Full wwPDB EM Validation Report

Oct 26, 2026 – 05:36 PM JST

PDB ID	:	26IX / pdb_000026ix
EMDB ID	:	EMD-80692
Title	:	Structure of recombinant RyR2 in complex with Ryanozole in the closed conformation (EGTA dataset, Local refinement of Core domain)
Authors	:	Otori, Y.; Takeuchi, S.; Ogawa, H.
Deposited on	:	2026-05-01
Resolution	:	2.65 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:

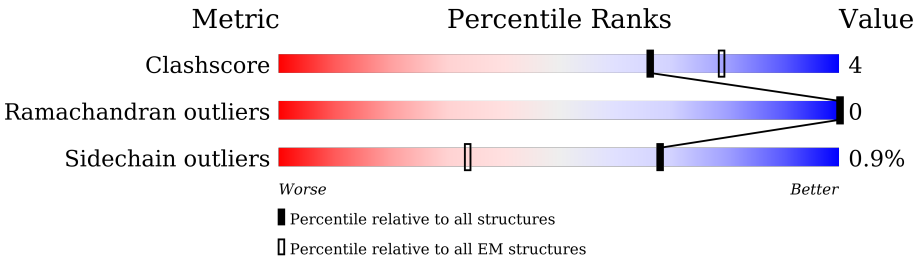
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

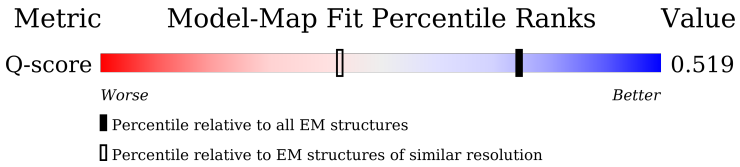
1 Overall quality at a glance

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

The reported resolution of this entry is 2.65 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9050 (2.15 - 3.15)

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	4966	6% 19% 79%
1	B	4966	6% 19% 79%
1	C	4966	6% 19% 79%
1	D	4966	6% 19% 79%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 67428 atoms, of which 33280 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.

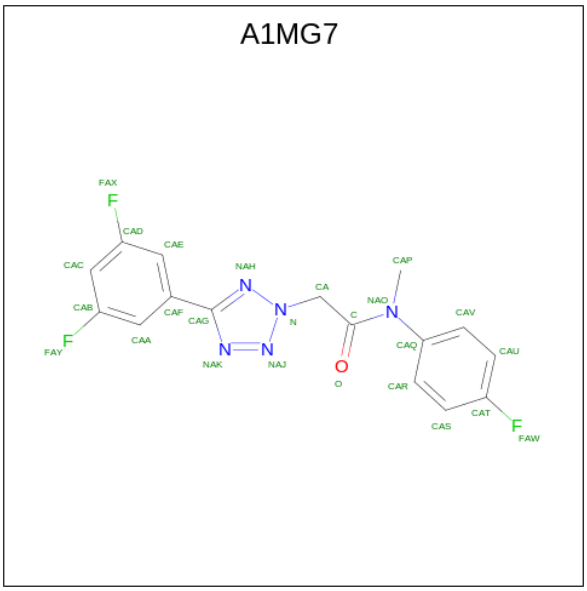
- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1042	Total	C	H	N	O	S	0	0
			16819	5477	8308	1371	1607	56		
1	B	1042	Total	C	H	N	O	S	0	0
			16819	5477	8308	1371	1607	56		
1	C	1042	Total	C	H	N	O	S	0	0
			16819	5477	8308	1371	1607	56		
1	D	1042	Total	C	H	N	O	S	0	0
			16819	5477	8308	1371	1607	56		

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	B	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	

- Molecule 3 is Ryanozole (CCD ID: A1MG7) (formula: $C_{16}H_{12}F_3N_5O$) (labeled as "Ligand of Interest" by depositor).



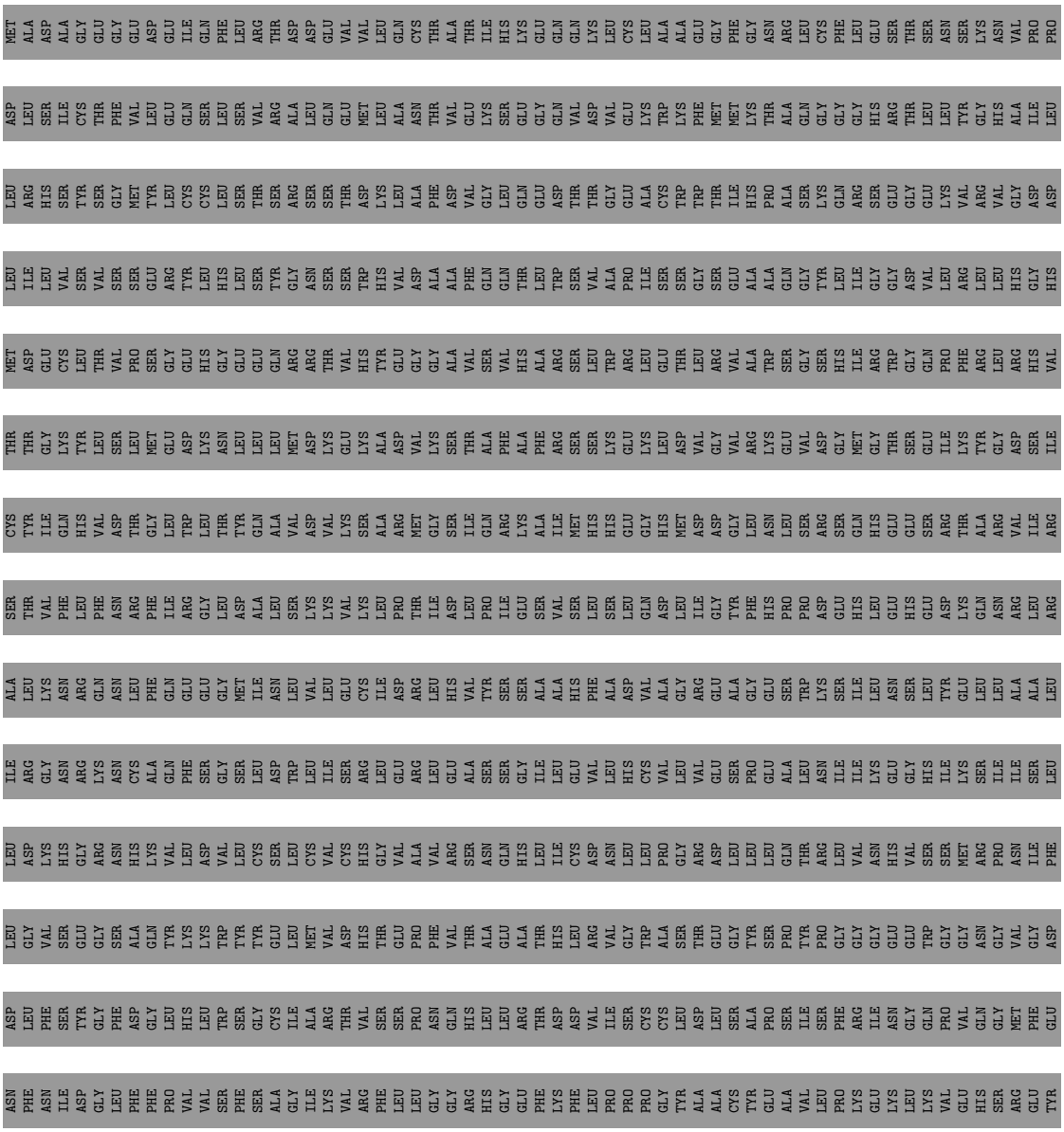
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
3	B	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
3	C	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	
3	D	1	Total	C	F	H	N	O	0
			37	16	3	12	5	1	

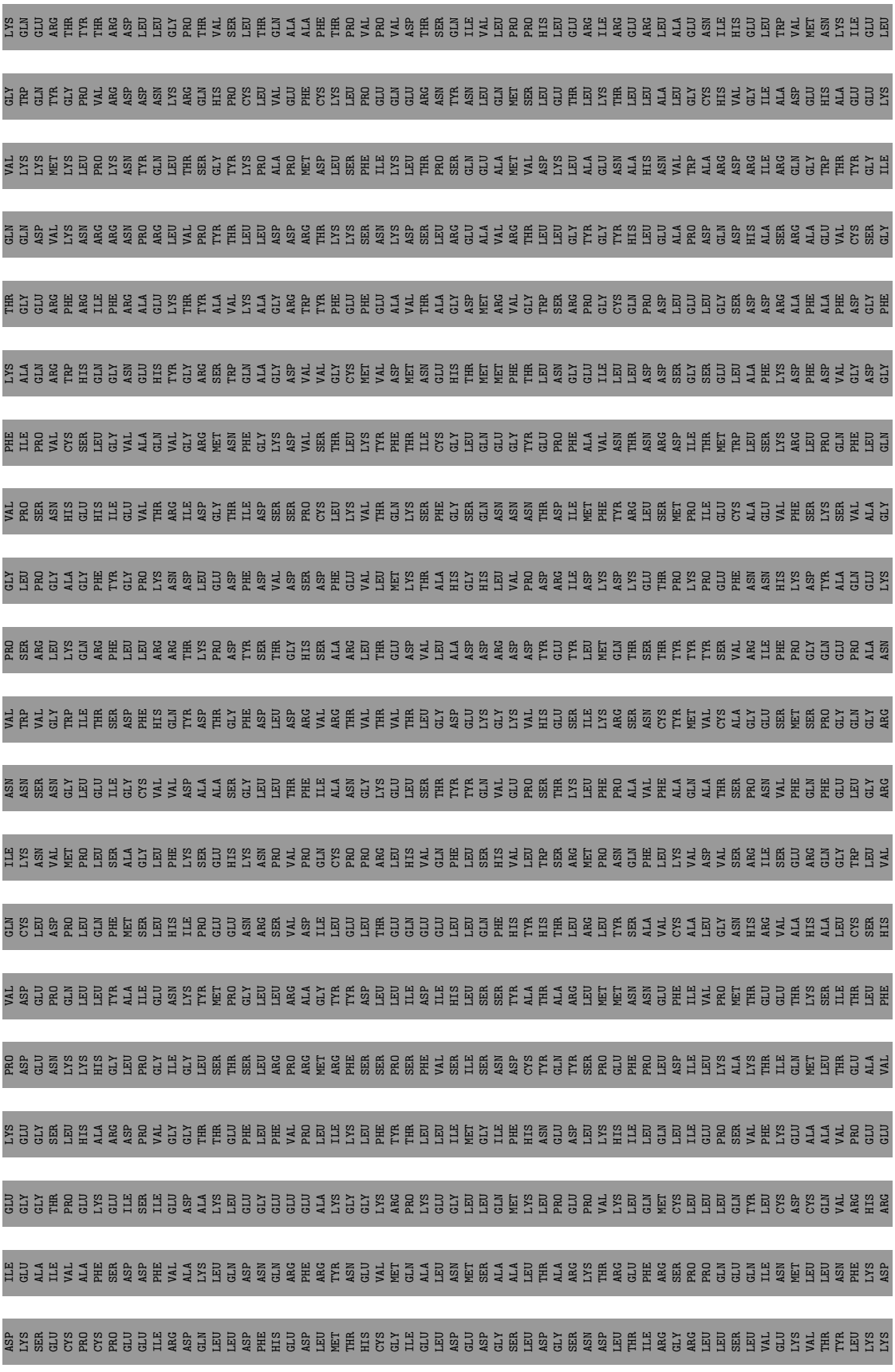
3 Residue-property plots (i)

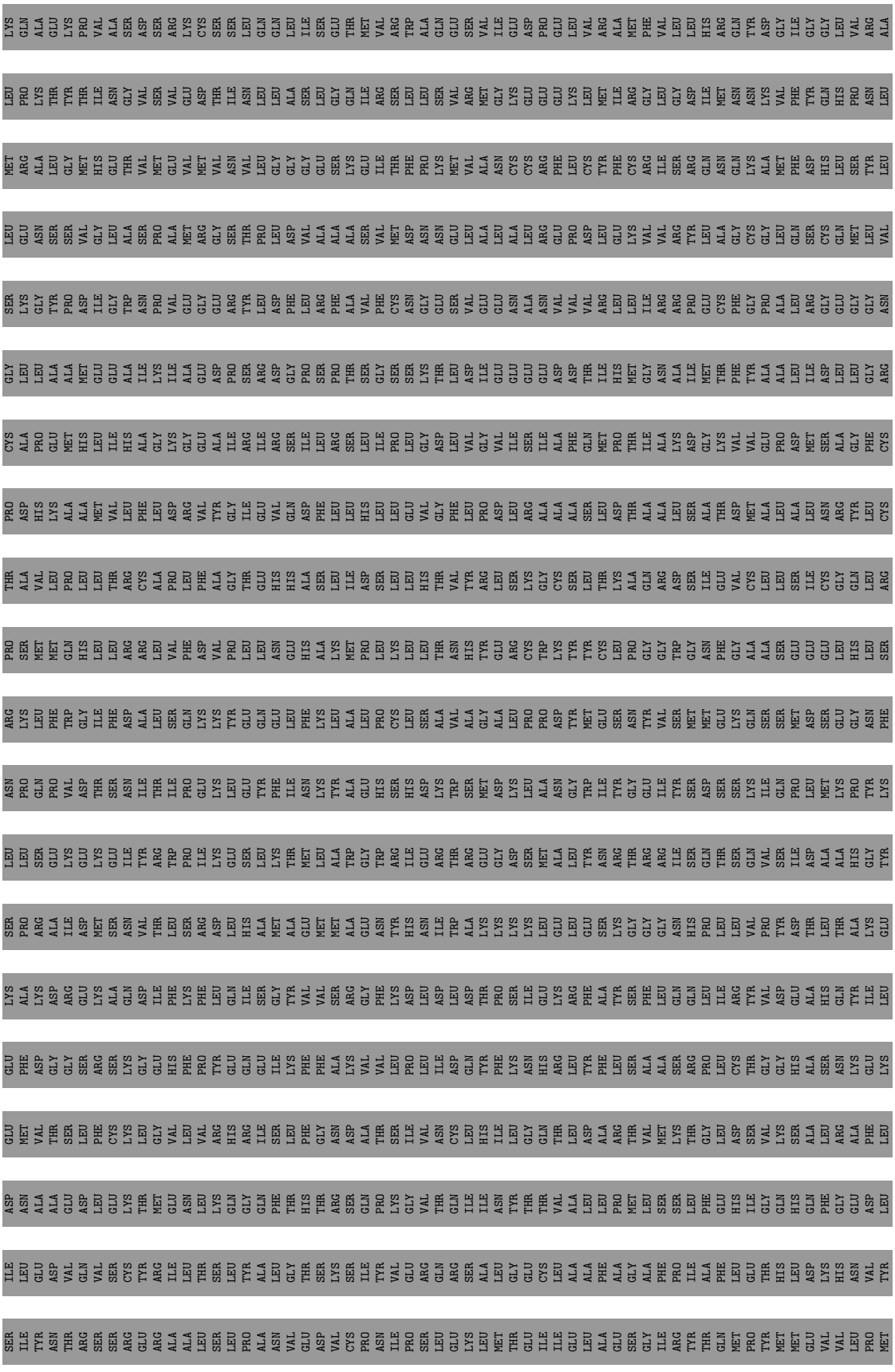
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

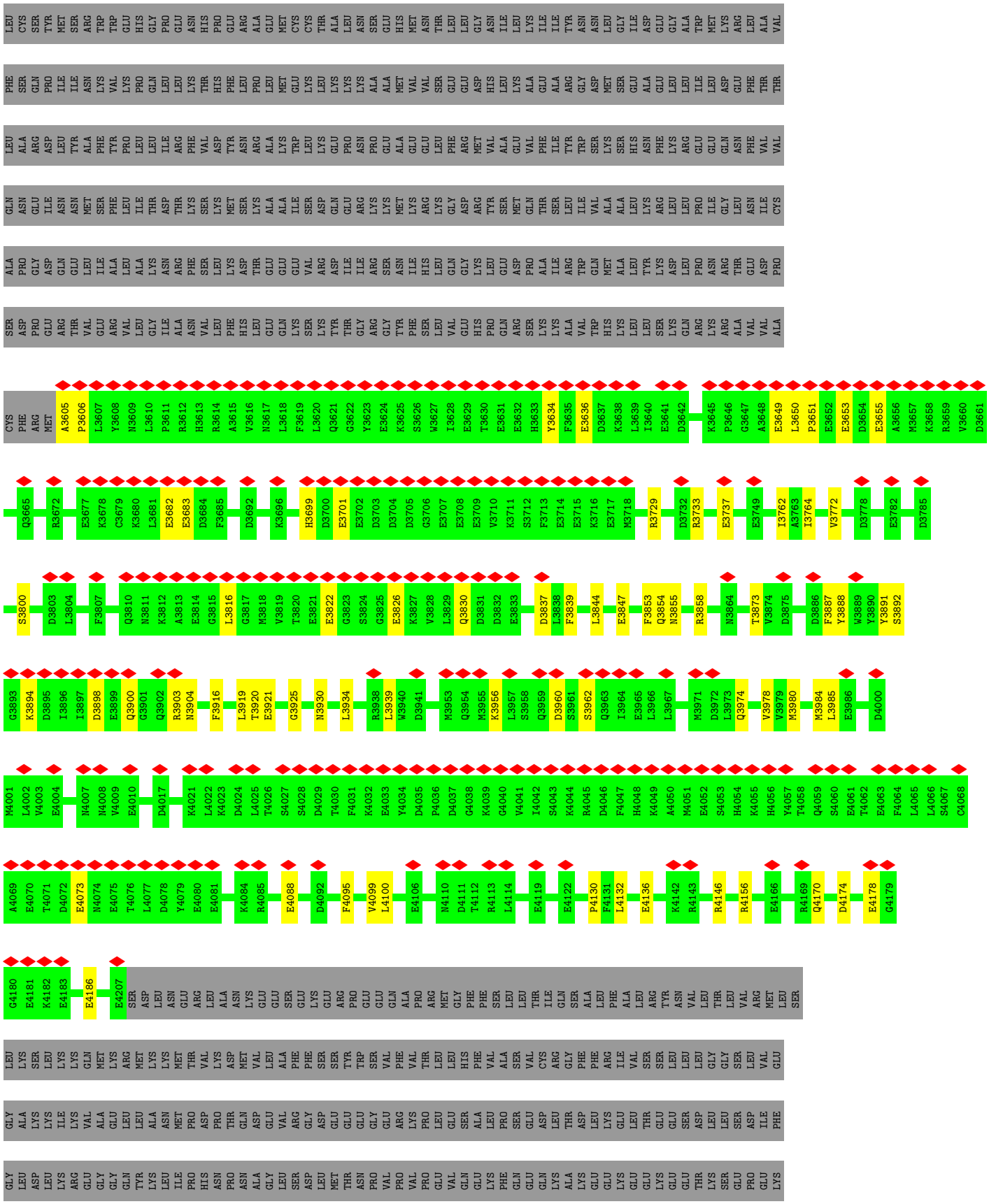
- Molecule 1: Ryanodine receptor 2

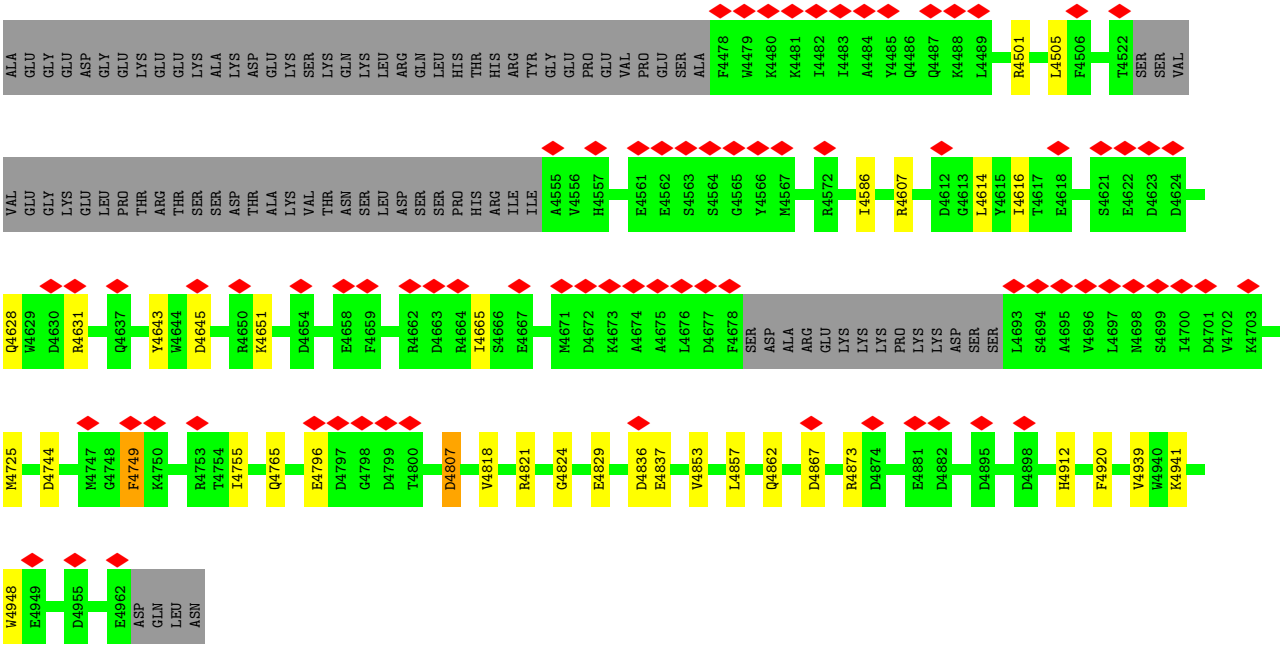





LYS GLN GLU ARG THR TYR THR ARG ASP LEU LEU GLY PRO THR VAL SER LEU THR GLN ALA ALA PHE THR PRO VAL PRO VAL ASP THR SER GLN ILE VAL LEU PRO PRO HIS LEU GLU ARG ILE ARG GLU ARG LEU ALA GLU ASN ILE HIS GLU LEU TRP VAL MET ASN LYS ILE GLU LEU
GLY TRP GLN TYR GLY PRO VAL ARG ASP ASP ASN LYS ARG GLN HIS PRO CYS LEU VAL GLU PHE CYS LYS LEU PRO GLU GLN GLU ARG ASN TYR ASN LEU GLN MET SER LEU GLU THR LEU LYS THR LEU LEU GLY CYS HIS VAL GLY ILE ALA ASP GLU HIS ALA GLU GLU LYS
VAL LYS LYS MET LYS LEU PRO LYS ASN TYR GLN LEU THR SER GLY TYR LYS PRO ALA PRO MET ASP LEU SER PHE ILE LYS LEU THR PRO SER GLN GLU GLN ALA MET VAL ASP LYS LEU ALA GLU ASN ALA HIS ASN VAL TRP ALA ARG ASP ARG ILE ARG GLN GLY TRP THR TYR GLY ILE
GLN GLN ASP VAL LYS ASN ARG ASN PRO ARG LEU VAL PRO TYR THR LEU LEU ASP ARG THR LYS LYS SER ASN LYS ASP SER LEU ARG GLU ALA VAL THR ALA GLY ASP MET ARG VAL GLY TRP SER ARG PRO GLY CYS GLN LEU PRO ASP PRO ASP GLN ASP GLY ASP SER ARG ALA GLU VAL CYS SER GLY
THR GLY GLU ARG PHE ILE PHE ARG ALA GLU LYS THR TYR ALA VAL LYS ALA GLY ARG TRP TYR PHE GLU PHE GLU GLU ALA VAL THR ALA GLY ASP MET ARG VAL GLY TRP SER ARG PRO GLY CYS GLN PRO ASP LEU GLU GLU LEU GLY SER ASP ASP ARG ALA PHE ALA PHE ASP GLY PHE
LYS ALA GLN ARG TRP HIS GLN GLY ASN GLU HIS TYR GLY ARG ASP VAL VAL GLY CYS MET VAL ASP MET MET ASN GLU HIS THR MET MET PHE THR LEU ASN GLY GLU ILE LEU LEU ASP ASP SER GLY SER LEU GLU LEU ALA PHE LYS ASP PHE ASP VAL GLY ASP
PHE ILE PRO VAL CYS SER LEU GLY VAL ALA GLN VAL GLY ARG MET ASN PHE GLY LYS ASP VAL SER THR LEU LYS TYR PHE THR LEU GLN GLU GLY TYR ALA VAL ASN THR ASN ARG ASP ILE THR MET TRP LEU GLN ILE LEU GLU CYS GLY LEU GLN GLU ALA ASP PHE ILE LEU
VAL PRO SER ASN HIS GLU HIS ILE GLU VAL THR ARG ILE ASP GLY THR ILE ASP SER SER PRO CYS LEU LYS VAL THR GLN LYS SER PHE GLY SER GLN ASN ASN ASN THR ASP ILE MET PHE TYR ARG LEU SER MET PRO ILE GLU CYS ALA GLU VAL PHE SER LYS SER VAL ALA GLY
GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU ASP PHE ASP VAL ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS
PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR GLU TYR LEU MET GLN THR SER THR TYR TYR TYR SER VAL ARG ILE PHE PRO GLY GLN GLU PRO ALA ASN
VAL TRP VAL GLY TRP ILE THR SER ASP PHE HIS GLN TYR ASP THR GLY PHE ASP LEU ASP ARG VAL ARG THR VAL THR VAL THR LEU LEU GLY ASP GLU LYS GLY LYS VAL HIS GLU SER ILE LYS ARG SER ASN CYS TYR MET VAL CYS ALA GLY GLU SER MET SER PRO GLY GLN GLY ARG
ASN ASN SER ASN GLY LEU GLU ILE GLY CYS VAL VAL ASP ALA ALA SER GLY LEU LEU THR PHE ILE ALA ASN GLY LYS GLU LEU SER THR SER VAL GLU THR ILE ALA ASN GLN ALA THR SER THR SER PRO ASN VAL PHE GLN PHE GLU LEU GLY LEU GLY ARG
ILE LYS ASN VAL MET PRO LEU SER ALA GLY LEU PHE LYS SER GLU HIS LYS ASN PRO VAL PRO GLN LEU CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER LEU GLN HIS VAL LEU TRP SER ARG MET PRO ASN GLN PHE LEU LYS VAL ASP VAL SER ARG LEU VAL LEU GLY GLN VAL
GLN CYS LEU ASP PRO LEU GLN PHE MET SER LEU HIS ILE PRO GLU GLU ASN ARG SER VAL ASP ILE LEU GLU GLN GLU GLU LEU LEU GLN PHE HIS TYR HIS THR LEU ARG LEU TYR SER ALA VAL CYS ALA LEU GLY ASN HIS ARG VAL ALA HIS ALA LEU CYS SER HIS
VAL ASP GLU PRO GLN LEU LEU ILE GLU ASN LYS TYR MET PRO GLY LEU LEU ARG ALA ALA GLY TYR TYR ASP LEU LEU ILE ASP ILE HIS LEU SER SER HIS TYR ALA THR ALA ARG LEU MET MET ASN ASN GLU PHE ILE VAL PRO MET THR GLU GLU THR LYS ALA HIS ALA LEU ILE THR LEU PHE
PRO ASP GLU ASN LYS HIS GLY PRO GLY ILE GLY LEU SER THR SER LEU ARG PRO ARG MET ARG PHE SER SER SER PRO SER PHE VAL SER ILE SER ASN ASP CYS TYR GLN TYR SER PRO GLU PHE PRO LEU ASP ILE LEU LEU LYS ALA LYS THR LYS HIS GLN PRO LEU LYS ASP
LYS GLU GLY SER LEU HIS ALA ARG PRO VAL GLY GLY THR THR GLU LEU PHE LEU LEU LEU ILE MET GLY ILE PHE HIS ASN GLU ASP LEU LYS HIS ILE LEU GLN LEU ILE GLU PRO GLU ALA ALA VAL PRO GLU GLU
GLU GLY GLY THR PRO GLU ILE SER ILE GLU GLY LYS ARG PRO LYS GLU GLY GLN LEU LEU GLU GLN MET LYS LEU PRO GLU PRO VAL LYS LEU GLN MET CYS LEU LEU LEU GLN GLN TYR GLU LEU CYS ASP CYS GLN VAL HIS ARG
ILE GLU ALA ILE VAL ALA PHE SER ASP ASP PHE VAL ALA LYS LEU GLN ASP ASN GLN ARG PHE ARG TYR ASN GLU VAL MET GLN ALA LEU ASN MET SER ALA LEU THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET ASN LEU LEU ASP LYS
ASP LYS SER GLU CYS PRO CYS HIS CYS GLY ILE GLU LEU ASP GLU GLU ASP PHE HIS GLU ASP GLY SER LEU ASP GLY THR ILE ARG GLY LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS

