Full wwPDB EM Validation Report (i)

Nov 2, 2022 – 06:45 AM EDT

PDB ID	:	5TAZ
EMDB ID	:	EMD-8390
Title	:	Structure of rabbit RyR1 (ryanodine dataset, class 3)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.30 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:

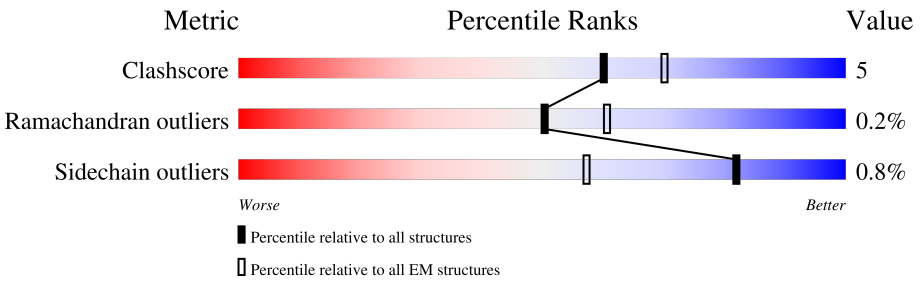
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.30 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	108	31% 87% 12% •
1	F	108	31% 89% 10% •
1	H	108	31% 88% 11% •
1	J	108	31% 89% 10% •
2	B	4416	38% 84% 10% 5%
2	E	4416	38% 84% 10% 5%
2	G	4416	38% 84% 10% 5%
2	I	4416	38% 85% 10% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 121276 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	F	107	818	516	144	154	4	0	0
1	A	107	818	516	144	154	4	0	0
1	H	107	818	516	144	154	4	0	0
1	J	107	818	516	144	154	4	0	0

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4194	29499	18686	5228	5428	157	0	0
2	I	4194	29499	18686	5228	5428	157	0	0
2	G	4194	29499	18686	5228	5428	157	0	0
2	E	4194	29499	18686	5228	5428	157	0	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	I	1	1	1	0
3	G	1	1	1	0
3	E	1	1	1	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

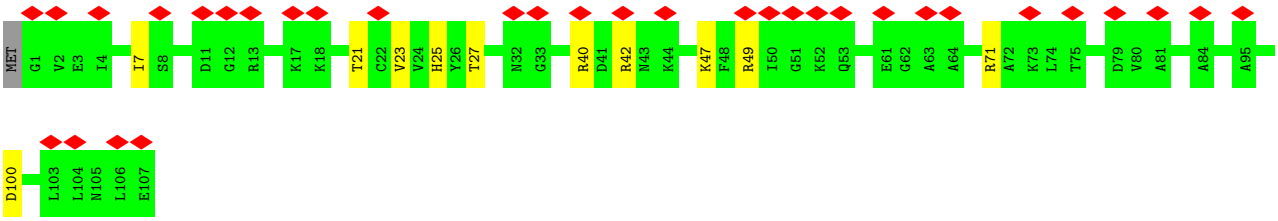
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	B	1	1	1	0
4	I	1	1	1	0
4	G	1	1	1	0
4	E	1	1	1	0

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.

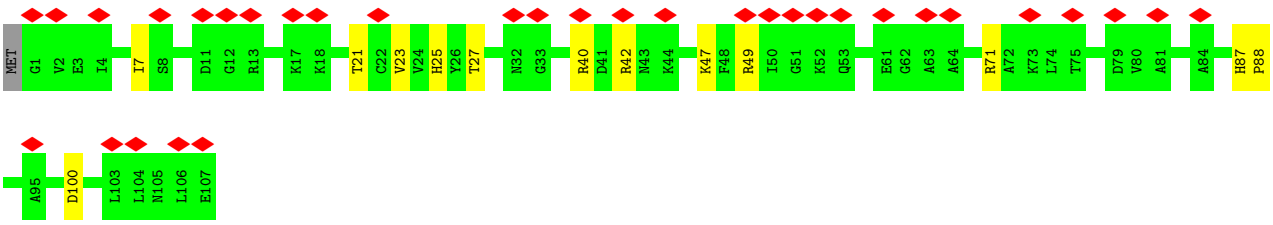
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



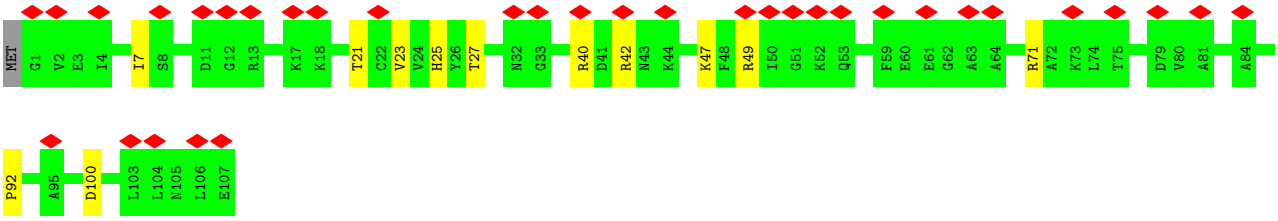
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



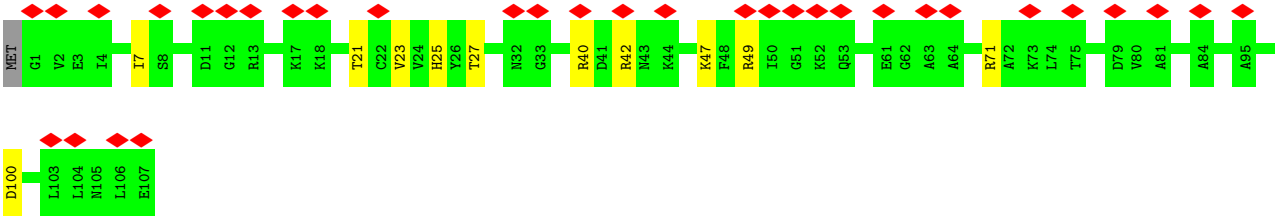
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



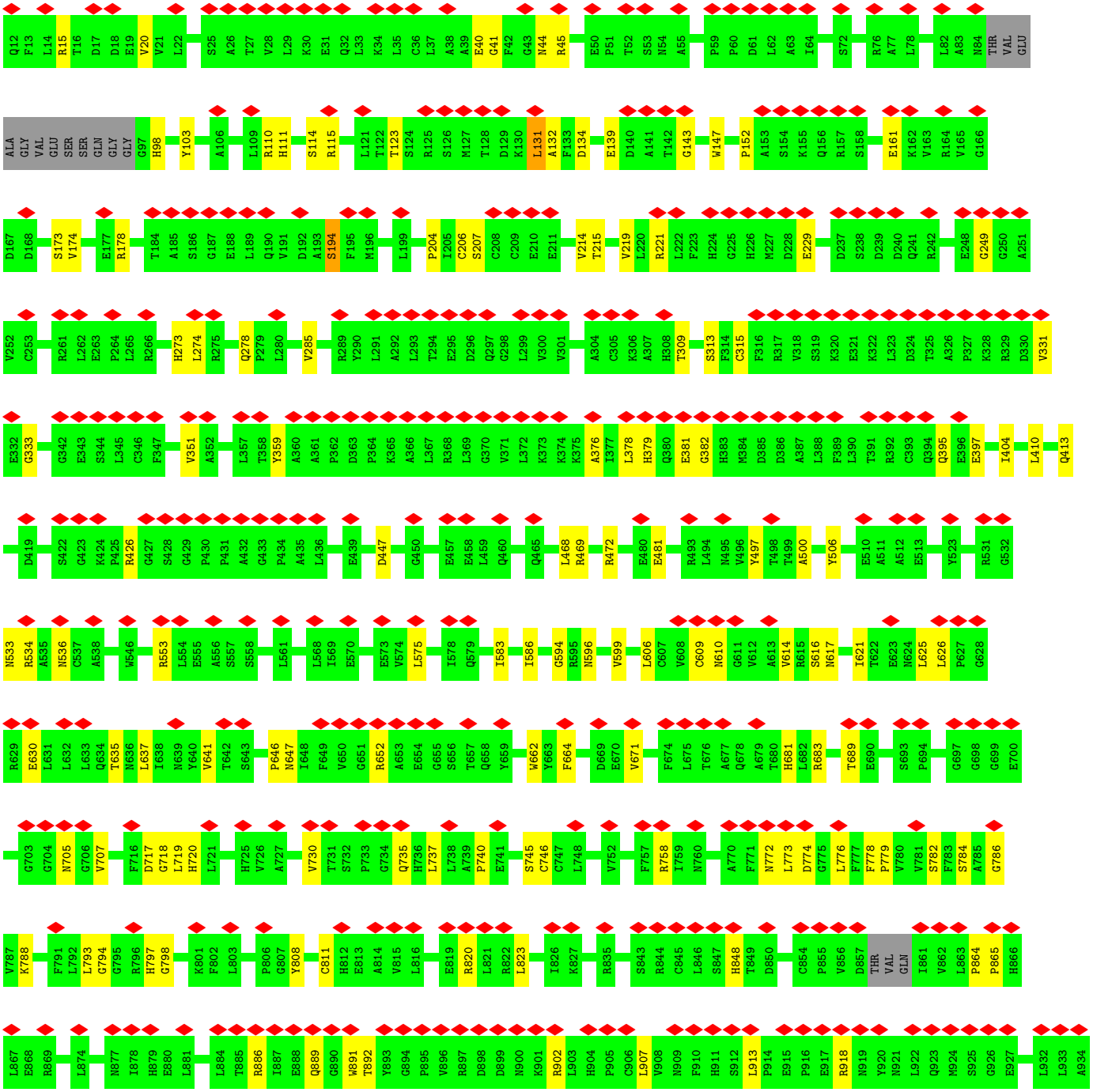
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

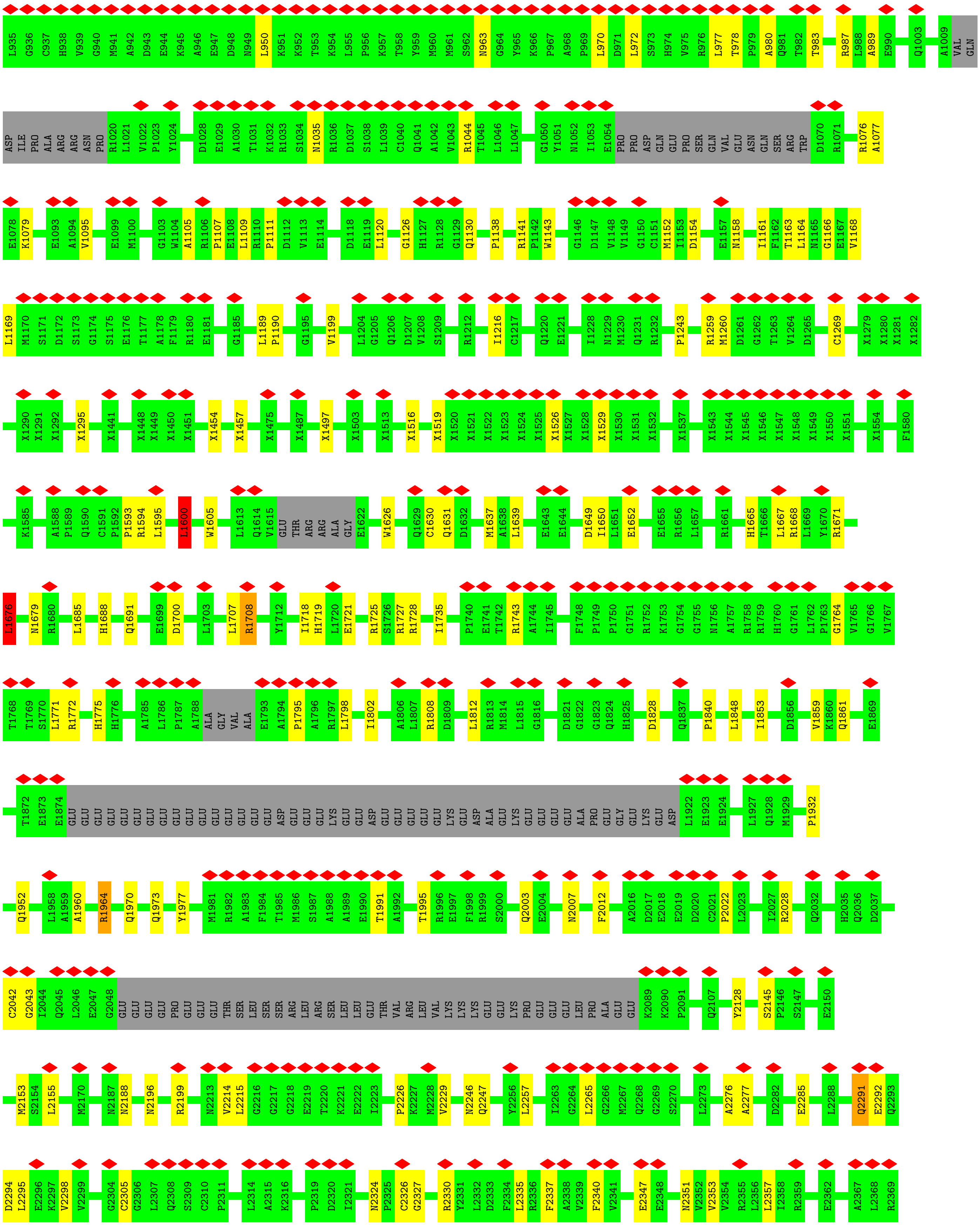
Chain J:



• Molecule 2: Ryanodine receptor 1

Chain B:

