Full wwPDB EM Validation Report (i)

Feb 25, 2024 – 12:56 PM EST

PDB ID	:	6X34
EMDB ID	:	EMD-22017
Title	:	Pig R615C RyR1 EGTA (all classes, open)
Authors	:	Woll, K.W.; Haji-Ghassemi, O.; Van Petegem, F.
Deposited on	:	2020-05-21
Resolution	:	4.70 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

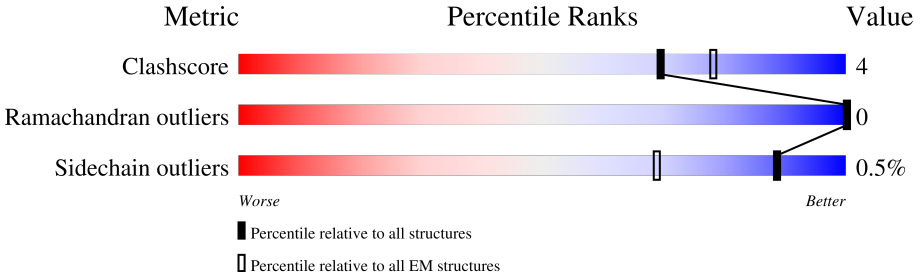
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 >=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 <=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	106	10% 88% 9% •
1	C	106	10% 88% 9% •
1	E	106	10% 88% 9% •
1	G	106	10% 88% 9% •
2	B	3716	16% 92% 8%
2	D	3716	16% 92% 8%
2	F	3716	16% 93% 7%
2	H	3716	16% 92% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 97888 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
			Total	C	N	O	S		
1	A	103	659	422	115	120	2	0	0
1	C	103	659	422	115	120	2	0	0
1	E	103	659	422	115	120	2	0	0
1	G	103	659	422	115	120	2	0	0

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	3715	23812	15199	4256	4267	90	6	0
2	D	3715	23812	15199	4256	4267	90	6	0
2	F	3715	23812	15199	4256	4267	90	6	0
2	H	3715	23812	15199	4256	4267	90	6	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

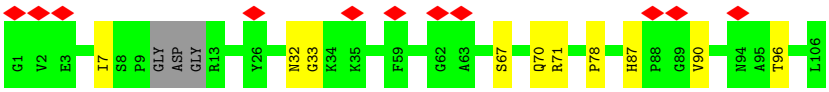
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	B	1	1	1	0
3	D	1	1	1	0
3	F	1	1	1	0
3	H	1	1	1	0

3 Residue-property plots (i)

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.

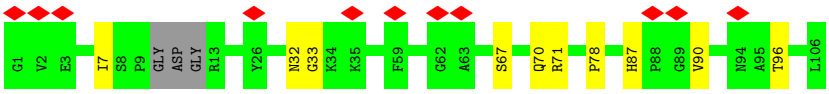
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



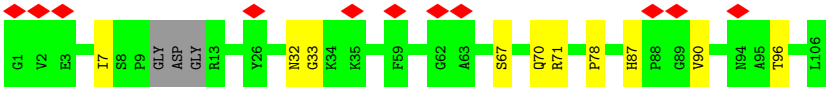
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C:



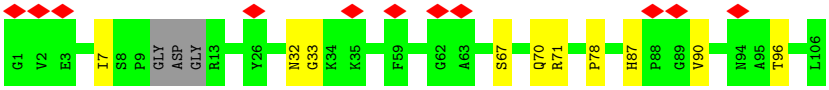
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



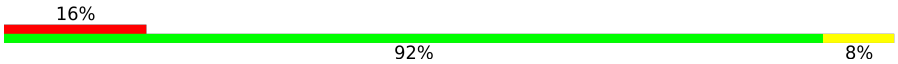
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

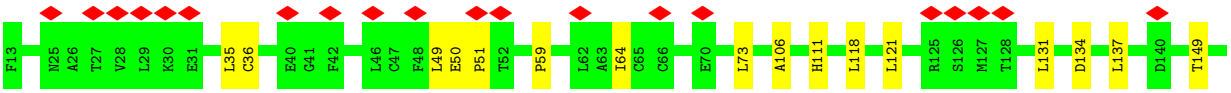
Chain G:

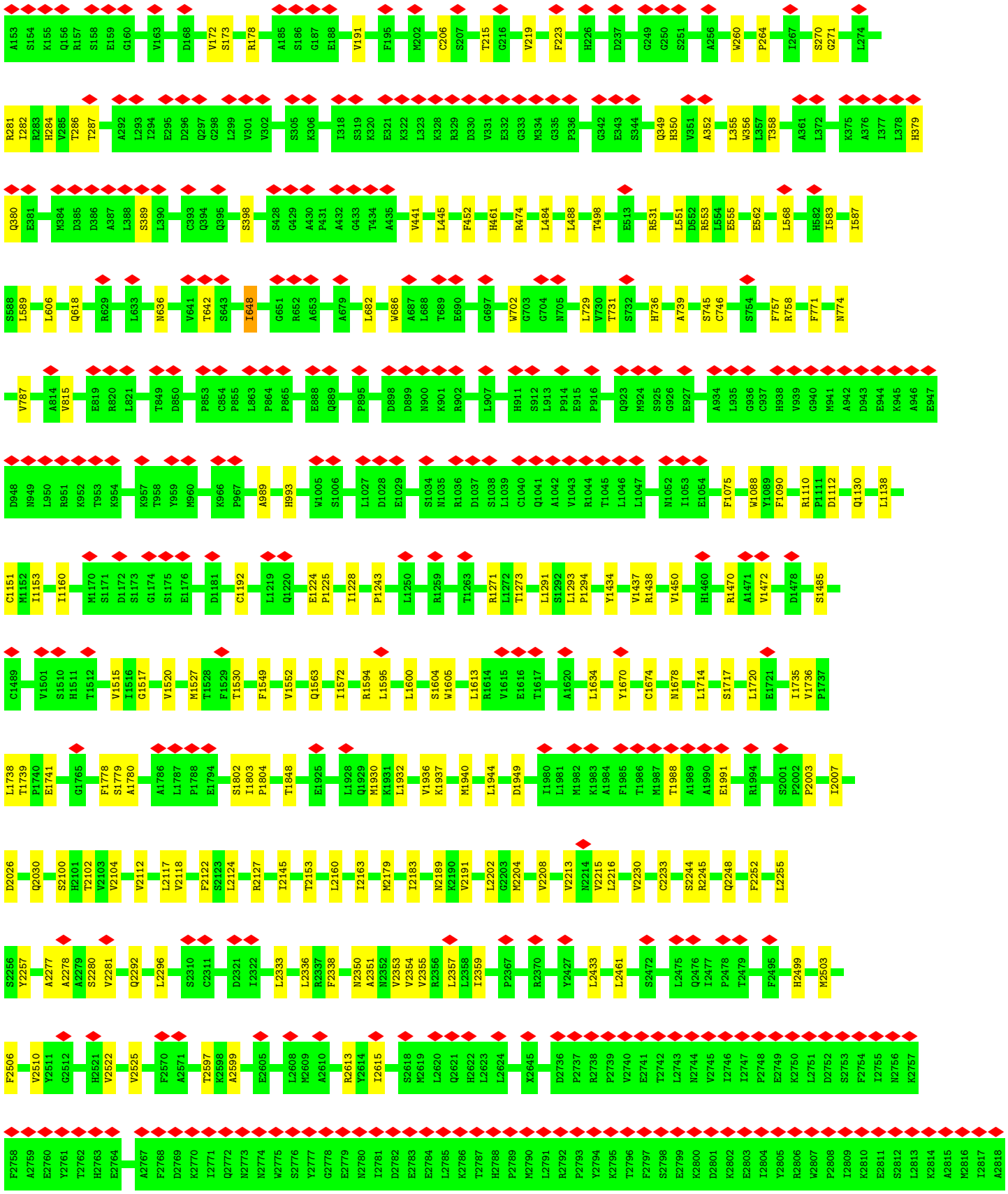


• Molecule 2: Ryanodine Receptor

Chain B:



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R281 I282 R283 H284 V285 T286 T287 A292 L293 I294 E295 D296 Q297 G298 L299 V301 V302 S305 K306 I318 S319 K320 E321 K322 L323 K328 R329 D330 V331 E332 G333 M334 G335 P336 G342 E343 S344 Q349 H350 V351 A352 L355 W356 L357 T358 A361 L372 K375 A376 I377 L378 H379
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V787 A814 V815 E819 R820 L821 T849 D850 P853 C854 P855 L863 P864 P865 E888 Q889 P895 D898 D899 N900 K901 R902 L907 H911 S912 L913 P914 E915 P916 Q923 M924 S925 G926 E927 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947
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L1738 T1739 P1740 E1741 G1765 F1778 S1779 A1780 A1786 L1787 P1788 E1794 S1802 I1803 P1804 T1848 E1925 L1928 Q1929 M1930 K1931 L1932 V1936 K1937 M1940 L1944 D1949 I1980 L1981 M1982 K1983 A1984 F1985 T1986 M1987 T1988 A1989 A1990 E1991 R1994 S2001 P2002 P2003 I2007
D2026 Q2030 S2100 H2101 T2102 V2103 V2104 V2112 L2117 V2118 F2122 S2123 L2124 R2127 I2145 T2153 L2160 I2163 M2179 I2183 N2189 K2190 V2191 L2202 G2203 M2204 V2208 V2213 N2214 V2215 L2216 V2230 C2233 S2244 R2245 Q2248 F2252 L2255
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F2506 V2510 Y2511 G2512 H2521 V2522 V2525 F2570 A2571 T2597 K2598 A2599 E2605 L2608 M2609 A2610 R2613 Y2614 I2615 S2618 M2619 L2620 Q2621 H2622 L2623 L2624 X2645 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 M2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 M2756 K2757
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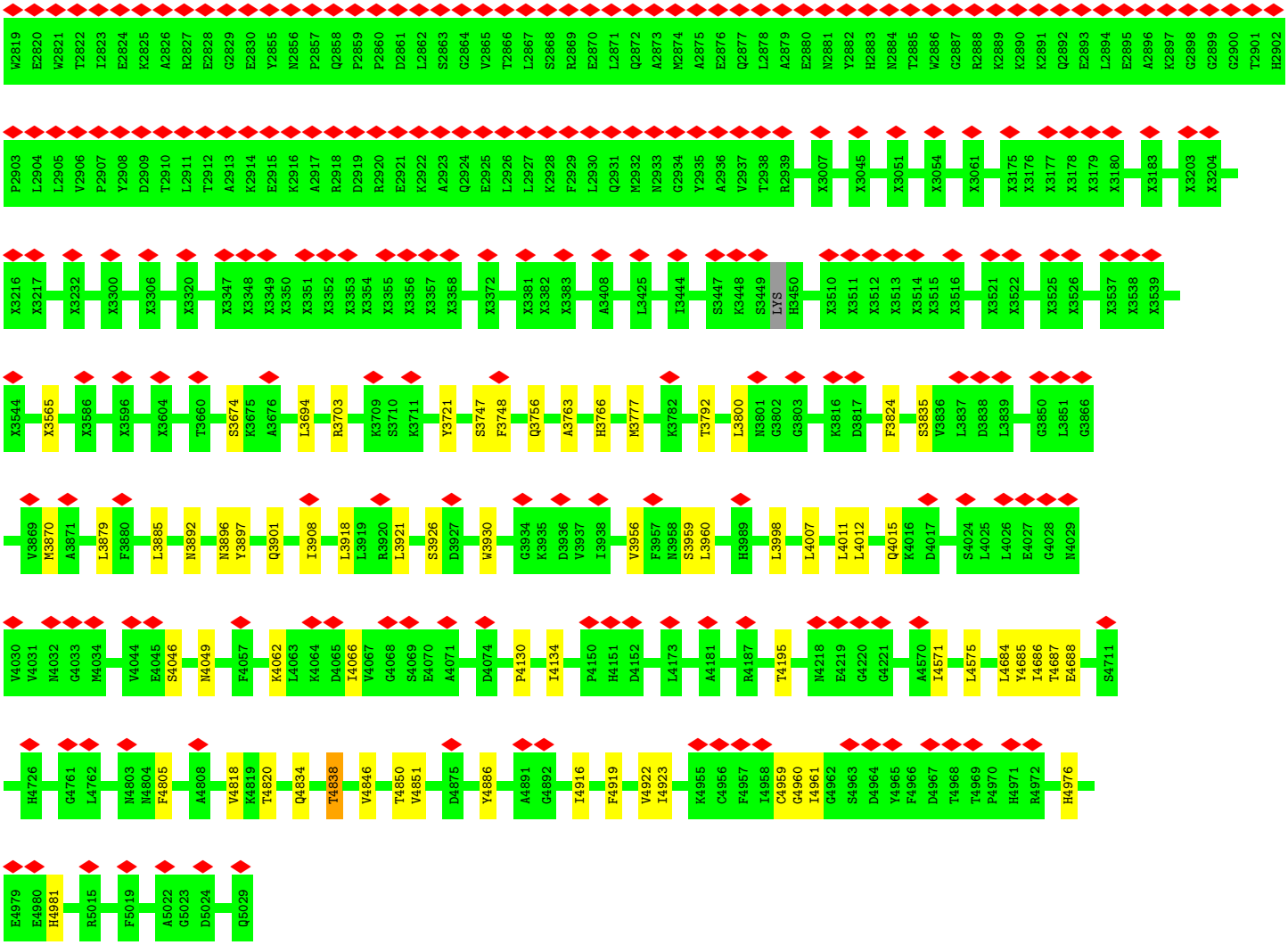
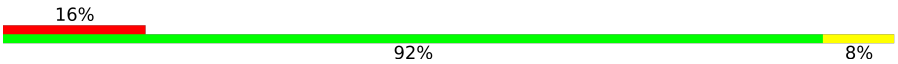
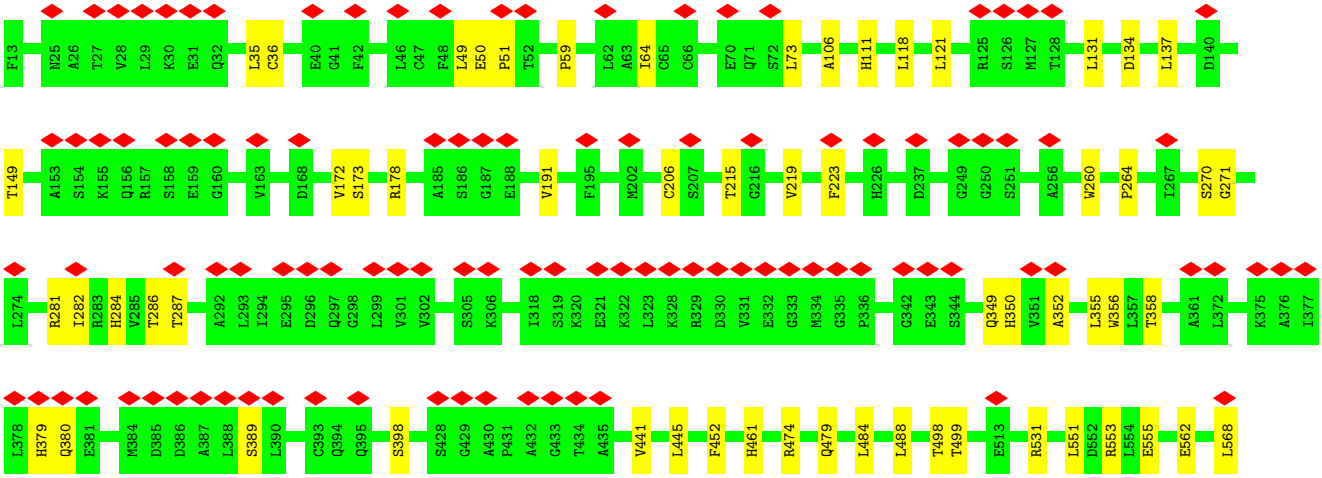
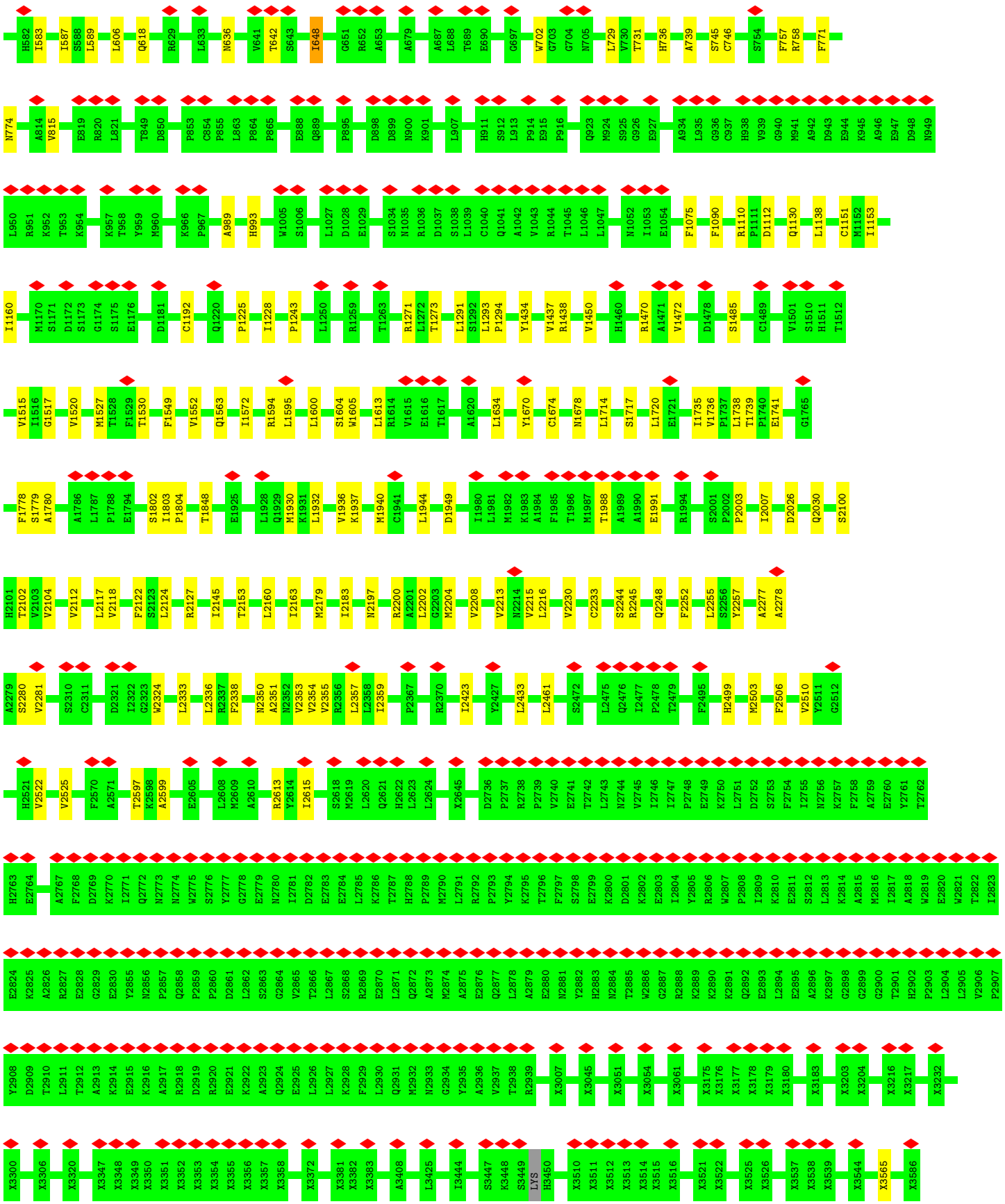


