | 1.98                     | 0.44              |
| 2:H:497:TYR:HB3   | 2:H:503:PHE:HB3   | 1.99                     | 0.44              |
| 1:J:27:THR:HB     | 1:J:100:ASP:HB3   | 1.99                     | 0.44              |
| 2:K:1257:VAL:HG12 | 2:K:1272:LEU:HD12 | 1.99                     | 0.44              |
| 2:B:35:LEU:HD13   | 2:B:49:LEU:HD13   | 1.99                     | 0.44              |
| 2:B:2462:VAL:O    | 2:B:2511:TYR:OH   | 2.34                     | 0.44              |
| 2:H:282:ILE:HB    | 2:H:291:LEU:HD21  | 2.00                     | 0.44              |
| 2:H:981:GLN:NE2   | 2:H:1053:ILE:O    | 2.48                     | 0.44              |
| 2:H:3637:LEU:HD12 | 2:H:3640:LEU:HD12 | 1.99                     | 0.44              |
| 2:B:845:CYS:SG    | 2:B:846:LEU:N     | 2.91                     | 0.44              |
| 1:D:9:PRO:HD3     | 2:E:736:HIS:HB2   | 2.00                     | 0.44              |
| 2:E:845:CYS:SG    | 2:E:846:LEU:N     | 2.91                     | 0.44              |
| 2:E:1431:THR:OG1  | 2:E:1521:ASP:OD1  | 2.29                     | 0.44              |
| 2:H:874:LEU:HD11  | 2:H:1042:ALA:HB1  | 1.99                     | 0.44              |
| 2:H:1974:GLN:HE22 | 2:H:3637:LEU:HB3  | 1.83                     | 0.44              |
| 2:K:282:ILE:HB    | 2:K:291:LEU:HD21  | 2.00                     | 0.44              |
| 2:B:978:THR:HG22  | 2:B:980:ALA:H     | 1.82                     | 0.44              |
| 2:B:2355:VAL:HG11 | 2:B:2454:ILE:HD12 | 2.00                     | 0.44              |
| 2:K:2355:VAL:HG11 | 2:K:2454:ILE:HD12 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:874:LEU:HD11  | 2:B:1042:ALA:HB1  | 1.99                     | 0.43              |
| 2:E:1974:GLN:HE22 | 2:E:3637:LEU:HB3  | 1.83                     | 0.43              |
| 2:K:845:CYS:SG    | 2:K:846:LEU:N     | 2.91                     | 0.43              |
| 2:K:874:LEU:HD11  | 2:K:1042:ALA:HB1  | 1.99                     | 0.43              |
| 2:K:4178:ILE:HD13 | 2:K:4188:ILE:HD11 | 2.00                     | 0.43              |
| 2:E:1716:ILE:O    | 2:E:1721:GLU:N    | 2.51                     | 0.43              |
| 2:H:3933:SER:OG   | 2:K:80:GLU:OE1    | 2.36                     | 0.43              |
| 2:B:282:ILE:HB    | 2:B:291:LEU:HD21  | 2.00                     | 0.43              |
| 2:B:1257:VAL:HG12 | 2:B:1272:LEU:HD12 | 1.99                     | 0.43              |
| 2:E:282:ILE:HB    | 2:E:291:LEU:HD21  | 2.00                     | 0.43              |
| 2:K:842:PRO:HG2   | 2:K:1196:PRO:HA   | 1.99                     | 0.43              |
| 2:K:497:TYR:HB3   | 2:K:503:PHE:HB3   | 1.99                     | 0.43              |
| 2:B:1716:ILE:O    | 2:B:1721:GLU:N    | 2.51                     | 0.43              |
| 2:B:4178:ILE:HD13 | 2:B:4188:ILE:HD11 | 2.00                     | 0.43              |
| 2:H:4178:ILE:HD13 | 2:H:4188:ILE:HD11 | 2.00                     | 0.43              |
| 2:K:1451:GLY:HA3  | 2:K:1494:MET:HA   | 1.99                     | 0.43              |
| 2:K:1716:ILE:O    | 2:K:1721:GLU:N    | 2.51                     | 0.43              |
| 2:B:639:ASN:OD1   | 2:B:640:TYR:N     | 2.52                     | 0.43              |
| 2:B:979:PRO:O     | 2:B:982:THR:OG1   | 2.36                     | 0.43              |
| 2:B:4234:GLU:OE2  | 2:B:5012:TYR:OH   | 2.33                     | 0.43              |
| 2:E:1110:ARG:NE   | 2:E:1112:ASP:OD2  | 2.52                     | 0.43              |
| 2:E:1236:THR:OG1  | 2:E:1608:MET:SD   | 2.67                     | 0.43              |
| 2:E:4178:ILE:HD13 | 2:E:4188:ILE:HD11 | 2.00                     | 0.43              |
| 2:H:232:THR:OG1   | 2:H:248:GLU:OE1   | 2.33                     | 0.43              |
| 2:H:1716:ILE:O    | 2:H:1721:GLU:N    | 2.51                     | 0.43              |
| 2:B:842:PRO:HG2   | 2:B:1196:PRO:HA   | 1.99                     | 0.43              |
| 2:B:1451:GLY:HA3  | 2:B:1494:MET:HA   | 1.99                     | 0.43              |
| 2:E:842:PRO:HG2   | 2:E:1196:PRO:HA   | 1.99                     | 0.43              |
| 2:H:1075:PHE:O    | 2:H:1192:CYS:N    | 2.46                     | 0.43              |
| 2:H:1451:GLY:HA3  | 2:H:1494:MET:HA   | 1.99                     | 0.43              |
| 2:E:214:VAL:HG11  | 2:E:390:LEU:HD13  | 2.01                     | 0.43              |
| 2:E:1708:ARG:NH1  | 2:E:1837:PHE:O    | 2.52                     | 0.43              |
| 2:E:2355:VAL:HG11 | 2:E:2454:ILE:HD12 | 2.00                     | 0.43              |
| 2:H:845:CYS:SG    | 2:H:846:LEU:N     | 2.91                     | 0.43              |
| 2:H:1110:ARG:NE   | 2:H:1112:ASP:OD2  | 2.52                     | 0.43              |
| 2:H:2369:LEU:H    | 2:H:2369:LEU:HD23 | 1.84                     | 0.43              |
| 2:B:214:VAL:HG11  | 2:B:390:LEU:HD13  | 2.01                     | 0.43              |
| 2:B:214:VAL:HB    | 2:B:339:ILE:HG13  | 2.01                     | 0.43              |
| 2:B:292:ALA:HB2   | 2:B:312:THR:HG22  | 1.99                     | 0.43              |
| 2:B:2369:LEU:HD23 | 2:B:2369:LEU:H    | 1.84                     | 0.43              |
| 2:E:292:ALA:HB2   | 2:E:312:THR:HG22  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:639:ASN:OD1   | 2:E:640:TYR:N     | 2.52                     | 0.43              |
| 2:E:874:LEU:HD11  | 2:E:1042:ALA:HB1  | 1.99                     | 0.43              |
| 2:E:981:GLN:NE2   | 2:E:1053:ILE:O    | 2.48                     | 0.43              |
| 2:E:1451:GLY:HA3  | 2:E:1494:MET:HA   | 1.99                     | 0.43              |
| 2:E:2239:TYR:OH   | 3:F:68:GLU:OE2    | 2.27                     | 0.43              |
| 2:K:396:GLU:OE2   | 2:K:470:SER:OG    | 2.33                     | 0.43              |
| 2:B:1286:MET:HE1  | 2:B:1464:PHE:HB3  | 2.01                     | 0.42              |
| 2:K:214:VAL:HB    | 2:K:339:ILE:HG13  | 2.01                     | 0.42              |
| 2:K:1286:MET:HE1  | 2:K:1464:PHE:HB3  | 2.01                     | 0.42              |
| 2:K:2369:LEU:HD23 | 2:K:2369:LEU:H    | 1.84                     | 0.42              |
| 2:B:894:GLY:HA3   | 2:B:903:LEU:HB3   | 2.01                     | 0.42              |
| 2:E:797:HIS:HA    | 2:E:1619:ARG:HH12 | 1.84                     | 0.42              |
| 2:E:2462:VAL:O    | 2:E:2511:TYR:OH   | 2.34                     | 0.42              |
| 1:G:9:PRO:HD3     | 2:H:736:HIS:HB2   | 2.00                     | 0.42              |
| 2:H:842:PRO:HG2   | 2:H:1196:PRO:HA   | 1.99                     | 0.42              |
| 2:H:1286:MET:HE1  | 2:H:1464:PHE:HB3  | 2.01                     | 0.42              |
| 2:H:2355:VAL:HG11 | 2:H:2454:ILE:HD12 | 2.00                     | 0.42              |
| 1:J:9:PRO:HD3     | 2:K:736:HIS:HB2   | 2.00                     | 0.42              |
| 2:K:1110:ARG:NE   | 2:K:1112:ASP:OD2  | 2.52                     | 0.42              |
| 2:B:80:GLU:OE1    | 2:K:3933:SER:OG   | 2.36                     | 0.42              |
| 2:E:2112:VAL:HG13 | 2:E:2117:LEU:HD23 | 2.01                     | 0.42              |
| 2:K:639:ASN:OD1   | 2:K:640:TYR:N     | 2.52                     | 0.42              |
| 2:K:1075:PHE:O    | 2:K:1192:CYS:N    | 2.46                     | 0.42              |
| 1:A:9:PRO:HD3     | 2:B:736:HIS:HB2   | 2.00                     | 0.42              |
| 2:B:929:LEU:HD13  | 2:B:932:LEU:HD12  | 2.02                     | 0.42              |
| 3:L:37:MET:HE2    | 3:L:37:MET:HB2    | 1.96                     | 0.42              |
| 2:E:3933:SER:OG   | 2:H:80:GLU:OE1    | 2.36                     | 0.42              |
| 2:H:797:HIS:HA    | 2:H:1619:ARG:HH12 | 1.84                     | 0.42              |
| 2:H:894:GLY:HA3   | 2:H:903:LEU:HB3   | 2.01                     | 0.42              |
| 2:H:2112:VAL:HG13 | 2:H:2117:LEU:HD23 | 2.01                     | 0.42              |
| 2:B:250:GLY:HA2   | 2:B:253:CYS:HB2   | 2.02                     | 0.42              |
| 2:B:3674:SER:OG   | 2:B:3768:ARG:NH2  | 2.53                     | 0.42              |
| 2:E:1286:MET:HE1  | 2:E:1464:PHE:HB3  | 2.01                     | 0.42              |
| 2:E:2369:LEU:HD23 | 2:E:2369:LEU:H    | 1.84                     | 0.42              |
| 2:H:103:TYR:OH    | 2:H:167:ASP:OD2   | 2.30                     | 0.42              |
| 2:B:1708:ARG:NH1  | 2:B:1837:PHE:O    | 2.52                     | 0.42              |
| 2:B:2189:ASN:OD1  | 2:B:2190:LYS:N    | 2.53                     | 0.42              |
| 2:B:3827:ILE:HG22 | 2:B:3831:MET:HE2  | 2.01                     | 0.42              |
| 2:E:214:VAL:HB    | 2:E:339:ILE:HG13  | 2.01                     | 0.42              |
| 2:E:894:GLY:HA3   | 2:E:903:LEU:HB3   | 2.01                     | 0.42              |
| 2:E:3674:SER:OG   | 2:E:3768:ARG:NH2  | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:K:2303:LEU:HD13 | 2:K:2332:TYR:HB2  | 2.02                     | 0.42              |
| 2:K:3827:ILE:HG22 | 2:K:3831:MET:HE2  | 2.01                     | 0.42              |
| 1:D:92:PRO:HG2    | 1:D:95:ALA:HB2    | 2.02                     | 0.42              |
| 2:H:639:ASN:OD1   | 2:H:640:TYR:N     | 2.52                     | 0.42              |
| 2:H:1143:TRP:CZ2  | 2:H:1149:VAL:HG21 | 2.55                     | 0.42              |
| 2:K:1478:ASP:N    | 2:K:1482:ASN:O    | 2.48                     | 0.42              |
| 2:K:2226:PHE:HB3  | 2:K:2229:MET:HG2  | 2.02                     | 0.42              |
| 2:B:1143:TRP:CZ2  | 2:B:1149:VAL:HG21 | 2.55                     | 0.42              |
| 2:B:2303:LEU:HD13 | 2:B:2332:TYR:HB2  | 2.02                     | 0.42              |
| 2:H:2462:VAL:O    | 2:H:2511:TYR:OH   | 2.34                     | 0.42              |
| 2:K:232:THR:OG1   | 2:K:248:GLU:OE1   | 2.33                     | 0.42              |
| 2:B:3933:SER:OG   | 2:E:80:GLU:OE1    | 2.36                     | 0.41              |
| 2:E:2229:MET:HE3  | 2:E:2229:MET:HB2  | 1.96                     | 0.41              |
| 2:H:214:VAL:HG11  | 2:H:390:LEU:HD13  | 2.01                     | 0.41              |
| 2:H:783:PHE:HZ    | 2:H:1615:VAL:HG22 | 1.85                     | 0.41              |
| 2:H:2226:PHE:HB3  | 2:H:2229:MET:HG2  | 2.02                     | 0.41              |
| 2:K:214:VAL:HG11  | 2:K:390:LEU:HD13  | 2.01                     | 0.41              |
| 2:K:894:GLY:HA3   | 2:K:903:LEU:HB3   | 2.01                     | 0.41              |
| 2:K:2239:TYR:OH   | 3:L:68:GLU:OE2    | 2.27                     | 0.41              |
| 2:H:214:VAL:HB    | 2:H:339:ILE:HG13  | 2.01                     | 0.41              |
| 2:H:250:GLY:HA2   | 2:H:253:CYS:HB2   | 2.02                     | 0.41              |
| 2:K:783:PHE:HZ    | 2:K:1615:VAL:HG22 | 1.85                     | 0.41              |
| 2:K:929:LEU:HD13  | 2:K:932:LEU:HD12  | 2.02                     | 0.41              |
| 2:K:2189:ASN:OD1  | 2:K:2190:LYS:N    | 2.53                     | 0.41              |
| 2:B:797:HIS:HA    | 2:B:1619:ARG:HH12 | 1.84                     | 0.41              |
| 2:E:250:GLY:HA2   | 2:E:253:CYS:HB2   | 2.02                     | 0.41              |
| 2:E:929:LEU:HD13  | 2:E:932:LEU:HD12  | 2.02                     | 0.41              |
| 2:E:1143:TRP:CZ2  | 2:E:1149:VAL:HG21 | 2.55                     | 0.41              |
| 2:K:250:GLY:HA2   | 2:K:253:CYS:HB2   | 2.02                     | 0.41              |
| 2:B:720:HIS:HB3   | 2:B:729:LEU:HA    | 2.02                     | 0.41              |
| 2:B:1074:ILE:HG23 | 2:B:1115:LEU:HD11 | 2.02                     | 0.41              |
| 2:B:2229:MET:HE3  | 2:B:2229:MET:HB2  | 1.96                     | 0.41              |
