Full wwPDB EM Validation Report (i)

Jul 10, 2023 – 04:33 PM EDT

PDB ID	:	8SEY
EMDB ID	:	EMD-40433
Title	:	Cryo-EM Structure of RyR1 + Adenosine (Local Refinement of TMD)
Authors	:	Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on	:	2023-04-10
Resolution	:	2.99 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

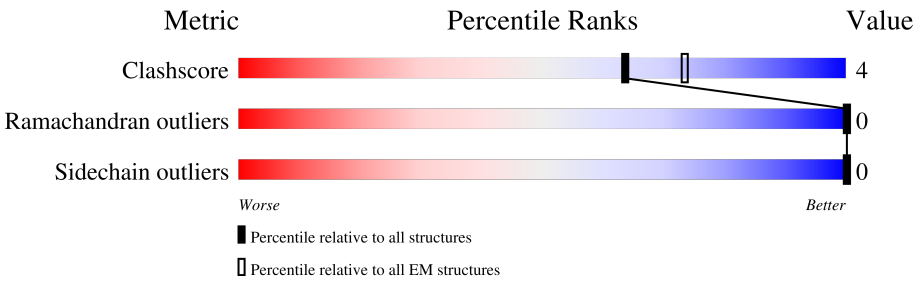
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.99 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	11% · 88%
1	B	5037	11% · 88%
1	C	5037	11% · 88%
1	D	5037	11% · 88%

2 Entry composition (i)

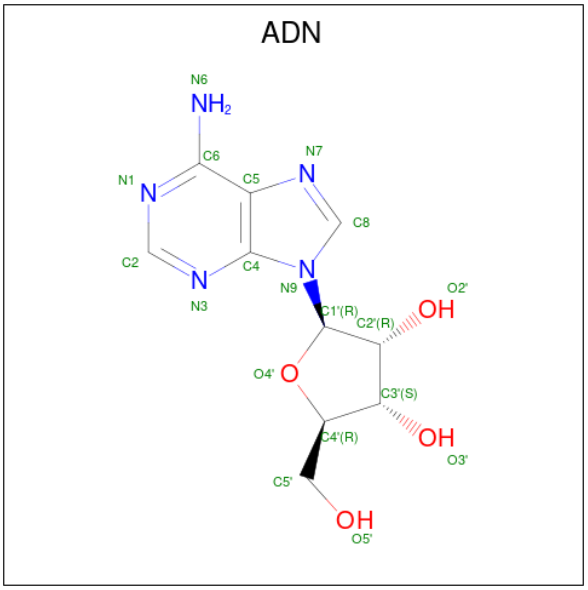
There are 3 unique types of molecules in this entry. The entry contains 20568 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	626	5122	3330	815	937	40	0	0
1	B	626	5122	3330	815	937	40	0	0
1	C	626	5122	3330	815	937	40	0	0
1	D	626	5122	3330	815	937	40	0	0

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	19	10	5	4	0
2	B	1	19	10	5	4	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	C	1	19	10	5	4	0
2	D	1	19	10	5	4	0

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

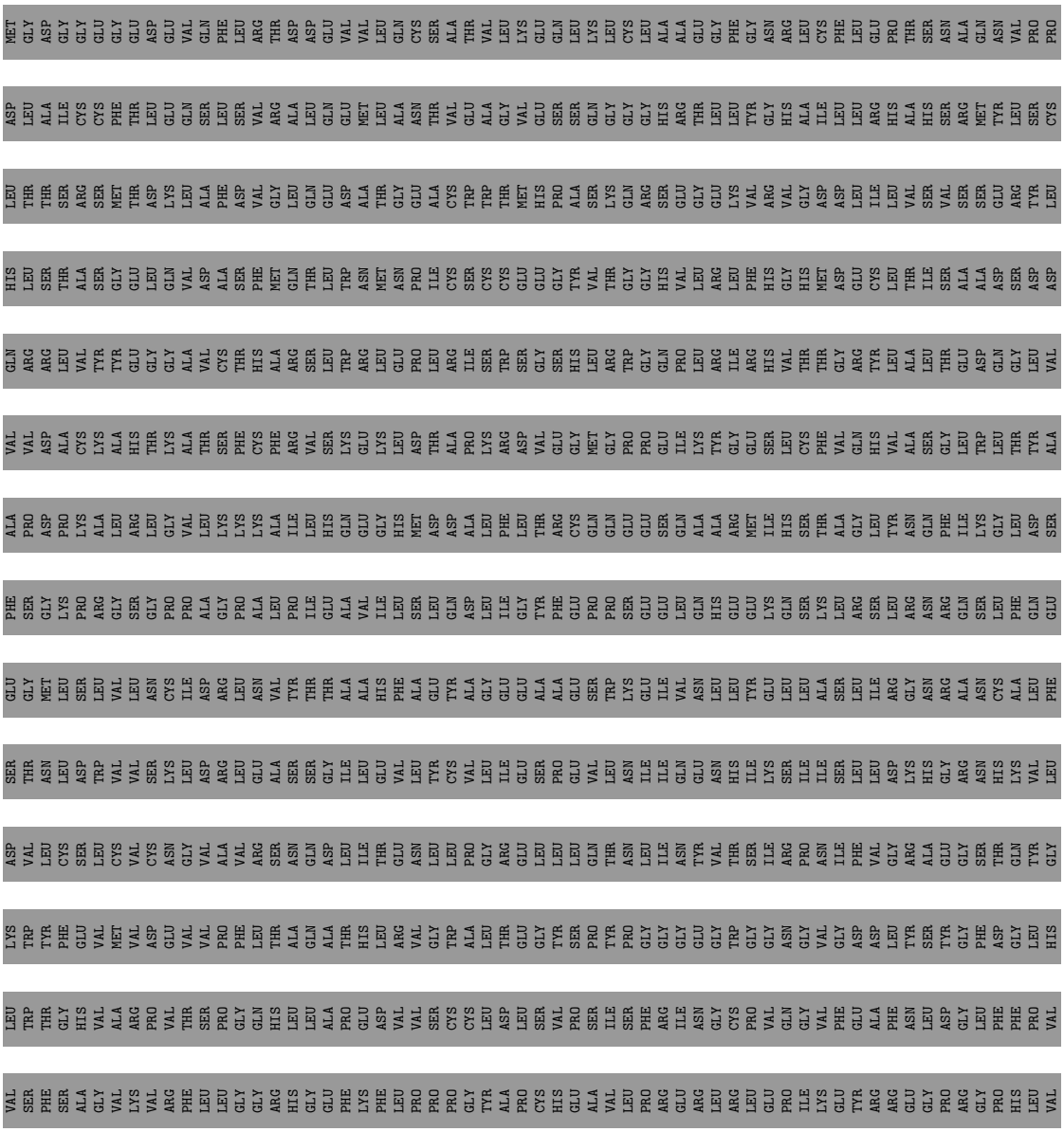
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0
3	B	1	1	1	0
3	C	1	1	1	0
3	D	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ryanodine receptor 1

Chain A:



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

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

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

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

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

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

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

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

ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR

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

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

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

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

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

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

GLU THR ARG ALA ILE THR LEU PHE PRO PRO GLY ARG LYS GLY GLY ASN ALA ARG ARG HIS GLY LEU PRO GLY VAL GLY VAL THR THR SER LEU ARG PRO PRO HIS HIS PHE SER PRO PRO CYS PHE VAL ALA ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG LEU SER PRO

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

GLN ILE LEU LYS MET ILE GLU PRO GLU VAL PHE THR GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU

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

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

HIS CYS GLY ILE GLN LEU GLU GLY GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN SER LEU GLN GLU LEU VAL SER HIS

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

GLN ILE ARG SER LEU LEU ILE VAL GLN MET GLY PRO GLN GLU GLU ASN LEU MET ILE GLN SER ILE GLY ASN 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 THR

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

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

VAL ASN GLY GLU SER VAL GLU GLU ASN ALA ASN VAL VAL VAL ARG LEU LEU ILE ARG LYS PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY SER GLY LEU LEU ALA ALA ILE GLU GLU ALA ILE ARG ILE SER GLU ASP PRO ALA ARG ASP GLY PRO GLY VAL ARG ARG ASP

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

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

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

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

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

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

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

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

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

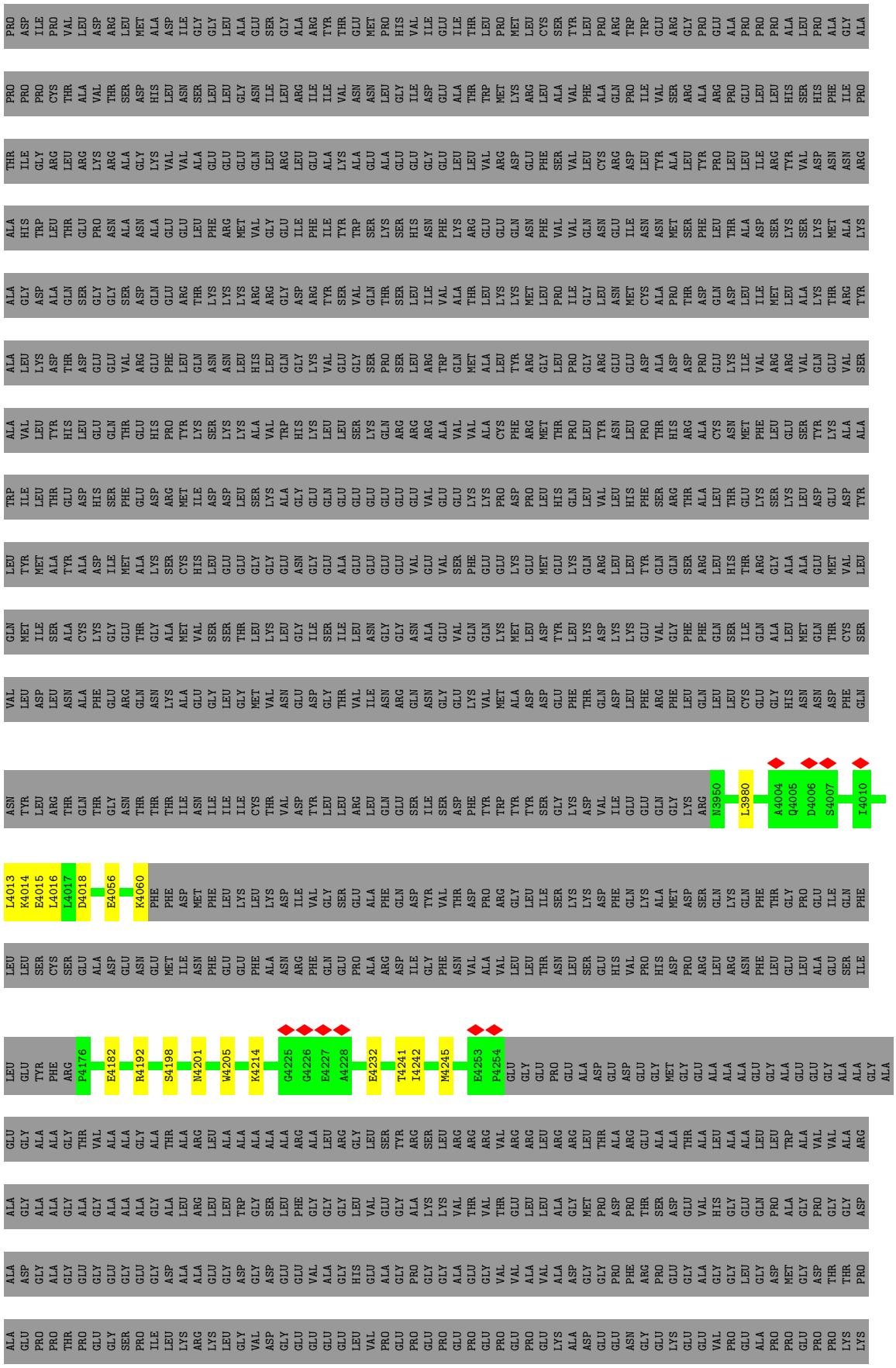
LEU LYS ASP MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU ILE LYS PHE PHE ALA LYS

