wwPDB EM Validation Summary Report (i)

Mar 10, 2026 – 01:43 AM UTC

PDB ID	:	8IAI / pdb_00008iai
EMDB ID	:	EMD-35302
Title	:	Structure of mammalian spectrin-actin junctional complex of membrane skeleton, State II, Global map
Authors	:	Li, N.; Chen, S.; Gao, N.
Deposited on	:	2023-02-08
Resolution	:	3.50 Å(reported)

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

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

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

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

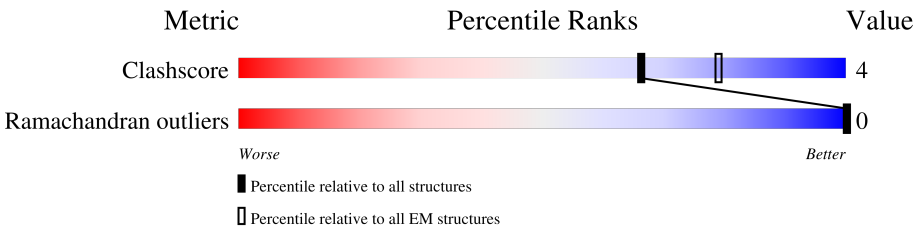
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

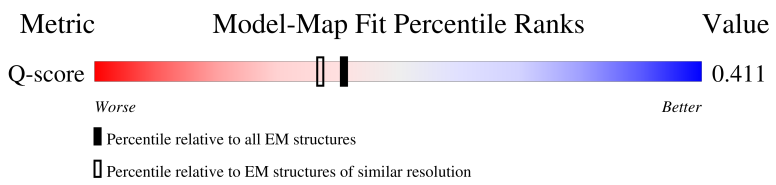
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	1	744	6% 38% 7% 55%
1	2	744	11% 32% 7% 61%
1	9	744	• 7% • 92%
2	3	724	12% 40% 6% 53%
2	4	724	10% 33% • 64%

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Mol	Chain	Length	Quality of chain
3	5	405	26% 71%
3	6	405	10% 25% 71%
3	7	405	5% 25% 71%
4	A	375	87% 13%
4	B	375	86% 13%
4	C	375	93% 7%
4	D	375	93% 7%
4	E	375	89% 11%
4	F	375	90% 9%
4	G	375	85% 15%
4	H	375	93% 6%
4	I	375	94% 6%
4	J	375	89% 10%
4	K	375	86% 13%
5	M	2148	6% 94%
5	N	2148	5% 95%
5	O	2148	5% 94%
5	P	2148	5% 95%
5	Q	2148	6% 94%
5	R	2148	5% 95%
5	S	2148	5% 94%
5	T	2148	5% 94%
6	U	248	90% 10%
7	V	248	6% 89% 10%
8	Y	359	68% 9% 23%

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Mol	Chain	Length	Quality of chain
9	Z	107	7% 82% 9% 8%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 60300 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
			Total	C	N	O	S		
1	1	334	2578	1641	447	478	12	0	0
1	2	290	2234	1426	386	412	10	0	0
1	9	62	530	328	94	102	6	0	0

- Molecule 2 is a protein called Beta-adducin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	338	2639	1669	457	495	18	0	0
2	4	262	2041	1296	351	378	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	5	119	974	625	171	176	2	0	0
3	6	119	927	595	157	173	2	0	0
3	7	116	946	606	166	172	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	374	2917	1845	490	560	22	0	0
4	B	374	2917	1845	490	560	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	374	2917	1845	490	560	22	0	0
4	D	374	2917	1845	490	560	22	0	0
4	E	374	2917	1845	490	560	22	0	0
4	F	374	2917	1845	490	560	22	0	0
4	G	374	2917	1845	490	560	22	0	0
4	H	374	2917	1845	490	560	22	0	0
4	I	374	2917	1845	490	560	22	0	0
4	J	371	2893	1833	487	551	22	0	0
4	K	371	2889	1828	487	552	22	0	0

- Molecule 5 is a protein called Spectrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	130	1065	671	200	188	6	0	0
5	N	117	960	609	181	164	6	0	0
5	O	131	1073	675	201	191	6	0	0
5	P	117	960	609	181	164	6	0	0
5	Q	129	1057	667	199	185	6	0	0
5	R	117	960	609	181	164	6	0	0
5	S	128	1048	660	197	185	6	0	0
5	T	128	1048	660	197	185	6	0	0

- Molecule 6 is a protein called Tropomyosin-1.9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	U	247	2000	1213	358	422	7	0	0

- Molecule 7 is a protein called Tropomyosin 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	V	246	2011	1218	362	421	10	0	0

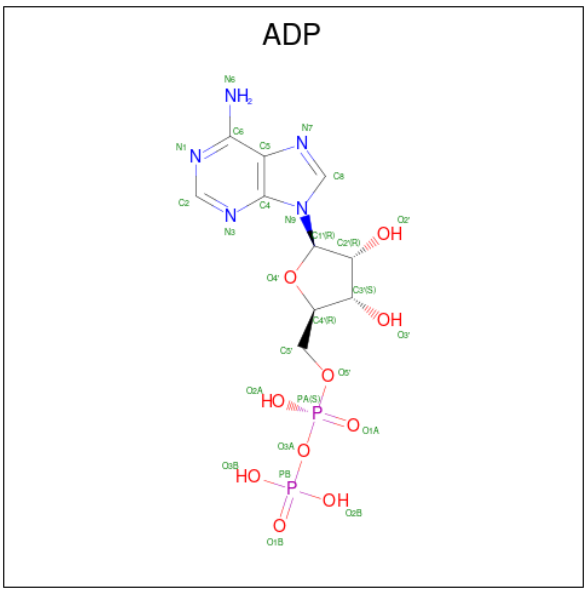
- Molecule 8 is a protein called Tropomodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Y	276	2119	1332	377	405	5	0	0

- Molecule 9 is a protein called SH3 domain-binding glutamic acid-rich-like protein.

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

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



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

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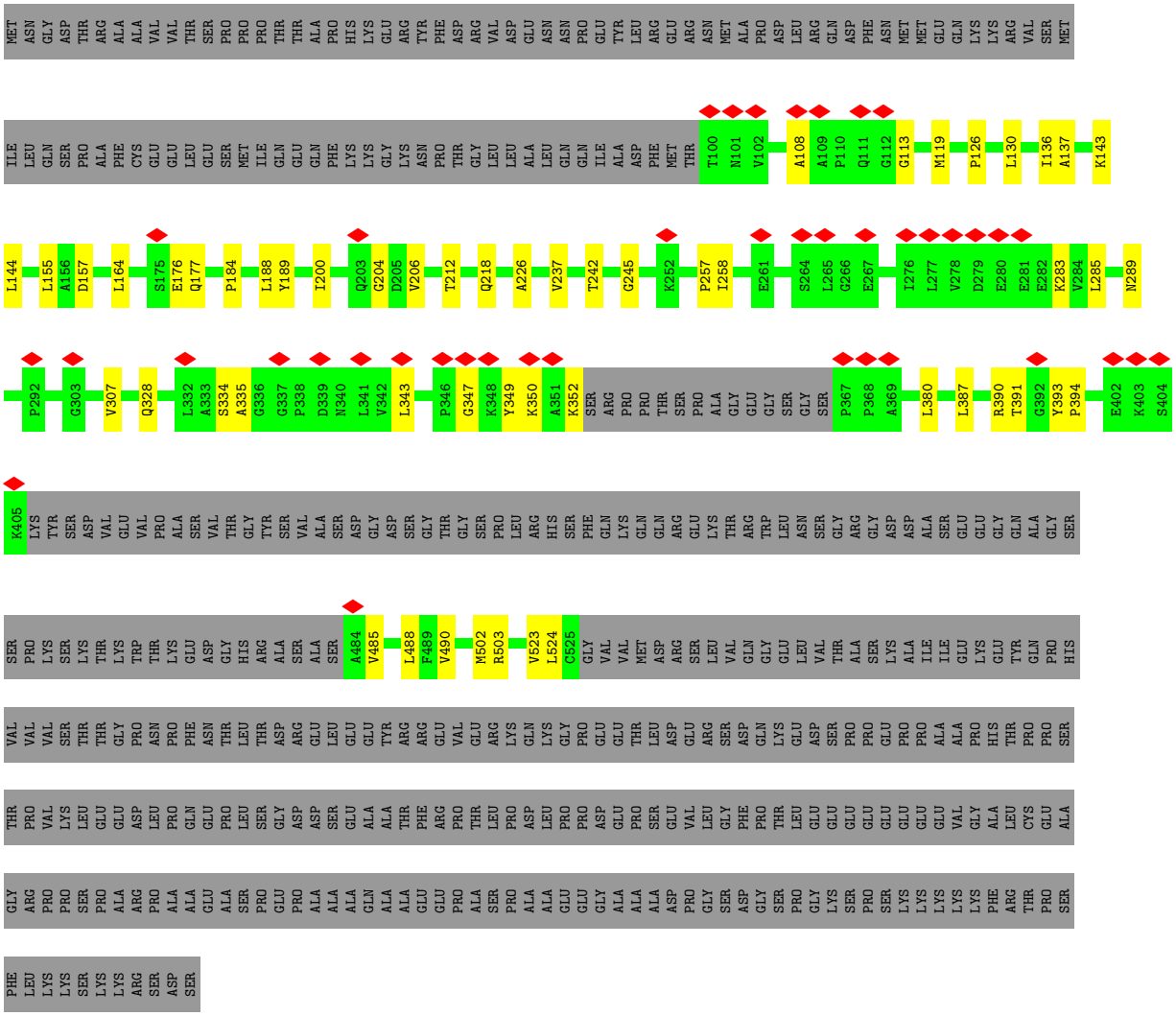
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	B	1	27	10	5	10	2	0
10	C	1	27	10	5	10	2	0
10	D	1	27	10	5	10	2	0
10	E	1	27	10	5	10	2	0
10	F	1	27	10	5	10	2	0
10	G	1	27	10	5	10	2	0
10	H	1	27	10	5	10	2	0
10	I	1	27	10	5	10	2	0
10	J	1	27	10	5	10	2	0
10	K	1	27	10	5	10	2	0

3 Residue-property plots (i)

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

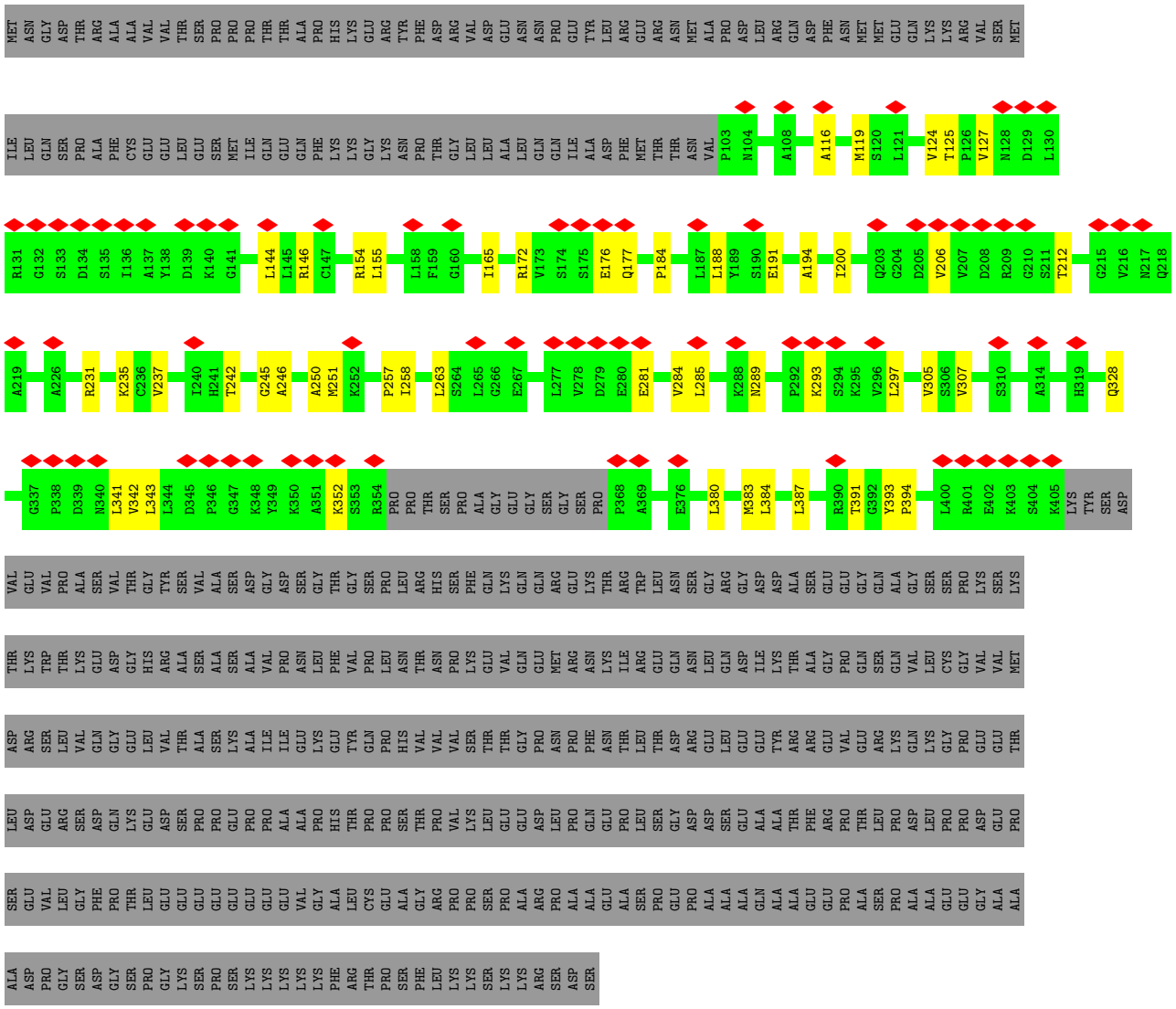
- Molecule 1: Adducin 1

Chain 1:



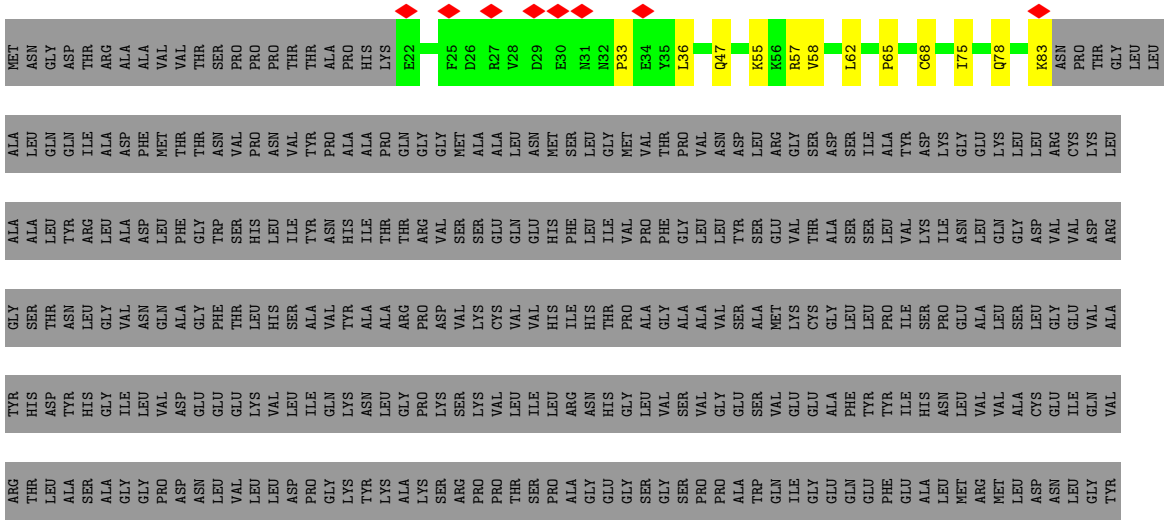
- Molecule 1: Adducin 1

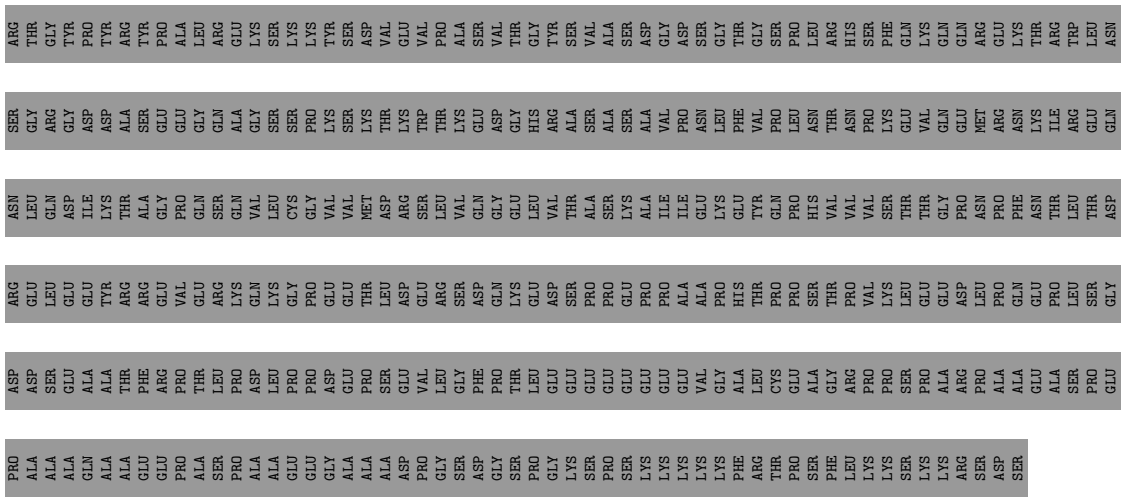
Chain 2:



- Molecule 1: Adducin 1

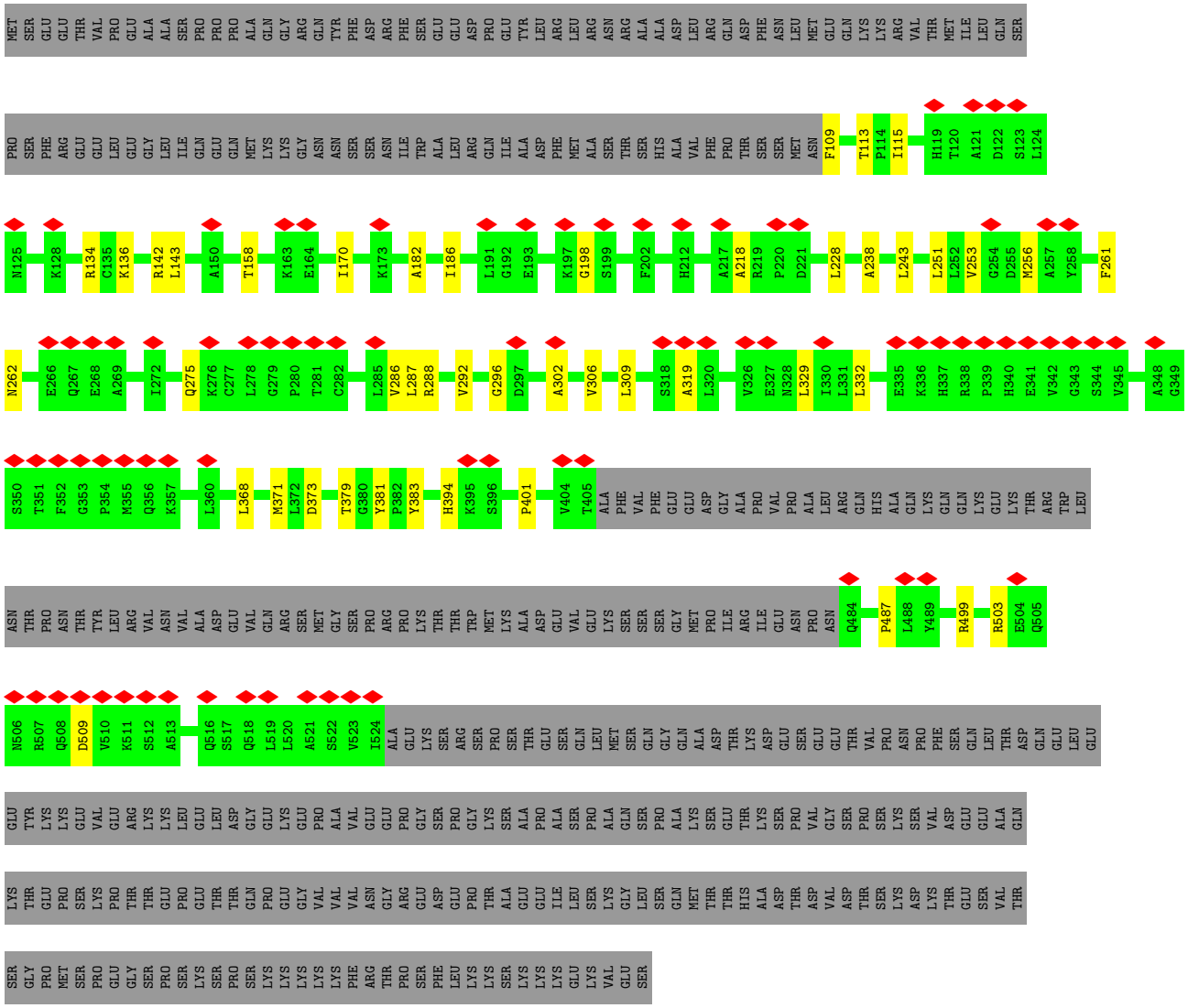
Chain 9: 7% 92%





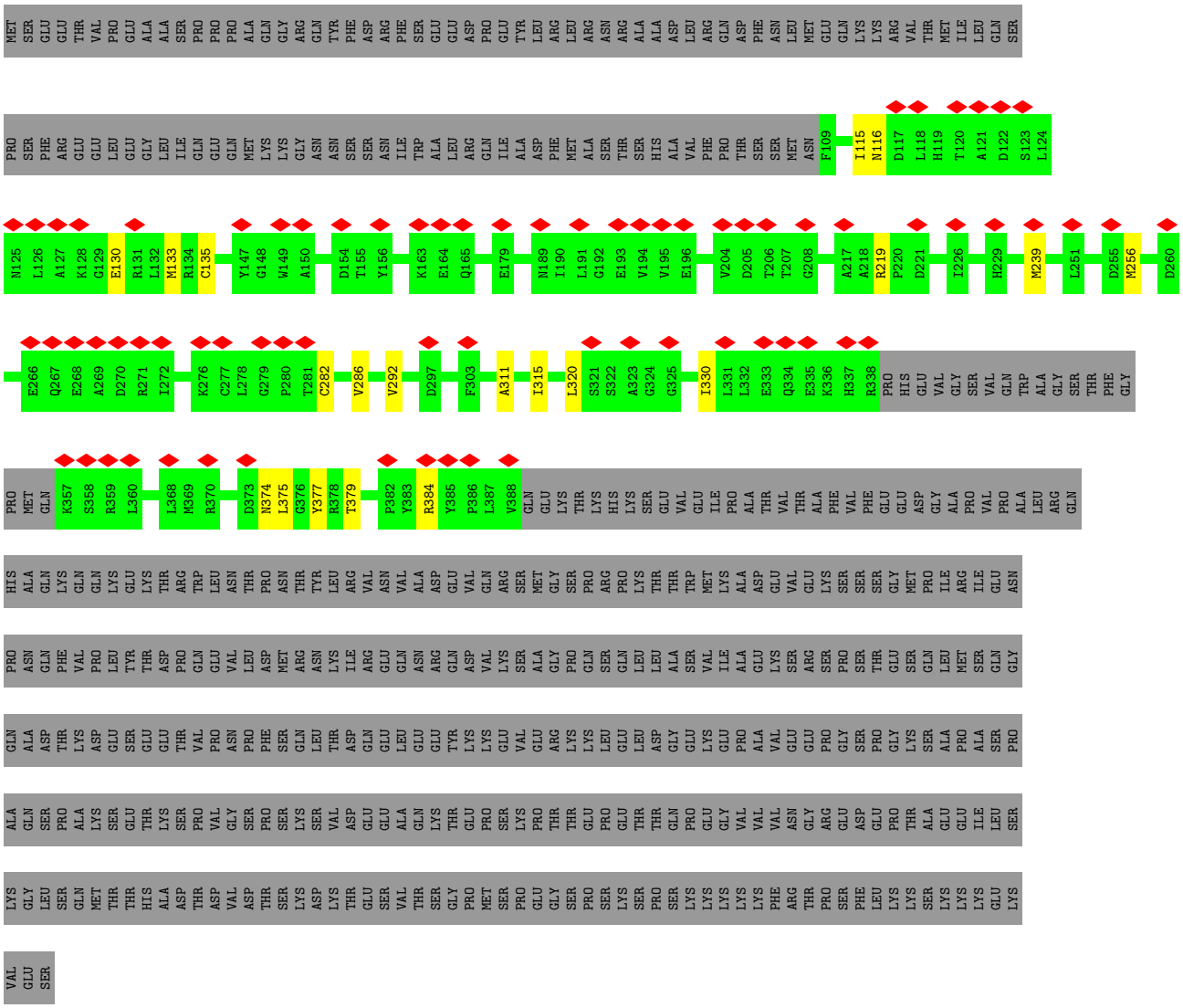
- Molecule 2: Beta-adducin

Chain 3:



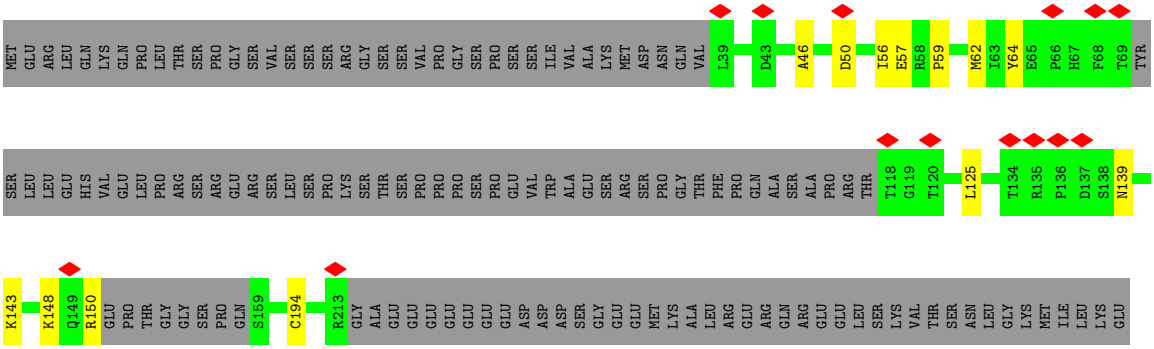
- Molecule 2: Beta-adducin

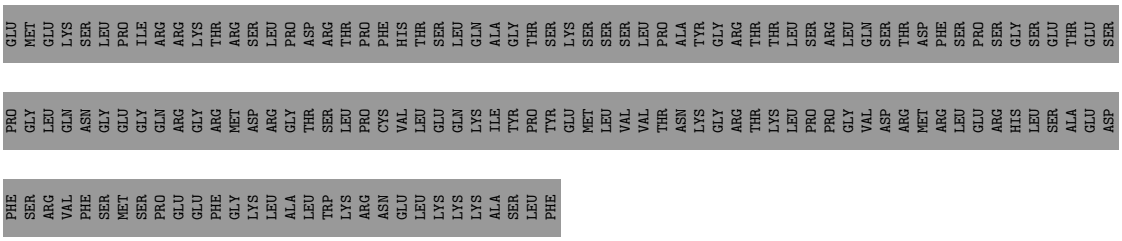
Chain 4:



- Molecule 3: Dematin actin binding protein

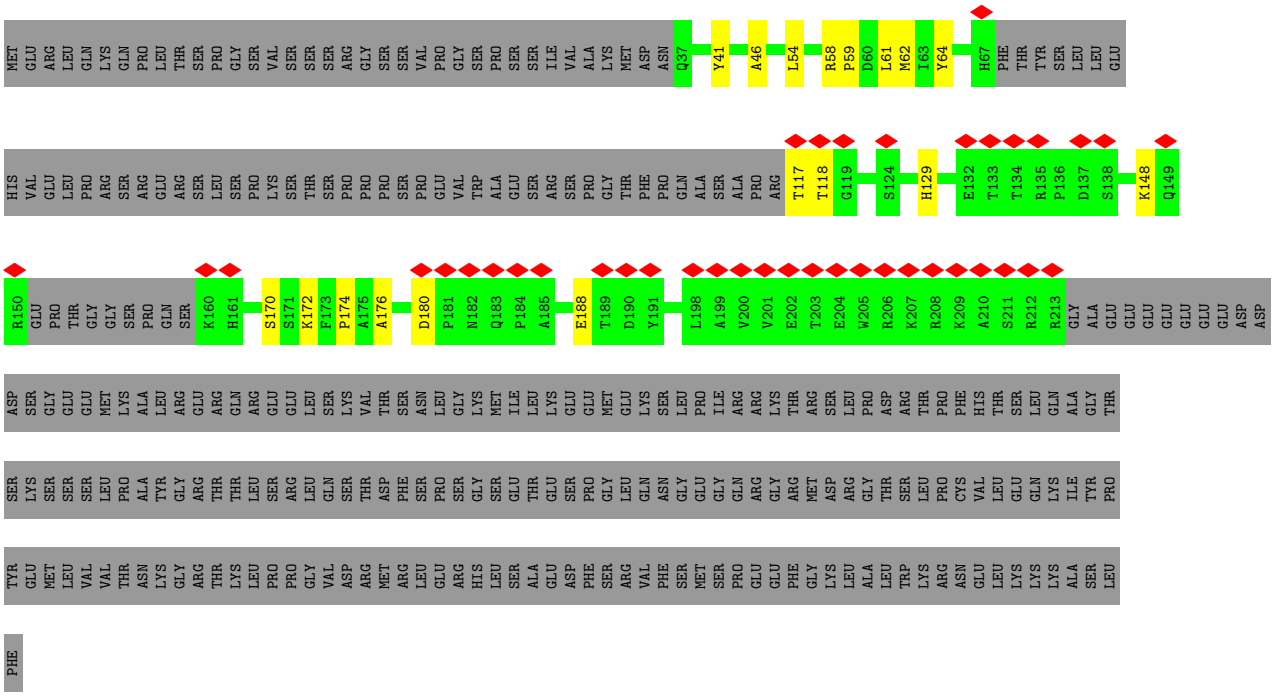
Chain 5:





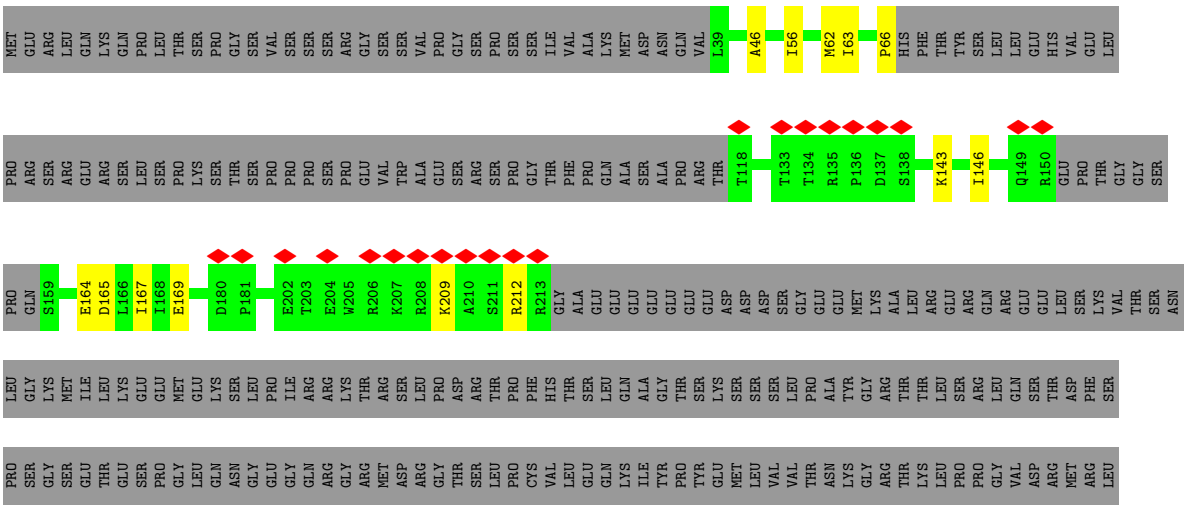
• Molecule 3: Dematin actin binding protein

Chain 6:



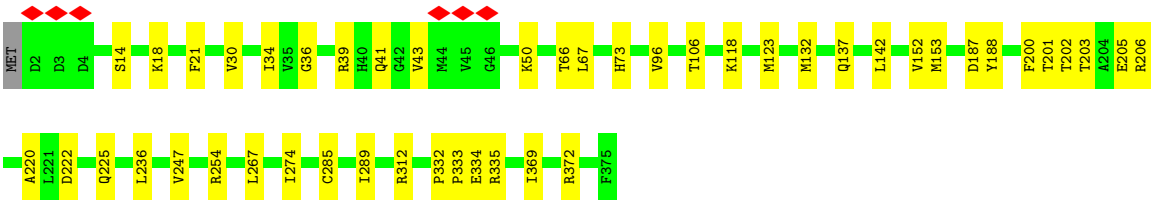
• Molecule 3: Dematin actin binding protein

Chain 7:



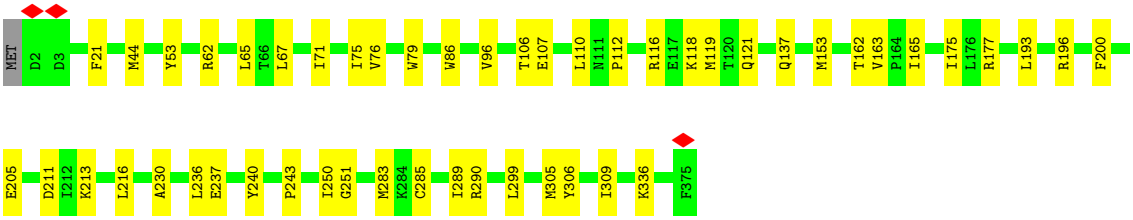
• Molecule 4: Actin, cytoplasmic 1

Chain A:



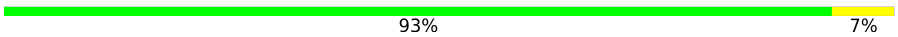
• Molecule 4: Actin, cytoplasmic 1

Chain B:



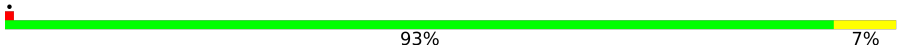
• Molecule 4: Actin, cytoplasmic 1

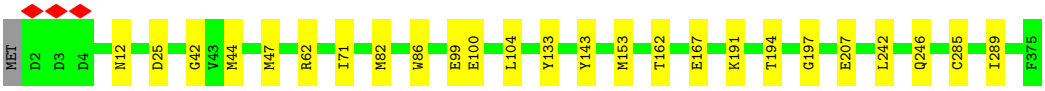
Chain C:



• Molecule 4: Actin, cytoplasmic 1

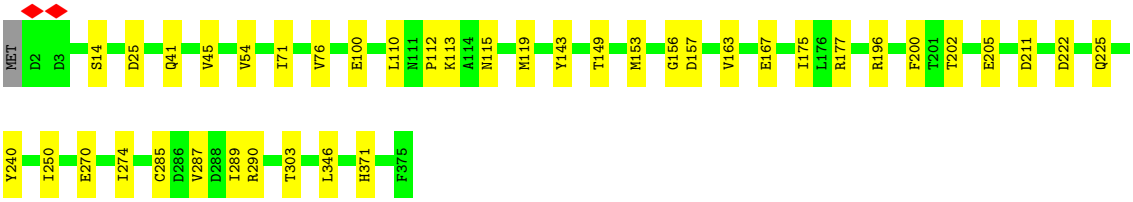
Chain D:





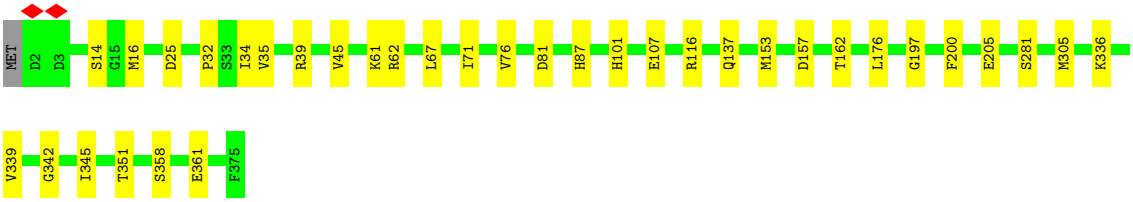
• Molecule 4: Actin, cytoplasmic 1

Chain E:



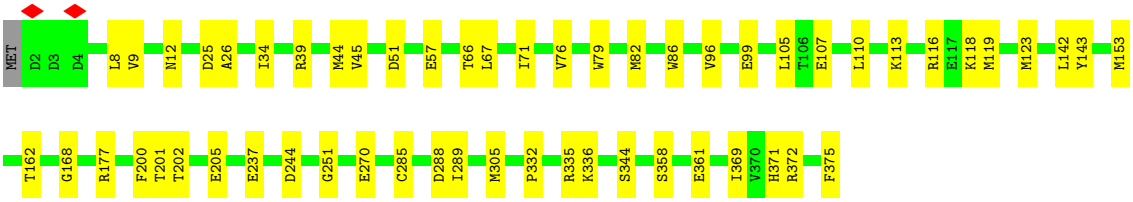
- Molecule 4: Actin, cytoplasmic 1

Chain F:



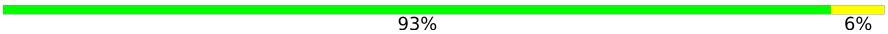
- Molecule 4: Actin, cytoplasmic 1

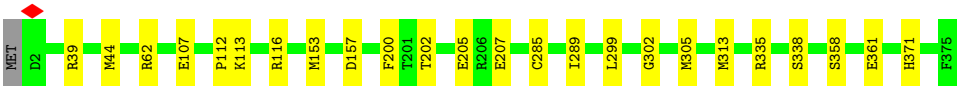
Chain G:



- Molecule 4: Actin, cytoplasmic 1

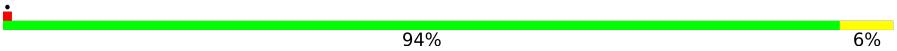
Chain H:





- Molecule 4: Actin, cytoplasmic 1

Chain I:

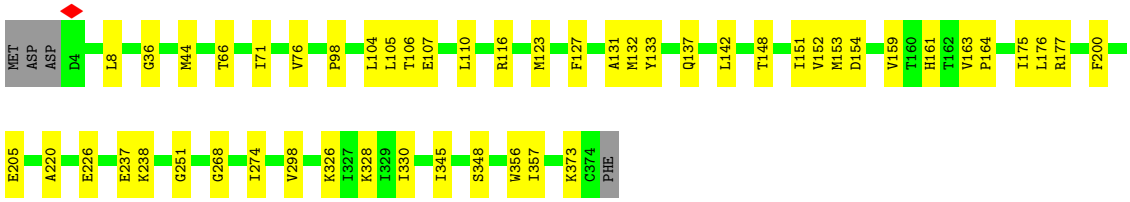


- Molecule 4: Actin, cytoplasmic 1

Chain J:

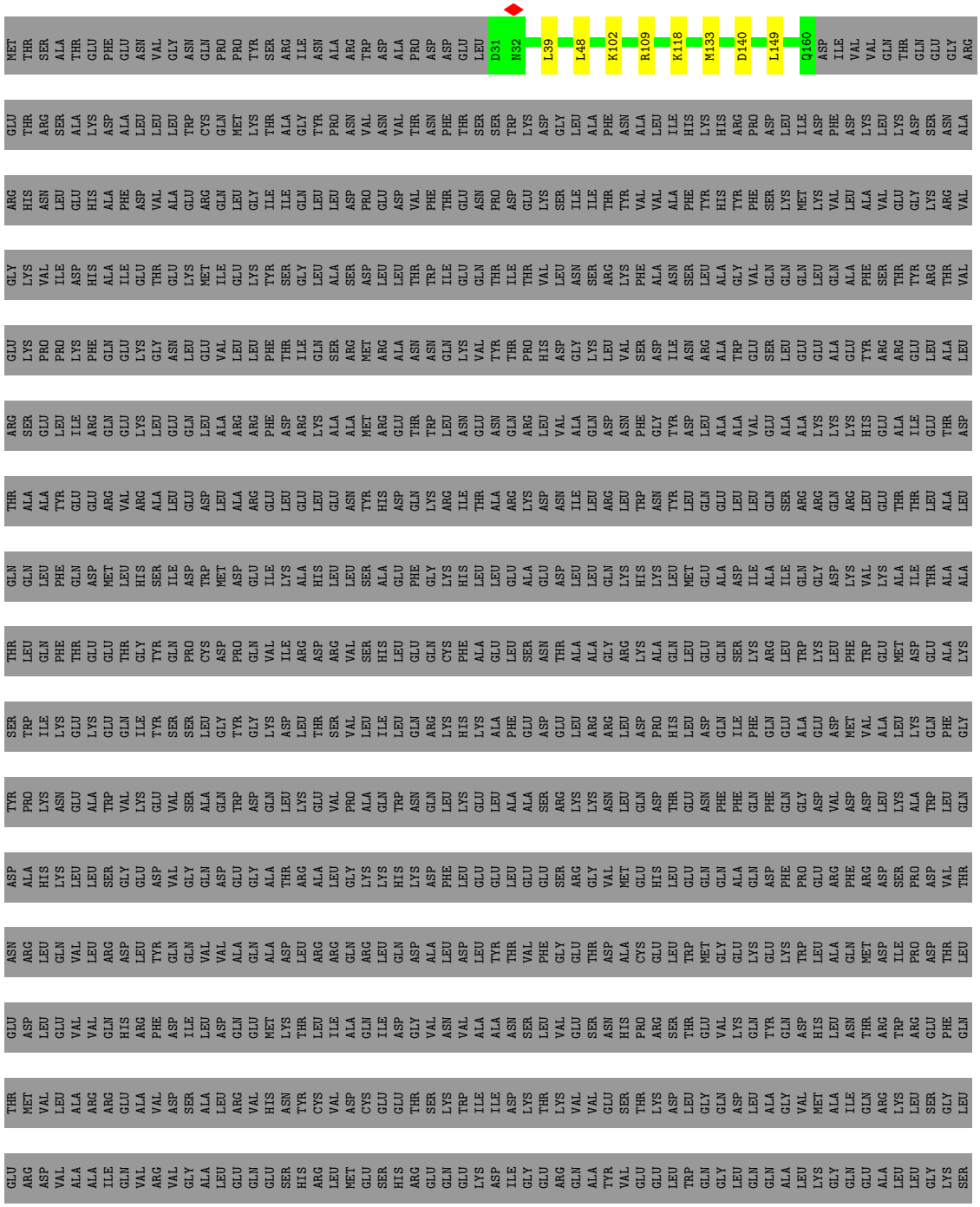
- Molecule 4: Actin, cytoplasmic 1

Chain K:



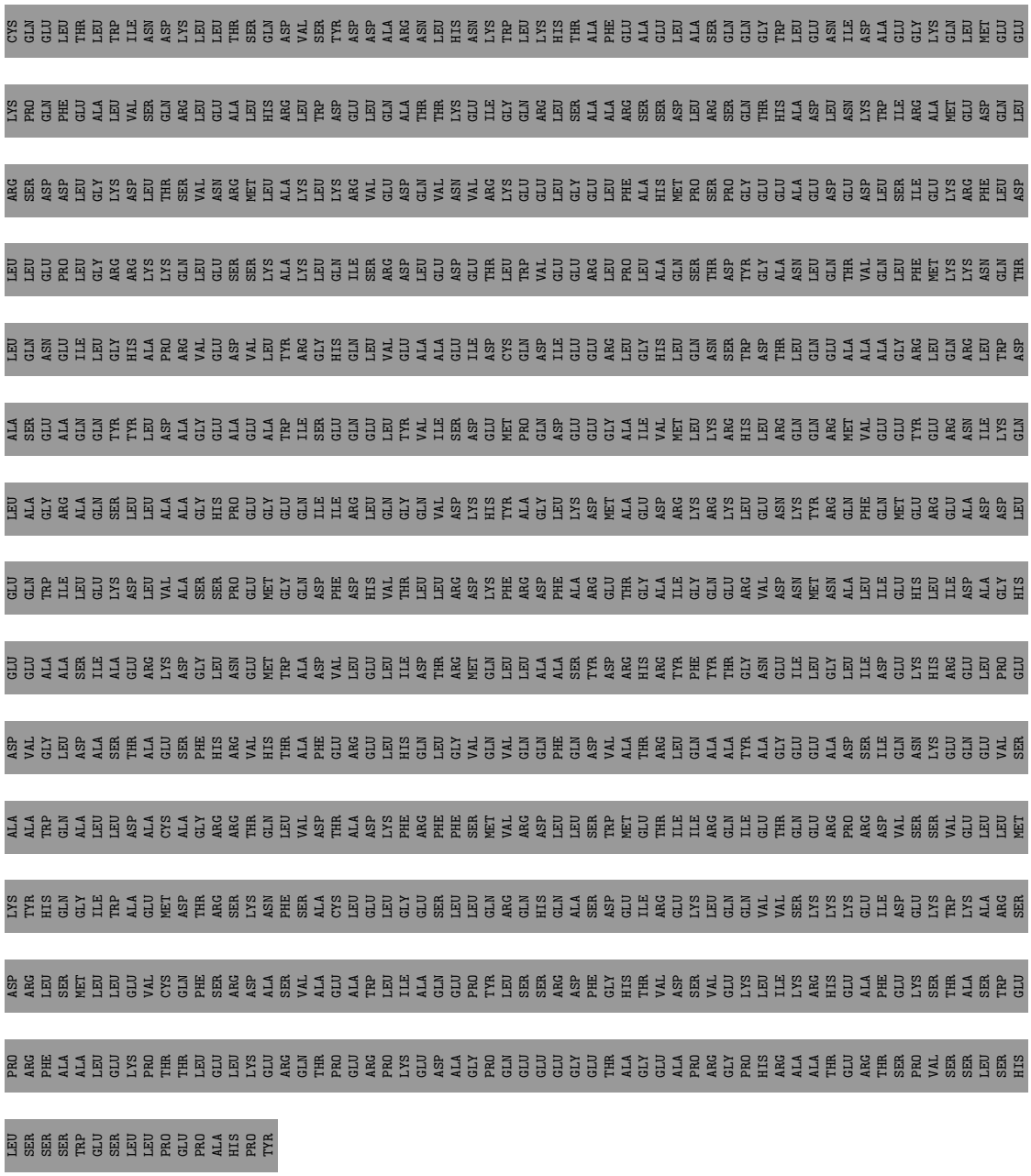
- Molecule 5: Spectrin beta chain

Chain M: 6% 94%



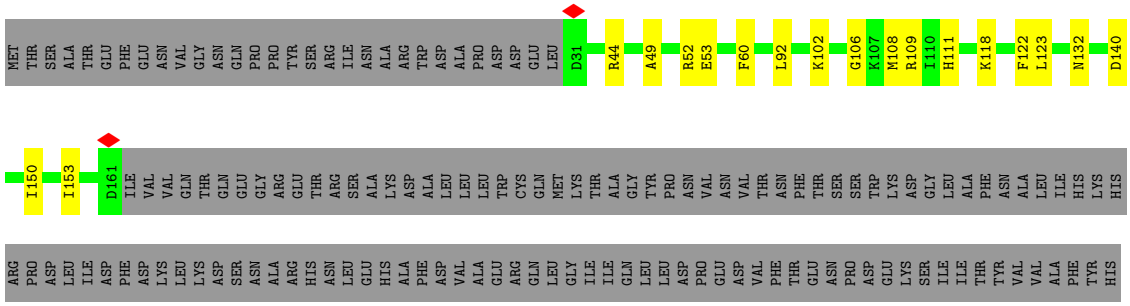
| | | |

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 ASP ASN ASP ASN SER SER ALA ARG LEU PHE GLU R42 D50 E51 R52 E53 L68 S72 R36 E93 M99 L100 K105
I110 L113 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 LEU LEU ALA ARG 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 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 SER LEU ASN SER ARG LYS PHE ALA ASN
SER LEU ALA GLY VAL GLN GLN GLN LEU GLN ALA 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 GLU LYS VAL TYR TRP HIS ASN VAL GLY ASP ILE
ASN ARG ALA TRP GLU SER LEU GLU GLU GLU ALA ALA GLU TYR ARG ARG GLU 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 TYR HIS ASP GLN LYS ARG ILE THR ALA ARG LYS ASP VAL ASN ALA LEU ASN PHE GLY TYR
ASP LEU ALA ALA VAL GLU ALA ALA LYS LYS LYS HIS GLU ALA ILE GLU THR ALA ASP THR ALA ALA TYR GLU GLU ARG VAL ARG ALA LEU GLU ASP LEU ALA ARG GLU LEU GLU ASN TYR HIS ASP GLN LYS ARG ILE THR ALA ARG LYS ASP VAL LEU ARG LEU TRP ASN TYR
LEU GLN GLU LEU GLN ARG ARG GLN ARG LEU GLU THR THR LEU ALA ALA LEU GLN 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 ASN ILE LEU ARG GLN LYS HIS HIS LYS LEU
MET GLU ALA ASP ILE ALA ILE GLN GLY ASP LYS VAL LYS ALA ILE THR ALA 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 GLU 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 GLU ALA GLU ASP ASP MET VAL ALA LEU LYS GLN PHE GLY TYR PRO LYS ASN GLU ALA TRP VAL LYS GLU VAL SER ALA GLN LEU LYS ASP 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 ALA ALA LEU ASP LEU SER GLY GLU ASP VAL GLY GLN ASP GLU GLY ALA THR ARG ALA LEU GLY GLY LYS LYS HIS LYS ASP PHE LEU GLU GLU LEU ALA PHE GLU 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 ALA ALA GLN ARG LEU GLN ASP ALA LEU ASP LEU TYR THR VAL PHE GLY GLU THR ASP LYS ASN ARG GLN GLN ILE GLN ASP ALA LEU ASP ALA ALA ARG PHE ILE ILE ASP GLY VAL ASN VAL ALA ALA ASN SER LEU LEU ARG SER LEU GLN
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 ALA ILE ASP GLY VAL ASN VAL ALA ALA ASN SER LEU VAL GLU THR ASP ALA HIS PRO GLN SER
THR GLU VAL LYS GLN TYR GLN ASP HIS LEU ASN THR ARG TRP ARG GLU PHE GLN THR MET VAL LEU GLU ALA ARG ARG GLU ALA VAL ASP SER ALA LEU ARG VAL ALA ASN TYR CYS VAL ASP CYS GLU GLU THR SER LYS TRP ILE ILE ASP LEU GLU 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 GLU ASP VAL ALA ALA ILE GLN VAL ARG VAL GLY ALA LEU GLU GLN GLU SER HIS ARG GLU GLN GLN VAL LYS ASP ILE GLY GLU ARG GLN ALA TYR VAL GLU LEU
TRP GLN GLY LEU GLN GLN ALA LEU LYS GLY GLN GLU ALA LEU GLN GLN LYS SER SER GLN LEU GLN ASP LEU ASP ALA PHE LEU GLN ASP LEU ASP ALA ALA PHE GLU ALA LEU SER THR ALA GLN LYS GLU VAL ALA SER LYS ASP MET PRO GLU SER LEU PRO GLU ALA GLU 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 SER ARG MET TRP GLU SER ARG HIS
THR LEU ALA GLN CYS LEU GLY PHE GLN GLU PHE GLN LYS ALA ALA LEU SER ASN GLN ALA GLU ALA GLY ILE LEU GLU TYR THR LEU ALA HIS LEU GLU GLU ASP ASP SER LEU GLU GLU ALA ALA ASP PRO GLU ALA ALA GLU LEU SER ASP LEU ILE ASP ILE GLU ILE ILE ASN GLN ILE ASP PHE PHE GLN ASP ALA LEU ASP ILE GLU ILE GLU ILE GLU



- Molecule 5: Spectrin beta chain

Chain O: 5% • 94%



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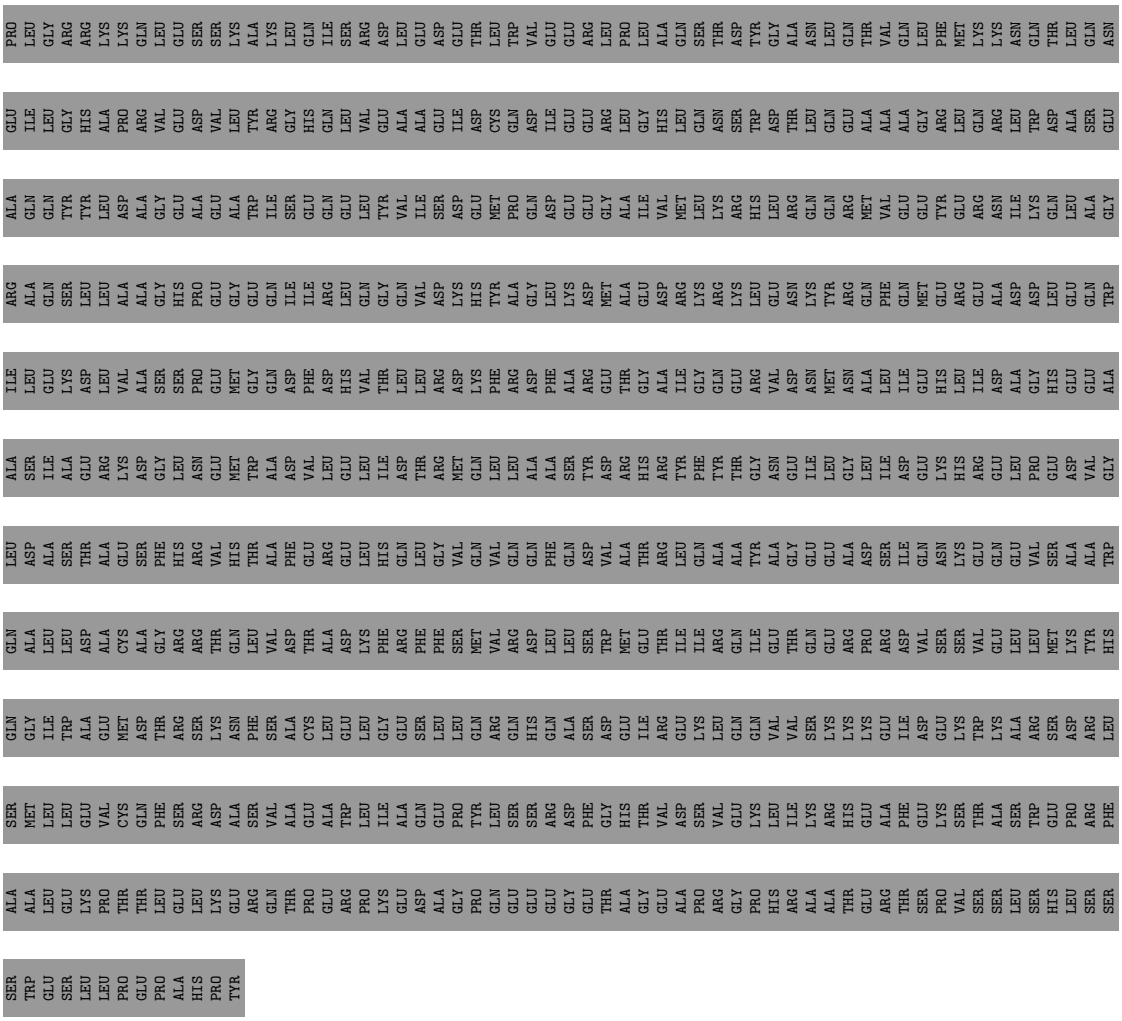
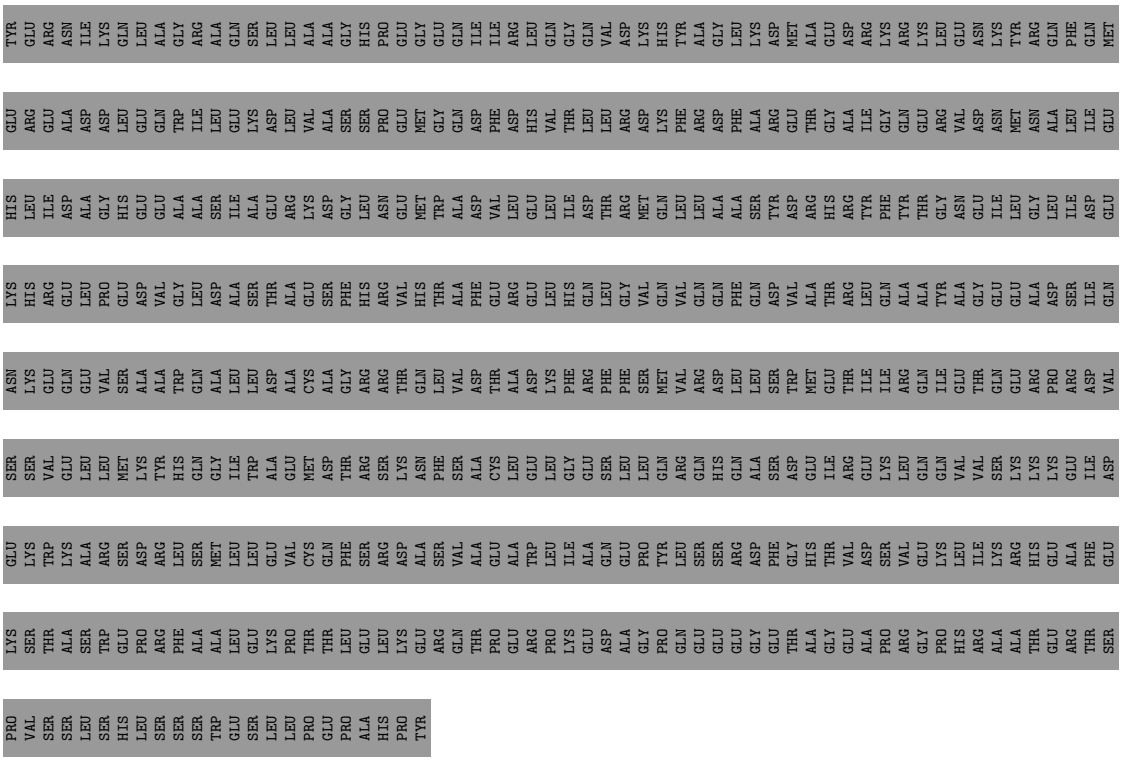