| 2:B:2365:PHE:HD1  | 2:B:2430:LEU:HD21 | 1.85                     | 0.41              |
| 2:B:3981:TRP:HB3  | 2:B:4042:MET:HG3  | 2.03                     | 0.41              |
| 2:E:2365:PHE:HD1  | 2:E:2430:LEU:HD21 | 1.85                     | 0.41              |
| 2:H:783:PHE:HB2   | 2:H:787:VAL:HB    | 2.02                     | 0.41              |
| 2:H:3674:SER:OG   | 2:H:3768:ARG:NH2  | 2.53                     | 0.41              |
| 2:K:1074:ILE:HG23 | 2:K:1115:LEU:HD11 | 2.02                     | 0.41              |
| 2:K:1143:TRP:CZ2  | 2:K:1149:VAL:HG21 | 2.55                     | 0.41              |
| 2:K:1708:ARG:NH1  | 2:K:1837:PHE:O    | 2.52                     | 0.41              |
| 2:K:2467:LEU:HD21 | 2:K:2506:PHE:HD2  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2112:VAL:HG13 | 2:B:2117:LEU:HD23 | 2.01                     | 0.41              |
| 1:D:38:SER:OG     | 1:D:41:ASP:OD2    | 2.38                     | 0.41              |
| 2:E:39:ALA:HB1    | 2:E:137:LEU:HD11  | 2.02                     | 0.41              |
| 2:E:1100:MET:HB2  | 2:E:1143:TRP:CZ3  | 2.56                     | 0.41              |
| 2:E:2189:ASN:OD1  | 2:E:2190:LYS:N    | 2.53                     | 0.41              |
| 2:E:4677:ARG:HE   | 2:E:5015:ARG:CZ   | 2.33                     | 0.41              |
| 2:H:21:VAL:HB     | 2:H:205:ILE:HD11  | 2.03                     | 0.41              |
| 2:H:39:ALA:HB1    | 2:H:137:LEU:HD11  | 2.02                     | 0.41              |
| 2:H:929:LEU:HD13  | 2:H:932:LEU:HD12  | 2.02                     | 0.41              |
| 2:H:1100:MET:HB2  | 2:H:1143:TRP:CZ3  | 2.56                     | 0.41              |
| 2:H:1708:ARG:NH1  | 2:H:1837:PHE:O    | 2.52                     | 0.41              |
| 2:H:4998:GLU:HA   | 2:H:5001:HIS:CE1  | 2.56                     | 0.41              |
| 1:J:38:SER:OG     | 1:J:41:ASP:OD2    | 2.38                     | 0.41              |
| 1:J:42:ARG:HD2    | 1:J:44:LYS:HE2    | 2.02                     | 0.41              |
| 2:K:2112:VAL:HG13 | 2:K:2117:LEU:HD23 | 2.01                     | 0.41              |
| 2:K:4677:ARG:HE   | 2:K:5015:ARG:CZ   | 2.33                     | 0.41              |
| 2:B:606:LEU:HD23  | 2:B:621:ILE:HD11  | 2.03                     | 0.41              |
| 2:B:4574:ILE:HG21 | 2:B:4641:LEU:HB2  | 2.03                     | 0.41              |
| 2:B:4677:ARG:HE   | 2:B:5015:ARG:CZ   | 2.33                     | 0.41              |
| 1:D:56:ILE:HG23   | 1:D:59:PHE:H      | 1.86                     | 0.41              |
| 2:E:1074:ILE:HG23 | 2:E:1115:LEU:HD11 | 2.02                     | 0.41              |
| 2:E:3725:MET:HE3  | 2:E:3765:LEU:HD22 | 2.02                     | 0.41              |
| 2:H:2189:ASN:OD1  | 2:H:2190:LYS:N    | 2.53                     | 0.41              |
| 2:K:3674:SER:OG   | 2:K:3768:ARG:NH2  | 2.53                     | 0.41              |
| 2:B:39:ALA:HB1    | 2:B:137:LEU:HD11  | 2.02                     | 0.41              |
| 2:B:596:ASN:HB3   | 2:B:599:VAL:HG23  | 2.02                     | 0.41              |
| 2:B:3725:MET:HE3  | 2:B:3765:LEU:HD22 | 2.02                     | 0.41              |
| 2:E:1252:HIS:HB3  | 2:E:1255:TYR:O    | 2.21                     | 0.41              |
| 2:E:4928:ALA:O    | 2:E:4932:GLY:N    | 2.52                     | 0.41              |
| 1:G:37:ASP:OD2    | 2:H:1783:PHE:HB2  | 2.21                     | 0.41              |
| 2:H:596:ASN:HB3   | 2:H:599:VAL:HG23  | 2.02                     | 0.41              |
| 2:H:606:LEU:HD23  | 2:H:621:ILE:HD11  | 2.03                     | 0.41              |
| 2:H:3827:ILE:HG22 | 2:H:3831:MET:HE2  | 2.01                     | 0.41              |
| 2:H:4575:LEU:HD11 | 2:H:4805:PHE:HA   | 2.03                     | 0.41              |
| 1:J:92:PRO:HG2    | 1:J:95:ALA:HB2    | 2.02                     | 0.41              |
| 2:K:606:LEU:HD23  | 2:K:621:ILE:HD11  | 2.03                     | 0.41              |
| 2:K:797:HIS:HA    | 2:K:1619:ARG:HH12 | 1.84                     | 0.41              |
| 2:K:4998:GLU:HA   | 2:K:5001:HIS:CE1  | 2.56                     | 0.41              |
| 1:D:42:ARG:HD2    | 1:D:44:LYS:HE2    | 2.02                     | 0.41              |
| 1:G:56:ILE:HG23   | 1:G:59:PHE:H      | 1.86                     | 0.41              |
| 1:G:92:PRO:HG2    | 1:G:95:ALA:HB2    | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:K:783:PHE:HB2   | 2:K:787:VAL:HB    | 2.02                     | 0.41              |
| 2:K:1236:THR:OG1  | 2:K:1608:MET:SD   | 2.67                     | 0.41              |
| 2:K:2560:LEU:HD23 | 2:K:2603:VAL:HG12 | 2.03                     | 0.41              |
| 2:K:4574:ILE:HG21 | 2:K:4641:LEU:HB2  | 2.03                     | 0.41              |
| 2:E:783:PHE:HZ    | 2:E:1615:VAL:HG22 | 1.85                     | 0.41              |
| 2:E:3961:THR:HG22 | 2:E:4021:MET:HA   | 2.03                     | 0.41              |
| 2:E:4998:GLU:HA   | 2:E:5001:HIS:CE1  | 2.56                     | 0.41              |
| 2:H:396:GLU:OE2   | 2:H:470:SER:OG    | 2.33                     | 0.41              |
| 2:H:1074:ILE:HG23 | 2:H:1115:LEU:HD11 | 2.02                     | 0.41              |
| 2:H:2560:LEU:HD23 | 2:H:2603:VAL:HG12 | 2.03                     | 0.41              |
| 2:K:21:VAL:HB     | 2:K:205:ILE:HD11  | 2.03                     | 0.41              |
| 2:K:720:HIS:HB3   | 2:K:729:LEU:HA    | 2.02                     | 0.41              |
| 2:K:2365:PHE:HD1  | 2:K:2430:LEU:HD21 | 1.85                     | 0.41              |
| 2:B:179:TYR:N     | 2:B:194:SER:O     | 2.54                     | 0.41              |
| 2:B:613:ALA:HB2   | 2:B:1676:LEU:HD12 | 2.03                     | 0.41              |
| 2:E:730:VAL:HA    | 2:E:1476:MET:HE1  | 2.03                     | 0.41              |
| 2:E:3827:ILE:HG22 | 2:E:3831:MET:HE2  | 2.01                     | 0.41              |
| 2:H:1988:THR:HG22 | 2:H:1990:ALA:H    | 1.86                     | 0.41              |
| 2:H:3961:THR:HG22 | 2:H:4021:MET:HA   | 2.03                     | 0.41              |
| 2:K:578:ILE:HG13  | 2:K:606:LEU:HD11  | 2.03                     | 0.41              |
| 1:A:38:SER:OG     | 1:A:41:ASP:OD2    | 2.38                     | 0.40              |
| 1:A:92:PRO:HG2    | 1:A:95:ALA:HB2    | 2.02                     | 0.40              |
| 2:B:1110:ARG:NE   | 2:B:1112:ASP:OD2  | 2.52                     | 0.40              |
| 2:B:4152:ASP:HB3  | 2:B:4155:LEU:HB3  | 2.03                     | 0.40              |
| 2:B:4966:PHE:HE1  | 2:B:5027:ARG:HD2  | 1.87                     | 0.40              |
| 2:B:4998:GLU:HA   | 2:B:5001:HIS:CE1  | 2.56                     | 0.40              |
| 2:E:606:LEU:HD23  | 2:E:621:ILE:HD11  | 2.03                     | 0.40              |
| 2:E:720:HIS:HB3   | 2:E:729:LEU:HA    | 2.02                     | 0.40              |
| 2:E:979:PRO:O     | 2:E:982:THR:OG1   | 2.36                     | 0.40              |
| 2:E:1288:PHE:HD2  | 2:E:1600:LEU:HD13 | 1.86                     | 0.40              |
| 2:E:4575:LEU:HD11 | 2:E:4805:PHE:HA   | 2.03                     | 0.40              |
| 2:H:179:TYR:N     | 2:H:194:SER:O     | 2.54                     | 0.40              |
| 2:H:730:VAL:HA    | 2:H:1476:MET:HE1  | 2.03                     | 0.40              |
| 2:H:2365:PHE:HD1  | 2:H:2430:LEU:HD21 | 1.85                     | 0.40              |
| 2:H:4574:ILE:HG21 | 2:H:4641:LEU:HB2  | 2.03                     | 0.40              |
| 2:K:1100:MET:HB2  | 2:K:1143:TRP:CZ3  | 2.56                     | 0.40              |
| 2:K:1252:HIS:HB3  | 2:K:1255:TYR:O    | 2.21                     | 0.40              |
| 2:K:1288:PHE:HD2  | 2:K:1600:LEU:HD13 | 1.86                     | 0.40              |
| 2:K:3961:THR:HG22 | 2:K:4021:MET:HA   | 2.03                     | 0.40              |
| 2:E:179:TYR:N     | 2:E:194:SER:O     | 2.54                     | 0.40              |
| 2:E:613:ALA:HB2   | 2:E:1676:LEU:HD12 | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4630:LEU:H    | 2:E:4630:LEU:HD23 | 1.86                     | 0.40              |
| 2:H:1130:GLN:HA   | 2:H:1139:PHE:H    | 1.87                     | 0.40              |
| 2:H:1439:VAL:HG21 | 2:H:1448:VAL:HG11 | 2.04                     | 0.40              |
| 2:K:20:VAL:HG12   | 2:K:204:PRO:HA    | 2.03                     | 0.40              |
| 2:K:730:VAL:HA    | 2:K:1476:MET:HE1  | 2.03                     | 0.40              |
| 2:K:4630:LEU:HD23 | 2:K:4630:LEU:H    | 1.86                     | 0.40              |
| 1:A:42:ARG:HD2    | 1:A:44:LYS:HE2    | 2.02                     | 0.40              |
| 2:B:578:ILE:HG13  | 2:B:606:LEU:HD11  | 2.03                     | 0.40              |
| 2:B:783:PHE:HZ    | 2:B:1615:VAL:HG22 | 1.85                     | 0.40              |
| 2:B:1988:THR:HG22 | 2:B:1990:ALA:H    | 1.86                     | 0.40              |
| 2:B:3961:THR:HG22 | 2:B:4021:MET:HA   | 2.03                     | 0.40              |
| 1:D:37:ASP:OD2    | 2:E:1783:PHE:HB2  | 2.21                     | 0.40              |
| 2:E:21:VAL:HB     | 2:E:205:ILE:HD11  | 2.03                     | 0.40              |
| 2:E:578:ILE:HG13  | 2:E:606:LEU:HD11  | 2.03                     | 0.40              |
| 2:E:596:ASN:HB3   | 2:E:599:VAL:HG23  | 2.02                     | 0.40              |
| 2:E:2226:PHE:HB3  | 2:E:2229:MET:HG2  | 2.02                     | 0.40              |
| 2:H:578:ILE:HG13  | 2:H:606:LEU:HD11  | 2.03                     | 0.40              |
| 2:H:720:HIS:HB3   | 2:H:729:LEU:HA    | 2.02                     | 0.40              |
| 2:H:1288:PHE:HD2  | 2:H:1600:LEU:HD13 | 1.86                     | 0.40              |
| 2:H:2303:LEU:HD13 | 2:H:2332:TYR:HB2  | 2.02                     | 0.40              |
| 2:H:2467:LEU:HD21 | 2:H:2506:PHE:HD2  | 1.86                     | 0.40              |
| 2:H:4677:ARG:HE   | 2:H:5015:ARG:CZ   | 2.33                     | 0.40              |
| 2:B:664:PHE:CZ    | 2:B:779:PRO:HB3   | 2.57                     | 0.40              |
| 2:B:730:VAL:HA    | 2:B:1476:MET:HE1  | 2.03                     | 0.40              |
| 2:B:1100:MET:HB2  | 2:B:1143:TRP:CZ3  | 2.56                     | 0.40              |
| 2:B:1288:PHE:HD2  | 2:B:1600:LEU:HD13 | 1.86                     | 0.40              |
| 2:B:2467:LEU:HD21 | 2:B:2506:PHE:HD2  | 1.86                     | 0.40              |
| 2:E:1435:TYR:O    | 2:E:1518:CYS:N    | 2.55                     | 0.40              |
| 2:E:4152:ASP:HB3  | 2:E:4155:LEU:HB3  | 2.03                     | 0.40              |
| 2:E:4234:GLU:OE2  | 2:E:5012:TYR:OH   | 2.33                     | 0.40              |
| 2:H:1252:HIS:HB3  | 2:H:1255:TYR:O    | 2.21                     | 0.40              |
| 2:K:39:ALA:HB1    | 2:K:137:LEU:HD11  | 2.02                     | 0.40              |
| 2:K:291:LEU:HB3   | 2:K:301:VAL:HG12  | 2.04                     | 0.40              |
| 2:B:4630:LEU:H    | 2:B:4630:LEU:HD23 | 1.86                     | 0.40              |
| 2:E:396:GLU:OE2   | 2:E:470:SER:OG    | 2.33                     | 0.40              |
| 2:E:886:ARG:HB3   | 2:E:891:TRP:HB2   | 2.04                     | 0.40              |
| 2:E:2303:LEU:HD13 | 2:E:2332:TYR:HB2  | 2.02                     | 0.40              |
| 1:G:38:SER:OG     | 1:G:41:ASP:OD2    | 2.38                     | 0.40              |
| 1:G:42:ARG:HD2    | 1:G:44:LYS:HE2    | 2.02                     | 0.40              |
| 2:H:3992:ALA:HB1  | 2:H:4052:MET:HE3  | 2.03                     | 0.40              |
| 2:K:613:ALA:HB2   | 2:K:1676:LEU:HD12 | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:3981:TRP:HB3 | 2:K:4042:MET:HG3 | 2.03                     | 0.40              |

