Full wwPDB EM Validation Report (i)

Mar 10, 2026 – 03:38 AM UTC

PDB ID	:	8SEX / pdb_00008sex
EMDB ID	:	EMD-40432
Title	:	Cryo-EM Structure of RyR1 + AMP (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	:	2.84 Å(reported)

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

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

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

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

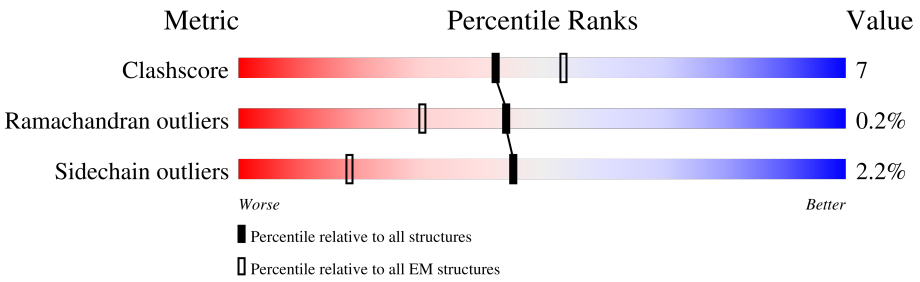
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.49

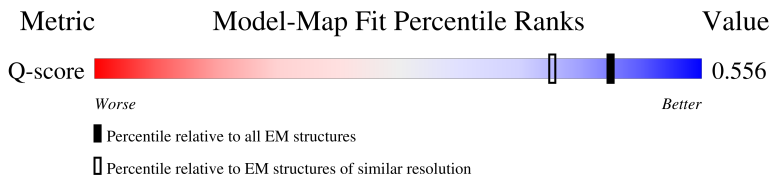
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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	11884 (2.34 - 3.34)

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	10% · 88%
1	B	5037	10% · 88%
1	C	5037	10% · 88%
1	D	5037	10% · 88%

2 Entry composition (i)

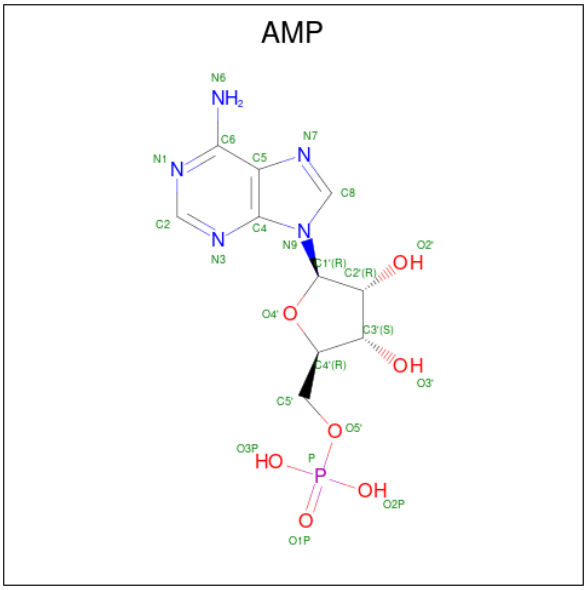
There are 3 unique types of molecules in this entry. The entry contains 20568 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	5118	3326	815	937	40	0	0
1	B	626	5118	3326	815	937	40	0	0
1	C	626	5118	3326	815	937	40	0	0
1	D	626	5118	3326	815	937	40	0	0

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	23	10	5	7	1	0
2	B	1	23	10	5	7	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	C	1	23	10	5	7	1	0
			Total	C	N	O	P	
2	D	1	23	10	5	7	1	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

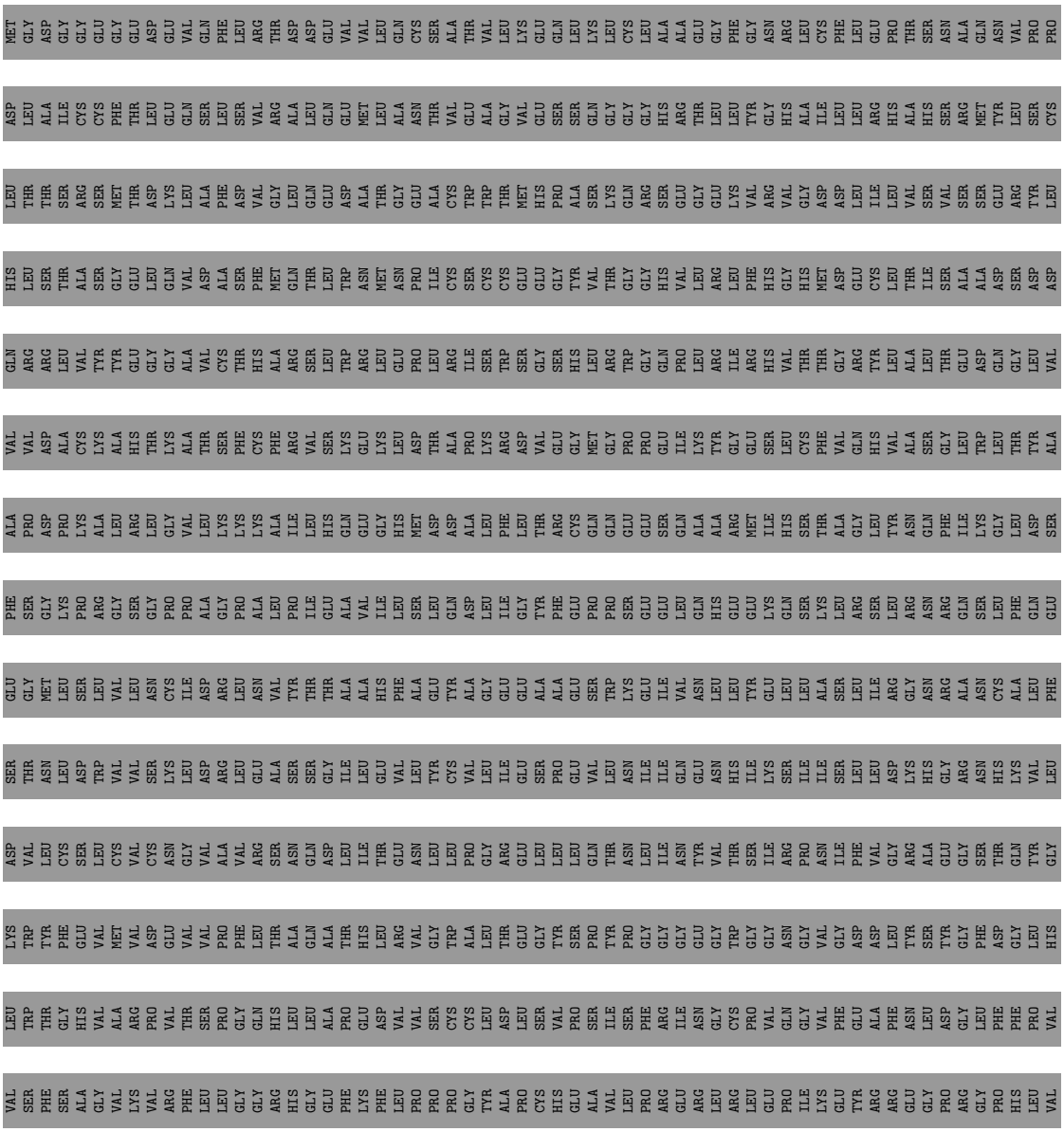
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0
			Total	Zn	
3	B	1	1	1	0
			Total	Zn	
3	C	1	1	1	0
			Total	Zn	
3	D	1	1	1	0

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:



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

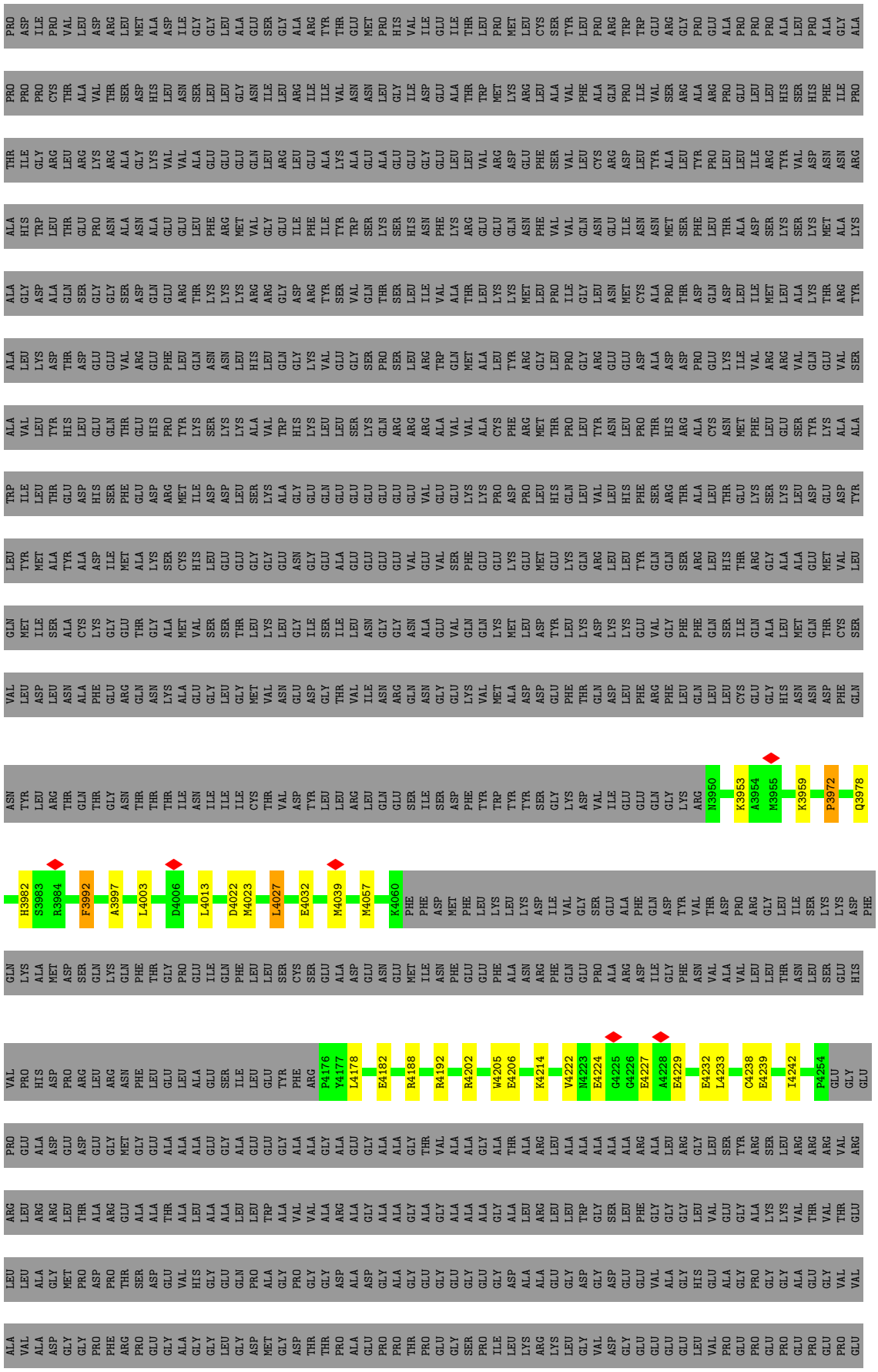
LEU LYS ASP MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU ILE LYS PHE PHE ALA LYS

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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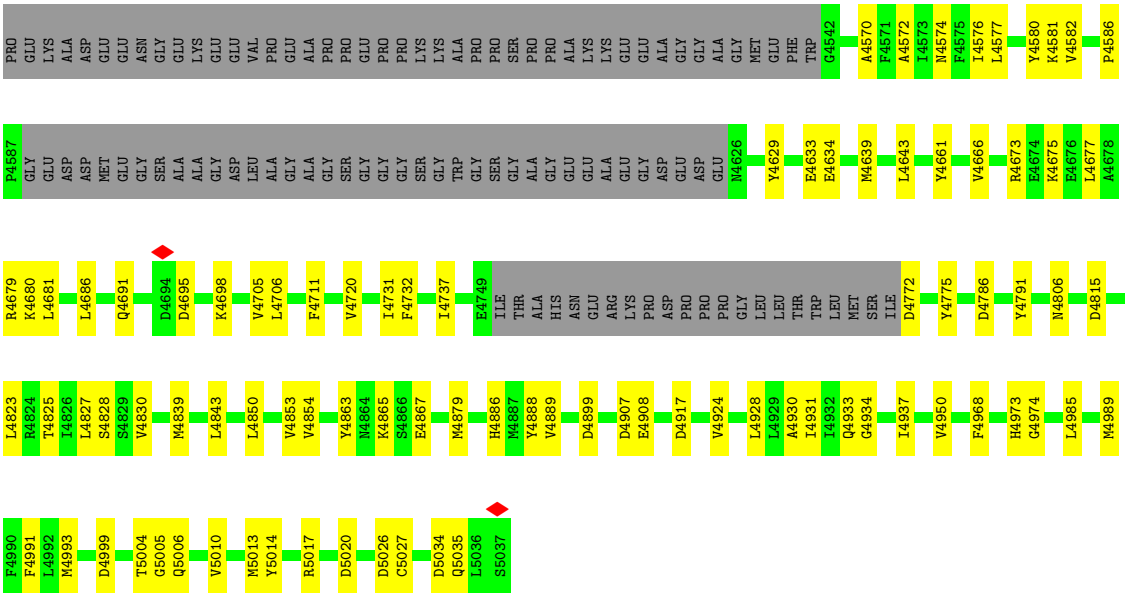
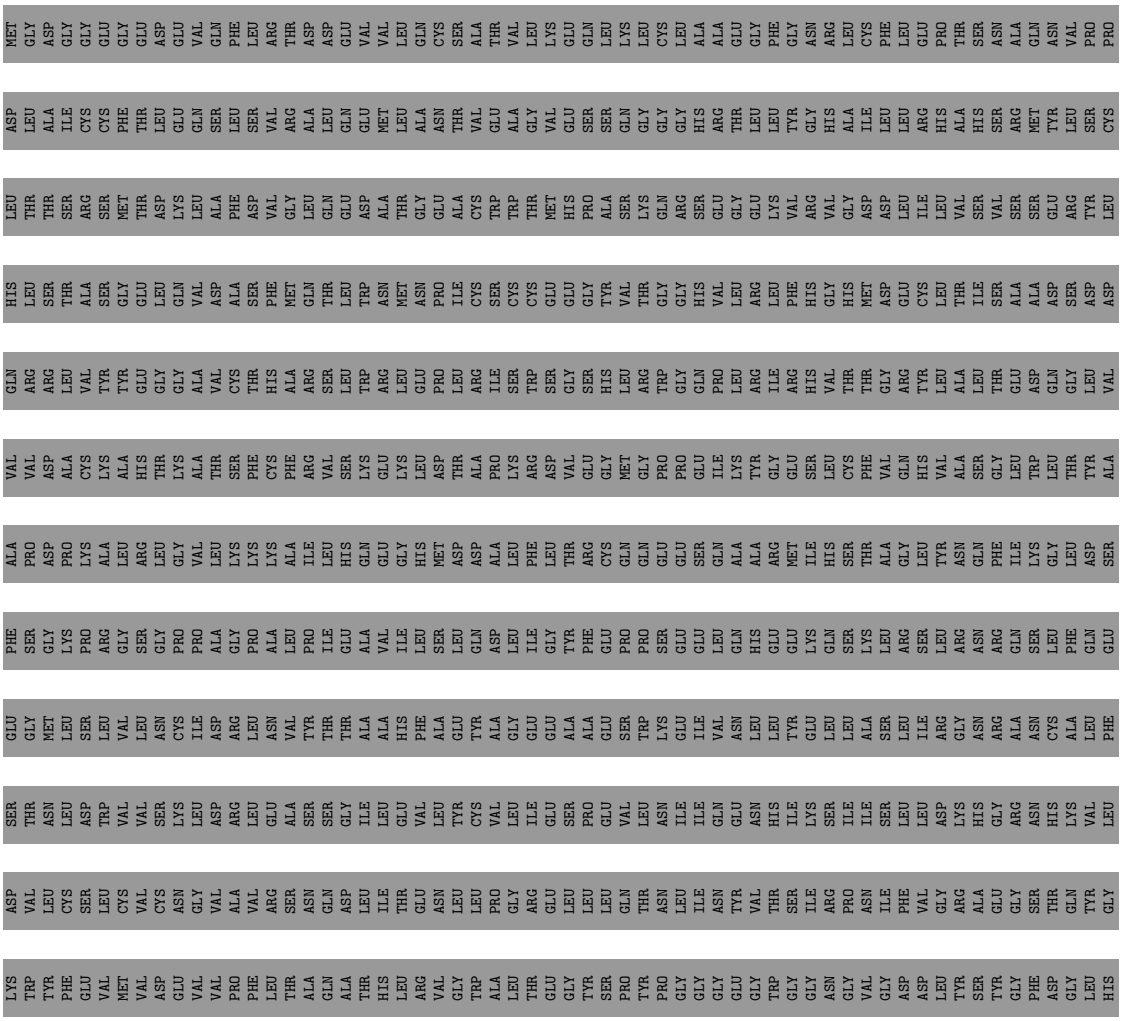


