Full wwPDB EM Validation Report

Feb 25, 2024 – 09:03 AM EST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

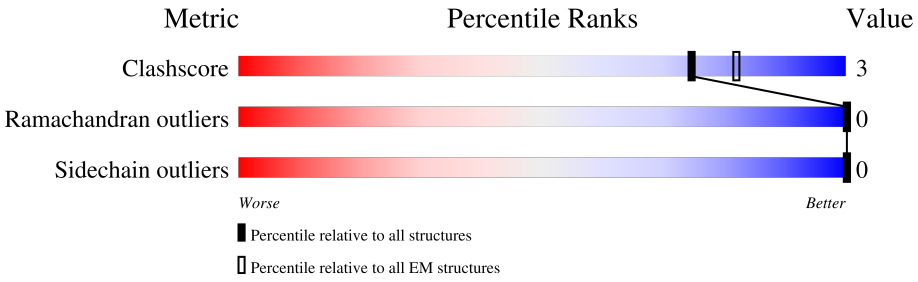
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.80 Å.

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



Metric	Whole archive (#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	110	83% 14%
1	D	110	80% 16%
1	G	110	5% 80% 16%
1	J	110	83% 14%
2	B	3800	23% 92% 8%
2	E	3800	23% 92% 8%
2	H	3800	23% 92% 8%
2	K	3800	23% 92% 8%

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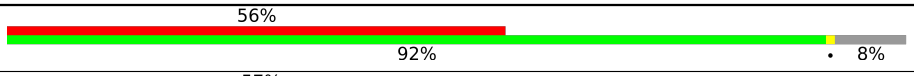
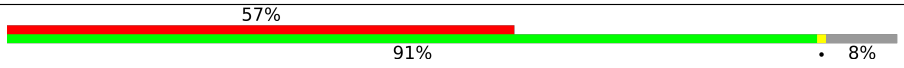
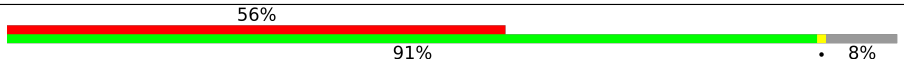
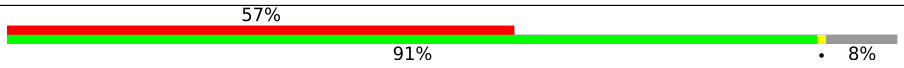
Mol	Chain	Length	Quality of chain
3	C	146	
3	F	146	
3	I	146	
3	L	146	

2 Entry composition (i)

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

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Ryanodine Receptor.

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

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

- Molecule 3 is a protein called Calmodulin-1.

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

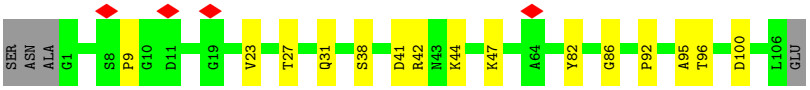
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Zn 1	0
4	E	1	Total 1	Zn 1	0
4	H	1	Total 1	Zn 1	0
4	K	1	Total 1	Zn 1	0

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.

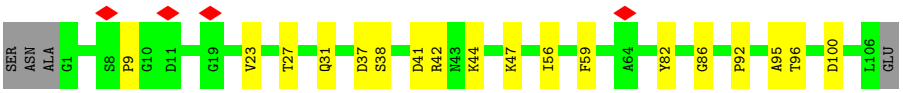
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



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

Chain D:

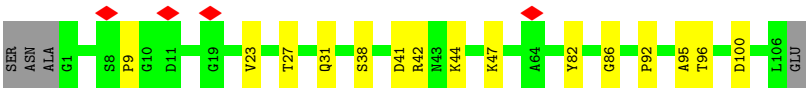


• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

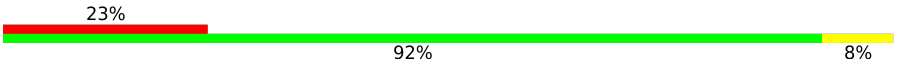
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

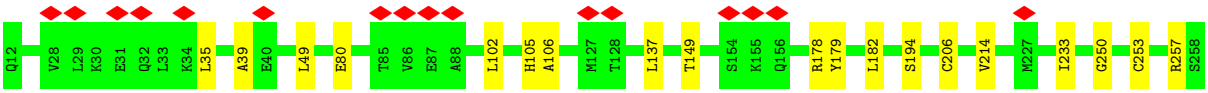
Chain J:

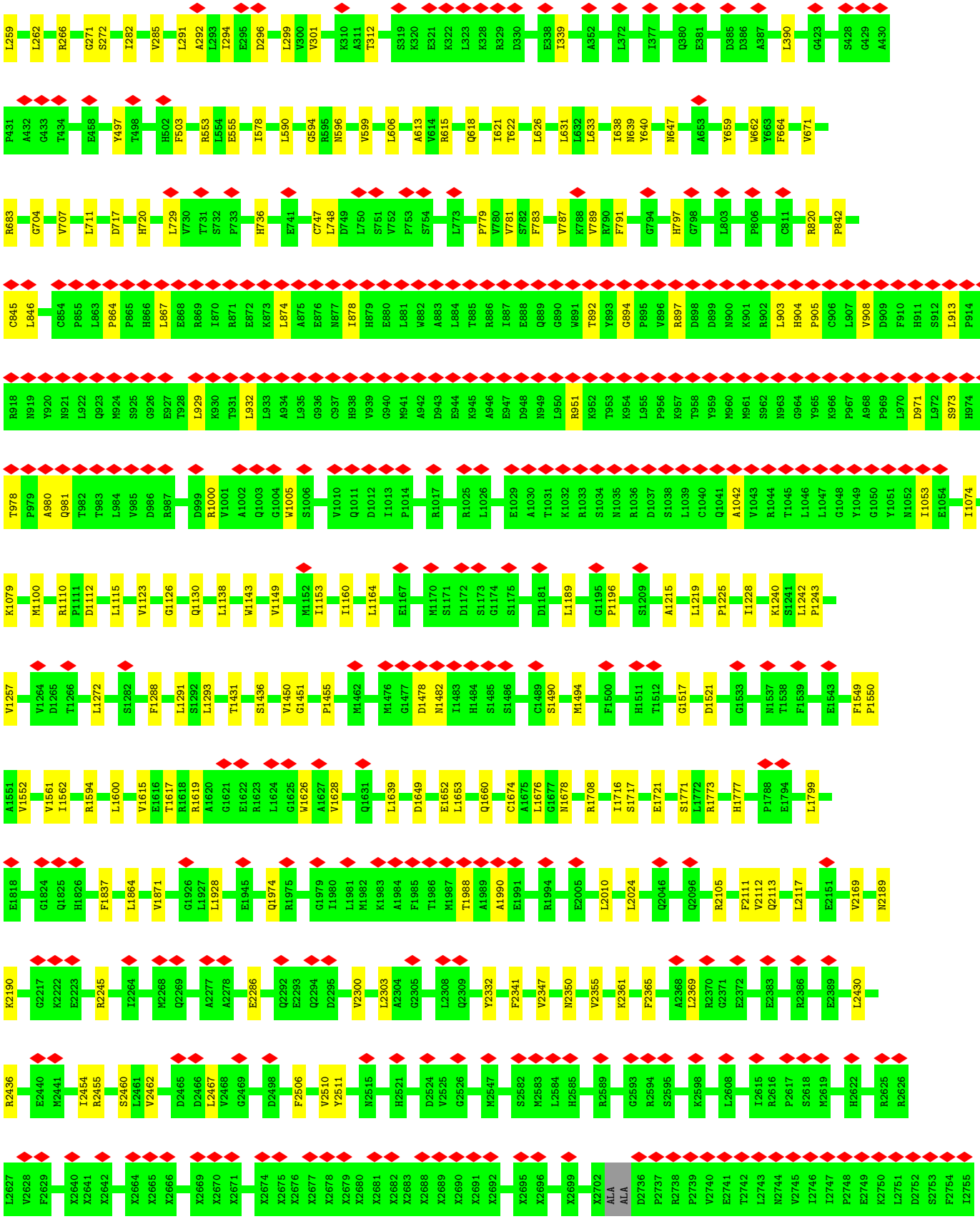


• Molecule 2: Ryanodine Receptor

Chain B:



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T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 D999 R1000 V1001 A1002 Q1003 G1004 W1005 S1006 V1010 Q1011 D1012 I1013 P1014 R1017 R1025 L1026 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 I1074
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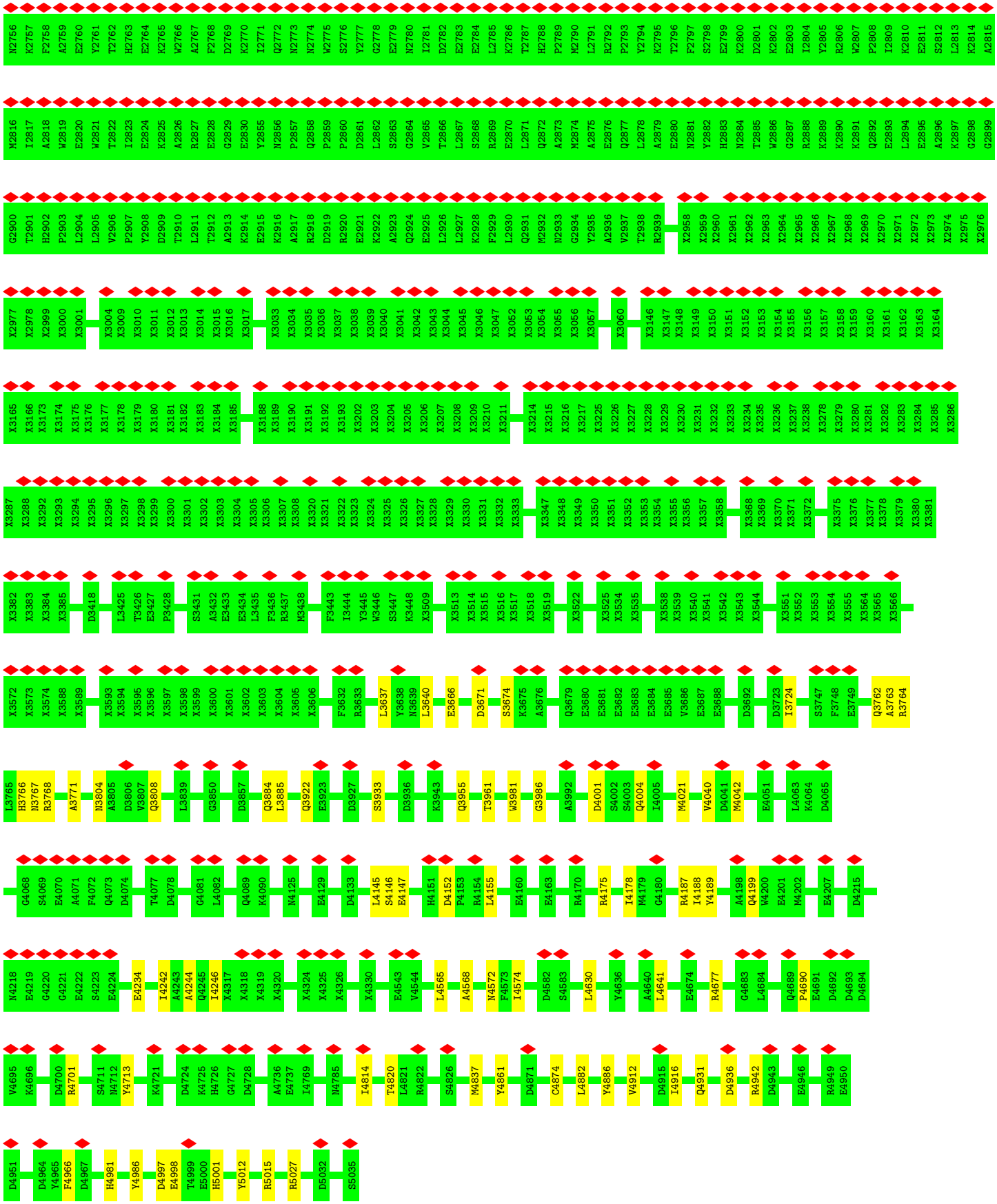
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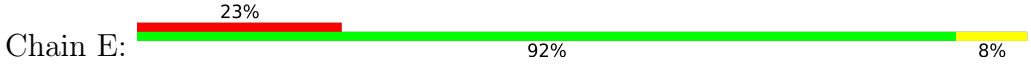
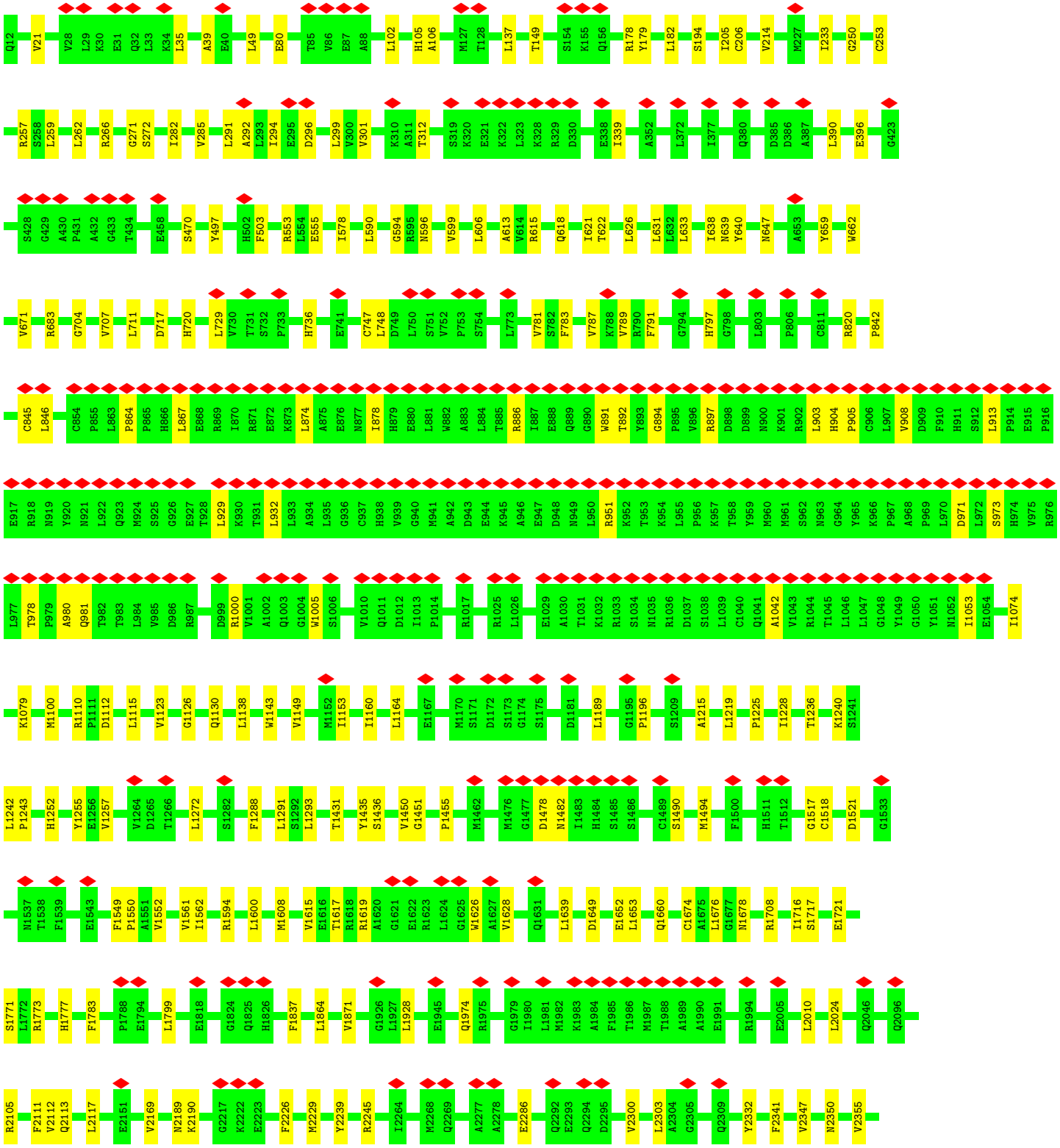
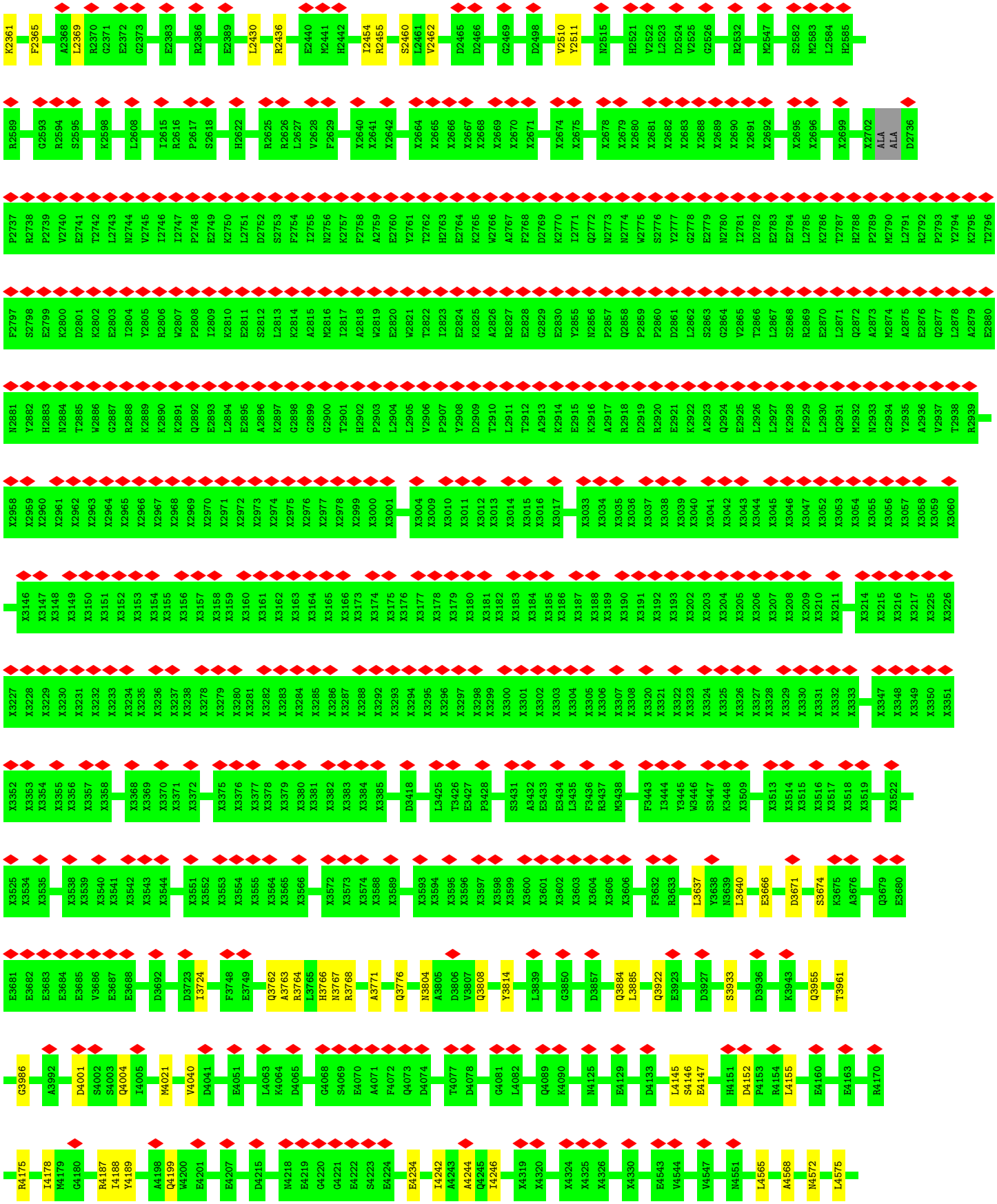
• Molecule 2: Ryanodine Receptor