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 PDB entries followed by that with respect to all EM entries.

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     | 104/110 (94%)     | 102 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | D     | 104/110 (94%)     | 102 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | G     | 104/110 (94%)     | 102 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 1   | J     | 104/110 (94%)     | 102 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 2   | B     | 3382/3800 (89%)   | 3336 (99%)  | 46 (1%)  | 0        | 100         | 100 |
| 2   | E     | 3382/3800 (89%)   | 3336 (99%)  | 46 (1%)  | 0        | 100         | 100 |
| 2   | H     | 3382/3800 (89%)   | 3336 (99%)  | 46 (1%)  | 0        | 100         | 100 |
| 2   | K     | 3382/3800 (89%)   | 3336 (99%)  | 46 (1%)  | 0        | 100         | 100 |
| 3   | C     | 129/146 (88%)     | 127 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 3   | F     | 129/146 (88%)     | 127 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 3   | I     | 129/146 (88%)     | 127 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 3   | L     | 129/146 (88%)     | 127 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| All | All   | 14460/16224 (89%) | 14260 (99%) | 200 (1%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM

entries.

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     | 71/90 (79%)      | 71 (100%)   | 0        | 100         | 100 |
| 1   | D     | 71/90 (79%)      | 71 (100%)   | 0        | 100         | 100 |
| 1   | G     | 71/90 (79%)      | 71 (100%)   | 0        | 100         | 100 |
| 1   | J     | 71/90 (79%)      | 71 (100%)   | 0        | 100         | 100 |
| 2   | B     | 2373/3010 (79%)  | 2373 (100%) | 0        | 100         | 100 |
| 2   | E     | 2373/3010 (79%)  | 2373 (100%) | 0        | 100         | 100 |
| 2   | H     | 2373/3010 (79%)  | 2373 (100%) | 0        | 100         | 100 |
| 2   | K     | 2373/3010 (79%)  | 2373 (100%) | 0        | 100         | 100 |
| 3   | C     | 44/125 (35%)     | 44 (100%)   | 0        | 100         | 100 |
| 3   | F     | 44/125 (35%)     | 44 (100%)   | 0        | 100         | 100 |
| 3   | I     | 44/125 (35%)     | 44 (100%)   | 0        | 100         | 100 |
| 3   | L     | 44/125 (35%)     | 44 (100%)   | 0        | 100         | 100 |
| All | All   | 9952/12900 (77%) | 9952 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 25   | HIS  |
| 1   | A     | 94   | ASN  |
| 2   | B     | 297  | GLN  |
| 2   | B     | 720  | HIS  |
| 2   | B     | 1443 | GLN  |
| 2   | B     | 1559 | GLN  |
| 2   | B     | 1693 | GLN  |
| 2   | B     | 2126 | HIS  |
| 2   | B     | 2170 | GLN  |
| 2   | B     | 2248 | GLN  |
| 2   | B     | 2352 | ASN  |
| 2   | B     | 2418 | HIS  |
| 2   | B     | 3429 | ASN  |
| 2   | B     | 3700 | HIS  |
| 2   | B     | 3955 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 4196 | ASN  |
| 2   | B     | 4199 | GLN  |
| 2   | B     | 4801 | HIS  |
| 2   | B     | 4945 | GLN  |
| 3   | C     | 50   | GLN  |
| 1   | D     | 25   | HIS  |
| 1   | D     | 94   | ASN  |
| 2   | E     | 297  | GLN  |
| 2   | E     | 720  | HIS  |
| 2   | E     | 921  | ASN  |
| 2   | E     | 1443 | GLN  |
| 2   | E     | 1559 | GLN  |
| 2   | E     | 2126 | HIS  |
| 2   | E     | 2170 | GLN  |
| 2   | E     | 2248 | GLN  |
| 2   | E     | 2352 | ASN  |
| 2   | E     | 2418 | HIS  |
| 2   | E     | 3429 | ASN  |
| 2   | E     | 3700 | HIS  |
| 2   | E     | 3955 | GLN  |
| 2   | E     | 4032 | ASN  |
| 2   | E     | 4196 | ASN  |
| 2   | E     | 4199 | GLN  |
| 2   | E     | 4801 | HIS  |
| 2   | E     | 4945 | GLN  |
| 3   | F     | 50   | GLN  |
| 1   | G     | 25   | HIS  |
| 1   | G     | 94   | ASN  |
| 2   | H     | 297  | GLN  |
| 2   | H     | 720  | HIS  |
| 2   | H     | 1443 | GLN  |
| 2   | H     | 1559 | GLN  |
| 2   | H     | 2126 | HIS  |
| 2   | H     | 2170 | GLN  |
| 2   | H     | 2248 | GLN  |
| 2   | H     | 2352 | ASN  |
| 2   | H     | 2418 | HIS  |
| 2   | H     | 3429 | ASN  |
| 2   | H     | 3700 | HIS  |
| 2   | H     | 3955 | GLN  |
| 2   | H     | 4196 | ASN  |
| 2   | H     | 4199 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | H     | 4801 | HIS  |
| 2   | H     | 4945 | GLN  |
| 3   | I     | 50   | GLN  |
| 1   | J     | 25   | HIS  |
| 1   | J     | 94   | ASN  |
| 2   | K     | 297  | GLN  |
| 2   | K     | 720  | HIS  |
| 2   | K     | 921  | ASN  |
| 2   | K     | 1443 | GLN  |
| 2   | K     | 1559 | GLN  |
| 2   | K     | 2126 | HIS  |
| 2   | K     | 2170 | GLN  |
| 2   | K     | 2248 | GLN  |
| 2   | K     | 2352 | ASN  |
| 2   | K     | 2418 | HIS  |
| 2   | K     | 3429 | ASN  |
| 2   | K     | 3700 | HIS  |
| 2   | K     | 3955 | GLN  |
| 2   | K     | 4196 | ASN  |
| 2   | K     | 4199 | GLN  |
| 2   | K     | 4801 | HIS  |
| 2   | K     | 4945 | GLN  |
| 3   | L     | 50   | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | B     | 57               |
| 2   | E     | 57               |
| 2   | H     | 57               |
| 2   | K     | 57               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 4333:UNK  | C      | 4543:GLU  | N      | 53.56        |
| 1     | E     | 4333:UNK  | C      | 4543:GLU  | N      | 53.56        |
| 1     | H     | 4333:UNK  | C      | 4543:GLU  | N      | 53.56        |
| 1     | K     | 4333:UNK  | C      | 4543:GLU  | N      | 53.56        |
| 1     | B     | 1054:GLU  | C      | 1071:ARG  | N      | 36.15        |
| 1     | E     | 1054:GLU  | C      | 1071:ARG  | N      | 36.15        |
| 1     | H     | 1054:GLU  | C      | 1071:ARG  | N      | 36.15        |
| 1     | K     | 1054:GLU  | C      | 1071:ARG  | N      | 36.15        |
| 1     | B     | 3606:UNK  | C      | 3625:ARG  | N      | 35.35        |
| 1     | E     | 3606:UNK  | C      | 3625:ARG  | N      | 35.35        |
| 1     | H     | 3606:UNK  | C      | 3625:ARG  | N      | 35.35        |
| 1     | K     | 3606:UNK  | C      | 3625:ARG  | N      | 35.35        |
| 1     | B     | 2939:ARG  | C      | 2956:UNK  | N      | 28.67        |
| 1     | E     | 2939:ARG  | C      | 2956:UNK  | N      | 28.67        |
| 1     | H     | 2939:ARG  | C      | 2956:UNK  | N      | 28.67        |
| 1     | K     | 2939:ARG  | C      | 2956:UNK  | N      | 28.67        |
| 1     | B     | 3385:UNK  | C      | 3411:PRO  | N      | 25.81        |
| 1     | E     | 3385:UNK  | C      | 3411:PRO  | N      | 25.81        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | H     | 3385:UNK  | C      | 3411:PRO  | N      | 25.81        |
| 1     | K     | 3385:UNK  | C      | 3411:PRO  | N      | 25.81        |
| 1     | B     | 4246:ILE  | C      | 4317:UNK  | N      | 25.72        |
| 1     | E     | 4246:ILE  | C      | 4317:UNK  | N      | 25.72        |
| 1     | H     | 4246:ILE  | C      | 4317:UNK  | N      | 25.72        |
| 1     | K     | 4246:ILE  | C      | 4317:UNK  | N      | 25.72        |
| 1     | B     | 3555:UNK  | C      | 3564:UNK  | N      | 24.65        |
| 1     | E     | 3555:UNK  | C      | 3564:UNK  | N      | 24.65        |
| 1     | H     | 3555:UNK  | C      | 3564:UNK  | N      | 24.65        |
| 1     | K     | 3555:UNK  | C      | 3564:UNK  | N      | 24.65        |
| 1     | B     | 2830:GLU  | C      | 2855:TYR  | N      | 23.94        |
| 1     | E     | 2830:GLU  | C      | 2855:TYR  | N      | 23.94        |
| 1     | H     | 2830:GLU  | C      | 2855:TYR  | N      | 23.94        |
| 1     | K     | 2830:GLU  | C      | 2855:TYR  | N      | 23.94        |
| 1     | B     | 855:PRO   | C      | 863:LEU   | N      | 22.50        |
| 1     | E     | 855:PRO   | C      | 863:LEU   | N      | 22.50        |
| 1     | H     | 855:PRO   | C      | 863:LEU   | N      | 22.50        |
| 1     | K     | 855:PRO   | C      | 863:LEU   | N      | 22.50        |
| 1     | B     | 1299:GLN  | C      | 1428:LEU  | N      | 21.48        |
| 1     | E     | 1299:GLN  | C      | 1428:LEU  | N      | 21.48        |
| 1     | H     | 1299:GLN  | C      | 1428:LEU  | N      | 21.48        |
| 1     | K     | 1299:GLN  | C      | 1428:LEU  | N      | 21.48        |
| 1     | B     | 4737:GLU  | C      | 4769:ILE  | N      | 20.98        |
| 1     | E     | 4737:GLU  | C      | 4769:ILE  | N      | 20.98        |
| 1     | H     | 4737:GLU  | C      | 4769:ILE  | N      | 20.98        |
| 1     | K     | 4737:GLU  | C      | 4769:ILE  | N      | 20.98        |
| 1     | B     | 3574:UNK  | C      | 3588:UNK  | N      | 20.52        |
| 1     | E     | 3574:UNK  | C      | 3588:UNK  | N      | 20.52        |
| 1     | H     | 3574:UNK  | C      | 3588:UNK  | N      | 20.52        |
| 1     | K     | 3574:UNK  | C      | 3588:UNK  | N      | 20.52        |
| 1     | B     | 2473:LEU  | C      | 2489:PRO  | N      | 19.14        |
| 1     | E     | 2473:LEU  | C      | 2489:PRO  | N      | 19.14        |
| 1     | H     | 2473:LEU  | C      | 2489:PRO  | N      | 19.14        |
| 1     | K     | 2473:LEU  | C      | 2489:PRO  | N      | 19.14        |
| 1     | B     | 2978:UNK  | C      | 2999:UNK  | N      | 18.10        |
| 1     | E     | 2978:UNK  | C      | 2999:UNK  | N      | 18.10        |
| 1     | H     | 2978:UNK  | C      | 2999:UNK  | N      | 18.10        |
| 1     | K     | 2978:UNK  | C      | 2999:UNK  | N      | 18.10        |
| 1     | B     | 2046:GLN  | C      | 2092:LEU  | N      | 17.97        |
| 1     | E     | 2046:GLN  | C      | 2092:LEU  | N      | 17.97        |
| 1     | H     | 2046:GLN  | C      | 2092:LEU  | N      | 17.97        |
| 1     | K     | 2046:GLN  | C      | 2092:LEU  | N      | 17.97        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 3358:UNK  | C      | 3365:UNK  | N      | 17.93        |
| 1     | E     | 3358:UNK  | C      | 3365:UNK  | N      | 17.93        |
| 1     | H     | 3358:UNK  | C      | 3365:UNK  | N      | 17.93        |
| 1     | K     | 3358:UNK  | C      | 3365:UNK  | N      | 17.93        |
| 1     | B     | 3731:LEU  | C      | 3747:SER  | N      | 17.86        |
| 1     | E     | 3731:LEU  | C      | 3747:SER  | N      | 17.86        |
| 1     | H     | 3731:LEU  | C      | 3747:SER  | N      | 17.86        |
| 1     | K     | 3731:LEU  | C      | 3747:SER  | N      | 17.86        |
| 1     | B     | 3193:UNK  | C      | 3202:UNK  | N      | 17.75        |
| 1     | E     | 3193:UNK  | C      | 3202:UNK  | N      | 17.75        |
| 1     | H     | 3193:UNK  | C      | 3202:UNK  | N      | 17.75        |
| 1     | K     | 3193:UNK  | C      | 3202:UNK  | N      | 17.75        |
| 1     | B     | 2650:UNK  | C      | 2664:UNK  | N      | 17.57        |
| 1     | E     | 2650:UNK  | C      | 2664:UNK  | N      | 17.57        |
| 1     | H     | 2650:UNK  | C      | 2664:UNK  | N      | 17.57        |
| 1     | K     | 2650:UNK  | C      | 2664:UNK  | N      | 17.57        |
| 1     | B     | 3238:UNK  | C      | 3278:UNK  | N      | 17.45        |
| 1     | E     | 3238:UNK  | C      | 3278:UNK  | N      | 17.45        |
| 1     | H     | 3238:UNK  | C      | 3278:UNK  | N      | 17.45        |
| 1     | K     | 3238:UNK  | C      | 3278:UNK  | N      | 17.45        |