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ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 P1023 Y1024 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 R1076 A1077
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T1768 T1769 S1770 L1771 R1772 H1775 H1776 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798 I1802 A1806 L1807 R1808 D1809 L1812 R1813 M1814 L1815 G1816 D1821 G1822 G1823 Q1824 H1825 D1828 Q1837 P1840 L1848 I1853 D1856 V1859 K1860 Q1861 E1869
T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 L1927 Q1928 M1929 P1932
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C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 K2090 P2091 Q2107 Y2128 S2145 P2146 S2147 E2150
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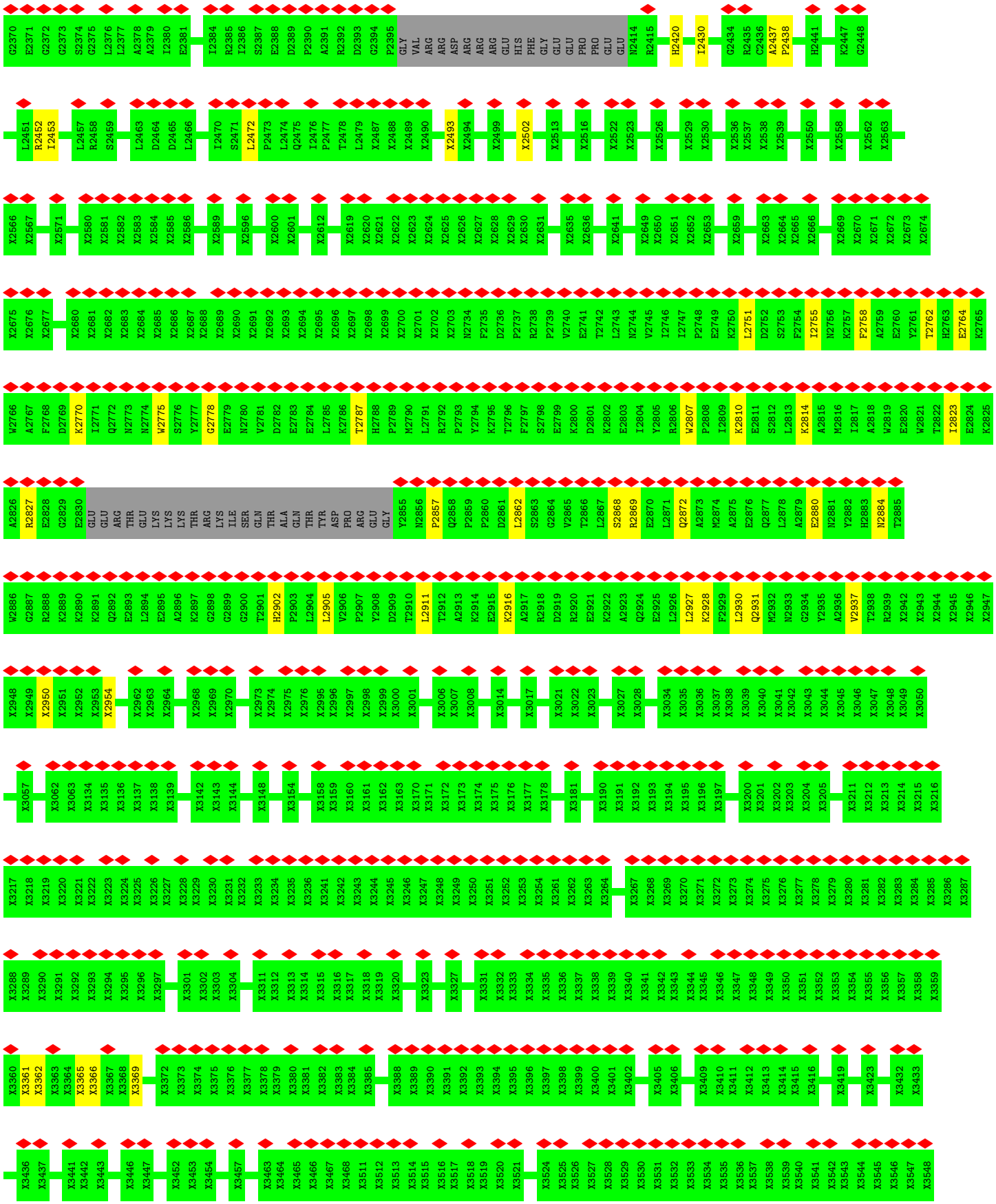
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L2451 R2452 I2453 L2457 R2458 S2459 L2463 D2464 D2465 L2466 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479 X2487 X2488 X2489 X2490 X2493 X2494 X2499 X2502 X2513 X2516 X2522 X2523 X2526 X2529 X2530 X2536 X2537 X2538 X2539 X2550 X2558 X2562 X2563
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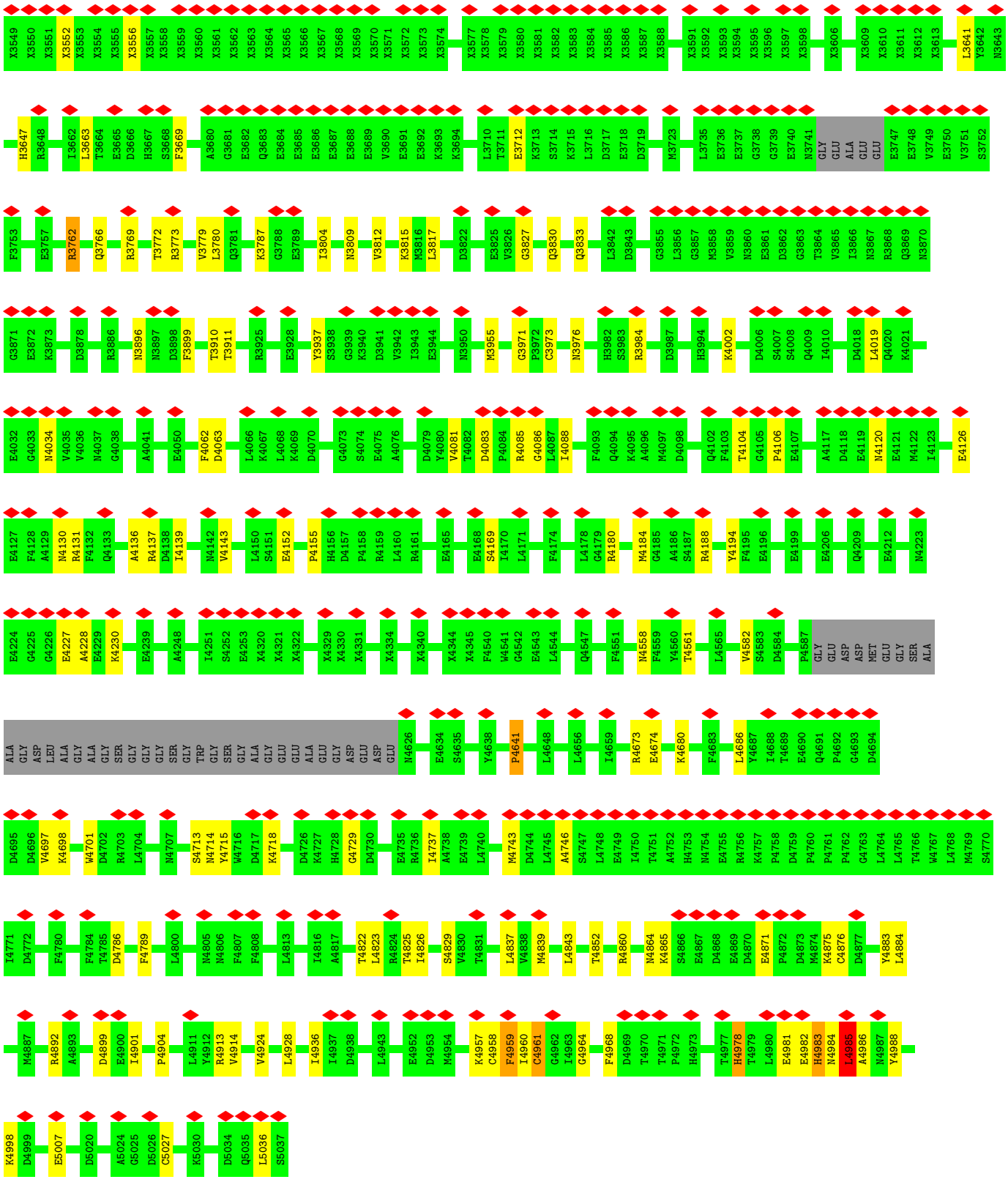
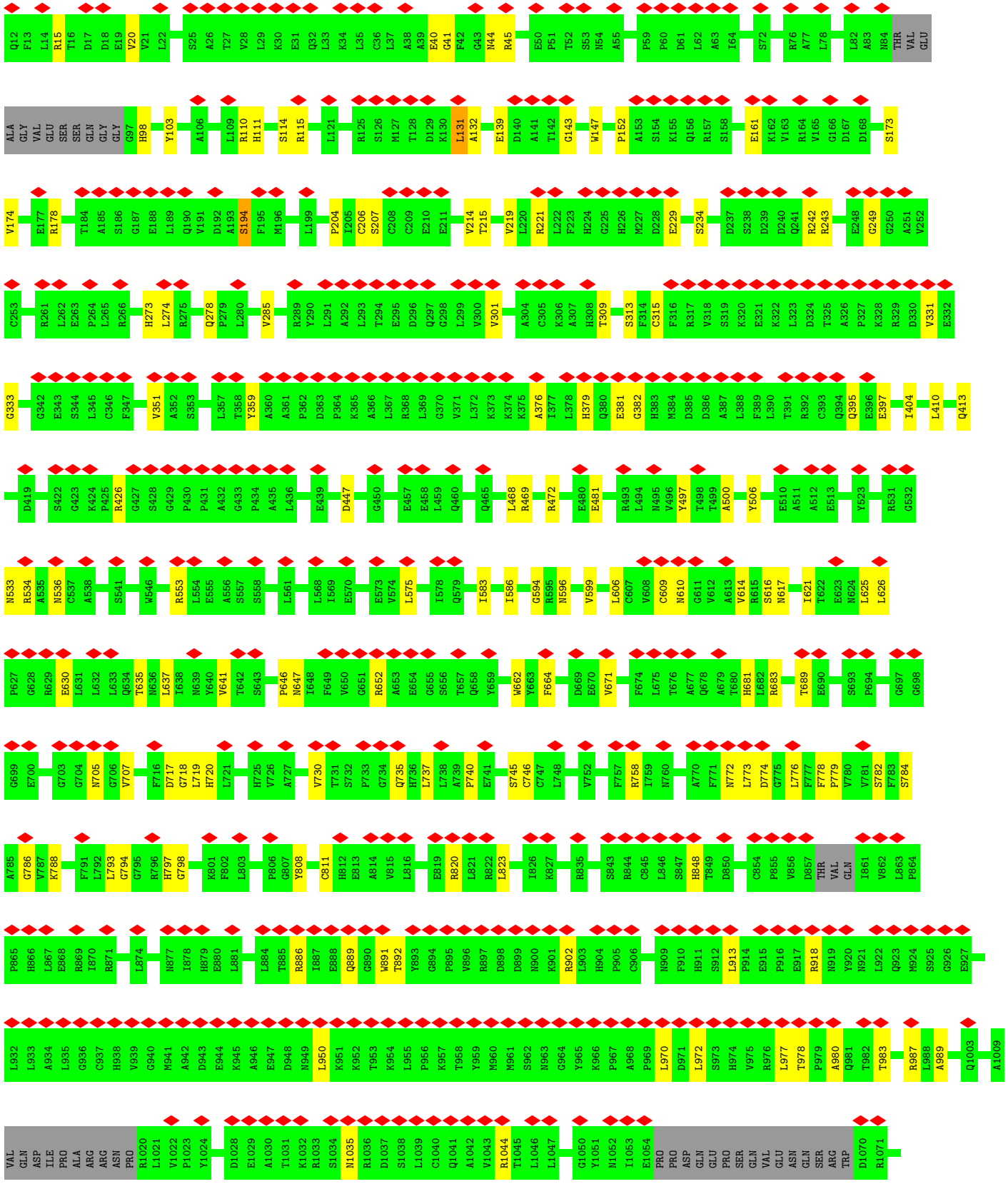


• Molecule 2: Ryanodine receptor 1

Chain I: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ALA GLY VAL GLU SER SER GLN GLY GLY G97 H98 Y103 A106 L109 R110 H111 S114 R115 L121 R125 S126 M127 T128 D129 K130 L131 A132 E139 D140 A141 T142 G143 W147 P152 A153 S154 K155 Q156 R157 S158 E161 K162 V163 R164 V165 G166 D167 D168 S173
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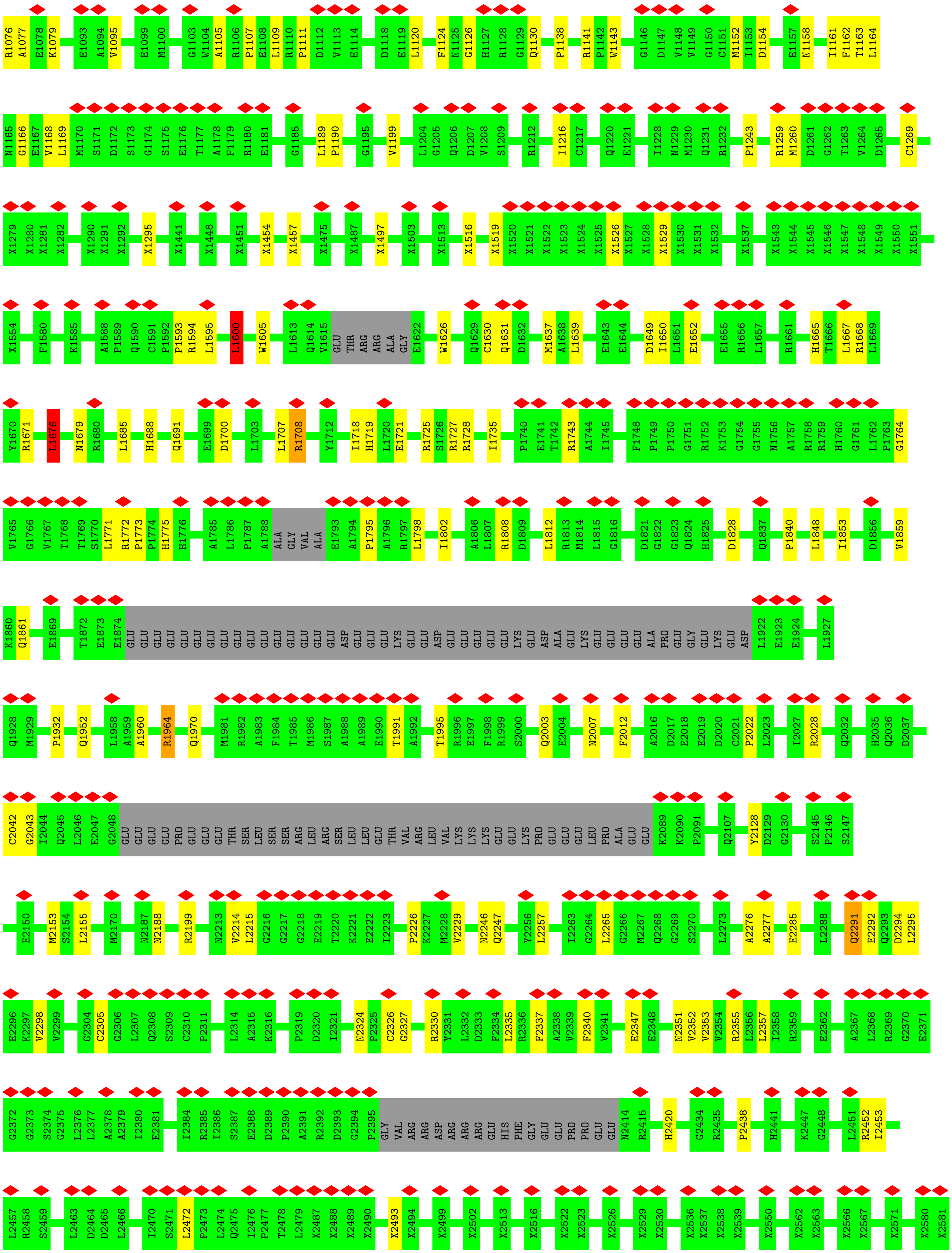
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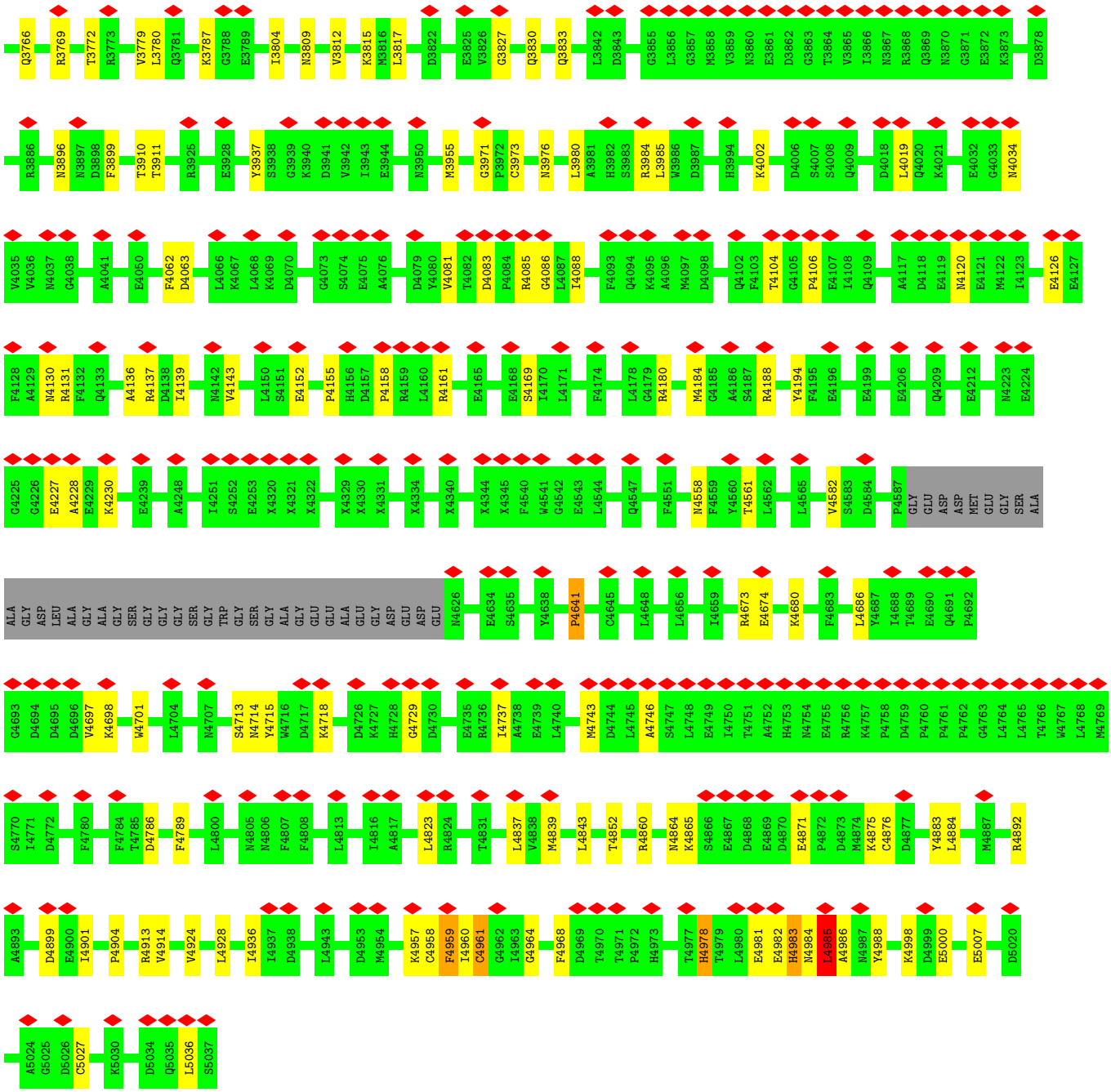

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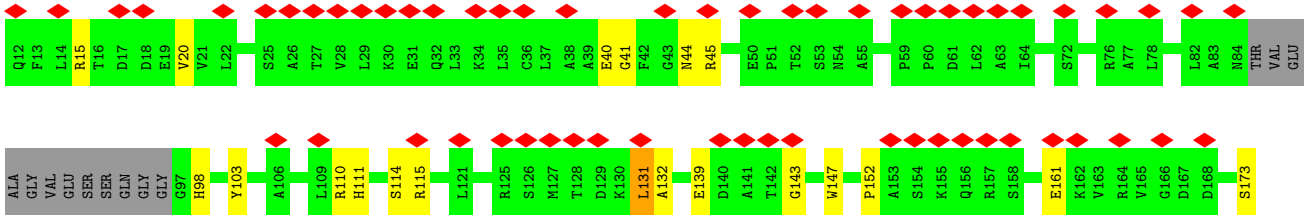