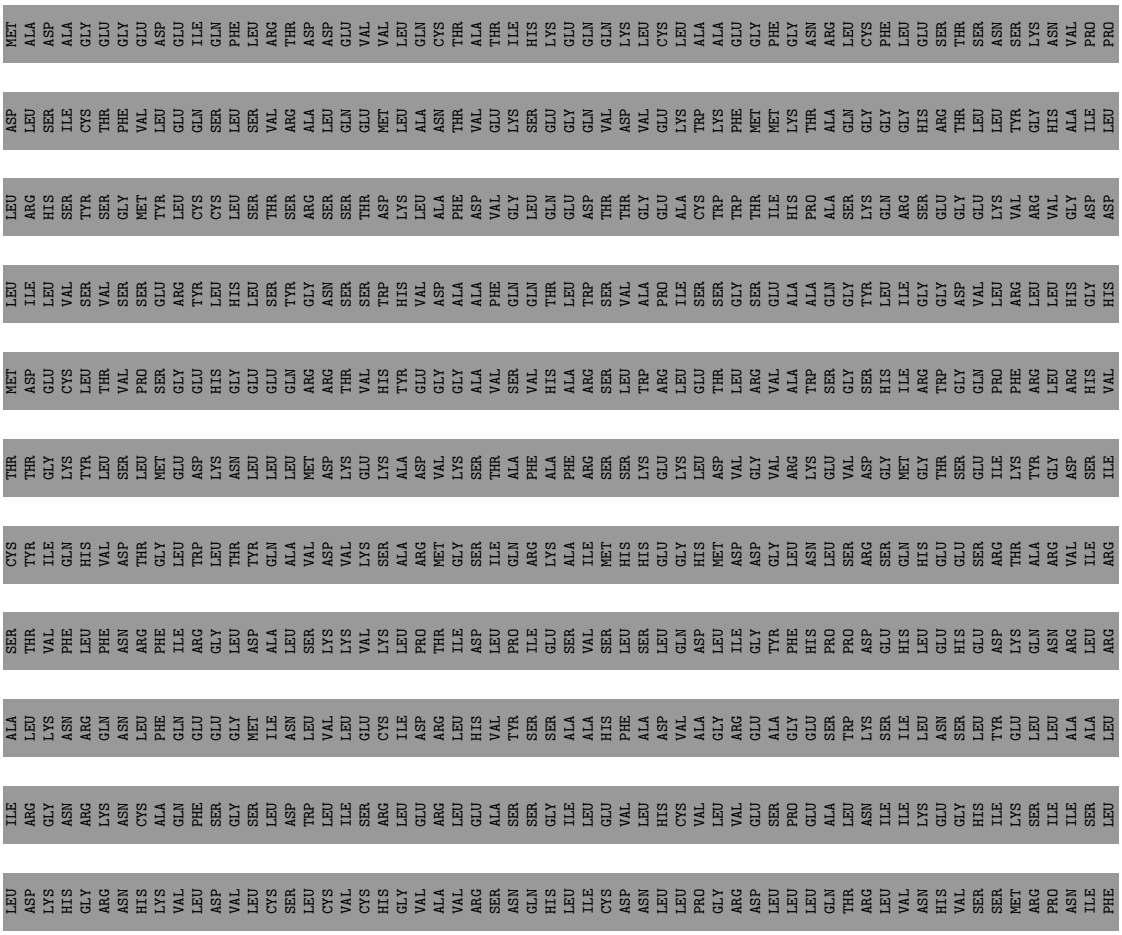


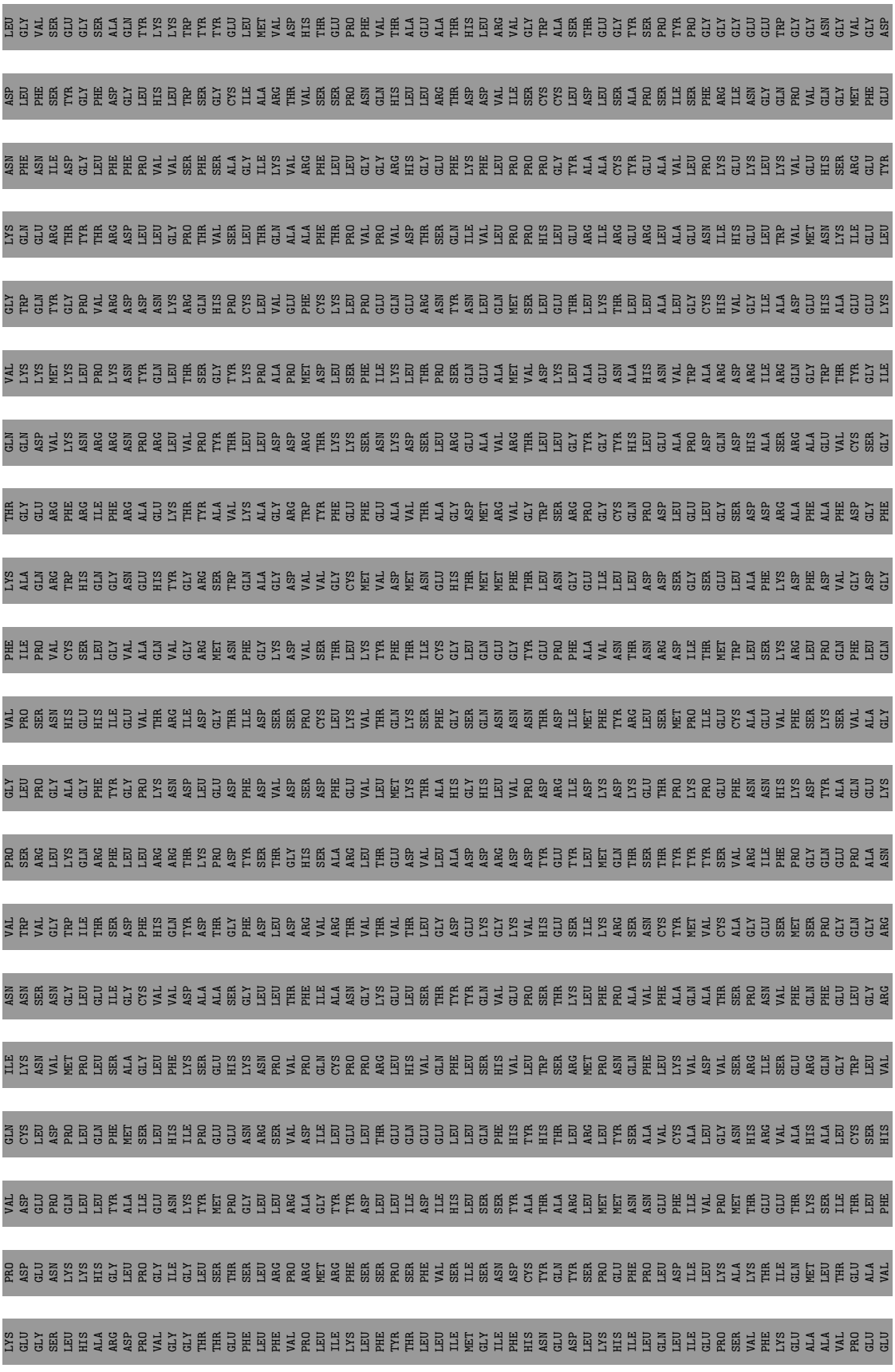

LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN HIS PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL
PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS ALA ALA MET ALA GLU LYS ALA GLU VAL ASP HIS LEU LYS ALA GLU LEU ILE LEU ASP GLU PHE THR THR
LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA ALA LYS TRP LEU LYS GLU ALA LYS LYS ARG GLU ILE ARG PRO ASN PRO GLU ALA MET GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL
GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA ILE SER ASP GLN GLU ARG GLY ASP ARG TYR SER MET GLN THR SER LEU ILE GLY LYS LYS MET LYS ARG LEU LEU PRO ILE GLY LEU ASN ASP PHE LEU ILE CYS
ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA ALA LYS ARG ASP ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU LEU PRO ASN ARG THR GLU ASP PRO
SER ASP PRO GLU ARG THR VAL GLU ARG VAL LEU LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN GLN LYS SER LYS TYR THR GLY ARG GLY TYR PHE SER LEU LEU GLN GLN THR SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA
CYS PHE ARG MET A3605 P3606 L3607 Y3608 N3609 L3610 P3611 R3612 H3613 R3614 A3615 V3616 N3617 L3618 F3619 L3620 Q3621 G3622 Y3623 E3624 K3625 S3626 W3627 I3628 E3629 T3630 E3631 E3632 H3633 Y3634 F3635 E3636 D3637 K3638 L3639 I3640 E3641 D3642 K3645 P3646 G3647 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 V3660 D3661
Q3665 R3672 E3677 K3678 C3679 K3680 L3681 E3682 E3683 D3684 F3685 D3692 K3696 H3699 D3700 E3701 E3702 D3703 D3704 D3705 G3706 E3707 E3708 E3709 V3710 K3711 S3712 F3713 E3714 E3715 K3716 E3717 M3718 R3729 D3732 R3733 E3737 E3749 I3762 A3763 I3764 V3772 D3778 E3782 D3785
S3800 D3803 L3804 F3807 Q3810 N3811 K3812 A3813 E3814 G3815 L3816 G3817 M3818 V3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 K3827 V3828 L3829 Q3830 D3831 D3832 E3833 D3837 L3838 F3839 L3844 E3847 F3853 Q3854 N3855 R3858 N3864 T3873 V3874 D3875 D3886 F3887 Y3888 W3889 Y3890 Y3891 S3892
G3893 K3894 D3895 I3896 I3897 D3898 E3899 Q3900 G3901 Q3902 R3903 N3904 F3916 L3919 T3920 E3921 G3925 N3930 L3934 R3938 L3939 W3940 D3941 M3953 Q3954 M3955 K3956 L3957 S3958 Q3959 D3960 S3961 S3962 Q3963 I3964 E3965 L3966 L3967 M3971 D3972 L3973 Q3974 V3978 Y3979 M3980 M3984 L3985 E3986 D4000
M4001 L4002 V4003 E4004 N4007 N4008 V4009 E4010 D4017 K4021 L4022 K4023 D4024 L4025 T4026 S4027 S4028 D4029 T4030 F4031 K4032 E4033 Y4034 D4035 P4036 D4037 G4038 K4039 G4040 V4041 I4042 S4043 K4044 R4045 D4046 F4047 H4048 K4049 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Y4057 T4058 Q4059 S4060 E4061 T4062 E4063 F4064 L4065 L4066 S4067 C4068
A4069 E4070 T4071 D4072 E4073 N4074 E4075 T4076 L4077 D4078 Y4079 E4080 E4081 K4084 R4085 E4088 D4092 F4095 V4099 L4100 E4106 N4110 D4111 T4112 R4113 L4114 E4119 E4122 P4130 F4131 L4132 E4136 K4142 R4143 R4146 R4156 E4166 R4169 Q4170 D4174 E4178 G4179
G4180 E4181 K4182 E4183 E4186 E4207 SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER
LEU LYS SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE VAL ALA SER VAL CYS ARG GLY PHE PHE ARG ILE VAL SER SER LEU LEU GLY GLY SER LEU VAL GLU
GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP ASP GLU VAL ARG GLY ASP GLU GLU TYR GLU GLU ARG LYS PRO LEU GLU GLU SER ALA LEU LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU LEU SER ASP ILE PHE
GLY LEU ASP LEU LYS ARG GLU GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET THR ASN PRO VAL PRO VAL PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU LYS GLU GLU THR LYS SER GLU PRO GLU LYS

