Full wwPDB EM Validation Report ⓘ

Aug 28, 2026 – 12:33 am BST

PDB ID	:	9HHL / pdb_00009hhl
EMDB ID	:	EMD-52171
Title	:	Structure of Dynein-Dynactin-NuMA-LIS1
Authors	:	d'Amico, E.A.; Carter, A.P.
Deposited on	:	2024-11-21
Resolution	:	6.53 Å(reported)

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

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

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

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

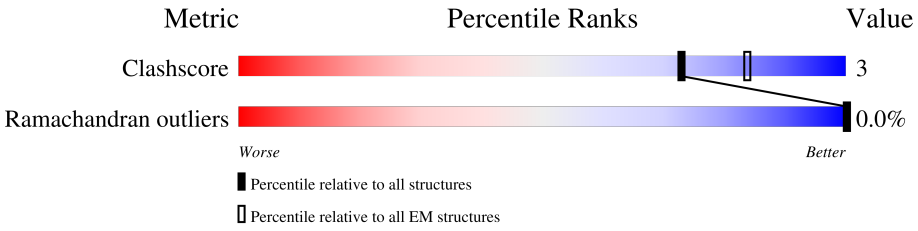
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

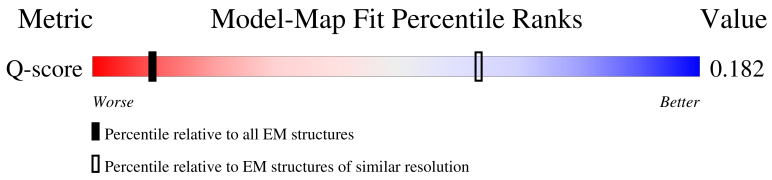
1 Overall quality at a glance

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

The reported resolution of this entry is 6.53 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.





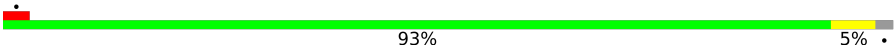
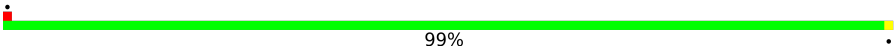
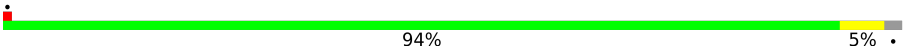
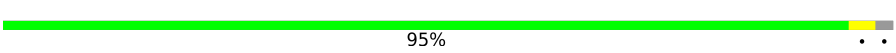
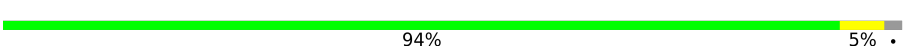
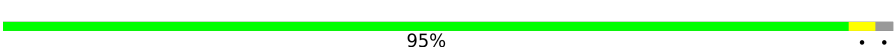
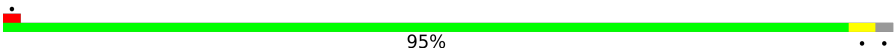
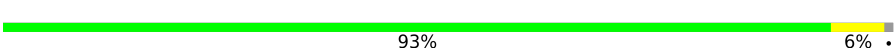
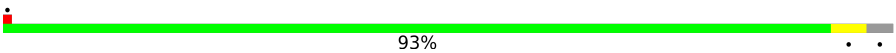
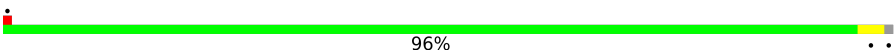
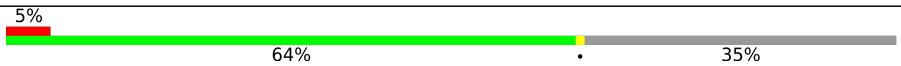
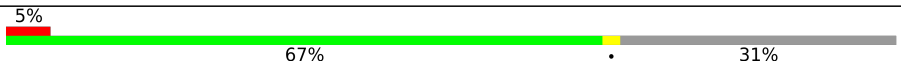
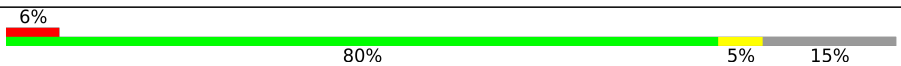
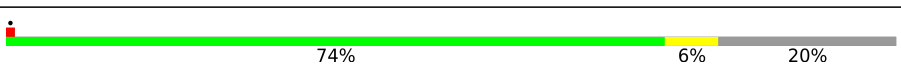
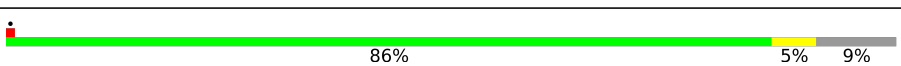
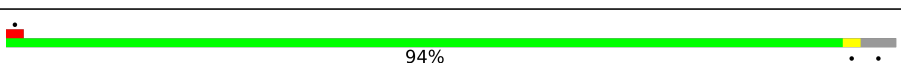
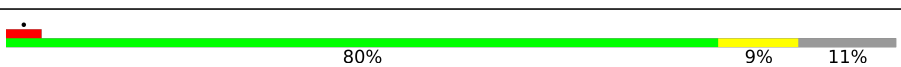
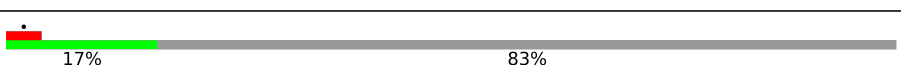
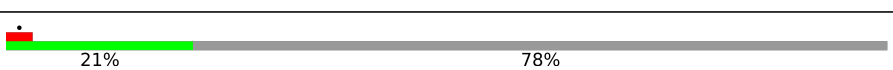
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	500 (6.03 - 7.02)

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	g	612	16% 59% 5% 36%
1	h	612	6% 61% · 35%
1	o	612	15% 58% 6% 36%
1	p	612	40% 65% · 34%
2	1	889	· 22% · 77%

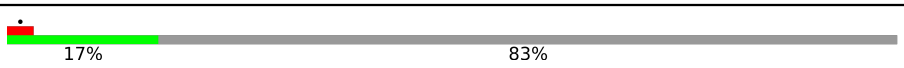
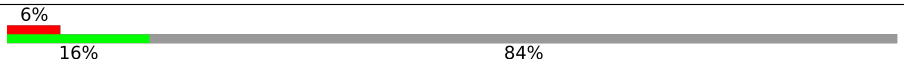
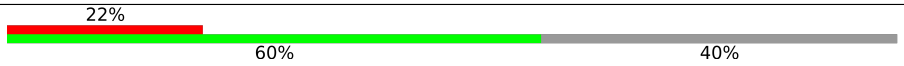
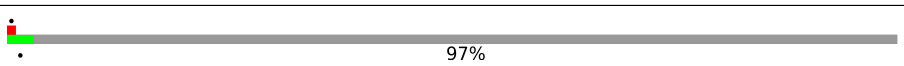
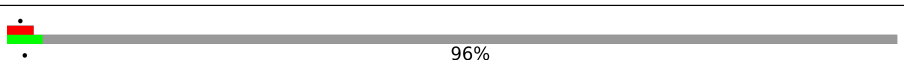
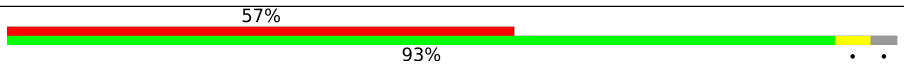
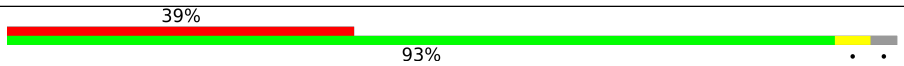
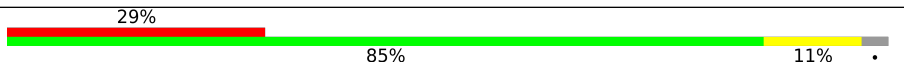
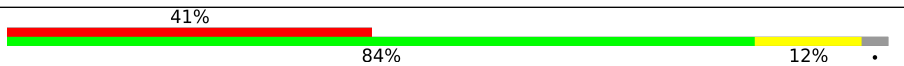
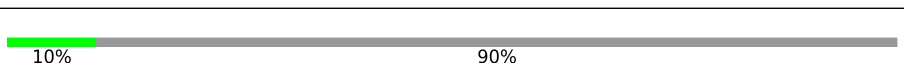
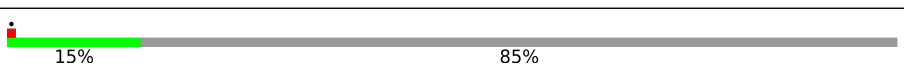
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Mol	Chain	Length	Quality of chain
2	2	889	
3	A	376	
3	B	376	
3	C	376	
3	D	376	
3	E	376	
3	F	376	
3	G	376	
3	I	376	
4	H	375	
5	J	417	
6	K	286	
7	L	272	
8	M	405	
8	N	405	
8	P	405	
8	Q	405	
8	V	405	
9	O	186	
9	R	186	
10	U	190	
11	W	182	
12	Y	467	
13	e	4646	
13	f	4646	

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Mol	Chain	Length	Quality of chain
13	m	4646	
13	n	4646	
14	j	492	
14	q	492	
14	u	492	
15	s	96	
15	t	96	
15	w	96	
15	z	96	
16	S	1281	
16	T	1281	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 64583 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 Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	p	401	Total 1980	C 1178	N 401	O 401	0	0
1	g	394	Total 1946	C 1158	N 394	O 394	0	0
1	h	396	Total 1955	C 1163	N 396	O 396	0	0
1	o	394	Total 1946	C 1158	N 394	O 394	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	484	SER	THR	conflict	UNP Q13409
p	499	GLY	ASP	conflict	UNP Q13409
g	510	SER	THR	conflict	UNP Q13409
g	525	GLY	ASP	conflict	UNP Q13409
h	510	SER	THR	conflict	UNP Q13409
h	525	GLY	ASP	conflict	UNP Q13409
o	510	SER	THR	conflict	UNP Q13409
o	525	GLY	ASP	conflict	UNP Q13409

- Molecule 2 is a protein called Nuclear mitotic apparatus protein 1,Methylated-DNA--protei n-cysteine methyltransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	205	Total 1021	C 611	N 205	O 205	0	0
2	2	193	Total 962	C 576	N 193	O 193	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	706	GLY	-	linker	UNP Q14980
1	707	SER	-	linker	UNP Q14980
1	737	ARG	GLU	engineered mutation	UNP P16455
1	739	ILE	LYS	engineered mutation	UNP P16455
1	740	PHE	LEU	engineered mutation	UNP P16455
1	769	ALA	CYS	engineered mutation	UNP P16455
1	822	SER	GLN	engineered mutation	UNP P16455
1	823	HIS	GLN	engineered mutation	UNP P16455
1	832	ALA	LYS	engineered mutation	UNP P16455
1	834	THR	ALA	engineered mutation	UNP P16455
1	835	ALA	ARG	engineered mutation	UNP P16455
1	838	LYS	GLY	engineered mutation	UNP P16455
1	839	THR	GLY	engineered mutation	UNP P16455
1	841	LEU	MET	engineered mutation	UNP P16455
1	842	SER	ARG	engineered mutation	UNP P16455
1	857	GLN	CYS	engineered mutation	UNP P16455
1	858	GLY	SER	engineered mutation	UNP P16455
1	859	ASP	SER	engineered mutation	UNP P16455
1	860	LEU	GLY	engineered mutation	UNP P16455
1	861	ASP	ALA	engineered mutation	UNP P16455
1	864	GLY	ASN	engineered mutation	UNP P16455
1	866	GLU	SER	engineered mutation	UNP P16455
2	706	GLY	-	linker	UNP Q14980
2	707	SER	-	linker	UNP Q14980
2	737	ARG	GLU	engineered mutation	UNP P16455
2	739	ILE	LYS	engineered mutation	UNP P16455
2	740	PHE	LEU	engineered mutation	UNP P16455
2	769	ALA	CYS	engineered mutation	UNP P16455
2	822	SER	GLN	engineered mutation	UNP P16455
2	823	HIS	GLN	engineered mutation	UNP P16455
2	832	ALA	LYS	engineered mutation	UNP P16455
2	834	THR	ALA	engineered mutation	UNP P16455
2	835	ALA	ARG	engineered mutation	UNP P16455
2	838	LYS	GLY	engineered mutation	UNP P16455
2	839	THR	GLY	engineered mutation	UNP P16455
2	841	LEU	MET	engineered mutation	UNP P16455
2	842	SER	ARG	engineered mutation	UNP P16455
2	857	GLN	CYS	engineered mutation	UNP P16455
2	858	GLY	SER	engineered mutation	UNP P16455
2	859	ASP	SER	engineered mutation	UNP P16455
2	860	LEU	GLY	engineered mutation	UNP P16455
2	861	ASP	ALA	engineered mutation	UNP P16455
2	864	GLY	ASN	engineered mutation	UNP P16455

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Chain	Residue	Modelled	Actual	Comment	Reference
2	866	GLU	SER	engineered mutation	UNP P16455

- Molecule 3 is a protein called ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	370	Total 1822	C 1082	N 370	O 370	0	0
3	B	370	Total 1822	C 1082	N 370	O 370	0	0
3	D	370	Total 1822	C 1082	N 370	O 370	0	0
3	E	370	Total 1822	C 1082	N 370	O 370	0	0
3	F	370	Total 1822	C 1082	N 370	O 370	0	0
3	G	370	Total 1822	C 1082	N 370	O 370	0	0
3	I	370	Total 1822	C 1082	N 370	O 370	0	0
3	C	375	Total 1847	C 1097	N 375	O 375	0	0

- Molecule 4 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	370	Total 1822	C 1082	N 370	O 370	0	0

- Molecule 5 is a protein called Arp11.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	379	Total 1868	C 1110	N 379	O 379	0	0

- Molecule 6 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	278	Total 1378	C 822	N 278	O 278	0	0

- Molecule 7 is a protein called F-actin-capping protein subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	269	Total 1327	C 789	N 269	O 269	0	0

- Molecule 8 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	M	265	Total 1320	C 790	N 265	O 265	0	0
8	N	280	Total 1394	C 834	N 280	O 280	0	0
8	P	343	Total 1707	C 1021	N 343	O 343	0	0
8	Q	325	Total 1612	C 962	N 325	O 325	0	0
8	V	75	Total 369	C 219	N 75	O 75	0	0

- Molecule 9 is a protein called Dynactin subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	O	170	Total 844	C 504	N 170	O 170	0	0
9	R	179	Total 888	C 530	N 179	O 179	0	0

- Molecule 10 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	169	Total 832	C 494	N 169	O 169	0	0

- Molecule 11 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	179	Total 881	C 523	N 179	O 179	0	0

- Molecule 12 is a protein called Dynactin subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Y	375	Total 1863	C 1113	N 375	O 375	0	0

- Molecule 13 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	807	Total	C	N	O	0	0
			4004	2390	807	807		
13	f	1017	Total	C	N	O	0	0
			5046	3012	1017	1017		
13	m	795	Total	C	N	O	0	0
			3946	2356	795	795		
13	n	744	Total	C	N	O	0	0
			3693	2205	744	744		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	1567	GLU	ARG	engineered mutation	UNP Q14204
e	1610	GLU	LYS	engineered mutation	UNP Q14204
f	1567	GLU	ARG	engineered mutation	UNP Q14204
f	1610	GLU	LYS	engineered mutation	UNP Q14204
m	1567	GLU	ARG	engineered mutation	UNP Q14204
m	1610	GLU	LYS	engineered mutation	UNP Q14204
n	1567	GLU	ARG	engineered mutation	UNP Q14204
n	1610	GLU	LYS	engineered mutation	UNP Q14204

- Molecule 14 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	j	296	Total	C	N	O	0	0
			1465	873	296	296		
14	q	15	Total	C	N	O	0	0
			75	45	15	15		
14	u	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 15 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	s	93	Total	C	N	O	0	0
			462	276	93	93		
15	t	93	Total	C	N	O	0	0
			462	276	93	93		
15	w	93	Total	C	N	O	0	0
			462	276	93	93		

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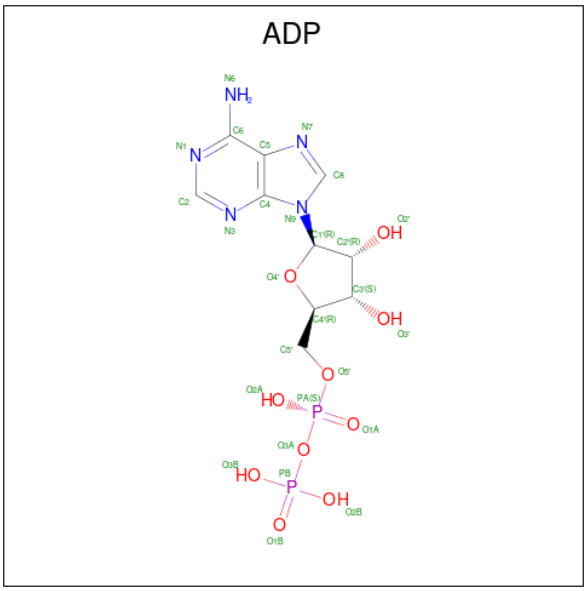
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Mol	Chain	Residues	Atoms				AltConf	Trace
15	z	93	Total	C	N	O	0	0
			462	276	93	93		

- Molecule 16 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	S	134	Total	C	N	O	0	0
			667	399	134	134		
16	T	192	Total	C	N	O	0	0
			952	568	192	192		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



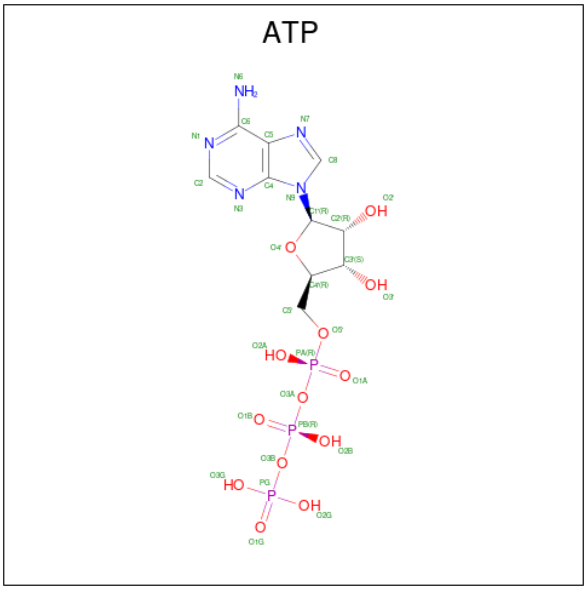
Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
17	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
18	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	Y	3	Total	Zn	0
			3	3	

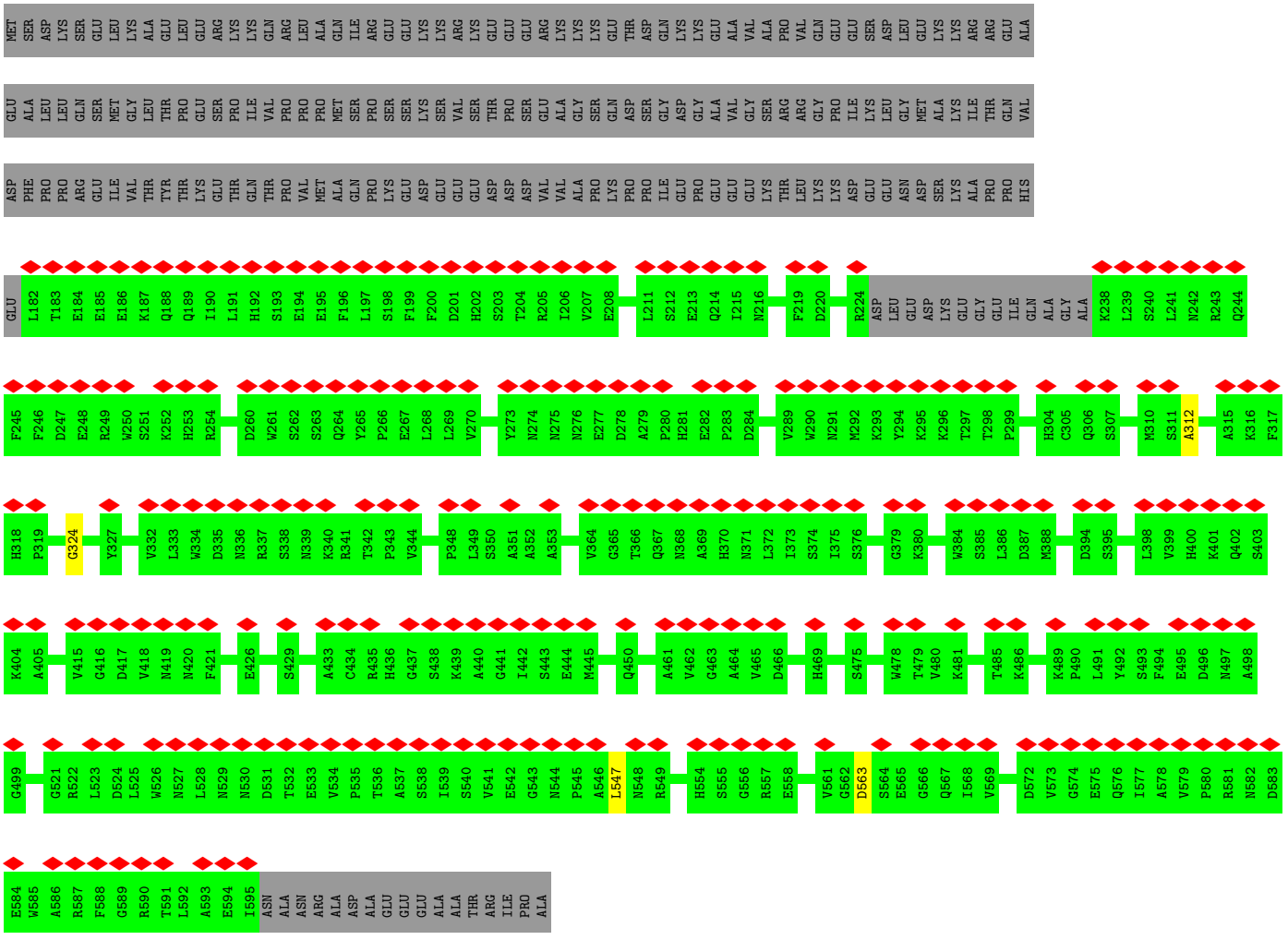
3 Residue-property plots (i)

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: Cytoplasmic dynein 1 intermediate chain 2

Chain p:

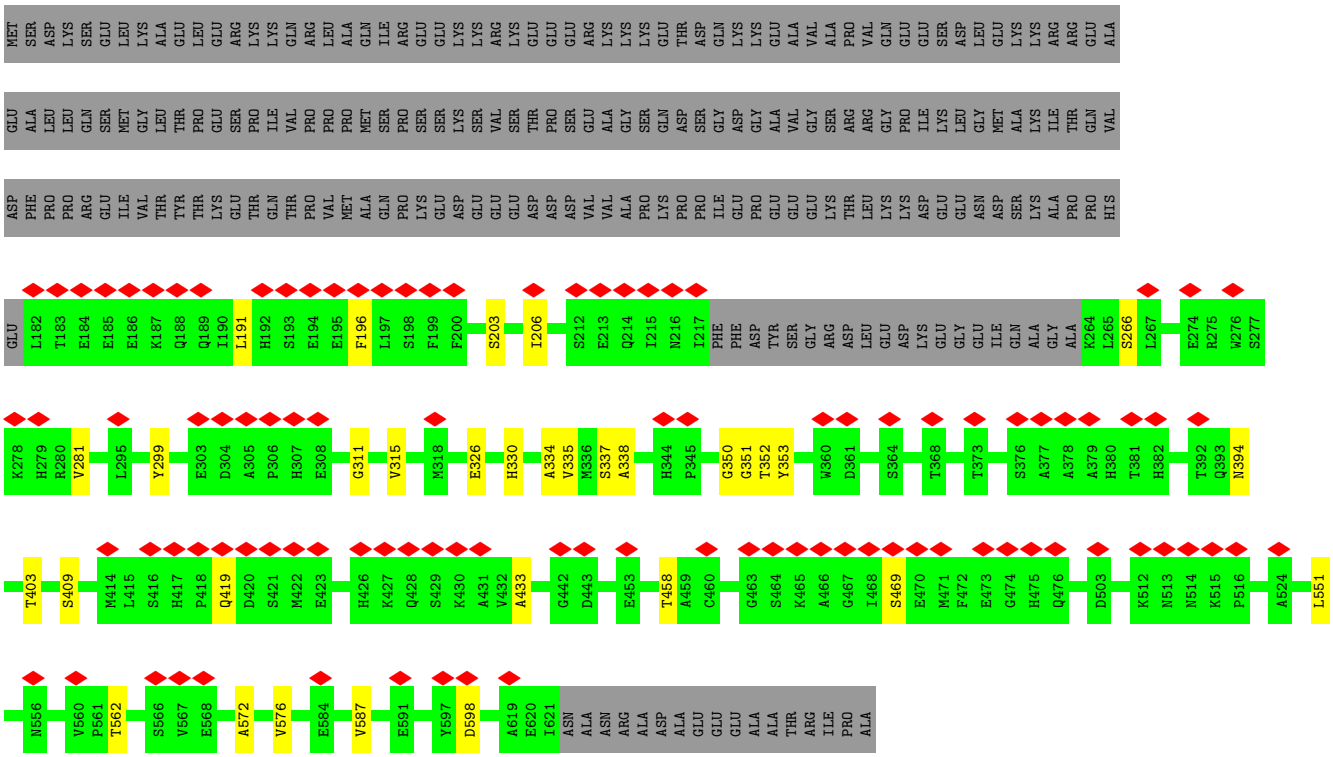




• Molecule 1: Cytoplasmic dynein 1 intermediate chain 2

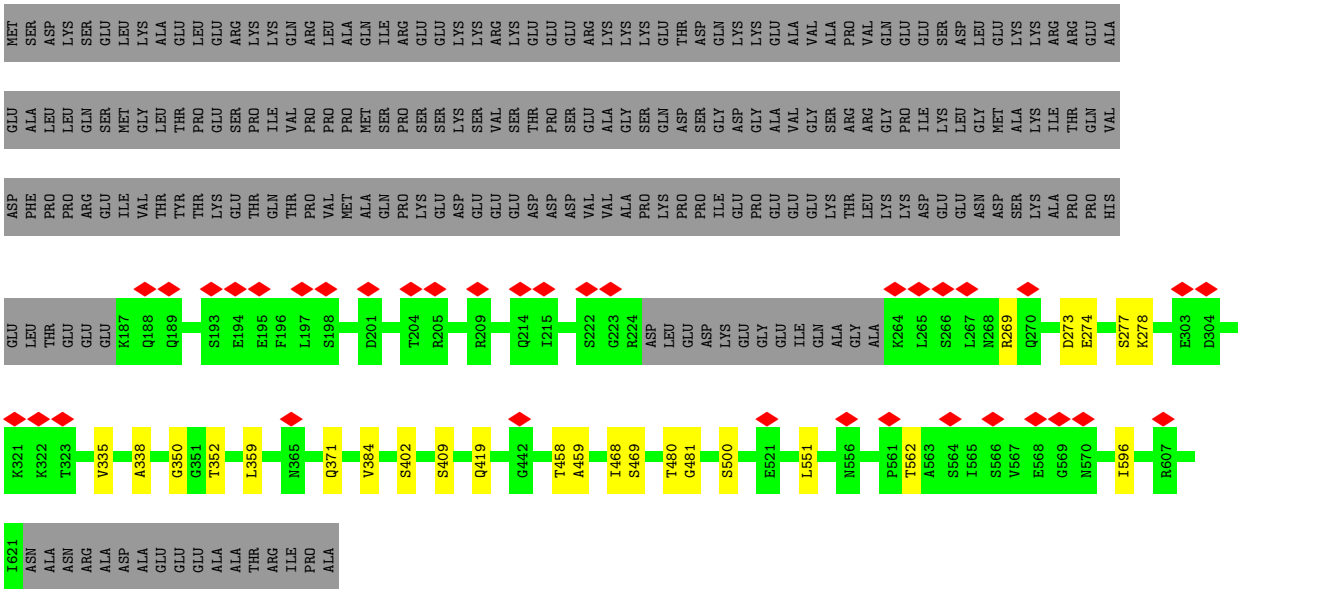
Chain g:





• Molecule 1: Cytoplasmic dynein 1 intermediate chain 2

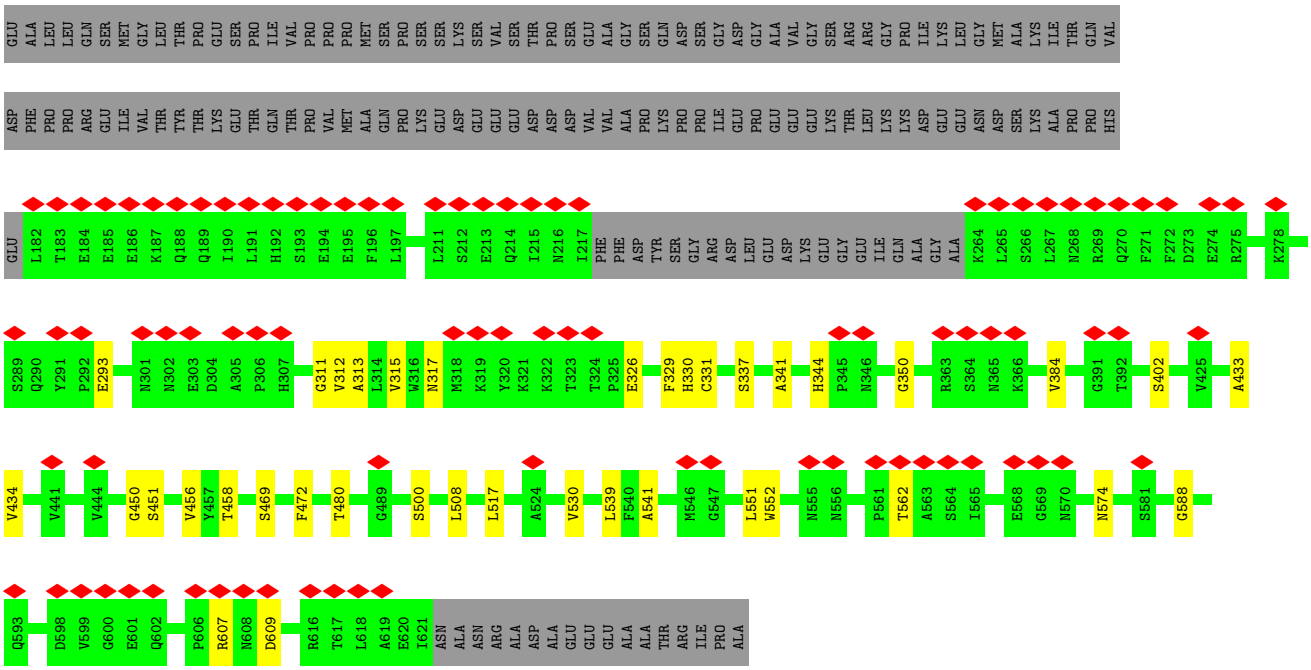




• Molecule 1: Cytoplasmic dynein 1 intermediate chain 2



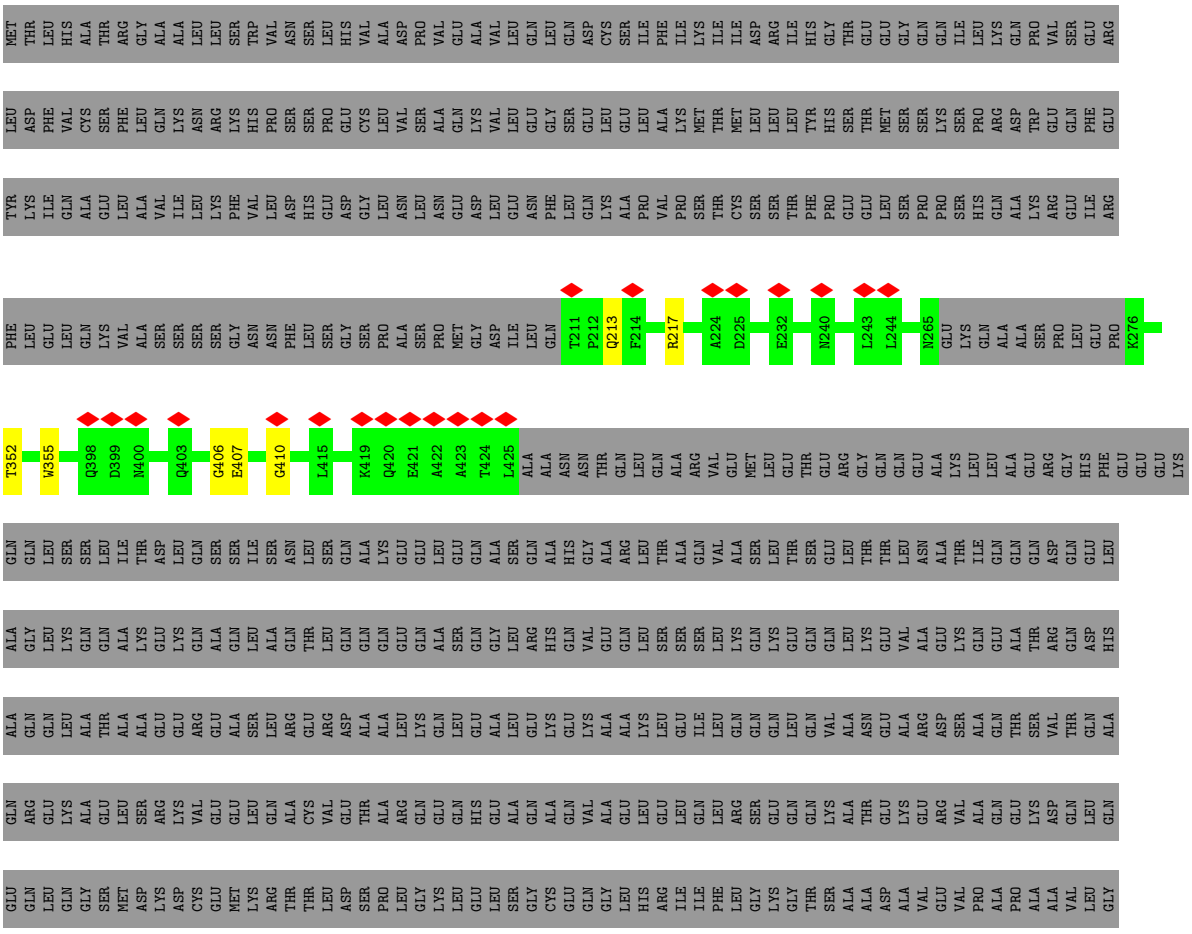


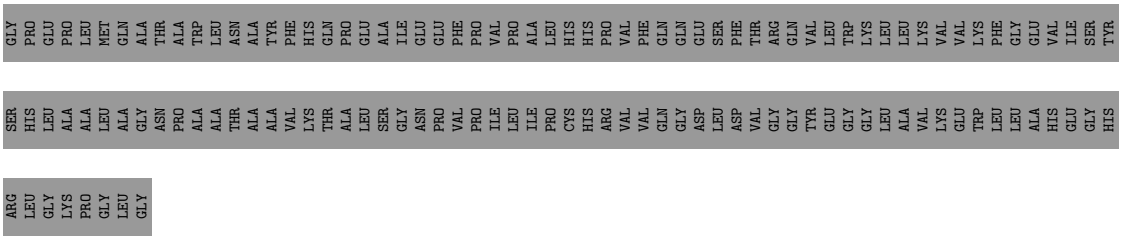


• Molecule 2: Nuclear mitotic apparatus protein 1,Methylated-DNA--protein-cysteine methyltransferase