- Molecule 2: Ryanodine Receptor

Chain D:



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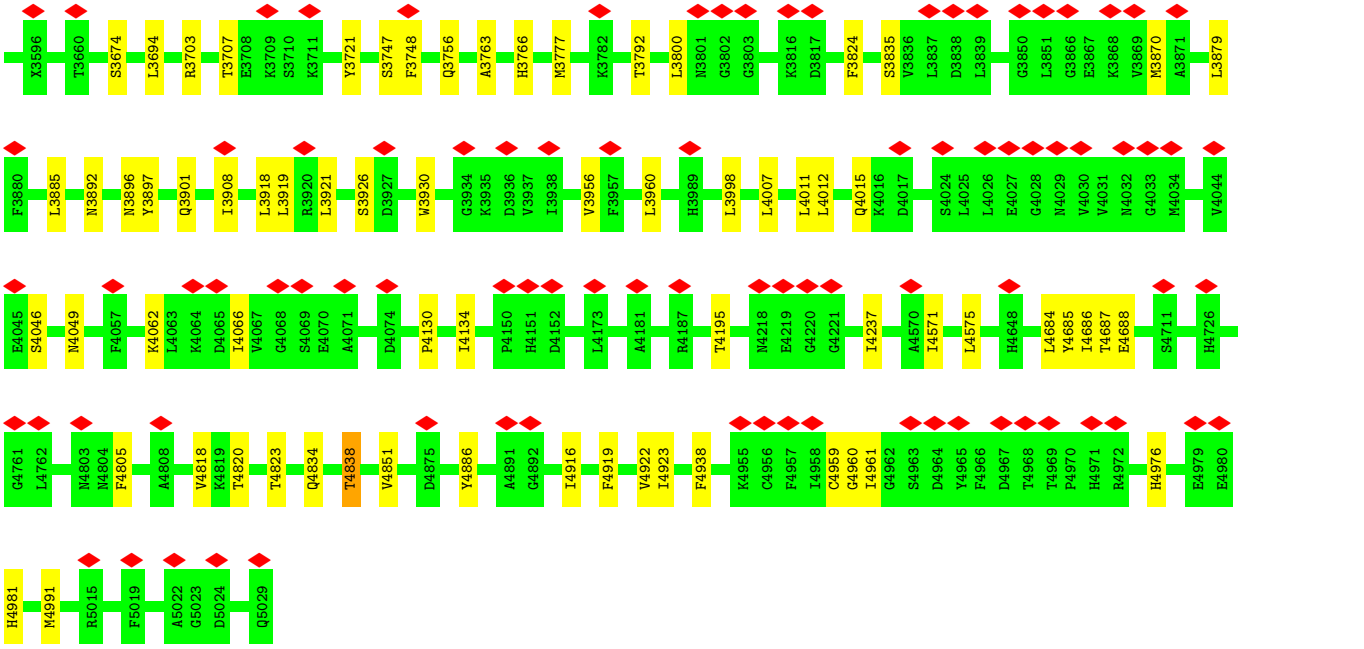
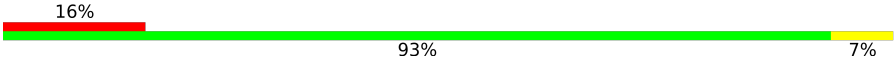
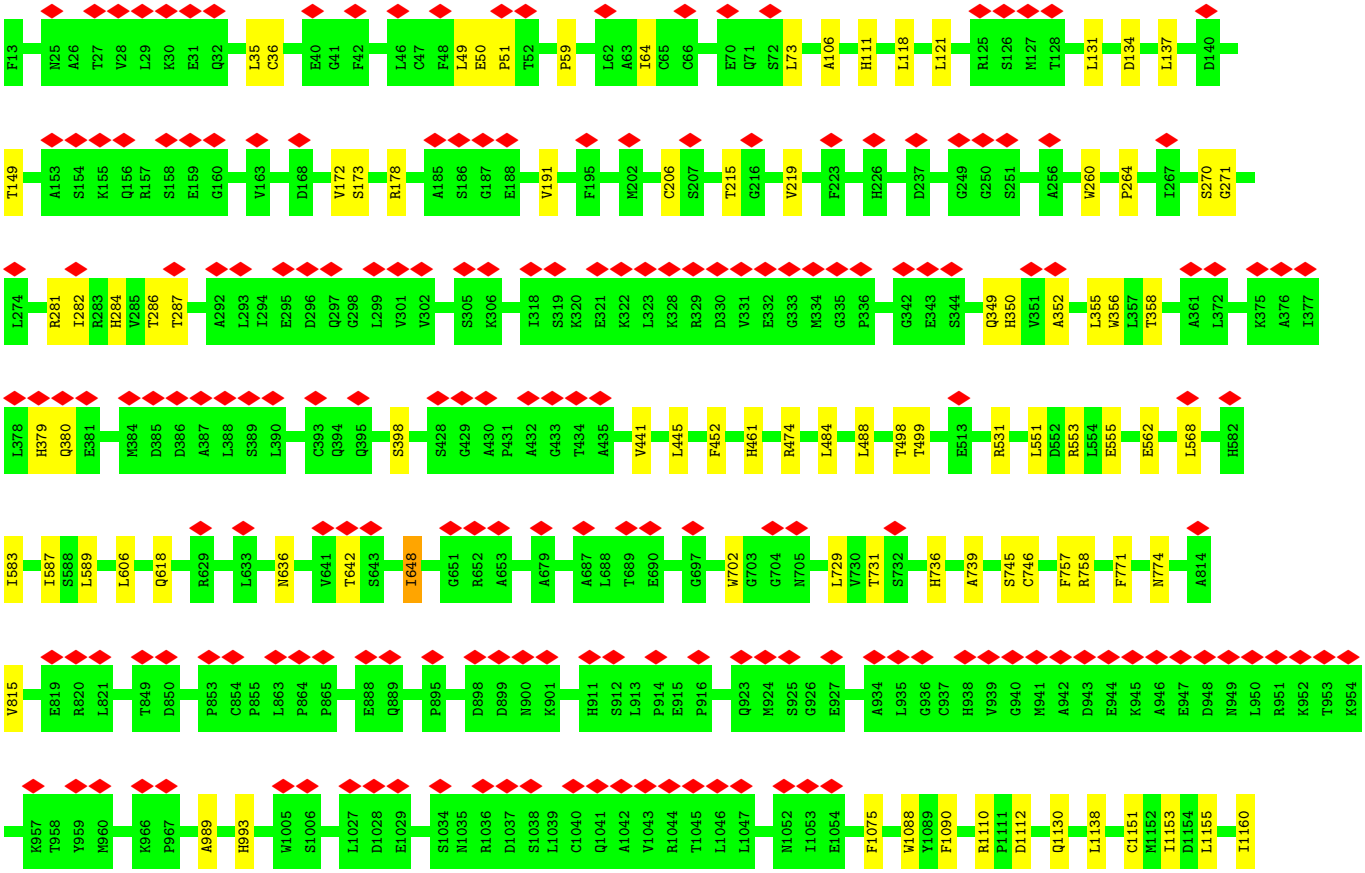


- Molecule 2: Ryanodine Receptor

Chain F:





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V2525 F2570 A2571 T2597 K2598 A2599 E2605 L2608 M2609 A2610 R2613 Y2614 I2615 S2618 M2619 L2620 Q2621 H2622 L2623 L2624 X2645 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764

A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 I2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826

R2827 E2828 G2829 E2830 Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910

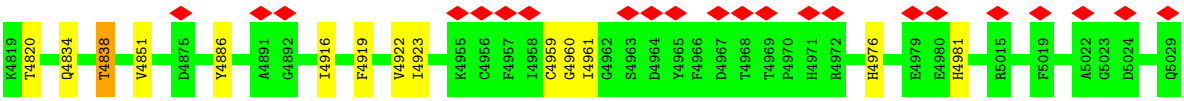
L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X3007 X3045 X3051 X3054 X3061 X3175 X3176 X3177 X3178 X3179 X3180 X3183 X3203 X3204 X3216 X3217 X3232 X3300 X3306

X3320 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3372 X3381 X3382 X3383 A3408 L3425 I3444 S3447 K3448 SER K3449 X3510 X3511 X3512 X3513 X3514 X3515 X3516 X3521 X3522 X3525 X3526 X3537 X3538 X3539 X3544 X3565 X3586 X3596 T3660

S3674 L3694 R3703 K3709 S3710 K3711 Y3721 S3747 F3748 Q3756 A3763 H3766 M3777 K3782 T3792 L3800 N3801 G3802 G3803 K3816 D3817 F3824 L3837 D3838 L3839 G3850 L3851 G3866 V3869 M3870 A3871 L3879 F3880 L3885 N3892 N3896 Y3897

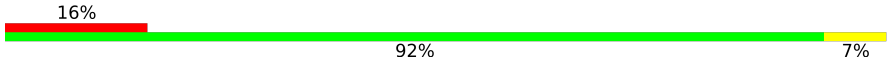
Q3901 I3908 L3918 L3919 R3920 L3921 S3926 D3927 W3930 G3934 K3935 D3936 V3937 I3938 V3956 F3957 M3958 S3959 L3960 H3989 L3998 L4007 L4011 L4012 Q4015 K4016 D4017 S4024 L4025 L4026 E4027 G4028 M4029 V4030 V4031 M4032 G4033 M4034 V4044 E4045 S4046 N4049 F4057 K4062

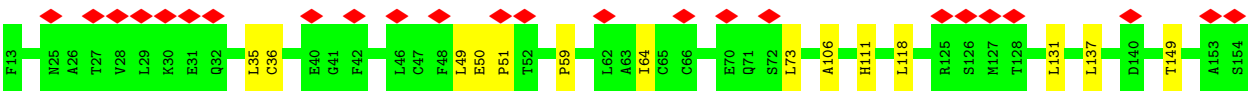
L4063 K4064 D4065 I4066 V4067 G4068 S4069 E4070 A4071 D4074 P4130 I4134 P4150 H4151 D4152 L4173 A4181 R4187 T4195 M4218 E4219 G4220 G4221 A4570 I4571 L4575 H4648 L4684 Y4685 I4686 T4687 E4688 S4711 H4726 G4761 L4762 N4803 N4804 F4805 A4808 V4818

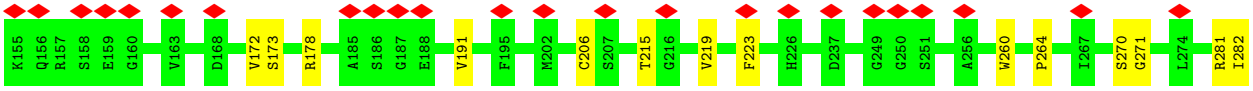


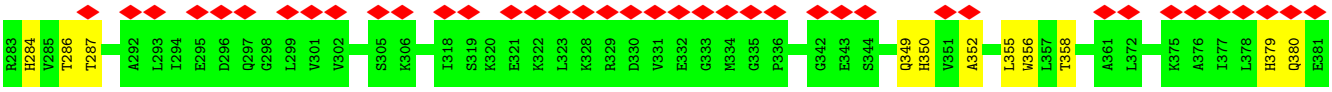
- Molecule 2: Ryanodine Receptor

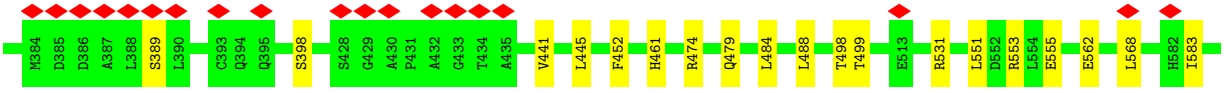
Chain H:

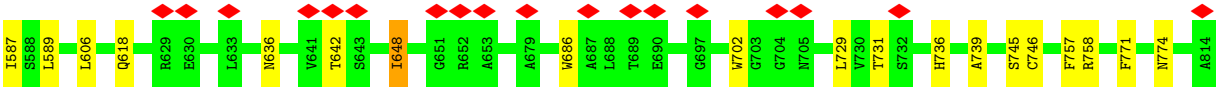


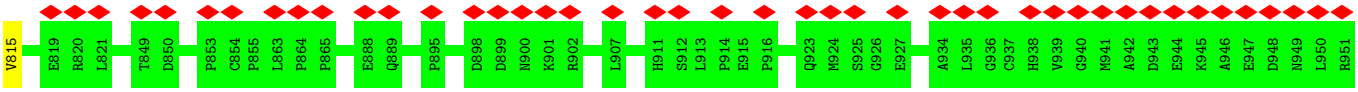


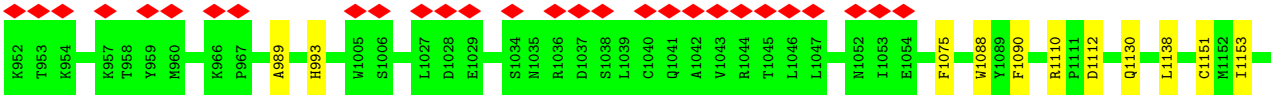


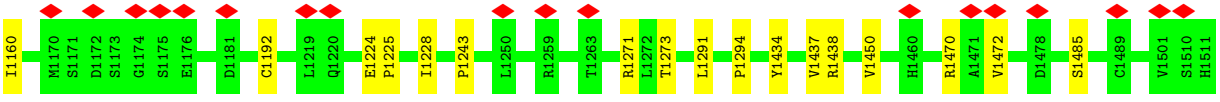


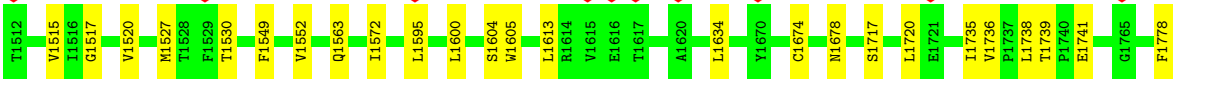


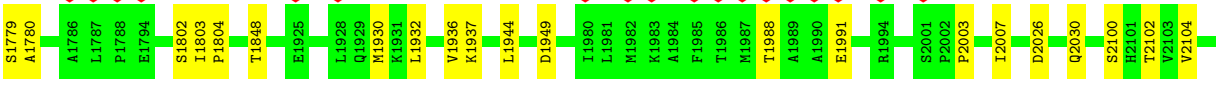


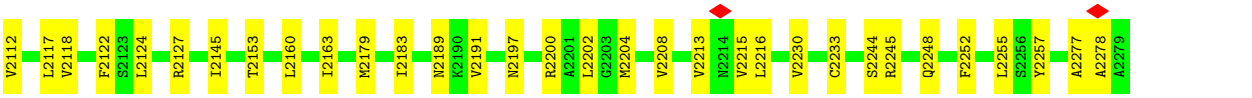


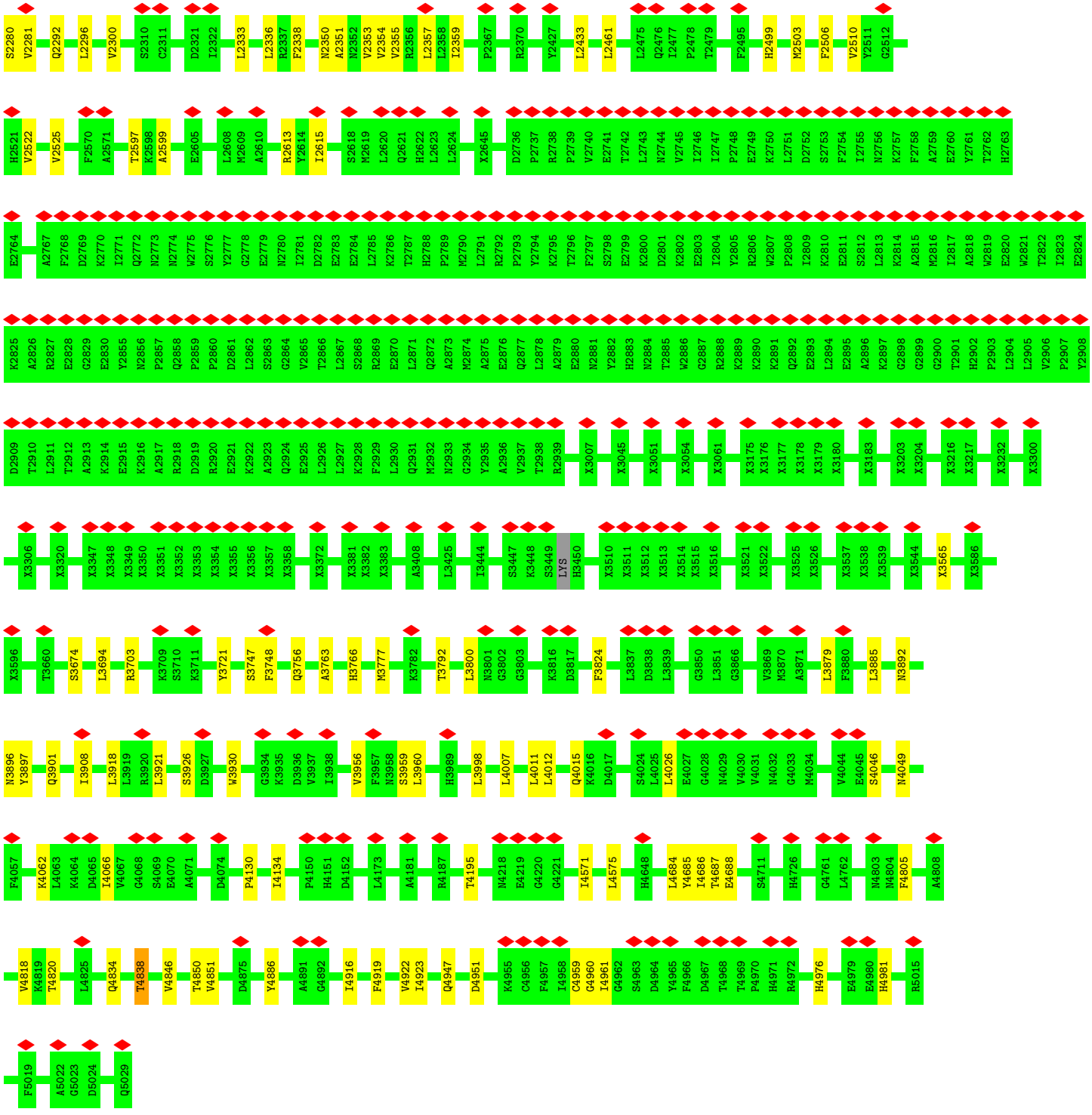








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H2521 V2522 V2525 F2570 A2571 T2597 K2598 A2599 E2605 L2608 M2609 A2610 R2613 Y2614 I2615 S2618 M2619 L2620 Q2621 H2622 L2623 L2624 X2645 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763
E2764 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 I2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824
K2825 A2826 R2827 E2828 G2829 E2830 Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908
D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X3007 X3045 X3051 X3054 X3061 X3175 X3176 X3177 X3178 X3179 X3180 X3183 X3203 X3204 X3216 X3217 X3232 X3300
X3306 X3320 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3372 X3381 X3382 X3383 A3408 L3425 I3444 S3447 K3448 S3449 LYS H3450 X3510 X3511 X3512 X3513 X3514 X3515 X3516 X3521 X3522 X3525 X3526 X3537 X3538 X3539 X3544 X3565 X3586
X3596 T3660 S3674 L3694 R3703 K3709 S3710 K3711 Y3721 S3747 F3748 Q3756 A3763 H3766 M3777 K3782 T3792 L3800 N3801 G3802 G3803 K3816 D3817 F3824 L3837 D3838 L3839 G3850 L3851 G3866 V3869 M3870 A3871 L3879 F3880 L3885 N3892
N3896 Y3897 Q3901 I3908 L3918 L3919 R3920 L3921 S3926 D3927 W3930 G3934 K3935 D3936 V3937 I3938 V3956 F3957 N3958 S3959 L3960 H3989 L3998 L4007 L4011 L4012 Q4015 K4016 D4017 S4024 L4025 L4026 E4027 G4028 N4029 V4030 V4031 N4032 G4033 M4034 V4044 E4045 S4046 N4049
F4057 K4062 L4063 K4064 D4065 I4066 V4067 G4068 S4069 E4070 A4071 D4074 P4130 I4134 P4150 H4151 D4152 L4173 A4181 R4187 T4195 N4218 E4219 G4220 G4221 I4571 L4575 H4648 L4684 Y4685 I4686 T4687 E4688 S4711 H4726 G4761 L4762 N4803 N4804 F4805 A4808
V4818 K4819 T4820 L4825 Q4834 T4838 V4846 T4850 V4851 D4875 Y4886 A4891 G4892 I4916 F4919 V4922 I4923 Q4947 D4951 K4955 C4956 F4957 I4958 C4959 G4960 I4961 G4962 S4963 D4964 Y4965 F4966 D4967 T4968 T4969 P4970 H4971 R4972 H4976 E4979 E4980 H4981 R5015
F5019 A5022 G5023 D5024 Q5029