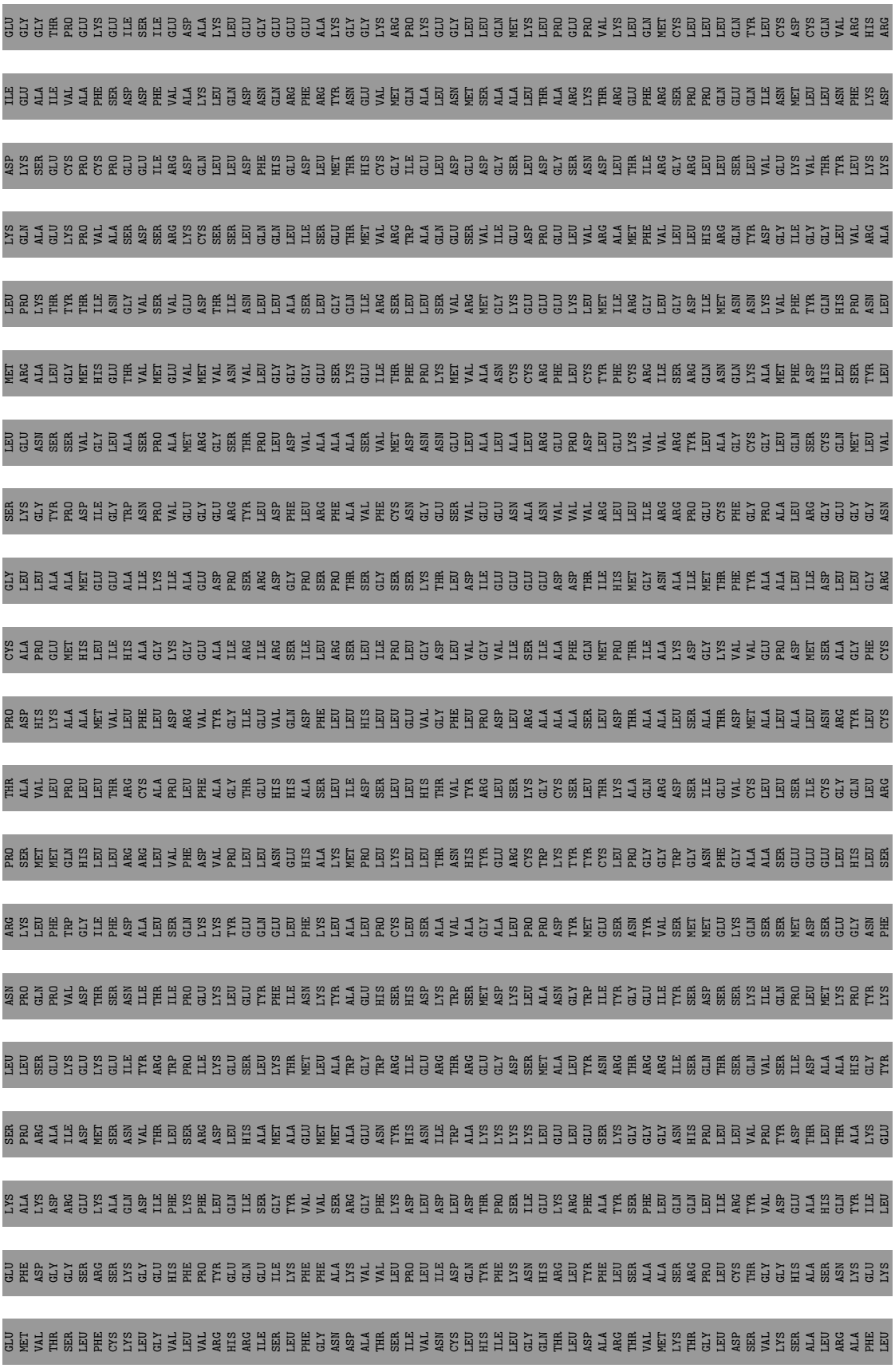


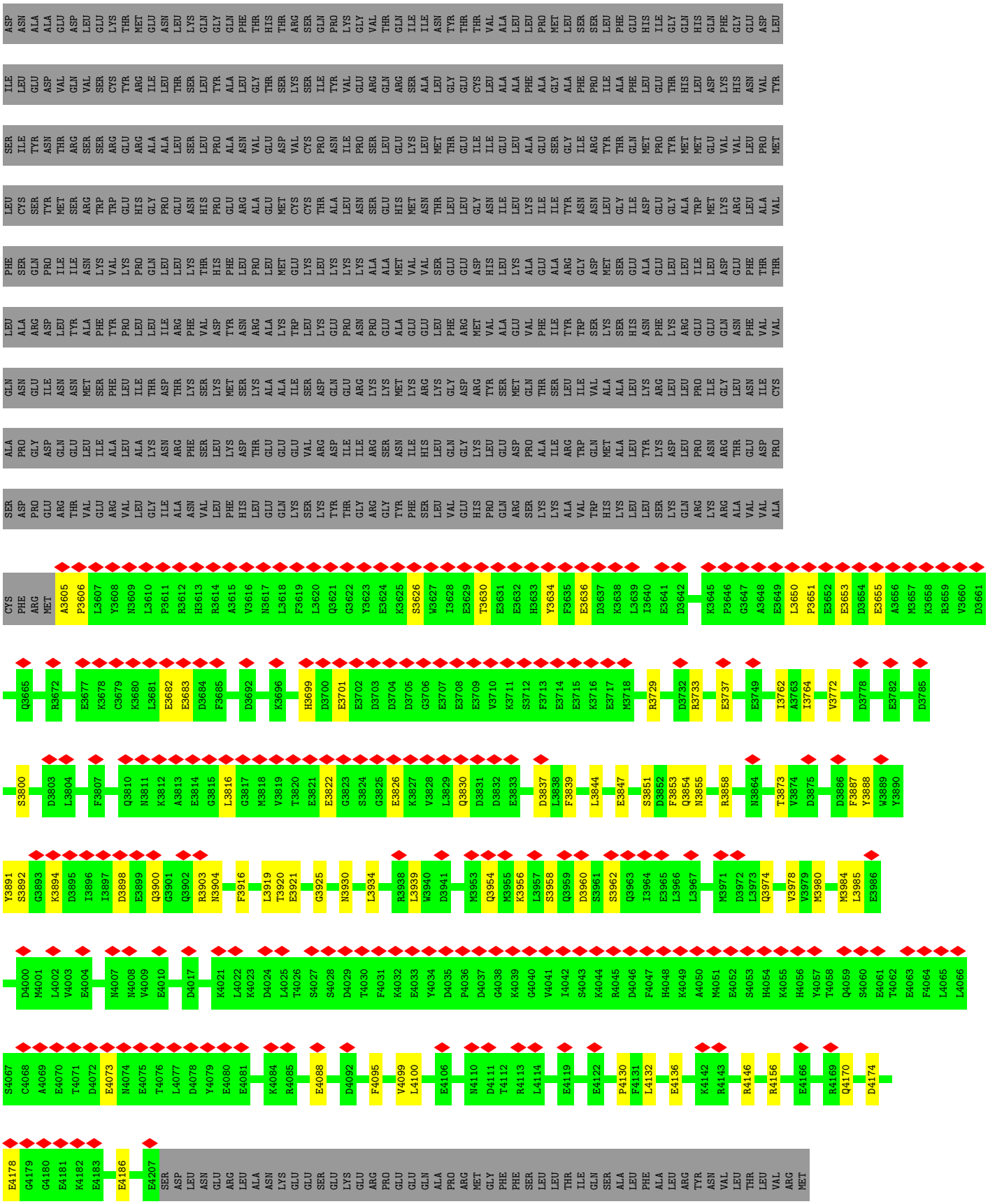
• Molecule 1: Ryanodine receptor 2

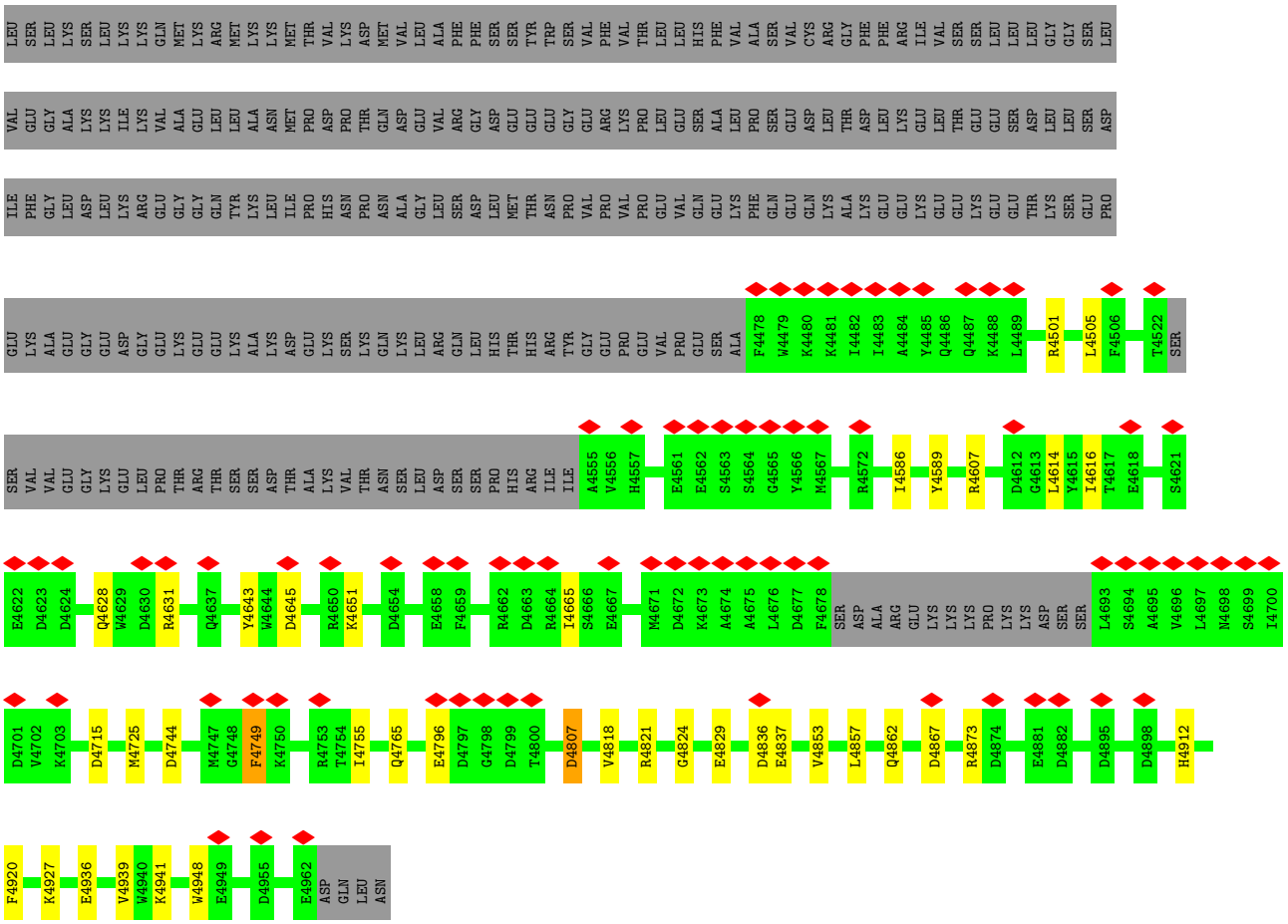
Chain B: 6% 19% 79%




LEU GLY VAL SER GLU GLY SER ALA GLN TYR LYS LYS TRP TYR TYR GLU LEU MET VAL ASP HIS THR GLU PRO PHE VAL THR ALA GLU ALA THR HIS LEU ARG VAL GLY TRP ALA SER THR GLU GLY TYR SER PRO TYR PRO GLY GLY GLY GLU GLU TRP GLY GLY ASN GLY VAL GLY ASP
ASP LEU PHE SER TYR GLY PHE ASP GLY LEU HIS LEU TRP SER GLY CYS ILE ALA ARG THR VAL SER SER PRO ASN GLN HIS LEU LEU ARG THR ASP ASP VAL ILE SER CYS CYS LEU ASP LEU SER ALA PRO SER ILE SER PHE ARG ILE ASN GLY GLN PRO VAL GLN GLY MET PHE GLU
ASN PHE ASN ILE ASP GLY LEU PHE PHE PRO VAL VAL SER PHE SER ALA GLY ILE LYS VAL ARG PHE LEU LEU GLY GLY ARG HIS GLY GLU PHE LYS PHE LEU PRO PRO GLY TYR ALA ALA CYS TYR GLU ALA VAL LEU PRO LYS GLU LYS LEU LYS VAL GLU HIS SER GLN GLY MET GLU TYR
LYS GLN GLU ARG THR TYR THR ARG ASP LEU LEU GLY PRO THR VAL SER LEU THR GLN ALA ALA PHE THR PRO VAL PRO GLY ASP LEU THR SER GLN ILE VAL LEU PRO PRO HIS LEU GLU GLN ARG ILE ARG GLU ARG LEU ALA GLU ASN ILE HIS GLU LEU TRP VAL MET ASN LYS ILE GLU GLU LEU
GLY TRP GLN TYR GLY PRO VAL ARG ASP ASP LEU ASN LYS ARG GLN HIS PRO CYS LEU VAL GLU PHE CYS LYS LEU PRO GLU GLN GLU ARG ASN TYR ASN LEU GLN MET SER LEU GLU THR LEU LYS THR LEU LEU ALA GLY CYS HIS VAL GLY ILE ALA ASP GLU HIS ALA GLU GLU LYS
VAL LYS LYS MET LYS LEU PRO LYS ASN TYR GLN LEU THR SER GLY TYR LYS PRO ALA PRO MET ASP LEU SER PHE ILE LYS LEU THR PRO SER GLN GLU MET VAL ASP LYS LEU ALA GLU ASN ALA HIS ASN VAL TRP ALA ARG ASP ARG ILE ARG GLN GLY TRP THR TYR GLY ILE
GLN GLN ASP VAL LYS ASN ARG ARG ASN PRO ARG LEU VAL PRO TYR THR LEU LEU ASP ASP ARG THR LYS LYS SER ASN LYS ASP SER LEU ARG GLU ALA VAL THR ALA GLY ASP MET THR LEU LEU GLY TYR GLY TYR HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY
THR GLY GLU ARG PHE ARG ILE PHE ARG ALA GLU LYS THR TYR ALA VAL LYS ALA GLY ARG TRP TYR PHE GLU PHE GLU ALA VAL THR ALA GLY ASP MET ARG VAL GLY TRP SER ARG PRO GLY CYS GLN PRO ASP LEU GLU LEU GLY SER ASP ASP ARG ALA PHE ALA GLU PHE ASP GLY GLY PHE
LYS ALA GLN ARG TRP HIS GLN GLY ASN GLU HIS TYR GLY ARG SER TRP GLN ALA GLY ASP VAL VAL GLY CYS MET VAL ASP MET ASN GLU HIS THR MET MET PHE THR LEU ASN GLY GLU ILE LEU LEU ASP ASP SER GLY SER GLU LEU ALA PHE LYS ASP PHE ASP VAL GLY ASP GLY
PHE ILE PRO VAL CYS SER LEU GLY VAL ALA GLN VAL GLY ARG MET ASN PHE GLY LYS ASP ASP VAL SER THR LEU LYS TYR PHE THR ILE CYS GLY LEU GLN GLU GLY TYR GLU PRO PHE ALA VAL ASN THR ASN ARG ASP ILE THR MET PHE TYR ARG LEU SER MET PRO ILE GLU CYS ALA GLU VAL PHE SER LYS SER VAL ALA GLY
VAL PRO SER ASN HIS GLU HIS ILE GLU VAL THR ARG ILE ASP GLY THR ILE ASP SER SER PRO CYS LEU LYS VAL THR GLN LYS SER PHE GLY SER GLN ASN ASN THR ASP ILE MET PHE TYR ARG LEU SER MET PRO ILE GLU GLU VAL ASP ASP ARG ILE ASP ASP ASP ARG ASP ASP
GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU GLU GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU GLU THR PRO LYS PRO GLU GLU CYS PHE ASN HIS LYS ASP SER LYS VAL ALA GLN GLU LYS
PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP TYR GLU TYR LEU MET GLN THR SER THR TYR TYR TYR SER VAL ARG LEU SER ASN PRO ILE PHE ASN ASN GLY
VAL TRP VAL GLY TRP ILE THR SER ASP PHE HIS GLN TYR ASP THR ARG VAL ARG THR VAL THR VAL THR LEU GLY ASP GLU LYS GLY LYS VAL HIS GLU SER ILE LYS SER ASN CYS TYR MET VAL CYS ALA GLY GLU SER MET SER PRO GLY GLN GLN ARG
ASN ASN SER ASN GLY CYS VAL VAL GLU GLU ILE GLY LEU LEU THR PHE ILE ALA ASN GLY LYS GLU LEU SER THR TYR GLN VAL GLU PRO SER THR LYS LEU PHE PRO ALA VAL PHE ALA GLN THR SER ALA PHE PRO ASN ASN VAL PHE GLN PHE GLU LEU GLY ARG
ILE LYS ASN VAL MET PRO LEU GLY CYS ALA PRO ARG LEU HIS VAL VAL GLN PHE LEU SER HIS VAL LEU TRP SER ARG MET PRO ASN GLN PHE LEU LYS VAL ASP VAL SER GLU ARG GLN GLY TRP LEU VAL
GLN CYS LEU ASP PRO LEU GLN PHE MET SER LEU HIS ILE PRO GLU GLU ASN ARG SER VAL ASP ILE LEU GLU LEU THR GLU GLN GLU GLU LEU LEU GLN PHE HIS TYR HIS THR LEU ARG LEU TYR SER ALA VAL CYS ALA LEU GLY ASN HIS ARG VAL ALA HIS ALA LEU CYS SER HIS
VAL ASP GLU PRO GLN LEU TYR ALA ILE GLU ASN LYS TYR MET PRO GLY LEU LEU ARG ALA GLY TYR TYR ASP LEU LEU ILE ASP ILE HIS LEU SER SER TYR ALA THR ALA ARG LEU MET MET ASN GLU PHE ILE VAL PRO MET THR GLU GLU THR LYS ALA LEU PHE
PRO ASP GLU ASN LYS HIS PHE SER SER PRO SER PHE VAL SER ILE SER ASN ASP CYS TYR GLN PHE PRO LEU ASP ILE LEU LYS GLU LYS
LYS GLU GLY SER LEU HIS ALA ARG ASP PRO VAL GLU PHE LEU PHE TYR THR THR LEU LEU ILE MET GLY ILE PHE HIS ASN GLU ASP LEU LYS HIS ILE LEU GLN LEU ILE GLU PRO SER VAL PHE LYS GLU ALA VAL PRO GLU GLU


GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU ASP ALA LYS LEU GLU GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS GLU GLY GLN LEU LEU GLN MET LYS LEU PRO GLU PRO VAL LYS LEU GLN MET CYS LEU LEU LEU LEU GLN TYR LEU CYS ASP CYS GLN VAL ARG HIS ARG
ILE GLU ALA ILE VAL ALA PHE SER ASP ASP PHE VAL ALA LYS LEU GLN ASP ASN GLN ARG PHE ARG TYR ASN GLU VAL MET GLN ALA LEU ASN MET SER ALA ALA LEU THR ALA ARG LYS THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASP SER LEU GLU ASP ALA ARG GLY LEU LEU ASP GLU GLU LEU ASN ASN MET LEU LEU ASN PHE LYS ASP
ASP LYS SER GLU CYS PRO CYS PRO GLU GLU ILE ARG ASP GLN LEU LEU ASP PHE HIS GLU ASP GLY MET HIS CYS GLY ILE GLU LEU ASP GLU SER LEU ASP GLY GLU LYS VAL THR TYR LEU LYS LYS
LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER SER LEU GLN GLU ASP ILE GLU GLU ASP PRO GLU LEU VAL ARG ALA MET PHE VAL LEU LEU HIS ARG GLN TYR ASP GLY ILE GLY LEU VAL ARG ALA
LEU PRO LYS THR TYR THR ILE ASN GLY VAL SER VAL GLU ASP THR ILE ASN LEU LEU ALA ALA SER LEU GLY GLN ILE ARG SER LEU LEU SER VAL ARG MET GLY LYS GLU GLU GLU LYS LEU MET ILE ARG GLY LEU GLY ASP ILE MET ASN ASN GLN LYS ALA MET PHE TYR GLN HIS PRO ASN LEU
MET ARG ALA LEU GLY MET HIS GLU THR VAL MET GLU VAL MET VAL ASN VAL LEU GLY GLY GLU SER LYS GLU ILE THR PHE PRO LYS MET VAL ALA ASN ASN CYS CYS ARG PHE LEU CYS TYR PHE CYS ARG ILE SER ARG GLN ASN GLN LYS ALA MET PHE LEU LEU VAL
LEU GLU ASN SER SER VAL GLY LEU ALA SER ALA ALA ALA SER VAL MET ASP ASN ASN GLU LEU LEU ALA LEU ARG GLU PRO ASP LEU GLU LYS VAL VAL ARG TYR LEU ALA GLY CYS GLY LEU GLN SER CYS GLN MET LEU VAL
SER LYS GLY TYR PRO ASP ILE GLY TRP ASN PRO VAL GLU GLY GLY GLU ARG TYR LEU ASP PHE ALA VAL PHE CYS ASN GLY GLU SER VAL GLU GLU ASN ALA ASN VAL VAL VAL ARG LEU LEU ILE ARG ARG PRO GLU CYS PHE GLY PRO ALA LEU GLN ARG GLY GLU GLY GLY ASN
GLY LEU LEU ALA ALA MET GLU GLU GLY ALA ILE LYS ILE ALA GLU ASP PRO SER PRO THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS MET GLY ASN ALA ILE MET THR PHE TYR ALA ALA LEU ILE ASP LEU LEU GLY ARG
CYS ALA PRO GLU MET HIS LEU ILE HIS ALA GLY LYS GLY GLU ALA ILE ARG ILE ARG SER LEU ILE PRO LEU GLY ASP LEU VAL GLY VAL ILE SER ILE ALA PHE GLN MET PRO THR ILE ALA LYS ASP GLY LYS VAL VAL GLU PRO ASP MET SER ALA GLY PHE CYS
PRO ASP HIS LYS ALA ALA MET VAL LEU PHE LEU GLU ASP ARG VAL TYR GLY ILE GLU VAL GLN ASP PHE LEU LEU HIS LEU LEU GLU VAL GLY PHE LEU PRO ASP LEU ARG ALA ALA SER LEU ASP THR ALA ILE ALA LEU SER ALA THR ASP MET ALA LEU LEU ASN ARG TYR LEU CYS
THR ALA VAL LEU PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU ILE ASP SER LEU LEU HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS VAL GLY GLN LEU LEU ARG
PRO SER MET MET GLN HIS LEU LEU ARG ARG LEU VAL PRO LEU LEU ASN GLU HIS ALA LYS MET PRO LEU LYS LEU LEU THR ASN HIS TYR GLU ARG CYS LEU PRO GLY GLY TRP GLY ASN PHE GLY ALA ALA GLU SER LEU HIS LEU SER
ARG LYS LEU PHE TRP ASP ALA LEU ALA LEU ALA LEU PRO CYS LEU SER ALA VAL ALA GLY ASP ALA LEU PRO PRO ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY ASN PHE
ASN PRO GLN PRO VAL ASP THR SER ASN ILE THR ILE PRO GLU LYS LEU GLU TYR PHE ILE ASN LYS TYR ALA GLU HIS SER HIS ASP LYS TRP SER MET ASP LYS LEU ALA ASN GLY TRP ILE TYR GLY GLU ILE TYR SER ASP SER SER LYS ILE GLN PRO LEU MET LYS PRO TYR LYS
LEU LEU SER GLU LYS GLU LYS ILE TYR ARG TRP PRO ILE LYS GLU SER LEU LYS THR MET LEU ALA ALA TRP GLY TRP ARG ILE GLU GLU ARG THR ARG GLU ILE GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE GLU SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY TYR
SER PRO ARG ALA ILE ASP MET SER MET VAL ASN ILE LEU ASN GLU ASN TYR HIS ASN ILE TRP ALA LYS LYS LYS LYS LEU GLU GLU SER LYS GLY GLY ASN HIS PRO LEU LEU LEU VAL PRO TYR ASP THR LEU THR ALA LYS GLU
LYS ALA LYS ASP ARG GLU ARG ILE LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LYS ASP LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU
GLU PHE ASP GLY SER LYS GLY VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU CYS THR GLY HIS ALA SER ASN LYS GLU LYS
GLU MET VAL THR SER LEU PHE CYS LYS LEU GLY VAL ASN ASP ALA ALA THR SER ILE VAL ASN CYS LEU HIS ILE LEU GLY GLN THR LEU ASP ALA ARG THR VAL MET LYS THR GLY LEU ASP SER VAL LYS SER ALA LEU ARG ALA PHE LEU

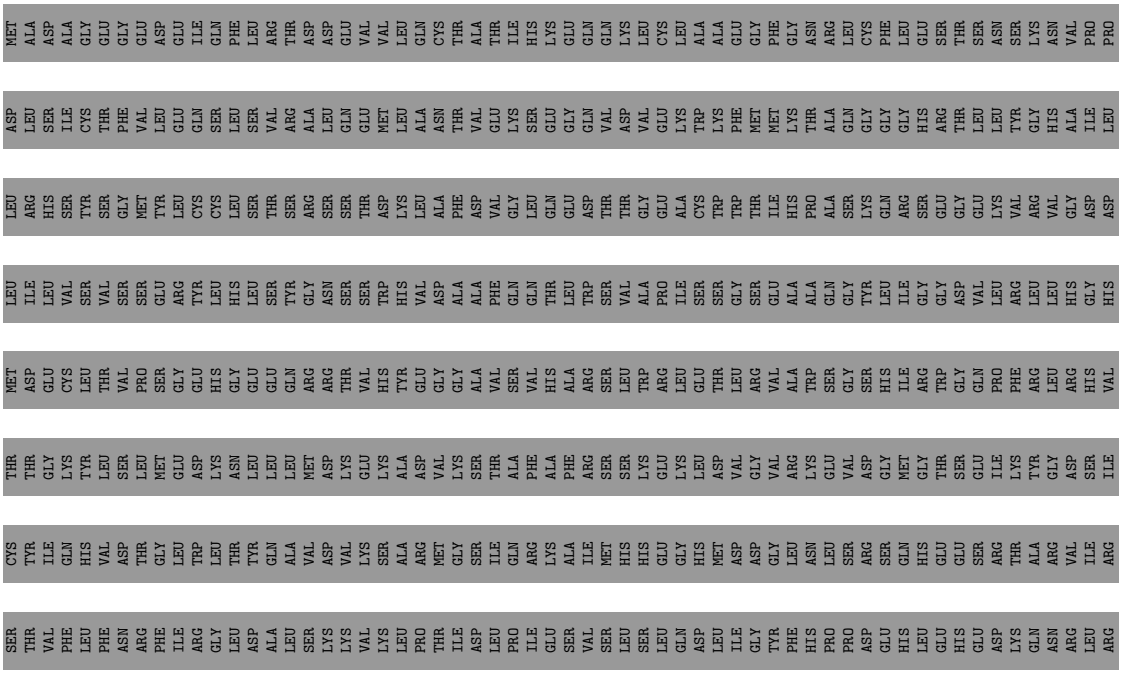

ASP ASN ALA ALA GLU ASP LEU GLU GLY THR MET GLU ASN LEU LYS GLN GLY GLN PHE THR HIS THR ARG SER GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR THR THR VAL ALA LEU LEU PRO MET LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU
ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR SER LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA PHE GLY ALA PHE PRO ILE ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN VAL TYR
SER ILE TYR ASN THR ARG GLU ARG ALA ALA LEU SER LEU PRO ALA ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU GLU LYS LEU MET THR GLU ILE ILE GLU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO TYR MET MET GLU VAL VAL LEU PRO MET
LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU GLY ASN HIS PRO GLU ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL
PHE SER GLN PRO ILE ILE ASN LYS VAL LYS LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU GLU ASP HIS LEU LYS ALA GLU VAL PHE ILE TYR TRP SER LYS SER MET GLN THR SER LEU ILE LEU ASP GLU ALA GLU ALA LEU
LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA ALA LYS TRP LEU LYS GLU GLU PRO ASN PRO GLU ALA GLU GLU GLU LEU PHE ARG MET VAL VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS LYS LEU LEU SER LEU ILE ARG GLY ASP MET SER GLU ALA GLU LEU LYS ARG GLU GLU GLN ASN PHE VAL VAL
GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA ILE SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS
ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ASP LYS ASN ARG PHE SER LEU LYS ASP THR GLU GLU GLU VAL ARG ASP ILE ILE ARG SER ASN ILE LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA ALA LEU TYR LYS ASP LEU PRO LEU ASN ARG THR GLU ASP PRO
SER ASP PRO GLU ARG THR VAL GLU ARG VAL LEU LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER LYS TYR THR GLY ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA
CYS PHE ARG MET A3605 P3606 L3607 Y3608 N3609 L3610 P3611 R3612 H3613 R3614 A3615 V3616 N3617 L3618 F3619 L3620 Q3621 G3622 Y3623 E3624 K3625 S3626 W3627 I3628 E3629 T3630 E3631 E3632 H3633 Y3634 F3635 E3636 D3637 K3638 L3639 I3640 E3641 D3642 K3645 P3646 G3647 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 V3660 D3661
Q3665 R3672 E3677 K3678 C3679 K3680 L3681 E3682 E3683 D3684 F3685 D3692 K3696 H3699 D3700 E3701 E3702 D3703 D3704 D3705 G3706 E3707 E3708 E3709 V3710 K3711 S3712 F3713 E3714 E3715 K3716 E3717 M3718 R3729 D3732 R3733 E3737 E3749 I3762 A3763 I3764 V3772 D3778 E3782 D3785
S3800 D3803 L3804 F3807 Q3810 N3811 K3812 A3813 E3814 G3815 L3816 G3817 M3818 V3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 K3827 V3828 L3829 Q3830 D3831 D3832 E3833 D3837 L3838 F3839 L3844 E3847 S3851 D3852 F3853 Q3854 N3855 R3858 N3864 T3873 V3874 D3875 D3886 F3887 Y3888 W3889 Y3890
Y3891 S3892 G3893 K3894 D3895 I3896 I3897 D3898 E3899 Q3900 G3901 Q3902 R3903 N3904 F3916 L3919 T3920 E3921 G3925 N3930 L3934 R3938 L3939 W3940 D3941 M3953 Q3954 M3955 K3956 L3957 S3958 Q3959 D3960 S3961 S3962 Q3963 I3964 E3965 L3966 L3967 M3971 D3972 L3973 Q3974 V3978 V3979 M3980 M3984 L3985 E3986
D4000 M4001 L4002 V4003 E4004 N4007 N4008 V4009 E4010 D4017 K4021 L4022 K4023 D4024 L4025 T4026 S4027 S4028 D4029 T4030 F4031 K4032 E4033 Y4034 D4035 P4036 D4037 G4038 K4039 G4040 V4041 I4042 S4043 K4044 R4045 D4046 F4047 H4048 K4049 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Y4057 T4058 Q4059 S4060 E4061 T4062 E4063 F4064 L4065 L4066
S4067 C4068 A4069 E4070 T4071 D4072 E4073 N4074 E4075 T4076 L4077 D4078 Y4079 E4080 E4081 K4084 R4085 E4088 D4092 F4095 V4099 L4100 E4106 N4110 D4111 T4112 R4113 L4114 E4119 E4122 P4130 F4131 L4132 E4136 K4142 R4143 R4146 R4156 E4166 R4169 Q4170 D4174
E4178 G4179 G4180 E4181 K4182 E4183 E4186 E4207 SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LEU LYS GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET

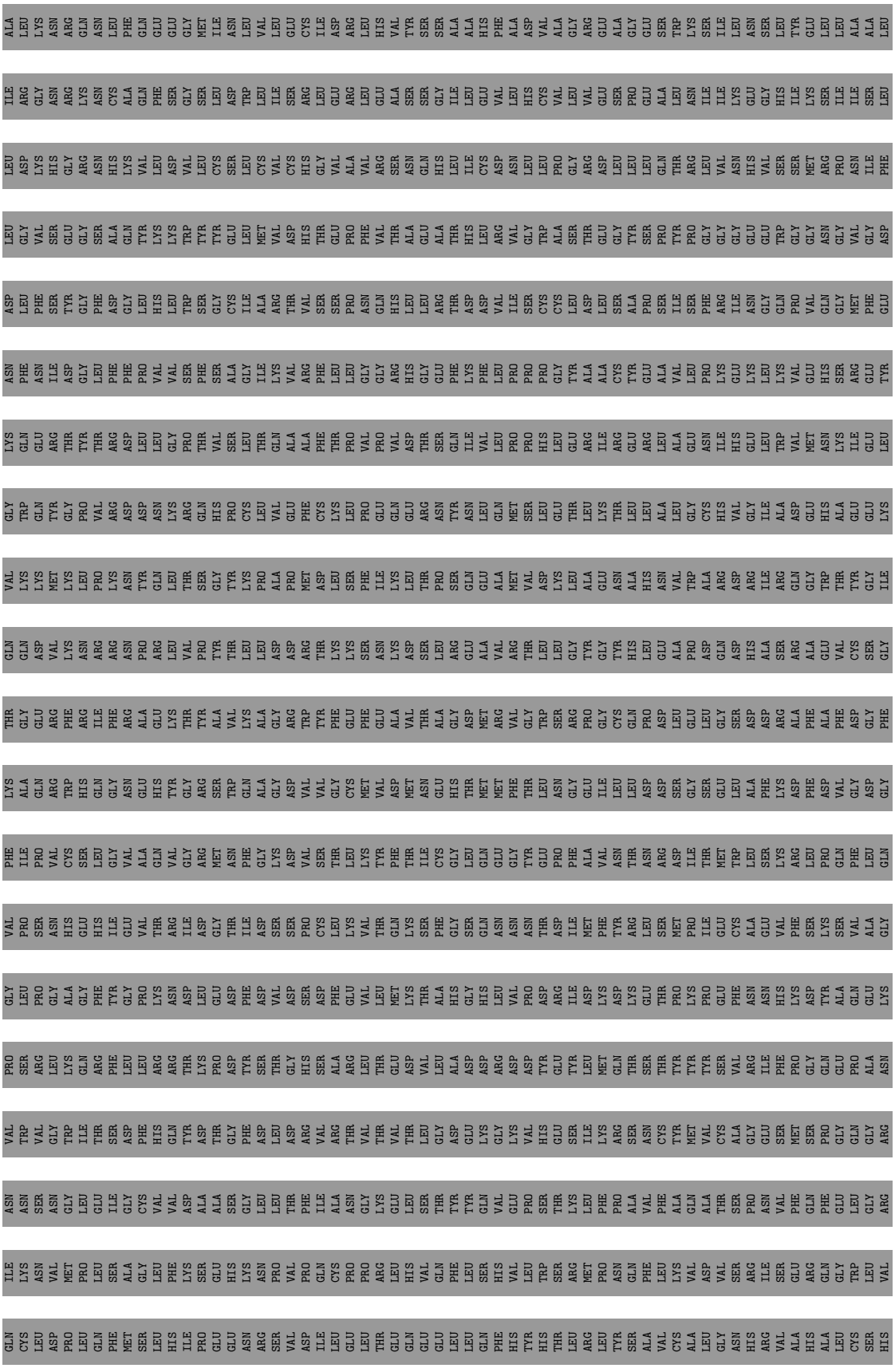


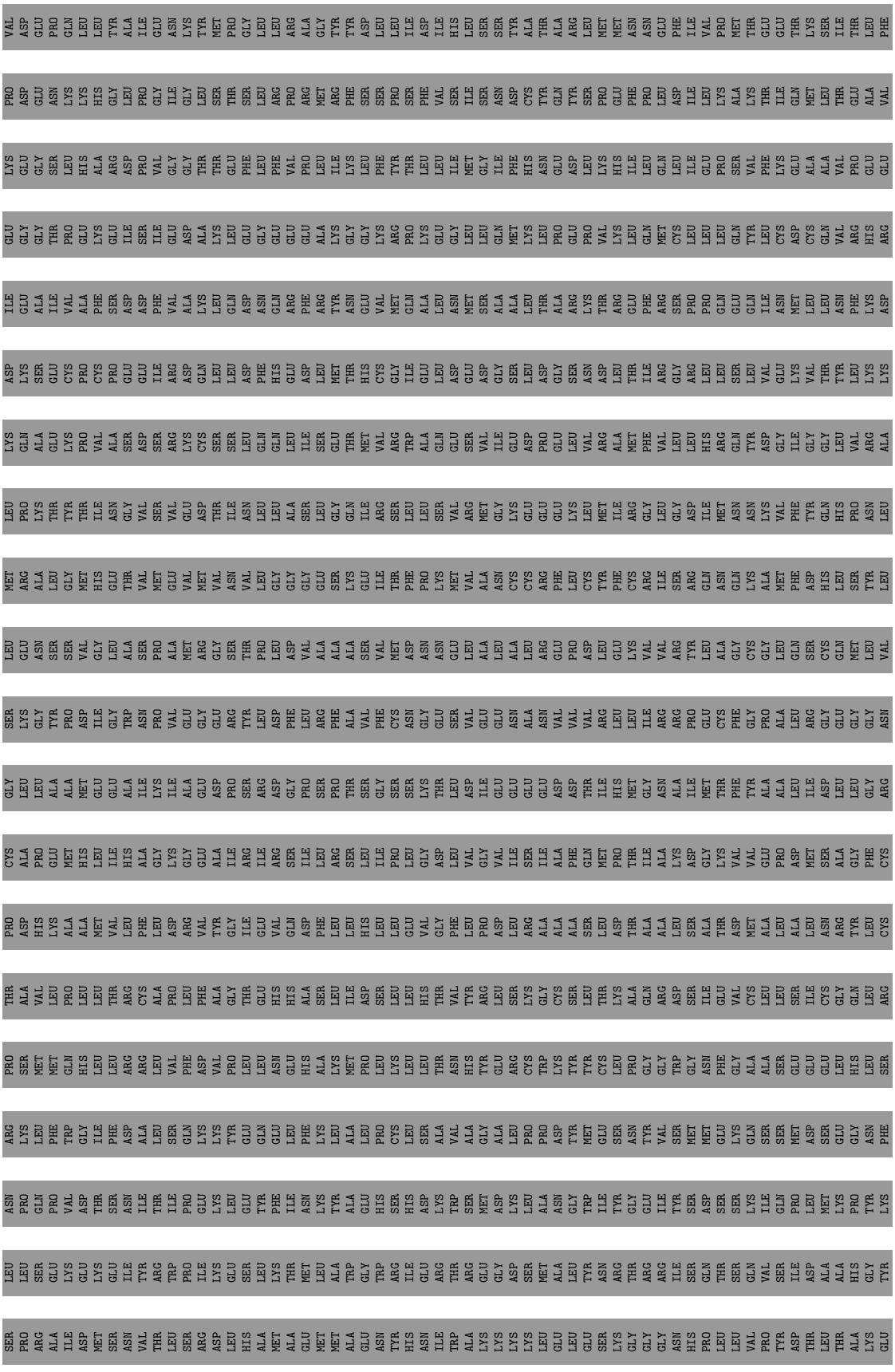
• Molecule 1: Ryanodine receptor 2

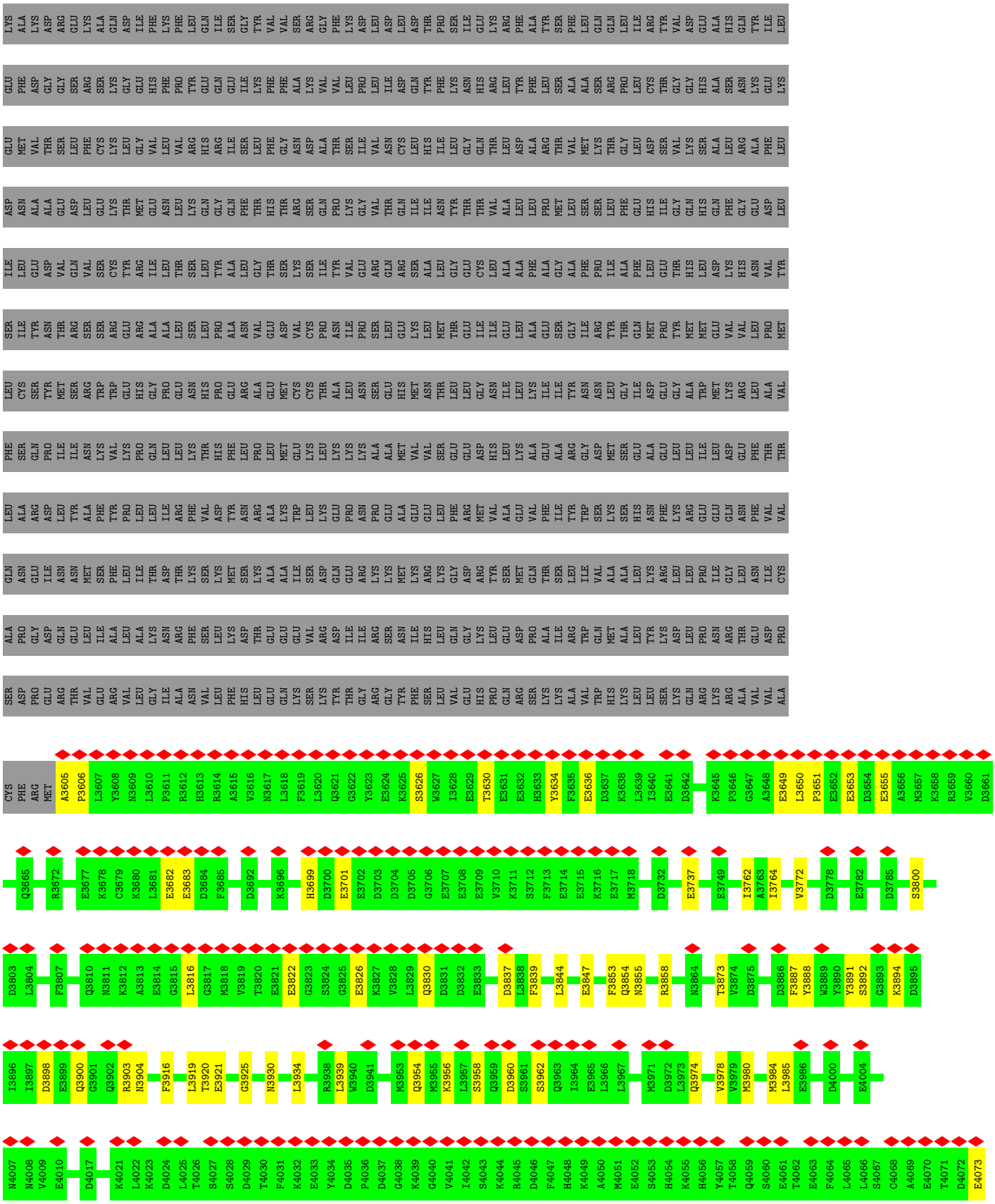
Chain C:



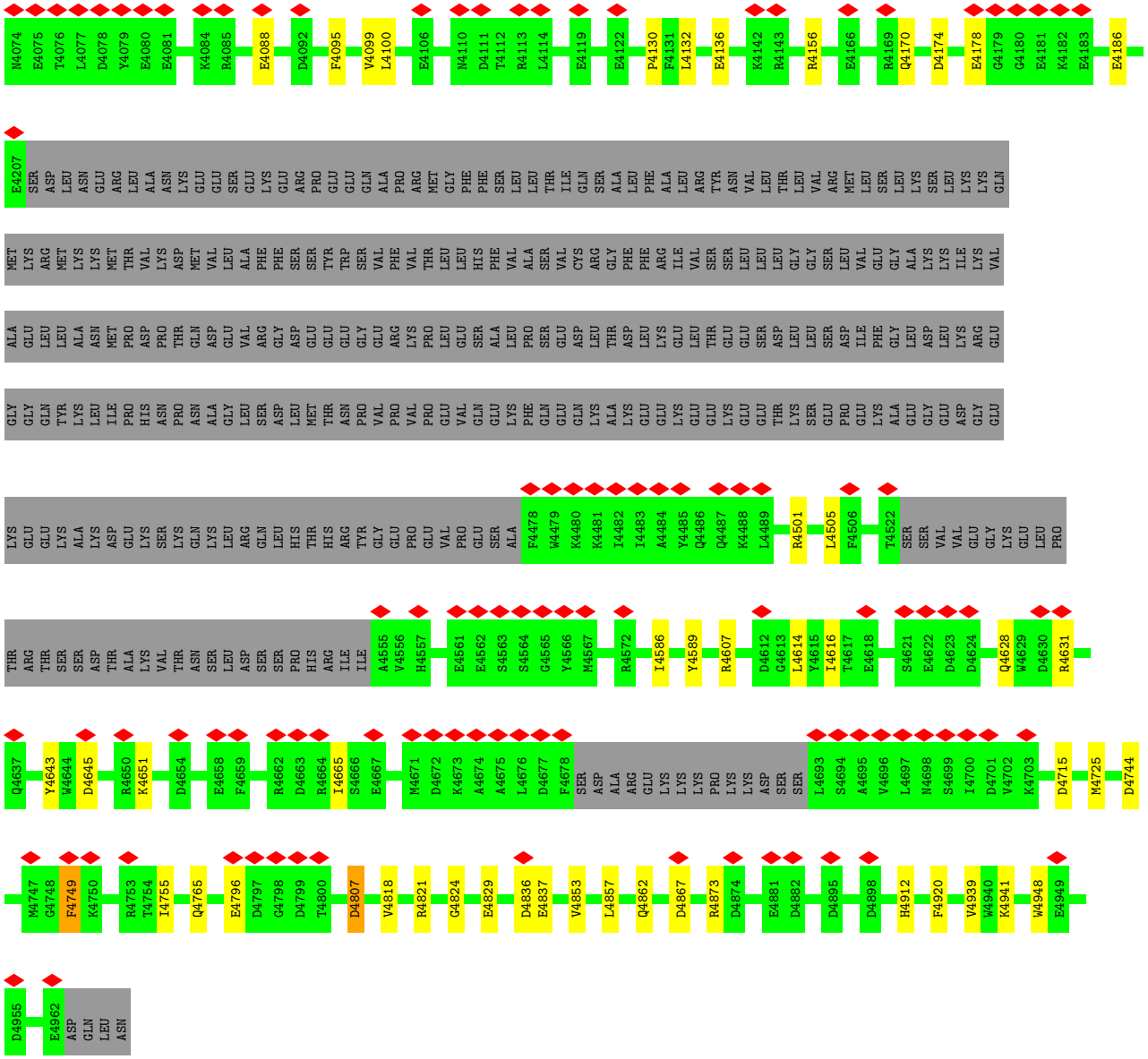



ALA LEU LYS ASN ARG GLN ASN LEU PHE GLN GLU GLU GLY MET ILE ASN LEU VAL LEU GLU CYS ILE ASP ARG LEU HIS VAL TYR SER SER ALA ALA HIS PHE ALA ASP VAL ALA GLY ARG GLU ALA GLY GLU SER TRP LYS SER ILE LEU ALA LEU
ILE ARG GLY ASN ARG LYS ASN CYS ALA GLN PHE SER GLY SER LEU ASP TRP LEU ILE SER ARG LEU GLU ARG LEU GLU ALA GLN PHE SER GLY ILE LEU ILE CYS ASP VAL LEU HIS CYS VAL ALA LEU GLU ALA GLY GLU ILE LEU ASN SER LEU TYR GLU LYS GLY HIS ILE LYS SER ILE ILE SER LEU
LEU ASP LYS HIS GLY ARG ASN HIS LYS VAL LEU ASP VAL LEU CYS SER LEU CYS VAL CYS HIS GLY VAL ALA VAL ARG SER ASN GLN HIS LEU ILE CYS ASP ASN LEU LEU PRO GLY ARG ASP LEU LEU LEU GLN THR ARG LEU VAL ASN HIS VAL SER SER MET ARG PRO ASN SER PHE
LEU GLY VAL SER GLU GLY SER ALA GLN TYR LYS LYS TRP TYR TYR GLU LEU MET VAL ASP HIS THR GLU PRO PHE VAL THR HIS LEU ALA GLU ALA THR HIS LEU ILE CYS ARG VAL GLY TRP ALA SER THR GLU GLY TYR SER PRO TYR PRO GLY GLY GLY GLU GLU TRP GLY GLY ASN GLY VAL GLY ASP
ASP LEU PHE SER TYR GLY PHE ASP GLY LEU HIS LEU TRP SER GLY CYS ILE ALA ARG THR VAL SER SER PRO ASN GLN HIS LEU LEU ARG THR ASP ASP VAL ILE SER CYS CYS LEU ASP LEU SER ALA PRO SER ILE SER PHE ARG ILE ASN GLY GLN LYS LEU LYS VAL GLU HIS SER ARG GLU GLU TYR
ASN PHE ASN ILE ASP GLY LEU PHE PHE PRO VAL PHE SER GLY ILE LYS VAL ARG PHE LEU LEU GLY GLY ARG HIS GLY GLU PHE LYS PHE LEU PRO PRO PRO GLY TYR ALA ALA CYS TYR GLU ALA VAL LEU PRO LYS GLU LYS LEU LYS VAL GLU HIS SER ARG GLU TYR
LYS GLN GLU ARG THR TYR THR ARG ASP LEU LEU GLY PRO THR VAL SER LEU THR GLN ALA ALA PHE THR PRO VAL PRO VAL ASP THR SER GLN ILE VAL LEU PRO PRO HIS LEU GLU ARG ILE ARG GLU ARG ASN LEU ALA GLU ASN ILE HIS GLU LEU TRP VAL MET ASN LYS ILE GLU GLU
GLY TRP GLN TYR GLY PRO VAL ARG ASP ASP ASN LYS ARG GLN HIS PRO CYS LEU VAL GLU PHE CYS LYS LEU PRO GLU GLN GLU ARG ASN TYR ASN LEU GLN MET SER LEU GLU THR LEU LYS THR LEU GLU ARG ALA ASP GLU HIS ALA GLU GLU LYS
VAL LYS LYS MET LYS LEU PRO LYS ASN TYR GLN LEU THR SER GLY TYR LYS PRO ALA PRO MET ASP LEU SER PHE ILE LYS LEU THR PRO SER GLN GLU ALA MET VAL ASP LYS LEU ALA GLU ASN ALA HIS ASN VAL TRP ALA ARG ASP ARG ILE ARG GLN GLY TRP THR TYR GLY ILE
GLN GLN ASP VAL LYS ASN ARG ARG ASN PRO ARG LEU VAL PRO TYR THR LEU LEU ASP ASP ARG THR LYS LYS SER ASN LYS ASP SER LEU ARG GLU ALA VAL THR ALA GLY ASP ARG GLU LEU LEU GLY TYR GLY TYR HIS LEU GLU ALA PRO ASP GLN ASP HIS ALA SER ARG ALA GLU VAL CYS SER GLY
THR GLY GLU ARG PHE ARG ILE PHE ARG ALA GLU LYS THR TYR ALA VAL LYS ALA GLY ARG TRP TYR PHE GLU PHE GLU ALA VAL THR ALA GLY ASP MET ARG VAL GLY TRP SER ARG PRO GLY CYS GLY LEU GLU LEU GLY SER GLY PHE ASP ARG ASP ARG ALA PHE ASP GLY GLY PHE
LYS ALA GLN ARG TRP HIS GLN GLY ASN GLU HIS TYR GLY ARG SER TRP GLN ALA GLY ASP ASP VAL VAL GLY CYS MET VAL ASP MET ASN GLU HIS THR MET MET PHE THR LEU ASN GLY GLU ILE LEU LEU ASP ASP SER GLY SER GLU LEU ALA PHE LYS ASP PHE ASP VAL ASP GLY
PHE ILE PRO VAL CYS SER LEU GLY VAL ALA GLN VAL GLY ARG MET ASN PHE GLY LYS ASP VAL SER THR LEU LYS TYR PHE THR ILE CYS GLY LEU GLN GLU GLY TYR GLU PRO ASP ALA VAL ASN THR ASN ARG ASP ILE THR MET TRP LEU SER LYS ARG LEU PRO GLN PHE LEU GLN
VAL PRO SER ASN HIS GLU VAL THR ARG ILE ASP GLY THR ILE ASP SER SER PRO CYS LEU LYS VAL THR GLN LYS SER PHE GLY SER GLN ASN ASN ASN THR ASP ILE MET PHE TYR ARG LEU SER MET PRO ILE GLU CYS ALA GLU VAL PHE SER LYS SER VAL ALA GLY
GLY LEU PRO GLY ALA GLY PHE TYR GLY PRO LYS ASN ASP LEU ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG ILE ASP LYS ASP LYS GLU THR PRO LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS
PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG THR LYS ASP ARG THR LYS GLY HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP TYR GLU TYR LEU MET GLN THR SER THR TYR TYR TYR SER VAL ARG LEU PHE PRO GLY GLN GLU PRO ALA ASN
VAL TRP VAL GLY TRP ILE THR SER ASP PHE HIS GLN LEU ASP PHE ASP LEU ARG THR VAL THR VAL THR LEU LEU GLY ASP GLU LYS VAL HIS GLU SER ILE LYS ARG SER ASN CYS TYR MET VAL CYS ALA GLY GLU SER MET VAL PHE PRO GLN PHE GLU GLN GLY ARG
ASN ASN SER ASN GLY LEU GLU ILE GLY CYS VAL VAL ASP PHE ILE ALA ASN GLY LYS GLU LEU SER THR TYR GLN VAL GLU PRO SER THR LYS LEU PHE PRO ALA VAL PHE ALA GLN ALA THR SER ASN VAL PHE GLN PHE GLU LEU GLY ARG
ILE LYS ASN VAL MET PRO LEU SER ALA GLY LEU SER GLU HIS LYS ASN PRO VAL PRO GLN CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER HIS VAL LEU TRP SER ARG MET PRO ASN GLN PHE LEU LYS VAL ASP VAL SER ARG ILE SER ARG GLY TRP LEU VAL
GLN CYS LEU ASP PRO LEU GLN PHE MET SER LEU HIS ILE PRO GLU GLU ASN ARG SER VAL ASP ILE LEU GLU LEU THR GLU GLN GLU GLU LEU LEU GLN PHE HIS TYR HIS THR LEU ARG LEU TYR SER ALA VAL CYS ALA LEU GLY ASN HIS ARG VAL ALA HIS ALA LEU GLU LEU


VAL ASP GLU PRO GLN LEU LEU TYR ALA ILE GLU ASN LYS TYR MET PRO GLY LEU LEU ARG ALA GLY TYR TYR ASP LEU LEU ILE ASP ILE HIS LEU SER SER TYR ALA THR ALA ARG LEU MET MET ASN ASN GLU PHE ILE VAL PRO MET THR GLU GLU THR LYS SER ILE THR LEU PHE
PRO ASP GLU ASN LYS LYS HIS GLY LEU PRO GLY ILE GLY LEU SER THR SER LEU ARG PRO ARG MET PHE SER SER PRO SER PHE VAL SER ILE SER ASN CYS TYR GLN TYR SER PRO GLU PHE PRO LEU ASP ILE LEU LYS ALA LYS THR ILE GLN MET LEU THR GLU ALA VAL
LYS GLU GLY SER LEU HIS ALA ARG ASP PRO VAL GLY GLY THR THR GLU PHE LEU PHE VAL PRO LEU ILE LYS LEU PHE TYR THR LEU LEU ILE MET GLY ILE PHE HIS ASN GLU ASP LEU LYS HIS ILE LEU GLN LEU ILE GLU PRO SER VAL PHE LYS GLU ALA ALA VAL PRO GLU GLU
GLU GLY GLY THR PRO GLU LYS GLU ILE SER ILE GLU GLY GLU ASP ALA LYS LEU GLU GLY GLU GLU ALA LYS GLY GLY LYS ARG PRO GLU PRO VAL LYS LEU GLN LEU LEU LEU LEU GLN TYR LEU CYS ASP CYS GLN VAL ARG HIS ARG
ILE GLU ALA ILE VAL ALA PHE SER ASP ASP PHE VAL ALA LYS LEU GLN ASP ASN GLN ARG PHE ARG TYR ASN GLU VAL MET GLN ALA LEU ASN MET SER ARG GLU PHE ARG SER PRO PRO GLN GLU GLU ASN MET LEU LEU ASN PHE LYS ASP
ASP LYS SER GLU CYS PRO CYS PRO GLU GLU ILE ARG ASP GLN LEU LEU ASP PHE HIS GLU ASP GLU CYS GLY ILE GLU LEU GLU ASP GLU ASP GLY SER ASN GLY LEU THR ILE ARG GLY ARG LEU GLU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS
LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER SER LEU GLU THR MET VAL ARG TRP ALA GLN GLU SER VAL ILE GLU ASP PRO GLU LEU VAL ARG ALA MET PHE VAL LEU LEU HIS ARG GLN TYR ASP GLY ILE GLY LEU GLY ASP ARG LEU ALA
LEU PRO LYS THR TYR THR ILE ASN GLY VAL SER VAL GLU ASP THR ILE ASN LEU LEU ALA LEU SER ARG SER LEU LEU SER VAL ARG MET GLY LYS GLU GLU ASP PRO GLU LEU LYS LEU MET ILE ARG GLY LEU GLY ASP ILE MET ASN ASN LYS VAL PHE TYR GLN HIS PRO ASN LEU
MET ARG ALA LEU GLY MET HIS GLU THR VAL MET GLU VAL MET VAL ASN VAL LEU GLY GLY GLY GLU SER LYS GLU ILE THR PHE PRO LYS MET VAL ALA ASN CYS CYS ARG PHE LEU CYS TYR PHE CYS ARG ILE SER ARG GLN ASN GLN LYS ALA MET PHE ASP HIS LEU SER TYR LEU
LEU GLU ASN SER SER VAL GLY LEU ALA SER PRO ALA MET ARG GLY SER THR PRO LEU ASP VAL ALA ALA ALA SER VAL MET ASP ASN ASN GLU LEU ALA LEU ARG GLU PRO ASP LEU GLU LYS VAL VAL ARG TYR LEU ALA GLY CYS GLY LEU GLN SER CYS GLN MET LEU VAL
SER LYS GLY TYR PRO ASP ILE GLY TRP ASN PRO VAL GLU GLY GLY GLU ARG TYR LEU ASP PHE LEU ARG PHE ALA VAL PHE CYS ASN GLY GLU SER VAL GLU GLU ASN ALA ASN VAL VAL VAL ARG LEU LEU ILE ARG ARG PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN
GLY LEU LEU ALA ALA MET GLU GLU GLU ALA ILE LYS ILE ALA GLU GLU ASP PRO SER ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU GLU ASN GLU GLU ASP ASP THR ILE HIS MET GLY ASN ALA ILE MET THR PHE TYR ALA GLY CYS GLY LEU GLN LEU LEU ASP ARG
CYS ALA PRO GLU MET HIS LEU ILE HIS ALA GLY LYS GLY GLU ALA ILE ARG ILE ARG SER ILE LEU ARG ILE HIS PRO LEU GLU VAL GLY ASP LEU VAL GLY VAL ILE SER ILE GLU ASP ALA PHE GLN MET PRO THR ILE ILE ALA ALA LYS ASP GLY LYS VAL PHE GLY ARG PHE CYS
PRO ASP HIS LYS ALA ALA MET VAL LEU PHE LEU ASP ARG VAL TYR GLY ILE GLU VAL GLN ASP PHE LEU LEU HIS LEU LEU LEU GLU VAL GLY PHE LEU PRO ASP LEU ARG LEU ASP THR ALA ALA LEU SER ALA THR ASP MET ALA LEU LEU ASN ARG TYR LEU CYS
THR ALA VAL LEU PRO LEU THR ARG CYS ALA ALA PRO LEU PHE ALA GLY THR GLU HIS HIS ALA SER LEU LEU HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU SER LEU LEU SER ILE CYS GLY GLN LEU ARG
PRO SER MET MET GLN HIS LEU LEU ARG LEU VAL PHE ASP VAL PRO LEU LEU ASN GLU HIS ALA LYS MET PRO LEU LYS LEU LEU THR ASN HIS TYR GLU ARG CYS TRP LYS TYR TYR CYS LEU PRO GLY GLY TRP GLY ASN PHE GLY ALA ALA SER GLU GLU LEU HIS LEU SER
ARG LYS LEU PHE TRP GLY ILE PHE ASP ALA LEU SER LEU ALA LEU PRO CYS LEU SER SER ALA VAL ALA GLY ALA ALA LEU PRO PRO ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY ASN PHE
ASN PRO GLN PRO VAL ASP THR SER ASN ILE THR ILE PRO GLU GLU TYR PHE ILE ASN LYS TYR ALA GLU HIS SER HIS ASP LYS TRP SER MET ASP LYS LEU ALA ASN GLY TRP ILE TYR GLY GLU ILE TYR SER ASP SER SER LYS HIS GLN PRO LEU MET LYS ILE PRO TYR LYS
LEU LEU SER GLU ILE TYR ARG TRP PRO ILE LYS LYS THR MET LEU ALA TRP GLY TRP ARG ILE GLU ARG THR ARG GLU GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN ILE ASP ALA ALA HIS GLY TYR
SER PRO ARG ALA ILE ASP LEU HIS MET MET ALA GLU ASN TYR HIS ASN ILE TRP ALA LYS LYS LYS LEU GLU LEU GLU SER LYS GLY GLY GLY ASN HIS PRO LEU LEU VAL PRO TYR ASP THR LEU THR ALA LYS GLU


LYS ALA LYS ASP ARG GLU LYS ALA GLN ASP ILE PHE LYS PHE LEU GLN ILE SER GLY TYR VAL VAL SER ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN ILE LEU
GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU CYS THR GLY GLY HIS ALA SER ASN LYS GLU LYS
GLU MET VAL THR SER LEU PHE CYS LYS LEU GLY VAL LEU VAL ARG HIS ARG ILE SER LEU LYS PHE PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE LEU GLY GLN THR LEU ASP ALA ARG THR VAL MET LYS THR GLY LEU ASP SER VAL LYS SER ALA LEU ARG ALA PHE LEU
ASP ASN ALA ALA GLU ASP LEU GLU LYS THR MET GLU ASN LEU LYS GLN GLY GLN PHE THR HIS THR ARG SER GLN PRO LYS GLY VAL THR GLN GLN ILE ILE ASN TYR THR THR VAL ALA LEU LEU PRO MET LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP LEU
ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY THR GLY VAL GLU ARG GLN ARG SER ILE TYR VAL GLU ARG GLN ARG SER ILE LEU GLU CYS LEU ALA ALA PHE ALA GLY ALA PHE PRO LEU ILE ALA PHE LEU GLU THR HIS LEU ASP LYS HIS ASN VAL TYR
SER ILE TYR ASN THR ARG GLU ARG ALA ALA LEU SER LEU PRO ALA ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET THR GLU ILE ILE GLU LEU ALA PHE ALA GLU SER GLY ILE ARG TYR THR MET PRO TYR MET MET GLU VAL VAL LEU PRO MET
LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN HIS PRO GLU ARG ALA ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU LEU GLY ASN ILE LEU LYS ALA GLU VAL GLY ASN ILE LEU ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA ALA VAL
PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU GLU ASP HIS LEU LYS ALA GLU ALA ALA ARG GLY ASP MET SER GLU ALA GLU LEU LEU LEU ILE LEU ASP GLU PHE THR THR
LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN GLN ASN PHE VAL VAL
GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA ILE SER ASP GLN GLU ARG ASP ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS
ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU GLU VAL ARG ASP ARG ILE ILE ARG SER ASN ILE HIS LEU GLN LEU GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU LEU TYR LYS ARG LEU LEU PRO ASN ARG THR GLU ASP PRO
SER ASP PRO GLU ARG ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA

CYS PHE ARG MET A3605 P3606 L3607 Y3608 N3609 L3610 P3611 R3612 H3613 R3614 A3615 V3616 N3617 L3618 F3619 L3620 Q3621 G3622 Y3623 E3624 K3625 S3626 W3627 I3628 E3629 T3630 E3631 E3632 H3633 Y3634 F3635 E3636 D3637 K3638 L3639 I3640 E3641 D3642 K3645 P3646 G3647 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 V3660 D3661
Q3665 R3672 E3677 K3678 C3679 K3680 L3681 E3682 E3683 D3684 F3685 D3692 K3696 H3699 D3700 E3701 E3702 D3703 D3704 D3705 G3706 E3707 E3708 E3709 V3710 K3711 S3712 F3713 E3714 E3715 K3716 E3717 M3718 D3732 E3737 E3749 I3762 A3763 I3764 V3772 D3778 E3782 D3785 S3800
D3803 L3804 F3807 Q3810 N3811 K3812 A3813 E3814 G3815 L3816 G3817 M3818 V3819 T3820 E3821 E3322 G3823 S3824 G3825 E3826 K3827 V3828 L3329 Q3830 D3831 D3832 E3333 D3837 L3838 F3839 L3844 E3847 F3853 Q3854 N3855 R3858 N3864 T3873 V3874 D3875 D3886 F3887 Y3888 W3889 Y3890 Y3891 S3392 G3393 K3894 D3895
I3896 I3897 D3898 E3899 Q3900 G3901 Q3902 R3903 N3904 F3916 L3919 T3920 E3921 G3925 N3930 L3934 R3938 L3939 W3940 D3941 M3953 Q3954 M3955 K3956 L3957 S3958 Q3959 D3960 S3961 S3962 Q3963 I3964 E3965 L3966 L3967 M3971 D3972 L3973 Q3974 V3978 V3979 M3980 M3984 L3985 E3986 P4000 E4004
N4007 N4008 V4009 E4010 D4017 K4021 L4022 K4023 D4024 L4025 T4026 S4027 S4028 D4029 T4030 F4031 K4032 E4033 Y4034 D4035 P4036 D4037 G4038 K4039 G4040 V4041 I4042 S4043 K4044 R4045 D4046 F4047 H4048 K4049 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Y4057 T4058 Q4059 S4060 E4061 T4062 E4063 F4064 L4065 L4066 S4067 C4068 A4069 E4070 T4071 D4072 E4073

