Full wwPDB EM Validation Report ⓘ

Jun 27, 2024 – 04:34 AM JST

PDB ID	:	8IAH
EMDB ID	:	EMD-35301
Title	:	Structure of mammalian spectrin-actin junctional complex of membrane skeleton, State I, Global map
Authors	:	Li, N.; Chen, S.; Gao, N.
Deposited on	:	2023-02-08
Resolution	:	3.60 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:

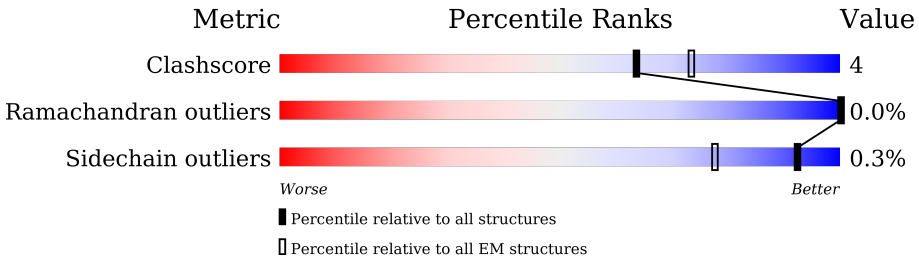
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	744	7% 93%
1	1	744	40% 5% 55%
1	2	744	32% 7% 60%
2	3	724	44% 6% 50%
2	4	724	33% 6% 61%
2	9	724	6% 93%
3	5	405	28% 70%
3	6	405	7% 28% 69%

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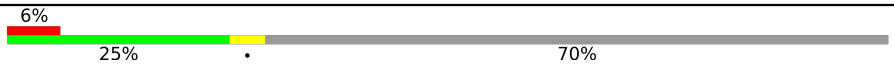
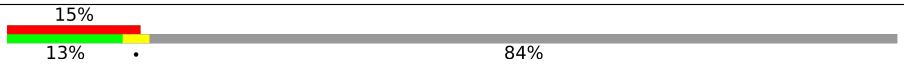
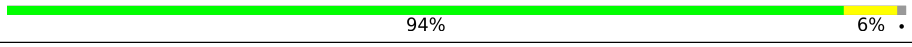
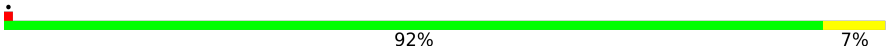
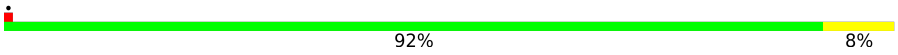
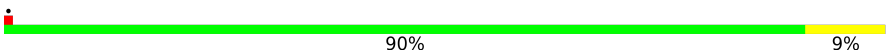
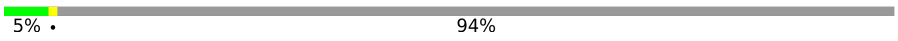
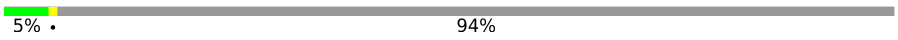
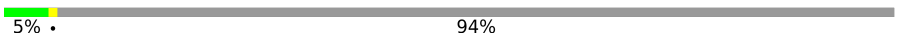
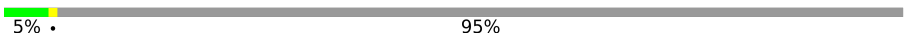
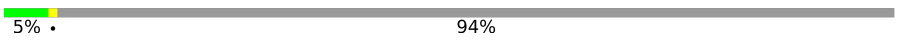
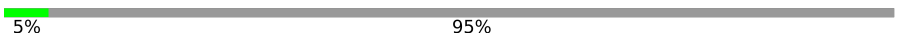
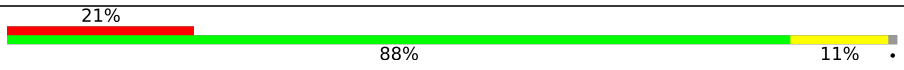
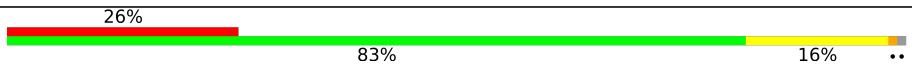
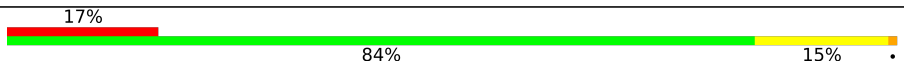
Mol	Chain	Length	Quality of chain
3	7	405	
4	8	2417	
5	A	375	
5	B	375	
5	C	375	
5	D	375	
5	E	375	
5	F	375	
5	G	375	
5	H	375	
5	I	375	
5	J	375	
5	K	375	
5	L	375	
6	M	2148	
6	N	2148	
6	O	2148	
6	P	2148	
6	Q	2148	
6	R	2148	
6	S	2148	
6	T	2148	
7	U	248	
8	V	248	
8	W	248	

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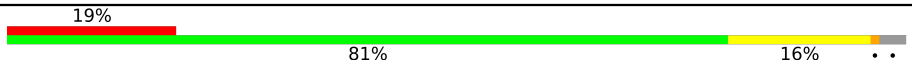
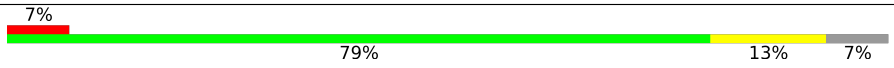
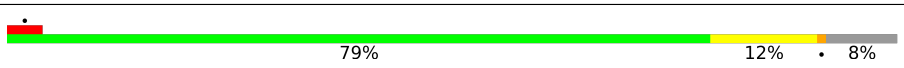
Mol	Chain	Length	Quality of chain
8	X	248	
9	Y	359	
10	Z	107	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 74320 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 Adducin 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	54	Total	C	N	O	S	0	0
			453	280	80	87	6		
1	1	334	Total	C	N	O	S	0	0
			2585	1647	448	478	12		
1	2	294	Total	C	N	O	S	0	0
			2263	1444	391	418	10		

- Molecule 2 is a protein called Beta-adducin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	365	Total	C	N	O	S	0	0
			2870	1812	500	538	20		
2	4	280	Total	C	N	O	S	0	0
			2157	1369	369	403	16		
2	9	54	Total	C	N	O	S	0	0
			455	280	84	88	3		

- Molecule 3 is a protein called Dematin actin binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	123	Total	C	N	O	S	0	0
			1008	649	175	182	2		
3	6	125	Total	C	N	O	S	0	0
			963	619	163	179	2		
3	7	121	Total	C	N	O	S	0	0
			976	624	173	177	2		

- Molecule 4 is a protein called Spectrin alpha, erythrocytic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	379	Total	C	N	O	S	0	0
			2799	1749	488	553	9		

- Molecule 5 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	374	Total	C	N	O	S	0	0
			2907	1837	490	560	20		
5	B	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
5	C	373	Total	C	N	O	S	0	0
			2909	1841	489	557	22		
5	D	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
5	E	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
5	F	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
5	G	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
5	H	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
5	I	373	Total	C	N	O	S	0	0
			2909	1841	489	557	22		
5	J	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
5	K	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		
5	L	374	Total	C	N	O	S	0	0
			2917	1845	490	560	22		

- Molecule 6 is a protein called Spectrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	130	Total	C	N	O	S	0	0
			1065	671	200	188	6		
6	N	122	Total	C	N	O	S	0	0
			1004	638	189	171	6		
6	O	131	Total	C	N	O	S	0	0
			1073	675	201	191	6		
6	P	117	Total	C	N	O	S	0	0
			960	609	181	164	6		
6	Q	129	Total	C	N	O	S	0	0
			1057	667	199	185	6		
6	R	117	Total	C	N	O	S	0	0
			960	609	181	164	6		
6	S	486	Total	C	N	O	S	0	0
			3983	2511	721	739	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	128	Total	C	N	O	S	0	0
			1048	660	197	185	6		

- Molecule 7 is a protein called Tropomyosin-1.9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	246	Total	C	N	O	S	0	0
			1992	1208	357	421	6		

- Molecule 8 is a protein called Tropomyosin 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	246	Total	C	N	O	S	0	0
			2011	1218	362	421	10		
8	W	248	Total	C	N	O	S	0	0
			2017	1222	364	421	10		
8	X	241	Total	C	N	O	S	0	0
			1974	1196	356	413	9		

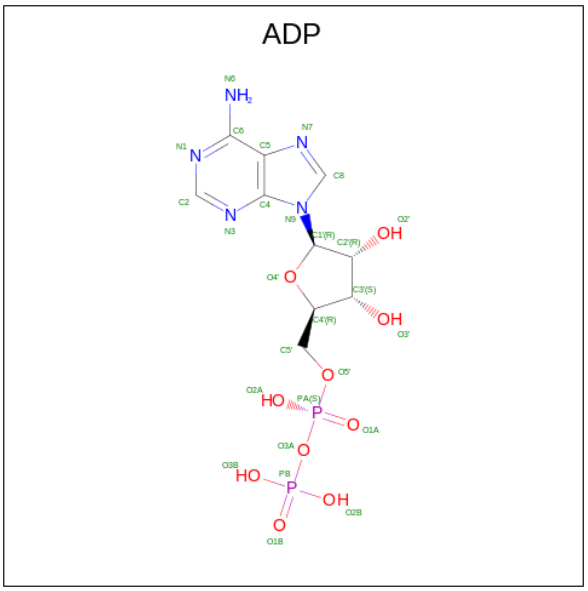
- Molecule 9 is a protein called Tropomodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Y	333	Total	C	N	O	S	0	0
			2547	1599	443	496	9		

- Molecule 10 is a protein called SH3 domain-binding glutamic acid-rich-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	98	Total	C	N	O	S	0	0
			798	513	131	151	3		

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



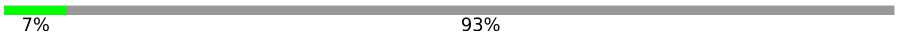
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

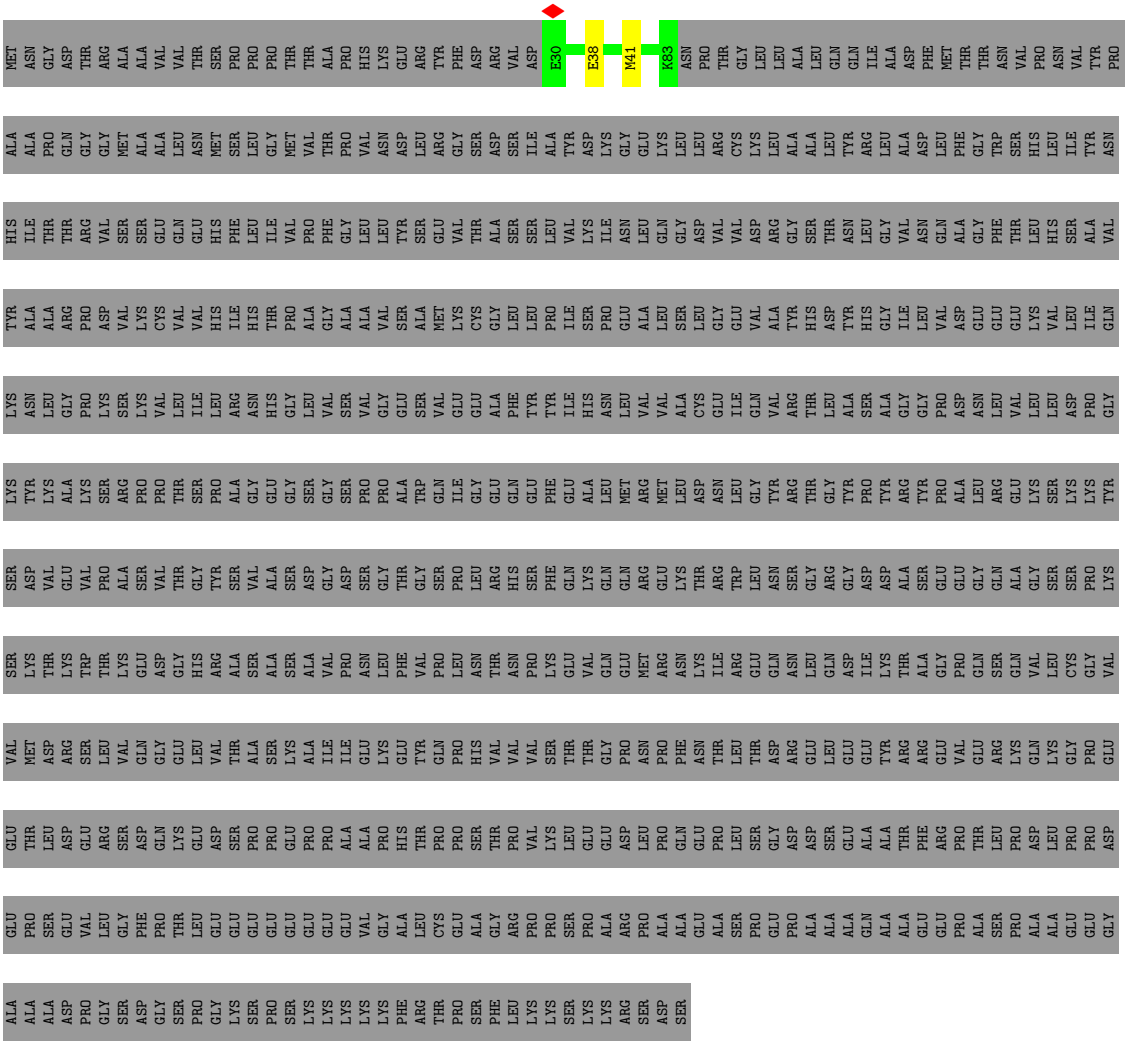
3 Residue-property plots (i)

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: Adducin 1

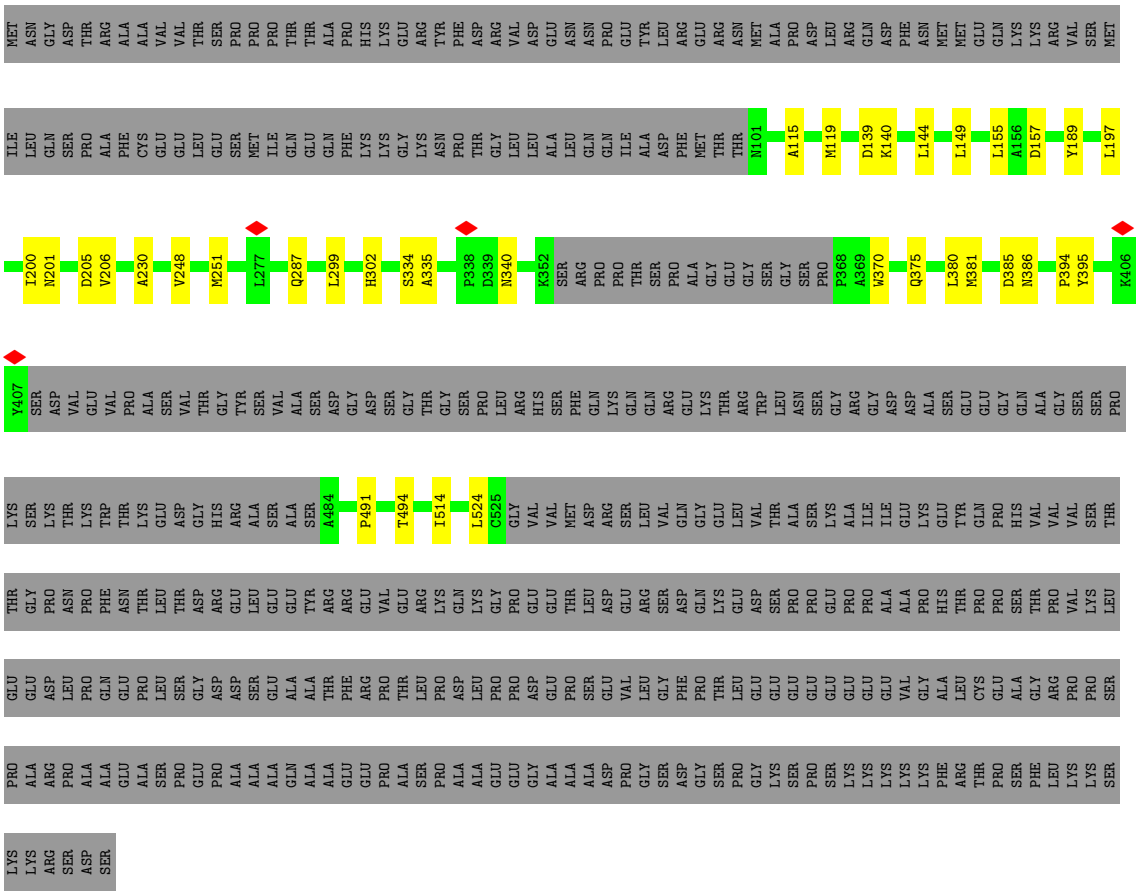
Chain 0:





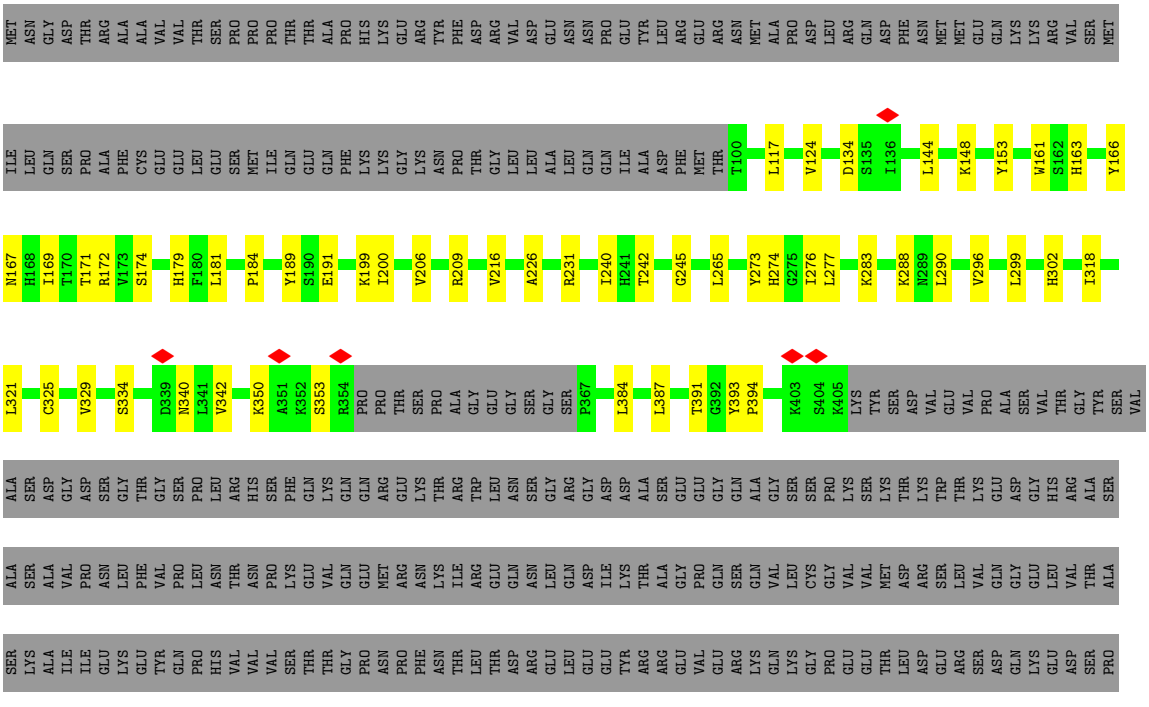
- Molecule 1: Adducin 1

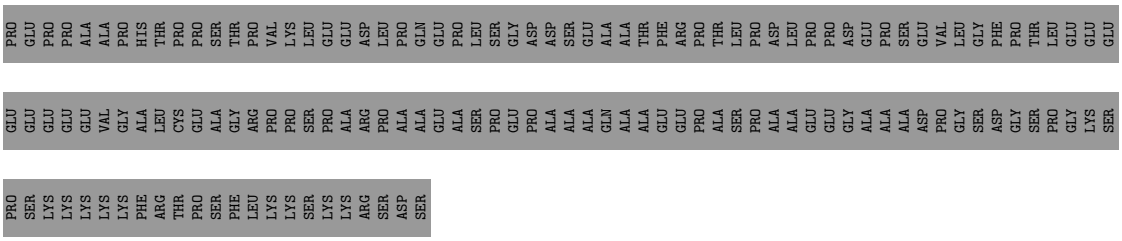
Chain 1:



• Molecule 1: Adducin 1

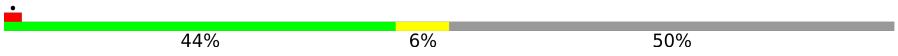
Chain 2:

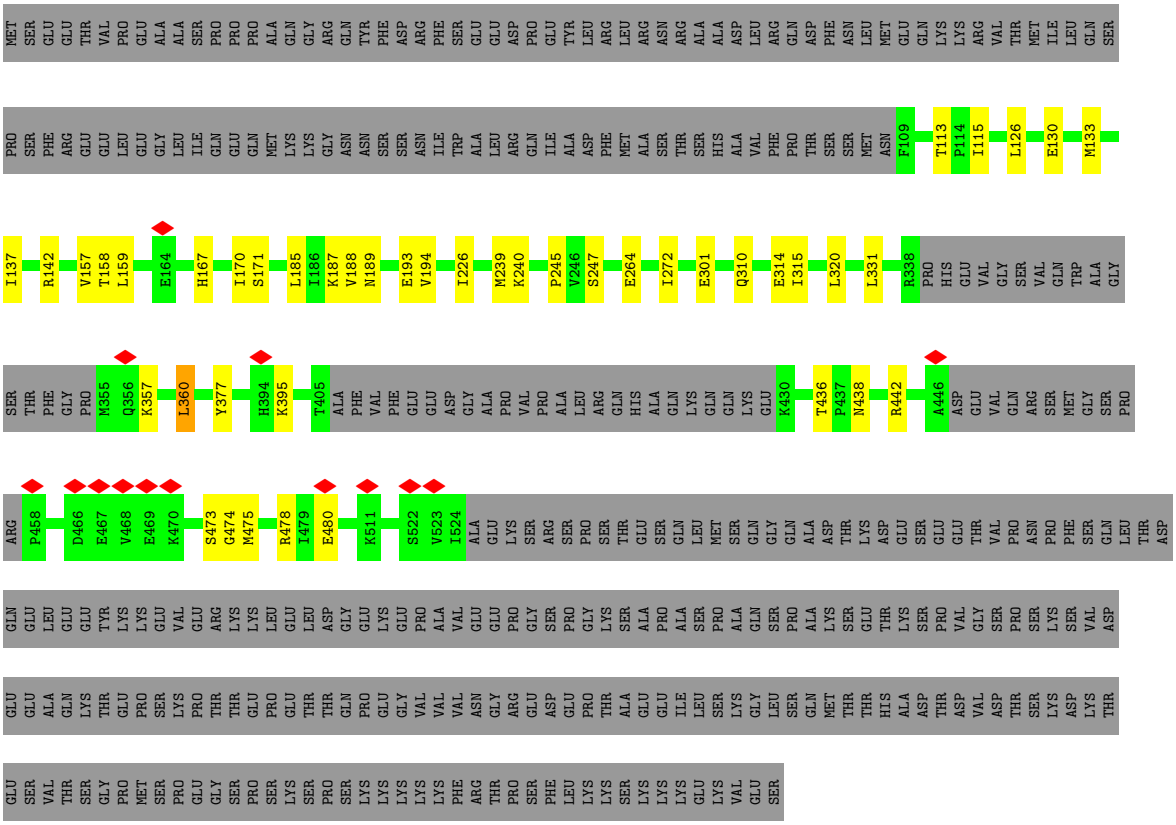




• Molecule 2: Beta-adducin

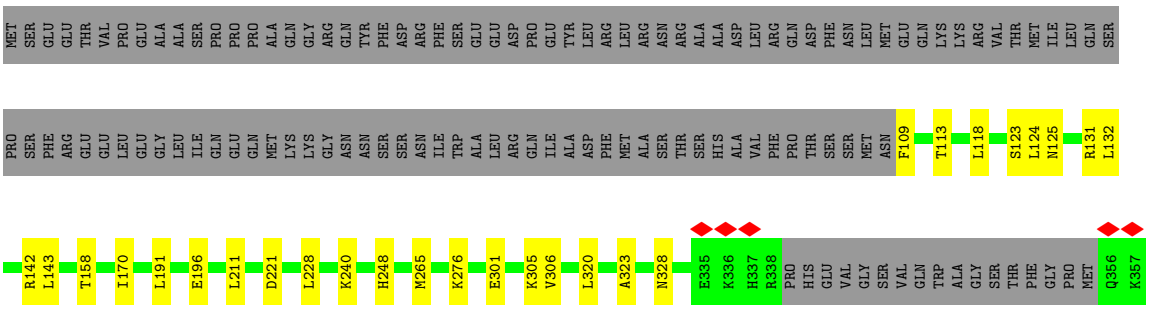
Chain 3:

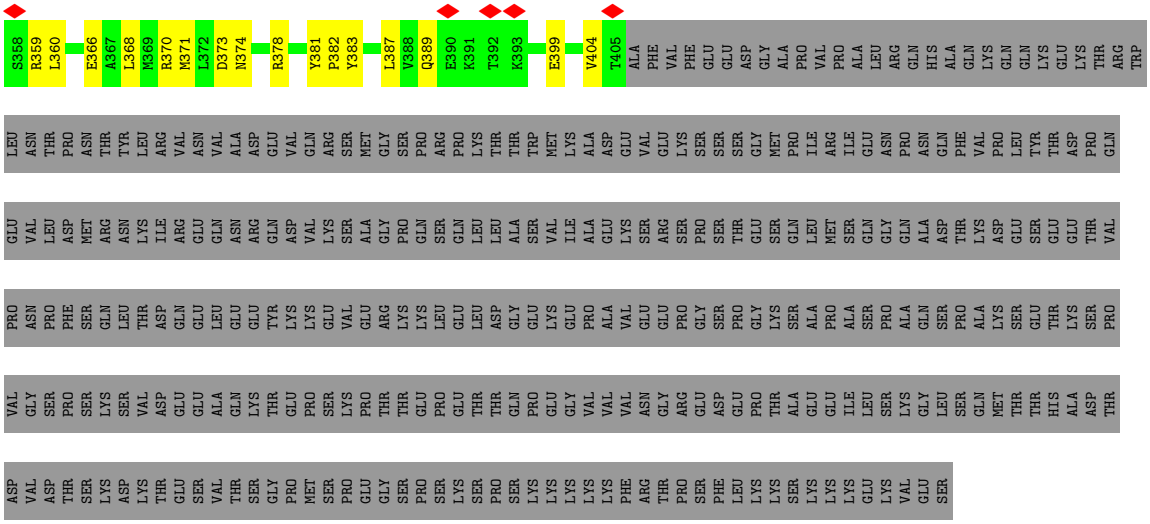




• Molecule 2: Beta-adducin

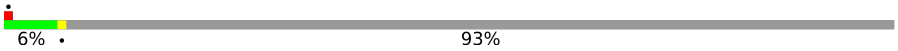
Chain 4:





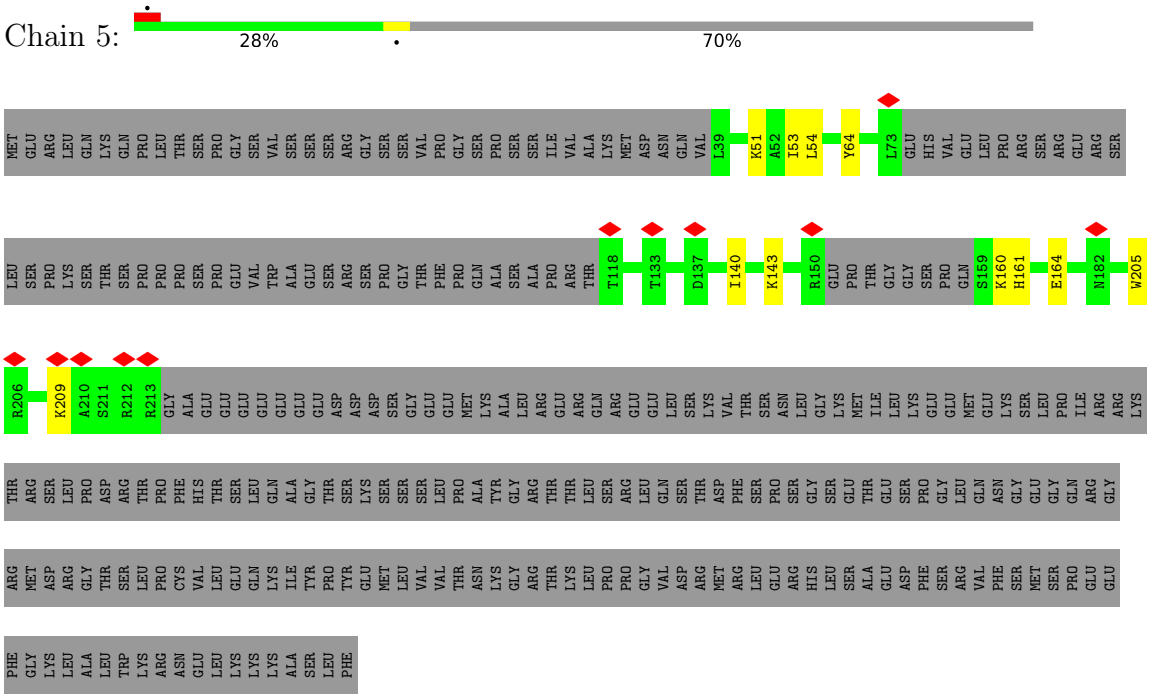
• Molecule 2: Beta-adducin

Chain 9:



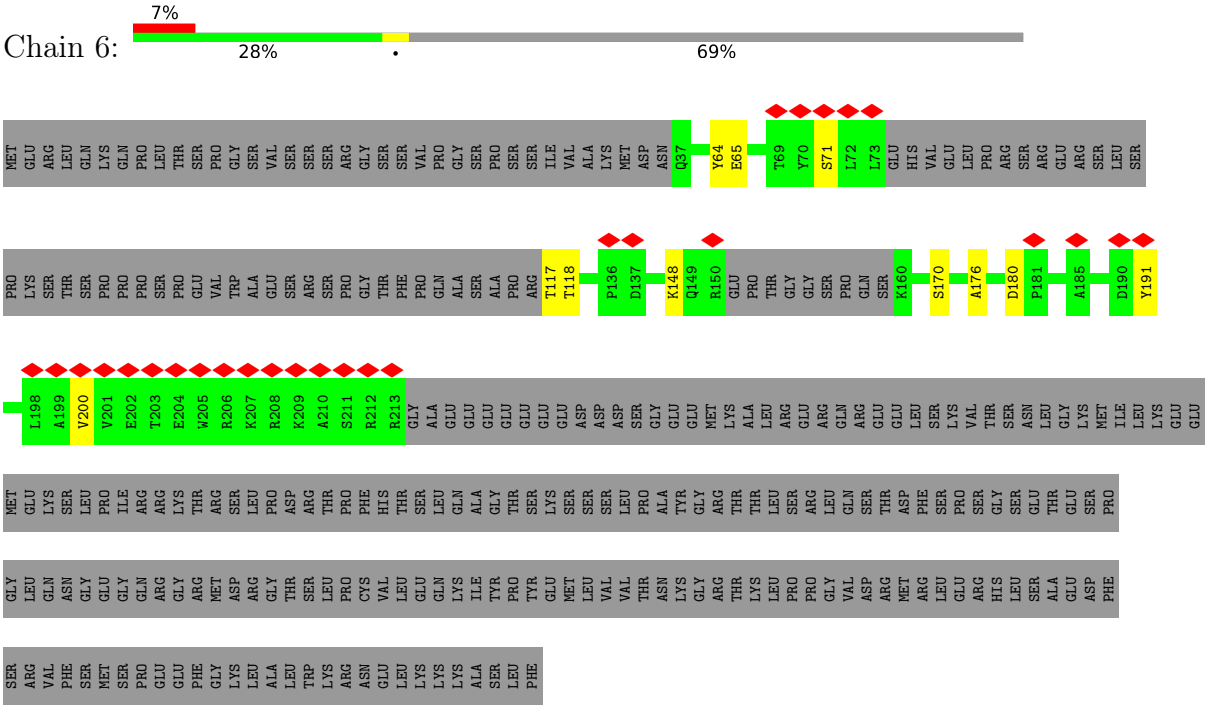
• Molecule 3: Dematin actin binding protein

Chain 5:



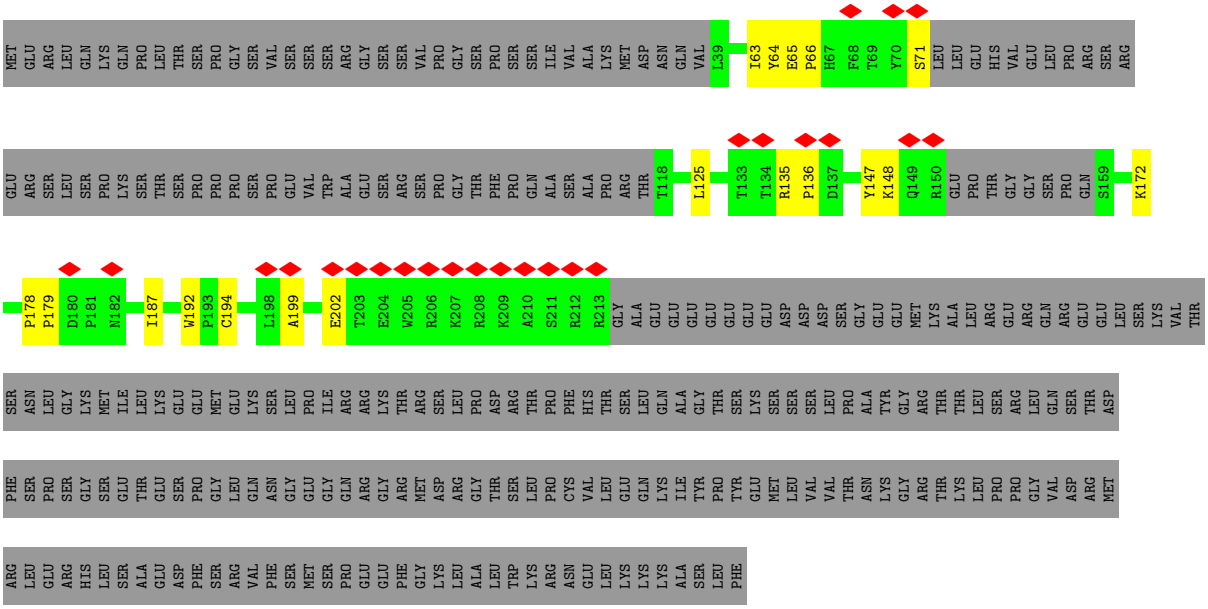
• Molecule 3: Dematin actin binding protein

Chain 6:



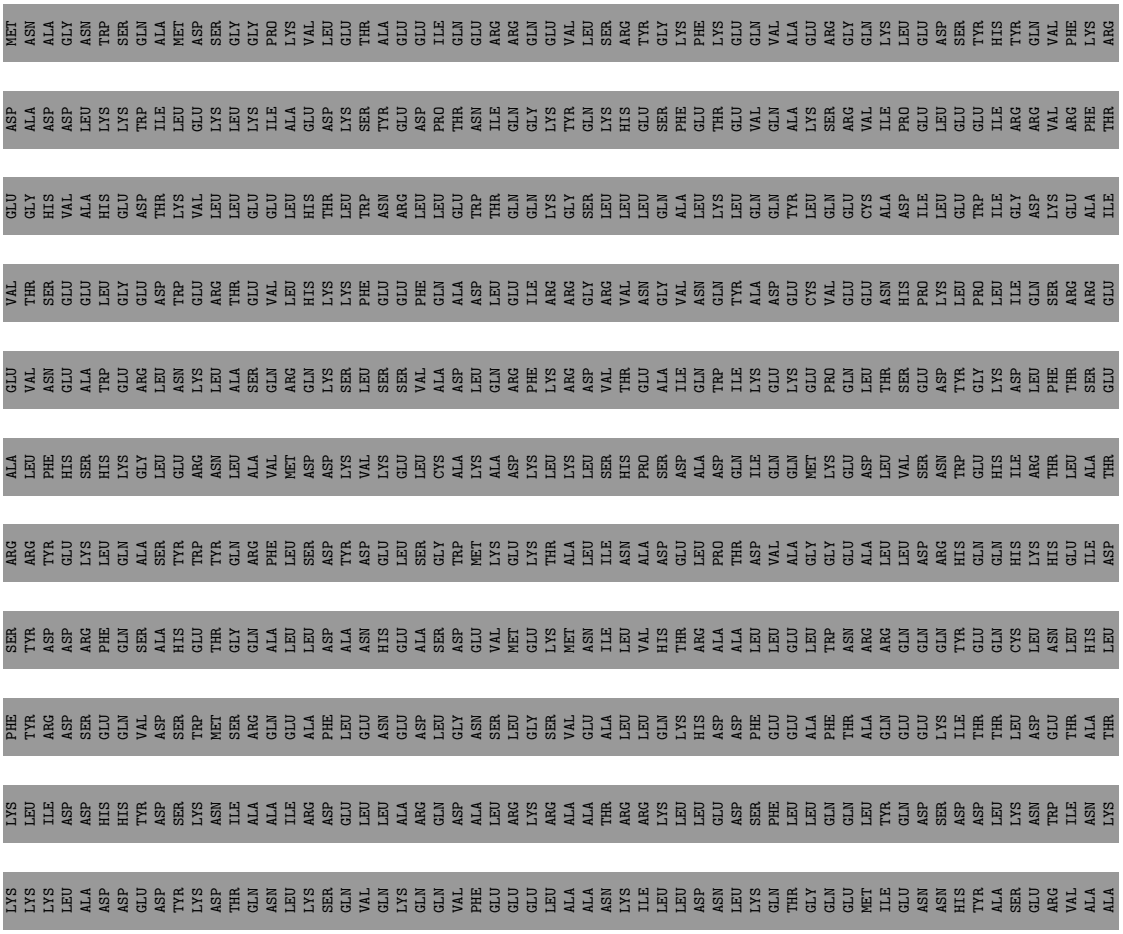
• Molecule 3: Dematin actin binding protein

Chain 7:



- Molecule 4: Spectrin alpha, erythrocytic 1

Chain 8:



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

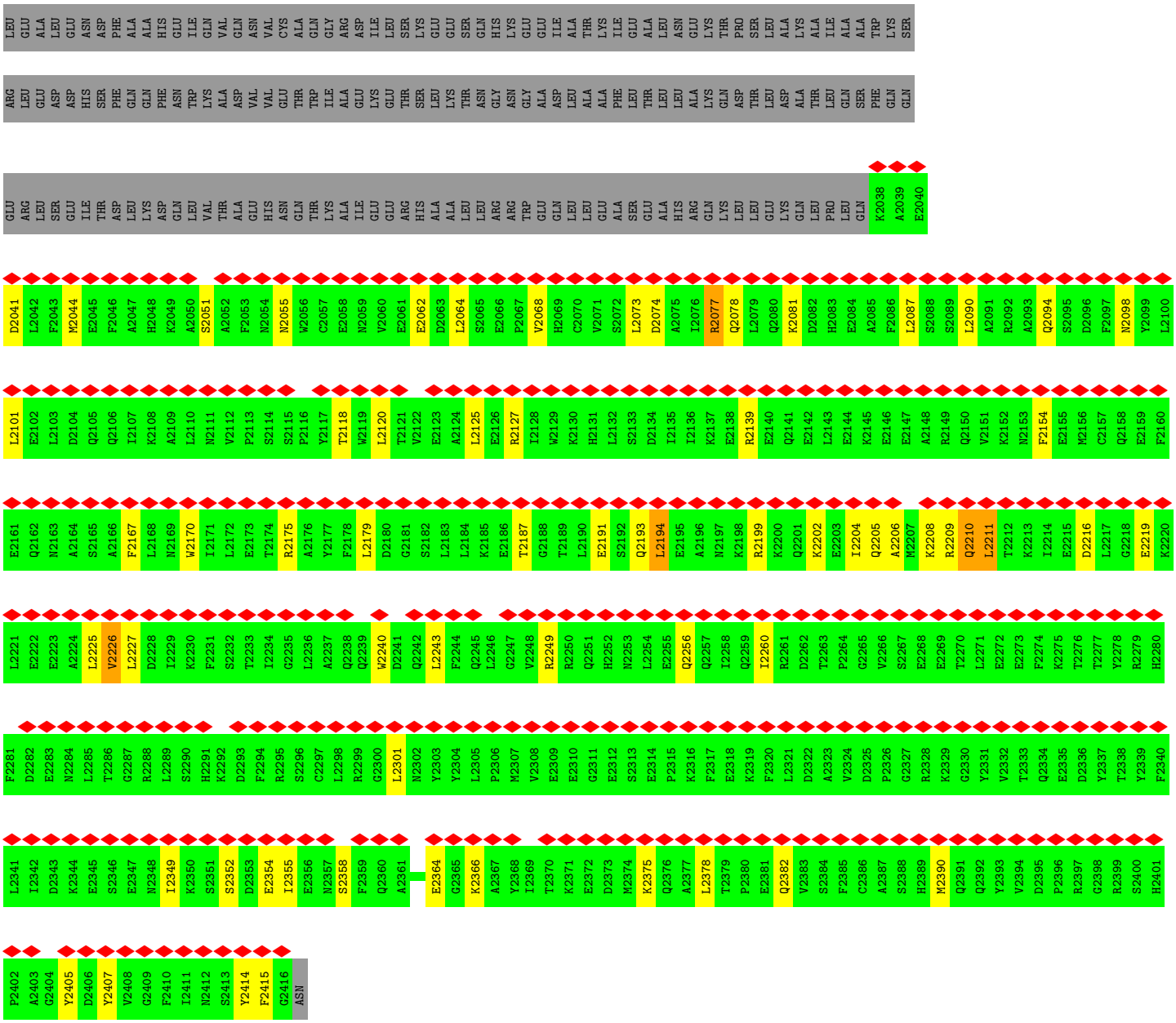
LEU GLY ASN ALA LEU VAL GLU ARG ARG ALA CYS ASP GLY ASN GLU GLU THR VAL LYS GLY GLN VAL GLU GLU LEU GLU LYS GLU TRP ASN HIS LEU LEU GLU ARG THR ALA ASP LYS GLY GLN LYS LEU ASN GLU ALA SER ARG GLN GLN ARG PHE ASN THR GLY ILE ARG ASP PHE GLU

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

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

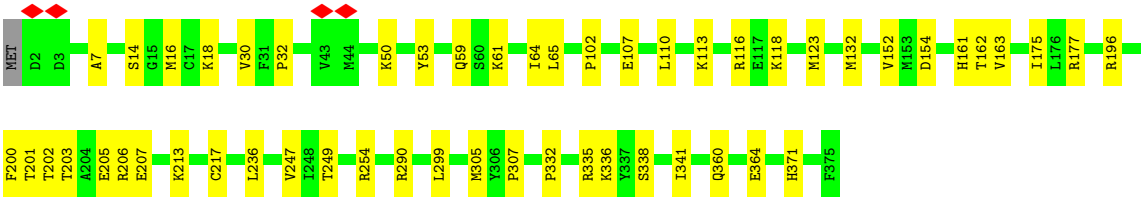
TYR GLY ARG ASP LEU HIS GLY VAL GLN ASN LEU LEU LYS LYS HIS LYS ARG LEU GLU GLY GLU LEU VAL ALA HIS GLU PRO ALA ILE GLN ASN VAL LEU ASP MET ALA ALA THR LEU GLY ASP LYS THR THR VAL GLY ARG GLU ALA ILE GLN GLU ARG LEU ASP GLN PHE VAL GLN HIS

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



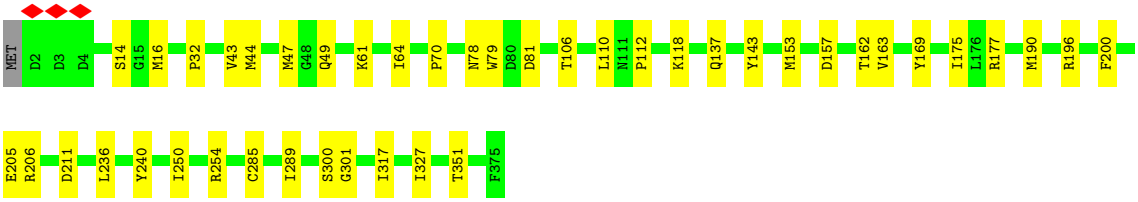
• Molecule 5: Actin, cytoplasmic 1

Chain A:



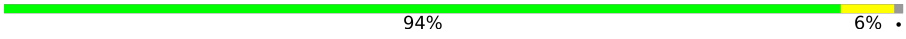
• Molecule 5: Actin, cytoplasmic 1

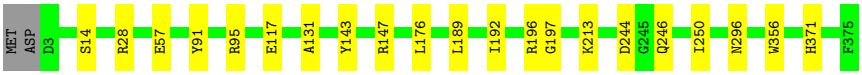
Chain B:



• Molecule 5: Actin, cytoplasmic 1

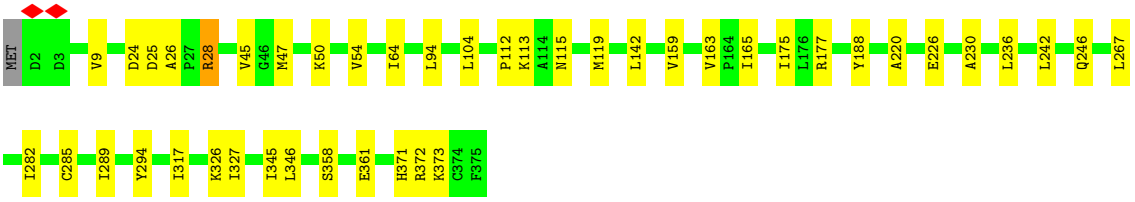
Chain C:





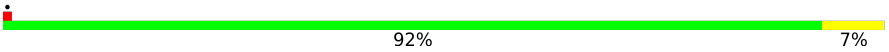
• Molecule 5: Actin, cytoplasmic 1

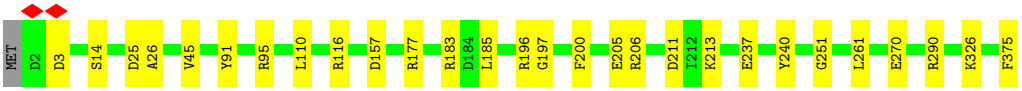
Chain D:



• Molecule 5: Actin, cytoplasmic 1

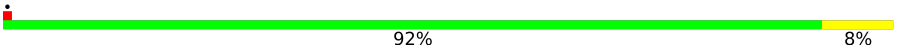
Chain E:

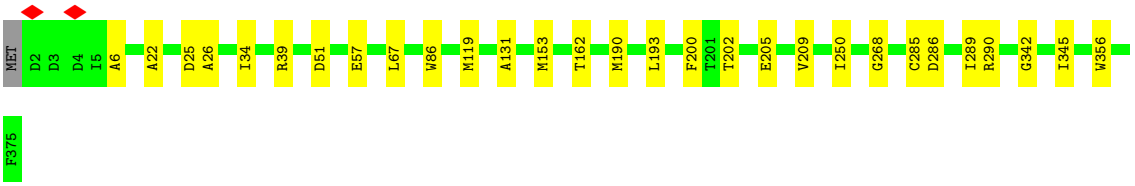




• Molecule 5: Actin, cytoplasmic 1

Chain F:



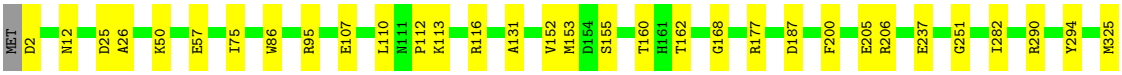


• Molecule 5: Actin, cytoplasmic 1

Chain G:

• Molecule 5: Actin, cytoplasmic 1

Chain H:

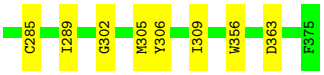


• Molecule 5: Actin, cytoplasmic 1

Chain I:

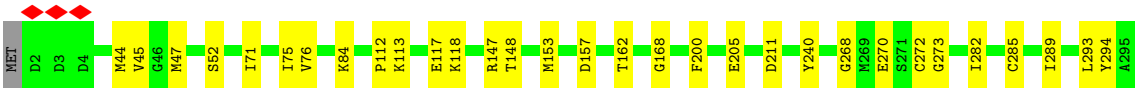
• Molecule 5: Actin, cytoplasmic 1

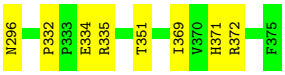
Chain J:



• Molecule 5: Actin, cytoplasmic 1

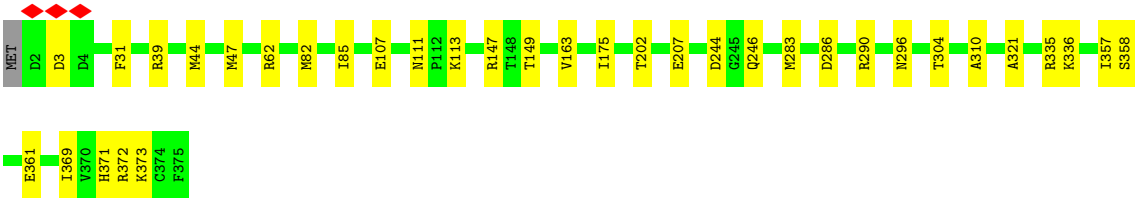
Chain K:





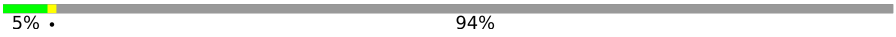
• Molecule 5: Actin, cytoplasmic 1

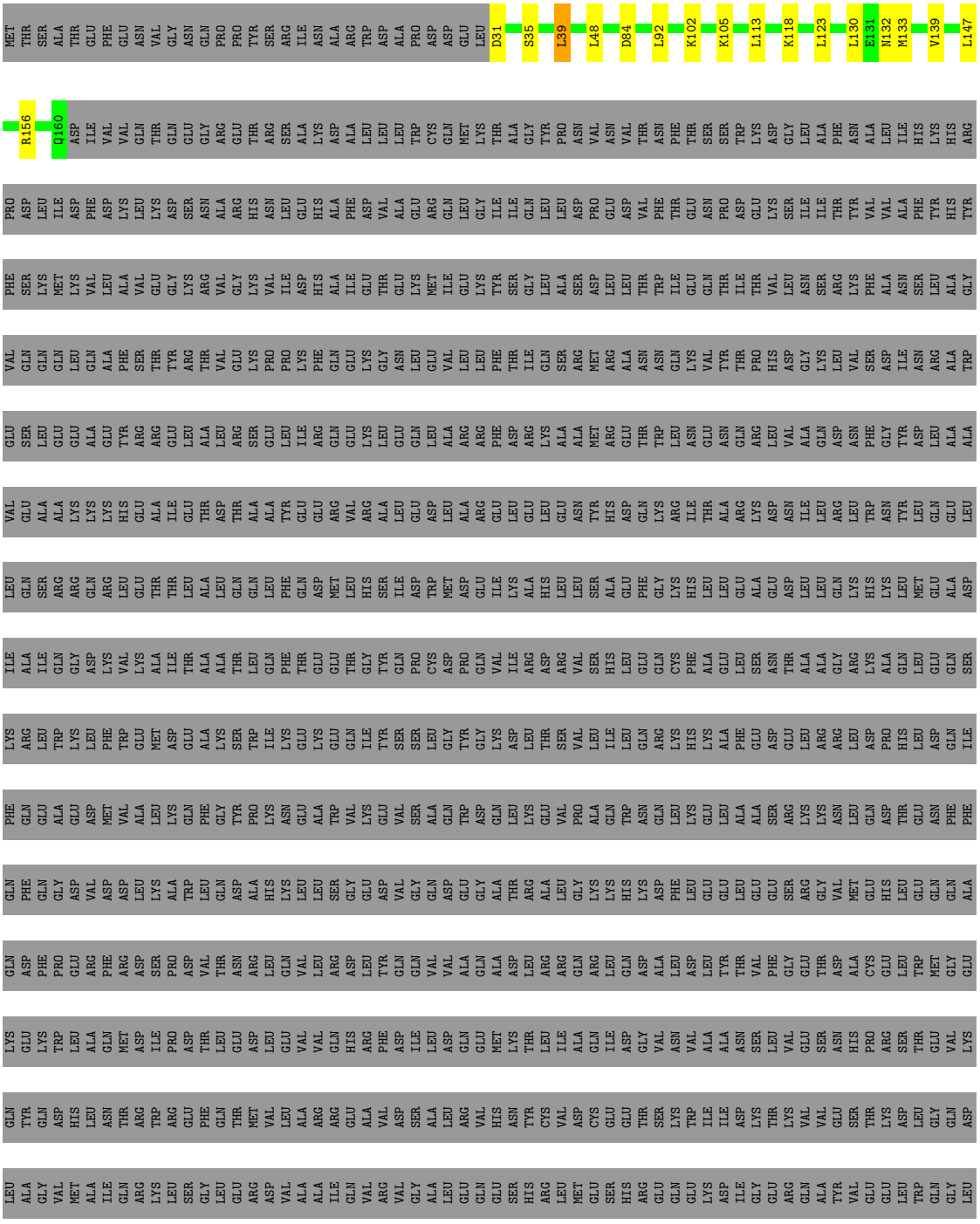
Chain L:

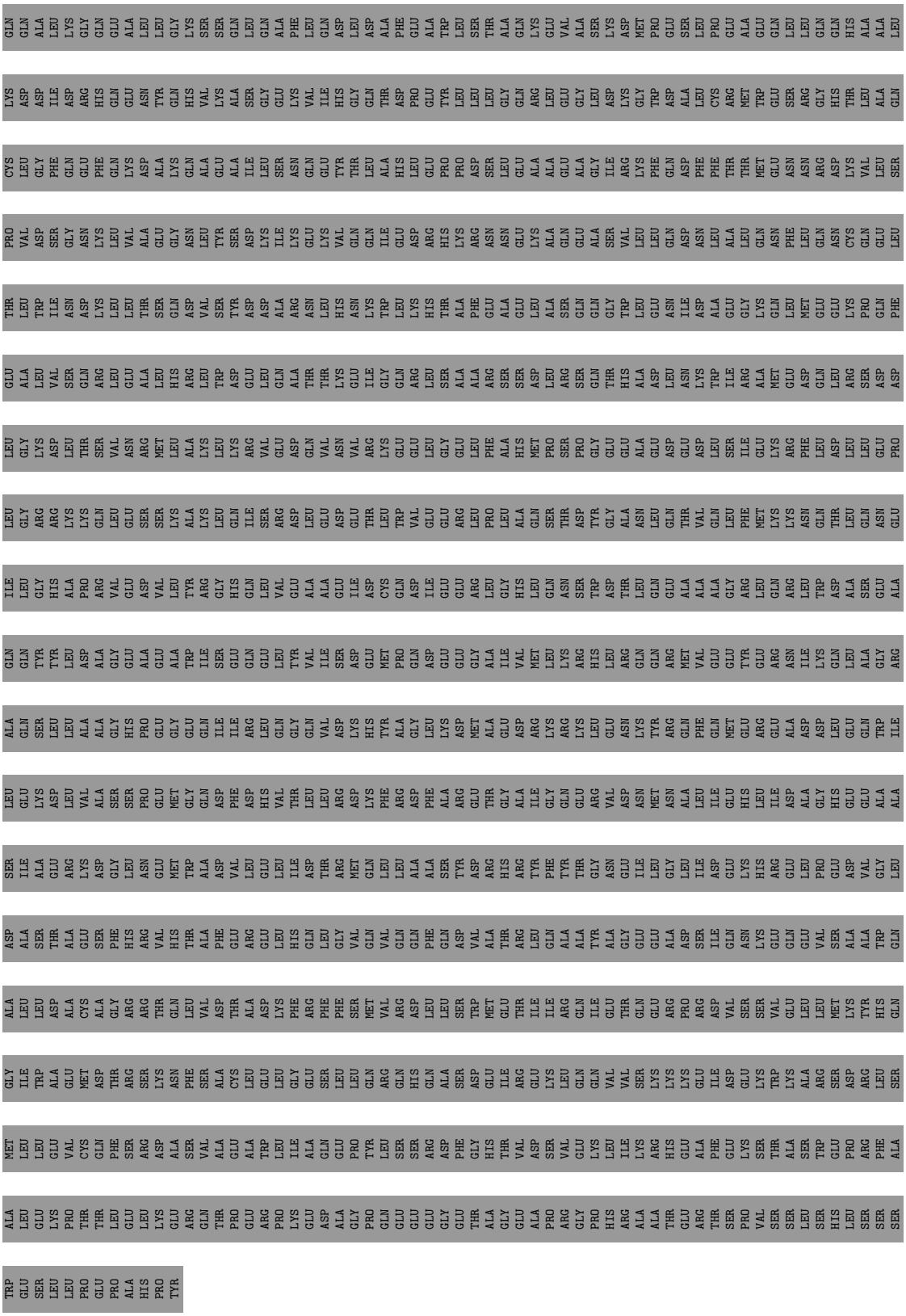


• Molecule 6: Spectrin beta chain

Chain M:

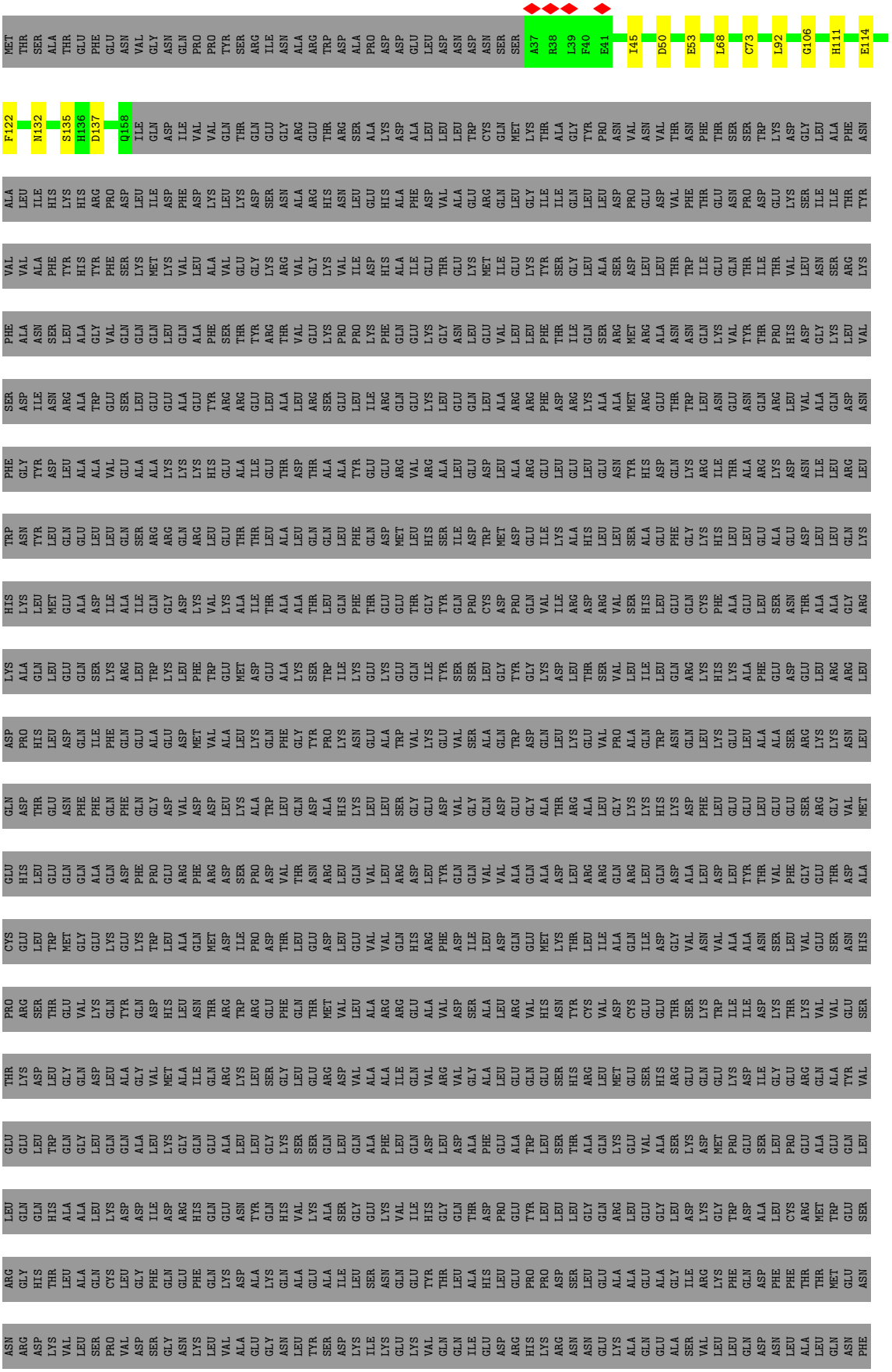


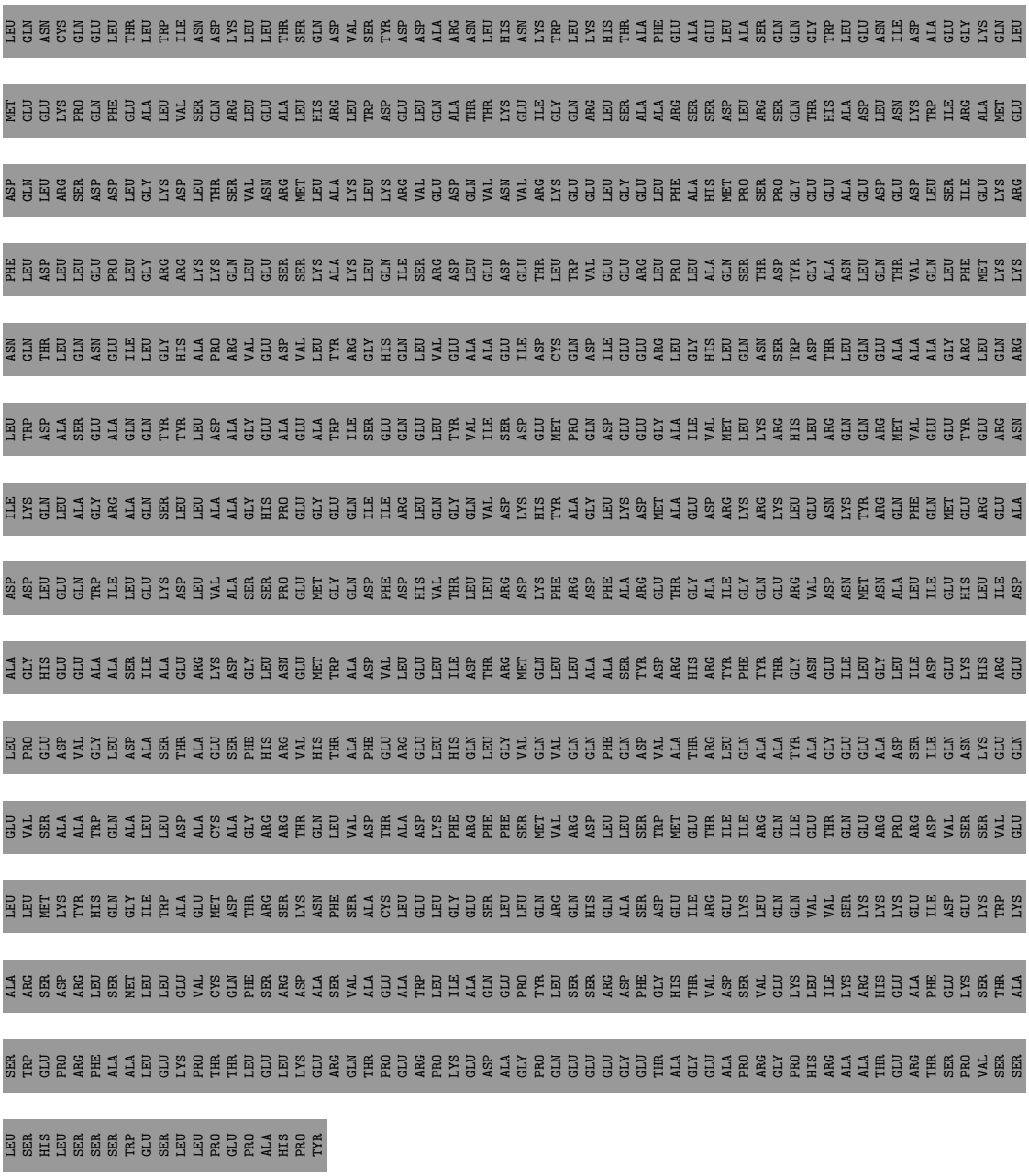




• Molecule 6: Spectrin beta chain

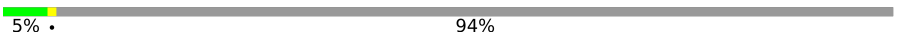
Chain N: 5% • 94%

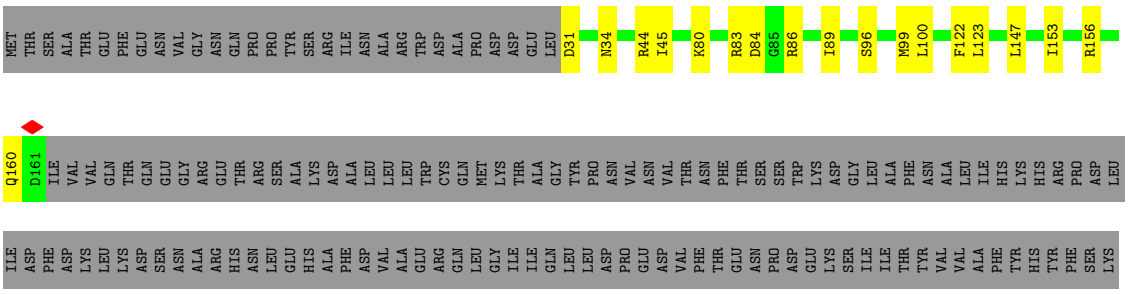

A37
R38
L39
F40
E41
I45
D50
E53
L68
C73
L92
G106
H111
E114
F122
N132
S135
H136
D137
Q158

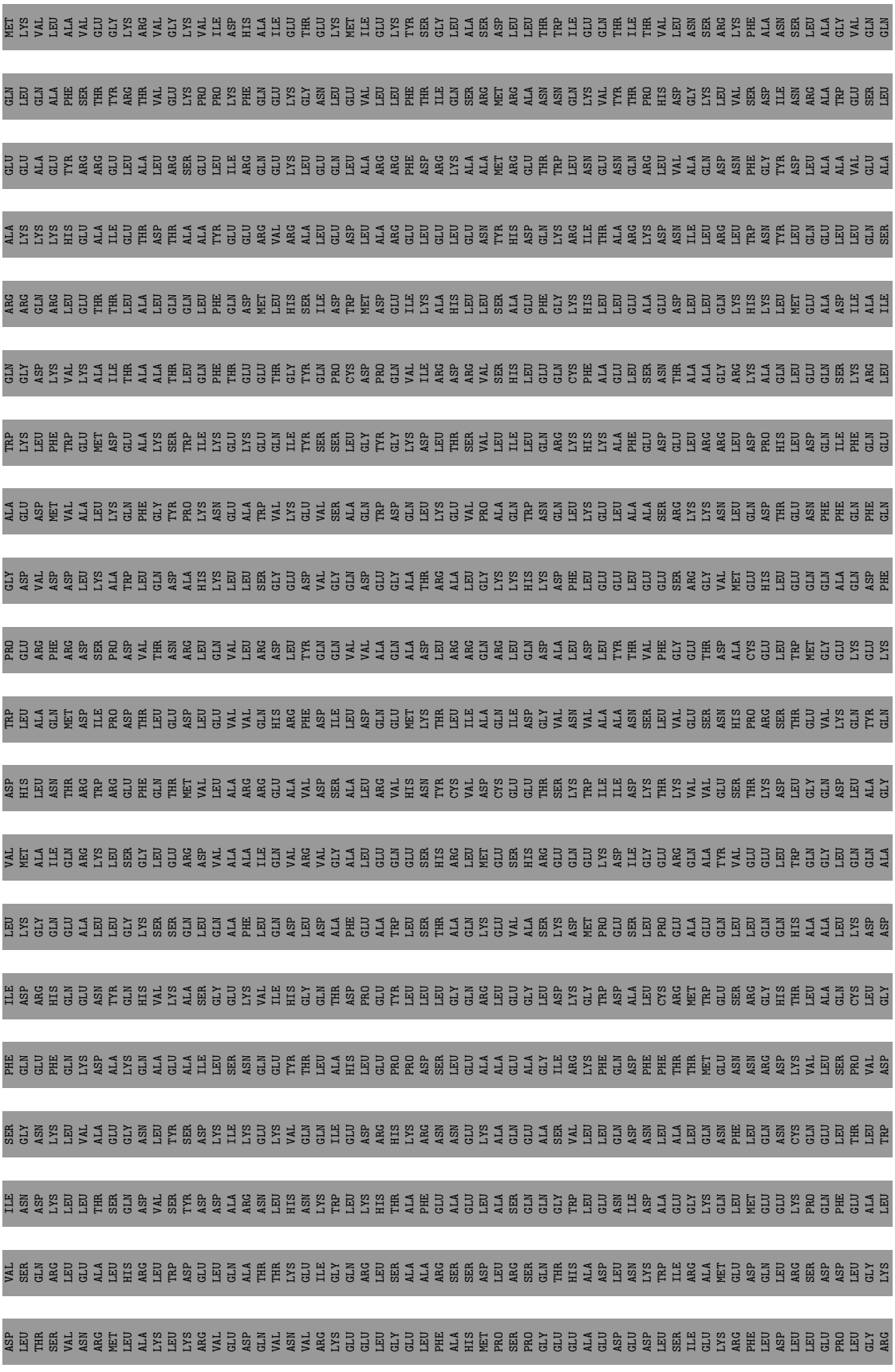


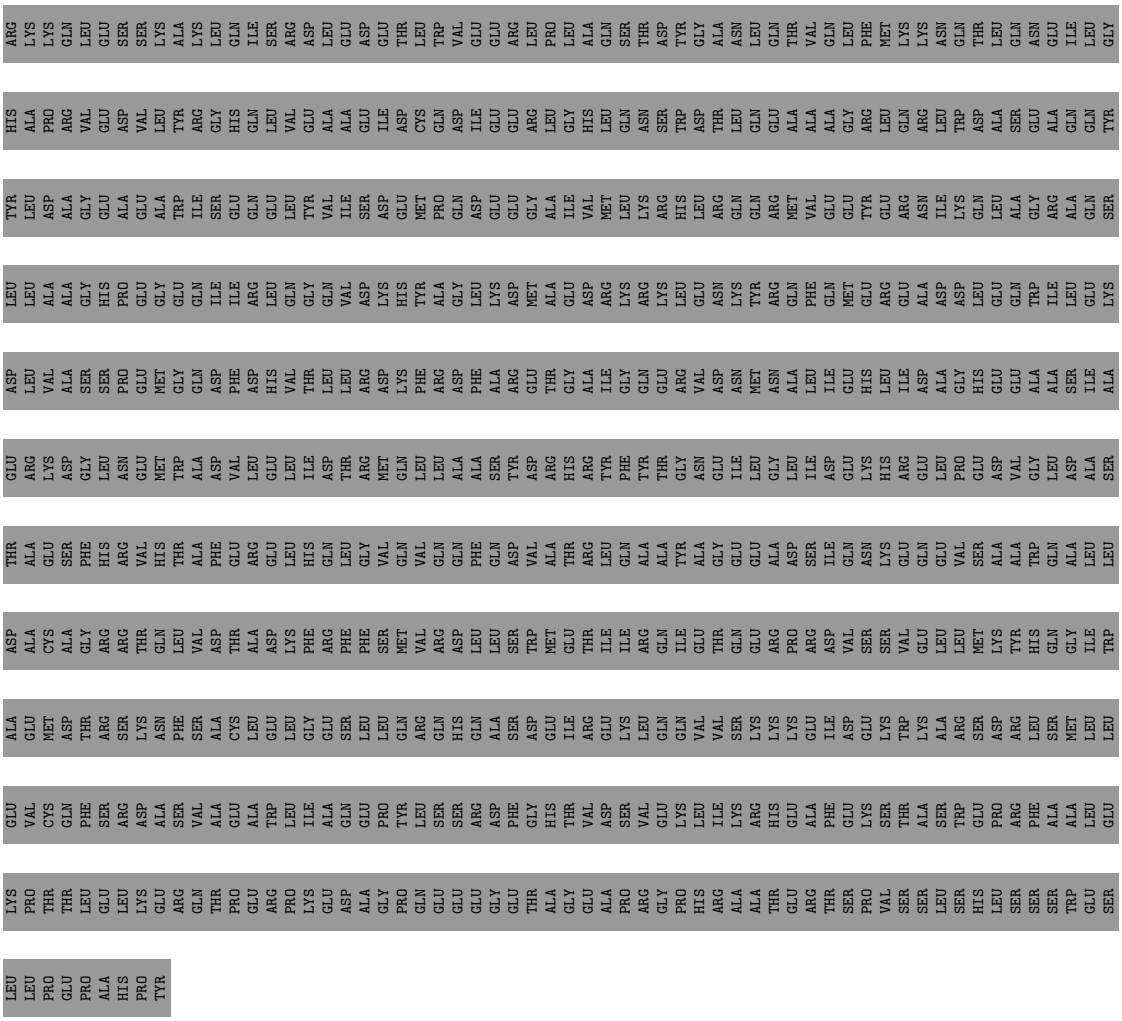
• Molecule 6: Spectrin beta chain

Chain O:



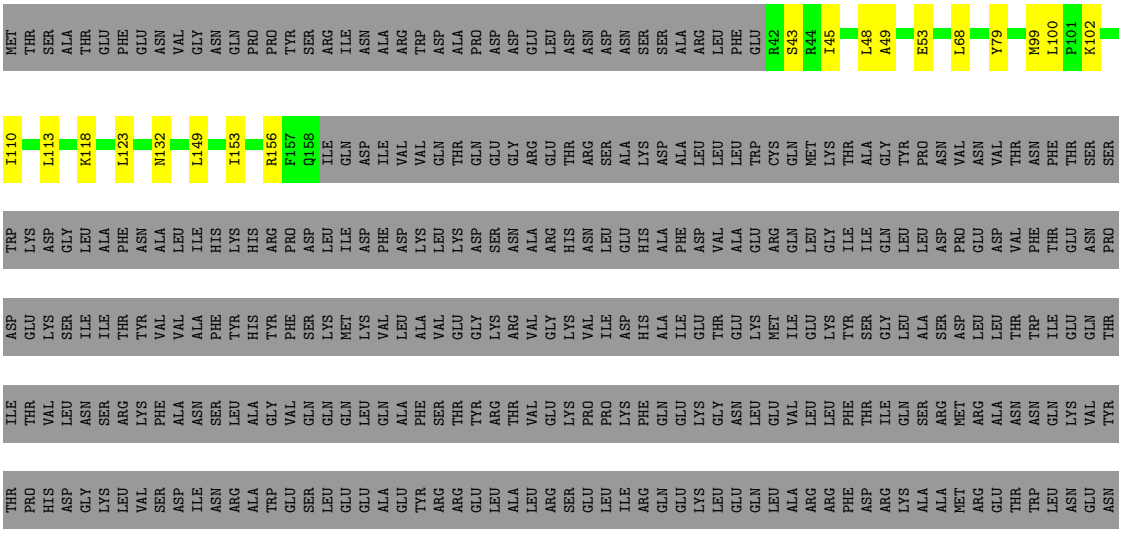


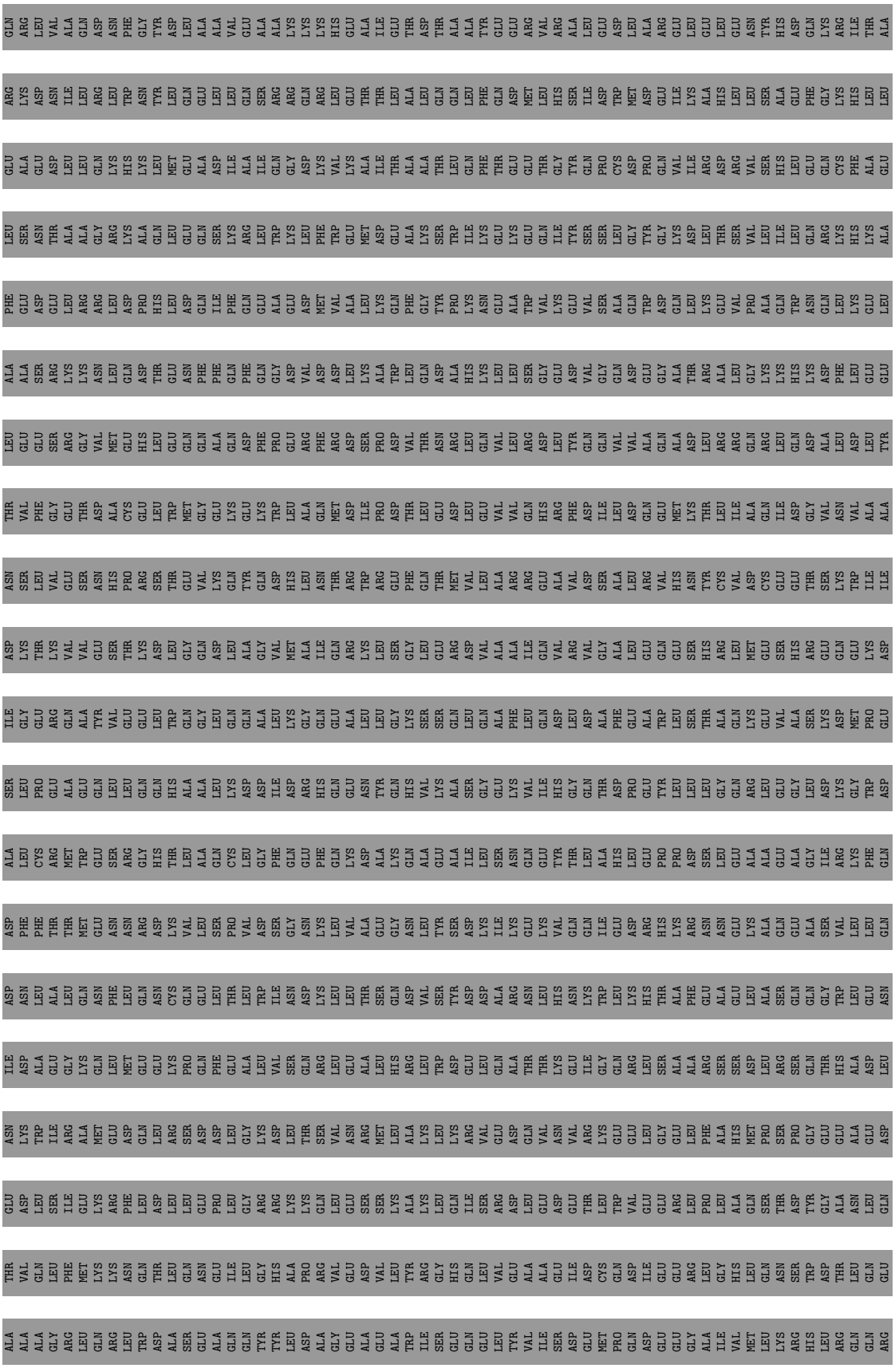


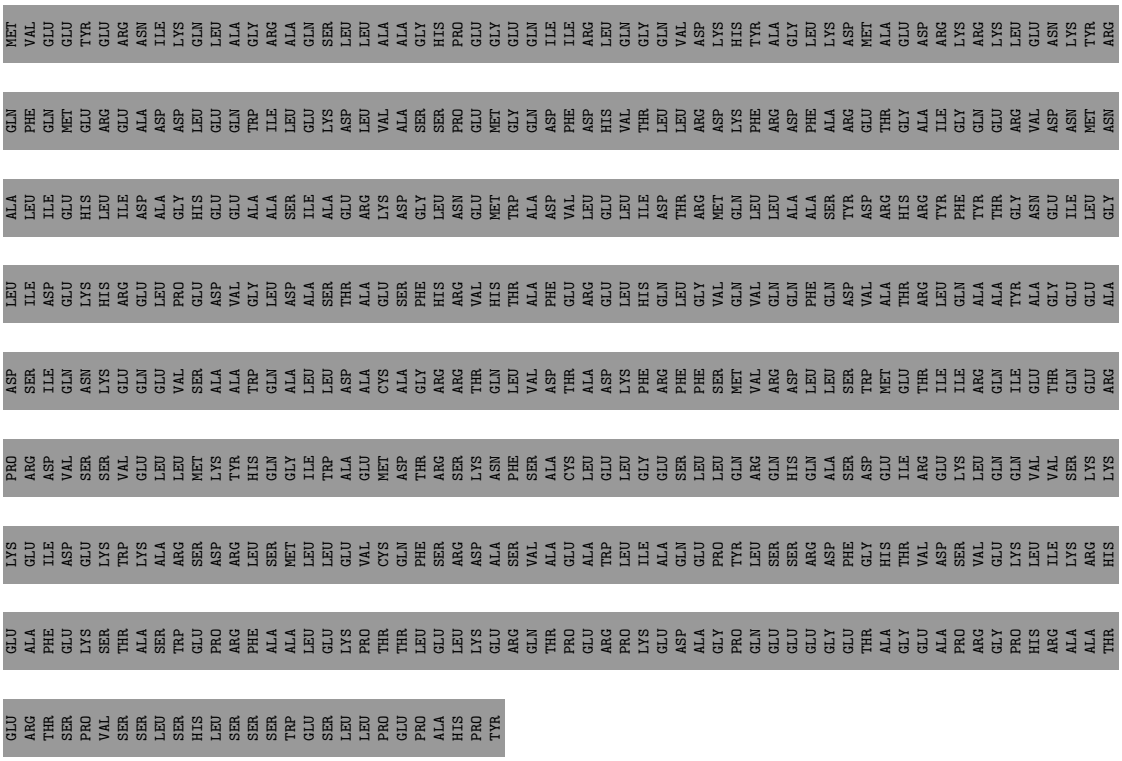


• Molecule 6: Spectrin beta chain

Chain P: 5% 95%

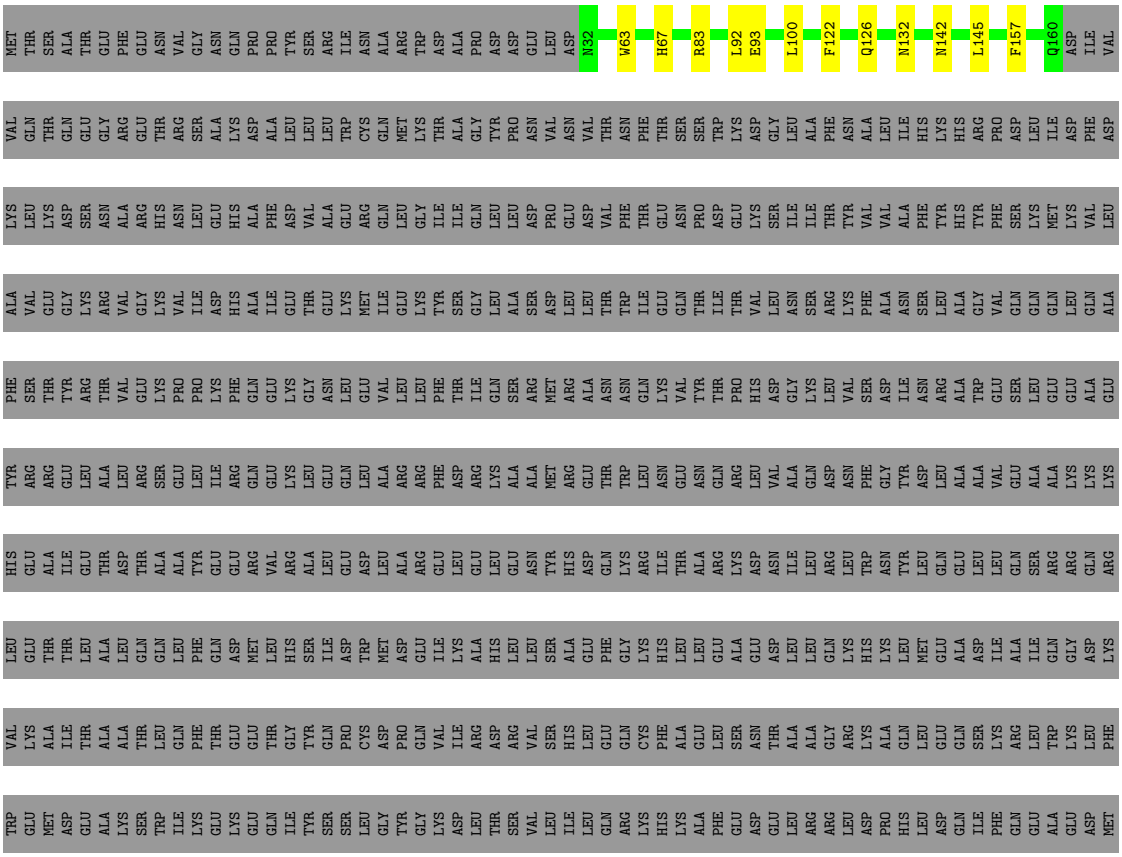


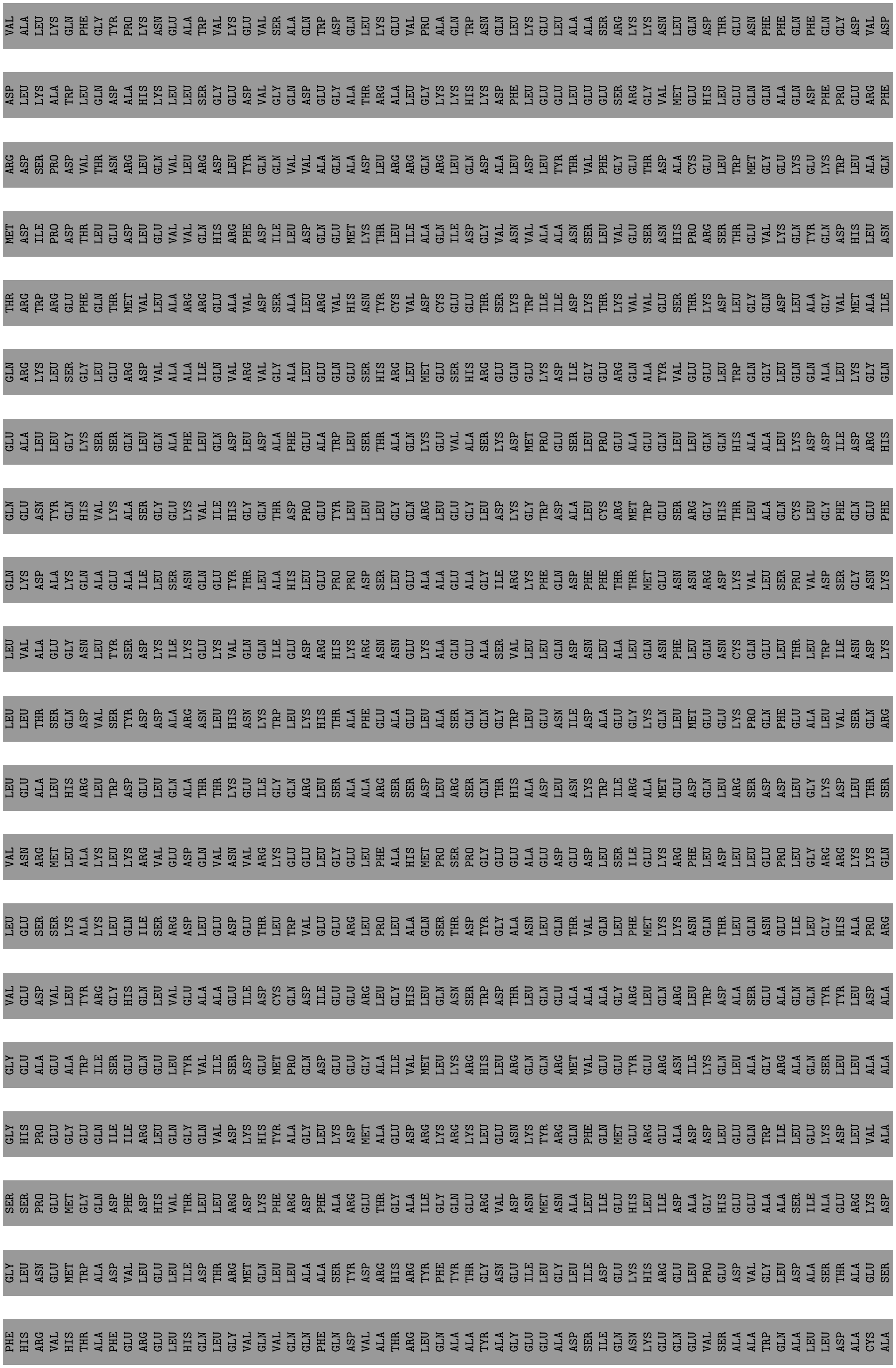


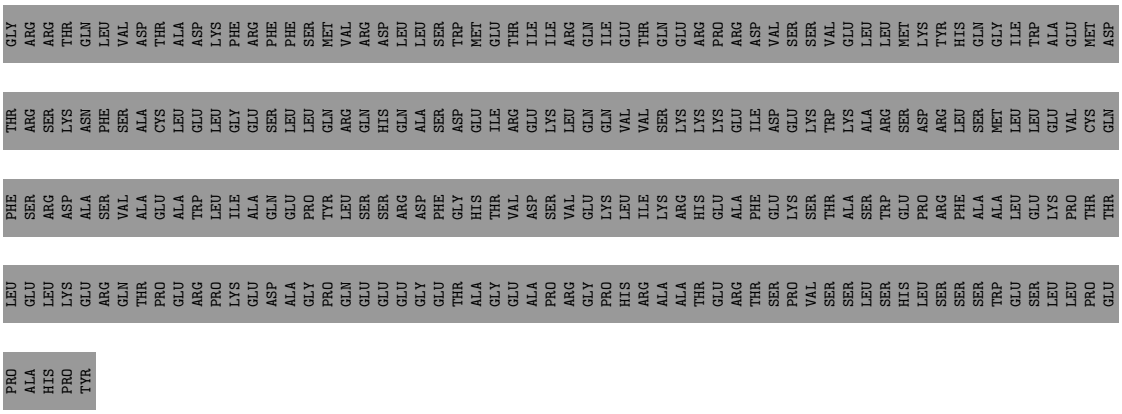


• Molecule 6: Spectrin beta chain

Chain Q: 5% • 94%

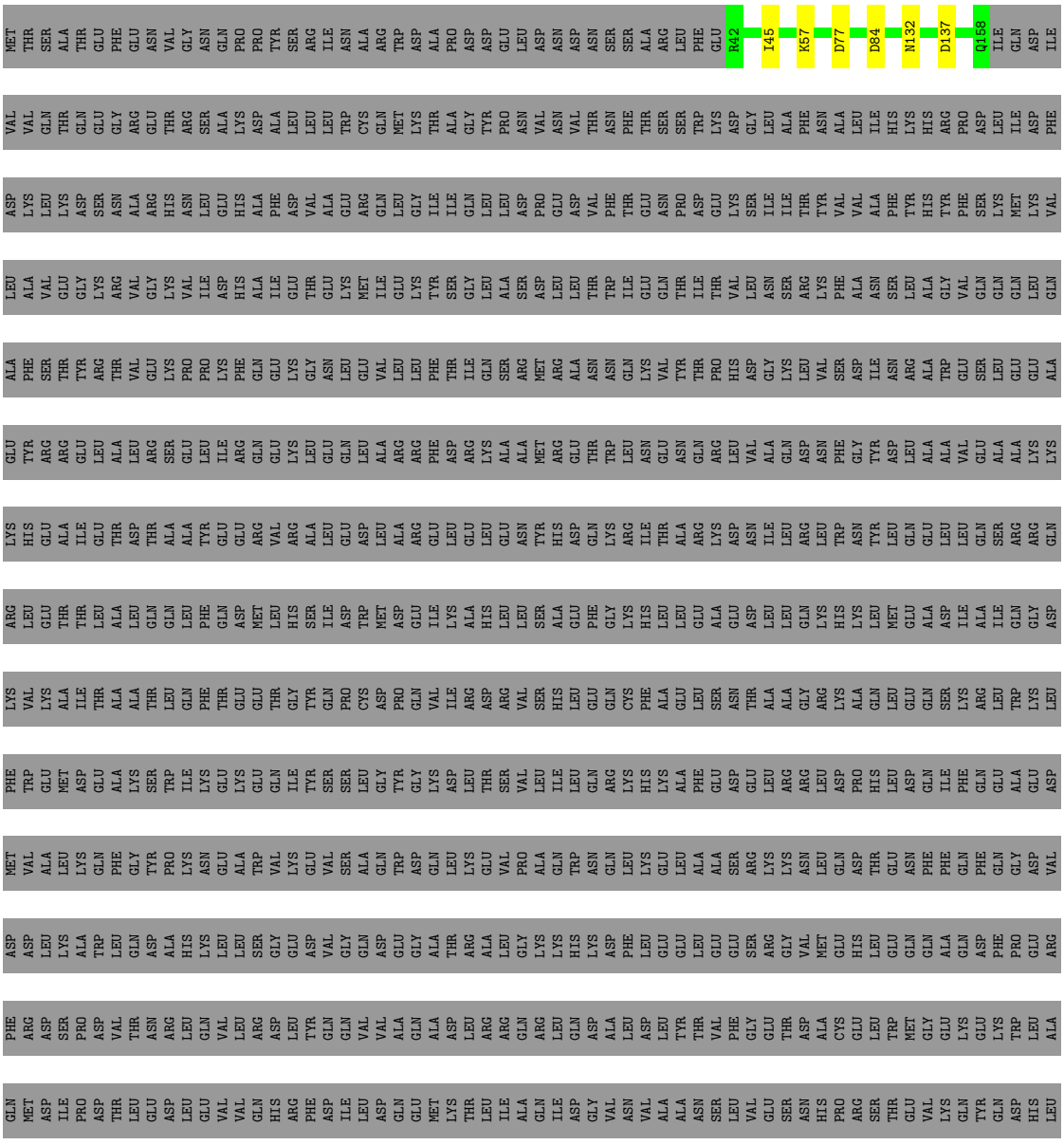


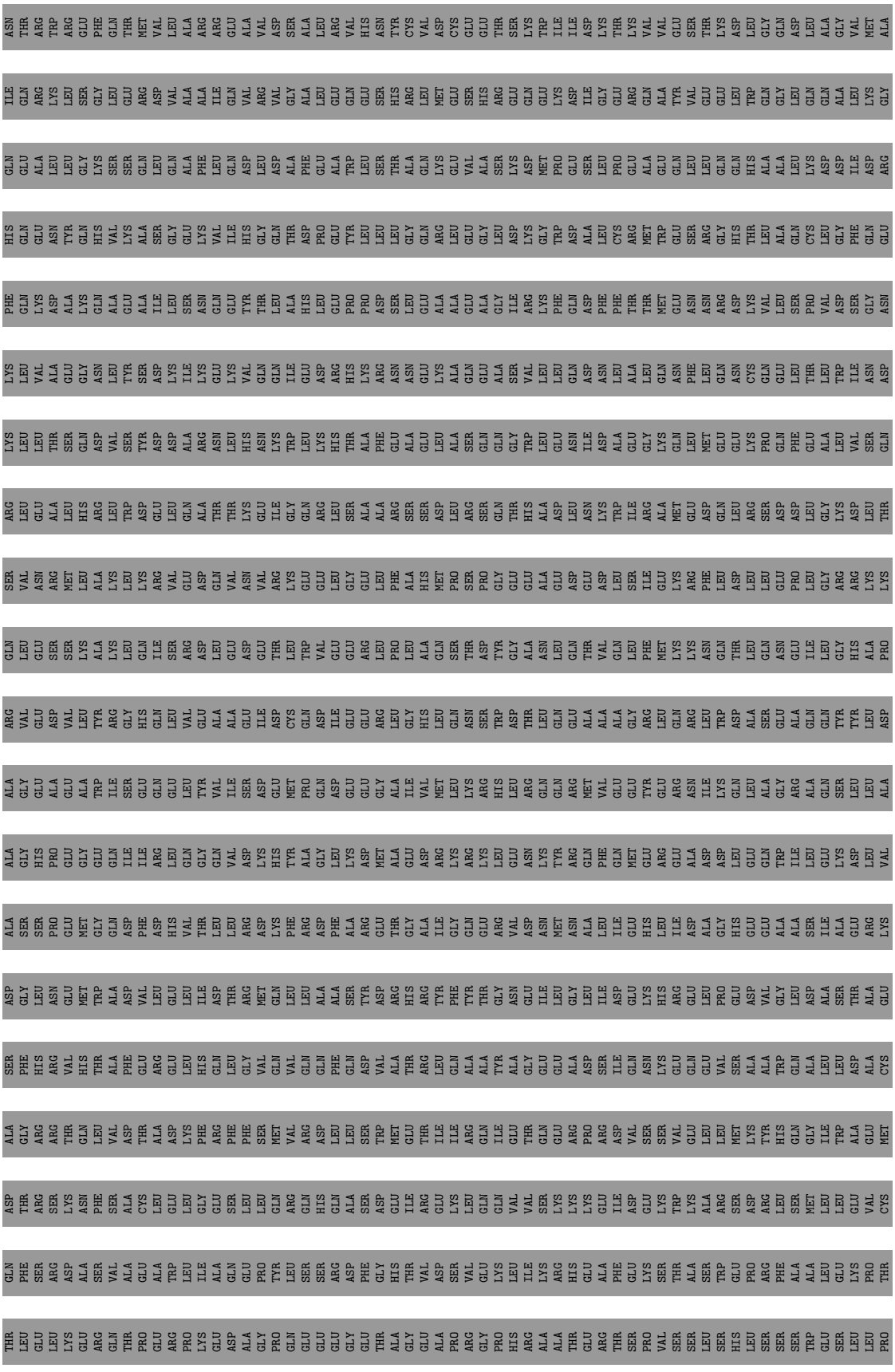

VAL ALA LEU LYS GLN PHE GLY TYR PRO LYS ASN GLU ALA TRP VAL LYS GLU VAL SER ALA GLN TRP ASP GLN LEU LYS GLU VAL PRO ALA GLN TRP ASN GLN LEU LYS GLU LEU ALA ALA SER ARG LYS LYS ASN LEU GLN ASP THR GLU ASN PHE PHE GLN PHE GLN GLY ASP VAL ASP
ASP LEU LYS ALA TRP LEU GLN ASP ALA HIS LYS LEU LEU SER GLY GLU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