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58822	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 ($e^-/Å^2$)	30	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	2.839	Depositor
Minimum map value	-1.092	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.702	Depositor
Map size (Å)	672.0, 672.0, 672.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	0.25	0/673	0.44	0/925
1	C	0.25	0/673	0.44	0/925
1	E	0.25	0/673	0.44	0/925
1	G	0.25	0/673	0.44	0/925
2	B	0.24	0/22632	0.39	0/31129
2	D	0.24	0/22632	0.39	0/31129
2	F	0.24	0/22632	0.39	0/31129
2	H	0.24	0/22632	0.39	0/31129
All	All	0.24	0/93220	0.39	0/128216

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	659	0	547	5	0
1	C	659	0	547	5	0
1	E	659	0	547	5	0
1	G	659	0	547	5	0
2	B	23812	0	18429	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	23812	0	18429	160	0
2	F	23812	0	18429	156	0
2	H	23812	0	18429	159	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	97888	0	75904	639	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 4.

All (639) 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:D:1225:PRO:HD2	2:D:1228:ILE:HD12	1.75	0.68
2:F:1225:PRO:HD2	2:F:1228:ILE:HD12	1.75	0.68
2:H:1225:PRO:HD2	2:H:1228:ILE:HD12	1.75	0.67
2:B:1225:PRO:HD2	2:B:1228:ILE:HD12	1.75	0.66
2:D:3926:SER:HB2	2:D:3930:TRP:HZ3	1.62	0.65
2:F:2336:LEU:HB2	2:F:2433:LEU:HD11	1.79	0.65
2:F:3926:SER:HB2	2:F:3930:TRP:HZ3	1.62	0.65
2:H:3926:SER:HB2	2:H:3930:TRP:HZ3	1.62	0.64
2:B:3926:SER:HB2	2:B:3930:TRP:HZ3	1.62	0.64
2:D:2336:LEU:HB2	2:D:2433:LEU:HD11	1.79	0.64
2:B:2336:LEU:HB2	2:B:2433:LEU:HD11	1.79	0.64
2:H:4046:SER:HA	2:H:4049:ASN:HD22	1.62	0.63
2:D:4046:SER:HA	2:D:4049:ASN:HD22	1.62	0.63
2:H:2336:LEU:HB2	2:H:2433:LEU:HD11	1.79	0.63
2:F:4046:SER:HA	2:F:4049:ASN:HD22	1.62	0.63
2:H:746:CYS:HA	2:H:757:PHE:HA	1.81	0.62
2:B:4046:SER:HA	2:B:4049:ASN:HD22	1.62	0.62
2:B:746:CYS:HA	2:B:757:PHE:HA	1.81	0.61
2:D:1090:PHE:HB3	2:D:1151:CYS:HB2	1.82	0.61
2:H:173:SER:HB3	2:H:178:ARG:H	1.66	0.61
2:H:1090:PHE:HB3	2:H:1151:CYS:HB2	1.82	0.61
2:D:746:CYS:HA	2:D:757:PHE:HA	1.81	0.61
2:F:746:CYS:HA	2:F:757:PHE:HA	1.81	0.61
2:D:173:SER:HB3	2:D:178:ARG:H	1.66	0.60
2:B:636:ASN:HD22	2:B:702:TRP:HE1	1.49	0.60
2:H:636:ASN:HD22	2:H:702:TRP:HE1	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1090:PHE:HB3	2:F:1151:CYS:HB2	1.82	0.60
2:H:358:THR:HG21	2:H:379:HIS:H	1.66	0.60
2:B:358:THR:HG21	2:B:379:HIS:H	1.66	0.60
2:F:173:SER:HB3	2:F:178:ARG:H	1.66	0.60
2:F:636:ASN:HD22	2:F:702:TRP:HE1	1.49	0.60
2:B:1090:PHE:HB3	2:B:1151:CYS:HB2	1.82	0.60
2:B:173:SER:HB3	2:B:178:ARG:H	1.66	0.59
2:F:358:THR:HG21	2:F:379:HIS:H	1.66	0.59
2:H:1130:GLN:HA	2:H:1138:LEU:HA	1.84	0.59
2:D:636:ASN:HD22	2:D:702:TRP:HE1	1.49	0.59
2:F:260:TRP:HE1	2:F:282:ILE:HG23	1.67	0.59
2:D:358:THR:HG21	2:D:379:HIS:H	1.66	0.59
2:H:260:TRP:HE1	2:H:282:ILE:HG23	1.67	0.59
2:B:260:TRP:HE1	2:B:282:ILE:HG23	1.67	0.59
2:B:4916:ILE:HD11	2:D:4886:TYR:HA	1.84	0.59
2:B:4886:TYR:HA	2:H:4916:ILE:HD11	1.84	0.59
2:D:4916:ILE:HD11	2:F:4886:TYR:HA	1.84	0.59
2:B:3674:SER:HB2	2:B:3694:LEU:HD22	1.85	0.58
2:D:2248:GLN:HE22	2:D:2280:SER:HA	1.68	0.58
2:F:441:VAL:O	2:F:445:LEU:HG	2.03	0.58
2:H:2248:GLN:HE22	2:H:2280:SER:HA	1.68	0.58
2:B:2248:GLN:HE22	2:B:2280:SER:HA	1.68	0.58
2:F:1130:GLN:HA	2:F:1138:LEU:HA	1.85	0.58
2:F:4916:ILE:HD11	2:H:4886:TYR:HA	1.84	0.58
2:H:3674:SER:HB2	2:H:3694:LEU:HD22	1.85	0.58
2:B:1130:GLN:HA	2:B:1138:LEU:HA	1.85	0.58
2:D:260:TRP:HE1	2:D:282:ILE:HG23	1.67	0.58
2:D:3674:SER:HB2	2:D:3694:LEU:HD22	1.85	0.58
2:B:441:VAL:O	2:B:445:LEU:HG	2.03	0.58
2:H:618:GLN:OE1	2:H:1678:ASN:ND2	2.37	0.58
2:H:441:VAL:O	2:H:445:LEU:HG	2.03	0.58
2:D:441:VAL:O	2:D:445:LEU:HG	2.03	0.58
2:D:618:GLN:OE1	2:D:1678:ASN:ND2	2.37	0.58
2:B:1153:ILE:HG13	2:B:1160:ILE:HG12	1.86	0.58
2:D:118:LEU:HA	2:D:137:LEU:HA	1.86	0.58
2:B:118:LEU:HA	2:B:137:LEU:HA	1.86	0.57
2:F:1153:ILE:HG13	2:F:1160:ILE:HG12	1.86	0.57
2:F:1932:LEU:HD12	2:F:1936:VAL:HG21	1.86	0.57
2:H:1153:ILE:HG13	2:H:1160:ILE:HG12	1.86	0.57
2:B:484:LEU:O	2:B:488:LEU:HG	2.04	0.57
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1932:LEU:HD12	2:B:1936:VAL:HG21	1.86	0.57
2:D:1130:GLN:HA	2:D:1138:LEU:HA	1.85	0.57
2:D:1153:ILE:HG13	2:D:1160:ILE:HG12	1.86	0.57
2:F:2248:GLN:HE22	2:F:2280:SER:HA	1.69	0.57
2:F:3674:SER:HB2	2:F:3694:LEU:HD22	1.85	0.57
2:D:484:LEU:O	2:D:488:LEU:HG	2.04	0.57
2:F:1944:LEU:HB2	2:F:2124:LEU:HD11	1.87	0.57
2:D:1932:LEU:HD12	2:D:1936:VAL:HG21	1.86	0.57
2:F:118:LEU:HA	2:F:137:LEU:HA	1.86	0.57
2:H:118:LEU:HA	2:H:137:LEU:HA	1.86	0.57
2:H:1932:LEU:HD12	2:H:1936:VAL:HG21	1.86	0.56
2:B:1932:LEU:HB2	2:B:1937:LYS:HE3	1.87	0.56
2:D:1932:LEU:HB2	2:D:1937:LYS:HE3	1.87	0.56
2:D:1944:LEU:HB2	2:D:2124:LEU:HD11	1.87	0.56
2:H:484:LEU:O	2:H:488:LEU:HG	2.04	0.56
2:H:1932:LEU:HB2	2:H:1937:LYS:HE3	1.87	0.56
2:H:1944:LEU:HB2	2:H:2124:LEU:HD11	1.87	0.56
2:B:35:LEU:HA	2:B:51:PRO:HA	1.88	0.56
2:F:35:LEU:HA	2:F:51:PRO:HA	1.88	0.56
2:F:1739:THR:HG22	2:F:1741:GLU:H	1.71	0.56
2:B:1944:LEU:HB2	2:B:2124:LEU:HD11	1.87	0.56
2:D:1434:TYR:HB2	2:D:1572:ILE:HD11	1.88	0.56
2:F:484:LEU:O	2:F:488:LEU:HG	2.04	0.56
2:F:1434:TYR:HB2	2:F:1572:ILE:HD11	1.88	0.56
2:F:1437:VAL:HG11	2:F:1450:VAL:HG21	1.88	0.56
2:F:3897:TYR:O	2:F:3901:GLN:NE2	2.32	0.56
2:H:1075:PHE:HB2	2:H:1192:CYS:HB2	1.88	0.56
2:H:3897:TYR:O	2:H:3901:GLN:NE2	2.32	0.56
2:B:1434:TYR:HB2	2:B:1572:ILE:HD11	1.88	0.56
2:F:618:GLN:OE1	2:F:1678:ASN:ND2	2.37	0.56
2:D:1437:VAL:HG11	2:D:1450:VAL:HG21	1.88	0.56
2:F:1932:LEU:HB2	2:F:1937:LYS:HE3	1.87	0.56
2:B:642:THR:HG23	2:B:1613:LEU:HD12	1.88	0.55
2:B:1075:PHE:HB2	2:B:1192:CYS:HB2	1.88	0.55
2:H:1437:VAL:HG11	2:H:1450:VAL:HG21	1.88	0.55
2:F:1075:PHE:HB2	2:F:1192:CYS:HB2	1.88	0.55
2:H:35:LEU:HA	2:H:51:PRO:HA	1.88	0.55
2:H:642:THR:HG23	2:H:1613:LEU:HD12	1.88	0.55
2:D:35:LEU:HA	2:D:51:PRO:HA	1.88	0.55
2:B:1739:THR:HG22	2:B:1741:GLU:H	1.71	0.55
2:F:2506:PHE:O	2:F:2510:VAL:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2506:PHE:O	2:H:2510:VAL:HG22	2.07	0.55
2:B:2215:VAL:HG13	2:B:2216:LEU:HD12	1.88	0.55
2:H:1434:TYR:HB2	2:H:1572:ILE:HD11	1.88	0.55
2:D:4011:LEU:HD23	2:D:4015:GLN:HE22	1.72	0.55
2:F:2160:LEU:HA	2:F:2163:ILE:HD12	1.89	0.55
2:B:1437:VAL:HG11	2:B:1450:VAL:HG21	1.88	0.55
2:D:1739:THR:HG22	2:D:1741:GLU:H	1.71	0.54
2:B:4959:CYS:SG	2:B:4960:GLY:N	2.81	0.54
2:F:642:THR:HG23	2:F:1613:LEU:HD12	1.88	0.54
2:H:4959:CYS:SG	2:H:4960:GLY:N	2.81	0.54
2:D:642:THR:HG23	2:D:1613:LEU:HD12	1.88	0.54
2:D:1075:PHE:HB2	2:D:1192:CYS:HB2	1.88	0.54
2:D:2160:LEU:HA	2:D:2163:ILE:HD12	1.89	0.54
2:B:4011:LEU:HD23	2:B:4015:GLN:HE22	1.72	0.54
2:H:1739:THR:HG22	2:H:1741:GLU:H	1.71	0.54
2:B:2506:PHE:O	2:B:2510:VAL:HG22	2.07	0.54
2:D:4959:CYS:SG	2:D:4960:GLY:N	2.81	0.54
2:H:2215:VAL:HG13	2:H:2216:LEU:HD12	1.89	0.54
2:B:1294:PRO:HB3	2:B:1549:PHE:HE1	1.73	0.54
2:F:4011:LEU:HD23	2:F:4015:GLN:HE22	1.72	0.54
2:D:2215:VAL:HG13	2:D:2216:LEU:HD12	1.88	0.54
1:E:7:ILE:HB	1:E:71:ARG:HG3	1.90	0.54
2:F:2215:VAL:HG13	2:F:2216:LEU:HD12	1.88	0.54
1:C:7:ILE:HB	1:C:71:ARG:HG3	1.90	0.53
2:H:2160:LEU:HA	2:H:2163:ILE:HD12	1.89	0.53
2:B:2160:LEU:HA	2:B:2163:ILE:HD12	1.89	0.53
2:D:2506:PHE:O	2:D:2510:VAL:HG22	2.07	0.53
2:F:4976:HIS:CE1	2:F:4981:HIS:ND1	2.77	0.53
2:H:1438:ARG:HA	2:H:1515:VAL:HG12	1.90	0.53
2:H:4011:LEU:HD23	2:H:4015:GLN:HE22	1.72	0.53
2:H:4686:ILE:HG23	2:H:4688:GLU:H	1.74	0.53
2:H:1294:PRO:HB3	2:H:1549:PHE:HE1	1.73	0.53
2:F:4686:ILE:HG23	2:F:4688:GLU:H	1.74	0.53
2:H:583:ILE:O	2:H:587:ILE:HG12	2.09	0.53
2:B:4686:ILE:HG23	2:B:4688:GLU:H	1.74	0.53
2:D:1294:PRO:HB3	2:D:1549:PHE:HE1	1.73	0.53
2:D:1438:ARG:HA	2:D:1515:VAL:HG12	1.90	0.53
2:D:4012:LEU:HD23	2:D:4130:PRO:HB2	1.90	0.53
2:B:4012:LEU:HD23	2:B:4130:PRO:HB2	1.90	0.53
2:F:583:ILE:O	2:F:587:ILE:HG12	2.09	0.53
1:G:7:ILE:HB	1:G:71:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:583:ILE:O	2:B:587:ILE:HG12	2.09	0.53
2:B:3897:TYR:O	2:B:3901:GLN:NE2	2.32	0.53
2:B:3956:VAL:O	2:B:3959:SER:OG	2.26	0.53
2:B:4976:HIS:CE1	2:B:4981:HIS:ND1	2.76	0.53
2:F:4959:CYS:SG	2:F:4960:GLY:N	2.81	0.53
1:A:7:ILE:HB	1:A:71:ARG:HG3	1.90	0.52
2:F:1438:ARG:HA	2:F:1515:VAL:HG12	1.90	0.52
2:F:2230:VAL:HA	2:F:2233:CYS:SG	2.49	0.52
2:H:4976:HIS:CE1	2:H:4981:HIS:ND1	2.77	0.52
2:B:1438:ARG:HA	2:B:1515:VAL:HG12	1.90	0.52
2:D:583:ILE:O	2:D:587:ILE:HG12	2.09	0.52
2:D:4919:PHE:HA	2:D:4923:ILE:HD13	1.91	0.52
2:D:4976:HIS:CE1	2:D:4981:HIS:ND1	2.77	0.52
2:H:2230:VAL:HA	2:H:2233:CYS:SG	2.49	0.52
2:B:1803:ILE:HD12	2:B:1804:PRO:HD2	1.92	0.52
2:B:2230:VAL:HA	2:B:2233:CYS:SG	2.49	0.52
2:B:4919:PHE:HA	2:B:4923:ILE:HD13	1.91	0.52
2:D:2230:VAL:HA	2:D:2233:CYS:SG	2.49	0.52
2:D:1803:ILE:HD12	2:D:1804:PRO:HD2	1.92	0.52
2:B:648:ILE:HG23	2:B:815:VAL:HB	1.93	0.51
2:D:4686:ILE:HG23	2:D:4688:GLU:H	1.74	0.51
2:F:1294:PRO:HB3	2:F:1549:PHE:HE1	1.73	0.51
2:F:2355:VAL:O	2:F:2359:ILE:HG12	2.11	0.51
2:H:4919:PHE:HA	2:H:4923:ILE:HD13	1.91	0.51
2:H:4012:LEU:HD23	2:H:4130:PRO:HB2	1.90	0.51
2:D:1735:ILE:HD11	2:D:2202:LEU:HD11	1.92	0.51
2:F:4012:LEU:HD23	2:F:4130:PRO:HB2	1.90	0.51
2:F:4919:PHE:HA	2:F:4923:ILE:HD13	1.91	0.51
2:H:2355:VAL:O	2:H:2359:ILE:HG12	2.11	0.51
2:B:1735:ILE:HD11	2:B:2202:LEU:HD11	1.92	0.51
1:C:67:SER:OG	1:C:70:GLN:OE1	2.29	0.51
2:H:648:ILE:HG23	2:H:815:VAL:HB	1.93	0.51
2:H:2333:LEU:HD22	2:H:2433:LEU:HD13	1.93	0.51
2:F:1803:ILE:HD12	2:F:1804:PRO:HD2	1.92	0.51
2:D:648:ILE:HG23	2:D:815:VAL:HB	1.93	0.50
2:D:2333:LEU:HD22	2:D:2433:LEU:HD13	1.93	0.50
2:F:4834:GLN:O	2:F:4838:THR:HG22	2.12	0.50
2:D:1720:LEU:HD22	2:D:1848:THR:HG22	1.94	0.50
2:B:3763:ALA:HA	2:B:3766:HIS:HB3	1.94	0.50
2:B:131:LEU:HD11	2:D:2461:LEU:HD22	1.94	0.50
2:B:1720:LEU:HD22	2:B:1848:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:SER:OG	1:G:70:GLN:OE1	2.29	0.50
2:B:2333:LEU:HD22	2:B:2433:LEU:HD13	1.93	0.50
2:D:64:ILE:O	2:D:111:HIS:NE2	2.45	0.50
2:H:1803:ILE:HD12	2:H:1804:PRO:HD2	1.92	0.50
2:B:2461:LEU:HD22	2:H:131:LEU:HD11	1.94	0.50
2:D:2355:VAL:O	2:D:2359:ILE:HG12	2.11	0.50
1:A:67:SER:OG	1:A:70:GLN:OE1	2.29	0.50
2:F:131:LEU:HD11	2:H:2461:LEU:HD22	1.94	0.50
2:F:648:ILE:HG23	2:F:815:VAL:HB	1.93	0.50
2:B:264:PRO:HG3	2:B:270:SER:HA	1.94	0.50
2:B:4834:GLN:O	2:B:4838:THR:HG22	2.12	0.50
2:F:1735:ILE:HD11	2:F:2202:LEU:HD11	1.92	0.50