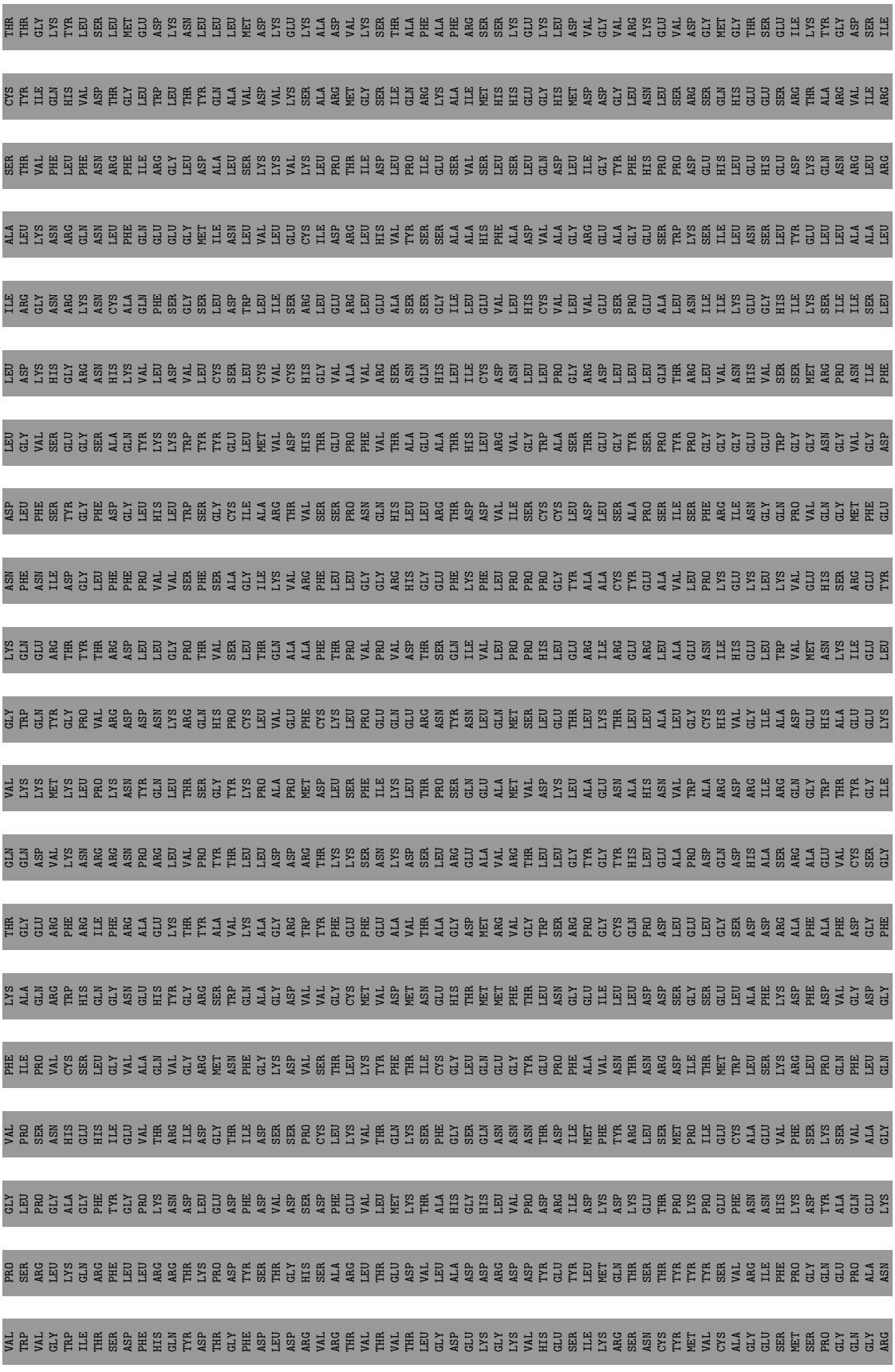


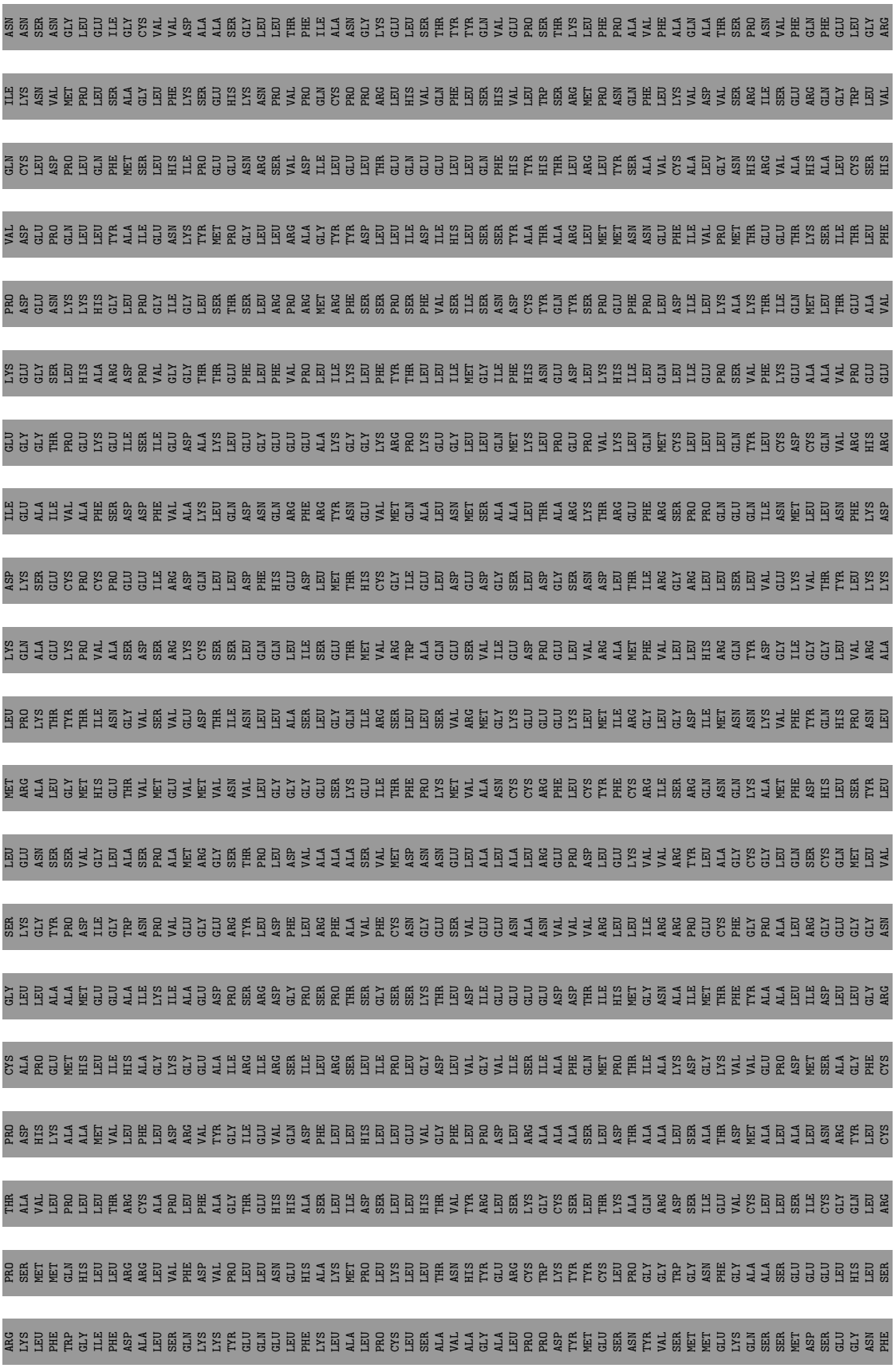
• Molecule 1: Ryanodine receptor 2

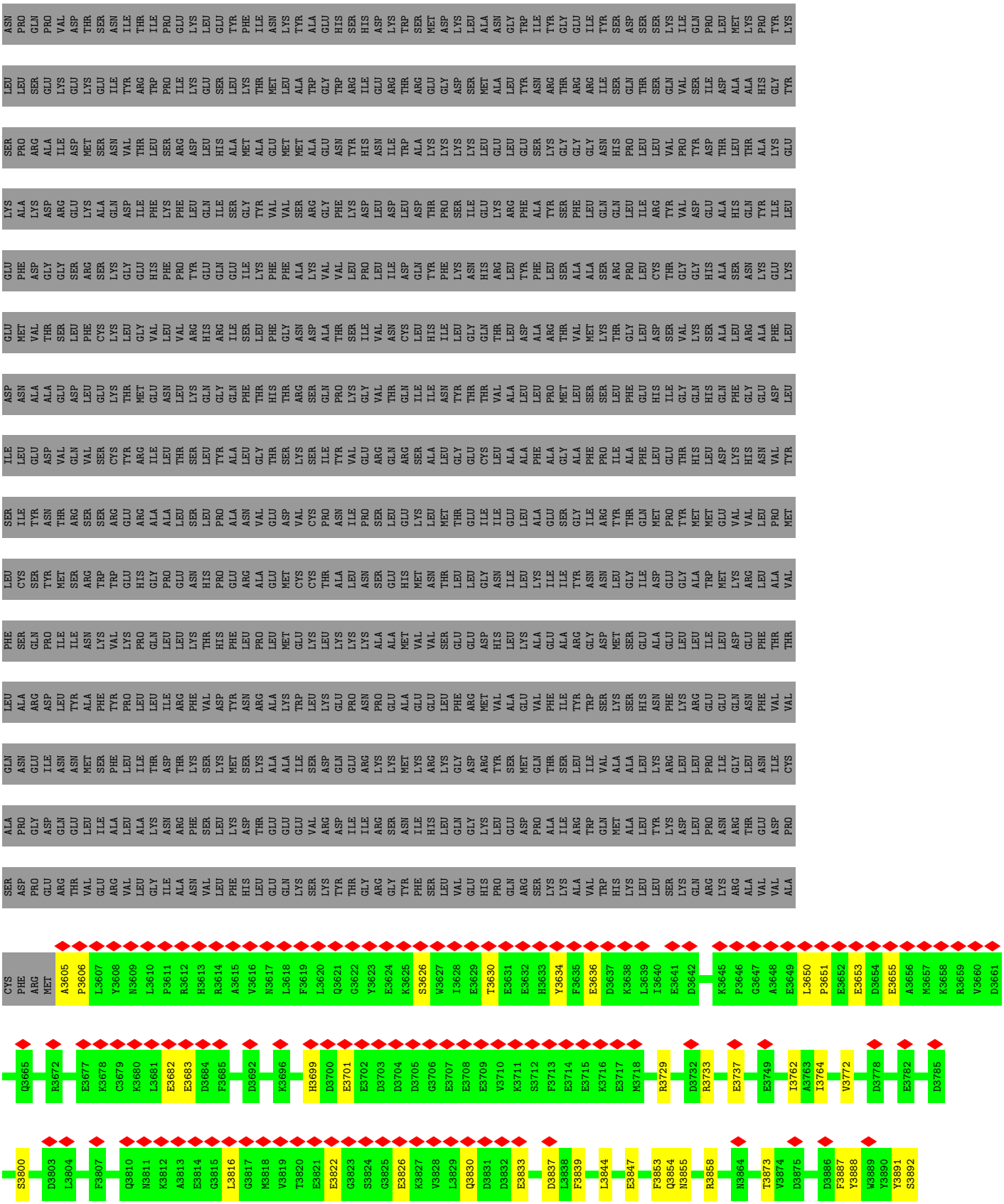
Chain D:



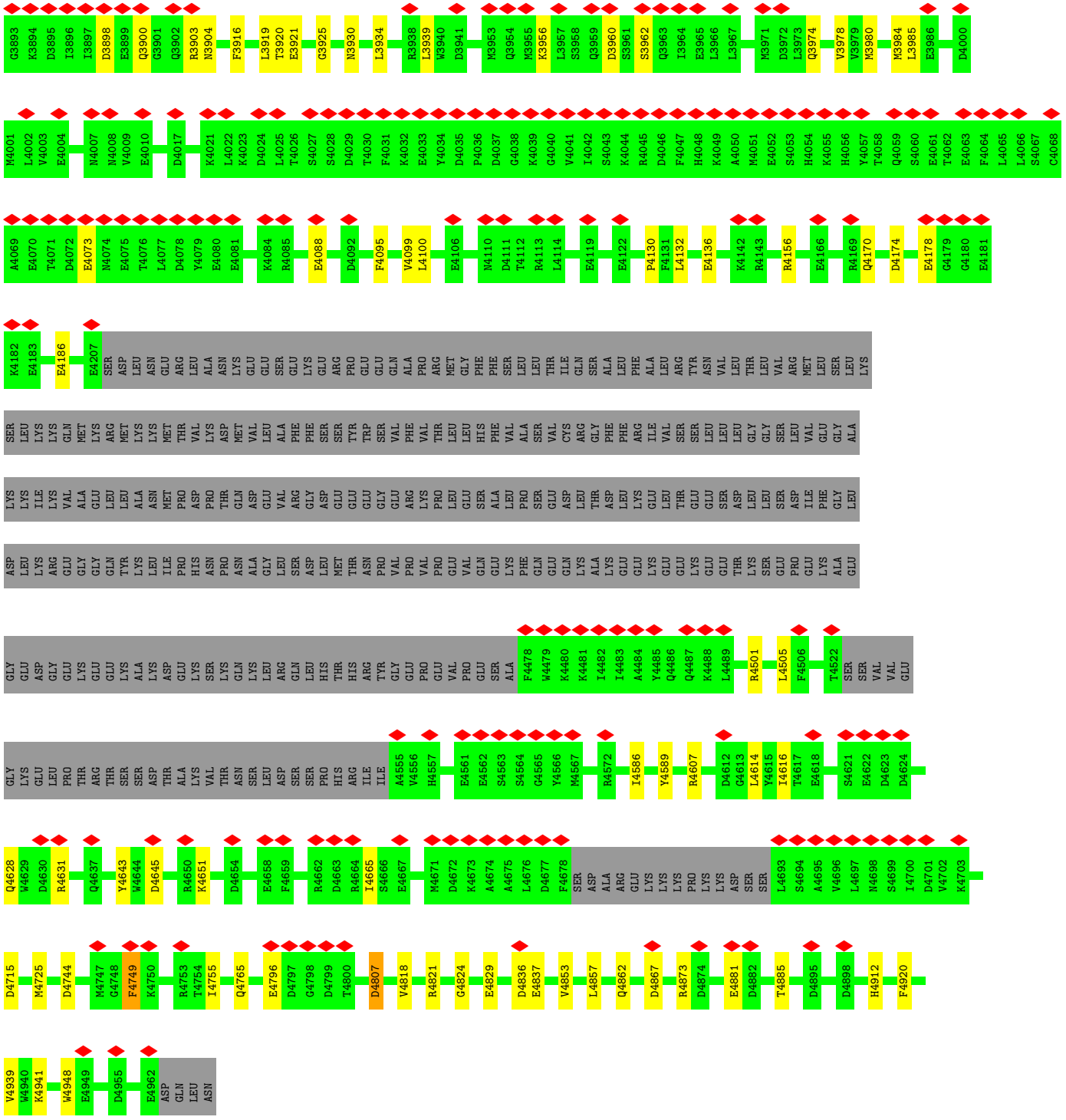





ASN ASN SER ASN GLY LEU GLU ILE GLY CYS VAL VAL ASP ALA ALA SER GLY LEU LEU THR PHE ILE ALA ASN GLY LYS GLU LEU SER THR TYR TYR GLN VAL GLU PRO SER THR LYS LEU PHE PRO ALA VAL PHE ALA GLN ALA THR SER PRO ASN VAL PHE GLN PHE GLU ARG
ILE LYS ASN VAL MET PRO LEU SER ALA GLY LEU PHE LYS SER GLU HIS LYS ASN PRO VAL PRO GLN CYS PRO PRO ARG LEU HIS VAL GLN PHE LEU SER HIS VAL LEU TRP SER ARG MET PRO ASN GLN PHE LEU LYS VAL ASP VAL SER ARG ILE SER GLU ARG GLN GLY TRP LEU VAL
GLN CYS LEU ASP PRO LEU GLN PHE MET SER LEU HIS ILE PRO GLU GLU ASN ARG SER VAL ASP ILE LEU GLU LEU GLU GLU LEU LEU GLN PHE HIS TYR HIS THR LEU THR GLU GLN GLU GLU LEU LEU GLN PHE HIS VAL LEU TYR SER ALA VAL CYS ALA LEU GLY ASN HIS ARG VAL ALA HIS ALA LEU CYS SER HIS
VAL ASP GLU PRO GLN LEU LEU TYR ALA ILE GLU ASN LYS TYR MET PRO GLY LEU LEU ARG ALA GLY TYR TYR ASP LEU LEU ILE ASP ILE HIS LEU SER SER TYR ALA THR ALA ARG LEU MET MET ASN ASN GLU PHE ILE VAL PRO MET THR GLU GLU THR LYS SER ILE THR LEU PHE
PRO ASP GLU ASN LYS LYS HIS GLY LEU PRO GLY ILE GLY LEU SER THR SER LEU ARG PRO ARG MET ARG PHE SER SER PHE VAL SER ILE LEU LYS ALA LYS THR ILE GLN MET ASP PHE GLU ALA VAL
LYS GLU GLY SER LEU HIS ALA ARG ASP PRO VAL GLY GLY THR THR GLU PHE LEU PHE VAL PRO LEU ILE LYS LEU PHE TYR THR LEU LEU LEU ILE MET GLY ILE PHE HIS ASN GLU ASP LEU LYS HIS ILE LEU GLN LEU ILE GLU PRO GLN GLU LYS ALA LYS THR PHE LYS GLU ALA VAL PRO GLU GLU
GLU GLY GLY THR PRO GLU ILE SER ASP PHE LYS LEU GLU GLY GLU GLU ALA LYS GLY GLY LYS ARG PRO LYS LEU GLY MET CYS LEU LEU LEU GLN TYR LEU CYS ASP CYS GLN VAL ARG HIS ARG
ILE GLU ALA ILE VAL ALA PHE SER ASP ASP PHE VAL ALA ALA PHE ARG TYR ASN GLU VAL MET GLN ALA LEU ASN MET SER ALA LYS THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLU LEU GLN ILE ASN MET ASP PHE ASN GLN ARG PHE ARG TYR THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASP LYS
ASP LYS SER GLU CYS PRO CYS PRO GLU GLU ILE ARG ASP GLN LEU LEU ASP PHE HIS GLU ASP LEU MET THR HIS CYS GLY ILE GLU LEU ASP GLU GLY SER LEU ASP GLY ARG LEU LEU SER LEU VAL GLU GLY LYS VAL THR TYR LEU LYS LYS
LYS GLN ALA GLU LYS PRO VAL ALA SER ASP SER ARG LYS CYS SER SER LEU GLN GLN LEU ILE SER GLU THR MET VAL ARG TRP ALA GLN GLU SER VAL ILE GLU ASP PRO GLU LEU VAL ARG ALA MET PHE VAL LEU HIS ARG GLN TYR ASP GLY ILE GLY LEU VAL ARG ALA
LEU PRO LYS THR TYR THR ILE ASN GLY VAL SER VAL ASN LEU LEU ALA SER LEU GLY GLN ILE ARG SER LEU LEU LEU SER VAL ARG MET GLY LYS GLU GLU ASP PRO GLU LEU LYS GLY ASP ILE MET ASN LEU GLN ILE ARG GLY LEU GLY ASP ILE MET ASN ASN LYS VAL PHE TYR GLN HIS PRO ASN LEU
MET ARG ALA LEU GLY MET HIS GLU GLU THR VAL MET GLU VAL MET MET VAL ASN VAL LEU GLY GLY GLU SER LYS GLU ILE THR PHE PHE PRO LYS MET VAL ALA ASN CYS CYS ARG PHE LEU CYS TYR PHE CYS ARG ILE SER ARG GLN ASN GLN LYS ALA MET PHE ASP HIS LEU SER TYR LEU
LEU GLU ASN SER SER VAL GLY LEU ALA SER ALA ALA ALA SER VAL MET ASP ASN ASN GLU LEU ALA LEU LEU GLU ARG GLU PRO ASP LEU GLU LYS VAL VAL ARG TYR LEU ALA GLY CYS GLY LEU GLN SER CYS GLN MET LEU VAL
SER LYS GLY TYR PRO ASP ILE GLY TRP ASN PRO VAL GLU GLY GLU ARG TYR LEU ASP PHE LEU ARG PHE ALA VAL PHE CYS ASN GLY GLU SER VAL GLU GLU ASN ALA ASN VAL VAL VAL ARG LEU LEU ILE ARG ARG PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN
GLY LEU LEU ALA ALA MET GLU GLU ALA ILE LYS ILE ALA GLU ASP PRO SER PRO THR SER GLY SER SER LYS THR LEU ASP ILE GLU GLU GLU GLU ASP ASP THR ILE HIS MET GLY ASN ALA ILE MET THR PHE TYR ALA ALA LEU ILE ASP LEU ILE GLY ARG
CYS ALA PRO GLU MET HIS LEU ILE HIS ALA GLY LYS ASP LEU VAL GLY ILE SER ILE ALA ALA PHE GLN MET PRO THR ILE ALA LYS ASP GLY LYS VAL LEU ASP THR ILE GLU GLY PRO ALA LEU GLN SER CYS GLN HIS LEU SER TYR
PRO ASP HIS LYS ALA MET VAL LEU ILE GLU VAL GLN ASP PHE LEU LEU LEU GLU VAL GLY PHE LEU PRO ASP LEU ARG ALA ALA ALA SER LEU LEU ASP THR ALA GLN ARG LEU SER ALA THR ASP MET ALA LEU PRO ALA LEU ASN ARG TYR LEU CYS
THR ALA VAL LEU PRO LEU THR ARG CYS ALA PRO LEU PHE ALA SER LEU HIS LEU ILE ASP SER LEU LEU HIS THR VAL TYR ARG LEU SER LYS GLY CYS SER LEU THR LYS ALA GLN ARG ASP SER ILE GLU VAL CYS LEU LEU GLU SER ILE CYS GLY GLN LEU LEU ARG
PRO SER MET MET GLN HIS LEU LEU ARG VAL PHE ASP VAL PRO LEU LEU ASN GLU HIS ALA LYS MET PRO LEU LYS LEU LEU THR ASN HIS TYR ARG GLU ARG CYS TRP LYS TYR TYR CYS LEU PRO GLY GLY TRP GLY ASN PHE GLY ALA ALA SER GLU GLU GLU LEU HIS LEU LEU
ARG LYS LEU PHE TRP GLY ILE PHE ASP ALA LEU GLN LYS TYR GLU GLN GLU LEU PHE LYS LEU ALA LEU PRO CYS LEU SER ALA VAL ALA GLY ALA LEU PRO ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER ASP SER GLU GLY ASN PHE


ASN PRO GLN PRO VAL ASP THR SER ASN ILE THR ILE PRO GLU LYS LEU GLU TYR PHE ILE ASN LYS TYR ALA GLU HIS SER HIS ASP LYS TRP SER MET ASP LYS LEU ALA ASN GLY TRP ILE TYR GLY GLU ILE TYR SER ASP SER SER LYS ILE GLN PRO LEU MET LYS PRO TYR LYS
LEU LEU SER GLU LYS GLU LYS GLU ILE TYR ARG TRP PRO ILE LYS GLU SER LEU LYS THR MET LEU ALA TRP GLY TRP ARG ILE GLU ARG THR ARG GLU GLY ASP SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER ILE ASP ALA ALA HIS GLY TYR
SER PRO ARG ALA ILE ASP MET SER ASN VAL THR LEU SER ARG ASP LEU HIS ALA MET ALA ALA GLU MET MET MET ALA GLU ASN TYR HIS ASN ILE TRP ALA LYS LYS LYS LYS LEU GLU GLU LEU GLU SER LYS GLY GLY GLY ASN HIS PRO LEU LEU VAL PRO TYR ASP THR LEU THR ALA LYS GLU
LYS ALA LYS ASP ARG GLU LYS ALA GLN ASP ILE PHE LYS PHE LEU GLN ILE SER GLY TYR VAL VAL SER ARG GLY PHE LYS ASP LEU ASP LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN ILE LEU
GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU TYR PHE LEU SER ALA ALA SER ARG PRO LEU CYS THR GLY GLY GLY HIS ALA SER ASN LYS GLU GLU
GLU MET VAL THR SER LEU PHE CYS LYS LEU GLY VAL HIS ARG ILE SER LEU PHE GLY ASN ASP ALA THR SER ILE VAL ASN CYS LEU HIS ILE LEU ASP GLN TYR THR THR VAL MET LYS THR GLY LEU ASP SER VAL LYS SER ALA LEU ARG ALA PHE LEU
ASP ASN ALA ALA GLU ASP LEU GLU LYS THR MET GLU ASN LEU LYS GLN GLY GLN PHE THR HIS THR ARG SER GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR THR GLN ILE ILE ASN TYR THR LEU ASP ALA ALA LEU LEU PRO MET LEU SER SER LEU PHE GLU HIS ILE GLY GLN HIS GLN PHE GLY GLU ASP GLU
ILE LEU GLU ASP VAL GLN VAL SER CYS TYR ARG ILE LEU THR SER LEU TYR ALA LEU GLY LYS SER ILE TYR VAL GLU ARG GLN ARG SER ALA LEU GLY GLU CYS LEU ALA ALA ALA PHE PRO ILE ALA PHE LEU GLU THR HIS LEU ASP ASN LYS HIS ASN VAL TYR
SER ILE TYR ASN THR ARG SER SER ARG GLU ARG ALA ALA LEU SER LEU PRO ALA ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET THR GLU ILE ILE GLU LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO TYR MET MET GLU VAL VAL LEU PRO MET
LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN HIS PRO GLU ARG ALA GLU MET CYS CYS THR ALA ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA ALA TRP MET LYS ARG LEU ALA VAL
PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU GLU LYS LEU LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU GLU ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP MET SER GLU ALA LEU ILE LEU ASP GLU PHE THR THR
LEU ALA ARG ASP LEU TYR PHE PRO LEU ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU GLN PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU VAL ASN PHE VAL VAL
GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA ILE SER ASP GLN GLU ARG LYS ASN ILE LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA LYS ARG LEU LEU PRO ILE GLN GLY LEU ASN ILE ASN CYS
ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU GLU GLU VAL ARG ASP ILE ILE ARG ASP ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN GLY ARG THR GLU ASP PRO
SER ASP PRO GLU ARG THR VAL GLU ARG VAL LEU GLY ILE ALA ASN VAL LEU PHE HIS LEU GLN GLN ARG GLY TYR PHE SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG LYS ARG ALA VAL VAL ALA

CYS PHE ARG MET A3605 P3606 L3607 Y3608 N3609 L3610 P3611 R3612 H3613 R3614 A3615 V3616 N3617 L3618 F3619 L3620 Q3621 G3622 Y3623 E3624 K3625 S3626 W3627 I3628 E3629 T3630 E3631 E3632 H3633 Y3634 F3635 E3636 D3637 K3638 L3639 I3640 E3641 D3642 K3645 P3646 G3647 A3648 E3649 L3650 P3651 E3652 E3653 D3654 E3655 A3656 M3657 K3658 R3659 V3660 D3661
Q3665 R3672 E3677 K3678 C3679 K3680 L3681 E3682 E3683 D3684 F3685 D3692 K3696 H3699 D3700 E3701 E3702 D3703 D3704 D3705 G3706 E3707 E3708 E3709 V3710 K3711 S3712 F3713 E3714 E3715 K3716 E3717 M3718 R3729 D3732 R3733 E3737 E3749 I3762 A3763 I3764 V3772 D3778 E3782 D3785
S3800 D3803 L3804 F3807 Q3810 N3811 K3812 A3813 E3814 G3815 L3816 G3817 M3818 V3819 T3820 E3821 E3822 G3823 S3824 G3825 E3826 K3827 V3828 L3829 Q3830 D3831 D3832 E3833 D3837 L3838 F3839 L3844 E3847 F3853 Q3854 N3855 R3858 N3864 T3873 Y3874 D3875 D3886 F3887 Y3888 W3889 Y3890 Y3891 S3892