• Molecule 6: Spectrin beta chain

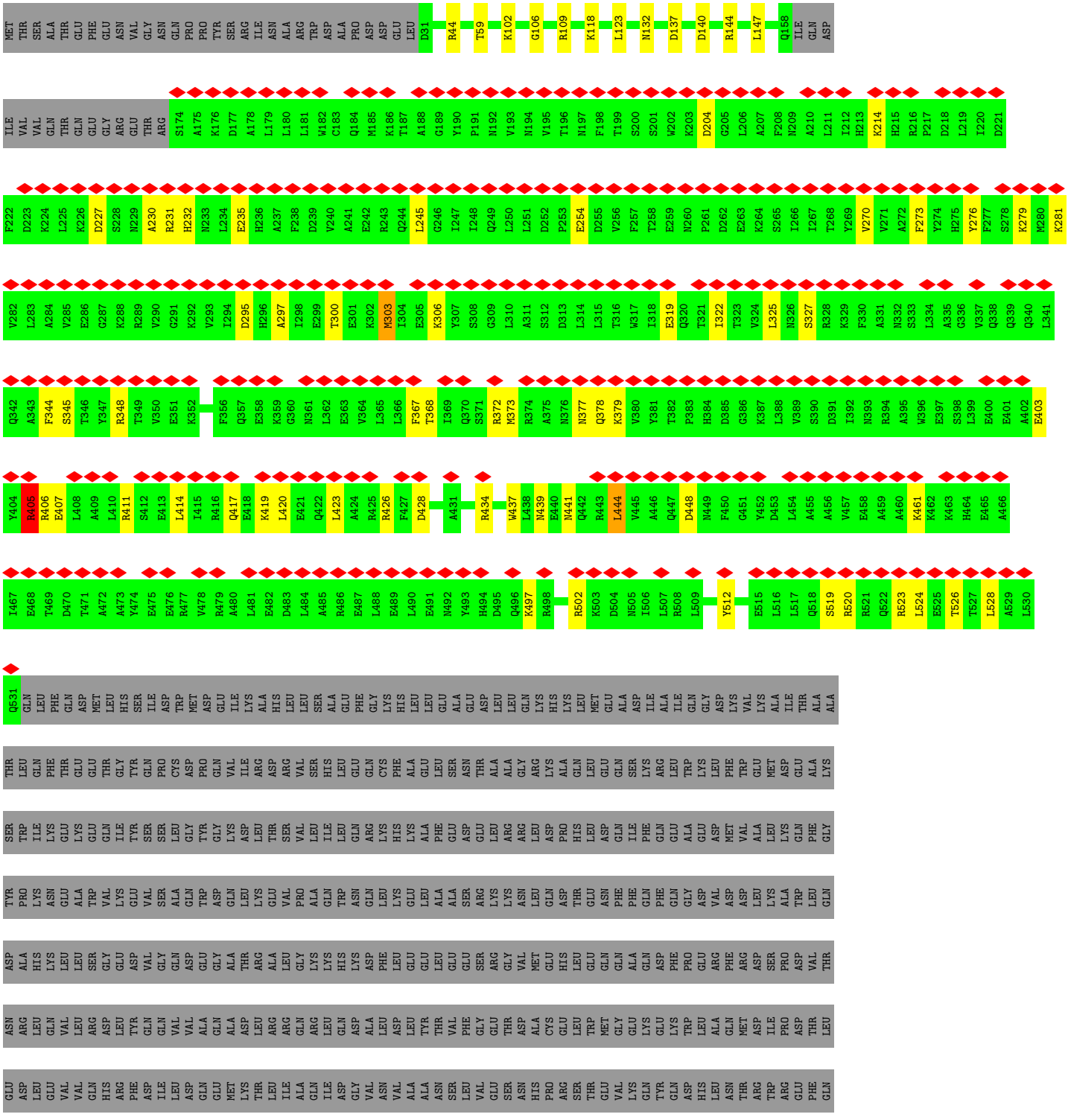
Chain R: 5% 95%

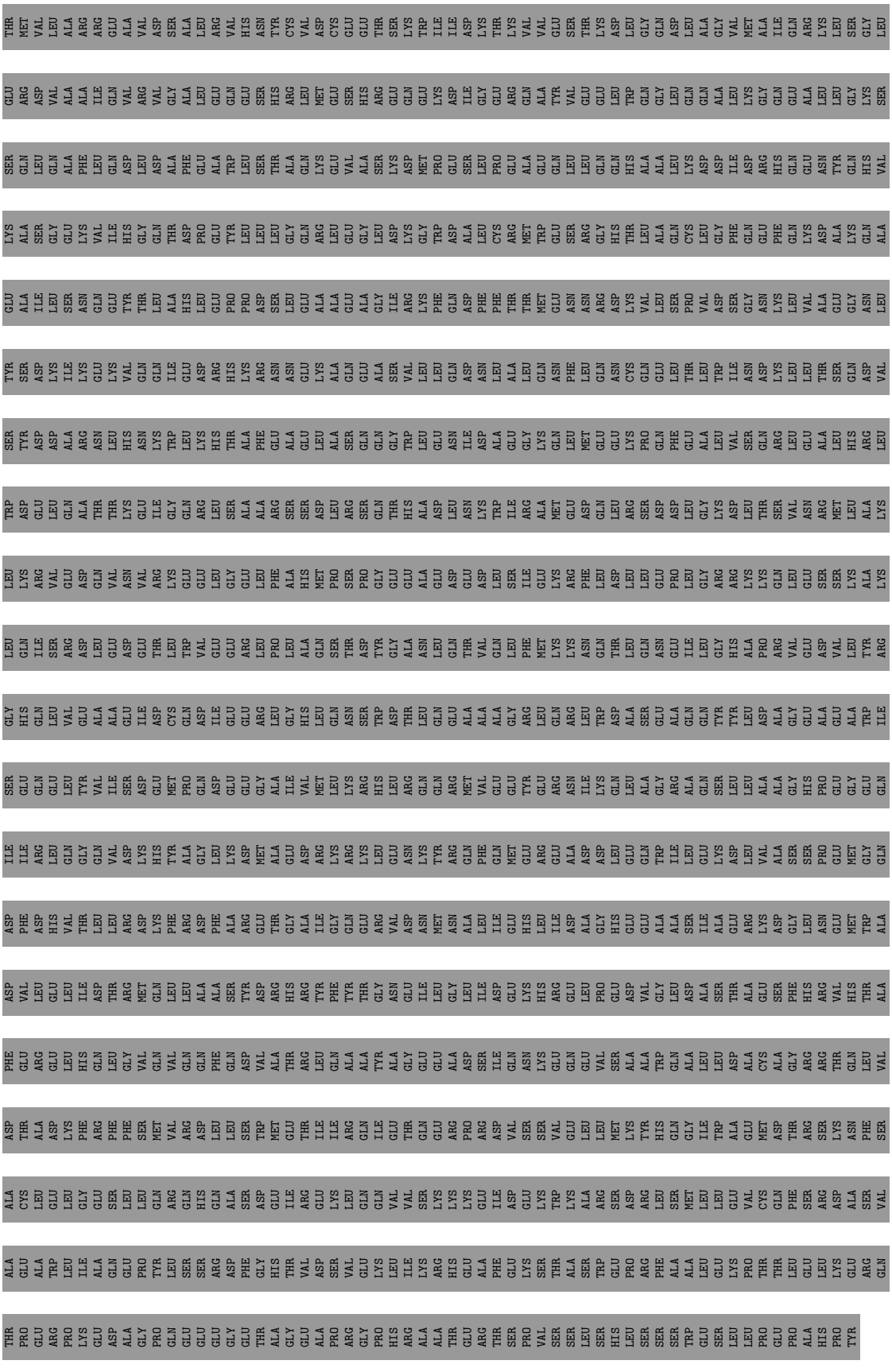




• Molecule 6: Spectrin beta chain

Chain S:





• Molecule 6: Spectrin beta chain

Chain T: 5% • 94%

MET THR SER ALA THR GLU PHE GLU ASN VAL GLY ASN GLN PRO PRO TYR SER ARG ILE ASN ALA ARG TRP ASP ALA PRO ASP ASP GLU LEU D31 R38 E41 D50 E53 Q56 L92 R109 F122 N132 M133 G134 D140 R156 F157 Q158 ILE GLN ASP

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

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

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

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

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

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

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

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

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

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

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

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

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

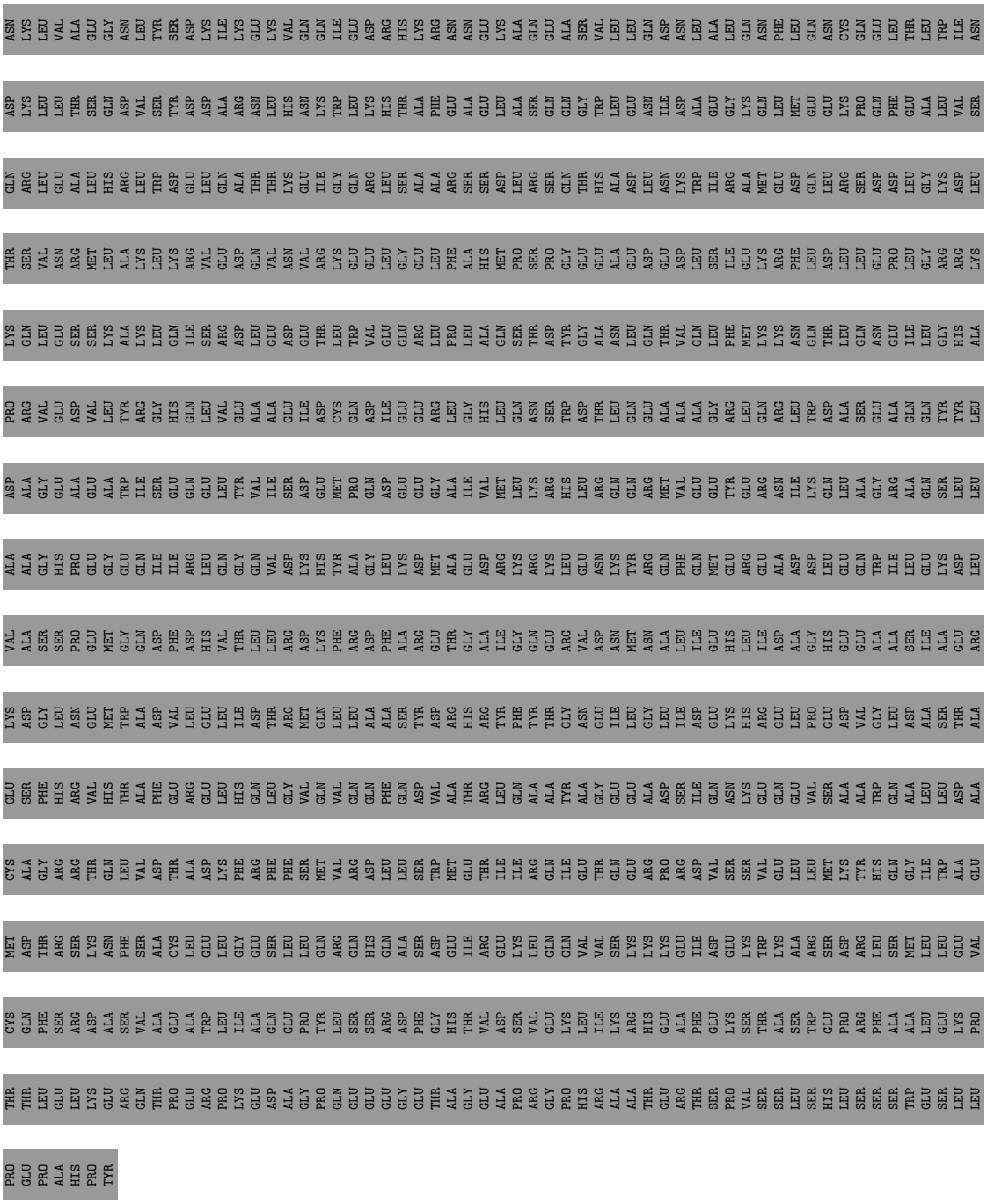
LEU ASN THR ARG TRP ARG GLU PHE GLN THR THR MET VAL LEU ALA ARG ARG GLU ALA VAL ASP SER ALA LEU ARG VAL HIS ASN TYR CYS VAL ASP CYS GLU GLU THR SER LYS TRP ILE ILE ASP LYS THR LYS VAL VAL GLU SER THR LYS ASP LEU GLY GLN ASP LEU ALA GLY VAL MET

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

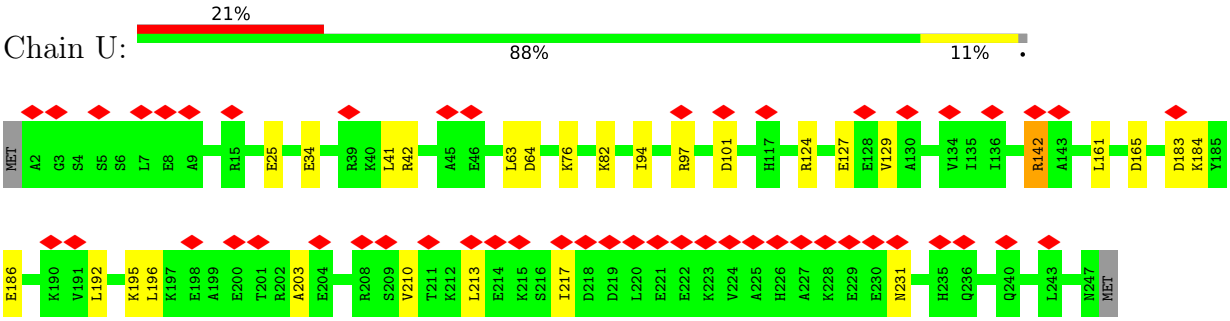
GLY GLN GLU ALA LEU LEU GLY LYS SER SER GLN LEU GLN ALA PHE LEU GLN ASP LEU ASP ALA PHE GLU ALA TRP LEU SER THR ALA GLN LYS GLU VAL ALA SER LYS ASP MET PRO GLU SER LEU PRO GLU ALA GLU GLN LEU LEU GLN GLN HIS ALA ALA LEU LYS ASP ILE ASP

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

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

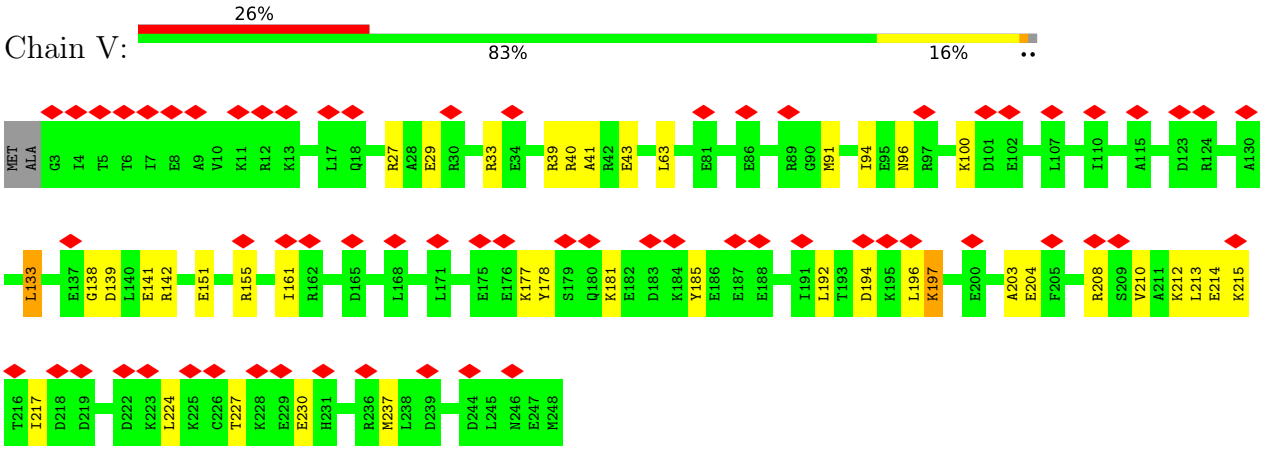


• Molecule 7: Tropomyosin-1.9



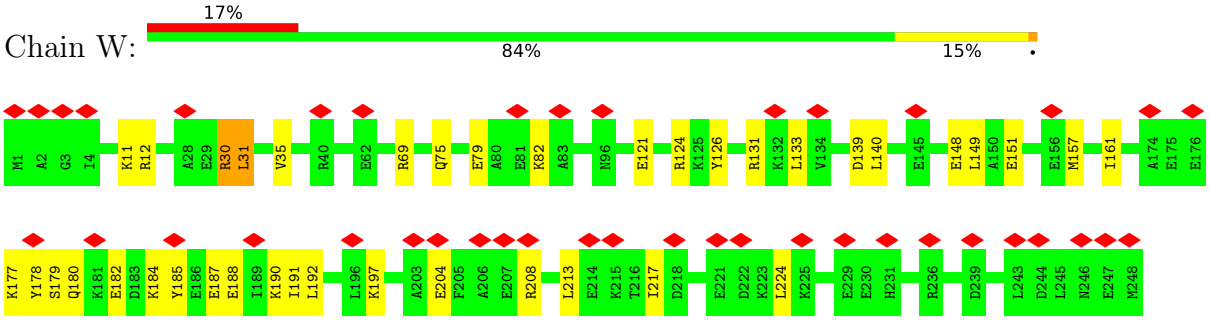
• Molecule 8: Tropomyosin 3

Chain V:



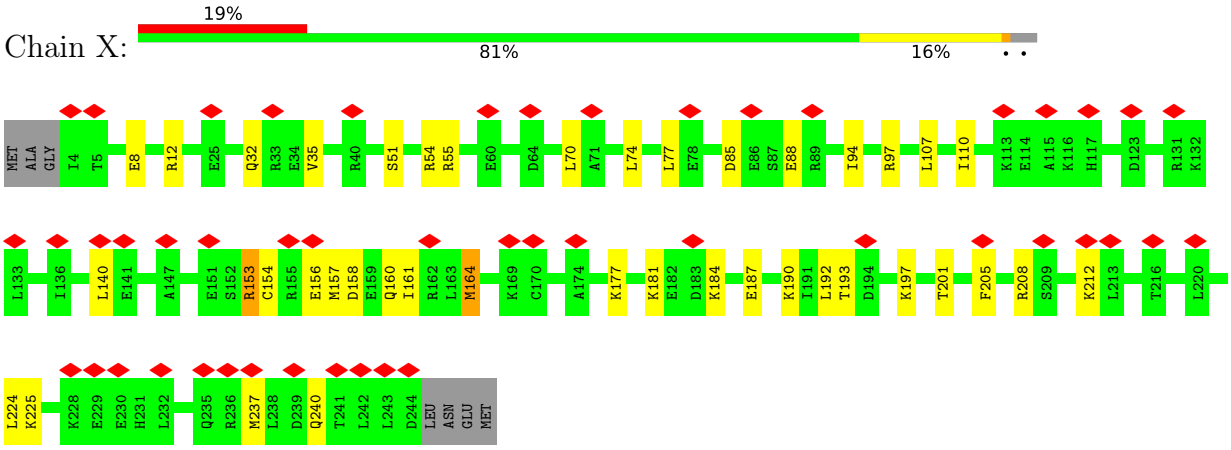
• Molecule 8: Tropomyosin 3

Chain W:



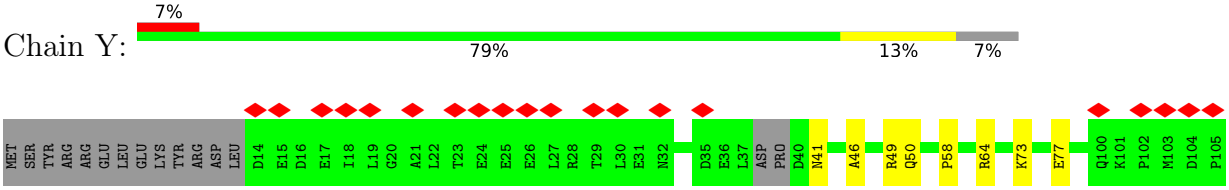
• Molecule 8: Tropomyosin 3

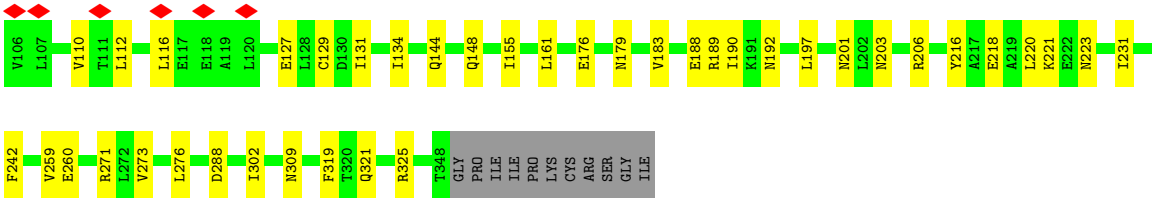
Chain X:



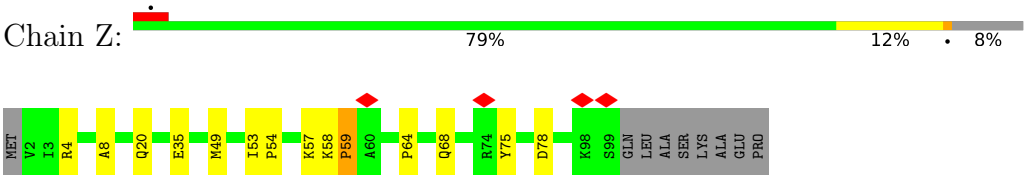
• Molecule 9: Tropomodulin-1

Chain Y:





• Molecule 10: SH3 domain-binding glutamic acid-rich-like protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34.4	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.839	Depositor
Minimum map value	-1.150	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	657.6, 657.6, 657.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality

5.1 Standard geometry

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

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	0	0.31	0/459	0.69	0/609
1	1	0.28	0/2638	0.54	0/3579
1	2	0.26	0/2312	0.51	0/3139
2	3	0.27	0/2924	0.56	0/3956
2	4	0.27	0/2198	0.54	0/2978
2	9	0.38	0/459	0.79	0/610
3	5	0.31	0/1040	0.62	0/1415
3	6	0.30	0/992	0.52	0/1358
3	7	0.29	0/1006	0.57	0/1369
4	8	0.32	0/2843	0.69	7/3851 (0.2%)
5	A	0.27	0/2970	0.51	0/4023
5	B	0.28	0/2980	0.49	0/4035
5	C	0.30	0/2972	0.50	0/4024
5	D	0.30	0/2980	0.53	2/4035 (0.0%)
5	E	0.30	0/2980	0.49	0/4035
5	F	0.30	0/2980	0.51	1/4035 (0.0%)
5	G	0.29	0/2980	0.49	0/4035
5	H	0.30	0/2980	0.51	0/4035
5	I	0.31	0/2972	0.51	0/4024
5	J	0.31	0/2980	0.52	1/4035 (0.0%)
5	K	0.29	0/2980	0.50	0/4035
5	L	0.27	0/2980	0.50	0/4035
6	M	0.28	0/1080	0.67	2/1448 (0.1%)
6	N	0.27	0/1019	0.59	0/1365
6	O	0.30	0/1088	0.55	0/1459
6	P	0.29	0/974	0.61	0/1305
6	Q	0.26	0/1072	0.56	0/1437
6	R	0.28	0/974	0.55	0/1305
6	S	0.32	0/4050	0.69	4/5458 (0.1%)
6	T	0.29	0/1063	0.55	0/1425
7	U	0.39	0/1999	0.72	3/2667 (0.1%)
8	V	0.41	0/2016	0.79	4/2687 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	W	0.43	0/2022	0.77	5/2696 (0.2%)
8	X	0.43	0/1979	0.74	3/2638 (0.1%)
9	Y	0.27	0/2584	0.54	0/3501
10	Z	0.56	1/817 (0.1%)	0.84	3/1099 (0.3%)
All	All	0.31	1/75342 (0.0%)	0.58	35/101740 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	59	PRO	CG-CD	-12.50	1.09	1.50

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Z	59	PRO	N-CD-CG	-15.33	80.20	103.20
10	Z	59	PRO	CA-CB-CG	-8.94	87.02	104.00
8	V	224	LEU	CA-CB-CG	8.05	133.83	115.30
6	M	39	LEU	CA-CB-CG	7.22	131.91	115.30
8	W	133	LEU	CA-CB-CG	6.99	131.38	115.30
8	X	55	ARG	CB-CG-CD	6.80	129.27	111.60
7	U	165	ASP	CB-CG-OD1	6.53	124.18	118.30
6	M	84	ASP	CB-CG-OD1	6.45	124.11	118.30
5	J	80	ASP	CB-CG-OD1	6.35	124.02	118.30
10	Z	59	PRO	CA-N-CD	-6.32	102.65	111.50
4	8	2225	LEU	CA-CB-CG	6.23	129.62	115.30
5	F	51	ASP	CB-CG-OD2	6.14	123.83	118.30
4	8	2154	PHE	CB-CG-CD2	-6.01	116.59	120.80
6	S	524	LEU	CA-CB-CG	5.94	128.96	115.30
8	W	30	ARG	CA-CB-CG	5.82	126.21	113.40
6	S	444	LEU	CA-CB-CG	5.75	128.53	115.30
7	U	142	ARG	CA-CB-CG	5.70	125.93	113.40
5	D	28	ARG	CA-CB-CG	5.60	125.72	113.40
4	8	2378	LEU	CA-CB-CG	5.45	127.83	115.30
5	D	28	ARG	CB-CG-CD	5.38	125.58	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	31	LEU	CB-CG-CD2	-5.27	102.05	111.00
8	X	164	MET	CB-CA-C	5.24	120.87	110.40
4	8	2211	LEU	CA-CB-CG	5.23	127.33	115.30
4	8	2194	LEU	CA-CB-CG	5.17	127.20	115.30
6	S	303	MET	CA-CB-CG	5.17	122.08	113.30
8	V	91	MET	CA-CB-CG	5.15	122.05	113.30
8	X	164	MET	CA-CB-CG	5.15	122.05	113.30
4	8	2077	ARG	CA-CB-CG	5.12	124.68	113.40
7	U	101	ASP	CB-CG-OD1	-5.11	113.70	118.30
4	8	2101	LEU	CA-CB-CG	5.07	126.97	115.30
8	W	133	LEU	CB-CG-CD1	-5.07	102.38	111.00
8	V	133	LEU	CA-CB-CG	5.04	126.89	115.30
8	V	237	MET	CA-CB-CG	5.03	121.86	113.30
8	W	149	LEU	CA-CB-CG	5.02	126.85	115.30
6	S	405	ARG	CA-CB-CG	5.02	124.44	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	405	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	453	0	446	1	0
1	1	2585	0	2610	21	0
1	2	2263	0	2279	37	0
2	3	2870	0	2884	31	0
2	4	2157	0	2149	31	0
2	9	455	0	456	9	0
3	5	1008	0	1009	8	0
3	6	963	0	914	9	0
3	7	976	0	965	14	0
4	8	2799	0	2478	45	0
5	A	2907	0	2851	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2917	0	2879	28	0
5	C	2909	0	2875	16	0
5	D	2917	0	2879	30	0
5	E	2917	0	2879	20	0
5	F	2917	0	2879	19	0
5	G	2917	0	2879	27	0
5	H	2917	0	2879	24	0
5	I	2909	0	2875	26	0
5	J	2917	0	2879	25	0
5	K	2917	0	2879	26	0
5	L	2917	0	2879	24	0
6	M	1065	0	1109	10	0
6	N	1004	0	1060	9	0
6	O	1073	0	1113	15	0
6	P	960	0	1016	13	0
6	Q	1057	0	1105	9	0
6	R	960	0	1016	5	0
6	S	3983	0	4009	50	0
6	T	1048	0	1090	8	0
7	U	1992	0	1988	25	0
8	V	2011	0	2017	29	0
8	W	2017	0	2023	28	0
8	X	1974	0	1982	28	0
9	Y	2547	0	2527	34	0
10	Z	798	0	781	8	0
11	A	27	0	12	2	0
11	B	27	0	12	0	0
11	C	27	0	12	2	0
11	D	27	0	12	0	0
11	E	27	0	12	0	0
11	F	27	0	12	0	0
11	G	27	0	12	1	0
11	H	27	0	12	0	0
11	I	27	0	12	0	0
11	J	27	0	12	1	0
11	K	27	0	12	1	0
11	L	27	0	12	0	0
All	All	74320	0	73682	643	0