2:B:219:VAL:HG21	2:B:398:SER:HB3	1.94	0.50
2:B:568:LEU:HD13	2:B:606:LEU:HD13	1.93	0.50
2:D:106:ALA:HA	2:D:149:THR:HA	1.94	0.50
2:B:2355:VAL:O	2:B:2359:ILE:HG12	2.11	0.49
2:D:4834:GLN:O	2:D:4838:THR:HG22	2.12	0.49
2:F:1988:THR:HG23	2:F:1991:GLU:H	1.77	0.49
2:H:264:PRO:HG3	2:H:270:SER:HA	1.94	0.49
2:H:1735:ILE:HD11	2:H:2202:LEU:HD11	1.92	0.49
2:B:64:ILE:O	2:B:111:HIS:NE2	2.45	0.49
2:D:219:VAL:HG21	2:D:398:SER:HB3	1.94	0.49
2:D:1988:THR:HG23	2:D:1991:GLU:H	1.77	0.49
2:F:2333:LEU:HD22	2:F:2433:LEU:HD13	1.93	0.49
2:H:219:VAL:HG21	2:H:398:SER:HB3	1.94	0.49
2:H:4834:GLN:O	2:H:4838:THR:HG22	2.12	0.49
2:D:568:LEU:HD13	2:D:606:LEU:HD13	1.93	0.49
2:F:106:ALA:HA	2:F:149:THR:HA	1.94	0.49
2:F:568:LEU:HD13	2:F:606:LEU:HD13	1.93	0.49
2:H:3763:ALA:HA	2:H:3766:HIS:HB3	1.94	0.49
2:B:106:ALA:HA	2:B:149:THR:HA	1.94	0.49
2:F:64:ILE:O	2:F:111:HIS:NE2	2.45	0.49
2:H:64:ILE:O	2:H:111:HIS:NE2	2.45	0.49
2:D:131:LEU:HD11	2:F:2461:LEU:HD22	1.94	0.49
2:F:219:VAL:HG21	2:F:398:SER:HB3	1.94	0.49
2:F:1720:LEU:HD22	2:F:1848:THR:HG22	1.94	0.49
2:H:1720:LEU:HD22	2:H:1848:THR:HG22	1.94	0.49
2:D:3763:ALA:HA	2:D:3766:HIS:HB3	1.94	0.49
2:B:1988:THR:HG23	2:B:1991:GLU:H	1.77	0.49
2:B:3777:MET:HG2	2:B:3792:THR:HG21	1.95	0.49
2:F:264:PRO:HG3	2:F:270:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1949:ASP:OD1	2:H:2127:ARG:NH2	2.46	0.49
2:H:3777:MET:HG2	2:H:3792:THR:HG21	1.95	0.49
2:H:1988:THR:HG23	2:H:1991:GLU:H	1.77	0.49
2:B:1949:ASP:OD1	2:B:2127:ARG:NH2	2.46	0.49
2:D:1949:ASP:OD1	2:D:2127:ARG:NH2	2.46	0.49
2:F:3763:ALA:HA	2:F:3766:HIS:HB3	1.94	0.49
2:H:1604:SER:OG	2:H:1605:TRP:N	2.46	0.48
2:D:1604:SER:OG	2:D:1605:TRP:N	2.46	0.48
2:F:1949:ASP:OD1	2:F:2127:ARG:NH2	2.46	0.48
2:H:568:LEU:HD13	2:H:606:LEU:HD13	1.93	0.48
2:D:264:PRO:HG3	2:D:270:SER:HA	1.94	0.48
2:F:59:PRO:HB3	2:F:281:ARG:HH11	1.78	0.48
2:F:1604:SER:OG	2:F:1605:TRP:N	2.46	0.48
2:H:106:ALA:HA	2:H:149:THR:HA	1.94	0.48
2:B:1604:SER:OG	2:B:1605:TRP:N	2.46	0.48
2:D:1291:LEU:HD12	2:D:1595:LEU:HD22	1.96	0.48
2:F:1291:LEU:HD12	2:F:1595:LEU:HD22	1.96	0.48
2:F:2522:VAL:HA	2:F:2525:VAL:HG12	1.96	0.48
2:H:2522:VAL:HA	2:H:2525:VAL:HG12	1.96	0.48
2:D:1613:LEU:HD23	2:D:1634:LEU:HD12	1.96	0.48
2:H:2244:SER:OG	2:H:2245:ARG:N	2.46	0.48
2:D:59:PRO:HB3	2:D:281:ARG:HH11	1.79	0.48
2:F:1613:LEU:HD23	2:F:1634:LEU:HD12	1.96	0.48
2:H:551:LEU:HD11	2:H:589:LEU:HD22	1.95	0.48
2:D:2244:SER:OG	2:D:2245:ARG:N	2.46	0.48
2:F:2244:SER:OG	2:F:2245:ARG:N	2.46	0.48
2:H:59:PRO:HB3	2:H:281:ARG:HH11	1.78	0.48
2:B:1291:LEU:HD12	2:B:1595:LEU:HD22	1.96	0.48
2:B:4959:CYS:HB2	2:B:4981:HIS:ND1	2.29	0.48
2:D:771:PHE:HB3	2:D:1472:VAL:HG23	1.96	0.48
2:D:3777:MET:HG2	2:D:3792:THR:HG21	1.95	0.48
2:F:551:LEU:HD11	2:F:589:LEU:HD22	1.95	0.48
2:F:745:SER:O	2:F:758:ARG:N	2.47	0.48
2:F:771:PHE:HB3	2:F:1472:VAL:HG23	1.96	0.47
2:H:1291:LEU:HD12	2:H:1595:LEU:HD22	1.96	0.47
2:B:2244:SER:OG	2:B:2245:ARG:N	2.46	0.47
2:D:4684:LEU:HG	2:D:4685:TYR:HD1	1.80	0.47
2:F:1674:CYS:O	2:F:1717:SER:OG	2.31	0.47
2:F:3777:MET:HG2	2:F:3792:THR:HG21	1.95	0.47
2:H:745:SER:O	2:H:758:ARG:N	2.47	0.47
2:H:771:PHE:HB3	2:H:1472:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:771:PHE:HB3	2:B:1472:VAL:HG23	1.96	0.47
2:B:1613:LEU:HD23	2:B:1634:LEU:HD12	1.96	0.47
2:D:4959:CYS:HB2	2:D:4981:HIS:ND1	2.29	0.47
1:E:67:SER:OG	1:E:70:GLN:OE1	2.29	0.47
2:H:355:LEU:HD22	2:H:380:GLN:HA	1.96	0.47
2:H:1674:CYS:O	2:H:1717:SER:OG	2.31	0.47
2:B:350:HIS:HD2	2:B:352:ALA:H	1.63	0.47
2:H:1779:SER:OG	2:H:1780:ALA:N	2.48	0.47
2:H:1613:LEU:HD23	2:H:1634:LEU:HD12	1.96	0.47
2:B:59:PRO:HB3	2:B:281:ARG:HH11	1.79	0.47
2:D:2522:VAL:HA	2:D:2525:VAL:HG12	1.96	0.47
2:H:3824:PHE:HB3	2:H:3908:ILE:HG21	1.96	0.47
2:B:551:LEU:HD11	2:B:589:LEU:HD22	1.95	0.47
2:D:350:HIS:HD2	2:D:352:ALA:H	1.63	0.47
2:F:3824:PHE:HB3	2:F:3908:ILE:HG21	1.96	0.47
2:B:1779:SER:OG	2:B:1780:ALA:N	2.48	0.47
2:B:4684:LEU:HG	2:B:4685:TYR:HD1	1.80	0.47
2:D:551:LEU:HD11	2:D:589:LEU:HD22	1.95	0.47
2:F:350:HIS:HD2	2:F:352:ALA:H	1.63	0.47
2:H:4684:LEU:HG	2:H:4685:TYR:HD1	1.80	0.47
2:H:4959:CYS:HB2	2:H:4981:HIS:ND1	2.29	0.47
2:F:1110:ARG:NH2	2:F:1112:ASP:OD1	2.48	0.47
2:F:1779:SER:OG	2:F:1780:ALA:N	2.48	0.47
2:H:1110:ARG:NH2	2:H:1112:ASP:OD1	2.48	0.47
2:B:2522:VAL:HA	2:B:2525:VAL:HG12	1.96	0.46
2:D:2277:ALA:O	2:D:2281:VAL:HG23	2.15	0.46
2:D:3756:GLN:OE1	2:D:3756:GLN:HA	2.15	0.46
2:F:4686:ILE:HG13	2:F:4687:THR:H	1.80	0.46
2:F:4959:CYS:HB2	2:F:4981:HIS:ND1	2.29	0.46
2:H:648:ILE:H	2:H:648:ILE:HG13	1.33	0.46
2:B:355:LEU:HD22	2:B:380:GLN:HA	1.96	0.46
2:B:4686:ILE:HG13	2:B:4687:THR:H	1.80	0.46
2:F:2277:ALA:O	2:F:2281:VAL:HG23	2.15	0.46
2:F:4684:LEU:HG	2:F:4685:TYR:HD1	1.80	0.46
2:B:2003:PRO:O	2:B:2007:ILE:HG12	2.16	0.46
2:D:349:GLN:HA	2:D:356:TRP:HA	1.97	0.46
2:D:2351:ALA:HA	2:D:2354:VAL:HG22	1.98	0.46
2:D:3824:PHE:HB3	2:D:3908:ILE:HG21	1.96	0.46
2:D:4686:ILE:HG13	2:D:4687:THR:H	1.80	0.46
2:D:355:LEU:HD22	2:D:380:GLN:HA	1.96	0.46
2:D:1779:SER:OG	2:D:1780:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:350:HIS:HD2	2:H:352:ALA:H	1.63	0.46
2:B:1110:ARG:NH2	2:B:1112:ASP:OD1	2.48	0.46
2:D:1110:ARG:NH2	2:D:1112:ASP:OD1	2.48	0.46
2:D:2003:PRO:O	2:D:2007:ILE:HG12	2.16	0.46
2:F:355:LEU:HD22	2:F:380:GLN:HA	1.96	0.46
2:H:2003:PRO:O	2:H:2007:ILE:HG12	2.16	0.46
2:B:1228:ILE:HD11	2:D:3565:UNK:H2	1.81	0.46
2:F:1228:ILE:HD11	2:H:3565:UNK:H2	1.81	0.46
2:F:3956:VAL:O	2:F:3959:SER:OG	2.26	0.46
2:B:3565:UNK:H2	2:H:1228:ILE:HD11	1.81	0.46
2:B:3824:PHE:HB3	2:B:3908:ILE:HG21	1.96	0.46
2:F:349:GLN:HA	2:F:356:TRP:HA	1.97	0.46
2:F:3756:GLN:OE1	2:F:3756:GLN:HA	2.15	0.46
2:H:349:GLN:HA	2:H:356:TRP:HA	1.97	0.46
2:H:2026:ASP:O	2:H:2030:GLN:HG2	2.16	0.46
2:H:3756:GLN:HA	2:H:3756:GLN:OE1	2.15	0.46
2:B:745:SER:O	2:B:758:ARG:N	2.47	0.46
2:B:2026:ASP:O	2:B:2030:GLN:HG2	2.16	0.46
2:H:2277:ALA:O	2:H:2281:VAL:HG23	2.15	0.46
2:D:2112:VAL:HG13	2:D:2117:LEU:HD22	1.98	0.46
2:D:4571:ILE:O	2:D:4575:LEU:HG	2.16	0.46
2:F:2351:ALA:HA	2:F:2354:VAL:HG22	1.98	0.46
2:F:4571:ILE:O	2:F:4575:LEU:HG	2.16	0.46
2:H:2278:ALA:HB1	2:H:2338:PHE:HD2	1.80	0.46
2:H:4686:ILE:HG13	2:H:4687:THR:H	1.80	0.46
2:B:989:ALA:O	2:B:993:HIS:ND1	2.46	0.45
2:B:2277:ALA:O	2:B:2281:VAL:HG23	2.15	0.45
2:D:149:THR:HG23	2:D:172:VAL:HB	1.98	0.45
2:D:2026:ASP:O	2:D:2030:GLN:HG2	2.16	0.45
2:F:2350:ASN:O	2:F:2354:VAL:HG13	2.16	0.45
2:H:774:ASN:HD21	2:H:1470:ARG:HH12	1.65	0.45
2:B:349:GLN:HA	2:B:356:TRP:HA	1.97	0.45
2:B:4571:ILE:O	2:B:4575:LEU:HG	2.16	0.45
1:C:87:HIS:HB2	1:C:90:VAL:HB	1.97	0.45
2:F:2003:PRO:O	2:F:2007:ILE:HG12	2.16	0.45
2:B:774:ASN:HD21	2:B:1470:ARG:HH12	1.65	0.45
2:D:745:SER:O	2:D:758:ARG:N	2.47	0.45
2:D:1674:CYS:O	2:D:1717:SER:OG	2.31	0.45
2:D:2350:ASN:O	2:D:2354:VAL:HG13	2.17	0.45
2:D:3897:TYR:O	2:D:3901:GLN:NE2	2.32	0.45
2:F:729:LEU:HG	2:F:731:THR:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2278:ALA:HB1	2:F:2338:PHE:HD2	1.80	0.45
2:H:2351:ALA:HA	2:H:2354:VAL:HG22	1.98	0.45
2:H:4571:ILE:O	2:H:4575:LEU:HG	2.16	0.45
2:B:2112:VAL:HG13	2:B:2117:LEU:HD22	1.98	0.45
2:B:2278:ALA:HB1	2:B:2338:PHE:HD2	1.80	0.45
2:D:553:ARG:HG2	2:D:555:GLU:H	1.82	0.45
2:D:1228:ILE:HD11	2:F:3565:UNK:H2	1.81	0.45
2:F:736:HIS:NE2	2:F:739:ALA:HB2	2.32	0.45
2:H:2145:ILE:HD12	2:H:2153:THR:HG21	1.99	0.45
2:B:498:THR:HA	2:B:553:ARG:HH22	1.81	0.45
2:B:3756:GLN:OE1	2:B:3756:GLN:HA	2.15	0.45
2:D:3703:ARG:O	2:D:3707:THR:OG1	2.32	0.45
2:F:149:THR:HG23	2:F:172:VAL:HB	1.98	0.45
2:B:2122:PHE:O	2:B:3721:TYR:OH	2.31	0.45
2:B:2351:ALA:HA	2:B:2354:VAL:HG22	1.98	0.45
2:B:3800:LEU:O	2:B:3885:LEU:HD23	2.17	0.45
2:D:498:THR:HA	2:D:553:ARG:HH22	1.81	0.45
2:D:4959:CYS:HB2	2:D:4981:HIS:HB3	1.99	0.45
2:F:1450:VAL:HG13	2:F:1552:VAL:HG22	1.99	0.45
2:F:4959:CYS:HB2	2:F:4981:HIS:HB3	1.99	0.45
2:H:498:THR:HA	2:H:553:ARG:HH22	1.82	0.45
2:H:729:LEU:HG	2:H:731:THR:H	1.81	0.45
2:D:2278:ALA:HB1	2:D:2338:PHE:HD2	1.80	0.45
2:F:774:ASN:HD21	2:F:1470:ARG:HH12	1.65	0.45
2:B:2597:THR:HG22	2:B:2599:ALA:H	1.82	0.45
2:D:736:HIS:NE2	2:D:739:ALA:HB2	2.32	0.45
2:D:3800:LEU:O	2:D:3885:LEU:HD23	2.17	0.45
2:F:2026:ASP:O	2:F:2030:GLN:HG2	2.16	0.45
1:G:87:HIS:HB2	1:G:90:VAL:HB	1.97	0.45
1:A:87:HIS:HB2	1:A:90:VAL:HB	1.97	0.45
2:B:2350:ASN:O	2:B:2354:VAL:HG13	2.16	0.45
2:D:729:LEU:HG	2:D:731:THR:H	1.81	0.45
2:D:774:ASN:HD21	2:D:1470:ARG:HH12	1.65	0.45
1:E:87:HIS:HB2	1:E:90:VAL:HB	1.97	0.45
2:F:553:ARG:HG2	2:F:555:GLU:H	1.82	0.45
2:B:2145:ILE:HD12	2:B:2153:THR:HG21	1.99	0.45
2:B:2353:VAL:O	2:B:2357:LEU:HG	2.17	0.45
2:F:2597:THR:HG22	2:F:2599:ALA:H	1.82	0.45
2:F:3747:SER:OG	2:F:3748:PHE:N	2.50	0.45
2:H:2350:ASN:O	2:H:2354:VAL:HG13	2.17	0.45
2:H:3800:LEU:O	2:H:3885:LEU:HD23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:THR:HG23	2:B:172:VAL:HB	1.98	0.44
2:D:2353:VAL:O	2:D:2357:LEU:HG	2.17	0.44
2:D:3956:VAL:O	2:D:3960:LEU:HD12	2.17	0.44
2:F:648:ILE:H	2:F:648:ILE:HG13	1.33	0.44
2:H:284:HIS:CD2	2:H:287:THR:H	2.35	0.44
2:H:3747:SER:OG	2:H:3748:PHE:N	2.50	0.44
2:B:4959:CYS:HB2	2:B:4981:HIS:HB3	1.99	0.44
2:D:2597:THR:HG22	2:D:2599:ALA:H	1.82	0.44
2:D:4062:LYS:O	2:D:4066:ILE:HG12	2.17	0.44
2:F:284:HIS:CD2	2:F:287:THR:H	2.35	0.44
2:F:498:THR:HA	2:F:553:ARG:HH22	1.82	0.44
2:F:2145:ILE:HD12	2:F:2153:THR:HG21	1.99	0.44
2:F:4684:LEU:H	2:F:4684:LEU:HD23	1.82	0.44
2:H:49:LEU:HD11	2:H:191:VAL:HG23	2.00	0.44
2:H:2112:VAL:HG13	2:H:2117:LEU:HD22	1.98	0.44
2:B:729:LEU:HG	2:B:731:THR:H	1.81	0.44
2:B:1450:VAL:HG13	2:B:1552:VAL:HG22	1.99	0.44
2:F:3800:LEU:O	2:F:3885:LEU:HD23	2.17	0.44
2:F:3956:VAL:O	2:F:3960:LEU:HD12	2.17	0.44
2:H:1450:VAL:HG13	2:H:1552:VAL:HG22	1.99	0.44
2:H:4684:LEU:H	2:H:4684:LEU:HD23	1.83	0.44
2:B:1517:GLY:N	2:B:1530:THR:O	2.49	0.44
2:D:531:ARG:NH2	2:D:562:GLU:OE2	2.51	0.44
2:D:2145:ILE:HD12	2:D:2153:THR:HG21	1.99	0.44
2:F:49:LEU:HD11	2:F:191:VAL:HG23	2.00	0.44
2:H:2353:VAL:O	2:H:2357:LEU:HG	2.17	0.44
2:B:284:HIS:CD2	2:B:287:THR:H	2.35	0.44
2:B:553:ARG:HG2	2:B:555:GLU:H	1.82	0.44
2:B:736:HIS:NE2	2:B:739:ALA:HB2	2.32	0.44
2:D:989:ALA:O	2:D:993:HIS:ND1	2.46	0.44
2:F:121:LEU:N	2:F:134:ASP:O	2.38	0.44
2:F:2353:VAL:O	2:F:2357:LEU:HG	2.17	0.44
2:F:4062:LYS:O	2:F:4066:ILE:HG12	2.17	0.44
2:F:2112:VAL:HG13	2:F:2117:LEU:HD22	1.98	0.44
2:H:149:THR:HG23	2:H:172:VAL:HB	1.98	0.44
2:H:3926:SER:HB2	2:H:3930:TRP:CZ3	2.48	0.44