- Molecule 5: Spectrin beta chain

Chain P: 5% 95%

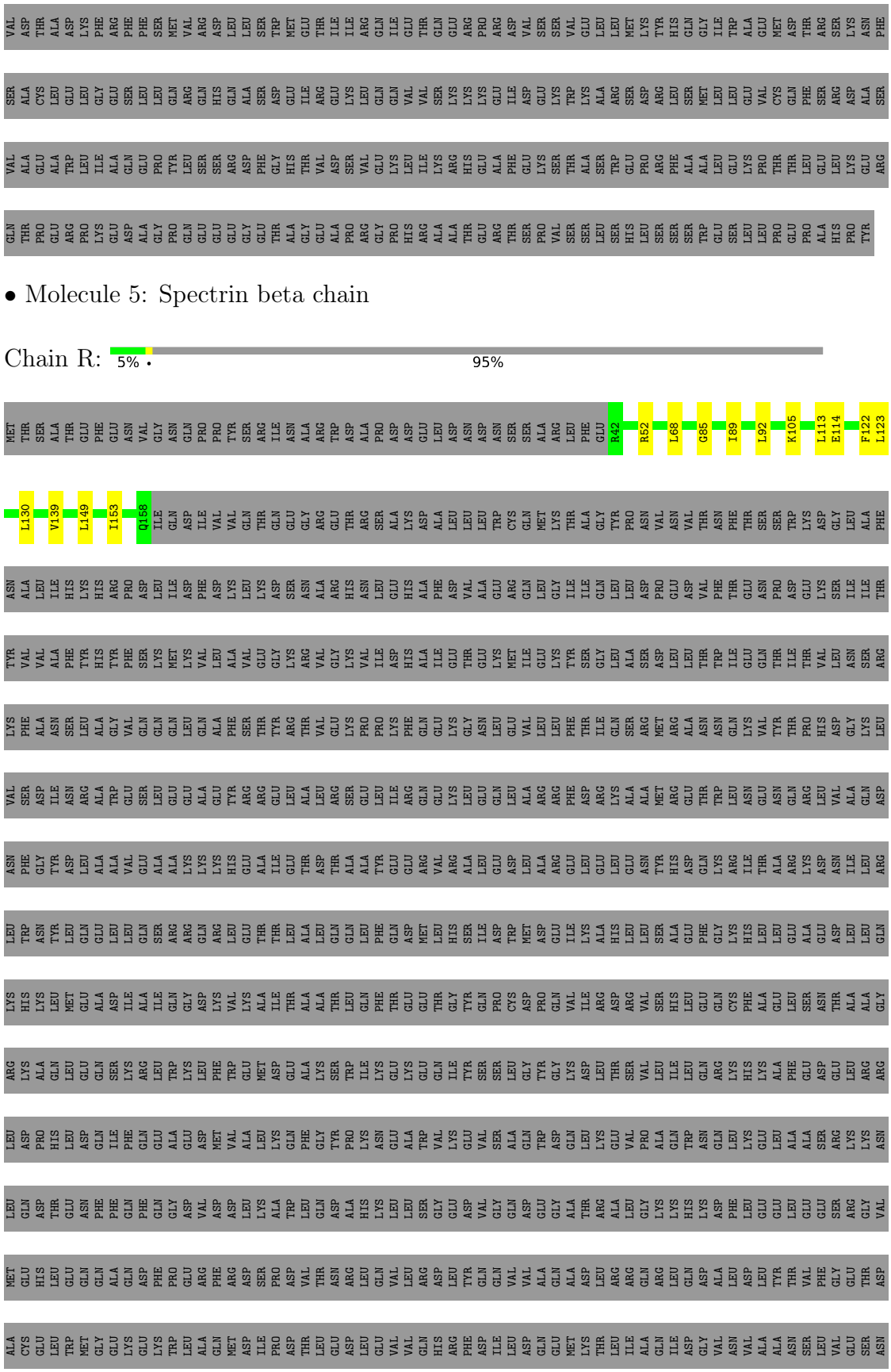
| | | |



- Molecule 5: Spectrin beta chain

Chain Q: 6% 94%

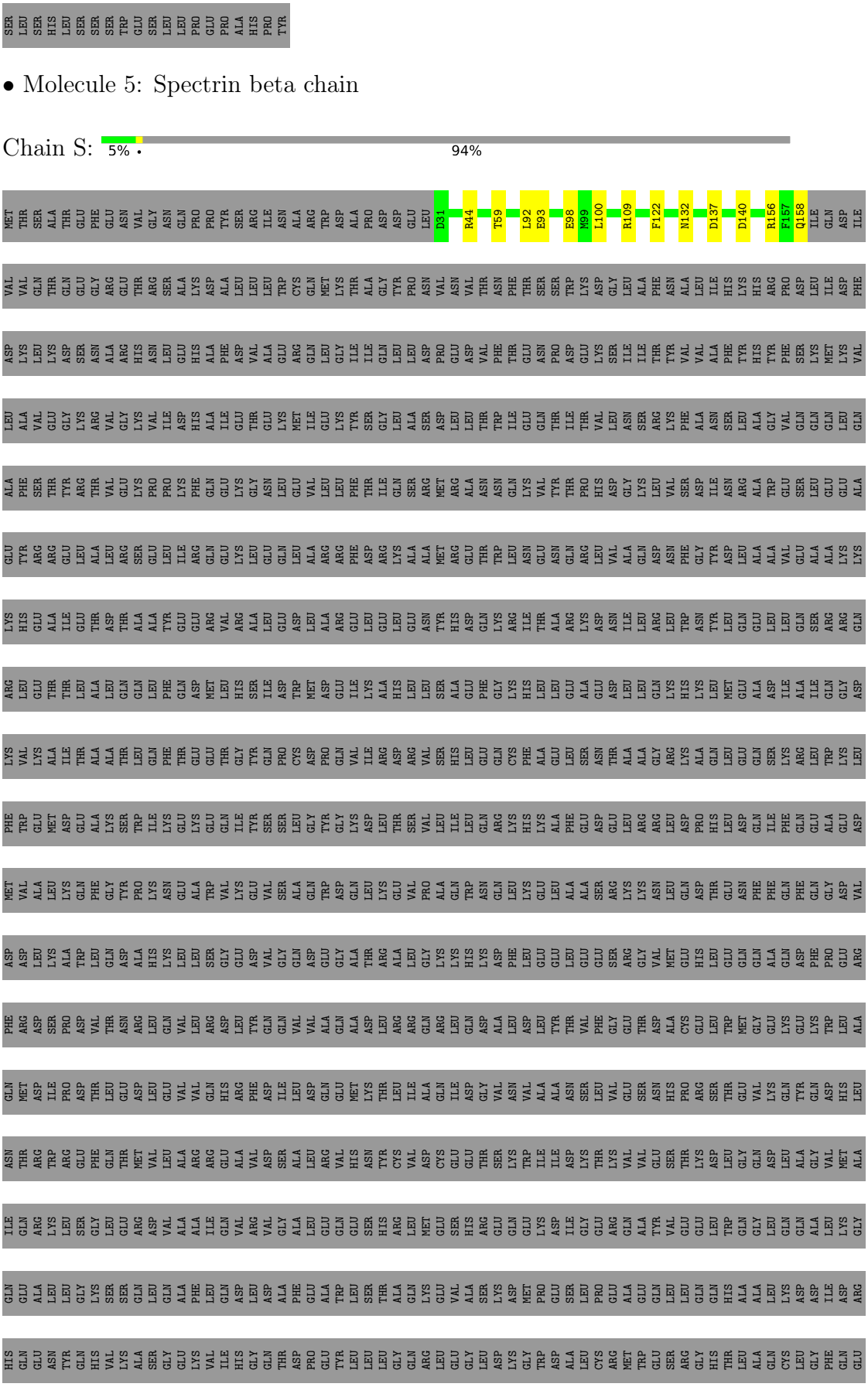
| | | |

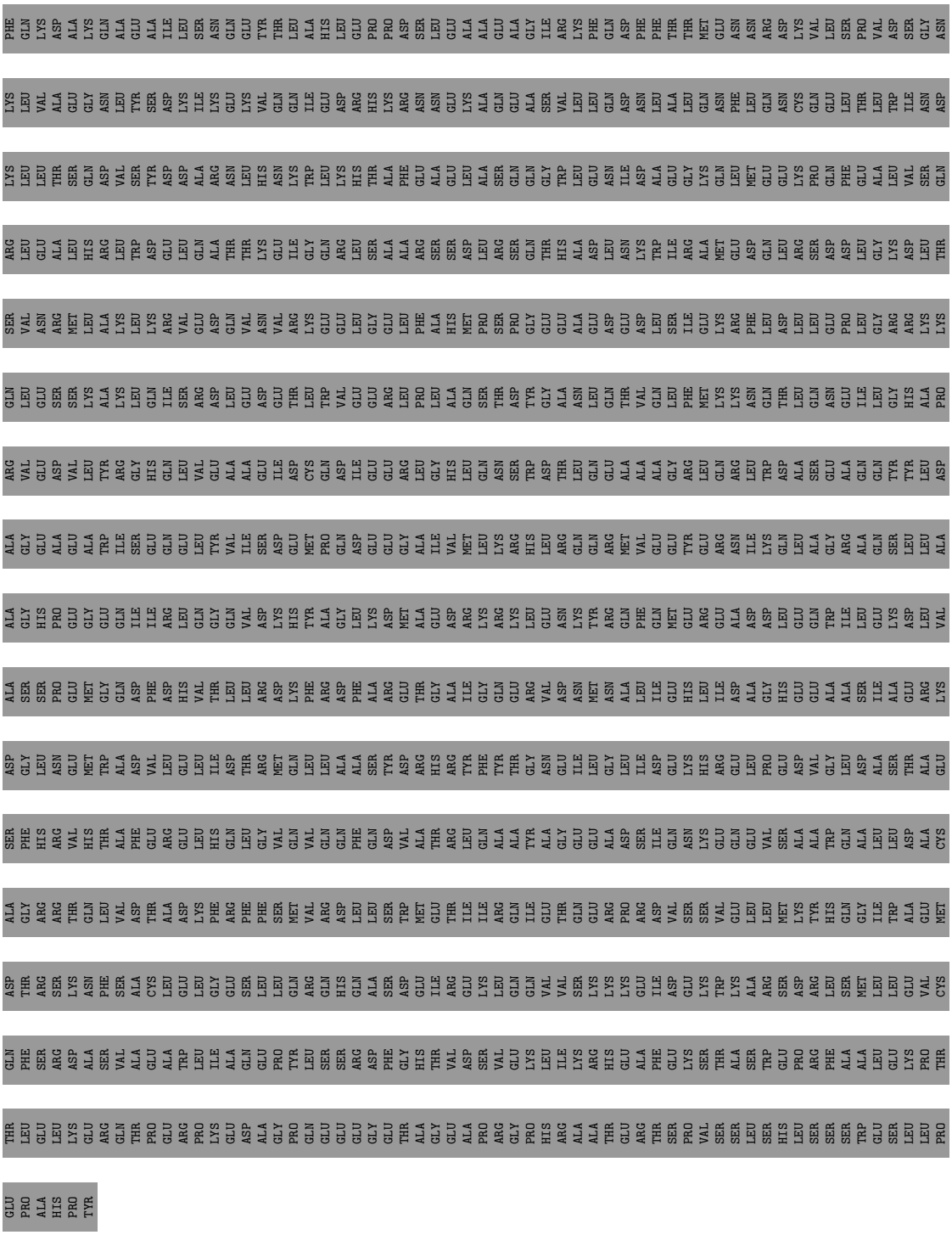


• Molecule 5: Spectrin beta chain

Chain R: 5% • 95%

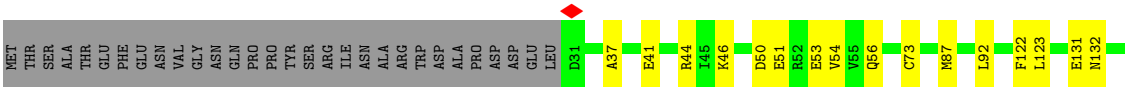
| | | |


SER LEU SER HIS LEU SER SER SER TRP GLU SER LEU LEU PRO GLU PRO ALA HIS PRO TYR
• Molecule 5: Spectrin beta chain
Chain S:
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 R44 T59 L92 E93 E98 M99 L100 R109 F122 N132 D137 D140 R156 F157 Q158 ILE GLN ASP ILE
VAL VAL GLN THR THR GLN GLU GLY 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 LEU GLY ILE ILE GLN LEU LEU ASP PRO GLU ASP VAL THR PHE THR GLU ASN PRO ASP GLU LYS SER ILE ILE THR TYR VAL VAL ALA PHE TYR HIS LYS SER LYS MET 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 GLN GLN GLN GLN 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 GLU ALA
GLU TYR ARG ARG GLU LEU ALA LEU ARG SER GLU LEU ILE ARG GLN GLU LYS LEU GLU GLN LEU ASP ARG LYS ALA 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 GLU GLY PHE GLY TYR ASP LEU ALA ALA VAL GLU GLU 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 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 GLU SER LYS 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 GLY LYS HIS LEU LEU GLU ALA ALA ASP ILE ALA ILE GLN 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 GLU LEU GLN SER LYS ARG LEU TRP LYS LEU
PHE TRP GLU MET ASP GLU ALA LYS SER TRP ILE LYS GLU LYS GLU 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 GLU ALA 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 LEU GLN ASP ALA HIS LYS LEU LEU LEU SER GLY GLU GLU ASP VAL GLY GLN ASP GLU GLY ALA ALA THR ARG ALA LEU GLY LYS LYS HIS LYS ASP PHE LEU GLU GLU GLU GLU SER ARG GLY VAL MET GLU HIS LEU GLU GLN GLN ALA GLN ASP PRO GLU GLU
PHE ARG ASP SER PRO ASP VAL THR ASN ARG LEU GLN VAL LEU ARG ARG ASP LEU LEU GLN GLN ARG LEU GLN ASP ALA LEU ASP LEU 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 GLN HIS ARG PHE ASP ILE LEU ASP GLU GLN GLU MET LYS THR LEU ILE ALA GLN LYS ASP ILE ALA ALA ASN VAL ALA 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 GLU ALA ARG ARG GLU ALA VAL ASP SER ALA LEU ARG GLU VAL HIS ASN TYR CYS VAL ASP CYS GLU GLU THR SER LYS TRP ILE ILE ASP LYS THR LYS VAL GLU SER THR LYS ASP LEU GLY GLN ASP LEU ALA
ILE GLN ARG LYS LEU SER GLY LEU GLU ARG ASP VAL ALA ALA ILE GLN VAL ARG VAL GLY ALA GLU GLU GLN GLN GLU GLN GLN GLU GLU GLN ARG LEU MET GLU SER GLU GLU LYS ASP ILE GLY GLU ARG GLN TYR VAL GLU LEU GLU LEU GLN GLN GLN GLN GLY LEU GLN GLN ALA GLY GLY
GLN GLU ALA LEU LEU GLY LYS SER LEU SER SER LEU ASP ALA PHE GLU ALA TRP LEU SER THR ALA GLN LYS GLU VAL ALA SER LYS ASP MET PRO GLU SER SER LEU PRO GLU ALA GLU GLN GLN LEU LEU GLN GLN 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