| 1     | B     | 88:ALA    | C      | 97:GLY    | N      | 16.98        |
| 1     | E     | 88:ALA    | C      | 97:GLY    | N      | 16.98        |
| 1     | H     | 88:ALA    | C      | 97:GLY    | N      | 16.98        |
| 1     | K     | 88:ALA    | C      | 97:GLY    | N      | 16.98        |
| 1     | B     | 3062:UNK  | C      | 3146:UNK  | N      | 15.60        |
| 1     | E     | 3062:UNK  | C      | 3146:UNK  | N      | 15.60        |
| 1     | H     | 3062:UNK  | C      | 3146:UNK  | N      | 15.60        |
| 1     | K     | 3062:UNK  | C      | 3146:UNK  | N      | 15.60        |
| 1     | B     | 3166:UNK  | C      | 3173:UNK  | N      | 15.53        |
| 1     | E     | 3166:UNK  | C      | 3173:UNK  | N      | 15.53        |
| 1     | H     | 3166:UNK  | C      | 3173:UNK  | N      | 15.53        |
| 1     | K     | 3166:UNK  | C      | 3173:UNK  | N      | 15.53        |
| 1     | B     | 3448:LYS  | C      | 3509:UNK  | N      | 14.65        |
| 1     | E     | 3448:LYS  | C      | 3509:UNK  | N      | 14.65        |
| 1     | H     | 3448:LYS  | C      | 3509:UNK  | N      | 14.65        |
| 1     | K     | 3448:LYS  | C      | 3509:UNK  | N      | 14.65        |
| 1     | B     | 3018:UNK  | C      | 3032:UNK  | N      | 14.33        |
| 1     | E     | 3018:UNK  | C      | 3032:UNK  | N      | 14.33        |
| 1     | H     | 3018:UNK  | C      | 3032:UNK  | N      | 14.33        |
| 1     | K     | 3018:UNK  | C      | 3032:UNK  | N      | 14.33        |
| 1     | B     | 3544:UNK  | C      | 3548:UNK  | N      | 13.83        |
| 1     | E     | 3544:UNK  | C      | 3548:UNK  | N      | 13.83        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | H     | 3544:UNK  | C      | 3548:UNK  | N      | 13.83        |
| 1     | K     | 3544:UNK  | C      | 3548:UNK  | N      | 13.83        |
| 1     | B     | 3860:VAL  | C      | 3867:GLU  | N      | 13.48        |
| 1     | E     | 3860:VAL  | C      | 3867:GLU  | N      | 13.48        |
| 1     | H     | 3860:VAL  | C      | 3867:GLU  | N      | 13.48        |
| 1     | K     | 3860:VAL  | C      | 3867:GLU  | N      | 13.48        |
| 1     | B     | 1871:VAL  | C      | 1924:GLU  | N      | 13.08        |
| 1     | E     | 1871:VAL  | C      | 1924:GLU  | N      | 13.08        |
| 1     | H     | 1871:VAL  | C      | 1924:GLU  | N      | 13.08        |
| 1     | K     | 1871:VAL  | C      | 1924:GLU  | N      | 13.08        |
| 1     | B     | 361:ALA   | C      | 372:LEU   | N      | 12.94        |
| 1     | E     | 361:ALA   | C      | 372:LEU   | N      | 12.94        |
| 1     | H     | 361:ALA   | C      | 372:LEU   | N      | 12.94        |
| 1     | K     | 361:ALA   | C      | 372:LEU   | N      | 12.94        |
| 1     | B     | 3047:UNK  | C      | 3052:UNK  | N      | 12.92        |
| 1     | E     | 3047:UNK  | C      | 3052:UNK  | N      | 12.92        |
| 1     | H     | 3047:UNK  | C      | 3052:UNK  | N      | 12.92        |
| 1     | K     | 3047:UNK  | C      | 3052:UNK  | N      | 12.92        |
| 1     | B     | 323:LEU   | C      | 328:LYS   | N      | 12.78        |
| 1     | E     | 323:LEU   | C      | 328:LYS   | N      | 12.78        |
| 1     | H     | 323:LEU   | C      | 328:LYS   | N      | 12.78        |
| 1     | K     | 323:LEU   | C      | 328:LYS   | N      | 12.78        |
| 1     | B     | 2389:GLU  | C      | 2418:HIS  | N      | 12.70        |
| 1     | E     | 2389:GLU  | C      | 2418:HIS  | N      | 12.70        |
| 1     | H     | 2389:GLU  | C      | 2418:HIS  | N      | 12.70        |
| 1     | K     | 2389:GLU  | C      | 2418:HIS  | N      | 12.70        |
| 1     | B     | 2310:SER  | C      | 2319:TYR  | N      | 12.60        |
| 1     | E     | 2310:SER  | C      | 2319:TYR  | N      | 12.60        |
| 1     | H     | 2310:SER  | C      | 2319:TYR  | N      | 12.60        |
| 1     | K     | 2310:SER  | C      | 2319:TYR  | N      | 12.60        |
| 1     | B     | 3308:UNK  | C      | 3320:UNK  | N      | 12.55        |
| 1     | E     | 3308:UNK  | C      | 3320:UNK  | N      | 12.55        |
| 1     | H     | 3308:UNK  | C      | 3320:UNK  | N      | 12.55        |
| 1     | K     | 3308:UNK  | C      | 3320:UNK  | N      | 12.55        |
| 1     | B     | 4585:PRO  | C      | 4626:VAL  | N      | 12.41        |
| 1     | E     | 4585:PRO  | C      | 4626:VAL  | N      | 12.41        |
| 1     | H     | 4585:PRO  | C      | 4626:VAL  | N      | 12.41        |
| 1     | K     | 4585:PRO  | C      | 4626:VAL  | N      | 12.41        |
| 1     | B     | 3217:UNK  | C      | 3225:UNK  | N      | 12.05        |
| 1     | E     | 3217:UNK  | C      | 3225:UNK  | N      | 12.05        |
| 1     | H     | 3217:UNK  | C      | 3225:UNK  | N      | 12.05        |
| 1     | K     | 3217:UNK  | C      | 3225:UNK  | N      | 12.05        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 3525:UNK  | C      | 3534:UNK  | N      | 12.04        |
| 1     | E     | 3525:UNK  | C      | 3534:UNK  | N      | 12.04        |
| 1     | H     | 3525:UNK  | C      | 3534:UNK  | N      | 12.04        |
| 1     | K     | 3525:UNK  | C      | 3534:UNK  | N      | 12.04        |
| 1     | B     | 4090:LYS  | C      | 4109:UNK  | N      | 11.97        |
| 1     | E     | 4090:LYS  | C      | 4109:UNK  | N      | 11.97        |
| 1     | H     | 4090:LYS  | C      | 4109:UNK  | N      | 11.97        |
| 1     | K     | 4090:LYS  | C      | 4109:UNK  | N      | 11.97        |
| 1     | B     | 1750:PRO  | C      | 1759:ARG  | N      | 11.44        |
| 1     | E     | 1750:PRO  | C      | 1759:ARG  | N      | 11.44        |
| 1     | H     | 1750:PRO  | C      | 1759:ARG  | N      | 11.44        |
| 1     | K     | 1750:PRO  | C      | 1759:ARG  | N      | 11.44        |
| 1     | B     | 2014:LYS  | C      | 2023:PRO  | N      | 11.36        |
| 1     | E     | 2014:LYS  | C      | 2023:PRO  | N      | 11.36        |
| 1     | H     | 2014:LYS  | C      | 2023:PRO  | N      | 11.36        |
| 1     | K     | 2014:LYS  | C      | 2023:PRO  | N      | 11.36        |
| 1     | B     | 1501:VAL  | C      | 1510:SER  | N      | 11.31        |
| 1     | E     | 1501:VAL  | C      | 1510:SER  | N      | 11.31        |
| 1     | H     | 1501:VAL  | C      | 1510:SER  | N      | 11.31        |
| 1     | K     | 1501:VAL  | C      | 1510:SER  | N      | 11.31        |
| 1     | B     | 1788:PRO  | C      | 1794:GLU  | N      | 11.03        |
| 1     | E     | 1788:PRO  | C      | 1794:GLU  | N      | 11.03        |
| 1     | H     | 1788:PRO  | C      | 1794:GLU  | N      | 11.03        |
| 1     | K     | 1788:PRO  | C      | 1794:GLU  | N      | 11.03        |
| 1     | B     | 4114:UNK  | C      | 4122:GLU  | N      | 10.80        |
| 1     | E     | 4114:UNK  | C      | 4122:GLU  | N      | 10.80        |
| 1     | H     | 4114:UNK  | C      | 4122:GLU  | N      | 10.80        |
| 1     | K     | 4114:UNK  | C      | 4122:GLU  | N      | 10.80        |
| 1     | B     | 3335:UNK  | C      | 3346:UNK  | N      | 10.61        |
| 1     | E     | 3335:UNK  | C      | 3346:UNK  | N      | 10.61        |
| 1     | H     | 3335:UNK  | C      | 3346:UNK  | N      | 10.61        |
| 1     | K     | 3335:UNK  | C      | 3346:UNK  | N      | 10.61        |
| 1     | B     | 3288:UNK  | C      | 3292:UNK  | N      | 9.91         |
| 1     | E     | 3288:UNK  | C      | 3292:UNK  | N      | 9.91         |
| 1     | H     | 3288:UNK  | C      | 3292:UNK  | N      | 9.91         |
| 1     | K     | 3288:UNK  | C      | 3292:UNK  | N      | 9.91         |
| 1     | B     | 2683:UNK  | C      | 2688:UNK  | N      | 9.67         |
| 1     | E     | 2683:UNK  | C      | 2688:UNK  | N      | 9.67         |
| 1     | H     | 2683:UNK  | C      | 2688:UNK  | N      | 9.67         |
| 1     | K     | 2683:UNK  | C      | 2688:UNK  | N      | 9.67         |
| 1     | B     | 2217:GLY  | C      | 2222:LYS  | N      | 9.51         |
| 1     | E     | 2217:GLY  | C      | 2222:LYS  | N      | 9.51         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | H     | 2217:GLY  | C      | 2222:LYS  | N      | 9.51         |
| 1     | K     | 2217:GLY  | C      | 2222:LYS  | N      | 9.51         |
| 1     | B     | 2571:ALA  | C      | 2579:MET  | N      | 8.61         |
| 1     | E     | 2571:ALA  | C      | 2579:MET  | N      | 8.61         |
| 1     | H     | 2571:ALA  | C      | 2579:MET  | N      | 8.61         |
| 1     | K     | 2571:ALA  | C      | 2579:MET  | N      | 8.61         |
| 1     | B     | 2632:PRO  | C      | 2638:UNK  | N      | 7.07         |
| 1     | E     | 2632:PRO  | C      | 2638:UNK  | N      | 7.07         |
| 1     | H     | 2632:PRO  | C      | 2638:UNK  | N      | 7.07         |
| 1     | K     | 2632:PRO  | C      | 2638:UNK  | N      | 7.07         |
| 1     | B     | 3004:UNK  | C      | 3009:UNK  | N      | 6.99         |
| 1     | E     | 3004:UNK  | C      | 3009:UNK  | N      | 6.99         |
| 1     | H     | 3004:UNK  | C      | 3009:UNK  | N      | 6.99         |
| 1     | K     | 3004:UNK  | C      | 3009:UNK  | N      | 6.99         |
| 1     | B     | 1478:ASP  | C      | 1482:ASN  | N      | 5.65         |
| 1     | E     | 1478:ASP  | C      | 1482:ASN  | N      | 5.65         |
| 1     | H     | 1478:ASP  | C      | 1482:ASN  | N      | 5.65         |
| 1     | K     | 1478:ASP  | C      | 1482:ASN  | N      | 5.65         |
| 1     | B     | 2535:ALA  | C      | 2541:THR  | N      | 5.55         |
| 1     | E     | 2535:ALA  | C      | 2541:THR  | N      | 5.55         |
| 1     | H     | 2535:ALA  | C      | 2541:THR  | N      | 5.55         |
| 1     | K     | 2535:ALA  | C      | 2541:THR  | N      | 5.55         |
| 1     | B     | 4863:LYS  | C      | 4871:ASP  | N      | 5.49         |
| 1     | E     | 4863:LYS  | C      | 4871:ASP  | N      | 5.49         |
| 1     | H     | 4863:LYS  | C      | 4871:ASP  | N      | 5.49         |
| 1     | K     | 4863:LYS  | C      | 4871:ASP  | N      | 5.49         |
| 1     | B     | 1275:ARG  | C      | 1282:SER  | N      | 5.47         |
| 1     | E     | 1275:ARG  | C      | 1282:SER  | N      | 5.47         |
| 1     | H     | 1275:ARG  | C      | 1282:SER  | N      | 5.47         |
| 1     | K     | 1275:ARG  | C      | 1282:SER  | N      | 5.47         |
| 1     | B     | 184:THR   | C      | 189:LEU   | N      | 4.54         |
| 1     | E     | 184:THR   | C      | 189:LEU   | N      | 4.54         |
| 1     | H     | 184:THR   | C      | 189:LEU   | N      | 4.54         |
| 1     | K     | 184:THR   | C      | 189:LEU   | N      | 4.54         |
| 1     | B     | 2383:GLU  | C      | 2384:ALA  | N      | 3.24         |
| 1     | B     | 4245:GLN  | C      | 4246:ILE  | N      | 3.24         |
| 1     | E     | 2383:GLU  | C      | 2384:ALA  | N      | 3.24         |
| 1     | E     | 4245:GLN  | C      | 4246:ILE  | N      | 3.24         |
| 1     | H     | 2383:GLU  | C      | 2384:ALA  | N      | 3.24         |
| 1     | H     | 4245:GLN  | C      | 4246:ILE  | N      | 3.24         |
| 1     | K     | 2383:GLU  | C      | 2384:ALA  | N      | 3.24         |
| 1     | K     | 4245:GLN  | C      | 4246:ILE  | N      | 3.24         |