- Molecule 1: Ryanodine receptor 1

Chain B: 10% 88%



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 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

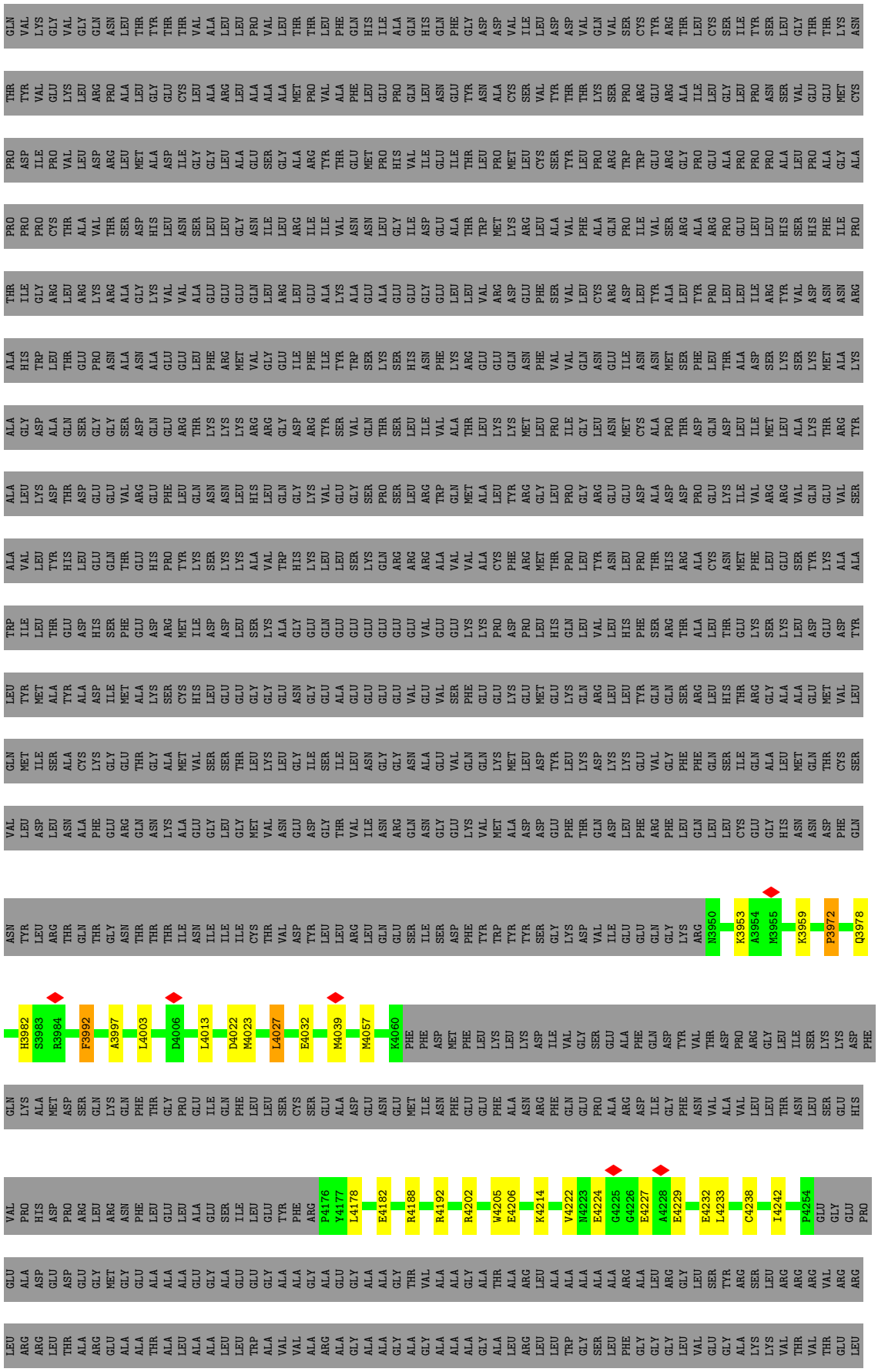
TRP THR ILE GLU LYS ALA ARG GLU GLY GLU GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY TYR ASN PRO GLN PRO PRO ASP LEU SER GLY VAL THR LEU SER ARG GLU LEU GLN ALA MET ALA GLU GLN LEU ALA GLU

ASN TYR HIS ASN THR TRP GLY ARG LYS LYS 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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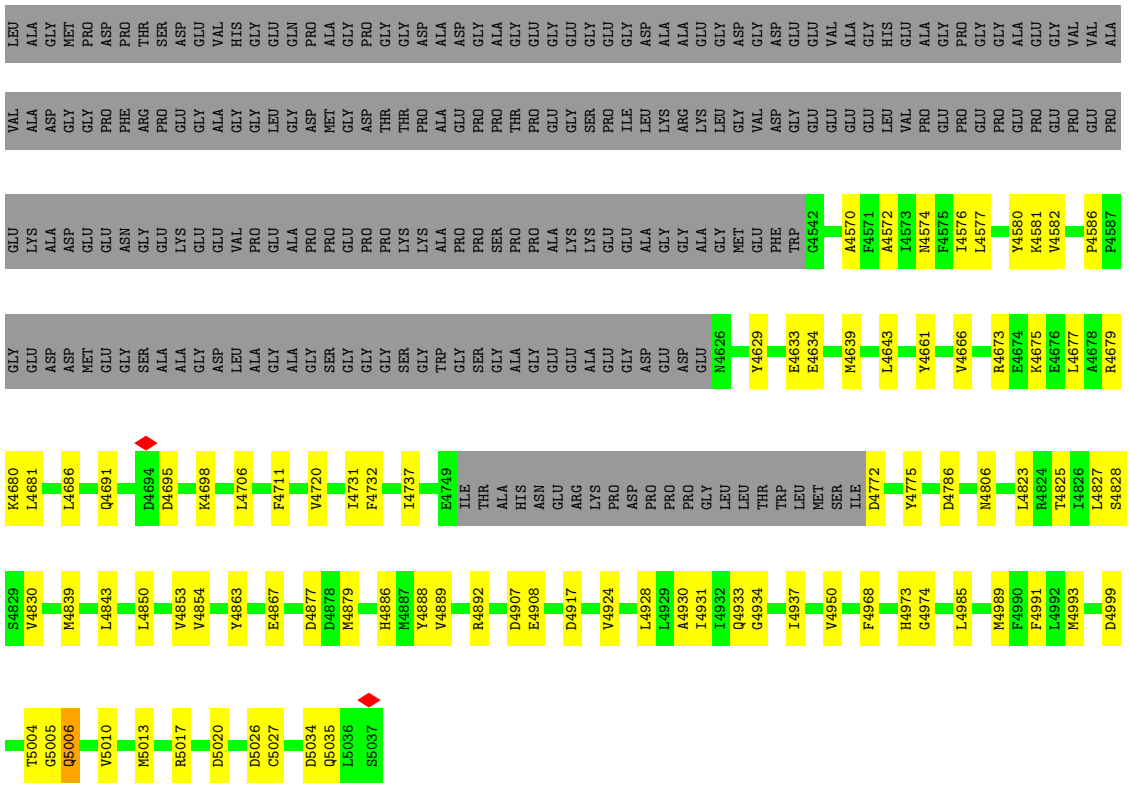


- Molecule 1: Ryanodine receptor 1

Chain C: 10% • 88%

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

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 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

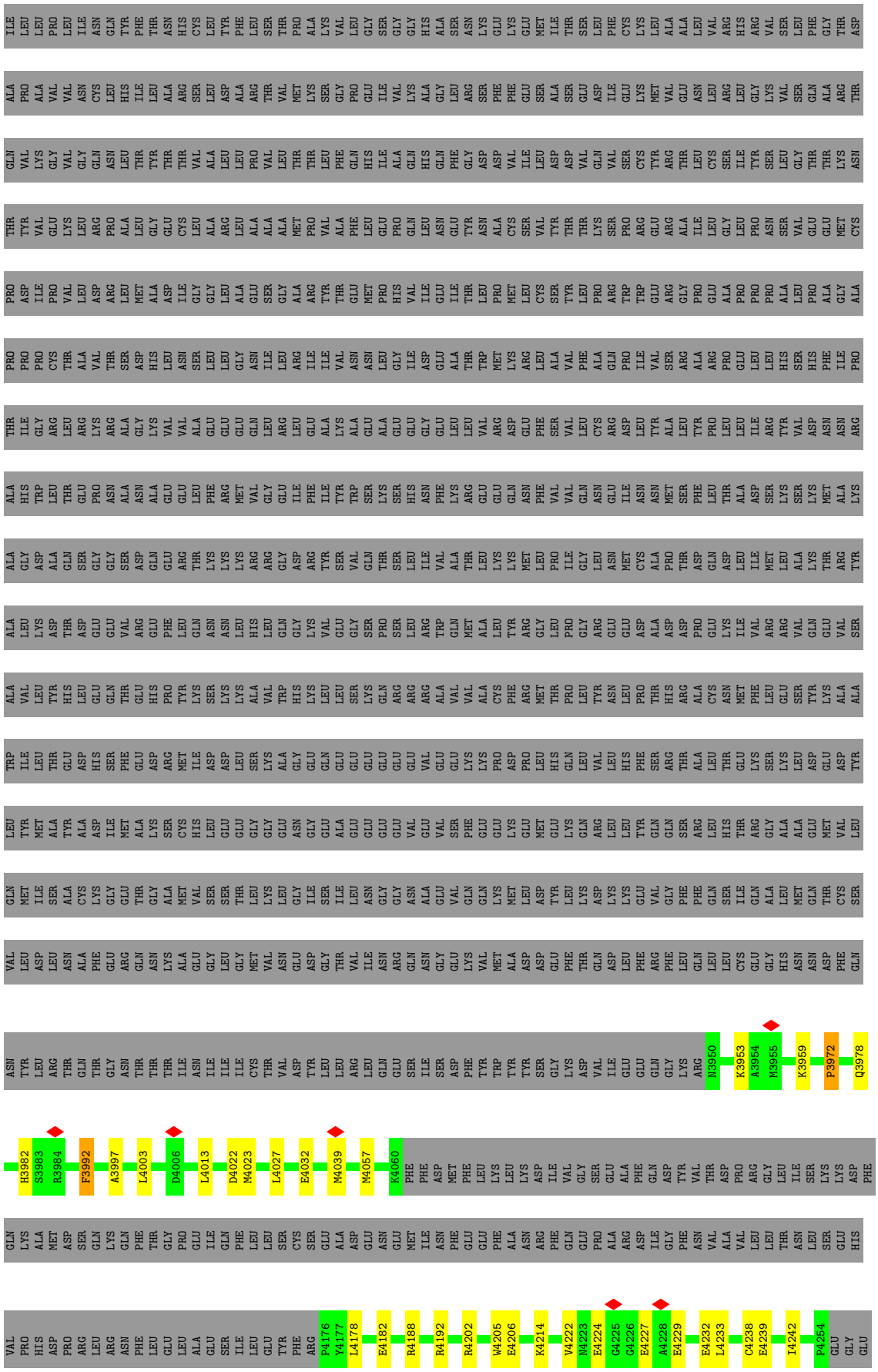
PRO CYS LEU CYS ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN PHE ASP PRO ARG PRO VAL GLU THR LEU ASN VAL ILE ILE PRO GLU LYS LEU ASP SER PHE ILE ASN LYS PHE ALA GLU

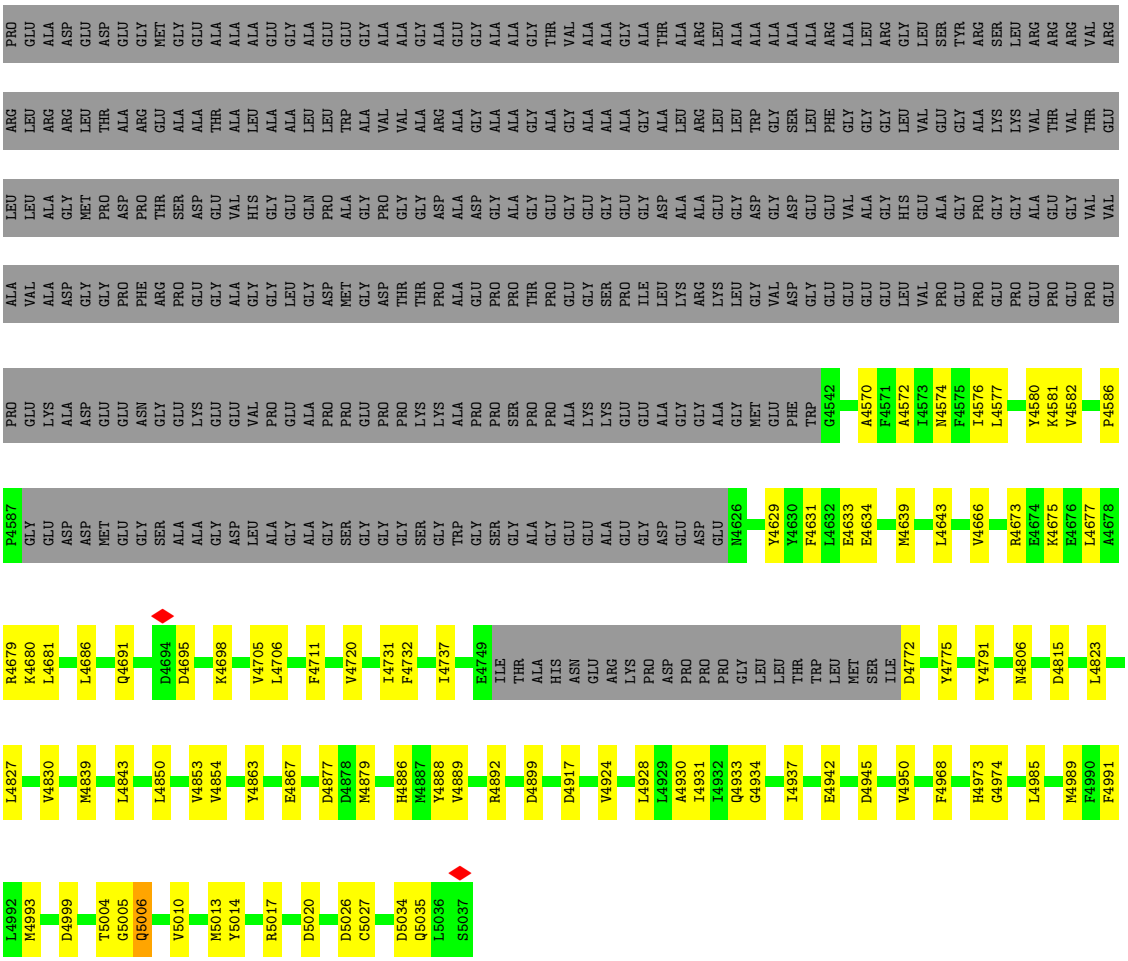
TYR THR HIS GLU LYS TRP ALA PHE ASP LYS ILE GLN ASN ASN TRP SER TYR GLY GLU ASN VAL ASP GLU GLU LEU LYS THR HIS PRO MET LEU ARG PRO TYR LYS THR PHE SER GLU LYS ASP LYS GLU ILE TYR ARG TRP PRO ILE LYS GLU SER LEU LYS ALA MET ILE ALA TRP GLU