2:B:3956:VAL:O	2:B:3960:LEU:HD12	2.17	0.44
2:F:531:ARG:NH2	2:F:562:GLU:OE2	2.51	0.44
2:H:736:HIS:NE2	2:H:739:ALA:HB2	2.32	0.44
2:H:3956:VAL:O	2:H:3960:LEU:HD12	2.17	0.44
2:B:49:LEU:HD11	2:B:191:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:HIS:CD2	2:D:287:THR:H	2.35	0.44
2:D:1450:VAL:HG13	2:D:1552:VAL:HG22	1.99	0.44
2:D:1520:VAL:HG22	2:D:1527:MET:HG2	1.99	0.44
2:D:2122:PHE:O	2:D:3721:TYR:OH	2.31	0.44
2:H:4959:CYS:HB2	2:H:4981:HIS:HB3	1.99	0.44
2:B:4062:LYS:O	2:B:4066:ILE:HG12	2.17	0.43
2:F:4818:VAL:HG22	2:F:4820:THR:H	1.83	0.43
2:B:531:ARG:NH2	2:B:562:GLU:OE2	2.51	0.43
2:D:4684:LEU:HD23	2:D:4684:LEU:H	1.82	0.43
2:H:2597:THR:HG22	2:H:2599:ALA:H	1.82	0.43
2:H:4062:LYS:O	2:H:4066:ILE:HG12	2.17	0.43
2:B:2204:MET:O	2:B:2208:VAL:HG23	2.18	0.43
2:B:4818:VAL:HG22	2:B:4820:THR:H	1.83	0.43
2:D:2252:PHE:HE1	2:D:2255:LEU:HD22	1.84	0.43
2:B:1520:VAL:HG22	2:B:1527:MET:HG2	1.99	0.43
2:B:4684:LEU:HD23	2:B:4684:LEU:H	1.82	0.43
2:H:4818:VAL:HG22	2:H:4820:THR:H	1.83	0.43
2:B:686:TRP:HE1	2:B:746:CYS:HG	1.66	0.43
2:B:1243:PRO:HB2	2:B:1600:LEU:HD11	2.00	0.43
2:D:49:LEU:HD11	2:D:191:VAL:HG23	2.00	0.43
2:D:1243:PRO:HB2	2:D:1600:LEU:HD11	2.00	0.43
2:H:553:ARG:HG2	2:H:555:GLU:H	1.82	0.43
2:H:1243:PRO:HB2	2:H:1600:LEU:HD11	2.00	0.43
2:D:284:HIS:NE2	2:D:286:THR:OG1	2.49	0.43
2:D:2204:MET:O	2:D:2208:VAL:HG23	2.18	0.43
2:H:2204:MET:O	2:H:2208:VAL:HG23	2.18	0.43
2:H:4846:VAL:O	2:H:4850:THR:OG1	2.29	0.43
2:B:2252:PHE:HE1	2:B:2255:LEU:HD22	1.84	0.43
2:D:3835:SER:OG	2:D:3870:MET:O	2.29	0.43
2:F:989:ALA:O	2:F:993:HIS:ND1	2.46	0.43
2:H:2499:HIS:O	2:H:2503:MET:HG2	2.19	0.43
2:B:284:HIS:NE2	2:B:286:THR:OG1	2.49	0.43
2:B:2499:HIS:O	2:B:2503:MET:HG2	2.19	0.43
2:B:3747:SER:OG	2:B:3748:PHE:N	2.50	0.43
2:F:452:PHE:HE1	2:F:474:ARG:HB3	1.84	0.43
2:F:2252:PHE:HE1	2:F:2255:LEU:HD22	1.84	0.43
2:H:1520:VAL:HG22	2:H:1527:MET:HG2	1.99	0.43
2:B:452:PHE:HE1	2:B:474:ARG:HB3	1.84	0.42
2:D:452:PHE:HE1	2:D:474:ARG:HB3	1.84	0.42
2:D:4818:VAL:HG22	2:D:4820:THR:H	1.83	0.42
2:D:4961:ILE:H	2:D:4981:HIS:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1520:VAL:HG22	2:F:1527:MET:HG2	1.99	0.42
2:H:284:HIS:NE2	2:H:286:THR:OG1	2.49	0.42
2:H:531:ARG:NH2	2:H:562:GLU:OE2	2.51	0.42
2:B:1930:MET:HG3	2:B:1932:LEU:HD21	2.02	0.42
2:B:2179:MET:O	2:B:2183:ILE:HG12	2.20	0.42
2:B:3926:SER:HB2	2:B:3930:TRP:CZ3	2.49	0.42
2:B:4846:VAL:O	2:B:4850:THR:OG1	2.29	0.42
2:D:2213:VAL:HG23	2:D:2257:TYR:OH	2.19	0.42
2:D:2499:HIS:O	2:D:2503:MET:HG2	2.19	0.42
2:F:1243:PRO:HB2	2:F:1600:LEU:HD11	2.00	0.42
2:F:2204:MET:O	2:F:2208:VAL:HG23	2.18	0.42
2:H:1517:GLY:N	2:H:1530:THR:O	2.49	0.42
2:H:1930:MET:HG3	2:H:1932:LEU:HD21	2.02	0.42
2:H:3918:LEU:HA	2:H:3921:LEU:HB3	2.01	0.42
2:B:4922:VAL:HG23	2:B:4923:ILE:HD12	2.01	0.42
2:D:4823:THR:HG1	2:D:4938:PHE:HE1	1.68	0.42
2:F:2213:VAL:HG23	2:F:2257:TYR:OH	2.19	0.42
2:F:4922:VAL:HG23	2:F:4923:ILE:HD12	2.01	0.42
2:B:1778:PHE:HB3	2:B:1802:SER:HB3	2.01	0.42
2:D:36:CYS:N	2:D:50:GLU:O	2.53	0.42
2:H:2189:ASN:OD1	2:H:2191:VAL:N	2.53	0.42
2:H:2213:VAL:HG23	2:H:2257:TYR:OH	2.19	0.42
2:B:1674:CYS:O	2:B:1717:SER:OG	2.31	0.42
2:B:2189:ASN:OD1	2:B:2191:VAL:N	2.53	0.42
2:B:4851:VAL:HB	2:D:4805:PHE:HE2	1.85	0.42
2:D:2179:MET:O	2:D:2183:ILE:HG12	2.19	0.42
2:D:3747:SER:OG	2:D:3748:PHE:N	2.50	0.42
1:E:32:ASN:OD1	1:E:33:GLY:N	2.53	0.42
2:F:2100:SER:O	2:F:2104:VAL:HG22	2.20	0.42
2:F:3918:LEU:HA	2:F:3921:LEU:HB3	2.02	0.42
2:F:4961:ILE:H	2:F:4981:HIS:CE1	2.37	0.42
2:H:36:CYS:N	2:H:50:GLU:O	2.53	0.42
2:H:4012:LEU:HD11	2:H:4134:ILE:HG21	2.02	0.42
2:B:36:CYS:N	2:B:50:GLU:O	2.53	0.42
2:B:3918:LEU:HA	2:B:3921:LEU:HB3	2.01	0.42
2:B:4686:ILE:HD12	2:B:4686:ILE:HA	1.96	0.42
2:D:1517:GLY:N	2:D:1530:THR:O	2.49	0.42
2:D:2613:ARG:O	2:D:2615:ILE:HD12	2.20	0.42
2:D:3892:ASN:O	2:D:3896:ASN:ND2	2.53	0.42
2:F:2499:HIS:O	2:F:2503:MET:HG2	2.19	0.42
2:F:4012:LEU:HD11	2:F:4134:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2179:MET:O	2:H:2183:ILE:HG12	2.19	0.42
2:H:2252:PHE:HE1	2:H:2255:LEU:HD22	1.84	0.42
2:B:2100:SER:O	2:B:2104:VAL:HG22	2.20	0.42
2:D:1670:TYR:HB3	2:D:1714:LEU:HD11	2.02	0.42
2:H:2100:SER:O	2:H:2104:VAL:HG22	2.20	0.42
2:D:223:PHE:O	2:D:389:SER:N	2.52	0.42
2:D:1930:MET:HG3	2:D:1932:LEU:HD21	2.02	0.42
2:D:4851:VAL:HB	2:F:4805:PHE:HE2	1.85	0.42
2:F:36:CYS:N	2:F:50:GLU:O	2.53	0.42
2:F:1930:MET:HG3	2:F:1932:LEU:HD21	2.02	0.42
1:C:32:ASN:OD1	1:C:33:GLY:N	2.53	0.42
2:D:2100:SER:O	2:D:2104:VAL:HG22	2.20	0.42
2:H:1736:VAL:HG12	2:H:1738:LEU:H	1.85	0.42
2:H:4947:GLN:O	2:H:4951:ASP:N	2.53	0.42
2:B:3892:ASN:O	2:B:3896:ASN:ND2	2.53	0.42
2:B:4961:ILE:H	2:B:4981:HIS:CE1	2.38	0.42
2:D:4012:LEU:HD11	2:D:4134:ILE:HG21	2.02	0.42
2:F:1736:VAL:HG12	2:F:1738:LEU:H	1.85	0.42
2:H:452:PHE:HE1	2:H:474:ARG:HB3	1.84	0.42
2:H:1778:PHE:HB3	2:H:1802:SER:HB3	2.01	0.42
2:H:4922:VAL:HG23	2:H:4923:ILE:HD12	2.01	0.42
2:B:2213:VAL:HG23	2:B:2257:TYR:OH	2.19	0.41
2:B:2613:ARG:O	2:B:2615:ILE:HD12	2.20	0.41
2:F:774:ASN:OD1	2:F:1470:ARG:NH2	2.50	0.41
2:F:1778:PHE:HB3	2:F:1802:SER:HB3	2.01	0.41
2:F:3892:ASN:O	2:F:3896:ASN:ND2	2.53	0.41
2:F:3998:LEU:HG	2:F:4007:LEU:HD22	2.02	0.41
2:B:206:CYS:HB2	2:B:271:GLY:HA3	2.01	0.41
2:B:774:ASN:OD1	2:B:1470:ARG:NH2	2.50	0.41
2:B:1736:VAL:HG12	2:B:1738:LEU:H	1.85	0.41
2:D:121:LEU:N	2:D:134:ASP:O	2.38	0.41
2:H:989:ALA:O	2:H:993:HIS:ND1	2.46	0.41
2:H:2122:PHE:O	2:H:3721:TYR:OH	2.31	0.41
2:B:4012:LEU:HD11	2:B:4134:ILE:HG21	2.02	0.41
2:F:1670:TYR:HB3	2:F:1714:LEU:HD11	2.02	0.41
1:G:32:ASN:OD1	1:G:33:GLY:N	2.53	0.41
2:H:3956:VAL:O	2:H:3959:SER:OG	2.26	0.41
2:B:223:PHE:O	2:B:389:SER:N	2.52	0.41
2:F:206:CYS:HB2	2:F:271:GLY:HA3	2.01	0.41
2:F:4851:VAL:HB	2:H:4805:PHE:HE2	1.84	0.41
2:H:206:CYS:HB2	2:H:271:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2112:VAL:HG11	2:H:2118:VAL:HB	2.02	0.41
1:C:78:PRO:HG3	1:C:96:THR:HG22	2.03	0.41
2:D:2197:ASN:OD1	2:D:2200:ARG:NH2	2.46	0.41
1:E:78:PRO:HG3	1:E:96:THR:HG22	2.03	0.41
2:F:2613:ARG:O	2:F:2615:ILE:HD12	2.20	0.41
2:H:3892:ASN:O	2:H:3896:ASN:ND2	2.53	0.41
2:H:4961:ILE:H	2:H:4981:HIS:CE1	2.38	0.41
2:B:1936:VAL:O	2:B:1940:MET:HG2	2.21	0.41
2:B:2112:VAL:HG11	2:B:2118:VAL:HB	2.02	0.41
2:B:4805:PHE:HE2	2:H:4851:VAL:HB	1.85	0.41
2:D:498:THR:HG23	2:D:499:THR:HG22	2.02	0.41
2:D:1778:PHE:HB3	2:D:1802:SER:HB3	2.01	0.41
2:D:3918:LEU:HA	2:D:3921:LEU:HB3	2.02	0.41
2:D:4237:ILE:HD12	2:D:4991:MET:HE2	2.03	0.41
2:D:4922:VAL:HG23	2:D:4923:ILE:HD12	2.01	0.41
2:F:2179:MET:O	2:F:2183:ILE:HG12	2.19	0.41
2:D:206:CYS:HB2	2:D:271:GLY:HA3	2.01	0.41
2:F:284:HIS:NE2	2:F:286:THR:OG1	2.49	0.41
2:F:2189:ASN:OD1	2:F:2191:VAL:N	2.53	0.41
2:H:461:HIS:CD2	2:H:3703:ARG:HG2	2.56	0.41
2:H:2292:GLN:O	2:H:2296:LEU:HD23	2.21	0.41
1:A:32:ASN:OD1	1:A:33:GLY:N	2.53	0.41
2:D:1736:VAL:HG12	2:D:1738:LEU:H	1.85	0.41
2:D:3998:LEU:HG	2:D:4007:LEU:HD22	2.02	0.41
2:F:2122:PHE:O	2:F:3721:TYR:OH	2.31	0.41
2:H:686:TRP:HE1	2:H:746:CYS:HG	1.66	0.41
2:H:2296:LEU:O	2:H:2300:VAL:HG13	2.21	0.41
2:B:121:LEU:N	2:B:134:ASP:O	2.38	0.41
2:B:1271:ARG:HA	2:B:1563:GLN:HA	2.03	0.41
2:B:1293:LEU:HD21	2:B:1594:ARG:HB3	2.03	0.41
2:B:3835:SER:OG	2:B:3870:MET:O	2.29	0.41
2:D:350:HIS:CD2	2:D:352:ALA:H	2.39	0.41
2:D:2351:ALA:O	2:D:2355:VAL:HG22	2.21	0.41
2:D:4961:ILE:N	2:D:4981:HIS:HE1	2.19	0.41
2:F:1271:ARG:HA	2:F:1563:GLN:HA	2.03	0.41
2:F:4961:ILE:N	2:F:4981:HIS:HE1	2.19	0.41
2:H:2506:PHE:CZ	2:H:2510:VAL:HG21	2.56	0.41
2:B:350:HIS:CD2	2:B:352:ALA:H	2.39	0.41
2:B:648:ILE:H	2:B:648:ILE:HG13	1.33	0.41
2:B:1670:TYR:HB3	2:B:1714:LEU:HD11	2.02	0.41
2:D:2506:PHE:CZ	2:D:2510:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2351:ALA:O	2:F:2355:VAL:HG22	2.21	0.41
2:F:2506:PHE:CZ	2:F:2510:VAL:HG21	2.56	0.41
1:G:78:PRO:HG3	1:G:96:THR:HG22	2.03	0.41
2:H:223:PHE:O	2:H:389:SER:N	2.52	0.41
2:H:2613:ARG:O	2:H:2615:ILE:HD12	2.20	0.41
2:B:1088:TRP:HA	2:B:1224:GLU:O	2.21	0.40
2:D:461:HIS:CD2	2:D:3703:ARG:HG2	2.56	0.40
2:D:1936:VAL:O	2:D:1940:MET:HG2	2.21	0.40
2:F:2292:GLN:O	2:F:2296:LEU:HD23	2.21	0.40
2:H:1088:TRP:HA	2:H:1224:GLU:O	2.21	0.40
2:H:1271:ARG:HA	2:H:1563:GLN:HA	2.03	0.40
2:H:2197:ASN:OD1	2:H:2200:ARG:NH2	2.46	0.40
1:A:78:PRO:HG3	1:A:96:THR:HG22	2.03	0.40
2:D:774:ASN:OD1	2:D:1470:ARG:NH2	2.50	0.40
2:D:3919:LEU:HD12	2:D:3919:LEU:HA	1.96	0.40
2:F:2296:LEU:O	2:F:2300:VAL:HG13	2.21	0.40
2:H:4686:ILE:HD12	2:H:4686:ILE:HA	1.96	0.40
2:B:2292:GLN:O	2:B:2296:LEU:HD23	2.21	0.40
2:B:4961:ILE:N	2:B:4981:HIS:HE1	2.19	0.40
2:D:1293:LEU:HD21	2:D:1594:ARG:HB3	2.03	0.40
2:F:498:THR:HG23	2:F:499:THR:HG22	2.03	0.40
2:F:1936:VAL:O	2:F:1940:MET:HG2	2.21	0.40
2:F:2112:VAL:HG11	2:F:2118:VAL:HB	2.02	0.40
2:F:3926:SER:HB2	2:F:3930:TRP:CZ3	2.49	0.40
2:H:479:GLN:HA	2:H:484:LEU:HD11	2.04	0.40
2:H:498:THR:HG23	2:H:499:THR:HG22	2.03	0.40
2:B:3998:LEU:HG	2:B:4007:LEU:HD22	2.02	0.40
2:D:1271:ARG:HA	2:D:1563:GLN:HA	2.03	0.40
2:D:2112:VAL:HG11	2:D:2118:VAL:HB	2.02	0.40
2:F:461:HIS:CD2	2:F:3703:ARG:HG2	2.56	0.40
2:F:1088:TRP:HA	2:F:1224:GLU:O	2.21	0.40
2:H:2351:ALA:O	2:H:2355:VAL:HG22	2.21	0.40
2:H:3998:LEU:HG	2:H:4007:LEU:HD22	2.02	0.40
2:B:461:HIS:CD2	2:B:3703:ARG:HG2	2.56	0.40
2:B:682:LEU:HD21	2:B:787:VAL:HG11	2.04	0.40
2:D:479:GLN:HA	2:D:484:LEU:HD11	2.04	0.40
2:D:2324:TRP:HH2	2:D:2423:ILE:HA	1.86	0.40
2:F:1155:LEU:HD23	2:F:1155:LEU:HA	1.95	0.40
2:H:4026:LEU:HD12	2:H:4026:LEU:HA	1.95	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	99/106 (93%)	97 (98%)	2 (2%)	0	100	100
1	C	99/106 (93%)	97 (98%)	2 (2%)	0	100	100
1	E	99/106 (93%)	97 (98%)	2 (2%)	0	100	100
1	G	99/106 (93%)	97 (98%)	2 (2%)	0	100	100
2	B	3316/3716 (89%)	3264 (98%)	52 (2%)	0	100	100
2	D	3316/3716 (89%)	3264 (98%)	52 (2%)	0	100	100
2	F	3316/3716 (89%)	3264 (98%)	52 (2%)	0	100	100
2	H	3316/3716 (89%)	3262 (98%)	54 (2%)	0	100	100
All	All	13660/15288 (89%)	13442 (98%)	218 (2%)	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	49/87 (56%)	49 (100%)	0	100	100
1	C	49/87 (56%)	49 (100%)	0	100	100
1	E	49/87 (56%)	49 (100%)	0	100	100
1	G	49/87 (56%)	49 (100%)	0	100	100
2	B	1599/2967 (54%)	1590 (99%)	9 (1%)	86	92
2	D	1599/2967 (54%)	1590 (99%)	9 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	1599/2967 (54%)	1590 (99%)	9 (1%)	86	92
2	H	1599/2967 (54%)	1590 (99%)	9 (1%)	86	92
All	All	6592/12216 (54%)	6556 (100%)	36 (0%)	89	93