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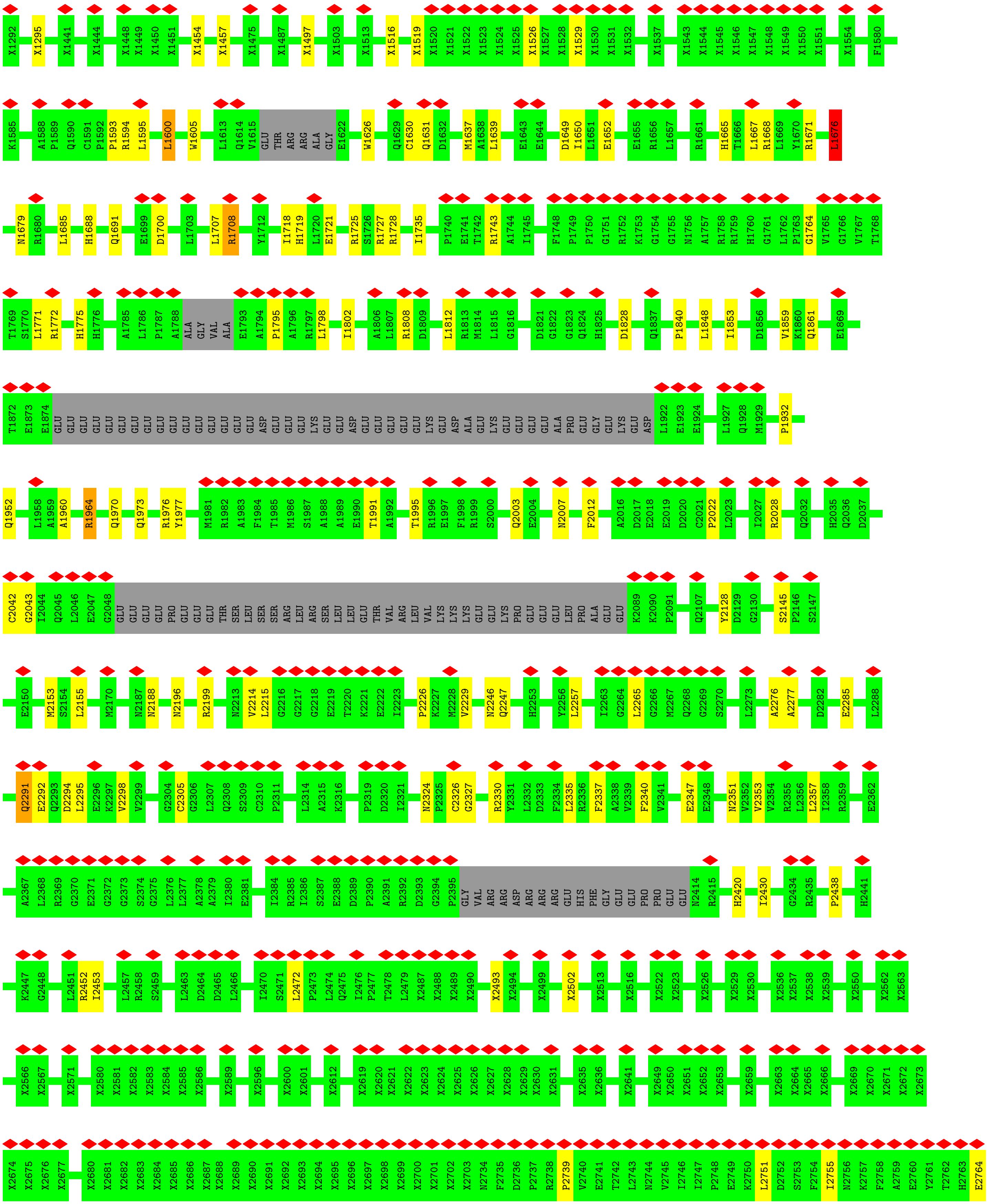
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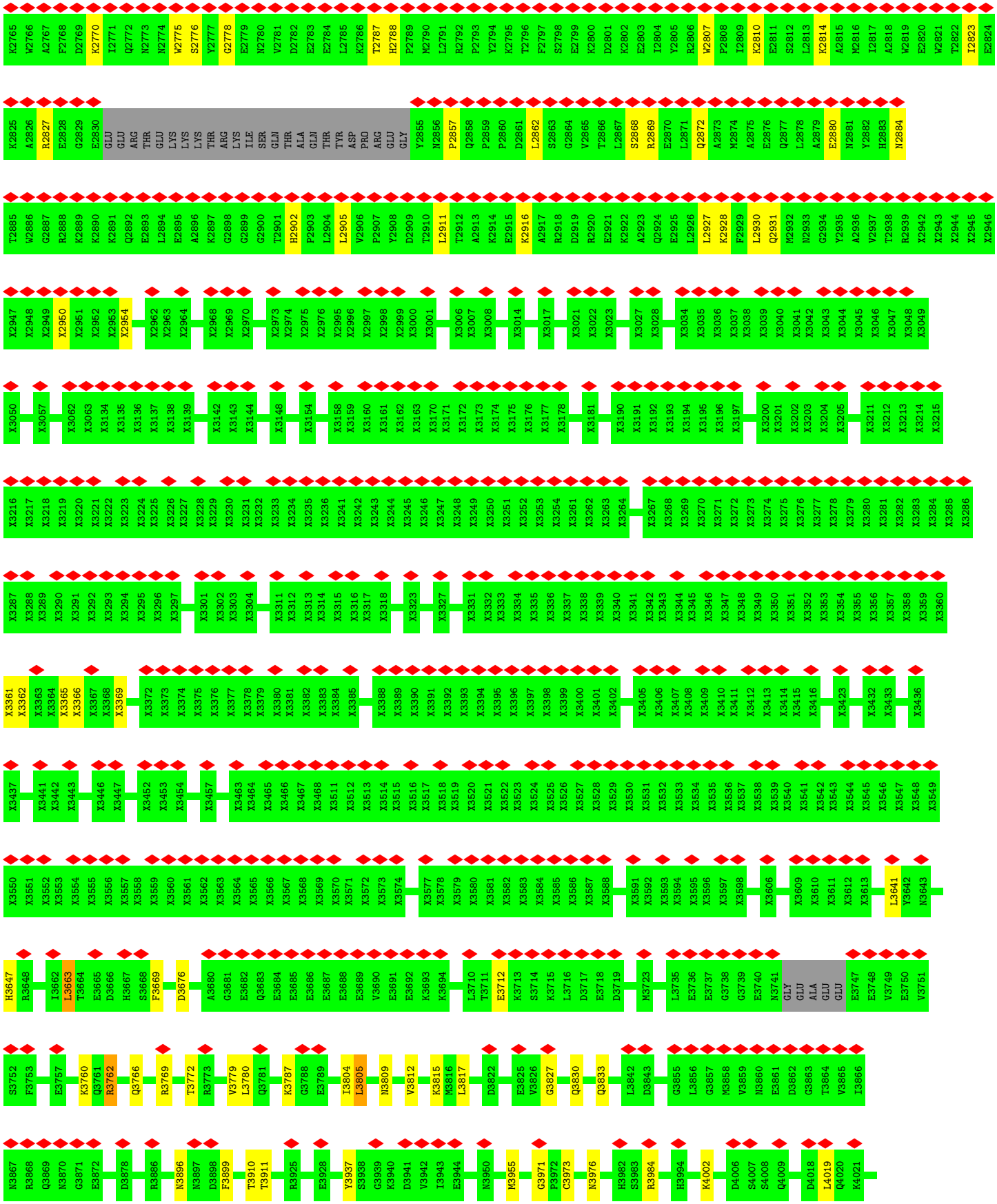
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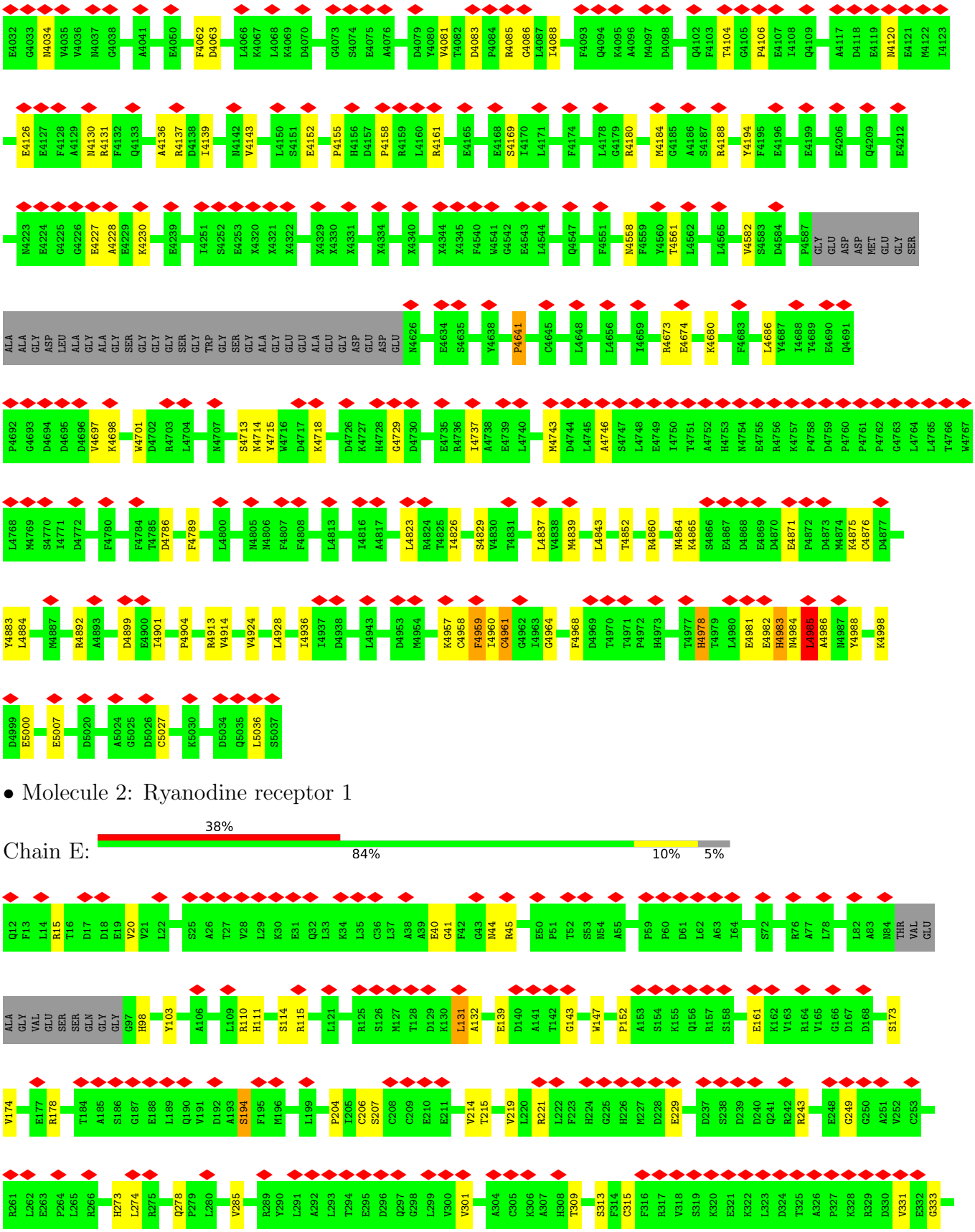

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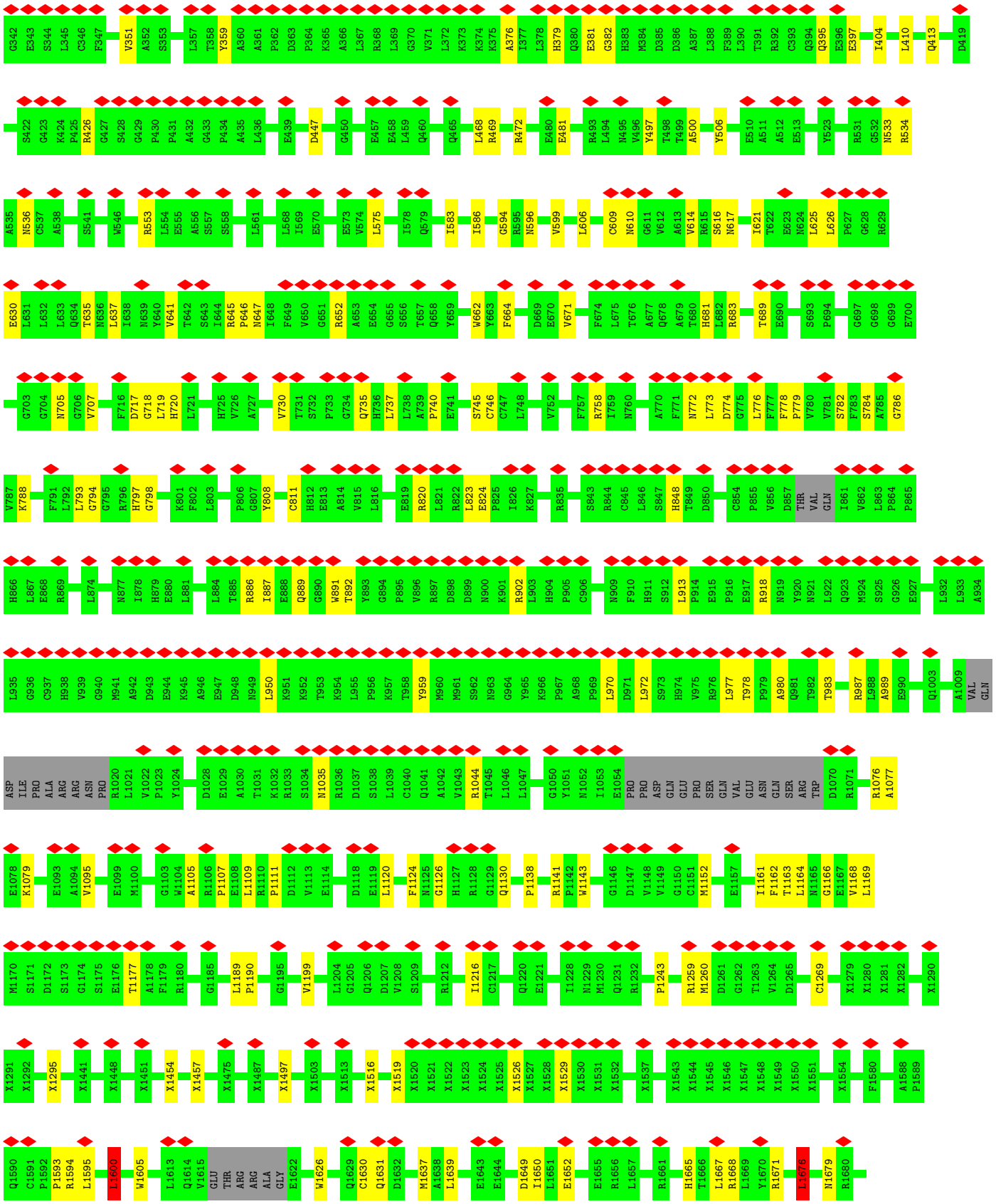
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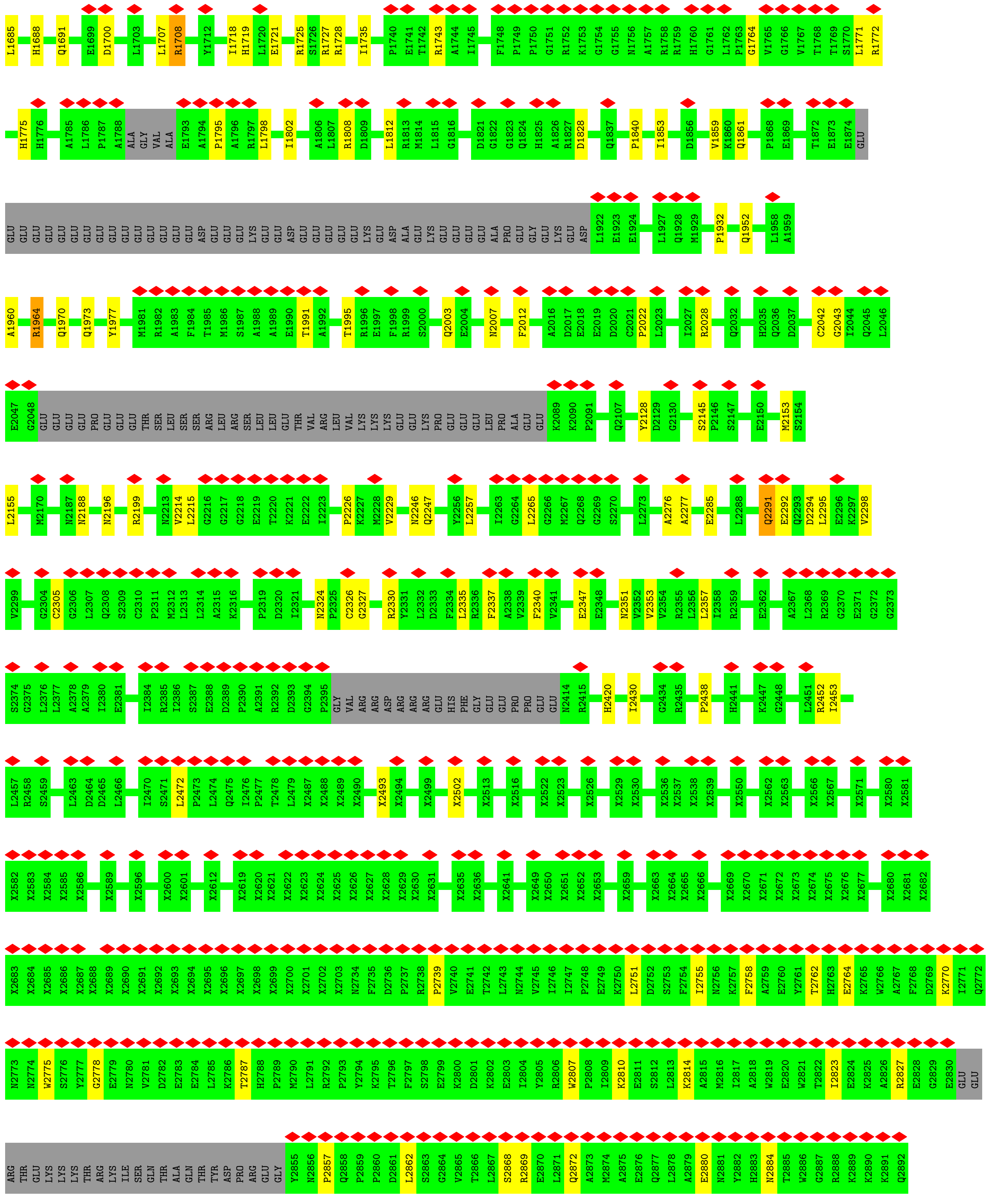
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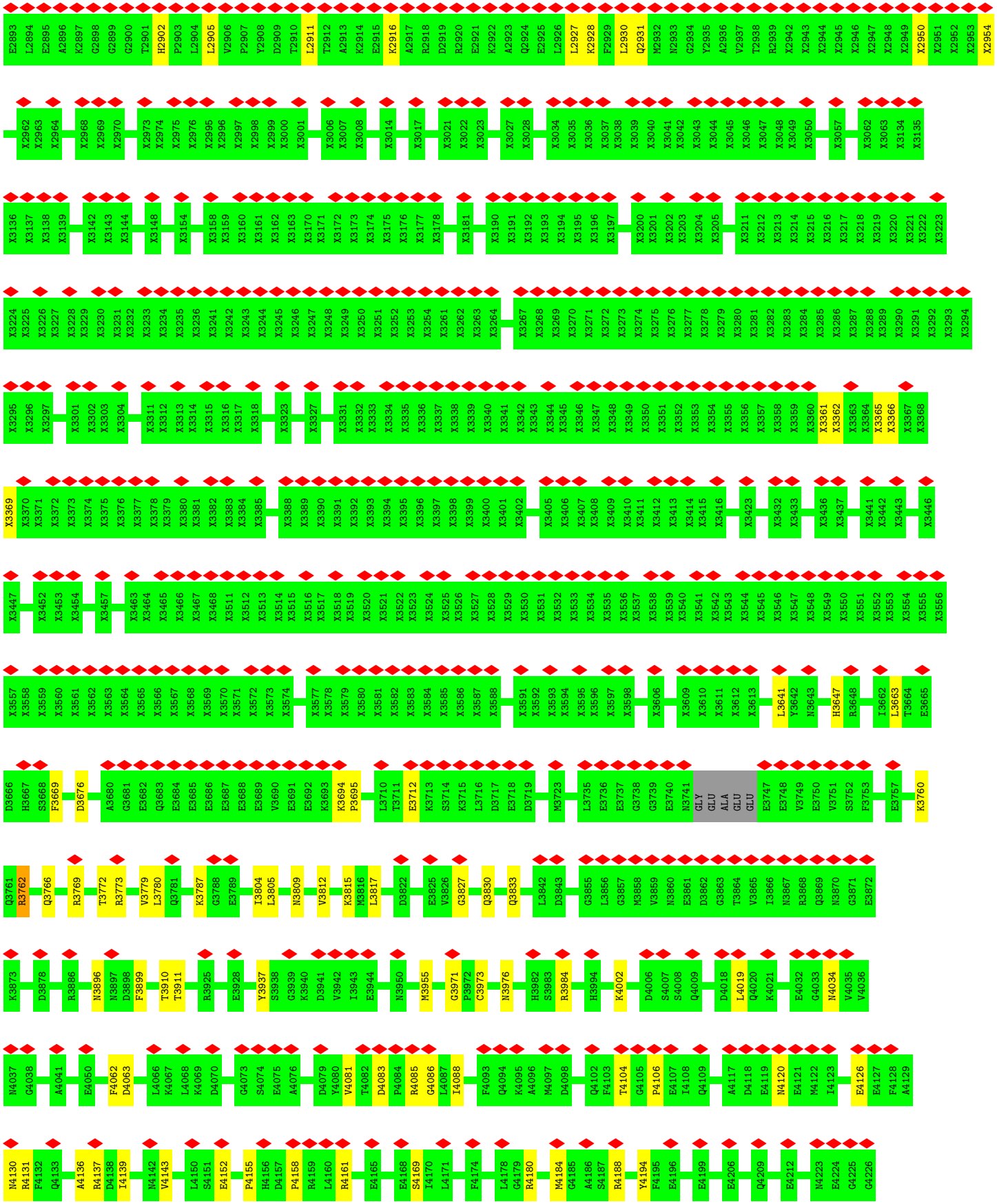
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D3666 H3667 S3668 F3669 D3676 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 M3723 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3757 K3760
Q3761 R3762 Q3766 R3769 T3772 R3773 V3779 L3780 Q3781 K3787 G3788 E3789 I3804 L3805 N3809 V3812 K3815 M3816 L3817 D3822 E3825 V3826 G3827 Q3830 Q3833 L3842 D3843 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872
K3873 D3878 R3886 N3896 N3897 D3898 F3899 T3910 T3911 R3925 E3928 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 E3944 N3950 M3955 G3971 P3972 C3973 N3976 H3982 S3983 R3984 H3994 K4002 D4006 S4007 S4008 Q4009 D4018 L4019 Q4020 K4021 E4032 G4033 N4034 V4035 V4036
N4037 G4038 A4041 E4050 F4062 D4063 L4066 K4067 L4068 K4069 D4070 G4073 S4074 E4075 A4076 D4079 Y4080 V4081 T4082 D4083 P4084 R4085 G4086 L4087 I4088 F4093 Q4094 K4095 A4096 M4097 D4098 Q4102 F4103 T4104 G4105 P4106 E4107 I4108 Q4109 A4117 D4118 E4119 M4120 E4121 M4122 I4123 E4126 E4127 F4128 A4129
N4130 R4131 F4132 Q4133 A4136 R4137 D4138 I4139 N4142 V4143 L4150 S4151 E4152 P4155 H4156 D4157 P4158 R4159 L4160 R4161 E4165 E4168 S4169 I4170 L4171 F4174 L4178 G4179 R4180 M4184 G4185 A4186 S4187 R4188 Y4194 F4195 E4196 E4199 E4206 Q4209 E4212 N4223 E4224 G4225 G4226