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

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

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

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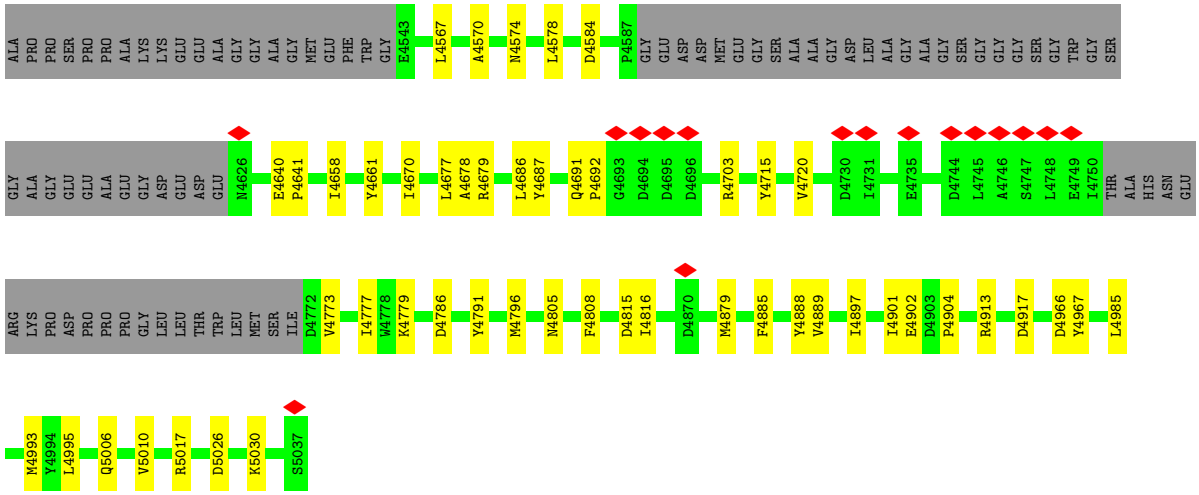
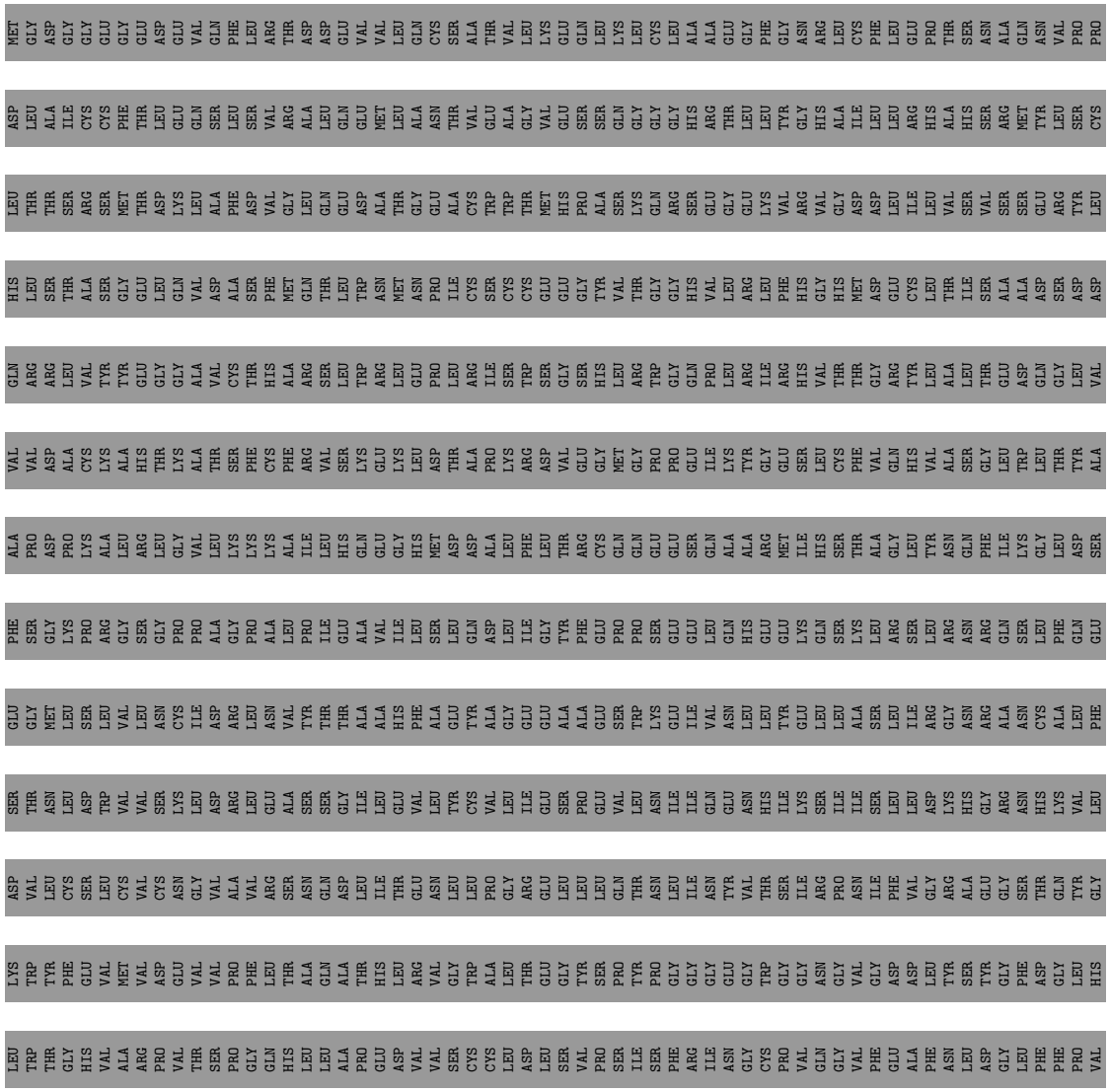
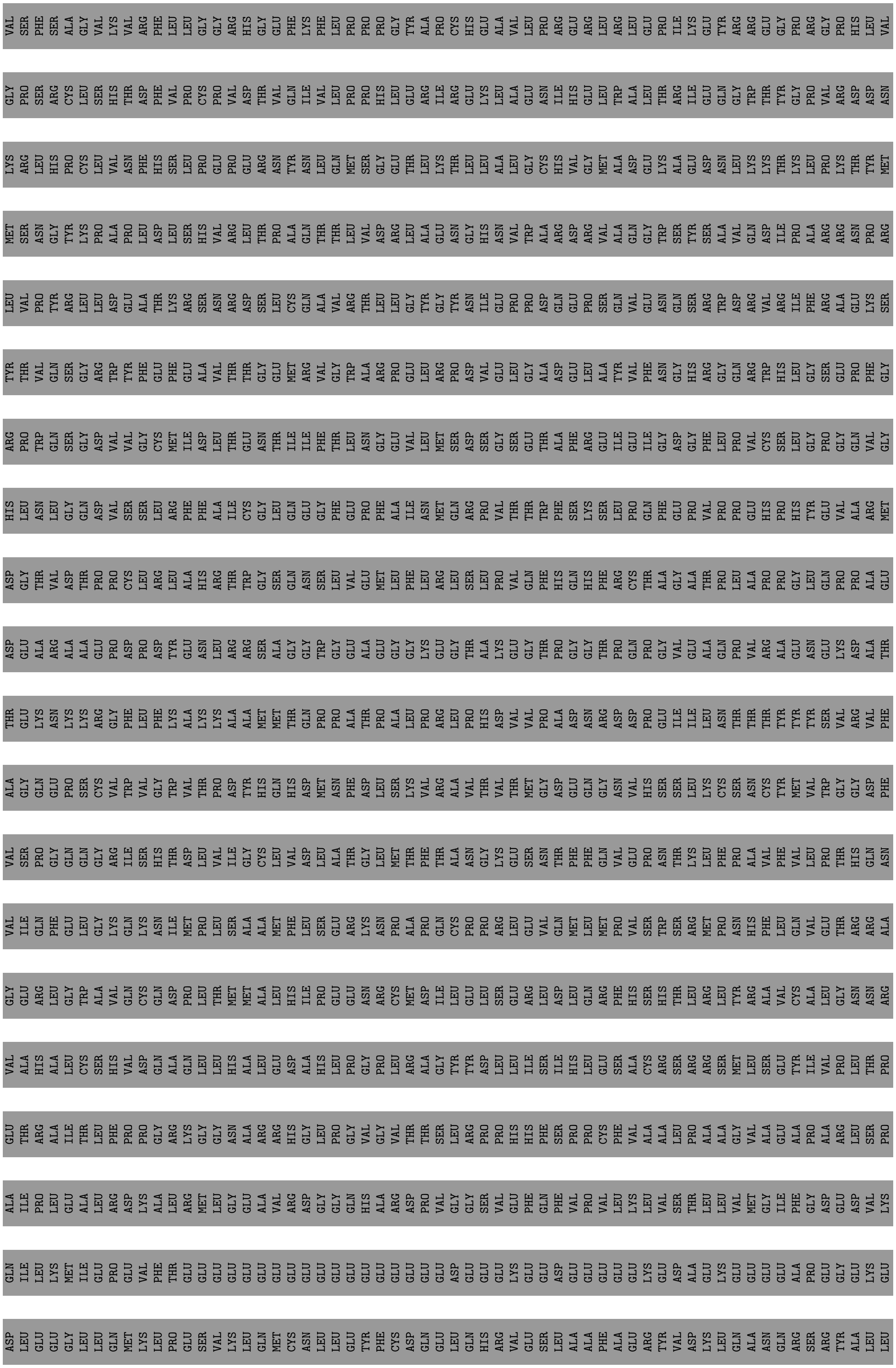
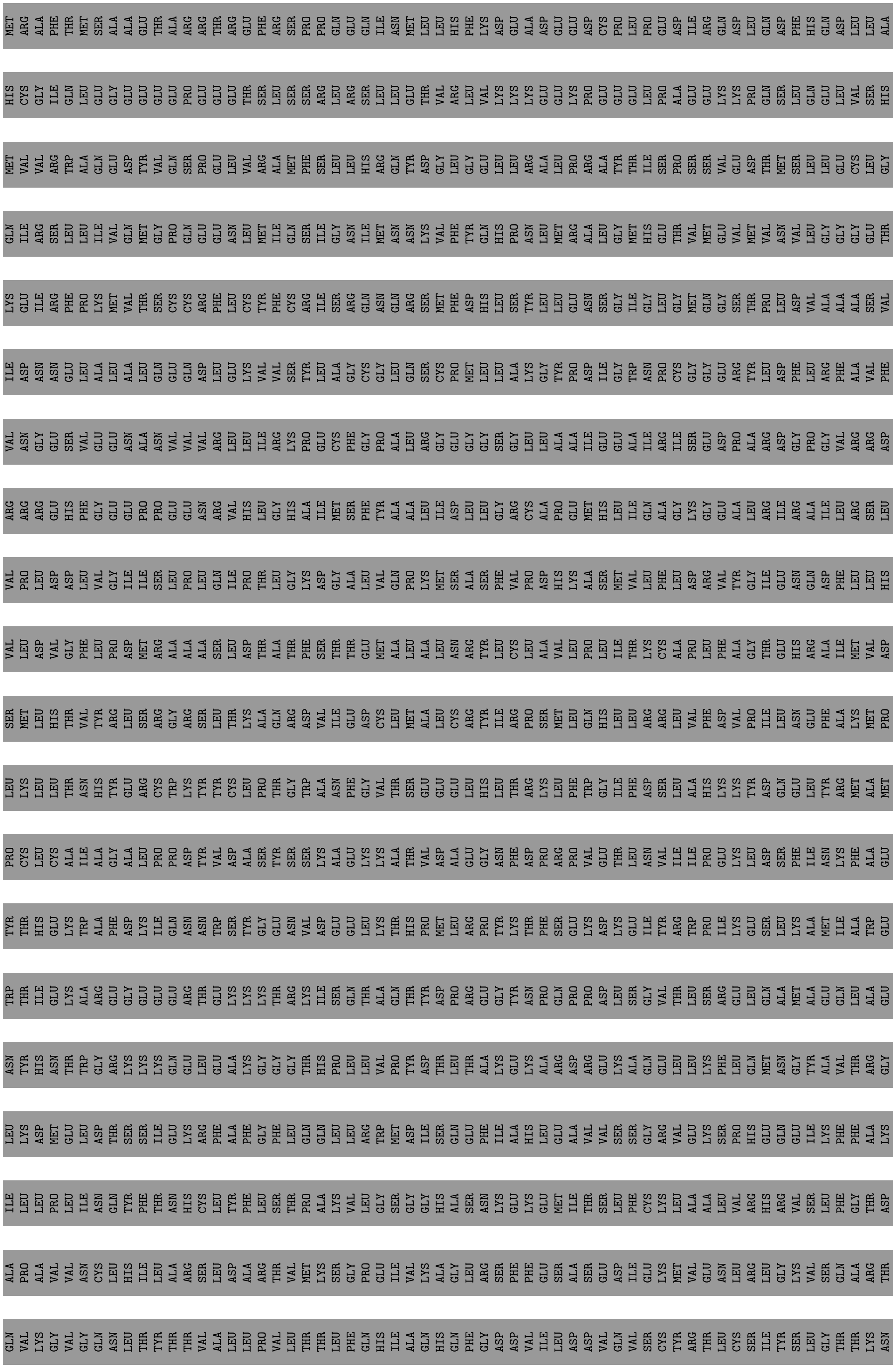


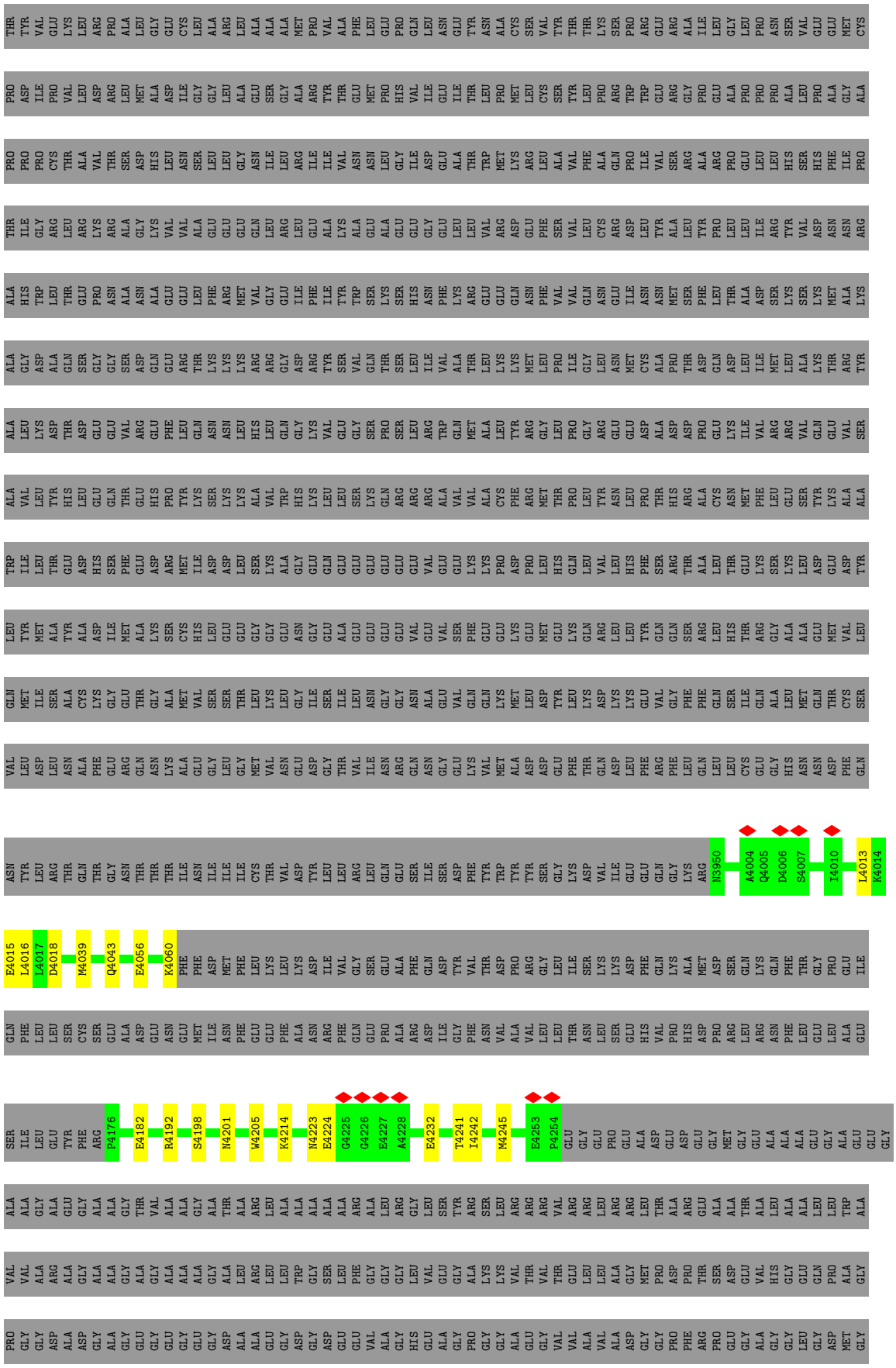
- Molecule 1: Ryanodine receptor 1

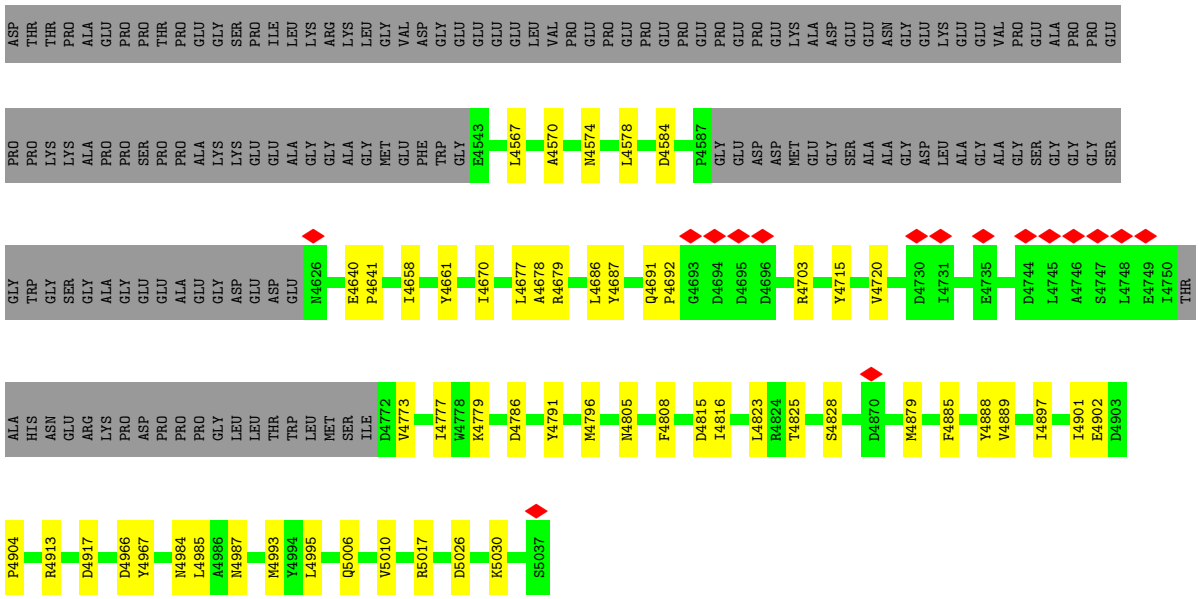
Chain B: 11% 88%





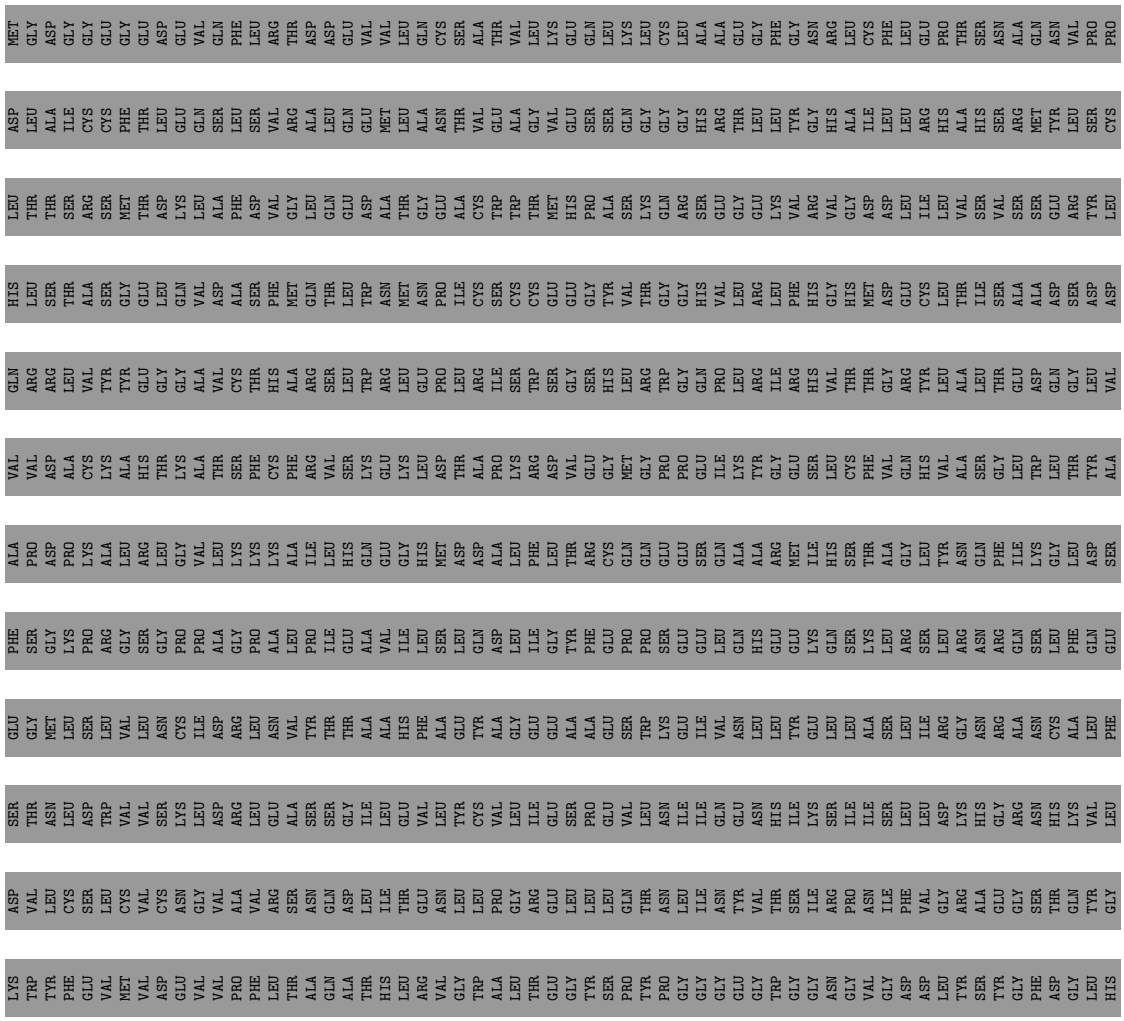

MET ARG ALA PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU ALA ASP GLU GLU ASP CYS PRO LEU PRO GLU ASP ILE ARG GLN ASP LEU GLN ASP PHE HIS GLN ASP LEU LEU ALA
HIS CYS GLY ILE GLN LEU GLU GLY GLU GLU GLU PRO GLU GLU GLU THR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