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

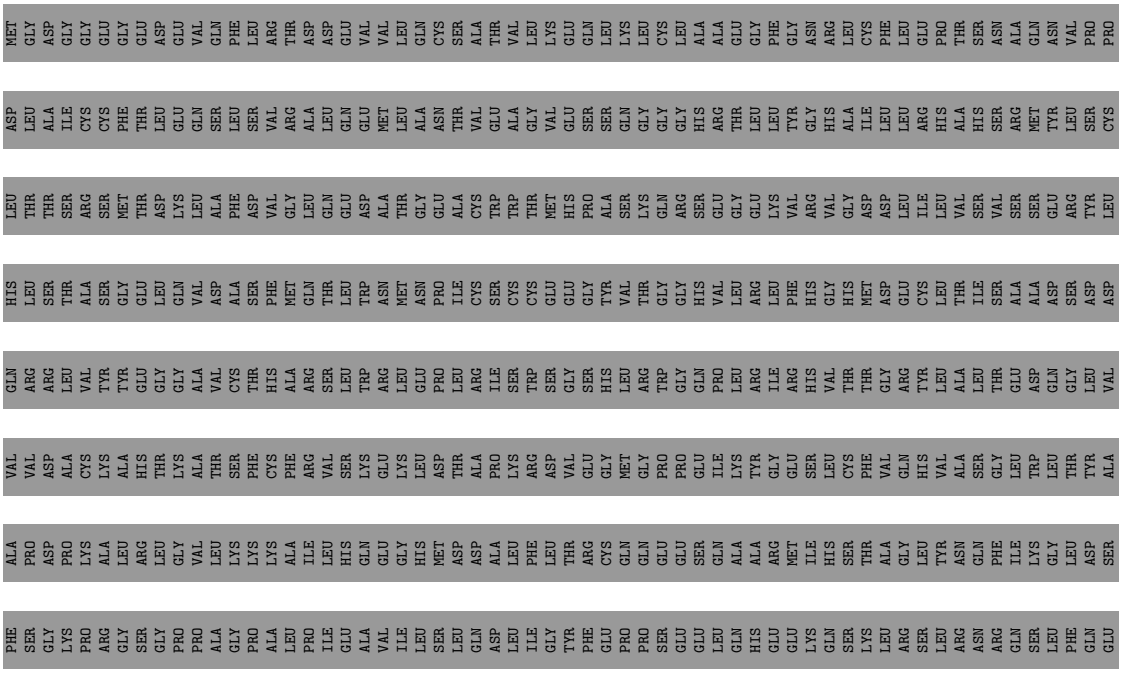
LEU LYS ASP MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU ILE LYS PHE PHE ALA LYS


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
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 ILE LYS MET VAL GLU ASN LEU ARG LEU LEU GLU SER ALA SER GLU ASP ILE GLU LYS LYS VAL SER GLN ALA ARG THR
GLN VAL LYS GLY VAL GLY GLN ASN LEU THR THR TYR THR THR THR ASP ALA LEU LEU PRO VAL LEU THR THR LEU PHE GLN HIS ILE ALA GLN HIS GLN PHE GLY ASP VAL ILE LEU ASP ASP VAL GLN VAL SER CYS TYR ARG THR LEU CYS SER ILE TYR SER LEU GLY THR THR 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 PRO ASN ASP VAL SER GLY ILE LEU GLU GLU ILE ASN ASN MET ILE ARG ARG ASN ASN
PRO ASP ILE PRO VAL LEU ASP ARG LEU MET MET ALA HIS LEU ASN SER LEU 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 THR LEU PRO ARG TRP TRP GLU ARG GLY PRO GLU ALA PRO PRO PRO ALA LEU ALA ILE ILE ARG 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 ILE VAL ASN ASN LEU GLY ILE ASP GLU ALA THR TRP MET LYS ARG LEU ALA VAL PHE ALA GLN PRO ILE VAL SER ARG ALA GLN PRO PRO PRO LEU LEU LEU ARG LEU HIS ASN ASN ASN PHE ILE PRO
THR ILE GLY ARG LEU ARG LYS ARG ALA GLY LYS VAL VAL ALA GLU GLU GLU GLN LEU GLU ALA ALA LYS ALA GLU GLU GLU GLU GLY GLU LEU VAL ARG ASP GLU PHE SER VAL LEU CYS ARG ASP LEU TYR TYR ALA LEU TYR TYR 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 LEU ASN MET CYS ALA PRO THR ASP GLN ASP LEU ILE ILE MET LEU ALA LYS THR ARG TYR
ALA LEU LYS ASP THR ASP GLU GLU VAL ARG GLU PHE LEU GLN ASN LEU HIS LEU GLN GLN GLY LYS VAL GLU GLY SER PRO SER LEU ARG TRP GLN MET ALA LEU TYR ARG GLY LEU PRO GLY LEU ARG GLU GLU ASP ALA ASP ASP PRO GLU LYS LYS ILE VAL ARG ARG VAL GLN GLU VAL 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 ARG ALA VAL VAL ALA CYS PHE ARG MET THR PRO GLY LEU TYR ASN LEU PRO THR HIS ARG ALA CYS ASN MET THR ILE LYS ALA ALA
TRP ILE LEU THR GLU ASP HIS SER PHE GLU ASP ARG MET ILE ASP ASP LEU SER LYS ALA GLY GLU GLU GLU GLU GLU GLU GLU GLU GLU VAL GLU GLU GLU LYS LYS PRO ASP PRO LEU HIS GLN LEU VAL LEU HIS PHE SER THR 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 GLY GLY GLY ASN GLY LEU ALA GLU GLU GLU GLU GLU GLU VAL GLU VAL LYS LYS GLU MET GLU LYS GLN ARG LEU LEU TYR GLN SER ARG LEU HIS THR THR ARG GLY ALA ALA LEU VAL THR GLN
GLN MET ILE SER ALA CYS LYS GLY GLU THR GLY ALA MET VAL SER SER THR LEU LYS LEU ASN GLY GLY ASN ALA GLU VAL GLN GLN LYS MET LEU ASP TYR LEU LYS ASP LYS LYS GLU LEU ILE SER ASP PHE TYR TYR TYR SER GLY LYS ASP VAL ILE GLU GLU GLN GLN GLY LYS ARG N3950 K3953 A3954 M3955 K3959 P3972 Q3978
VAL LEU ASP LEU ASN ALA PHE GLU ARG GLN ASN LYS ALA GLU GLY GLU LYS VAL MET ALA ASP ASP GLU PHE THR GLN ASN ASP LEU PHE ARG PHE LEU GLN LEU LEU LEU CYS GLU GLY HIS ASN ASN ASP PHE GLN
H3982 S3983 R3984 F3992 A3997 L4003 D4006 L4013 D4022 M4023 L4027 E4032 M4039 M4057 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 ILE ALA 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 SER PHE GLU GLU PHE ALA ASN ARG PHE GLN GLU PRO ALA ARG ASP ILE GLY PHE ASN VAL ALA ASP LEU LEU GLU HIS GLU
VAL PRO HIS ASP PRO ARG LEU ARG ASN PHE LEU GLU LEU ALA GLU SER ILE LEU GLU TYR PHE ARG P4176 V4177 L4178 E4182 R4188 R4192 R4202 W4205 E4206 K4214 V4222 N4223 E4224 G4225 G4226 E4227 A4228 E4229 E4232 L4233 C4238 E4239 I4242 P4254 GLU GLY GLU
WORLDWIDE PDB PROTEIN DATA BANK



• Molecule 1: Ryanodine receptor 1

Chain D: 10% • 88%



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

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

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 SER ASN GLU LYS ASP ALA THR

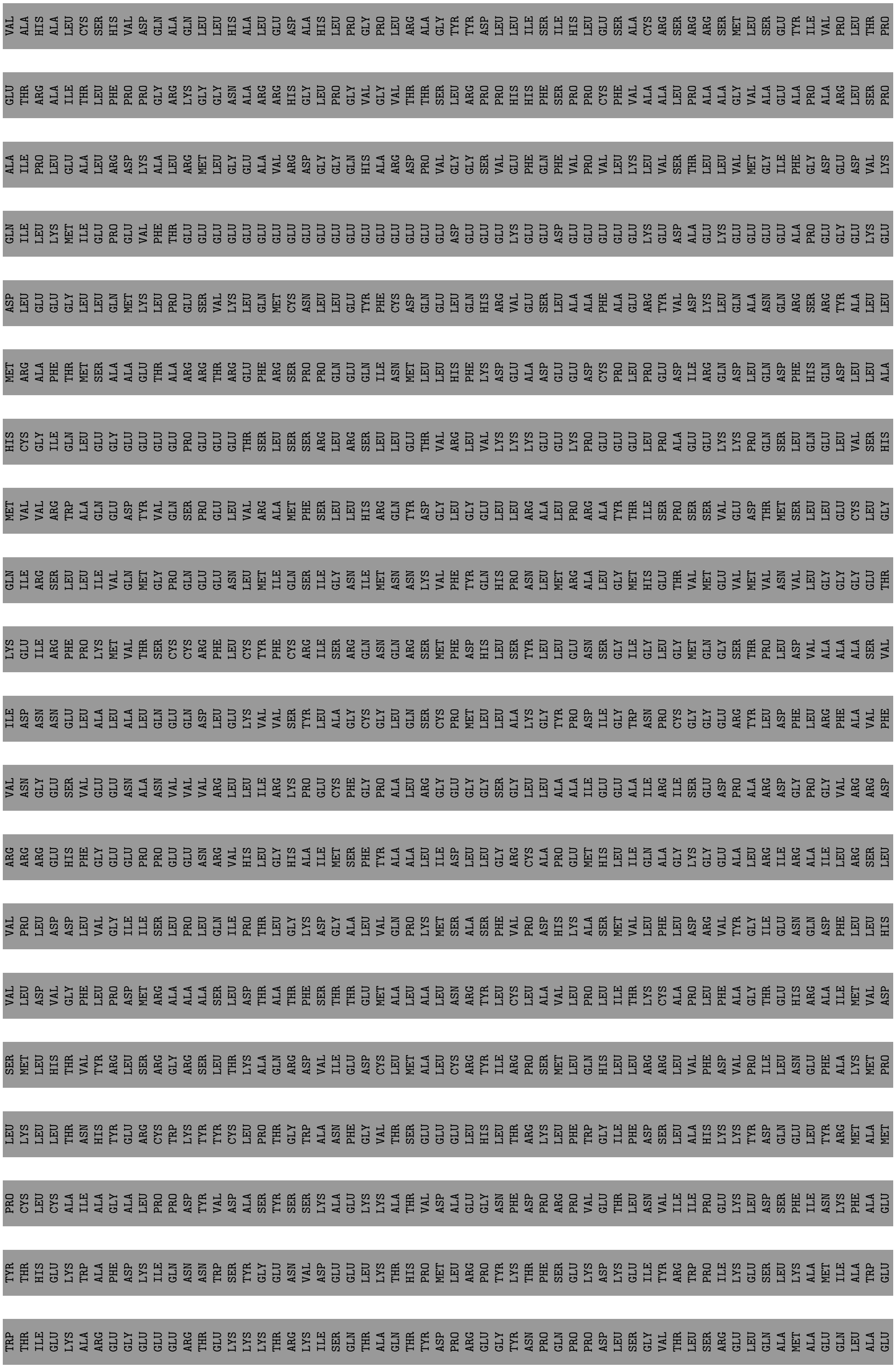
THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP PRO GLU ILE ILE LEU ASN THR THR THR TYR TYR TYR SER VAL ARG VAL PHE