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

All (643) 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)
6:O:31:ASP:N	6:O:34:ASN:HD22	1.46	1.12
4:8:2206:ALA:O	4:8:2209:ARG:HB3	1.48	1.11
2:3:167:HIS:HA	2:3:188:VAL:O	1.81	0.80
5:I:159:VAL:HG21	5:I:177:ARG:HE	1.50	0.77
5:L:283:MET:HA	5:L:290:ARG:HH12	1.52	0.75
8:W:157:MET:HE1	8:X:158:ASP:HA	1.71	0.73
6:O:31:ASP:N	6:O:34:ASN:ND2	2.31	0.72
7:U:25:GLU:OE2	8:V:27:ARG:NH2	2.23	0.71
7:U:210:VAL:HG11	8:V:210:VAL:HB	1.72	0.69
7:U:231:ASN:ND2	8:V:230:GLU:OE2	2.26	0.68
5:F:57:GLU:OE2	6:P:132:ASN:ND2	2.27	0.68
5:C:213:LYS:NZ	11:C:401:ADP:O2'	2.27	0.67
3:7:192:TRP:HD1	3:7:194:CYS:H	1.40	0.67
5:A:110:LEU:O	5:A:177:ARG:NH1	2.28	0.67
1:2:340:ASN:HB3	2:3:239:MET:HE3	1.76	0.66
1:2:172:ARG:HG2	1:2:174:SER:H	1.61	0.66
5:A:213:LYS:NZ	11:A:401:ADP:O2'	2.29	0.66
9:Y:46:ALA:HA	9:Y:49:ARG:HE	1.60	0.66
1:2:242:THR:HG23	1:2:245:GLY:H	1.62	0.65
6:S:373:MET:O	6:S:377:ASN:N	2.27	0.65
8:W:157:MET:CE	8:X:158:ASP:HA	2.27	0.64
5:C:117:GLU:OE2	5:C:371:HIS:NE2	2.32	0.63
2:4:132:LEU:HD11	2:4:382:PRO:HD3	1.81	0.63
5:A:18:LYS:HG2	5:A:30:VAL:HG22	1.80	0.63
6:Q:63:TRP:NE1	6:Q:67:HIS:HE1	1.96	0.63
5:A:307:PRO:HB3	9:Y:49:ARG:HD2	1.80	0.63
2:3:157:VAL:HG22	2:3:226:ILE:HG23	1.80	0.62
8:V:29:GLU:OE2	8:V:33:ARG:NH1	2.32	0.62
9:Y:41:ASN:O	9:Y:49:ARG:NH1	2.31	0.62
8:X:51:SER:HA	8:X:54:ARG:HH11	1.65	0.62
1:1:144:LEU:HD21	1:1:394:PRO:HG3	1.82	0.62
6:M:113:LEU:HD22	6:M:139:VAL:HG21	1.81	0.62
8:W:192:LEU:HD23	8:X:192:LEU:HB3	1.81	0.62
1:1:491:PRO:HD2	5:K:45:VAL:HG23	1.82	0.61
5:H:12:ASN:HD21	5:H:86:TRP:HE1	1.48	0.61
6:P:53:GLU:OE2	6:P:79:TYR:OH	2.19	0.61
2:3:301:GLU:HG3	2:3:360:LEU:HD23	1.83	0.61
2:4:399:GLU:OE1	5:L:147:ARG:NH1	2.34	0.61
4:8:2208:LYS:HA	4:8:2211:LEU:HG	1.83	0.61
5:A:217:CYS:O	9:Y:50:GLN:NE2	2.34	0.60
6:M:102:LYS:O	6:M:118:LYS:NZ	2.34	0.60
5:I:168:GLY:HA2	5:K:44:MET:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:149:THR:O	5:L:296:ASN:ND2	2.35	0.60
6:S:437:TRP:NE1	6:S:441:ASN:OD1	2.33	0.60
6:O:96:SER:O	6:O:160:GLN:NE2	2.34	0.60
5:A:290:ARG:NH1	5:C:244:ASP:OD2	2.34	0.60
5:F:342:GLY:HA2	5:F:345:ILE:HD12	1.82	0.60
1:1:524:LEU:HD21	6:S:59:THR:HG21	1.83	0.60
5:D:9:VAL:HG12	5:D:104:LEU:HB3	1.82	0.60
6:S:407:GLU:OE1	6:S:411:ARG:NH1	2.34	0.60
5:A:360:GLN:NE2	5:A:364:GLU:OE2	2.35	0.59
5:F:200:PHE:HB3	5:F:205:GLU:HB3	1.84	0.59
5:H:358:SER:HB3	5:H:361:GLU:HG3	1.84	0.59
8:V:214:GLU:HA	8:V:217:ILE:HD12	1.84	0.59
6:T:38:ARG:HA	6:T:41:GLU:HG3	1.84	0.59
5:I:50:LYS:NZ	6:S:137:ASP:OD2	2.34	0.59
5:B:47:MET:HA	9:Y:176:GLU:HB3	1.84	0.59
6:S:428:ASP:OD1	6:S:502:ARG:NH1	2.36	0.58
8:V:151:GLU:OE2	8:V:155:ARG:NH1	2.36	0.58
3:7:71:SER:O	8:W:131:ARG:NH2	2.36	0.58
5:A:61:LYS:HD3	5:A:64:ILE:HD11	1.85	0.58
5:F:6:ALA:HB1	5:F:22:ALA:HB3	1.85	0.58
5:J:139:VAL:HG22	5:J:165:ILE:HD11	1.84	0.58
5:A:59:GLN:NE2	5:A:207:GLU:OE1	2.37	0.58
5:G:57:GLU:OE1	6:Q:132:ASN:ND2	2.36	0.58
5:I:110:LEU:O	5:I:177:ARG:NH1	2.37	0.58
9:Y:112:LEU:HD11	9:Y:116:LEU:HD23	1.85	0.58
2:3:167:HIS:HB3	2:3:187:LYS:HD2	1.85	0.58
5:B:169:TYR:HB2	5:D:64:ILE:HD11	1.84	0.58
5:F:202:THR:OG1	5:F:205:GLU:OE1	2.22	0.58
6:S:519:SER:OG	6:S:523:ARG:NH2	2.37	0.58
8:X:94:ILE:HG12	8:X:97:ARG:HH12	1.68	0.57
8:X:74:LEU:HA	8:X:77:LEU:HD12	1.85	0.57
3:6:71:SER:HA	8:W:82:LYS:HG2	1.85	0.57
4:8:2199:ARG:HA	4:8:2202:LYS:HD2	1.86	0.57
5:B:44:MET:HG3	5:B:47:MET:HG2	1.86	0.57
5:A:201:THR:OG1	9:Y:64:ARG:NH2	2.38	0.57
5:G:202:THR:OG1	5:G:205:GLU:OE1	2.18	0.57
5:J:106:THR:HB	5:J:137:GLN:HG2	1.85	0.57
3:5:209:LYS:NZ	7:U:64:ASP:OD1	2.37	0.57
5:F:190:MET:HG3	5:F:209:VAL:HG11	1.86	0.57
2:4:228:LEU:HD11	2:4:306:VAL:HG13	1.85	0.57
4:8:2064:LEU:HG	4:8:2139:ARG:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:161:TRP:HB3	1:2:240:ILE:HD11	1.85	0.56
7:U:34:GLU:OE2	8:V:39:ARG:NH2	2.38	0.56
1:1:335:ALA:HA	1:1:340:ASN:HB3	1.87	0.56
2:3:310:GLN:NE2	2:3:314:GLU:OE2	2.38	0.56
5:B:61:LYS:HE3	5:B:64:ILE:HD11	1.86	0.56
5:B:250:ILE:HD12	5:B:254:ARG:HB3	1.88	0.56
5:D:361:GLU:OE1	5:D:373:LYS:NZ	2.38	0.56
6:S:303:MET:HA	6:S:306:LYS:HB2	1.88	0.56
6:S:344:PHE:HZ	6:S:403:GLU:HG2	1.71	0.56
5:B:110:LEU:O	5:B:177:ARG:NH1	2.38	0.56
5:C:57:GLU:OE1	6:M:132:ASN:ND2	2.39	0.56
3:5:53:ILE:HG21	5:D:345:ILE:HG12	1.87	0.56
3:5:64:TYR:OH	5:D:25:ASP:O	2.22	0.56
5:B:14:SER:HB2	5:B:157:ASP:HB3	1.88	0.56
4:8:2078:GLN:HA	4:8:2081:LYS:HG2	1.87	0.56
6:P:110:ILE:HA	6:P:113:LEU:HD12	1.88	0.56
1:0:38:GLU:HA	1:0:41:MET:HG3	1.88	0.56
2:3:137:ILE:HB	2:3:159:LEU:HD12	1.87	0.56
2:9:53:ARG:NH2	5:K:334:GLU:OE2	2.38	0.56
8:X:184:LYS:HA	8:X:187:GLU:HG2	1.88	0.56
5:C:91:TYR:OH	6:M:156:ARG:NH2	2.39	0.56
5:E:196:ARG:HH12	5:E:251:GLY:HA3	1.70	0.56
7:U:129:VAL:HG13	8:V:133:LEU:HD11	1.88	0.56
5:D:24:ASP:OD2	5:D:28:ARG:NH2	2.32	0.55
5:A:14:SER:N	11:A:401:ADP:O2B	2.36	0.55
5:J:190:MET:HG3	5:J:209:VAL:HG11	1.87	0.55
5:B:49:GLN:OE1	9:Y:201:ASN:ND2	2.39	0.55
5:E:25:ASP:OD2	6:O:44:ARG:NH1	2.40	0.55
5:L:244:ASP:OD2	5:L:246:GLN:NE2	2.39	0.55
8:W:161:ILE:HD13	8:X:161:ILE:HD11	1.89	0.55
5:E:270:GLU:OE2	5:F:39:ARG:NH1	2.40	0.55
5:G:107:GLU:OE1	5:G:111:ASN:ND2	2.36	0.55
9:Y:273:VAL:HA	9:Y:276:LEU:HD23	1.88	0.55
2:4:211:LEU:HA	2:4:265:MET:SD	2.46	0.54
9:Y:127:GLU:HB2	9:Y:155:ILE:HD13	1.89	0.54
10:Z:54:PRO:O	10:Z:58:LYS:NZ	2.35	0.54
1:1:230:ALA:HB2	1:1:287:GLN:HG2	1.89	0.54
5:A:123:MET:HG3	5:A:132:MET:HG3	1.90	0.54
5:A:236:LEU:O	5:A:254:ARG:NH1	2.38	0.54
6:S:270:VAL:HA	6:S:273:PHE:CE1	2.41	0.54
5:E:110:LEU:O	5:E:177:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:285:CYS:HB3	5:F:289:ILE:HD11	1.89	0.54
6:N:50:ASP:HA	6:N:53:GLU:HB3	1.90	0.54
8:W:35:VAL:HB	8:X:35:VAL:HG22	1.88	0.54
5:C:143:TYR:OH	5:E:45:VAL:O	2.25	0.54
6:Q:63:TRP:NE1	6:Q:67:HIS:CE1	2.75	0.54
1:2:200:ILE:HG22	1:2:206:VAL:HA	1.89	0.54
5:B:106:THR:HB	5:B:137:GLN:HG2	1.89	0.54
6:T:109:ARG:NH2	6:T:140:ASP:OD1	2.41	0.54
9:Y:189:ARG:HH21	9:Y:197:LEU:HD13	1.73	0.54
9:Y:273:VAL:HG21	9:Y:302:ILE:HG12	1.90	0.54
4:8:2041:ASP:HA	4:8:2044:MET:HG3	1.89	0.54
4:8:2175:ARG:HG3	4:8:2243:LEU:HD21	1.90	0.54
5:L:357:ILE:HG12	5:L:373:LYS:HG2	1.89	0.54
1:2:384:LEU:HD12	1:2:387:LEU:HD12	1.90	0.54
5:G:358:SER:HB3	5:G:361:GLU:HG3	1.88	0.54
5:E:14:SER:HB2	5:E:157:ASP:HB3	1.90	0.54
5:L:44:MET:HB3	5:L:47:MET:HG2	1.89	0.53
6:S:325:LEU:O	6:S:406:ARG:NH2	2.33	0.53
4:8:2179:LEU:HA	6:S:367:PHE:HZ	1.73	0.53
5:D:317:ILE:HG22	5:D:327:ILE:HD13	1.90	0.53
10:Z:4:ARG:HG2	10:Z:35:GLU:HB2	1.89	0.53
1:1:514:ILE:O	6:S:44:ARG:NH2	2.39	0.53
1:2:342:VAL:HG23	2:3:240:LYS:HG2	1.91	0.53
2:3:113:THR:OG1	2:3:142:ARG:NH2	2.41	0.53
2:4:123:SER:OG	2:4:124:LEU:N	2.42	0.53
4:8:2354:GLU:O	4:8:2358:SER:HB3	2.09	0.53
3:6:117:THR:OG1	3:6:118:THR:N	2.42	0.53
5:E:237:GLU:HG2	5:E:251:GLY:HA2	1.91	0.53
7:U:203:ALA:HB2	8:V:203:ALA:HB2	1.91	0.53
5:G:200:PHE:HB3	5:G:205:GLU:HB3	1.89	0.53
2:4:323:ALA:HB1	2:4:328:ASN:HB2	1.91	0.53
5:I:237:GLU:HA	5:I:251:GLY:HA2	1.90	0.53
9:Y:188:GLU:OE2	9:Y:192:ASN:ND2	2.40	0.53
2:4:301:GLU:HG2	2:4:305:LYS:HE2	1.90	0.53
1:2:167:ASN:O	1:2:189:TYR:OH	2.25	0.52
4:8:2051:SER:O	4:8:2055:ASN:ND2	2.42	0.52
6:P:49:ALA:O	6:P:53:GLU:HB2	2.09	0.52
5:A:196:ARG:NH2	5:A:249:THR:O	2.42	0.52
5:G:14:SER:HB2	5:G:157:ASP:HB3	1.90	0.52
6:M:130:LEU:HD12	6:M:133:MET:HG3	1.91	0.52
7:U:195:LYS:HG3	8:V:196:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:33:ARG:HE	2:9:37:ARG:HD3	1.75	0.52
5:F:26:ALA:HB1	6:P:45:ILE:HD13	1.91	0.52
7:U:192:LEU:HD23	8:V:192:LEU:HD23	1.91	0.52
8:V:204:GLU:O	8:V:208:ARG:HG2	2.09	0.52
5:C:246:GLN:NE2	9:Y:321:GLN:OE1	2.42	0.52
5:J:215:LYS:HD3	5:J:240:TYR:HE1	1.74	0.52
3:5:51:LYS:HB2	3:5:54:LEU:HB2	1.92	0.52
5:K:268:GLY:O	5:L:39:ARG:NH2	2.43	0.52
5:L:31:PHE:HE2	5:L:85:ILE:HD11	1.75	0.52
3:5:161:HIS:ND1	3:5:164:GLU:OE2	2.43	0.52
5:K:272:CYS:SG	5:K:273:GLY:N	2.80	0.52
5:D:26:ALA:HB1	6:N:45:ILE:HD13	1.92	0.52
6:S:441:ASN:HA	6:S:444:LEU:HG	1.92	0.52
7:U:210:VAL:HA	7:U:213:LEU:HB2	1.91	0.52
1:1:115:ALA:O	1:1:119:MET:HG2	2.10	0.51
1:1:200:ILE:HG22	1:1:206:VAL:HA	1.91	0.51
2:4:323:ALA:O	2:4:328:ASN:ND2	2.41	0.51
5:L:62:ARG:HH11	5:L:207:GLU:HB2	1.75	0.51
2:3:171:SER:HA	2:3:185:LEU:HD22	1.91	0.51
5:A:202:THR:OG1	5:A:205:GLU:OE1	2.21	0.51
5:D:220:ALA:HB1	5:D:226:GLU:HG3	1.92	0.51
5:F:34:ILE:HD12	5:F:67:LEU:HD22	1.92	0.51
4:8:2226:VAL:HG23	4:8:2227:LEU:H	1.76	0.51
5:L:82:MET:HA	5:L:85:ILE:HG22	1.92	0.51
5:J:153:MET:HG3	5:J:162:THR:HG22	1.92	0.51
5:K:52:SER:OG	5:K:84:LYS:NZ	2.37	0.51
8:X:177:LYS:O	8:X:181:LYS:HG2	2.10	0.51
5:D:142:LEU:HD12	5:D:165:ILE:HD12	1.93	0.51
5:C:28:ARG:NH1	6:M:48:LEU:O	2.44	0.51
5:D:54:VAL:O	6:N:132:ASN:ND2	2.43	0.51
5:J:285:CYS:HB3	5:J:289:ILE:HD11	1.93	0.51
6:S:461:LYS:HD2	6:S:528:LEU:HD11	1.93	0.51
9:Y:319:PHE:HB2	9:Y:325:ARG:HB2	1.92	0.51
1:2:191:GLU:OE1	2:4:374:ASN:ND2	2.43	0.51
2:4:378:ARG:NH1	5:L:321:ALA:O	2.39	0.51
5:B:43:VAL:HG21	9:Y:206:ARG:HD3	1.93	0.51
5:D:358:SER:HB3	5:D:361:GLU:HG3	1.93	0.51
5:H:187:ASP:OD1	5:H:206:ARG:NH1	2.44	0.51
4:8:2249:ARG:NH1	6:S:368:THR:OG1	2.44	0.51
5:H:152:VAL:O	5:H:162:THR:HA	2.11	0.50
5:I:131:ALA:HB1	5:I:356:TRP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:436:THR:HB	2:3:475:MET:HB3	1.93	0.50
4:8:2187:THR:OG1	4:8:2193:GLN:NE2	2.38	0.50
5:B:317:ILE:HG22	5:B:327:ILE:HD13	1.93	0.50
5:D:115:ASN:O	5:D:119:MET:HG3	2.11	0.50
2:4:301:GLU:HG3	2:4:360:LEU:HD23	1.93	0.50
8:X:154:CYS:O	8:X:157:MET:HG2	2.12	0.50
5:F:268:GLY:O	5:G:39:ARG:NH2	2.45	0.50
8:X:153:ARG:O	8:X:156:GLU:HG2	2.11	0.50
4:8:2382:GLN:NE2	6:S:295:ASP:OD1	2.45	0.50
5:L:369:ILE:HG13	5:L:372:ARG:HH21	1.77	0.50
3:7:135:ARG:HD3	3:7:136:PRO:HD2	1.94	0.50
5:D:47:MET:O	6:N:135:SER:OG	2.23	0.50
5:G:110:LEU:O	5:G:177:ARG:NH1	2.45	0.50
5:D:47:MET:SD	5:D:47:MET:N	2.85	0.50
5:F:153:MET:HG2	5:F:162:THR:HG22	1.94	0.50
8:W:30:ARG:HG3	8:W:31:LEU:HD12	1.94	0.50
2:4:366:GLU:HG2	2:4:381:TYR:HE2	1.76	0.50
5:I:106:THR:HB	5:I:137:GLN:HG2	1.94	0.49
8:W:69:ARG:HB2	8:X:70:LEU:HD11	1.93	0.49
1:1:299:LEU:HB2	1:1:302:HIS:HB3	1.93	0.49
5:H:107:GLU:OE2	5:H:116:ARG:NE	2.44	0.49
9:Y:218:GLU:HG3	9:Y:221:LYS:HE3	1.95	0.49
1:2:273:TYR:HH	2:4:248:HIS:HD1	1.39	0.49
5:B:196:ARG:NH1	5:B:250:ILE:O	2.45	0.49
5:D:112:PRO:HG3	5:E:197:GLY:HA2	1.95	0.49
5:E:91:TYR:OH	6:O:156:ARG:NH2	2.42	0.49
5:I:202:THR:OG1	5:I:205:GLU:OE1	2.26	0.49
5:K:117:GLU:OE2	5:K:371:HIS:NE2	2.43	0.49
6:O:100:LEU:HD11	6:O:122:PHE:CG	2.47	0.49
6:Q:92:LEU:HD13	6:Q:122:PHE:HD2	1.77	0.49
2:3:188:VAL:HG12	2:3:194:VAL:HA	1.95	0.49
5:B:300:SER:OG	5:B:301:GLY:N	2.45	0.49
6:O:99:MET:N	6:O:99:MET:SD	2.80	0.49
5:B:70:PRO:HB3	5:B:81:ASP:HB3	1.94	0.49
6:S:227:ASP:O	6:S:230:ALA:HB2	2.12	0.49
7:U:217:ILE:HG13	8:V:217:ILE:HG12	1.95	0.49
5:D:159:VAL:HG11	5:D:177:ARG:HE	1.78	0.49
5:L:107:GLU:OE1	5:L:111:ASN:ND2	2.38	0.49
6:S:231:ARG:NH1	6:S:254:GLU:OE2	2.46	0.49
8:W:224:LEU:HD22	8:X:224:LEU:HD13	1.94	0.49
4:8:2216:ASP:HA	4:8:2219:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:157:ASP:OD1	11:G:401:ADP:O3'	2.30	0.49
9:Y:190:ILE:HG23	9:Y:223:ASN:HD22	1.78	0.49
1:2:391:THR:HG23	1:2:393:TYR:H	1.77	0.49
5:K:270:GLU:HG3	5:L:202:THR:HB	1.95	0.49
3:7:187:ILE:HG21	6:S:106:GLY:HA2	1.95	0.49
4:8:2062:GLU:OE1	6:S:434:ARG:NH2	2.45	0.49
5:I:143:TYR:CE2	5:I:346:LEU:HD13	2.47	0.49
2:3:157:VAL:HG13	2:3:226:ILE:HG12	1.95	0.48
5:B:44:MET:SD	5:B:44:MET:N	2.82	0.48
1:1:149:LEU:HD23	1:1:197:LEU:HD13	1.95	0.48
6:T:92:LEU:HD13	6:T:122:PHE:HD2	1.78	0.48
4:8:2205:GLN:HA	4:8:2208:LYS:HG2	1.94	0.48
4:8:2364:GLU:OE2	6:S:279:LYS:NZ	2.41	0.48
5:C:189:LEU:HA	5:C:192:ILE:HG22	1.95	0.48
5:J:107:GLU:OE2	5:J:116:ARG:NE	2.45	0.48
2:4:221:ASP:OD1	2:4:221:ASP:N	2.46	0.48
5:A:200:PHE:HB3	5:A:205:GLU:HB3	1.96	0.48
8:V:138:GLY:HA2	8:V:141:GLU:HG2	1.95	0.48
1:2:134:ASP:N	1:2:134:ASP:OD1	2.46	0.48
1:2:144:LEU:HG	1:2:148:LYS:HE3	1.96	0.48
1:2:226:ALA:HB2	1:2:283:LYS:HG2	1.95	0.48
5:E:26:ALA:HB1	6:O:45:ILE:HD13	1.94	0.48
5:G:143:TYR:OH	5:I:45:VAL:N	2.45	0.48
4:8:2120:LEU:HD23	4:8:2125:LEU:HD21	1.96	0.48
6:O:123:LEU:HD11	6:O:153:ILE:HD11	1.95	0.48
4:8:2211:LEU:HD11	4:8:2240:TRP:CD2	2.49	0.48
2:9:68:GLU:OE1	5:K:351:THR:OG1	2.22	0.48
5:E:290:ARG:NH1	5:G:244:ASP:OD1	2.46	0.48
5:F:286:ASP:O	5:F:290:ARG:NE	2.46	0.48
4:8:2206:ALA:O	4:8:2209:ARG:CB	2.40	0.48
5:B:163:VAL:HG23	5:B:175:ILE:HG12	1.95	0.48
5:G:357:ILE:HG12	5:G:373:LYS:HG2	1.94	0.48
5:J:91:TYR:OH	6:T:156:ARG:NH2	2.46	0.48
6:N:92:LEU:HD13	6:N:122:PHE:HD2	1.79	0.48
6:S:245:LEU:HD12	6:S:276:TYR:HE2	1.79	0.48
5:F:193:LEU:HD21	5:F:250:ILE:HG22	1.95	0.47
5:G:149:THR:HG22	5:G:167:GLU:H	1.78	0.47
5:K:211:ASP:OD2	5:K:240:TYR:OH	2.31	0.47
6:R:57:LYS:NZ	6:R:77:ASP:OD1	2.39	0.47
9:Y:144:GLN:HG2	9:Y:148:GLN:NE2	2.29	0.47
5:A:332:PRO:O	5:A:335:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:201:THR:HG23	5:G:202:THR:HG23	1.95	0.47
5:H:57:GLU:OE1	6:R:132:ASN:ND2	2.48	0.47
5:J:2:ASP:OD1	5:J:2:ASP:N	2.46	0.47
2:3:442:ARG:NH1	5:J:363:ASP:O	2.47	0.47
2:4:191:LEU:HD12	6:S:497:LYS:HB3	1.95	0.47
5:L:358:SER:HB3	5:L:361:GLU:HG3	1.95	0.47
7:U:94:ILE:O	7:U:97:ARG:HB2	2.15	0.47
8:W:179:SER:O	8:W:182:GLU:HG3	2.14	0.47
5:B:236:LEU:O	5:B:254:ARG:NH1	2.46	0.47
5:D:188:TYR:HB2	5:D:267:LEU:HD21	1.96	0.47
5:J:99:GLU:HG2	5:J:128:ASN:HB3	1.96	0.47
1:1:157:ASP:HB2	1:1:189:TYR:HB3	1.95	0.47
1:1:370:TRP:NE1	1:1:375:GLN:HB2	2.29	0.47
4:8:2352:SER:HA	4:8:2355:ILE:HD13	1.97	0.47
1:1:201:ASN:OD1	1:1:205:ASP:N	2.47	0.47
3:7:147:TYR:HE2	5:G:5:ILE:HD11	1.80	0.47
2:9:65:GLU:HA	2:9:68:GLU:HB2	1.96	0.47
5:B:285:CYS:HB3	5:B:289:ILE:HD11	1.96	0.47
5:G:153:MET:HG3	5:G:162:THR:HG22	1.97	0.47
5:K:148:THR:O	5:K:168:GLY:N	2.48	0.47
8:V:178:TYR:HA	8:V:181:LYS:HB3	1.97	0.47
10:Z:57:LYS:HZ1	10:Z:75:TYR:HE2	1.62	0.47
4:8:2205:GLN:HA	4:8:2208:LYS:HE3	1.96	0.47
5:B:351:THR:OG1	6:N:114:GLU:OE2	2.31	0.47
5:L:286:ASP:OD1	5:L:286:ASP:N	2.43	0.47
6:M:31:ASP:N	6:M:31:ASP:OD1	2.48	0.47
6:N:68:LEU:HD12	6:N:73:CYS:HB2	1.96	0.47
5:J:57:GLU:HB3	6:T:132:ASN:HD21	1.80	0.47
6:S:319:GLU:HA	6:S:322:ILE:HG12	1.97	0.47
1:2:144:LEU:HD11	1:2:394:PRO:HD3	1.96	0.46
4:8:2118:THR:HG22	4:8:2120:LEU:H	1.80	0.46
5:A:107:GLU:OE2	5:A:116:ARG:NE	2.36	0.46
5:B:200:PHE:HB3	5:B:205:GLU:HB3	1.97	0.46
2:3:478:ARG:NH2	2:3:480:GLU:OE2	2.48	0.46
3:7:64:TYR:OH	5:H:25:ASP:O	2.30	0.46
4:8:2256:GLN:O	4:8:2260:ILE:HG12	2.15	0.46
5:J:95:ARG:HD2	6:T:56:GLN:HG2	1.97	0.46
6:M:35:SER:O	6:M:39:LEU:HB2	2.15	0.46
5:H:26:ALA:HB1	6:R:45:ILE:HD13	1.96	0.46
8:V:213:LEU:O	8:V:217:ILE:HG13	2.14	0.46
8:W:187:GLU:HA	8:W:190:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:8:2208:LYS:HE2	4:8:2240:TRP:HH2	1.80	0.46
5:G:51:ASP:OD1	5:G:51:ASP:N	2.47	0.46
5:G:191:LYS:HB2	5:G:191:LYS:HE2	1.69	0.46
1:1:386:ASN:O	2:4:109:PHE:N	2.49	0.46
3:7:65:GLU:HG3	3:7:66:PRO:HD3	1.98	0.46
5:I:358:SER:HB3	5:I:361:GLU:HG3	1.98	0.46
5:H:200:PHE:HB3	5:H:205:GLU:HB3	1.97	0.46
5:I:220:ALA:HB1	5:I:226:GLU:HG3	1.97	0.46
9:Y:183:VAL:O	9:Y:216:TYR:OH	2.33	0.46
1:2:163:HIS:HE1	1:2:166:TYR:HD2	1.62	0.46
5:G:193:LEU:HD23	5:G:193:LEU:HA	1.83	0.46
6:S:523:ARG:O	6:S:526:THR:OG1	2.32	0.46
10:Z:53:ILE:HG13	10:Z:58:LYS:HZ1	1.80	0.46
2:3:158:THR:HG22	2:3:170:ILE:HG22	1.98	0.46
5:F:26:ALA:HB3	6:P:48:LEU:HD12	1.98	0.46
5:K:113:LYS:HG2	5:K:371:HIS:CE1	2.51	0.46
3:6:148:LYS:NZ	5:E:3:ASP:OD1	2.48	0.46
4:8:2073:LEU:HD23	4:8:2077:ARG:HH12	1.80	0.46
6:S:297:ALA:O	6:S:300:THR:OG1	2.20	0.46
4:8:2167:PHE:HA	4:8:2170:TRP:CD1	2.51	0.45
7:U:161:LEU:HD13	8:V:161:ILE:HG22	1.98	0.45
2:4:404:VAL:HG11	5:L:310:ALA:HB1	1.96	0.45
3:7:125:LEU:HD23	5:I:41:GLN:HE21	1.81	0.45
5:D:113:LYS:HB3	5:D:371:HIS:CE1	2.52	0.45
7:U:42:ARG:NH2	8:V:41:ALA:HB3	2.31	0.45
8:W:12:ARG:HA	9:Y:110:VAL:HG11	1.97	0.45
1:2:274:HIS:HD2	1:2:277:LEU:H	1.63	0.45
2:3:126:LEU:HD22	2:3:130:GLU:HG2	1.97	0.45
5:C:95:ARG:HD3	6:M:147:LEU:HB3	1.99	0.45
5:D:163:VAL:HG23	5:D:175:ILE:HG12	1.97	0.45
5:H:113:LYS:HE2	5:H:371:HIS:CE1	2.50	0.45
8:W:139:ASP:HB2	8:X:140:LEU:HD11	1.97	0.45
5:D:285:CYS:HB3	5:D:289:ILE:HD11	1.98	0.45
5:I:57:GLU:OE2	6:S:144:ARG:NH2	2.50	0.45
5:K:369:ILE:HD12	5:K:372:ARG:HD3	1.99	0.45
6:S:411:ARG:HA	6:S:414:LEU:HB3	1.98	0.45
7:U:124:ARG:HA	7:U:127:GLU:HG3	1.97	0.45
1:2:231:ARG:HH21	1:2:290:LEU:HD21	1.81	0.45
5:H:168:GLY:HA2	5:J:44:MET:HG3	1.99	0.45
5:I:138:ALA:HB1	5:I:152:VAL:HG13	1.98	0.45
5:I:346:LEU:HD12	5:I:346:LEU:HA	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:189:ASN:ND2	2:3:193:GLU:OE1	2.45	0.45
2:3:473:SER:OG	2:3:474:GLY:N	2.50	0.45
3:6:64:TYR:OH	5:F:25:ASP:O	2.20	0.45
4:8:2074:ASP:OD1	4:8:2074:ASP:N	2.50	0.45
5:A:152:VAL:O	5:A:162:THR:HA	2.16	0.45
5:I:190:MET:HG2	5:I:209:VAL:HG21	1.97	0.45
8:W:213:LEU:O	8:W:217:ILE:HG13	2.16	0.45
3:6:65:GLU:HB3	6:P:43:SER:HA	1.98	0.45
2:9:70:LEU:HD11	5:K:168:GLY:HA3	1.99	0.45
5:G:374:CYS:SG	5:G:375:PHE:N	2.90	0.45
5:J:157:ASP:HB2	11:J:401:ADP:H4'	1.99	0.45
8:W:140:LEU:HD13	8:X:140:LEU:HA	1.99	0.45
4:8:2301:LEU:O	6:S:281:LYS:NZ	2.46	0.45
5:D:25:ASP:OD1	5:D:25:ASP:N	2.47	0.45
3:6:170:SER:OG	3:6:176:ALA:O	2.35	0.45
6:P:102:LYS:O	6:P:118:LYS:NZ	2.46	0.45
8:X:160:GLN:O	8:X:164:MET:HG3	2.17	0.45
1:2:209:ARG:HH22	2:4:389:GLN:NE2	2.15	0.44
5:A:50:LYS:HG3	5:A:53:TYR:HE1	1.81	0.44
5:A:338:SER:HA	5:A:341:ILE:HD12	1.98	0.44
5:D:346:LEU:HD12	5:D:346:LEU:HA	1.81	0.44
5:H:131:ALA:HB1	5:H:356:TRP:HB3	1.99	0.44
5:K:75:ILE:HD12	5:K:112:PRO:HD2	1.99	0.44
8:W:75:GLN:O	8:W:79:GLU:HG2	2.17	0.44
2:3:189:ASN:OD1	2:3:193:GLU:N	2.50	0.44
2:4:125:ASN:N	2:4:196:GLU:OE2	2.38	0.44
5:D:242:LEU:HD12	5:D:246:GLN:HB2	1.98	0.44
5:G:168:GLY:HA2	5:I:44:MET:HG3	1.99	0.44
5:H:200:PHE:HD1	5:H:205:GLU:HG2	1.82	0.44
5:J:122:ILE:O	5:J:126:THR:OG1	2.32	0.44
8:W:121:GLU:O	8:W:124:ARG:HB2	2.16	0.44
8:X:85:ASP:HA	8:X:88:GLU:HG2	1.98	0.44
2:4:158:THR:HG22	2:4:170:ILE:HG22	1.98	0.44
3:5:53:ILE:HD11	5:D:25:ASP:HA	1.99	0.44
4:8:2366:LYS:O	4:8:2407:TYR:OH	2.29	0.44
5:H:237:GLU:HG2	5:H:251:GLY:HA2	2.00	0.44
9:Y:179:ASN:ND2	9:Y:203:ASN:O	2.46	0.44
1:1:385:ASP:OD2	1:1:395:TYR:OH	2.29	0.44
1:2:124:VAL:HG11	5:L:290:ARG:HH21	1.82	0.44
5:H:282:ILE:HG21	5:H:294:TYR:CE1	2.52	0.44
3:7:178:PRO:HA	3:7:179:PRO:HD3	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:8:2087:LEU:HD13	4:8:2090:LEU:HD12	2.00	0.44
5:H:2:ASP:OD1	5:H:2:ASP:N	2.49	0.44
5:J:306:TYR:HD2	5:J:309:ILE:HD11	1.83	0.44
5:K:332:PRO:O	5:K:335:ARG:NH1	2.50	0.44
6:S:204:ASP:OD1	6:S:204:ASP:N	2.51	0.44
5:B:211:ASP:OD2	5:B:240:TYR:OH	2.35	0.44
6:S:232:HIS:HA	6:S:235:GLU:HG2	1.99	0.44
8:W:188:GLU:O	8:W:191:ILE:HG12	2.17	0.44
1:2:299:LEU:HD22	1:2:302:HIS:HB3	2.00	0.44
3:5:140:ILE:HA	3:5:143:LYS:HE3	2.00	0.44
5:E:185:LEU:HD11	5:E:261:LEU:HG	1.99	0.44
5:F:25:ASP:N	5:F:25:ASP:OD1	2.48	0.44
6:S:102:LYS:O	6:S:118:LYS:NZ	2.47	0.44
8:V:177:LYS:HE3	8:V:177:LYS:HB3	1.77	0.44
3:5:205:TRP:O	3:5:209:LYS:HG2	2.18	0.44
5:E:183:ARG:HD2	5:E:206:ARG:HH12	1.83	0.44
5:J:302:GLY:O	5:J:305:MET:HB2	2.18	0.44
6:P:99:MET:SD	6:P:99:MET:N	2.87	0.44
5:B:153:MET:HG2	5:B:162:THR:HG22	1.99	0.44
5:C:14:SER:N	11:C:401:ADP:O2B	2.51	0.44
5:E:326:LYS:HA	5:E:326:LYS:HD3	1.80	0.44
5:H:155:SER:HB3	5:H:160:THR:HG23	2.00	0.44
8:W:182:GLU:HA	8:W:185:TYR:HD1	1.83	0.44
8:X:237:MET:O	8:X:240:GLN:HG3	2.18	0.44
9:Y:231:ILE:HD11	9:Y:259:VAL:HG12	2.00	0.44
2:4:276:LYS:HD2	6:S:512:TYR:HE1	1.83	0.43
2:4:359:ARG:HD2	2:4:359:ARG:HA	1.72	0.43
5:B:143:TYR:OH	5:D:45:VAL:N	2.50	0.43
5:D:28:ARG:HG3	5:D:94:LEU:HD23	2.00	0.43
6:Q:93:GLU:HB3	6:Q:100:LEU:HD13	2.00	0.43
8:W:180:GLN:HE21	8:W:184:LYS:HE2	1.83	0.43
8:W:184:LYS:O	8:W:187:GLU:HG3	2.17	0.43
1:1:155:LEU:HD11	1:1:380:LEU:HB3	2.01	0.43
1:2:124:VAL:HG13	5:L:286:ASP:HA	2.00	0.43
2:9:37:ARG:HH12	2:9:42:ARG:HG3	1.83	0.43
5:G:285:CYS:HB3	5:G:289:ILE:HD11	2.00	0.43
6:S:300:THR:HG22	6:S:372:ARG:HD3	2.00	0.43
8:W:31:LEU:HD21	8:X:32:GLN:HB2	2.01	0.43
1:1:139:ASP:OD1	1:1:140:LYS:N	2.51	0.43
5:C:176:LEU:HD23	5:C:176:LEU:HA	1.87	0.43
4:8:2216:ASP:O	4:8:2219:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:8:2390:MET:SD	4:8:2405:TYR:HB3	2.59	0.43
6:O:80:LYS:HA	6:O:83:ARG:HD2	1.99	0.43
1:1:334:SER:HB2	2:4:320:LEU:HB2	2.00	0.43
4:8:2094:GLN:O	4:8:2098:ASN:ND2	2.51	0.43
4:8:2375:LYS:HB3	4:8:2375:LYS:HE3	1.83	0.43
5:L:113:LYS:HE2	5:L:113:LYS:HB2	1.88	0.43
6:P:149:LEU:O	6:P:153:ILE:HG13	2.18	0.43
9:Y:73:LYS:O	9:Y:77:GLU:HG2	2.18	0.43
9:Y:131:ILE:HA	9:Y:134:ILE:HG22	1.99	0.43
3:7:172:LYS:HE3	5:G:100:GLU:HB3	2.01	0.43
5:A:113:LYS:HG2	5:A:371:HIS:CE1	2.54	0.43
10:Z:8:ALA:H	10:Z:20:GLN:NE2	2.16	0.43
3:7:66:PRO:HG3	8:W:126:TYR:HE2	1.83	0.43
4:8:2349:ILE:HG21	4:8:2355:ILE:HD11	2.01	0.43
5:D:282:ILE:HG21	5:D:294:TYR:CE1	2.54	0.43
6:O:123:LEU:HD23	6:O:123:LEU:HA	1.87	0.43
9:Y:260:GLU:HG2	9:Y:288:ASP:H	1.83	0.43
10:Z:78:ASP:OD1	10:Z:78:ASP:N	2.49	0.43
1:2:325:CYS:O	1:2:329:VAL:HG23	2.19	0.43
5:A:16:MET:HA	5:A:32:PRO:HA	2.00	0.43
5:H:325:MET:SD	5:H:325:MET:N	2.92	0.43
5:I:163:VAL:HG23	5:I:175:ILE:HG12	2.01	0.43
7:U:183:ASP:OD1	7:U:184:LYS:N	2.52	0.43
1:1:248:VAL:HA	1:1:251:MET:HG2	2.01	0.43
5:G:113:LYS:HE2	5:G:113:LYS:HB2	1.80	0.43
8:V:96:ASN:O	8:V:100:LYS:HG2	2.18	0.43
5:B:79:TRP:CE2	5:B:118:LYS:HG2	2.53	0.43
6:S:147:LEU:HD23	6:S:147:LEU:HA	1.87	0.43
8:V:139:ASP:HA	8:V:142:ARG:HE	1.84	0.43
9:Y:129:CYS:SG	9:Y:161:LEU:N	2.92	0.43
1:2:274:HIS:CD2	1:2:277:LEU:H	2.37	0.42
2:9:40:ASP:OD2	2:9:40:ASP:N	2.52	0.42
5:H:153:MET:HG2	5:H:162:THR:HG22	2.01	0.42
5:K:200:PHE:HB3	5:K:205:GLU:HB3	2.01	0.42
5:L:3:ASP:OD1	5:L:3:ASP:N	2.51	0.42
5:L:113:LYS:HG3	5:L:371:HIS:NE2	2.34	0.42
6:S:109:ARG:NH2	6:S:140:ASP:OD1	2.51	0.42
9:Y:116:LEU:HD12	9:Y:116:LEU:HA	1.85	0.42
4:8:2167:PHE:HE2	4:8:2210:GLN:HE22	1.63	0.42
4:8:2204:ILE:O	4:8:2208:LYS:N	2.50	0.42
5:A:118:LYS:HA	5:A:118:LYS:HD2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:200:PHE:HB3	5:E:205:GLU:HB3	2.01	0.42
5:K:153:MET:HG3	5:K:162:THR:HG22	2.00	0.42
8:X:187:GLU:O	8:X:190:LYS:HG2	2.19	0.42
5:I:57:GLU:OE1	6:S:132:ASN:ND2	2.52	0.42
5:I:282:ILE:HG21	5:I:294:TYR:CE1	2.53	0.42
5:J:50:LYS:HD2	6:T:134:GLY:HA3	2.01	0.42
6:T:50:ASP:O	6:T:53:GLU:HG2	2.19	0.42
1:2:117:LEU:HD21	2:4:371:MET:SD	2.59	0.42
5:A:53:TYR:HD2	5:A:65:LEU:HD11	1.84	0.42
5:F:86:TRP:HH2	5:F:119:MET:HG3	1.82	0.42
5:J:15:GLY:HA2	5:J:69:TYR:HE2	1.84	0.42
5:K:285:CYS:HB3	5:K:289:ILE:HD11	2.01	0.42
5:L:304:THR:O	5:L:335:ARG:NE	2.50	0.42
7:U:196:LEU:HG	8:V:196:LEU:HA	2.02	0.42
1:1:494:THR:OG1	5:K:47:MET:O	2.38	0.42
2:4:143:LEU:HD11	2:4:368:LEU:HD22	2.01	0.42
3:7:187:ILE:HD13	3:7:192:TRP:CZ3	2.54	0.42
5:A:203:THR:HA	5:A:206:ARG:HB2	2.01	0.42
5:G:39:ARG:HD2	5:G:66:THR:HG23	2.01	0.42
5:K:282:ILE:HG21	5:K:294:TYR:CE1	2.54	0.42
5:L:163:VAL:HG12	5:L:175:ILE:HG23	2.02	0.42
1:2:273:TYR:OH	2:4:248:HIS:ND1	2.31	0.42
6:S:345:SER:O	6:S:348:ARG:HB3	2.20	0.42
8:X:51:SER:HA	8:X:54:ARG:HD3	2.01	0.42
2:4:113:THR:HB	2:4:142:ARG:HH22	1.85	0.42
5:H:25:ASP:OD1	5:H:25:ASP:N	2.51	0.42
6:M:92:LEU:HD11	6:M:123:LEU:HD21	2.01	0.42
1:2:153:TYR:OH	1:2:169:ILE:O	2.32	0.42
2:4:373:ASP:OD2	2:4:383:TYR:OH	2.29	0.42
3:6:180:ASP:OD1	3:6:180:ASP:N	2.53	0.42
6:S:420:LEU:HA	6:S:423:LEU:HG	2.02	0.42
7:U:63:LEU:HA	8:V:63:LEU:HD13	2.02	0.42
1:2:353:SER:HA	2:3:264:GLU:HG3	2.02	0.42
5:H:75:ILE:HD12	5:H:112:PRO:HD2	2.02	0.42
6:S:123:LEU:HD23	6:S:123:LEU:HA	1.92	0.42
8:X:107:LEU:O	8:X:110:ILE:HG22	2.20	0.42
8:X:197:LYS:O	8:X:201:THR:HG23	2.19	0.42
1:2:265:LEU:HD22	1:2:296:VAL:HG21	2.01	0.42
1:2:350:LYS:HD2	1:2:350:LYS:HA	1.81	0.42
5:F:131:ALA:HB1	5:F:356:TRP:HB3	2.01	0.42
5:H:50:LYS:NZ	6:R:137:ASP:OD1	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:63:TRP:CE2	6:Q:67:HIS:CE1	3.08	0.42
6:S:327:SER:O	6:S:406:ARG:NH2	2.52	0.42
8:V:40:ARG:O	8:V:43:GLU:HG3	2.20	0.42
8:W:204:GLU:O	8:W:208:ARG:HG2	2.20	0.42
2:3:245:PRO:HD2	2:3:331:LEU:HD12	2.01	0.41
2:4:118:LEU:HD13	2:4:131:ARG:HB2	2.02	0.41
5:B:112:PRO:HG3	5:C:197:GLY:HA2	2.02	0.41
5:C:147:ARG:HD3	5:C:296:ASN:HD22	1.85	0.41
5:I:193:LEU:HD23	5:I:193:LEU:HA	1.89	0.41
6:S:227:ASP:N	6:S:227:ASP:OD1	2.53	0.41
7:U:82:LYS:HE3	7:U:82:LYS:HB2	1.74	0.41
1:1:381:MET:HE3	1:1:381:MET:HA	2.01	0.41
5:K:147:ARG:HD3	5:K:296:ASN:HD22	1.84	0.41
8:V:194:ASP:O	8:V:197:LYS:HG3	2.21	0.41
1:2:171:THR:HG22	1:2:181:LEU:HB2	2.01	0.41
1:2:184:PRO:HA	1:2:216:VAL:HG12	2.03	0.41
4:8:2191:GLU:HA	4:8:2194:LEU:HD23	2.01	0.41
4:8:2414:TYR:O	6:S:379:LYS:N	2.43	0.41
5:B:16:MET:HA	5:B:32:PRO:HA	2.03	0.41
5:K:157:ASP:OD2	11:K:401:ADP:O3'	2.25	0.41
5:K:293:LEU:HD23	5:K:293:LEU:HA	1.92	0.41
8:X:193:THR:O	8:X:197:LYS:HG2	2.20	0.41
5:D:230:ALA:HA	5:D:236:LEU:HD21	2.02	0.41
5:E:95:ARG:HD3	6:O:147:LEU:HB3	2.03	0.41
7:U:213:LEU:O	7:U:217:ILE:HG12	2.19	0.41
3:7:63:ILE:HG22	3:7:66:PRO:HD2	2.03	0.41
5:A:247:VAL:HB	9:Y:58:PRO:HA	2.02	0.41
5:J:131:ALA:HB1	5:J:356:TRP:HB3	2.02	0.41
7:U:41:LEU:HD23	7:U:41:LEU:HA	1.94	0.41
9:Y:190:ILE:HG21	9:Y:220:LEU:HD22	2.03	0.41
1:2:288:LYS:HE2	1:2:288:LYS:HB3	1.89	0.41
3:6:200:VAL:HG23	6:Q:83:ARG:NH2	2.36	0.41
3:7:199:ALA:HA	3:7:202:GLU:HG2	2.03	0.41
5:B:78:ASN:HB3	5:B:81:ASP:HB2	2.02	0.41
5:C:131:ALA:HB1	5:C:356:TRP:HB3	2.02	0.41
5:C:196:ARG:NH1	5:C:250:ILE:O	2.52	0.41
5:I:153:MET:HG2	5:I:162:THR:HG22	2.01	0.41
5:J:211:ASP:OD2	5:J:240:TYR:OH	2.38	0.41
8:V:212:LYS:HG3	8:V:215:LYS:HE2	2.03	0.41
10:Z:59:PRO:HG2	10:Z:64:PRO:HA	2.02	0.41
5:J:191:LYS:HE3	5:J:191:LYS:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:215:LYS:HB3	5:J:215:LYS:HE2	1.89	0.41
6:O:84:ASP:OD2	6:O:86:ARG:HD3	2.20	0.41
2:3:272:ILE:HD12	2:3:272:ILE:HA	1.92	0.41
5:H:110:LEU:O	5:H:177:ARG:NH1	2.54	0.41
6:O:89:ILE:HD12	6:O:89:ILE:HA	1.91	0.41
6:P:123:LEU:HD23	6:P:123:LEU:HA	1.85	0.41
1:2:318:ILE:HD12	1:2:321:LEU:HD23	2.03	0.41
2:3:159:LEU:HD23	2:3:159:LEU:HA	1.94	0.41
2:3:395:LYS:HA	2:3:395:LYS:HD2	1.81	0.41
2:4:191:LEU:HD23	2:4:191:LEU:HA	1.88	0.41
2:4:370:ARG:HD3	2:4:387:LEU:HD22	2.03	0.41
4:8:2074:ASP:O	4:8:2077:ARG:HB2	2.20	0.41
2:9:65:GLU:O	2:9:68:GLU:HB2	2.21	0.41
5:A:163:VAL:HG12	5:A:175:ILE:HG23	2.03	0.41
5:D:50:LYS:NZ	6:N:137:ASP:OD2	2.44	0.41
5:H:290:ARG:HD2	5:J:244:ASP:OD1	2.19	0.41
5:I:113:LYS:HG3	5:I:371:HIS:CE1	2.56	0.41
5:K:71:ILE:HG12	5:K:76:VAL:HG22	2.02	0.41
5:K:118:LYS:HD2	5:K:118:LYS:HA	1.97	0.41
6:Q:126:GLN:HG3	6:Q:157:PHE:HE1	1.86	0.41
6:S:214:LYS:HB2	6:S:214:LYS:HE3	1.78	0.41
6:S:417:GLN:HA	6:S:420:LEU:HG	2.02	0.41
6:S:448:ASP:OD1	6:S:520:ARG:NH1	2.54	0.41
7:U:94:ILE:HG22	8:V:94:ILE:HG22	2.03	0.41
7:U:186:GLU:HA	8:V:185:TYR:OH	2.21	0.41
8:X:8:GLU:OE2	8:X:12:ARG:NH2	2.54	0.41
8:X:208:ARG:HG3	8:X:212:LYS:HZ1	1.86	0.41
9:Y:276:LEU:O	9:Y:309:ASN:ND2	2.54	0.41
2:3:115:ILE:HD13	2:3:377:TYR:HB3	2.03	0.41
2:3:357:LYS:HD3	2:3:357:LYS:HA	1.73	0.41
2:3:436:THR:HG22	2:3:438:ASN:H	1.86	0.41
5:A:299:LEU:HD23	5:A:299:LEU:HA	1.95	0.41
6:S:419:LYS:HE3	6:S:419:LYS:HB3	1.95	0.41
7:U:231:ASN:ND2	8:V:227:THR:HG23	2.36	0.41
4:8:2073:LEU:HD23	4:8:2077:ARG:NH1	2.35	0.40
5:A:305:MET:HE2	5:A:336:LYS:H	1.86	0.40
5:E:116:ARG:NH2	5:E:375:PHE:O	2.44	0.40
5:E:211:ASP:OD2	5:E:240:TYR:OH	2.30	0.40
6:N:106:GLY:HA3	6:N:111:HIS:CG	2.56	0.40
6:P:68:LEU:HD23	6:P:68:LEU:HA	1.95	0.40
6:Q:142:ASN:HD22	6:Q:145:LEU:HD12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:426:ARG:HD3	6:S:426:ARG:HA	1.69	0.40
1:2:179:HIS:HB3	1:2:199:LYS:HD2	2.03	0.40
1:2:334:SER:HB3	2:3:320:LEU:HD23	2.04	0.40
3:6:191:TYR:HB3	6:O:44:ARG:HH12	1.86	0.40
4:8:2415:PHE:HA	6:S:378:GLN:HA	2.02	0.40
5:I:285:CYS:HB3	5:I:289:ILE:HD11	2.02	0.40
6:R:84:ASP:N	6:R:84:ASP:OD1	2.54	0.40
8:W:11:LYS:HZ2	9:Y:110:VAL:HG23	1.86	0.40
8:W:11:LYS:NZ	9:Y:110:VAL:HG23	2.37	0.40
8:W:148:GLU:O	8:W:151:GLU:HG3	2.20	0.40
10:Z:49:MET:SD	10:Z:68:GLN:HG3	2.61	0.40
1:2:274:HIS:HD2	1:2:276:ILE:H	1.69	0.40
4:8:2354:GLU:O	4:8:2358:SER:CB	2.69	0.40
2:9:58:LEU:HD23	2:9:58:LEU:HA	1.89	0.40
5:A:154:ASP:HB3	5:A:161:HIS:CE1	2.55	0.40
5:B:190:MET:HE1	5:B:206:ARG:HG2	2.02	0.40
5:G:237:GLU:HG2	5:G:251:GLY:HA2	2.03	0.40
9:Y:242:PHE:CE1	9:Y:271:ARG:HG3	2.56	0.40
2:3:133:MET:SD	2:3:159:LEU:HD13	2.62	0.40
5:A:7:ALA:HA	5:A:102:PRO:HD2	2.03	0.40
5:G:68:LYS:HB2	5:G:68:LYS:HE2	1.94	0.40
5:I:200:PHE:HB3	5:I:205:GLU:HB3	2.04	0.40
2:3:247:SER:HB3	2:3:315:ILE:HG21	2.03	0.40
5:E:213:LYS:HE3	5:E:213:LYS:HB3	1.84	0.40
6:P:100:LEU:HD23	6:P:100:LEU:HA	1.96	0.40
7:U:76:LYS:HE3	7:U:76:LYS:HB2	1.86	0.40
8:X:205:PHE:O	8:X:208:ARG:HG2	2.22	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	0	52/744 (7%)	50 (96%)	2 (4%)	0	100	100
1	1	328/744 (44%)	317 (97%)	11 (3%)	0	100	100
1	2	290/744 (39%)	278 (96%)	12 (4%)	0	100	100
2	3	357/724 (49%)	335 (94%)	21 (6%)	1 (0%)	41	75
2	4	276/724 (38%)	262 (95%)	14 (5%)	0	100	100
2	9	52/724 (7%)	50 (96%)	2 (4%)	0	100	100
3	5	117/405 (29%)	114 (97%)	3 (3%)	0	100	100
3	6	119/405 (29%)	112 (94%)	7 (6%)	0	100	100
3	7	115/405 (28%)	105 (91%)	10 (9%)	0	100	100
4	8	377/2417 (16%)	356 (94%)	19 (5%)	2 (0%)	29	68
5	A	372/375 (99%)	355 (95%)	17 (5%)	0	100	100
5	B	372/375 (99%)	365 (98%)	7 (2%)	0	100	100
5	C	371/375 (99%)	363 (98%)	8 (2%)	0	100	100
5	D	372/375 (99%)	360 (97%)	12 (3%)	0	100	100
5	E	372/375 (99%)	361 (97%)	11 (3%)	0	100	100
5	F	372/375 (99%)	359 (96%)	13 (4%)	0	100	100
5	G	372/375 (99%)	363 (98%)	9 (2%)	0	100	100
5	H	372/375 (99%)	360 (97%)	12 (3%)	0	100	100
5	I	371/375 (99%)	359 (97%)	11 (3%)	1 (0%)	41	75
5	J	372/375 (99%)	363 (98%)	9 (2%)	0	100	100
5	K	372/375 (99%)	358 (96%)	14 (4%)	0	100	100
5	L	372/375 (99%)	360 (97%)	12 (3%)	0	100	100
6	M	128/2148 (6%)	124 (97%)	4 (3%)	0	100	100
6	N	120/2148 (6%)	119 (99%)	1 (1%)	0	100	100
6	O	129/2148 (6%)	127 (98%)	2 (2%)	0	100	100
6	P	115/2148 (5%)	112 (97%)	3 (3%)	0	100	100
6	Q	127/2148 (6%)	124 (98%)	3 (2%)	0	100	100
6	R	115/2148 (5%)	110 (96%)	5 (4%)	0	100	100
6	S	482/2148 (22%)	473 (98%)	9 (2%)	0	100	100
6	T	126/2148 (6%)	124 (98%)	2 (2%)	0	100	100
7	U	244/248 (98%)	242 (99%)	2 (1%)	0	100	100
8	V	244/248 (98%)	243 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	W	246/248 (99%)	243 (99%)	3 (1%)	0	100	100
8	X	239/248 (96%)	239 (100%)	0	0	100	100
9	Y	329/359 (92%)	318 (97%)	11 (3%)	0	100	100
10	Z	96/107 (90%)	94 (98%)	2 (2%)	0	100	100
All	All	9285/31178 (30%)	8997 (97%)	284 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	8	2068	VAL
5	I	4	ASP
4	8	2226	VAL
2	3	360	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	51/626 (8%)	51 (100%)	0	100	100
1	1	280/626 (45%)	280 (100%)	0	100	100
1	2	243/626 (39%)	243 (100%)	0	100	100
2	3	320/637 (50%)	320 (100%)	0	100	100
2	4	235/637 (37%)	234 (100%)	1 (0%)	91	97
2	9	50/637 (8%)	49 (98%)	1 (2%)	55	79
3	5	113/364 (31%)	112 (99%)	1 (1%)	78	90
3	6	101/364 (28%)	101 (100%)	0	100	100
3	7	107/364 (29%)	106 (99%)	1 (1%)	78	90
4	8	257/2118 (12%)	255 (99%)	2 (1%)	81	91
5	A	313/318 (98%)	313 (100%)	0	100	100
5	B	317/318 (100%)	317 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	C	316/318 (99%)	316 (100%)	0	100 100
5	D	317/318 (100%)	315 (99%)	2 (1%)	86 94
5	E	317/318 (100%)	317 (100%)	0	100 100
5	F	317/318 (100%)	317 (100%)	0	100 100
5	G	317/318 (100%)	317 (100%)	0	100 100
5	H	317/318 (100%)	316 (100%)	1 (0%)	92 97
5	I	316/318 (99%)	315 (100%)	1 (0%)	92 97
5	J	317/318 (100%)	317 (100%)	0	100 100
5	K	317/318 (100%)	317 (100%)	0	100 100
5	L	317/318 (100%)	316 (100%)	1 (0%)	92 97
6	M	119/1870 (6%)	118 (99%)	1 (1%)	81 91
6	N	111/1870 (6%)	111 (100%)	0	100 100
6	O	120/1870 (6%)	120 (100%)	0	100 100
6	P	107/1870 (6%)	106 (99%)	1 (1%)	78 90
6	Q	118/1870 (6%)	118 (100%)	0	100 100
6	R	107/1870 (6%)	107 (100%)	0	100 100
6	S	429/1870 (23%)	427 (100%)	2 (0%)	88 95
6	T	117/1870 (6%)	117 (100%)	0	100 100
7	U	212/214 (99%)	211 (100%)	1 (0%)	88 95
8	V	215/216 (100%)	214 (100%)	1 (0%)	88 95
8	W	214/216 (99%)	211 (99%)	3 (1%)	67 85
8	X	211/216 (98%)	209 (99%)	2 (1%)	78 90
9	Y	271/318 (85%)	271 (100%)	0	100 100
10	Z	89/96 (93%)	89 (100%)	0	100 100
All	All	7995/27051 (30%)	7973 (100%)	22 (0%)	92 97