THR TYR VAL GLU LYS LEU ARG PRO ALA LEU GLY GLU CYS LEU ALA ARG LEU ALA ALA MET PRO VAL ALA PHE LEU GLU PRO GLN LEU ASN GLU TYR ASN ALA CYS SER VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS
PRO ASP ILE PRO VAL LEU ASP ARG LEU MET ALA ASP ILE GLY GLY LEU ALA GLU SER GLY ALA ARG TYR THR GLU MET PRO HIS VAL ILE GLU ILE THR LEU PRO MET LEU CYS SER TYR LEU PRO ARG TRP TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA LEU PRO ALA GLY ALA
PRO PRO PRO CYS THR ALA VAL THR SER ASP HIS LEU ASN SER LEU LEU GLY ASN ILE LEU ARG ILE ILE VAL ASN ASN LEU GLY VAL ASP GLU ALA THR TRP MET LYS ARG LEU ALA VAL PHE ALA GLN PRO ILE VAL SER ARG ALA ARG PRO GLU LEU LEU HIS SER HIS PHE ILE PRO
THR ILE GLY ARG LEU ARG LYS ARG ALA GLY LYS VAL VAL ALA GLU GLU GLU GLN LEU ARG GLU GLU ALA LYS ALA GLU ALA GLU GLU GLY GLU GLU LEU ARG ASP GLU PHE SER VAL LEU CYS ARG ASP LEU TYR ALA LEU TYR PRO LEU LEU ILE ARG TYR VAL ASP ASN ASN ARG
ALA HIS TRP LEU THR GLU PRO ASN ALA ASN ALA GLU GLU LEU PHE ARG MET VAL GLY GLU ILE PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU THR ALA ASP SER LYS SER LYS MET ALA LYS
ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG LYS LYS ARG ARG GLY ASP ARG TYR SER VAL GLN THR SER LEU ILE VAL ALA THR LEU LYS LYS MET LEU PRO ILE GLY ARG LEU ASN MET CYS ALA PRO THR ASP LEU LEU ILE MET LEU ALA LYS THR ARG TYR
ALA LEU LYS ASP THR ASP GLU GLU VAL ARG GLU PHE LEU GLN ASN ASN LEU HIS LEU GLN LYS SER PRO SER LEU ARG TRP GLN MET ALA ALA LEU LYS VAL GLU GLY SER LYS GLN ARG GLU GLU ASP ALA PRO SER LEU ILE VAL ALA VAL ARG ARG GLU LYS ILE VAL ARG GLU ARG ASP PRO THR ASP GLN GLU LYS ASP SER SER
ALA VAL LEU TYR HIS LEU GLU GLN THR GLU HIS PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET THR PRO LEU TYR ASN LEU PRO THR HIS ARG ALA CYS ASN MET PHE LEU GLU LYS ILE VAL ARG ARG VAL ALA LYS SER
TRP ILE LEU THR GLU ASP HIS SER PHE GLU ASP ARG MET ILE ASP ASP LEU SER LYS ALA GLY GLU GLN GLU GLU GLU GLU GLU VAL GLU GLU LYS LYS PRO ASP PRO LEU HIS GLN LEU VAL LEU HIS PHE SER ARG THR ALA LEU THR GLU LYS SER LYS LEU ASP GLU ASP TYR
LEU TYR MET ALA TYR ALA ASP ILE MET ALA LYS SER CYS HIS LEU GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL GLU VAL SER PHE GLU GLU GLU LYS GLN GLN ARG LEU LEU TYR GLN GLN SER ARG LEU HIS THR ARG GLY ALA ALA GLU MET VAL LEU
GLN MET ILE SER ALA CYS LYS GLY GLU THR GLY ALA MET VAL SER SER THR LEU LYS LEU GLY ILE SER ILE LEU ASN GLY GLY ASN ALA GLU VAL GLN GLN LYS MET LEU ASP TYR LEU LYS ASP LYS LYS GLU VAL GLY PHE PHE GLN SER ILE GLN LEU MET GLN THR CYS SER
VAL LEU ASP LEU ASN ALA PHE GLU ARG GLN ASN LYS ALA GLU GLY GLU MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY GLU LYS VAL GLU GLU ALA THR ASP ASP GLU PHE THR GLN ASP LEU PHE ARG PHE LEU GLN LEU LEU LEU CYS ASN GLU ASP ASP PHE GLN
ASN TYR LEU ARG THR GLN THR GLY ASN THR THR THR ILE ASN ILE ILE ILE CYS THR VAL ASP TYR LEU LEU ARG LEU GLN GLU SER ILE SER ASP PHE TYR TRP TYR TYR SER GLY LYS ASP VAL ILE GLU GLU GLN GLY LYS ARG N3950 A4004 Q4005 D4006 S4007 I4010 L4013 K4014
E4015 L4016 L4017 D4018 M4039 Q4043 E4056 K4060 PHE PHE ASP MET PHE LEU LYS LEU LYS ASP ILE VAL GLY SER GLU ALA PHE GLN ASP TYR VAL THR ASP PRO ARG GLY LEU ILE SER LYS LYS ASP PHE GLN LYS ALA MET ASP SER GLN LYS GLN PHE THR GLY PRO GLU ILE
GLN PHE LEU LEU SER CYS SER GLU ALA ASP GLU ASN GLU MET ILE ASN PHE GLU GLU PHE ALA ASN ARG PHE GLN GLU PRO ALA ARG ASP ILE GLY PHE ASN VAL ALA LEU LEU THR ASN LEU SER GLU HIS VAL PRO HIS ASP PRO ARG LEU ARG ASN PHE LEU GLU GLU LEU GLU LEU
SER ILE LEU GLU TYR PHE ARG P4176 E4182 R4192 S4198 N4201 W4205 K4214 N4223 E4224 G4225 G4226 E4227 A4228 E4232 T4241 I4242 M4245 E4253 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLY ALA ALA ALA GLU GLY ALA GLU GLU GLY
ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ARG ARG LEU ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG GLU ALA ALA THR ALA LEU ALA ALA ALA LEU LEU TRP ALA
VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA ALA GLY GLY GLY ALA LEU LEU ALA LEU VAL GLU GLY LYS LYS VAL THR VAL THR GLU LEU LEU ALA ALA MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN GLU GLY LEU ALA GLY
PRO GLY GLY ASP ALA ASP GLY GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA GLY PRO PHE ARG PRO GLU GLY GLY ALA GLY GLY ASP PRO GLU GLU GLY ASP MET GLY



- Molecule 1: Ryanodine receptor 1

Chain C:



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

VAL SER PHE SER ALA GLY VAL LYS VAL ARG PHE LEU LEU GLY GLY ARG HIS GLY GLU PHE LYS PHE LEU PRO PRO PRO GLY TYR ALA PRO CYS HIS GLU ALA VAL LEU PRO ARG GLU ARG LEU ARG LEU GLU PRO ILE LYS GLU TYR ARG ARG GLU GLY PRO ARG GLY PRO HIS LEU VAL

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

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

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

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

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

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

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

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

ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR

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

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

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

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

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

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

GLU THR ARG ALA ILE THR LEU PHE PRO PRO GLY ARG LYS GLY GLY ASN ALA ARG ARG HIS GLY LEU PRO GLY VAL GLY VAL THR THR SER LEU ARG PRO PRO HIS HIS PHE SER PRO PRO CYS PHE VAL ALA ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG LEU SER PRO

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

GLN ILE LEU LYS MET ILE GLU PRO GLU VAL PHE THR GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU

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

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

HIS CYS GLY ILE GLN LEU GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN SER LEU GLN GLU LEU VAL SER HIS

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

GLN ILE ARG SER LEU LEU ILE VAL GLN MET GLY PRO GLN GLU GLU ASN LEU MET ILE GLN SER ILE GLY ASN 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 GLU THR

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

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

VAL ASN GLY GLU SER VAL GLU GLU ASN ALA ASN VAL VAL ARG LEU LEU ILE ARG LYS PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY SER GLY LEU LEU ALA ALA ILE GLU ALA ILE ARG ILE SER GLU ASP PRO ALA ARG ASP GLY PRO GLY VAL ARG ARG ASP

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

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

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

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

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

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

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

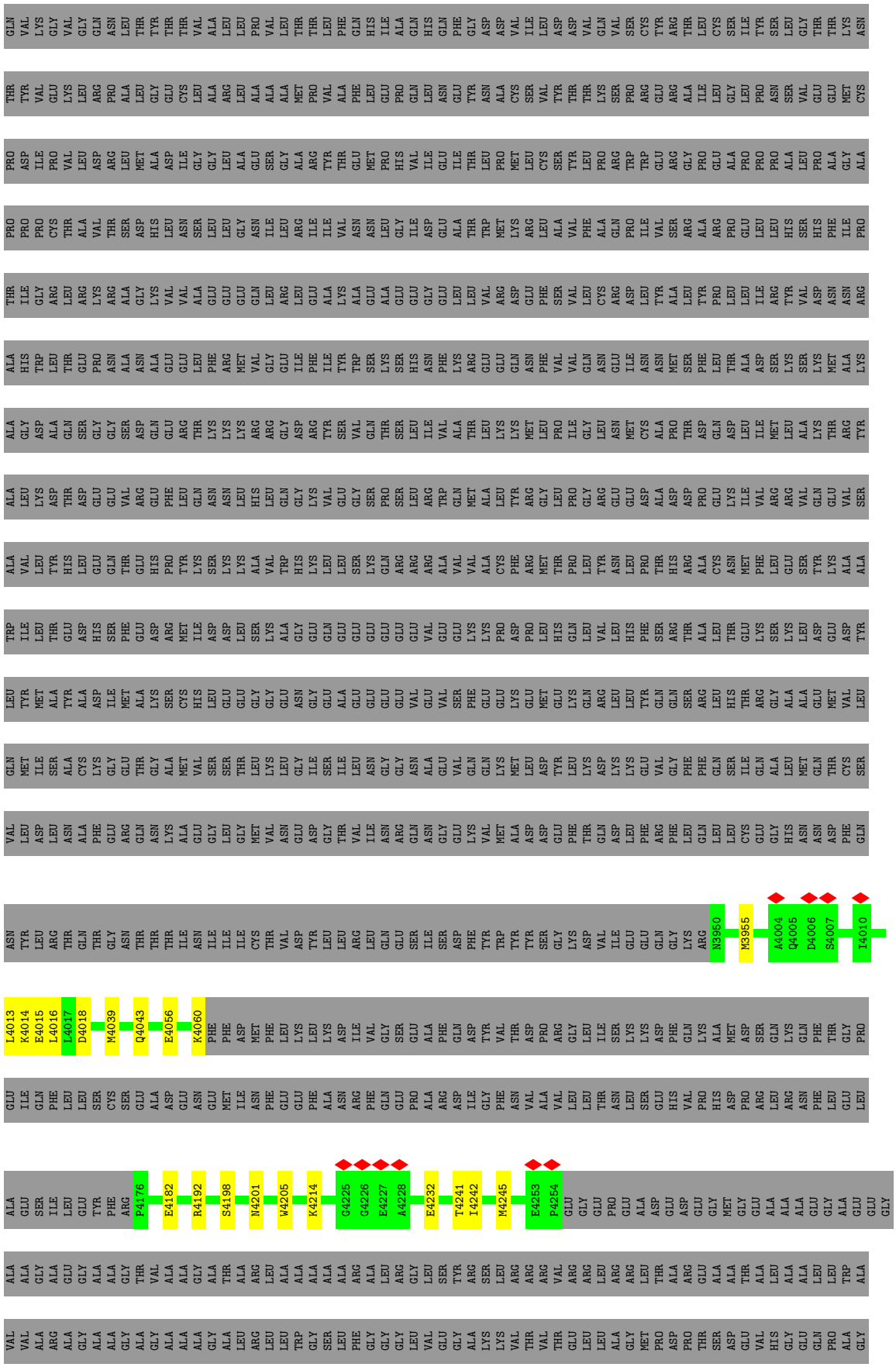
TRP THR ILE GLU LYS ALA ARG GLU GLY GLU GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY TYR ASN PRO GLN PRO PRO ASP LEU SER GLY VAL THR LEU SER ARG GLU LEU GLN ALA MET ALA GLU GLN LEU ALA GLU