Chain 1:



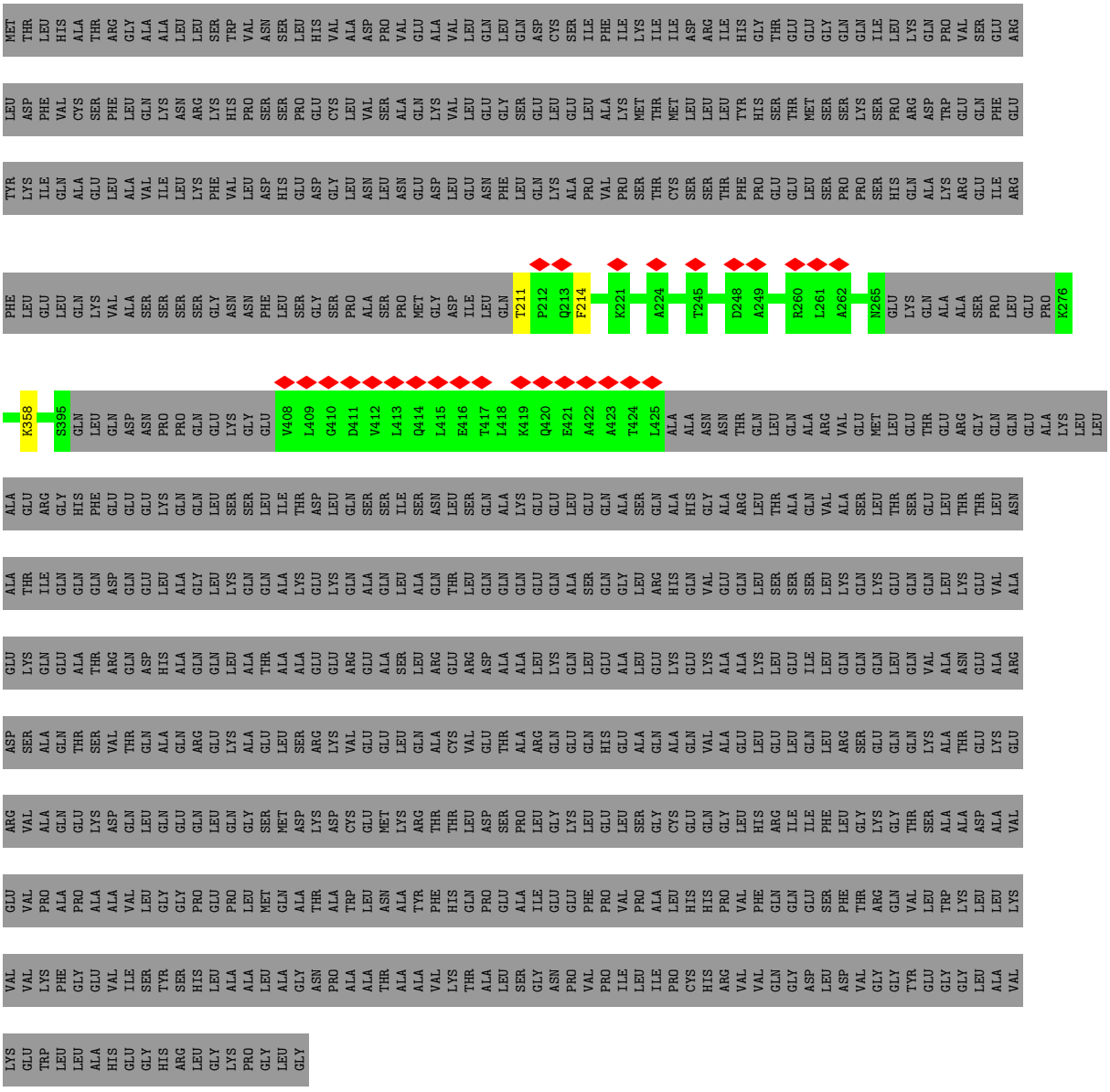




• Molecule 2: Nuclear mitotic apparatus protein 1,Methylated-DNA--protein-cysteine methyltransferase

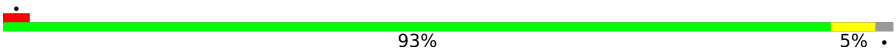
Chain 2:

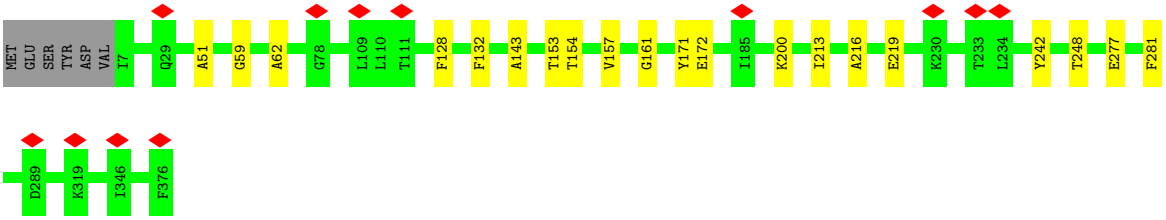




• Molecule 3: ARP1 actin related protein 1 homolog A

Chain A:

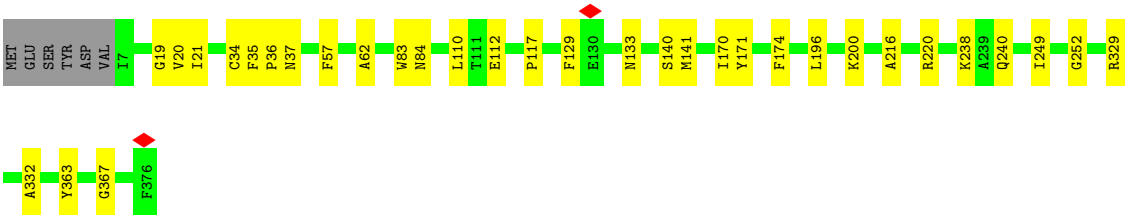




• Molecule 3: ARP1 actin related protein 1 homolog A

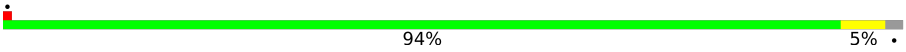
Chain B:

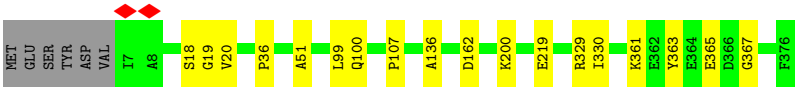




• Molecule 3: ARP1 actin related protein 1 homolog A

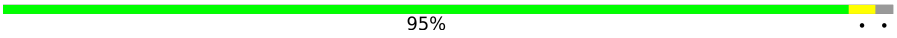
Chain D:





• Molecule 3: ARP1 actin related protein 1 homolog A

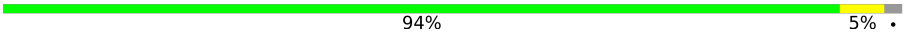
Chain E:

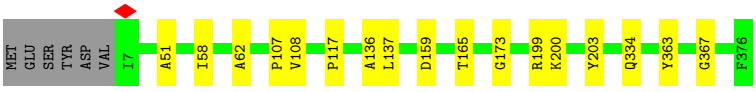




• Molecule 3: ARP1 actin related protein 1 homolog A

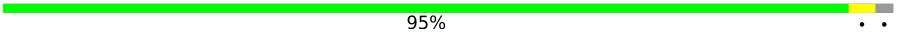
Chain F:

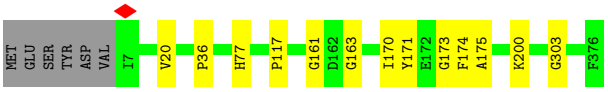




• Molecule 3: ARP1 actin related protein 1 homolog A

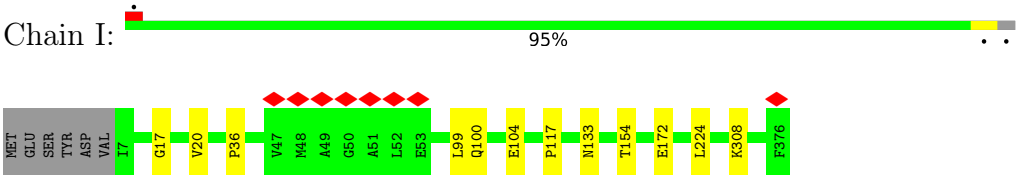
Chain G:





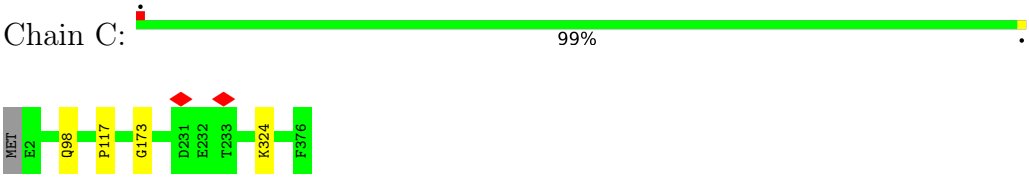
• Molecule 3: ARP1 actin related protein 1 homolog A

Chain I:



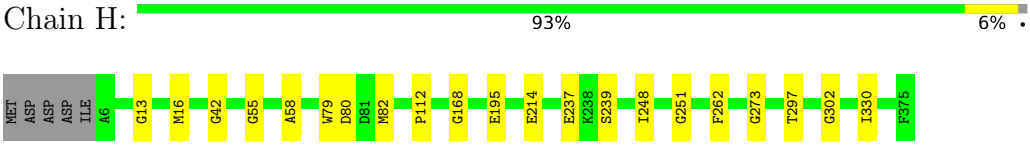
• Molecule 3: ARP1 actin related protein 1 homolog A

Chain C:



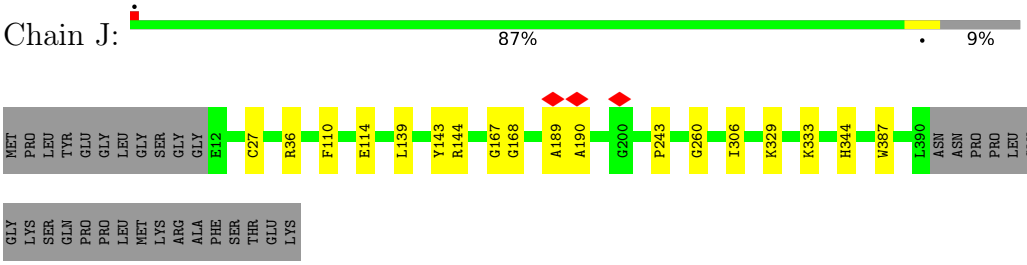
• Molecule 4: Actin, cytoplasmic 1

Chain H:



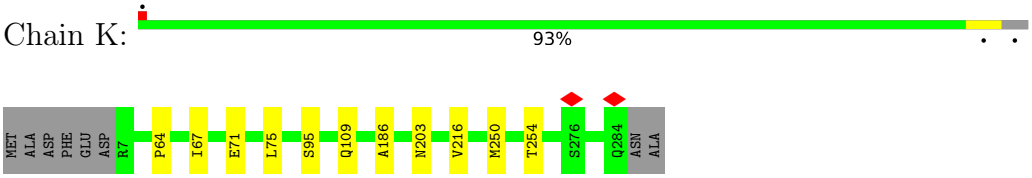
• Molecule 5: Arp11

Chain J:



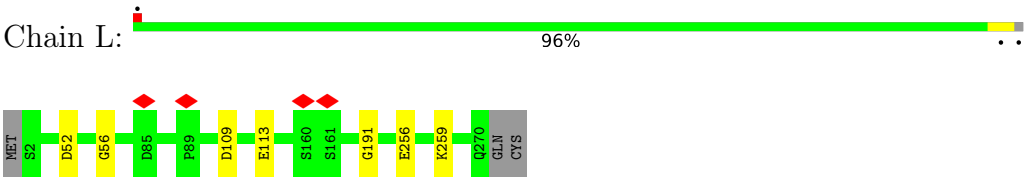
• Molecule 6: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K:



• Molecule 7: F-actin-capping protein subunit beta

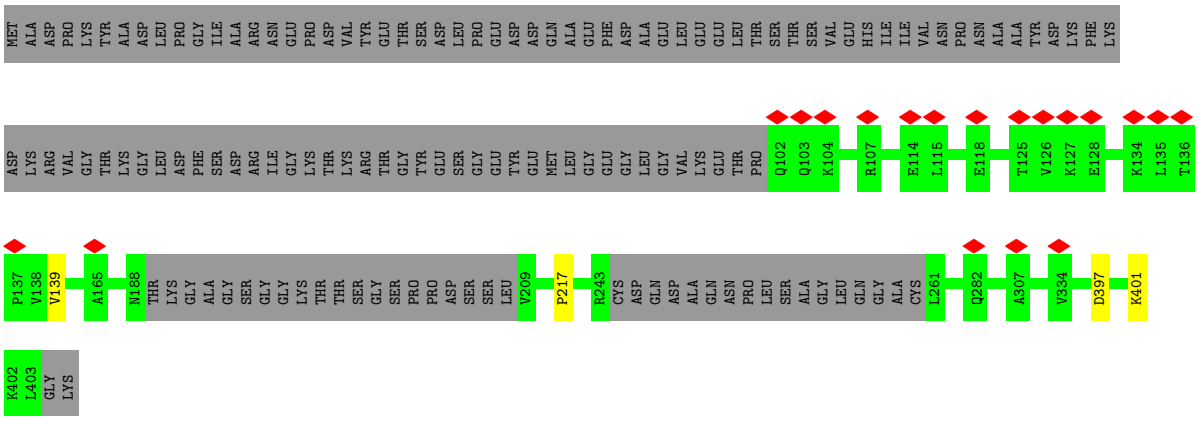
Chain L:



• Molecule 8: Dynactin subunit 2

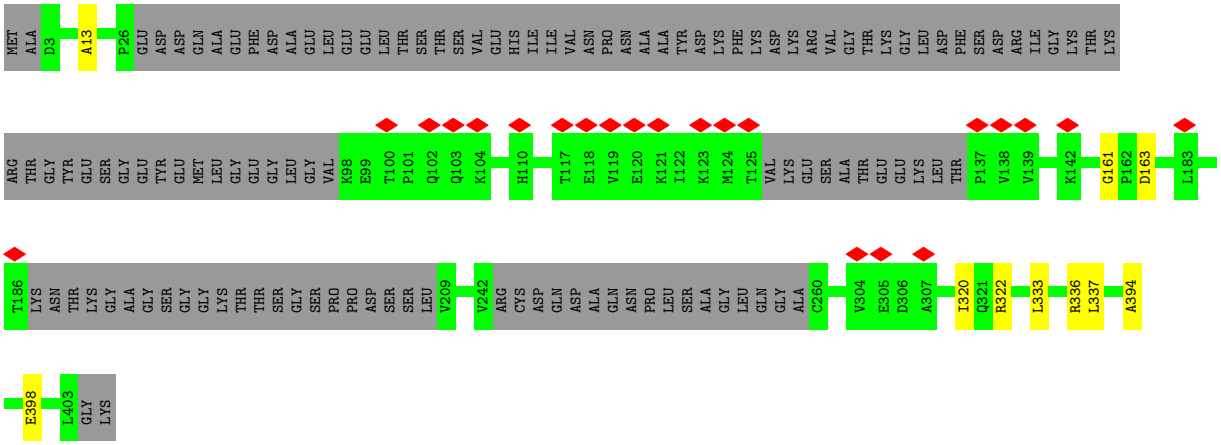
Chain M:



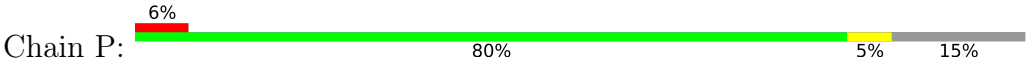


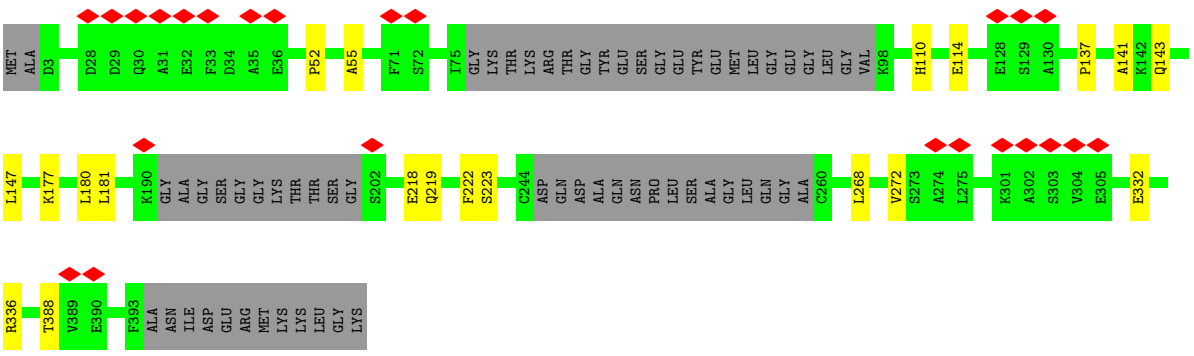
• Molecule 8: Dynactin subunit 2





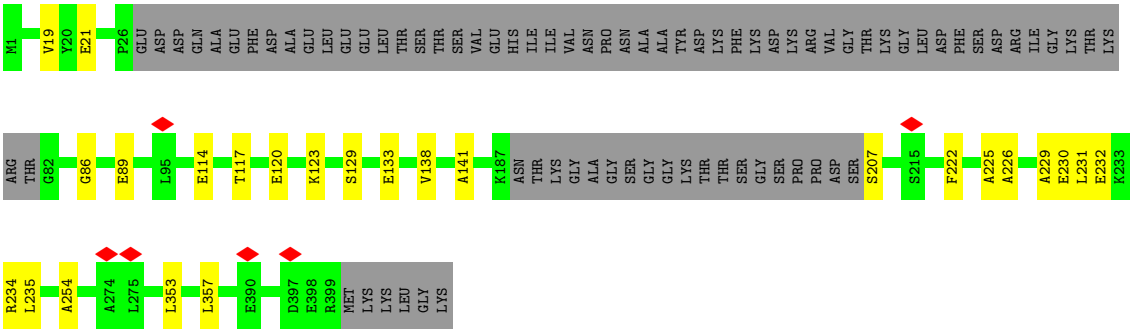
• Molecule 8: Dynactin subunit 2





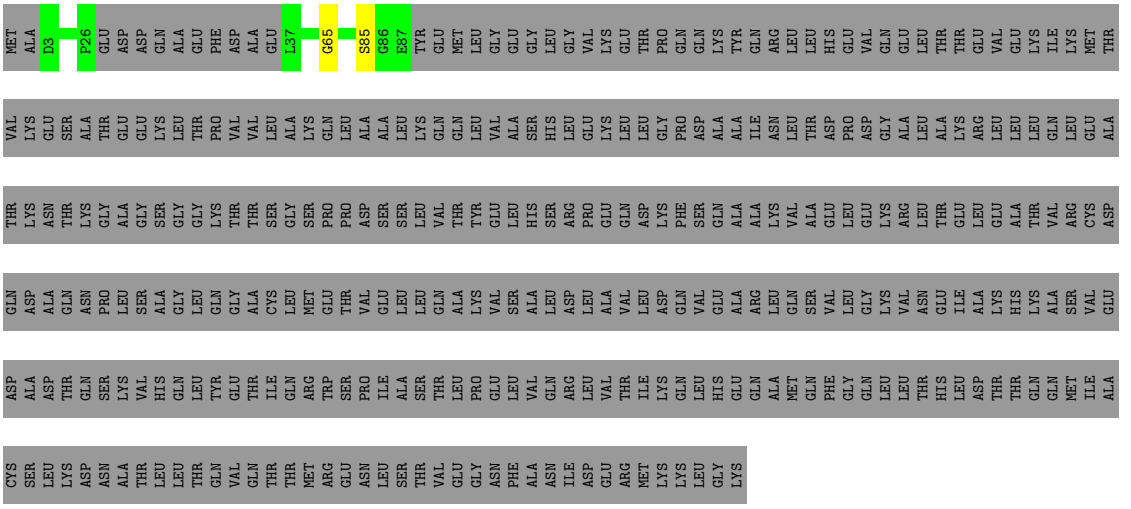
• Molecule 8: Dynactin subunit 2



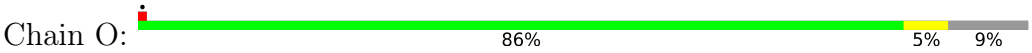


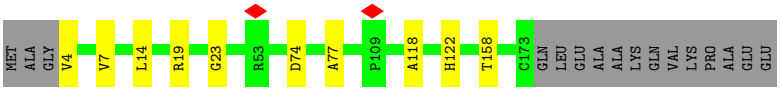
• Molecule 8: Dynactin subunit 2



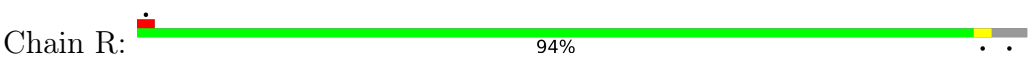


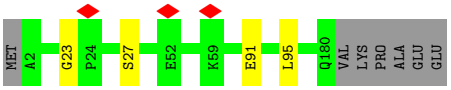
• Molecule 9: Dynactin subunit 3





• Molecule 9: Dynactin subunit 3





• Molecule 10: Dynactin 6

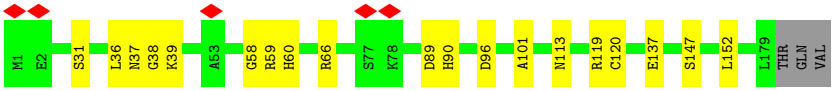




• Molecule 11: Dynactin subunit 5

Chain W:

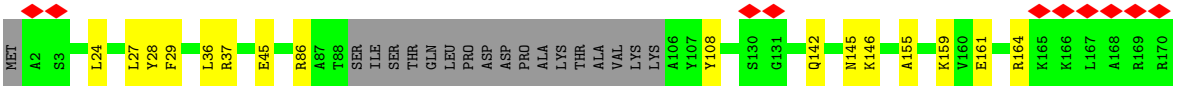


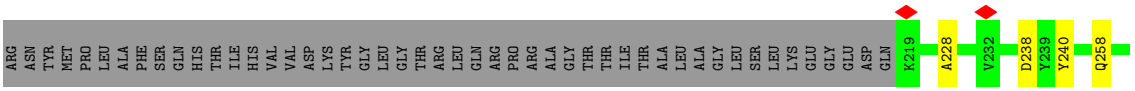


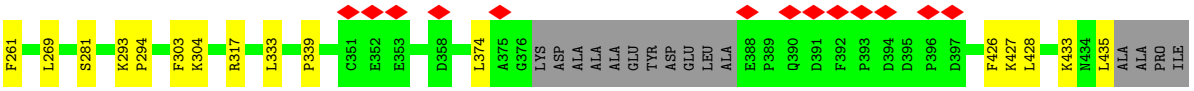
• Molecule 12: Dynactin subunit 4

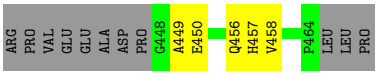
Chain Y:







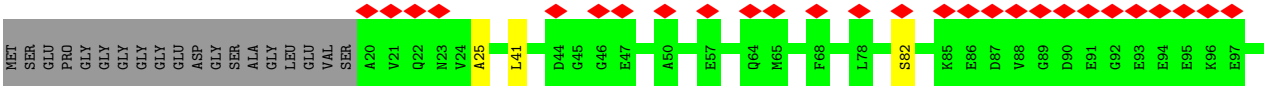


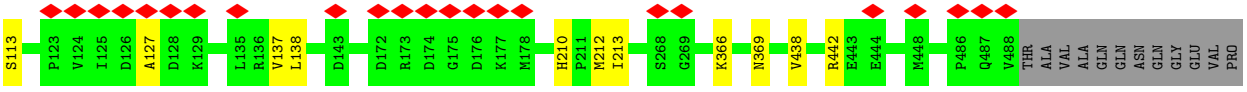


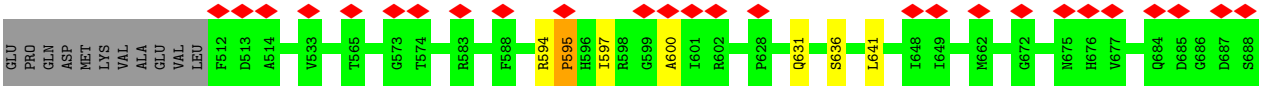
• Molecule 13: Cytoplasmic dynein 1 heavy chain 1

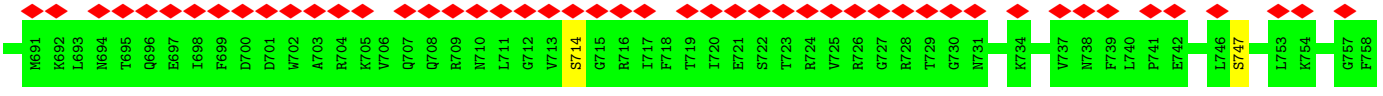
Chain e:

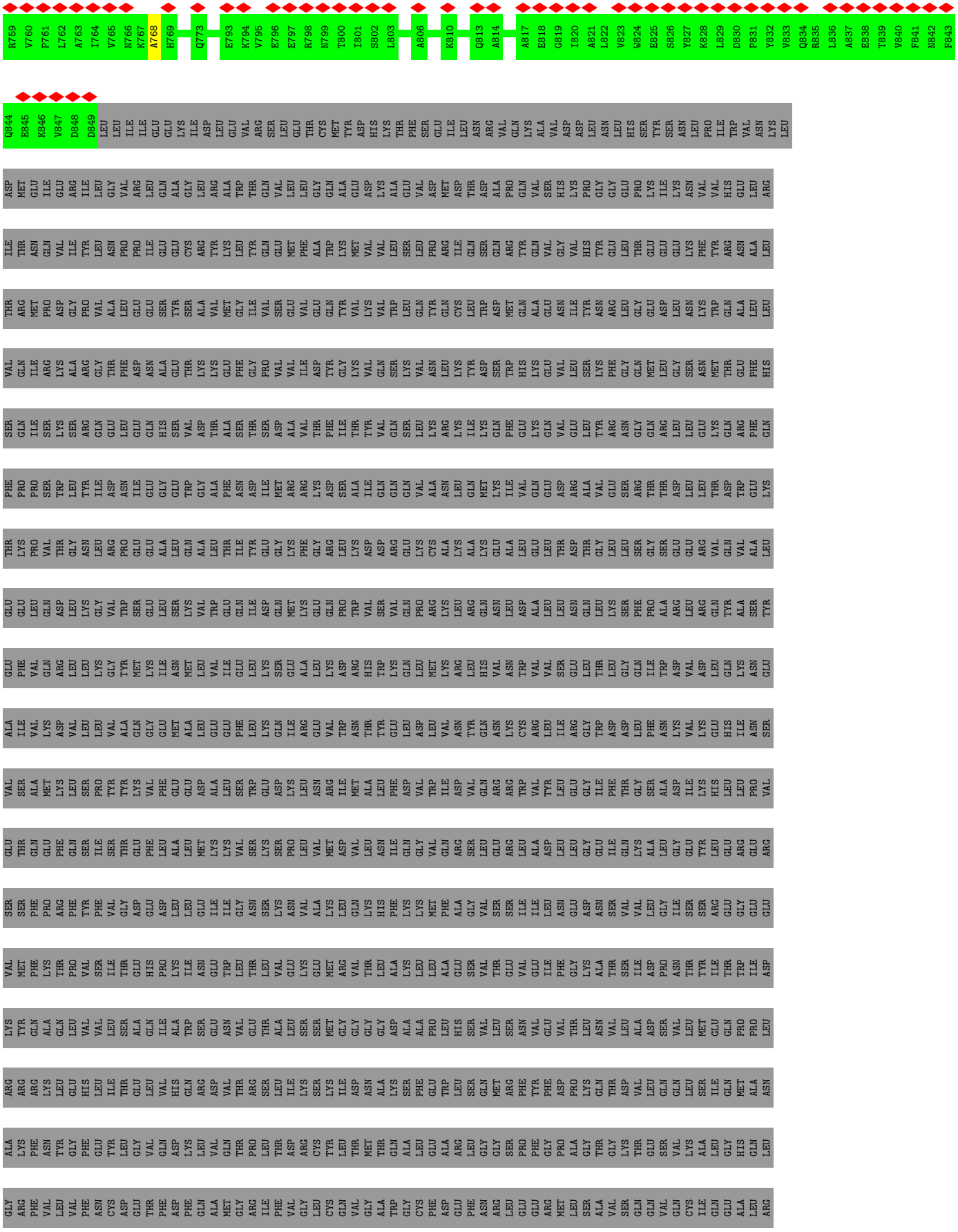


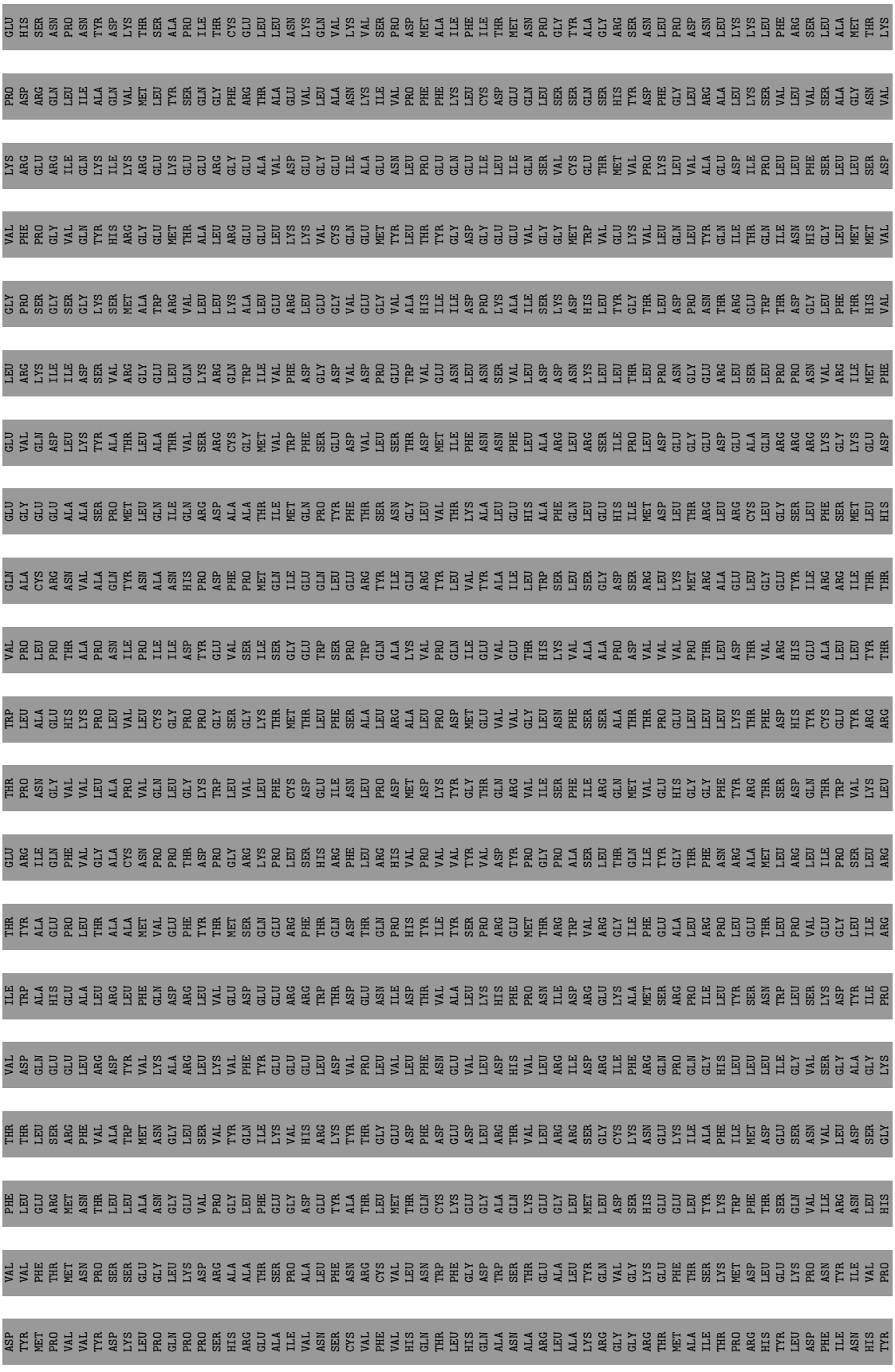


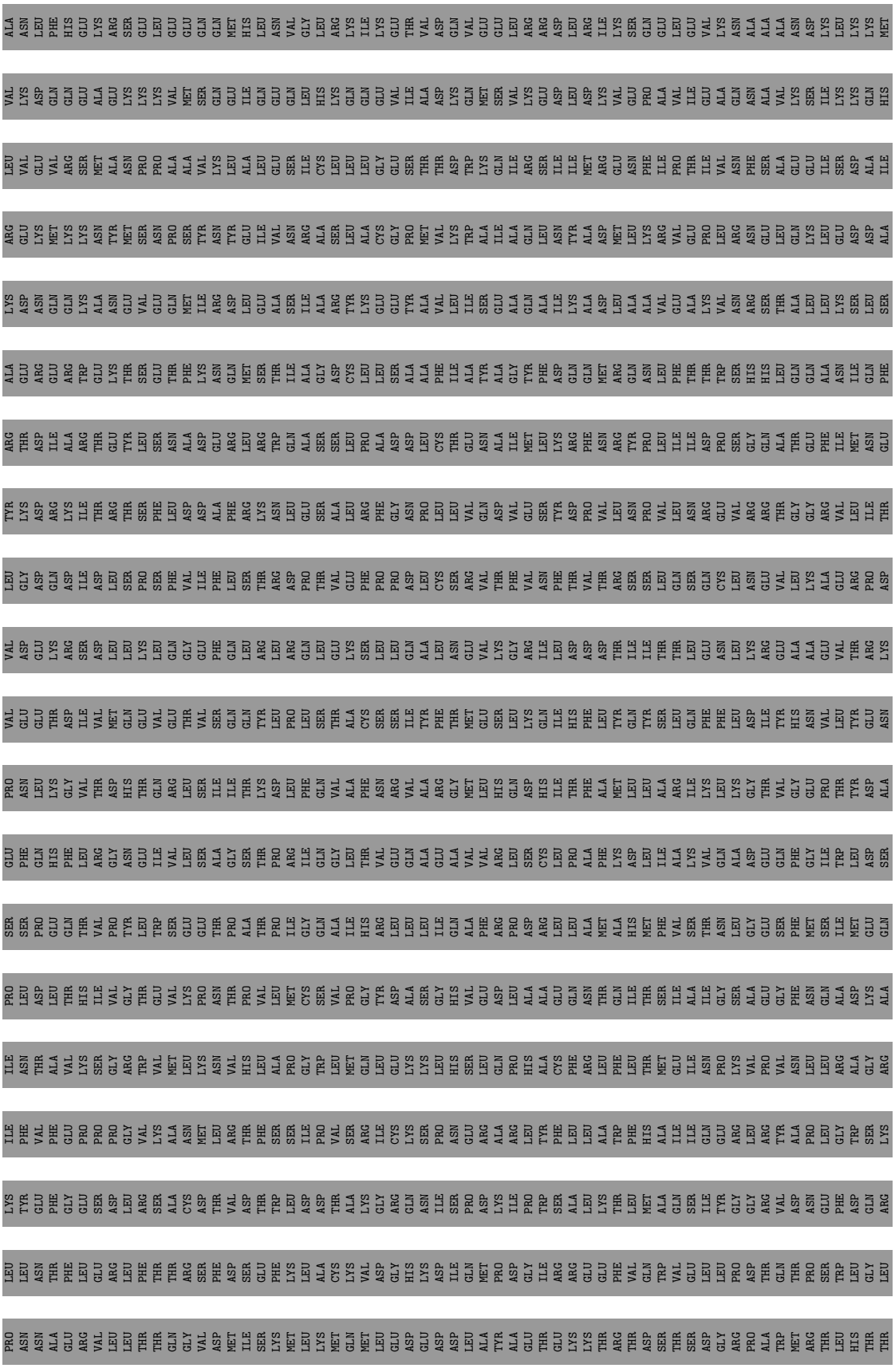


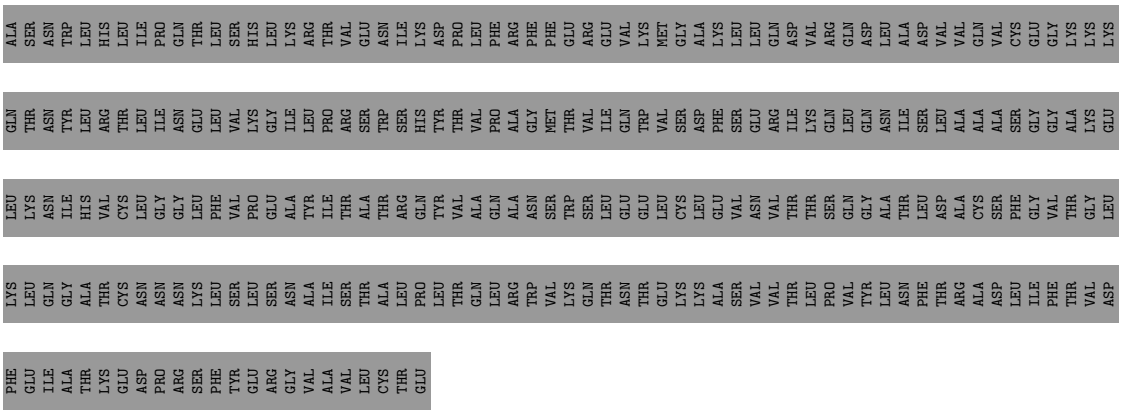





R759 V760 P761 L762 A763 I764 V765 N766 K767 A768 H769 Q773 E793 K794 V795 E796 E797 R798 N799 T800 I801 S802 L803 A806 K810 Q813 A814 A817 E818 G819 I820 A821 L822 V823 W824 E825 S826 Y827 K828 L829 D830 P831 Y832 V833 Q834 R835 L836 A837 E838 T839 V840 F841 N842 F843
Q844 E845 K846 V847 D848 D849 LEU LEU ILE ILE GLU GLU LYS ILE ASP LEU GLU VAL ARG SER LEU GLU LEU THR CYS MET TYR ASP HIS LYS THR PHE SER GLU ILE LEU ASN ARG VAL GLN LYS ALA VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN VAL VAL HIS GLU LEU ARG
ASP MET GLU ILE GLU ARG ILE LEU GLY VAL ARG LEU GLN GLN ALA GLY LEU ARG ALA TRP THR GLN VAL LEU LEU GLY GLN ALA GLU ASP LYS ALA GLU VAL ASP ASP MET ASP THR ASP ALA PRO GLN VAL ALA SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN LEU HIS SER TYR SER ASN LEU PRO ILE TRP VAL ASN LYS LEU
ILE THR ASN GLN VAL ILE TYR LEU ASN PRO PRO ILE GLU GLU CYS ARG TYR LYS LEU TYR GLN GLU MET PHE ALA TRP LYS MET VAL VAL LEU SER LEU SER GLN ARG TYR GLN VAL GLY VAL HIS TYR GLU LEU THR GLU GLU GLU LYS PHE TYR ARG ASN ALA LEU
THR ARG MET PRO ASP GLY PRO VAL ALA LEU GLU GLU SER TYR SER ALA VAL MET GLY ILE VAL SER GLU VAL GLU GLN TYR VAL LYS VAL TRP LEU GLN TYR GLN CYS LEU TRP ASP MET GLN ALA GLU ASN ILE TYR ASN ARG LEU GLY GLU ASP LEU ASN LYS TRP GLN ALA LEU LEU
VAL GLN ILE ARG LYS ALA ARG GLY THR PHE ASP ASN ALA GLU THR LYS LYS GLU PHE GLY PRO VAL VAL ILE ASP TYR GLY LYS VAL GLN SER LYS VAL ASN LEU LYS TYR ASP SER TRP HIS LYS GLU VAL LEU SER LYS PHE GLY GLN MET LEU GLY SER ASN MET THR GLU PHE HIS
SER GLN ILE SER LYS SER ARG GLN GLU LEU GLU GLN HIS SER VAL ASP THR ALA SER THR SER ASP ALA VAL THR PHE ILE THR TYR VAL GLN SER LEU LYS ARG LYS ILE LYS GLN PHE GLU LYS GLN VAL GLU LEU TYR ARG ASN GLY GLN ARG LEU GLU LEU GLU LYS GLN PHE
PHE PRO PRO SER TRP LEU TYR ILE ASP ASN ILE GLU GLY GLU TRP GLY ALA PHE ASN ASP ILE MET ARG ARG LYS ASP SER ALA ILE GLN GLN GLN VAL ALA ASN LEU GLN MET LYS ILE VAL GLN GLU ASP ARG ALA VAL GLU SER ARG THR THR ASP LEU LEU THR ASP TRP GLU LYS
THR LYS PRO VAL THR GLY ASN LEU ARG PRO GLU GLU ALA LEU GLN ALA LEU THR ILE TYR GLU GLY LYS PHE GLY ARG LEU LYS ASP ASP ARG GLU LYS CYS ALA LYS ALA LYS GLU ALA LEU GLU LEU GLU LEU THR ASP THR GLY LEU LEU SER GLY SER GLU GLU ARG VAL GLN VAL ALA LEU
GLU GLU LEU GLN ASP LEU LYS GLY VAL TRP SER GLU LEU SER LYS VAL TRP GLU GLN ILE ASP GLN MET LYS GLU GLN PRO TRP VAL SER VAL GLN PRO ARG LYS LEU ARG GLN ASN LEU ASP ALA LEU LEU ASN GLN LEU LYS SER PHE PRO ALA ARG LEU ARG GLN TYR ALA SER TYR
GLU PHE VAL GLN ARG LEU LEU LEU LYS GLY TYR MET LYS ILE ASN MET LEU VAL ILE GLU LEU LEU LYS SER GLU ALA LEU LYS ASP ARG HIS TRP LYS GLN LEU MET LYS LYS ARG LEU HIS VAL ASN TRP VAL SER GLU LEU THR LEU GLY GLN ILE TRP ASP VAL ASP LEU GLN LEU GLU
ALA ILE VAL LYS ASP VAL LEU LEU VAL ALA GLN GLY GLU MET ALA LEU GLU GLU GLU PHE LEU LEU LYS GLN ILE ARG GLU VAL TRP ASN THR TYR GLU LEU ASP VAL LYS ASP LEU VAL ASN TYR GLN ASN LYS CYS ARG LEU ILE ARG GLY TRP ASP ASP LEU GLU LEU PHE ASP LYS VAL LYS GLU HIS ILE ASN SER
VAL SER ALA MET LYS LEU SER PRO TYR TYR LYS VAL PHE GLU GLU ASP ALA LEU SER TRP GLU ASP LYS LEU ASN ARG ILE MET ALA LEU PHE ASP VAL TRP ILE ASP VAL GLN ARG ARG TRP VAL TYR LEU LEU GLU GLY ILE PHE THR GLY SER ALA ASP ILE LYS HIS LEU LEU PRO VAL
GLU THR GLN GLU PHE GLN SER THR GLU PHE LEU ALA LEU MET LYS LYS VAL SER LYS SER PRO LEU VAL MET ASP VAL THR ASN ILE GLN GLY VAL GLN ARG SER LEU GLU ARG LEU LEU ALA ASP LEU LEU GLY GLU ILE GLN LYS ALA LEU GLY GLU TYR LEU GLU LEU GLU ARG GLU
SER SER PHE PRO ARG PHE TYR PHE VAL GLY ASP GLU ASP LEU LEU GLU ILE ILE GLY ASN SER LYS ASN VAL ALA LYS LEU GLN LYS HIS PHE LYS LYS MET PHE ALA GLY VAL SER LEU GLU ILE LEU ASN GLU ASP ASN SER VAL LEU ILE SER SER ARG GLU LEU GLY GLU
VAL MET PHE LYS THR PRO VAL SER ILE THR GLU HIS PRO LYS ILE ASN GLU TRP LEU THR LEU VAL GLU LYS GLU MET ARG VAL THR LEU ALA LYS LYS LEU LEU ALA GLU SER VAL THR GLU VAL GLU ILE PHE GLY LYS ALA THR SER ILE GLN LYS ALA ASP PRO ASN THR TYR ILE THR TRP ILE ASP
LYS TYR GLN ALA GLN LEU VAL VAL LEU SER ALA GLN ILE ALA TRP SER GLU GLU ASN VAL LEU SER SER MET GLY GLY GLY GLY ASP ALA ALA ALA PRO LEU HIS SER VAL LEU SER ASN VAL GLU VAL LEU ALA ASP SER VAL LEU MET GLU GLN PRO PRO LEU
ARG ARG ARG LYS LEU GLU ILE THR GLU LEU VAL HIS GLN ARG ASP VAL THR ARG SER LEU ILE LYS SER LYS ILE ASP ASN ALA LYS SER PHE GLU TRP LEU SER GLN MET ARG PHE TYR PHE ASP PRO LYS GLN THR ASP VAL ILE SER GLN ILE GLN LEU ASN ALA
ALA LYS PHE ASN TYR GLY LEU GLN VAL THR PRO LEU THR ASP ARG CYS TYR LEU THR MET THR GLN ALA LEU GLU ALA ARG LEU GLY GLY SER PRO PHE GLY PRO ALA GLY THR GLY LYS THR ALA LEU VAL LYS ALA LEU GLY HIS GLN LEU
GLY ARG PHE VAL LEU VAL PHE ASP GLU THR PHE ASP PHE VAL GLY LEU CYS GLN VAL GLY ALA TRP GLY CYS PHE ASP GLU PHE ASN ARG LEU GLU GLU ARG MET LEU SER ALA VAL SER GLN GLN VAL GLN CYS ILE GLN GLU ALA LEU ARG


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

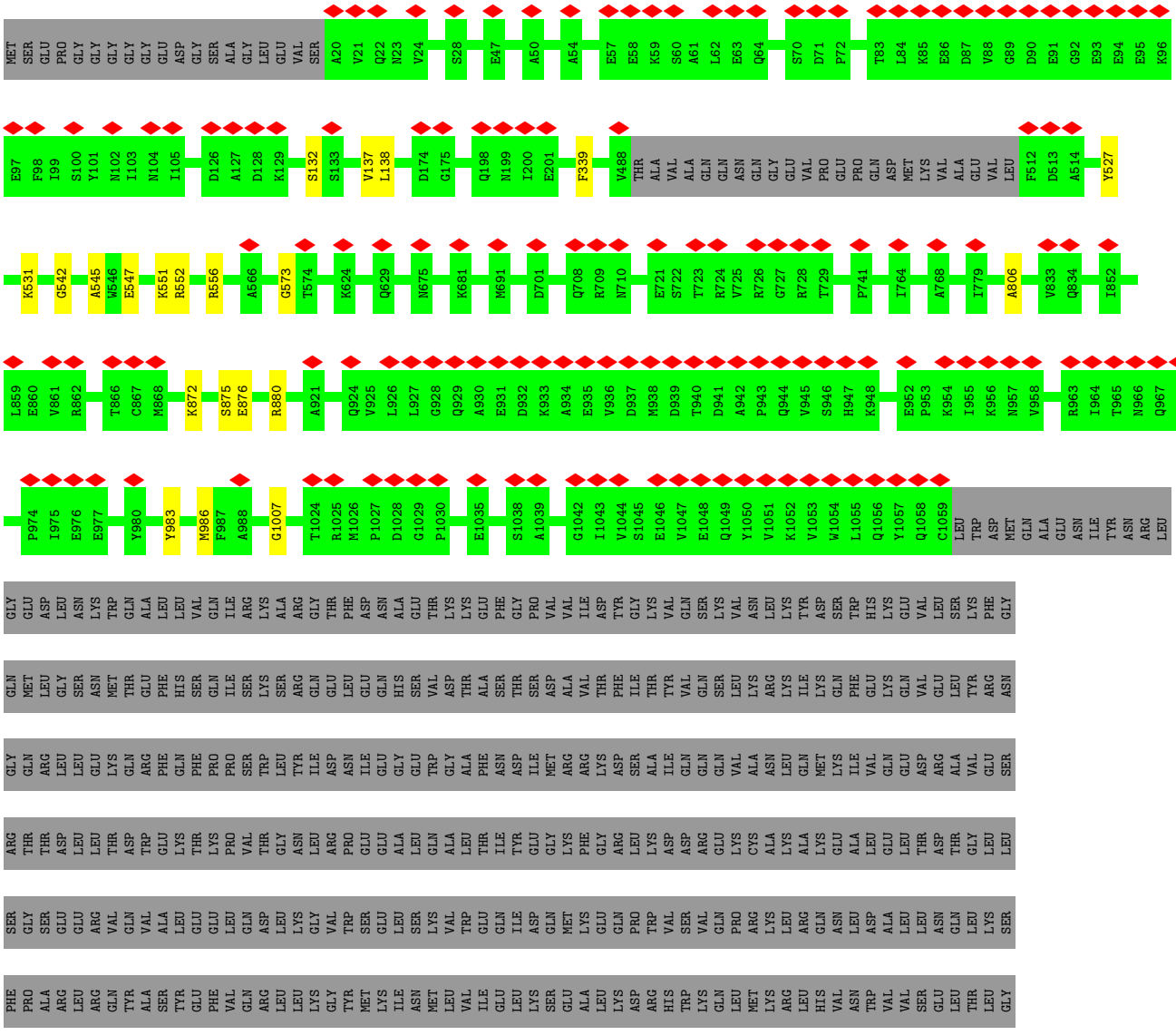

ALA ASN LEU PHE HIS GLU LYS ARG SER GLU LEU GLU GLU GLN GLN MET HIS LEU ASN VAL GLY LEU ARG LYS ILE LYS SER GLN GLU GLU VAL LYS ASP GLN VAL GLU GLU LEU ARG ARG ASP LEU ARG ILE LYS SER GLN GLU LEU VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS VAL MET SER GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN GLN GLU GLU VAL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

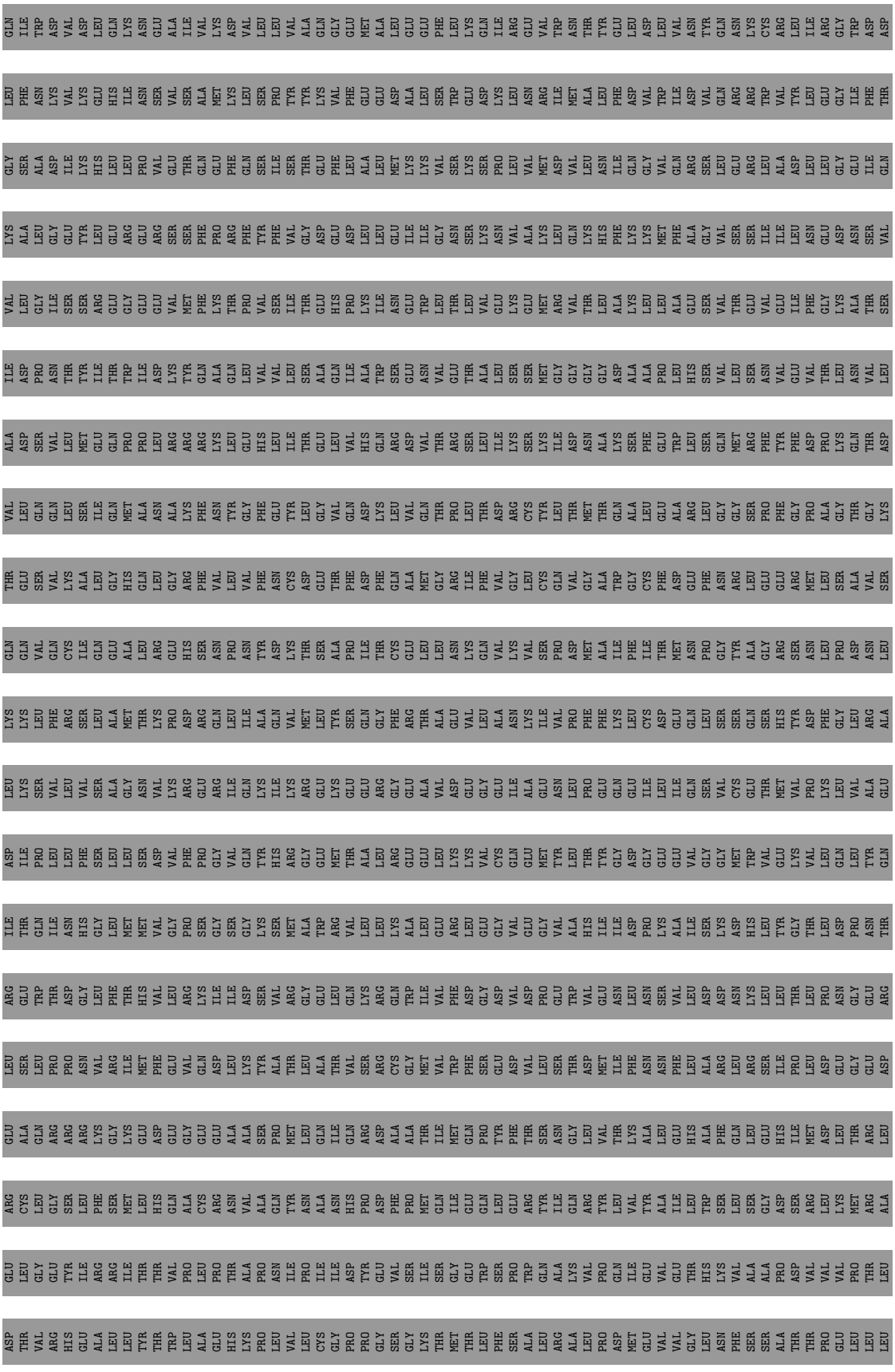


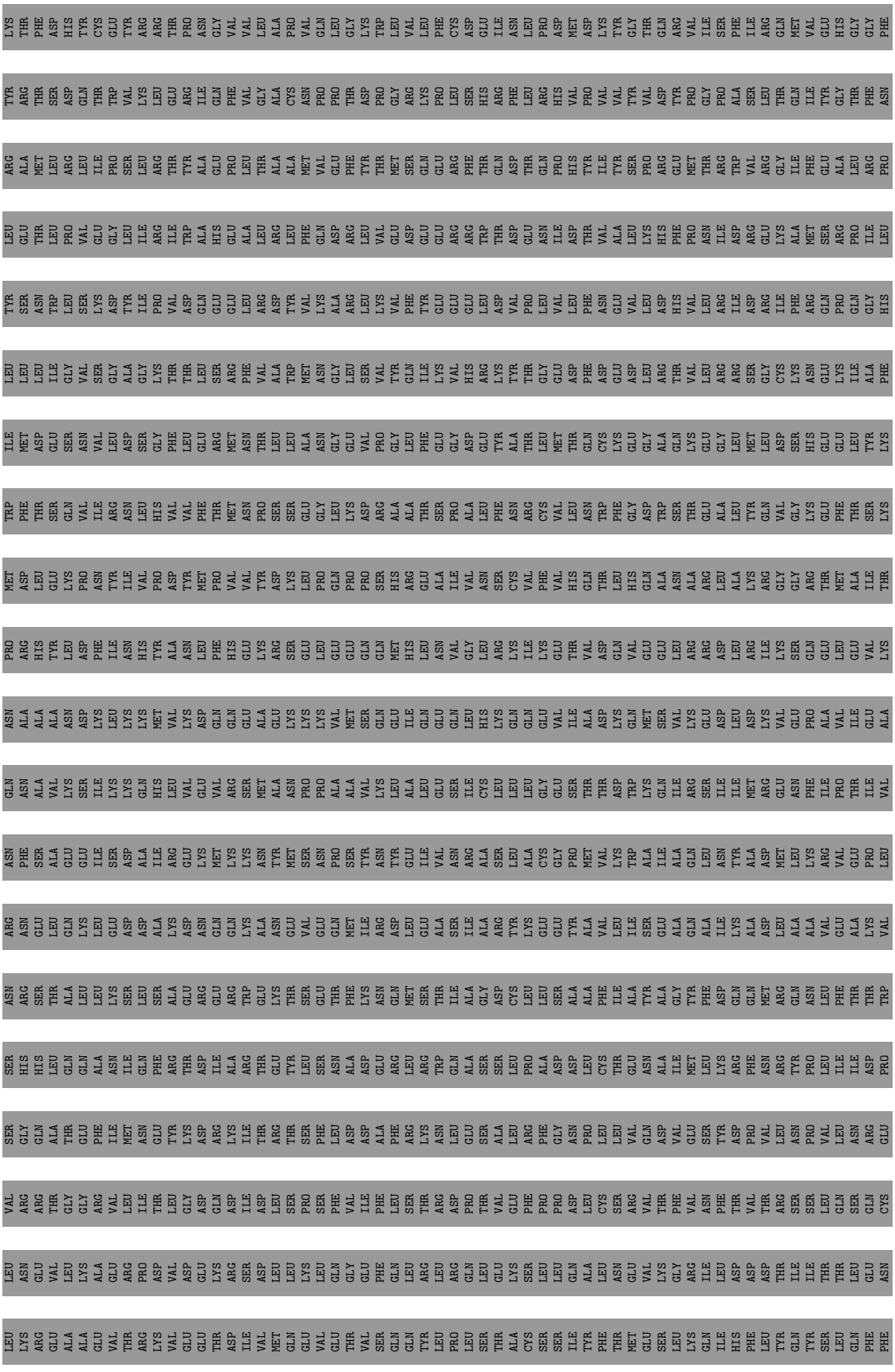
• Molecule 13: Cytoplasmic dynein 1 heavy chain 1

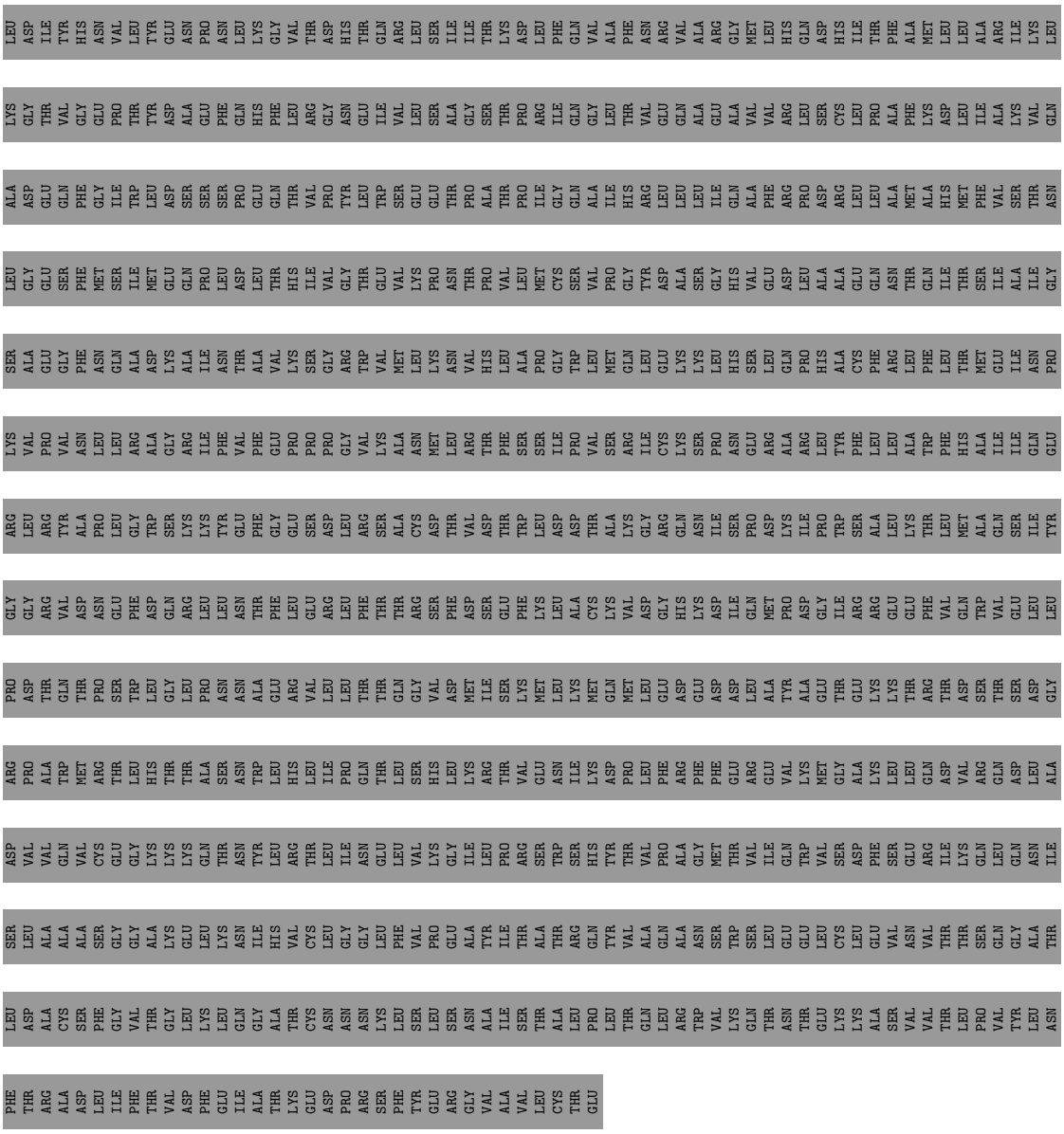
Chain f:






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

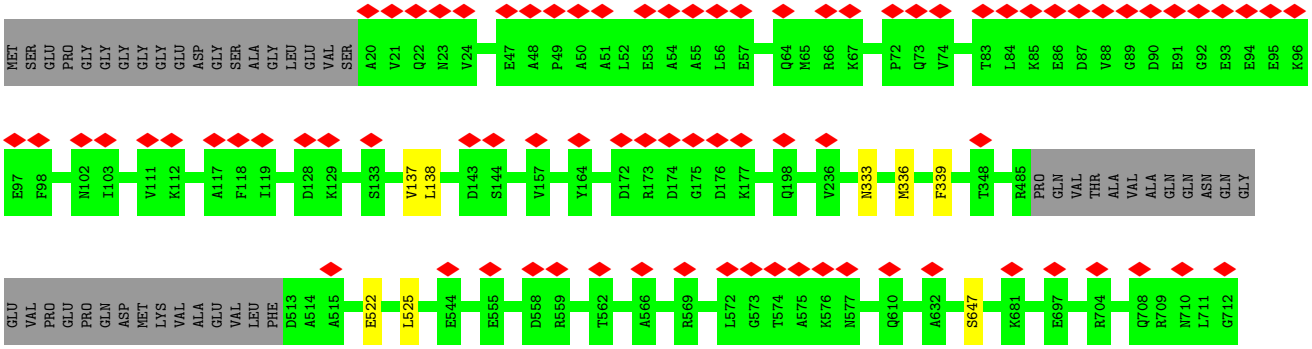

LYS THR PHE ASP HIS TYR CYS GLU TYR ARG ARG THR PRO ASN GLY VAL VAL LEU ALA PRO VAL GLN LEU GLY LYS TRP LEU VAL LEU PHE CYS ASP GLU ILE ASN LEU PRO ASP MET ASP LYS TYR GLY THR GLN ARG VAL ILE SER PHE ILE ARG GLN MET VAL GLU HIS GLY GLY PHE
TYR ARG THR SER ASP GLN THR TRP VAL LYS LEU GLU ARG ILE GLN PHE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

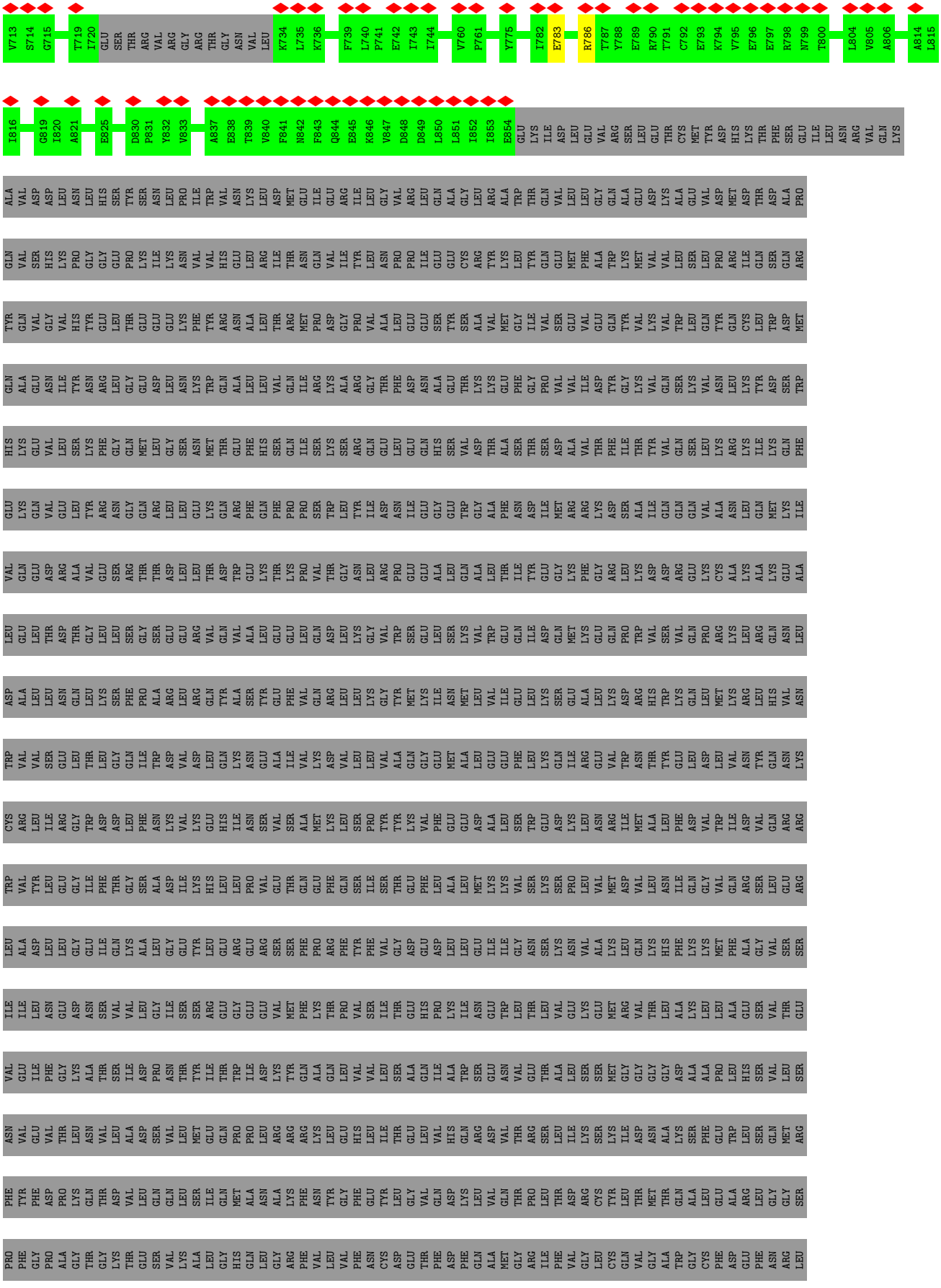


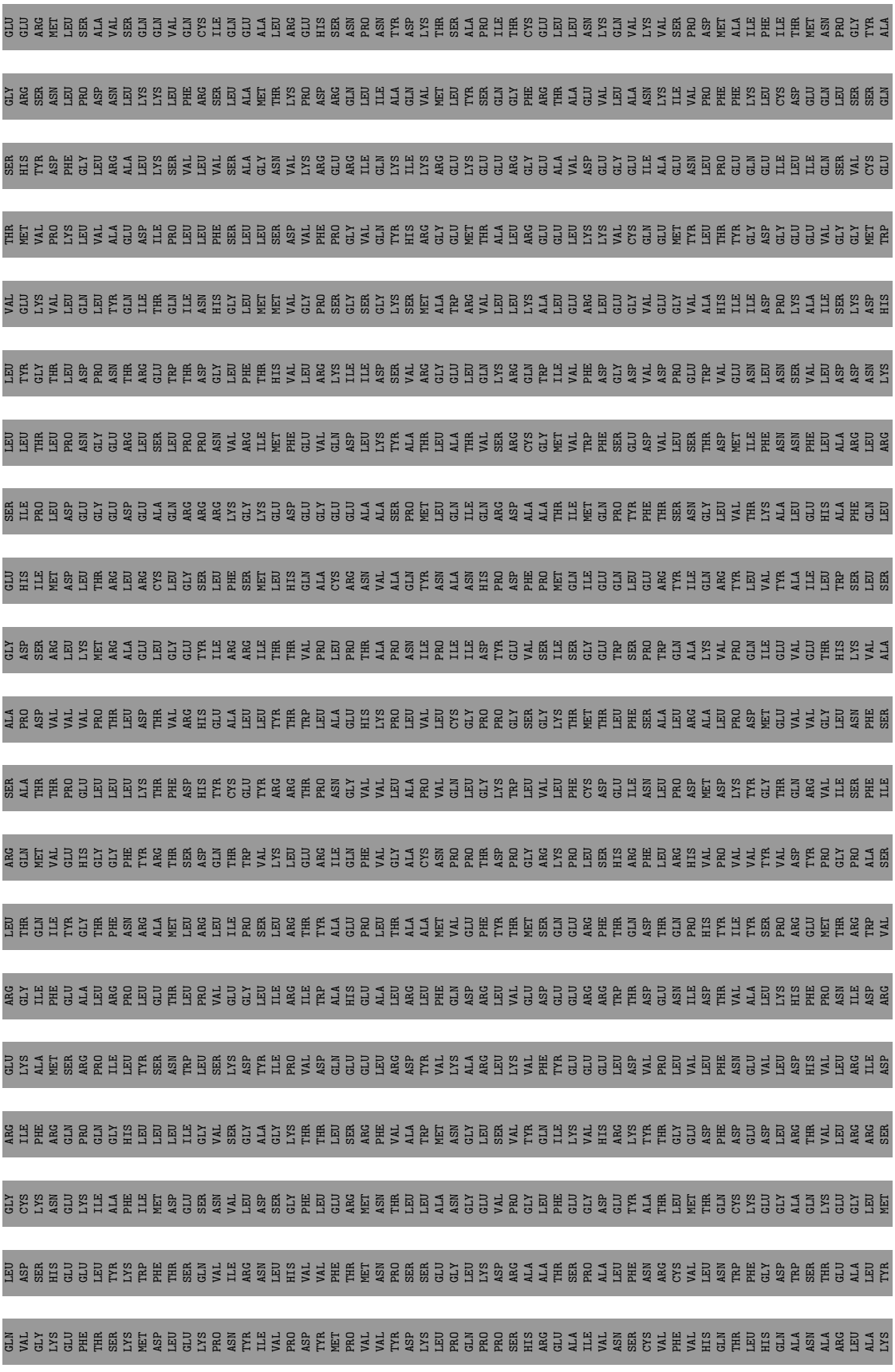
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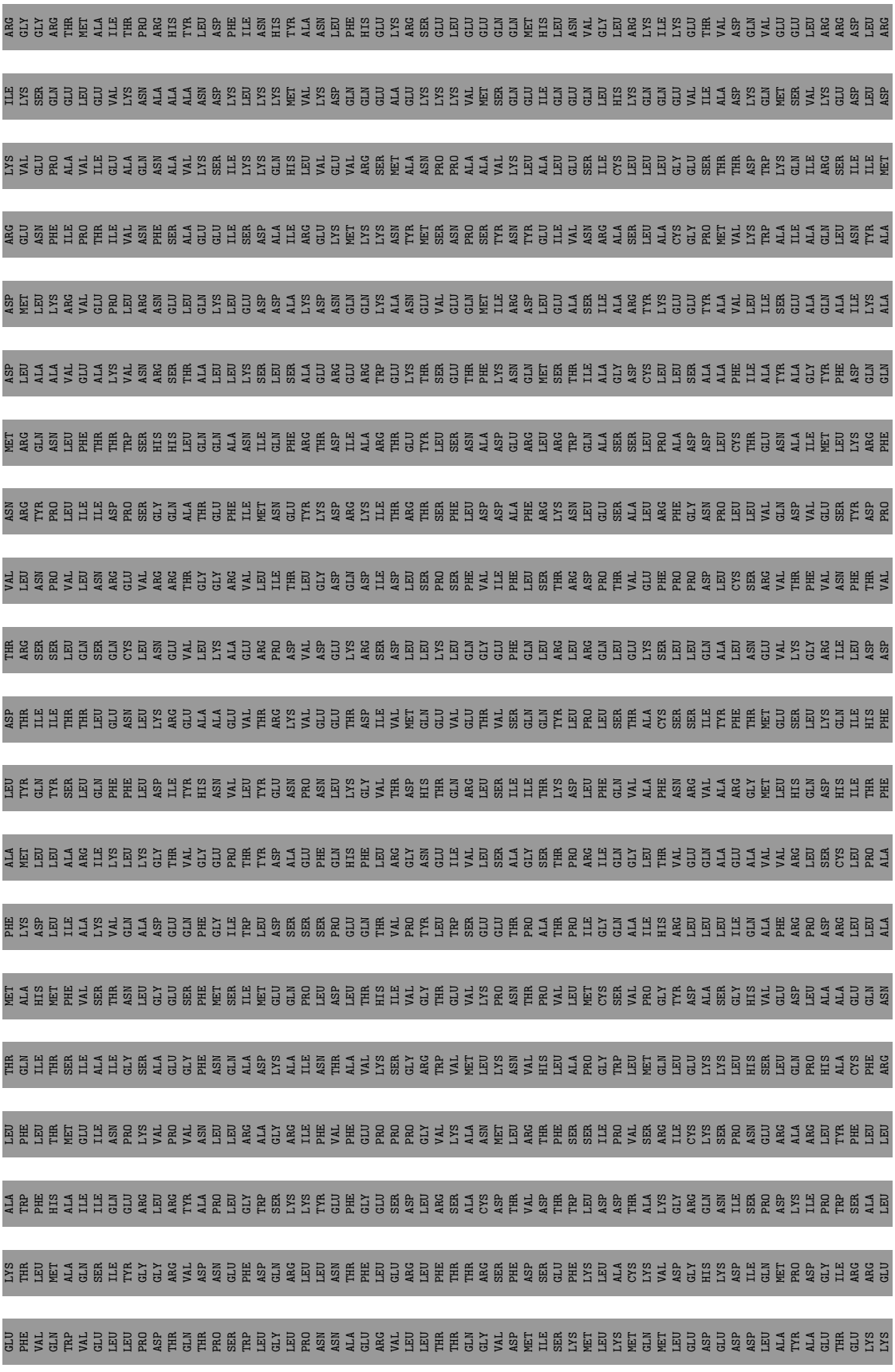
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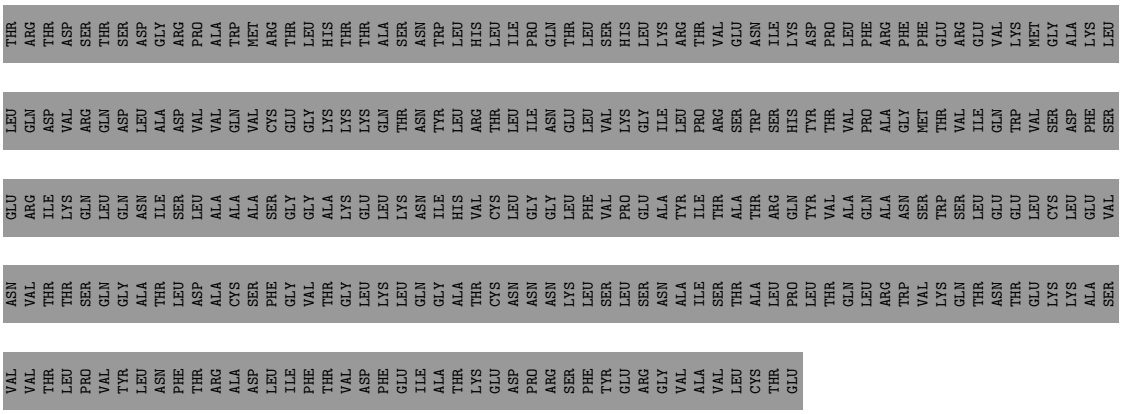





V713 S714 G715 T719 I720 GLU SER THR ARG VAL ARG GLY ARG THR GLY ASN VAL LEU K734 L735 K736 F739 L740 P741 E742 I743 I744 V760 P761 Y775 I782 E783 R786 T787 Y788 E789 R790 T791 C792 E793 K794 V795 E796 E797 R798 N799 T800 L804 V805 A806 A814 L815
I816 G819 I820 A821 E825 D830 P831 Y832 V833 A837 E838 T839 V840 F841 N842 F843 Q844 E845 K846 V847 D848 D849 L850 L851 I852 I853 E854 GLU LYS ILE ASP LEU GLU VAL ARG SER LEU GLU GLY GLN ALA GLU ASP LYS ALA GLU VAL ASP MET ASP SER GLU ILE LEU ASN ARG VAL GLN LYS
ALA VAL ASP ASP LEU ASN LEU HIS SER TYR SER ASN LEU PRO ILE TRP VAL ASN LYS LEU ASP MET GLU ILE GLU ARG ILE LEU GLY VAL ASP ARG ALA TRP THR GLN VAL LEU LEU GLU GLY GLN ALA GLU ASP LYS ALA GLU VAL ASP MET ASP SER GLU ILE LEU ASN ARG VAL GLN LYS
GLN VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN VAL VAL HIS GLU LEU ARG ILE THR ASN GLN VAL ILE TYR LEU ASN PRO PRO ILE GLU GLU CYS ARG TYR LYS LEU TYR GLN GLU MET PHE ALA TRP LYS MET VAL VAL LEU SER LEU LEU PRO ARG ILE GLN SER GLN ARG
TYR GLN VAL GLY VAL HIS TYR GLU LEU THR GLU GLU GLU GLU LYS PHE TYR ARG ASN ASN ALA LEU THR ARG MET PRO ASP GLY PRO VAL ALA ALA LEU GLU GLU SER TYR SER ALA VAL MET GLY ILE GLU VAL SER GLU VAL GLU GLN TYR VAL LYS VAL TRP LEU GLN TYR GLN CYS LEU TRP ASP MET
GLN ALA GLU ASN ILE TYR ASN ARG LEU GLY GLU ASP LEU ASN LYS TRP GLN ALA LEU LEU VAL GLN ILE ILE ARG LYS ALA ARG GLY THR PHE ASP ASN ALA GLU THR LYS LYS GLU PHE GLY PRO VAL VAL ILE ASP TYR GLY LYS VAL GLN SER LYS VAL VAL ASN LEU LYS TYR ASP SER TRP
HIS LYS GLU VAL LEU SER LYS PHE GLY GLN MET LEU GLY SER ASN MET THR GLU PHE HIS SER GLN ILE SER LYS SER ARG GLN GLU LEU GLU ILE GLN HIS SER VAL ASP THR ALA SER THR SER ASP ALA VAL THR PHE ILE THR TYR VAL GLN SER LEU LEU LYS ARG LYS ILE LYS GLN PHE
GLU LYS GLN VAL GLU LEU TYR ARG ASN GLY GLN ARG LEU GLU LYS GLN ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ASN ILE GLU GLY GLU TRP GLY ALA PHE ASN ASP ILE MET ARG ARG LYS ASP SER ALA ILE GLN GLN GLN VAL LYS ILE
VAL GLN GLU ASP ARG ALA VAL GLU SER ARG THR THR ASP LEU LEU THR ASP TRP GLU LYS THR LYS PRO VAL THR GLY ASN LEU ARG PRO GLU GLU ALA LEU GLN ALA ALA LEU THR ILE TYR GLU GLY LYS PHE GLY ARG LEU LYS ASP ASP ARG GLU LYS CYS ALA LYS ALA LYS GLU ALA
LEU GLU LEU THR ASP GLY SER GLY SER GLU GLU ARG VAL GLN VAL ALA LEU GLU GLU LEU GLN ASP LEU LYS GLY VAL TRP SER GLU LEU SER LYS VAL TRP GLU GLN ILE ASP GLN MET LYS GLU GLN PRO TRP VAL SER VAL GLN PRO ARG LYS LEU ARG GLN ASN LEU
ASP ALA LEU LEU ASN GLN LEU LYS SER PHE PRO ALA ARG LEU ARG GLN TYR ALA SER TYR GLU PHE VAL GLN ARG LEU LEU LYS GLY GLY TYR MET LYS ILE ASN MET LEU VAL ILE GLU LEU LYS SER GLU ALA LEU LYS ASP ASP ARG HIS TRP TRP LYS GLU ALA LEU ARG GLN ASN VAL
TRP VAL VAL SER GLU LEU THR LEU GLY GLN ILE TRP ASP VAL LEU LEU LEU ALA GLN GLY GLU MET ALA LEU GLU GLU PHE LEU LYS GLN ILE ARG GLU VAL TRP ASN THR TYR GLU LEU ASP VAL LEU ASP VAL LEU GLN LYS HIS TRP TYR LYS GLU ASN TYR GLN ASN ASN LYS
CYS ARG LEU ILE ARG GLY TRP ASP ASP LEU PHE ASN LYS VAL LYS GLU HIS ILE ASN SER VAL SER ALA MET LYS LEU SER PRO TYR TYR LYS VAL PHE GLU GLU ASP ALA LEU SER TRP GLU ASP LYS LEU ASN ARG ILE MET ALA LEU PHE ASP VAL TRP ILE ASP VAL GLN ARG ARG
TRP VAL TYR LEU GLU GLY SER ALA ASP ILE LYS HIS LEU LEU PRO VAL GLU THR GLN GLU PHE PHE THR GLY SER ILE SER THR GLU PHE LEU ALA LEU GLU MET LYS LYS VAL SER LYS SER PRO LEU VAL MET ASP VAL LEU ASN ILE HIS LEU VAL GLN GLY VAL GLN ARG
LEU ALA ASP LEU LEU GLU ILE GLN LYS ALA LEU GLY GLU ARG SER SER PHE PRO ARG PHE TYR PHE VAL GLY ASP GLU ASP LEU LEU GLU ILE ILE GLY ASN SER LYS ASN VAL ALA LYS LEU GLN LYS HIS PHE LYS LYS MET PHE ALA GLY VAL SER SER
ILE ILE LEU ASN GLU ASP ASN SER VAL VAL ASP ARG GLU GLY GLU SER VAL SER ILE THR GLU HIS PRO LYS ILE ASN GLU TRP LEU THR LEU LEU VAL GLU LYS MET ARG VAL THR LEU GLU HIS ALA LYS LEU LEU ALA GLU SER VAL THR GLU
VAL GLU ILE PHE GLY LYS ALA THR SER ILE ASP PRO GLN ILE THR TRP SER ALA GLN LEU VAL SER ILE LEU SER ALA GLN ILE ASP GLU TRP SER GLU ASN VAL GLU THR ALA LEU SER SER MET GLY GLY GLY GLY ASP ALA ALA ALA PRO LEU HIS SER VAL LEU SER
ASN VAL GLU VAL THR LEU ALA ASP SER VAL LEU MET GLU GLN PRO PRO LEU ARG ARG LYS LEU GLU HIS GLN ARG ASP VAL THR ARG SER LEU ILE LYS SER LYS ILE ASP ASN ALA LYS SER PHE GLU TRP LEU SER GLN MET ARG
PHE TYR PHE ASP PRO LYS GLN THR GLY GLN LEU ILE GLN LEU GLN MET ALA ASN ALA LYS PHE ASN TYR GLY PHE GLU TYR LEU GLY VAL GLN GLN LEU ASP LYS PHE GLU TYR LEU THR ASP ARG CYS TYR LEU THR MET THR GLN ALA GLN LEU GLY GLU ALA ARG LEU GLY GLY SER
PRO PHE GLY PRO ALA GLY LYS THR GLY GLU HIS GLN LEU GLY ARG PHE VAL LEU VAL PHE ASN CYS ASP GLU THR PHE ASP PHE GLN ALA MET GLY ARG ILE PHE VAL GLY LEU CYS GLN VAL GLY ALA TRP GLY CYS PHE ASP GLU PHE ASN ARG LEU

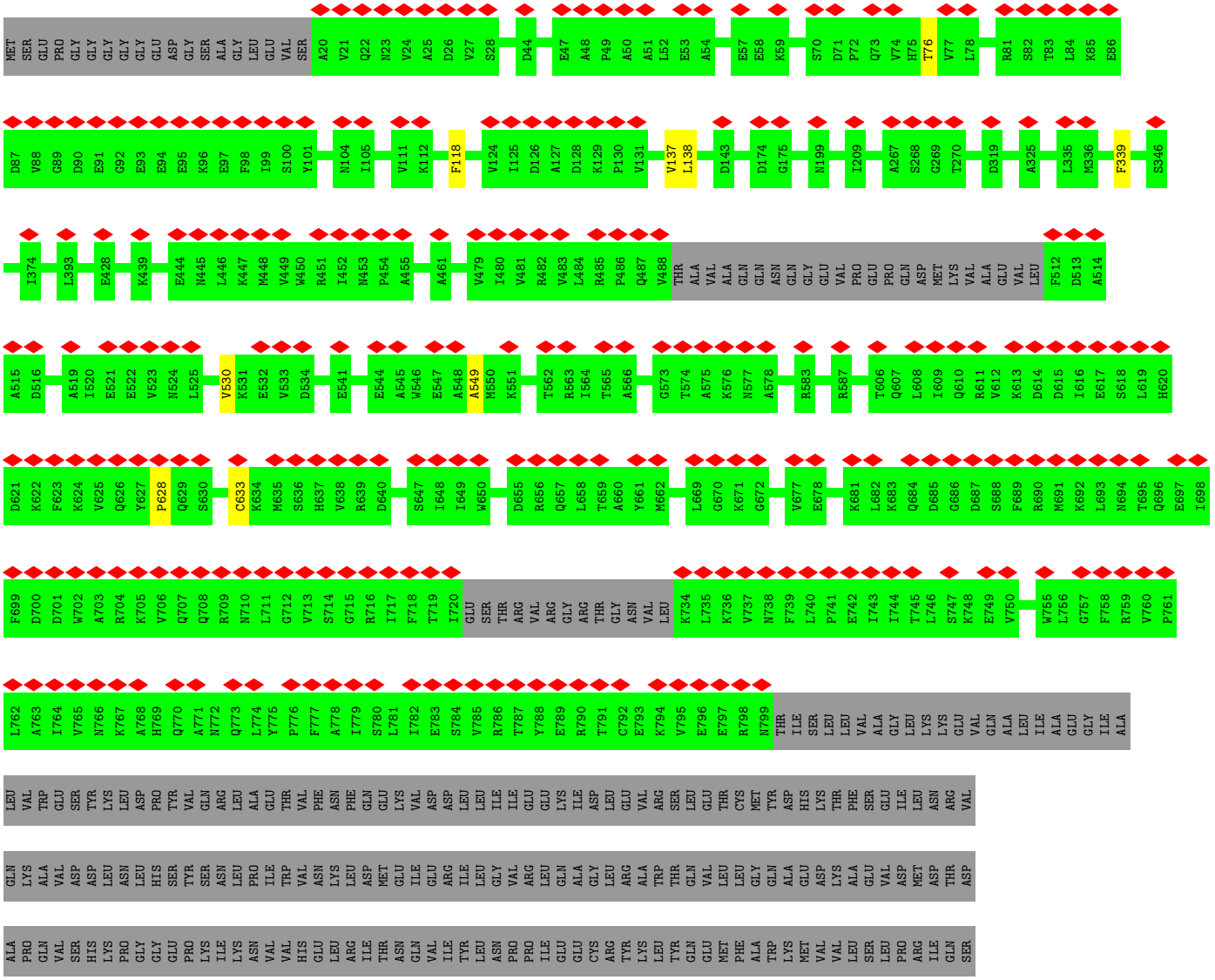

GLU GLU ARG MET LEU SER ALA VAL SER GLN GLN VAL GLN CYS ILE GLN GLU ALA LEU ARG GLU HIS SER ASN PRO ASN TYR ASP THR SER ALA PRO ILE THR CYS GLU LEU LEU ASN LYS GLN VAL LYS VAL SER PRO ASP MET ALA ILE PHE ILE THR MET ASN PRO GLY TYR ALA
GLY ARG SER ASN LEU PRO ASP ASN LEU LYS LYS LEU PHE ARG SER LEU ALA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


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



• Molecule 13: Cytoplasmic dynein 1 heavy chain 1

Chain n: 6% 16% 84%



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

LEU ARG ILE LYS SER GLN GLU VAL LYS ASN ALA ALA ALA ASN ASP LYS LEU LYS LYS MET VAL LYS ASP GLN GLN GLU ALA GLU LYS LYS LYS VAL MET SER GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN ILE ALA ASP LYS GLN MET SER VAL LYS GLU

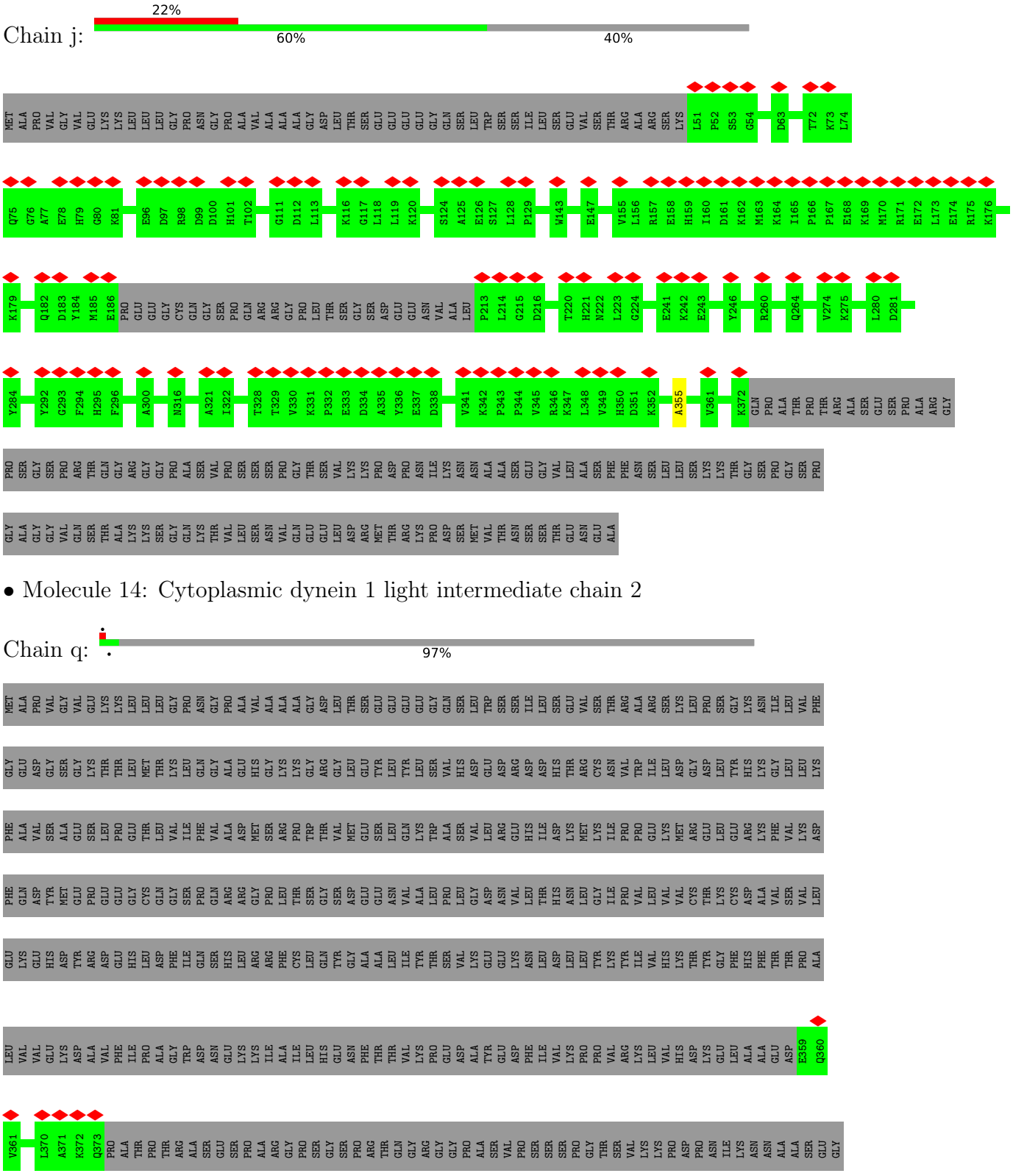
LEU ASP LYS VAL GLU PRO ALA ALA VAL ILE CYS LEU LEU GLU SER ILE LEU GLU GLU SER ILE LYS LYS LEU ALA GLU LEU GLU VAL LYS LEU ILE ARG SER ILE

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



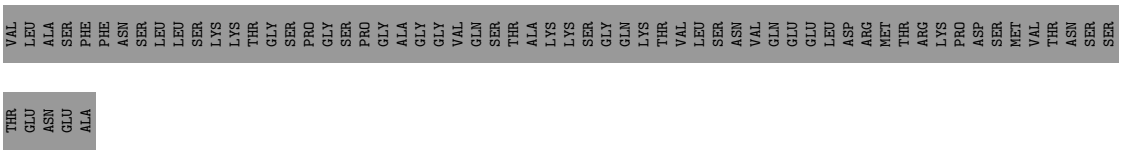
• Molecule 14: Cytoplasmic dynein 1 light intermediate chain 2

Chain j:



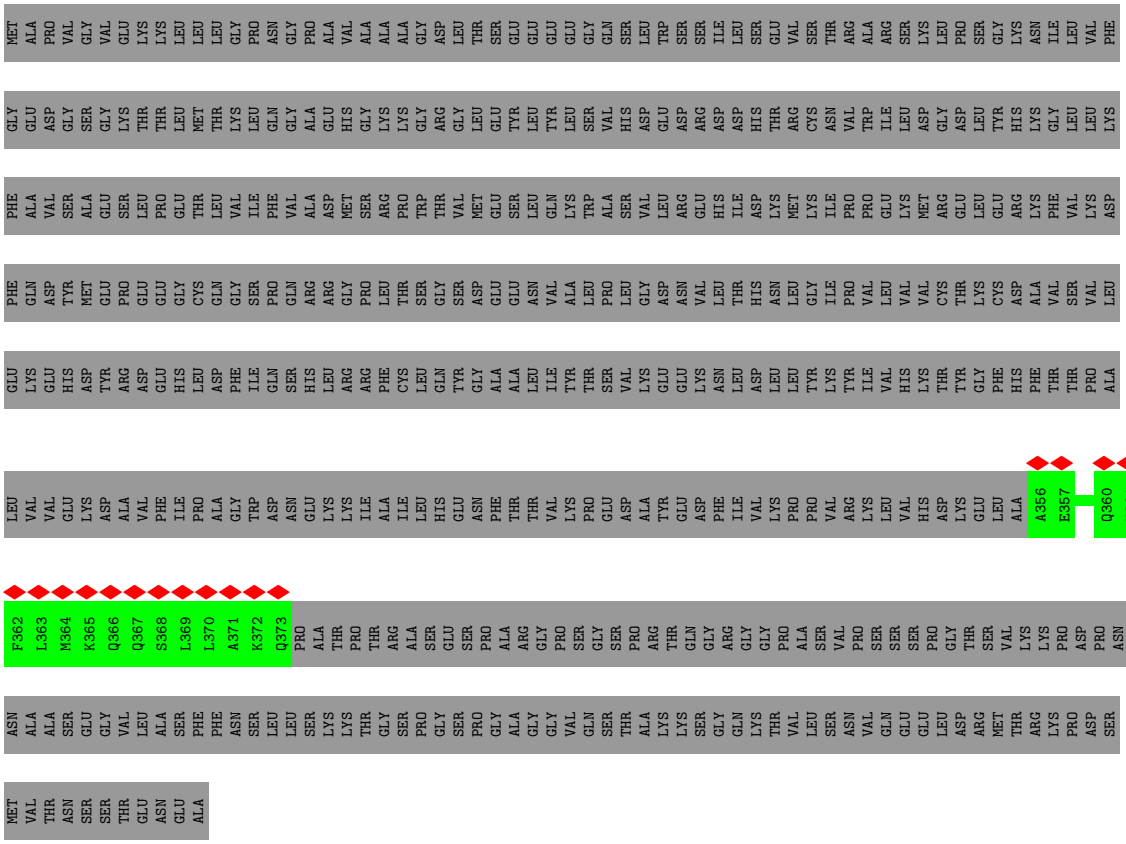
• Molecule 14: Cytoplasmic dynein 1 light intermediate chain 2

Chain q:

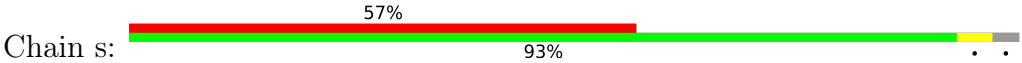


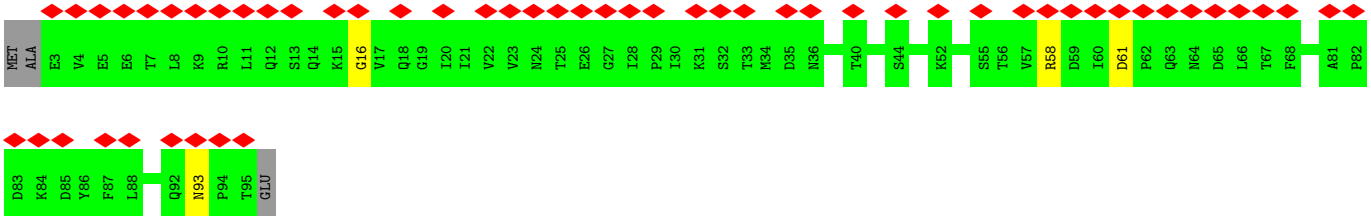
• Molecule 14: Cytoplasmic dynein 1 light intermediate chain 2





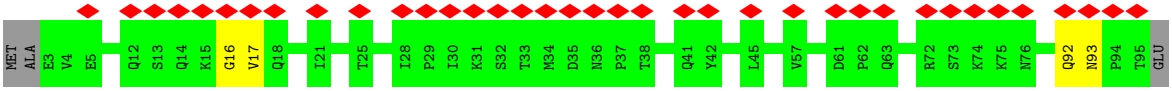
• Molecule 15: Dynein light chain roadblock-type 1



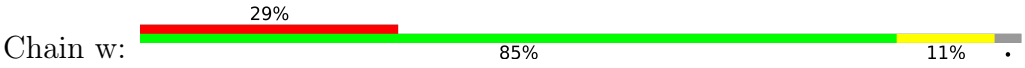


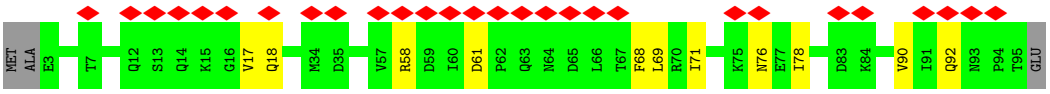
• Molecule 15: Dynein light chain roadblock-type 1



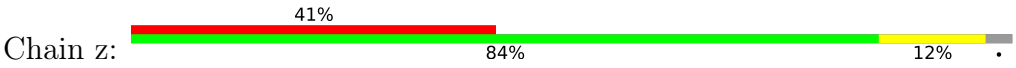


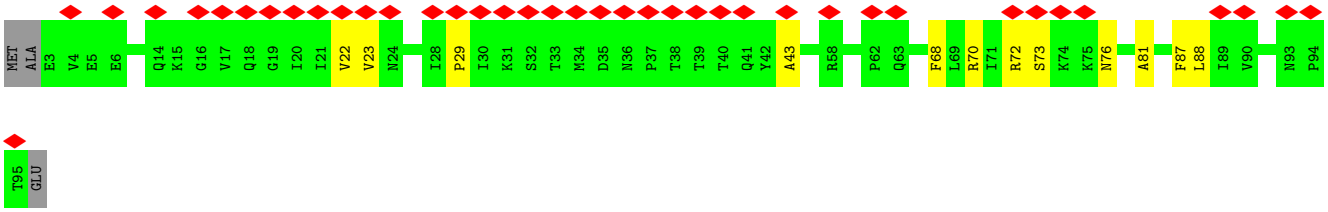
• Molecule 15: Dynein light chain roadblock-type 1





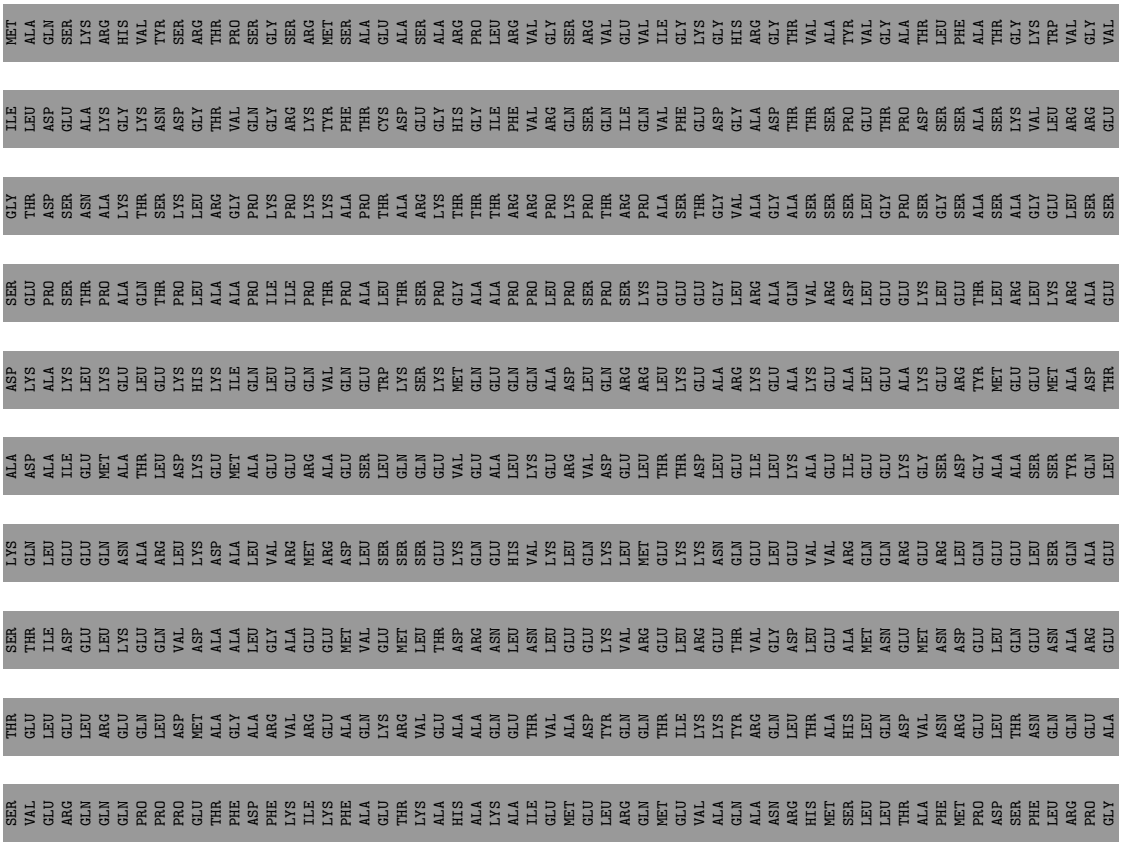
• Molecule 15: Dynein light chain roadblock-type 1

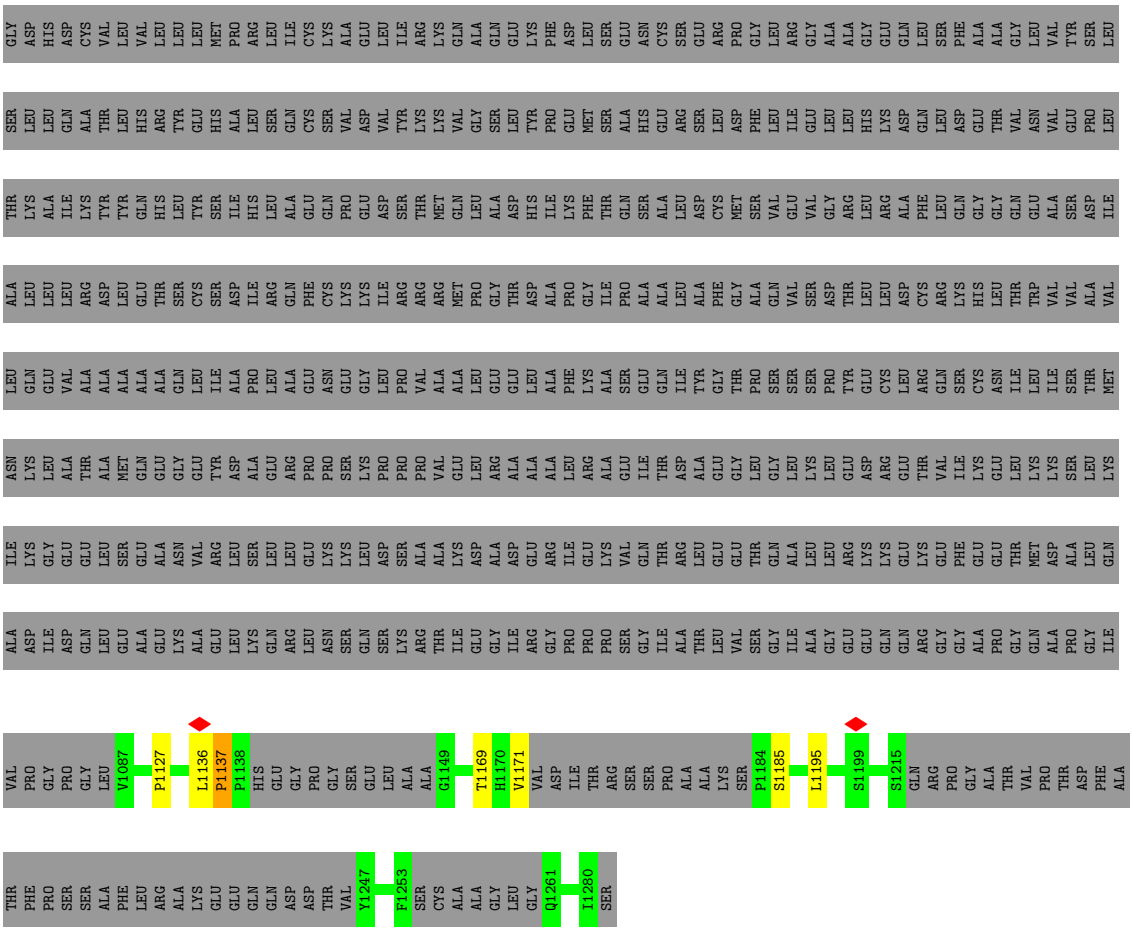




• Molecule 16: Dynactin subunit 1



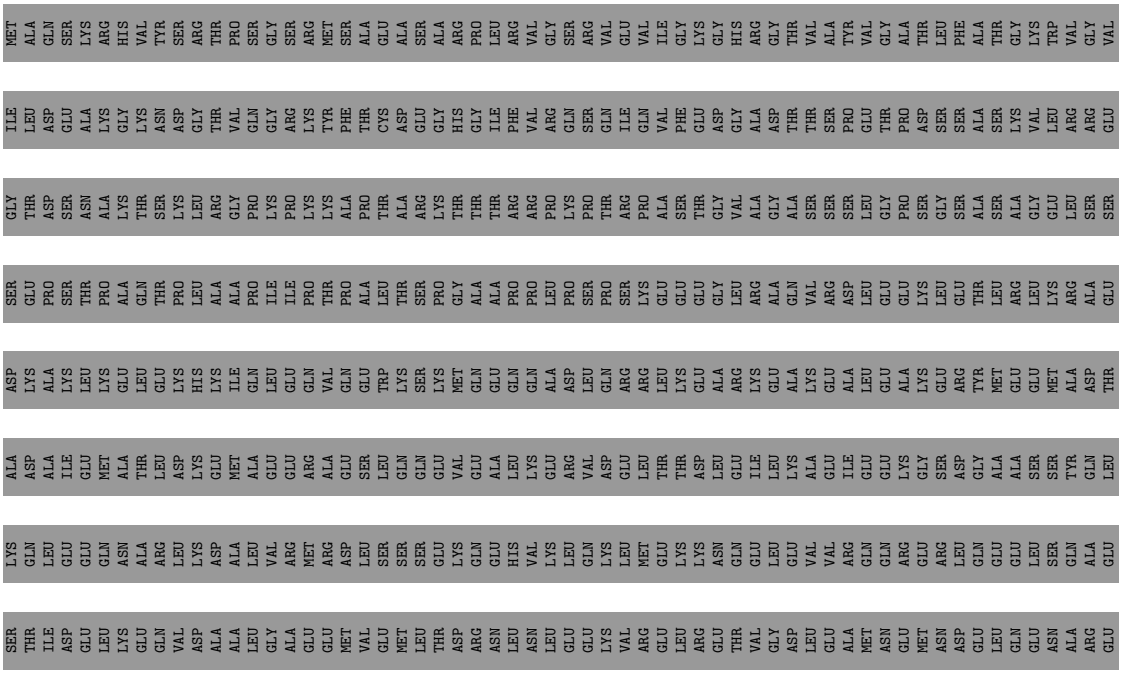


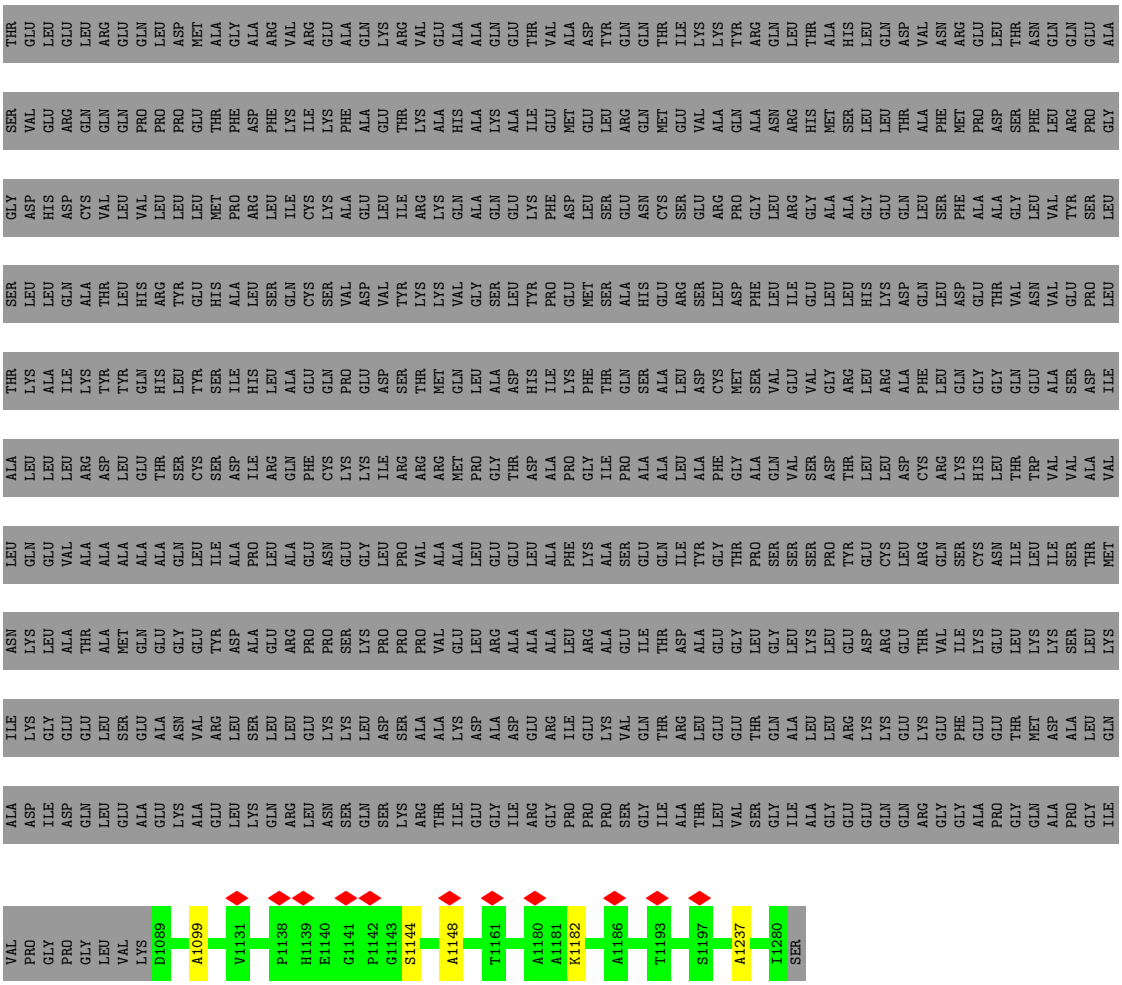


• Molecule 16: Dynactin subunit 1

Chain T:






THR GLU LEU GLU LEU ARG GLU GLN LEU ASP MET ALA GLY ALA ARG VAL ARG GLU ALA GLN LYS ARG VAL GLU ALA ALA GLN GLU THR VAL ALA ASP TYR GLN GLN THR ILE LYS LYS TYR ARG GLN LEU THR ALA HIS LEU GLN ASP VAL ASN ARG GLU LEU THR ASN GLN GLN GLU ALA
SER VAL GLU ARG GLN GLN GLN PRO PRO PRO PRO GLU THR PHE ASP PHE LYS ILE LYS PHE ALA GLU THR LYS ALA HIS ALA LYS ALA ILE GLU MET GLU LEU ARG GLN MET GLU VAL ALA GLN ALA ASN ARG HIS MET SER LEU LEU THR ALA PHE MET PRO ASP SER PHE LEU ARG PRO GLY
GLY ASP HIS ASP CYS VAL LEU VAL LEU LEU LEU LEU MET PRO ARG LEU ILE CYS LYS ALA GLU LEU ILE ARG LYS GLN ALA GLN GLU LYS PHE ASP LEU SER GLU ASN CYS SER GLU ARG PRO GLY LEU ARG GLY ALA GLY GLU GLN GLN LEU SER PHE ALA ALA GLY LEU VAL TYR SER LEU
SER LEU LEU GLN ALA THR LEU HIS ARG TYR GLU HIS ALA LEU SER GLN CYS SER VAL ASP VAL TYR LYS LYS VAL GLY SER LEU TYR PRO GLU MET SER ALA HIS GLU ARG SER LEU ASP PHE LEU ILE GLU GLU LEU LEU HIS LYS ASP GLN LEU SER PHE GLU ASP GLU THR VAL ASN VAL GLU PRO LEU
THR LYS ALA ILE LYS TYR TYR GLN HIS LEU TYR SER ILE HIS LEU ALA GLU GLN PRO GLU ASP SER THR MET GLN LEU ALA ASP HIS ILE LYS PHE THR GLN SER ALA LEU ASP CYS MET SER VAL GLU VAL GLY ARG LEU ARG LEU ILE ALA ALA GLY GLN GLU ALA SER ASP ILE
ALA LEU LEU LEU ARG ASP LEU GLU THR SER CYS SER ASP ILE ARG GLN PHE CYS LYS LYS ILE ARG ARG ARG MET PRO GLY THR ASP ALA PRO GLY ILE PRO ALA ALA LEU ALA PHE GLY ALA ALA GLN VAL SER ASP THR LEU LEU ARG ALA PHE LEU ASP CYS ARG GLN SER LYS HIS LEU THR TRP VAL VAL ALA ALA VAL
LEU GLN GLU VAL ALA ALA ALA GLN LEU ILE ALA PRO LEU ALA GLU GLU ASN GLU GLY LEU PRO VAL ALA ALA LEU GLU LEU ALA PHE LYS ALA SER GLU GLN ILE TYR GLY THR PRO SER SER SER PRO TYR GLU CYS LEU ARG GLN SER CYS ASN ILE LEU LEU ILE SER THR MET
ASN LYS LEU ALA THR ALA MET GLN GLU GLY GLU TYR ASP ALA GLU ARG PRO PRO SER LYS PRO PRO PRO VAL GLU LEU ARG ALA ALA ALA LEU ARG ALA GLU ILE THR ASP ALA GLU GLY LEU LYS LEU GLU LEU LYS GLU LEU LYS LYS SER LEU
ILE LYS GLY GLU GLU LEU SER GLU GLU ALA ASN VAL ARG LEU SER LEU LEU GLU GLU LYS LYS LEU ASP SER ALA ALA LYS ASP ALA ASP GLU ARG ILE GLU LYS VAL GLN THR ARG LEU GLU GLU THR GLN ALA LEU LEU LYS GLU LEU LYS LEU GLN
ALA ASP ILE ASP GLN LEU GLU ALA GLU LYS ALA GLU LEU SER GLN ARG LEU ASN SER GLN SER LYS ARG THR ILE GLU GLY ILE ARG GLY PRO PRO PRO SER GLY ILE ALA THR LEU VAL SER GLY ILE ALA GLY GLU GLU GLN GLN ARG GLY GLY ALA PRO GLY GLN ALA PRO GLY ILE
VAL PRO GLY PRO GLY LEU VAL LYS D1089 A1099 V1131 P1138 H1139 E1140 G1141 P1142 G1143 S1144 A1148 T1161 A1180 A1181 K1182 A1186 T1193 S1197 A1237 I1280 SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8092	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.195	Depositor
Minimum map value	-0.758	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	878.39996, 878.39996, 878.39996	wwPDB
Map dimensions	488, 488, 488	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.8, 1.8, 1.8	Depositor

5 Model quality

5.1 Standard geometry

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

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	g	0.12	0/1944	0.34	0/2704
1	h	0.12	0/1953	0.37	0/2716
1	o	0.12	0/1944	0.36	0/2704
1	p	0.30	0/1978	0.70	0/2751
2	1	0.29	0/1019	0.66	0/1421
2	2	0.25	0/959	0.64	1/1336 (0.1%)
3	A	0.19	0/1821	0.66	0/2531
3	B	0.21	0/1821	0.67	0/2531
3	C	0.35	0/1846	0.80	4/2566 (0.2%)
3	D	0.19	0/1821	0.60	0/2531
3	E	0.47	1/1821 (0.1%)	0.68	3/2531 (0.1%)
3	F	0.19	0/1821	0.62	0/2531
3	G	0.16	0/1821	0.56	0/2531
3	I	0.16	0/1821	0.56	0/2531
4	H	0.16	0/1821	0.55	0/2531
5	J	0.15	0/1867	0.53	0/2596
6	K	0.15	0/1377	0.51	0/1919
7	L	0.24	0/1326	0.59	0/1844
8	M	0.12	0/1317	0.42	0/1836
8	N	0.11	0/1389	0.40	0/1933
8	P	0.16	0/1703	0.53	0/2373
8	Q	0.33	1/1609 (0.1%)	0.61	0/2240
8	V	0.15	0/367	0.52	0/507
9	O	0.19	0/843	0.60	2/1175 (0.2%)
9	R	0.20	0/887	0.59	0/1236
10	U	0.16	0/830	0.45	0/1151
11	W	0.12	0/880	0.35	0/1222
12	Y	0.17	0/1858	0.51	2/2586 (0.1%)
13	e	0.15	0/4002	0.46	1/5581 (0.0%)
13	f	0.18	1/5044 (0.0%)	0.46	0/7035
13	m	0.19	1/3943 (0.0%)	0.51	0/5498
13	n	0.16	1/3690 (0.0%)	0.45	0/5145

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
14	j	0.14	0/1463	0.39	0/2036
14	q	0.10	0/74	0.34	0/102
14	u	0.15	0/89	0.48	0/123
15	s	0.16	0/461	0.50	0/642
15	t	0.15	0/461	0.39	0/642
15	w	0.13	0/461	0.34	0/642
15	z	0.17	0/461	0.38	0/642
16	S	0.68	0/662	1.36	6/917 (0.7%)
16	T	0.31	0/951	0.76	0/1325
All	All	0.22	5/64226 (0.0%)	0.55	19/89394 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	41	ARG	C-N	17.63	1.51	1.33
8	Q	207	SER	C-N	-9.07	1.21	1.33
13	f	339	PHE	C-N	6.93	1.39	1.33
13	m	339	PHE	C-N	5.20	1.37	1.33
13	n	339	PHE	C-N	5.12	1.45	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	S	1127	PRO	CA-C-N	8.64	128.27	118.85
16	S	1127	PRO	C-N-CA	8.64	128.27	118.85
3	E	41	ARG	O-C-N	-7.70	114.10	121.57
16	S	1136	LEU	CA-C-N	7.03	127.62	120.38
16	S	1136	LEU	C-N-CA	7.03	127.62	120.38
3	C	324	LYS	CA-C-N	5.88	132.76	121.54
3	C	324	LYS	C-N-CA	5.88	132.76	121.54
16	S	1137	PRO	N-CA-CB	5.69	108.60	103.08
3	E	41	ARG	CA-C-N	5.61	127.14	120.23
3	E	41	ARG	C-N-CA	5.61	127.14	120.23
12	Y	269	LEU	CA-C-N	-5.61	115.05	122.56
12	Y	269	LEU	C-N-CA	-5.61	115.05	122.56
9	O	14	LEU	CA-C-N	-5.41	112.59	122.38
9	O	14	LEU	C-N-CA	-5.41	112.59	122.38
3	C	98	GLN	CA-C-N	5.27	131.61	121.54
3	C	98	GLN	C-N-CA	5.27	131.61	121.54
2	2	358	LYS	N-CA-CB	5.18	118.31	110.28
16	S	1127	PRO	N-CA-CB	5.17	108.10	103.08
13	e	714	SER	CB-CA-C	-5.02	109.81	115.79

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	g	1946	0	874	18	0
1	h	1955	0	879	13	0
1	o	1946	0	874	19	0
1	p	1980	0	889	2	0
2	1	1021	0	448	7	0
2	2	962	0	424	1	0
3	A	1822	0	820	14	0
3	B	1822	0	820	23	0
3	C	1847	0	830	2	0
3	D	1822	0	820	15	0
3	E	1822	0	820	7	0
3	F	1822	0	820	12	0
3	G	1822	0	820	9	0
3	I	1822	0	820	8	0
4	H	1822	0	835	15	0
5	J	1868	0	823	12	0
6	K	1378	0	611	7	0
7	L	1327	0	585	4	0
8	M	1320	0	604	2	0
8	N	1394	0	632	6	0
8	P	1707	0	769	12	0
8	Q	1612	0	747	15	0
8	V	369	0	161	1	0
9	O	844	0	385	5	0
9	R	888	0	413	2	0
10	U	832	0	371	10	0
11	W	881	0	379	14	0
12	Y	1863	0	794	23	0
13	e	4004	0	1786	15	0
13	f	5046	0	2235	13	0
13	m	3946	0	1760	6	0
13	n	3693	0	1641	5	0
14	j	1465	0	642	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	q	75	0	32	0	0
14	u	90	0	41	0	0
15	s	462	0	192	2	0
15	t	462	0	192	4	0
15	w	462	0	192	8	0
15	z	462	0	192	10	0
16	S	667	0	285	4	0
16	T	952	0	434	3	0
17	A	27	0	12	2	0
17	B	27	0	12	0	0
17	C	27	0	12	0	0
17	D	27	0	12	5	0
17	E	27	0	12	0	0
17	F	27	0	12	0	0
17	G	27	0	12	2	0
17	I	27	0	12	1	0
18	H	31	0	12	2	0
18	J	31	0	12	1	0
19	Y	3	0	0	0	0
All	All	64583	0	28811	304	0