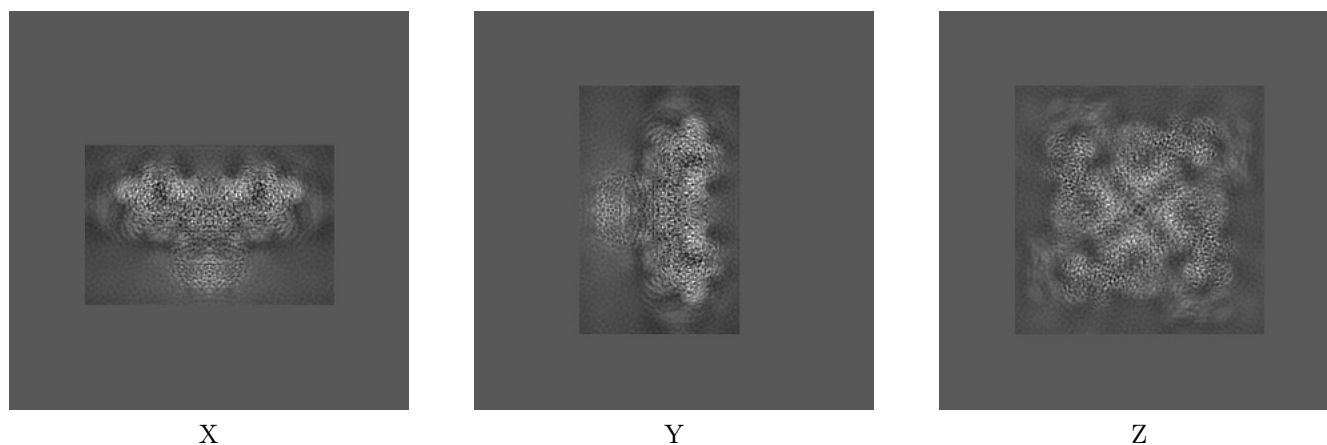
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22015. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