Chain E:



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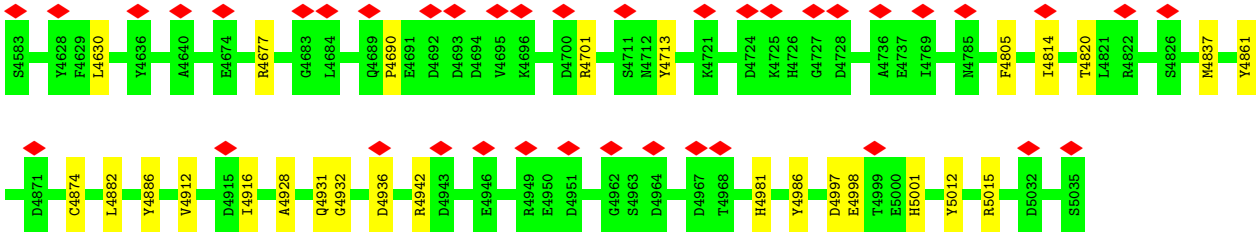
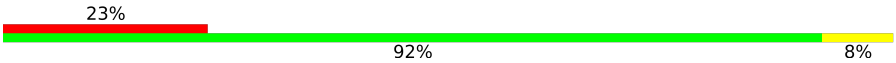
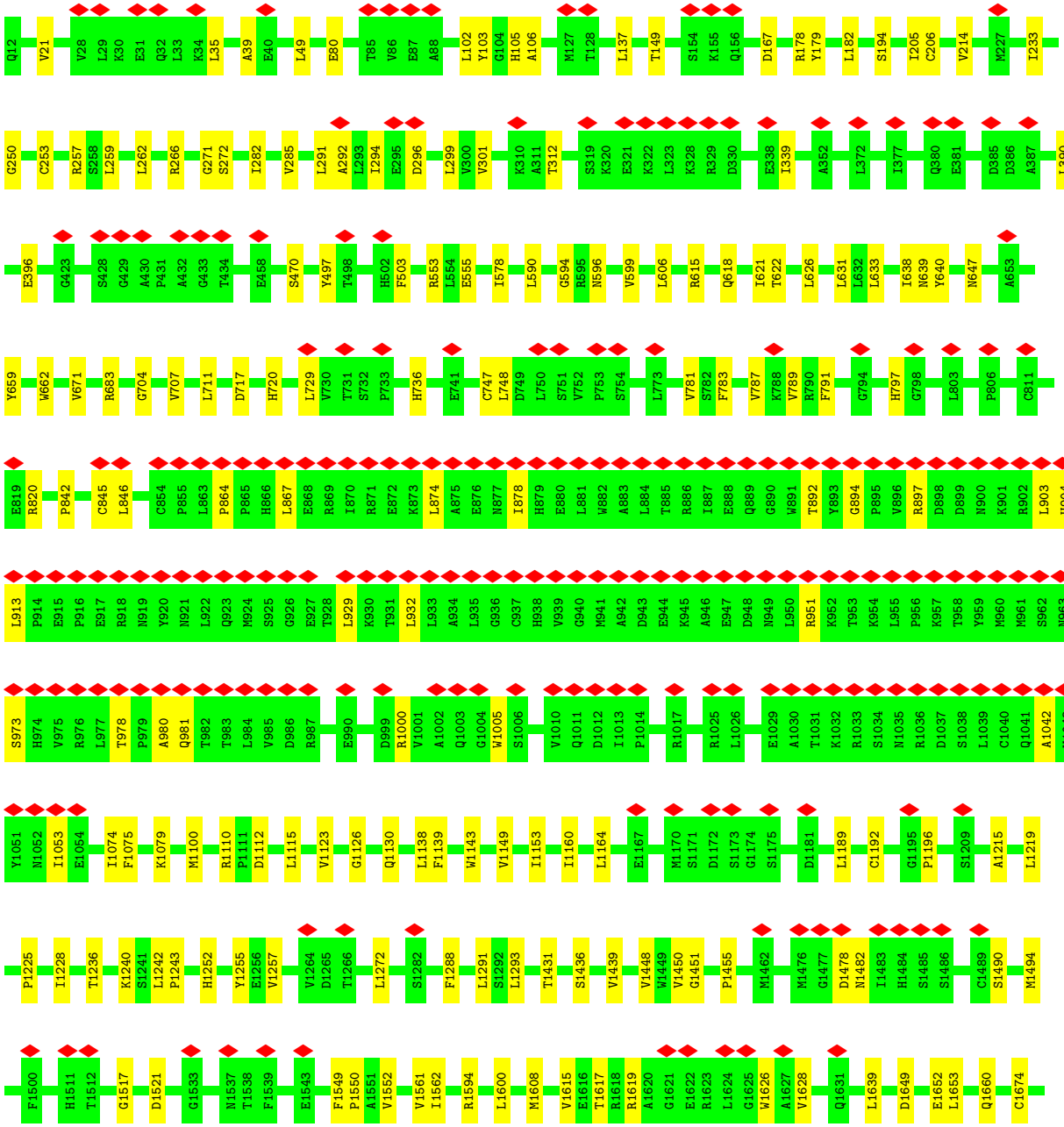
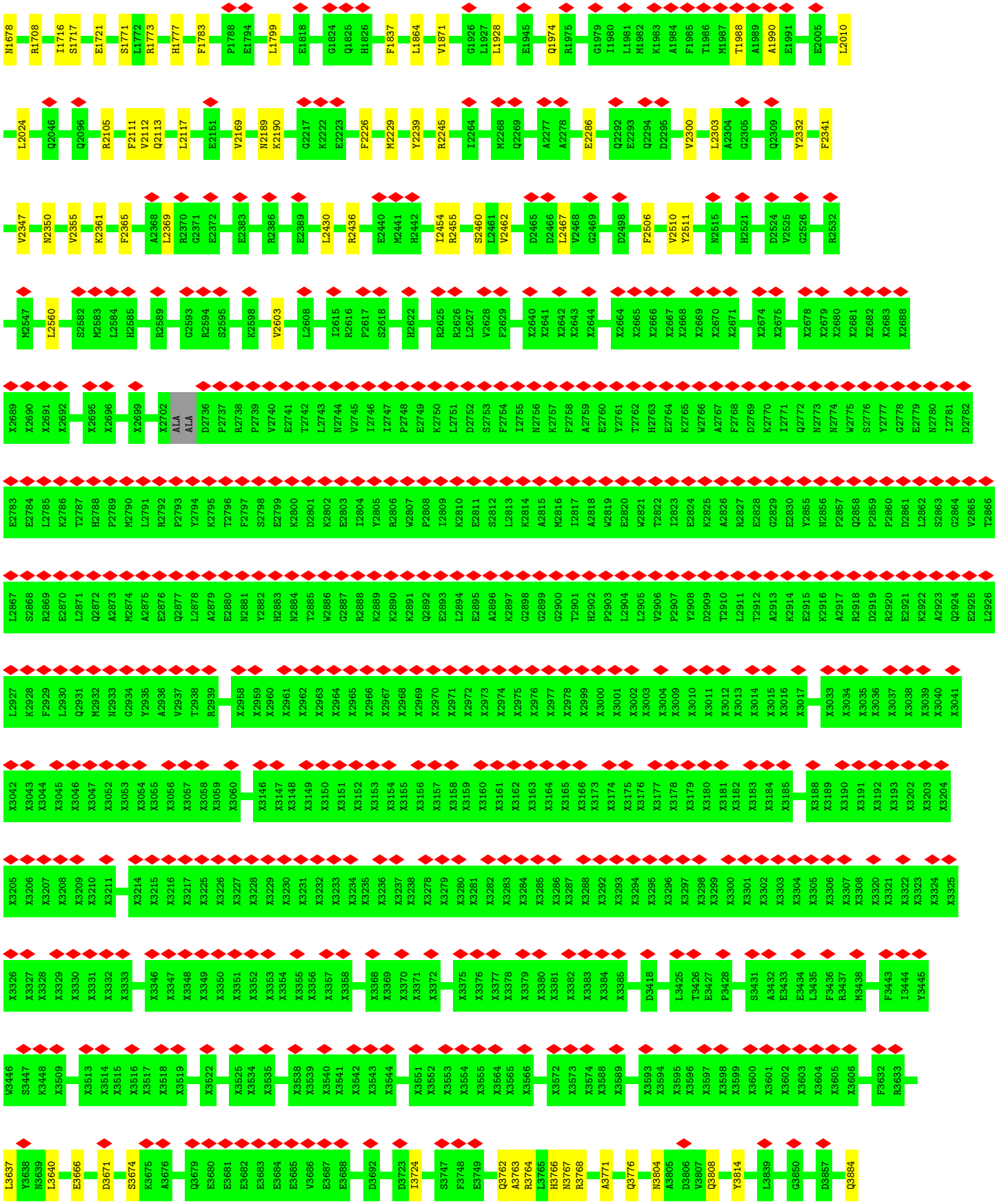


• Molecule 2: Ryanodine Receptor

Chain H:



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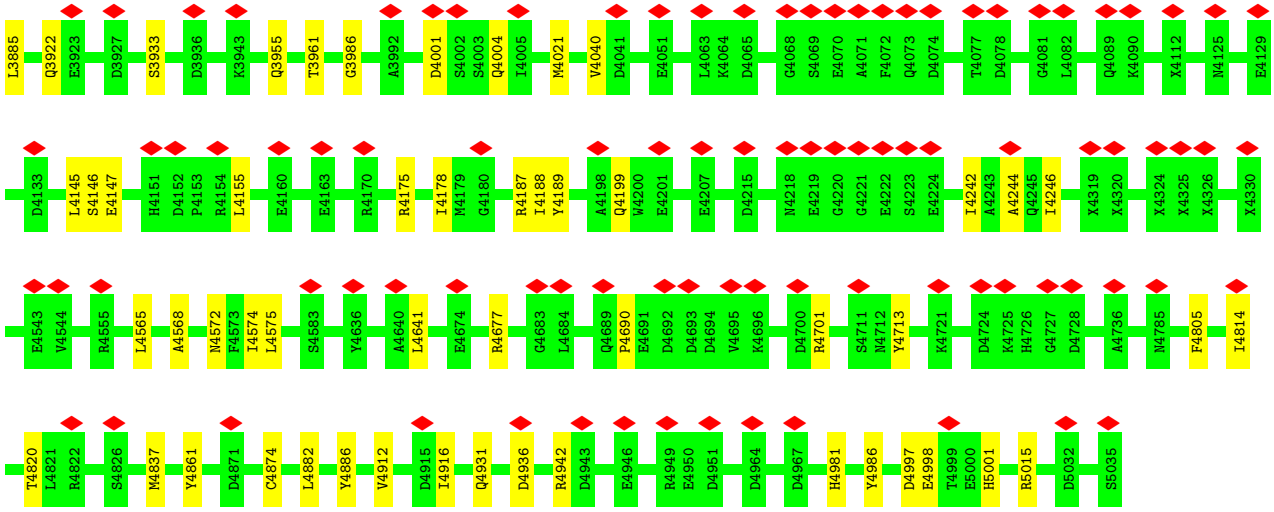
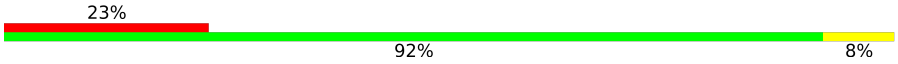
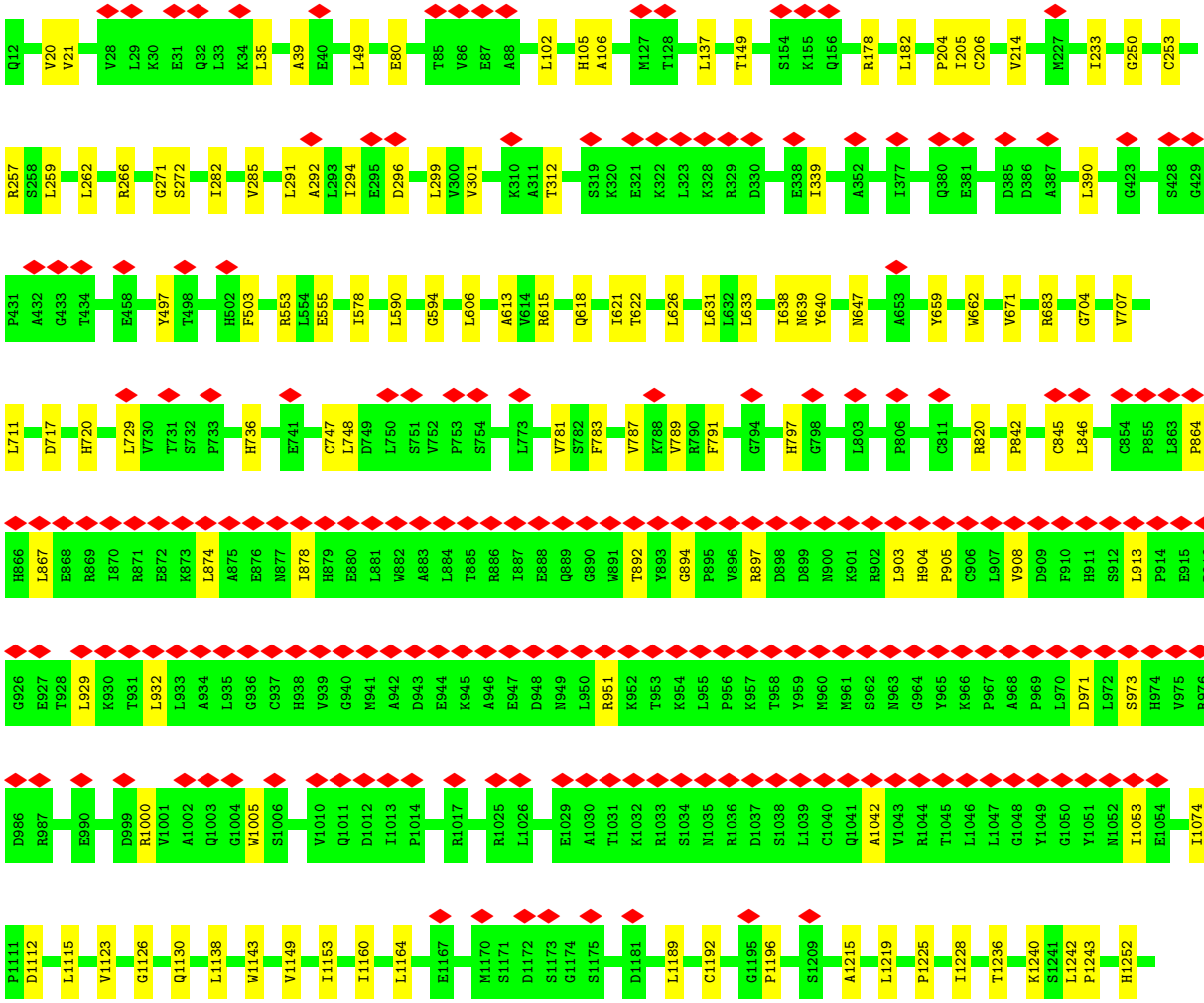
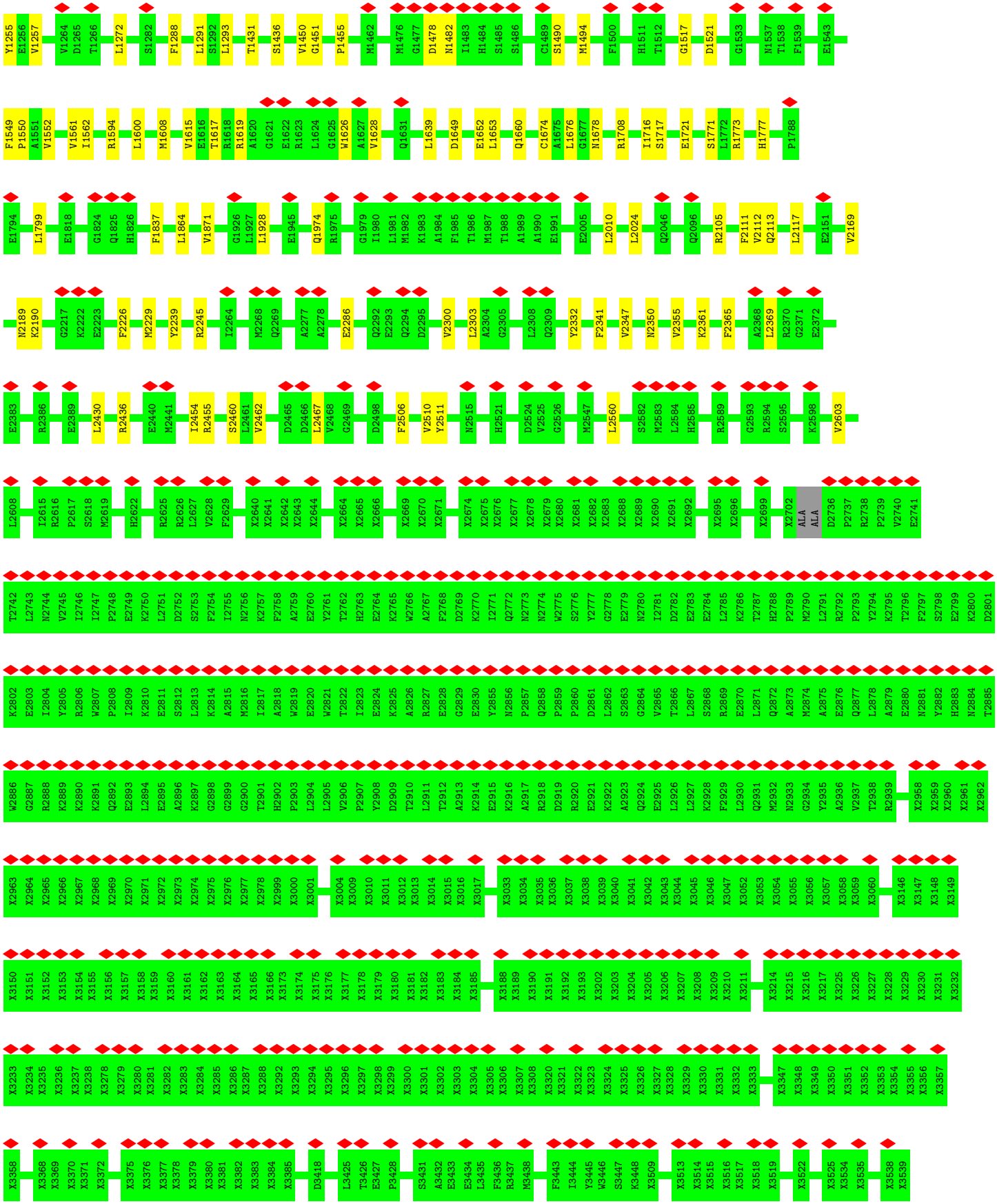


• Molecule 2: Ryanodine Receptor

Chain K:



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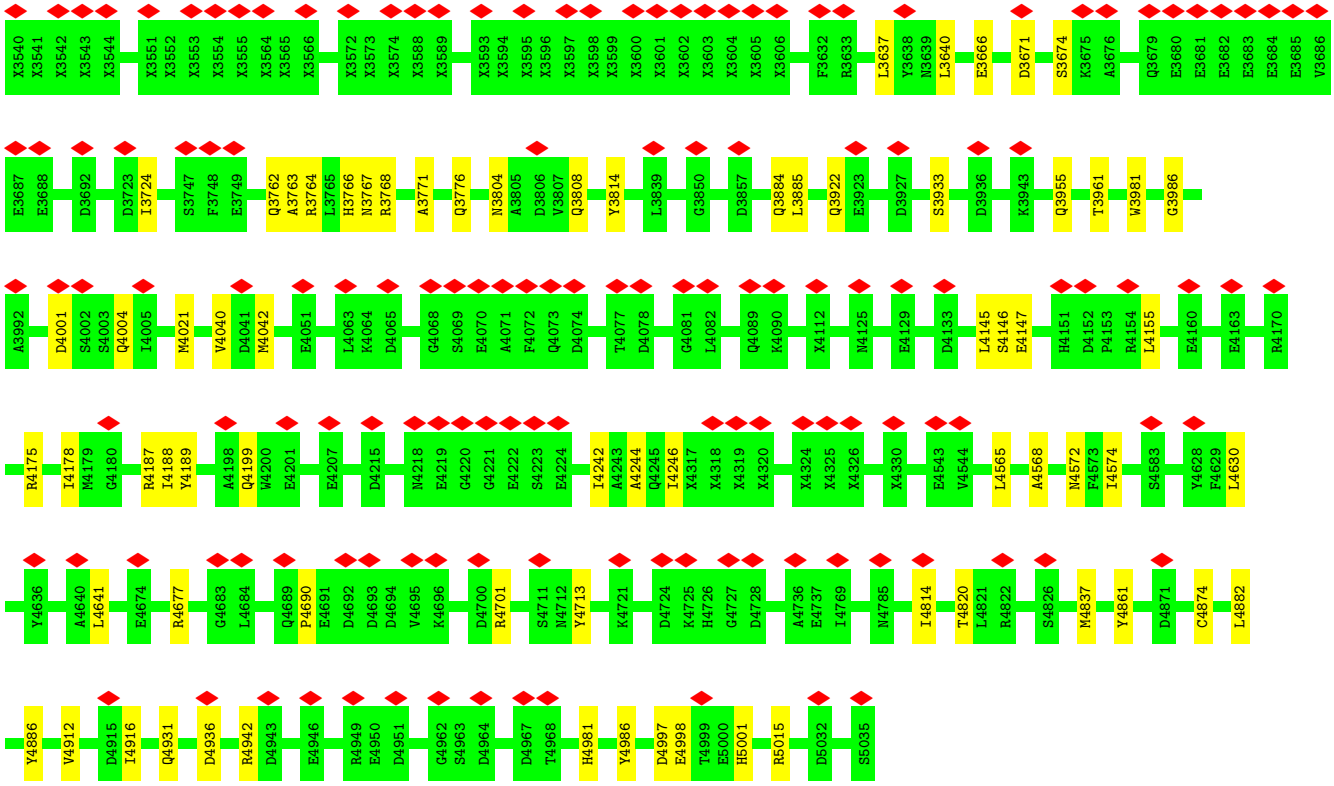
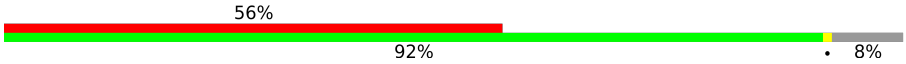
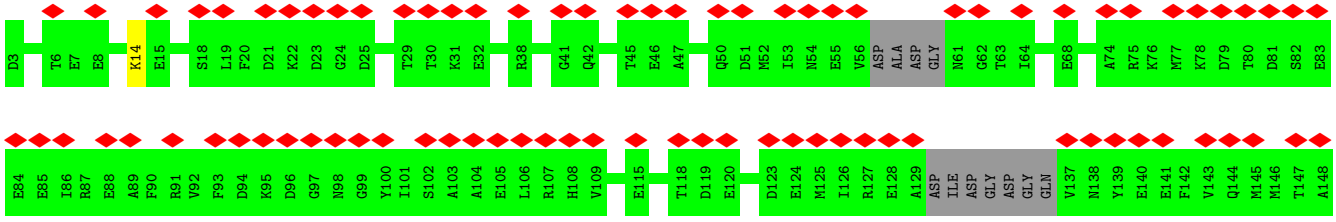


• Molecule 3: Calmodulin-1

Chain C:





• Molecule 3: Calmodulin-1

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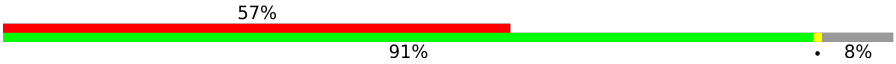
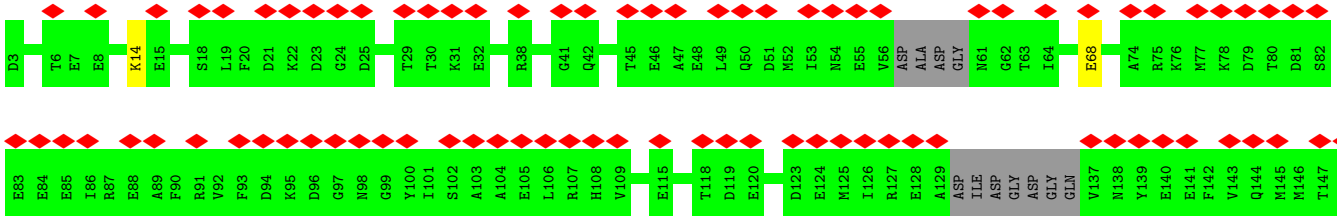
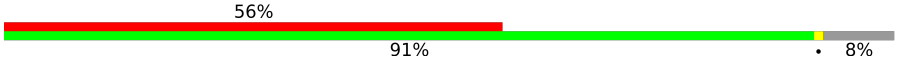
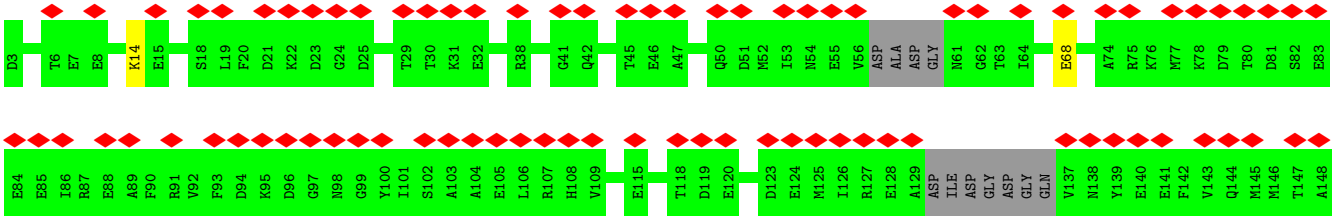




• Molecule 3: Calmodulin-1

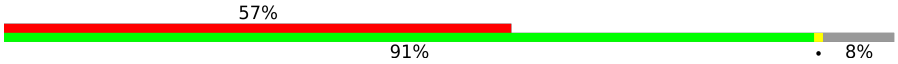
Chain I:

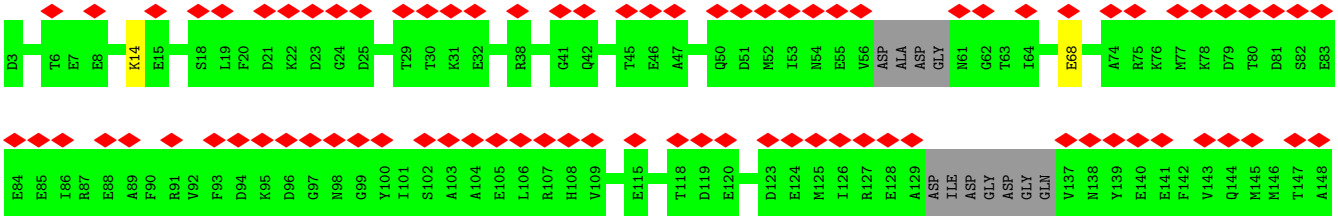




• Molecule 3: Calmodulin-1

Chain L:





4 Experimental information (i)

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

5 Model quality

5.1 Standard geometry

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	0/758	0.43	0/1033
1	D	0.25	0/758	0.43	0/1033
1	G	0.25	0/758	0.43	0/1033
1	J	0.25	0/758	0.43	0/1033
2	B	0.23	0/25809	0.37	0/35154
2	E	0.23	0/25809	0.37	0/35154
2	H	0.23	0/25809	0.37	0/35154
2	K	0.23	0/25809	0.37	0/35154
3	C	0.24	0/820	0.37	0/1120
3	F	0.24	0/820	0.37	0/1120
3	I	0.24	0/820	0.37	0/1120
3	L	0.24	0/820	0.37	0/1120
All	All	0.23	0/109548	0.37	0/149228

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	742	0	702	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	742	0	702	10	0
1	G	742	0	702	10	0
1	J	742	0	702	8	0
2	B	27011	0	23901	165	0
2	E	27011	0	23901	171	0
2	H	27011	0	23901	173	0
2	K	27011	0	23901	169	0
3	C	816	0	573	1	0
3	F	816	0	573	2	0
3	I	816	0	573	2	0
3	L	816	0	573	2	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
All	All	114280	0	100704	680	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (680) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2460:SER:OG	2:E:178:ARG:NH1	2.40	0.54
2:E:2460:SER:OG	2:H:178:ARG:NH1	2.40	0.54
2:K:1450:VAL:HA	2:K:1552:VAL:HG22	1.89	0.54
2:B:1450:VAL:HA	2:B:1552:VAL:HG22	1.89	0.54
2:B:1674:CYS:HA	2:B:1678:ASN:HB3	1.90	0.54
2:E:2347:VAL:HG12	2:E:2350:ASN:H	1.73	0.54
2:B:1436:SER:HA	2:B:1517:GLY:HA2	1.89	0.53
2:B:2347:VAL:HG12	2:B:2350:ASN:H	1.73	0.53
2:B:4886:TYR:HA	2:E:4916:ILE:HD11	1.90	0.53
2:H:4882:LEU:HD11	2:K:4912:VAL:HG11	1.89	0.53
2:K:4199:GLN:HE22	2:K:4244:ALA:HB2	1.72	0.53
2:K:878:ILE:HD11	2:K:1042:ALA:HB2	1.90	0.53
2:B:878:ILE:HD11	2:B:1042:ALA:HB2	1.90	0.53
2:E:4175:ARG:NH1	2:E:4189:TYR:OH	2.42	0.53
2:B:3666:GLU:HA	2:B:3724:ILE:HG23	1.91	0.53
2:E:2111:PHE:HD2	2:E:2113:GLN:HG2	1.74	0.53
2:K:2111:PHE:HD2	2:K:2113:GLN:HG2	1.74	0.53
2:E:3666:GLU:HA	2:E:3724:ILE:HG23	1.91	0.53
2:H:2347:VAL:HG12	2:H:2350:ASN:H	1.73	0.53
2:H:4175:ARG:NH1	2:H:4189:TYR:OH	2.42	0.53
2:B:4199:GLN:HE22	2:B:4244:ALA:HB2	1.72	0.53
2:E:3762:GLN:OE1	2:E:3804:ASN:ND2	2.40	0.53
2:H:233:ILE:O	2:H:257:ARG:NH1	2.41	0.53
2:H:2111:PHE:HD2	2:H:2113:GLN:HG2	1.74	0.53
2:K:1293:LEU:HD11	2:K:1594:ARG:HG2	1.90	0.53
2:H:1293:LEU:HD11	2:H:1594:ARG:HG2	1.90	0.52
2:H:4886:TYR:HA	2:K:4916:ILE:HD11	1.90	0.52
2:K:2347:VAL:HG12	2:K:2350:ASN:H	1.73	0.52
2:B:259:LEU:HB2	2:B:285:VAL:HG21	1.91	0.52
2:B:4175:ARG:NH1	2:B:4189:TYR:OH	2.42	0.52
2:B:4916:ILE:HD11	2:K:4886:TYR:HA	1.90	0.52
2:B:4997:ASP:OD1	2:B:4997:ASP:N	2.42	0.52
2:E:4886:TYR:HA	2:H:4916:ILE:HD11	1.90	0.52
2:H:1149:VAL:HG22	2:H:1164:LEU:HD13	1.92	0.52
2:K:259:LEU:HB2	2:K:285:VAL:HG21	1.91	0.52
2:K:4175:ARG:NH1	2:K:4189:TYR:OH	2.42	0.52
2:H:4997:ASP:N	2:H:4997:ASP:OD1	2.42	0.52
2:E:233:ILE:O	2:E:257:ARG:NH1	2.41	0.52
2:E:878:ILE:HD11	2:E:1042:ALA:HB2	1.90	0.52
1:D:82:TYR:HB3	1:D:86:GLY:HA2	1.92	0.52
2:E:633:LEU:HD13	2:E:1639:LEU:HD21	1.91	0.52