E4227 A4228 E4229 K4230 E4239 A4248 I4251 S4252 E4253 X4320 X4321 X4322 X4329 X4330 X4331 X4334 X4340 X4344 X4345 F4540 W4541 G4542 E4543 L4544 Q4547 F4551 N4558 F4559 Y4560 T4561 L4562 L4565 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY
ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 E4634 S4635 Y4638 P4641 C4645 L4648 L4656 I4659 E4674 K4680 F4683 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695
D4696 V4697 K4698 W4701 D4702 R4703 L4704 N4707 S4713 N4714 Y4715 W4716 D4717 K4718 D4726 K4727 H4728 G4729 D4730 E4735 R4736 I4737 A4738 E4739 L4740 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 S4770 I4771
D4772 F4780 F4784 T4785 D4786 F4789 L4800 H4803 Y4804 N4805 N4806 F4807 F4808 L4813 I4816 A4817 T4822 L4823 R4824 T4825 T4831 L4837 V4838 M4839 L4843 T4852 R4860 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876 D4877 Y4883 L4884 M4887
R4892 A4893 D4899 E4900 I4901 P4904 R4913 V4914 V4924 L4928 I4936 I4937 D4938 L4943 E4952 D4953 M4954 K4957 C4958 F4959 I4960 C4961 G4962 I4963 G4964 F4968 D4969 T4970 T4971 P4972 H4973 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 K4998 D4999 E5000
E5007 D5020 A5024 G5025 D5026 C5027 K5030 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.147	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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: CA, 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	0.30	0/834	0.54	0/1123
1	F	0.30	0/834	0.54	0/1123
1	H	0.30	0/834	0.54	0/1123
1	J	0.30	0/834	0.54	0/1123
2	B	0.29	0/25428	0.53	6/34534 (0.0%)
2	E	0.29	0/25428	0.53	6/34534 (0.0%)
2	G	0.29	0/25428	0.53	6/34534 (0.0%)
2	I	0.29	0/25428	0.53	6/34534 (0.0%)
All	All	0.29	0/105048	0.53	24/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	131	LEU	CA-CB-CG	7.91	133.50	115.30
2	G	131	LEU	CA-CB-CG	7.91	133.49	115.30
2	B	131	LEU	CA-CB-CG	7.90	133.47	115.30
2	E	131	LEU	CA-CB-CG	7.89	133.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1600	LEU	CA-CB-CG	6.81	130.95	115.30
2	G	1600	LEU	CA-CB-CG	6.81	130.95	115.30
2	B	1600	LEU	CA-CB-CG	6.80	130.93	115.30
2	E	1600	LEU	CA-CB-CG	6.79	130.91	115.30
2	I	1676	LEU	CA-CB-CG	6.69	130.69	115.30
2	G	1676	LEU	CA-CB-CG	6.69	130.69	115.30
2	B	1676	LEU	CA-CB-CG	6.69	130.68	115.30
2	E	1676	LEU	CA-CB-CG	6.68	130.67	115.30
2	E	977	LEU	CA-CB-CG	6.00	129.09	115.30
2	G	977	LEU	CA-CB-CG	5.98	129.06	115.30
2	B	977	LEU	CA-CB-CG	5.97	129.03	115.30
2	I	977	LEU	CA-CB-CG	5.95	128.98	115.30
2	E	4985	LEU	CA-CB-CG	5.40	127.72	115.30
2	B	4985	LEU	CA-CB-CG	5.40	127.71	115.30
2	I	4985	LEU	CA-CB-CG	5.40	127.71	115.30
2	G	4985	LEU	CA-CB-CG	5.40	127.71	115.30
2	B	4901	ILE	CG1-CB-CG2	-5.18	100.01	111.40
2	I	4901	ILE	CG1-CB-CG2	-5.18	100.01	111.40
2	G	4901	ILE	CG1-CB-CG2	-5.18	100.01	111.40
2	E	4901	ILE	CG1-CB-CG2	-5.17	100.03	111.40

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	194	SER	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	194	SER	Peptide
2	E	2291	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	808	TYR	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	194	SER	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	808	TYR	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	194	SER	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	808	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	7	0
1	F	818	0	824	6	0
1	H	818	0	824	7	0
1	J	818	0	824	6	0
2	B	29499	0	24749	265	0
2	E	29499	0	24749	262	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	29499	0	24749	265	0
2	I	29499	0	24748	262	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102291	1047	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 5.