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

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

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

ALA PRO ALA VAL VAL ASN CYS LEU HIS ILE LEU ALA ARG SER LEU ASP ALA ARG THR VAL MET LYS SER GLY PRO GLU ILE VAL LYS ALA GLY LEU ARG SER PHE PHE GLU SER ALA SER GLU ASP ILE GLU LYS MET VAL GLU ASN LEU ARG LEU GLY LYS VAL SER GLN ALA ARG THR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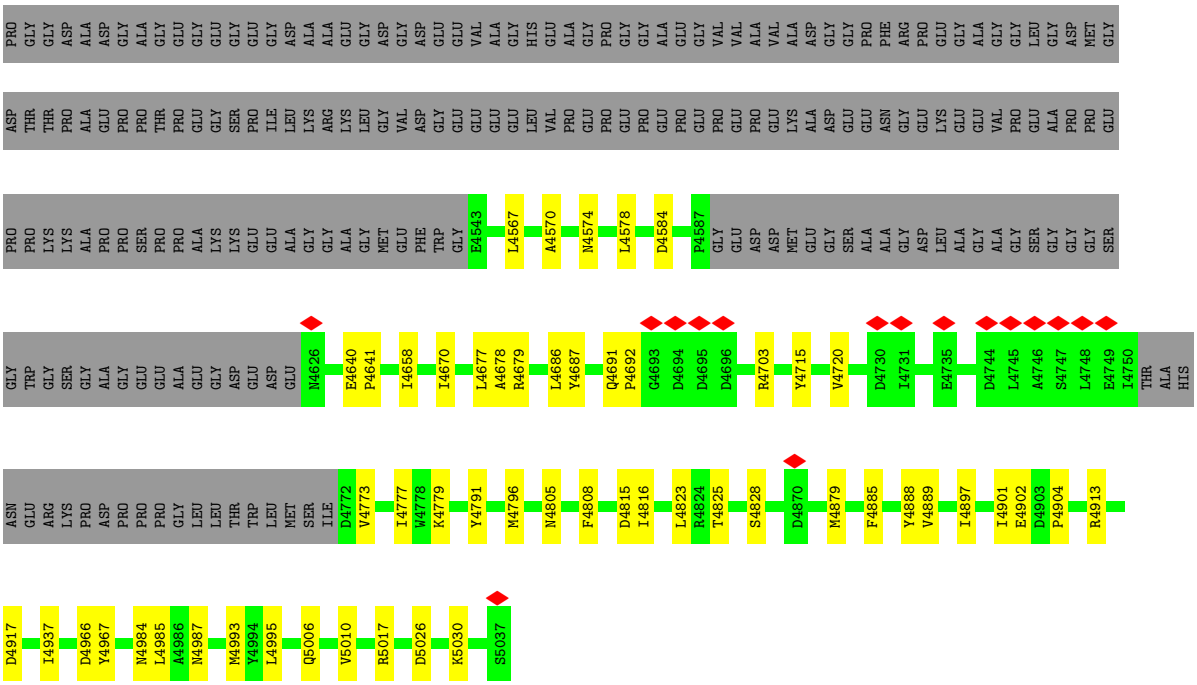
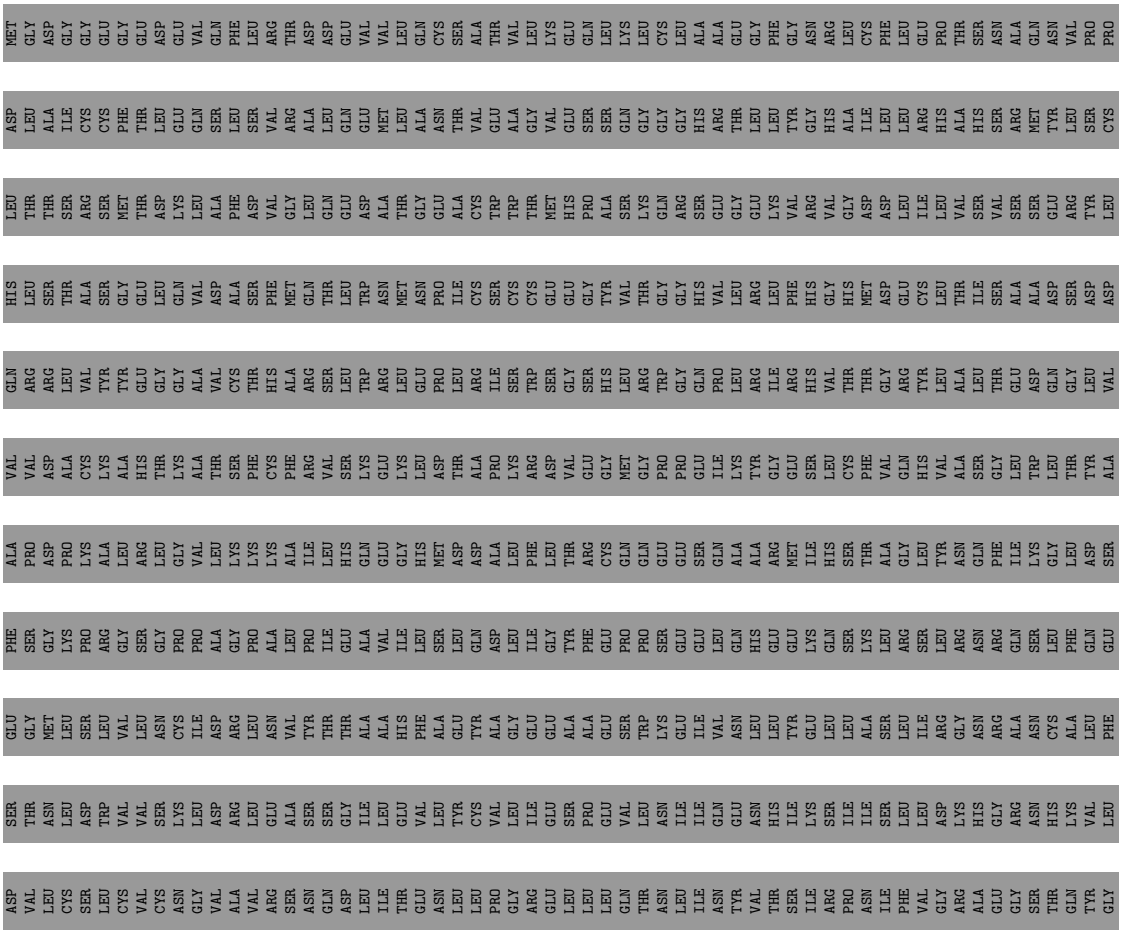
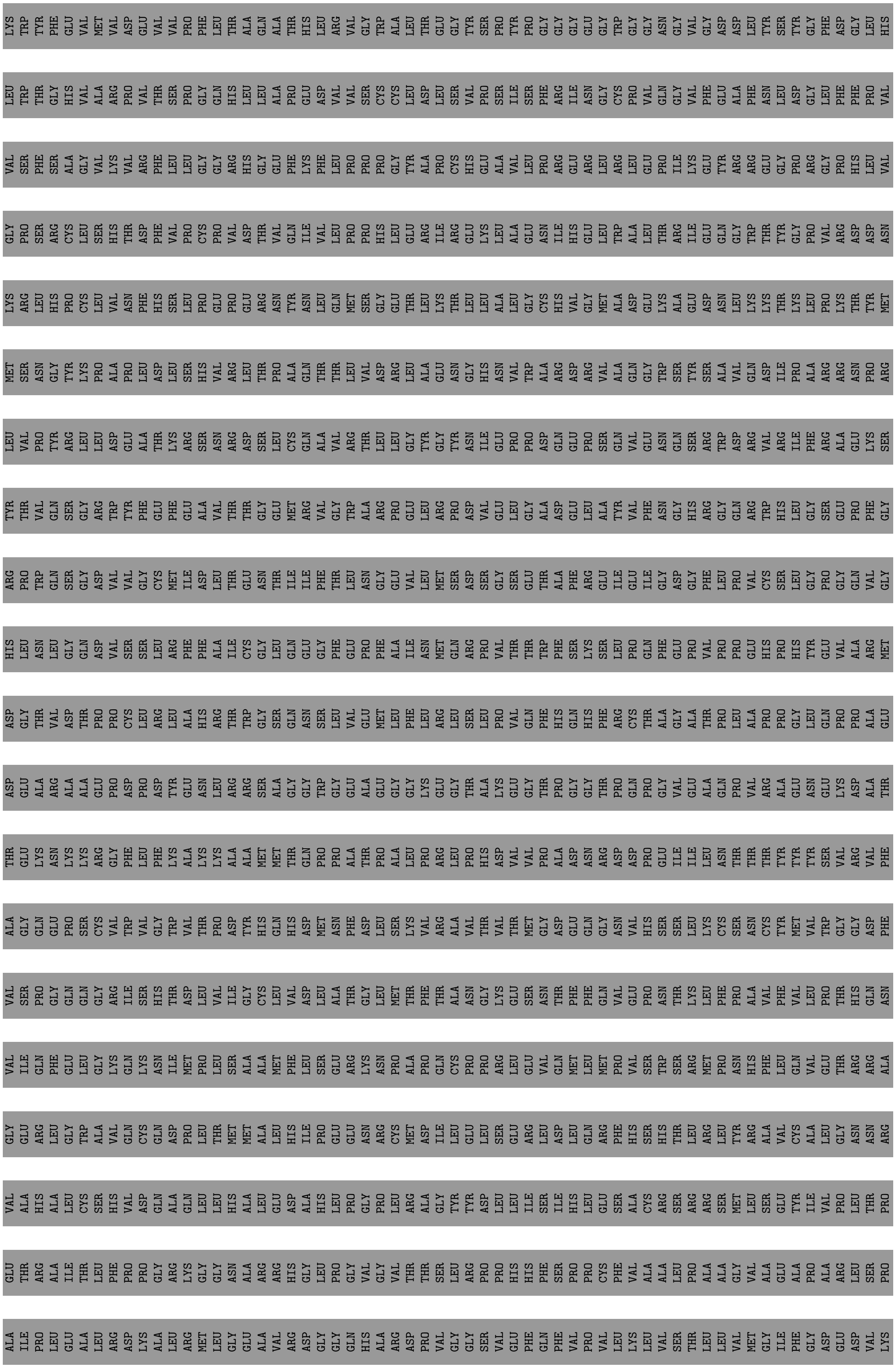
P4254



• Molecule 1: Ryanodine receptor 1

Chain D: 11% 88%




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

GLN ILE LEU LYS MET ILE GLU PRO GLU VAL PHE THR GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU

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

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

HIS CYS GLY ILE GLN LEU GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN SER LEU GLN GLU LEU VAL SER HIS

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

GLN ILE ARG SER LEU LEU ILE VAL GLN MET GLY PRO GLN GLU GLU ASN LEU MET ILE GLN SER ILE GLY ASN 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 THR

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

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

VAL ASN GLY GLU SER VAL GLU GLU ASN ALA ASN VAL VAL VAL ARG LEU LEU ILE ARG LYS PRO GLU CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY SER GLY LEU LEU ALA ALA ILE GLU GLU ALA ILE ARG ILE SER GLU ASP PRO ALA ARG ASP GLY PRO GLY VAL ARG ARG ASP

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

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

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

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

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

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

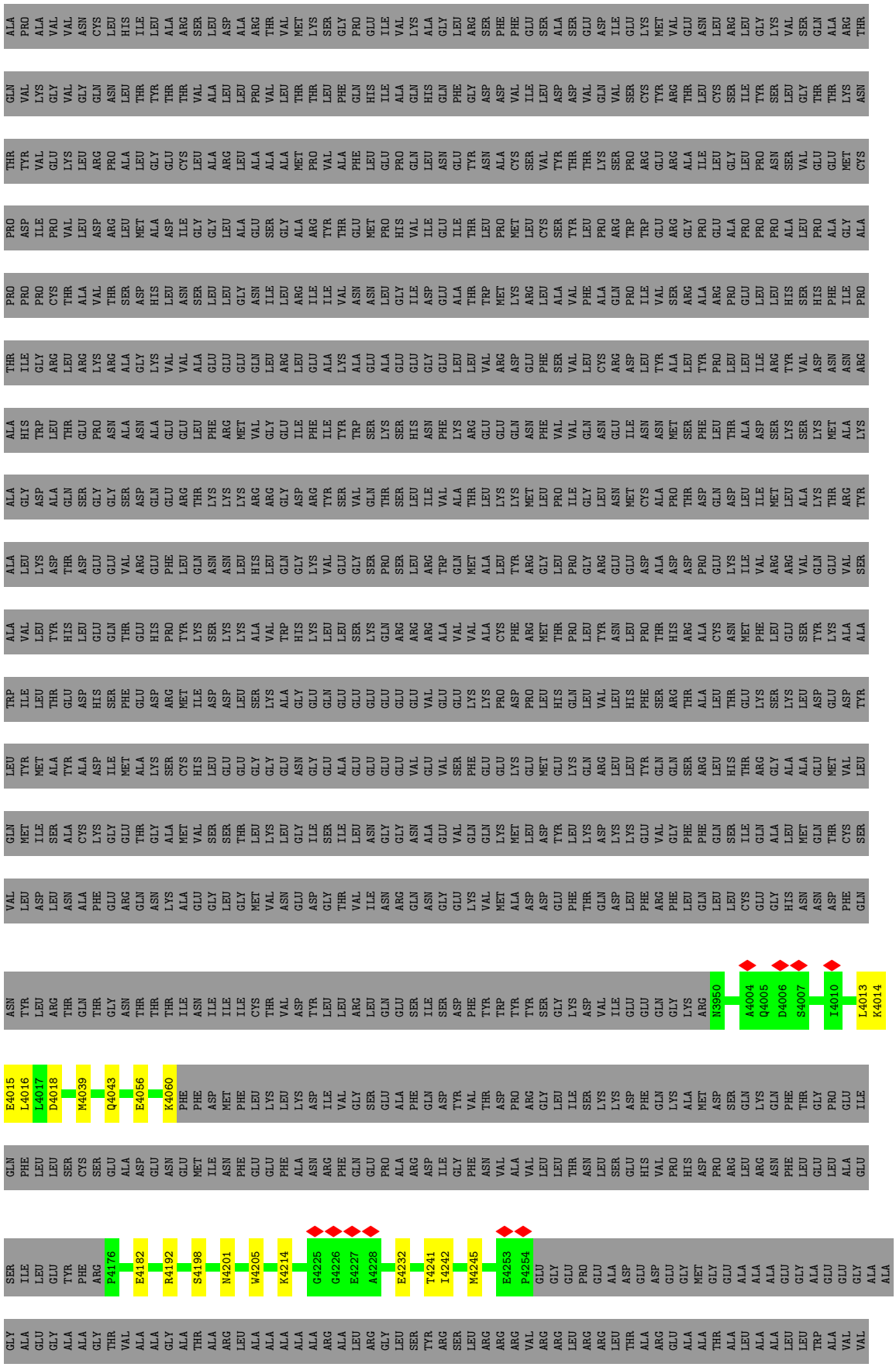
TYR THR HIS GLU LYS TRP ALA PHE ASP LYS ILE GLN ASN ASN TRP SER TYR GLY GLU ASN VAL ASP GLU GLU LEU LYS THR HIS PRO MET LEU ARG PRO TYR LYS THR PHE SER GLU LYS ASP LYS GLU ILE TYR ARG TRP PRO ILE LYS GLU SER LEU LYS ALA MET ILE ALA TRP GLU

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

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

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

ILE LEU LEU PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU TYR PHE LEU SER THR PRO ALA LYS VAL LEU GLY SER GLY GLY HIS ALA SER ASN LYS GLU LYS GLU MET ILE THR SER LEU PHE CYS LYS LEU ALA ALA LEU VAL ARG HIS ARG VAL SER LEU PHE GLY THR ASP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L4013
K4014
P4176
E4182
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S4198
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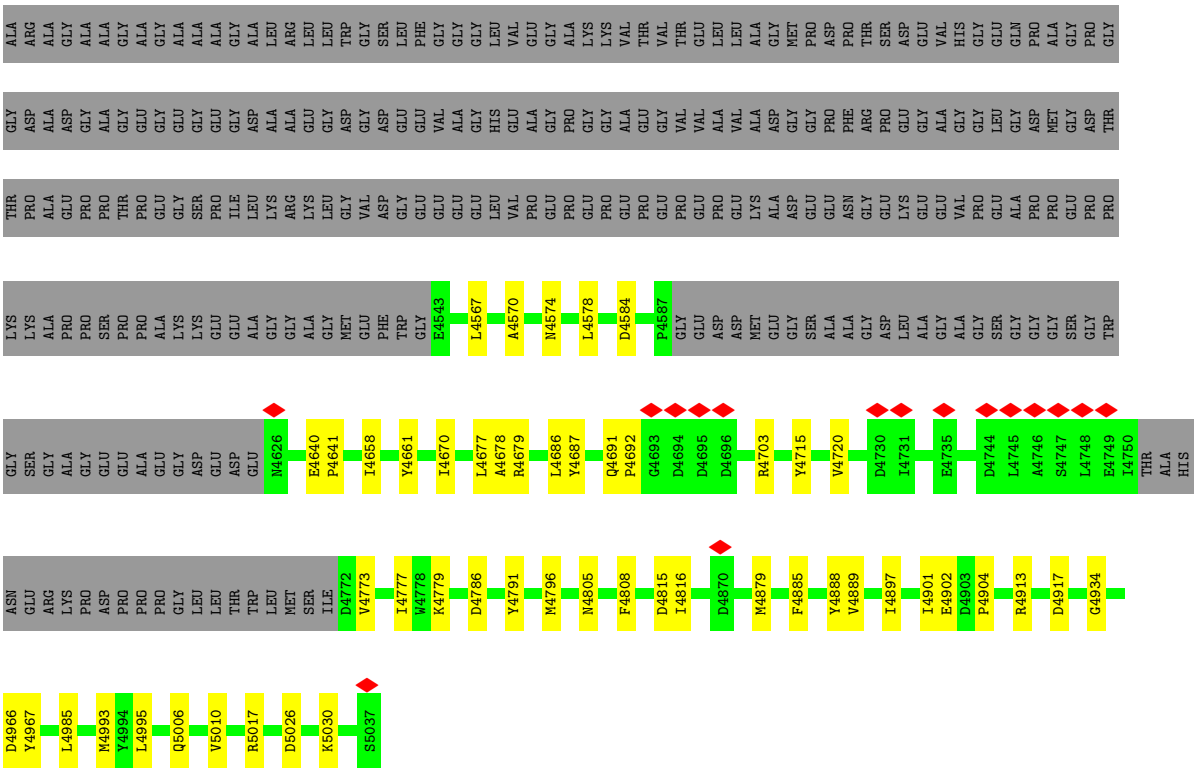
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GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLU GLY GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR
THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU GLU LYS ALA ASP GLY GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO
LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU PHE TRP GLY E4543 L4567 A4570 N4574 L4578 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP
GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 E4640 P4641 I4658 Y4661 I4670 L4677 A4678 R4679 L4686 Y4687 Q4691 P4692 G4693 D4694 D4695 D4696 R4703 Y4715 V4720 D4730 I4731 E4735 D4744 L4745 A4746 S4747 L4748 E4749 I4750 THR ALA HIS
ASN GLU ARG LYS PRO ASP PRO PRO PRO GLY LEU LEU THR TRP LEU MET SER ILE D4772 V4773 I4777 W4778 K4779 D4786 Y4791 M4796 N4805 F4808 D4815 I4816 D4870 M4879 F4885 Y4888 V4889 I4897 I4901 E4902 D4903 P4904 R4913 D4917 G4934
D4966 Y4967 L4985 M4993 Y4994 L4995 Q5006 V5010 R5017 D5026 K5030 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51504	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.677	Depositor
Minimum map value	-2.569	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.585	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.25	0/5241	0.43	0/7072
1	B	0.25	0/5241	0.42	0/7072
1	C	0.25	0/5241	0.42	0/7072
1	D	0.25	0/5241	0.42	0/7072
All	All	0.25	0/20964	0.42	0/28288