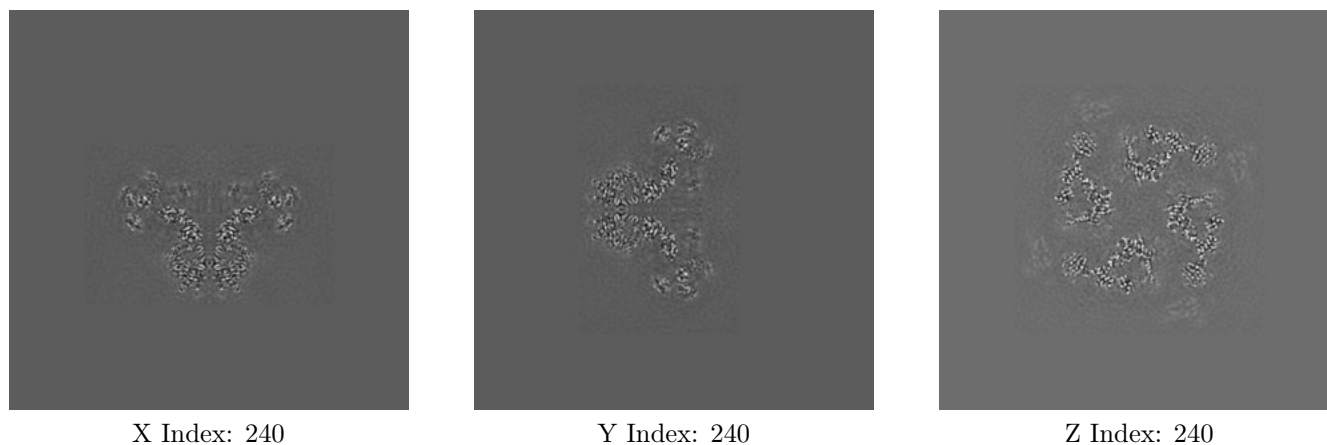
#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

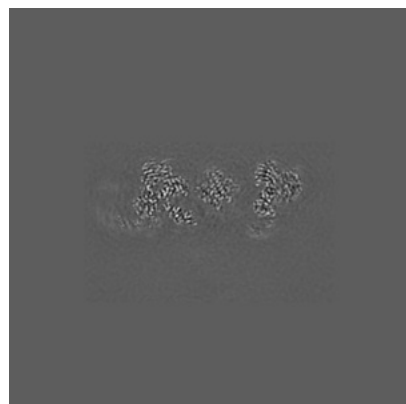
#### 6.2.1 Primary map



The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

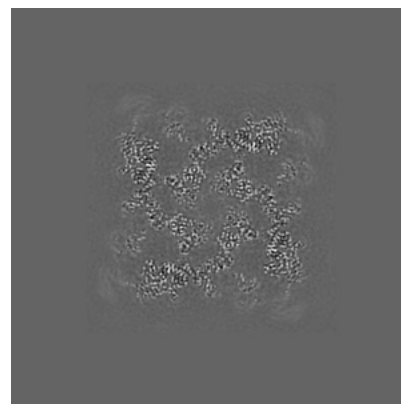
### 6.3.1 Primary map



X Index: 311



Y Index: 311

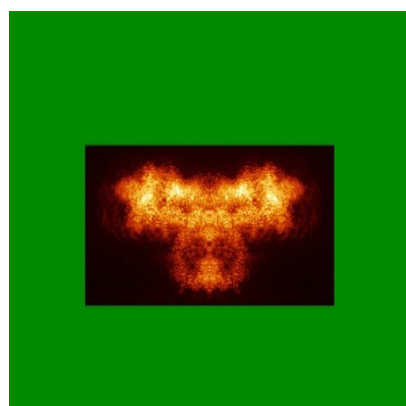


Z Index: 258

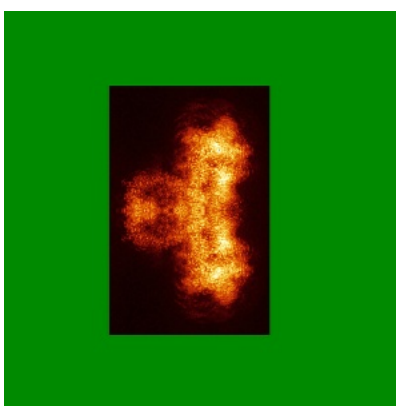
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