G3393 K3894 D3895 I3896 I3897 D3898 E3899 Q3900 G3901 Q3902 R3903 N3904 F3916 L3919 T3920 E3921 G3925 N3930 L3934 R3938 L3939 W3940 D3941 M3953 Q3954 M3955 K3956 L3957 S3958 Q3959 D3960 S3961 S3962 Q3963 I3964 E3965 L3966 L3967 M3971 D3972 L3973 Q3974 V3978 V3979 M3980 M3984 L3985 E3986 D4000
M4001 L4002 V4003 E4004 N4007 N4008 V4009 E4010 D4017 K4021 L4022 K4023 D4024 L4025 T4026 S4027 S4028 D4029 T4030 F4031 K4032 E4033 Y4034 D4035 P4036 D4037 G4038 K4039 G4040 V4041 I4042 S4043 K4044 R4045 D4046 F4047 H4048 K4049 A4050 M4051 E4052 S4053 H4054 K4055 H4056 Y4057 T4058 Q4059 S4060 E4061 T4062 E4063 F4064 L4065 L4066 S4067 C4068
A4069 E4070 T4071 D4072 E4073 N4074 E4075 T4076 L4077 D4078 Y4079 E4080 E4081 K4084 R4085 E4088 D4092 F4095 V4099 L4100 E4106 N4110 D4111 T4112 R4113 L4114 E4119 E4122 P4130 F4131 L4132 E4136 K4142 R4143 R4156 E4166 R4169 Q4170 D4174 E4178 G4179 G4180 E4181
K4182 E4183 E4186 E4207 SER ASP LEU ASN GLU ARG LEU ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN ALA PRO ARG MET GLY PHE PHE SER LEU LEU THR ILE GLN SER ALA LEU PHE ALA LEU ARG TYR ASN VAL LEU THR LEU VAL ARG MET LEU SER LEU LYS
SER LEU LYS LYS GLN MET LYS ARG MET LYS LYS MET THR VAL LYS ASP MET VAL LEU ALA PHE PHE SER SER TYR TRP SER VAL PHE VAL THR LEU LEU HIS PHE PHE VAL ALA SER VAL CYS ARG GLY PHE PHE ARG ILE VAL SER SER LEU LEU LEU GLY GLY SER LEU VAL ARG GLU GLY ALA
LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLU GLU GLU GLY GLU ARG LYS PRO LEU GLU SER ALA LEU PRO SER GLU ASP LEU THR ASP LEU LYS GLU LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU
ASP LEU LYS ARG GLU GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET THR ASN PRO VAL PRO VAL PRO GLU GLU VAL GLN GLU GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU LYS GLU GLU LYS GLU GLU THR LYS SER GLU PRO GLU LYS ALA GLU
GLY GLU ASP GLY GLU LYS GLU GLU LYS ALA LYS ASP GLU LYS SER LYS GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU PRO GLU VAL PRO GLU SER ALA F4478 W4479 K4480 K4481 I4482 I4483 A4484 Y4485 Q4486 K4487 K4488 L4489 R4501 L4505 F4506 T4522 SER SER VAL VAL GLU
GLY LYS GLU LEU PRO THR ARG THR SER SER ASP THR ALA LYS VAL THR ASN SER LEU ASP SER SER PRO HIS ARG ILE ILE A4555 V4556 H4557 E4561 E4562 S4563 S4564 G4565 Y4566 M4567 R4572 I4586 Y4589 R4607 D4612 G4613 L4614 Y4615 T4616 T4617 E4618 S4621 E4622 D4623 D4624
Q4628 W4629 D4630 R4631 Q4637 Y4643 W4644 D4645 R4650 K4651 D4654 E4658 F4659 R4662 D4663 R4664 I4665 S4666 E4667 M4671 D4672 K4673 A4674 A4675 L4676 D4677 F4678 SER ASP ALA ARG GLU LYS LYS PRO LYS LYS ASP SER L4693 S4694 A4695 V4696 L4697 N4698 S4699 I4700 D4701 V4702 K4703
D4715 M4725 D4744 M4747 G4748 F4749 K4750 R4753 T4754 I4755 Q4765 E4796 D4797 G4798 D4799 T4800 D4807 V4818 R4821 G4824 E4829 D4836 E4837 V4853 L4857 Q4862 D4867 R4873 D4874 E4881 D4882 T4885 D4895 D4898 H4912 F4920
V4939 W4940 K4941 W4948 E4949 D4965 E4962 ASP GLN LEU ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	102955	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	471.04, 471.04, 471.04	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	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, A1MG7

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	0.20	0/8695	0.31	0/11721
1	B	0.20	0/8695	0.31	0/11721
1	C	0.20	0/8695	0.31	0/11721
1	D	0.20	0/8695	0.31	0/11721
All	All	0.20	0/34780	0.31	0/46884

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3925	GLY	Peptide
1	A	4749	PHE	Peptide
1	B	3925	GLY	Peptide
1	B	4749	PHE	Peptide
1	C	3925	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	C	4749	PHE	Peptide
1	D	3925	GLY	Peptide
1	D	4749	PHE	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	8511	8308	8305	67	0
1	B	8511	8308	8305	71	0
1	C	8511	8308	8305	68	0
1	D	8511	8308	8305	68	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	25	12	0	0	0
3	B	25	12	0	0	0
3	C	25	12	0	0	0
3	D	25	12	0	0	0
All	All	34148	33280	33220	262	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3800:SER:OG	1:D:3830:GLN:O	2.05	0.74
1:D:3891:TYR:O	1:D:3956:LYS:NZ	2.20	0.74
1:C:3800:SER:OG	1:C:3830:GLN:O	2.05	0.74
1:B:3891:TYR:O	1:B:3956:LYS:NZ	2.21	0.73
1:A:3891:TYR:O	1:A:3956:LYS:NZ	2.21	0.73
1:B:3800:SER:OG	1:B:3830:GLN:O	2.05	0.73
1:C:3891:TYR:O	1:C:3956:LYS:NZ	2.21	0.72
1:A:4867:ASP:OD1	1:B:4873:ARG:NH1	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4873:ARG:NH1	1:D:4867:ASP:OD1	2.23	0.72
1:A:3800:SER:OG	1:A:3830:GLN:O	2.05	0.71
1:C:4867:ASP:OD1	1:D:4873:ARG:NH1	2.23	0.71
1:B:4867:ASP:OD1	1:C:4873:ARG:NH1	2.23	0.70
1:D:3634:TYR:OH	1:D:3701:GLU:OE1	2.10	0.70
1:A:3634:TYR:OH	1:A:3701:GLU:OE1	2.10	0.70
1:C:3634:TYR:OH	1:C:3701:GLU:OE1	2.10	0.69
1:B:3634:TYR:OH	1:B:3701:GLU:OE1	2.10	0.68
1:C:3900:GLN:OE1	1:C:3903:ARG:NH2	2.30	0.65
1:B:3900:GLN:OE1	1:B:3903:ARG:NH2	2.30	0.65
1:A:3900:GLN:OE1	1:A:3903:ARG:NH2	2.30	0.64
1:D:3900:GLN:OE1	1:D:3903:ARG:NH2	2.30	0.64
1:B:3653:GLU:OE1	1:B:3653:GLU:N	2.31	0.64
1:D:3653:GLU:OE1	1:D:3653:GLU:N	2.31	0.64
1:A:3653:GLU:N	1:A:3653:GLU:OE1	2.31	0.63
1:C:3653:GLU:N	1:C:3653:GLU:OE1	2.31	0.63
1:A:3920:THR:HG22	1:A:3980:MET:HA	1.85	0.58
1:C:3920:THR:HG22	1:C:3980:MET:HA	1.85	0.58
1:C:4607:ARG:NH2	1:C:4643:TYR:OH	2.37	0.58
1:D:3920:THR:HG22	1:D:3980:MET:HA	1.85	0.58
1:A:4607:ARG:NH2	1:A:4643:TYR:OH	2.37	0.58
1:B:3920:THR:HG22	1:B:3980:MET:HA	1.85	0.58
1:B:4607:ARG:NH2	1:B:4643:TYR:OH	2.37	0.57
1:D:4607:ARG:NH2	1:D:4643:TYR:OH	2.37	0.57
1:B:3683:GLU:N	1:B:3683:GLU:OE1	2.39	0.56
1:C:3683:GLU:OE1	1:C:3683:GLU:N	2.39	0.56
1:B:4136:GLU:OE1	1:B:4912:HIS:NE2	2.38	0.56
1:D:3934:LEU:HD12	1:D:3939:LEU:HD22	1.88	0.56
1:A:4136:GLU:OE1	1:A:4912:HIS:NE2	2.38	0.56
1:A:3683:GLU:OE1	1:A:3683:GLU:N	2.39	0.56
1:A:3934:LEU:HD12	1:A:3939:LEU:HD22	1.88	0.56
1:D:3683:GLU:N	1:D:3683:GLU:OE1	2.39	0.56
1:D:4136:GLU:OE1	1:D:4912:HIS:NE2	2.38	0.56
1:D:3916:PHE:O	1:D:3920:THR:HG23	2.06	0.55
1:A:3894:LYS:O	1:A:3956:LYS:NZ	2.23	0.55
1:A:3916:PHE:O	1:A:3920:THR:HG23	2.06	0.55
1:C:3916:PHE:O	1:C:3920:THR:HG23	2.06	0.55
1:B:3764:ILE:HG22	1:B:3772:VAL:HG21	1.89	0.55
1:A:3764:ILE:HG22	1:A:3772:VAL:HG21	1.89	0.55
1:C:3934:LEU:HD12	1:C:3939:LEU:HD22	1.87	0.55
1:C:4136:GLU:OE1	1:C:4912:HIS:NE2	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3934:LEU:HD12	1:B:3939:LEU:HD22	1.88	0.54
1:B:3916:PHE:O	1:B:3920:THR:HG23	2.06	0.54
1:C:3919:LEU:HD22	1:C:3934:LEU:HD11	1.90	0.54
1:B:3919:LEU:HD22	1:B:3934:LEU:HD11	1.90	0.54
1:D:3764:ILE:HG22	1:D:3772:VAL:HG21	1.89	0.54
1:D:3919:LEU:HD22	1:D:3934:LEU:HD11	1.90	0.54
1:C:3764:ILE:HG22	1:C:3772:VAL:HG21	1.89	0.53
1:D:4796:GLU:N	1:D:4796:GLU:OE1	2.42	0.53
1:A:3919:LEU:HD22	1:A:3934:LEU:HD11	1.90	0.53
1:C:4796:GLU:N	1:C:4796:GLU:OE1	2.42	0.52
1:C:3737:GLU:N	1:C:3737:GLU:OE1	2.43	0.52
1:A:3822:GLU:N	1:A:3822:GLU:OE1	2.42	0.52
1:D:3822:GLU:N	1:D:3822:GLU:OE1	2.42	0.52
1:D:4836:ASP:OD1	1:D:4837:GLU:N	2.43	0.52
1:B:3762:ILE:HD11	1:B:3837:ASP:O	2.10	0.52
1:D:3762:ILE:HD11	1:D:3837:ASP:O	2.10	0.52
1:B:3822:GLU:N	1:B:3822:GLU:OE1	2.42	0.52
1:B:4836:ASP:OD1	1:B:4837:GLU:N	2.43	0.52
1:C:3891:TYR:OH	1:C:3898:ASP:OD1	2.26	0.52
1:C:4836:ASP:OD1	1:C:4837:GLU:N	2.43	0.52
1:C:3762:ILE:HD11	1:C:3837:ASP:O	2.10	0.52
1:C:3822:GLU:N	1:C:3822:GLU:OE1	2.42	0.52
1:D:4178:GLU:N	1:D:4178:GLU:OE1	2.43	0.52
1:A:3737:GLU:OE1	1:A:3737:GLU:N	2.43	0.51
1:B:4178:GLU:N	1:B:4178:GLU:OE1	2.43	0.51
1:B:3737:GLU:OE1	1:B:3737:GLU:N	2.43	0.51
1:A:3762:ILE:HD11	1:A:3837:ASP:O	2.10	0.51
1:C:4178:GLU:OE1	1:C:4178:GLU:N	2.43	0.51
1:B:3626:SER:O	1:B:3630:THR:OG1	2.22	0.51
1:A:3891:TYR:OH	1:A:3898:ASP:OD1	2.26	0.51
1:B:4796:GLU:OE1	1:B:4796:GLU:N	2.42	0.51
1:A:4178:GLU:N	1:A:4178:GLU:OE1	2.43	0.51
1:A:4836:ASP:OD1	1:A:4837:GLU:N	2.43	0.50
1:D:3655:GLU:N	1:D:3655:GLU:OE1	2.44	0.50
1:B:3655:GLU:OE1	1:B:3655:GLU:N	2.44	0.50
1:D:3839:PHE:CE1	1:D:3873:THR:HG23	2.46	0.50
1:D:3891:TYR:OH	1:D:3898:ASP:OD1	2.26	0.50
1:D:3737:GLU:OE1	1:D:3737:GLU:N	2.43	0.50
1:A:3844:LEU:HD23	1:A:3847:GLU:OE1	2.12	0.49
1:A:4796:GLU:N	1:A:4796:GLU:OE1	2.42	0.49
1:B:3839:PHE:CE1	1:B:3873:THR:HG23	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3839:PHE:CE1	1:C:3873:THR:HG23	2.47	0.49
1:C:3844:LEU:HD23	1:C:3847:GLU:OE1	2.12	0.49
1:A:3839:PHE:CE1	1:A:3873:THR:HG23	2.47	0.49
1:D:3844:LEU:HD23	1:D:3847:GLU:OE1	2.12	0.49
1:B:3844:LEU:HD23	1:B:3847:GLU:OE1	2.12	0.49
1:B:3891:TYR:OH	1:B:3898:ASP:OD1	2.26	0.49
1:C:3650:LEU:HD12	1:C:3651:PRO:N	2.27	0.49
1:D:3650:LEU:HD12	1:D:3651:PRO:N	2.27	0.49
1:A:3655:GLU:N	1:A:3655:GLU:OE1	2.44	0.49
1:B:3650:LEU:HD12	1:B:3651:PRO:N	2.27	0.49
1:C:3655:GLU:N	1:C:3655:GLU:OE1	2.44	0.49
1:B:4095:PHE:O	1:B:4099:VAL:HG23	2.13	0.48
1:A:3650:LEU:HD12	1:A:3651:PRO:N	2.27	0.48
1:A:3682:GLU:N	1:A:3682:GLU:OE1	2.47	0.48
1:C:4095:PHE:O	1:C:4099:VAL:HG23	2.13	0.48
1:A:4505:LEU:HD22	1:A:4749:PHE:CE2	2.49	0.48
1:D:4095:PHE:O	1:D:4099:VAL:HG23	2.13	0.48
1:B:4099:VAL:HG22	1:B:4132:LEU:HD13	1.96	0.48
1:C:4505:LEU:HD22	1:C:4749:PHE:CE2	2.49	0.48
1:D:4099:VAL:HG22	1:D:4132:LEU:HD13	1.96	0.48
1:B:3682:GLU:OE1	1:B:3682:GLU:N	2.47	0.48
1:B:4645:ASP:OD2	1:B:4651:LYS:NZ	2.47	0.48
1:C:4088:GLU:N	1:C:4088:GLU:OE1	2.47	0.48
1:B:4853:VAL:HA	1:B:4857:LEU:HD12	1.96	0.48
1:C:4186:GLU:OE1	1:C:4948:TRP:NE1	2.45	0.48
1:C:4645:ASP:OD2	1:C:4651:LYS:NZ	2.47	0.48
1:D:4645:ASP:OD2	1:D:4651:LYS:NZ	2.47	0.48
1:C:4853:VAL:HA	1:C:4857:LEU:HD12	1.96	0.48
1:B:3888:TYR:O	1:B:3892:SER:N	2.47	0.47
1:A:4095:PHE:O	1:A:4099:VAL:HG23	2.13	0.47
1:B:4170:GLN:NE2	1:B:4174:ASP:OD1	2.47	0.47
1:D:4170:GLN:NE2	1:D:4174:ASP:OD1	2.47	0.47
1:B:3894:LYS:O	1:B:3956:LYS:NZ	2.23	0.47
1:A:3839:PHE:HE1	1:A:3873:THR:HG23	1.79	0.47
1:A:3888:TYR:O	1:A:3892:SER:N	2.47	0.47
1:B:4088:GLU:N	1:B:4088:GLU:OE1	2.47	0.47
1:C:3682:GLU:N	1:C:3682:GLU:OE1	2.47	0.47
1:C:4170:GLN:NE2	1:C:4174:ASP:OD1	2.47	0.47
1:D:4088:GLU:N	1:D:4088:GLU:OE1	2.47	0.47
1:A:4645:ASP:OD2	1:A:4651:LYS:NZ	2.47	0.47
1:A:4824:GLY:O	1:B:4821:ARG:NH1	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3888:TYR:O	1:D:3892:SER:N	2.47	0.47
1:A:4170:GLN:NE2	1:A:4174:ASP:OD1	2.47	0.47
1:A:4616:ILE:HD12	1:A:4665:ILE:HD13	1.97	0.47
1:A:4821:ARG:NH1	1:D:4824:GLY:O	2.46	0.47
1:B:4505:LEU:HD22	1:B:4749:PHE:CE2	2.49	0.47
1:D:4505:LEU:HD22	1:D:4749:PHE:CE2	2.49	0.47
1:D:4616:ILE:HD12	1:D:4665:ILE:HD13	1.97	0.47
1:A:3855:ASN:OD1	1:A:3858:ARG:NH2	2.48	0.47
1:A:3900:GLN:O	1:A:3904:ASN:ND2	2.48	0.47
1:B:3855:ASN:OD1	1:B:3858:ARG:NH2	2.48	0.47
1:B:4824:GLY:O	1:C:4821:ARG:NH1	2.46	0.47
1:C:4099:VAL:HG22	1:C:4132:LEU:HD13	1.96	0.47
1:D:3682:GLU:OE1	1:D:3682:GLU:N	2.47	0.47
1:A:4088:GLU:N	1:A:4088:GLU:OE1	2.47	0.47
1:D:3855:ASN:OD1	1:D:3858:ARG:NH2	2.48	0.47
1:A:4186:GLU:OE1	1:A:4948:TRP:NE1	2.45	0.47
1:B:3839:PHE:HE1	1:B:3873:THR:HG23	1.79	0.47
1:B:4073:GLU:OE1	1:B:4073:GLU:N	2.45	0.47
1:B:4186:GLU:OE1	1:B:4948:TRP:NE1	2.45	0.47
1:C:3888:TYR:O	1:C:3892:SER:N	2.47	0.47
1:C:3900:GLN:O	1:C:3904:ASN:ND2	2.48	0.47
1:D:3605:ALA:HB3	1:D:3606:PRO:HD3	1.97	0.47
1:A:3636:GLU:OE1	1:A:3636:GLU:N	2.47	0.47
1:C:4616:ILE:HD12	1:C:4665:ILE:HD13	1.97	0.47
1:C:4824:GLY:O	1:D:4821:ARG:NH1	2.46	0.47
1:D:3839:PHE:HE1	1:D:3873:THR:HG23	1.79	0.47
1:A:4099:VAL:HG22	1:A:4132:LEU:HD13	1.96	0.46
1:B:3900:GLN:O	1:B:3904:ASN:ND2	2.48	0.46
1:C:3839:PHE:HE1	1:C:3873:THR:HG23	1.79	0.46
1:D:4186:GLU:OE1	1:D:4948:TRP:NE1	2.45	0.46
1:D:3636:GLU:OE1	1:D:3636:GLU:N	2.47	0.46
1:A:3826:GLU:OE2	1:A:3830:GLN:NE2	2.49	0.46
1:C:3636:GLU:OE1	1:C:3636:GLU:N	2.47	0.46
1:C:3855:ASN:OD1	1:C:3858:ARG:NH2	2.48	0.46
1:C:3605:ALA:HB3	1:C:3606:PRO:HD3	1.97	0.46
1:C:3626:SER:O	1:C:3630:THR:OG1	2.23	0.46
1:D:4853:VAL:HA	1:D:4857:LEU:HD12	1.96	0.46
1:A:4853:VAL:HA	1:A:4857:LEU:HD12	1.96	0.46
1:B:3826:GLU:OE2	1:B:3830:GLN:NE2	2.49	0.46
1:C:3960:ASP:OD1	1:C:3962:SER:OG	2.25	0.46
1:C:3974:GLN:O	1:C:3978:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3605:ALA:HB3	1:A:3606:PRO:HD3	1.97	0.46
1:B:3985:LEU:HD12	1:B:4100:LEU:HD12	1.98	0.46
1:A:4765:GLN:OE1	1:B:4755:ILE:HD11	2.16	0.46
1:A:4628:GLN:OE1	1:A:4631:ARG:NH1	2.49	0.46
1:B:3605:ALA:HB3	1:B:3606:PRO:HD3	1.97	0.46
1:B:4616:ILE:HD12	1:B:4665:ILE:HD13	1.97	0.46
1:B:4765:GLN:OE1	1:C:4755:ILE:HD11	2.16	0.46
1:C:4073:GLU:OE1	1:C:4073:GLU:N	2.45	0.46
1:C:4628:GLN:OE1	1:C:4631:ARG:NH1	2.49	0.46
1:D:3985:LEU:HD12	1:D:4100:LEU:HD12	1.98	0.46
1:D:4099:VAL:HG22	1:D:4132:LEU:CD1	2.46	0.46
1:A:3985:LEU:HD12	1:A:4100:LEU:HD12	1.98	0.45
1:B:4628:GLN:OE1	1:B:4631:ARG:NH1	2.49	0.45
1:D:3900:GLN:O	1:D:3904:ASN:ND2	2.48	0.45
1:A:3974:GLN:O	1:A:3978:VAL:HG23	2.16	0.45
1:A:4755:ILE:HD11	1:D:4765:GLN:OE1	2.16	0.45
1:C:3985:LEU:HD12	1:C:4100:LEU:HD12	1.98	0.45
1:A:4099:VAL:HG22	1:A:4132:LEU:CD1	2.46	0.45
1:B:3974:GLN:O	1:B:3978:VAL:HG23	2.16	0.45
1:C:3826:GLU:OE2	1:C:3830:GLN:NE2	2.49	0.45
1:C:4099:VAL:HG22	1:C:4132:LEU:CD1	2.46	0.45
1:B:4099:VAL:HG22	1:B:4132:LEU:CD1	2.46	0.45
1:D:4628:GLN:OE1	1:D:4631:ARG:NH1	2.49	0.45
1:A:4501:ARG:NH2	1:A:4744:ASP:OD1	2.50	0.45
1:B:4130:PRO:O	1:B:4156:ARG:NH1	2.50	0.45
1:C:4501:ARG:NH2	1:C:4744:ASP:OD1	2.50	0.45
1:D:4073:GLU:OE1	1:D:4073:GLU:N	2.45	0.45
1:A:4130:PRO:O	1:A:4156:ARG:NH1	2.50	0.45
1:C:4765:GLN:OE1	1:D:4755:ILE:HD11	2.16	0.45
1:D:3826:GLU:OE2	1:D:3830:GLN:NE2	2.49	0.45
1:D:4818:VAL:HG12	1:D:4829:GLU:HG3	2.00	0.44
1:D:4501:ARG:NH2	1:D:4744:ASP:OD1	2.50	0.44
1:B:4589:TYR:OH	1:B:4715:ASP:OD2	2.32	0.44
1:B:4818:VAL:HG12	1:B:4829:GLU:HG3	2.00	0.44
1:B:3960:ASP:OD1	1:B:3962:SER:OG	2.25	0.44
1:C:4130:PRO:O	1:C:4156:ARG:NH1	2.50	0.44
1:D:4130:PRO:O	1:D:4156:ARG:NH1	2.50	0.44
1:A:4073:GLU:OE1	1:A:4073:GLU:N	2.45	0.44
1:A:4818:VAL:HG12	1:A:4829:GLU:HG3	2.00	0.44
1:D:3626:SER:O	1:D:3630:THR:OG1	2.22	0.44
1:B:3636:GLU:OE1	1:B:3636:GLU:N	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4501:ARG:NH2	1:B:4744:ASP:OD1	2.50	0.44
1:D:4920:PHE:HE2	1:D:4939:VAL:HG11	1.83	0.44
1:C:3894:LYS:O	1:C:3956:LYS:NZ	2.24	0.44
1:D:3974:GLN:O	1:D:3978:VAL:HG23	2.16	0.44
1:D:4589:TYR:OH	1:D:4715:ASP:OD2	2.32	0.44
1:B:4927:LYS:NZ	1:B:4936:GLU:OE1	2.38	0.43
1:C:4818:VAL:HG12	1:C:4829:GLU:HG3	2.00	0.43
1:A:4920:PHE:HE2	1:A:4939:VAL:HG11	1.83	0.43
1:C:4920:PHE:HE2	1:C:4939:VAL:HG11	1.83	0.43
1:B:3729:ARG:O	1:B:3733:ARG:NH1	2.52	0.43
1:A:4505:LEU:HD22	1:A:4749:PHE:CD2	2.54	0.43
1:D:3729:ARG:O	1:D:3733:ARG:NH1	2.52	0.43
1:B:3854:GLN:NE2	1:B:3921:GLU:O	2.52	0.42
1:B:4920:PHE:HE2	1:B:4939:VAL:HG11	1.83	0.42
1:A:4807:ASP:OD1	1:A:4807:ASP:N	2.52	0.42
1:C:4505:LEU:HD22	1:C:4749:PHE:CD2	2.54	0.42
1:D:4505:LEU:HD22	1:D:4749:PHE:CD2	2.54	0.42
1:B:3954:GLN:O	1:B:3958:SER:OG	2.33	0.42
1:B:4505:LEU:HD22	1:B:4749:PHE:CD2	2.54	0.42
1:D:4807:ASP:OD1	1:D:4807:ASP:N	2.51	0.42
1:C:4807:ASP:OD1	1:C:4807:ASP:N	2.52	0.42
1:A:3729:ARG:O	1:A:3733:ARG:NH1	2.52	0.42
1:B:4807:ASP:OD1	1:B:4807:ASP:N	2.52	0.42
1:A:4586:ILE:HD11	1:A:4725:MET:HB2	2.01	0.42
1:C:3854:GLN:NE2	1:C:3921:GLU:O	2.52	0.42
1:D:3833:GLU:OE1	1:D:3833:GLU:N	2.49	0.42
1:D:4586:ILE:HD11	1:D:4725:MET:HB2	2.01	0.42
1:B:4586:ILE:HD11	1:B:4725:MET:HB2	2.01	0.41
1:A:3854:GLN:NE2	1:A:3921:GLU:O	2.52	0.41
1:A:3960:ASP:OD1	1:A:3962:SER:OG	2.25	0.41
1:B:3851:SER:O	1:B:3855:ASN:ND2	2.51	0.41
1:A:4136:GLU:OE2	1:A:4146:ARG:NH1	2.54	0.41
1:D:3854:GLN:NE2	1:D:3921:GLU:O	2.52	0.41
1:D:4881:GLU:O	1:D:4885:THR:HG22	2.21	0.41
1:A:3939:LEU:CD2	1:A:3984:MET:HE3	2.51	0.41
1:C:3649:GLU:OE1	1:C:3649:GLU:N	2.50	0.41
1:C:4586:ILE:HD11	1:C:4725:MET:HB2	2.01	0.41
1:C:4589:TYR:OH	1:C:4715:ASP:OD2	2.32	0.41
1:D:3930:ASN:O	1:D:3934:LEU:HD23	2.21	0.41
1:D:3939:LEU:CD2	1:D:3984:MET:HE3	2.51	0.41
1:A:3649:GLU:OE1	1:A:3649:GLU:N	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4136:GLU:OE2	1:B:4146:ARG:NH1	2.54	0.40
1:C:3930:ASN:O	1:C:3934:LEU:HD23	2.21	0.40
1:A:3930:ASN:O	1:A:3934:LEU:HD23	2.21	0.40
1:D:3960:ASP:OD1	1:D:3962:SER:OG	2.25	0.40
1:C:3954:GLN:O	1:C:3958:SER:OG	2.33	0.40
1:B:3930:ASN:O	1:B:3934:LEU:HD23	2.21	0.40
1:B:3939:LEU:CD2	1:B:3984:MET:HE3	2.51	0.40
1:C:3939:LEU:CD2	1:C:3984:MET:HE3	2.51	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	1034/4966 (21%)	1007 (97%)	27 (3%)	0	100	100
1	B	1034/4966 (21%)	1007 (97%)	27 (3%)	0	100	100
1	C	1034/4966 (21%)	1007 (97%)	27 (3%)	0	100	100
1	D	1034/4966 (21%)	1005 (97%)	29 (3%)	0	100	100
All	All	4136/19864 (21%)	4026 (97%)	110 (3%)	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	929/4355 (21%)	921 (99%)	8 (1%)	70 82
1	B	929/4355 (21%)	921 (99%)	8 (1%)	70 82
1	C	929/4355 (21%)	921 (99%)	8 (1%)	70 82
1	D	929/4355 (21%)	921 (99%)	8 (1%)	70 82
All	All	3716/17420 (21%)	3684 (99%)	32 (1%)	68 82