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5122	0	5019	44	0
1	B	5122	0	5019	46	0
1	C	5122	0	5019	48	0
1	D	5122	0	5019	45	0
2	A	19	0	13	0	0
2	B	19	0	13	0	0
2	C	19	0	13	0	0
2	D	19	0	13	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	20568	0	20128	174	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 (174) 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:B:4995:LEU:HD11	1:B:5010:VAL:HG13	1.76	0.68
1:C:4995:LEU:HD11	1:C:5010:VAL:HG13	1.76	0.67
1:D:4995:LEU:HD11	1:D:5010:VAL:HG13	1.76	0.66
1:A:4995:LEU:HD11	1:A:5010:VAL:HG13	1.76	0.66
1:D:4902:GLU:O	1:D:4913:ARG:NH1	2.27	0.63
1:B:4902:GLU:O	1:B:4913:ARG:NH1	2.27	0.59
1:D:4904:PRO:HB3	1:D:4913:ARG:HG2	1.85	0.58
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.85	0.58
1:B:4241:THR:O	1:B:4245:MET:HG3	2.04	0.58
1:C:4678:ALA:HB1	1:C:4720:VAL:HG21	1.86	0.58
1:B:4678:ALA:HB1	1:B:4720:VAL:HG21	1.86	0.57
1:C:4241:THR:O	1:C:4245:MET:HG3	2.04	0.57
1:C:4214:LYS:HE2	1:C:4985:LEU:HD11	1.87	0.57
1:D:4214:LYS:HE2	1:D:4985:LEU:HD11	1.87	0.57
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.85	0.57
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.86	0.57
1:A:4241:THR:O	1:A:4245:MET:HG3	2.04	0.57
1:B:4214:LYS:HE2	1:B:4985:LEU:HD11	1.87	0.57
1:D:4241:THR:O	1:D:4245:MET:HG3	2.04	0.57
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.85	0.57
1:B:4888:TYR:OH	1:C:4917:ASP:OD2	2.22	0.56
1:A:4214:LYS:HE2	1:A:4985:LEU:HD11	1.87	0.56
1:C:4888:TYR:OH	1:D:4917:ASP:OD2	2.22	0.56
1:A:4678:ALA:HB1	1:A:4720:VAL:HG21	1.86	0.56
1:B:4885:PHE:O	1:B:4889:VAL:HG22	2.06	0.56
1:C:4885:PHE:O	1:C:4889:VAL:HG22	2.06	0.56
1:A:4888:TYR:OH	1:B:4917:ASP:OD2	2.22	0.55
1:A:4902:GLU:O	1:A:4913:ARG:NH1	2.27	0.55
1:D:4885:PHE:O	1:D:4889:VAL:HG22	2.06	0.55
1:A:4917:ASP:OD2	1:D:4888:TYR:OH	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4885:PHE:O	1:A:4889:VAL:HG22	2.06	0.55
1:C:4902:GLU:O	1:C:4913:ARG:NH1	2.27	0.54
1:C:4966:ASP:OD1	1:C:4967:TYR:N	2.41	0.54
1:D:4966:ASP:OD1	1:D:4967:TYR:N	2.40	0.54
1:A:4966:ASP:OD1	1:A:4967:TYR:N	2.40	0.54
1:B:4966:ASP:OD1	1:B:4967:TYR:N	2.41	0.53
1:C:4013:LEU:HD12	1:C:4016:LEU:HD23	1.91	0.53
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.38	0.53
1:B:4013:LEU:HD12	1:B:4016:LEU:HD23	1.91	0.52
1:B:5026:ASP:HA	1:B:5030:LYS:HD2	1.92	0.52
1:C:5026:ASP:HA	1:C:5030:LYS:HD2	1.92	0.52
1:A:4056:GLU:OE2	1:A:4060:LYS:NZ	2.42	0.52
1:D:4013:LEU:HD12	1:D:4016:LEU:HD23	1.91	0.52
1:D:5026:ASP:HA	1:D:5030:LYS:HD2	1.92	0.51
1:A:5026:ASP:HA	1:A:5030:LYS:HD2	1.92	0.51
1:D:4056:GLU:OE2	1:D:4060:LYS:NZ	2.43	0.51
1:C:4056:GLU:OE2	1:C:4060:LYS:NZ	2.43	0.51
1:D:4686:LEU:O	1:D:4691:GLN:N	2.40	0.51
1:A:4013:LEU:HD12	1:A:4016:LEU:HD23	1.91	0.50
1:D:4773:VAL:O	1:D:4777:ILE:HG12	2.12	0.50
1:A:4773:VAL:O	1:A:4777:ILE:HG12	2.12	0.50
1:C:4232:GLU:OE2	1:C:5017:ARG:NH2	2.45	0.49
1:D:4658:ILE:HD11	1:D:4796:MET:HB2	1.95	0.49
1:B:4791:TYR:OH	1:B:4815:ASP:OD1	2.24	0.49
1:A:4791:TYR:OH	1:A:4815:ASP:OD1	2.24	0.49
1:B:4232:GLU:OE2	1:B:5017:ARG:NH2	2.46	0.49
1:A:4658:ILE:HD11	1:A:4796:MET:HB2	1.95	0.49
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.38	0.49
1:B:4773:VAL:O	1:B:4777:ILE:HG12	2.12	0.49
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.45	0.48
1:C:4658:ILE:HD11	1:C:4796:MET:HB2	1.95	0.48
1:C:4773:VAL:O	1:C:4777:ILE:HG12	2.12	0.48
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.45	0.48
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.38	0.48
1:B:4056:GLU:OE2	1:B:4060:LYS:NZ	2.43	0.48
1:B:4658:ILE:HD11	1:B:4796:MET:HB2	1.95	0.48
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.38	0.48
1:C:4677:LEU:HD11	1:C:4687:TYR:HE2	1.79	0.48
1:B:4677:LEU:HD11	1:B:4687:TYR:HE2	1.79	0.47
1:D:4913:ARG:NE	1:D:4917:ASP:OD2	2.47	0.47
1:B:4198:SER:OG	1:B:4201:ASN:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4640:GLU:HB3	1:B:4641:PRO:HD3	1.97	0.47
1:A:4198:SER:OG	1:A:4201:ASN:OD1	2.33	0.47
1:A:4677:LEU:HD11	1:A:4687:TYR:HE2	1.79	0.47
1:B:4578:LEU:HA	1:C:4879:MET:HG2	1.97	0.47
1:C:4198:SER:OG	1:C:4201:ASN:OD1	2.33	0.47
1:C:4825:THR:O	1:C:4828:SER:OG	2.24	0.47
1:C:4913:ARG:NE	1:C:4917:ASP:OD2	2.47	0.47
1:D:4677:LEU:HD11	1:D:4687:TYR:HE2	1.79	0.47
1:A:4913:ARG:NE	1:A:4917:ASP:OD2	2.47	0.47
1:B:4913:ARG:NE	1:B:4917:ASP:OD2	2.47	0.47
1:A:4578:LEU:HA	1:B:4879:MET:HG2	1.97	0.47
1:C:4584:ASP:N	1:C:4584:ASP:OD1	2.48	0.47
1:D:4198:SER:OG	1:D:4201:ASN:OD1	2.33	0.47
1:A:4182:GLU:OE2	1:A:4192:ARG:NH2	2.38	0.46
1:A:4640:GLU:HB3	1:A:4641:PRO:HD3	1.97	0.46
1:C:4640:GLU:HB3	1:C:4641:PRO:HD3	1.97	0.46
1:B:4584:ASP:N	1:B:4584:ASP:OD1	2.48	0.46
1:B:4182:GLU:OE2	1:B:4192:ARG:NH2	2.38	0.46
1:B:4242:ILE:HG12	1:B:4993:MET:HB3	1.98	0.46
1:A:4661:TYR:OH	1:A:4786:ASP:OD2	2.26	0.46
1:A:4686:LEU:O	1:A:4691:GLN:N	2.40	0.46
1:C:4242:ILE:HG12	1:C:4993:MET:HB3	1.98	0.46
1:A:4879:MET:HG2	1:D:4578:LEU:HA	1.97	0.46
1:B:4039:MET:O	1:B:4043:GLN:HG2	2.16	0.46
1:D:4039:MET:O	1:D:4043:GLN:HG2	2.16	0.46
1:D:4640:GLU:HB3	1:D:4641:PRO:HD3	1.97	0.46
1:D:4679:ARG:NH1	1:D:4715:TYR:OH	2.37	0.46
1:C:4039:MET:O	1:C:4043:GLN:HG2	2.16	0.45
1:C:4578:LEU:HA	1:D:4879:MET:HG2	1.97	0.45
1:C:4791:TYR:OH	1:C:4815:ASP:OD1	2.24	0.45
1:B:5006:GLN:O	1:B:5010:VAL:HG12	2.17	0.45
1:D:4791:TYR:OH	1:D:4815:ASP:OD1	2.24	0.45
1:A:4205:TRP:CZ2	1:A:4214:LYS:HD2	2.52	0.45
1:C:4205:TRP:CZ2	1:C:4214:LYS:HD2	2.52	0.45
1:B:4205:TRP:CZ2	1:B:4214:LYS:HD2	2.51	0.45
1:C:5006:GLN:O	1:C:5010:VAL:HG12	2.17	0.45
1:A:5006:GLN:O	1:A:5010:VAL:HG12	2.17	0.45
1:D:4205:TRP:CZ2	1:D:4214:LYS:HD2	2.51	0.45
1:D:4687:TYR:HA	1:D:4691:GLN:HG2	1.99	0.45
1:A:4692:PRO:HD2	1:A:4703:ARG:NH2	2.32	0.45
1:B:4686:LEU:O	1:B:4691:GLN:N	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4242:ILE:HG12	1:A:4993:MET:HB3	1.98	0.44
1:C:4687:TYR:HA	1:C:4691:GLN:HG2	1.99	0.44
1:D:4661:TYR:OH	1:D:4786:ASP:OD2	2.26	0.44
1:D:5006:GLN:O	1:D:5010:VAL:HG12	2.17	0.44
1:C:4686:LEU:O	1:C:4691:GLN:N	2.40	0.44
1:D:4242:ILE:HG12	1:D:4993:MET:HB3	1.98	0.44
1:A:4015:GLU:HA	1:A:4018:ASP:OD2	2.18	0.44
1:A:4687:TYR:HA	1:A:4691:GLN:HG2	1.99	0.44
1:B:4687:TYR:HA	1:B:4691:GLN:HG2	1.99	0.44
1:C:4679:ARG:NH1	1:C:4715:TYR:OH	2.37	0.44
1:C:4897:ILE:O	1:C:4901:ILE:HG12	2.18	0.44
1:D:4692:PRO:HD2	1:D:4703:ARG:NH2	2.33	0.44
1:A:4897:ILE:O	1:A:4901:ILE:HG12	2.18	0.44
1:B:4015:GLU:HA	1:B:4018:ASP:OD2	2.18	0.44
1:C:4015:GLU:HA	1:C:4018:ASP:OD2	2.18	0.44
1:A:4584:ASP:OD1	1:A:4584:ASP:N	2.48	0.44
1:B:4567:LEU:HD11	1:B:4816:ILE:HG22	2.00	0.44
1:B:4897:ILE:O	1:B:4901:ILE:HG12	2.18	0.44
1:C:4692:PRO:HD2	1:C:4703:ARG:NH2	2.32	0.44
1:B:4661:TYR:OH	1:B:4786:ASP:OD2	2.26	0.43
1:B:4692:PRO:HD2	1:B:4703:ARG:NH2	2.32	0.43
1:B:4825:THR:O	1:B:4828:SER:OG	2.24	0.43
1:D:4670:ILE:HG13	1:D:4779:LYS:NZ	2.33	0.43
1:A:4670:ILE:HG13	1:A:4779:LYS:NZ	2.33	0.43
1:B:4805:ASN:HB3	1:B:4808:PHE:CD2	2.54	0.43
1:D:4015:GLU:HA	1:D:4018:ASP:OD2	2.18	0.43
1:D:4584:ASP:OD1	1:D:4584:ASP:N	2.48	0.43
1:C:4567:LEU:HD11	1:C:4816:ILE:HG22	2.01	0.43
1:D:4014:LYS:HD3	1:D:4014:LYS:HA	1.84	0.43
1:A:4805:ASN:HB3	1:A:4808:PHE:CD2	2.54	0.43
1:B:4679:ARG:NH1	1:B:4715:TYR:OH	2.37	0.43
1:C:4670:ILE:HG13	1:C:4779:LYS:NZ	2.34	0.43
1:C:4805:ASN:HB3	1:C:4808:PHE:CD2	2.54	0.43
1:D:4567:LEU:HD11	1:D:4816:ILE:HG22	2.00	0.43
1:A:4014:LYS:HD3	1:A:4014:LYS:HA	1.84	0.43
1:B:4823:LEU:HD23	1:B:4823:LEU:HA	1.90	0.43
1:A:4567:LEU:HD11	1:A:4816:ILE:HG22	2.01	0.43
1:A:4679:ARG:NH1	1:A:4715:TYR:OH	2.37	0.43
1:B:4670:ILE:HG13	1:B:4779:LYS:NZ	2.34	0.43
1:D:4182:GLU:OE2	1:D:4192:ARG:NH2	2.37	0.42
1:D:4805:ASN:HB3	1:D:4808:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4897:ILE:O	1:D:4901:ILE:HG12	2.18	0.42
1:D:4901:ILE:HG13	1:D:4913:ARG:NH2	2.35	0.42
1:A:4901:ILE:HG13	1:A:4913:ARG:NH2	2.35	0.42
1:C:4182:GLU:OE2	1:C:4192:ARG:NH2	2.37	0.42
1:C:4823:LEU:HD23	1:C:4823:LEU:HA	1.90	0.42
1:D:4805:ASN:HB3	1:D:4808:PHE:HD2	1.85	0.42
1:B:4805:ASN:HB3	1:B:4808:PHE:HD2	1.85	0.42
1:B:4901:ILE:HG13	1:B:4913:ARG:NH2	2.35	0.42
1:C:4901:ILE:HG13	1:C:4913:ARG:NH2	2.35	0.41
1:A:4805:ASN:HB3	1:A:4808:PHE:HD2	1.85	0.41
1:C:3955:MET:HE1	1:C:4016:LEU:HA	2.03	0.41
1:D:4679:ARG:HH21	1:D:5017:ARG:NH1	2.19	0.41
1:A:4679:ARG:HH21	1:A:5017:ARG:NH1	2.19	0.41
1:C:4014:LYS:HA	1:C:4014:LYS:HD3	1.84	0.40
1:B:4984:ASN:HB3	1:B:4987:ASN:HB2	2.04	0.40
1:C:4995:LEU:HD23	1:C:4995:LEU:HA	1.96	0.40
1:A:3980:LEU:HD23	1:A:3980:LEU:HA	1.95	0.40
1:B:4223:ASN:HB3	1:B:4224:GLU:OE2	2.22	0.40
1:C:4679:ARG:HH21	1:C:5017:ARG:NH1	2.19	0.40
1:C:4937:ILE:HG12	1:D:4934:GLY:HA2	2.04	0.40
1:C:4984:ASN:HB3	1:C:4987:ASN:HB2	2.04	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	616/5037 (12%)	600 (97%)	16 (3%)	0	100	100
1	B	616/5037 (12%)	601 (98%)	15 (2%)	0	100	100
1	C	616/5037 (12%)	601 (98%)	15 (2%)	0	100	100
1	D	616/5037 (12%)	601 (98%)	15 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2464/20148 (12%)	2403 (98%)	61 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/4276 (13%)	559 (100%)	0	100	100
1	B	559/4276 (13%)	559 (100%)	0	100	100
1	C	559/4276 (13%)	559 (100%)	0	100	100
1	D	559/4276 (13%)	559 (100%)	0	100	100
All	All	2236/17104 (13%)	2236 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 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	$\#\|Z\| > 2$
2	ADN	B	5101	-	18,21,21	0.65	0	18,31,31	0.79	1 (5%)
2	ADN	A	5101	-	18,21,21	0.66	0	18,31,31	0.79	1 (5%)
2	ADN	C	5101	-	18,21,21	0.66	0	18,31,31	0.79	1 (5%)
2	ADN	D	5101	-	18,21,21	0.65	0	18,31,31	0.78	1 (5%)