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4861:TYR:HD2	2:E:4874:CYS:HB3	1.76	0.51
2:H:266:ARG:NH1	2:H:272:SER:OG	2.44	0.51
2:B:266:ARG:NH1	2:B:272:SER:OG	2.44	0.51
2:E:266:ARG:NH1	2:E:272:SER:OG	2.44	0.51
2:H:106:ALA:HA	2:H:149:THR:HA	1.92	0.51
2:H:2341:PHE:HB2	2:H:2436:ARG:HD3	1.93	0.51
2:K:106:ALA:HA	2:K:149:THR:HA	1.92	0.51
2:B:1777:HIS:HB3	2:B:1799:LEU:HD13	1.92	0.50
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.93	0.50
2:H:3762:GLN:OE1	2:H:3804:ASN:ND2	2.40	0.50
2:K:3766:HIS:HB2	2:K:3771:ALA:HB2	1.93	0.50
2:K:4242:ILE:O	2:K:4246:ILE:N	2.44	0.50
1:A:82:TYR:HB3	1:A:86:GLY:HA2	1.92	0.50
2:B:683:ARG:HB2	2:B:707:VAL:HG21	1.94	0.50
2:B:3762:GLN:OE1	2:B:3804:ASN:ND2	2.40	0.50
2:E:106:ALA:HA	2:E:149:THR:HA	1.92	0.50
2:H:683:ARG:HB2	2:H:707:VAL:HG21	1.94	0.50
2:H:1130:GLN:HG2	2:H:1138:LEU:HA	1.92	0.50
2:K:4997:ASP:OD1	2:K:4997:ASP:N	2.42	0.50
2:K:1130:GLN:HG2	2:K:1138:LEU:HA	1.92	0.50
2:E:897:ARG:HE	2:E:905:PRO:HD2	1.75	0.50
1:J:82:TYR:HB3	1:J:86:GLY:HA2	1.92	0.50
2:E:683:ARG:HB2	2:E:707:VAL:HG21	1.94	0.50
2:K:864:PRO:HD2	2:K:867:LEU:HD12	1.93	0.50
2:B:897:ARG:HE	2:B:905:PRO:HD2	1.75	0.50
2:E:2341:PHE:HB2	2:E:2436:ARG:HD3	1.93	0.50
2:H:892:THR:O	2:H:904:HIS:N	2.45	0.50
2:K:4861:TYR:HD2	2:K:4874:CYS:HB3	1.76	0.50
2:E:1243:PRO:HB3	2:E:1600:LEU:HD21	1.94	0.50
2:H:4861:TYR:HD2	2:H:4874:CYS:HB3	1.76	0.50
2:K:683:ARG:HB2	2:K:707:VAL:HG21	1.94	0.50
2:B:4861:TYR:HD2	2:B:4874:CYS:HB3	1.76	0.49
2:B:2341:PHE:HB2	2:B:2436:ARG:HD3	1.93	0.49
2:H:864:PRO:HD2	2:H:867:LEU:HD12	1.93	0.49
2:K:102:LEU:HB2	2:K:105:HIS:CD2	2.48	0.49
2:K:1455:PRO:HB3	2:K:1549:PHE:HE2	1.78	0.49
2:B:102:LEU:HB2	2:B:105:HIS:CD2	2.48	0.49
2:B:1455:PRO:HB3	2:B:1549:PHE:HE2	1.78	0.49
2:H:4040:VAL:HG22	2:H:4145:LEU:HD21	1.95	0.49
2:E:102:LEU:HB2	2:E:105:HIS:CD2	2.48	0.49
2:H:1431:THR:OG1	2:H:1521:ASP:OD1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.48	0.49
2:H:3763:ALA:O	2:H:3767:ASN:ND2	2.46	0.49
2:H:3776:GLN:NE2	2:H:3814:TYR:OH	2.37	0.49
2:K:892:THR:O	2:K:904:HIS:N	2.45	0.49
2:K:3763:ALA:HA	2:K:3766:HIS:CE1	2.48	0.49
2:K:3763:ALA:O	2:K:3767:ASN:ND2	2.46	0.49
2:E:3776:GLN:NE2	2:E:3814:TYR:OH	2.37	0.49
2:K:1243:PRO:HB3	2:K:1600:LEU:HD21	1.94	0.49
2:B:2300:VAL:HG12	2:B:2361:LYS:HD2	1.96	0.48
2:H:1455:PRO:HB3	2:H:1549:PHE:HE2	1.78	0.48
2:H:1561:VAL:HG12	2:H:1562:ILE:HG12	1.95	0.48
2:K:1126:GLY:HA3	2:K:1143:TRP:CE2	2.48	0.48
2:K:4040:VAL:HG22	2:K:4145:LEU:HD21	1.95	0.48
2:H:2300:VAL:HG12	2:H:2361:LYS:HD2	1.96	0.48
2:H:3763:ALA:HA	2:H:3766:HIS:CE1	2.48	0.48
2:K:2300:VAL:HG12	2:K:2361:LYS:HD2	1.96	0.48
2:E:3884:GLN:OE1	2:E:3955:GLN:NE2	2.47	0.48
2:H:618:GLN:OE1	2:H:1678:ASN:ND2	2.39	0.48
2:H:659:TYR:O	2:H:662:TRP:NE1	2.47	0.48
2:B:3763:ALA:HA	2:B:3766:HIS:CE1	2.48	0.48
2:B:3884:GLN:OE1	2:B:3955:GLN:NE2	2.47	0.48
2:E:671:VAL:HG23	2:E:787:VAL:HG22	1.96	0.48
2:E:892:THR:O	2:E:904:HIS:N	2.45	0.48
2:E:1561:VAL:HG12	2:E:1562:ILE:HG12	1.95	0.48
2:E:3763:ALA:O	2:E:3767:ASN:ND2	2.46	0.48
2:B:892:THR:O	2:B:904:HIS:N	2.45	0.48
2:E:1455:PRO:HB3	2:E:1549:PHE:HE2	1.78	0.48
2:K:2341:PHE:HB2	2:K:2436:ARG:HD3	1.93	0.48
1:D:31:GLN:HB2	1:D:96:THR:HB	1.95	0.48
2:E:2300:VAL:HG12	2:E:2361:LYS:HD2	1.96	0.48
2:K:3762:GLN:OE1	2:K:3804:ASN:ND2	2.40	0.48
2:B:618:GLN:OE1	2:B:1678:ASN:ND2	2.39	0.48
2:E:1653:LEU:HD23	2:E:1660:GLN:HA	1.96	0.48
2:H:1243:PRO:HB3	2:H:1600:LEU:HD21	1.94	0.48
2:K:781:VAL:HG11	2:K:789:VAL:HG21	1.96	0.48
2:B:671:VAL:HG23	2:B:787:VAL:HG22	1.96	0.48
2:B:1561:VAL:HG12	2:B:1562:ILE:HG12	1.95	0.48
2:H:3884:GLN:OE1	2:H:3955:GLN:NE2	2.47	0.48
2:K:659:TYR:O	2:K:662:TRP:NE1	2.47	0.48
1:A:31:GLN:HB2	1:A:96:THR:HB	1.95	0.48
2:B:1243:PRO:HB3	2:B:1600:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4040:VAL:HG22	2:E:4145:LEU:HD21	1.95	0.48
1:J:31:GLN:HB2	1:J:96:THR:HB	1.95	0.48
2:K:1561:VAL:HG12	2:K:1562:ILE:HG12	1.95	0.48
2:B:3763:ALA:O	2:B:3767:ASN:ND2	2.46	0.48
2:E:3763:ALA:HA	2:E:3766:HIS:CE1	2.48	0.48
2:H:1079:LYS:HA	2:H:1189:LEU:HD11	1.96	0.48
2:H:1126:GLY:HA3	2:H:1143:TRP:CE2	2.48	0.48
2:H:1653:LEU:HD23	2:H:1660:GLN:HA	1.96	0.48
2:K:1079:LYS:HA	2:K:1189:LEU:HD11	1.96	0.48
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.48	0.47
2:H:102:LEU:HB2	2:H:105:HIS:CD2	2.48	0.47
2:K:4690:PRO:HB2	2:K:4701:ARG:HH11	1.79	0.47
2:B:4040:VAL:HG22	2:B:4145:LEU:HD21	1.95	0.47
2:B:4690:PRO:HB2	2:B:4701:ARG:HH11	1.79	0.47
2:E:659:TYR:O	2:E:662:TRP:NE1	2.47	0.47
2:E:1079:LYS:HA	2:E:1189:LEU:HD11	1.96	0.47
2:K:1431:THR:OG1	2:K:1521:ASP:OD1	2.29	0.47
2:K:3776:GLN:NE2	2:K:3814:TYR:OH	2.37	0.47
2:B:659:TYR:O	2:B:662:TRP:NE1	2.47	0.47
2:K:2455:ARG:HG3	2:K:2510:VAL:HG23	1.97	0.47
2:B:1864:LEU:HB3	2:B:1871:VAL:HG11	1.97	0.47
2:B:1079:LYS:HA	2:B:1189:LEU:HD11	1.96	0.47
2:E:781:VAL:HG11	2:E:789:VAL:HG21	1.96	0.47
2:H:671:VAL:HG23	2:H:787:VAL:HG22	1.96	0.47
2:H:781:VAL:HG11	2:H:789:VAL:HG21	1.96	0.47
2:K:1653:LEU:HD23	2:K:1660:GLN:HA	1.96	0.47
2:E:1478:ASP:N	2:E:1482:ASN:O	2.48	0.47
2:E:2455:ARG:HG3	2:E:2510:VAL:HG23	1.97	0.47
2:K:671:VAL:HG23	2:K:787:VAL:HG22	1.96	0.47
2:K:3884:GLN:OE1	2:K:3955:GLN:NE2	2.47	0.47
2:B:781:VAL:HG11	2:B:789:VAL:HG21	1.96	0.47
2:B:1653:LEU:HD23	2:B:1660:GLN:HA	1.96	0.47
2:H:4690:PRO:HB2	2:H:4701:ARG:HH11	1.79	0.47
2:E:4690:PRO:HB2	2:E:4701:ARG:HH11	1.79	0.46
2:E:4981:HIS:HB2	2:E:4986:TYR:HE2	1.81	0.46
2:E:2010:LEU:HB3	2:E:2024:LEU:HD11	1.97	0.46
1:G:31:GLN:HB2	1:G:96:THR:HB	1.95	0.46
2:H:1864:LEU:HB3	2:H:1871:VAL:HG11	1.97	0.46
2:H:2010:LEU:HB3	2:H:2024:LEU:HD11	1.97	0.46
2:H:4981:HIS:HB2	2:H:4986:TYR:HE2	1.81	0.46
2:K:594:GLY:HA2	2:K:1594:ARG:HE	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:908:VAL:HG23	2:K:913:LEU:HD23	1.98	0.46
2:B:1717:SER:HA	2:B:1721:GLU:HB2	1.98	0.46
2:H:594:GLY:HA2	2:H:1594:ARG:HE	1.81	0.46
2:B:2455:ARG:HG3	2:B:2510:VAL:HG23	1.97	0.46
2:E:553:ARG:HG3	2:E:555:GLU:H	1.80	0.46
2:H:262:LEU:HD23	2:H:262:LEU:H	1.80	0.46
2:K:262:LEU:HD23	2:K:262:LEU:H	1.80	0.46
2:B:908:VAL:HG23	2:B:913:LEU:HD23	1.98	0.46
2:B:1153:ILE:HG13	2:B:1160:ILE:HG12	1.98	0.46
2:B:1225:PRO:HD2	2:B:1228:ILE:HD12	1.97	0.46
2:B:4981:HIS:HB2	2:B:4986:TYR:HE2	1.81	0.46
2:E:594:GLY:HA2	2:E:1594:ARG:HE	1.81	0.46
2:K:683:ARG:HG2	2:K:717:ASP:HB3	1.98	0.46
2:B:2010:LEU:HB3	2:B:2024:LEU:HD11	1.97	0.46
2:B:4565:LEU:HG	2:B:4814:ILE:HG22	1.98	0.46
2:E:1717:SER:HA	2:E:1721:GLU:HB2	1.98	0.46
2:K:1225:PRO:HD2	2:K:1228:ILE:HD12	1.97	0.46
2:K:1864:LEU:HB3	2:K:1871:VAL:HG11	1.97	0.46
2:K:4981:HIS:HB2	2:K:4986:TYR:HE2	1.81	0.46
2:B:553:ARG:HG3	2:B:555:GLU:H	1.80	0.46
2:B:594:GLY:HA2	2:B:1594:ARG:HE	1.81	0.46
2:E:4565:LEU:HG	2:E:4814:ILE:HG22	1.98	0.46
2:H:908:VAL:HG23	2:H:913:LEU:HD23	1.98	0.46
2:B:1478:ASP:N	2:B:1482:ASN:O	2.48	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46
2:E:1864:LEU:HB3	2:E:1871:VAL:HG11	1.97	0.46
2:H:1225:PRO:HD2	2:H:1228:ILE:HD12	1.97	0.46
2:B:981:GLN:NE2	2:B:1053:ILE:O	2.48	0.45
2:E:711:LEU:HD21	2:E:1490:SER:HA	1.98	0.45
2:E:1153:ILE:HG13	2:E:1160:ILE:HG12	1.98	0.45
2:H:711:LEU:HD21	2:H:1490:SER:HA	1.98	0.45
2:H:553:ARG:HG3	2:H:555:GLU:H	1.80	0.45
2:K:2010:LEU:HB3	2:K:2024:LEU:HD11	1.97	0.45
2:H:2455:ARG:HG3	2:H:2510:VAL:HG23	1.97	0.45
2:H:4820:THR:HB	2:K:4837:MET:HG3	1.98	0.45
2:B:262:LEU:H	2:B:262:LEU:HD23	1.80	0.45
2:B:3922:GLN:HE21	2:B:3986:GLY:HA3	1.82	0.45
2:E:908:VAL:HG23	2:E:913:LEU:HD23	1.98	0.45
2:H:1478:ASP:N	2:H:1482:ASN:O	2.48	0.45
2:K:553:ARG:HG3	2:K:555:GLU:H	1.80	0.45
2:K:981:GLN:NE2	2:K:1053:ILE:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1431:THR:OG1	2:B:1521:ASP:OD1	2.29	0.45
2:B:3637:LEU:HD12	2:B:3640:LEU:HD12	1.99	0.45
2:E:618:GLN:OE1	2:E:1678:ASN:ND2	2.39	0.45
2:H:683:ARG:HG2	2:H:717:ASP:HB3	1.98	0.45
2:H:1153:ILE:HG13	2:H:1160:ILE:HG12	1.98	0.45
2:K:1717:SER:HA	2:K:1721:GLU:HB2	1.98	0.45
2:B:615:ARG:HH21	2:B:2169:VAL:HG11	1.82	0.45
1:D:27:THR:HB	1:D:100:ASP:HB3	1.99	0.45
2:E:1225:PRO:HD2	2:E:1228:ILE:HD12	1.97	0.45
2:H:1717:SER:HA	2:H:1721:GLU:HB2	1.98	0.45
1:A:27:THR:HB	1:A:100:ASP:HB3	1.99	0.45
2:E:262:LEU:HD23	2:E:262:LEU:H	1.80	0.45
2:H:978:THR:HG22	2:H:980:ALA:H	1.82	0.45
2:K:622:THR:HG23	2:K:626:LEU:HD12	1.99	0.45
2:K:3637:LEU:HD12	2:K:3640:LEU:HD12	1.99	0.45
2:B:4820:THR:HB	2:E:4837:MET:HG3	1.98	0.45
2:E:1257:VAL:HG12	2:E:1272:LEU:HD12	1.99	0.45
2:E:3922:GLN:HE21	2:E:3986:GLY:HA3	1.82	0.45
2:H:35:LEU:HD13	2:H:49:LEU:HD13	1.99	0.45
2:H:292:ALA:HB2	2:H:312:THR:HG22	1.99	0.45
2:H:2239:TYR:OH	3:I:68:GLU:OE2	2.27	0.45
1:G:27:THR:HB	1:G:100:ASP:HB3	1.99	0.45
2:K:1153:ILE:HG13	2:K:1160:ILE:HG12	1.98	0.45
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.44
2:B:711:LEU:HD21	2:B:1490:SER:HA	1.98	0.44
2:H:1257:VAL:HG12	2:H:1272:LEU:HD12	1.99	0.44
2:K:3922:GLN:HE21	2:K:3986:GLY:HA3	1.82	0.44
2:B:622:THR:HG23	2:B:626:LEU:HD12	1.99	0.44
2:E:978:THR:HG22	2:E:980:ALA:H	1.82	0.44
2:H:615:ARG:HH21	2:H:2169:VAL:HG11	1.82	0.44
2:K:35:LEU:HD13	2:K:49:LEU:HD13	1.99	0.44
2:K:978:THR:HG22	2:K:980:ALA:H	1.82	0.44
2:K:2462:VAL:O	2:K:2511:TYR:OH	2.34	0.44
2:B:497:TYR:HB3	2:B:503:PHE:HB3	1.99	0.44
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.99	0.44
2:H:3922:GLN:HE21	2:H:3986:GLY:HA3	1.82	0.44
2:K:292:ALA:HB2	2:K:312:THR:HG22	1.99	0.44
2:K:711:LEU:HD21	2:K:1490:SER:HA	1.98	0.44
2:E:615:ARG:HH21	2:E:2169:VAL:HG11	1.82	0.44
2:H:4565:LEU:HG	2:H:4814:ILE:HG22	1.98	0.44
2:K:615:ARG:HH21	2:K:2169:VAL:HG11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1974:GLN:HE22	2:K:3637:LEU:HB3	1.83	0.44
2:K:4565:LEU:HG	2:K:4814:ILE:HG22	1.98	0.44
2:B:1974:GLN:HE22	2:B:3637:LEU:HB3	1.83	0.44
2:E:622:THR:HG23	2:E:626:LEU:HD12	1.99	0.44
2:H:622:THR:HG23	2:H:626:LEU:HD12	1.99	0.44
2:B:4837:MET:HG3	2:K:4820:THR:HB	1.98	0.44
2:E:497:TYR:HB3	2:E:503:PHE:HB3	1.99	0.44
2:E:3637:LEU:HD12	2:E:3640:LEU:HD12	1.99	0.44
2:E:4820:THR:HB	2:H:4837:MET:HG3	1.98	0.44
2:H:497:TYR:HB3	2:H:503:PHE:HB3	1.99	0.44
1:J:27:THR:HB	1:J:100:ASP:HB3	1.99	0.44
2:K:1257:VAL:HG12	2:K:1272:LEU:HD12	1.99	0.44
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.99	0.44
2:B:2462:VAL:O	2:B:2511:TYR:OH	2.34	0.44
2:H:282:ILE:HB	2:H:291:LEU:HD21	2.00	0.44
2:H:981:GLN:NE2	2:H:1053:ILE:O	2.48	0.44
2:H:3637:LEU:HD12	2:H:3640:LEU:HD12	1.99	0.44
2:B:845:CYS:SG	2:B:846:LEU:N	2.91	0.44
1:D:9:PRO:HD3	2:E:736:HIS:HB2	2.00	0.44
2:E:845:CYS:SG	2:E:846:LEU:N	2.91	0.44
2:E:1431:THR:OG1	2:E:1521:ASP:OD1	2.29	0.44
2:H:874:LEU:HD11	2:H:1042:ALA:HB1	1.99	0.44
2:H:1974:GLN:HE22	2:H:3637:LEU:HB3	1.83	0.44