- Molecule 5: Spectrin beta chain

Chain T: 5% 94%



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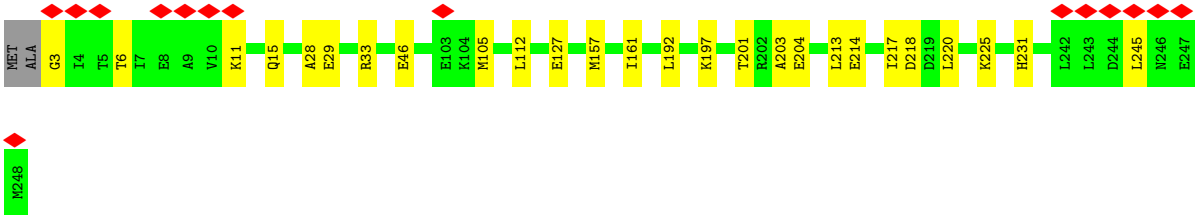
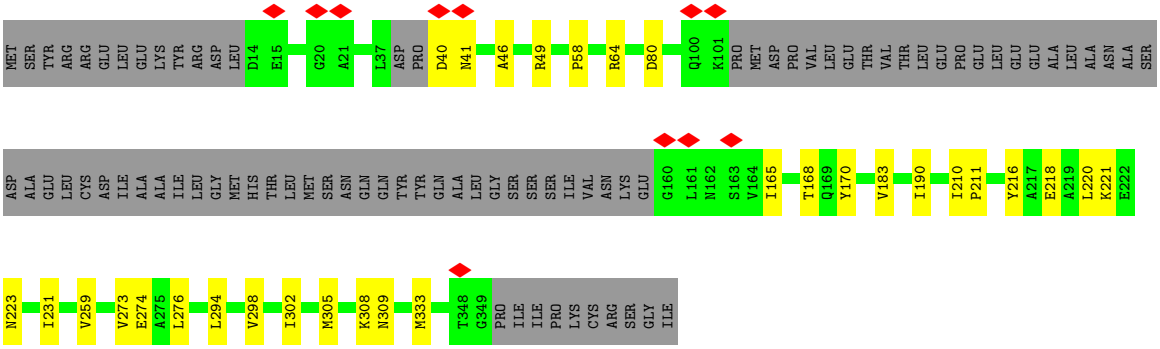


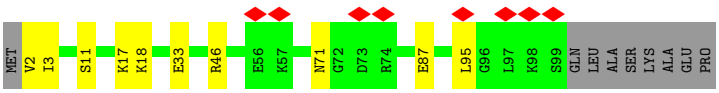
• Molecule 8: Tropomodulin-1

Chain Y:



• Molecule 9: SH3 domain-binding glutamic acid-rich-like protein

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68000	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	3.014	Depositor
Minimum map value	-1.436	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.4	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 (i)

5.1 Standard geometry (i)

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	1	0.17	0/2631	0.45	0/3572
1	2	0.18	0/2282	0.47	0/3095
1	9	0.27	0/538	0.72	0/715
2	3	0.16	0/2692	0.41	0/3646
2	4	0.18	0/2081	0.46	0/2816
3	5	0.15	0/1005	0.42	0/1367
3	6	0.17	0/955	0.46	0/1307
3	7	0.17	0/975	0.46	0/1326
4	A	0.14	0/2980	0.38	0/4035
4	B	0.14	0/2980	0.38	0/4035
4	C	0.14	0/2980	0.36	0/4035
4	D	0.15	0/2980	0.37	0/4035
4	E	0.14	0/2980	0.35	0/4035
4	F	0.14	0/2980	0.37	0/4035
4	G	0.13	0/2980	0.33	0/4035
4	H	0.14	0/2980	0.36	0/4035
4	I	0.13	0/2980	0.34	0/4035
4	J	0.15	0/2956	0.35	0/4002
4	K	0.14	0/2951	0.39	0/3997
5	M	0.17	0/1080	0.44	0/1448
5	N	0.18	0/974	0.51	0/1305
5	O	0.18	0/1088	0.42	0/1459
5	P	0.21	0/974	0.60	1/1305 (0.1%)
5	Q	0.16	0/1072	0.41	0/1437
5	R	0.17	0/974	0.41	0/1305
5	S	0.17	0/1063	0.39	0/1425
5	T	0.19	0/1063	0.54	1/1425 (0.1%)
6	U	0.30	0/2007	0.47	0/2677
7	V	0.32	0/2016	0.51	0/2687
8	Y	0.18	0/2149	0.43	0/2905
9	Z	0.22	0/817	0.57	0/1099
All	All	0.17	0/61163	0.42	2/82635 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	53	GLU	CA-CB-CG	5.20	124.49	114.10
5	T	53	GLU	CA-CB-CG	5.09	124.28	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2578	0	2602	35	0
1	2	2234	0	2251	31	0
1	9	530	0	513	8	0
2	3	2639	0	2636	28	0
2	4	2041	0	2043	14	0
3	5	974	0	973	10	0
3	6	927	0	895	16	0
3	7	946	0	950	9	0
4	A	2917	0	2879	30	0
4	B	2917	0	2879	30	0
4	C	2917	0	2879	17	0
4	D	2917	0	2879	16	0
4	E	2917	0	2879	31	0
4	F	2917	0	2879	22	0
4	G	2917	0	2879	40	0
4	H	2917	0	2879	16	0
4	I	2917	0	2879	18	0
4	J	2893	0	2867	22	0
4	K	2889	0	2862	31	0
5	M	1065	0	1109	5	0
5	N	960	0	1016	6	0
5	O	1073	0	1113	11	0
5	P	960	0	1016	10	0
5	Q	1057	0	1105	7	0
5	R	960	0	1016	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1048	0	1090	11	0
5	T	1048	0	1090	12	0
6	U	2000	0	1997	22	0
7	V	2011	0	2017	22	0
8	Y	2119	0	2109	22	0
9	Z	798	0	781	8	0
10	A	27	0	12	1	0
10	B	27	0	12	1	0
10	C	27	0	12	1	0
10	D	27	0	12	0	0
10	E	27	0	12	1	0
10	F	27	0	12	0	0
10	G	27	0	12	0	0
10	H	27	0	12	1	0
10	I	27	0	12	0	0
10	J	27	0	12	0	0
10	K	27	0	12	0	0
All	All	60300	0	60094	471	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.

The worst 5 of 471 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:U:231:ASN:HA	6:U:234:MET:HE2	1.73	0.70
2:3:218:ALA:HB2	2:3:275:GLN:HG2	1.74	0.69
5:N:93:GLU:HB3	5:N:100:LEU:HD13	1.74	0.69
4:D:153:MET:HG2	4:D:162:THR:HG22	1.76	0.67
6:U:161:LEU:HD13	7:V:161:ILE:HG22	1.75	0.67

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	1	328/744 (44%)	319 (97%)	9 (3%)	0	100	100
1	2	286/744 (38%)	273 (96%)	13 (4%)	0	100	100
1	9	60/744 (8%)	57 (95%)	3 (5%)	0	100	100
2	3	334/724 (46%)	322 (96%)	12 (4%)	0	100	100
2	4	258/724 (36%)	249 (96%)	9 (4%)	0	100	100
3	5	113/405 (28%)	108 (96%)	5 (4%)	0	100	100
3	6	113/405 (28%)	106 (94%)	7 (6%)	0	100	100
3	7	110/405 (27%)	104 (94%)	6 (6%)	0	100	100
4	A	372/375 (99%)	359 (96%)	13 (4%)	0	100	100
4	B	372/375 (99%)	365 (98%)	7 (2%)	0	100	100
4	C	372/375 (99%)	364 (98%)	8 (2%)	0	100	100
4	D	372/375 (99%)	364 (98%)	8 (2%)	0	100	100
4	E	372/375 (99%)	362 (97%)	10 (3%)	0	100	100
4	F	372/375 (99%)	362 (97%)	10 (3%)	0	100	100
4	G	372/375 (99%)	368 (99%)	4 (1%)	0	100	100
4	H	372/375 (99%)	363 (98%)	9 (2%)	0	100	100
4	I	372/375 (99%)	365 (98%)	7 (2%)	0	100	100
4	J	369/375 (98%)	359 (97%)	10 (3%)	0	100	100
4	K	369/375 (98%)	359 (97%)	10 (3%)	0	100	100
5	M	128/2148 (6%)	125 (98%)	3 (2%)	0	100	100
5	N	115/2148 (5%)	113 (98%)	2 (2%)	0	100	100
5	O	129/2148 (6%)	128 (99%)	1 (1%)	0	100	100
5	P	115/2148 (5%)	111 (96%)	4 (4%)	0	100	100
5	Q	127/2148 (6%)	123 (97%)	4 (3%)	0	100	100
5	R	115/2148 (5%)	113 (98%)	2 (2%)	0	100	100
5	S	126/2148 (6%)	124 (98%)	2 (2%)	0	100	100
5	T	126/2148 (6%)	125 (99%)	1 (1%)	0	100	100
6	U	245/248 (99%)	245 (100%)	0	0	100	100
7	V	244/248 (98%)	244 (100%)	0	0	100	100
8	Y	270/359 (75%)	260 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Z	96/107 (90%)	93 (97%)	3 (3%)	0	100	100
All	All	7524/27166 (28%)	7332 (97%)	192 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	$\#\|Z\| > 2$
10	ADP	B	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.84	8 (18%)
10	ADP	F	401	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)
10	ADP	D	401	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	ADP	C	401	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
10	ADP	I	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	8 (18%)
10	ADP	A	401	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	8 (18%)
10	ADP	J	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.83	8 (18%)
10	ADP	K	401	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
10	ADP	G	401	-	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
10	ADP	H	401	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)
10	ADP	E	401	-	28,29,29	1.38	4 (14%)	43,45,45	1.84	8 (18%)

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
10	ADP	B	401	-	-	3/16/32/32	0/3/3/3
10	ADP	F	401	-	-	5/16/32/32	0/3/3/3
10	ADP	D	401	-	-	3/16/32/32	0/3/3/3
10	ADP	C	401	-	-	4/16/32/32	0/3/3/3
10	ADP	I	401	-	-	5/16/32/32	0/3/3/3
10	ADP	A	401	-	-	6/16/32/32	0/3/3/3
10	ADP	J	401	-	-	5/16/32/32	0/3/3/3
10	ADP	K	401	-	-	5/16/32/32	0/3/3/3
10	ADP	G	401	-	-	4/16/32/32	0/3/3/3
10	ADP	H	401	-	-	5/16/32/32	0/3/3/3
10	ADP	E	401	-	-	4/16/32/32	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	401	ADP	C5-C4	4.72	1.47	1.39
10	A	401	ADP	C5-C4	4.71	1.47	1.39
10	F	401	ADP	C5-C4	4.70	1.47	1.39
10	K	401	ADP	C5-C4	4.70	1.47	1.39
10	G	401	ADP	C5-C4	4.70	1.47	1.39

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	401	ADP	C5-C4-N3	-5.89	118.60	126.72
10	C	401	ADP	C5-C4-N3	-5.88	118.62	126.72
10	A	401	ADP	C5-C4-N3	-5.87	118.63	126.72
10	B	401	ADP	C5-C4-N3	-5.86	118.65	126.72
10	F	401	ADP	C5-C4-N3	-5.86	118.65	126.72

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

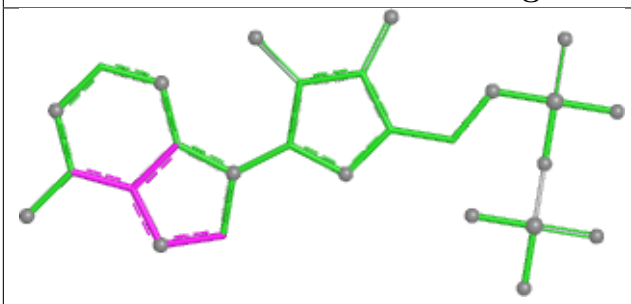
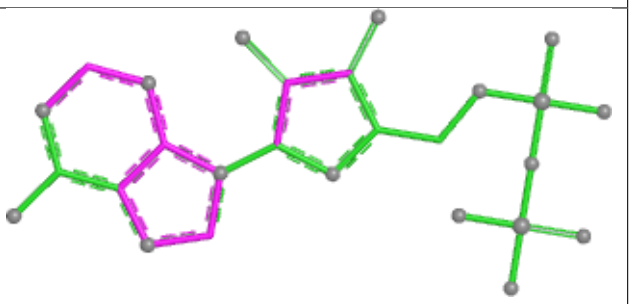
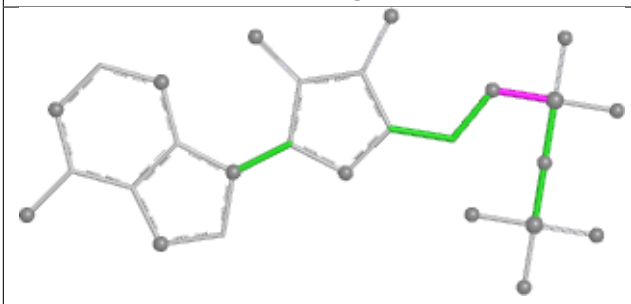
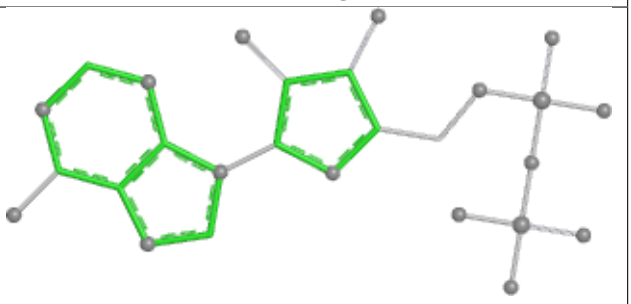
Mol	Chain	Res	Type	Atoms
10	A	401	ADP	PA-O3A-PB-O3B
10	A	401	ADP	C5'-O5'-PA-O1A
10	A	401	ADP	C5'-O5'-PA-O2A
10	A	401	ADP	C5'-O5'-PA-O3A
10	B	401	ADP	C5'-O5'-PA-O1A

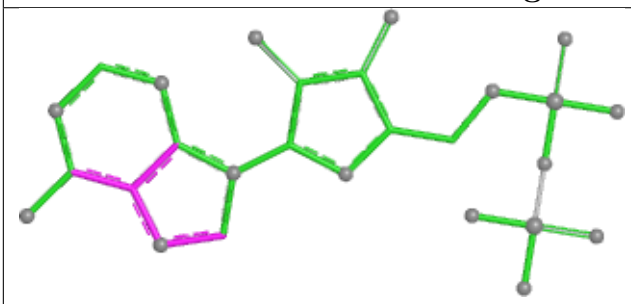
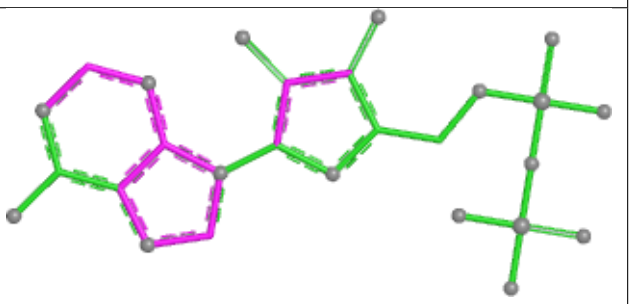
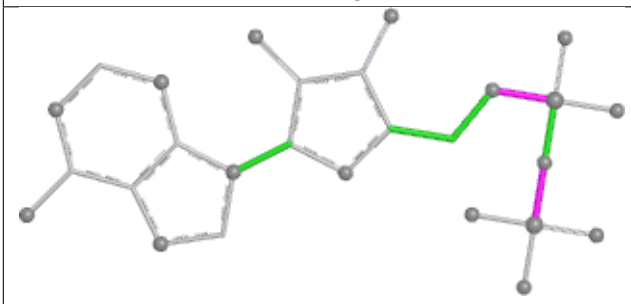
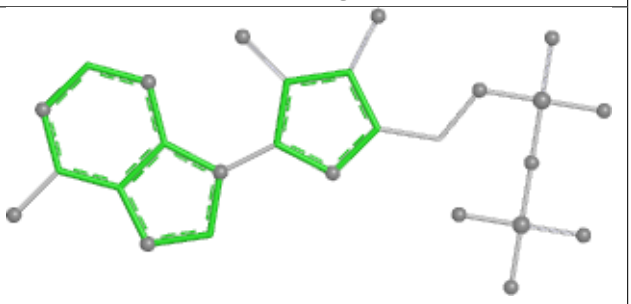
There are no ring outliers.

5 monomers are involved in 5 short contacts:

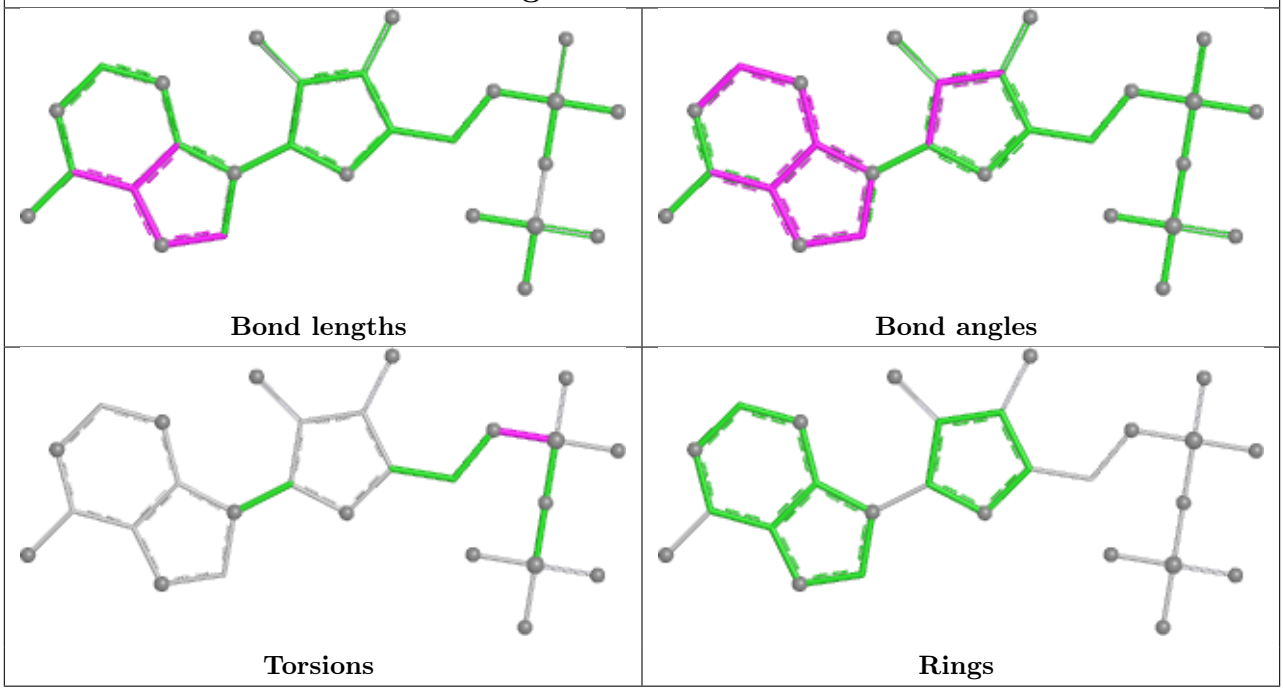
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	401	ADP	1	0
10	C	401	ADP	1	0
10	A	401	ADP	1	0
10	H	401	ADP	1	0
10	E	401	ADP	1	0