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
2	ADN	B	5101	-	-	2/2/22/22	0/3/3/3
2	ADN	A	5101	-	-	2/2/22/22	0/3/3/3
2	ADN	C	5101	-	-	2/2/22/22	0/3/3/3
2	ADN	D	5101	-	-	2/2/22/22	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5101	ADN	C5-C6-N6	2.30	123.85	120.35
2	B	5101	ADN	C5-C6-N6	2.28	123.81	120.35
2	C	5101	ADN	C5-C6-N6	2.28	123.81	120.35
2	D	5101	ADN	C5-C6-N6	2.28	123.81	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

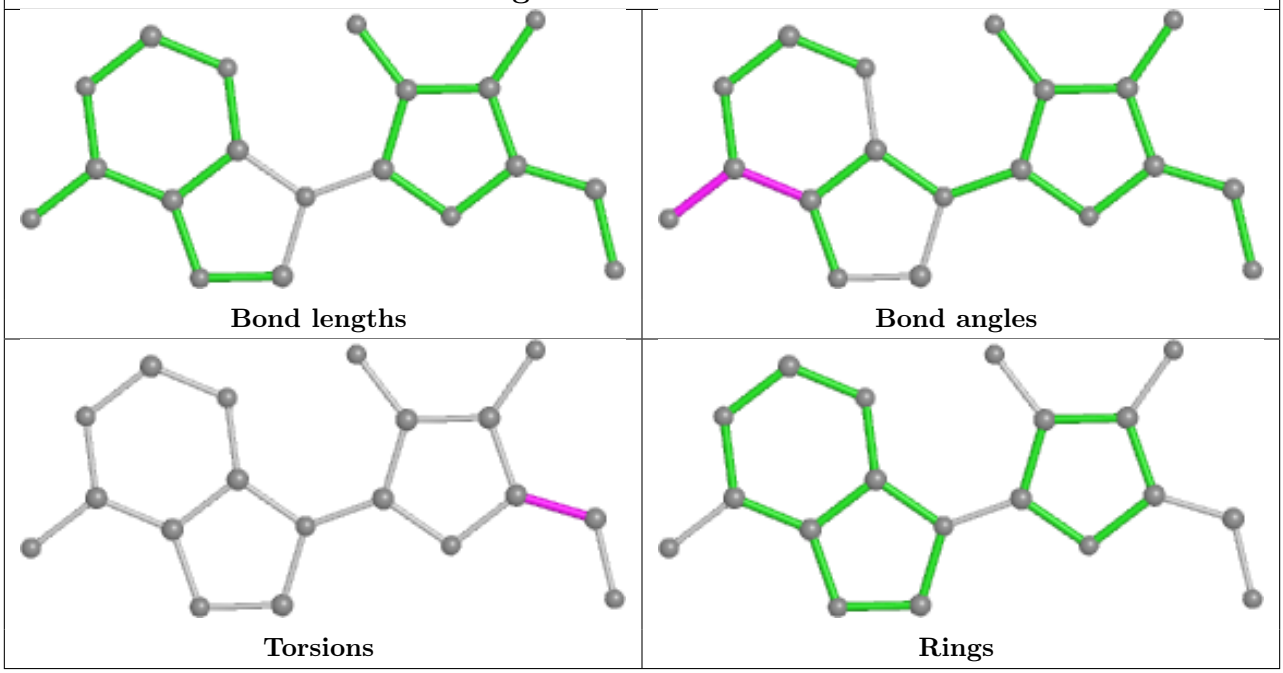
Mol	Chain	Res	Type	Atoms
2	A	5101	ADN	O4'-C4'-C5'-O5'
2	C	5101	ADN	O4'-C4'-C5'-O5'
2	D	5101	ADN	O4'-C4'-C5'-O5'
2	B	5101	ADN	O4'-C4'-C5'-O5'
2	C	5101	ADN	C3'-C4'-C5'-O5'
2	D	5101	ADN	C3'-C4'-C5'-O5'
2	A	5101	ADN	C3'-C4'-C5'-O5'
2	B	5101	ADN	C3'-C4'-C5'-O5'

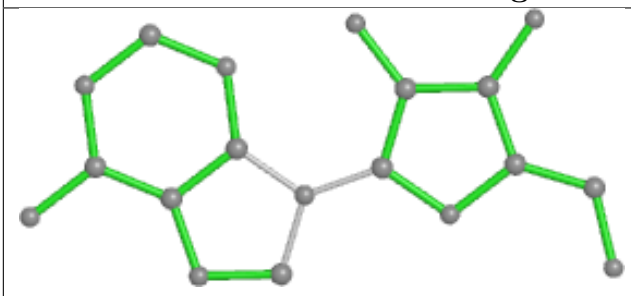
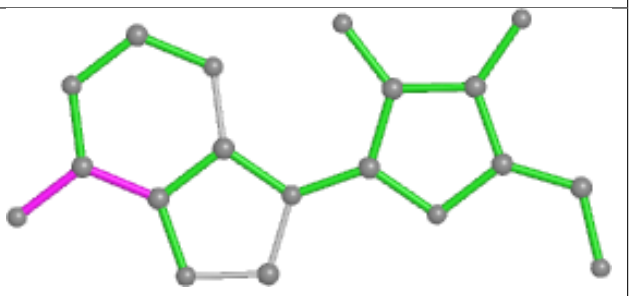
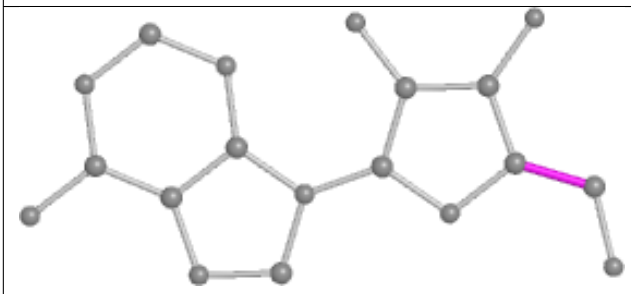
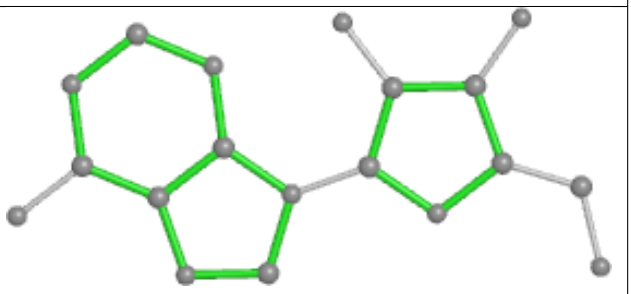
There are no ring outliers.

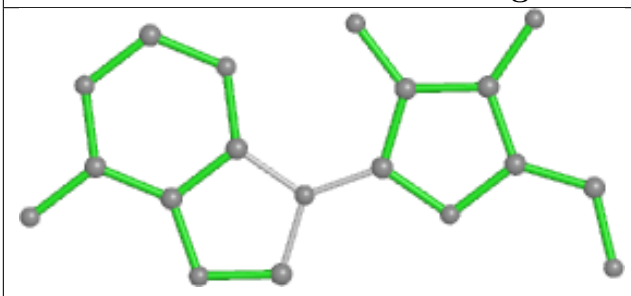
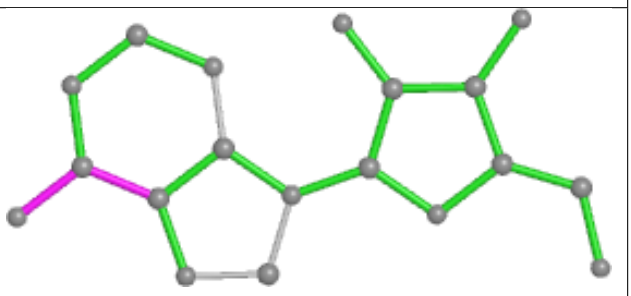
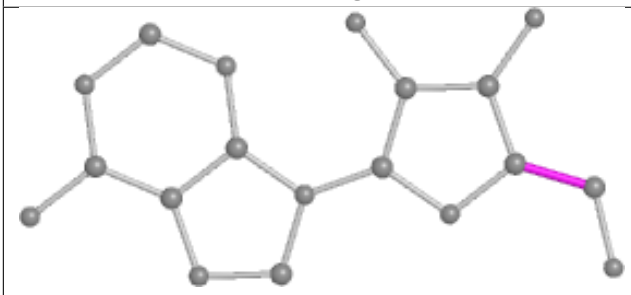
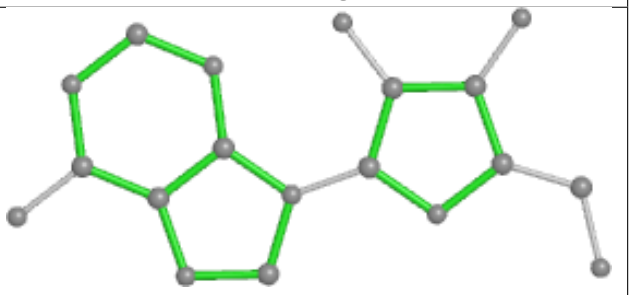
No monomer is involved in short contacts.

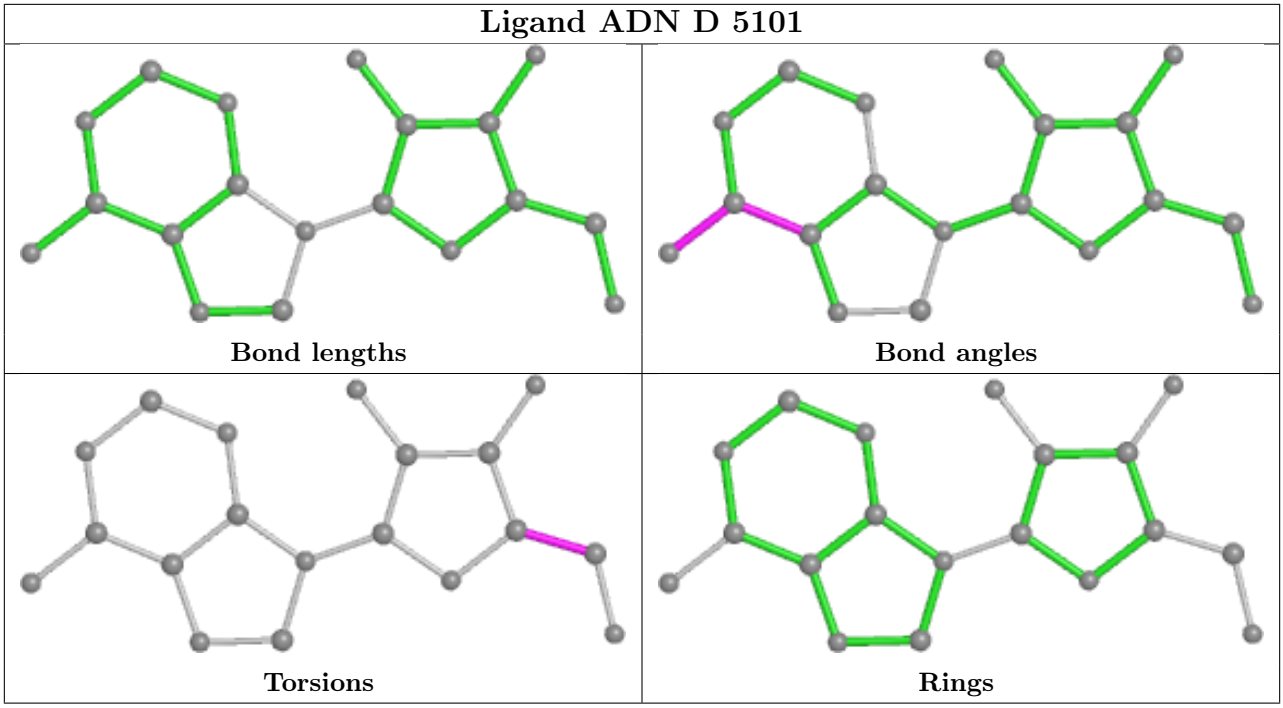
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ADN B 5101



Ligand ADN A 5101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADN C 5101	
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

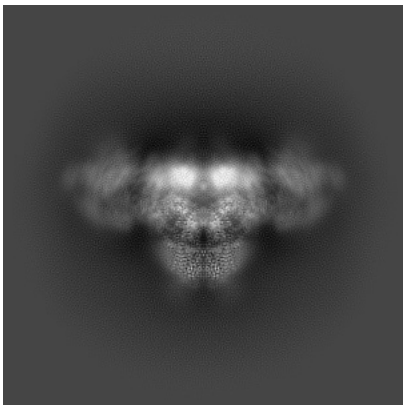
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-40433. These allow visual inspection of the internal detail of the map and identification of artifacts.

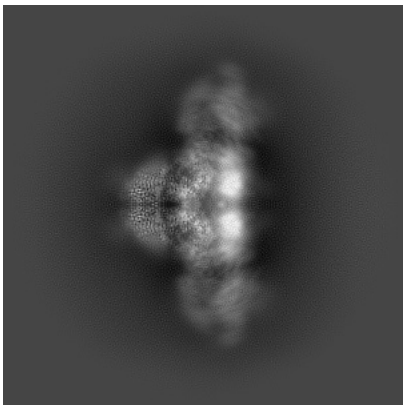
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

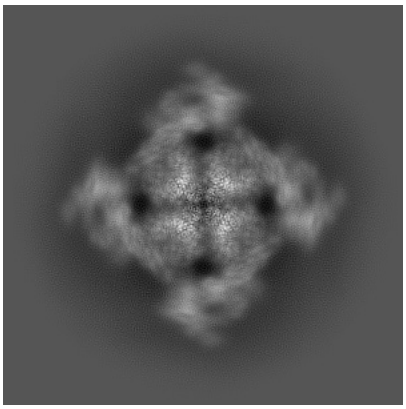
6.1.1 Primary map



X

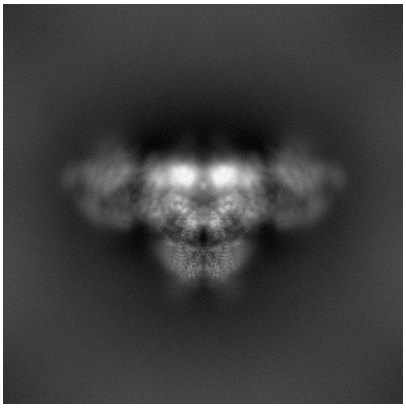


Y

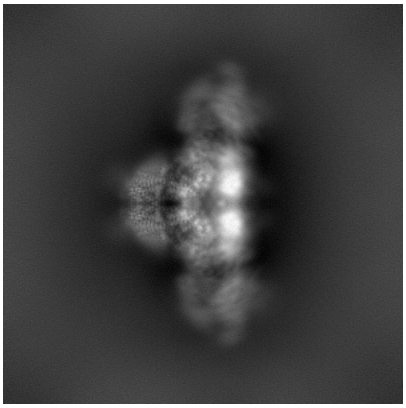


Z

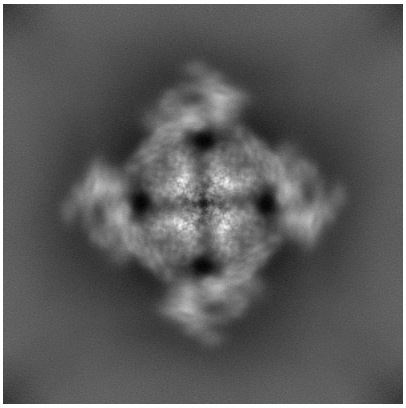
6.1.2 Raw map



X



Y

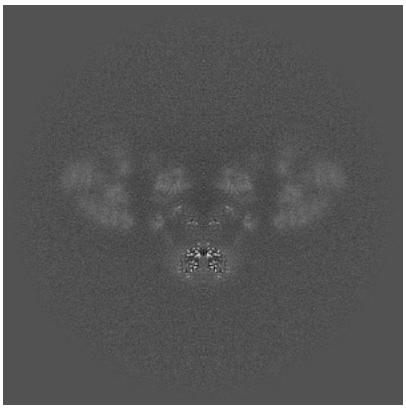


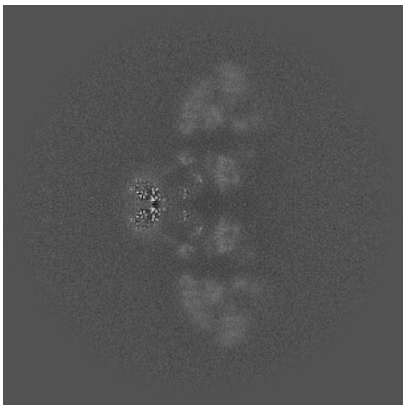
Z

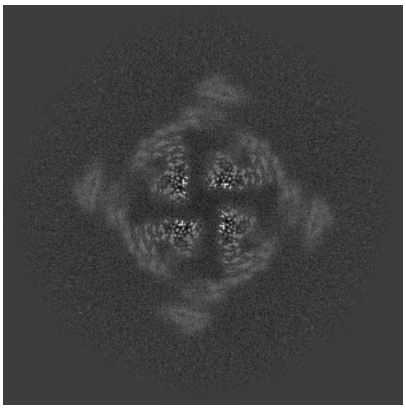
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