2:K:282:ILE:HB	2:K:291:LEU:HD21	2.00	0.44
2:B:978:THR:HG22	2:B:980:ALA:H	1.82	0.44
2:B:2355:VAL:HG11	2:B:2454:ILE:HD12	2.00	0.44
2:K:2355:VAL:HG11	2:K:2454:ILE:HD12	2.00	0.44
2:B:874:LEU:HD11	2:B:1042:ALA:HB1	1.99	0.43
2:E:1974:GLN:HE22	2:E:3637:LEU:HB3	1.83	0.43
2:K:845:CYS:SG	2:K:846:LEU:N	2.91	0.43
2:K:874:LEU:HD11	2:K:1042:ALA:HB1	1.99	0.43
2:K:4178:ILE:HD13	2:K:4188:ILE:HD11	2.00	0.43
2:E:1716:ILE:O	2:E:1721:GLU:N	2.51	0.43
2:H:3933:SER:OG	2:K:80:GLU:OE1	2.36	0.43
2:B:282:ILE:HB	2:B:291:LEU:HD21	2.00	0.43
2:B:1257:VAL:HG12	2:B:1272:LEU:HD12	1.99	0.43
2:E:282:ILE:HB	2:E:291:LEU:HD21	2.00	0.43
2:K:842:PRO:HG2	2:K:1196:PRO:HA	1.99	0.43
2:K:497:TYR:HB3	2:K:503:PHE:HB3	1.99	0.43
2:B:1716:ILE:O	2:B:1721:GLU:N	2.51	0.43
2:B:4178:ILE:HD13	2:B:4188:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4178:ILE:HD13	2:H:4188:ILE:HD11	2.00	0.43
2:K:1451:GLY:HA3	2:K:1494:MET:HA	1.99	0.43
2:K:1716:ILE:O	2:K:1721:GLU:N	2.51	0.43
2:B:639:ASN:OD1	2:B:640:TYR:N	2.52	0.43
2:B:4234:GLU:OE2	2:B:5012:TYR:OH	2.33	0.43
2:E:1110:ARG:NE	2:E:1112:ASP:OD2	2.52	0.43
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.67	0.43
2:E:4178:ILE:HD13	2:E:4188:ILE:HD11	2.00	0.43
2:H:1716:ILE:O	2:H:1721:GLU:N	2.51	0.43
2:B:842:PRO:HG2	2:B:1196:PRO:HA	1.99	0.43
2:B:1451:GLY:HA3	2:B:1494:MET:HA	1.99	0.43
2:E:842:PRO:HG2	2:E:1196:PRO:HA	1.99	0.43
2:H:1075:PHE:O	2:H:1192:CYS:N	2.46	0.43
2:H:1451:GLY:HA3	2:H:1494:MET:HA	1.99	0.43
2:E:214:VAL:HG11	2:E:390:LEU:HD13	2.01	0.43
2:E:1708:ARG:NH1	2:E:1837:PHE:O	2.52	0.43
2:E:2355:VAL:HG11	2:E:2454:ILE:HD12	2.00	0.43
2:H:845:CYS:SG	2:H:846:LEU:N	2.91	0.43
2:H:1110:ARG:NE	2:H:1112:ASP:OD2	2.52	0.43
2:H:2369:LEU:H	2:H:2369:LEU:HD23	1.84	0.43
2:B:214:VAL:HG11	2:B:390:LEU:HD13	2.01	0.43
2:B:214:VAL:HB	2:B:339:ILE:HG13	2.01	0.43
2:B:292:ALA:HB2	2:B:312:THR:HG22	1.99	0.43
2:B:2369:LEU:HD23	2:B:2369:LEU:H	1.84	0.43
2:E:292:ALA:HB2	2:E:312:THR:HG22	1.99	0.43
2:E:639:ASN:OD1	2:E:640:TYR:N	2.52	0.43
2:E:874:LEU:HD11	2:E:1042:ALA:HB1	1.99	0.43
2:E:981:GLN:NE2	2:E:1053:ILE:O	2.48	0.43
2:E:1451:GLY:HA3	2:E:1494:MET:HA	1.99	0.43
2:E:2239:TYR:OH	3:F:68:GLU:OE2	2.27	0.43
2:K:214:VAL:HB	2:K:339:ILE:HG13	2.01	0.42
2:K:2369:LEU:HD23	2:K:2369:LEU:H	1.84	0.42
2:B:894:GLY:HA3	2:B:903:LEU:HB3	2.01	0.42
2:E:797:HIS:HA	2:E:1619:ARG:HH12	1.84	0.42
2:E:2462:VAL:O	2:E:2511:TYR:OH	2.34	0.42
1:G:9:PRO:HD3	2:H:736:HIS:HB2	2.00	0.42
2:H:842:PRO:HG2	2:H:1196:PRO:HA	1.99	0.42
2:H:2355:VAL:HG11	2:H:2454:ILE:HD12	2.00	0.42
1:J:9:PRO:HD3	2:K:736:HIS:HB2	2.00	0.42
2:K:1110:ARG:NE	2:K:1112:ASP:OD2	2.52	0.42
2:E:2112:VAL:HG13	2:E:2117:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:639:ASN:OD1	2:K:640:TYR:N	2.52	0.42
2:K:1075:PHE:O	2:K:1192:CYS:N	2.46	0.42
1:A:9:PRO:HD3	2:B:736:HIS:HB2	2.00	0.42
2:B:929:LEU:HD13	2:B:932:LEU:HD12	2.02	0.42
2:E:3933:SER:OG	2:H:80:GLU:OE1	2.36	0.42
2:H:797:HIS:HA	2:H:1619:ARG:HH12	1.84	0.42
2:H:894:GLY:HA3	2:H:903:LEU:HB3	2.01	0.42
2:H:2112:VAL:HG13	2:H:2117:LEU:HD23	2.01	0.42
2:B:250:GLY:HA2	2:B:253:CYS:HB2	2.02	0.42
2:B:3674:SER:OG	2:B:3768:ARG:NH2	2.53	0.42
2:E:2369:LEU:HD23	2:E:2369:LEU:H	1.84	0.42
2:H:103:TYR:OH	2:H:167:ASP:OD2	2.30	0.42
2:B:1708:ARG:NH1	2:B:1837:PHE:O	2.52	0.42
2:B:2189:ASN:OD1	2:B:2190:LYS:N	2.53	0.42
2:E:214:VAL:HB	2:E:339:ILE:HG13	2.01	0.42
2:E:894:GLY:HA3	2:E:903:LEU:HB3	2.01	0.42
2:E:3674:SER:OG	2:E:3768:ARG:NH2	2.53	0.42
2:K:2303:LEU:HD13	2:K:2332:TYR:HB2	2.02	0.42
1:D:92:PRO:HG2	1:D:95:ALA:HB2	2.02	0.42
2:H:639:ASN:OD1	2:H:640:TYR:N	2.52	0.42
2:H:1143:TRP:CZ2	2:H:1149:VAL:HG21	2.55	0.42
2:K:1478:ASP:N	2:K:1482:ASN:O	2.48	0.42
2:K:2226:PHE:HB3	2:K:2229:MET:HG2	2.02	0.42
2:B:1143:TRP:CZ2	2:B:1149:VAL:HG21	2.55	0.42
2:B:2303:LEU:HD13	2:B:2332:TYR:HB2	2.02	0.42
2:H:1236:THR:OG1	2:H:1608:MET:SD	2.67	0.42
2:H:2462:VAL:O	2:H:2511:TYR:OH	2.34	0.42
2:H:214:VAL:HG11	2:H:390:LEU:HD13	2.01	0.41
2:H:783:PHE:HZ	2:H:1615:VAL:HG22	1.85	0.41
2:H:2226:PHE:HB3	2:H:2229:MET:HG2	2.02	0.41
2:K:214:VAL:HG11	2:K:390:LEU:HD13	2.01	0.41
2:K:894:GLY:HA3	2:K:903:LEU:HB3	2.01	0.41
2:K:2239:TYR:OH	3:L:68:GLU:OE2	2.27	0.41
2:H:214:VAL:HB	2:H:339:ILE:HG13	2.01	0.41
2:H:250:GLY:HA2	2:H:253:CYS:HB2	2.02	0.41
2:K:783:PHE:HZ	2:K:1615:VAL:HG22	1.85	0.41
2:K:929:LEU:HD13	2:K:932:LEU:HD12	2.02	0.41
2:K:2189:ASN:OD1	2:K:2190:LYS:N	2.53	0.41
2:B:797:HIS:HA	2:B:1619:ARG:HH12	1.84	0.41
2:E:250:GLY:HA2	2:E:253:CYS:HB2	2.02	0.41
2:E:929:LEU:HD13	2:E:932:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1143:TRP:CZ2	2:E:1149:VAL:HG21	2.55	0.41
2:K:250:GLY:HA2	2:K:253:CYS:HB2	2.02	0.41
2:B:720:HIS:HB3	2:B:729:LEU:HA	2.02	0.41
2:B:1074:ILE:HG23	2:B:1115:LEU:HD11	2.02	0.41
2:B:2365:PHE:HD1	2:B:2430:LEU:HD21	1.85	0.41
2:B:3933:SER:OG	2:E:80:GLU:OE1	2.36	0.41
2:B:3981:TRP:HB3	2:B:4042:MET:HG3	2.03	0.41
2:E:2365:PHE:HD1	2:E:2430:LEU:HD21	1.85	0.41
2:H:783:PHE:HB2	2:H:787:VAL:HB	2.02	0.41
2:H:3674:SER:OG	2:H:3768:ARG:NH2	2.53	0.41
2:K:1074:ILE:HG23	2:K:1115:LEU:HD11	2.02	0.41
2:K:1143:TRP:CZ2	2:K:1149:VAL:HG21	2.55	0.41
2:K:1708:ARG:NH1	2:K:1837:PHE:O	2.52	0.41
2:K:2467:LEU:HD21	2:K:2506:PHE:HD2	1.86	0.41
2:B:2112:VAL:HG13	2:B:2117:LEU:HD23	2.01	0.41
1:D:38:SER:OG	1:D:41:ASP:OD2	2.38	0.41
2:E:39:ALA:HB1	2:E:137:LEU:HD11	2.02	0.41
2:E:1100:MET:HB2	2:E:1143:TRP:CZ3	2.56	0.41
2:E:2189:ASN:OD1	2:E:2190:LYS:N	2.53	0.41
2:E:4677:ARG:HE	2:E:5015:ARG:CZ	2.33	0.41
2:H:21:VAL:HB	2:H:205:ILE:HD11	2.03	0.41
2:H:39:ALA:HB1	2:H:137:LEU:HD11	2.02	0.41
2:H:929:LEU:HD13	2:H:932:LEU:HD12	2.02	0.41
2:H:1100:MET:HB2	2:H:1143:TRP:CZ3	2.56	0.41
2:H:1708:ARG:NH1	2:H:1837:PHE:O	2.52	0.41
2:H:4998:GLU:HA	2:H:5001:HIS:CE1	2.56	0.41
1:J:38:SER:OG	1:J:41:ASP:OD2	2.38	0.41
1:J:42:ARG:HD2	1:J:44:LYS:HE2	2.02	0.41
2:K:2112:VAL:HG13	2:K:2117:LEU:HD23	2.01	0.41
2:K:4677:ARG:HE	2:K:5015:ARG:CZ	2.33	0.41
2:B:606:LEU:HD23	2:B:621:ILE:HD11	2.03	0.41
2:B:4574:ILE:HG21	2:B:4641:LEU:HB2	2.03	0.41
2:B:4677:ARG:HE	2:B:5015:ARG:CZ	2.33	0.41
1:D:56:ILE:HG23	1:D:59:PHE:H	1.86	0.41
2:E:1074:ILE:HG23	2:E:1115:LEU:HD11	2.02	0.41
2:H:2189:ASN:OD1	2:H:2190:LYS:N	2.53	0.41
2:K:3674:SER:OG	2:K:3768:ARG:NH2	2.53	0.41
2:B:39:ALA:HB1	2:B:137:LEU:HD11	2.02	0.41
2:B:596:ASN:HB3	2:B:599:VAL:HG23	2.02	0.41
2:E:1252:HIS:HB3	2:E:1255:TYR:O	2.21	0.41
2:E:4928:ALA:O	2:E:4932:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:ASP:OD2	2:H:1783:PHE:HB2	2.21	0.41
2:H:596:ASN:HB3	2:H:599:VAL:HG23	2.02	0.41
2:H:606:LEU:HD23	2:H:621:ILE:HD11	2.03	0.41
2:H:4575:LEU:HD11	2:H:4805:PHE:HA	2.03	0.41
1:J:92:PRO:HG2	1:J:95:ALA:HB2	2.02	0.41
2:K:606:LEU:HD23	2:K:621:ILE:HD11	2.03	0.41
2:K:797:HIS:HA	2:K:1619:ARG:HH12	1.84	0.41
2:K:4998:GLU:HA	2:K:5001:HIS:CE1	2.56	0.41
2:B:80:GLU:OE1	2:K:3933:SER:OG	2.36	0.41
1:D:42:ARG:HD2	1:D:44:LYS:HE2	2.02	0.41
1:G:56:ILE:HG23	1:G:59:PHE:H	1.86	0.41
1:G:92:PRO:HG2	1:G:95:ALA:HB2	2.02	0.41
2:K:783:PHE:HB2	2:K:787:VAL:HB	2.02	0.41
2:K:1236:THR:OG1	2:K:1608:MET:SD	2.67	0.41
2:K:2560:LEU:HD23	2:K:2603:VAL:HG12	2.03	0.41
2:K:4574:ILE:HG21	2:K:4641:LEU:HB2	2.03	0.41
2:E:783:PHE:HZ	2:E:1615:VAL:HG22	1.85	0.41
2:E:3961:THR:HG22	2:E:4021:MET:HA	2.03	0.41
2:E:4998:GLU:HA	2:E:5001:HIS:CE1	2.56	0.41
2:H:396:GLU:OE2	2:H:470:SER:OG	2.33	0.41
2:H:1074:ILE:HG23	2:H:1115:LEU:HD11	2.02	0.41
2:H:2560:LEU:HD23	2:H:2603:VAL:HG12	2.03	0.41
2:K:21:VAL:HB	2:K:205:ILE:HD11	2.03	0.41
2:K:720:HIS:HB3	2:K:729:LEU:HA	2.02	0.41
2:K:2365:PHE:HD1	2:K:2430:LEU:HD21	1.85	0.41
2:B:179:TYR:N	2:B:194:SER:O	2.54	0.41
2:B:613:ALA:HB2	2:B:1676:LEU:HD12	2.03	0.41
2:H:1988:THR:HG22	2:H:1990:ALA:H	1.86	0.41
2:H:3961:THR:HG22	2:H:4021:MET:HA	2.03	0.41
2:K:578:ILE:HG13	2:K:606:LEU:HD11	2.03	0.41
1:A:38:SER:OG	1:A:41:ASP:OD2	2.38	0.40
1:A:92:PRO:HG2	1:A:95:ALA:HB2	2.02	0.40
2:B:1110:ARG:NE	2:B:1112:ASP:OD2	2.52	0.40
2:B:4152:ASP:HB3	2:B:4155:LEU:HB3	2.03	0.40
2:B:4966:PHE:HE1	2:B:5027:ARG:HD2	1.87	0.40
2:B:4998:GLU:HA	2:B:5001:HIS:CE1	2.56	0.40
2:E:606:LEU:HD23	2:E:621:ILE:HD11	2.03	0.40
2:E:720:HIS:HB3	2:E:729:LEU:HA	2.02	0.40
2:E:1288:PHE:HD2	2:E:1600:LEU:HD13	1.86	0.40
2:E:4575:LEU:HD11	2:E:4805:PHE:HA	2.03	0.40
2:H:179:TYR:N	2:H:194:SER:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2365:PHE:HD1	2:H:2430:LEU:HD21	1.85	0.40
2:H:4574:ILE:HG21	2:H:4641:LEU:HB2	2.03	0.40
2:K:1100:MET:HB2	2:K:1143:TRP:CZ3	2.56	0.40
2:K:1252:HIS:HB3	2:K:1255:TYR:O	2.21	0.40
2:K:1288:PHE:HD2	2:K:1600:LEU:HD13	1.86	0.40
2:K:3961:THR:HG22	2:K:4021:MET:HA	2.03	0.40
2:E:179:TYR:N	2:E:194:SER:O	2.54	0.40
2:E:613:ALA:HB2	2:E:1676:LEU:HD12	2.03	0.40
2:E:4630:LEU:H	2:E:4630:LEU:HD23	1.86	0.40
2:H:1130:GLN:HA	2:H:1139:PHE:H	1.87	0.40
2:H:1439:VAL:HG21	2:H:1448:VAL:HG11	2.04	0.40
2:K:20:VAL:HG12	2:K:204:PRO:HA	2.03	0.40
2:K:4630:LEU:HD23	2:K:4630:LEU:H	1.86	0.40
1:A:42:ARG:HD2	1:A:44:LYS:HE2	2.02	0.40
2:B:578:ILE:HG13	2:B:606:LEU:HD11	2.03	0.40
2:B:783:PHE:HZ	2:B:1615:VAL:HG22	1.85	0.40
2:B:1988:THR:HG22	2:B:1990:ALA:H	1.86	0.40
2:B:3961:THR:HG22	2:B:4021:MET:HA	2.03	0.40
1:D:37:ASP:OD2	2:E:1783:PHE:HB2	2.21	0.40
2:E:21:VAL:HB	2:E:205:ILE:HD11	2.03	0.40
2:E:578:ILE:HG13	2:E:606:LEU:HD11	2.03	0.40
2:E:596:ASN:HB3	2:E:599:VAL:HG23	2.02	0.40
2:E:2226:PHE:HB3	2:E:2229:MET:HG2	2.02	0.40
2:H:578:ILE:HG13	2:H:606:LEU:HD11	2.03	0.40
2:H:720:HIS:HB3	2:H:729:LEU:HA	2.02	0.40
2:H:1288:PHE:HD2	2:H:1600:LEU:HD13	1.86	0.40
2:H:2303:LEU:HD13	2:H:2332:TYR:HB2	2.02	0.40
2:H:2467:LEU:HD21	2:H:2506:PHE:HD2	1.86	0.40
2:H:4677:ARG:HE	2:H:5015:ARG:CZ	2.33	0.40
2:B:664:PHE:CZ	2:B:779:PRO:HB3	2.57	0.40
2:B:1100:MET:HB2	2:B:1143:TRP:CZ3	2.56	0.40
2:B:1288:PHE:HD2	2:B:1600:LEU:HD13	1.86	0.40
2:B:2467:LEU:HD21	2:B:2506:PHE:HD2	1.86	0.40
2:E:1435:TYR:O	2:E:1518:CYS:N	2.55	0.40
2:E:4152:ASP:HB3	2:E:4155:LEU:HB3	2.03	0.40
2:E:4234:GLU:OE2	2:E:5012:TYR:OH	2.33	0.40
2:H:1252:HIS:HB3	2:H:1255:TYR:O	2.21	0.40
2:K:39:ALA:HB1	2:K:137:LEU:HD11	2.02	0.40
2:K:291:LEU:HB3	2:K:301:VAL:HG12	2.04	0.40
2:B:4630:LEU:H	2:B:4630:LEU:HD23	1.86	0.40
2:E:396:GLU:OE2	2:E:470:SER:OG	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.04	0.40
2:E:2303:LEU:HD13	2:E:2332:TYR:HB2	2.02	0.40
1:G:38:SER:OG	1:G:41:ASP:OD2	2.38	0.40
1:G:42:ARG:HD2	1:G:44:LYS:HE2	2.02	0.40
2:K:613:ALA:HB2	2:K:1676:LEU:HD12	2.03	0.40
2:K:3981:TRP:HB3	2:K:4042:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3955	GLN
2	B	4199	GLN
2	E	3955	GLN
2	H	3955	GLN
2	K	3955	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	57
2	E	57
2	H	57
2	K	57