All (1047) 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:4968:PHE:CE2	2:E:4978:HIS:CE1	2.18	1.32
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.18	1.32
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.18	1.30
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.18	1.30
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.67	1.02
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	1.67	0.96
2:G:4968:PHE:CE2	2:G:4978:HIS:HE1	1.81	0.95
2:I:4968:PHE:CE2	2:I:4978:HIS:HE1	1.81	0.94
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	1.67	0.93
2:E:4968:PHE:CE2	2:E:4978:HIS:HE1	1.81	0.92
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	1.67	0.91
2:B:4968:PHE:CE2	2:B:4978:HIS:HE1	1.81	0.91
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.43	0.87
2:I:4982:GLU:HG3	2:I:5027:CYS:SG	2.15	0.86
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.43	0.86
2:E:4982:GLU:HG3	2:E:5027:CYS:SG	2.15	0.86
2:G:4982:GLU:HG3	2:G:5027:CYS:SG	2.15	0.85
2:B:4982:GLU:HG3	2:B:5027:CYS:SG	2.15	0.85
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.43	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.43	0.84
2:G:4968:PHE:CD2	2:G:4978:HIS:ND1	2.52	0.78
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.66	0.77
2:I:4968:PHE:CD2	2:I:4978:HIS:ND1	2.52	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.66	0.77
2:B:4968:PHE:CD2	2:B:4978:HIS:ND1	2.52	0.77
2:E:4968:PHE:CD2	2:E:4978:HIS:ND1	2.52	0.76
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.66	0.76
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.66	0.76
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.25	0.72
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.25	0.71
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.25	0.70
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.25	0.70
2:E:379:HIS:HD2	2:E:382:GLY:H	1.39	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.39	0.68
2:I:4230:LYS:HG3	2:I:4959:PHE:HE1	1.57	0.68
2:G:4230:LYS:HG3	2:G:4959:PHE:HE1	1.57	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.39	0.68
2:B:4230:LYS:HG3	2:B:4959:PHE:HE1	1.57	0.67
2:E:4230:LYS:HG3	2:E:4959:PHE:HE1	1.57	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.39	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.67
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.77	0.67
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.77	0.66
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.77	0.66
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.61	0.65
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.61	0.65
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.61	0.65
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.79	0.65
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.79	0.65
2:B:4983:HIS:HD2	2:B:4988:TYR:OH	1.80	0.65
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.61	0.64
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.30	0.64
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.30	0.64
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.30	0.64
2:I:4957:LYS:HE2	2:I:4964:GLY:CA	2.27	0.64
2:B:4957:LYS:HE2	2:B:4964:GLY:CA	2.27	0.64
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.80	0.64
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.79	0.63
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.79	0.63
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.30	0.63
2:E:4957:LYS:HE2	2:E:4964:GLY:CA	2.27	0.63
2:E:4983:HIS:HD2	2:E:4988:TYR:OH	1.80	0.63
2:I:4983:HIS:HD2	2:I:4988:TYR:OH	1.80	0.63
2:G:4957:LYS:HE2	2:G:4964:GLY:CA	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.80	0.63
2:G:4983:HIS:HD2	2:G:4988:TYR:OH	1.80	0.63
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.80	0.63
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.81	0.63
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.81	0.63
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.80	0.62
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.81	0.62
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.81	0.62
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.81	0.62
2:B:313:SER:HB3	2:B:351:VAL:HB	1.82	0.61
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.73	0.61
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.74	0.61
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.82	0.61
2:G:313:SER:HB3	2:G:351:VAL:HB	1.82	0.61
2:I:313:SER:HB3	2:I:351:VAL:HB	1.82	0.61
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.74	0.61
2:E:359:TYR:HA	2:E:376:ALA:HA	1.83	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.61
2:E:313:SER:HB3	2:E:351:VAL:HB	1.82	0.61
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.34	0.60
2:G:359:TYR:HA	2:G:376:ALA:HA	1.83	0.60
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.83	0.60
2:B:331:VAL:HG12	2:B:333:GLY:H	1.66	0.60
2:I:4984:ASN:C	2:I:4986:ALA:H	2.04	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:G:4230:LYS:HD2	2:G:4959:PHE:HD1	1.66	0.60
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.74	0.60
2:G:4984:ASN:C	2:G:4986:ALA:H	2.04	0.60
2:I:331:VAL:HG12	2:I:333:GLY:H	1.66	0.60
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.67	0.60
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.84	0.60
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.83	0.60
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.83	0.60
2:E:4984:ASN:C	2:E:4986:ALA:H	2.04	0.60
2:I:4984:ASN:O	2:I:4986:ALA:N	2.35	0.60
2:E:4230:LYS:HD2	2:E:4959:PHE:HD1	1.67	0.60
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.67	0.60
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.82	0.60
2:G:4984:ASN:O	2:G:4986:ALA:N	2.35	0.60
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.67	0.60
2:B:359:TYR:HA	2:B:376:ALA:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4984:ASN:C	2:B:4986:ALA:H	2.04	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.84	0.59
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.83	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.84	0.59
2:I:359:TYR:HA	2:I:376:ALA:HA	1.83	0.59
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.84	0.59
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.85	0.59
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.84	0.59
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.36	0.59
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.85	0.59
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.35	0.59
2:E:4984:ASN:O	2:E:4986:ALA:N	2.35	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.85	0.59
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.35	0.59
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.20	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.85	0.59
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.67	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.34	0.59
2:E:331:VAL:HG12	2:E:333:GLY:H	1.66	0.59
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.84	0.59
2:E:111:HIS:HD2	2:E:114:SER:H	1.50	0.59
2:B:111:HIS:HD2	2:B:114:SER:H	1.50	0.59
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.85	0.59
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.34	0.59
2:E:4968:PHE:CZ	2:E:4978:HIS:HE1	2.20	0.59
2:G:111:HIS:HD2	2:G:114:SER:H	1.50	0.59
2:G:331:VAL:HG12	2:G:333:GLY:H	1.66	0.59
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.84	0.59
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.85	0.58
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.35	0.58
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.58
2:B:4984:ASN:O	2:B:4986:ALA:N	2.35	0.58
2:I:4230:LYS:HD2	2:I:4959:PHE:HD1	1.67	0.58
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.68	0.58
2:G:978:THR:HB	2:G:980:ALA:H	1.67	0.58
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.58
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.68	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.34	0.58
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.36	0.58
2:I:4968:PHE:CZ	2:I:4978:HIS:HE1	2.20	0.58
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4968:PHE:CZ	2:G:4978:HIS:HE1	2.20	0.58
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.84	0.58
2:I:978:THR:HB	2:I:980:ALA:H	1.68	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.58
2:I:173:SER:HB3	2:I:178:ARG:H	1.69	0.58
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.35	0.58
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.36	0.58
2:B:978:THR:HB	2:B:980:ALA:H	1.67	0.58
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.85	0.58
2:B:2827:ARG:HH21	2:B:2931:GLN:HG3	1.69	0.58
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.58
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.36	0.58
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.85	0.58
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.58
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.34	0.58
2:I:2827:ARG:HH21	2:I:2931:GLN:HG3	1.69	0.58
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.57
2:G:173:SER:HB3	2:G:178:ARG:H	1.69	0.57
2:E:978:THR:HB	2:E:980:ALA:H	1.68	0.57
2:B:173:SER:HB3	2:B:178:ARG:H	1.69	0.57
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.86	0.57
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.86	0.57
2:I:111:HIS:HD2	2:I:114:SER:H	1.50	0.57
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.86	0.57
2:E:173:SER:HB3	2:E:178:ARG:H	1.69	0.57
2:B:4230:LYS:HD2	2:B:4959:PHE:HD1	1.67	0.57
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.68	0.57
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.87	0.57
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.68	0.57
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.87	0.57
2:G:2827:ARG:HH21	2:G:2931:GLN:HG3	1.69	0.57
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.87	0.57
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.38	0.57
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.38	0.57
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.38	0.57
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.57
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.87	0.56
2:I:889:GLN:O	2:I:902:ARG:NH1	2.39	0.56
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.86	0.56
2:E:889:GLN:O	2:E:902:ARG:NH1	2.38	0.56
2:E:2827:ARG:HH21	2:E:2931:GLN:HG3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.79	0.56
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.87	0.56
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.38	0.56
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.79	0.56
2:B:889:GLN:O	2:B:902:ARG:NH1	2.38	0.56
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.88	0.56
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.87	0.56
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.79	0.56
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.87	0.56
2:I:2347:GLU:O	2:I:2351:ASN:N	2.39	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.79	0.56
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.39	0.56
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.79	0.56
2:E:2347:GLU:O	2:E:2351:ASN:N	2.39	0.56
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.87	0.56
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.87	0.55
2:G:889:GLN:O	2:G:902:ARG:NH1	2.38	0.55
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.39	0.55
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.39	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.39	0.55
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.87	0.55
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.39	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.39	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.72	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.79	0.55
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.40	0.55
2:G:609:CYS:SG	2:G:610:ASN:N	2.79	0.55
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.39	0.55
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.34	0.55
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.89	0.55
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.55
2:G:2452:ARG:NH1	2:E:174:VAL:O	2.40	0.55
2:E:609:CYS:SG	2:E:610:ASN:N	2.79	0.55
2:E:4957:LYS:HE2	2:E:4964:GLY:HA2	1.88	0.55
1:A:21:THR:HA	1:A:49:ARG:HA	1.89	0.54
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.34	0.54
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.89	0.54
2:I:4957:LYS:HE2	2:I:4964:GLY:HA2	1.88	0.54
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.39	0.54
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.89	0.54
1:H:21:THR:HA	1:H:49:ARG:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.54
2:G:4957:LYS:HE2	2:G:4964:GLY:HA2	1.88	0.54
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.72	0.54
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.72	0.54
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.39	0.54
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.90	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.90	0.54
2:I:4184:MET:HE1	2:I:4188:ARG:HE	1.73	0.54
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.54
2:B:4184:MET:HE1	2:B:4188:ARG:HE	1.73	0.54
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.72	0.54
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.89	0.54
1:F:21:THR:HA	1:F:49:ARG:HA	1.89	0.54
2:B:4957:LYS:HE2	2:B:4964:GLY:HA2	1.88	0.54
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.89	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.41	0.54
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.39	0.54
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.90	0.53
2:B:4823:LEU:HD23	2:I:4843:LEU:HD12	1.91	0.53
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.89	0.53
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.41	0.53
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.90	0.53
1:J:21:THR:HA	1:J:49:ARG:HA	1.89	0.53
2:I:730:VAL:O	2:I:735:GLN:NE2	2.41	0.53
2:B:730:VAL:O	2:B:735:GLN:NE2	2.41	0.53
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.39	0.53
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.91	0.53
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.41	0.53
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.91	0.53
2:B:4839:MET:HB3	2:E:4823:LEU:HD11	1.89	0.53
2:G:730:VAL:O	2:G:735:GLN:NE2	2.41	0.53
2:B:4843:LEU:HD12	2:E:4823:LEU:HD23	1.90	0.53
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.89	0.53
2:E:730:VAL:O	2:E:735:GLN:NE2	2.41	0.53
2:B:111:HIS:CD2	2:B:114:SER:H	2.27	0.53
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.42	0.53
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.91	0.53
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.74	0.53
2:G:4184:MET:HE1	2:G:4188:ARG:HE	1.74	0.53
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.42	0.53
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.90	0.52
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.89	0.52
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.41	0.52
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.34	0.52
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.52
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.91	0.52
2:B:4823:LEU:HD11	2:I:4839:MET:HB3	1.91	0.52
2:I:4823:LEU:HD23	2:G:4843:LEU:HD12	1.91	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.42	0.52
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	1.91	0.52
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.42	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.42	0.52
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.90	0.52
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.91	0.52
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.43	0.52
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.91	0.52
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.74	0.52
2:G:4823:LEU:HD23	2:E:4843:LEU:HD12	1.92	0.52
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.43	0.52
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	1.91	0.52
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.90	0.52
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.52
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.75	0.52
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.92	0.52
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.75	0.52
2:I:111:HIS:CD2	2:I:114:SER:H	2.27	0.52
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.42	0.52
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.42	0.52
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.74	0.52
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.42	0.52
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.92	0.52
2:I:4823:LEU:HD11	2:G:4839:MET:HB3	1.91	0.52
2:G:111:HIS:CD2	2:G:114:SER:H	2.27	0.52
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.43	0.52
2:E:2868:SER:O	2:E:2872:GLN:N	2.43	0.52
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.92	0.51
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.92	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.92	0.51
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.75	0.51
2:G:2868:SER:O	2:G:2872:GLN:N	2.43	0.51
2:E:621:ILE:O	2:E:625:LEU:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.51
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.92	0.51
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.92	0.51
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.75	0.51
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.92	0.51
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.90	0.51
2:I:132:ALA:HA	2:I:194:SER:HB2	1.92	0.51
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.43	0.51
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.39	0.51
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.92	0.51
2:G:4823:LEU:HD11	2:E:4839:MET:HB3	1.92	0.51
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.43	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.92	0.51
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	1.91	0.51
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.51
2:E:4184:MET:HE1	2:E:4188:ARG:HE	1.74	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.92	0.51
2:B:621:ILE:O	2:B:625:LEU:N	2.40	0.51
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.92	0.51
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.93	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.27	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.92	0.51
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.92	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.51
2:B:2868:SER:O	2:B:2872:GLN:N	2.43	0.51
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.75	0.51
2:I:621:ILE:O	2:I:625:LEU:N	2.40	0.51
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.43	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.51
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.44	0.51
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.43	0.50
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.92	0.50
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.93	0.50
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	1.91	0.50
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.76	0.50
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.93	0.50
2:G:4984:ASN:C	2:G:4986:ALA:N	2.64	0.50
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.93	0.50
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.93	0.50
2:E:4984:ASN:C	2:E:4986:ALA:N	2.65	0.50
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.93	0.50
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.50
2:B:614:VAL:HG22	2:B:616:SER:H	1.76	0.50
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.44	0.50
2:I:4984:ASN:C	2:I:4986:ALA:N	2.64	0.50
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.94	0.50
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.94	0.50
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.94	0.50
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.91	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.50
2:I:2868:SER:O	2:I:2872:GLN:N	2.43	0.50
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	2.24	0.50
2:G:621:ILE:O	2:G:625:LEU:N	2.40	0.50
2:I:278:GLN:N	2:I:315:CYS:SG	2.85	0.50
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.94	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.50
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.75	0.50
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.92	0.50
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.94	0.50
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.94	0.50
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.50
2:E:614:VAL:HG22	2:E:616:SER:H	1.76	0.50
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.94	0.50
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.42	0.50
2:E:4983:HIS:ND1	2:E:4983:HIS:N	2.60	0.50
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	2.24	0.50
2:B:4984:ASN:C	2:B:4986:ALA:N	2.64	0.50
2:I:683:ARG:NH1	2:I:707:VAL:O	2.43	0.50
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.94	0.50
2:I:4837:LEU:HD22	2:I:4936:ILE:HD11	1.93	0.50
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.74	0.50
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.44	0.50
2:B:4837:LEU:HD22	2:B:4936:ILE:HD11	1.93	0.50
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.77	0.50
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.94	0.50
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.76	0.50
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.76	0.49
2:I:4983:HIS:ND1	2:I:4983:HIS:N	2.60	0.49
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.44	0.49
2:G:4837:LEU:HD22	2:G:4936:ILE:HD11	1.93	0.49
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.49
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.95	0.49
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.45	0.49
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.44	0.49
2:G:3984:ARG:HH22	2:E:161:GLU:HA	1.76	0.49
2:B:278:GLN:N	2:B:315:CYS:SG	2.85	0.49
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.94	0.49
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.94	0.49
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.94	0.49
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.78	0.49
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.94	0.49
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.92	0.49
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.94	0.49
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.94	0.49
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.94	0.49
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.45	0.49
2:G:4983:HIS:ND1	2:G:4983:HIS:N	2.60	0.49
2:E:626:LEU:HD23	2:E:630:GLU:H	1.77	0.49
2:E:4837:LEU:HD22	2:E:4936:ILE:HD11	1.93	0.49
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.29	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.49
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.93	0.49
2:B:626:LEU:HD23	2:B:630:GLU:H	1.78	0.49
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.49
2:B:4958:CYS:SG	2:B:4961:CYS:N	2.85	0.49
2:G:626:LEU:HD23	2:G:630:GLU:H	1.78	0.49
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.45	0.49
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.44	0.49
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.78	0.49
2:I:626:LEU:HD23	2:I:630:GLU:H	1.78	0.49
2:I:2778:GLY:HA3	2:I:2787:THR:HB	1.95	0.49
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.95	0.49
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.95	0.49
2:E:4958:CYS:SG	2:E:4961:CYS:N	2.85	0.49
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.95	0.49
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.93	0.49
2:G:786:GLY:HA2	2:G:1631:GLN:HA	1.95	0.49
2:E:786:GLY:HA2	2:E:1631:GLN:HA	1.95	0.49
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.49
2:B:4697:VAL:O	2:B:4701:TRP:N	2.46	0.48
2:B:4983:HIS:ND1	2:B:4983:HIS:N	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:683:ARG:NH1	2:E:707:VAL:O	2.43	0.48
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.94	0.48
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.95	0.48
2:G:614:VAL:HG22	2:G:616:SER:H	1.76	0.48
2:B:2214:VAL:HG23	2:B:2215:LEU:HD12	1.96	0.48
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.78	0.48
2:E:1991:THR:O	2:E:1995:THR:OG1	2.31	0.48
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.95	0.48
2:I:614:VAL:HG22	2:I:616:SER:H	1.76	0.48
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.78	0.48
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.96	0.48
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.40	0.48
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.45	0.48
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.96	0.48
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.48
2:G:2778:GLY:HA3	2:G:2787:THR:HB	1.95	0.48
2:B:4914:VAL:HG21	2:E:4884:LEU:HD11	1.96	0.48
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.95	0.48
2:E:278:GLN:N	2:E:315:CYS:SG	2.85	0.48
2:B:786:GLY:HA2	2:B:1631:GLN:HA	1.95	0.48
2:I:786:GLY:HA2	2:I:1631:GLN:HA	1.95	0.48
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.96	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.31	0.47
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.96	0.47
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.96	0.47
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.29	0.47
2:I:4697:VAL:O	2:I:4701:TRP:N	2.46	0.47
2:E:41:GLY:O	2:E:45:ARG:NH1	2.47	0.47
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.43	0.47
2:E:4697:VAL:O	2:E:4701:TRP:N	2.47	0.47
2:B:41:GLY:O	2:B:45:ARG:NH1	2.47	0.47
2:I:41:GLY:O	2:I:45:ARG:NH1	2.47	0.47
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.47
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.96	0.47
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.47
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.78	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.50	0.47
2:I:2214:VAL:HG23	2:I:2215:LEU:HD12	1.96	0.47
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.48	0.47
2:G:2214:VAL:HG23	2:G:2215:LEU:HD12	1.96	0.47
2:G:278:GLN:N	2:G:315:CYS:SG	2.85	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:983:THR:O	2:G:987:ARG:N	2.46	0.47
2:E:1457:UNK:N	2:E:1497:UNK:O	2.48	0.47
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.97	0.47
2:B:1772:ARG:HH21	2:B:1952:GLN:HE22	1.63	0.47
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.96	0.47
2:G:41:GLY:O	2:G:45:ARG:NH1	2.47	0.47
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.97	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.50	0.47
2:E:2214:VAL:HG23	2:E:2215:LEU:HD12	1.96	0.47
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.97	0.47
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.97	0.47
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.47
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.47
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.48	0.47
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.96	0.47
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.48	0.47
2:E:1772:ARG:HH21	2:E:1952:GLN:HE22	1.63	0.47
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.97	0.47
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	2.24	0.47
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.79	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.97	0.47
2:I:983:THR:O	2:I:987:ARG:N	2.46	0.47
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.97	0.47
2:G:4697:VAL:O	2:G:4701:TRP:N	2.46	0.47
2:E:2778:GLY:HA3	2:E:2787:THR:HB	1.95	0.47
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.50	0.47
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.80	0.47
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.44	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.48	0.47
2:I:1457:UNK:N	2:I:1497:UNK:O	2.48	0.47
2:I:1772:ARG:HH21	2:I:1952:GLN:HE22	1.63	0.47
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.96	0.47
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.97	0.47
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.80	0.47
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.96	0.47
2:G:1457:UNK:N	2:G:1497:UNK:O	2.48	0.47
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	1.97	0.47
2:E:983:THR:O	2:E:987:ARG:N	2.46	0.47
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	1.97	0.47
2:E:3361:UNK:O	2:E:3365:UNK:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.97	0.47
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.97	0.47
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.97	0.47
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.80	0.47
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.97	0.47
2:B:1457:UNK:N	2:B:1497:UNK:O	2.48	0.46
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.96	0.46
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.50	0.46
2:G:1772:ARG:HH21	2:G:1952:GLN:HE22	1.63	0.46
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.97	0.46
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.80	0.46
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.48	0.46
2:B:2778:GLY:HA3	2:B:2787:THR:HB	1.95	0.46
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.97	0.46
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.98	0.46
2:G:4884:LEU:HD11	2:E:4914:VAL:HG21	1.97	0.46
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.98	0.46
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.97	0.46
2:I:3361:UNK:O	2:I:3365:UNK:N	2.48	0.46
2:E:1130:GLN:HG2	2:E:1138:PRO:HA	1.98	0.46
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.98	0.46
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.78	0.46
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.46
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	1.98	0.46
2:B:3361:UNK:O	2:B:3365:UNK:N	2.48	0.46
2:B:4998:LYS:NZ	2:B:5007:GLU:OE1	2.43	0.46
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.98	0.46
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.98	0.46
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.98	0.46
2:E:243:ARG:NH1	2:E:301:VAL:O	2.42	0.46
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.48	0.46
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.46
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.98	0.46
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.98	0.46
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.98	0.46
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.97	0.46
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.46
2:E:2902:HIS:HB3	2:E:2905:LEU:HG	1.98	0.46
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.97	0.46
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.97	0.46
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.48	0.46
2:I:2810:LYS:O	2:I:2814:LYS:N	2.42	0.46
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.29	0.46
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.48	0.46
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.98	0.46
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	1.97	0.46
2:I:913:LEU:O	2:I:918:ARG:NH2	2.49	0.46
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.46
2:I:4884:LEU:HD11	2:G:4914:VAL:HG21	1.97	0.46
2:G:606:LEU:O	2:G:617:ASN:ND2	2.49	0.46
2:G:2810:LYS:O	2:G:2814:LYS:N	2.42	0.46
2:G:3361:UNK:O	2:G:3365:UNK:N	2.48	0.46
2:E:606:LEU:O	2:E:617:ASN:ND2	2.49	0.46
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.97	0.46
2:B:1295:UNK:N	2:B:1454:UNK:O	2.49	0.46
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.97	0.46
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.98	0.46
2:I:606:LEU:O	2:I:617:ASN:ND2	2.49	0.46
2:I:1105:ALA:N	2:I:1189:LEU:O	2.49	0.46
2:G:1295:UNK:N	2:G:1454:UNK:O	2.49	0.46
2:G:2810:LYS:HE2	2:G:2814:LYS:HE3	1.98	0.46
2:E:2810:LYS:HE2	2:E:2814:LYS:HE3	1.98	0.46
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.96	0.46
2:B:913:LEU:O	2:B:918:ARG:NH2	2.49	0.46
2:B:1105:ALA:N	2:B:1189:LEU:O	2.49	0.46
2:B:1130:GLN:HG2	2:B:1138:PRO:HA	1.97	0.46
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.49	0.46
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	1.97	0.46
2:I:4852:THR:HG21	2:I:4883:TYR:HB2	1.99	0.46
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.45
2:I:776:LEU:HG	2:I:848:HIS:HA	1.99	0.45
2:I:2880:GLU:O	2:I:2884:ASN:N	2.49	0.45
2:I:4713:SER:HA	2:I:4718:LYS:HE2	1.99	0.45
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.45
2:I:1295:UNK:N	2:I:1454:UNK:O	2.49	0.45
2:I:1771:LEU:HB3	2:I:2153:MET:HE1	1.99	0.45
2:I:2902:HIS:HB3	2:I:2905:LEU:HG	1.98	0.45
2:G:221:ARG:NH2	2:G:397:GLU:OE2	2.48	0.45
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.43	0.45
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.45
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.45
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.45
2:B:4713:SER:HA	2:B:4718:LYS:HE2	1.98	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.98	0.45
2:G:776:LEU:HG	2:G:848:HIS:HA	1.98	0.45
2:G:3760:LYS:NZ	2:G:5000:GLU:OE1	2.40	0.45
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	2.25	0.45
2:G:4852:THR:HG21	2:G:4883:TYR:HB2	1.99	0.45
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.98	0.45
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.98	0.45
2:B:606:LEU:O	2:B:617:ASN:ND2	2.49	0.45
2:B:683:ARG:NH1	2:B:707:VAL:O	2.43	0.45
2:I:243:ARG:NH1	2:I:301:VAL:O	2.42	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.99	0.45
2:I:1130:GLN:HG2	2:I:1138:PRO:HA	1.98	0.45
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.97	0.45
2:I:3760:LYS:NZ	2:I:5000:GLU:OE1	2.40	0.45
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.45
2:E:913:LEU:O	2:E:918:ARG:NH2	2.49	0.45
2:E:1295:UNK:N	2:E:1454:UNK:O	2.49	0.45
2:E:776:LEU:HG	2:E:848:HIS:HA	1.99	0.45
2:B:776:LEU:HG	2:B:848:HIS:HA	1.99	0.45
2:B:4978:HIS:CE1	2:B:5027:CYS:HG	2.35	0.45
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.99	0.45
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.50	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.50	0.45
2:G:243:ARG:NH1	2:G:301:VAL:O	2.42	0.45
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.99	0.45
2:G:2902:HIS:HB3	2:G:2905:LEU:HG	1.98	0.45
2:G:3973:CYS:SG	2:G:3976:ASN:ND2	2.90	0.45
2:E:3760:LYS:NZ	2:E:5000:GLU:OE1	2.40	0.45
2:B:2880:GLU:O	2:B:2884:ASN:N	2.49	0.45
2:I:2810:LYS:HE2	2:I:2814:LYS:HE3	1.98	0.45
2:I:3973:CYS:SG	2:I:3976:ASN:ND2	2.90	0.45
2:G:913:LEU:O	2:G:918:ARG:NH2	2.49	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.99	0.45
2:B:3766:GLN:HG3	2:B:3769:ARG:HH12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4852:THR:HG21	2:E:4883:TYR:HB2	1.99	0.45
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.98	0.45
2:I:3766:GLN:HG3	2:I:3769:ARG:HH12	1.82	0.45
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.45
2:G:647:ASN:ND2	2:G:820:ARG:O	2.49	0.45
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.50	0.45
2:G:2880:GLU:O	2:G:2884:ASN:N	2.49	0.45
2:G:3766:GLN:HG3	2:G:3769:ARG:HH12	1.82	0.45
2:G:4713:SER:HA	2:G:4718:LYS:HE2	1.98	0.45
2:E:647:ASN:ND2	2:E:820:ARG:O	2.49	0.45
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.82	0.45
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.50	0.45
2:B:2810:LYS:HE2	2:B:2814:LYS:HE3	1.98	0.45
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.99	0.45
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.50	0.45
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.50	0.45
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.45
2:E:3766:GLN:HG3	2:E:3769:ARG:HH12	1.82	0.45
2:B:3973:CYS:SG	2:B:3976:ASN:ND2	2.90	0.44
2:B:4852:THR:HG21	2:B:4883:TYR:HB2	1.99	0.44
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.81	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.99	0.44
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.82	0.44
2:G:2305:CYS:HA	2:G:2324:ASN:HD22	1.82	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.44
2:G:4826:ILE:O	2:G:4829:SER:OG	2.31	0.44
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.82	0.44
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.99	0.44
2:B:2950:UNK:O	2:B:2954:UNK:N	2.50	0.44
2:B:4959:PHE:CD1	2:B:4959:PHE:O	2.70	0.44
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.44
2:G:1130:GLN:HG2	2:G:1138:PRO:HA	1.97	0.44
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.44
2:E:3973:CYS:SG	2:E:3976:ASN:ND2	2.90	0.44
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.99	0.44
2:B:1973:GLN:O	2:B:1977:TYR:N	2.46	0.44
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.44
2:I:2305:CYS:HA	2:I:2324:ASN:HD22	1.82	0.44
2:G:683:ARG:NH1	2:G:707:VAL:O	2.43	0.44
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4959:PHE:CD1	2:G:4959:PHE:O	2.70	0.44
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.99	0.44
2:E:2880:GLU:O	2:E:2884:ASN:N	2.49	0.44
2:B:647:ASN:ND2	2:B:820:ARG:O	2.49	0.44
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.99	0.44
2:B:2305:CYS:HA	2:B:2324:ASN:HD22	1.82	0.44
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	1.98	0.44
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.51	0.44
2:G:20:VAL:HG12	2:G:204:PRO:HA	2.00	0.44
2:G:1771:LEU:HB3	2:G:2153:MET:HE1	1.99	0.44
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:E:583:ILE:HA	2:E:586:ILE:HD12	1.99	0.44
2:E:1105:ALA:N	2:E:1189:LEU:O	2.49	0.44
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.51	0.44
2:B:1771:LEU:HB3	2:B:2153:MET:HE1	2.00	0.44
2:G:379:HIS:CD2	2:G:381:GLU:H	2.36	0.44
2:E:20:VAL:HG12	2:E:204:PRO:HA	2.00	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.36	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.44
2:B:583:ILE:HA	2:B:586:ILE:HD12	1.99	0.44
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.50	0.44
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.36	0.44
2:B:4928:LEU:HD13	2:B:4928:LEU:HA	1.89	0.44
2:I:583:ILE:HA	2:I:586:ILE:HD12	1.99	0.44
2:I:594:GLY:H	2:I:1594:ARG:HD3	1.82	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.44
2:G:594:GLY:H	2:G:1594:ARG:HD3	1.82	0.44
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.51	0.44
2:E:635:THR:HB	2:E:1639:LEU:HD23	2.00	0.44
2:E:4713:SER:HA	2:E:4718:LYS:HE2	1.98	0.44
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.44
2:I:4998:LYS:NZ	2:I:5007:GLU:OE1	2.43	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.83	0.44
2:G:4892:ARG:NH2	2:E:4899:ASP:OD1	2.48	0.44
2:E:594:GLY:H	2:E:1594:ARG:HD3	1.82	0.44
2:E:892:THR:N	2:E:902:ARG:O	2.50	0.44
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.43	0.44
2:E:2305:CYS:HA	2:E:2324:ASN:HD22	1.82	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1166:GLY:HA3	2:I:1216:ILE:HD13	2.00	0.44
2:I:4959:PHE:CD1	2:I:4959:PHE:O	2.70	0.44
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.51	0.44
2:B:594:GLY:H	2:B:1594:ARG:HD3	1.82	0.44
2:I:20:VAL:HG12	2:I:204:PRO:HA	2.00	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.36	0.44
2:I:4958:CYS:SG	2:I:4961:CYS:N	2.85	0.44
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.36	0.44
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.49	0.44
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.43	0.44
2:B:635:THR:HB	2:B:1639:LEU:HD23	2.00	0.43
2:B:662:TRP:HZ3	2:B:811:CYS:HA	1.83	0.43
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.49	0.43
2:B:1166:GLY:HA3	2:B:1216:ILE:HD13	1.99	0.43
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.01	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:I:219:VAL:HG13	2:I:285:VAL:HG21	2.00	0.43
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.82	0.43
2:I:4892:ARG:NH2	2:G:4899:ASP:OD1	2.47	0.43
2:G:583:ILE:HA	2:G:586:ILE:HD12	1.99	0.43
2:G:1166:GLY:HA3	2:G:1216:ILE:HD13	1.99	0.43
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.29	0.43
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.43
2:E:1771:LEU:HB3	2:E:2153:MET:HE1	1.99	0.43
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.01	0.43
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.83	0.43
2:B:2810:LYS:O	2:B:2814:LYS:N	2.42	0.43
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	2.00	0.43
2:I:2012:PHE:CG	2:I:2022:PRO:HD3	2.54	0.43
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.43
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.99	0.43
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.99	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.01	0.43
2:B:379:HIS:CD2	2:B:381:GLU:H	2.36	0.43
2:I:652:ARG:HB3	2:I:773:LEU:HD13	2.01	0.43
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.53	0.43
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.44	0.43
2:G:219:VAL:HG13	2:G:285:VAL:HG21	2.00	0.43
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.49	0.43
2:E:1166:GLY:HA3	2:E:1216:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.83	0.43
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.83	0.43
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	2.01	0.43
2:B:4826:ILE:O	2:B:4829:SER:OG	2.31	0.43
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.83	0.43
2:G:2012:PHE:CG	2:G:2022:PRO:HD3	2.54	0.43
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.53	0.43
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.36	0.43
1:A:25:HIS:HB3	1:A:40:ARG:HD3	2.01	0.43
2:B:20:VAL:HG12	2:B:204:PRO:HA	2.00	0.43
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.83	0.43
2:B:652:ARG:HB3	2:B:773:LEU:HD13	2.01	0.43
2:I:647:ASN:ND2	2:I:820:ARG:O	2.49	0.43
2:G:2353:VAL:O	2:G:2357:LEU:N	2.49	0.43
2:E:15:ARG:HD3	2:E:98:HIS:HB3	2.00	0.43
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.01	0.43
1:A:27:THR:HB	1:A:100:ASP:HB3	2.01	0.43
2:B:892:THR:N	2:B:902:ARG:O	2.50	0.43
2:I:221:ARG:NH2	2:I:397:GLU:OE2	2.48	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.35	0.43
2:G:635:THR:HB	2:G:1639:LEU:HD23	2.00	0.43
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.43
2:B:794:GLY:H	2:B:798:GLY:HA3	1.84	0.43
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.53	0.43
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.43
2:I:15:ARG:HD3	2:I:98:HIS:HB3	2.00	0.43
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.83	0.43
2:G:1105:ALA:N	2:G:1189:LEU:O	2.49	0.43
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.38	0.43
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.84	0.43
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	2.01	0.43
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.01	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.42	0.43
2:E:221:ARG:NH2	2:E:397:GLU:OE2	2.48	0.43
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.01	0.43
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.52	0.43
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.01	0.43
2:I:2758:PHE:O	2:I:2762:THR:N	2.51	0.43
2:G:15:ARG:HD3	2:G:98:HIS:HB3	2.00	0.43
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.01	0.43
2:E:652:ARG:HB3	2:E:773:LEU:HD13	2.01	0.43
1:H:25:HIS:HB3	1:H:40:ARG:HD3	2.01	0.43
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.01	0.43
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.43
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.43
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.83	0.43
2:E:794:GLY:H	2:E:798:GLY:HA3	1.84	0.43
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.01	0.43
2:B:2012:PHE:CG	2:B:2022:PRO:HD3	2.54	0.43
2:B:2758:PHE:O	2:B:2762:THR:N	2.51	0.43
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	2.01	0.43
2:I:4928:LEU:HD13	2:I:4928:LEU:HA	1.89	0.43
2:G:664:PHE:HB2	2:G:746:CYS:HB2	2.01	0.43
2:G:4083:ASP:HB3	2:G:4086:GLY:H	1.84	0.43
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.83	0.43
2:E:4083:ASP:HB3	2:E:4086:GLY:H	1.84	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.42
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.52	0.42
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.42
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.01	0.42
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.01	0.42
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.44	0.42
2:I:635:THR:HB	2:I:1639:LEU:HD23	2.00	0.42
2:I:664:PHE:HB2	2:I:746:CYS:HB2	2.01	0.42
2:G:652:ARG:HB3	2:G:773:LEU:HD13	2.01	0.42
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.42
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.38	0.42
2:B:468:LEU:HB3	2:B:472:ARG:HH12	1.85	0.42
2:B:983:THR:O	2:B:987:ARG:N	2.46	0.42
2:B:3804:ILE:HG22	2:B:3812:VAL:HG21	2.02	0.42
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	2.01	0.42
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
2:G:3804:ILE:HG22	2:G:3812:VAL:HG21	2.01	0.42
2:G:4558:ASN:HB2	2:G:4561:THR:HB	2.02	0.42
2:E:2012:PHE:CG	2:E:2022:PRO:HD3	2.54	0.42
1:F:27:THR:HB	1:F:100:ASP:HB3	2.01	0.42
2:I:794:GLY:H	2:I:798:GLY:HA3	1.84	0.42
2:I:4558:ASN:HB2	2:I:4561:THR:HB	2.01	0.42
2:G:794:GLY:H	2:G:798:GLY:HA3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.83	0.42
2:E:219:VAL:HG13	2:E:285:VAL:HG21	2.00	0.42
2:E:468:LEU:HB3	2:E:472:ARG:HH12	1.85	0.42
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.83	0.42
2:I:662:TRP:HZ3	2:I:811:CYS:HA	1.83	0.42
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.53	0.42
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.84	0.42
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.01	0.42
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.53	0.42
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.01	0.42
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.42
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.52	0.42
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	2.01	0.42
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.01	0.42
1:J:25:HIS:HB3	1:J:40:ARG:HD3	2.01	0.42
2:B:15:ARG:HD3	2:B:98:HIS:HB3	2.00	0.42
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.01	0.42
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.38	0.42
2:G:468:LEU:HB3	2:G:472:ARG:HH12	1.85	0.42
2:E:3804:ILE:HG22	2:E:3812:VAL:HG21	2.01	0.42
1:H:27:THR:HB	1:H:100:ASP:HB3	2.01	0.42
1:J:27:THR:HB	1:J:100:ASP:HB3	2.01	0.42
2:B:219:VAL:HG13	2:B:285:VAL:HG21	2.00	0.42
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.42	0.42
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.02	0.42
2:I:2128:TYR:HB3	2:I:3669:PHE:HB3	2.02	0.42
2:G:662:TRP:HZ3	2:G:811:CYS:HA	1.83	0.42
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	2.00	0.42
2:B:2128:TYR:HB3	2:B:3669:PHE:HB3	2.02	0.42
2:B:4083:ASP:HB3	2:B:4086:GLY:H	1.84	0.42
2:E:2128:TYR:HB3	2:E:3669:PHE:HB3	2.02	0.42
2:E:2298:VAL:HG21	2:E:2335:LEU:HD21	2.02	0.42
2:E:2758:PHE:O	2:E:2762:THR:N	2.51	0.42
2:B:1163:THR:HG22	2:B:1168:VAL:HA	2.02	0.42
2:B:2353:VAL:O	2:B:2357:LEU:N	2.49	0.42
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.01	0.42
2:I:1163:THR:HG22	2:I:1168:VAL:HA	2.02	0.42
2:I:3804:ILE:HG22	2:I:3812:VAL:HG21	2.02	0.42
2:I:4083:ASP:HB3	2:I:4086:GLY:H	1.84	0.42
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.02	0.42
2:E:664:PHE:HB2	2:E:746:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.84	0.42
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.83	0.42
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.01	0.42
2:E:719:LEU:HA	2:E:730:VAL:HG22	2.02	0.42
2:E:2353:VAL:O	2:E:2357:LEU:N	2.49	0.42
2:E:4136:ALA:HA	2:E:4139:ILE:HG22	2.02	0.42
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.48	0.42
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.42
2:G:1163:THR:HG22	2:G:1168:VAL:HA	2.02	0.42
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	2.01	0.42
2:B:2291:GLN:HE21	2:B:2294:ASP:H	1.68	0.41
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.38	0.41
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.85	0.41
2:B:4136:ALA:HA	2:B:4139:ILE:HG22	2.02	0.41
2:G:892:THR:N	2:G:902:ARG:O	2.50	0.41
2:G:2128:TYR:HB3	2:G:3669:PHE:HB3	2.02	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.41
2:E:2810:LYS:O	2:E:2814:LYS:N	2.42	0.41
2:B:664:PHE:HB2	2:B:746:CYS:HB2	2.01	0.41
2:I:2353:VAL:O	2:I:2357:LEU:N	2.49	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.01	0.41
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.52	0.41
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.01	0.41
2:E:1163:THR:HG22	2:E:1168:VAL:HA	2.02	0.41
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.02	0.41
2:I:2291:GLN:HE21	2:I:2294:ASP:H	1.69	0.41
2:G:907:LEU:O	2:G:963:ASN:ND2	2.41	0.41
2:G:1154:ASP:O	2:G:1158:ASN:N	2.53	0.41
2:G:3663:LEU:H	2:G:3663:LEU:HG	1.72	0.41
2:G:4984:ASN:OD1	2:G:4986:ALA:HB3	2.21	0.41
2:E:689:THR:H	2:E:778:PHE:HE2	1.68	0.41
2:E:793:LEU:HB2	2:E:797:HIS:H	1.85	0.41
2:E:1259:ARG:NH2	2:E:1595:LEU:O	2.54	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.41
2:I:950:LEU:HB3	2:I:970:LEU:HD22	2.01	0.41
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.53	0.41
2:G:1973:GLN:O	2:G:1977:TYR:N	2.46	0.41
2:E:950:LEU:HB3	2:E:970:LEU:HD22	2.01	0.41
2:E:2291:GLN:HE21	2:E:2294:ASP:H	1.69	0.41
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.53	0.41
2:E:3773:ARG:HG3	2:E:3815:LYS:HZ3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:719:LEU:HA	2:B:730:VAL:HG22	2.02	0.41
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.02	0.41
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.41
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	2.03	0.41
2:I:4158:PRO:HA	2:I:4161:ARG:HB2	2.02	0.41
2:I:4984:ASN:OD1	2:I:4986:ALA:HB3	2.21	0.41
2:G:395:GLN:HG3	2:G:397:GLU:H	1.86	0.41
2:E:4984:ASN:OD1	2:E:4986:ALA:HB3	2.21	0.41
2:B:221:ARG:NH2	2:B:397:GLU:OE2	2.48	0.41
2:B:689:THR:H	2:B:778:PHE:HE2	1.68	0.41
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.84	0.41
2:B:4062:PHE:HE2	2:B:4143:VAL:HG21	1.86	0.41
2:I:234:SER:O	2:I:242:ARG:NE	2.52	0.41
2:I:2298:VAL:HG21	2:I:2335:LEU:HD21	2.02	0.41
2:I:4062:PHE:HE2	2:I:4143:VAL:HG21	1.86	0.41
2:G:719:LEU:HA	2:G:730:VAL:HG22	2.02	0.41
2:G:2291:GLN:HE21	2:G:2294:ASP:H	1.68	0.41
2:G:2298:VAL:HG21	2:G:2335:LEU:HD21	2.02	0.41
2:G:4136:ALA:HA	2:G:4139:ILE:HG22	2.02	0.41
2:G:4958:CYS:SG	2:G:4961:CYS:N	2.85	0.41
2:E:4558:ASN:HB2	2:E:4561:THR:HB	2.01	0.41
1:F:25:HIS:HB3	1:F:40:ARG:HD3	2.01	0.41
2:B:1259:ARG:NH2	2:B:1595:LEU:O	2.54	0.41
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.86	0.41
2:I:45:ARG:NH2	2:I:447:ASP:OD1	2.54	0.41
2:I:793:LEU:HB2	2:I:797:HIS:H	1.85	0.41
2:I:1970:GLN:HB3	2:I:3641:LEU:HG	2.03	0.41
2:G:3676:ASP:N	2:G:3676:ASP:OD1	2.53	0.41
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.02	0.41
2:B:378:LEU:HD23	2:B:378:LEU:HA	1.94	0.41
2:B:4558:ASN:HB2	2:B:4561:THR:HB	2.02	0.41
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.86	0.41
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.41
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.41
2:G:1970:GLN:HB3	2:G:3641:LEU:HG	2.03	0.41
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.43	0.41
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.03	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.41
2:B:2298:VAL:HG21	2:B:2335:LEU:HD21	2.02	0.41
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.02	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41
2:I:468:LEU:HB3	2:I:472:ARG:HH12	1.85	0.41
2:I:719:LEU:HA	2:I:730:VAL:HG22	2.02	0.41
2:I:892:THR:N	2:I:902:ARG:O	2.50	0.41
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.41
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.03	0.41
2:I:3662:ILE:H	2:I:3662:ILE:HG13	1.77	0.41
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.86	0.41
2:G:793:LEU:HB2	2:G:797:HIS:H	1.85	0.41
2:G:950:LEU:HB3	2:G:970:LEU:HD22	2.01	0.41
2:G:1725:ARG:HH21	2:G:1725:ARG:HD2	1.74	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.02	0.41
2:G:4062:PHE:HE2	2:G:4143:VAL:HG21	1.86	0.41
2:G:4158:PRO:HA	2:G:4161:ARG:HB2	2.02	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.02	0.41
2:E:1970:GLN:HB3	2:E:3641:LEU:HG	2.03	0.41
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	2.03	0.41
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	2.03	0.41
2:E:4062:PHE:HE2	2:E:4143:VAL:HG21	1.86	0.41
2:E:4158:PRO:HA	2:E:4161:ARG:HB2	2.02	0.41
2:B:793:LEU:HB2	2:B:797:HIS:H	1.85	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.41
2:B:1970:GLN:HB3	2:B:3641:LEU:HG	2.03	0.41
2:B:2437:ALA:HA	2:B:2438:PRO:HD3	1.97	0.41
2:B:4984:ASN:OD1	2:B:4986:ALA:HB3	2.21	0.41
2:I:1154:ASP:O	2:I:1158:ASN:N	2.54	0.41
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.41
2:G:1161:ILE:HA	2:G:1177:THR:HB	2.02	0.41
2:G:2145:SER:HB2	2:G:3647:HIS:CE1	2.56	0.41
2:E:645:ARG:N	2:E:824:GLU:O	2.45	0.41
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.56	0.41
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.93	0.40
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.94	0.40
2:B:950:LEU:HB3	2:B:970:LEU:HD22	2.01	0.40
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.43	0.40
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.03	0.40
2:I:4136:ALA:HA	2:I:4139:ILE:HG22	2.02	0.40
2:G:1259:ARG:NH2	2:G:1595:LEU:O	2.54	0.40
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1124:PHE:HB2	2:E:1162:PHE:CE2	2.56	0.40
2:E:1161:ILE:HA	2:E:1177:THR:HB	2.02	0.40
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	2.03	0.40
2:E:1973:GLN:O	2:E:1977:TYR:N	2.46	0.40
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.40
2:B:2927:LEU:HA	2:B:2930:LEU:HD12	2.04	0.40
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	2.03	0.40
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.03	0.40
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.86	0.40
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.86	0.40
2:B:45:ARG:NH2	2:B:447:ASP:OD1	2.54	0.40
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.37	0.40
2:B:907:LEU:O	2:B:963:ASN:ND2	2.41	0.40
2:B:1154:ASP:O	2:B:1158:ASN:N	2.53	0.40
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	2.03	0.40
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.03	0.40
2:B:3552:UNK:O	2:B:3556:UNK:N	2.55	0.40
2:I:1124:PHE:HB2	2:I:1162:PHE:CE2	2.56	0.40
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	2.03	0.40
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.04	0.40
2:E:395:GLN:HG3	2:E:397:GLU:H	1.86	0.40
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.03	0.40
2:G:45:ARG:NH2	2:G:447:ASP:OD1	2.54	0.40
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.04	0.40
2:G:1124:PHE:HB2	2:G:1162:PHE:CE2	2.56	0.40
2:B:2145:SER:HB2	2:B:3647:HIS:CE1	2.56	0.40
2:B:4822:THR:O	2:B:4825:THR:OG1	2.36	0.40
2:I:689:THR:H	2:I:778:PHE:HE2	1.68	0.40
2:I:1259:ARG:NH2	2:I:1595:LEU:O	2.54	0.40
2:I:2352:VAL:HG12	2:I:2355:ARG:HH11	1.86	0.40
2:I:3552:UNK:O	2:I:3556:UNK:N	2.55	0.40
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	2.04	0.40
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.03	0.40
2:G:2776:SER:O	2:G:2788:HIS:N	2.55	0.40
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	2.03	0.40
2:E:45:ARG:NH2	2:E:447:ASP:OD1	2.54	0.40
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.04	0.40
2:E:2927:LEU:HA	2:E:2930:LEU:HD12	2.04	0.40
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.96	0.40
2:E:4822:THR:O	2:E:4825:THR:OG1	2.36	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	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	47	81
2	E	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	47	81
2	G	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	47	81
2	I	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	11973 (90%)	1363 (10%)	24 (0%)	50	81