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	4	240	LYS
3	5	160	LYS
3	7	148	LYS
4	8	2127	ARG
4	8	2210	GLN

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Mol	Chain	Res	Type
2	9	64	ARG
5	D	326	LYS
5	D	372	ARG
5	H	95	ARG
5	I	95	ARG
5	L	336	LYS
6	M	105	LYS
6	P	156	ARG
6	S	405	ARG
6	S	439	ASN
7	U	142	ARG
8	V	197	LYS
8	W	177	LYS
8	W	178	TYR
8	W	197	LYS
8	X	153	ARG
8	X	225	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	274	HIS
2	3	334	GLN
2	4	389	GLN
4	8	2055	ASN
4	8	2098	ASN
6	Q	67	HIS
7	U	231	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
11	ADP	A	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
11	ADP	K	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.46	4 (13%)
11	ADP	B	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.40	5 (17%)
11	ADP	I	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)
11	ADP	H	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.48	4 (13%)
11	ADP	L	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.47	4 (13%)
11	ADP	C	401	-	24,29,29	0.93	1 (4%)	29,45,45	1.47	4 (13%)
11	ADP	J	401	-	24,29,29	0.92	1 (4%)	29,45,45	1.56	4 (13%)
11	ADP	G	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.46	4 (13%)
11	ADP	F	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.49	4 (13%)
11	ADP	E	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
11	ADP	D	401	-	24,29,29	0.92	1 (4%)	29,45,45	1.47	4 (13%)

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
11	ADP	A	401	-	-	7/12/32/32	0/3/3/3
11	ADP	K	401	-	-	5/12/32/32	0/3/3/3
11	ADP	B	401	-	-	6/12/32/32	0/3/3/3
11	ADP	I	401	-	-	5/12/32/32	0/3/3/3
11	ADP	H	401	-	-	5/12/32/32	0/3/3/3
11	ADP	L	401	-	-	3/12/32/32	0/3/3/3
11	ADP	C	401	-	-	6/12/32/32	0/3/3/3
11	ADP	J	401	-	-	5/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	G	401	-	-	5/12/32/32	0/3/3/3
11	ADP	F	401	-	-	5/12/32/32	0/3/3/3
11	ADP	E	401	-	-	3/12/32/32	0/3/3/3
11	ADP	D	401	-	-	5/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	401	ADP	C5-C4	2.44	1.47	1.40
11	F	401	ADP	C5-C4	2.42	1.47	1.40
11	L	401	ADP	C5-C4	2.42	1.47	1.40
11	B	401	ADP	C5-C4	2.42	1.47	1.40
11	D	401	ADP	C5-C4	2.40	1.47	1.40
11	G	401	ADP	C5-C4	2.37	1.47	1.40
11	H	401	ADP	C5-C4	2.36	1.47	1.40
11	E	401	ADP	C5-C4	2.35	1.47	1.40
11	I	401	ADP	C5-C4	2.34	1.47	1.40
11	C	401	ADP	C5-C4	2.33	1.47	1.40
11	K	401	ADP	C5-C4	2.33	1.47	1.40
11	J	401	ADP	C5-C4	2.30	1.47	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	E	401	ADP	PA-O3A-PB	-4.23	118.32	132.83
11	J	401	ADP	PA-O3A-PB	-4.10	118.77	132.83
11	H	401	ADP	PA-O3A-PB	-3.87	119.54	132.83
11	I	401	ADP	PA-O3A-PB	-3.75	119.97	132.83
11	K	401	ADP	PA-O3A-PB	-3.69	120.16	132.83
11	F	401	ADP	PA-O3A-PB	-3.62	120.39	132.83
11	J	401	ADP	C3'-C2'-C1'	3.59	106.39	100.98
11	D	401	ADP	PA-O3A-PB	-3.51	120.77	132.83
11	L	401	ADP	C3'-C2'-C1'	3.49	106.23	100.98
11	F	401	ADP	C3'-C2'-C1'	3.48	106.21	100.98
11	D	401	ADP	C3'-C2'-C1'	3.46	106.19	100.98
11	E	401	ADP	C3'-C2'-C1'	3.44	106.16	100.98
11	C	401	ADP	C3'-C2'-C1'	3.44	106.16	100.98
11	G	401	ADP	C3'-C2'-C1'	3.44	106.15	100.98
11	A	401	ADP	C3'-C2'-C1'	3.43	106.14	100.98
11	A	401	ADP	PA-O3A-PB	-3.41	121.13	132.83
11	G	401	ADP	PA-O3A-PB	-3.40	121.16	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	401	ADP	PA-O3A-PB	-3.33	121.40	132.83
11	H	401	ADP	C3'-C2'-C1'	3.31	105.97	100.98
11	L	401	ADP	PA-O3A-PB	-3.30	121.52	132.83
11	K	401	ADP	C3'-C2'-C1'	3.26	105.88	100.98
11	B	401	ADP	PA-O3A-PB	-3.24	121.71	132.83
11	I	401	ADP	C3'-C2'-C1'	3.24	105.85	100.98
11	A	401	ADP	N3-C2-N1	-3.20	123.68	128.68
11	L	401	ADP	N3-C2-N1	-3.15	123.76	128.68
11	B	401	ADP	N3-C2-N1	-3.12	123.80	128.68
11	C	401	ADP	N3-C2-N1	-3.09	123.84	128.68
11	B	401	ADP	C3'-C2'-C1'	3.09	105.63	100.98
11	I	401	ADP	N3-C2-N1	-3.00	123.99	128.68
11	J	401	ADP	N3-C2-N1	-2.98	124.02	128.68
11	D	401	ADP	N3-C2-N1	-2.97	124.03	128.68
11	H	401	ADP	N3-C2-N1	-2.92	124.12	128.68
11	F	401	ADP	N3-C2-N1	-2.92	124.12	128.68
11	K	401	ADP	N3-C2-N1	-2.91	124.13	128.68
11	G	401	ADP	N3-C2-N1	-2.89	124.17	128.68
11	E	401	ADP	N3-C2-N1	-2.86	124.21	128.68
11	E	401	ADP	C4-C5-N7	-2.69	106.60	109.40
11	F	401	ADP	C4-C5-N7	-2.61	106.68	109.40
11	H	401	ADP	C4-C5-N7	-2.59	106.70	109.40
11	B	401	ADP	C4-C5-N7	-2.57	106.72	109.40
11	I	401	ADP	C4-C5-N7	-2.56	106.73	109.40
11	C	401	ADP	C4-C5-N7	-2.55	106.74	109.40
11	A	401	ADP	C4-C5-N7	-2.53	106.77	109.40
11	J	401	ADP	C4-C5-N7	-2.50	106.79	109.40
11	L	401	ADP	C4-C5-N7	-2.49	106.80	109.40
11	G	401	ADP	C4-C5-N7	-2.49	106.81	109.40
11	K	401	ADP	C4-C5-N7	-2.49	106.81	109.40
11	D	401	ADP	C4-C5-N7	-2.47	106.82	109.40
11	B	401	ADP	O3B-PB-O2B	2.02	115.37	107.64

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	401	ADP	PA-O3A-PB-O3B
11	A	401	ADP	C5'-O5'-PA-O1A
11	A	401	ADP	C5'-O5'-PA-O2A
11	B	401	ADP	PA-O3A-PB-O3B
11	B	401	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
11	B	401	ADP	C5'-O5'-PA-O2A
11	C	401	ADP	PA-O3A-PB-O3B
11	C	401	ADP	C5'-O5'-PA-O1A
11	C	401	ADP	C5'-O5'-PA-O2A
11	D	401	ADP	PA-O3A-PB-O3B
11	D	401	ADP	C5'-O5'-PA-O2A
11	E	401	ADP	C5'-O5'-PA-O1A
11	E	401	ADP	C5'-O5'-PA-O2A
11	F	401	ADP	PA-O3A-PB-O3B
11	F	401	ADP	C5'-O5'-PA-O1A
11	F	401	ADP	C5'-O5'-PA-O2A
11	G	401	ADP	PA-O3A-PB-O3B
11	G	401	ADP	C5'-O5'-PA-O1A
11	G	401	ADP	C5'-O5'-PA-O2A
11	H	401	ADP	PA-O3A-PB-O3B
11	H	401	ADP	C5'-O5'-PA-O1A
11	H	401	ADP	C5'-O5'-PA-O2A
11	I	401	ADP	PA-O3A-PB-O3B
11	I	401	ADP	C5'-O5'-PA-O1A
11	I	401	ADP	C5'-O5'-PA-O2A
11	J	401	ADP	C5'-O5'-PA-O1A
11	J	401	ADP	C5'-O5'-PA-O2A
11	K	401	ADP	PA-O3A-PB-O3B
11	K	401	ADP	C5'-O5'-PA-O1A
11	K	401	ADP	C5'-O5'-PA-O2A
11	L	401	ADP	C5'-O5'-PA-O3A
11	J	401	ADP	PA-O3A-PB-O1B
11	H	401	ADP	PA-O3A-PB-O1B
11	A	401	ADP	PA-O3A-PB-O2B
11	J	401	ADP	PA-O3A-PB-O3B
11	A	401	ADP	C5'-O5'-PA-O3A
11	D	401	ADP	C5'-O5'-PA-O3A
11	F	401	ADP	C5'-O5'-PA-O3A
11	I	401	ADP	C5'-O5'-PA-O3A
11	K	401	ADP	C5'-O5'-PA-O3A
11	D	401	ADP	C5'-O5'-PA-O1A
11	L	401	ADP	C5'-O5'-PA-O1A
11	B	401	ADP	PA-O3A-PB-O1B
11	I	401	ADP	PA-O3A-PB-O1B
11	A	401	ADP	C3'-C4'-C5'-O5'
11	A	401	ADP	PA-O3A-PB-O1B
11	C	401	ADP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
11	G	401	ADP	PA-O3A-PB-O1B
11	B	401	ADP	PA-O3A-PB-O2B
11	C	401	ADP	PA-O3A-PB-O2B
11	F	401	ADP	PA-O3A-PB-O2B
11	K	401	ADP	PA-O3A-PB-O2B
11	L	401	ADP	PA-O3A-PB-O2B
11	B	401	ADP	C5'-O5'-PA-O3A
11	C	401	ADP	C5'-O5'-PA-O3A
11	E	401	ADP	C5'-O5'-PA-O3A
11	G	401	ADP	C5'-O5'-PA-O3A
11	H	401	ADP	C5'-O5'-PA-O3A
11	J	401	ADP	C5'-O5'-PA-O3A
11	D	401	ADP	PA-O3A-PB-O1B

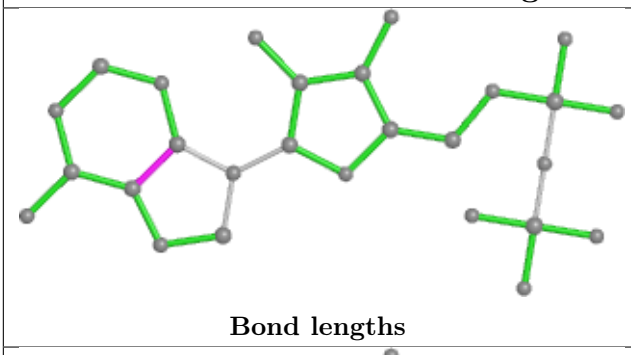
There are no ring outliers.