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4333:UNK	C	4543:GLU	N	53.56
1	E	4333:UNK	C	4543:GLU	N	53.56
1	H	4333:UNK	C	4543:GLU	N	53.56
1	K	4333:UNK	C	4543:GLU	N	53.56

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1054:GLU	C	1071:ARG	N	36.15
1	E	1054:GLU	C	1071:ARG	N	36.15
1	H	1054:GLU	C	1071:ARG	N	36.15
1	K	1054:GLU	C	1071:ARG	N	36.15
1	B	3606:UNK	C	3625:ARG	N	35.35
1	E	3606:UNK	C	3625:ARG	N	35.35
1	H	3606:UNK	C	3625:ARG	N	35.35
1	K	3606:UNK	C	3625:ARG	N	35.35
1	B	2939:ARG	C	2956:UNK	N	28.67
1	E	2939:ARG	C	2956:UNK	N	28.67
1	H	2939:ARG	C	2956:UNK	N	28.67
1	K	2939:ARG	C	2956:UNK	N	28.67
1	B	3385:UNK	C	3411:PRO	N	25.81
1	E	3385:UNK	C	3411:PRO	N	25.81
1	H	3385:UNK	C	3411:PRO	N	25.81
1	K	3385:UNK	C	3411:PRO	N	25.81
1	B	4246:ILE	C	4317:UNK	N	25.72
1	E	4246:ILE	C	4317:UNK	N	25.72
1	H	4246:ILE	C	4317:UNK	N	25.72
1	K	4246:ILE	C	4317:UNK	N	25.72
1	B	3555:UNK	C	3564:UNK	N	24.65
1	E	3555:UNK	C	3564:UNK	N	24.65
1	H	3555:UNK	C	3564:UNK	N	24.65
1	K	3555:UNK	C	3564:UNK	N	24.65
1	B	2830:GLU	C	2855:TYR	N	23.94
1	E	2830:GLU	C	2855:TYR	N	23.94
1	H	2830:GLU	C	2855:TYR	N	23.94
1	K	2830:GLU	C	2855:TYR	N	23.94
1	B	855:PRO	C	863:LEU	N	22.50
1	E	855:PRO	C	863:LEU	N	22.50
1	H	855:PRO	C	863:LEU	N	22.50
1	K	855:PRO	C	863:LEU	N	22.50
1	B	1299:GLN	C	1428:LEU	N	21.48
1	E	1299:GLN	C	1428:LEU	N	21.48
1	H	1299:GLN	C	1428:LEU	N	21.48
1	K	1299:GLN	C	1428:LEU	N	21.48
1	B	4737:GLU	C	4769:ILE	N	20.98
1	E	4737:GLU	C	4769:ILE	N	20.98
1	H	4737:GLU	C	4769:ILE	N	20.98
1	K	4737:GLU	C	4769:ILE	N	20.98
1	B	3574:UNK	C	3588:UNK	N	20.52
1	E	3574:UNK	C	3588:UNK	N	20.52

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	3574:UNK	C	3588:UNK	N	20.52
1	K	3574:UNK	C	3588:UNK	N	20.52
1	B	2473:LEU	C	2489:PRO	N	19.14
1	E	2473:LEU	C	2489:PRO	N	19.14
1	H	2473:LEU	C	2489:PRO	N	19.14
1	K	2473:LEU	C	2489:PRO	N	19.14
1	B	2978:UNK	C	2999:UNK	N	18.10
1	E	2978:UNK	C	2999:UNK	N	18.10
1	H	2978:UNK	C	2999:UNK	N	18.10
1	K	2978:UNK	C	2999:UNK	N	18.10
1	B	2046:GLN	C	2092:LEU	N	17.97
1	E	2046:GLN	C	2092:LEU	N	17.97
1	H	2046:GLN	C	2092:LEU	N	17.97
1	K	2046:GLN	C	2092:LEU	N	17.97
1	B	3358:UNK	C	3365:UNK	N	17.93
1	E	3358:UNK	C	3365:UNK	N	17.93
1	H	3358:UNK	C	3365:UNK	N	17.93
1	K	3358:UNK	C	3365:UNK	N	17.93
1	B	3731:LEU	C	3747:SER	N	17.86
1	E	3731:LEU	C	3747:SER	N	17.86
1	H	3731:LEU	C	3747:SER	N	17.86
1	K	3731:LEU	C	3747:SER	N	17.86
1	B	3193:UNK	C	3202:UNK	N	17.75
1	E	3193:UNK	C	3202:UNK	N	17.75
1	H	3193:UNK	C	3202:UNK	N	17.75
1	K	3193:UNK	C	3202:UNK	N	17.75
1	B	2650:UNK	C	2664:UNK	N	17.57
1	E	2650:UNK	C	2664:UNK	N	17.57
1	H	2650:UNK	C	2664:UNK	N	17.57
1	K	2650:UNK	C	2664:UNK	N	17.57
1	B	3238:UNK	C	3278:UNK	N	17.45
1	E	3238:UNK	C	3278:UNK	N	17.45
1	H	3238:UNK	C	3278:UNK	N	17.45
1	K	3238:UNK	C	3278:UNK	N	17.45
1	B	88:ALA	C	97:GLY	N	16.98
1	E	88:ALA	C	97:GLY	N	16.98
1	H	88:ALA	C	97:GLY	N	16.98
1	K	88:ALA	C	97:GLY	N	16.98
1	B	3062:UNK	C	3146:UNK	N	15.60
1	E	3062:UNK	C	3146:UNK	N	15.60
1	H	3062:UNK	C	3146:UNK	N	15.60
1	K	3062:UNK	C	3146:UNK	N	15.60

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3166:UNK	C	3173:UNK	N	15.53
1	E	3166:UNK	C	3173:UNK	N	15.53
1	H	3166:UNK	C	3173:UNK	N	15.53
1	K	3166:UNK	C	3173:UNK	N	15.53
1	B	3448:LYS	C	3509:UNK	N	14.65
1	E	3448:LYS	C	3509:UNK	N	14.65
1	H	3448:LYS	C	3509:UNK	N	14.65
1	K	3448:LYS	C	3509:UNK	N	14.65
1	B	3018:UNK	C	3032:UNK	N	14.33
1	E	3018:UNK	C	3032:UNK	N	14.33
1	H	3018:UNK	C	3032:UNK	N	14.33
1	K	3018:UNK	C	3032:UNK	N	14.33
1	B	3544:UNK	C	3548:UNK	N	13.83
1	E	3544:UNK	C	3548:UNK	N	13.83
1	H	3544:UNK	C	3548:UNK	N	13.83
1	K	3544:UNK	C	3548:UNK	N	13.83
1	B	3860:VAL	C	3867:GLU	N	13.48
1	E	3860:VAL	C	3867:GLU	N	13.48
1	H	3860:VAL	C	3867:GLU	N	13.48
1	K	3860:VAL	C	3867:GLU	N	13.48
1	B	1871:VAL	C	1924:GLU	N	13.08
1	E	1871:VAL	C	1924:GLU	N	13.08
1	H	1871:VAL	C	1924:GLU	N	13.08
1	K	1871:VAL	C	1924:GLU	N	13.08
1	B	361:ALA	C	372:LEU	N	12.94
1	E	361:ALA	C	372:LEU	N	12.94
1	H	361:ALA	C	372:LEU	N	12.94
1	K	361:ALA	C	372:LEU	N	12.94
1	B	3047:UNK	C	3052:UNK	N	12.92
1	E	3047:UNK	C	3052:UNK	N	12.92
1	H	3047:UNK	C	3052:UNK	N	12.92
1	K	3047:UNK	C	3052:UNK	N	12.92
1	B	323:LEU	C	328:LYS	N	12.78
1	E	323:LEU	C	328:LYS	N	12.78
1	H	323:LEU	C	328:LYS	N	12.78
1	K	323:LEU	C	328:LYS	N	12.78
1	B	2389:GLU	C	2418:HIS	N	12.70
1	E	2389:GLU	C	2418:HIS	N	12.70
1	H	2389:GLU	C	2418:HIS	N	12.70
1	K	2389:GLU	C	2418:HIS	N	12.70
1	B	2310:SER	C	2319:TYR	N	12.60
1	E	2310:SER	C	2319:TYR	N	12.60