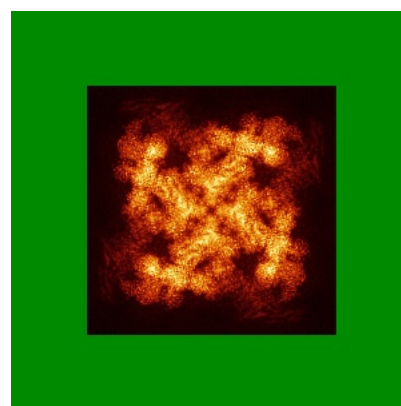
### 6.4.1 Primary map



X



Y

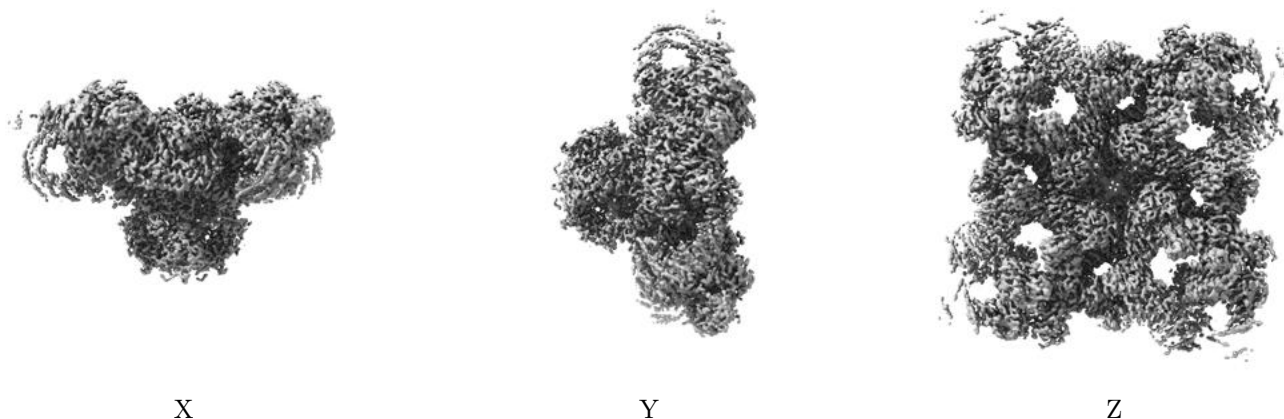


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

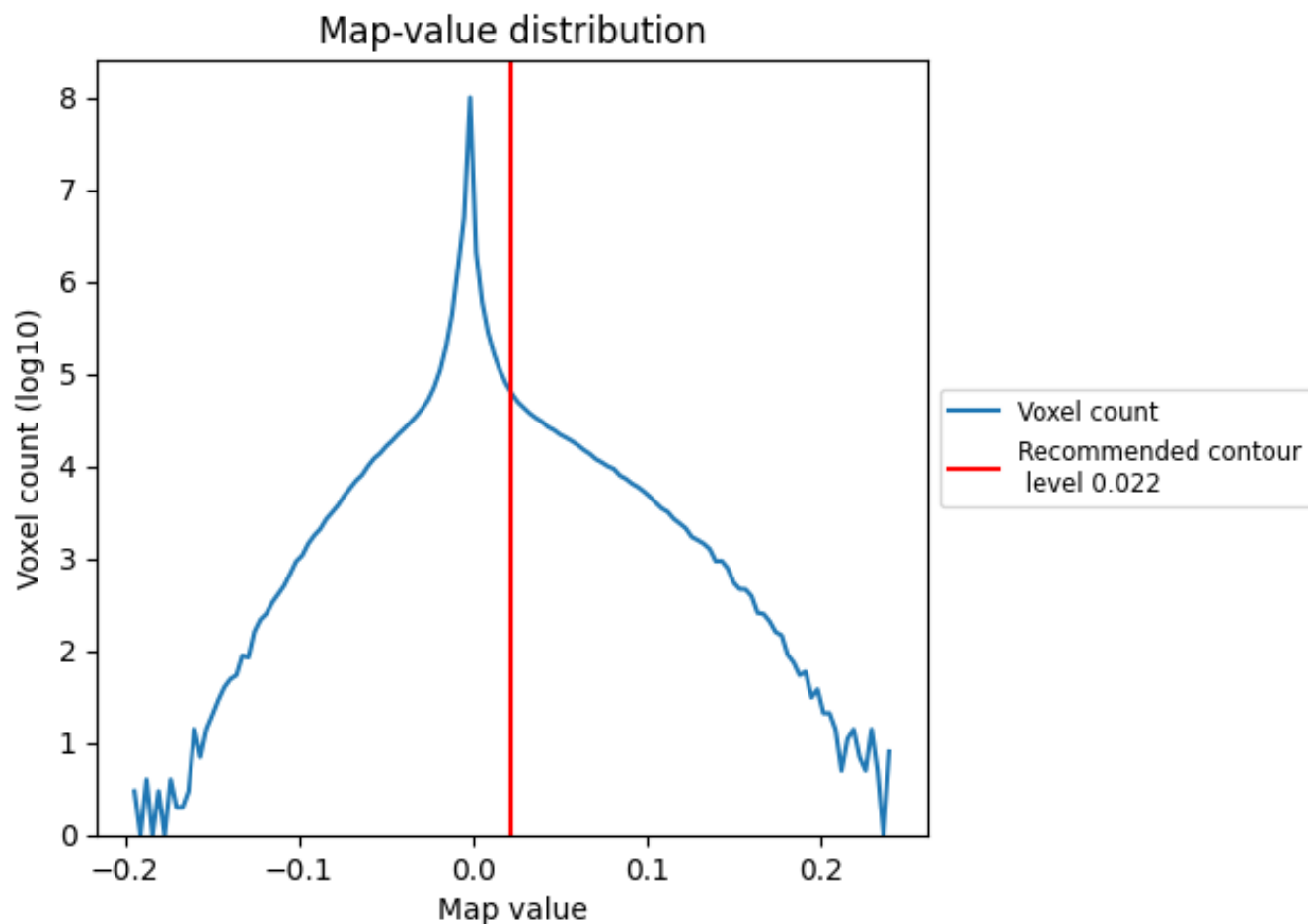
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

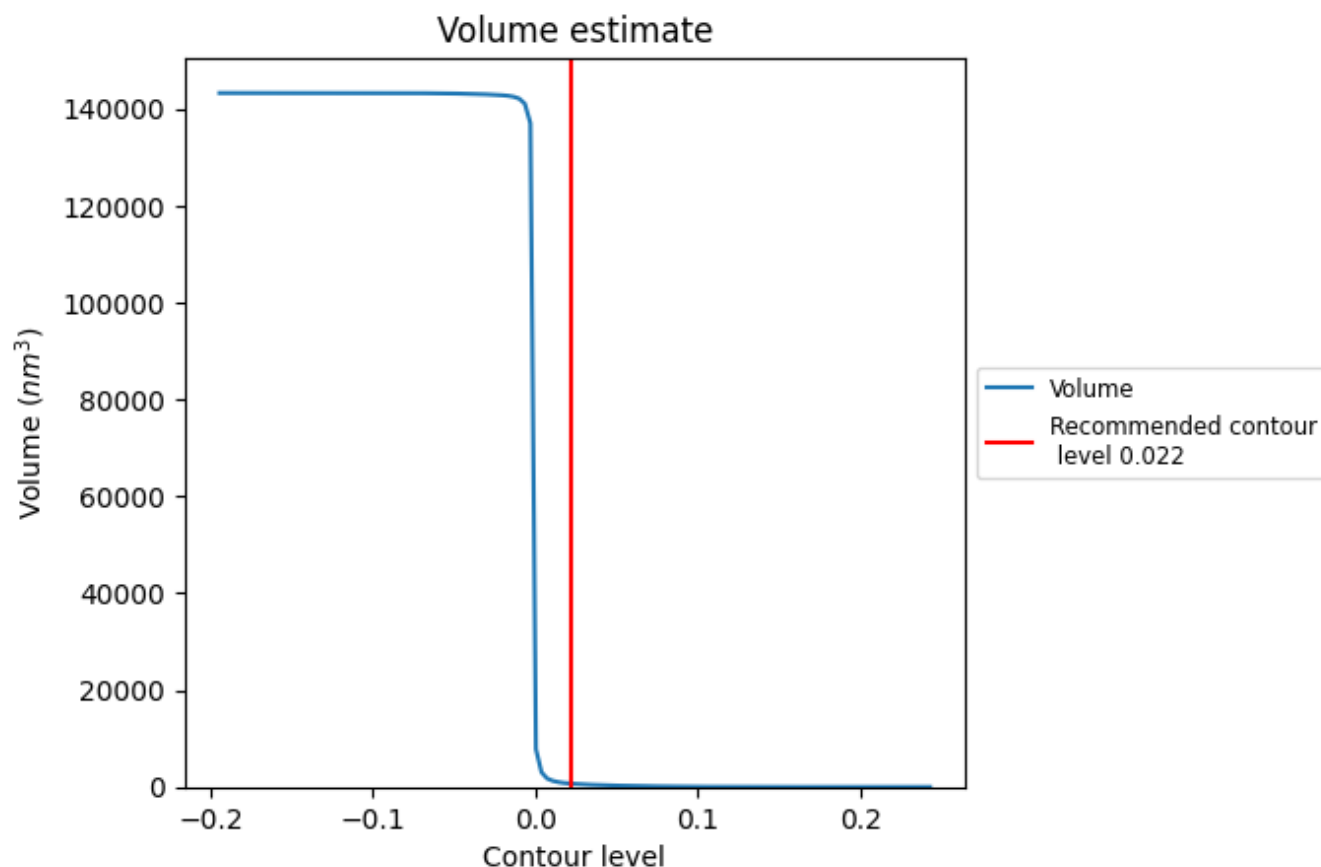
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

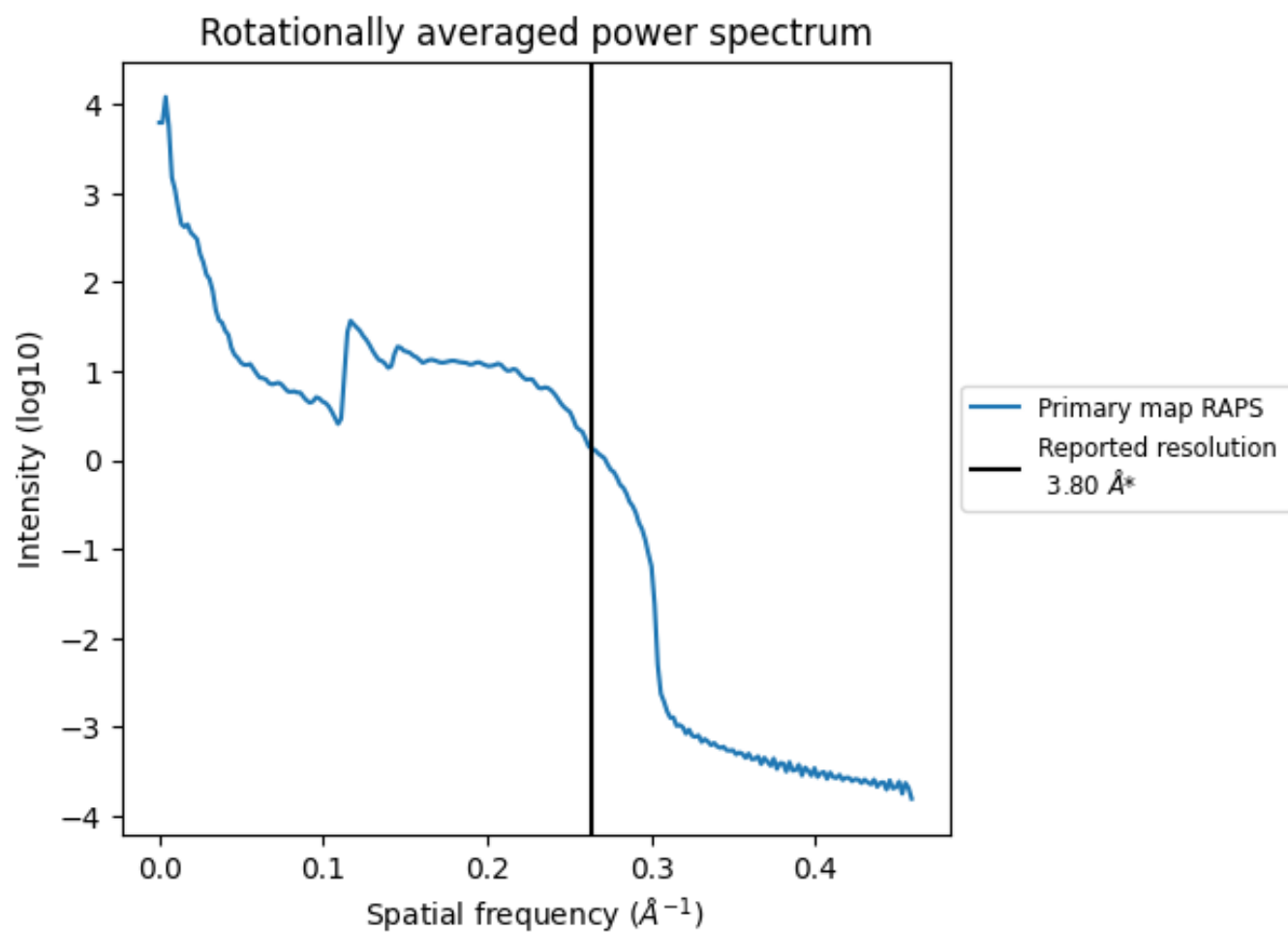
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 692  $\text{nm}^3$ ; this corresponds to an approximate mass of 625 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