5 monomers are involved in 7 short contacts:

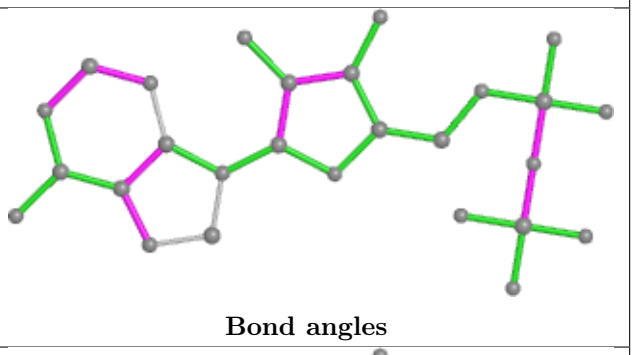
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	401	ADP	2	0
11	K	401	ADP	1	0
11	C	401	ADP	2	0
11	J	401	ADP	1	0
11	G	401	ADP	1	0

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 ADP A 401



Bond lengths



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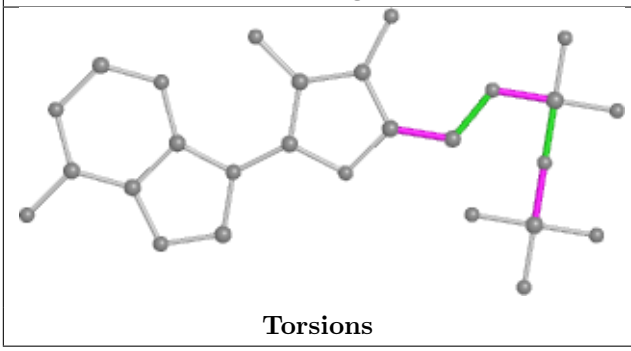
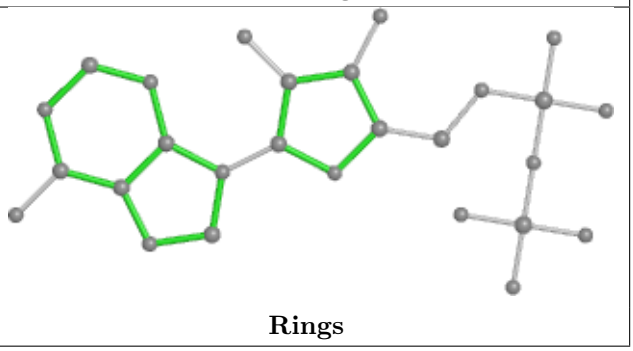
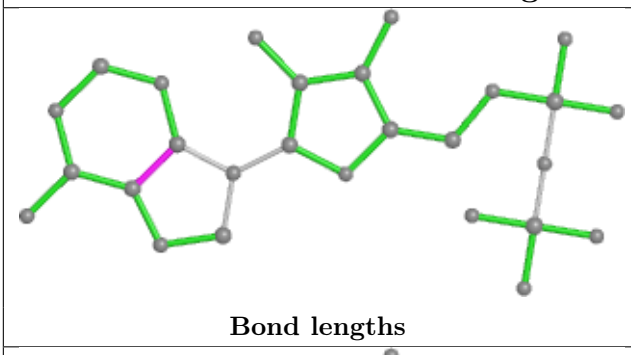


Torsions



Rings

Ligand ADP K 401



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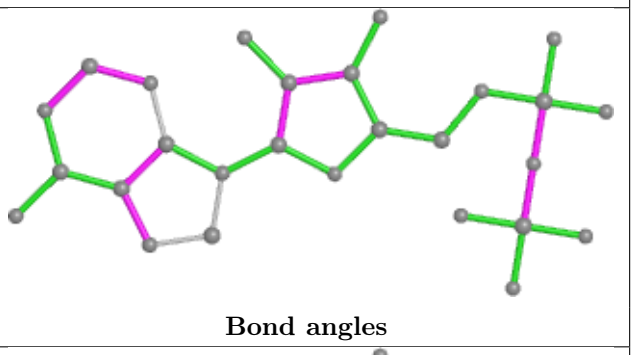

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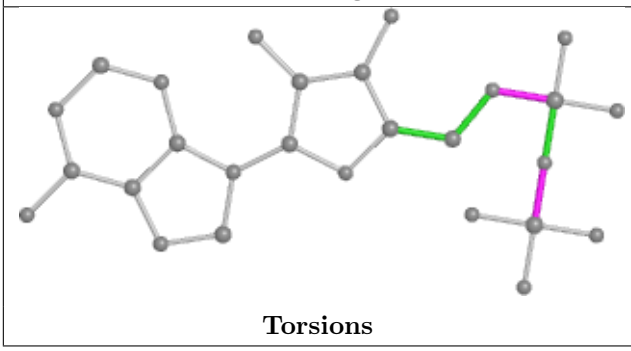

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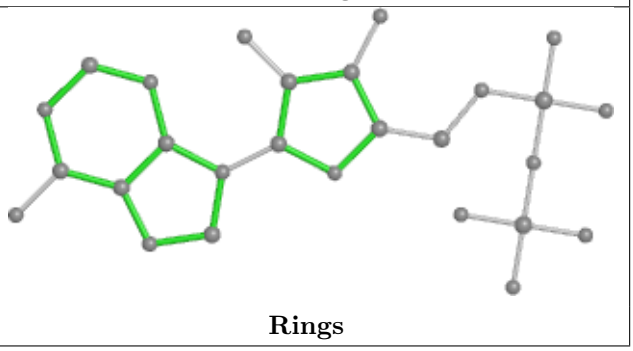
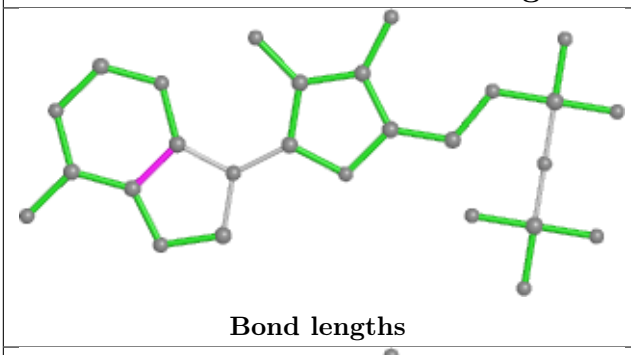
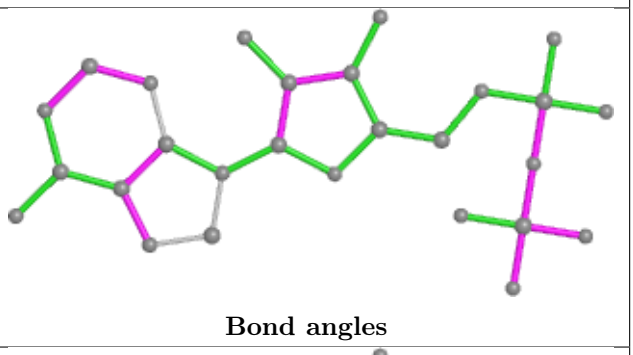


Rings

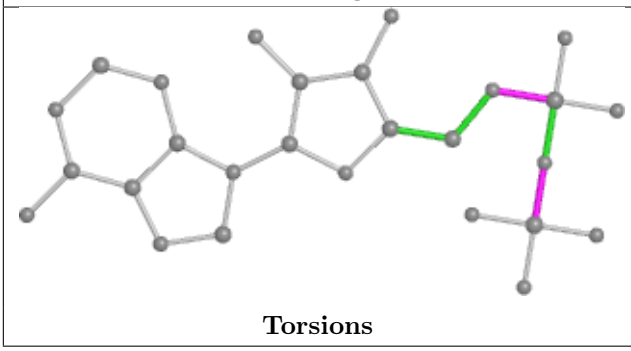
Ligand ADP B 401



Bond lengths



Bond angles



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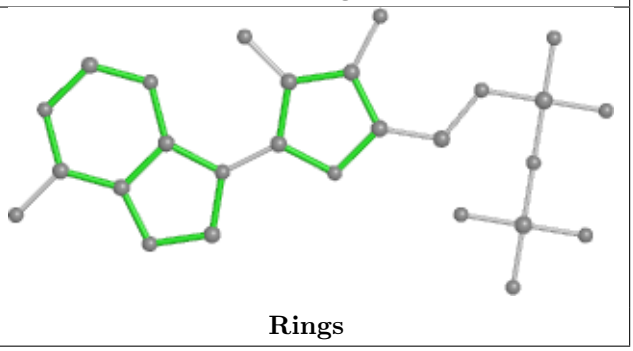
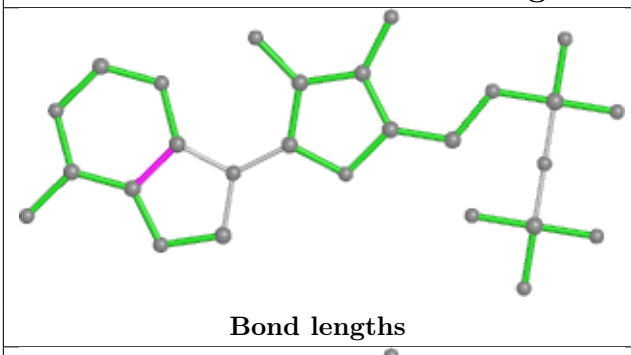


Rings

Ligand ADP I 401



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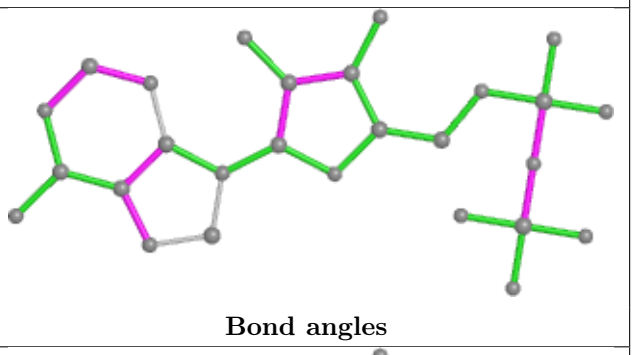
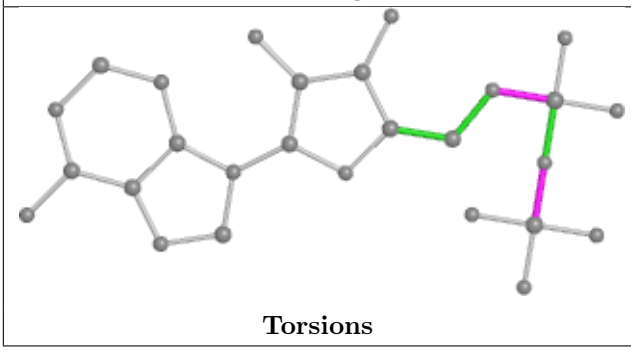


Bond angles



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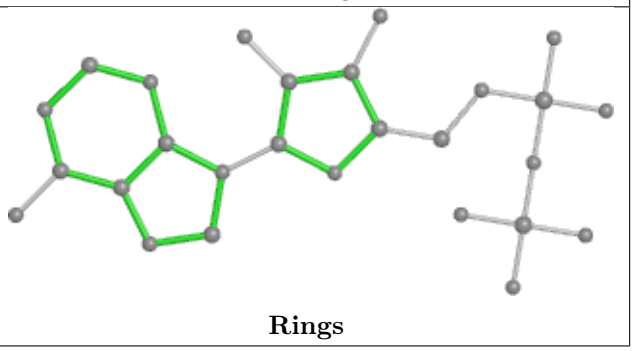

Rings

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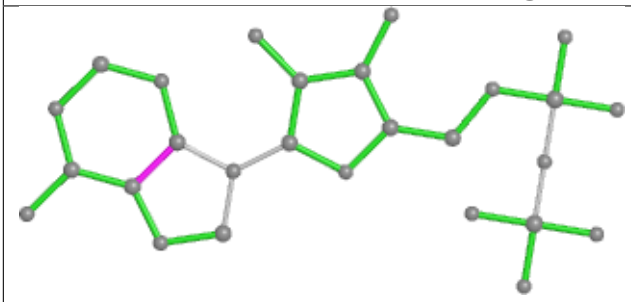
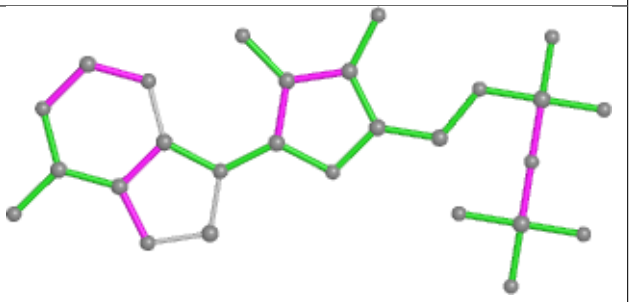
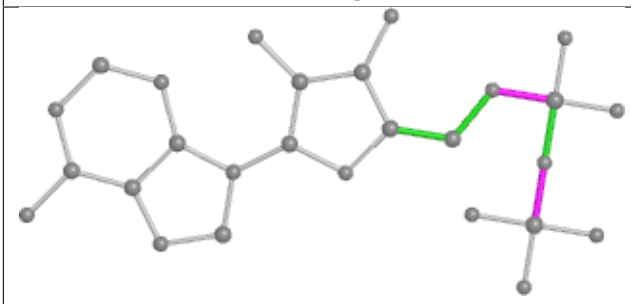
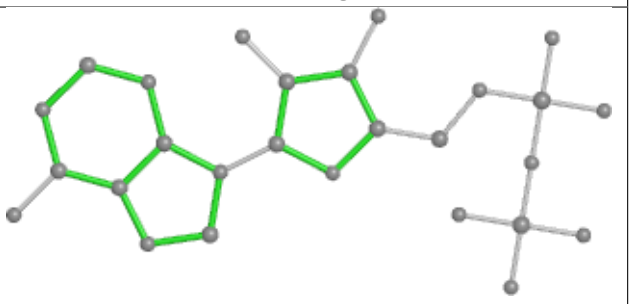
 Bond lengths	 Bond angles
 Torsions	 Rings

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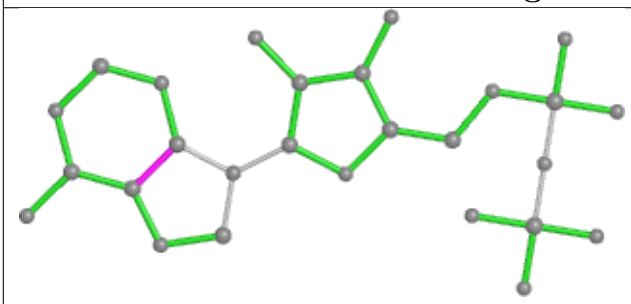
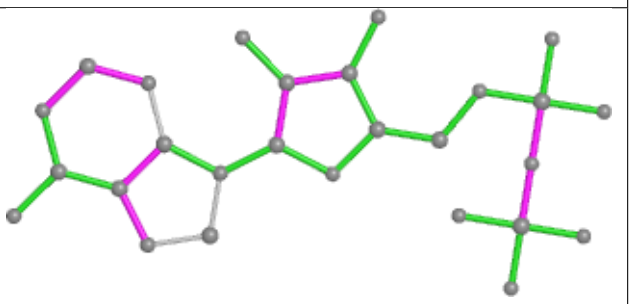
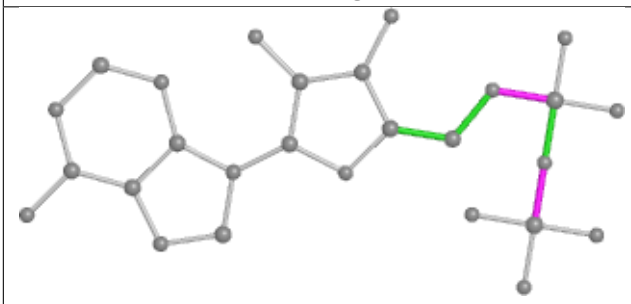
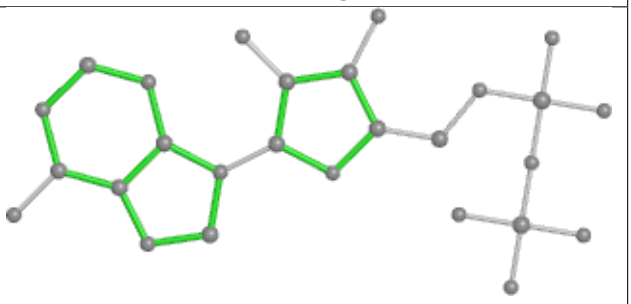
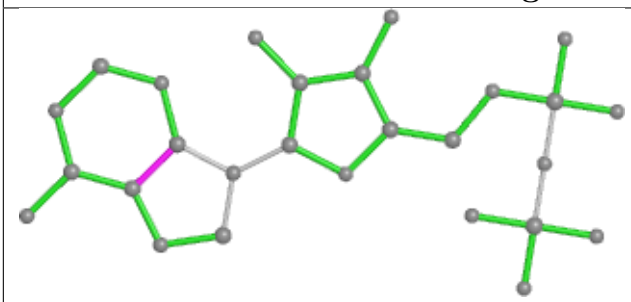
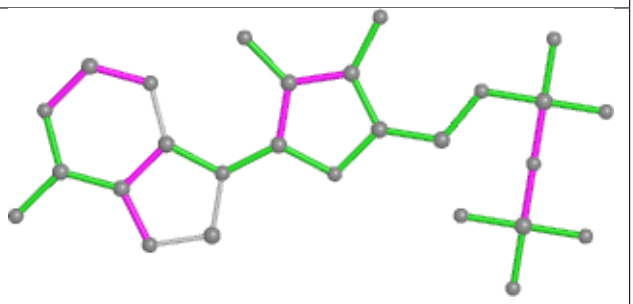
 Bond lengths	 Bond angles
 Torsions	 Rings

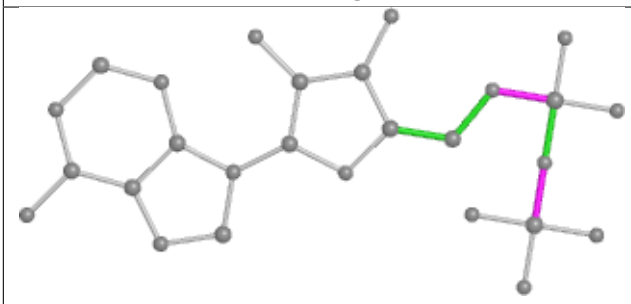
Ligand ADP C 401



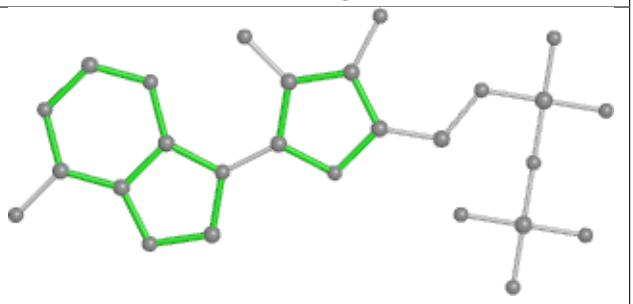
Bond lengths



Bond angles

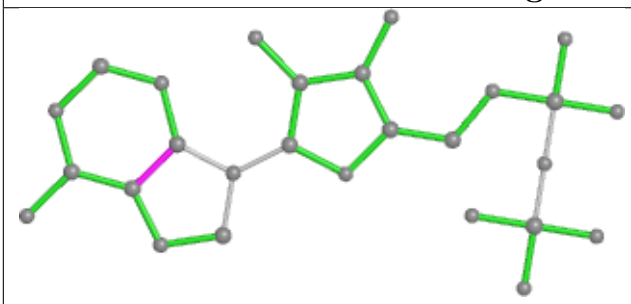


Torsions

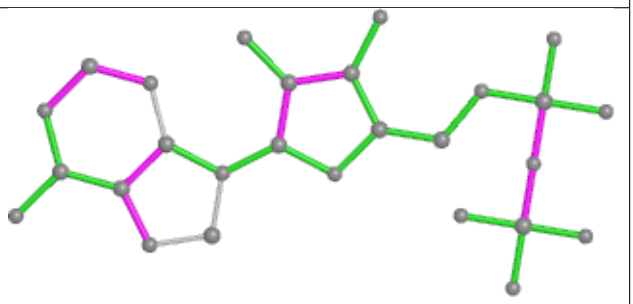


Rings

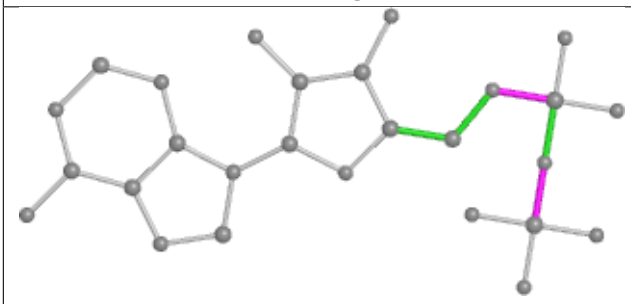
Ligand ADP J 401



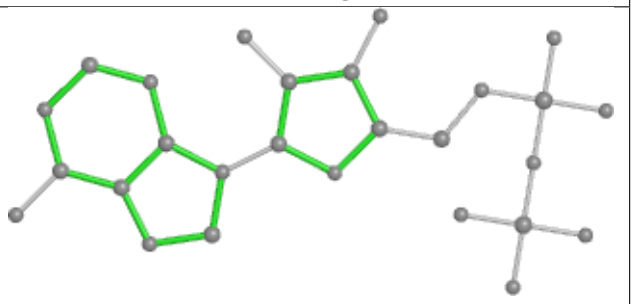
Bond lengths



Bond angles

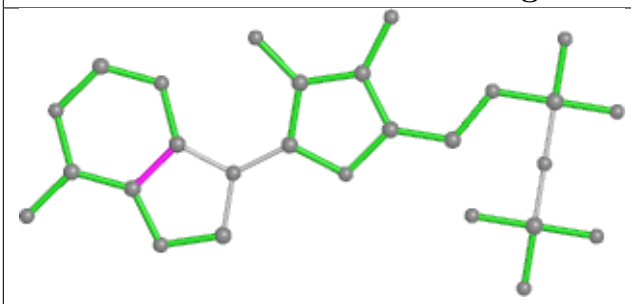


Torsions

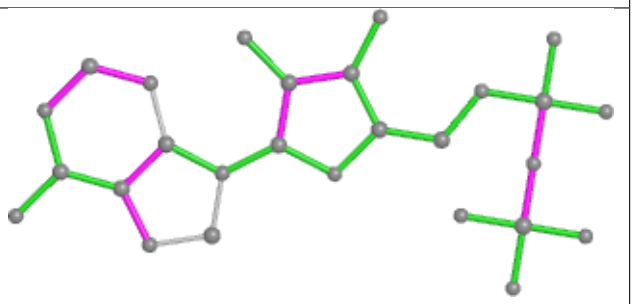


Rings

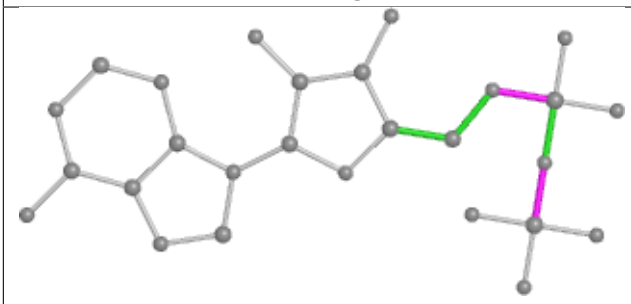
Ligand ADP G 401



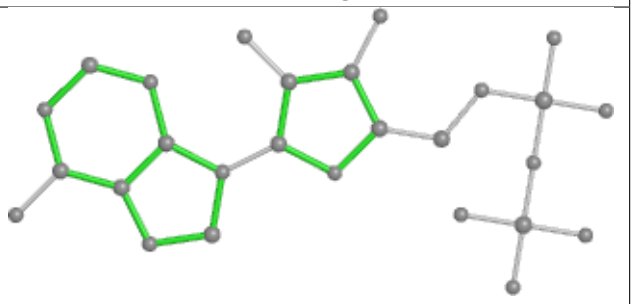
Bond lengths



Bond angles

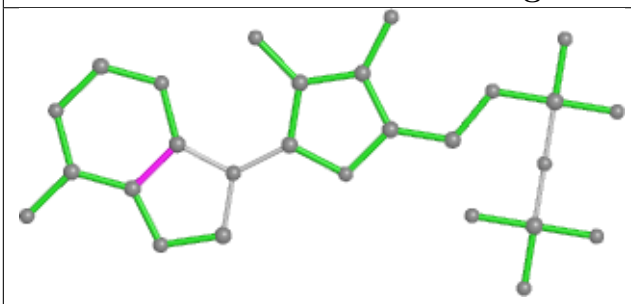


Torsions

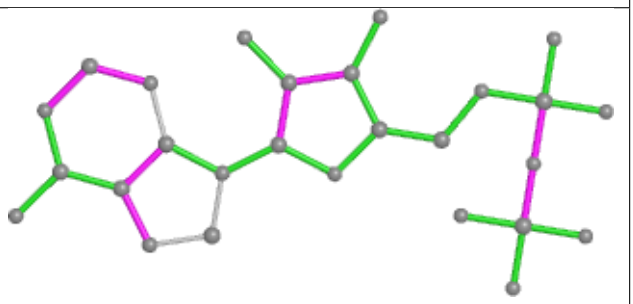


Rings

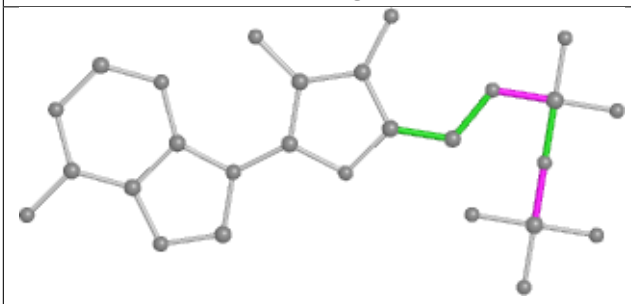
Ligand ADP F 401



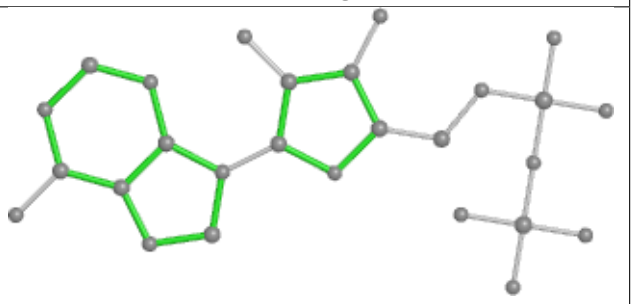
Bond lengths



Bond angles

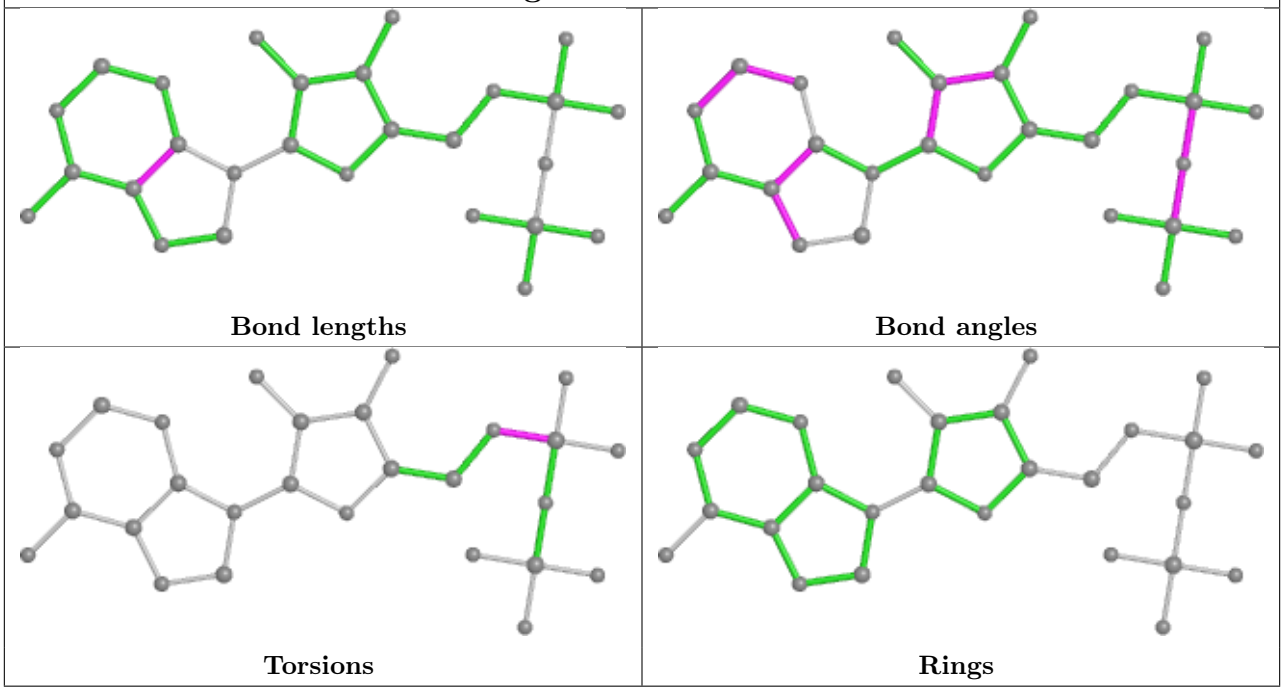


Torsions

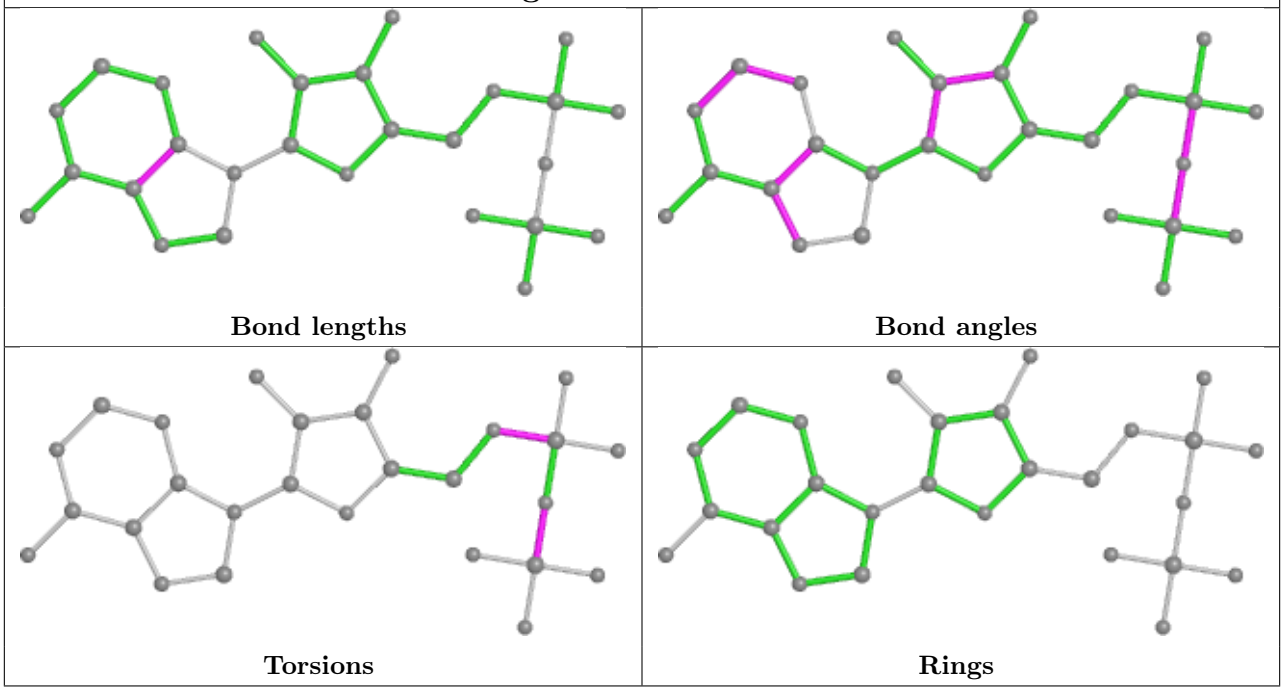


Rings

Ligand ADP E 401



Ligand ADP D 401



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.

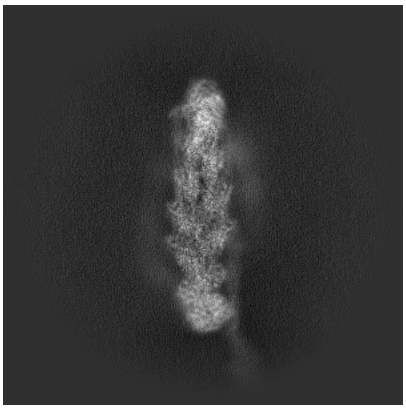
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35301. These allow visual inspection of the internal detail of the map and identification of artifacts.