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	2310:SER	C	2319:TYR	N	12.60
1	K	2310:SER	C	2319:TYR	N	12.60
1	B	3308:UNK	C	3320:UNK	N	12.55
1	E	3308:UNK	C	3320:UNK	N	12.55
1	H	3308:UNK	C	3320:UNK	N	12.55
1	K	3308:UNK	C	3320:UNK	N	12.55
1	B	4585:PRO	C	4626:VAL	N	12.41
1	E	4585:PRO	C	4626:VAL	N	12.41
1	H	4585:PRO	C	4626:VAL	N	12.41
1	K	4585:PRO	C	4626:VAL	N	12.41
1	B	3217:UNK	C	3225:UNK	N	12.05
1	E	3217:UNK	C	3225:UNK	N	12.05
1	H	3217:UNK	C	3225:UNK	N	12.05
1	K	3217:UNK	C	3225:UNK	N	12.05
1	B	3525:UNK	C	3534:UNK	N	12.04
1	E	3525:UNK	C	3534:UNK	N	12.04
1	H	3525:UNK	C	3534:UNK	N	12.04
1	K	3525:UNK	C	3534:UNK	N	12.04
1	B	4090:LYS	C	4109:UNK	N	11.97
1	E	4090:LYS	C	4109:UNK	N	11.97
1	H	4090:LYS	C	4109:UNK	N	11.97
1	K	4090:LYS	C	4109:UNK	N	11.97
1	B	1750:PRO	C	1759:ARG	N	11.44
1	E	1750:PRO	C	1759:ARG	N	11.44
1	H	1750:PRO	C	1759:ARG	N	11.44
1	K	1750:PRO	C	1759:ARG	N	11.44
1	B	2014:LYS	C	2023:PRO	N	11.36
1	E	2014:LYS	C	2023:PRO	N	11.36
1	H	2014:LYS	C	2023:PRO	N	11.36
1	K	2014:LYS	C	2023:PRO	N	11.36
1	B	1501:VAL	C	1510:SER	N	11.31
1	E	1501:VAL	C	1510:SER	N	11.31
1	H	1501:VAL	C	1510:SER	N	11.31
1	K	1501:VAL	C	1510:SER	N	11.31
1	B	1788:PRO	C	1794:GLU	N	11.03
1	E	1788:PRO	C	1794:GLU	N	11.03
1	H	1788:PRO	C	1794:GLU	N	11.03
1	K	1788:PRO	C	1794:GLU	N	11.03
1	B	4114:UNK	C	4122:GLU	N	10.80
1	E	4114:UNK	C	4122:GLU	N	10.80
1	H	4114:UNK	C	4122:GLU	N	10.80
1	K	4114:UNK	C	4122:GLU	N	10.80

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3335:UNK	C	3346:UNK	N	10.61
1	E	3335:UNK	C	3346:UNK	N	10.61
1	H	3335:UNK	C	3346:UNK	N	10.61
1	K	3335:UNK	C	3346:UNK	N	10.61
1	B	3288:UNK	C	3292:UNK	N	9.91
1	E	3288:UNK	C	3292:UNK	N	9.91
1	H	3288:UNK	C	3292:UNK	N	9.91
1	K	3288:UNK	C	3292:UNK	N	9.91
1	B	2683:UNK	C	2688:UNK	N	9.67
1	E	2683:UNK	C	2688:UNK	N	9.67
1	H	2683:UNK	C	2688:UNK	N	9.67
1	K	2683:UNK	C	2688:UNK	N	9.67
1	B	2217:GLY	C	2222:LYS	N	9.51
1	E	2217:GLY	C	2222:LYS	N	9.51
1	H	2217:GLY	C	2222:LYS	N	9.51
1	K	2217:GLY	C	2222:LYS	N	9.51
1	B	2571:ALA	C	2579:MET	N	8.61
1	E	2571:ALA	C	2579:MET	N	8.61
1	H	2571:ALA	C	2579:MET	N	8.61
1	K	2571:ALA	C	2579:MET	N	8.61
1	B	2632:PRO	C	2638:UNK	N	7.07
1	E	2632:PRO	C	2638:UNK	N	7.07
1	H	2632:PRO	C	2638:UNK	N	7.07
1	K	2632:PRO	C	2638:UNK	N	7.07
1	B	3004:UNK	C	3009:UNK	N	6.99
1	E	3004:UNK	C	3009:UNK	N	6.99
1	H	3004:UNK	C	3009:UNK	N	6.99
1	K	3004:UNK	C	3009:UNK	N	6.99
1	B	1478:ASP	C	1482:ASN	N	5.65
1	E	1478:ASP	C	1482:ASN	N	5.65
1	H	1478:ASP	C	1482:ASN	N	5.65
1	K	1478:ASP	C	1482:ASN	N	5.65
1	B	2535:ALA	C	2541:THR	N	5.55
1	E	2535:ALA	C	2541:THR	N	5.55
1	H	2535:ALA	C	2541:THR	N	5.55
1	K	2535:ALA	C	2541:THR	N	5.55
1	B	4863:LYS	C	4871:ASP	N	5.49
1	E	4863:LYS	C	4871:ASP	N	5.49
1	H	4863:LYS	C	4871:ASP	N	5.49
1	K	4863:LYS	C	4871:ASP	N	5.49
1	B	1275:ARG	C	1282:SER	N	5.47
1	E	1275:ARG	C	1282:SER	N	5.47

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1275:ARG	C	1282:SER	N	5.47
1	K	1275:ARG	C	1282:SER	N	5.47
1	B	184:THR	C	189:LEU	N	4.54
1	E	184:THR	C	189:LEU	N	4.54
1	H	184:THR	C	189:LEU	N	4.54
1	K	184:THR	C	189:LEU	N	4.54
1	B	2383:GLU	C	2384:ALA	N	3.24
1	B	4245:GLN	C	4246:ILE	N	3.24
1	E	2383:GLU	C	2384:ALA	N	3.24
1	E	4245:GLN	C	4246:ILE	N	3.24
1	H	2383:GLU	C	2384:ALA	N	3.24
1	H	4245:GLN	C	4246:ILE	N	3.24
1	K	2383:GLU	C	2384:ALA	N	3.24
1	K	4245:GLN	C	4246:ILE	N	3.24

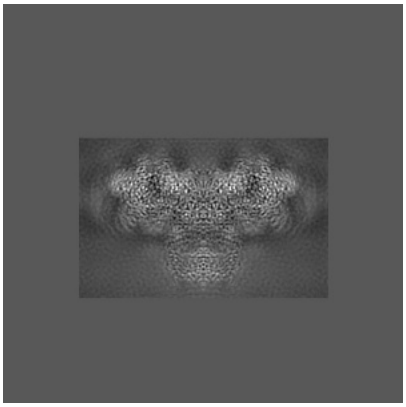
6 Map visualisation

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

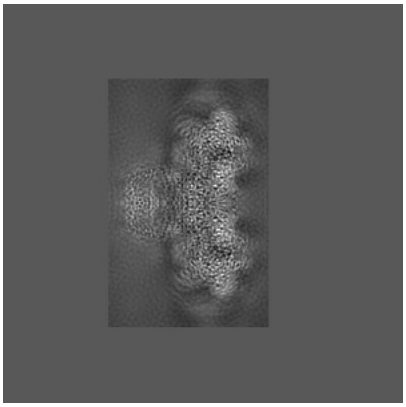
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

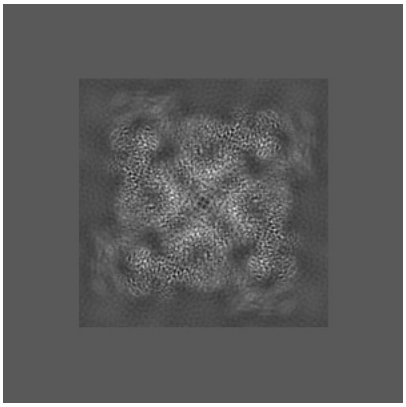
6.1.1 Primary map



X



Y

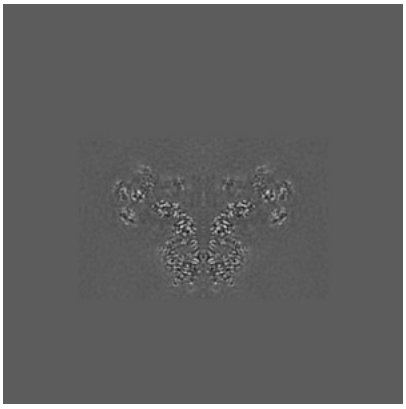


Z

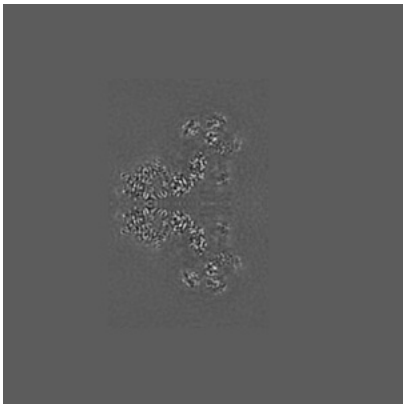
The images above show the map projected in three orthogonal directions.

6.2 Central slices

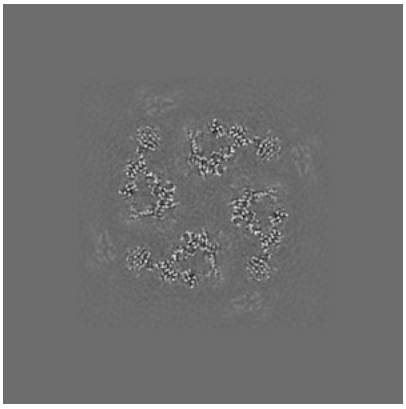
6.2.1 Primary map



X Index: 240



Y Index: 240

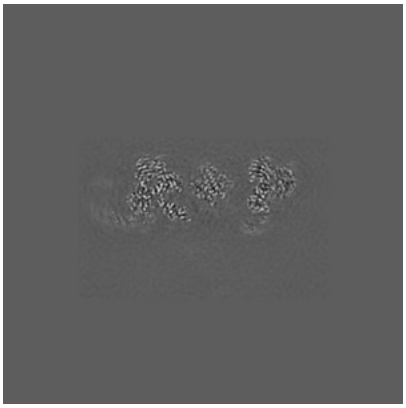


Z Index: 240

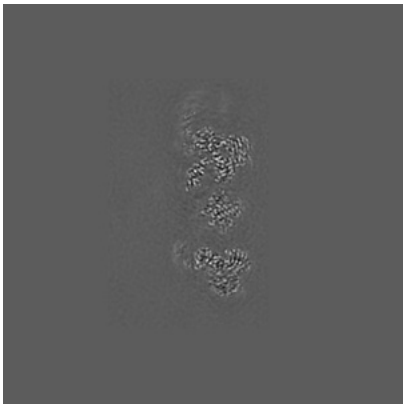
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

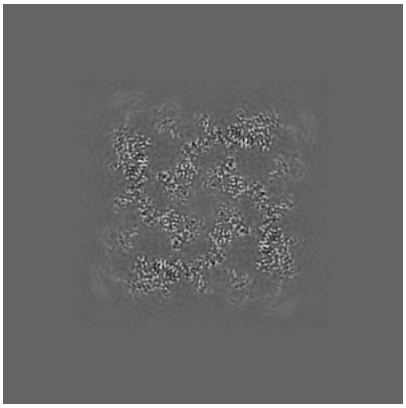
6.3.1 Primary map



X Index: 311



Y Index: 311

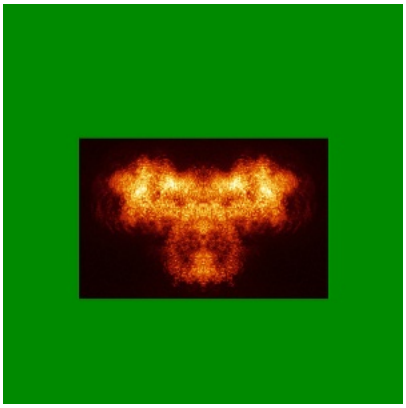


Z Index: 258

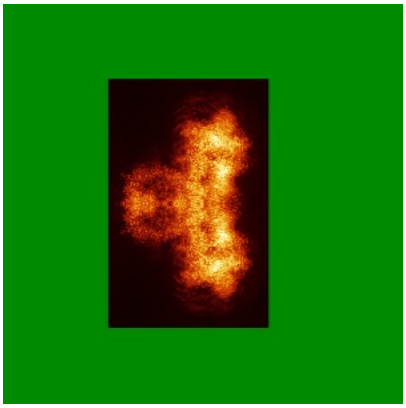
The images above show the largest variance slices of the map in three orthogonal directions.

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

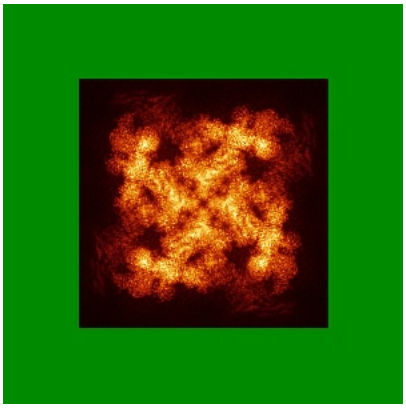
6.4.1 Primary map



X



Y

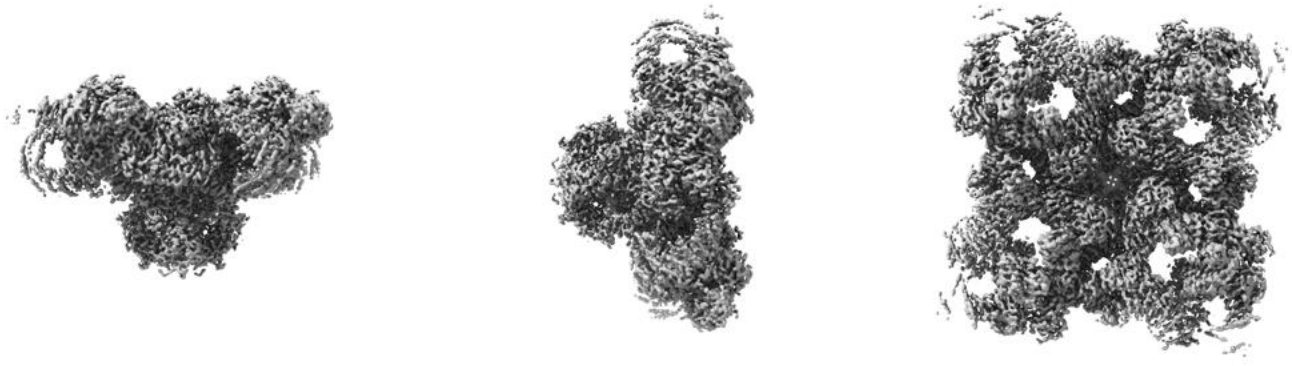


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

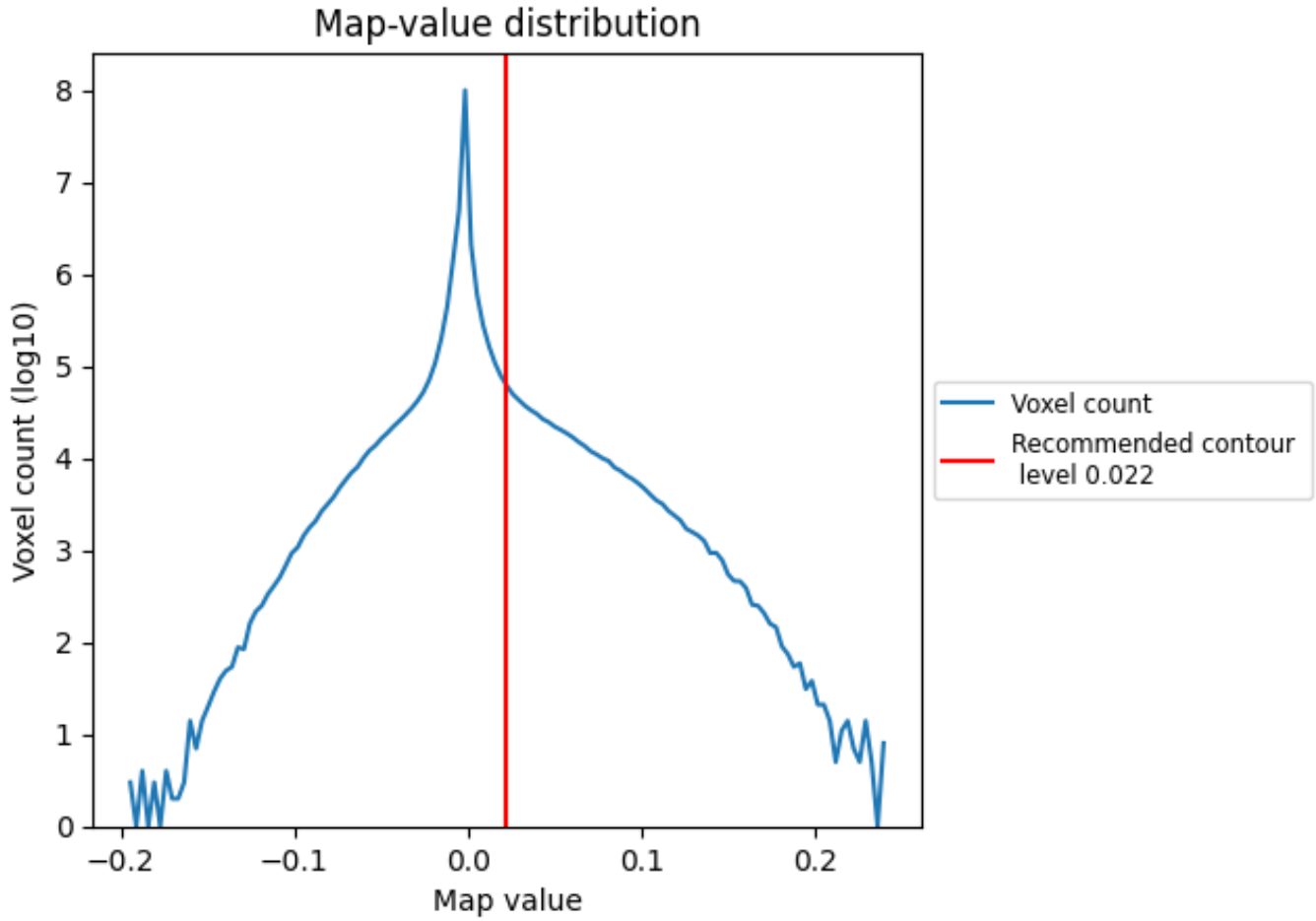
6.6 Mask visualisation (i)