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3699	HIS
1	A	3816	LEU
1	A	3853	PHE
1	A	3887	PHE
1	A	4614	LEU
1	A	4807	ASP
1	A	4862	GLN
1	A	4941	LYS
1	B	3699	HIS
1	B	3816	LEU
1	B	3853	PHE
1	B	3887	PHE
1	B	4614	LEU
1	B	4807	ASP
1	B	4862	GLN
1	B	4941	LYS
1	C	3699	HIS
1	C	3816	LEU
1	C	3853	PHE
1	C	3887	PHE
1	C	4614	LEU
1	C	4807	ASP
1	C	4862	GLN
1	C	4941	LYS
1	D	3699	HIS
1	D	3816	LEU
1	D	3853	PHE
1	D	3887	PHE
1	D	4614	LEU
1	D	4807	ASP
1	D	4862	GLN
1	D	4941	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3774	GLN
1	A	3810	GLN
1	A	3849	HIS
1	A	3952	HIS
1	A	4487	GLN
1	A	4698	ASN
1	A	4786	ASN
1	B	3810	GLN
1	B	3849	HIS
1	B	3952	HIS
1	B	4487	GLN
1	B	4698	ASN
1	B	4786	ASN
1	C	3810	GLN
1	C	3849	HIS
1	C	4487	GLN
1	C	4698	ASN
1	D	3810	GLN
1	D	3849	HIS
1	D	4487	GLN
1	D	4698	ASN
1	D	4786	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	A1MG7	A	5002	-	27,27,27	1.62	5 (18%)	36,38,38	2.53	10 (27%)
3	A1MG7	C	5002	-	27,27,27	1.63	5 (18%)	36,38,38	2.53	10 (27%)
3	A1MG7	D	5002	-	27,27,27	1.63	6 (22%)	36,38,38	2.53	10 (27%)
3	A1MG7	B	5002	-	27,27,27	1.63	5 (18%)	36,38,38	2.54	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1MG7	A	5002	-	-	0/16/16/16	0/3/3/3
3	A1MG7	C	5002	-	-	0/16/16/16	0/3/3/3
3	A1MG7	D	5002	-	-	0/16/16/16	0/3/3/3
3	A1MG7	B	5002	-	-	0/16/16/16	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5002	A1MG7	C-NAO	4.96	1.45	1.35
3	C	5002	A1MG7	C-NAO	4.94	1.45	1.35
3	B	5002	A1MG7	C-NAO	4.93	1.45	1.35
3	A	5002	A1MG7	C-NAO	4.89	1.45	1.35
3	A	5002	A1MG7	N-NAH	3.13	1.37	1.33
3	B	5002	A1MG7	N-NAH	3.13	1.37	1.33
3	D	5002	A1MG7	N-NAH	3.13	1.37	1.33
3	C	5002	A1MG7	N-NAH	3.12	1.37	1.33
3	A	5002	A1MG7	N-NAJ	2.91	1.36	1.32
3	B	5002	A1MG7	N-NAJ	2.91	1.36	1.32
3	A	5002	A1MG7	NAK-NAJ	2.90	1.36	1.32
3	B	5002	A1MG7	NAK-NAJ	2.90	1.36	1.32
3	C	5002	A1MG7	NAK-NAJ	2.90	1.36	1.32
3	D	5002	A1MG7	N-NAJ	2.89	1.36	1.32
3	C	5002	A1MG7	CAF-CAG	2.87	1.52	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5002	A1MG7	NAK-NAJ	2.87	1.36	1.32
3	C	5002	A1MG7	N-NAJ	2.85	1.36	1.32
3	D	5002	A1MG7	CAF-CAG	2.81	1.52	1.47
3	A	5002	A1MG7	CAF-CAG	2.80	1.52	1.47
3	B	5002	A1MG7	CAF-CAG	2.78	1.52	1.47
3	D	5002	A1MG7	O-C	-2.03	1.18	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	5002	A1MG7	CAG-NAH-N	7.91	107.96	101.70
3	A	5002	A1MG7	CAG-NAH-N	7.90	107.95	101.70
3	B	5002	A1MG7	CAG-NAH-N	7.90	107.95	101.70
3	C	5002	A1MG7	CAG-NAH-N	7.87	107.93	101.70
3	D	5002	A1MG7	NAH-N-NAJ	-7.03	108.07	114.03
3	A	5002	A1MG7	NAH-N-NAJ	-7.03	108.07	114.03
3	B	5002	A1MG7	NAH-N-NAJ	-7.03	108.07	114.03
3	C	5002	A1MG7	NAH-N-NAJ	-6.99	108.11	114.03
3	D	5002	A1MG7	CA-N-NAJ	5.88	127.16	122.59
3	C	5002	A1MG7	CA-N-NAJ	5.86	127.14	122.59
3	A	5002	A1MG7	CA-N-NAJ	5.85	127.13	122.59
3	B	5002	A1MG7	CA-N-NAJ	5.85	127.13	122.59
3	D	5002	A1MG7	NAH-CAG-NAK	-3.81	108.44	112.00
3	C	5002	A1MG7	NAH-CAG-NAK	-3.81	108.45	112.00
3	A	5002	A1MG7	NAH-CAG-NAK	-3.80	108.45	112.00
3	B	5002	A1MG7	NAH-CAG-NAK	-3.80	108.45	112.00
3	B	5002	A1MG7	CAE-CAD-CAC	-2.88	119.88	123.52
3	A	5002	A1MG7	CAE-CAD-CAC	-2.87	119.90	123.52
3	D	5002	A1MG7	CAE-CAD-CAC	-2.85	119.92	123.52
3	C	5002	A1MG7	CAE-CAD-CAC	-2.84	119.93	123.52
3	C	5002	A1MG7	CAC-CAB-CAA	-2.67	120.14	123.52
3	A	5002	A1MG7	CAC-CAB-CAA	-2.66	120.15	123.52
3	B	5002	A1MG7	CAC-CAB-CAA	-2.66	120.15	123.52
3	D	5002	A1MG7	CAC-CAB-CAA	-2.61	120.22	123.52
3	B	5002	A1MG7	CAF-CAG-NAK	2.55	126.93	123.96
3	A	5002	A1MG7	CAF-CAG-NAK	2.53	126.91	123.96
3	A	5002	A1MG7	CAD-CAC-CAB	2.52	120.06	116.13
3	B	5002	A1MG7	CAD-CAC-CAB	2.52	120.06	116.13
3	C	5002	A1MG7	CAF-CAG-NAK	2.51	126.89	123.96
3	D	5002	A1MG7	CAF-CAG-NAK	2.50	126.88	123.96
3	C	5002	A1MG7	CAD-CAC-CAB	2.49	120.00	116.13
3	D	5002	A1MG7	CAD-CAC-CAB	2.47	119.97	116.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	5002	A1MG7	CAG-NAK-NAJ	2.27	107.73	105.91
3	A	5002	A1MG7	CAG-NAK-NAJ	2.25	107.71	105.91
3	B	5002	A1MG7	CAG-NAK-NAJ	2.25	107.71	105.91
3	C	5002	A1MG7	CAG-NAK-NAJ	2.25	107.71	105.91
3	A	5002	A1MG7	N-NAJ-NAK	2.22	107.81	105.99
3	B	5002	A1MG7	N-NAJ-NAK	2.22	107.81	105.99
3	C	5002	A1MG7	N-NAJ-NAK	2.21	107.81	105.99
3	D	5002	A1MG7	N-NAJ-NAK	2.21	107.80	105.99

There are no chirality outliers.

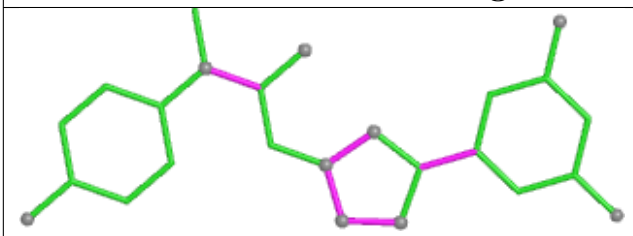
There are no torsion outliers.

There are no ring outliers.

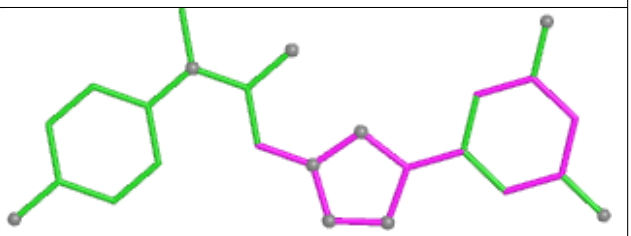
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

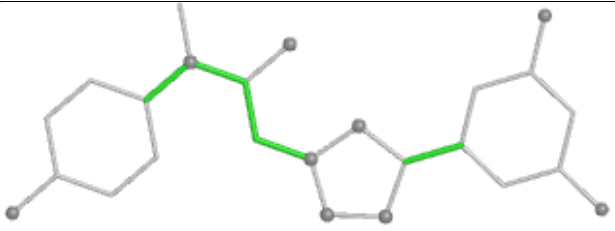
Ligand A1MG7 A 5002



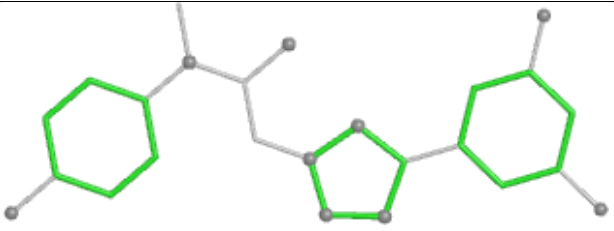
Bond lengths



Bond angles

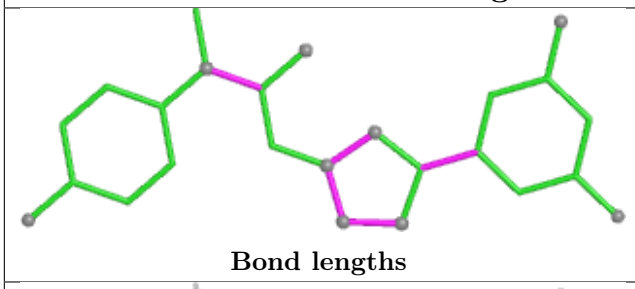


Torsions

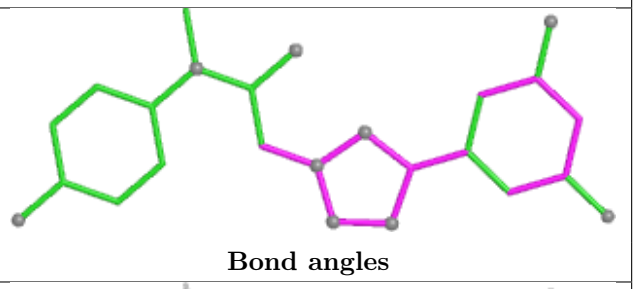


Rings

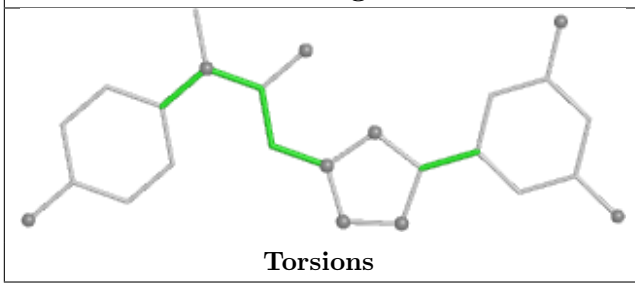
Ligand A1MG7 C 5002



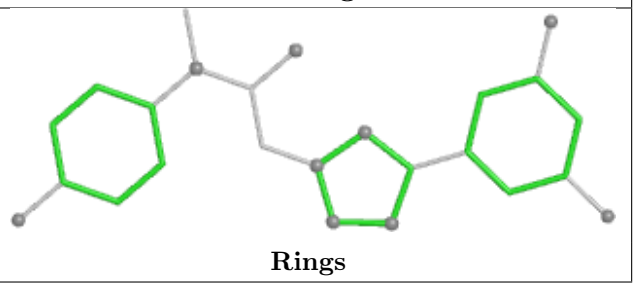
Bond lengths



Bond angles

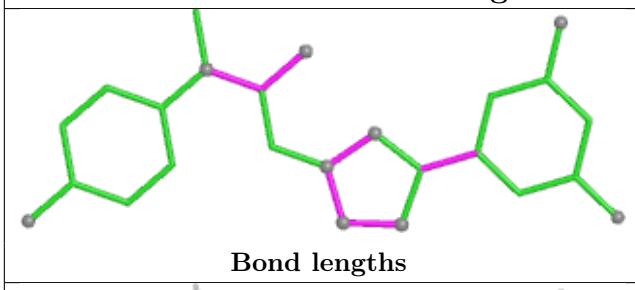


Torsions

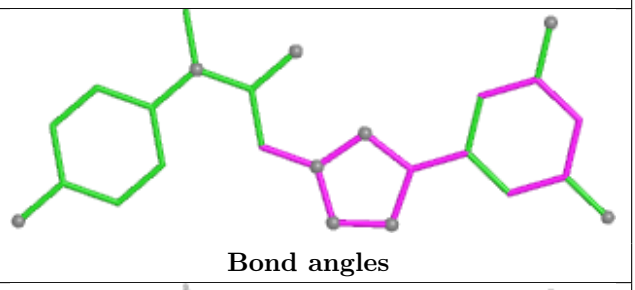


Rings

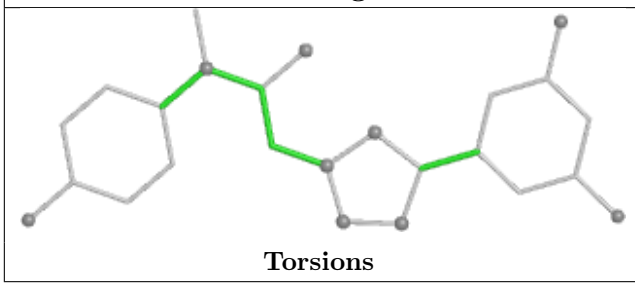
Ligand A1MG7 D 5002



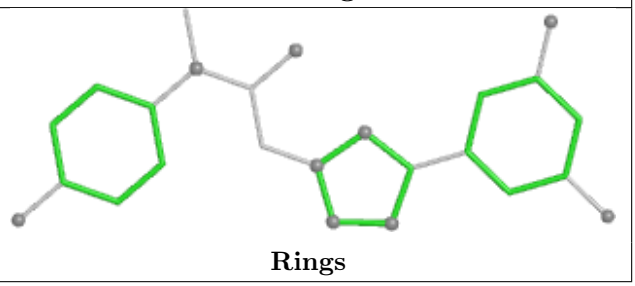
Bond lengths



Bond angles

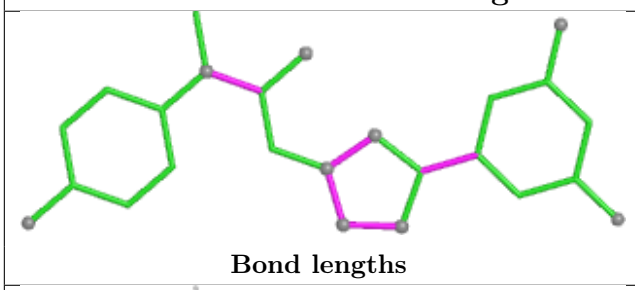


Torsions

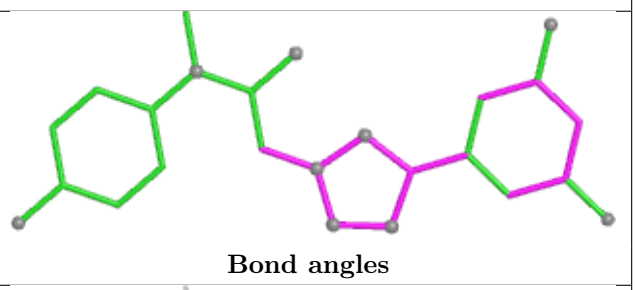


Rings

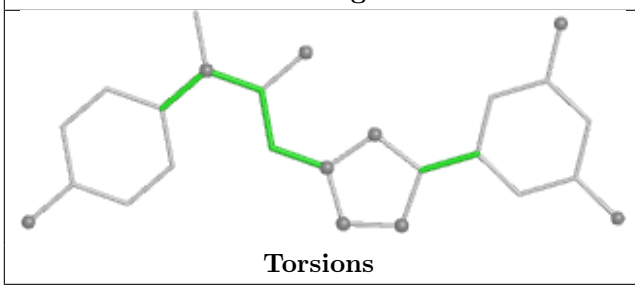
Ligand A1MG7 B 5002



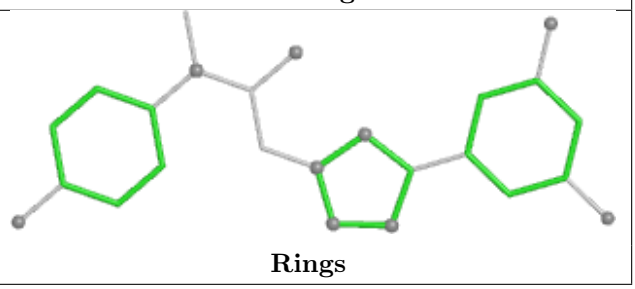
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

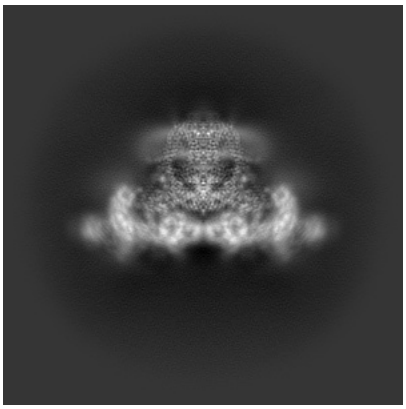
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-80692. These allow visual inspection of the internal detail of the map and identification of artifacts.

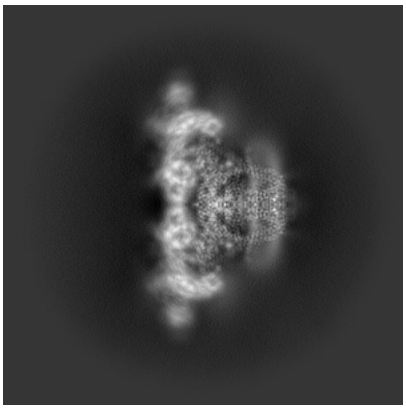
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

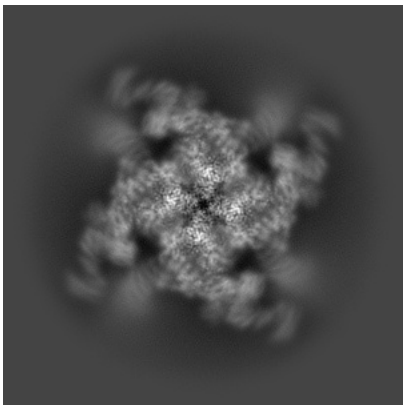
6.1.1 Primary map



X

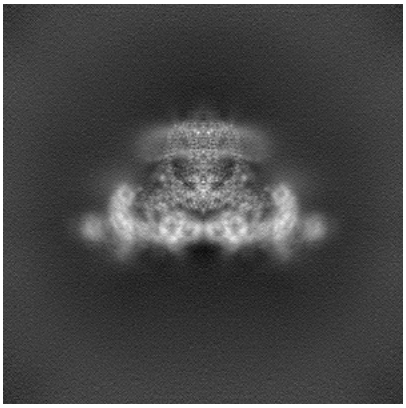


Y

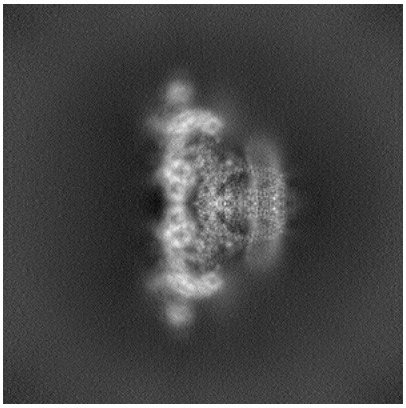


Z

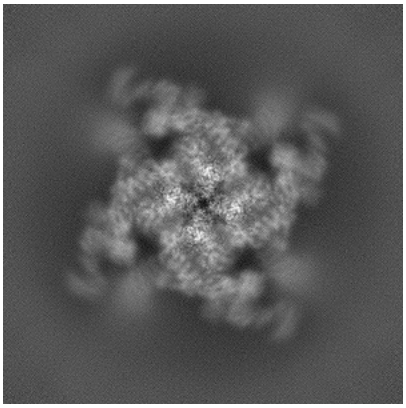
6.1.2 Raw map



X



Y

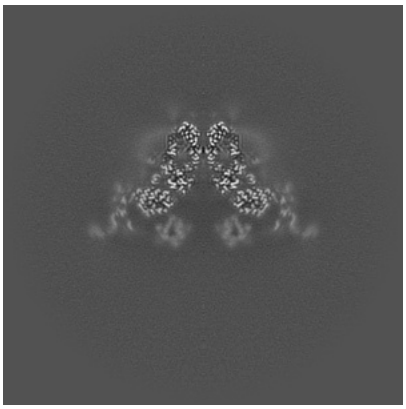


Z

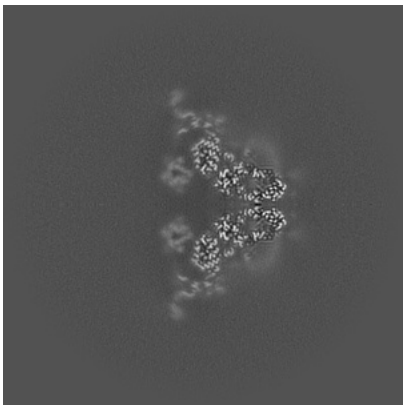
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

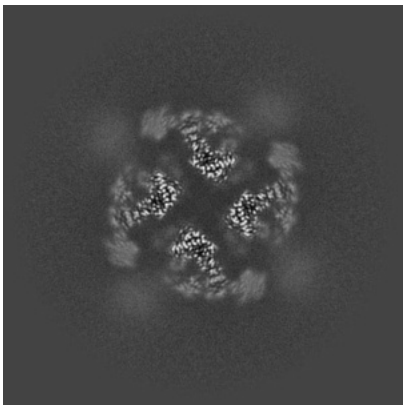
6.2.1 Primary map



X Index: 256

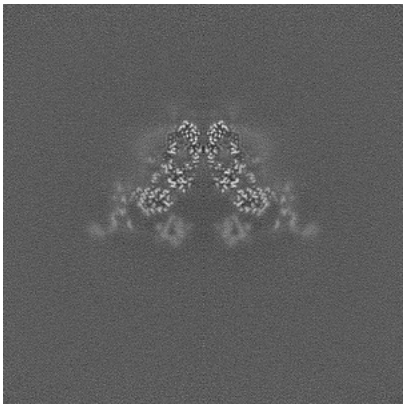


Y Index: 256

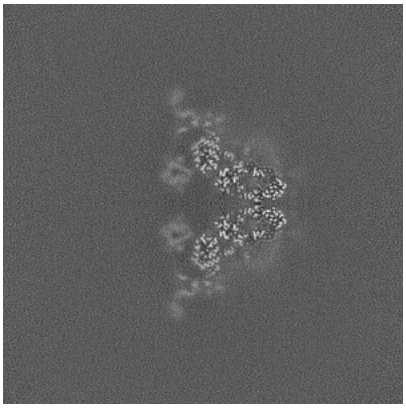


Z Index: 256

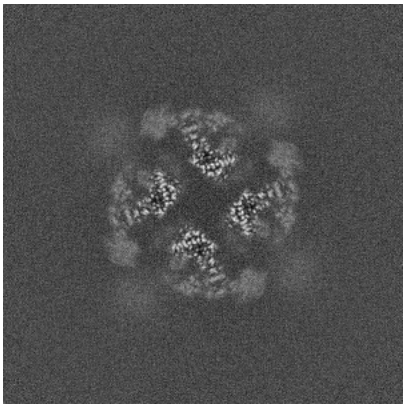
6.2.2 Raw map



X Index: 256



Y Index: 256

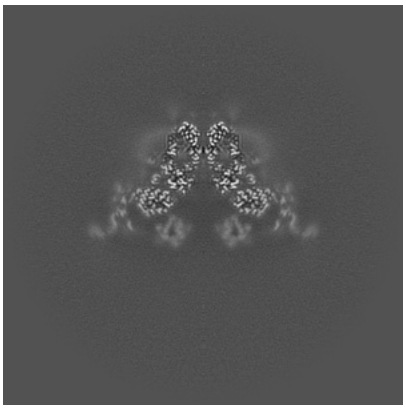


Z Index: 256

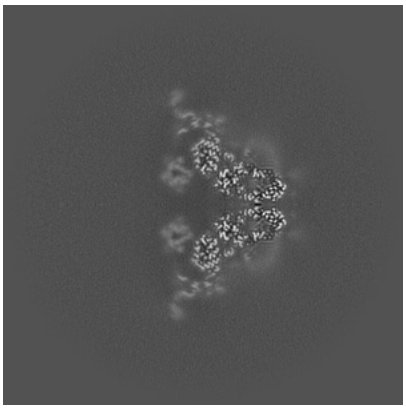
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

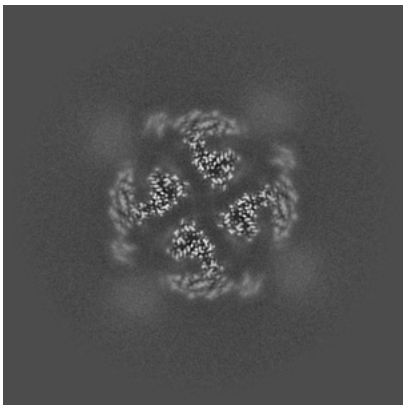
6.3.1 Primary map



X Index: 256

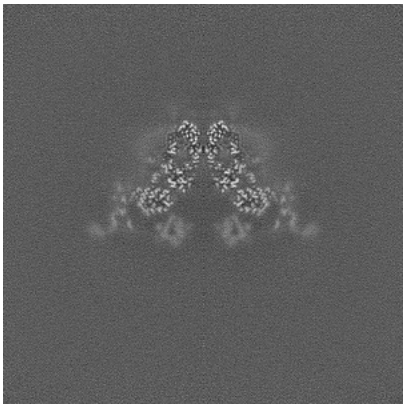


Y Index: 256

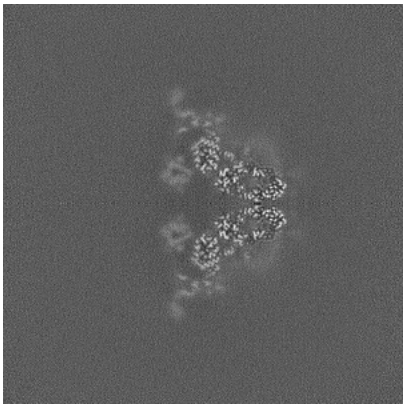


Z Index: 262

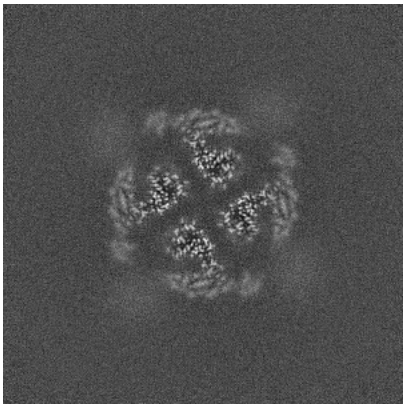
6.3.2 Raw map



X Index: 256



Y Index: 256

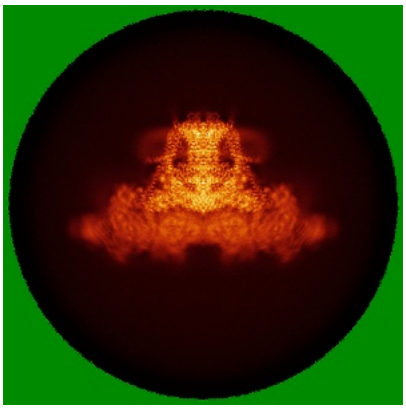


Z Index: 262

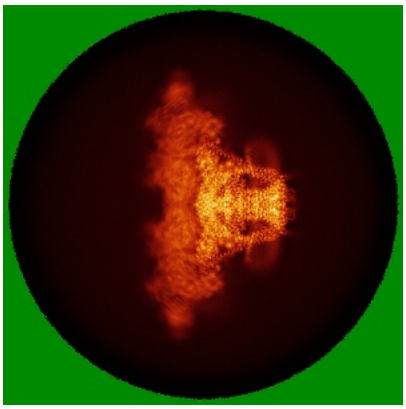
The images above show the largest variance slices of the map in three orthogonal directions.