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

All (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:406:GLY:HA2	11:W:37:ASN:HA	1.48	0.96
8:P:388:THR:CB	16:S:1171:VAL:CB	2.48	0.90
3:A:154:THR:HA	3:A:171:TYR:HA	1.55	0.89
3:A:153:THR:CB	3:A:172:GLU:HA	2.03	0.87
2:1:213:GLN:O	2:1:217:ARG:N	2.12	0.82
3:D:162:ASP:N	17:D:800:ADP:O1B	2.11	0.81
10:U:82:MET:CB	10:U:99:MET:HA	2.13	0.79
15:z:22:VAL:HA	15:z:88:LEU:HA	1.65	0.78
12:Y:433:LYS:HA	12:Y:450:GLU:HA	1.66	0.77
3:A:200:LYS:O	3:B:117:PRO:HA	1.85	0.76
5:J:144:ARG:O	5:J:167:GLY:N	2.16	0.76
2:1:407:GLU:N	11:W:36:LEU:O	2.18	0.76
15:t:16:GLY:O	15:t:93:ASN:N	2.18	0.76
5:J:143:TYR:O	5:J:168:GLY:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:219:GLN:O	8:P:223:SER:N	2.19	0.76
3:E:200:LYS:O	3:F:117:PRO:HA	1.87	0.74
8:P:110:HIS:O	8:P:114:GLU:N	2.16	0.74
13:f:573:GLY:HA3	1:g:394:ASN:CB	2.19	0.73
13:e:138:LEU:HA	13:f:137:VAL:O	1.89	0.72
3:B:170:ILE:HA	3:B:174:PHE:O	1.89	0.72
8:N:333:LEU:HA	8:N:336:ARG:CB	2.20	0.72
13:f:806:ALA:HB1	14:j:355:ALA:HA	1.72	0.71
3:A:277:GLU:O	3:A:281:PHE:CB	2.39	0.71
13:e:137:VAL:O	13:f:138:LEU:HA	1.91	0.71
13:e:631:GLN:CB	1:g:572:ALA:HB2	2.22	0.69
8:Q:232:GLU:HA	8:Q:235:LEU:CB	2.23	0.69
11:W:58:GLY:HA3	11:W:89:ASP:HA	1.75	0.69
3:F:200:LYS:O	3:G:117:PRO:HA	1.93	0.68
12:Y:435:LEU:H	12:Y:449:ALA:HB1	1.58	0.68
1:g:335:VAL:HA	1:g:352:THR:HA	1.74	0.68
10:U:118:ILE:O	10:U:137:ILE:N	2.23	0.67
15:w:76:ASN:HA	15:w:92:GLN:O	1.94	0.67
3:D:19:GLY:N	17:D:800:ADP:O2B	2.24	0.67
12:Y:294:PRO:HA	12:Y:303:PHE:CB	2.25	0.67
1:h:551:LEU:O	1:h:562:THR:N	2.26	0.66
2:1:406:GLY:HA2	11:W:37:ASN:CA	2.23	0.66
3:F:334:GLN:HA	8:N:13:ALA:HB3	1.76	0.66
12:Y:427:LYS:HA	12:Y:457:HIS:HA	1.77	0.66
15:s:58:ARG:HA	15:s:61:ASP:O	1.96	0.66
13:e:597:ILE:HA	13:e:600:ALA:HB3	1.77	0.66
12:Y:428:LEU:N	12:Y:456:GLN:O	2.29	0.65
3:D:18:SER:N	17:D:800:ADP:O2B	2.29	0.65
11:W:38:GLY:HA3	11:W:59:ARG:HA	1.77	0.65
13:m:138:LEU:HA	13:n:137:VAL:O	1.97	0.65
15:s:16:GLY:O	15:s:93:ASN:N	2.25	0.65
15:z:23:VAL:HA	15:z:29:PRO:HA	1.79	0.65
11:W:147:SER:O	11:W:152:LEU:N	2.29	0.65
7:L:256:GLU:HA	7:L:259:LYS:CB	2.27	0.64
11:W:96:ASP:O	11:W:113:ASN:HA	1.97	0.64
3:G:200:LYS:O	4:H:112:PRO:HA	1.98	0.64
3:G:171:TYR:N	3:G:174:PHE:O	2.27	0.63
3:B:129:PHE:O	3:B:133:ASN:HA	1.98	0.63
1:o:313:ALA:N	1:o:329:PHE:O	2.27	0.63
5:J:143:TYR:N	18:J:800:ATP:O1G	2.30	0.63
1:g:206:ILE:CB	15:z:81:ALA:HB1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:480:THR:N	1:h:500:SER:O	2.29	0.62
3:A:59:GLY:O	3:A:62:ALA:HB3	1.99	0.62
1:g:191:LEU:HA	1:g:196:PHE:CB	2.29	0.62
1:g:337:SER:O	1:g:351:GLY:N	2.27	0.62
3:F:363:TYR:O	3:F:367:GLY:N	2.30	0.62
1:g:315:VAL:O	1:g:326:GLU:N	2.32	0.62
15:w:78:ILE:HA	15:w:90:VAL:O	2.00	0.62
3:B:112:GLU:N	3:B:140:SER:O	2.30	0.61
3:B:196:LEU:O	3:B:200:LYS:CB	2.48	0.61
3:B:20:VAL:HA	3:B:35:PHE:O	2.00	0.61
13:f:527:TYR:O	13:f:531:LYS:N	2.34	0.61
3:A:219:GLU:HA	17:A:800:ADP:C2	2.35	0.61
1:g:551:LEU:O	1:g:562:THR:N	2.34	0.60
1:o:574:ASN:N	1:o:588:GLY:O	2.32	0.60
8:M:397:ASP:O	8:M:401:LYS:N	2.33	0.60
11:W:60:HIS:O	11:W:90:HIS:HA	2.02	0.60
4:H:237:GLU:CB	4:H:251:GLY:HA2	2.32	0.60
9:O:158:THR:CB	16:S:1169:THR:O	2.49	0.60
13:n:628:PRO:HA	13:n:633:CYS:CB	2.31	0.60
3:F:199:ARG:HA	3:F:203:TYR:O	2.02	0.60
15:w:17:VAL:HA	15:w:92:GLN:CB	2.31	0.60
8:Q:114:GLU:HA	8:Q:117:THR:CB	2.32	0.59
8:Q:226:ALA:O	8:Q:229:ALA:HB3	2.02	0.59
3:A:153:THR:O	3:A:172:GLU:N	2.36	0.59
3:D:219:GLU:HA	17:D:800:ADP:C2	2.37	0.59
8:Q:222:PHE:HA	8:Q:225:ALA:HB3	1.84	0.59
1:o:458:THR:O	1:o:469:SER:N	2.24	0.59
9:O:118:ALA:O	9:O:122:HIS:N	2.35	0.59
15:w:68:PHE:O	15:z:72:ARG:N	2.36	0.59
3:D:20:VAL:HA	3:D:36:PRO:HA	1.84	0.59
3:E:51:ALA:HB2	3:G:173:GLY:HA3	1.85	0.59
3:F:107:PRO:CB	3:F:136:ALA:HB3	2.34	0.58
12:Y:45:GLU:N	12:Y:281:SER:O	2.36	0.58
3:D:51:ALA:CB	3:F:173:GLY:HA3	2.33	0.58
3:D:107:PRO:CB	3:D:136:ALA:HB3	2.34	0.58
8:Q:120:GLU:O	8:Q:123:LYS:N	2.36	0.58
12:Y:28:TYR:O	12:Y:37:ARG:N	2.23	0.57
3:F:58:ILE:N	3:F:62:ALA:HB2	2.20	0.57
4:H:42:GLY:HA3	5:J:387:TRP:HA	1.86	0.57
5:J:110:PHE:O	5:J:114:GLU:HA	2.03	0.57
6:K:67:ILE:H	6:K:71:GLU:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:983:TYR:HA	13:f:986:MET:CB	2.34	0.57
3:B:171:TYR:N	3:B:174:PHE:O	2.33	0.57
1:o:480:THR:N	1:o:500:SER:O	2.37	0.57
3:D:363:TYR:O	3:D:367:GLY:N	2.37	0.56
11:W:101:ALA:HB1	11:W:120:CYS:O	2.05	0.56
12:Y:339:PRO:O	12:Y:374:LEU:N	2.24	0.56
3:B:332:ALA:H	8:Q:86:GLY:HA3	1.70	0.56
4:H:55:GLY:O	4:H:58:ALA:HB3	2.06	0.56
13:n:530:VAL:HA	13:n:549:ALA:HB1	1.88	0.56
5:J:243:PRO:O	5:J:260:GLY:HA3	2.06	0.56
8:N:161:GLY:O	16:S:1185:SER:O	2.24	0.56
12:Y:29:PHE:HA	12:Y:36:LEU:HA	1.88	0.56
3:D:200:LYS:O	3:E:117:PRO:HA	2.05	0.55
1:o:311:GLY:O	1:o:331:CYS:N	2.32	0.55
4:H:79:TRP:O	4:H:82:MET:N	2.40	0.55
3:D:219:GLU:HA	17:D:800:ADP:N1	2.21	0.55
7:L:109:ASP:O	7:L:113:GLU:HA	2.06	0.55
1:o:315:VAL:O	1:o:326:GLU:N	2.40	0.55
1:o:341:ALA:HB3	1:o:344:HIS:O	2.06	0.55
13:e:747:SER:HA	13:e:768:ALA:HB1	1.88	0.54
1:o:551:LEU:O	1:o:562:THR:N	2.38	0.54
3:D:361:LYS:O	3:D:365:GLU:CB	2.55	0.54
3:I:20:VAL:HA	3:I:36:PRO:HA	1.90	0.54
3:B:110:LEU:O	3:B:140:SER:N	2.32	0.54
12:Y:161:GLU:HA	12:Y:164:ARG:CB	2.37	0.54
13:m:522:GLU:HA	13:m:525:LEU:CB	2.38	0.54
3:B:112:GLU:O	3:B:141:MET:HA	2.08	0.54
12:Y:428:LEU:O	12:Y:456:GLN:N	2.31	0.54
1:g:334:ALA:O	1:g:353:TYR:N	2.39	0.53
12:Y:86:ARG:N	12:Y:108:TYR:O	2.40	0.53
3:B:21:ILE:N	3:B:35:PHE:O	2.38	0.53
13:e:636:SER:O	13:e:641:LEU:N	2.35	0.53
3:I:154:THR:HA	3:I:172:GLU:H	1.74	0.53
8:P:218:GLU:O	8:P:222:PHE:N	2.28	0.53
3:E:77:HIS:HA	3:E:163:GLY:HA3	1.91	0.52
4:H:79:TRP:O	4:H:80:ASP:C	2.52	0.52
6:K:67:ILE:O	6:K:71:GLU:N	2.42	0.52
1:g:338:ALA:HA	1:g:350:GLY:HA2	1.91	0.52
3:B:216:ALA:O	3:B:220:ARG:CB	2.58	0.52
10:U:82:MET:HA	10:U:99:MET:O	2.10	0.52
10:U:114:GLY:HA3	10:U:132:ASN:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:269:ARG:O	1:h:596:ILE:N	2.28	0.52
2:2:211:THR:O	2:2:214:PHE:N	2.42	0.52
11:W:39:LYS:N	11:W:59:ARG:O	2.43	0.52
3:A:161:GLY:HA3	17:A:800:ADP:O2B	2.10	0.51
1:o:456:VAL:O	1:o:472:PHE:N	2.41	0.51
13:f:872:LYS:O	13:f:875:SER:N	2.42	0.51
3:A:242:TYR:HA	3:A:248:THR:HA	1.93	0.50
15:z:23:VAL:N	15:z:87:PHE:O	2.44	0.50
3:G:77:HIS:HA	3:G:163:GLY:O	2.12	0.50
8:Q:254:ALA:HB2	16:T:1099:ALA:HB2	1.93	0.50
3:A:143:ALA:HB1	3:A:157:VAL:CB	2.42	0.49
3:I:17:GLY:HA2	17:I:800:ADP:O3B	2.12	0.49
1:o:312:VAL:HA	1:o:330:HIS:HA	1.94	0.49
6:K:95:SER:N	6:K:109:GLN:O	2.40	0.49
7:L:52:ASP:O	7:L:56:GLY:N	2.43	0.49
2:1:410:GLY:N	11:W:31:SER:O	2.43	0.49
12:Y:161:GLU:O	12:Y:164:ARG:CB	2.61	0.49
1:g:266:SER:O	1:g:598:ASP:N	2.40	0.49
10:U:122:GLY:O	10:U:140:ASN:HA	2.12	0.49
15:t:16:GLY:O	15:t:92:GLN:HA	2.12	0.49
1:h:273:ASP:O	1:h:277:SER:N	2.45	0.49
6:K:203:ASN:O	7:L:191:GLY:HA2	2.12	0.49
8:Q:230:GLU:O	8:Q:234:ARG:N	2.38	0.49
3:B:19:GLY:O	3:B:37:ASN:N	2.40	0.48
9:R:23:GLY:HA2	9:R:27:SER:HA	1.95	0.48
13:m:783:GLU:HA	13:m:786:ARG:CB	2.43	0.48
12:Y:24:LEU:HA	12:Y:27:LEU:CB	2.43	0.48
13:f:876:GLU:O	13:f:880:ARG:N	2.31	0.48
8:M:139:VAL:CB	16:S:1195:LEU:CB	2.91	0.48
8:P:52:PRO:HA	8:P:55:ALA:HB3	1.95	0.48
13:m:137:VAL:O	13:n:138:LEU:HA	2.13	0.48
1:g:409:SER:O	1:g:419:GLN:N	2.47	0.48
8:P:177:LYS:HA	8:P:180:LEU:CB	2.43	0.48
3:B:238:LYS:HA	3:B:252:GLY:HA2	1.96	0.48
3:I:104:GLU:HA	3:I:133:ASN:O	2.13	0.48
13:e:366:LYS:O	13:e:369:ASN:N	2.46	0.48
3:F:108:VAL:O	3:F:137:LEU:HA	2.15	0.47
8:P:137:PRO:O	8:P:141:ALA:N	2.47	0.47
13:e:41:LEU:HA	13:f:132:SER:CB	2.44	0.47
1:g:403:THR:O	1:g:433:ALA:HA	2.15	0.47
4:H:297:THR:O	4:H:330:ILE:N	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:82:SER:HA	13:e:113:SER:CB	2.44	0.47
8:P:177:LYS:O	8:P:181:LEU:N	2.47	0.47
10:U:126:GLY:N	10:U:143:ILE:O	2.48	0.47
1:g:311:GLY:O	1:g:330:HIS:HA	2.15	0.47
1:g:458:THR:O	1:g:469:SER:N	2.30	0.47
10:U:121:SER:O	10:U:139:GLU:CB	2.63	0.47
1:o:433:ALA:O	1:o:451:SER:HA	2.15	0.47
2:1:352:THR:O	2:1:355:TRP:CB	2.63	0.46
3:I:99:LEU:O	3:I:100:GLN:C	2.58	0.46
8:N:320:ILE:C	8:N:322:ARG:H	2.23	0.46
15:w:71:ILE:HA	15:z:68:PHE:O	2.14	0.46
15:t:16:GLY:C	15:t:93:ASN:H	2.18	0.46
3:D:330:ILE:O	8:Q:19:VAL:HA	2.16	0.46
3:D:51:ALA:HB2	3:F:173:GLY:HA3	1.97	0.46
3:E:145:LEU:O	3:E:343:GLY:HA3	2.16	0.46
1:o:293:GLU:O	1:o:317:ASN:HA	2.15	0.46
5:J:189:ALA:O	5:J:190:ALA:HB3	2.15	0.46
1:o:508:LEU:O	1:o:517:LEU:N	2.48	0.46
3:F:51:ALA:HB2	4:H:168:GLY:HA3	1.97	0.46
1:h:458:THR:O	1:h:469:SER:N	2.24	0.46
1:o:607:ARG:CB	1:o:609:ASP:H	2.29	0.46
13:e:210:HIS:O	13:e:212:MET:N	2.49	0.46
15:w:58:ARG:HA	15:w:61:ASP:O	2.16	0.46
1:h:335:VAL:HA	1:h:352:THR:HA	1.98	0.46
1:h:481:GLY:O	1:h:500:SER:N	2.48	0.46
3:E:301:SER:HA	3:E:336:ARG:CB	2.46	0.45
3:I:154:THR:CA	3:I:172:GLU:H	2.28	0.45
13:f:1007:GLY:HA2	13:m:647:SER:CB	2.47	0.45
8:P:332:GLU:O	8:P:336:ARG:CB	2.64	0.45
11:W:119:ARG:O	11:W:137:GLU:HA	2.16	0.45
12:Y:293:LYS:O	12:Y:304:LYS:N	2.49	0.45
12:Y:317:ARG:O	12:Y:333:LEU:N	2.41	0.45
3:B:19:GLY:O	3:B:36:PRO:HA	2.17	0.45
12:Y:155:ALA:O	12:Y:159:LYS:N	2.48	0.45
1:h:359:LEU:N	1:h:371:GLN:O	2.47	0.45
3:G:20:VAL:HA	3:G:36:PRO:HA	1.98	0.45
4:H:237:GLU:HA	4:H:251:GLY:HA2	1.98	0.45
13:e:594:ARG:O	13:e:595:PRO:C	2.60	0.45
6:K:186:ALA:N	6:K:216:VAL:O	2.49	0.45
8:P:268:LEU:O	8:P:272:VAL:N	2.44	0.45
3:B:363:TYR:O	3:B:367:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:224:LEU:N	3:I:308:LYS:O	2.31	0.45
8:Q:138:VAL:O	8:Q:141:ALA:HB3	2.17	0.45
1:g:576:VAL:HA	1:g:587:VAL:HA	1.99	0.45
13:m:333:ASN:HA	13:m:336:MET:CB	2.47	0.45
1:o:530:VAL:HA	1:o:541:ALA:O	2.17	0.45
12:Y:238:ASP:C	12:Y:240:TYR:H	2.25	0.44
1:o:337:SER:O	1:o:350:GLY:HA2	2.16	0.44
5:J:139:LEU:O	5:J:306:ILE:N	2.33	0.44
9:R:91:GLU:O	9:R:95:LEU:N	2.47	0.44
15:z:73:SER:N	15:z:76:ASN:O	2.44	0.44
11:W:66:ARG:O	11:W:96:ASP:HA	2.17	0.44
10:U:110:LYS:O	10:U:128:CYS:HA	2.18	0.44
9:O:74:ASP:O	9:O:77:ALA:HB3	2.18	0.44
1:h:274:GLU:HA	1:h:278:LYS:CB	2.47	0.44
1:p:312:ALA:HA	1:p:324:GLY:HA2	2.00	0.44
4:H:302:GLY:HA3	18:H:401:ATP:H5'2	2.00	0.44
3:B:240:GLN:HA	3:B:249:ILE:O	2.18	0.43
1:h:409:SER:O	1:h:419:GLN:N	2.51	0.43
15:w:18:GLN:H	15:w:92:GLN:HA	1.83	0.43
3:B:83:TRP:O	3:B:84:ASN:C	2.60	0.43
1:h:384:VAL:HA	1:h:402:SER:HA	2.00	0.43
1:h:459:ALA:HB2	1:h:468:ILE:HA	1.99	0.43
8:P:219:GLN:CB	16:T:1237:ALA:HB1	2.48	0.43
4:H:262:PHE:O	4:H:273:GLY:HA3	2.17	0.43
8:N:394:ALA:O	8:N:398:GLU:CB	2.66	0.43
1:o:434:VAL:HA	1:o:450:GLY:O	2.18	0.43
3:B:329:ARG:HA	8:Q:89:GLU:HA	2.01	0.43
8:Q:231:LEU:O	8:Q:235:LEU:N	2.51	0.43
3:A:51:ALA:HA	3:C:173:GLY:HA2	2.00	0.43
13:e:25:ALA:HA	13:e:127:ALA:HB2	1.99	0.43
1:g:281:VAL:O	1:g:299:TYR:HA	2.19	0.43
13:e:210:HIS:O	13:e:213:ILE:N	2.49	0.43
3:G:161:GLY:HA3	17:G:800:ADP:O1B	2.19	0.43
12:Y:142:GLN:HA	12:Y:145:ASN:CB	2.49	0.42
3:B:57:PHE:C	3:B:62:ALA:HB2	2.44	0.42
6:K:250:MET:O	6:K:254:THR:N	2.53	0.42
13:f:542:GLY:HA2	13:f:545:ALA:HB3	2.01	0.42
1:o:539:LEU:HA	1:o:552:TRP:O	2.19	0.42
13:e:597:ILE:HA	13:e:600:ALA:CB	2.47	0.42
13:e:438:VAL:O	13:e:442:ARG:CB	2.67	0.42
3:B:200:LYS:O	3:C:117:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:129:SER:O	8:Q:133:GLU:CB	2.68	0.42
8:V:65:GLY:N	8:V:85:SER:O	2.53	0.42
12:Y:142:GLN:O	12:Y:146:LYS:N	2.34	0.42
15:z:23:VAL:CB	15:z:43:ALA:HB1	2.49	0.42
4:H:239:SER:HA	4:H:248:ILE:O	2.20	0.42
6:K:64:PRO:HA	6:K:75:LEU:HA	2.02	0.42
12:Y:258:GLN:O	12:Y:261:PHE:O	2.37	0.42
3:F:159:ASP:O	3:F:165:THR:HA	2.20	0.42
15:w:69:LEU:HA	15:z:70:ARG:O	2.19	0.42
2:1:410:GLY:HA2	11:W:31:SER:CB	2.50	0.42
3:A:213:ILE:O	3:A:216:ALA:HB3	2.20	0.42
12:Y:426:PHE:O	12:Y:458:VAL:N	2.48	0.42
13:f:552:ARG:O	13:f:556:ARG:N	2.48	0.42
1:h:338:ALA:HA	1:h:350:GLY:HA2	2.01	0.42
16:T:1144:SER:O	16:T:1148:ALA:HB2	2.20	0.42
4:H:195:GLU:O	3:I:117:PRO:HA	2.20	0.42
9:O:4:VAL:O	9:O:7:VAL:N	2.51	0.42
3:A:128:PHE:O	3:A:132:PHE:O	2.38	0.41
3:D:99:LEU:O	3:D:100:GLN:C	2.63	0.41
10:U:114:GLY:N	10:U:131:LEU:O	2.53	0.41
3:D:329:ARG:HA	8:Q:21:GLU:HA	2.02	0.41
5:J:329:LYS:O	5:J:333:LYS:N	2.52	0.41
5:J:144:ARG:C	5:J:167:GLY:HA3	2.46	0.41
1:g:203:SER:HA	15:z:81:ALA:O	2.20	0.41
3:B:238:LYS:HA	3:B:252:GLY:CA	2.51	0.41
8:P:143:GLN:O	8:P:147:LEU:N	2.38	0.41
3:E:160:SER:HA	3:E:165:THR:HA	2.01	0.41
13:n:76:THR:HA	13:n:118:PHE:O	2.21	0.41
1:p:547:LEU:HA	1:p:563:ASP:HA	2.02	0.41
3:G:170:ILE:CB	3:G:175:ALA:HB2	2.50	0.41
4:H:13:GLY:HA3	4:H:16:MET:O	2.21	0.41
5:J:27:CYS:O	5:J:36:ARG:N	2.54	0.41
5:J:344:HIS:HA	12:Y:228:ALA:HA	2.03	0.41
8:N:333:LEU:O	8:N:337:LEU:N	2.51	0.41
9:O:19:ARG:O	9:O:23:GLY:HA2	2.20	0.41
15:t:17:VAL:HA	15:t:92:GLN:HA	2.03	0.41
3:A:153:THR:C	3:A:172:GLU:H	2.29	0.41
3:B:21:ILE:O	3:B:34:CYS:HA	2.20	0.40
3:G:303:GLY:HA3	17:G:800:ADP:H5'2	2.02	0.40
13:f:547:GLU:O	13:f:551:LYS:N	2.55	0.40
4:H:214:GLU:HA	18:H:401:ATP:N1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:59:GLN:CB	10:U:93:GLY:H	2.35	0.40
8:Q:353:LEU:O	8:Q:357:LEU:N	2.54	0.40
1:o:384:VAL:HA	1:o:402:SER:HA	2.02	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	g	390/612 (64%)	386 (99%)	4 (1%)	0	100	100
1	h	392/612 (64%)	388 (99%)	4 (1%)	0	100	100
1	o	390/612 (64%)	380 (97%)	10 (3%)	0	100	100
1	p	397/612 (65%)	383 (96%)	14 (4%)	0	100	100
2	1	201/889 (23%)	195 (97%)	6 (3%)	0	100	100
2	2	187/889 (21%)	187 (100%)	0	0	100	100
3	A	368/376 (98%)	359 (98%)	9 (2%)	0	100	100
3	B	368/376 (98%)	354 (96%)	14 (4%)	0	100	100
3	C	373/376 (99%)	358 (96%)	15 (4%)	0	100	100
3	D	368/376 (98%)	360 (98%)	8 (2%)	0	100	100
3	E	368/376 (98%)	350 (95%)	18 (5%)	0	100	100
3	F	368/376 (98%)	353 (96%)	15 (4%)	0	100	100
3	G	368/376 (98%)	357 (97%)	11 (3%)	0	100	100
3	I	368/376 (98%)	351 (95%)	17 (5%)	0	100	100
4	H	368/375 (98%)	354 (96%)	14 (4%)	0	100	100
5	J	377/417 (90%)	364 (97%)	13 (3%)	0	100	100
6	K	276/286 (96%)	266 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	L	267/272 (98%)	265 (99%)	2 (1%)	0	100	100
8	M	259/405 (64%)	253 (98%)	5 (2%)	1 (0%)	30	67
8	N	270/405 (67%)	262 (97%)	7 (3%)	1 (0%)	30	67
8	P	335/405 (83%)	320 (96%)	15 (4%)	0	100	100
8	Q	319/405 (79%)	310 (97%)	9 (3%)	0	100	100
8	V	71/405 (18%)	69 (97%)	2 (3%)	0	100	100
9	O	168/186 (90%)	159 (95%)	9 (5%)	0	100	100
9	R	177/186 (95%)	164 (93%)	13 (7%)	0	100	100
10	U	165/190 (87%)	154 (93%)	11 (7%)	0	100	100
11	W	177/182 (97%)	172 (97%)	5 (3%)	0	100	100
12	Y	365/467 (78%)	343 (94%)	22 (6%)	0	100	100
13	e	803/4646 (17%)	779 (97%)	23 (3%)	1 (0%)	48	83
13	f	1013/4646 (22%)	989 (98%)	24 (2%)	0	100	100
13	m	789/4646 (17%)	782 (99%)	7 (1%)	0	100	100
13	n	738/4646 (16%)	724 (98%)	14 (2%)	0	100	100
14	j	292/492 (59%)	286 (98%)	6 (2%)	0	100	100
14	q	13/492 (3%)	13 (100%)	0	0	100	100
14	u	16/492 (3%)	16 (100%)	0	0	100	100
15	s	91/96 (95%)	85 (93%)	6 (7%)	0	100	100
15	t	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
15	w	91/96 (95%)	85 (93%)	6 (7%)	0	100	100
15	z	91/96 (95%)	82 (90%)	9 (10%)	0	100	100
16	S	124/1281 (10%)	117 (94%)	6 (5%)	1 (1%)	16	54
16	T	190/1281 (15%)	180 (95%)	9 (5%)	1 (0%)	24	63
All	All	12842/34826 (37%)	12440 (97%)	397 (3%)	5 (0%)	100	100

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	M	217	PRO
16	S	1137	PRO
8	N	163	ASP
16	T	1182	LYS
13	e	595	PRO

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
18	ATP	H	401	-	29,33,33	0.26	0	44,52,52	0.45	1 (2%)
18	ATP	J	800	-	29,33,33	0.27	0	44,52,52	0.48	1 (2%)
17	ADP	B	800	-	27,29,29	1.37	4 (14%)	42,45,45	1.96	10 (23%)
17	ADP	E	800	-	27,29,29	1.36	4 (14%)	42,45,45	1.95	10 (23%)
17	ADP	A	800	-	27,29,29	1.36	4 (14%)	42,45,45	1.96	11 (26%)
17	ADP	G	800	-	27,29,29	1.37	4 (14%)	42,45,45	1.97	10 (23%)
17	ADP	C	800	-	27,29,29	1.38	4 (14%)	42,45,45	1.96	11 (26%)
17	ADP	D	800	-	27,29,29	1.36	4 (14%)	42,45,45	1.96	10 (23%)
17	ADP	I	800	-	27,29,29	1.36	4 (14%)	42,45,45	1.98	10 (23%)
17	ADP	F	800	-	27,29,29	1.37	4 (14%)	42,45,45	1.95	10 (23%)

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
18	ATP	H	401	-	-	10/22/38/38	0/3/3/3
18	ATP	J	800	-	-	7/22/38/38	0/3/3/3
17	ADP	B	800	-	-	1/16/32/32	0/3/3/3
17	ADP	E	800	-	-	4/16/32/32	0/3/3/3
17	ADP	A	800	-	-	1/16/32/32	0/3/3/3
17	ADP	G	800	-	-	6/16/32/32	0/3/3/3
17	ADP	C	800	-	-	2/16/32/32	0/3/3/3
17	ADP	D	800	-	-	7/16/32/32	0/3/3/3
17	ADP	I	800	-	-	4/16/32/32	0/3/3/3
17	ADP	F	800	-	-	2/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	800	ADP	C5-C4	4.66	1.47	1.39
17	G	800	ADP	C5-C4	4.64	1.47	1.39
17	I	800	ADP	C5-C4	4.62	1.47	1.39
17	B	800	ADP	C5-C4	4.60	1.47	1.39
17	E	800	ADP	C5-C4	4.60	1.47	1.39
17	F	800	ADP	C5-C4	4.59	1.47	1.39
17	D	800	ADP	C5-C4	4.57	1.47	1.39
17	A	800	ADP	C5-C4	4.54	1.47	1.39
17	C	800	ADP	C5-C6	2.73	1.48	1.41
17	E	800	ADP	C5-C6	2.73	1.48	1.41
17	F	800	ADP	C5-C6	2.71	1.48	1.41
17	B	800	ADP	C5-C6	2.71	1.48	1.41
17	G	800	ADP	C5-C6	2.70	1.48	1.41
17	I	800	ADP	C5-C6	2.70	1.48	1.41
17	D	800	ADP	C5-C6	2.70	1.48	1.41
17	A	800	ADP	C5-C6	2.69	1.48	1.41
17	A	800	ADP	C8-N7	2.43	1.36	1.31
17	F	800	ADP	C8-N7	2.41	1.36	1.31
17	B	800	ADP	C8-N7	2.41	1.36	1.31
17	E	800	ADP	C8-N7	2.40	1.36	1.31
17	G	800	ADP	C8-N7	2.38	1.36	1.31
17	D	800	ADP	C8-N7	2.38	1.36	1.31
17	I	800	ADP	C8-N7	2.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	800	ADP	C8-N7	2.35	1.36	1.31
17	C	800	ADP	C5-N7	-2.26	1.34	1.39
17	B	800	ADP	C5-N7	-2.21	1.34	1.39
17	I	800	ADP	C5-N7	-2.19	1.34	1.39
17	D	800	ADP	C5-N7	-2.17	1.34	1.39
17	F	800	ADP	C5-N7	-2.16	1.34	1.39
17	G	800	ADP	C5-N7	-2.14	1.35	1.39
17	A	800	ADP	C5-N7	-2.14	1.35	1.39
17	E	800	ADP	C5-N7	-2.13	1.35	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	800	ADP	C5-C4-N3	-6.39	118.41	126.75
17	D	800	ADP	C5-C4-N3	-6.35	118.47	126.75
17	B	800	ADP	C5-C4-N3	-6.34	118.48	126.75
17	E	800	ADP	C5-C4-N3	-6.34	118.48	126.75
17	I	800	ADP	C5-C4-N3	-6.34	118.48	126.75
17	G	800	ADP	C5-C4-N3	-6.32	118.50	126.75
17	A	800	ADP	C5-C4-N3	-6.16	118.72	126.75
17	C	800	ADP	C5-C4-N3	-6.11	118.78	126.75
17	F	800	ADP	N3-C4-N9	5.02	135.35	127.08
17	G	800	ADP	N3-C4-N9	5.02	135.35	127.08
17	I	800	ADP	N3-C4-N9	5.00	135.32	127.08
17	D	800	ADP	N3-C4-N9	4.98	135.28	127.08
17	E	800	ADP	N3-C4-N9	4.93	135.21	127.08
17	B	800	ADP	N3-C4-N9	4.92	135.18	127.08
17	C	800	ADP	N3-C4-N9	4.80	134.99	127.08
17	A	800	ADP	N3-C4-N9	4.79	134.98	127.08
17	C	800	ADP	C2-N3-C4	3.89	120.94	111.75
17	F	800	ADP	C2-N3-C4	3.88	120.91	111.75
17	G	800	ADP	C2-N3-C4	3.87	120.90	111.75
17	I	800	ADP	C2-N3-C4	3.86	120.87	111.75
17	D	800	ADP	C2-N3-C4	3.85	120.85	111.75
17	A	800	ADP	C2-N3-C4	3.85	120.84	111.75
17	E	800	ADP	C2-N3-C4	3.84	120.81	111.75
17	B	800	ADP	C2-N3-C4	3.73	120.56	111.75
17	B	800	ADP	PA-O3A-PB	-3.72	120.07	132.83
17	I	800	ADP	PA-O3A-PB	-3.52	120.73	132.83
17	A	800	ADP	PA-O3A-PB	-3.51	120.78	132.83
17	E	800	ADP	PA-O3A-PB	-3.37	121.25	132.83
17	B	800	ADP	C4-C5-N7	-3.34	106.55	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	800	ADP	PA-O3A-PB	-3.32	121.42	132.83
17	D	800	ADP	PA-O3A-PB	-3.30	121.50	132.83
17	E	800	ADP	C4-C5-N7	-3.28	106.62	110.62
17	A	800	ADP	C4-C5-N7	-3.28	106.62	110.62
17	D	800	ADP	C4-C5-N7	-3.25	106.66	110.62
17	I	800	ADP	C4-C5-N7	-3.24	106.68	110.62
17	G	800	ADP	PA-O3A-PB	-3.21	121.79	132.83
17	F	800	ADP	C4-C5-N7	-3.21	106.71	110.62
17	G	800	ADP	C4-C5-N7	-3.21	106.71	110.62
17	C	800	ADP	C4-C5-N7	-3.19	106.74	110.62
17	C	800	ADP	N3-C2-N1	-3.17	123.65	128.60
17	A	800	ADP	N3-C2-N1	-3.16	123.67	128.60
17	C	800	ADP	PA-O3A-PB	-3.09	122.23	132.83
17	G	800	ADP	N3-C2-N1	-3.07	123.80	128.60
17	I	800	ADP	N3-C2-N1	-3.05	123.83	128.60
17	F	800	ADP	N3-C2-N1	-3.04	123.85	128.60
17	D	800	ADP	N3-C2-N1	-3.03	123.87	128.60
17	E	800	ADP	N3-C2-N1	-2.99	123.92	128.60
17	B	800	ADP	C5-N7-C8	2.80	107.49	103.51
17	I	800	ADP	C5-N7-C8	2.79	107.47	103.51
17	A	800	ADP	C5-N7-C8	2.78	107.45	103.51
17	D	800	ADP	C5-N7-C8	2.76	107.43	103.51
17	B	800	ADP	N3-C2-N1	-2.75	124.29	128.60
17	E	800	ADP	C5-N7-C8	2.75	107.42	103.51
17	G	800	ADP	C5-N7-C8	2.72	107.38	103.51
17	F	800	ADP	C5-N7-C8	2.71	107.35	103.51
17	C	800	ADP	C5-N7-C8	2.66	107.29	103.51
17	A	800	ADP	C4-N9-C8	2.55	108.49	105.73
17	G	800	ADP	C4-N9-C8	2.54	108.48	105.73
17	D	800	ADP	C4-N9-C8	2.53	108.47	105.73
17	I	800	ADP	C4-N9-C8	2.49	108.42	105.73
17	F	800	ADP	C4-N9-C8	2.48	108.41	105.73
17	B	800	ADP	C4-N9-C8	2.47	108.40	105.73
17	C	800	ADP	C3'-C2'-C1'	2.46	106.11	101.43
17	B	800	ADP	C3'-C2'-C1'	2.42	106.02	101.43
17	E	800	ADP	C4-N9-C8	2.41	108.34	105.73
17	I	800	ADP	C3'-C2'-C1'	2.41	106.00	101.43
17	G	800	ADP	C3'-C2'-C1'	2.40	105.99	101.43
17	C	800	ADP	C4-N9-C8	2.39	108.32	105.73
17	D	800	ADP	C3'-C2'-C1'	2.38	105.95	101.43
17	C	800	ADP	C6-C5-N7	2.28	136.28	132.02
17	E	800	ADP	C3'-C2'-C1'	2.28	105.75	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	800	ADP	C3'-C2'-C1'	2.26	105.71	101.43
17	A	800	ADP	C6-C5-N7	2.17	136.07	132.02
17	A	800	ADP	C3'-C2'-C1'	2.13	105.47	101.43
17	B	800	ADP	C6-C5-N7	2.09	135.92	132.02
17	E	800	ADP	C6-C5-N7	2.08	135.89	132.02
17	D	800	ADP	C6-C5-N7	2.07	135.88	132.02
17	I	800	ADP	C6-C5-N7	2.06	135.87	132.02
17	G	800	ADP	C6-C5-N7	2.06	135.86	132.02
17	C	800	ADP	C2'-C1'-N9	-2.05	108.12	113.30
18	J	800	ATP	PB-O3B-PG	2.04	139.81	132.83
18	H	401	ATP	PB-O3B-PG	2.04	139.81	132.83
17	A	800	ADP	N9-C8-N7	-2.03	111.13	113.91
17	F	800	ADP	C6-C5-N7	2.01	135.76	132.02