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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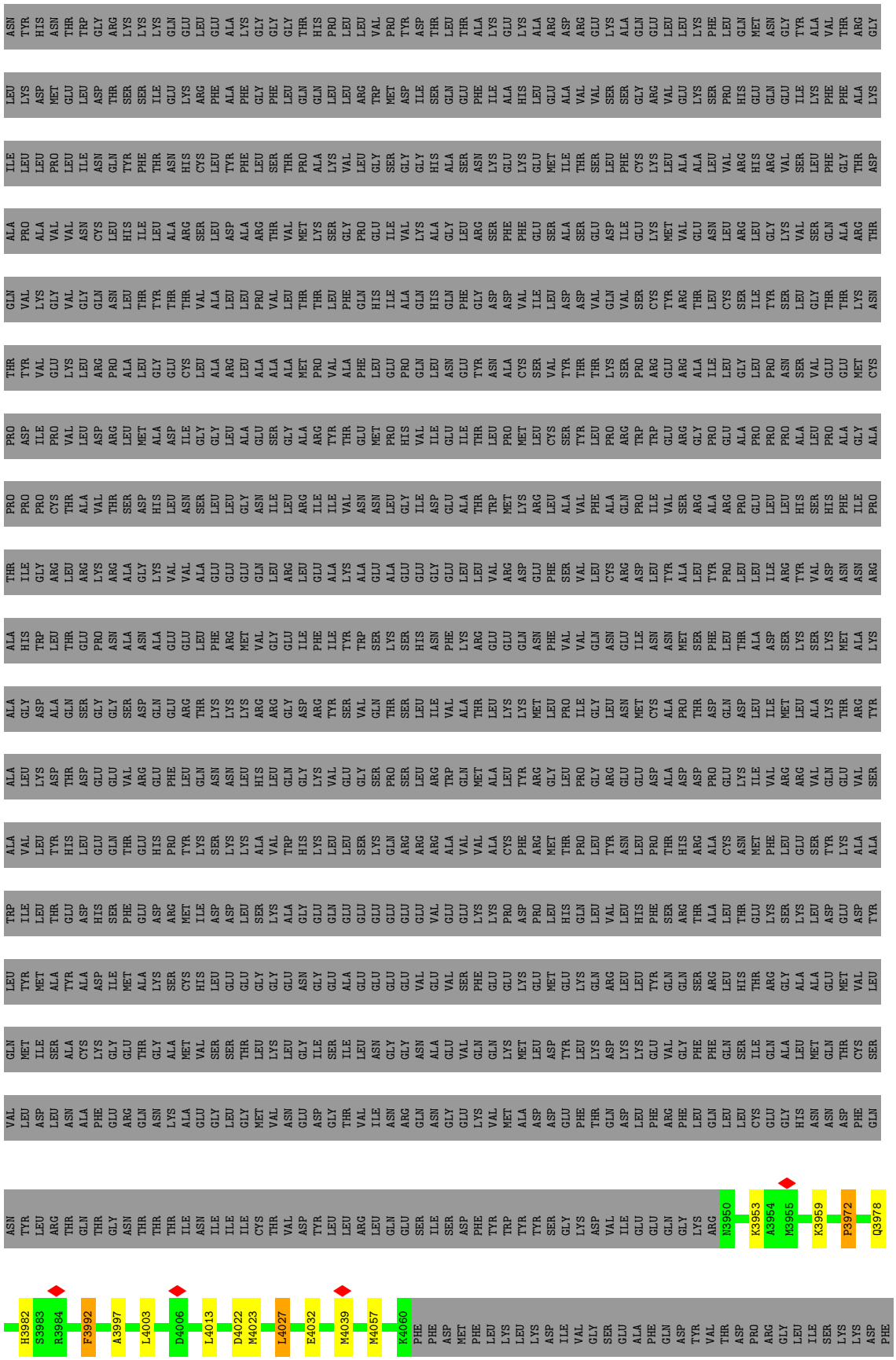
GLU THR ARG ALA ILE THR LEU PHE PRO PRO GLY ARG LYS GLY GLY ASN ALA ARG ARG HIS GLY LEU PRO GLY VAL GLY VAL THR THR SER LEU ARG PRO PRO HIS HIS PHE SER PRO PRO CYS PHE VAL ALA ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG LEU SER PRO
ALA ILE PRO LEU GLU ALA LEU ARG ASP LYS ALA LEU ARG MET LEU GLY 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 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 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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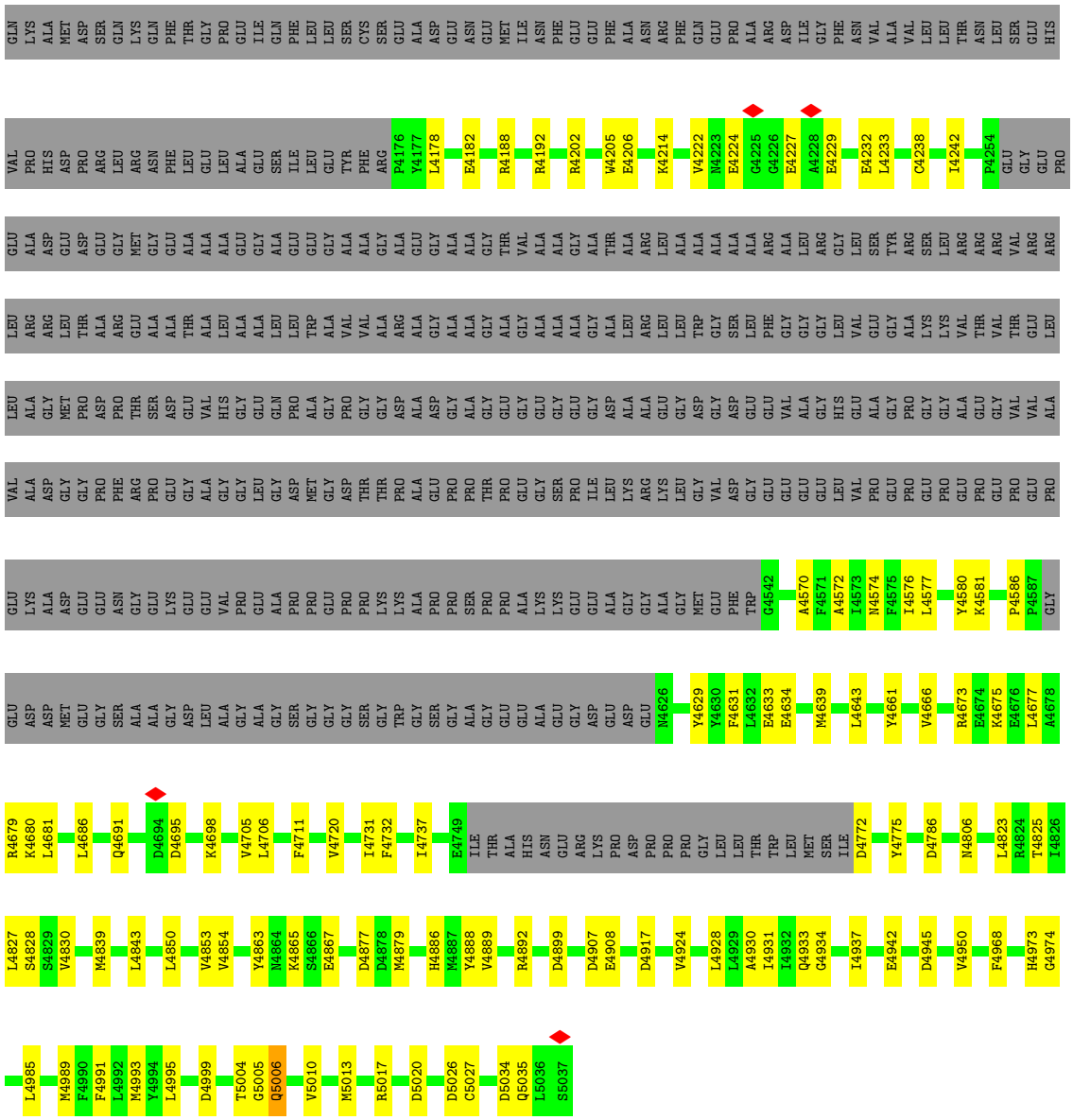
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VAL PRO HIS ASP PRO ARG LEU ARG ASN PHE LEU GLU LEU ALA GLU SER ILE LEU GLU TYR PHE ARG P4176 Y4177 L4178 E4182 R4188 R4192 R4202 W4205 E4206 K4214 V4222 M4223 E4224 G4225 G4226 E4227 A4228 E4229 E4232 L4233 C4238 I4242 P4254 GLU GLY GLU PRO
GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA ALA GLU GLU GLU GLY ALA GLU GLU GLY ALA ALA GLU GLY ALA ALA ALA GLY ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ALA LEU ARG ARG ARG ARG ARG VAL ARG ARG
LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU LEU TRP ALA VAL VAL ALA ARG ALA ALA GLY ALA GLY ALA ALA GLY ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR GLU LEU
LEU ALA GLY MET PRO ASP PRO PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLU GLY GLU GLU GLY GLU GLY GLU GLU GLY ASP ALA ALA GLU GLY VAL ALA ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA 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 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 PRO GLU PRO ALA
GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU PHE TRP G4542 A4570 F4571 A4572 I4573 N4574 F4575 I4576 L4577 Y4580 K4581 P4586 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 GLU GLU GLU ASP GLU N4626 Y4629 Y4630 F4631 L4632 E4633 E4634 M4639 L4643 Y4661 V4666 R4673 E4674 K4675 E4676 L4677 A4678
R4679 K4680 L4681 L4686 Q4691 D4694 D4695 K4698 V4705 L4706 F4711 V4720 I4731 F4732 I4737 E4749 ILE THR ALA HIS ASN GLU ARG LYS PRO ASP PRO PRO PRO GLY LEU LEU LEU THR TRP LEU MET SER ILE D4772 Y4775 D4786 N4806 L4823 R4824 T4825 I4826
L4827 S4828 S4829 V4830 M4839 L4843 L4850 V4853 V4854 Y4863 N4864 K4865 S4866 E4867 D4877 D4878 M4879 H4886 M4887 Y4888 V4889 R4892 D4899 D4907 E4908 D4917 V4924 L4928 L4929 A4930 I4931 I4932 Q4933 G4934 I4937 E4942 D4945 V4950 F4968 H4973 G4974
L4985 M4989 F4990 F4991 L4992 M4993 Y4994 L4995 D4999 T5004 G5005 Q5006 V5010 M5013 R5017 D5020 D5026 C5027 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133836	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	3.058	Depositor
Minimum map value	-1.891	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.059	Depositor
Recommended contour level	0.192	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: AMP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.20	0/5237	0.30	0/7066
1	B	0.20	0/5237	0.30	0/7066
1	C	0.20	0/5237	0.30	0/7066
1	D	0.20	0/5237	0.30	0/7066
All	All	0.20	0/20948	0.30	0/28264

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	5118	0	5009	79	0
1	B	5118	0	5009	77	0
1	C	5118	0	5009	80	0
1	D	5118	0	5009	82	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	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	20084	272	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 7.