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 B 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP F 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 401



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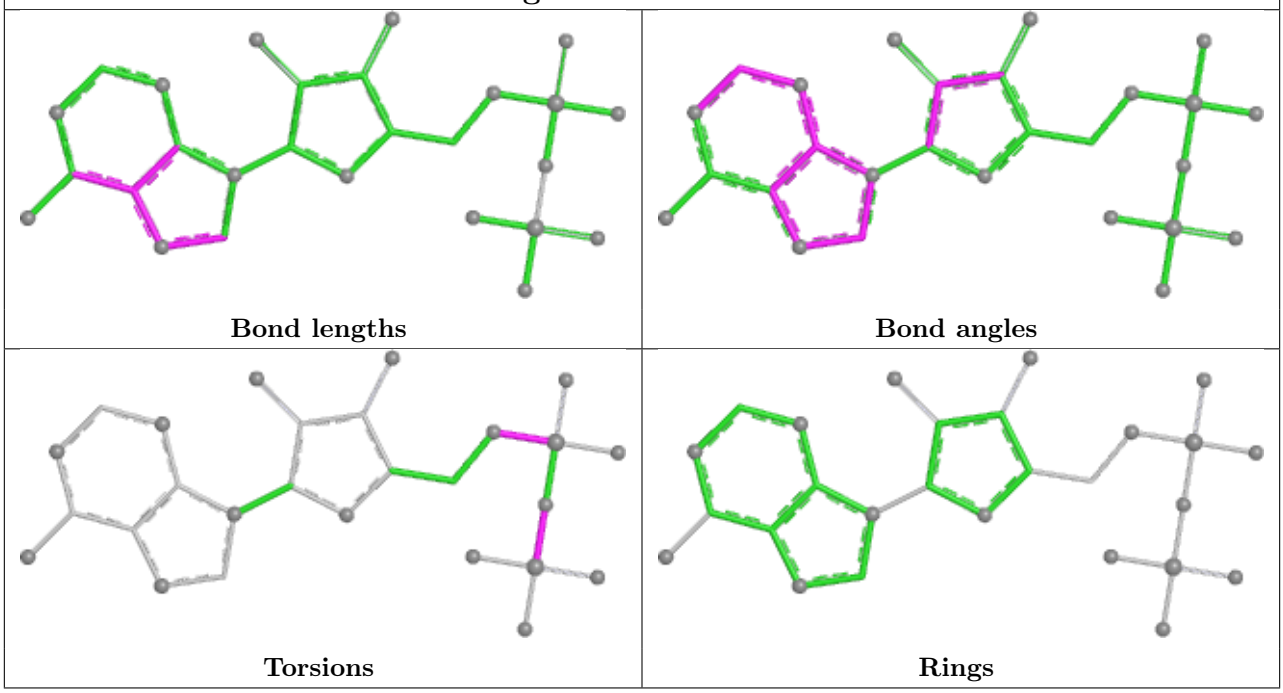
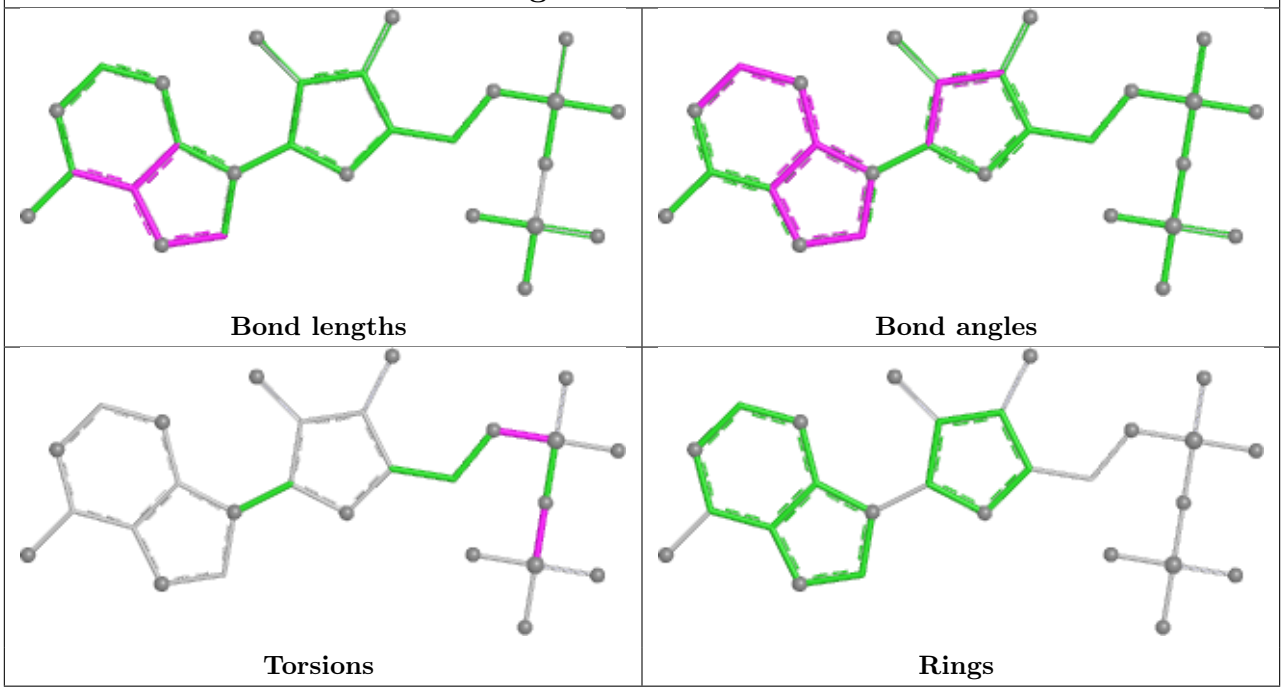


Ligand ADP I 401



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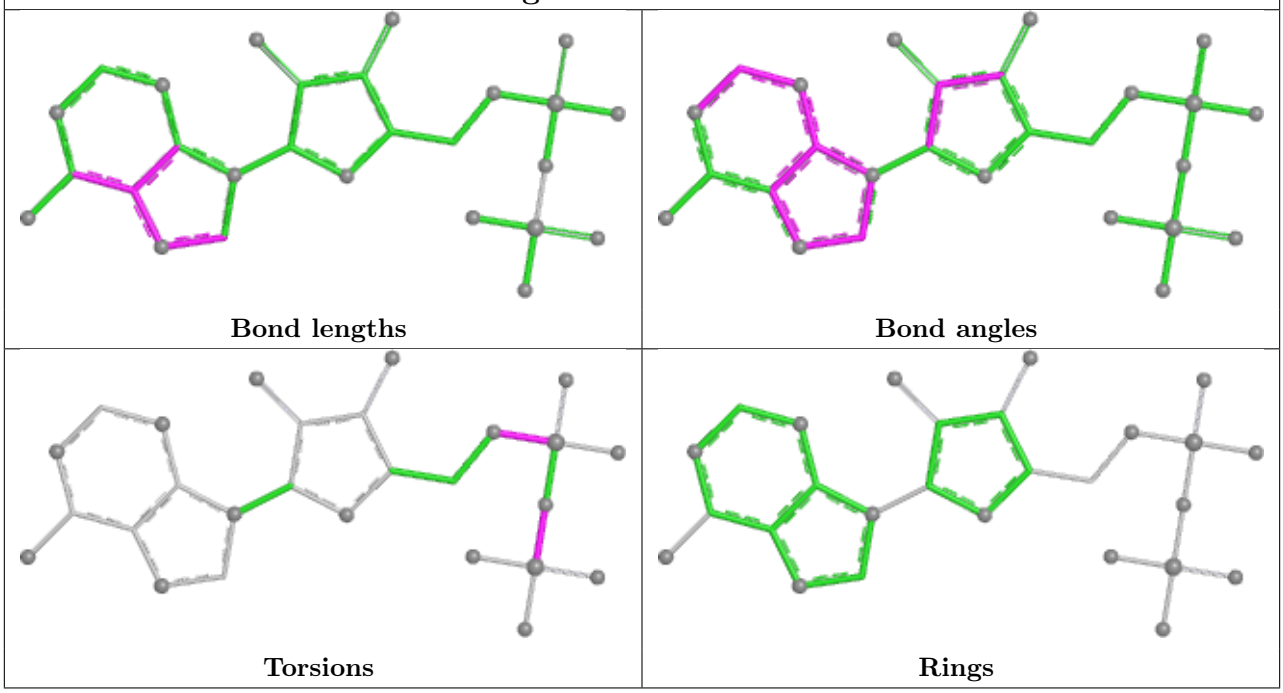
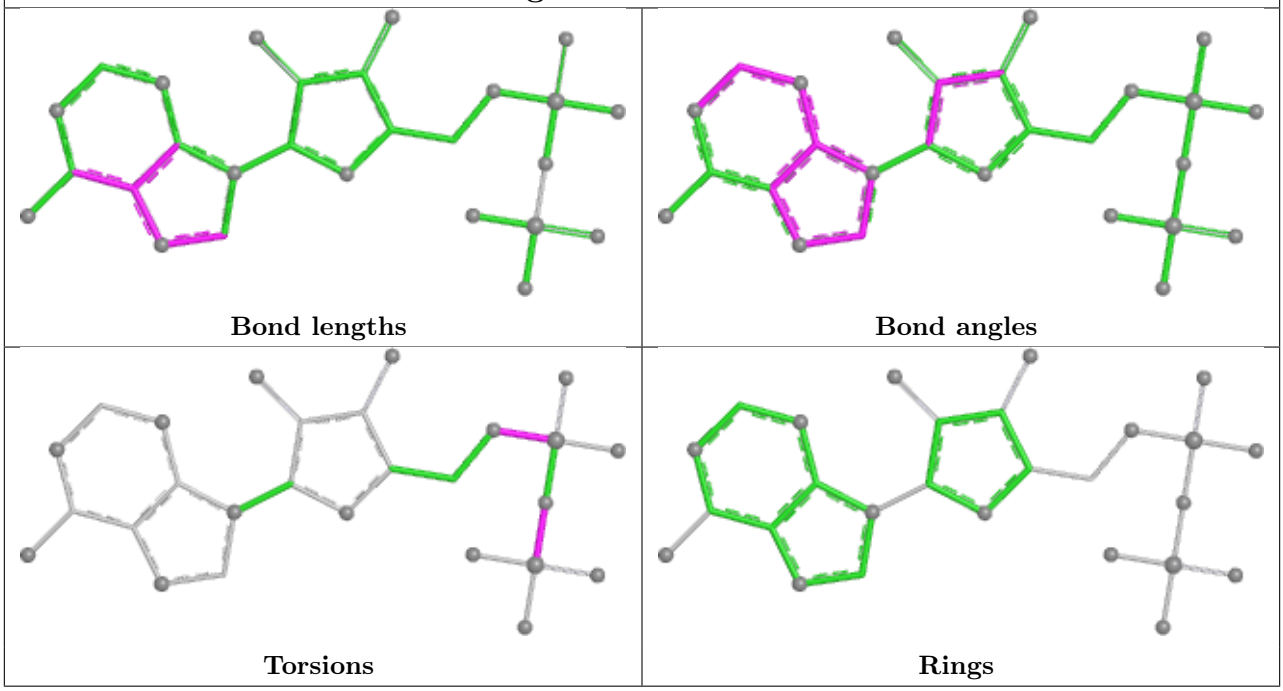
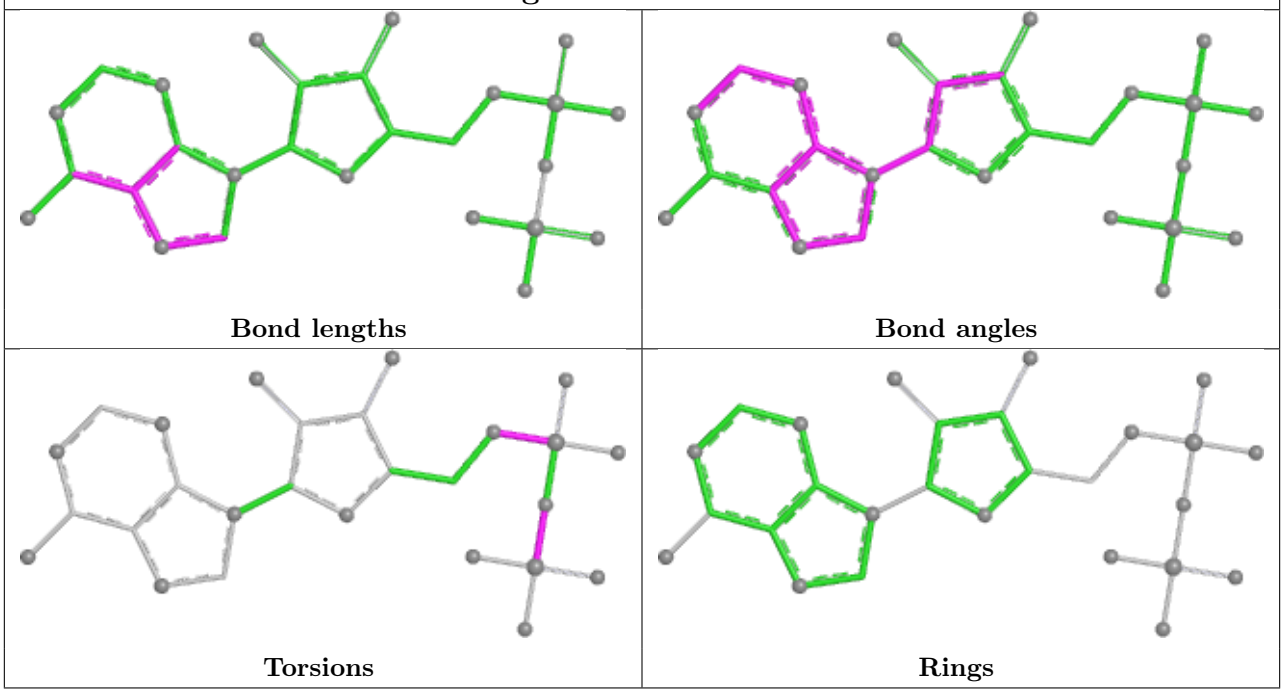