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

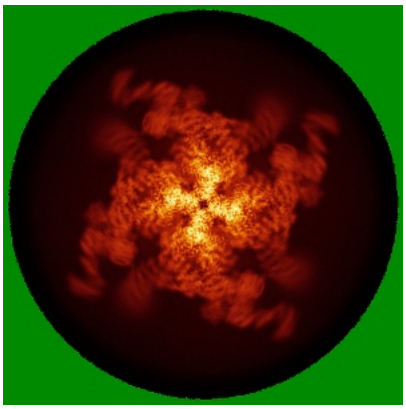
6.4.1 Primary map



X

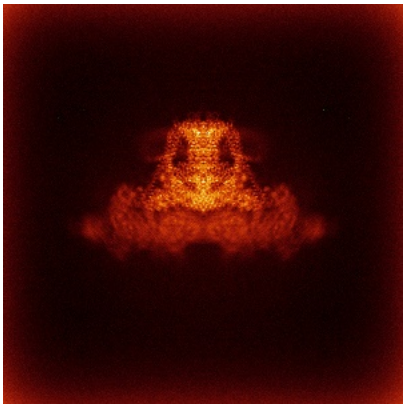


Y

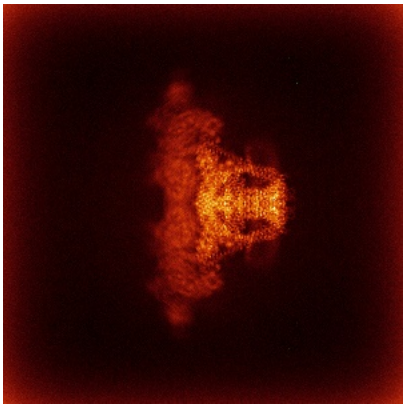


Z

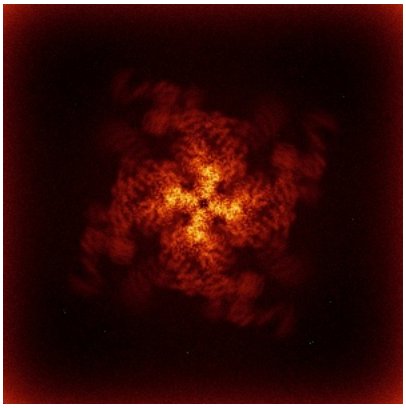
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

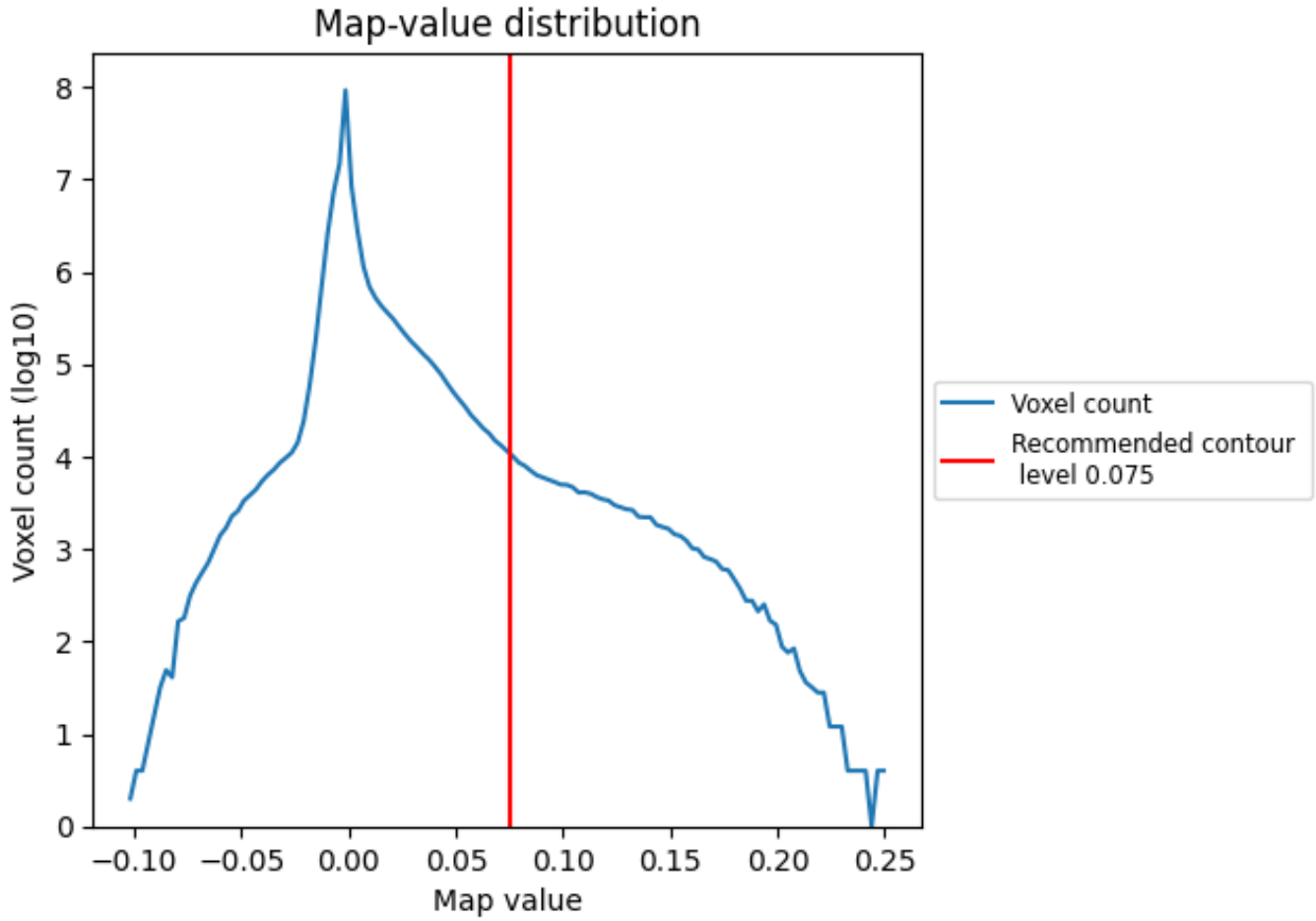
6.6 Mask visualisation (i)

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

7 Map analysis

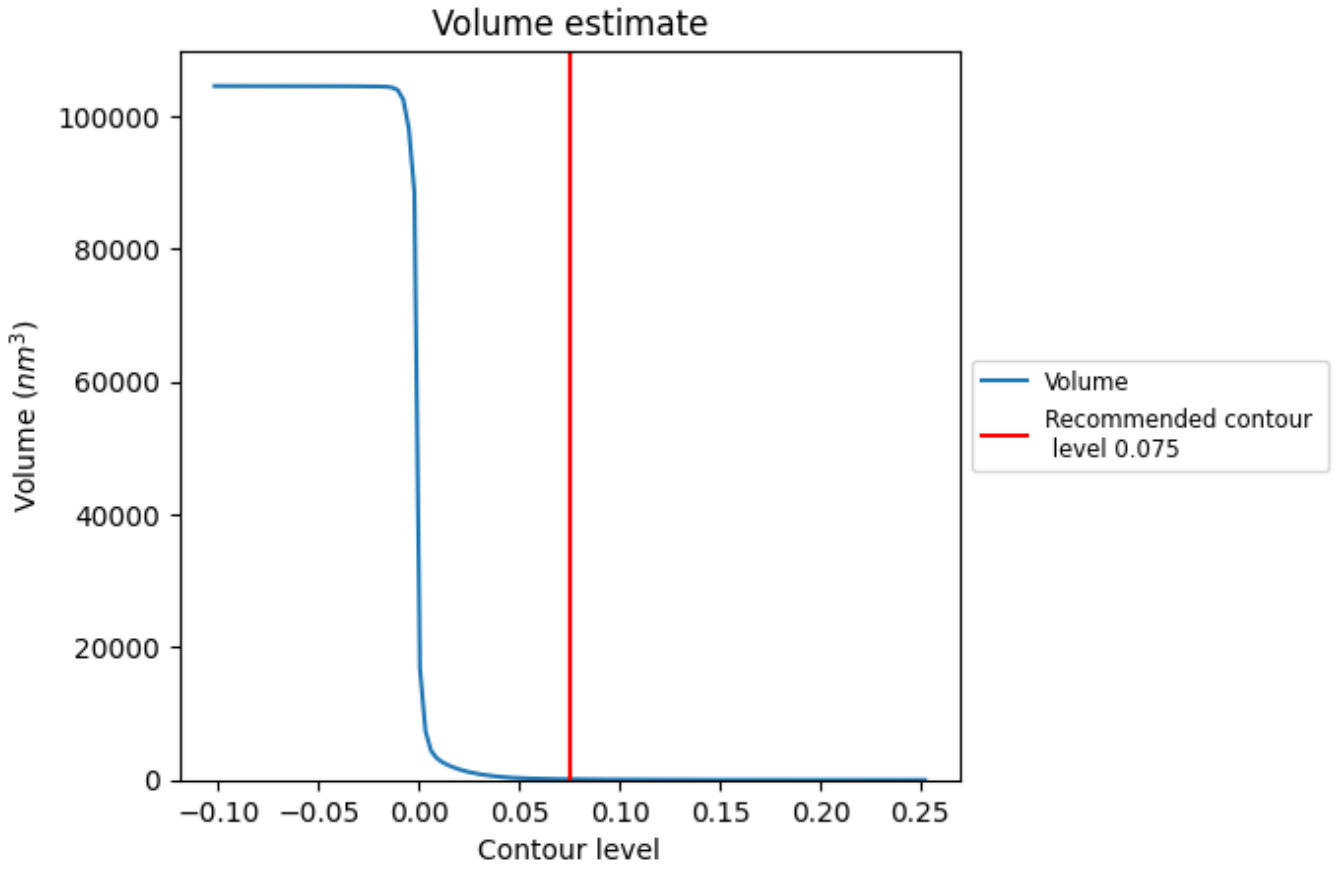
This section contains the results of statistical analysis of the map.

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.

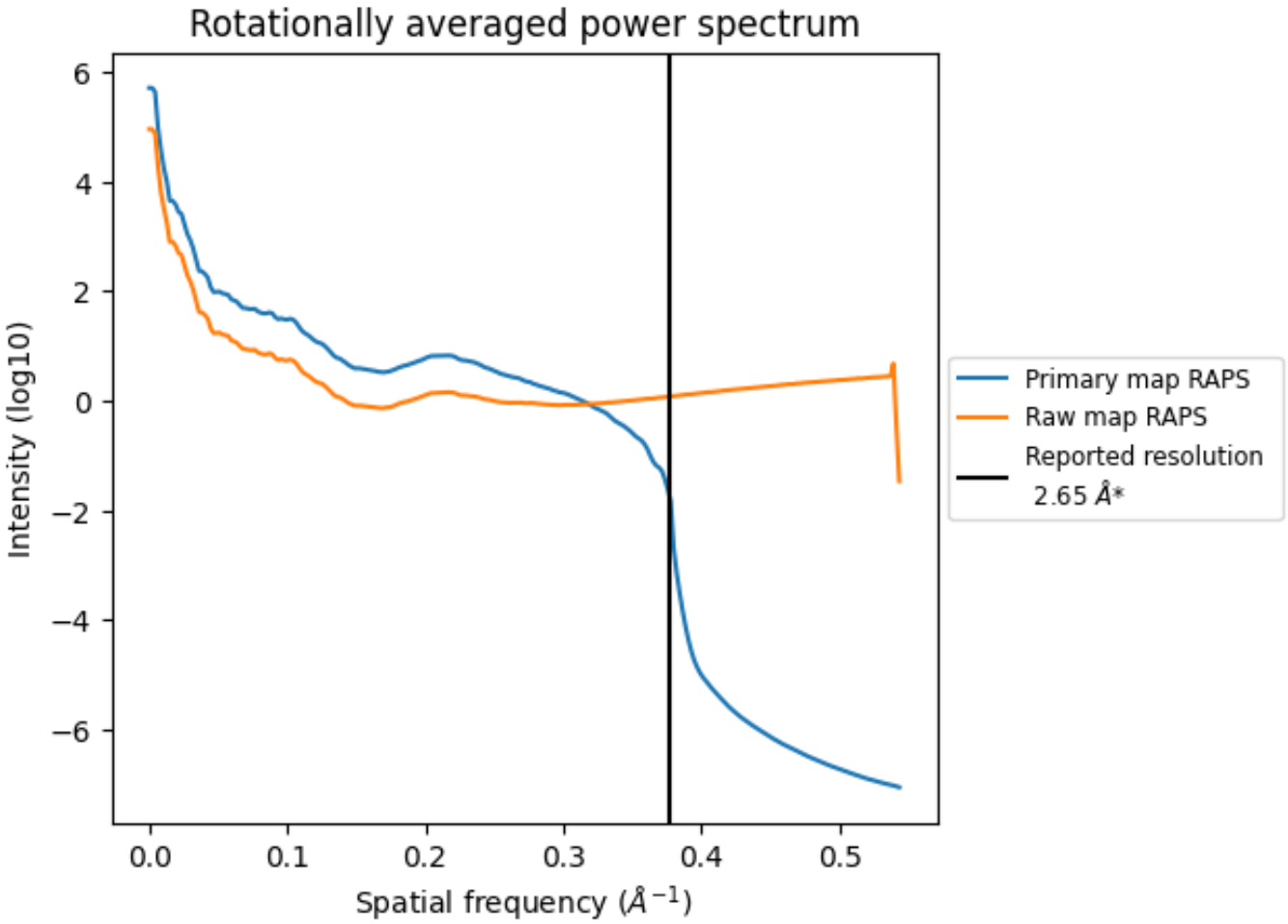
7.2 Volume estimate (i)



The volume at the recommended contour level is 106 nm^3; this corresponds to an approximate mass of 96 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)

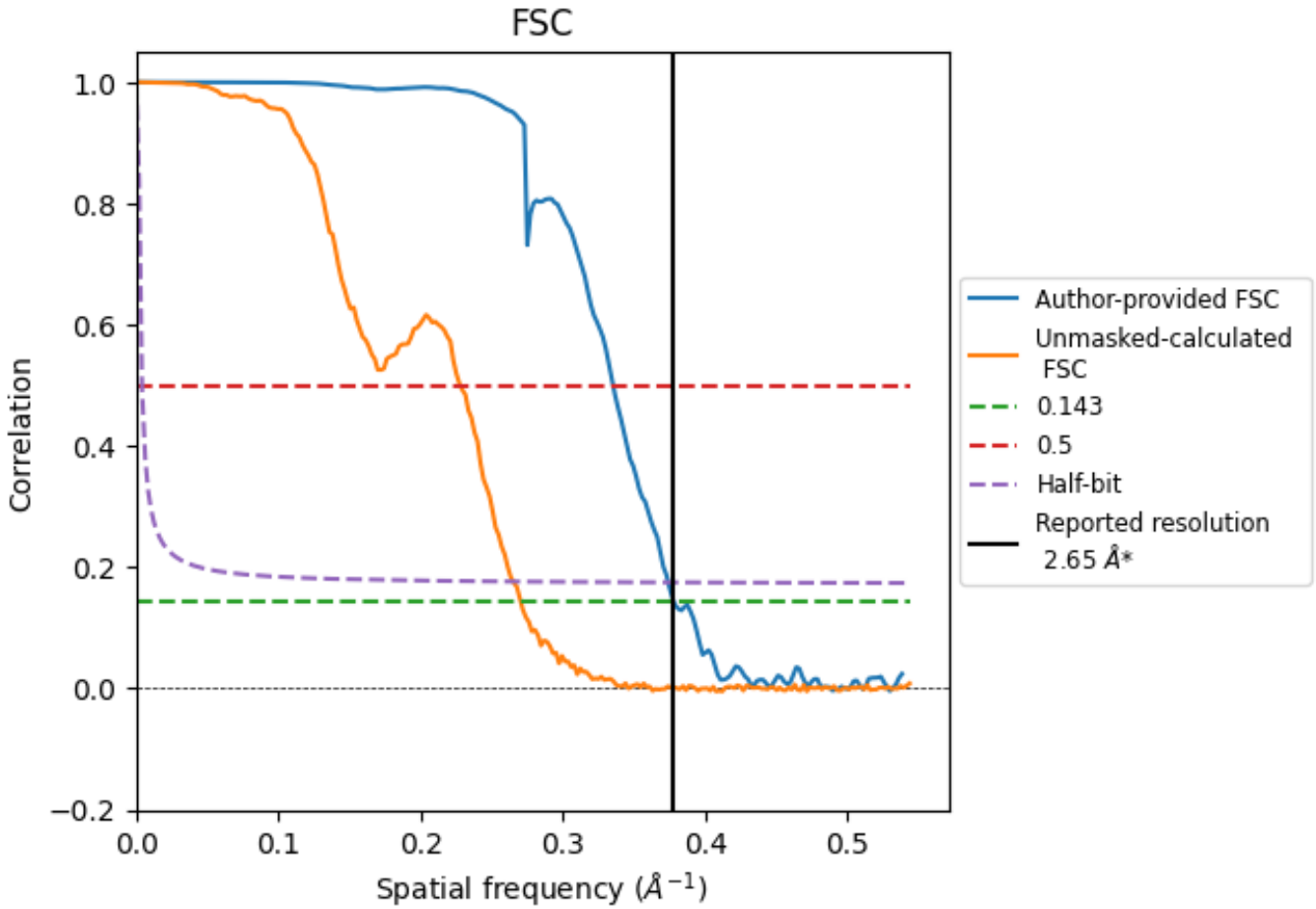


*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.377 Å^{-1}

8.2 Resolution estimates (i)

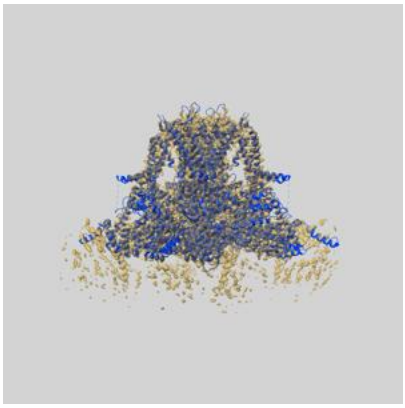
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	2.98	2.67
Unmasked-calculated*	3.70	4.39	3.78

*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 3.70 differs from the reported value 2.65 by more than 10 %

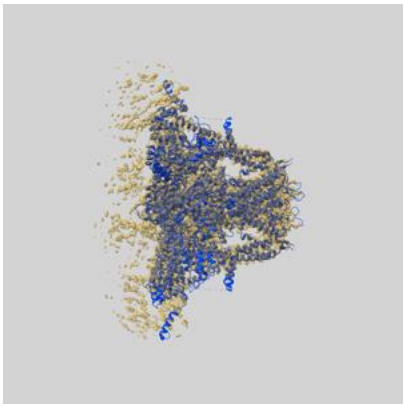
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-80692 and PDB model 26IX. Per-residue inclusion information can be found in section 3 on page 5.

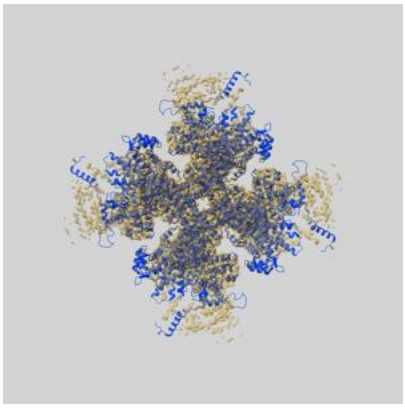
9.1 Map-model overlay



X



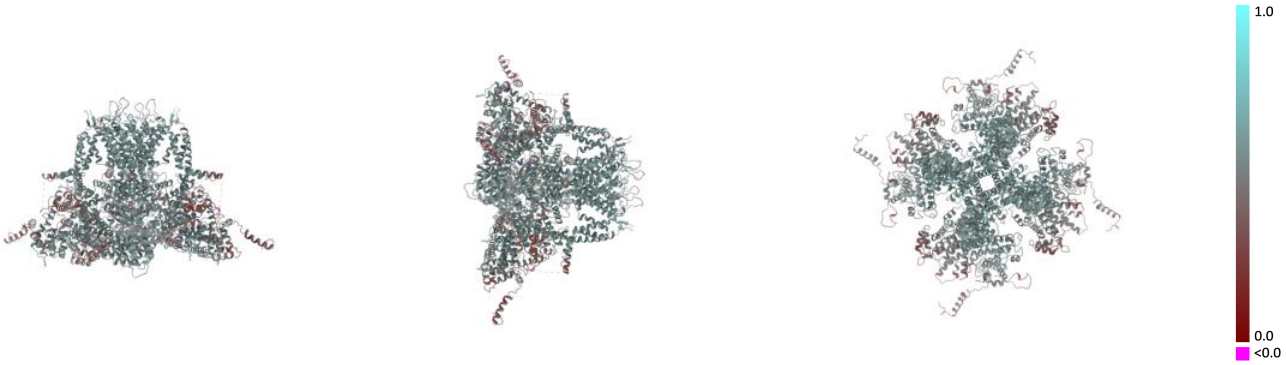
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.075 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.

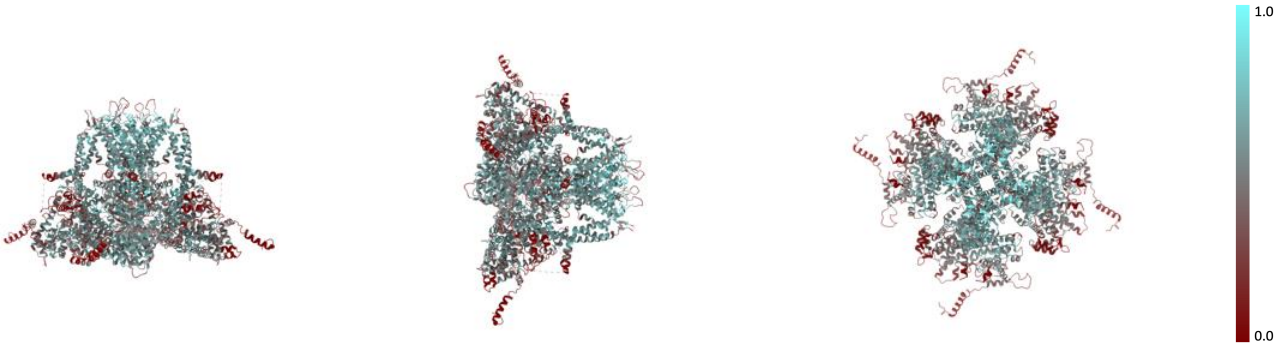
9.2 Q-score mapped to coordinate model (i)



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.

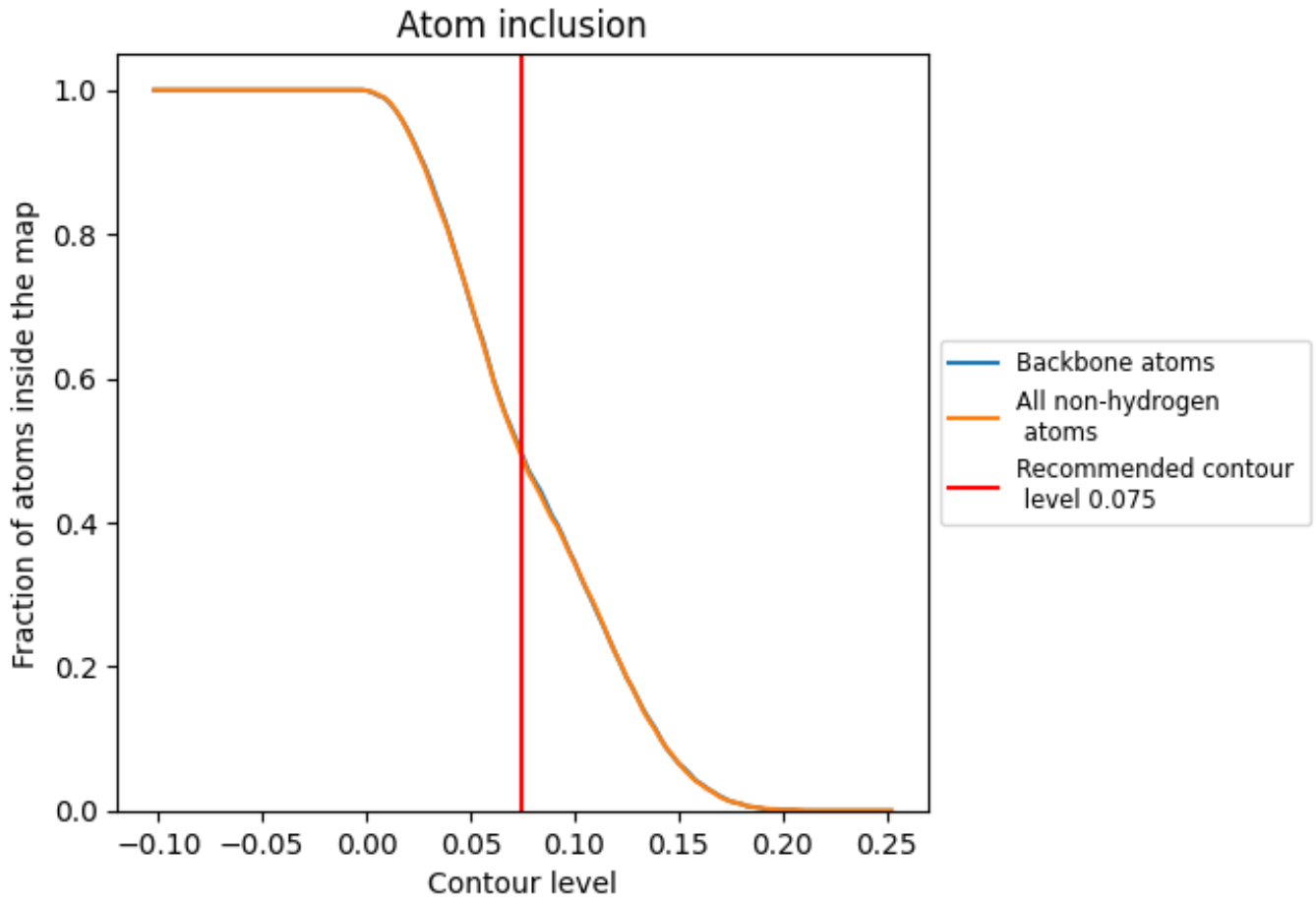
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.075).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 49% 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 (0.075) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.4890	0.5190
A	0.4980	0.5200
B	0.4980	0.5200
C	0.4980	0.5190
D	0.4980	0.5190