All (272) 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:C:4888:TYR:OH	1:D:4917:ASP:OD2	1.96	0.84
1:A:4888:TYR:OH	1:B:4917:ASP:OD2	1.96	0.84
1:A:4917:ASP:OD2	1:D:4888:TYR:OH	1.96	0.84
1:B:4888:TYR:OH	1:C:4917:ASP:OD2	1.96	0.82
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.75	0.68
1:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.75	0.68
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.75	0.68
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.75	0.66
1:A:4827:LEU:HD21	1:B:4843:LEU:HD21	1.79	0.64
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.30	0.64
1:A:4843:LEU:HD21	1:D:4827:LEU:HD21	1.79	0.63
1:C:4827:LEU:HD21	1:D:4843:LEU:HD21	1.79	0.63
1:B:4827:LEU:HD21	1:C:4843:LEU:HD21	1.79	0.63
1:C:4182:GLU:OE2	1:C:4192:ARG:NH2	2.30	0.62
1:B:3959:LYS:NZ	1:B:4022:ASP:OD2	2.31	0.62
1:B:4182:GLU:OE2	1:B:4192:ARG:NH2	2.30	0.61
1:D:4182:GLU:OE2	1:D:4192:ARG:NH2	2.30	0.61
1:A:4182:GLU:OE2	1:A:4192:ARG:NH2	2.30	0.61
1:C:3978:GLN:HG3	1:C:4039:MET:HE1	1.83	0.61
1:D:3978:GLN:HG3	1:D:4039:MET:HE1	1.83	0.61
1:D:3959:LYS:NZ	1:D:4022:ASP:OD2	2.31	0.61
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.30	0.61
1:C:3959:LYS:NZ	1:C:4022:ASP:OD2	2.31	0.60
1:B:3978:GLN:HG3	1:B:4039:MET:HE1	1.83	0.60
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.30	0.60
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.30	0.60
1:A:3978:GLN:HG3	1:A:4039:MET:HE1	1.83	0.60
1:A:3959:LYS:NZ	1:A:4022:ASP:OD2	2.31	0.60
1:A:4227:GLU:OE1	1:D:4973:HIS:CE1	2.55	0.60
1:B:4973:HIS:CE1	1:C:4227:GLU:OE1	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4973:HIS:CE1	1:D:4227:GLU:OE1	2.55	0.59
1:A:4973:HIS:CE1	1:B:4227:GLU:OE1	2.55	0.59
1:C:4634:GLU:HG3	1:C:4639:MET:HG3	1.85	0.59
1:C:4823:LEU:CD2	1:D:4839:MET:HG3	2.33	0.59
1:A:4823:LEU:CD2	1:B:4839:MET:HG3	2.33	0.59
1:A:4839:MET:HG3	1:D:4823:LEU:CD2	2.33	0.58
1:B:4634:GLU:HG3	1:B:4639:MET:HG3	1.85	0.58
1:B:4823:LEU:CD2	1:C:4839:MET:HG3	2.33	0.58
1:A:4634:GLU:HG3	1:A:4639:MET:HG3	1.85	0.58
1:D:4232:GLU:OE2	1:D:5017:ARG:NH2	2.33	0.58
1:B:4232:GLU:OE2	1:B:5017:ARG:NH2	2.33	0.58
1:A:4731:ILE:HG23	1:A:4732:PHE:HD1	1.69	0.58
1:B:5013:MET:HE1	1:B:5020:ASP:HB2	1.86	0.57
1:C:5013:MET:HE1	1:C:5020:ASP:HB2	1.86	0.57
1:D:4634:GLU:HG3	1:D:4639:MET:HG3	1.85	0.57
1:B:4731:ILE:HG23	1:B:4732:PHE:HD1	1.69	0.57
1:D:4731:ILE:HG23	1:D:4732:PHE:HD1	1.69	0.56
1:C:4731:ILE:HG23	1:C:4732:PHE:HD1	1.69	0.56
1:A:5013:MET:HE1	1:A:5020:ASP:HB2	1.86	0.56
1:C:4232:GLU:OE2	1:C:5017:ARG:NH2	2.33	0.56
1:A:4232:GLU:OE2	1:A:5017:ARG:NH2	2.33	0.56
1:D:5013:MET:HE1	1:D:5020:ASP:HB2	1.86	0.56
1:C:4863:TYR:HH	1:C:4886:HIS:HE2	1.45	0.55
1:D:3972:PRO:HD2	1:D:5005:GLY:HA3	1.89	0.55
1:B:3972:PRO:HD2	1:B:5005:GLY:HA3	1.89	0.54
1:A:4680:LYS:HD2	1:A:4686:LEU:HD22	1.90	0.54
1:A:4772:ASP:HB3	1:A:4775:TYR:HB3	1.89	0.54
1:D:4772:ASP:HB3	1:D:4775:TYR:HB3	1.89	0.54
1:C:3972:PRO:HD2	1:C:5005:GLY:HA3	1.89	0.54
1:C:4772:ASP:HB3	1:C:4775:TYR:HB3	1.89	0.54
1:B:4680:LYS:HD2	1:B:4686:LEU:HD22	1.90	0.54
1:B:4772:ASP:HB3	1:B:4775:TYR:HB3	1.89	0.54
1:A:3972:PRO:HD2	1:A:5005:GLY:HA3	1.89	0.53
1:D:4680:LYS:HD2	1:D:4686:LEU:HD22	1.90	0.53
1:B:4991:PHE:HE2	1:B:5010:VAL:HG11	1.74	0.53
1:C:4991:PHE:HE2	1:C:5010:VAL:HG11	1.74	0.52
1:C:4680:LYS:HD2	1:C:4686:LEU:HD22	1.90	0.52
1:A:4991:PHE:HE2	1:A:5010:VAL:HG11	1.74	0.52
1:C:4791:TYR:OH	1:C:4815:ASP:OD1	2.26	0.52
1:B:4238:CYS:O	1:B:4242:ILE:HG13	2.10	0.52
1:D:4681:LEU:HD11	1:D:4706:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4238:CYS:O	1:C:4242:ILE:HG13	2.10	0.52
1:A:4681:LEU:HD11	1:A:4706:LEU:HD22	1.92	0.51
1:A:4863:TYR:OH	1:A:4886:HIS:NE2	2.39	0.51
1:A:4238:CYS:O	1:A:4242:ILE:HG13	2.10	0.51
1:D:4238:CYS:O	1:D:4242:ILE:HG13	2.10	0.51
1:D:4991:PHE:HE2	1:D:5010:VAL:HG11	1.74	0.51
1:D:4853:VAL:HA	1:D:4879:MET:HE1	1.93	0.51
1:A:4863:TYR:HH	1:A:4886:HIS:HE2	1.49	0.50
1:B:4681:LEU:HD11	1:B:4706:LEU:HD22	1.92	0.50
1:C:4681:LEU:HD11	1:C:4706:LEU:HD22	1.92	0.50
1:A:4853:VAL:HA	1:A:4879:MET:HE1	1.93	0.50
1:B:4853:VAL:HA	1:B:4879:MET:HE1	1.93	0.49
1:A:4222:VAL:HG11	1:A:4950:VAL:HA	1.94	0.49
1:B:4686:LEU:O	1:B:4691:GLN:N	2.41	0.49
1:B:4863:TYR:OH	1:B:4886:HIS:NE2	2.39	0.49
1:C:4222:VAL:HG11	1:C:4950:VAL:HA	1.94	0.49
1:C:4853:VAL:HA	1:C:4879:MET:HE1	1.93	0.49
1:D:4677:LEU:HD23	1:D:4711:PHE:CE1	2.48	0.49
1:C:4677:LEU:HD23	1:C:4711:PHE:CE1	2.48	0.49
1:A:4677:LEU:HD23	1:A:4711:PHE:CE1	2.48	0.48
1:D:4863:TYR:OH	1:D:4886:HIS:NE2	2.39	0.48
1:B:4222:VAL:HG11	1:B:4950:VAL:HA	1.94	0.48
1:B:4677:LEU:HD23	1:B:4711:PHE:CE1	2.48	0.48
1:A:4686:LEU:O	1:A:4691:GLN:N	2.41	0.48
1:C:4863:TYR:OH	1:C:4886:HIS:NE2	2.39	0.48
1:A:4675:LYS:O	1:A:4679:ARG:HD3	2.14	0.48
1:B:4850:LEU:O	1:B:4854:VAL:HG23	2.14	0.48
1:C:4850:LEU:O	1:C:4854:VAL:HG23	2.14	0.48
1:D:4222:VAL:HG11	1:D:4950:VAL:HA	1.94	0.48
1:C:4823:LEU:HD21	1:D:4839:MET:HG3	1.96	0.47
1:A:4931:ILE:HD11	1:D:4830:VAL:CG2	2.44	0.47
1:A:4839:MET:HG3	1:D:4823:LEU:HD21	1.96	0.47
1:A:4850:LEU:O	1:A:4854:VAL:HG23	2.14	0.47
1:B:4003:LEU:HB2	1:B:4013:LEU:HD13	1.96	0.47
1:A:4576:ILE:HG21	1:A:4643:LEU:HB2	1.96	0.47
1:D:4675:LYS:O	1:D:4679:ARG:HD3	2.14	0.47
1:C:4830:VAL:CG2	1:D:4931:ILE:HD11	2.44	0.47
1:B:4675:LYS:O	1:B:4679:ARG:HD3	2.14	0.47
1:C:4003:LEU:HB2	1:C:4013:LEU:HD13	1.96	0.47
1:C:4576:ILE:HG21	1:C:4643:LEU:HB2	1.96	0.47
1:D:4673:ARG:CZ	1:D:4698:LYS:HG3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4850:LEU:O	1:D:4854:VAL:HG23	2.14	0.47
1:A:4003:LEU:HB2	1:A:4013:LEU:HD13	1.96	0.47
1:A:4830:VAL:CG2	1:B:4931:ILE:HD11	2.44	0.47
1:B:4830:VAL:CG2	1:C:4931:ILE:HD11	2.44	0.47
1:C:3997:ALA:HB1	1:C:4057:MET:HE3	1.97	0.47
1:B:3992:PHE:HB3	1:B:4023:MET:HE1	1.97	0.46
1:A:3992:PHE:HB3	1:A:4023:MET:HE1	1.97	0.46
1:A:3997:ALA:HB1	1:A:4057:MET:HE3	1.97	0.46
1:A:4823:LEU:HD21	1:B:4839:MET:HG3	1.96	0.46
1:B:4673:ARG:CZ	1:B:4698:LYS:HG3	2.45	0.46
1:C:4675:LYS:O	1:C:4679:ARG:HD3	2.14	0.46
1:D:4576:ILE:HG21	1:D:4643:LEU:HB2	1.96	0.46
1:D:5006:GLN:H	1:D:5006:GLN:HG2	1.48	0.46
1:A:4673:ARG:CZ	1:A:4698:LYS:HG3	2.45	0.46
1:B:4576:ILE:HG21	1:B:4643:LEU:HB2	1.96	0.46
1:C:3992:PHE:HB3	1:C:4023:MET:HE1	1.97	0.46
1:B:4188:ARG:HA	1:B:4188:ARG:HH11	1.81	0.46
1:B:4823:LEU:HD21	1:C:4839:MET:HG3	1.96	0.46
1:C:4673:ARG:CZ	1:C:4698:LYS:HG3	2.45	0.46
1:D:4003:LEU:HB2	1:D:4013:LEU:HD13	1.96	0.46
1:D:4863:TYR:HH	1:D:4886:HIS:HE2	1.49	0.46
1:B:3997:ALA:HB1	1:B:4057:MET:HE3	1.97	0.45
1:A:4989:MET:HE3	1:A:4989:MET:HB3	1.86	0.45
1:A:4188:ARG:HA	1:A:4188:ARG:HH11	1.81	0.45
1:A:4825:THR:O	1:A:4828:SER:OG	2.32	0.45
1:B:3972:PRO:HD3	1:B:4032:GLU:OE1	2.17	0.45
1:C:3972:PRO:HD3	1:C:4032:GLU:OE1	2.17	0.45
1:D:3997:ALA:HB1	1:D:4057:MET:HE3	1.97	0.45
1:A:4867:GLU:CD	1:A:4867:GLU:H	2.25	0.45
1:C:4973:HIS:ND1	1:D:4227:GLU:OE1	2.50	0.45
1:D:4825:THR:O	1:D:4828:SER:OG	2.32	0.45
1:A:4973:HIS:ND1	1:B:4227:GLU:OE1	2.50	0.45
1:C:4867:GLU:CD	1:C:4867:GLU:H	2.25	0.45
1:D:4581:LYS:HD3	1:D:4633:GLU:HG3	1.99	0.45
1:A:4968:PHE:O	1:A:4974:GLY:HA3	2.17	0.45
1:A:4227:GLU:OE1	1:D:4973:HIS:ND1	2.50	0.45
1:A:4791:TYR:OH	1:A:4815:ASP:OD1	2.26	0.45
1:B:4968:PHE:O	1:B:4974:GLY:HA3	2.17	0.45
1:C:4239:GLU:OE2	1:C:5014:TYR:OH	2.30	0.45
1:C:4968:PHE:O	1:C:4974:GLY:HA3	2.17	0.45
1:A:3972:PRO:HD3	1:A:4032:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5035:GLN:OE1	1:A:5035:GLN:N	2.49	0.45
1:B:4577:LEU:HD21	1:B:4806:ASN:HB3	1.99	0.45
1:C:4577:LEU:HD21	1:C:4806:ASN:HB3	1.99	0.45
1:D:3992:PHE:HB3	1:D:4023:MET:HE1	1.97	0.45
1:D:4188:ARG:HA	1:D:4188:ARG:HH11	1.81	0.45
1:D:4867:GLU:H	1:D:4867:GLU:CD	2.25	0.45
1:A:4581:LYS:HD3	1:A:4633:GLU:HG3	1.99	0.44
1:B:4867:GLU:CD	1:B:4867:GLU:H	2.25	0.44
1:C:4581:LYS:HD3	1:C:4633:GLU:HG3	1.99	0.44
1:D:4577:LEU:HD21	1:D:4806:ASN:HB3	1.99	0.44
1:B:5035:GLN:OE1	1:B:5035:GLN:N	2.49	0.44
1:B:4973:HIS:ND1	1:C:4227:GLU:OE1	2.50	0.44
1:C:5035:GLN:N	1:C:5035:GLN:OE1	2.49	0.44
1:A:4924:VAL:HA	1:A:4928:LEU:HD12	2.00	0.44
1:D:4968:PHE:O	1:D:4974:GLY:HA3	2.17	0.44
1:B:4581:LYS:HD3	1:B:4633:GLU:HG3	1.99	0.44
1:B:4581:LYS:HE3	1:B:4581:LYS:HB3	1.82	0.44
1:B:4933:GLN:HG2	1:C:4930:ALA:HB2	2.00	0.44
1:B:5006:GLN:H	1:B:5006:GLN:HG2	1.48	0.44
1:A:4577:LEU:HD21	1:A:4806:ASN:HB3	1.99	0.44
1:D:3972:PRO:HD3	1:D:4032:GLU:OE1	2.17	0.44
1:B:4924:VAL:HA	1:B:4928:LEU:HD12	2.00	0.44
1:C:4933:GLN:HG2	1:D:4930:ALA:HB2	2.00	0.44
1:B:3953:LYS:HE2	1:B:3953:LYS:HB3	1.88	0.44
1:C:4188:ARG:HH11	1:C:4188:ARG:HA	1.81	0.44
1:C:5006:GLN:H	1:C:5006:GLN:HG2	1.48	0.44
1:D:4924:VAL:HA	1:D:4928:LEU:HD12	2.00	0.44
1:D:5035:GLN:OE1	1:D:5035:GLN:N	2.49	0.44
1:A:4933:GLN:HG2	1:B:4930:ALA:HB2	2.00	0.43
1:C:3953:LYS:HE2	1:C:3953:LYS:HB3	1.88	0.43
1:C:4823:LEU:HD23	1:C:4823:LEU:HA	1.84	0.43
1:A:4930:ALA:HB2	1:D:4933:GLN:HG2	2.00	0.43
1:C:4686:LEU:O	1:C:4691:GLN:N	2.41	0.43
1:A:4214:LYS:HE2	1:A:4985:LEU:HD11	2.01	0.43
1:A:4229:GLU:HG3	1:A:4233:LEU:HG	2.01	0.43
1:B:4214:LYS:HE2	1:B:4985:LEU:HD11	2.01	0.43
1:B:4229:GLU:HG3	1:B:4233:LEU:HG	2.01	0.43
1:B:4695:ASP:OD1	1:B:4695:ASP:N	2.51	0.43
1:D:5026:ASP:OD1	1:D:5027:CYS:N	2.52	0.43
1:A:4695:ASP:N	1:A:4695:ASP:OD1	2.51	0.43
1:C:4993:MET:HE2	1:C:4993:MET:HB3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4027:LEU:HD13	1:B:4027:LEU:HA	1.92	0.43
1:C:4581:LYS:HE3	1:C:4581:LYS:HB3	1.82	0.43
1:D:4214:LYS:HE2	1:D:4985:LEU:HD11	2.01	0.43
1:D:4686:LEU:O	1:D:4691:GLN:N	2.41	0.43
1:A:4999:ASP:N	1:A:4999:ASP:OD1	2.52	0.43
1:B:5026:ASP:OD1	1:B:5027:CYS:N	2.52	0.43
1:B:4823:LEU:HD23	1:B:4823:LEU:HA	1.84	0.43
1:C:4229:GLU:HG3	1:C:4233:LEU:HG	2.01	0.43
1:C:5026:ASP:OD1	1:C:5027:CYS:N	2.52	0.43
1:A:4239:GLU:OE2	1:A:5014:TYR:OH	2.30	0.43
1:A:4572:ALA:O	1:A:4576:ILE:HG12	2.19	0.43
1:A:5026:ASP:OD1	1:A:5027:CYS:N	2.52	0.42
1:B:4572:ALA:O	1:B:4576:ILE:HG12	2.19	0.42
1:C:4214:LYS:HE2	1:C:4985:LEU:HD11	2.01	0.42
1:A:4661:TYR:OH	1:A:4786:ASP:OD2	2.30	0.42
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.84	0.42
1:B:4661:TYR:OH	1:B:4786:ASP:OD2	2.30	0.42
1:C:3982:HIS:NE2	1:C:4039:MET:SD	2.92	0.42
1:C:4586:PRO:HG3	1:C:4629:TYR:CZ	2.54	0.42
1:C:4892:ARG:NH1	1:D:4899:ASP:OD1	2.51	0.42
1:D:4989:MET:HE3	1:D:4989:MET:HB3	1.86	0.42
1:C:4924:VAL:HA	1:C:4928:LEU:HD12	2.00	0.42
1:A:4586:PRO:HG3	1:A:4629:TYR:CZ	2.54	0.42
1:A:4917:ASP:HB2	1:D:4888:TYR:HE1	1.85	0.42
1:B:3982:HIS:NE2	1:B:4039:MET:SD	2.92	0.42
1:D:4572:ALA:O	1:D:4576:ILE:HG12	2.19	0.42
1:D:4205:TRP:CE3	1:D:4989:MET:HE2	2.55	0.42
1:A:4907:ASP:OD1	1:A:4908:GLU:N	2.52	0.42
1:B:4586:PRO:HG3	1:B:4629:TYR:CZ	2.54	0.42
1:A:3953:LYS:HE2	1:A:3953:LYS:HB3	1.88	0.42
1:A:4865:LYS:HA	1:A:4865:LYS:HD2	1.85	0.42
1:B:4205:TRP:CE3	1:B:4989:MET:HE2	2.55	0.42
1:C:4572:ALA:O	1:C:4576:ILE:HG12	2.19	0.42
1:D:4999:ASP:OD1	1:D:4999:ASP:N	2.52	0.42
1:B:4907:ASP:OD1	1:B:4908:GLU:N	2.52	0.42
1:C:4695:ASP:OD1	1:C:4695:ASP:N	2.51	0.42
1:C:4888:TYR:HE1	1:D:4917:ASP:HB2	1.85	0.42
1:D:4661:TYR:OH	1:D:4786:ASP:OD2	2.30	0.42
1:A:4888:TYR:HE1	1:B:4917:ASP:HB2	1.85	0.42
1:B:4888:TYR:HE1	1:C:4917:ASP:HB2	1.85	0.42
1:D:4229:GLU:HG3	1:D:4233:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4205:TRP:CE3	1:A:4989:MET:HE2	2.55	0.42
1:A:4899:ASP:OD1	1:D:4892:ARG:NH1	2.51	0.42
1:D:3982:HIS:NE2	1:D:4039:MET:SD	2.92	0.42
1:A:4202:ARG:O	1:A:4206:GLU:HG2	2.20	0.41
1:B:4892:ARG:NH1	1:C:4899:ASP:OD1	2.51	0.41
1:D:4907:ASP:OD1	1:D:4908:GLU:N	2.52	0.41
1:B:4999:ASP:OD1	1:B:4999:ASP:N	2.52	0.41
1:A:4582:VAL:HG12	1:B:4877:ASP:O	2.21	0.41
1:C:4205:TRP:CE3	1:C:4989:MET:HE2	2.55	0.41
1:D:4586:PRO:HG3	1:D:4629:TYR:CZ	2.54	0.41
1:A:3982:HIS:NE2	1:A:4039:MET:SD	2.92	0.41
1:D:4705:VAL:HG23	1:D:4775:TYR:HD1	1.86	0.41
1:C:4202:ARG:O	1:C:4206:GLU:HG2	2.20	0.41
1:D:4027:LEU:HD13	1:D:4027:LEU:HA	1.92	0.41
1:A:4027:LEU:HD13	1:A:4027:LEU:HA	1.92	0.41
1:D:4865:LYS:HD2	1:D:4865:LYS:HA	1.85	0.41
1:B:4202:ARG:O	1:B:4206:GLU:HG2	2.20	0.41
1:C:4937:ILE:HG12	1:D:4934:GLY:HA2	2.03	0.41
1:D:4202:ARG:O	1:D:4206:GLU:HG2	2.20	0.41
1:A:4934:GLY:HA2	1:D:4937:ILE:HG12	2.03	0.41
1:A:4937:ILE:HG12	1:B:4934:GLY:HA2	2.03	0.41
1:B:4582:VAL:HG12	1:C:4877:ASP:O	2.21	0.41
1:B:4825:THR:O	1:B:4828:SER:OG	2.32	0.41
1:C:4705:VAL:HG23	1:C:4775:TYR:HD1	1.86	0.41
1:C:4942:GLU:HA	1:C:4945:ASP:OD2	2.21	0.41
1:D:3953:LYS:HE2	1:D:3953:LYS:HB3	1.88	0.41
1:D:4695:ASP:OD1	1:D:4695:ASP:N	2.51	0.41
1:D:4995:LEU:HD23	1:D:4995:LEU:HA	1.95	0.41
1:D:4993:MET:HE2	1:D:4993:MET:HB3	1.85	0.40
1:B:4937:ILE:HG12	1:C:4934:GLY:HA2	2.03	0.40
1:C:4582:VAL:HG12	1:D:4877:ASP:O	2.21	0.40
1:C:4631:PHE:HE2	1:C:4633:GLU:HG2	1.87	0.40
1:D:4631:PHE:HE2	1:D:4633:GLU:HG2	1.87	0.40
1:A:4705:VAL:HG23	1:A:4775:TYR:HD1	1.86	0.40
1:B:4989:MET:HE3	1:B:4989:MET:HB3	1.86	0.40
1:C:4999:ASP:N	1:C:4999:ASP:OD1	2.52	0.40
1:D:4942:GLU:HA	1:D:4945:ASP:OD2	2.21	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%)	598 (97%)	17 (3%)	1 (0%)	43	62
1	B	616/5037 (12%)	598 (97%)	17 (3%)	1 (0%)	43	62
1	C	567/5037 (11%)	549 (97%)	17 (3%)	1 (0%)	43	62
1	D	616/5037 (12%)	598 (97%)	17 (3%)	1 (0%)	43	62
All	All	2415/20148 (12%)	2343 (97%)	68 (3%)	4 (0%)	44	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3972	PRO
1	B	3972	PRO
1	C	3972	PRO
1	D	3972	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	558/4276 (13%)	546 (98%)	12 (2%)	45	69
1	B	558/4276 (13%)	546 (98%)	12 (2%)	45	69
1	C	558/4276 (13%)	546 (98%)	12 (2%)	45	69
1	D	558/4276 (13%)	546 (98%)	12 (2%)	45	69
All	All	2232/17104 (13%)	2184 (98%)	48 (2%)	45	69

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3992	PHE
1	A	4027	LEU
1	A	4178	LEU
1	A	4224	GLU
1	A	4580	TYR
1	A	4666	VAL
1	A	4720	VAL
1	A	4737	ILE
1	A	4889	VAL
1	A	5004	THR
1	A	5006	GLN
1	A	5034	ASP
1	B	3992	PHE
1	B	4027	LEU
1	B	4178	LEU
1	B	4224	GLU
1	B	4580	TYR
1	B	4666	VAL
1	B	4720	VAL
1	B	4737	ILE
1	B	4889	VAL
1	B	5004	THR
1	B	5006	GLN
1	B	5034	ASP
1	C	3992	PHE
1	C	4027	LEU
1	C	4178	LEU
1	C	4224	GLU
1	C	4580	TYR
1	C	4666	VAL
1	C	4720	VAL
1	C	4737	ILE
1	C	4889	VAL
1	C	5004	THR
1	C	5006	GLN
1	C	5034	ASP
1	D	3992	PHE
1	D	4027	LEU
1	D	4178	LEU
1	D	4224	GLU
1	D	4580	TYR
1	D	4666	VAL