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	73	LEU
2	B	215	THR
2	B	648	ILE
2	B	1273	THR
2	B	1485	SER
2	B	2102	THR
2	B	3879	LEU
2	B	4195	THR
2	B	4838	THR
2	D	73	LEU
2	D	215	THR
2	D	648	ILE
2	D	1273	THR
2	D	1485	SER
2	D	2102	THR
2	D	3879	LEU
2	D	4195	THR
2	D	4838	THR
2	F	73	LEU
2	F	215	THR
2	F	648	ILE
2	F	1273	THR
2	F	1485	SER
2	F	2102	THR
2	F	3879	LEU
2	F	4195	THR
2	F	4838	THR
2	H	73	LEU
2	H	215	THR
2	H	648	ILE
2	H	1273	THR
2	H	1485	SER
2	H	2102	THR
2	H	3879	LEU

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Mol	Chain	Res	Type
2	H	4195	THR
2	H	4838	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
2	B	57	ASN
2	B	350	HIS
2	B	379	HIS
2	B	636	ASN
2	B	848	HIS
2	B	1678	ASN
2	B	1702	HIS
2	B	2194	GLN
2	B	3663	HIS
2	B	3766	HIS
2	B	3972	GLN
2	B	4015	GLN
2	B	4049	ASN
2	B	4931	GLN
1	C	87	HIS
2	D	57	ASN
2	D	350	HIS
2	D	379	HIS
2	D	636	ASN
2	D	848	HIS
2	D	1678	ASN
2	D	1702	HIS
2	D	2194	GLN
2	D	3663	HIS
2	D	3766	HIS
2	D	3972	GLN
2	D	4015	GLN
2	D	4049	ASN
2	D	4931	GLN
1	E	87	HIS
2	F	57	ASN
2	F	350	HIS
2	F	379	HIS
2	F	636	ASN
2	F	848	HIS

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Mol	Chain	Res	Type
2	F	1678	ASN
2	F	1702	HIS
2	F	2162	GLN
2	F	2194	GLN
2	F	3663	HIS
2	F	3766	HIS
2	F	3972	GLN
2	F	4015	GLN
2	F	4049	ASN
2	F	4931	GLN
1	G	87	HIS
2	H	57	ASN
2	H	350	HIS
2	H	379	HIS
2	H	636	ASN
2	H	848	HIS
2	H	1678	ASN
2	H	1702	HIS
2	H	2162	GLN
2	H	2194	GLN
2	H	3663	HIS
2	H	3766	HIS
2	H	3828	GLN
2	H	3972	GLN
2	H	4015	GLN
2	H	4049	ASN
2	H	4931	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	58
2	D	58
2	F	58
2	H	58

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3606:UNK	C	3636:PRO	N	48.84
1	D	3606:UNK	C	3636:PRO	N	48.84
1	F	3606:UNK	C	3636:PRO	N	48.84
1	H	3606:UNK	C	3636:PRO	N	48.84
1	B	1054:GLU	C	1071:ARG	N	39.53
1	D	1054:GLU	C	1071:ARG	N	39.53
1	F	1054:GLU	C	1071:ARG	N	39.53
1	H	1054:GLU	C	1071:ARG	N	39.53
1	B	2700:UNK	C	2736:ASP	N	30.16
1	B	4737:GLU	C	4761:GLY	N	30.16
1	D	2700:UNK	C	2736:ASP	N	30.16
1	D	4737:GLU	C	4761:GLY	N	30.16
1	F	2700:UNK	C	2736:ASP	N	30.16

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	4737:GLU	C	4761:GLY	N	30.16
1	H	2700:UNK	C	2736:ASP	N	30.16
1	H	4737:GLU	C	4761:GLY	N	30.16
1	B	3238:UNK	C	3292:UNK	N	27.65
1	D	3238:UNK	C	3292:UNK	N	27.65
1	F	3238:UNK	C	3292:UNK	N	27.65
1	H	3238:UNK	C	3292:UNK	N	27.65
1	B	3555:UNK	C	3565:UNK	N	27.02
1	D	3555:UNK	C	3565:UNK	N	27.02
1	F	3555:UNK	C	3565:UNK	N	27.02
1	H	3555:UNK	C	3565:UNK	N	27.02
1	B	4239:GLU	C	4543:GLU	N	25.66
1	D	4239:GLU	C	4543:GLU	N	25.66
1	F	4239:GLU	C	4543:GLU	N	25.66
1	H	4239:GLU	C	4543:GLU	N	25.66
1	B	2939:ARG	C	2956:UNK	N	24.97
1	D	2939:ARG	C	2956:UNK	N	24.97
1	F	2939:ARG	C	2956:UNK	N	24.97
1	H	2939:ARG	C	2956:UNK	N	24.96
1	B	2830:GLU	C	2855:TYR	N	24.07
1	D	2830:GLU	C	2855:TYR	N	24.06
1	F	2830:GLU	C	2855:TYR	N	24.06
1	H	2830:GLU	C	2855:TYR	N	24.06
1	B	1299:GLN	C	1428:LEU	N	22.11
1	D	1299:GLN	C	1428:LEU	N	22.11
1	F	1299:GLN	C	1428:LEU	N	22.11
1	H	1299:GLN	C	1428:LEU	N	22.11
1	B	971:ASP	C	980:ALA	N	20.32
1	D	971:ASP	C	980:ALA	N	20.32
1	F	971:ASP	C	980:ALA	N	20.32
1	H	971:ASP	C	980:ALA	N	20.32
1	B	2653:UNK	C	2664:UNK	N	19.61
1	B	3193:UNK	C	3202:UNK	N	19.61
1	D	2653:UNK	C	2664:UNK	N	19.61
1	D	3193:UNK	C	3202:UNK	N	19.61
1	F	2653:UNK	C	2664:UNK	N	19.61
1	F	3193:UNK	C	3202:UNK	N	19.61
1	H	2653:UNK	C	2664:UNK	N	19.61
1	H	3193:UNK	C	3202:UNK	N	19.61
1	B	3731:LEU	C	3747:SER	N	19.49
1	D	3731:LEU	C	3747:SER	N	19.49
1	F	3731:LEU	C	3747:SER	N	19.49

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	3731:LEU	C	3747:SER	N	19.49
1	B	84:ASN	C	97:GLY	N	18.90
1	D	84:ASN	C	97:GLY	N	18.90
1	F	84:ASN	C	97:GLY	N	18.90
1	H	84:ASN	C	97:GLY	N	18.90
1	B	855:PRO	C	863:LEU	N	18.87
1	D	855:PRO	C	863:LEU	N	18.87
1	F	855:PRO	C	863:LEU	N	18.87
1	H	855:PRO	C	863:LEU	N	18.87
1	B	2527:PHE	C	2548:ALA	N	18.11
1	D	2527:PHE	C	2548:ALA	N	18.11
1	F	2527:PHE	C	2548:ALA	N	18.11
1	H	2527:PHE	C	2548:ALA	N	18.11
1	B	3574:UNK	C	3586:UNK	N	17.76
1	D	3574:UNK	C	3586:UNK	N	17.76
1	F	3574:UNK	C	3586:UNK	N	17.76
1	H	3574:UNK	C	3586:UNK	N	17.76
1	B	2046:GLN	C	2092:LEU	N	17.69
1	D	2046:GLN	C	2092:LEU	N	17.69
1	F	2046:GLN	C	2092:LEU	N	17.69
1	H	2046:GLN	C	2092:LEU	N	17.69
1	B	3062:UNK	C	3146:UNK	N	16.16
1	D	3062:UNK	C	3146:UNK	N	16.16
1	F	3062:UNK	C	3146:UNK	N	16.15
1	H	3062:UNK	C	3146:UNK	N	16.15
1	B	3166:UNK	C	3173:UNK	N	15.90
1	D	3166:UNK	C	3173:UNK	N	15.90
1	F	3166:UNK	C	3173:UNK	N	15.90
1	H	3166:UNK	C	3173:UNK	N	15.90
1	B	323:LEU	C	328:LYS	N	15.44
1	D	323:LEU	C	328:LYS	N	15.44
1	F	323:LEU	C	328:LYS	N	15.44
1	H	323:LEU	C	328:LYS	N	15.44
1	B	4090:LYS	C	4109:UNK	N	15.01
1	D	4090:LYS	C	4109:UNK	N	15.01
1	F	4090:LYS	C	4109:UNK	N	15.01
1	H	4090:LYS	C	4109:UNK	N	15.01
1	B	3461:VAL	C	3509:UNK	N	14.54
1	D	3461:VAL	C	3509:UNK	N	14.54
1	F	3461:VAL	C	3509:UNK	N	14.54
1	H	3461:VAL	C	3509:UNK	N	14.54
1	B	2629:PHE	C	2641:UNK	N	14.36

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	2629:PHE	C	2641:UNK	N	14.36
1	F	2629:PHE	C	2641:UNK	N	14.36
1	H	2629:PHE	C	2641:UNK	N	14.36
1	B	2263:GLY	C	2271:SER	N	14.28
1	D	2263:GLY	C	2271:SER	N	14.28
1	F	2263:GLY	C	2271:SER	N	14.28
1	H	2263:GLY	C	2271:SER	N	14.28
1	B	3358:UNK	C	3366:UNK	N	13.72
1	D	3358:UNK	C	3366:UNK	N	13.72
1	F	3358:UNK	C	3366:UNK	N	13.72
1	H	3358:UNK	C	3366:UNK	N	13.72
1	B	1628:VAL	C	1633:PRO	N	13.63
1	D	1628:VAL	C	1633:PRO	N	13.63
1	F	1628:VAL	C	1633:PRO	N	13.63
1	H	1628:VAL	C	1633:PRO	N	13.63
1	B	3018:UNK	C	3032:UNK	N	13.56
1	D	3018:UNK	C	3032:UNK	N	13.56
1	F	3018:UNK	C	3032:UNK	N	13.56
1	H	3018:UNK	C	3032:UNK	N	13.56
1	B	3335:UNK	C	3346:UNK	N	13.39
1	D	3335:UNK	C	3346:UNK	N	13.39
1	F	3335:UNK	C	3346:UNK	N	13.39
1	H	3335:UNK	C	3346:UNK	N	13.39
1	B	2512:GLY	C	2518:PHE	N	13.27
1	F	2512:GLY	C	2518:PHE	N	13.27
1	H	2512:GLY	C	2518:PHE	N	13.27
1	D	2512:GLY	C	2518:PHE	N	13.26
1	B	3676:ALA	C	3689:LYS	N	13.14
1	D	3676:ALA	C	3689:LYS	N	13.14
1	F	3676:ALA	C	3689:LYS	N	13.14
1	H	3676:ALA	C	3689:LYS	N	13.14
1	B	1871:VAL	C	1924:GLU	N	13.11
1	D	1871:VAL	C	1924:GLU	N	13.11
1	F	1871:VAL	C	1924:GLU	N	13.11
1	H	1871:VAL	C	1924:GLU	N	13.11
1	B	1501:VAL	C	1510:SER	N	12.64
1	D	1501:VAL	C	1510:SER	N	12.64
1	F	1501:VAL	C	1510:SER	N	12.64
1	H	1501:VAL	C	1510:SER	N	12.64
1	B	3851:LEU	C	3866:GLY	N	12.53
1	D	3851:LEU	C	3866:GLY	N	12.53
1	F	3851:LEU	C	3866:GLY	N	12.53

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	3851:LEU	C	3866:GLY	N	12.53
1	B	3385:UNK	C	3398:GLU	N	12.42
1	D	3385:UNK	C	3398:GLU	N	12.42
1	F	3385:UNK	C	3398:GLU	N	12.42
1	H	3385:UNK	C	3398:GLU	N	12.42
1	B	3217:UNK	C	3225:UNK	N	12.32
1	D	3217:UNK	C	3225:UNK	N	12.32
1	F	3217:UNK	C	3225:UNK	N	12.32
1	H	3217:UNK	C	3225:UNK	N	12.32
1	B	2479:THR	C	2491:MET	N	12.18
1	D	2479:THR	C	2491:MET	N	12.18
1	F	2479:THR	C	2491:MET	N	12.18
1	H	2479:THR	C	2491:MET	N	12.18
1	B	2571:ALA	C	2579:MET	N	11.70
1	D	2385:ILE	C	2422:ALA	N	11.70
1	D	2571:ALA	C	2579:MET	N	11.70
1	F	2385:ILE	C	2422:ALA	N	11.70
1	F	2571:ALA	C	2579:MET	N	11.70
1	H	2571:ALA	C	2579:MET	N	11.70
1	B	2385:ILE	C	2422:ALA	N	11.69
1	H	2385:ILE	C	2422:ALA	N	11.69
1	B	4584:PRO	C	4626:VAL	N	11.60
1	D	4584:PRO	C	4626:VAL	N	11.60
1	F	4584:PRO	C	4626:VAL	N	11.60
1	H	4584:PRO	C	4626:VAL	N	11.60
1	B	2978:UNK	C	2999:UNK	N	11.39
1	D	2978:UNK	C	2999:UNK	N	11.39
1	F	2978:UNK	C	2999:UNK	N	11.39
1	H	2978:UNK	C	2999:UNK	N	11.39
1	B	2014:LYS	C	2023:PRO	N	11.34
1	D	2014:LYS	C	2023:PRO	N	11.34
1	F	2014:LYS	C	2023:PRO	N	11.34
1	H	2014:LYS	C	2023:PRO	N	11.34
1	B	3308:UNK	C	3320:UNK	N	11.21
1	D	3308:UNK	C	3320:UNK	N	11.21
1	H	3308:UNK	C	3320:UNK	N	11.21
1	F	3308:UNK	C	3320:UNK	N	11.20
1	D	2683:UNK	C	2688:UNK	N	11.04
1	B	2683:UNK	C	2688:UNK	N	11.03
1	F	2683:UNK	C	2688:UNK	N	11.03
1	H	2683:UNK	C	2688:UNK	N	11.03
1	B	1788:PRO	C	1794:GLU	N	10.94

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1788:PRO	C	1794:GLU	N	10.94
1	F	1788:PRO	C	1794:GLU	N	10.94
1	H	1788:PRO	C	1794:GLU	N	10.94
1	B	1750:PRO	C	1760:ARG	N	10.39
1	D	1750:PRO	C	1760:ARG	N	10.39
1	F	1750:PRO	C	1760:ARG	N	10.39
1	H	1750:PRO	C	1760:ARG	N	10.39
1	B	4690:PRO	C	4695:VAL	N	9.67
1	D	4690:PRO	C	4695:VAL	N	9.67
1	F	4690:PRO	C	4695:VAL	N	9.67
1	H	4690:PRO	C	4695:VAL	N	9.67
1	B	4114:UNK	C	4122:GLU	N	9.61
1	D	4114:UNK	C	4122:GLU	N	9.61
1	F	4114:UNK	C	4122:GLU	N	9.61
1	H	4114:UNK	C	4122:GLU	N	9.61
1	B	3526:UNK	C	3534:UNK	N	9.55
1	D	3526:UNK	C	3534:UNK	N	9.55
1	F	3526:UNK	C	3534:UNK	N	9.55
1	H	3526:UNK	C	3534:UNK	N	9.55
1	B	361:ALA	C	372:LEU	N	9.53
1	D	361:ALA	C	372:LEU	N	9.53
1	F	361:ALA	C	372:LEU	N	9.53
1	H	361:ALA	C	372:LEU	N	9.53
1	B	3544:UNK	C	3548:UNK	N	9.38
1	D	3544:UNK	C	3548:UNK	N	9.38
1	F	3544:UNK	C	3548:UNK	N	9.38
1	H	3544:UNK	C	3548:UNK	N	9.38
1	B	2370:ARG	C	2377:LEU	N	8.90
1	D	2370:ARG	C	2377:LEU	N	8.90
1	F	2370:ARG	C	2377:LEU	N	8.90
1	H	2370:ARG	C	2377:LEU	N	8.90
1	B	2216:LEU	C	2225:ARG	N	8.03
1	D	2216:LEU	C	2225:ARG	N	8.03
1	F	2216:LEU	C	2225:ARG	N	8.03
1	H	2216:LEU	C	2225:ARG	N	8.03
1	B	3047:UNK	C	3051:UNK	N	6.30
1	D	3047:UNK	C	3051:UNK	N	6.30
1	F	3047:UNK	C	3051:UNK	N	6.30
1	H	3047:UNK	C	3051:UNK	N	6.30
1	B	299:LEU	C	301:VAL	N	5.74
1	D	299:LEU	C	301:VAL	N	5.74
1	F	299:LEU	C	301:VAL	N	5.74

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	299:LEU	C	301:VAL	N	5.74
1	B	1478:ASP	C	1482:ASN	N	5.49
1	D	1478:ASP	C	1482:ASN	N	5.49
1	F	1478:ASP	C	1482:ASN	N	5.49
1	H	1478:ASP	C	1482:ASN	N	5.49
1	B	1275:ARG	C	1282:SER	N	4.75
1	D	1275:ARG	C	1282:SER	N	4.75
1	F	1275:ARG	C	1282:SER	N	4.75
1	H	1275:ARG	C	1282:SER	N	4.75

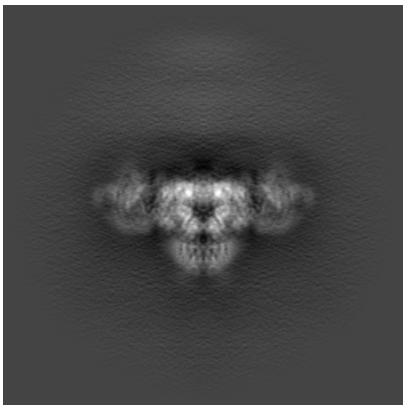
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22017. These allow visual inspection of the internal detail of the map and identification of artifacts.