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	D	800	ADP	C5'-O5'-PA-O1A
17	D	800	ADP	C5'-O5'-PA-O2A
17	D	800	ADP	C5'-O5'-PA-O3A
17	E	800	ADP	C5'-O5'-PA-O2A
17	E	800	ADP	C5'-O5'-PA-O3A
17	G	800	ADP	C5'-O5'-PA-O3A
17	G	800	ADP	C3'-C4'-C5'-O5'
17	I	800	ADP	C5'-O5'-PA-O1A
17	C	800	ADP	C5'-O5'-PA-O2A
17	C	800	ADP	C5'-O5'-PA-O3A
18	H	401	ATP	PB-O3B-PG-O2G
18	H	401	ATP	C5'-O5'-PA-O1A
18	H	401	ATP	C3'-C4'-C5'-O5'
18	J	800	ATP	C5'-O5'-PA-O1A
18	J	800	ATP	C5'-O5'-PA-O2A
18	J	800	ATP	C5'-O5'-PA-O3A
18	J	800	ATP	O4'-C4'-C5'-O5'
18	J	800	ATP	C3'-C4'-C5'-O5'
17	D	800	ADP	O4'-C4'-C5'-O5'
17	D	800	ADP	C3'-C4'-C5'-O5'
17	F	800	ADP	O4'-C4'-C5'-O5'
17	G	800	ADP	O4'-C4'-C5'-O5'
18	H	401	ATP	O4'-C4'-C5'-O5'
18	H	401	ATP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
18	J	800	ATP	PB-O3B-PG-O1G
18	H	401	ATP	PG-O3B-PB-O1B
17	E	800	ADP	C3'-C4'-C5'-O5'
18	H	401	ATP	PB-O3A-PA-O5'
17	F	800	ADP	C3'-C4'-C5'-O5'
17	I	800	ADP	PA-O3A-PB-O3B
18	J	800	ATP	PB-O3B-PG-O2G
17	I	800	ADP	C5'-O5'-PA-O3A
17	D	800	ADP	PB-O3A-PA-O2A
17	G	800	ADP	C5'-O5'-PA-O2A
17	I	800	ADP	C5'-O5'-PA-O2A
18	H	401	ATP	C5'-O5'-PA-O2A
17	G	800	ADP	PB-O3A-PA-O2A
18	H	401	ATP	PA-O3A-PB-O2B
17	E	800	ADP	PA-O3A-PB-O2B
18	H	401	ATP	C5'-O5'-PA-O3A
17	A	800	ADP	O4'-C4'-C5'-O5'
17	D	800	ADP	PB-O3A-PA-O1A
17	G	800	ADP	PB-O3A-PA-O1A
17	B	800	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

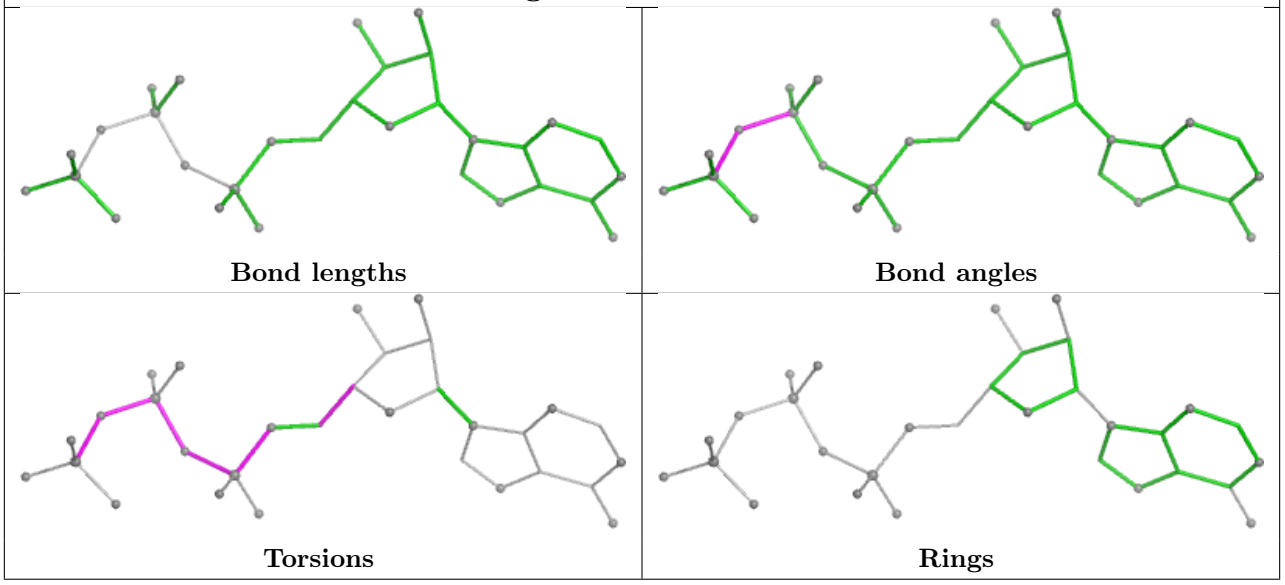
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	H	401	ATP	2	0
18	J	800	ATP	1	0
17	A	800	ADP	2	0
17	G	800	ADP	2	0
17	D	800	ADP	5	0
17	I	800	ADP	1	0

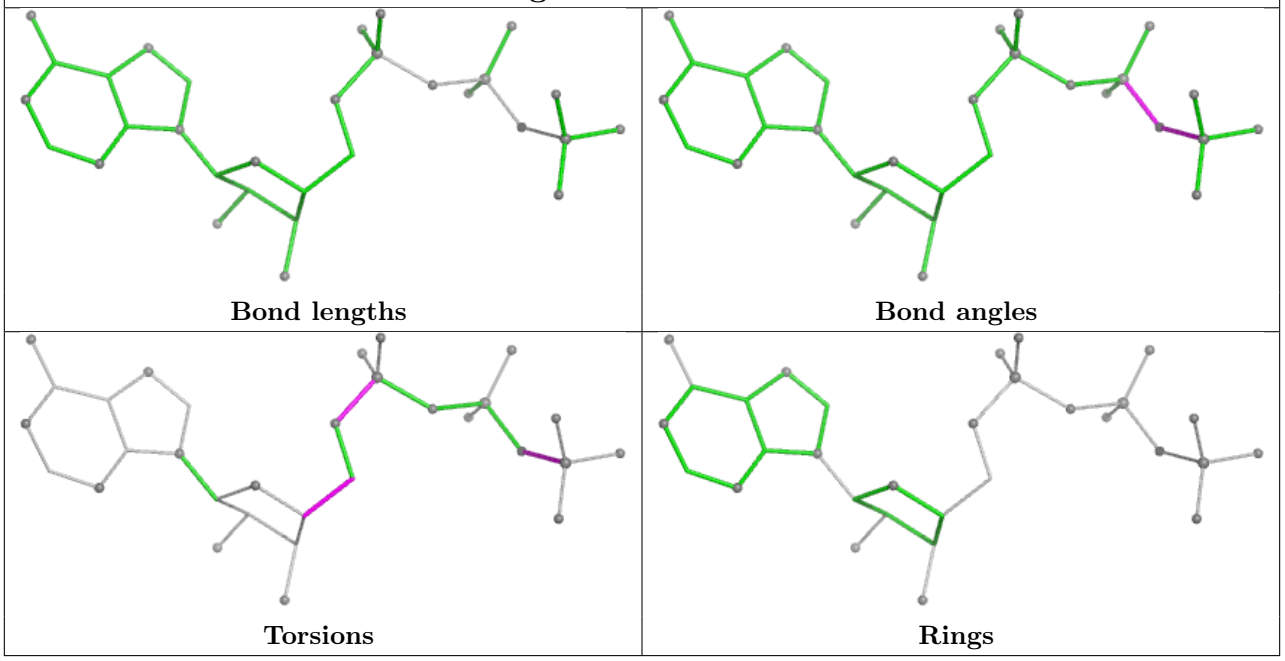
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

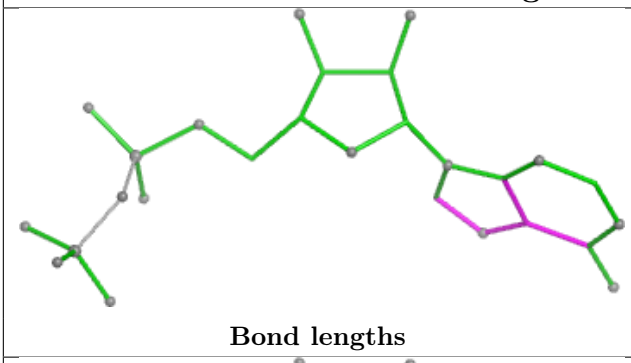
Ligand ATP H 401



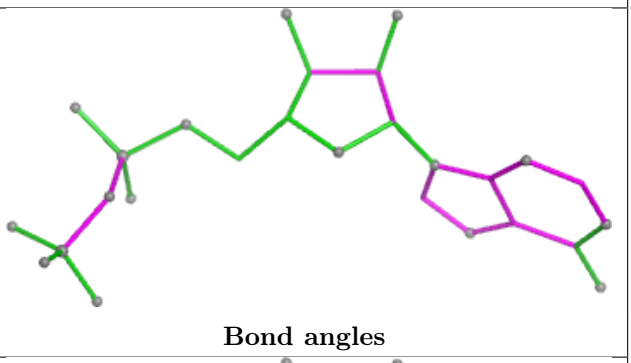
Ligand ATP J 800



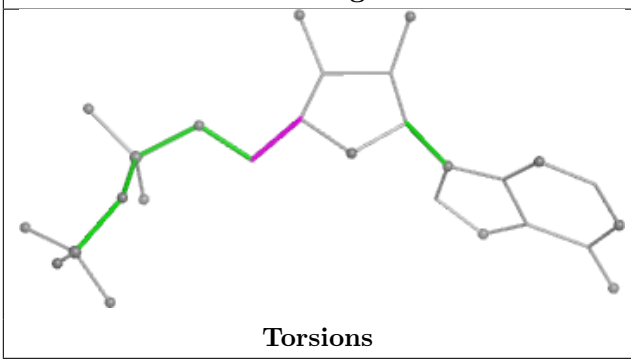
Ligand ADP B 800



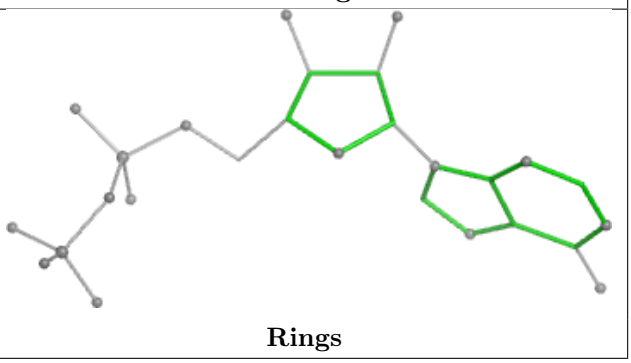
Bond lengths



Bond angles

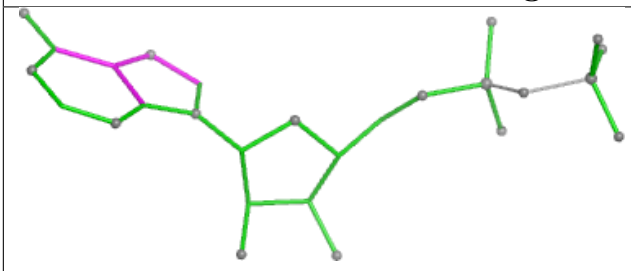


Torsions

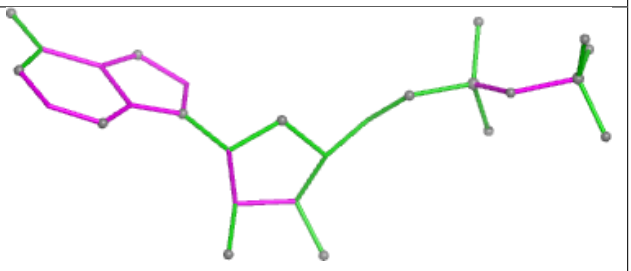


Rings

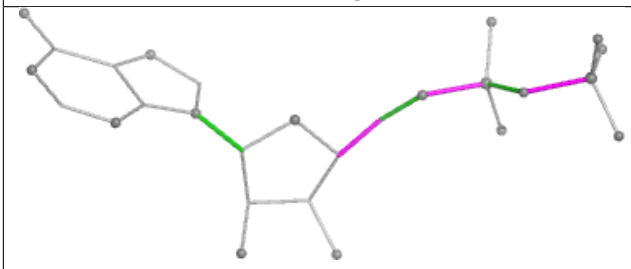
Ligand ADP E 800



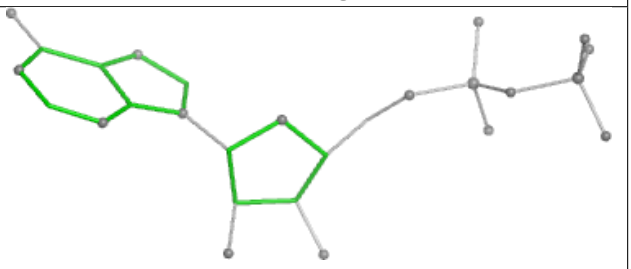
Bond lengths



Bond angles

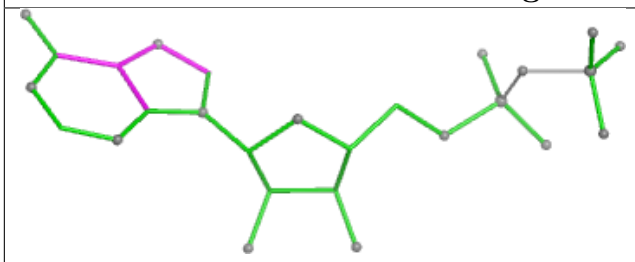


Torsions

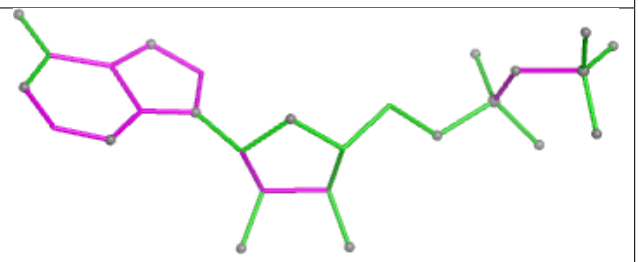


Rings

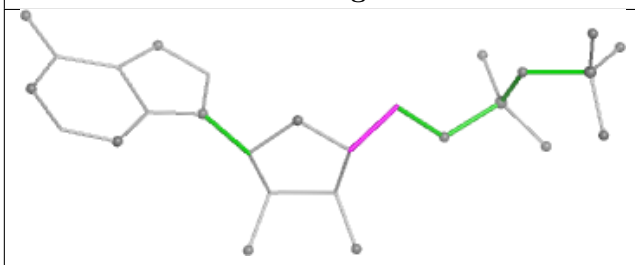
Ligand ADP A 800



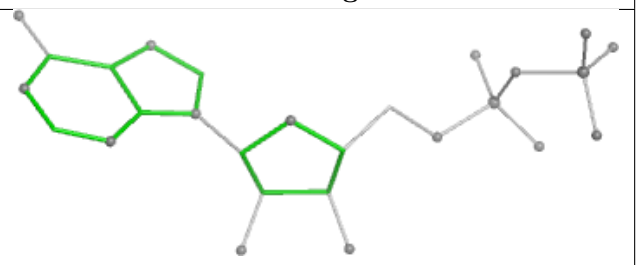
Bond lengths



Bond angles

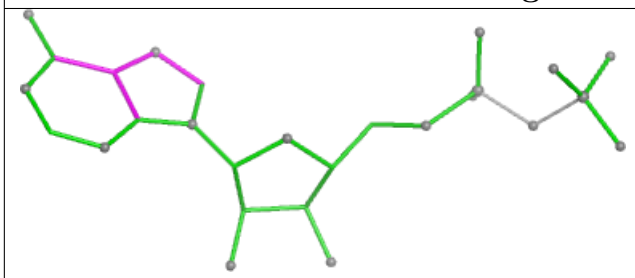


Torsions

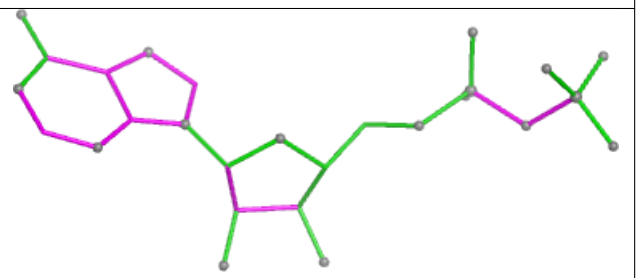


Rings

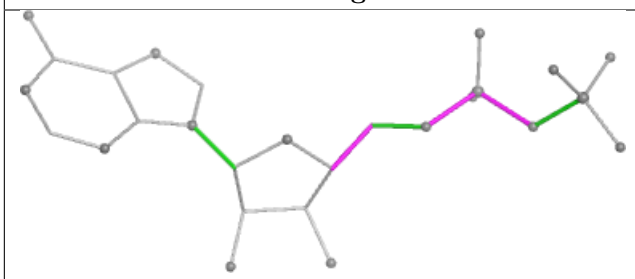
Ligand ADP G 800



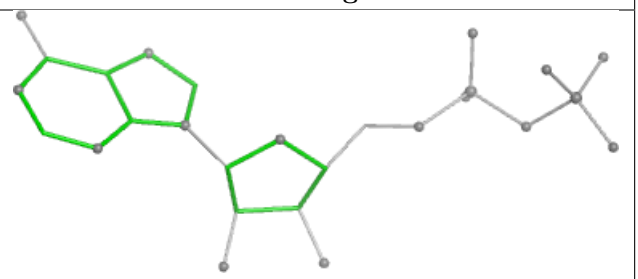
Bond lengths



Bond angles

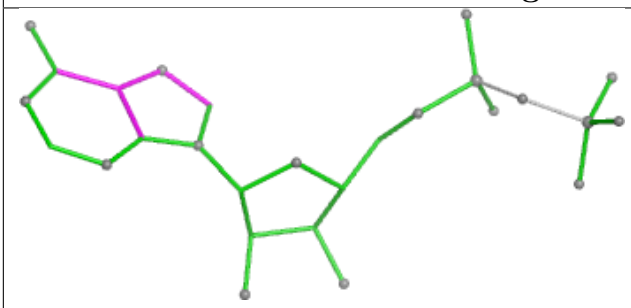


Torsions



Rings

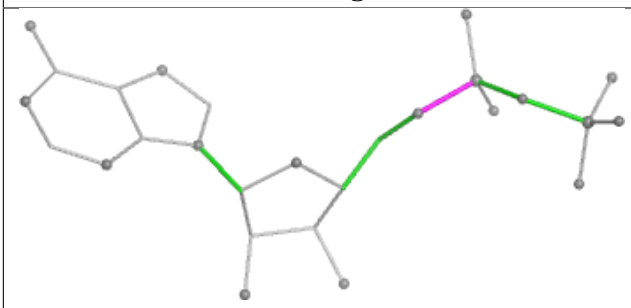
Ligand ADP C 800



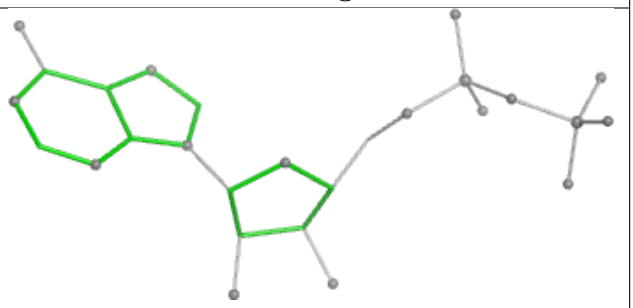
Bond lengths



Bond angles

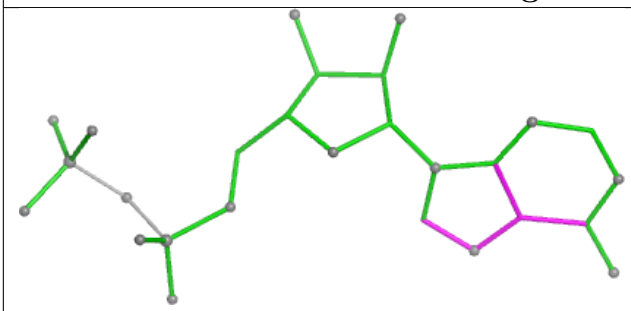


Torsions

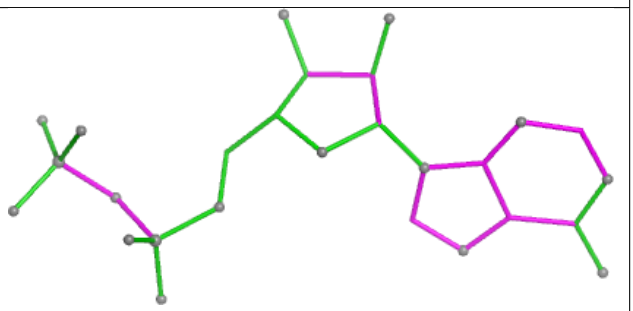


Rings

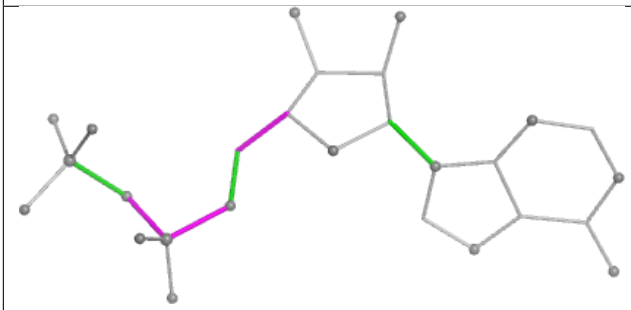
Ligand ADP D 800



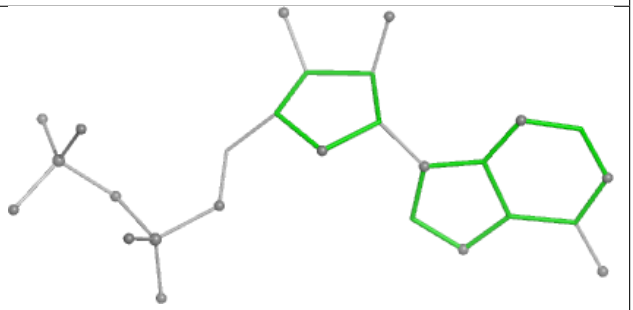
Bond lengths



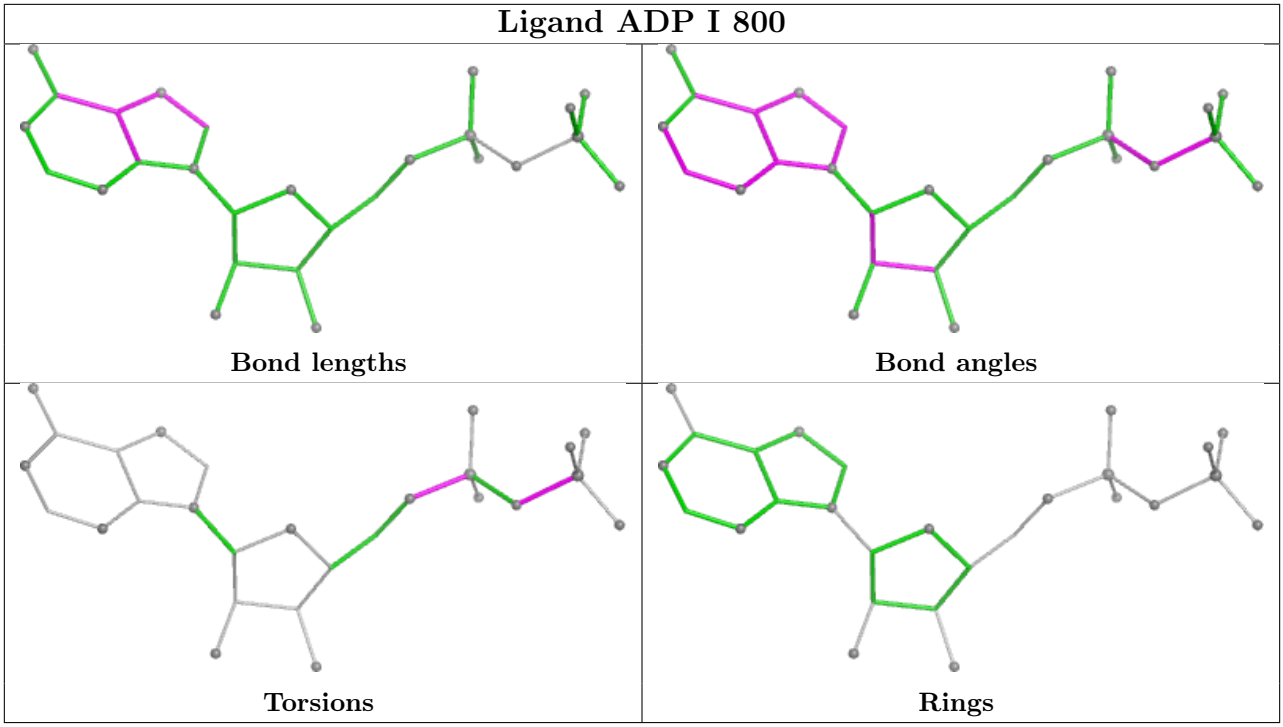
Bond angles

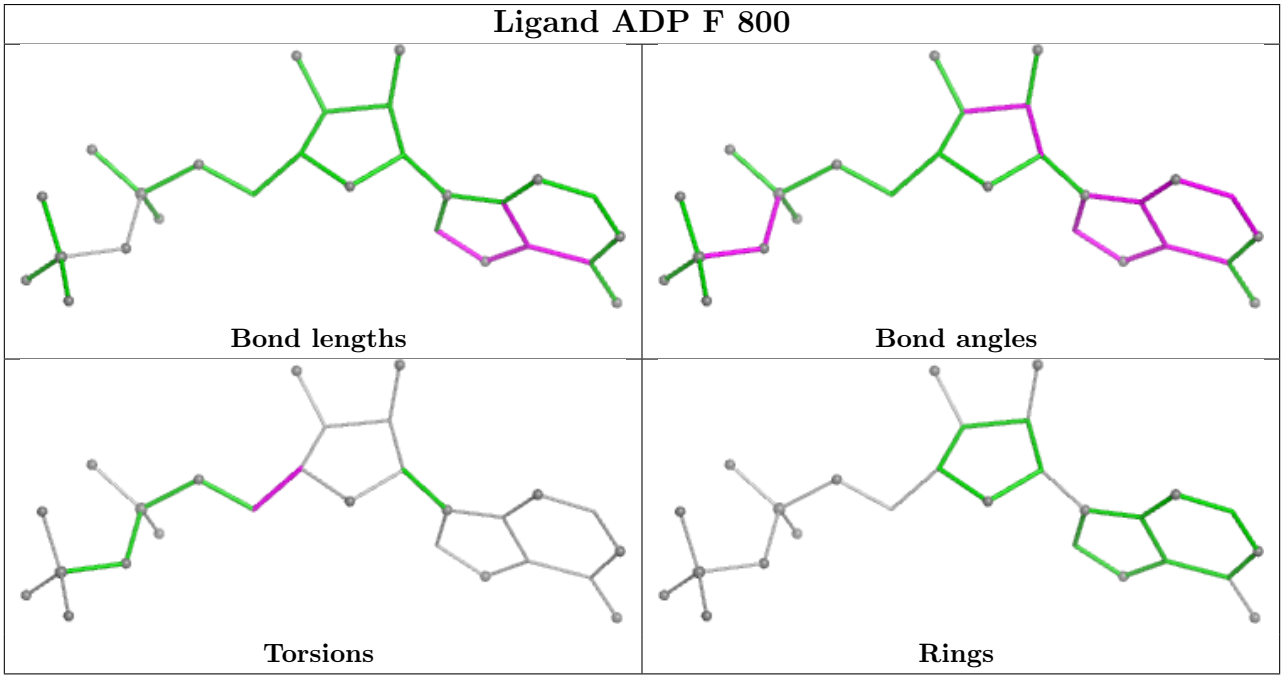


Torsions



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.

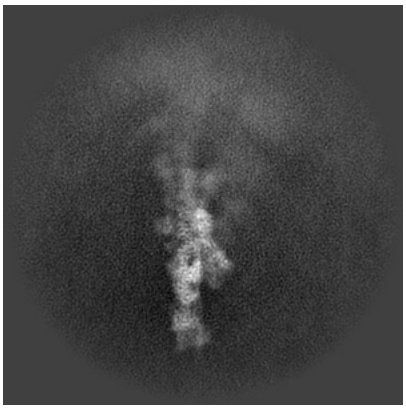
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52171. These allow visual inspection of the internal detail of the map and identification of artifacts.