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

7 Map analysis

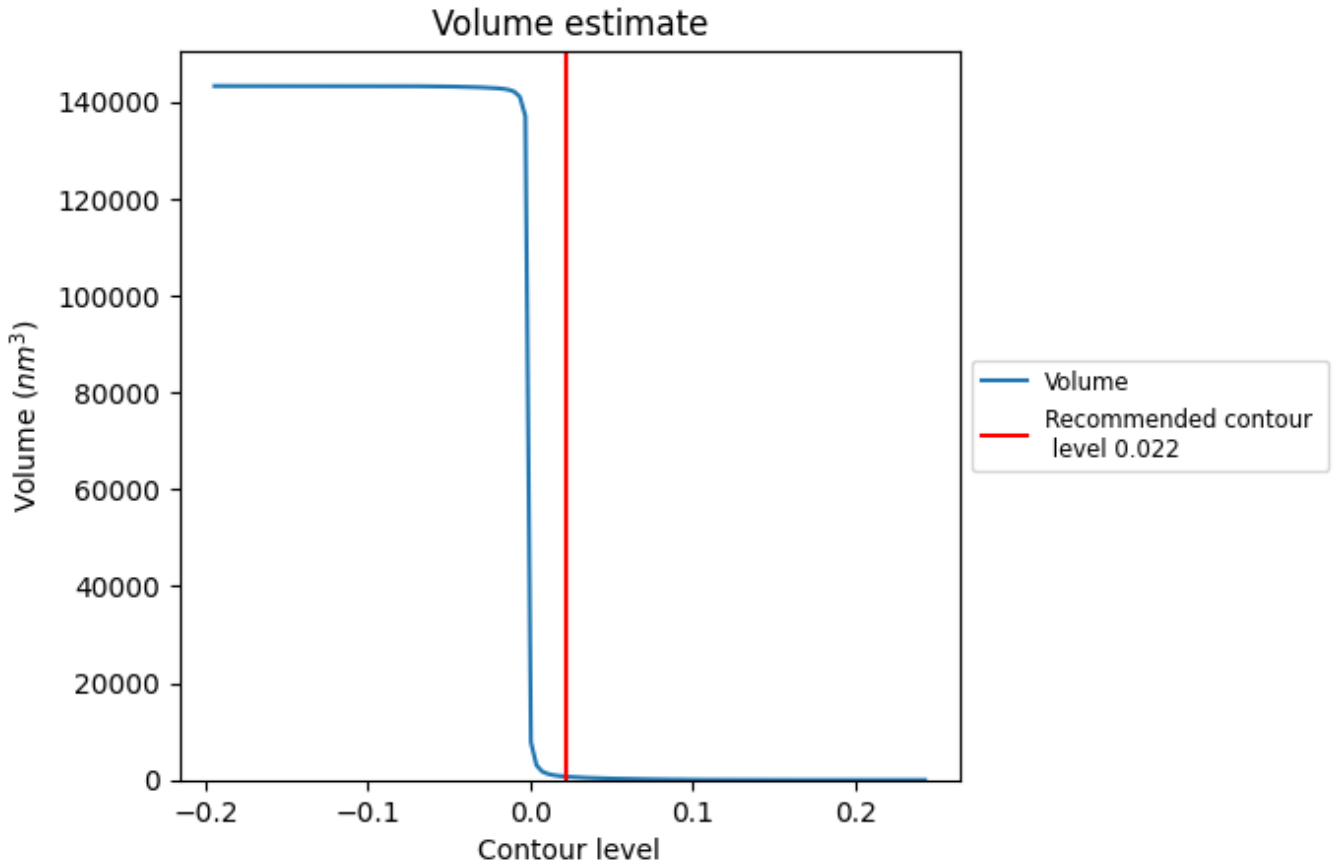
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

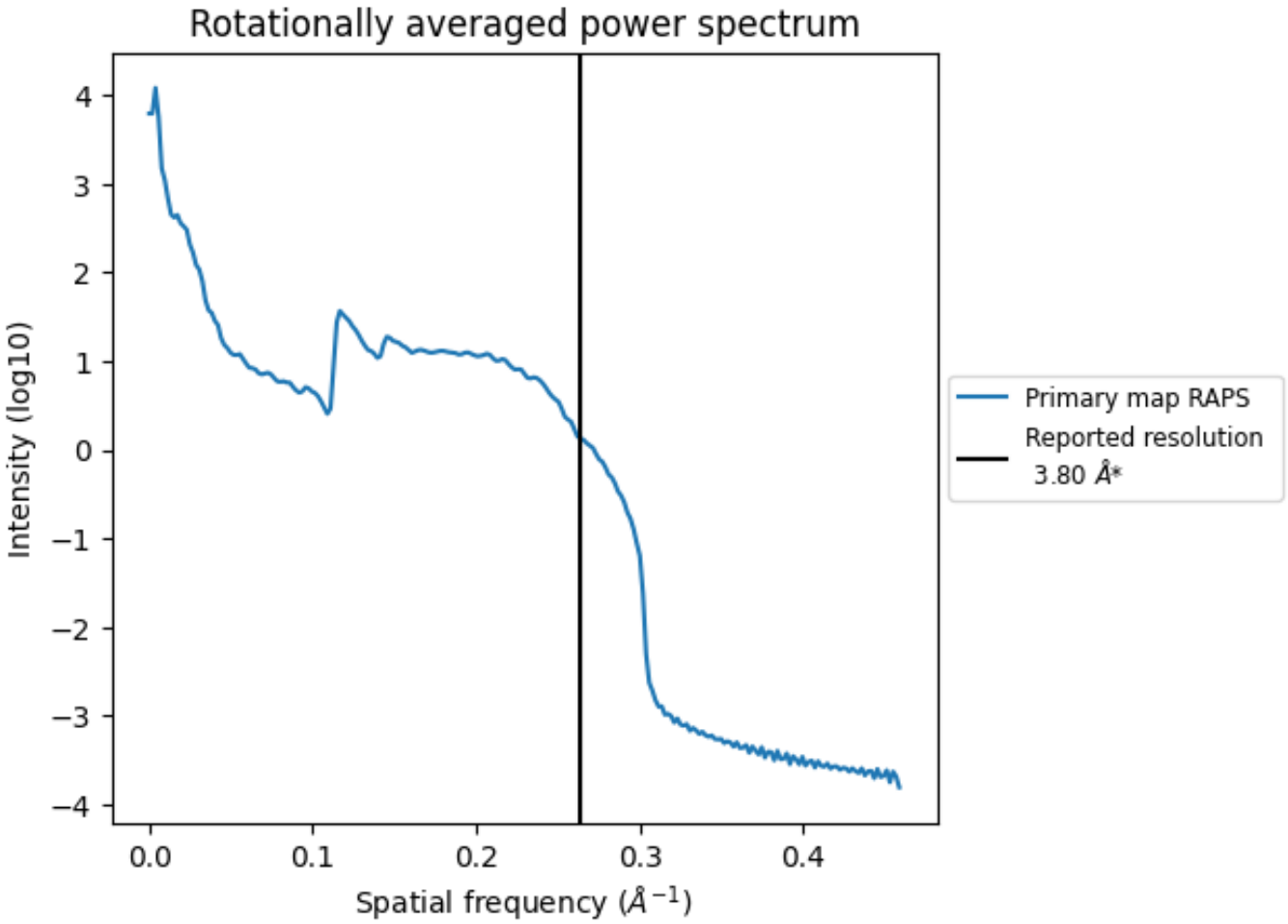
7.2 Volume estimate



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

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

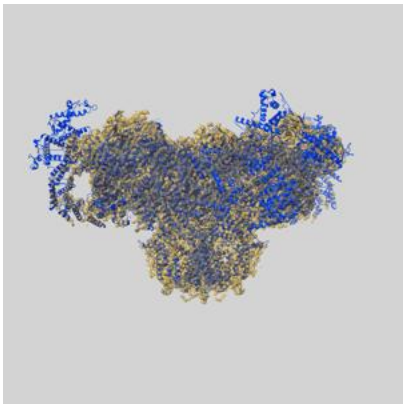
8 Fourier-Shell correlation

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

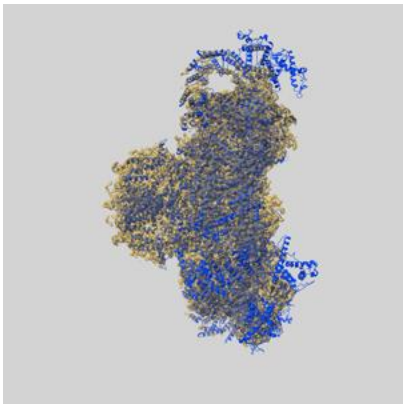
9 Map-model fit

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

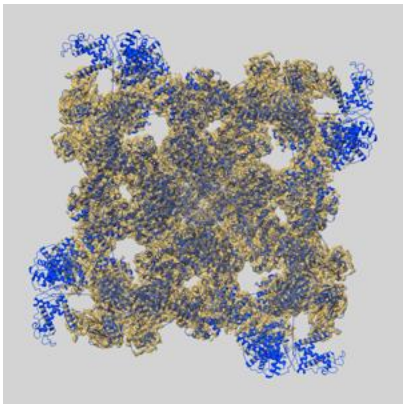
9.1 Map-model overlay



X



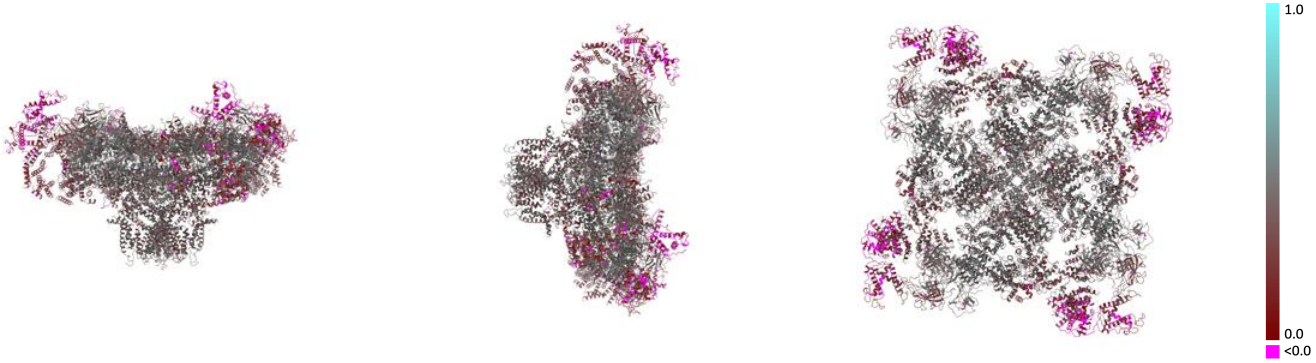
Y



Z

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

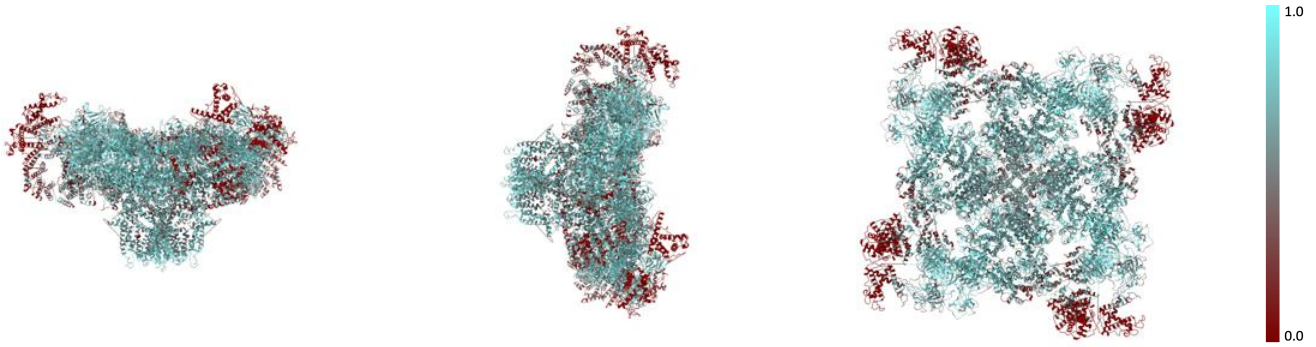
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

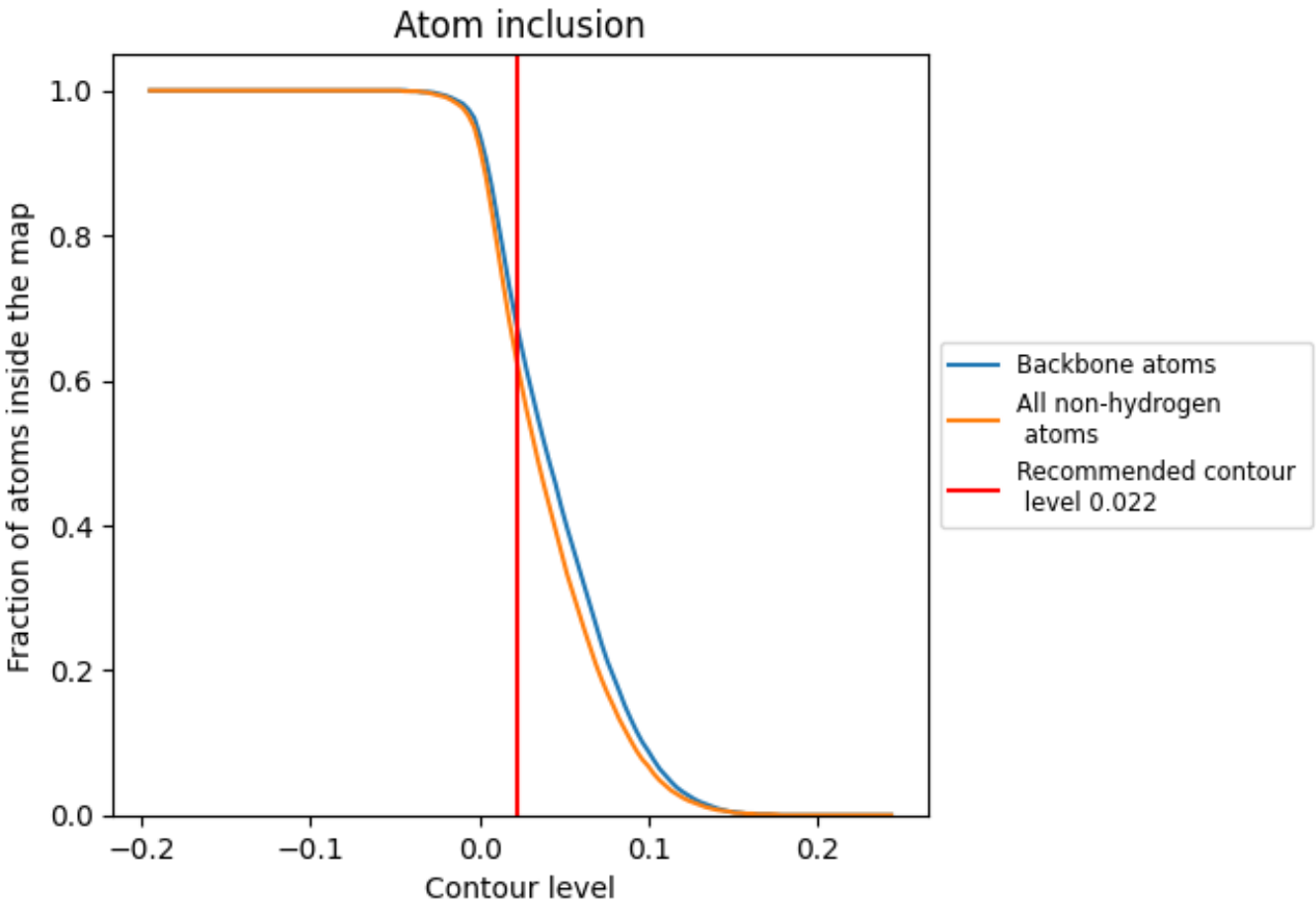
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

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

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