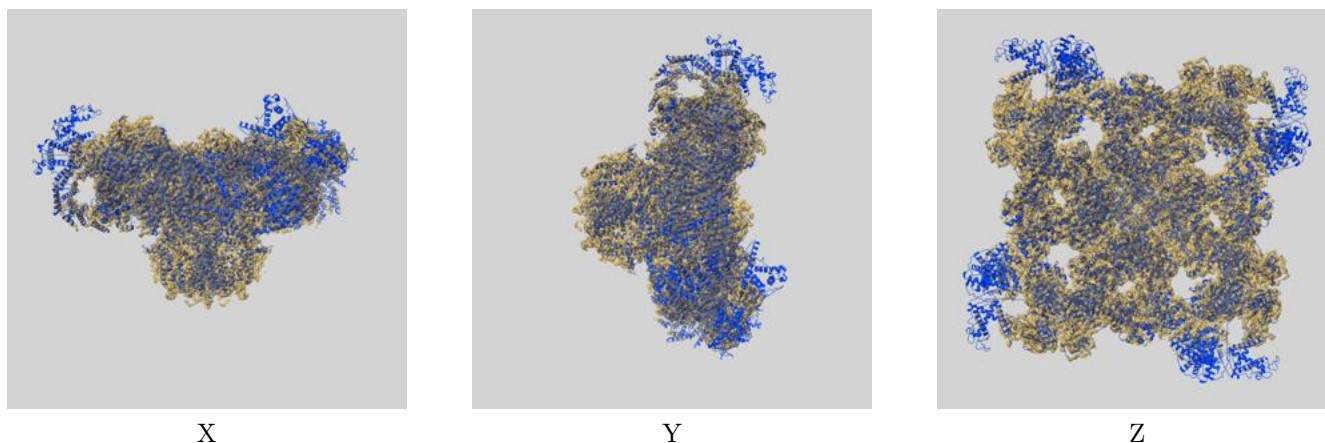
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

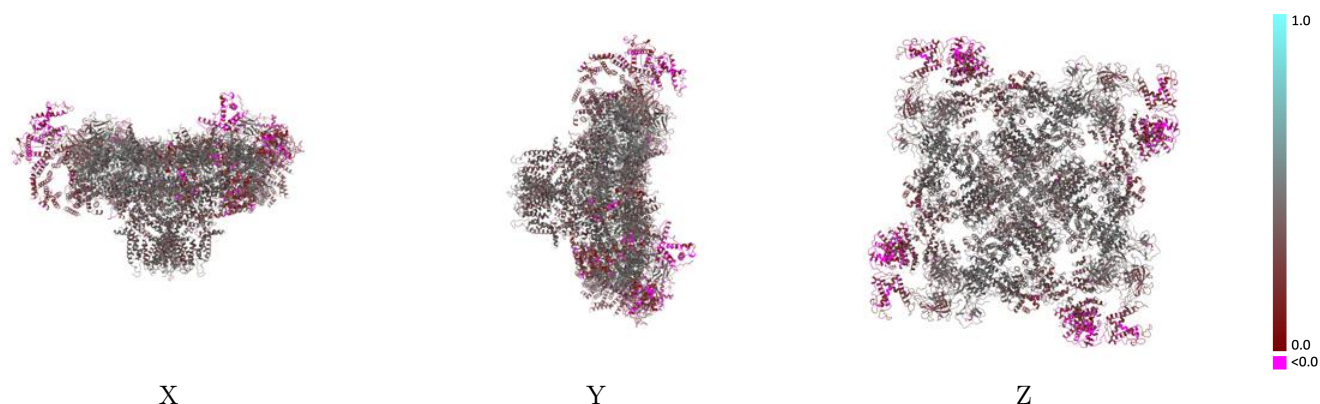
This section contains information regarding the fit between EMDB map EMD-22015 and PDB model 6X32. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



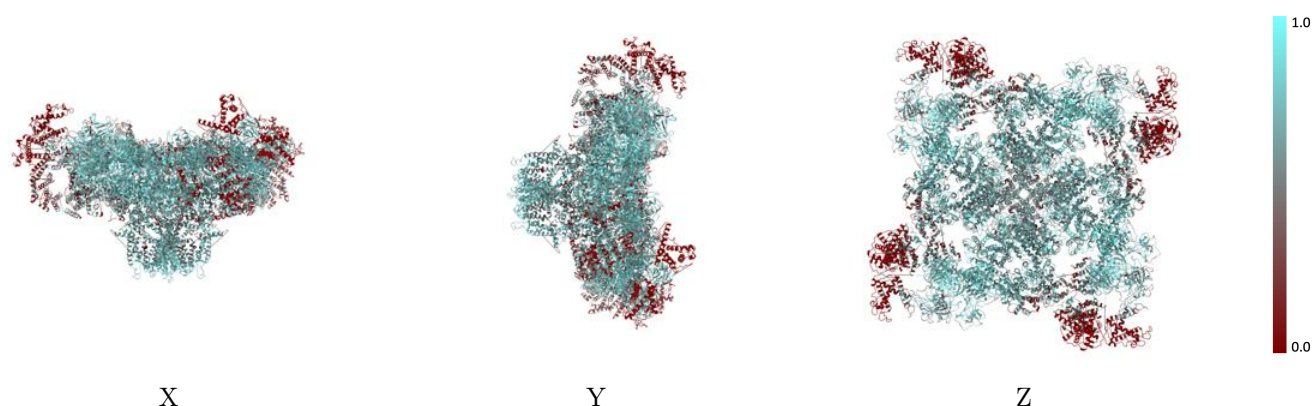
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



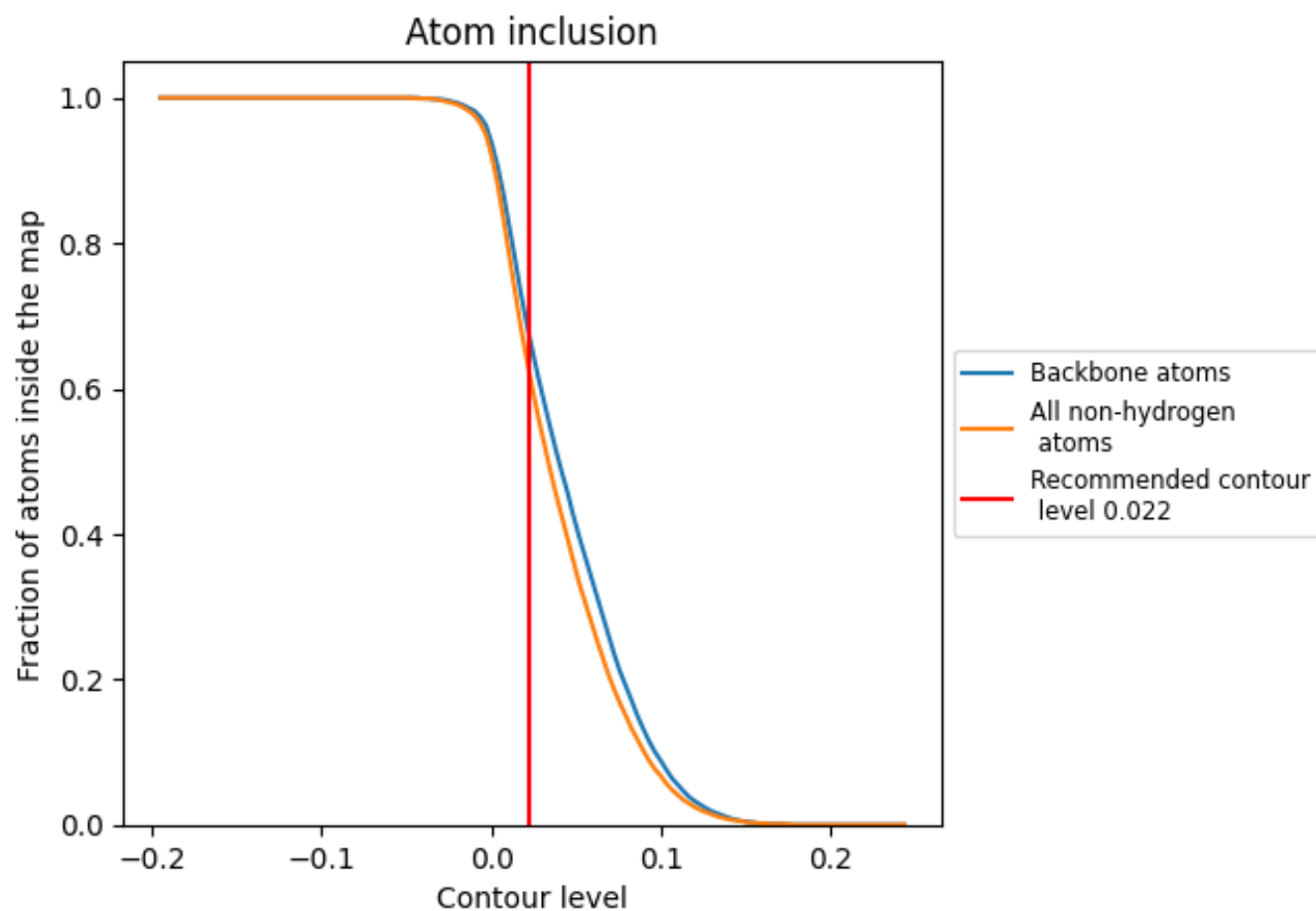
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| All   |  0.6270 |  0.3740 |
| A     |  0.7080 |  0.4070 |
| B     |  0.6330 |  0.3770 |
| C     |  0.3970 |  0.2520 |
| D     |  0.7050 |  0.4060 |
| E     |  0.6320 |  0.3770 |
| F     |  0.3960 |  0.2510 |
| G     |  0.7050 |  0.4060 |
| H     |  0.6310 |  0.3760 |
| I     |  0.3960 |  0.2540 |
| J     |  0.7080 |  0.4040 |
| K     |  0.6320 |  0.3760 |
| L     |  0.3920 |  0.2510 |