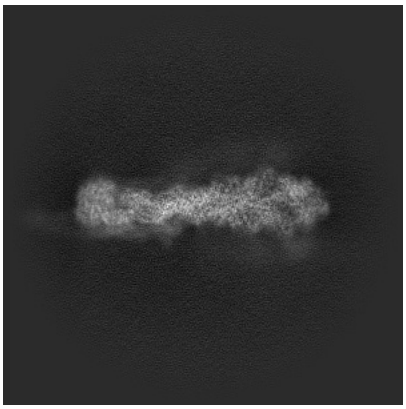
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

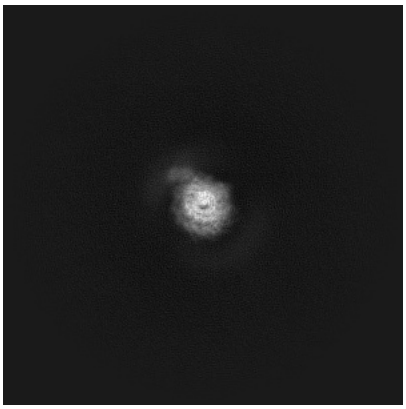
6.1.1 Primary map



X

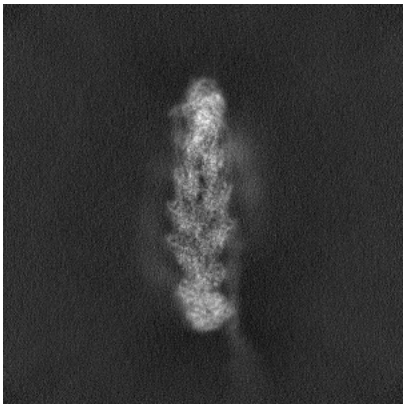


Y

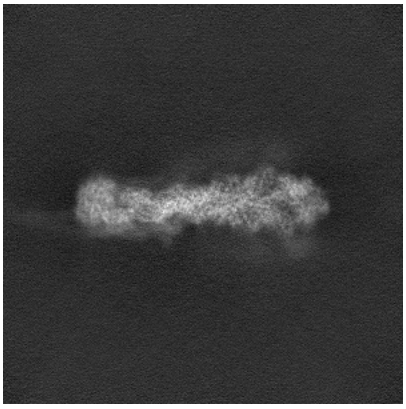


Z

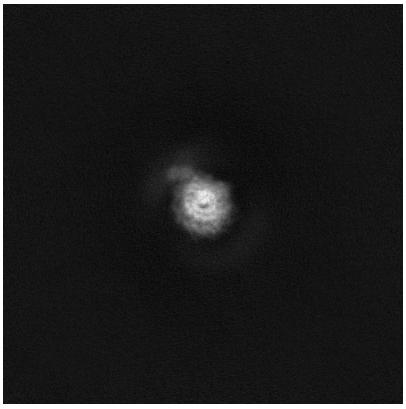
6.1.2 Raw map



X



Y

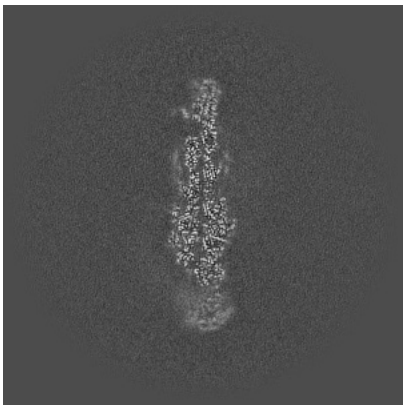


Z

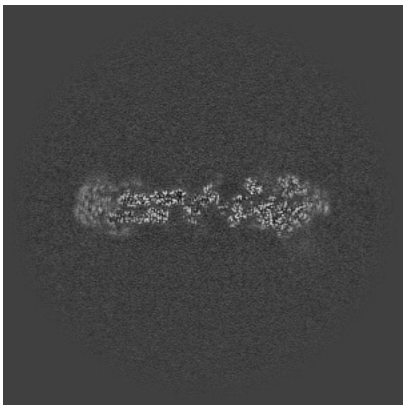
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

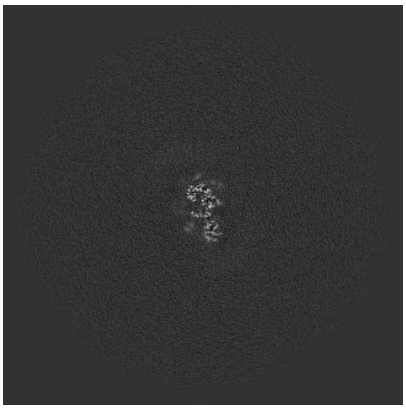
6.2.1 Primary map



X Index: 240

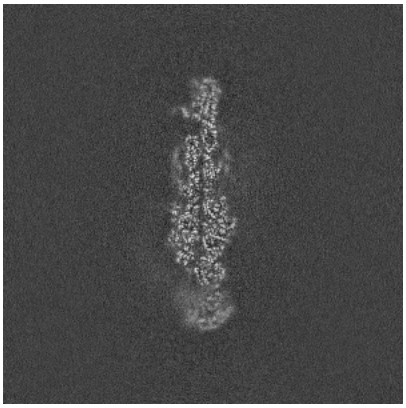


Y Index: 240

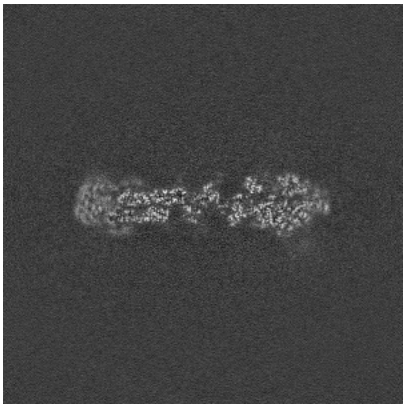


Z Index: 240

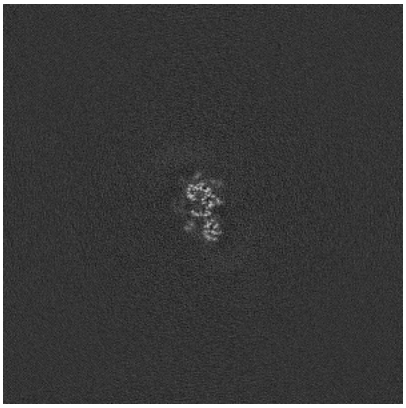
6.2.2 Raw map



X Index: 240



Y Index: 240

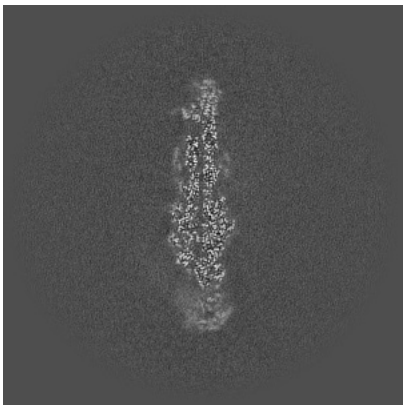


Z Index: 240

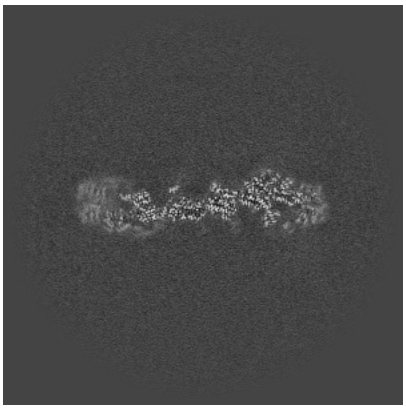
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

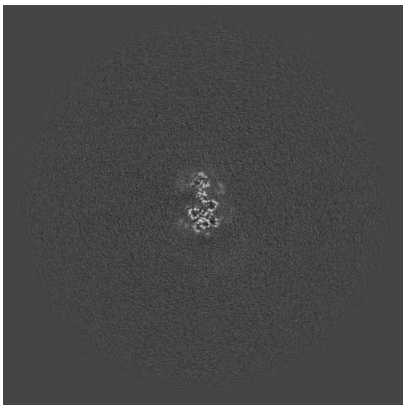
6.3.1 Primary map



X Index: 241

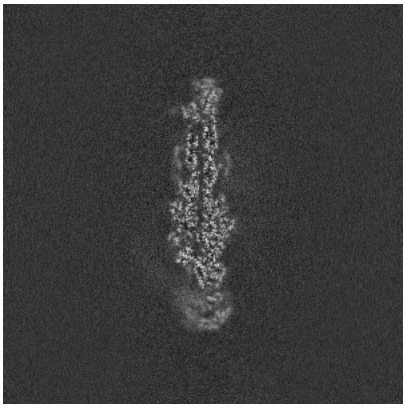


Y Index: 231

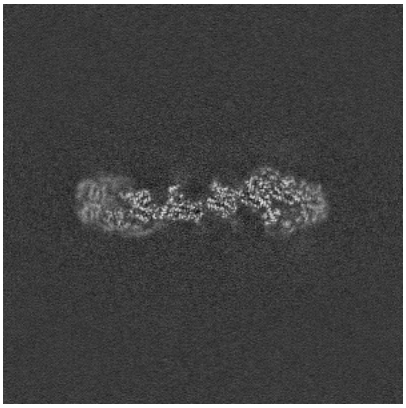


Z Index: 214

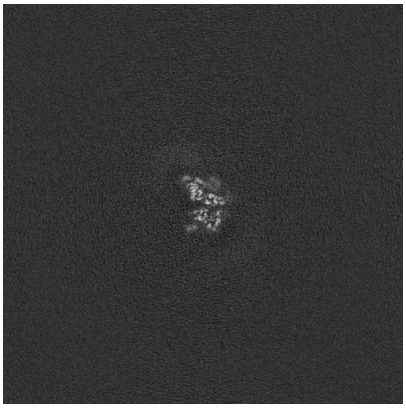
6.3.2 Raw map



X Index: 242



Y Index: 232

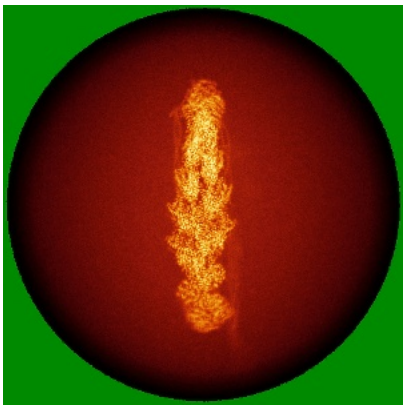


Z Index: 249

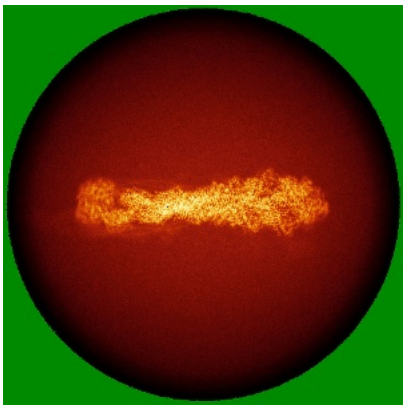
The images above show the largest variance slices of the map in three orthogonal directions.

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

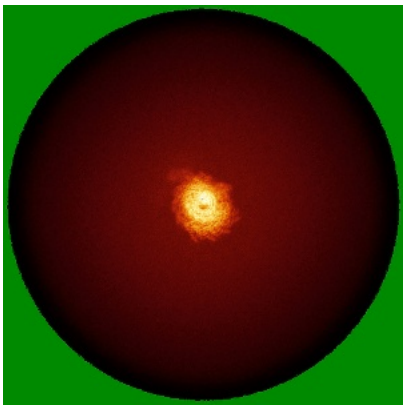
6.4.1 Primary map



X

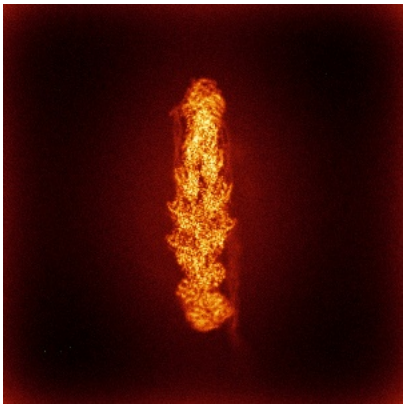


Y

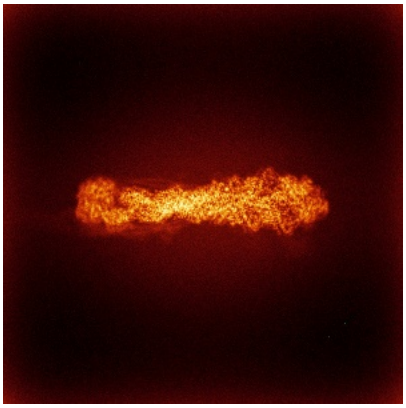


Z

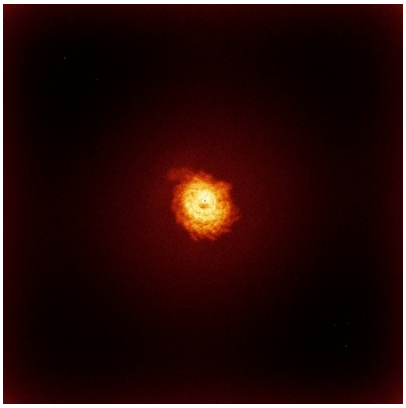
6.4.2 Raw map



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 0.35. 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.

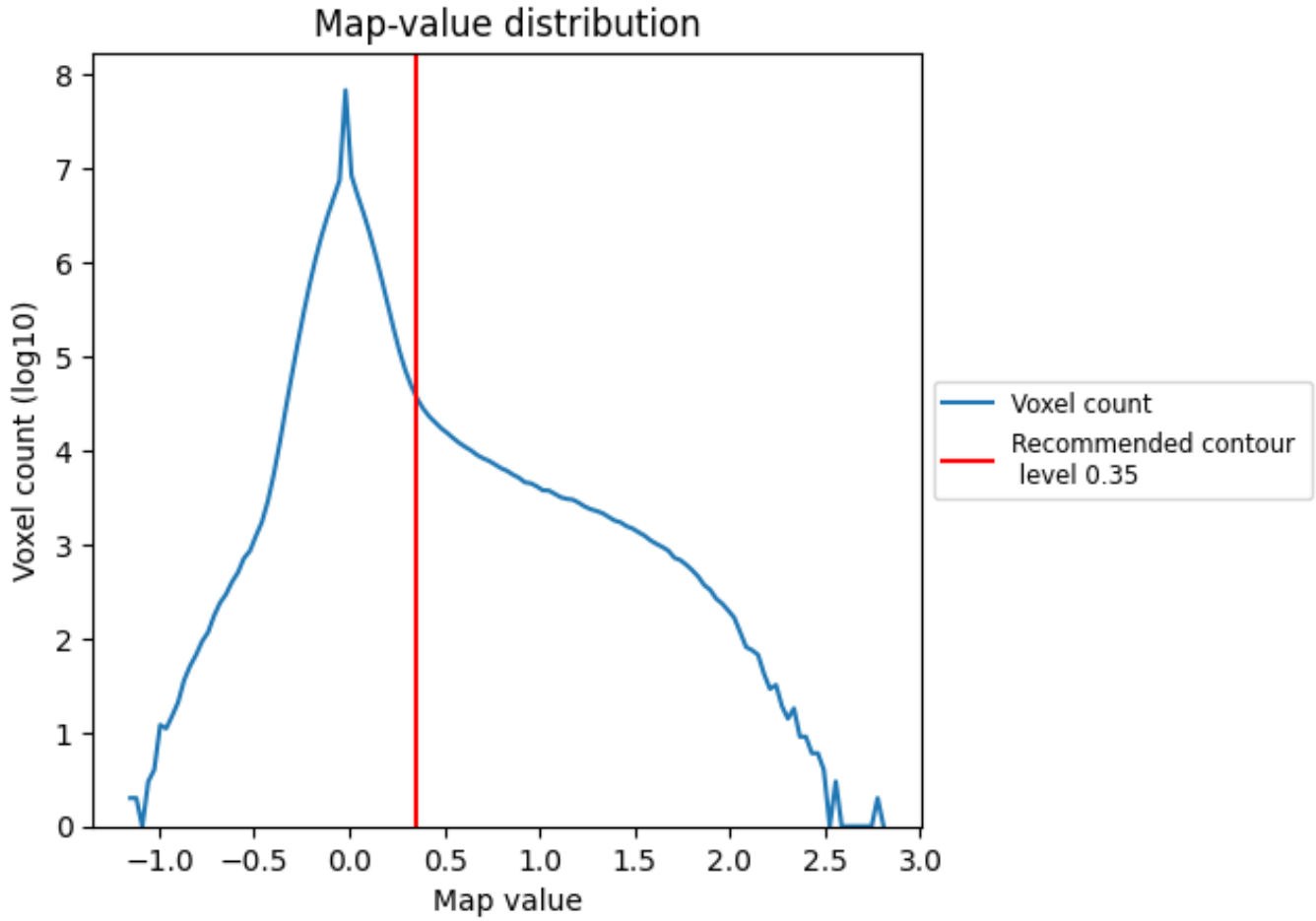
6.6 Mask visualisation (i)

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

7 Map analysis

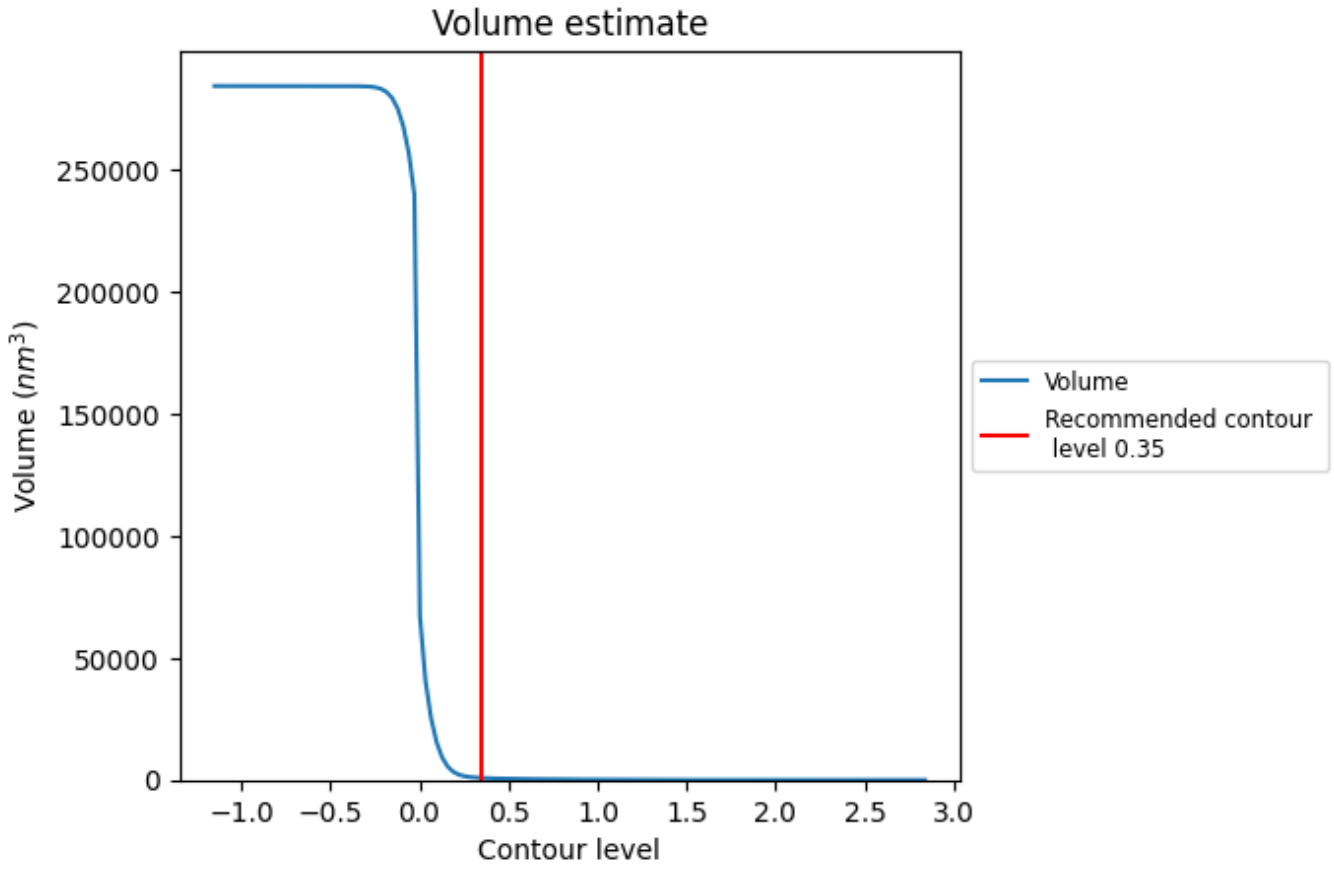
This section contains the results of statistical analysis of the map.

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.

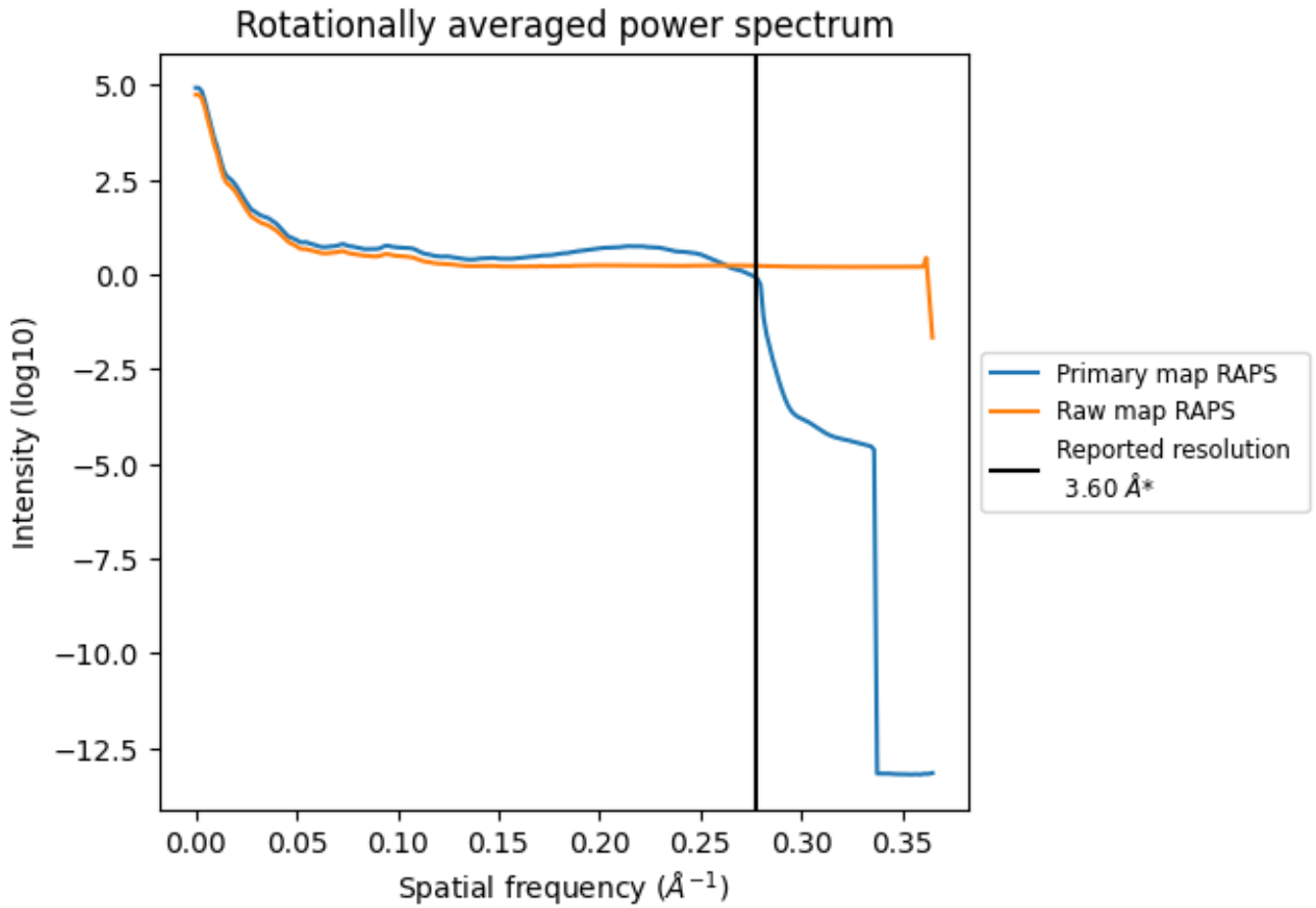
7.2 Volume estimate



The volume at the recommended contour level is 817 nm^3; this corresponds to an approximate mass of 738 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)

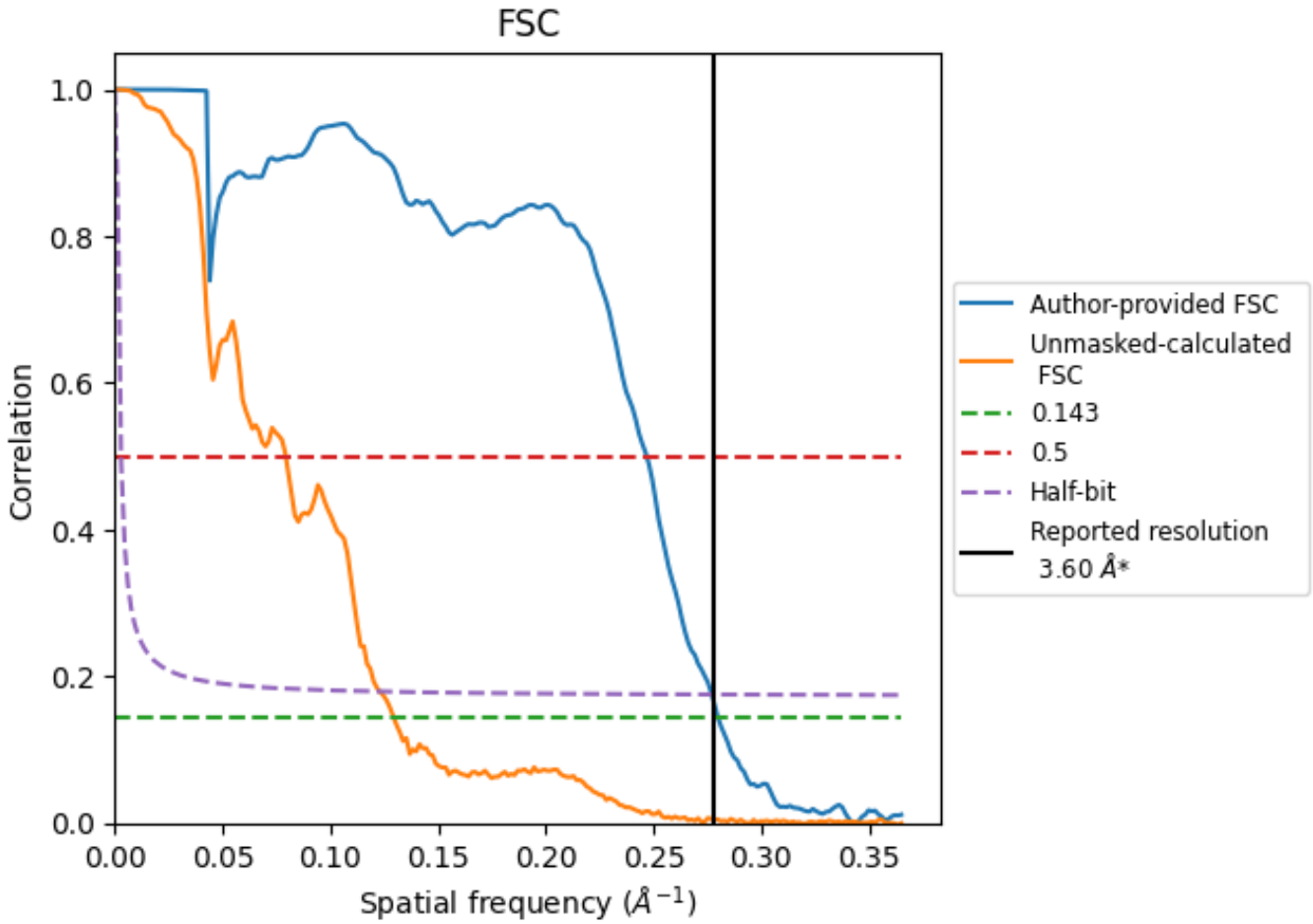


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

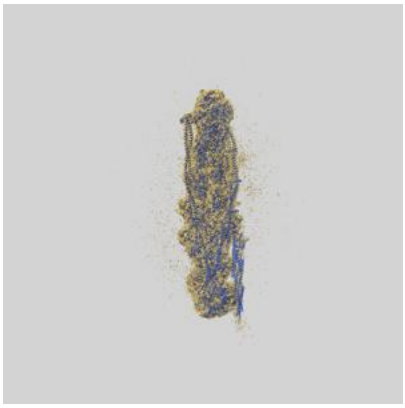
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.05	3.61
Unmasked-calculated*	7.73	12.61	8.13

*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 7.73 differs from the reported value 3.6 by more than 10 %

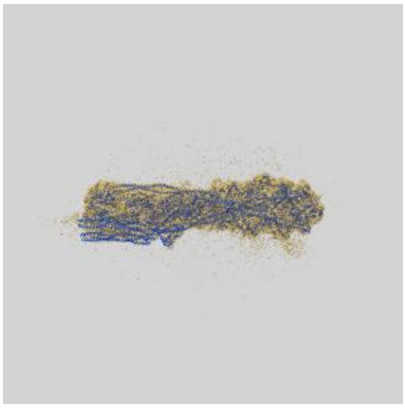
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35301 and PDB model 8IAH. Per-residue inclusion information can be found in section 3 on page 9.

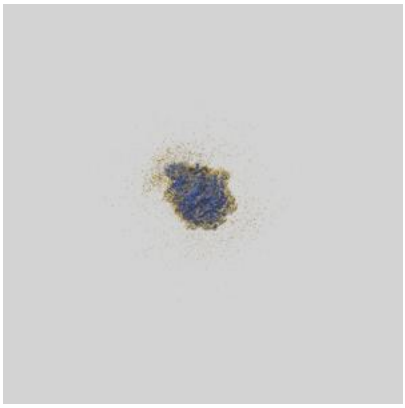
9.1 Map-model overlay



X



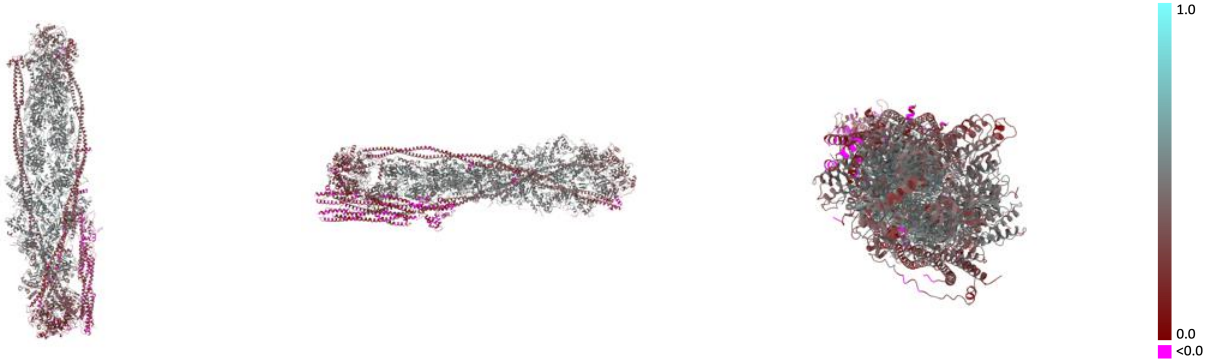
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

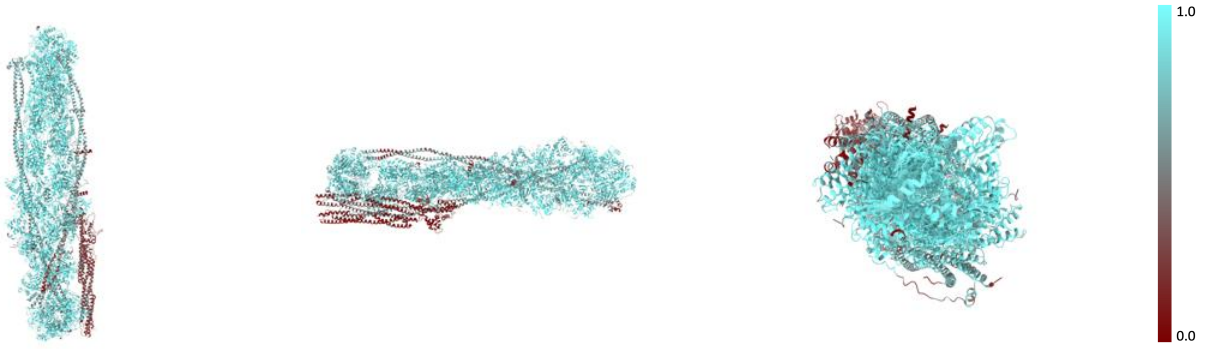
9.2 Q-score mapped to coordinate model



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.

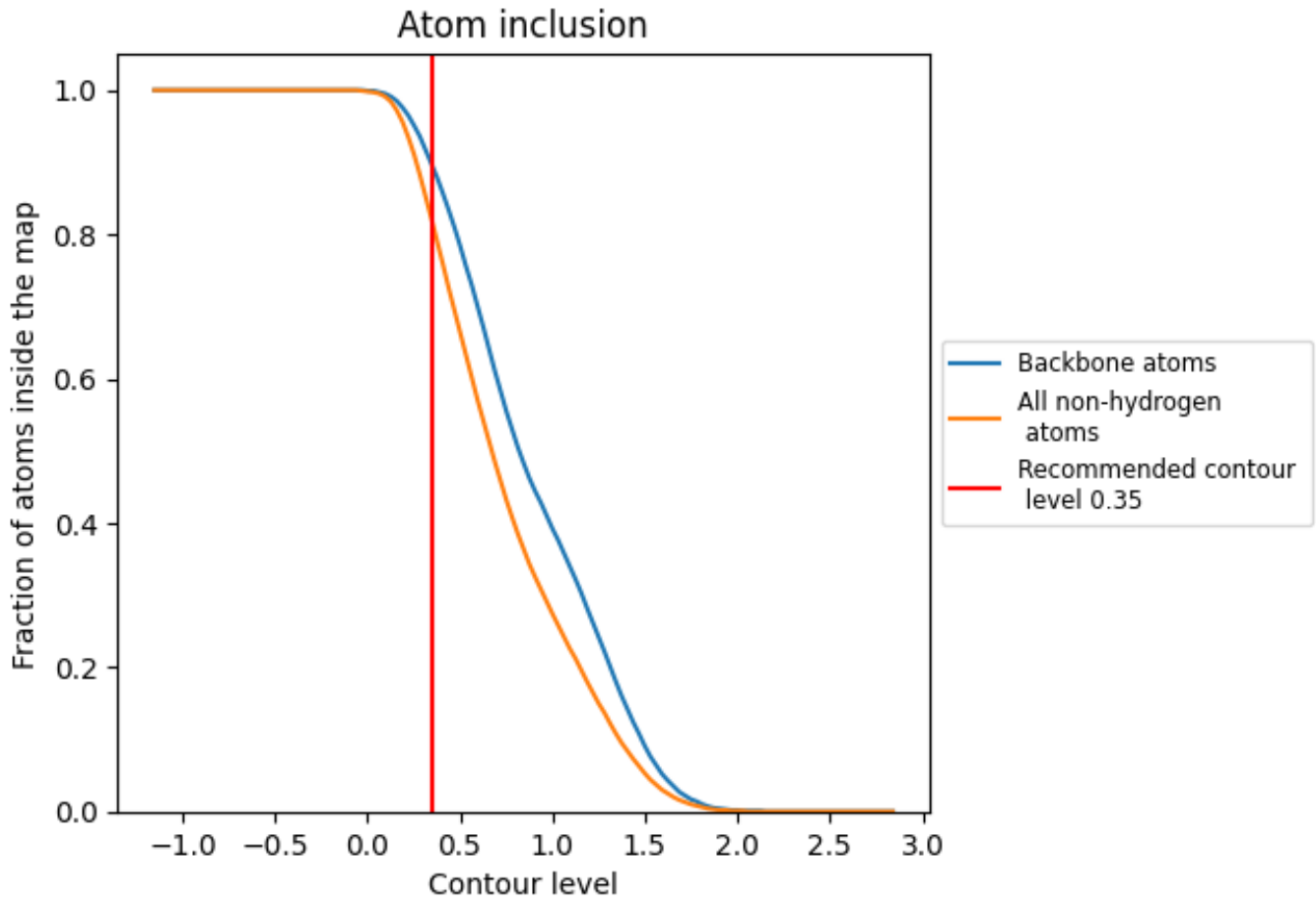
9.3 Atom inclusion mapped to coordinate model



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.3850
0	0.8490	0.2980
1	0.8800	0.3370
2	0.8640	0.2550
3	0.8300	0.2810
4	0.8390	0.2770
5	0.7780	0.3820
6	0.6920	0.3810
7	0.7140	0.3650
8	0.1040	0.0700
9	0.8150	0.3460
A	0.9340	0.4030
B	0.9500	0.4640
C	0.9550	0.4970
D	0.9520	0.4980
E	0.9600	0.5090
F	0.9550	0.5030
G	0.9640	0.5080
H	0.9580	0.5040
I	0.9570	0.5030
J	0.9500	0.5010
K	0.9490	0.4800
L	0.9270	0.4330
M	0.9340	0.4210
N	0.8710	0.4340
O	0.9470	0.4680
P	0.9370	0.4610
Q	0.9610	0.4690
R	0.9520	0.4720
S	0.3960	0.2030
T	0.9450	0.4540
U	0.5690	0.2710
V	0.5340	0.2430
W	0.5970	0.2320
X	0.5750	0.2260

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Chain	Atom inclusion	Q-score
Y	0.8280	0.3220
Z	0.8400	0.3540