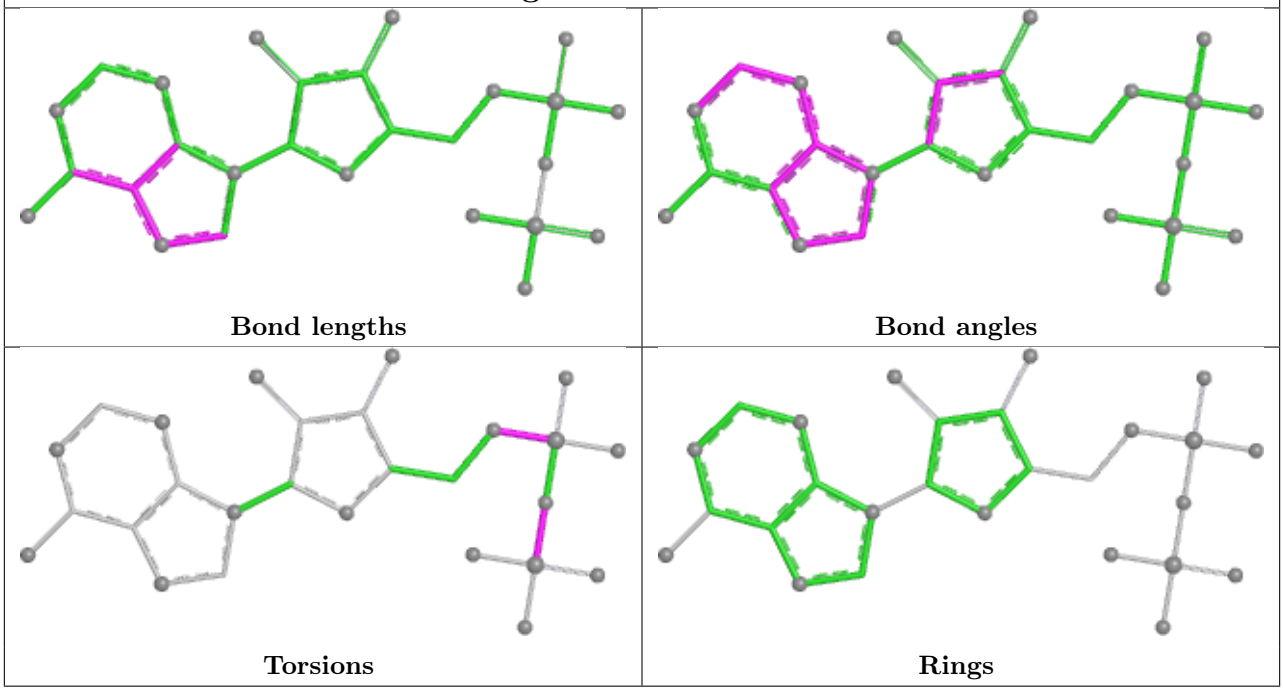
Ligand ADP J 401



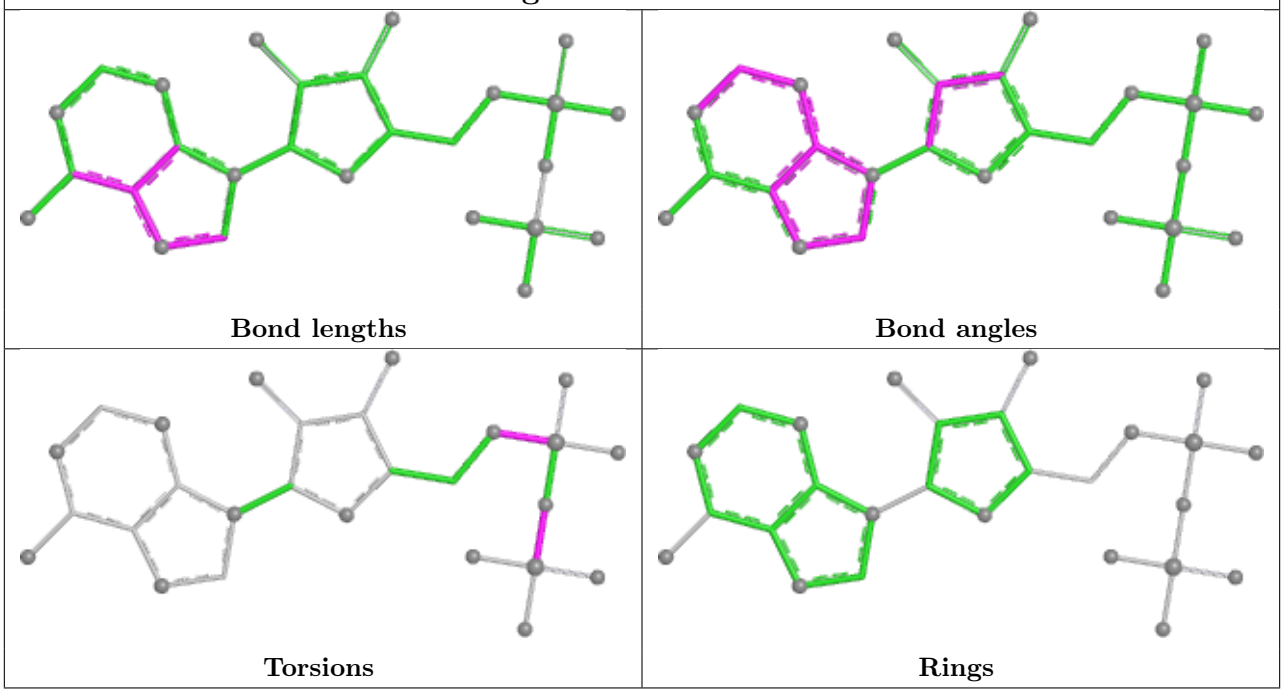
Ligand ADP K 401

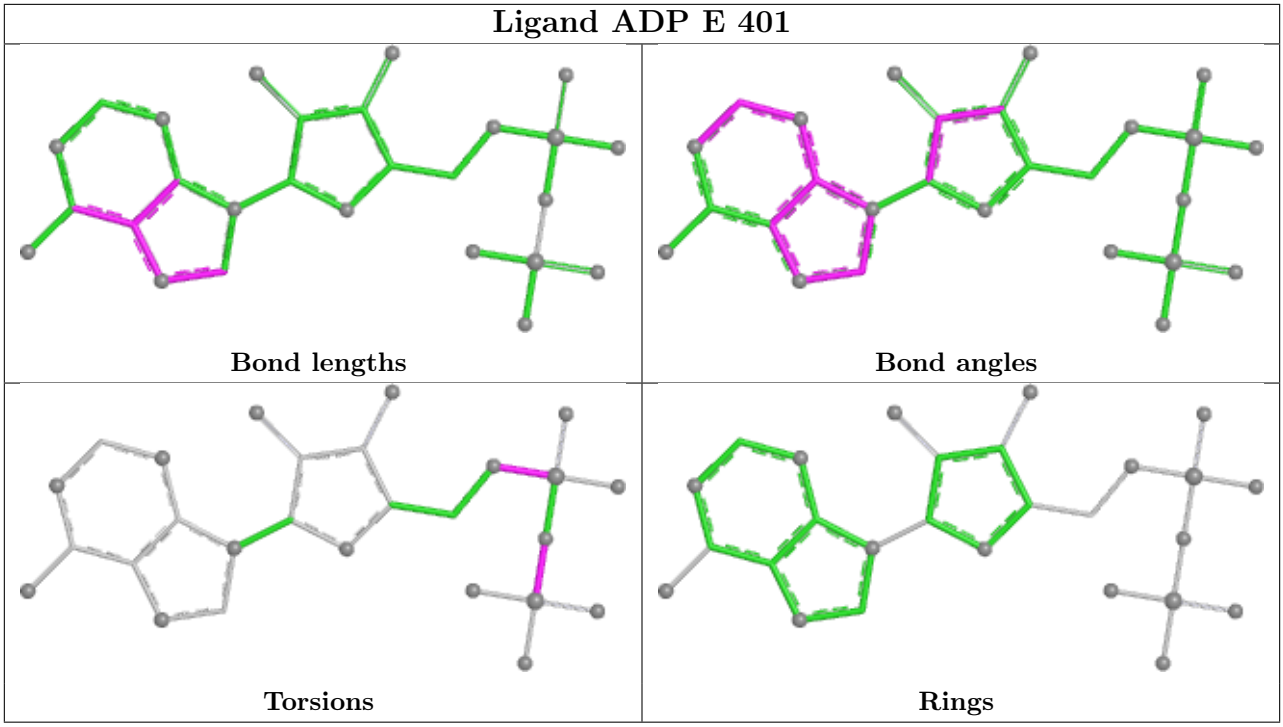


Ligand ADP G 401



Ligand ADP H 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.

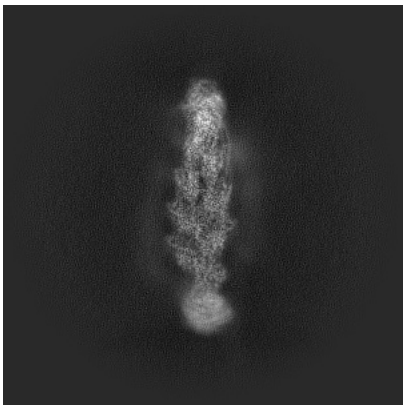
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35302. These allow visual inspection of the internal detail of the map and identification of artifacts.

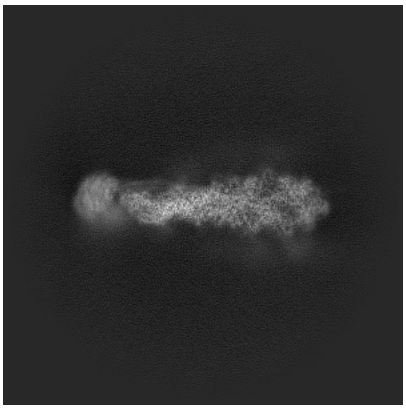
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

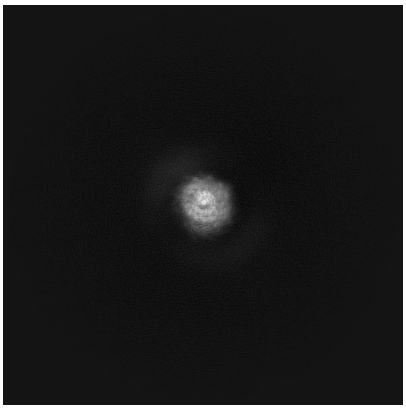
6.1.1 Primary map



X

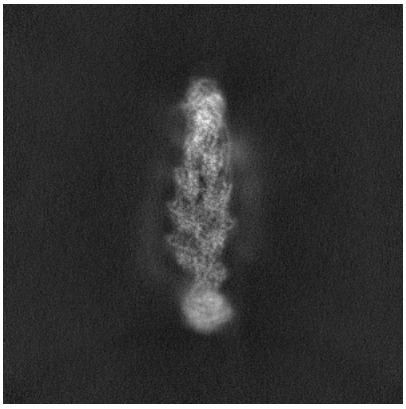


Y

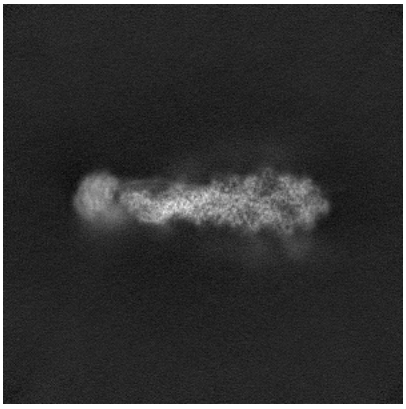


Z

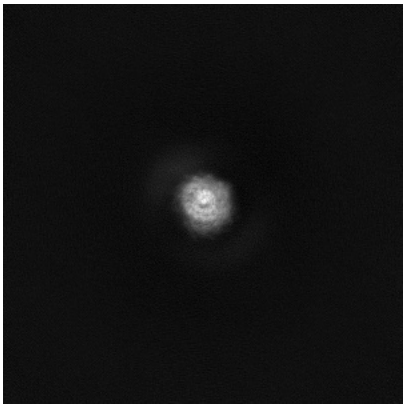
6.1.2 Raw map



X



Y

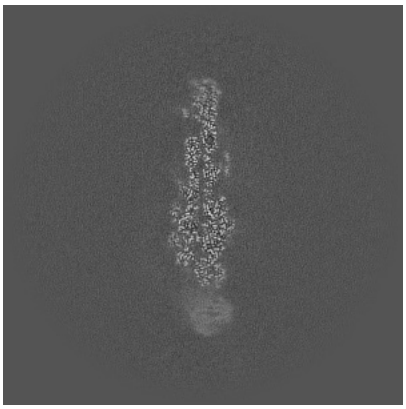


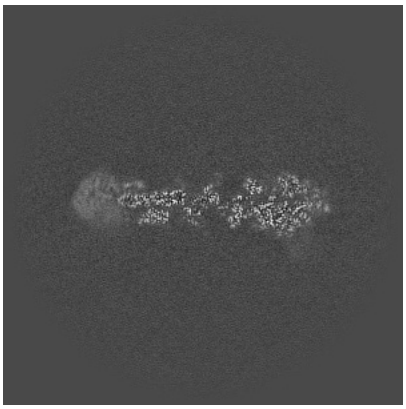
Z

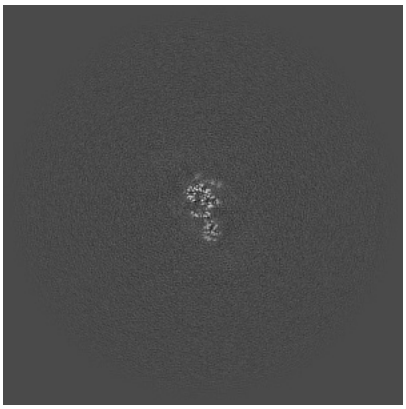
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

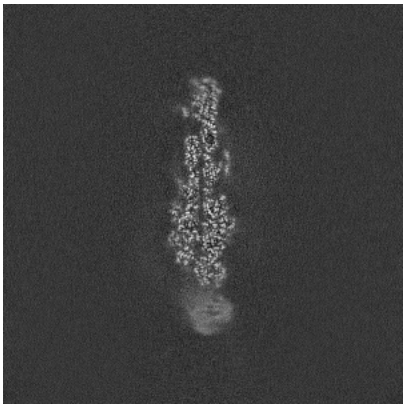
6.2.1 Primary map

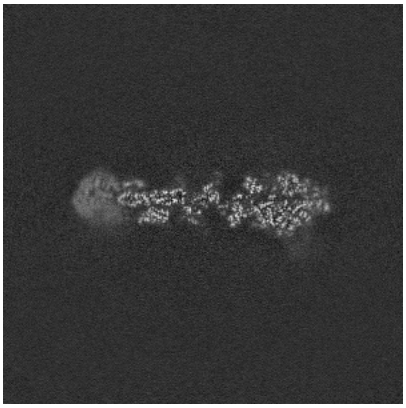

X Index: 240


Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240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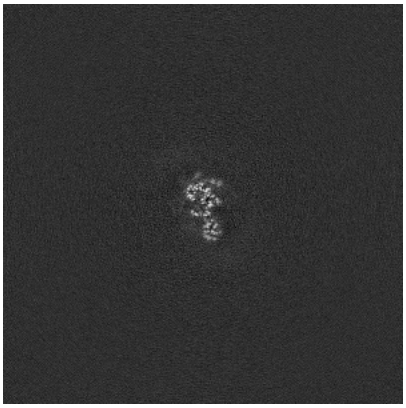
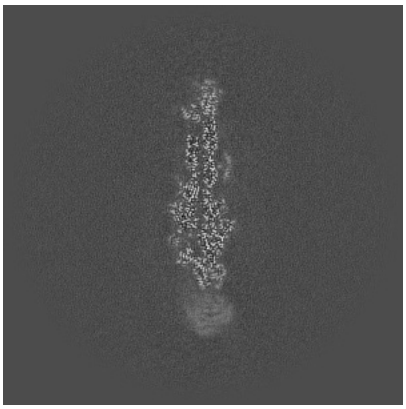
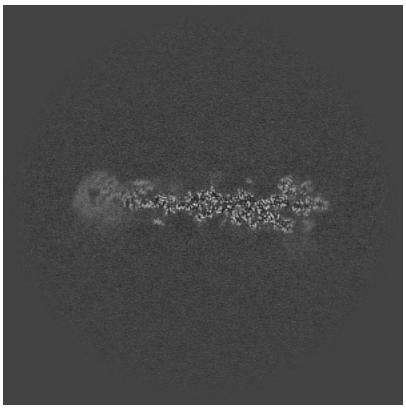

Z Index: 240

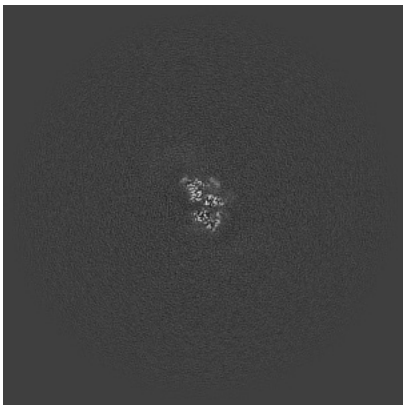
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

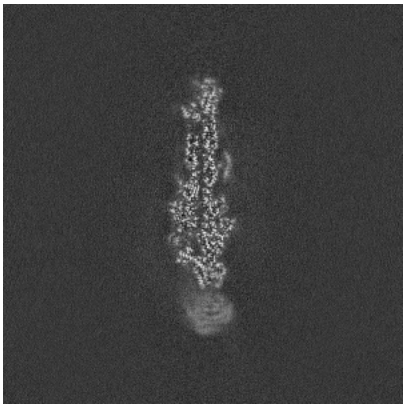
6.3.1 Primary map

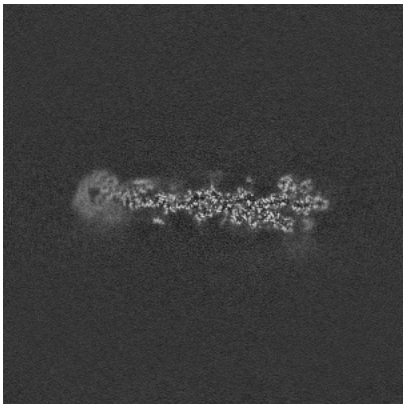

X Index: 242

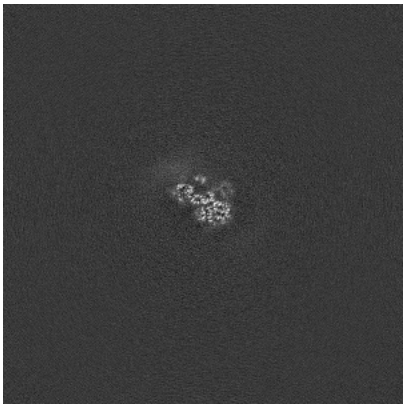

Y Index: 247


Z Index: 249

6.3.2 Raw map


X Index: 242

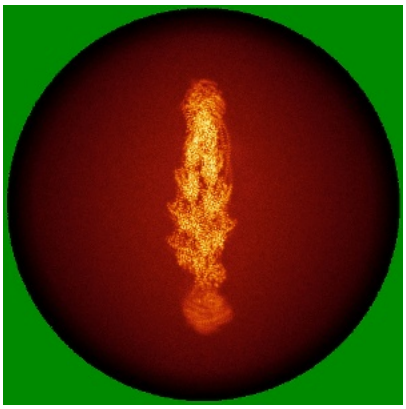

Y Index: 247

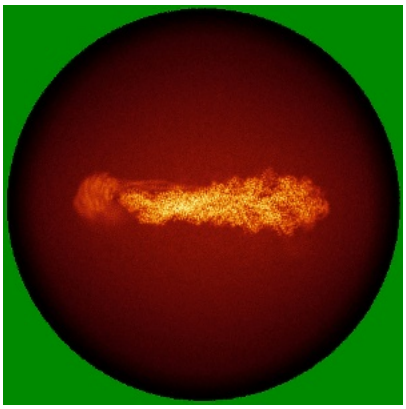

Z Index: 298

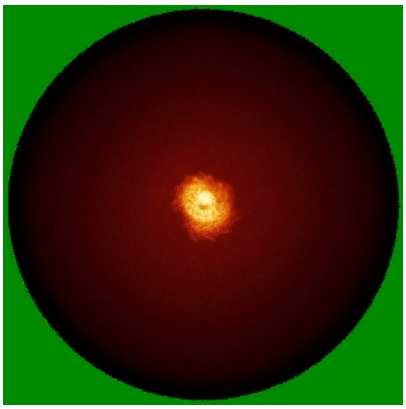
The images above show the largest variance slices of the map in three orthogonal directions.