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Mol	Chain	Res	Type
1	D	4720	VAL
1	D	4737	ILE
1	D	4889	VAL
1	D	5004	THR
1	D	5006	GLN
1	D	5034	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3950	ASN
1	A	4009	GLN
1	A	4037	ASN
1	A	4700	GLN
1	A	4832	HIS
1	A	5015	GLN
1	B	4009	GLN
1	B	4037	ASN
1	B	4700	GLN
1	B	4832	HIS
1	B	5015	GLN
1	C	3950	ASN
1	C	4009	GLN
1	C	4037	ASN
1	C	4832	HIS
1	C	5015	GLN
1	D	4009	GLN
1	D	4037	ASN
1	D	4832	HIS
1	D	5015	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
2	AMP	D	5101	-	25,25,25	0.35	0	37,38,38	0.48	0
2	AMP	C	5101	-	25,25,25	0.35	0	37,38,38	0.48	0
2	AMP	A	5101	-	25,25,25	0.35	0	37,38,38	0.48	0
2	AMP	B	5101	-	25,25,25	0.35	0	37,38,38	0.48	0

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	AMP	D	5101	-	-	2/10/26/26	0/3/3/3
2	AMP	C	5101	-	-	2/10/26/26	0/3/3/3
2	AMP	A	5101	-	-	2/10/26/26	0/3/3/3
2	AMP	B	5101	-	-	2/10/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5101	AMP	O4'-C4'-C5'-O5'
2	B	5101	AMP	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

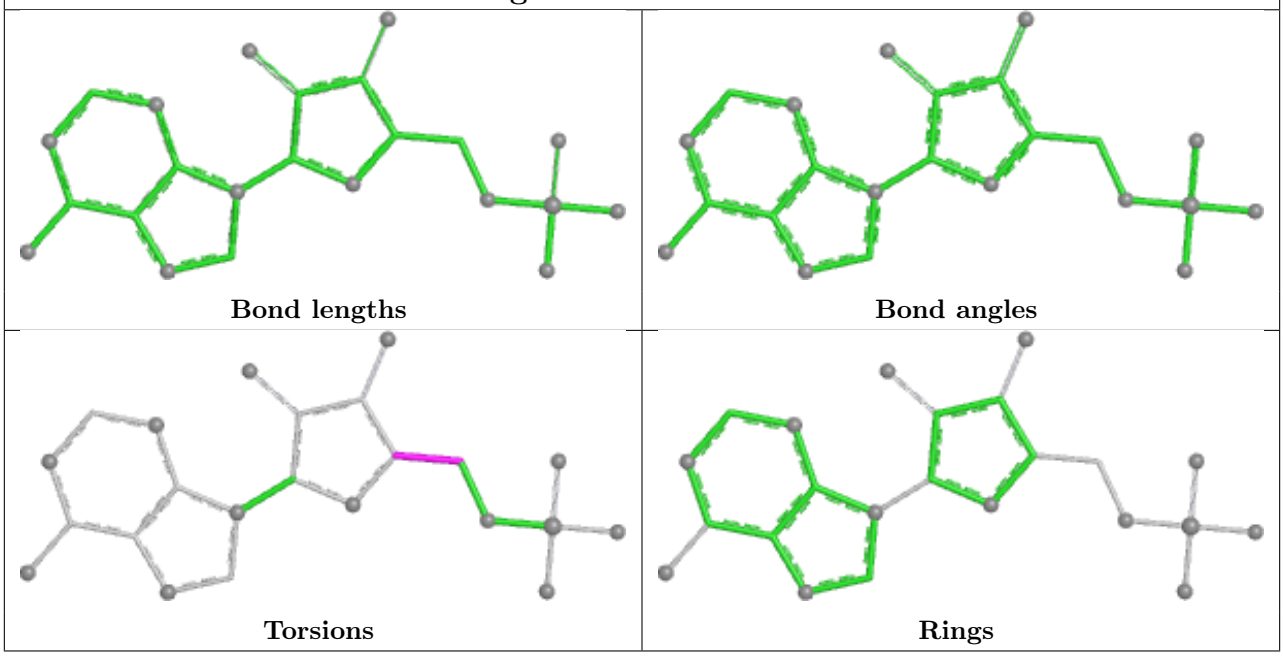
Mol	Chain	Res	Type	Atoms
2	C	5101	AMP	O4'-C4'-C5'-O5'
2	D	5101	AMP	O4'-C4'-C5'-O5'
2	A	5101	AMP	C3'-C4'-C5'-O5'
2	B	5101	AMP	C3'-C4'-C5'-O5'
2	C	5101	AMP	C3'-C4'-C5'-O5'
2	D	5101	AMP	C3'-C4'-C5'-O5'

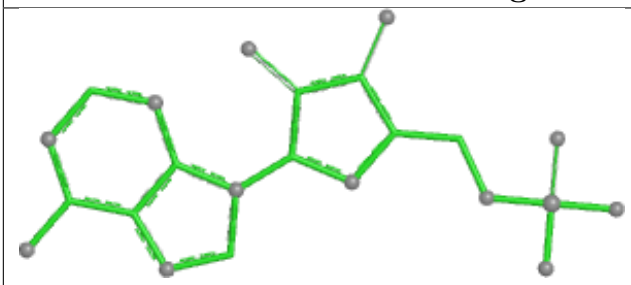
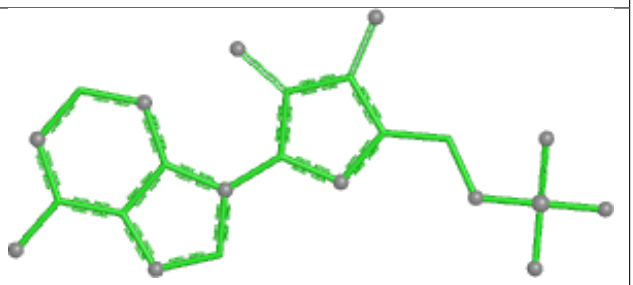
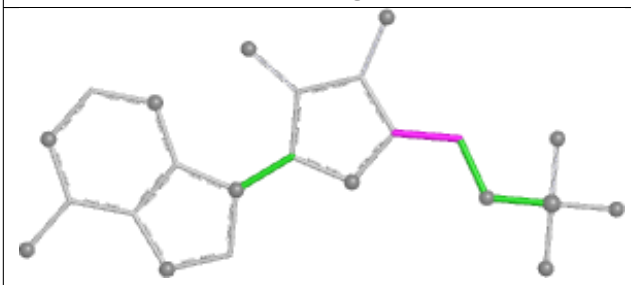
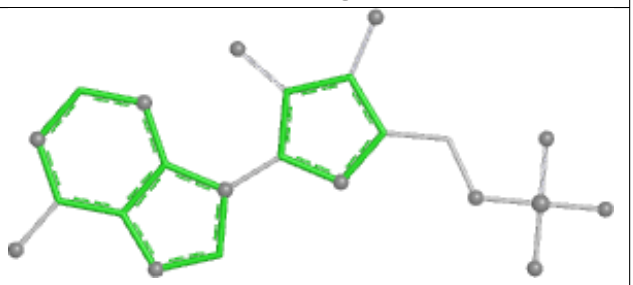
There are no ring outliers.

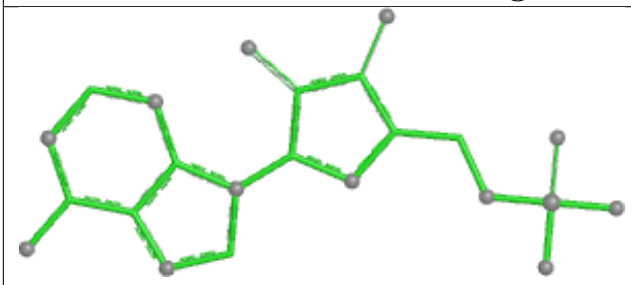
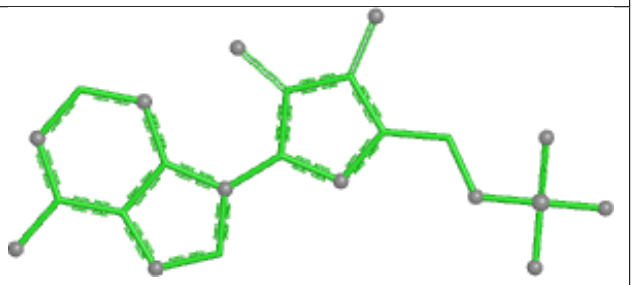
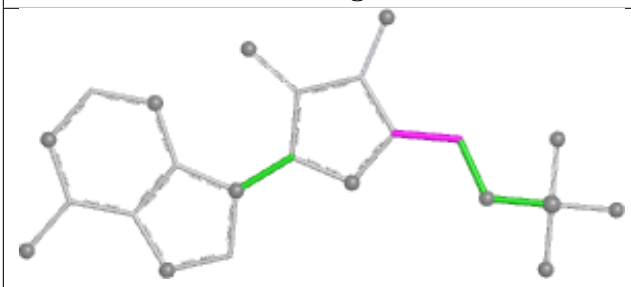
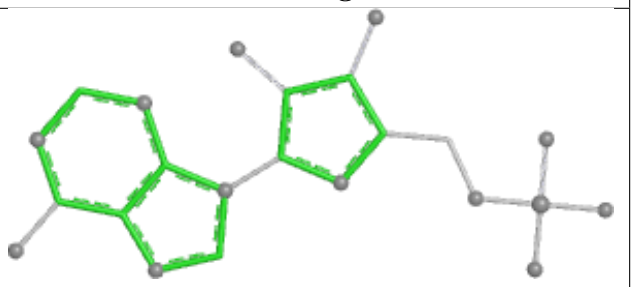
No monomer is involved in short contacts.

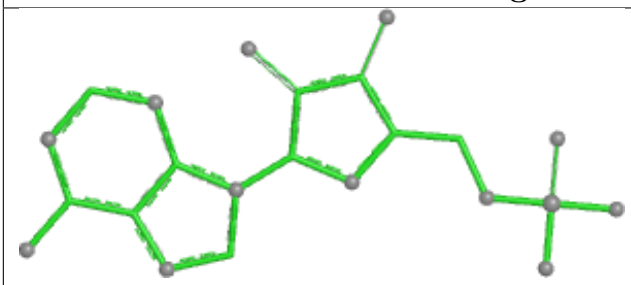
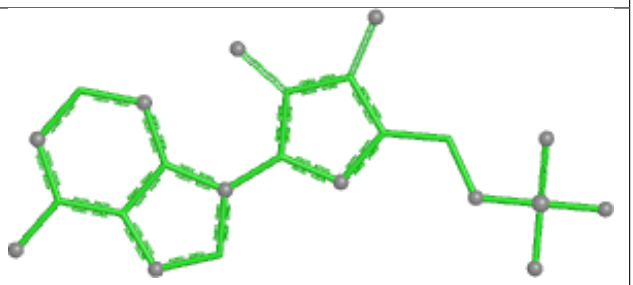
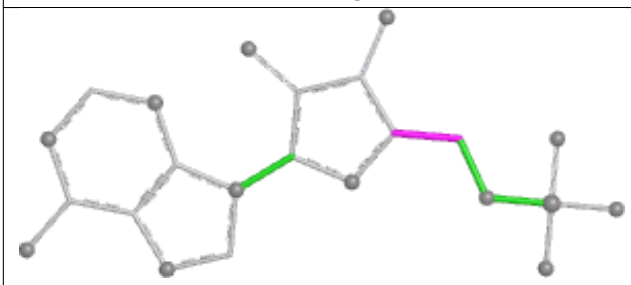
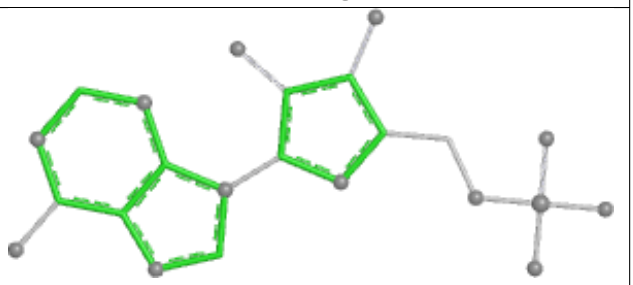
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand AMP C 5101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP A 5101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP B 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)

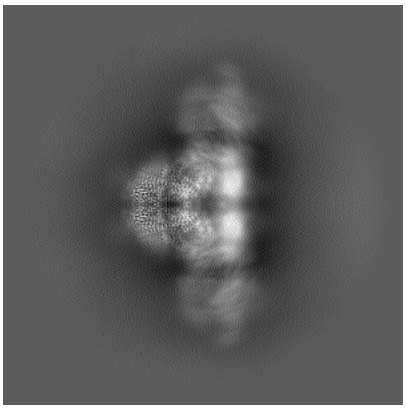
This section contains visualisations of the EMDB entry EMD-40432. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

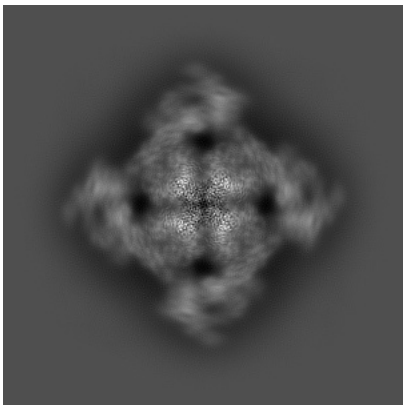
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

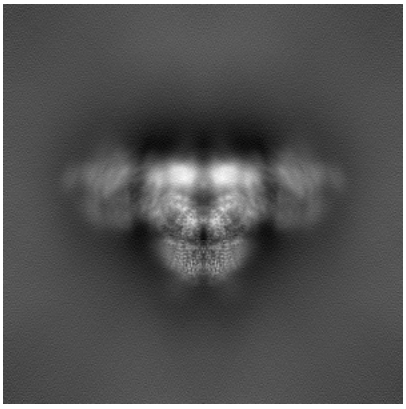


Y

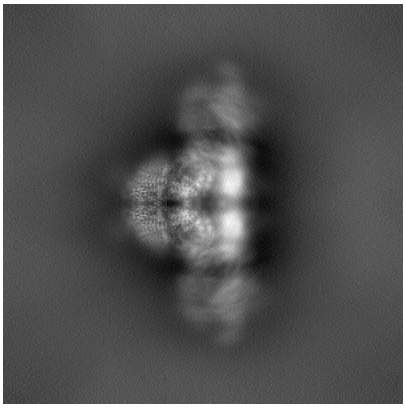


Z

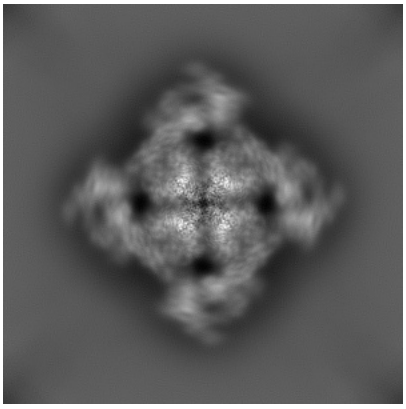
6.1.2 Raw map



X



Y

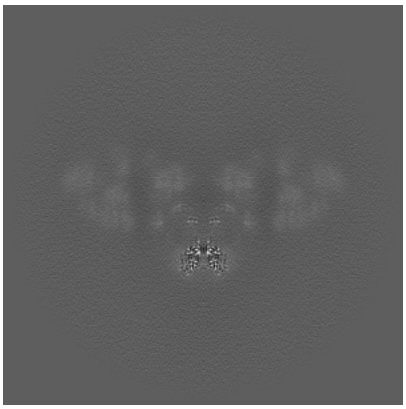


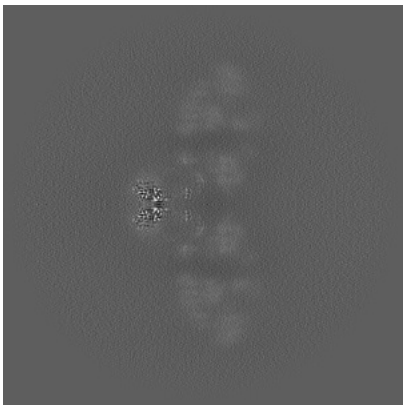
Z

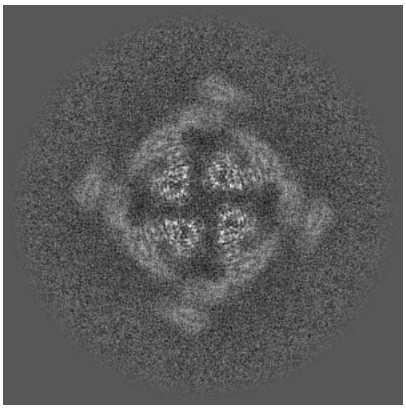
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