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU
2	I	4985	LEU
2	G	4985	LEU
2	E	4985	LEU
2	B	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	E	1708	ARG
2	B	1932	PRO
2	B	2292	GLU
2	B	4641	PRO
2	I	1932	PRO
2	I	2292	GLU
2	I	4641	PRO
2	G	1932	PRO
2	G	2292	GLU
2	G	4641	PRO

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Mol	Chain	Res	Type
2	E	1932	PRO
2	E	2292	GLU
2	E	4641	PRO
2	B	1840	PRO
2	I	1840	PRO
2	G	1840	PRO
2	E	1840	PRO

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
2	E	2493/3022 (82%)	2471 (99%)	22 (1%)	78	88
2	G	2493/3022 (82%)	2471 (99%)	22 (1%)	78	88
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	81	89
All	All	10324/12444 (83%)	10238 (99%)	86 (1%)	82	89

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG

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Mol	Chain	Res	Type
2	B	3663	LEU
2	B	3762	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4137	ARG
2	B	4959	PHE
2	B	4961	CYS
2	B	4978	HIS
2	B	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3762	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4137	ARG
2	I	4959	PHE
2	I	4961	CYS
2	I	4978	HIS
2	I	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG

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Mol	Chain	Res	Type
2	G	3663	LEU
2	G	3762	ARG
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4137	ARG
2	G	4959	PHE
2	G	4961	CYS
2	G	4978	HIS
2	G	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU
2	E	3762	ARG
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4137	ARG
2	E	4959	PHE
2	E	4961	CYS
2	E	4978	HIS
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS

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Mol	Chain	Res	Type
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	413	GLN
2	B	725	HIS
2	B	797	HIS
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1952	GLN
2	B	2005	GLN
2	B	2041	HIS
2	B	2127	GLN
2	B	2291	GLN
2	B	3771	HIS
2	B	3781	GLN
2	B	3809	ASN
2	B	3830	GLN
2	B	3896	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	3976	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4806	ASN
2	B	4983	HIS
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS

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Mol	Chain	Res	Type
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	725	HIS
2	I	797	HIS
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1952	GLN
2	I	2005	GLN
2	I	2041	HIS
2	I	2127	GLN
2	I	2291	GLN
2	I	3771	HIS
2	I	3781	GLN
2	I	3809	ASN
2	I	3830	GLN
2	I	3896	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	3976	ASN
2	I	4034	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4983	HIS
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN
2	G	725	HIS
2	G	797	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN

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Mol	Chain	Res	Type
2	G	1719	HIS
2	G	1775	HIS
2	G	1952	GLN
2	G	2005	GLN
2	G	2041	HIS
2	G	2127	GLN
2	G	2291	GLN
2	G	3771	HIS
2	G	3781	GLN
2	G	3809	ASN
2	G	3830	GLN
2	G	3896	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	3976	ASN
2	G	4034	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4983	HIS
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	725	HIS
2	E	797	HIS
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1952	GLN
2	E	2005	GLN
2	E	2041	HIS
2	E	2127	GLN
2	E	2291	GLN
2	E	3771	HIS
2	E	3781	GLN
2	E	3809	ASN

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Mol	Chain	Res	Type
2	E	3830	GLN
2	E	3896	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	3976	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4806	ASN
2	E	4983	HIS

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 8 ligands modelled in this entry, 8 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	14
2	I	14
2	G	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.83
1	I	4345:UNK	C	4540:PHE	N	73.83
1	G	4345:UNK	C	4540:PHE	N	73.83
1	E	4345:UNK	C	4540:PHE	N	73.83
1	B	3613:UNK	C	3639:THR	N	45.16
1	I	3613:UNK	C	3639:THR	N	45.16
1	G	3613:UNK	C	3639:THR	N	45.16
1	E	3613:UNK	C	3639:THR	N	45.16
1	B	4253:GLU	C	4320:UNK	N	28.14
1	I	4253:GLU	C	4320:UNK	N	28.14
1	G	4253:GLU	C	4320:UNK	N	28.14
1	E	4253:GLU	C	4320:UNK	N	28.14
1	B	3163:UNK	C	3170:UNK	N	16.17
1	I	3163:UNK	C	3170:UNK	N	16.17
1	G	3163:UNK	C	3170:UNK	N	16.17
1	E	3163:UNK	C	3170:UNK	N	16.17
1	B	3063:UNK	C	3134:UNK	N	14.94
1	I	3063:UNK	C	3134:UNK	N	14.94
1	G	3063:UNK	C	3134:UNK	N	14.94
1	E	3063:UNK	C	3134:UNK	N	14.94
1	B	3468:UNK	C	3511:UNK	N	14.40
1	I	3468:UNK	C	3511:UNK	N	14.40
1	G	3468:UNK	C	3511:UNK	N	14.40
1	E	3468:UNK	C	3511:UNK	N	14.40
1	B	2703:UNK	C	2734:ASN	N	13.12
1	I	2703:UNK	C	2734:ASN	N	13.12
1	G	2703:UNK	C	2734:ASN	N	13.12
1	E	2703:UNK	C	2734:ASN	N	13.12
1	B	3236:UNK	C	3241:UNK	N	12.96
1	I	3236:UNK	C	3241:UNK	N	12.96
1	G	3236:UNK	C	3241:UNK	N	12.96
1	E	3236:UNK	C	3241:UNK	N	12.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1564:UNK	C	1573:MET	N	12.42
1	I	1564:UNK	C	1573:MET	N	12.42
1	G	1564:UNK	C	1573:MET	N	12.42
1	E	1564:UNK	C	1573:MET	N	12.42
1	B	2976:UNK	C	2995:UNK	N	12.17
1	I	2976:UNK	C	2995:UNK	N	12.17
1	G	2976:UNK	C	2995:UNK	N	12.17
1	E	2976:UNK	C	2995:UNK	N	12.17
1	B	3254:UNK	C	3261:UNK	N	8.29
1	I	3254:UNK	C	3261:UNK	N	8.29
1	G	3254:UNK	C	3261:UNK	N	8.29
1	E	3254:UNK	C	3261:UNK	N	8.29
1	G	1297:UNK	C	1430:UNK	N	6.05
1	B	1297:UNK	C	1430:UNK	N	6.04
1	I	1297:UNK	C	1430:UNK	N	6.04
1	E	1297:UNK	C	1430:UNK	N	6.04
1	I	2939:ARG	C	2942:UNK	N	3.73
1	G	2939:ARG	C	2942:UNK	N	3.73
1	E	2939:ARG	C	2942:UNK	N	3.73
1	B	2939:ARG	C	2942:UNK	N	3.72
1	G	2479:LEU	C	2487:UNK	N	3.51
1	B	2479:LEU	C	2487:UNK	N	3.50
1	I	2479:LEU	C	2487:UNK	N	3.50
1	E	2479:LEU	C	2487:UNK	N	3.50

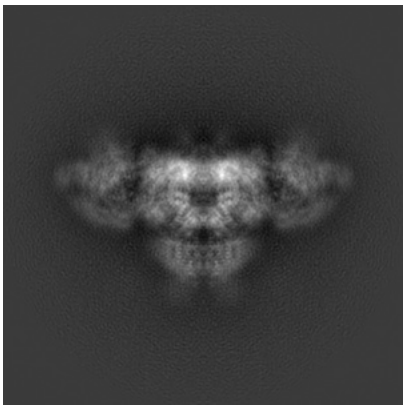
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8390. These allow visual inspection of the internal detail of the map and identification of artifacts.