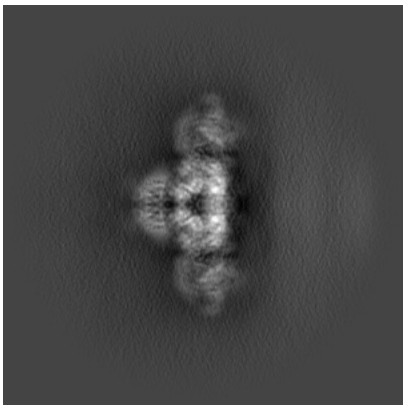
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

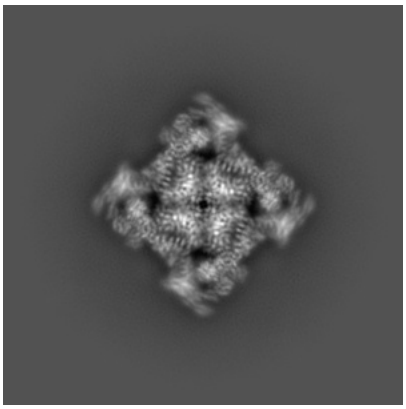
6.1.1 Primary map



X

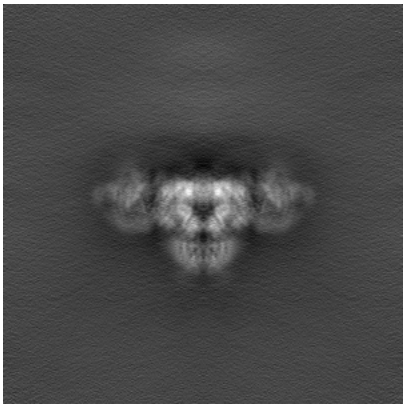


Y

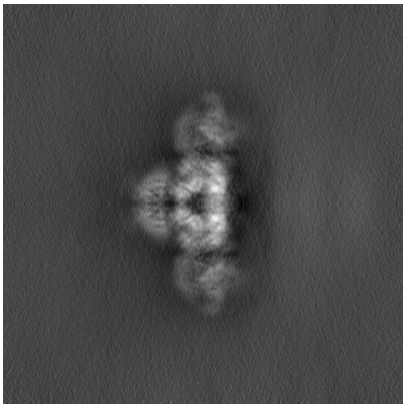


Z

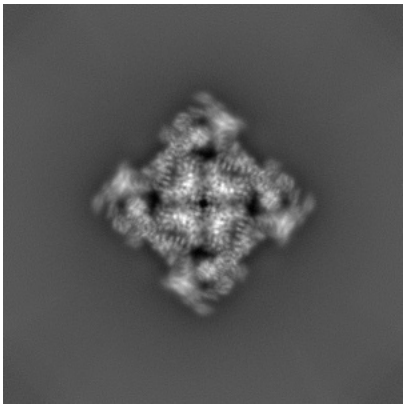
6.1.2 Raw map



X



Y

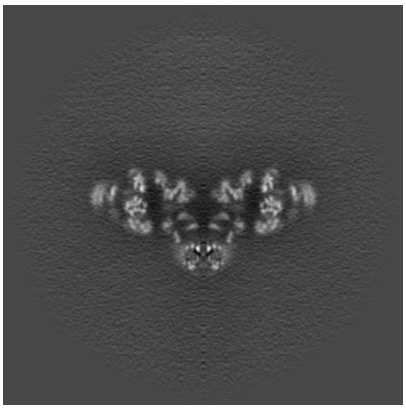


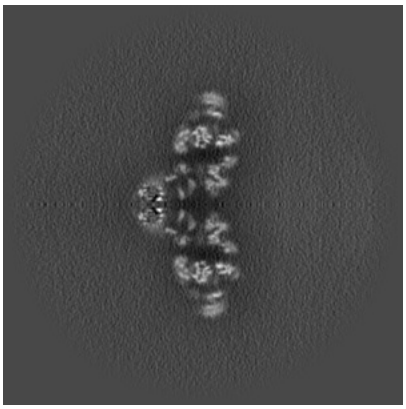
Z

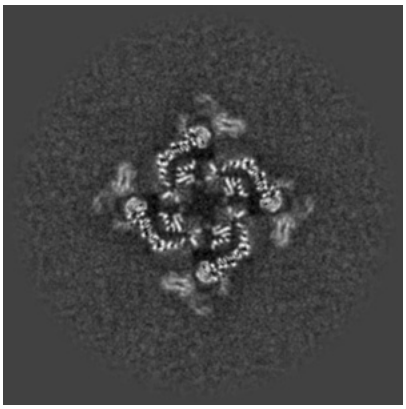
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

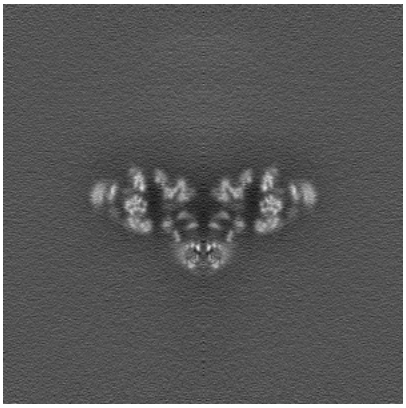
6.2.1 Primary map

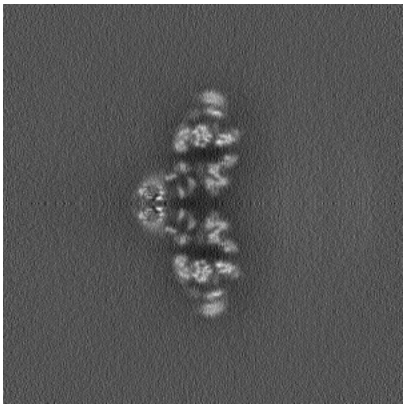

X Index: 240

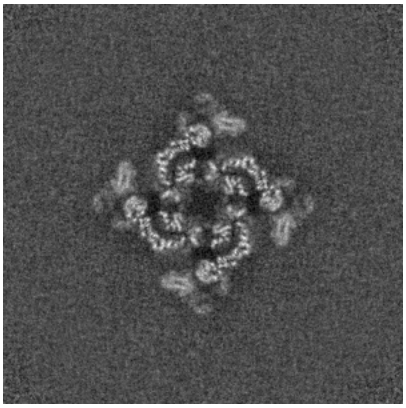

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

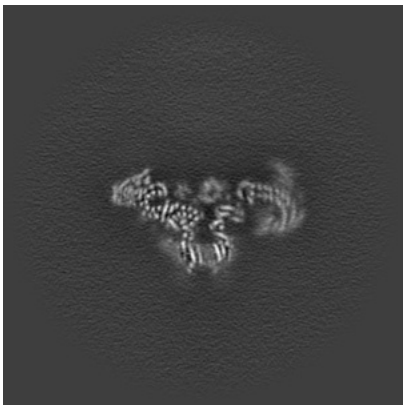

Y Index: 240


Z Index: 240

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

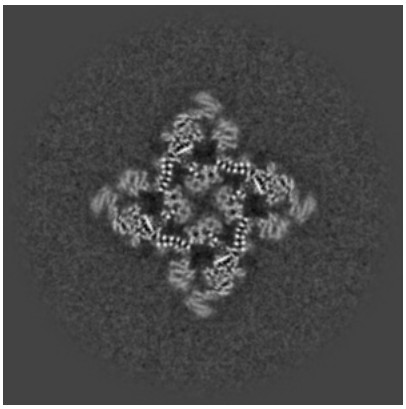
6.3 Largest variance slices (i)

6.3.1 Primary map



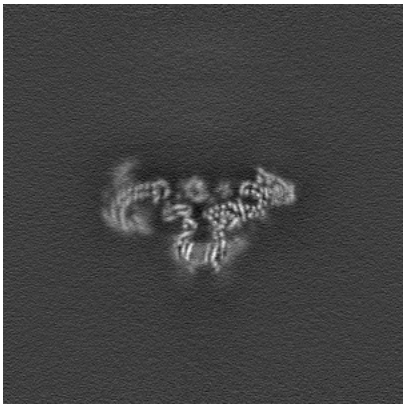
X Index: 262

Y Index: 218

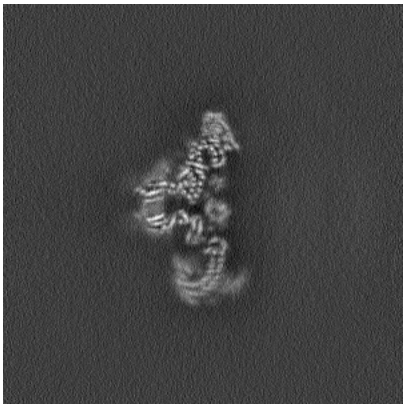


Z Index: 250

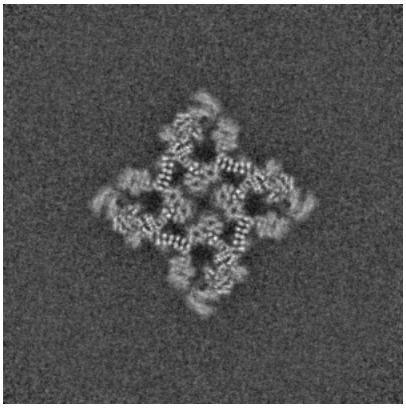
6.3.2 Raw map



X Index: 218



Y Index: 262

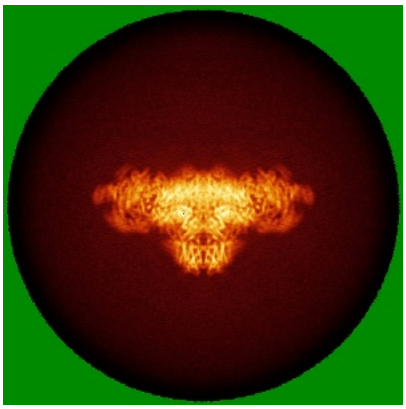


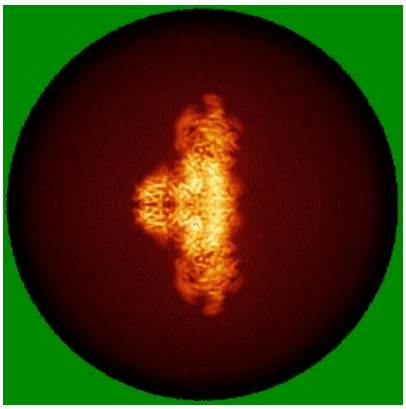
Z Index: 252

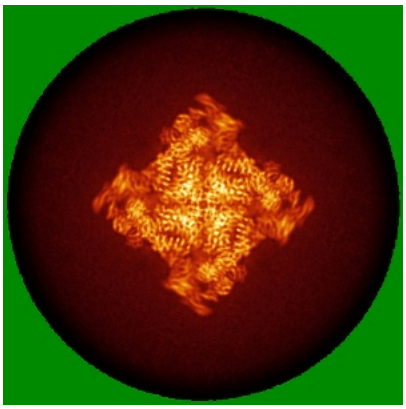
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

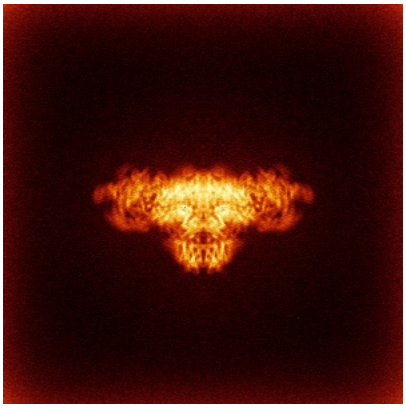
6.4.1 Primary map

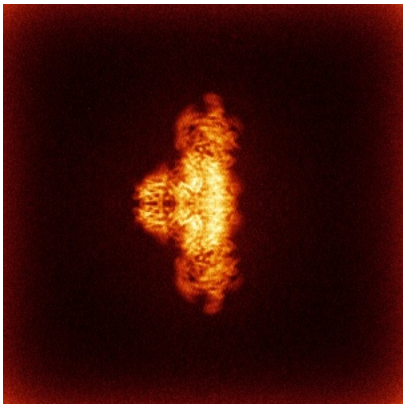

X

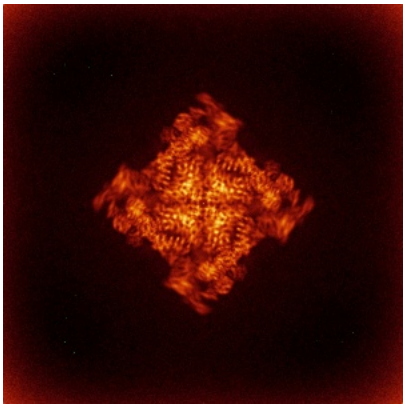

Y


Z

6.4.2 Raw 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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.702. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

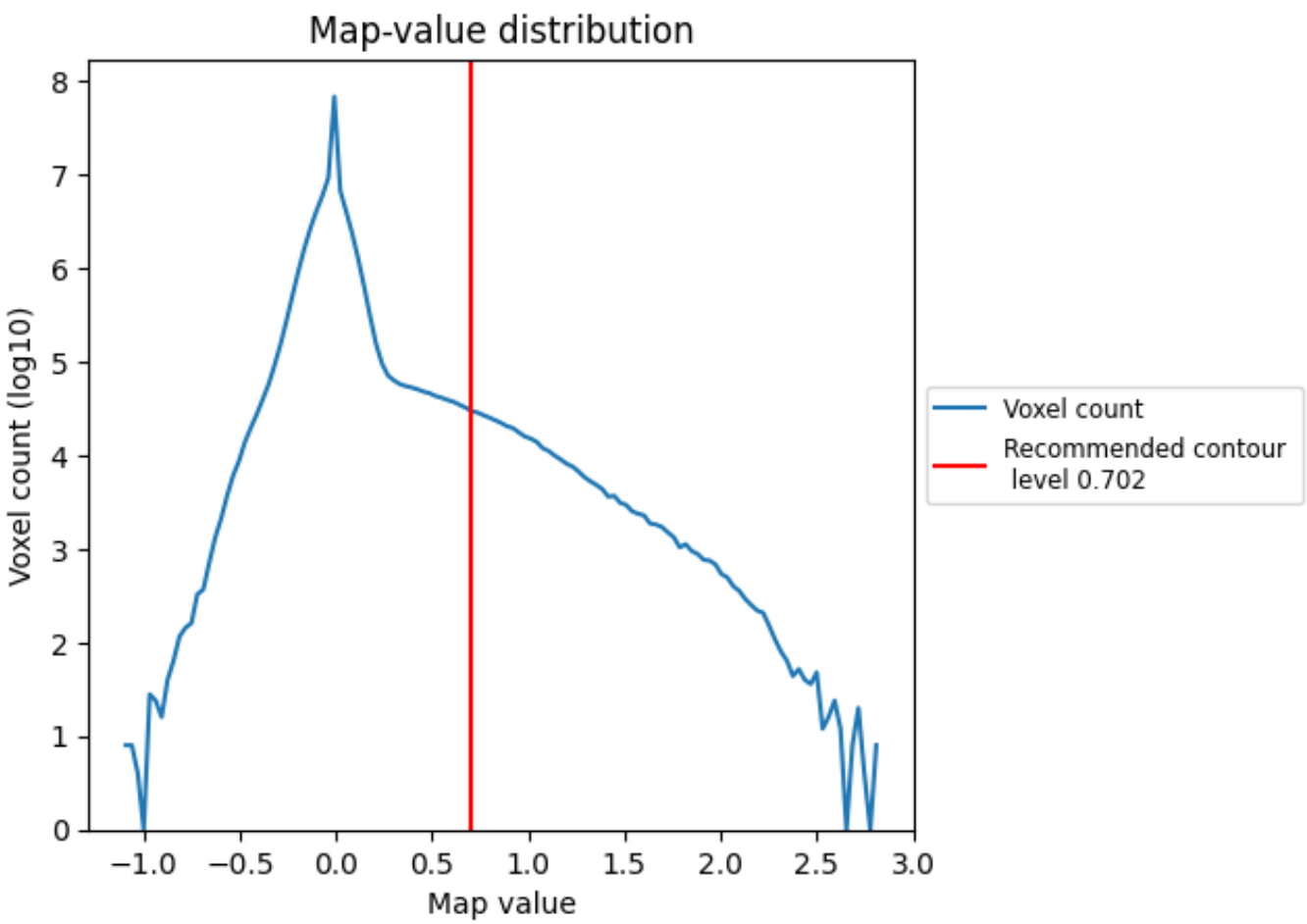
6.6 Mask visualisation (i)

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

7 Map analysis (i)

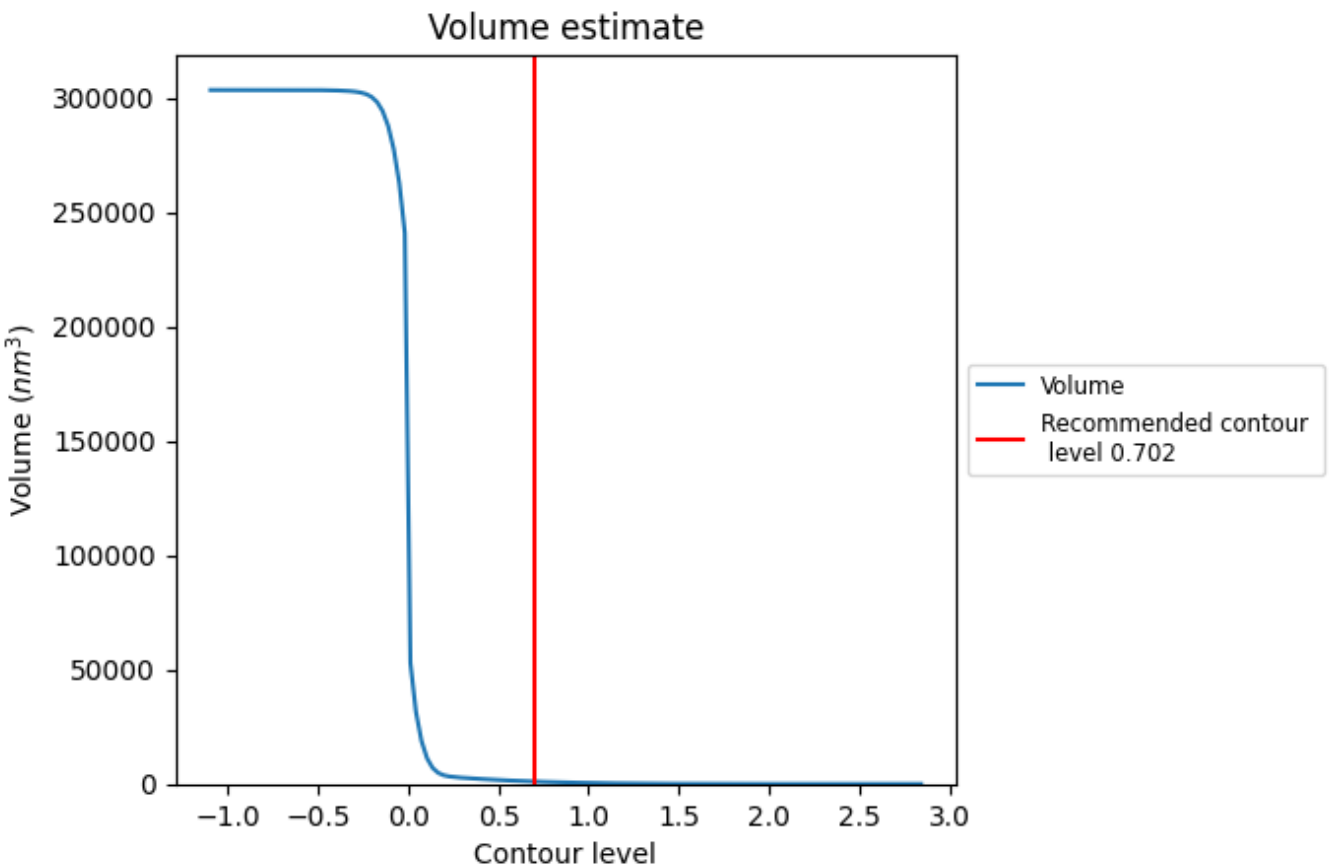
This section contains the results of statistical analysis of the map.