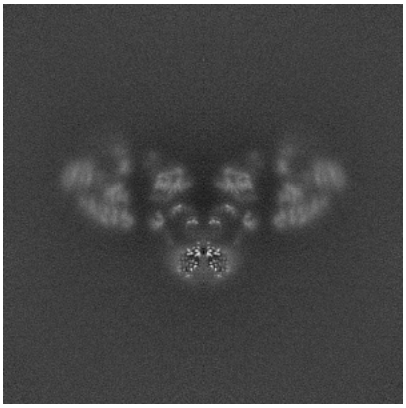
6.2.1 Primary map

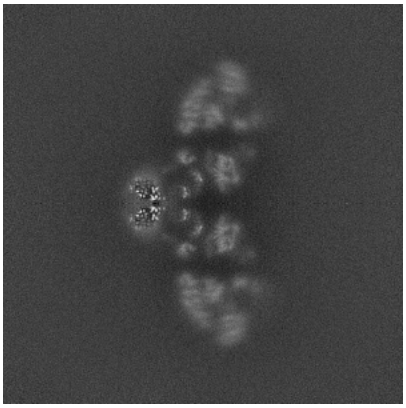

X Index: 200

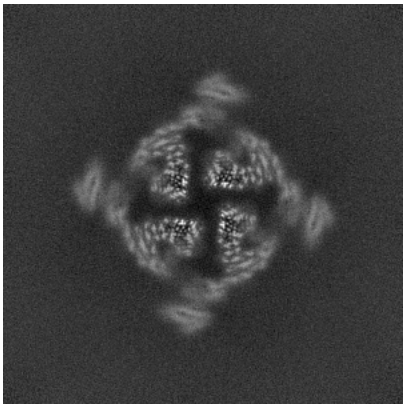

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

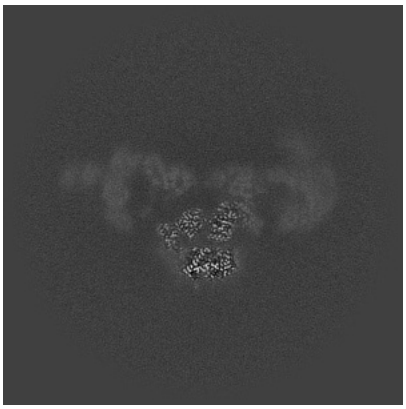

Y Index: 200

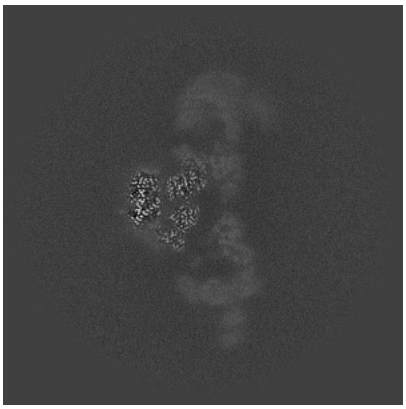

Z Index: 200

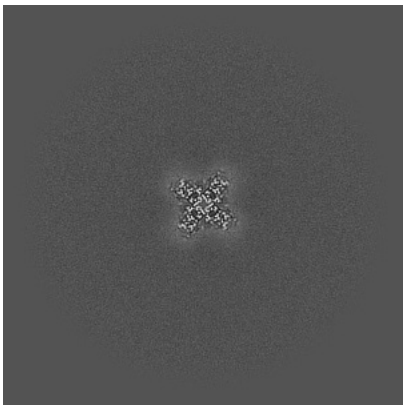
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

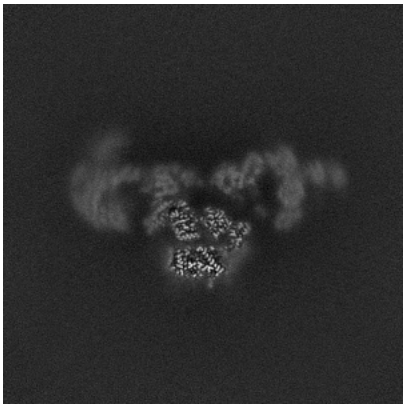
6.3.1 Primary map

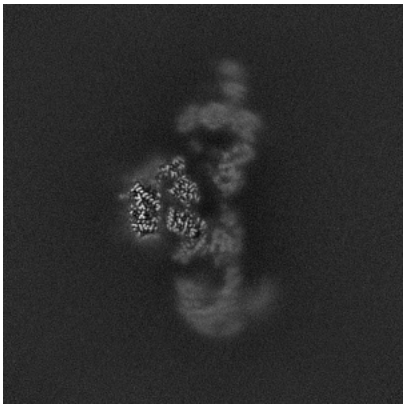

X Index: 212

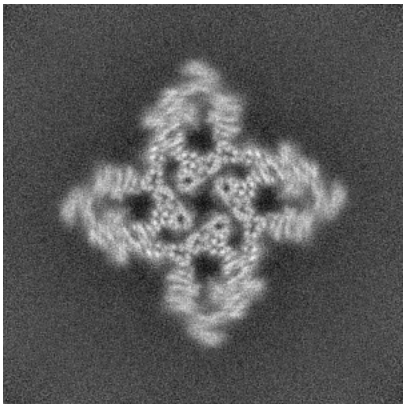

Y Index: 188


Z Index: 137

6.3.2 Raw map


X Index: 188

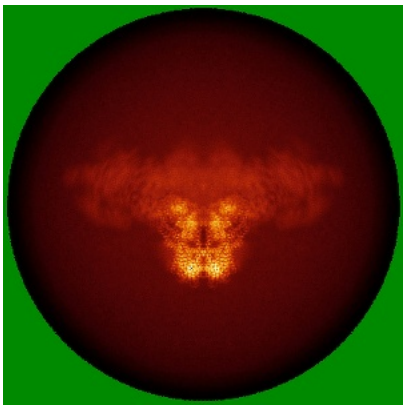

Y Index: 212

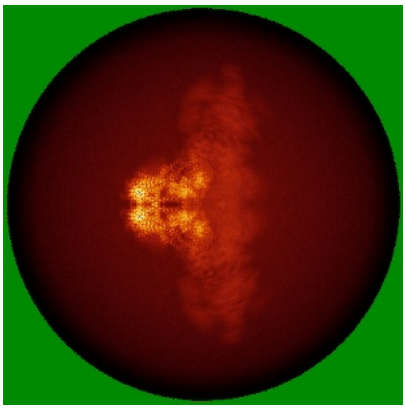

Z Index: 225

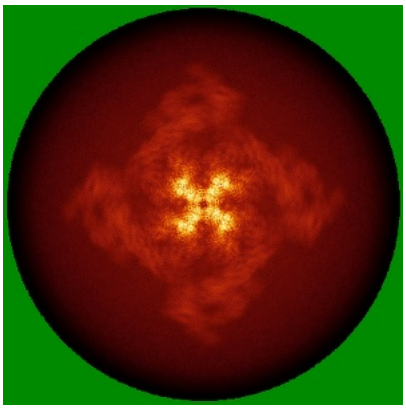
The images above show the largest variance slices of the map in three orthogonal directions.

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

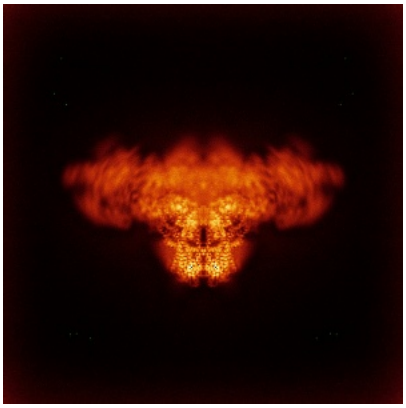
6.4.1 Primary map

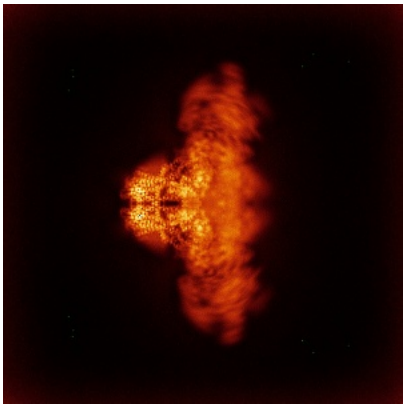

X

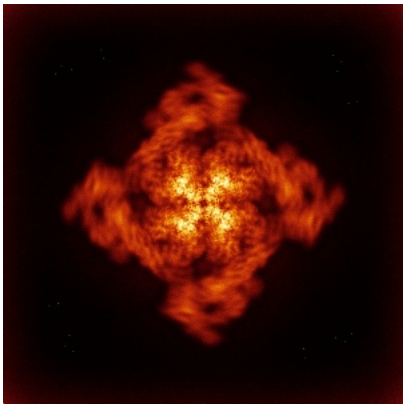

Y


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 0.585. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

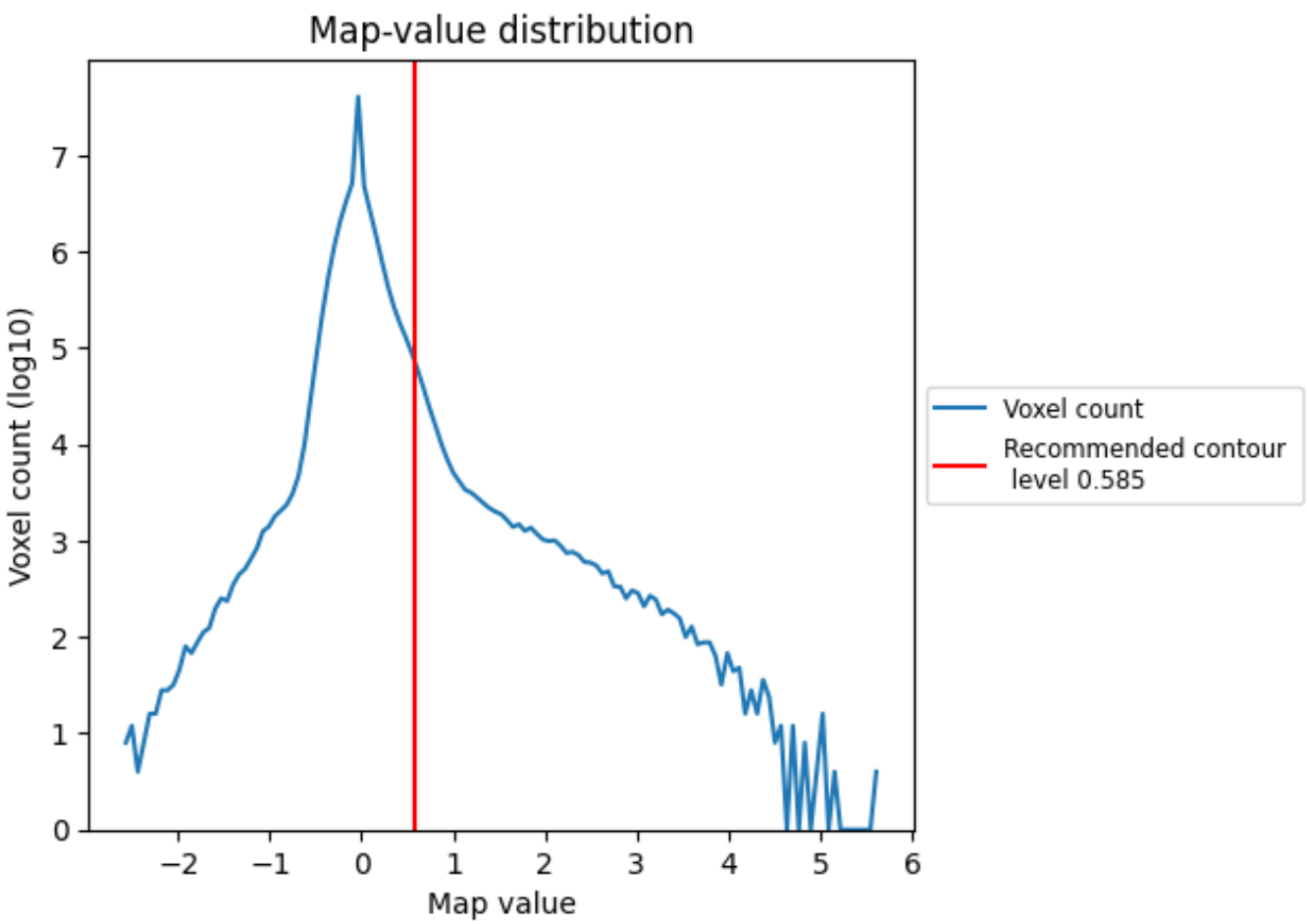
6.6 Mask visualisation (i)

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

7 Map analysis (i)

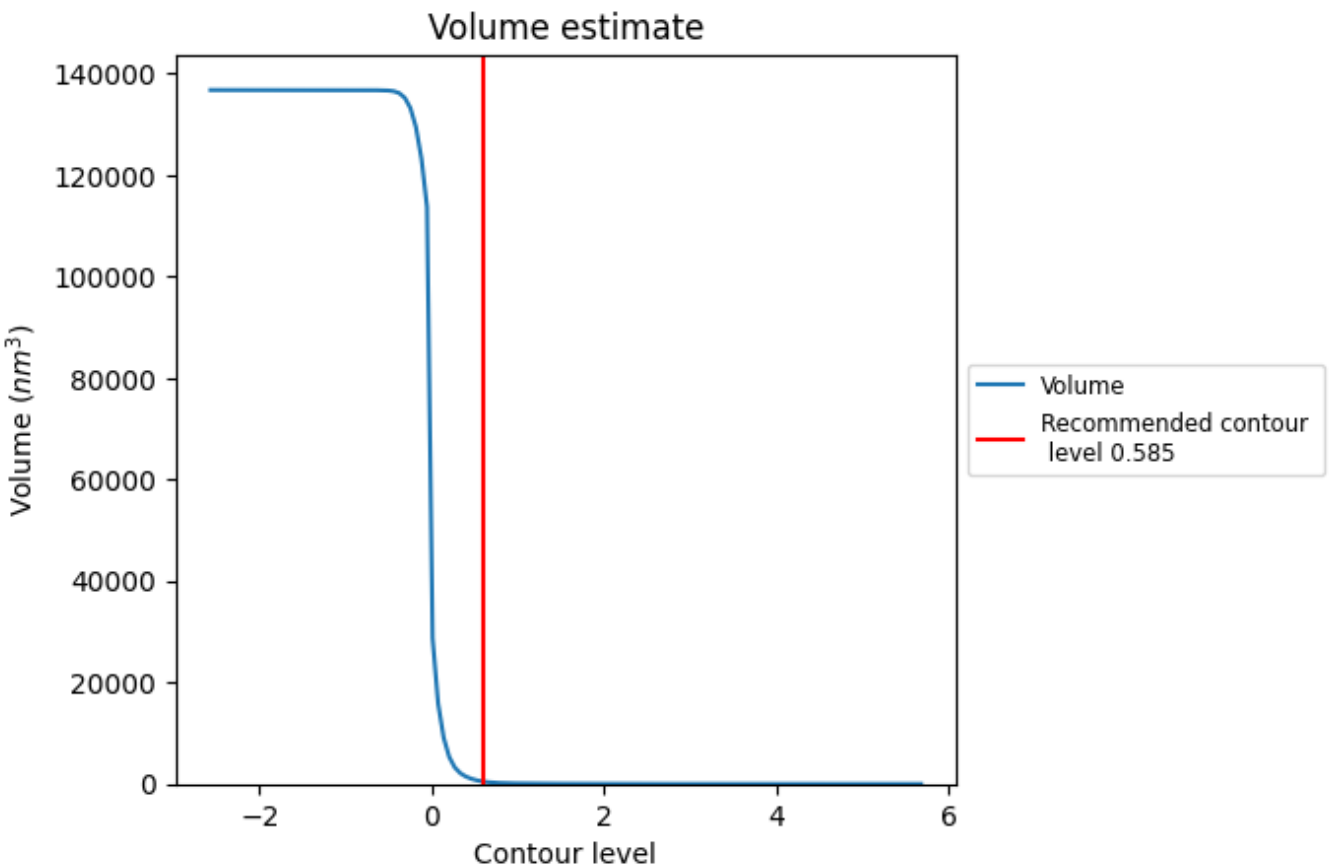
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