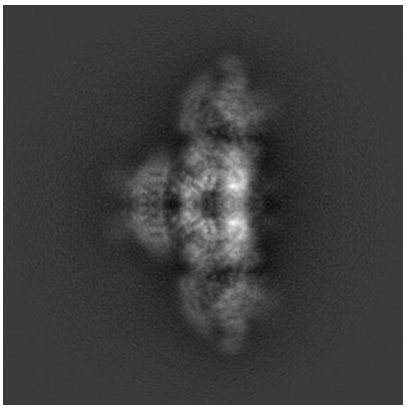
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

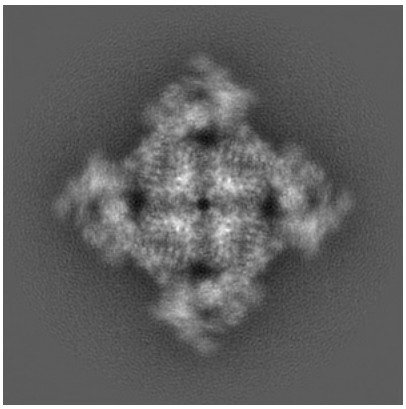
6.1.1 Primary map



X

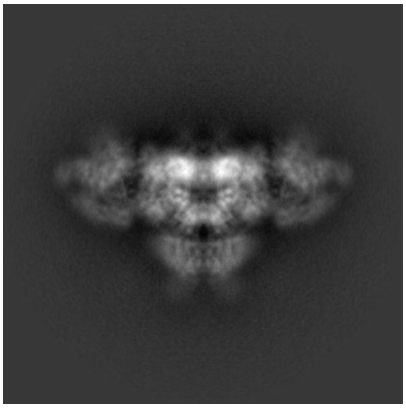


Y

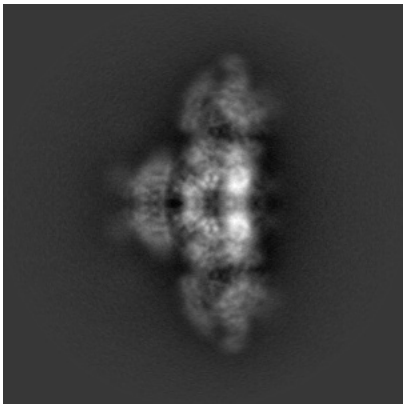


Z

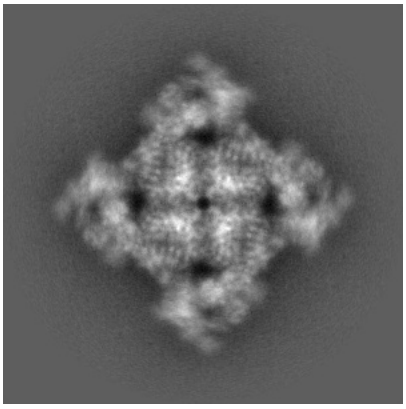
6.1.2 Raw map



X



Y

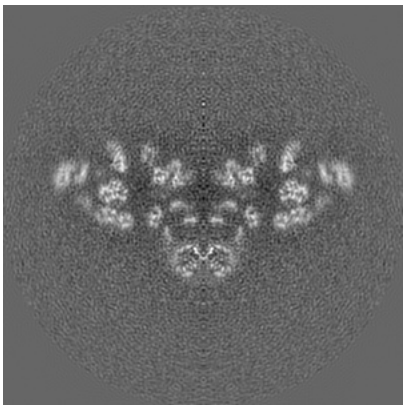


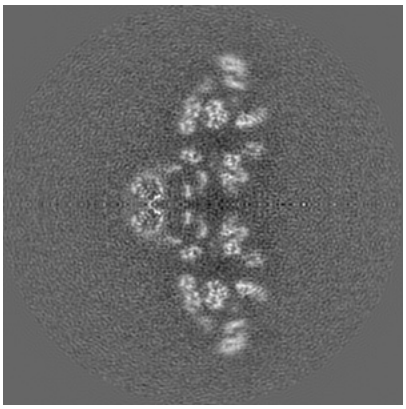
Z

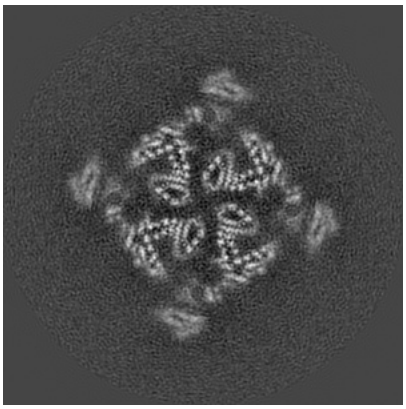
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

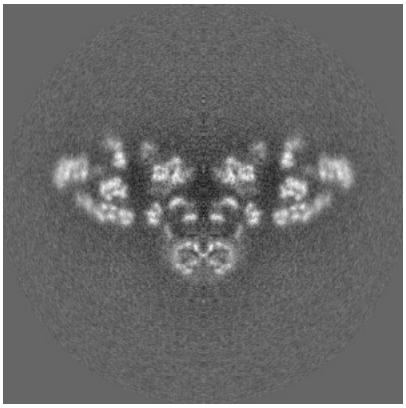
6.2.1 Primary map

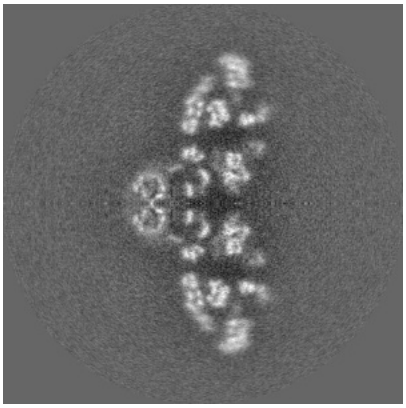

X Index: 200

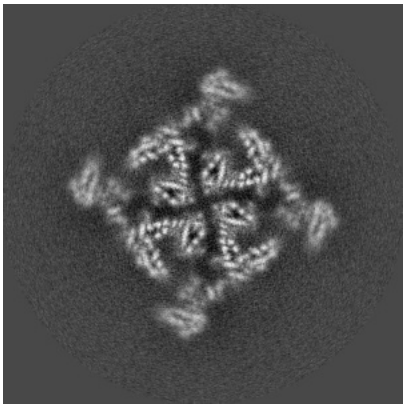

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

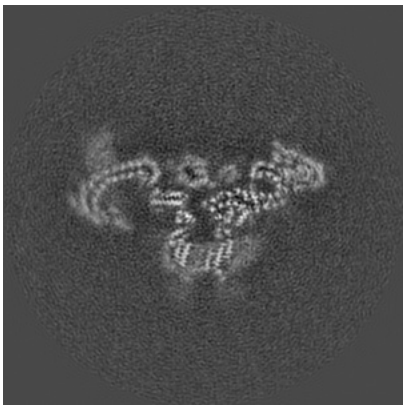

Y Index: 200

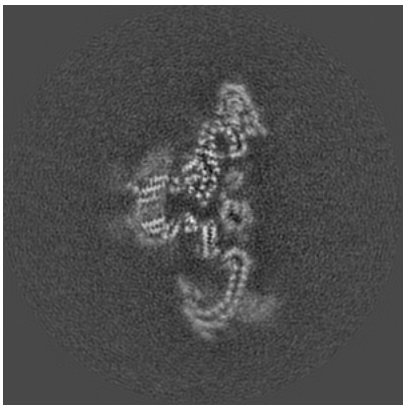

Z Index: 200

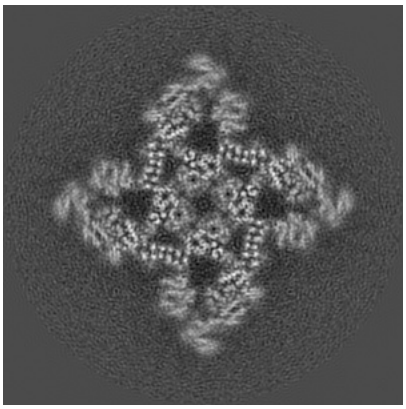
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

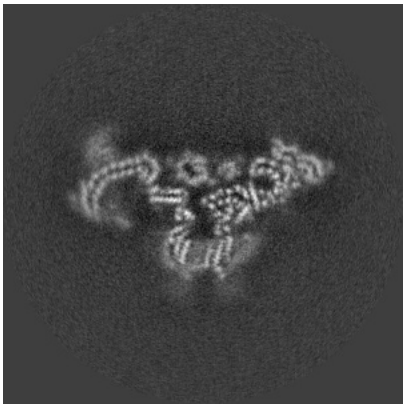
6.3.1 Primary map

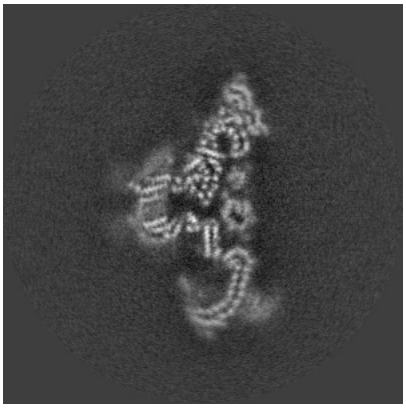

X Index: 175

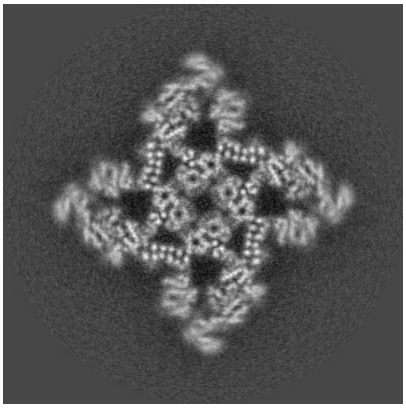

Y Index: 225


Z Index: 227

6.3.2 Raw map


X Index: 175

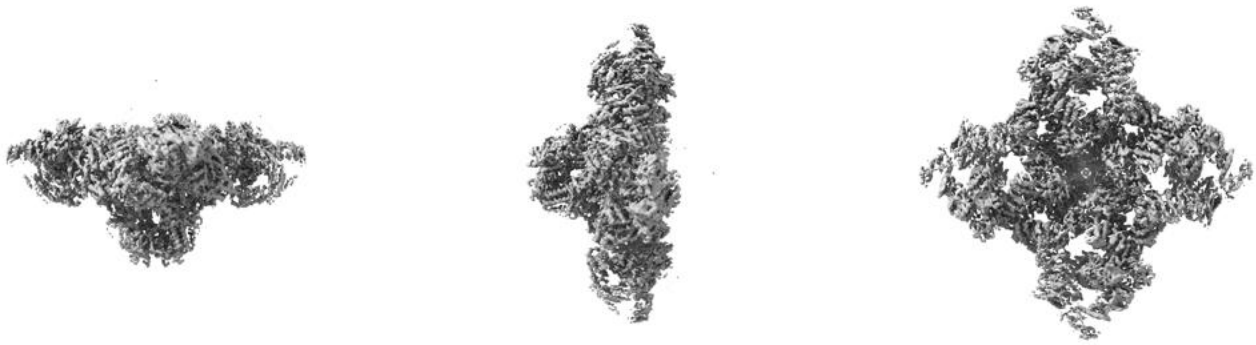

Y Index: 225


Z Index: 229

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

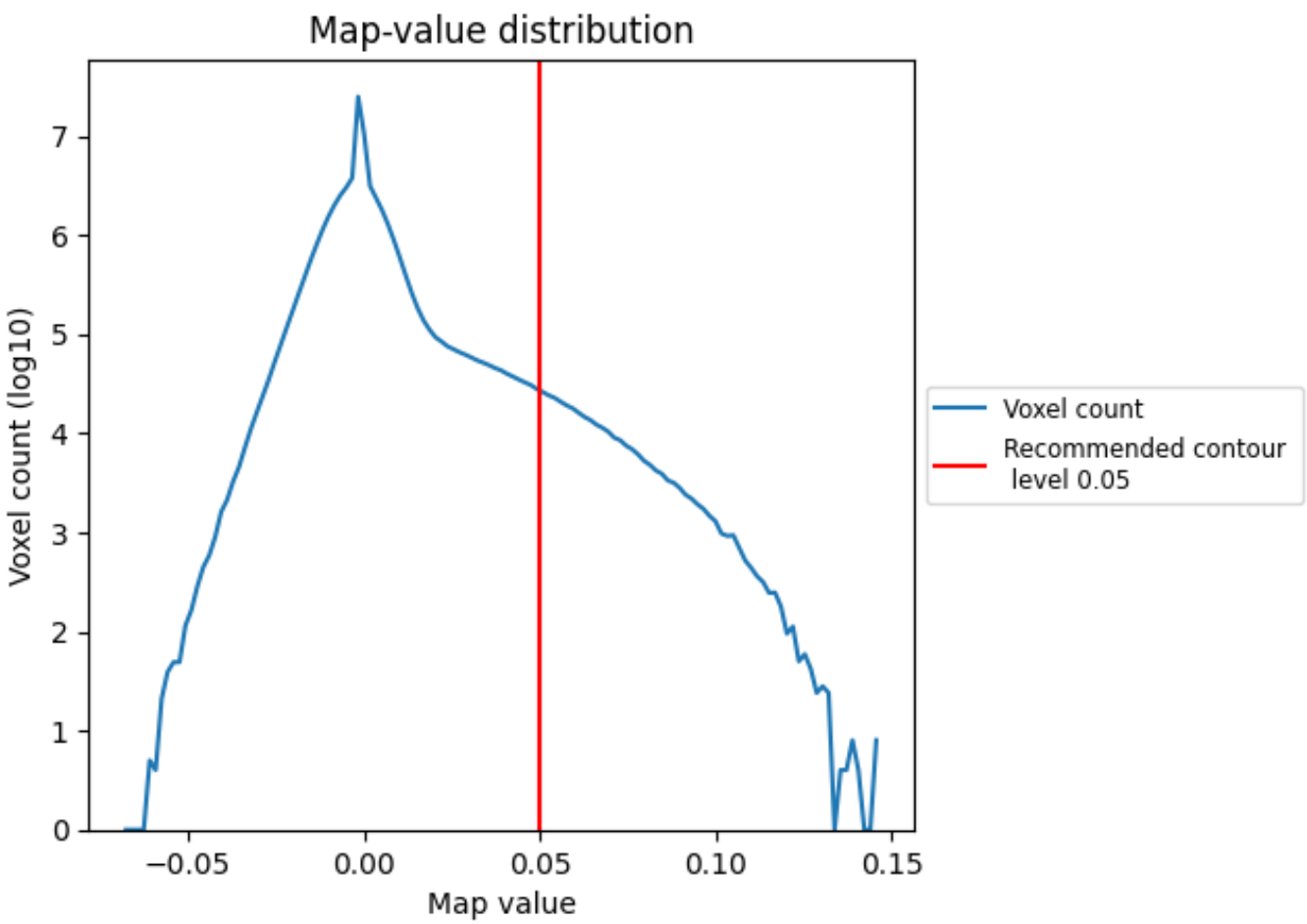
6.5 Mask visualisation (i)

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

7 Map analysis (i)

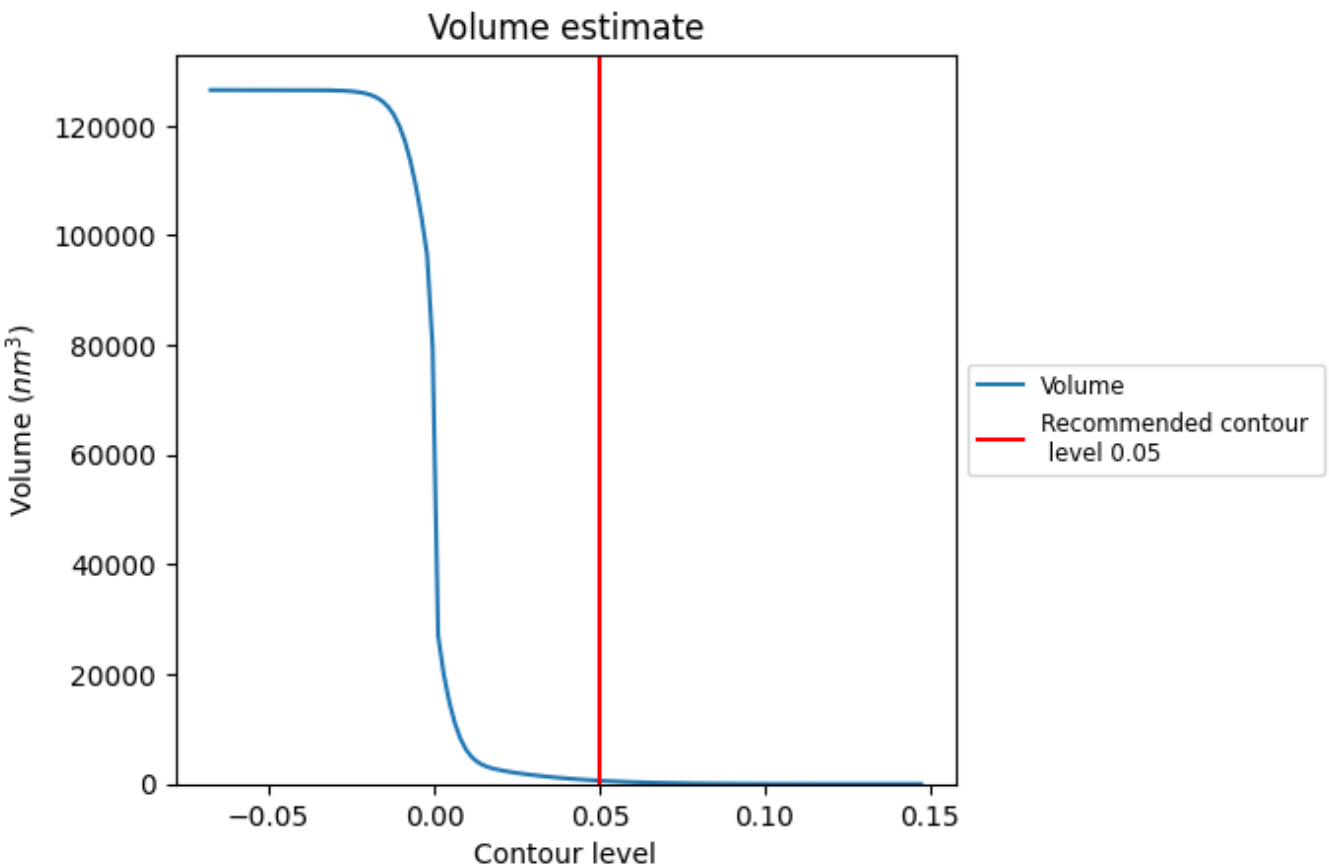
This section contains the results of statistical analysis of the map.