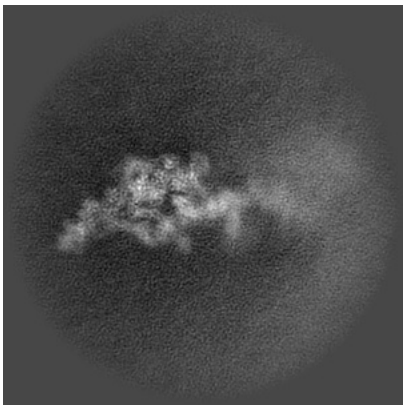
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

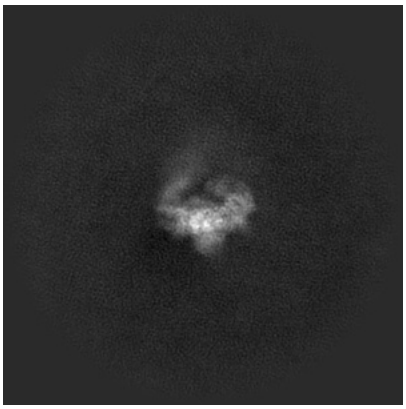
6.1.1 Primary map



X

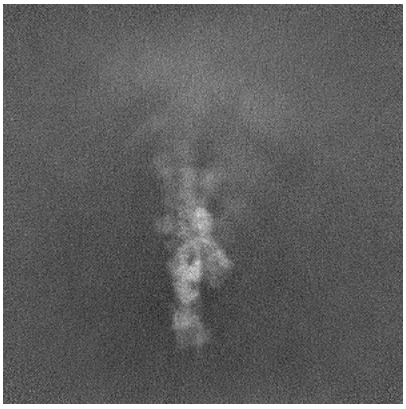


Y

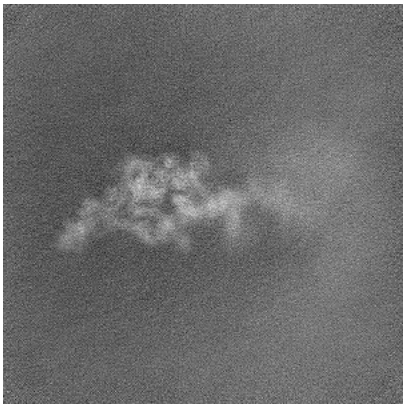


Z

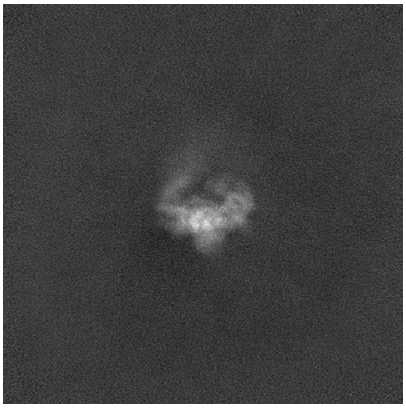
6.1.2 Raw map



X



Y



Z

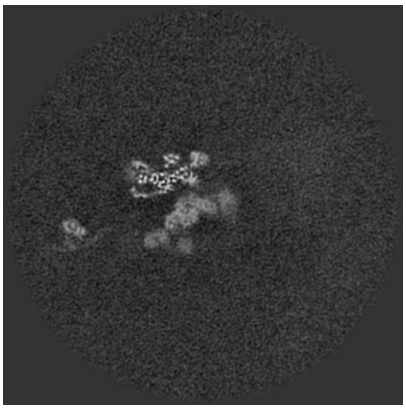
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

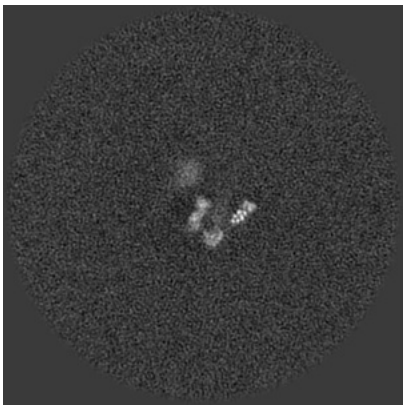
6.2.1 Primary map



X Index: 244



Y Index: 244

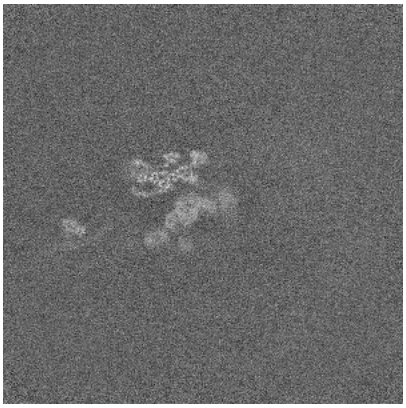


Z Index: 244

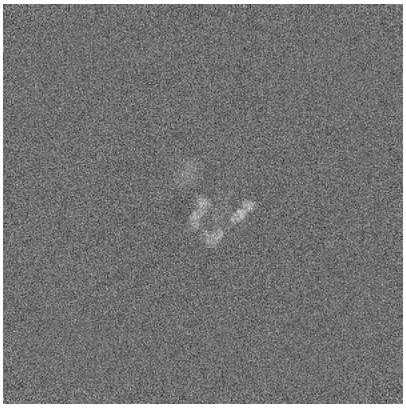
6.2.2 Raw map



X Index: 244



Y Index: 244



Z Index: 244

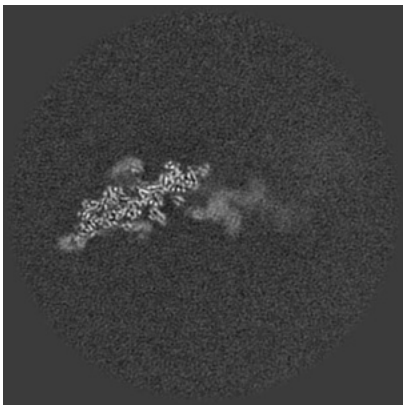
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

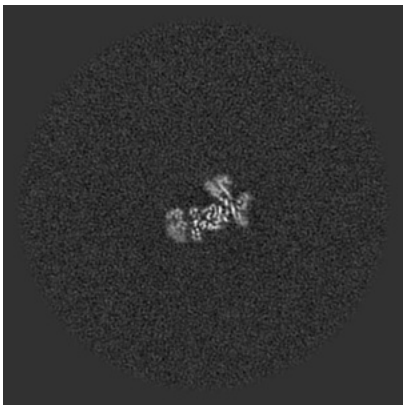
6.3.1 Primary map



X Index: 251

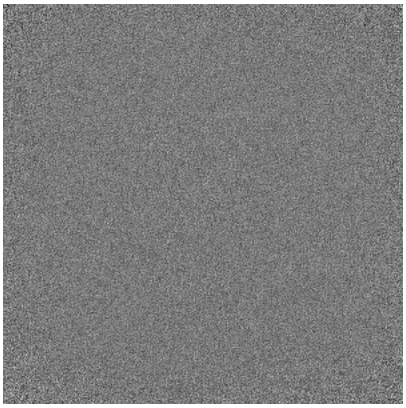


Y Index: 223

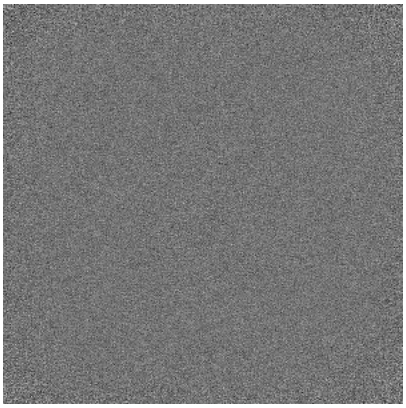


Z Index: 166

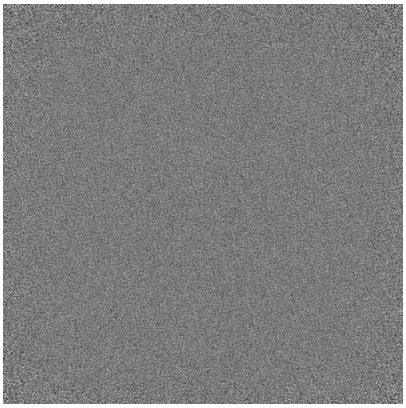
6.3.2 Raw map



X Index: 0



Y Index: 0

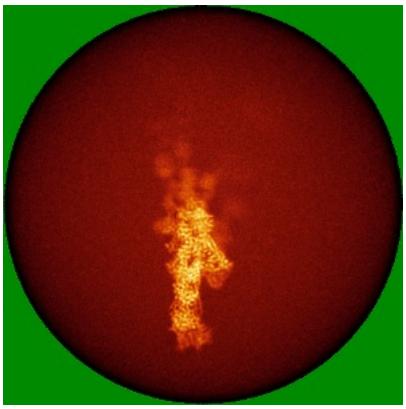


Z Index: 0

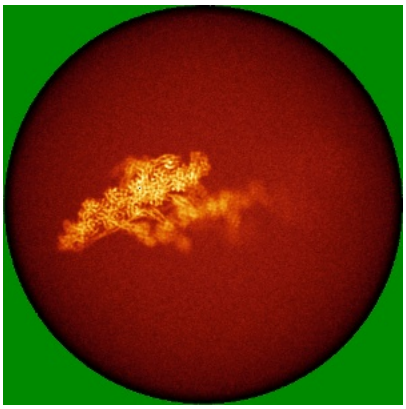
The images above show the largest variance slices of the map in three orthogonal directions.

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

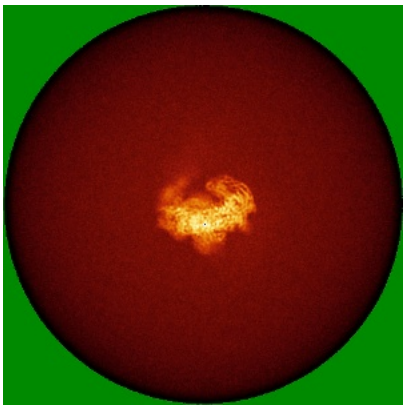
6.4.1 Primary map



X

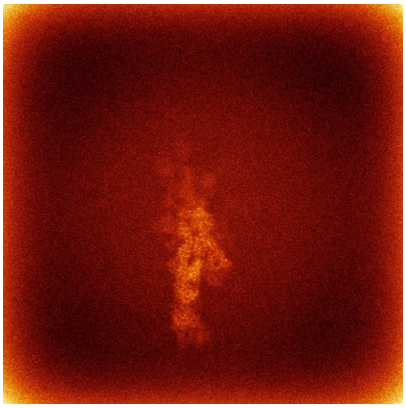


Y

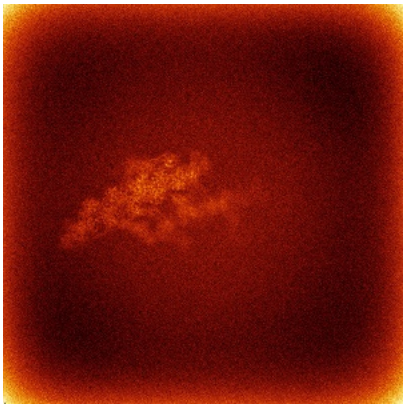


Z

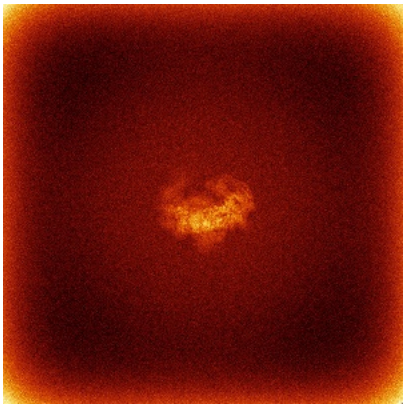
6.4.2 Raw map



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

6.5.2 Raw map



X Y Z

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

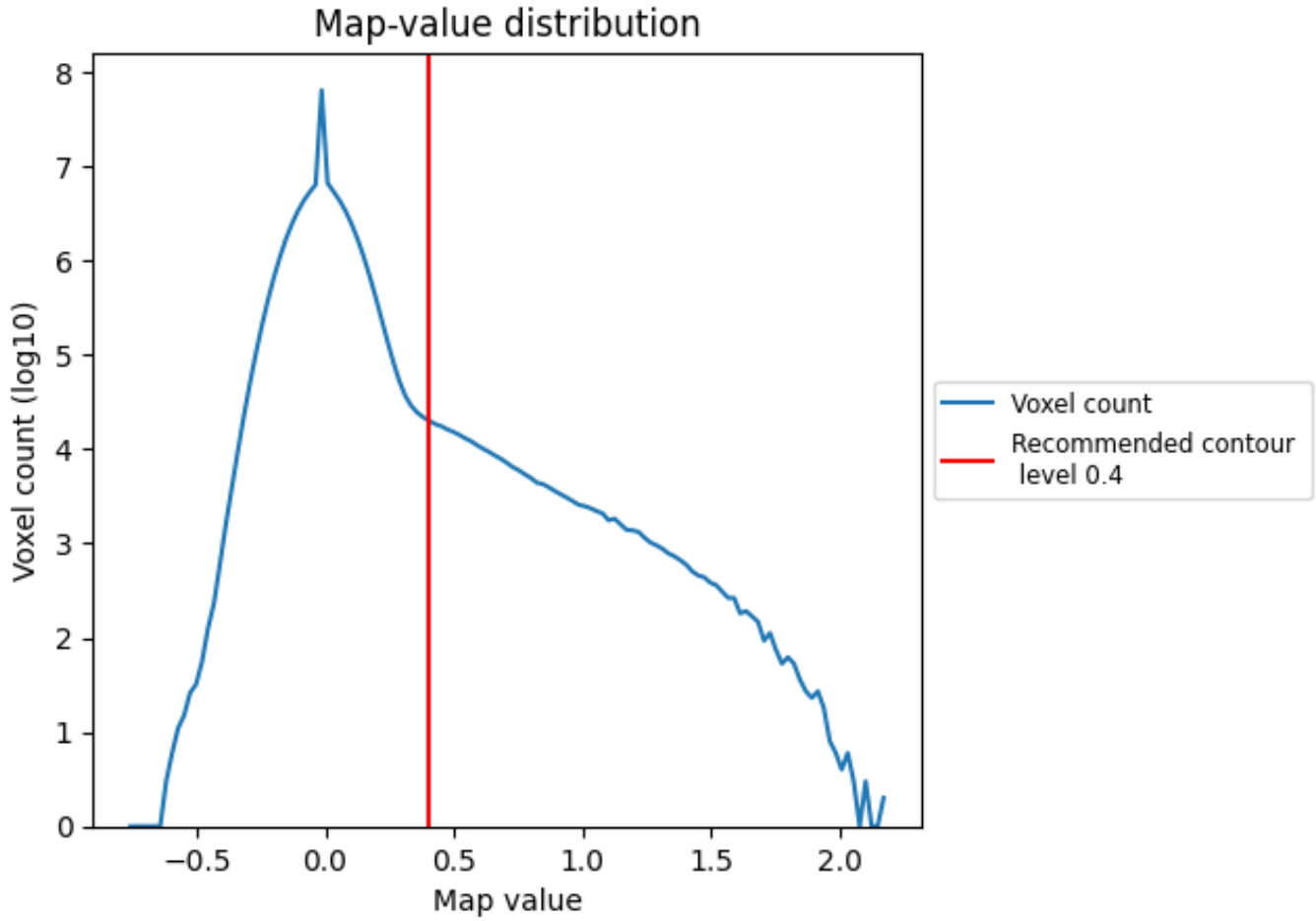
6.6 Mask visualisation (i)

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

7 Map analysis

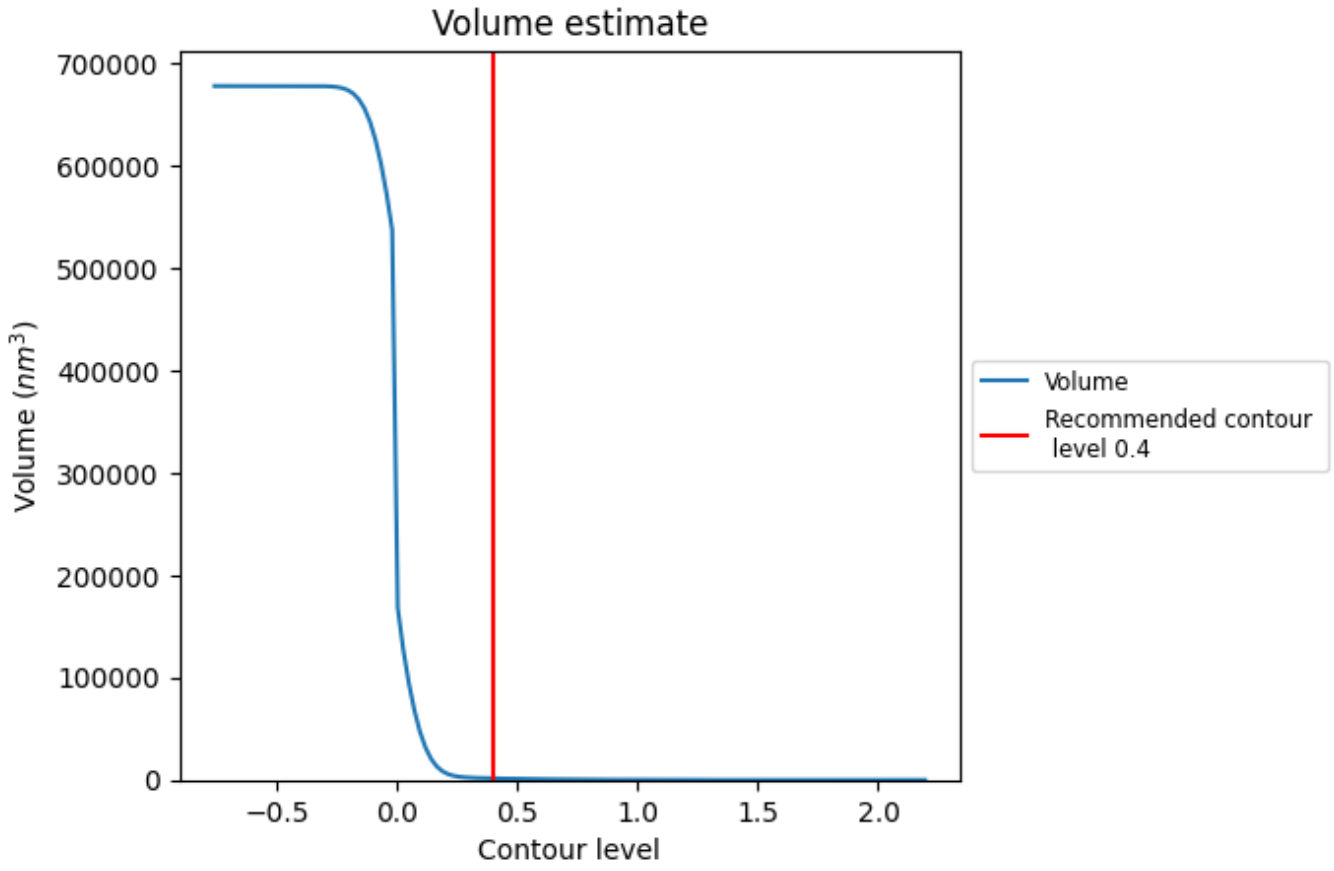
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

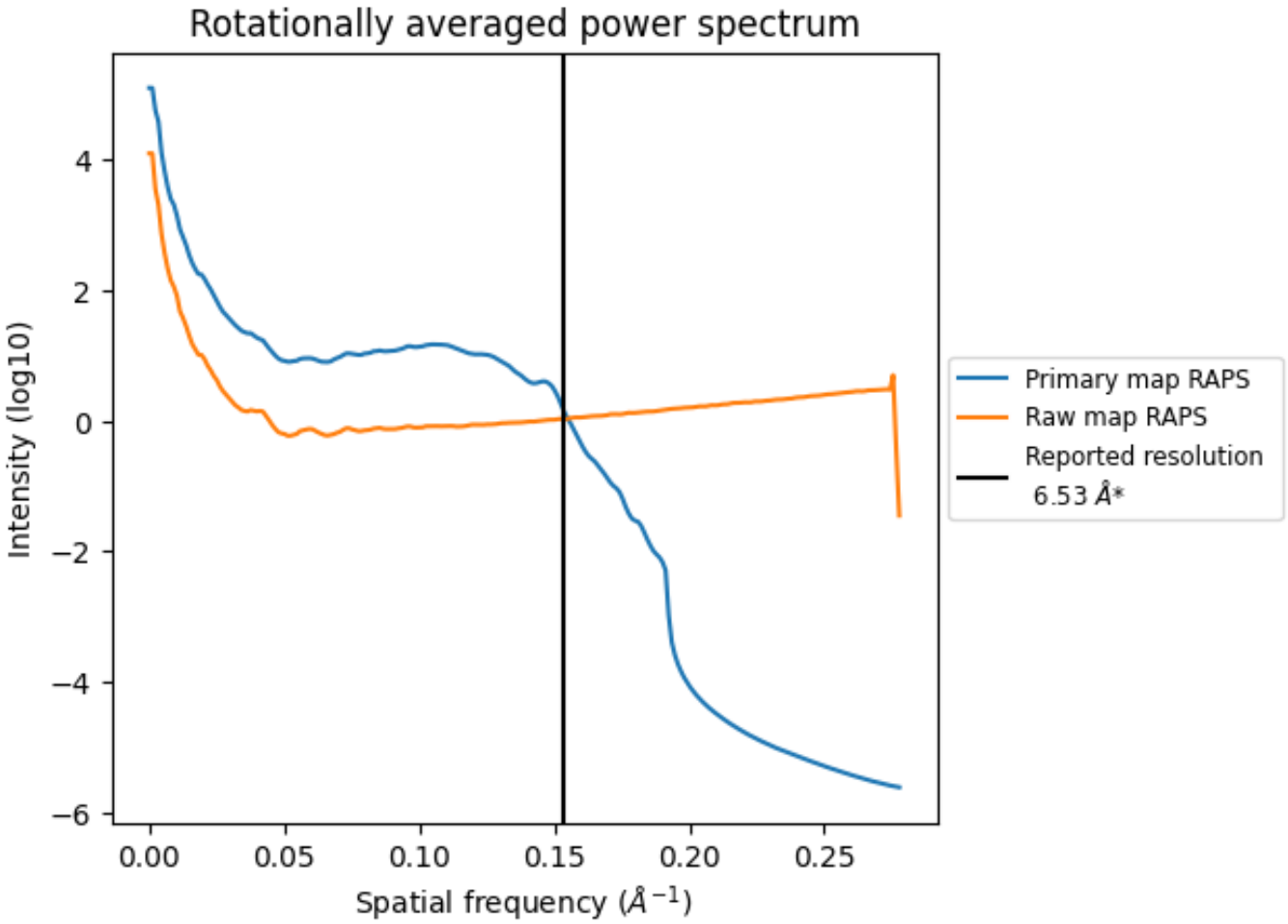
7.2 Volume estimate



The volume at the recommended contour level is 1541 nm^3; this corresponds to an approximate mass of 1392 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)

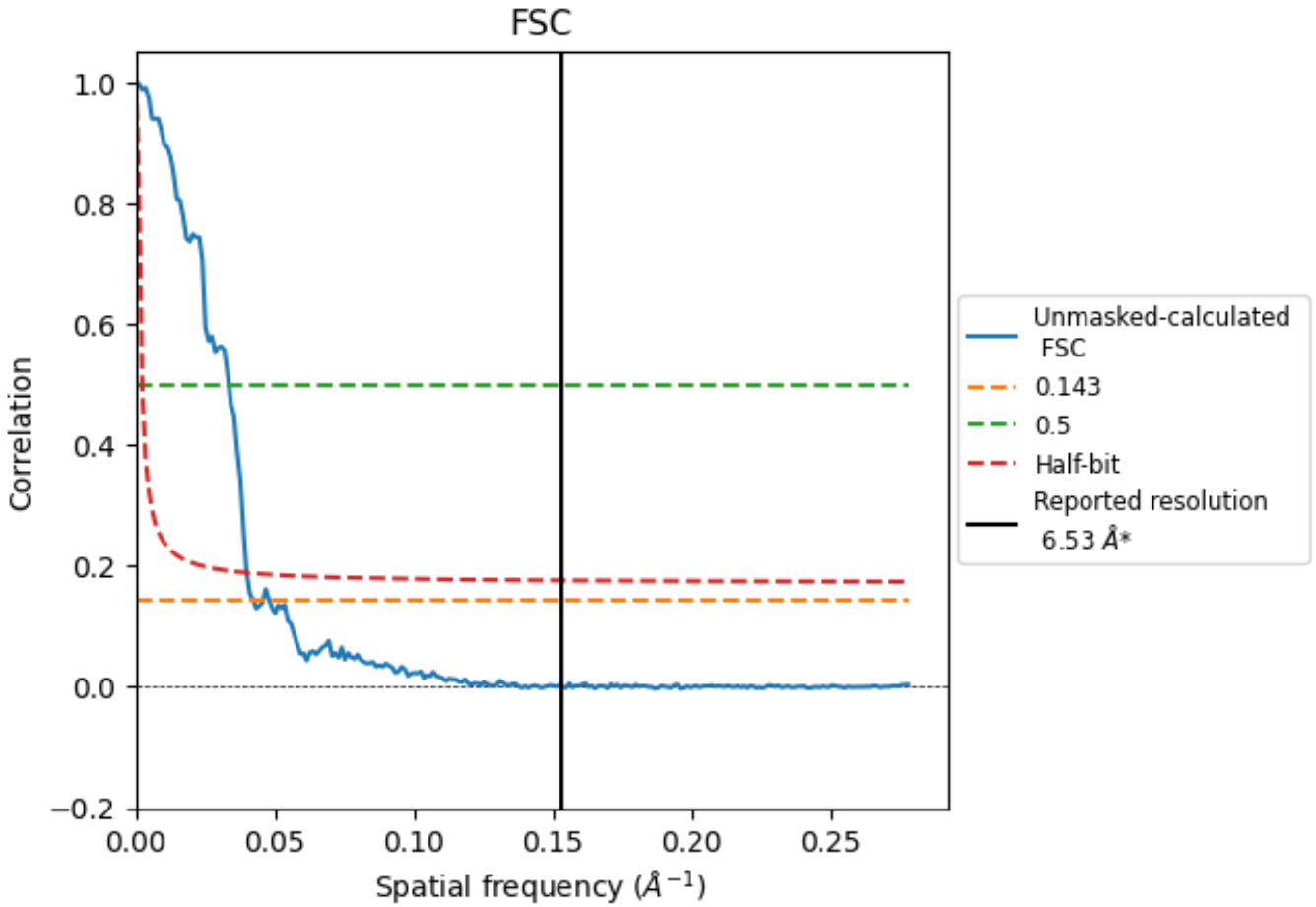


*Reported resolution corresponds to spatial frequency of 0.153 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.153 Å^{-1}

8.2 Resolution estimates (i)

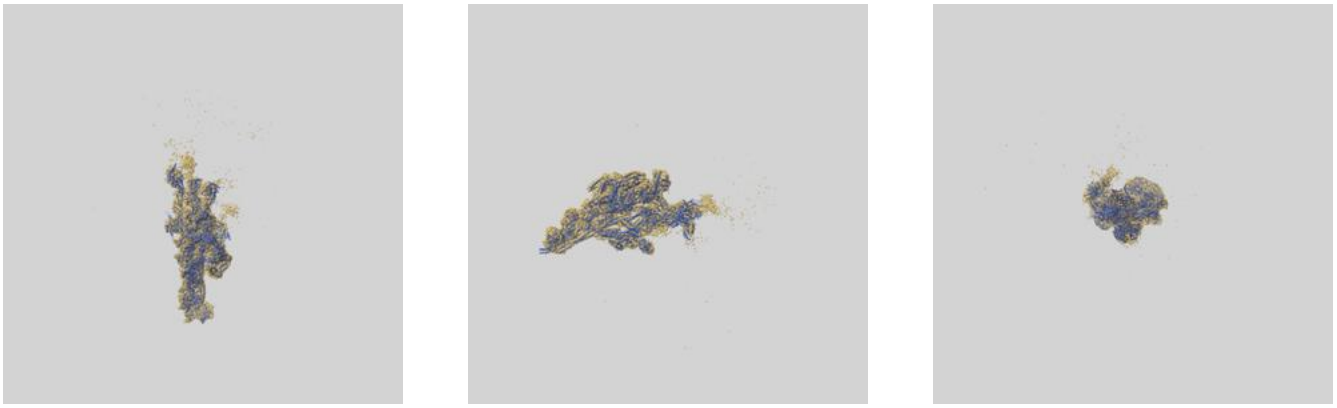
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	23.70	29.94	25.06

*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 23.70 differs from the reported value 6.53 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52171 and PDB model 9HHL. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

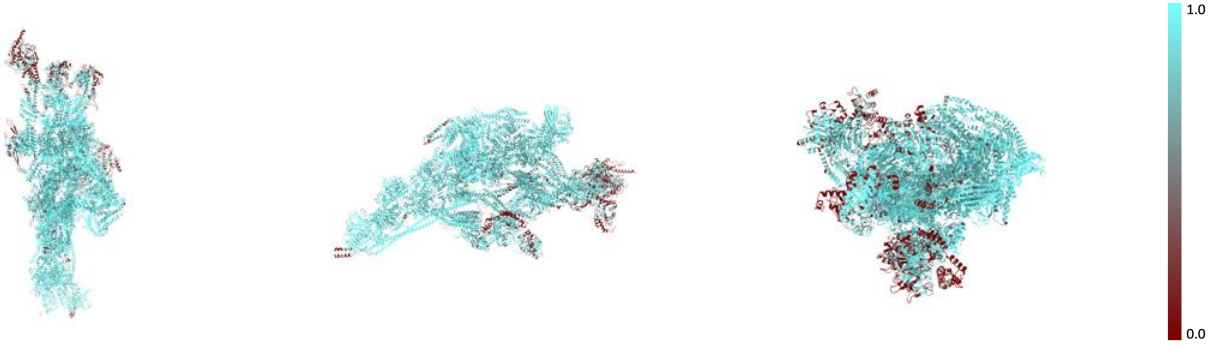
9.2 Q-score mapped to coordinate model (i)



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.

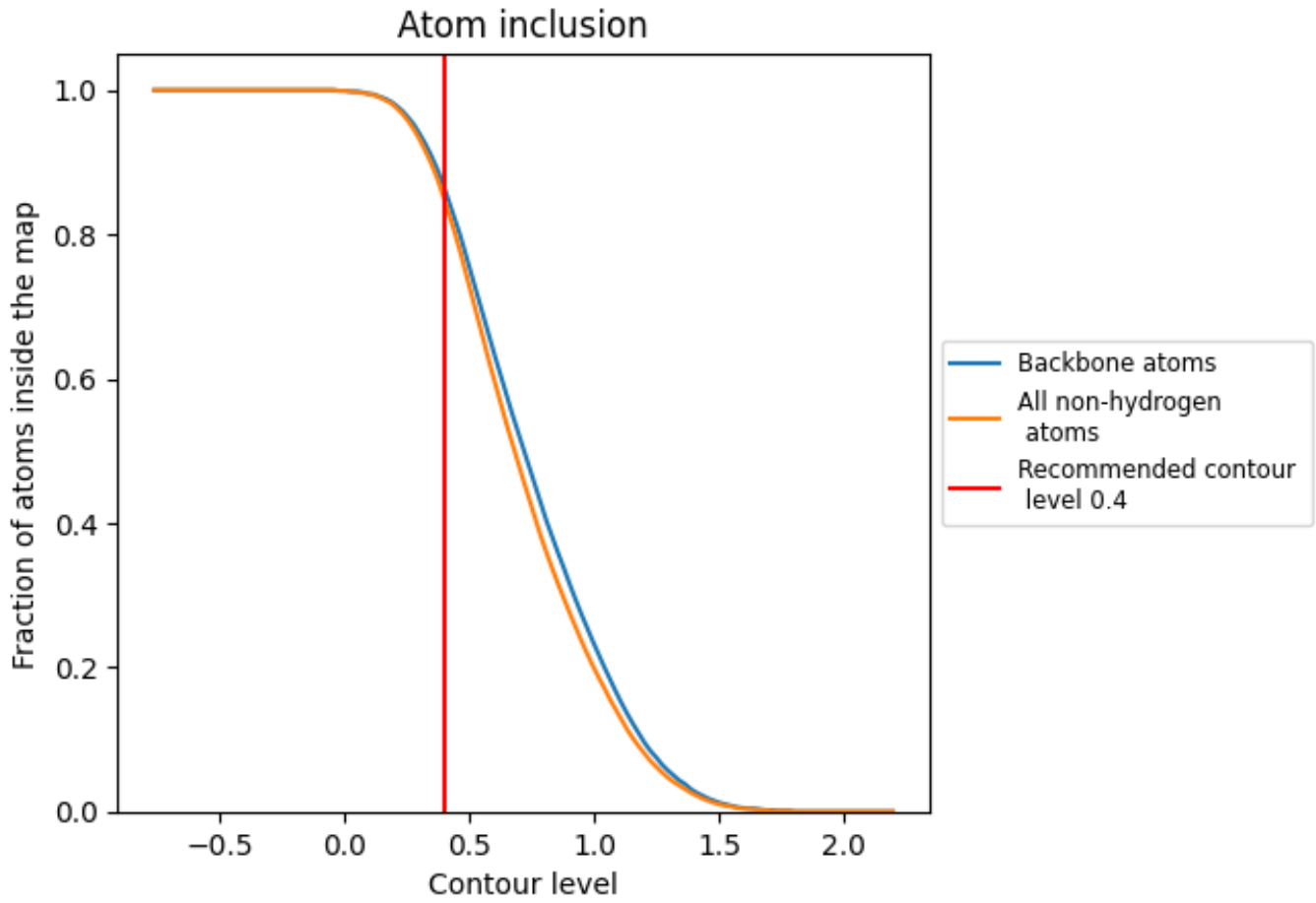
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.1820
1	0.8750	0.2260
2	0.8470	0.2370
A	0.9350	0.2240
B	0.9600	0.2420
C	0.9620	0.2430
D	0.9780	0.2620
E	0.9850	0.2690
F	0.9870	0.2710
G	0.9860	0.2690
H	0.9830	0.2740
I	0.9660	0.2570
J	0.9750	0.2570
K	0.9640	0.2080
L	0.9550	0.2370
M	0.8950	0.2020
N	0.8970	0.1900
O	0.9680	0.2120
P	0.8930	0.2300
Q	0.9520	0.2480
R	0.9540	0.2080
S	0.9730	0.2140
T	0.9080	0.2190
U	0.9240	0.1740
V	0.9730	0.2950
W	0.9500	0.1840
Y	0.9200	0.2120
e	0.7730	0.1540
f	0.8340	0.1670
g	0.7310	0.0350
h	0.8970	0.1160
j	0.6180	0.0570
m	0.8020	0.1460
n	0.6270	0.1060
o	0.7520	0.0530



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
p	0.4010	0.0390
q	0.6000	0.1290
s	0.4180	0.0560
t	0.5910	0.0880
u	0.1110	-0.0180
w	0.6930	0.0120
z	0.5430	0.0260