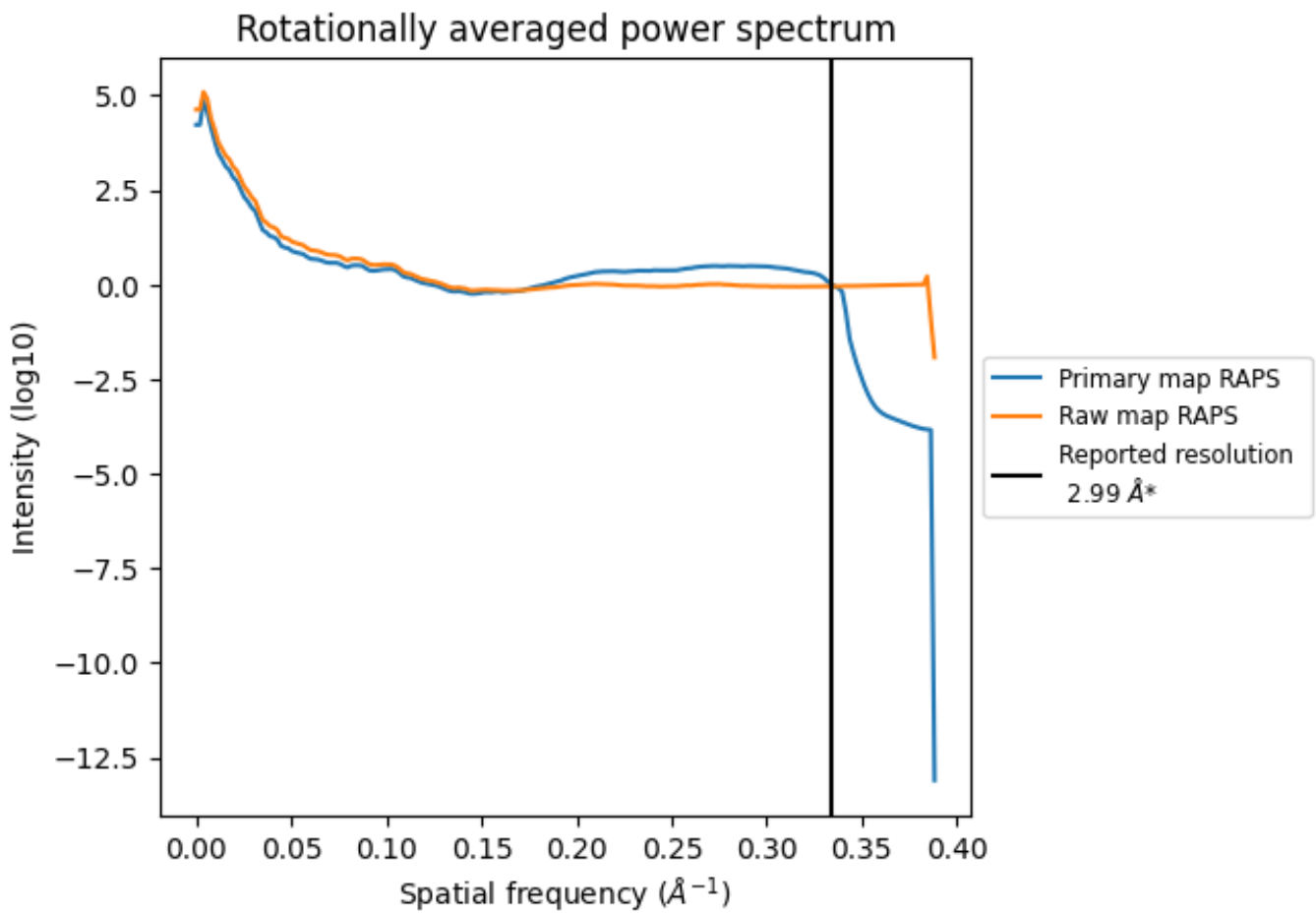
7.2 Volume estimate (i)



The volume at the recommended contour level is 502 nm^3; this corresponds to an approximate mass of 453 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)

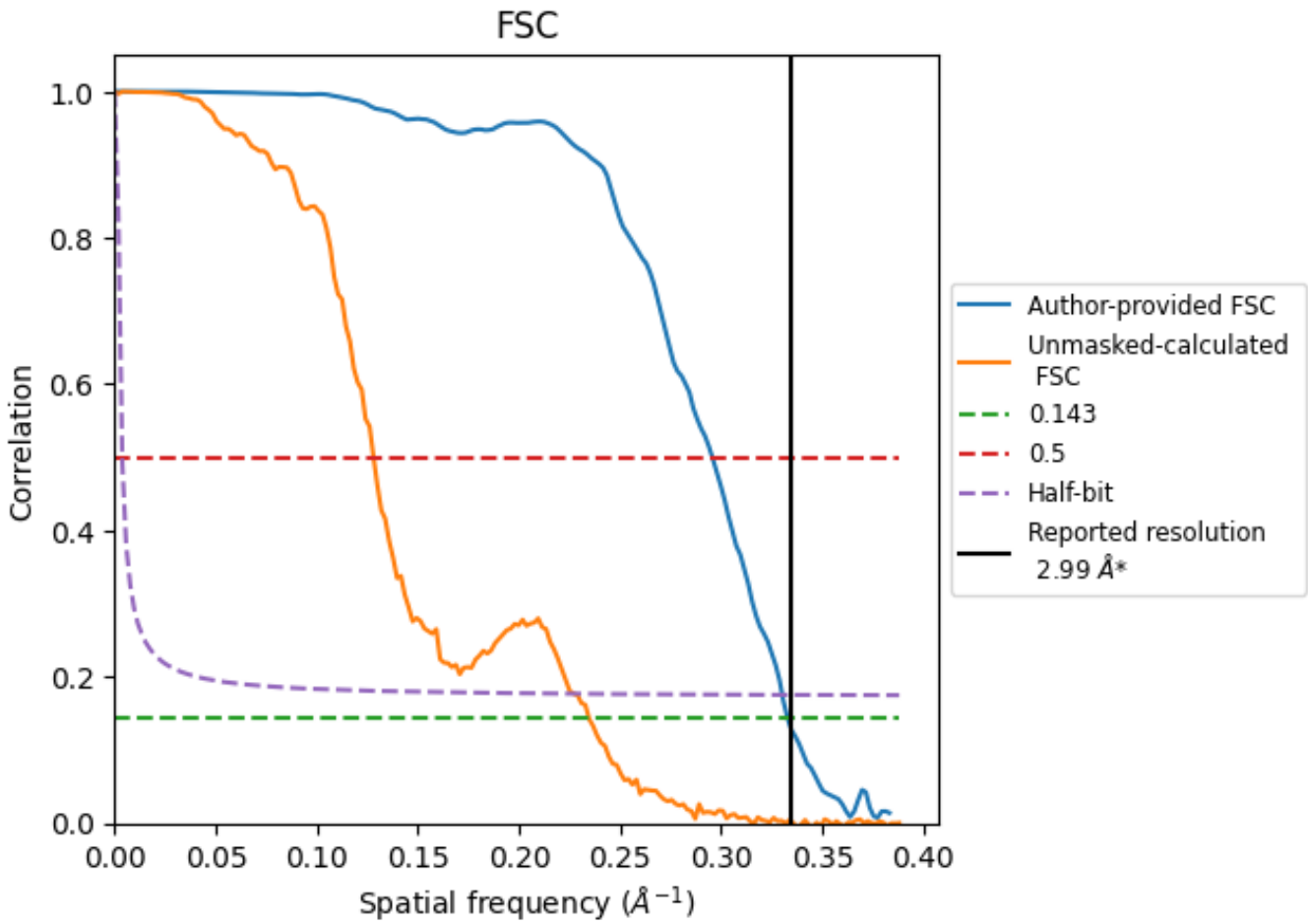


*Reported resolution corresponds to spatial frequency of 0.334 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.334 Å^{-1}

8.2 Resolution estimates (i)

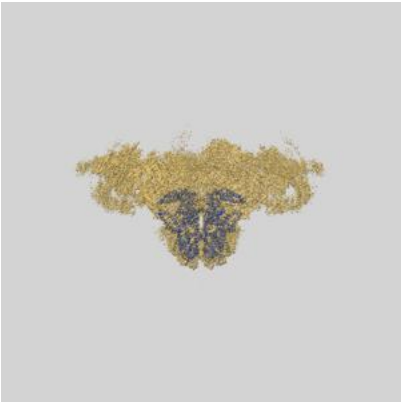
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	3.00	3.38	3.03
Unmasked-calculated*	4.26	7.80	4.40

*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 4.26 differs from the reported value 2.99 by more than 10 %

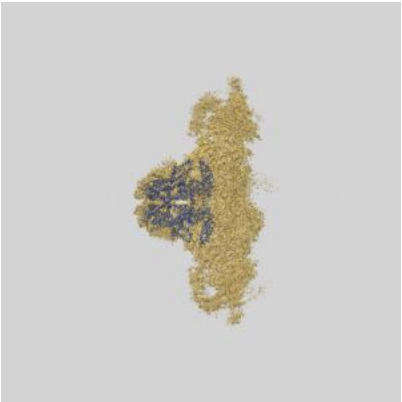
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-40433 and PDB model 8SEY. Per-residue inclusion information can be found in section 3 on page 5.

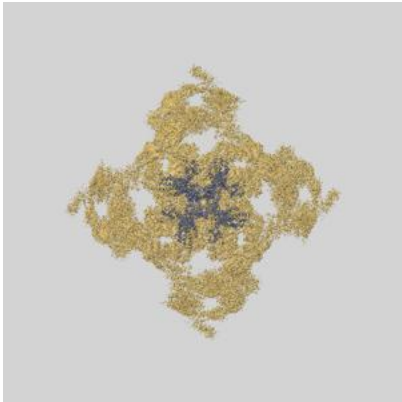
9.1 Map-model overlay (i)



X



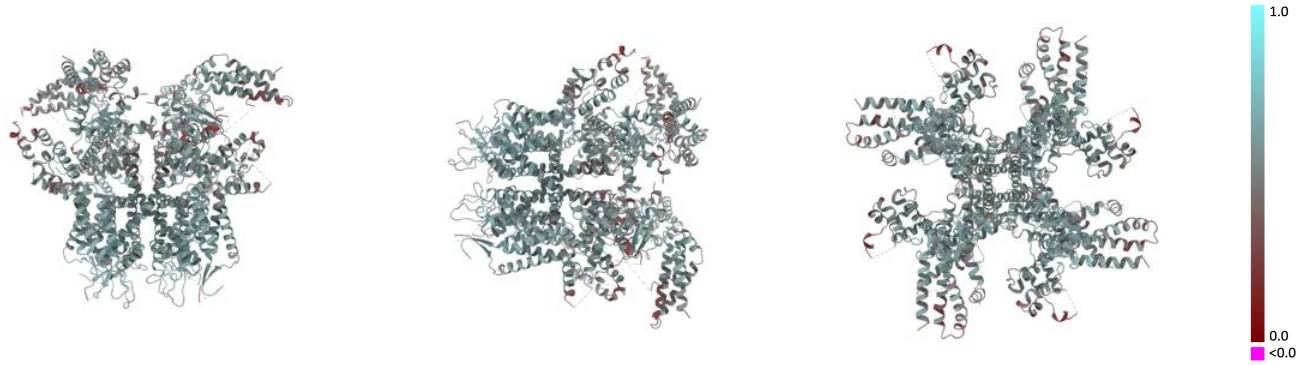
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.585 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.

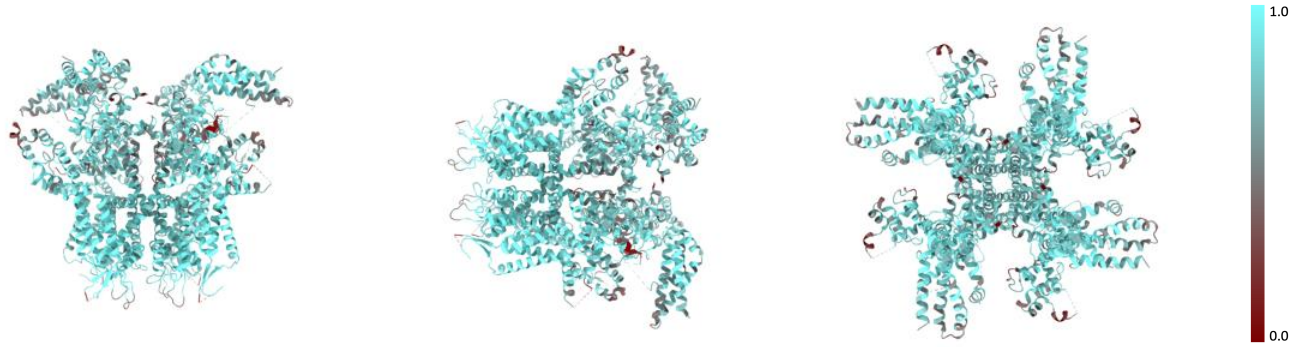
9.2 Q-score mapped to coordinate model (i)



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.

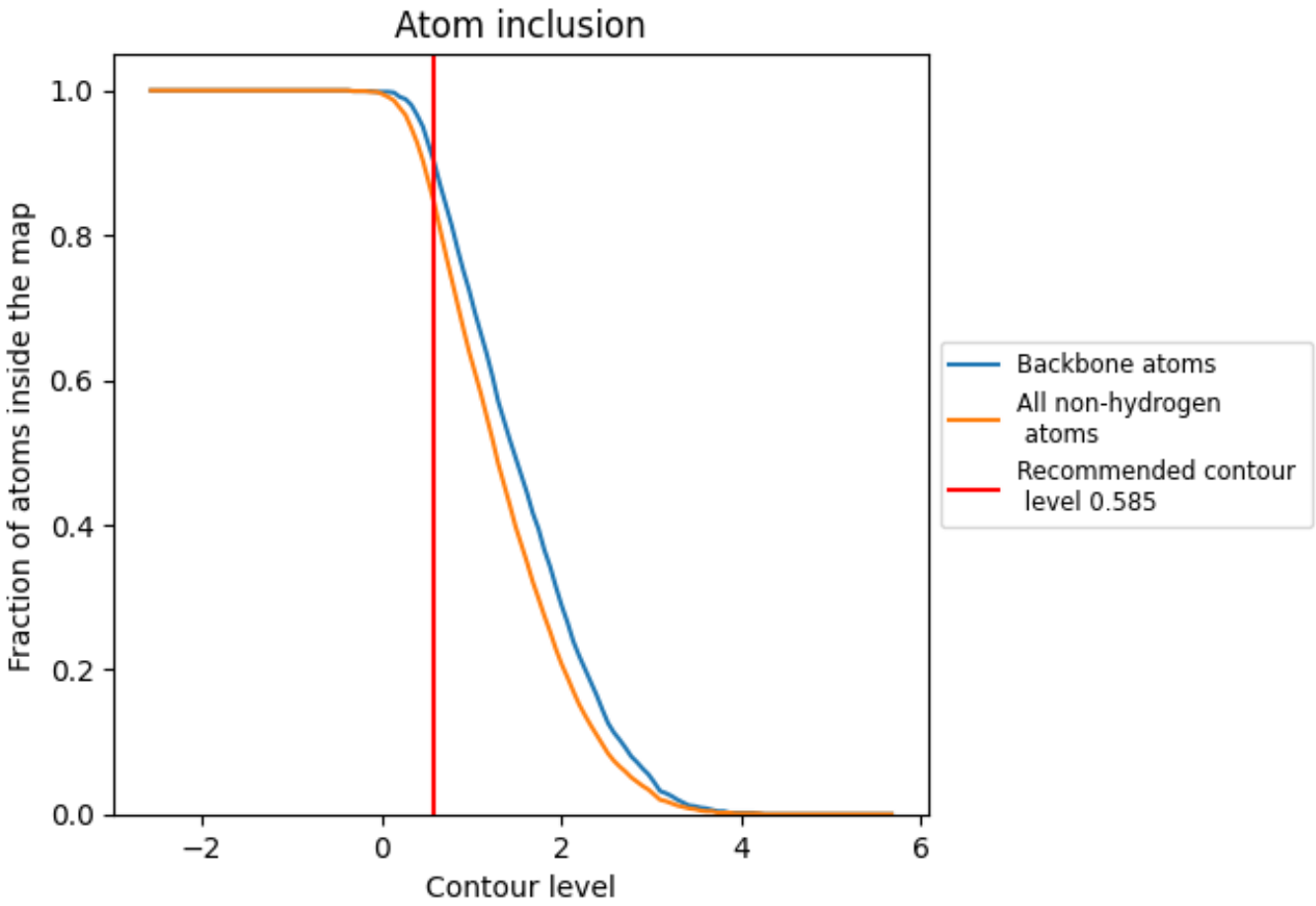
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.585).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.585) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.5450
A	0.8450	0.5450
B	0.8450	0.5440
C	0.8450	0.5450
D	0.8450	0.5450