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.

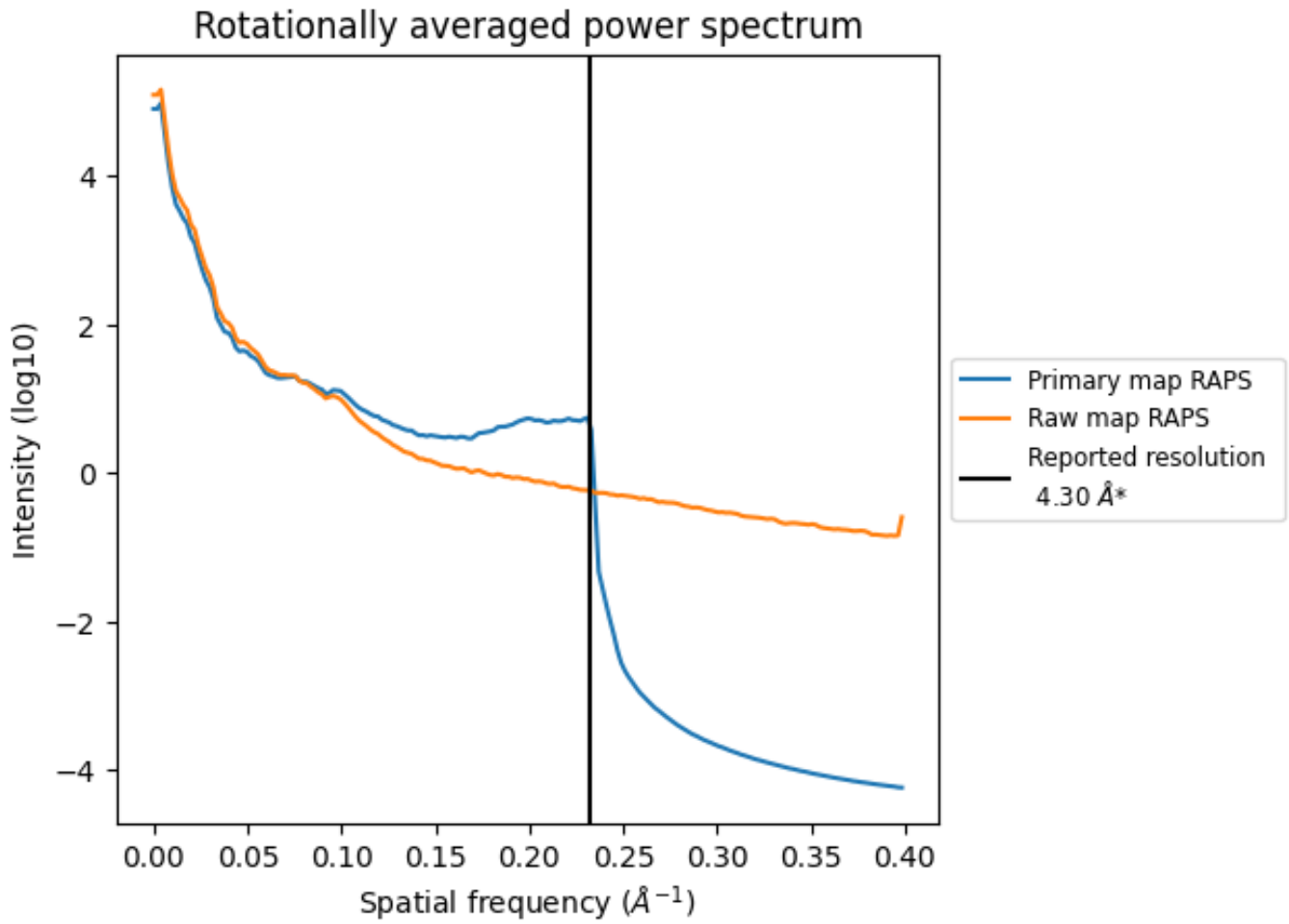
7.2 Volume estimate (i)



The volume at the recommended contour level is 603 nm^3; this corresponds to an approximate mass of 545 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)

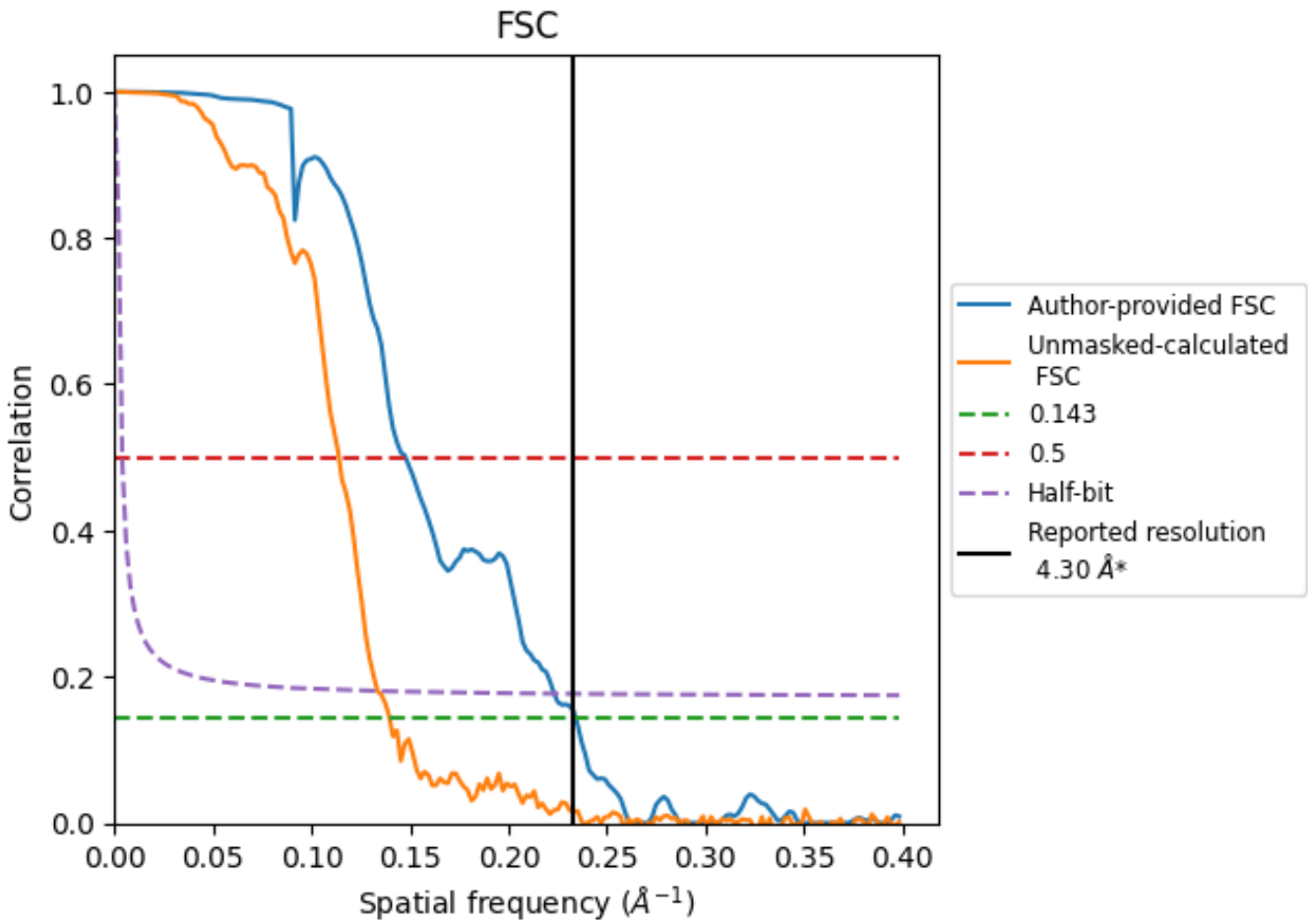


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

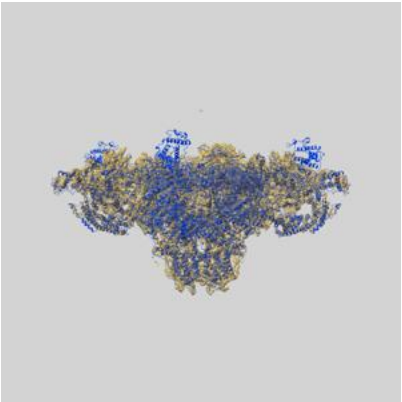
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.27	6.77	4.48
Unmasked-calculated*	7.16	8.77	7.49

*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 7.16 differs from the reported value 4.3 by more than 10 %

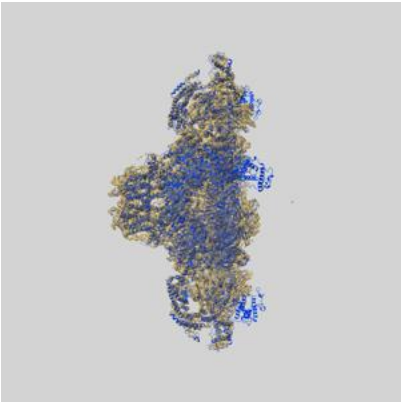
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8390 and PDB model 5TAZ. Per-residue inclusion information can be found in section 3 on page 5.

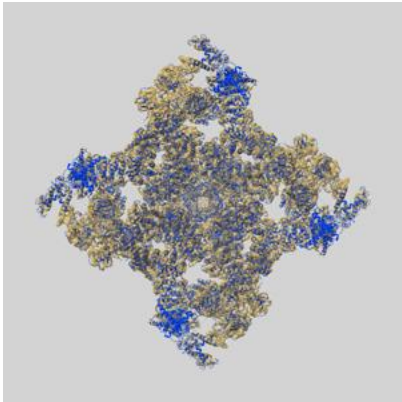
9.1 Map-model overlay (i)



X



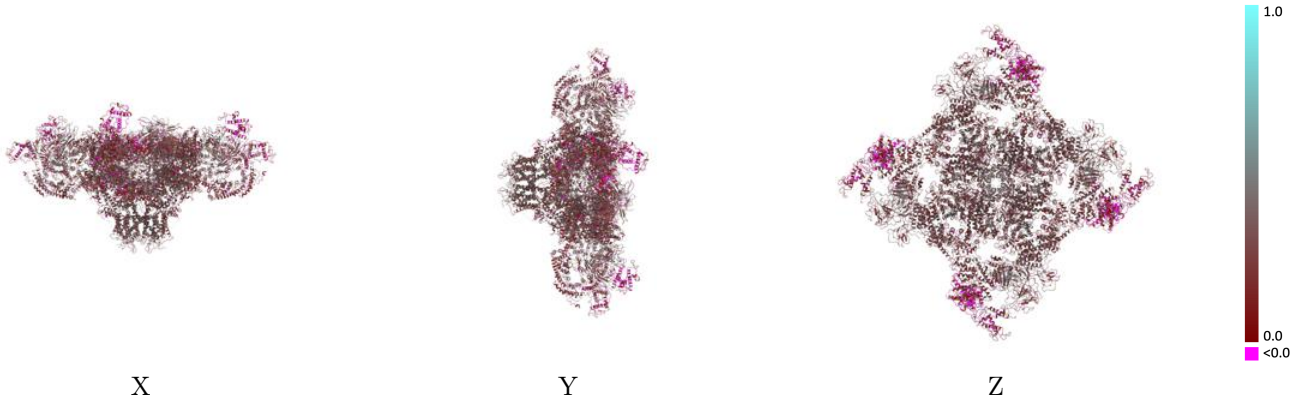
Y



Z

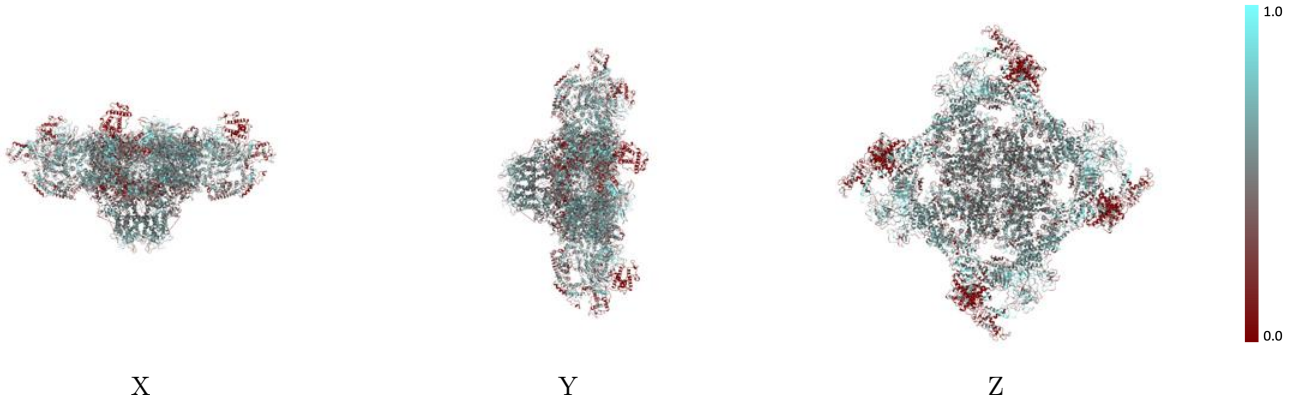
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



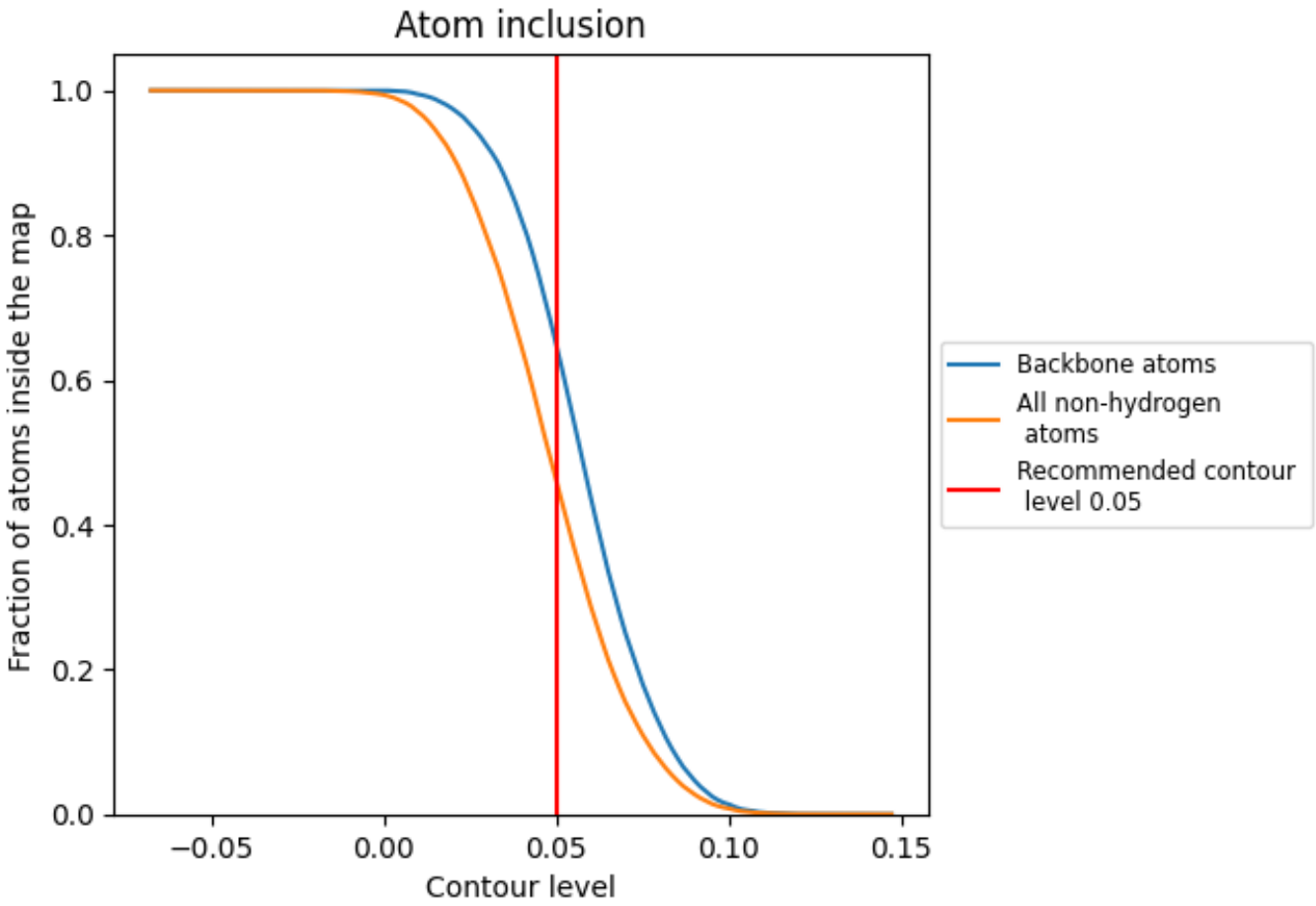
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 46% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4617	0.2730
A	0.4876	0.2880
B	0.4607	0.2730
E	0.4608	0.2730
F	0.4864	0.2930
G	0.4614	0.2730
H	0.4851	0.2930
I	0.4609	0.2730
J	0.4913	0.2910