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.

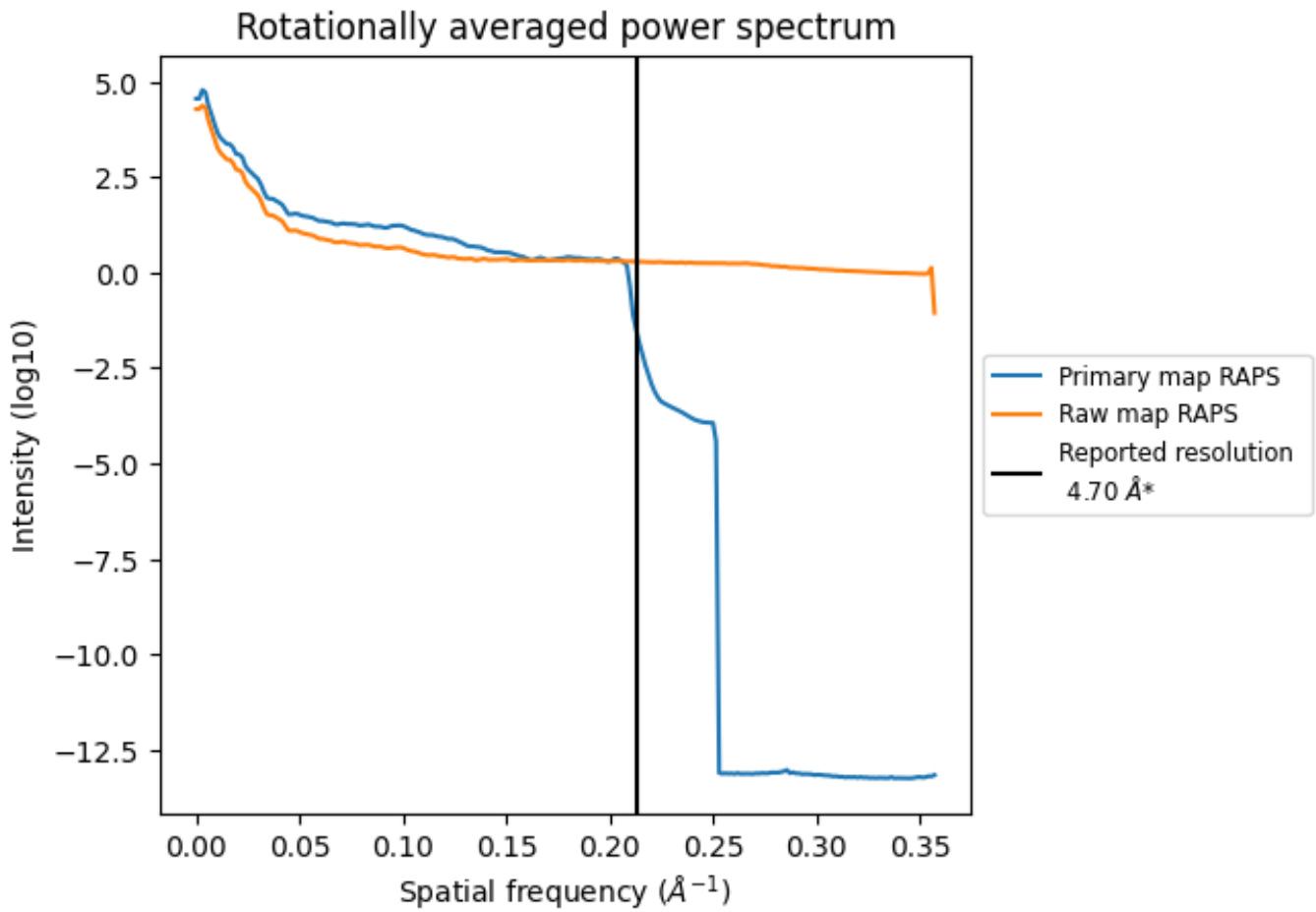
7.2 Volume estimate (i)



The volume at the recommended contour level is 1056 nm^3; this corresponds to an approximate mass of 954 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 (i)

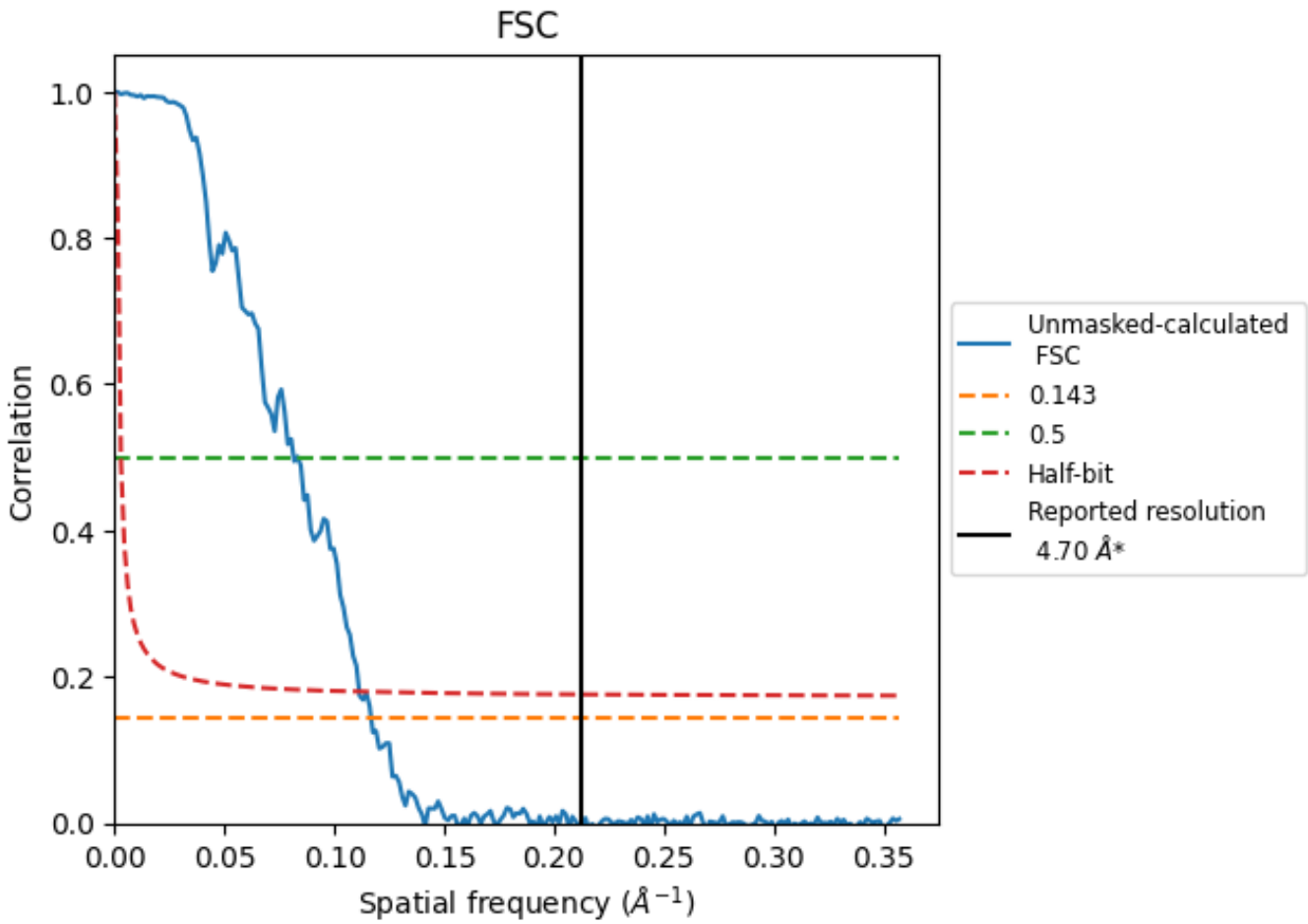


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8.2 Resolution estimates (i)

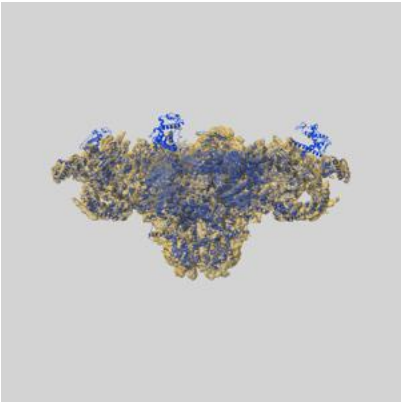
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.56	12.25	8.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.56 differs from the reported value 4.7 by more than 10 %

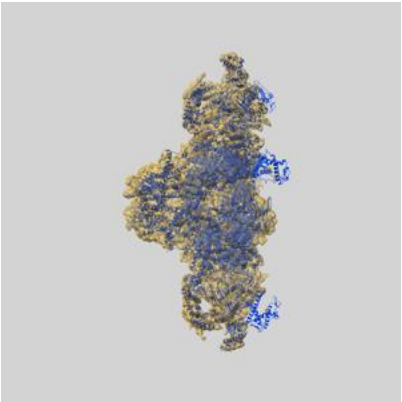
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22017 and PDB model 6X34. Per-residue inclusion information can be found in section 3 on page 4.

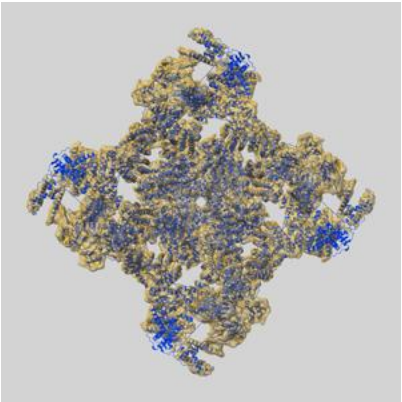
9.1 Map-model overlay (i)



X



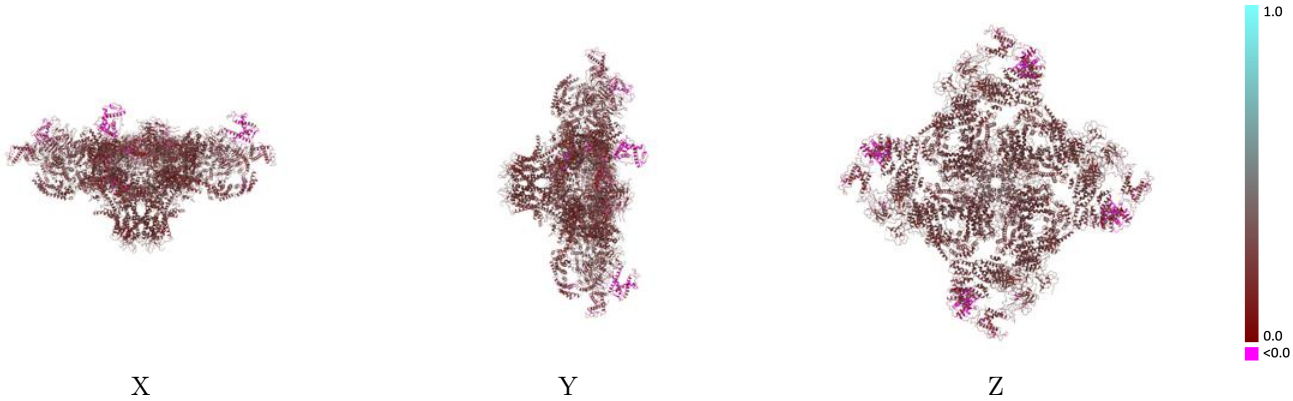
Y



Z

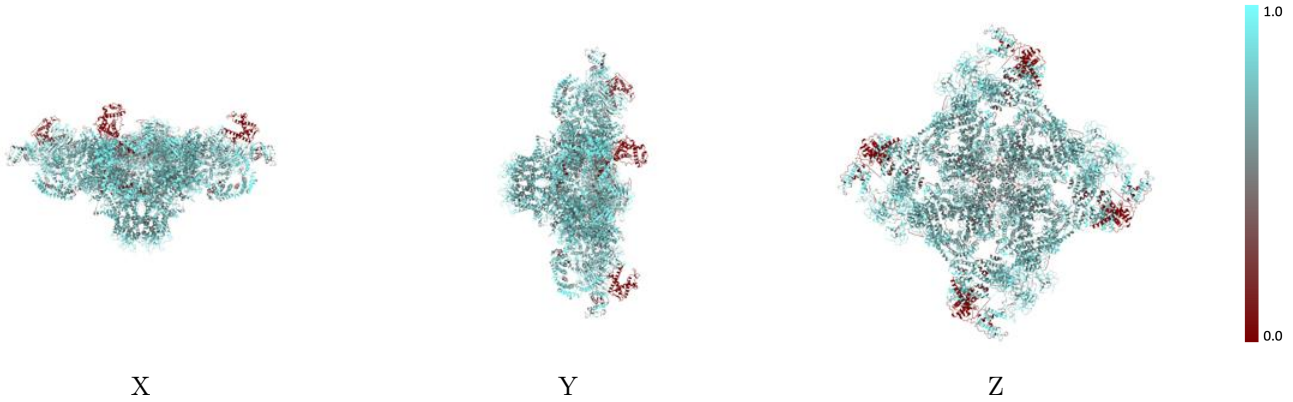
The images above show the 3D surface view of the map at the recommended contour level 0.702 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



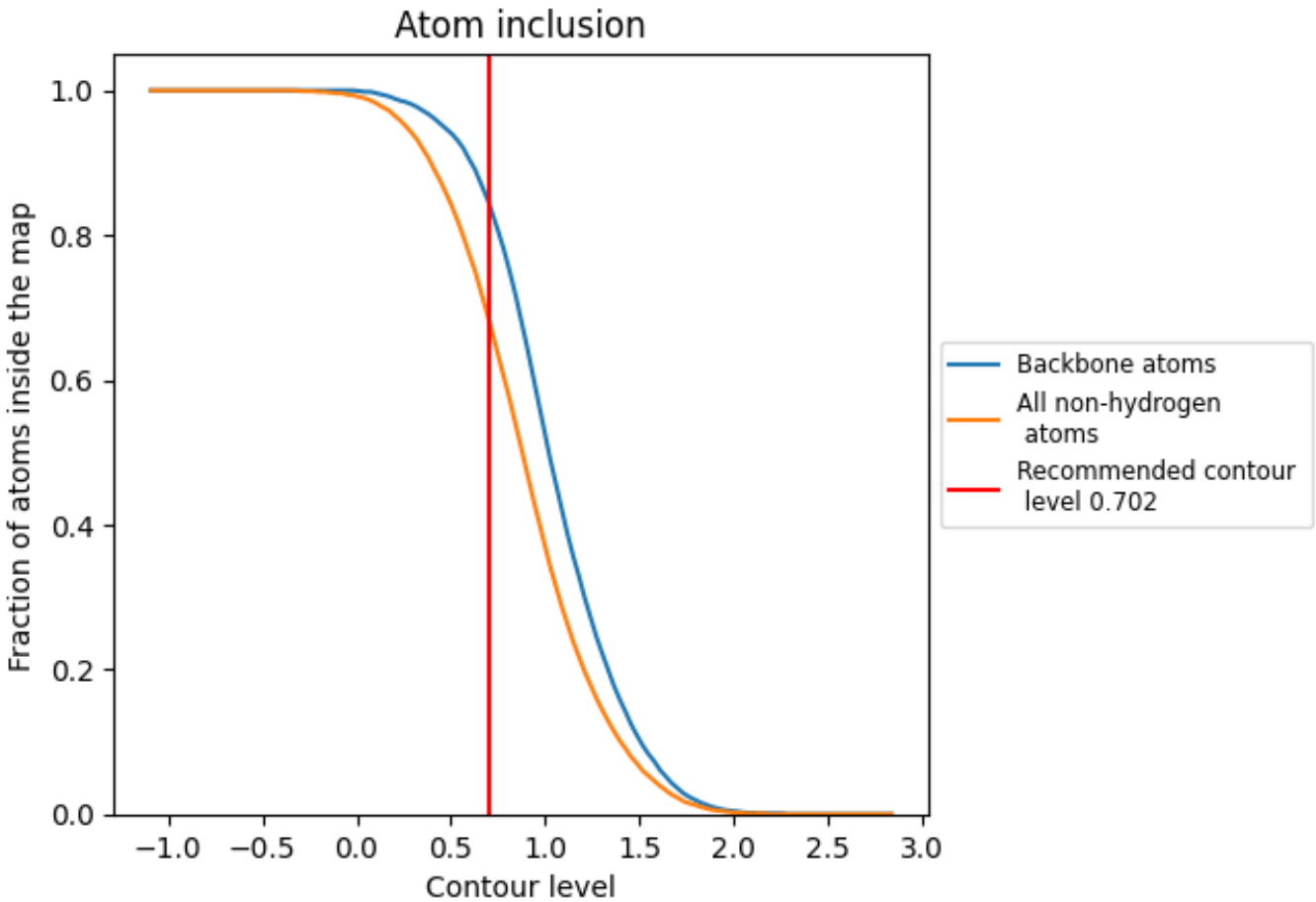
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.702).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.702) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.2430
A	0.7130	0.2800
B	0.6820	0.2420
C	0.7200	0.2800
D	0.6820	0.2410
E	0.7200	0.2800
F	0.6820	0.2410
G	0.7200	0.2830
H	0.6810	0.2410