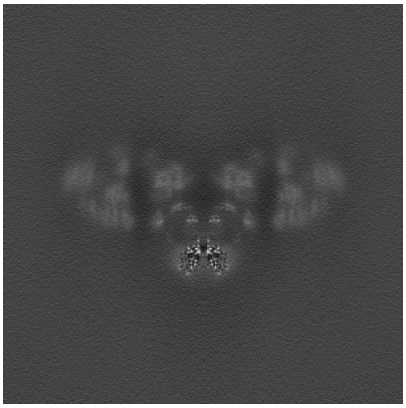
6.2.1 Primary map

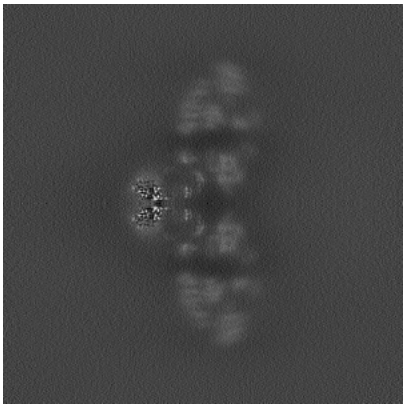

X Index: 200

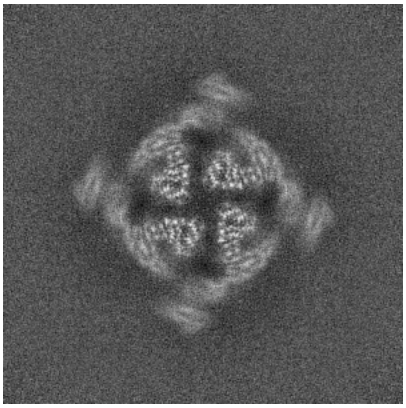

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

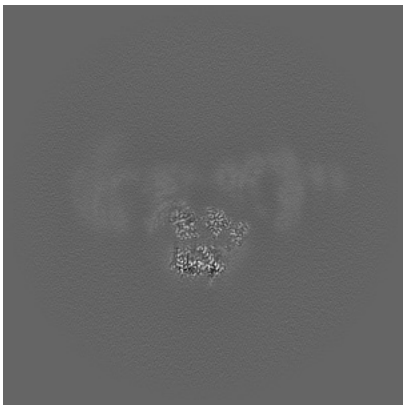

Y Index: 200


Z Index: 200

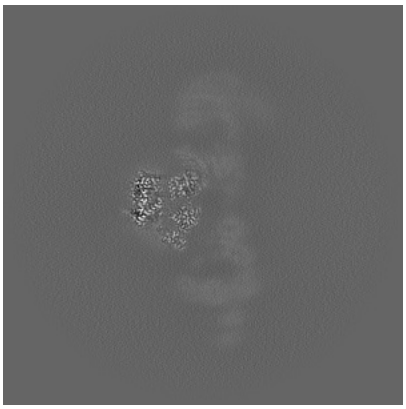
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

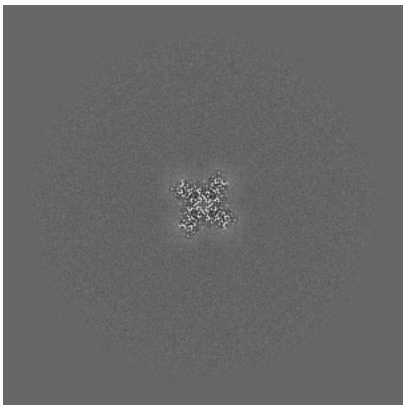
6.3.1 Primary map



X Index: 188

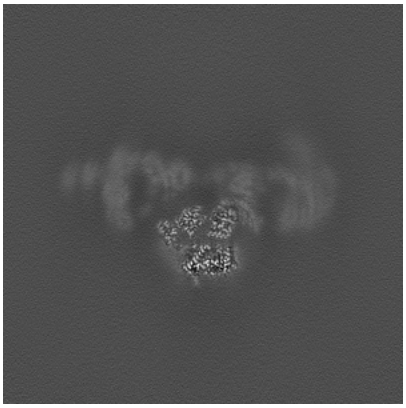


Y Index: 188

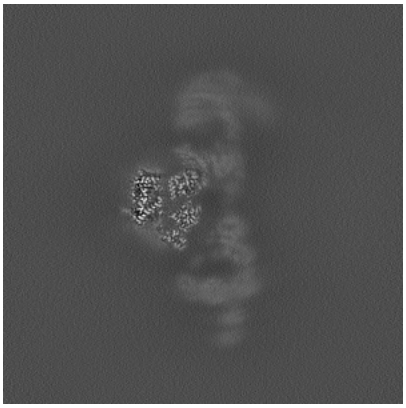


Z Index: 139

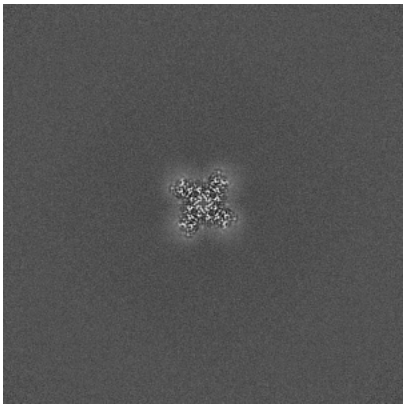
6.3.2 Raw map



X Index: 212



Y Index: 188

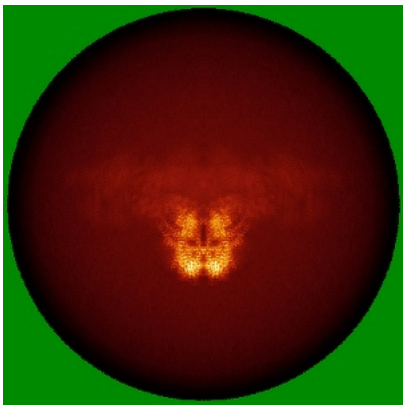


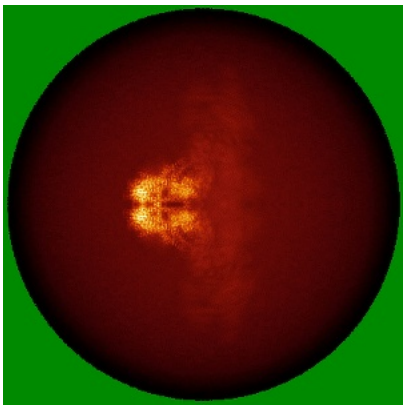
Z Index: 139

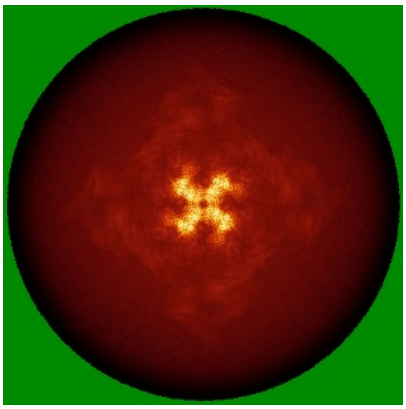
The images above show the largest variance slices of the map in three orthogonal directions.

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

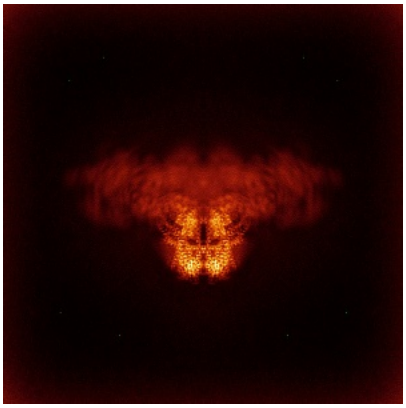
6.4.1 Primary map

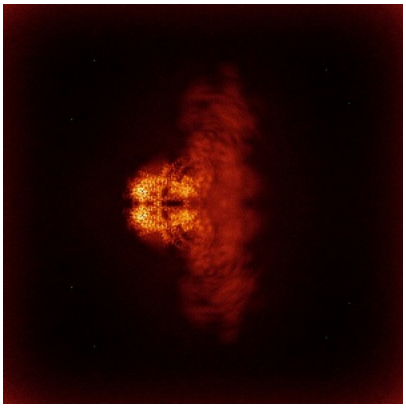

X

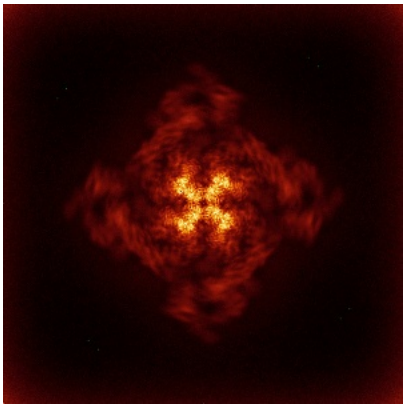

Y


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 0.192. 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.

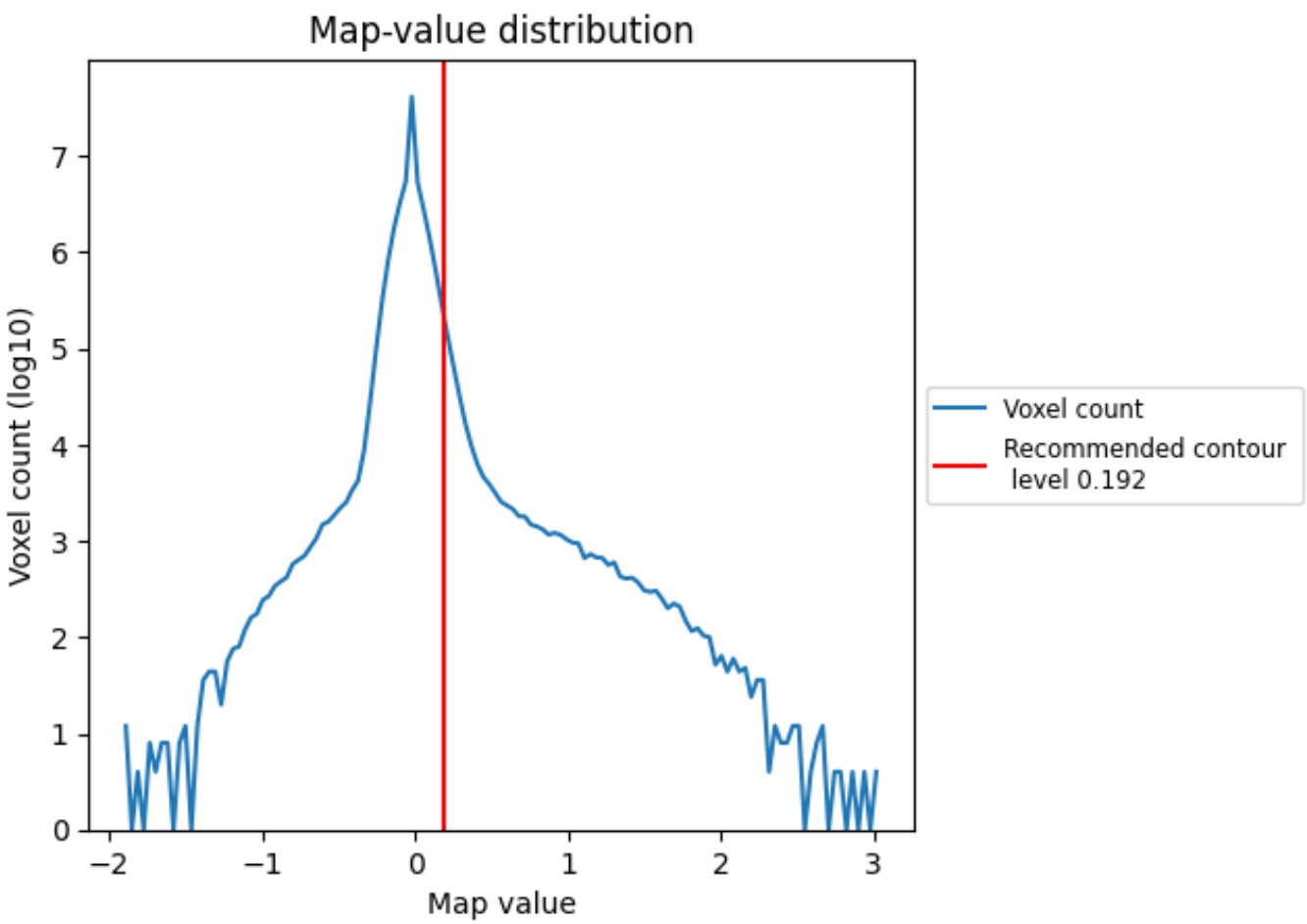
6.6 Mask visualisation (i)

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

7 Map analysis (i)

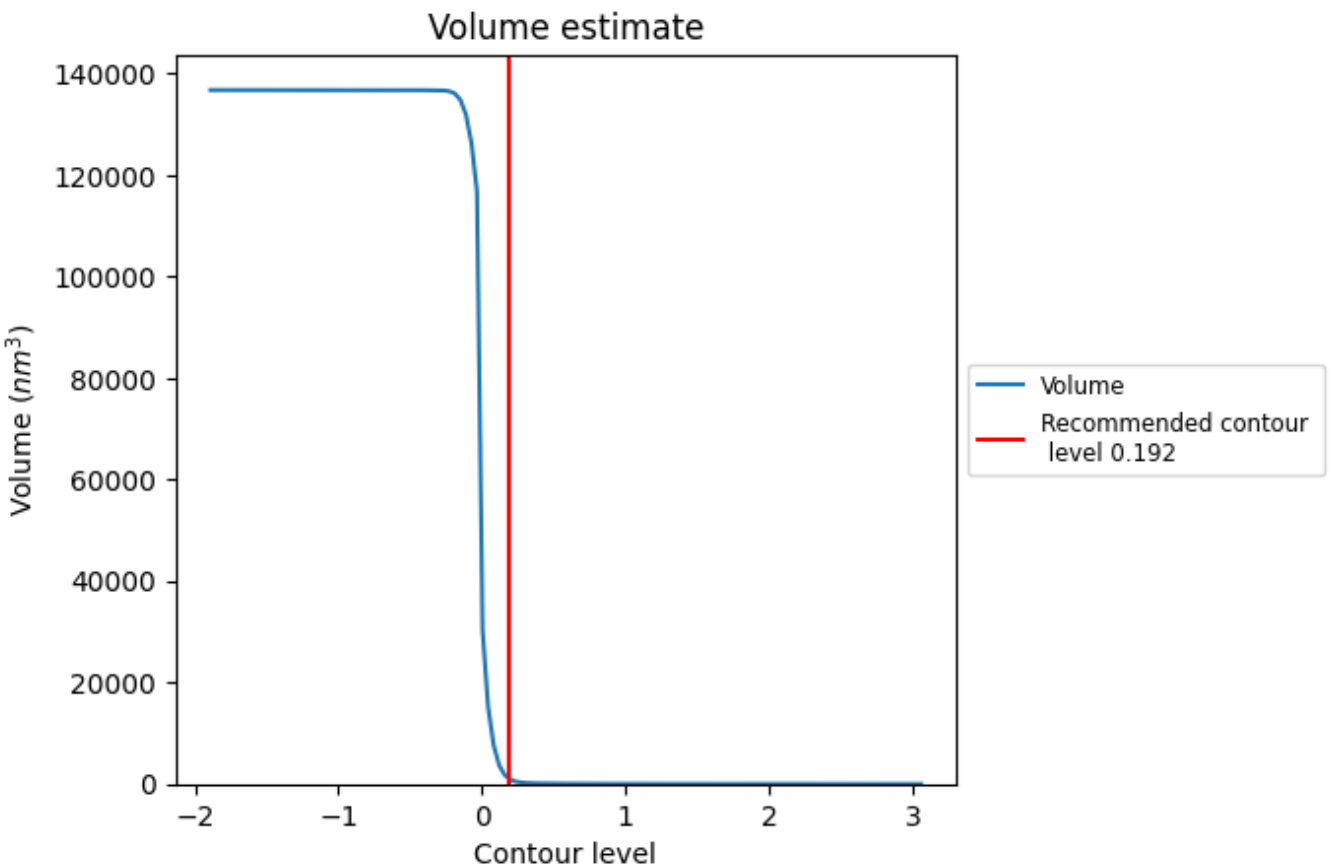
This section contains the results of statistical analysis of the map.

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.

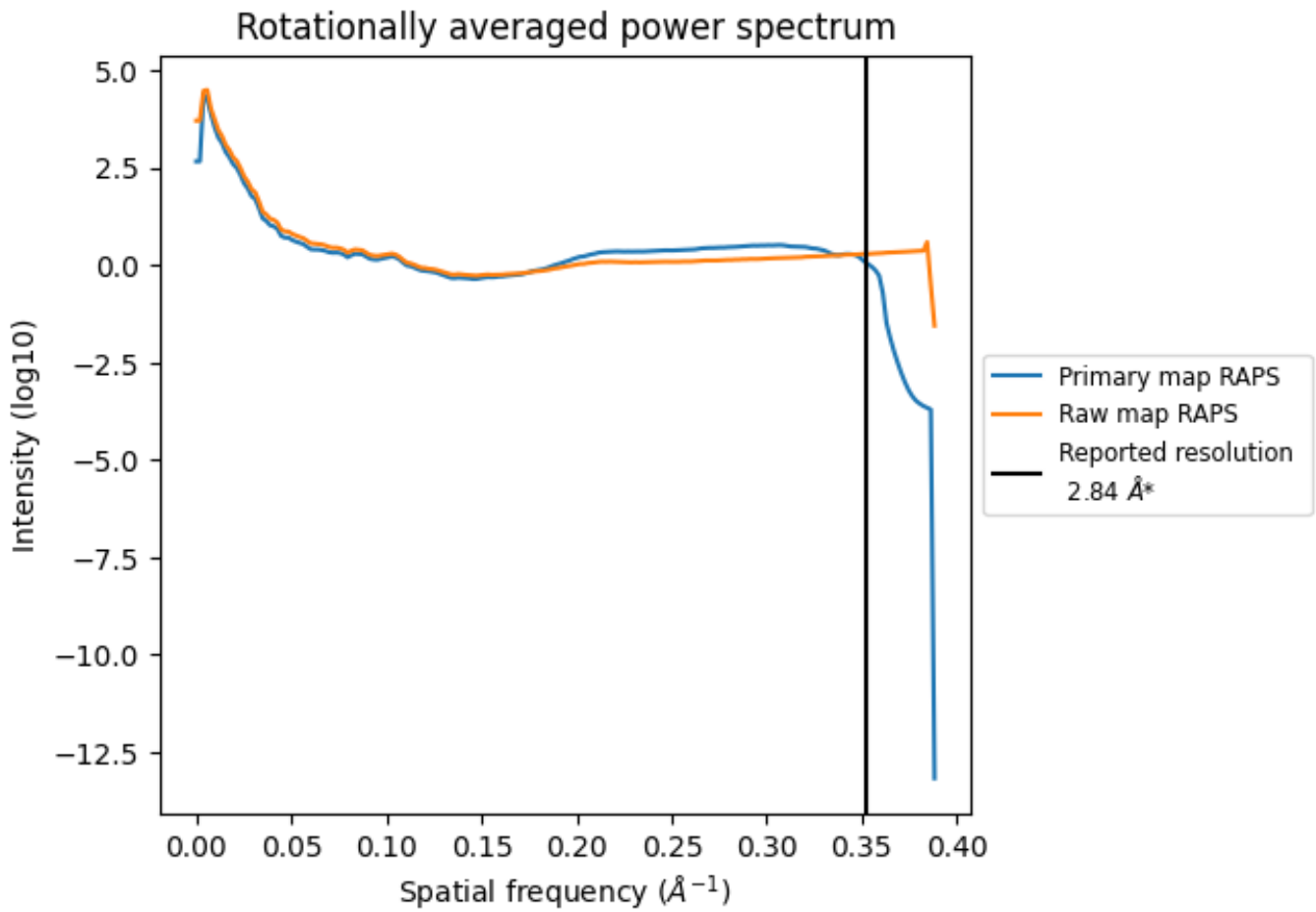
7.2 Volume estimate (i)



The volume at the recommended contour level is 973 nm^3; this corresponds to an approximate mass of 879 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)

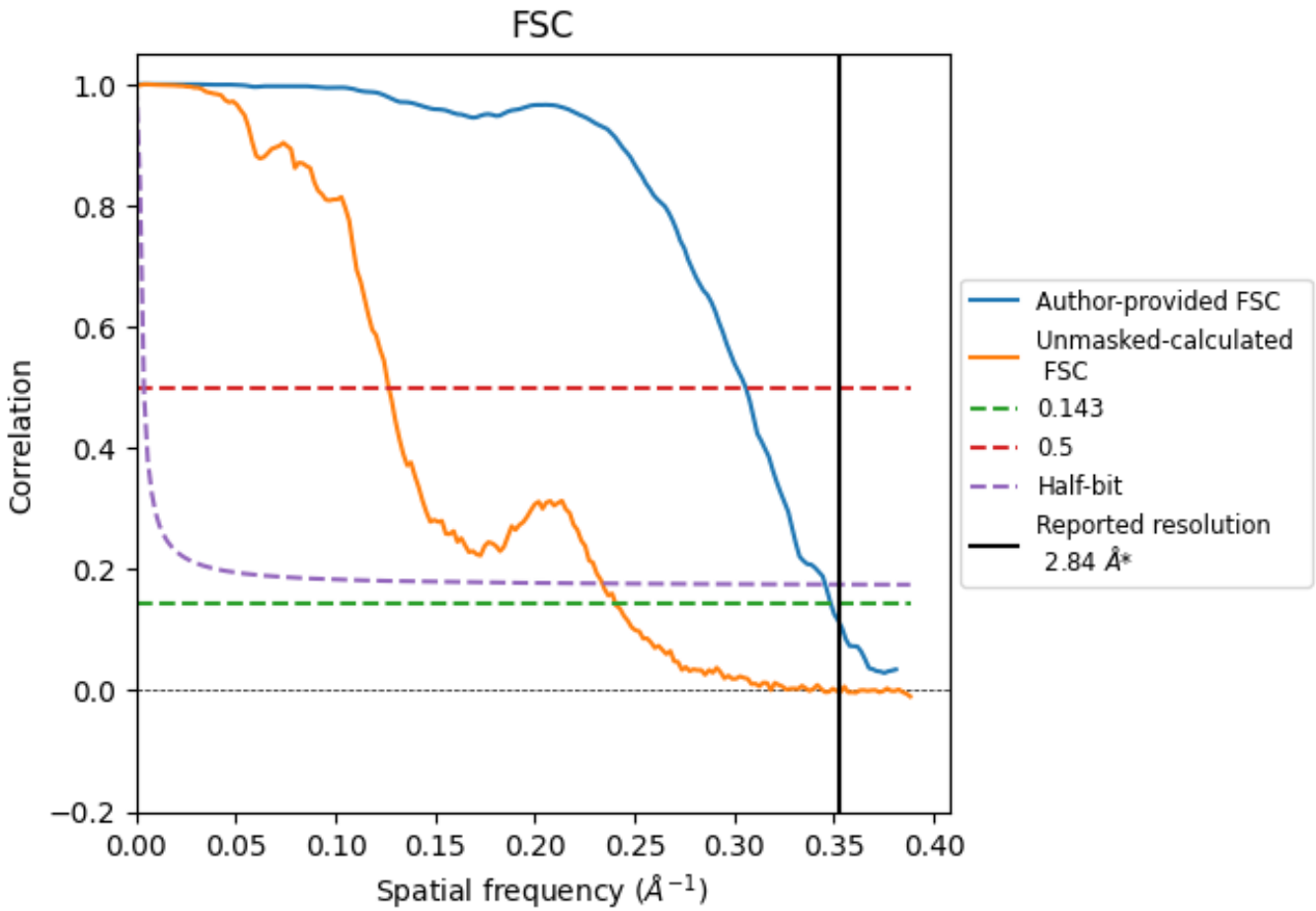


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

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 0.352 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.87	3.27	2.89
Unmasked-calculated*	4.16	7.90	4.28

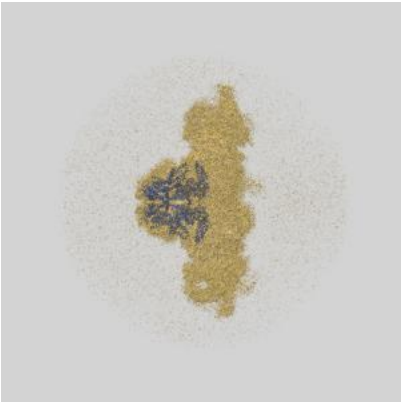
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.16 differs from the reported value 2.84 by more than 10 %

9 Map-model fit (i)

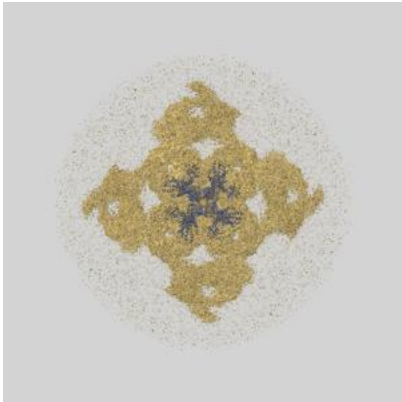
This section contains information regarding the fit between EMDB map EMD-40432 and PDB model 8SEX. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay (i)

X



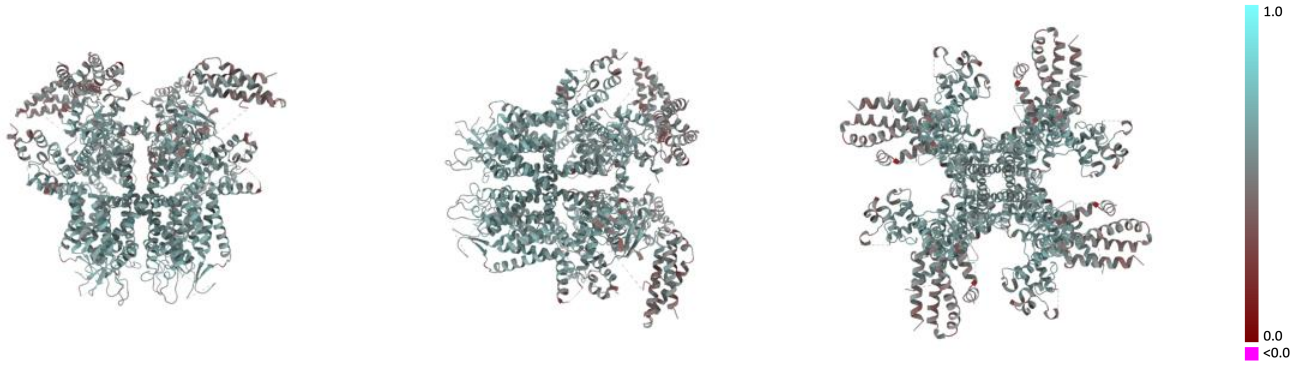
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.192 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)



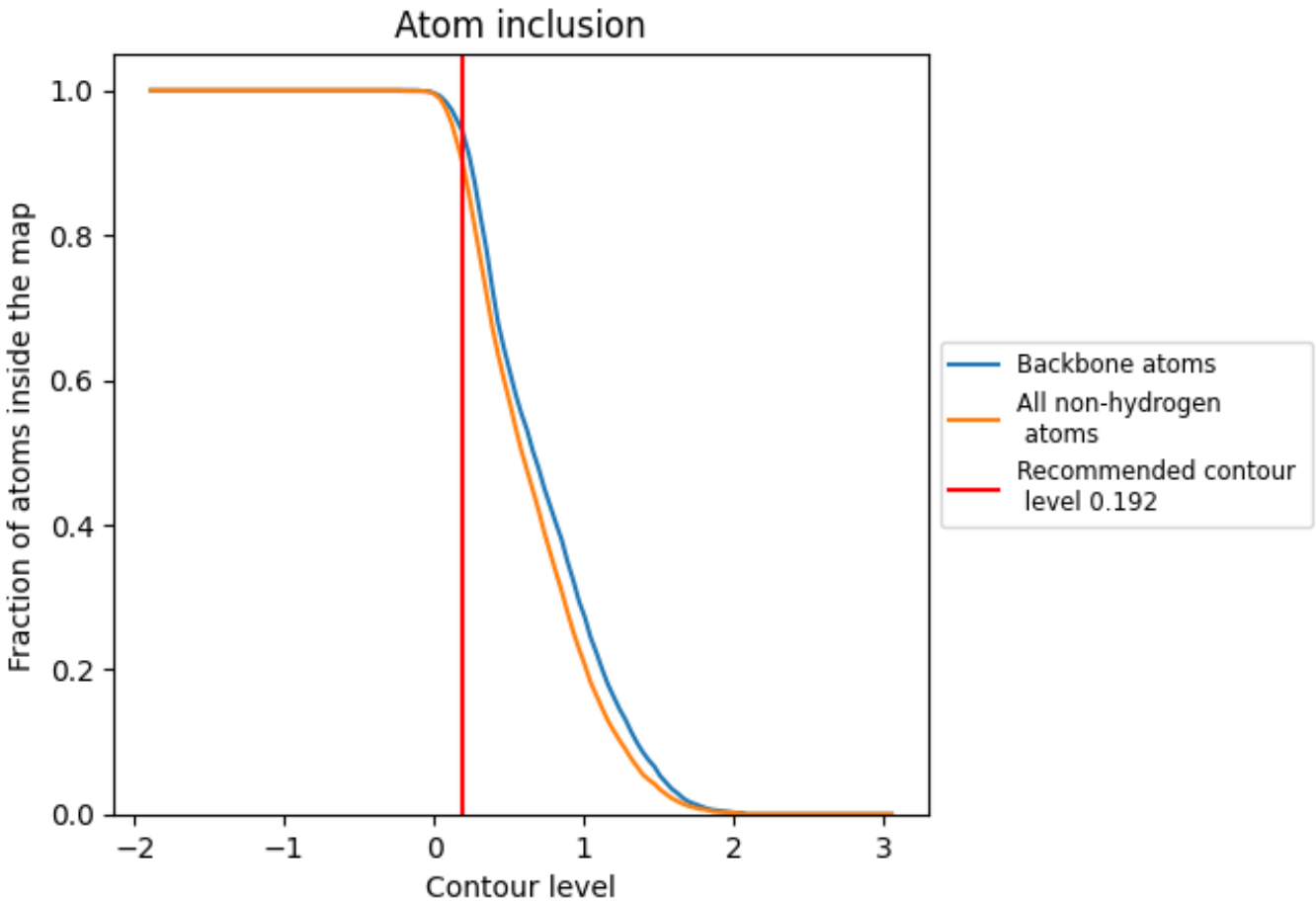
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.192) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.5560
A	0.9000	0.5570
B	0.9000	0.5570
C	0.9000	0.5570
D	0.9000	0.5560