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

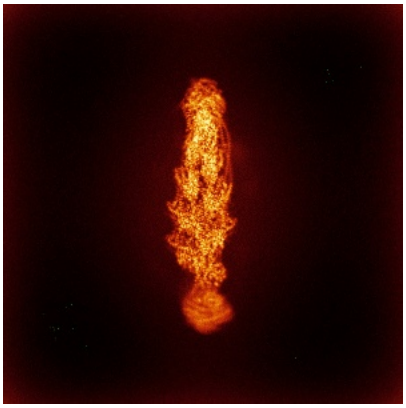
6.4.1 Primary map

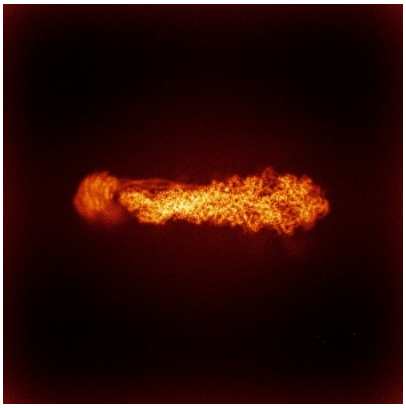

X

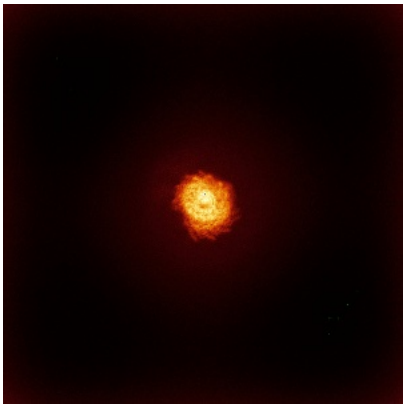

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

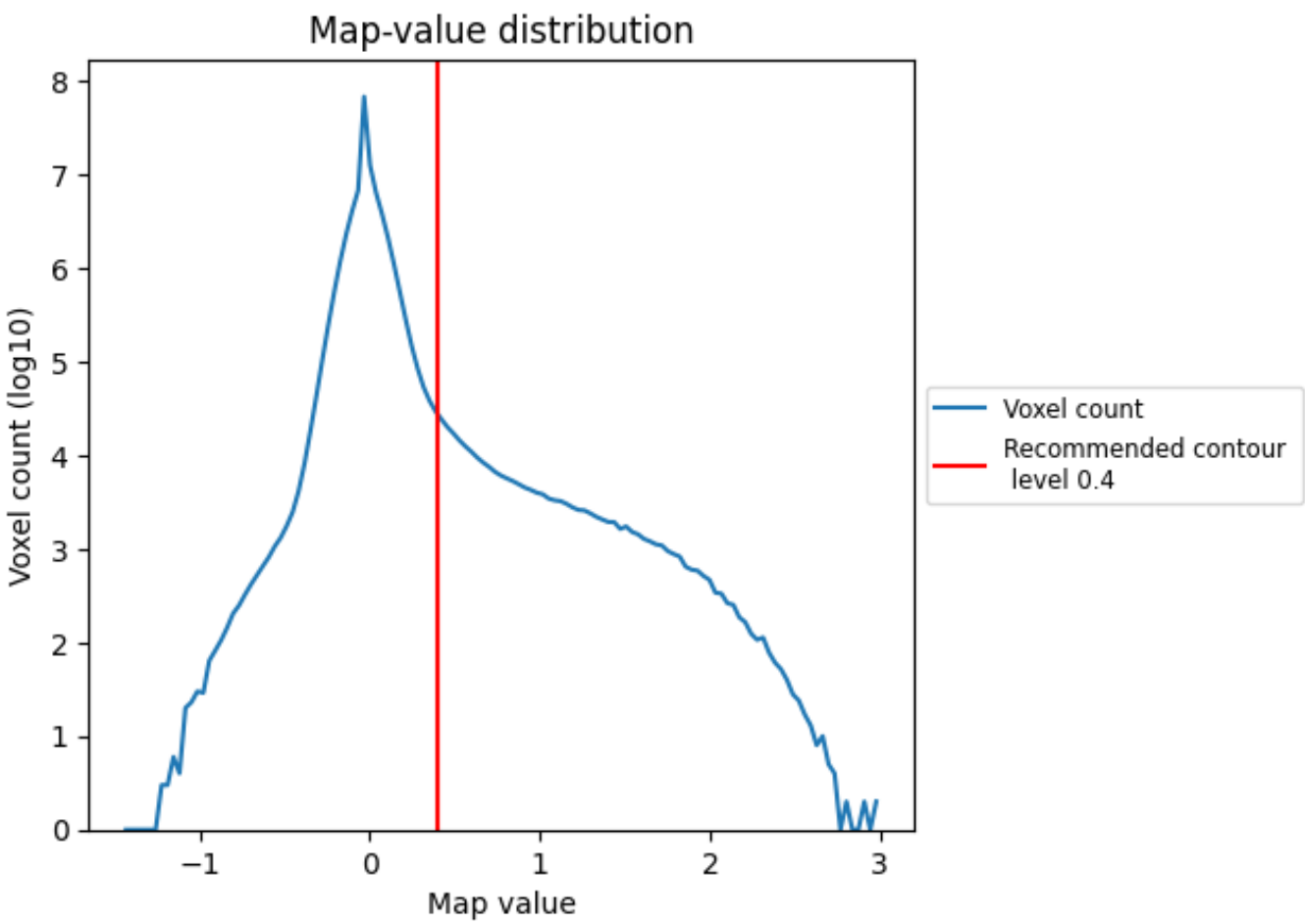
6.6 Mask visualisation (i)

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

7 Map analysis (i)

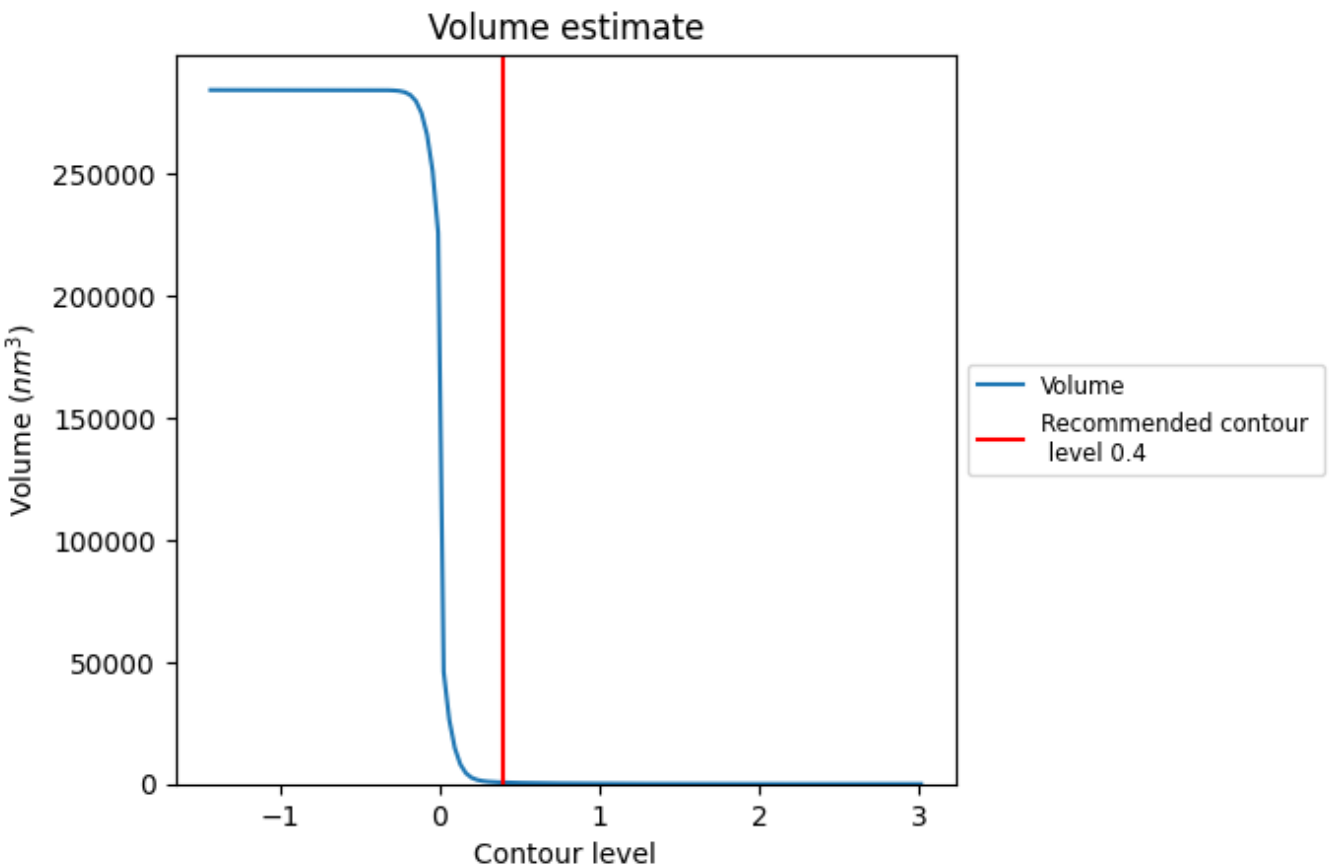
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

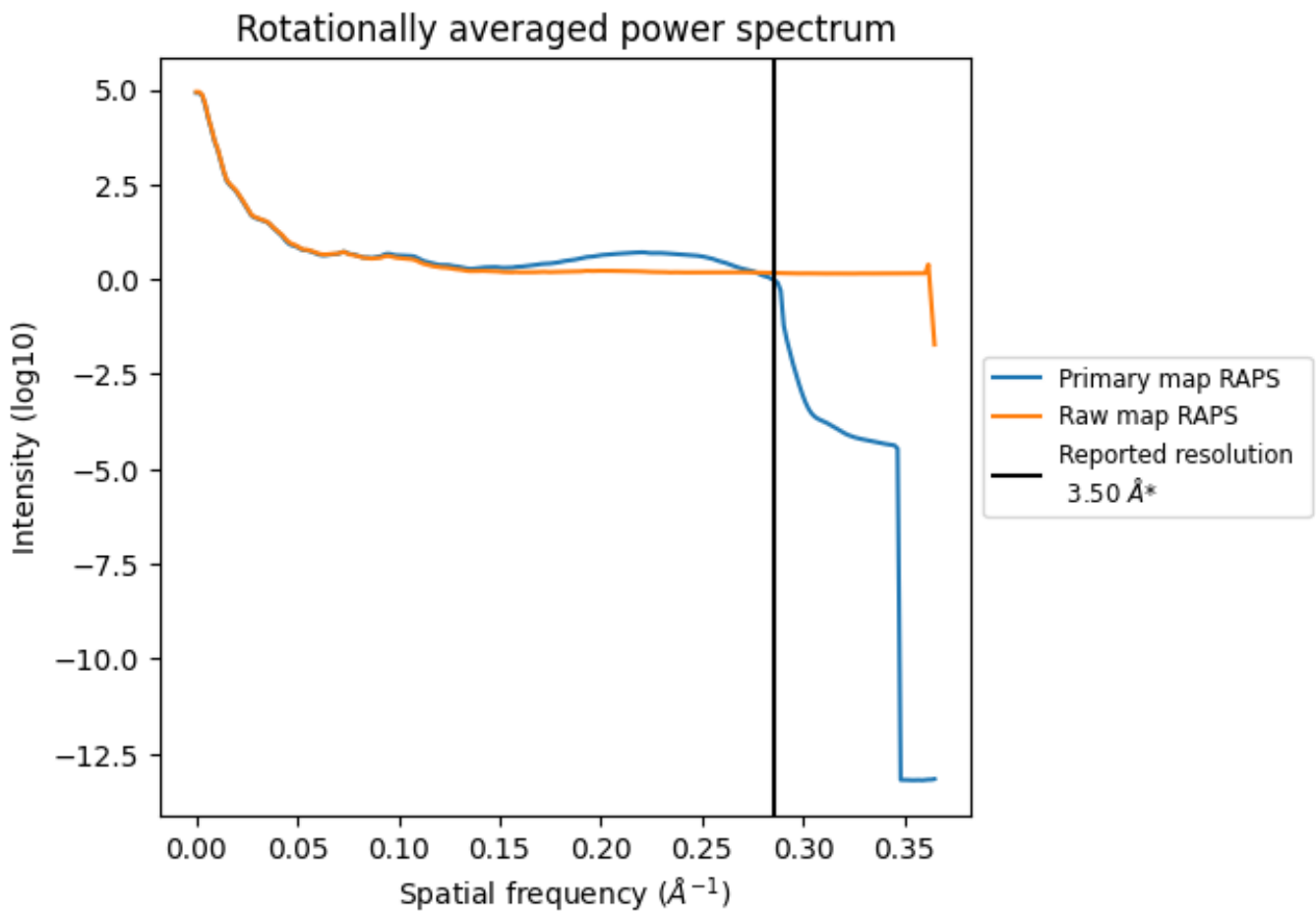
7.2 Volume estimate (i)



The volume at the recommended contour level is 611 nm^3; this corresponds to an approximate mass of 552 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)

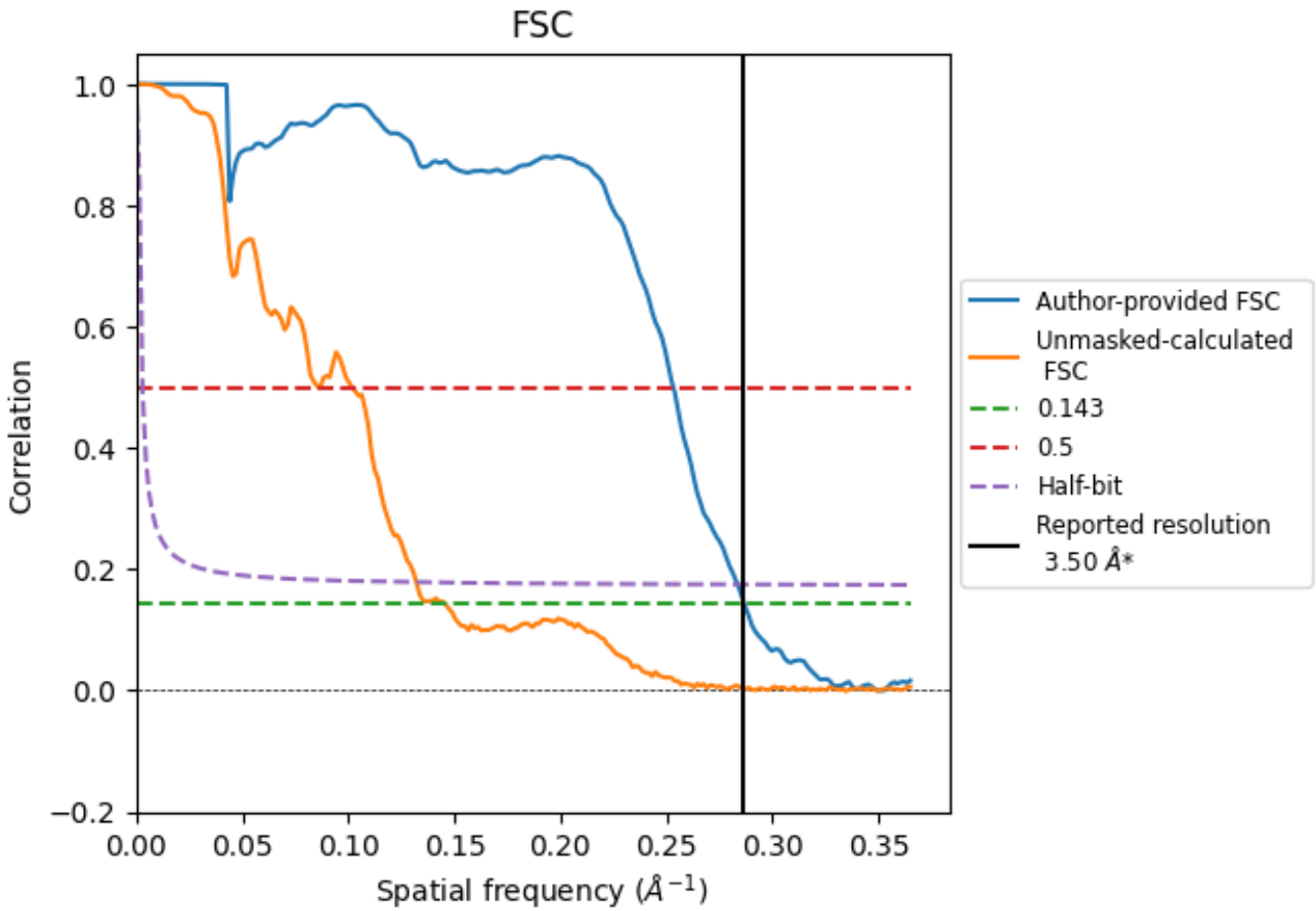


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	3.95	3.53
Unmasked-calculated*	6.87	11.63	7.57

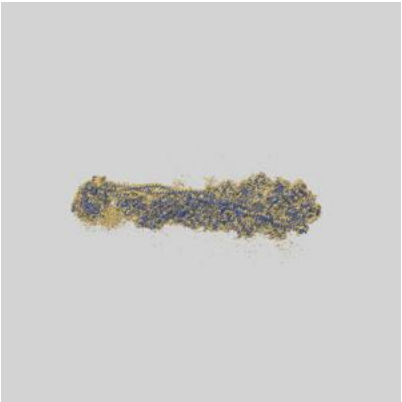
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.87 differs from the reported value 3.5 by more than 10 %

9 Map-model fit (i)

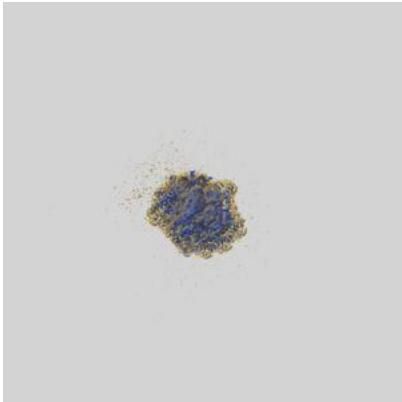
This section contains information regarding the fit between EMDB map EMD-35302 and PDB model 8IAI. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)

X



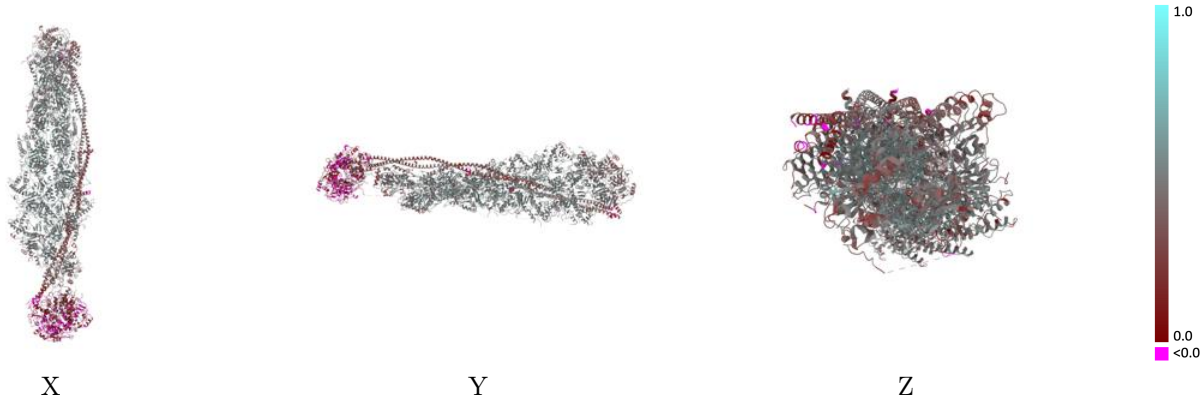
Y



Z

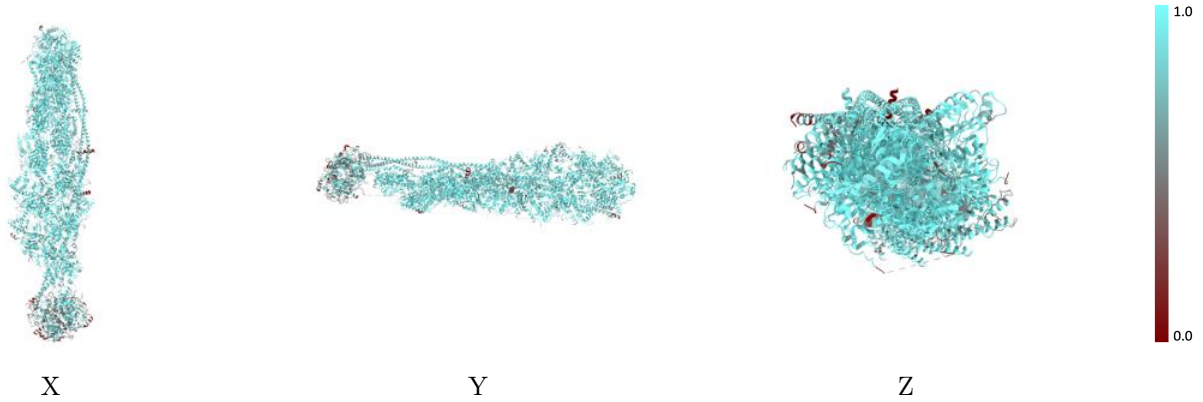
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



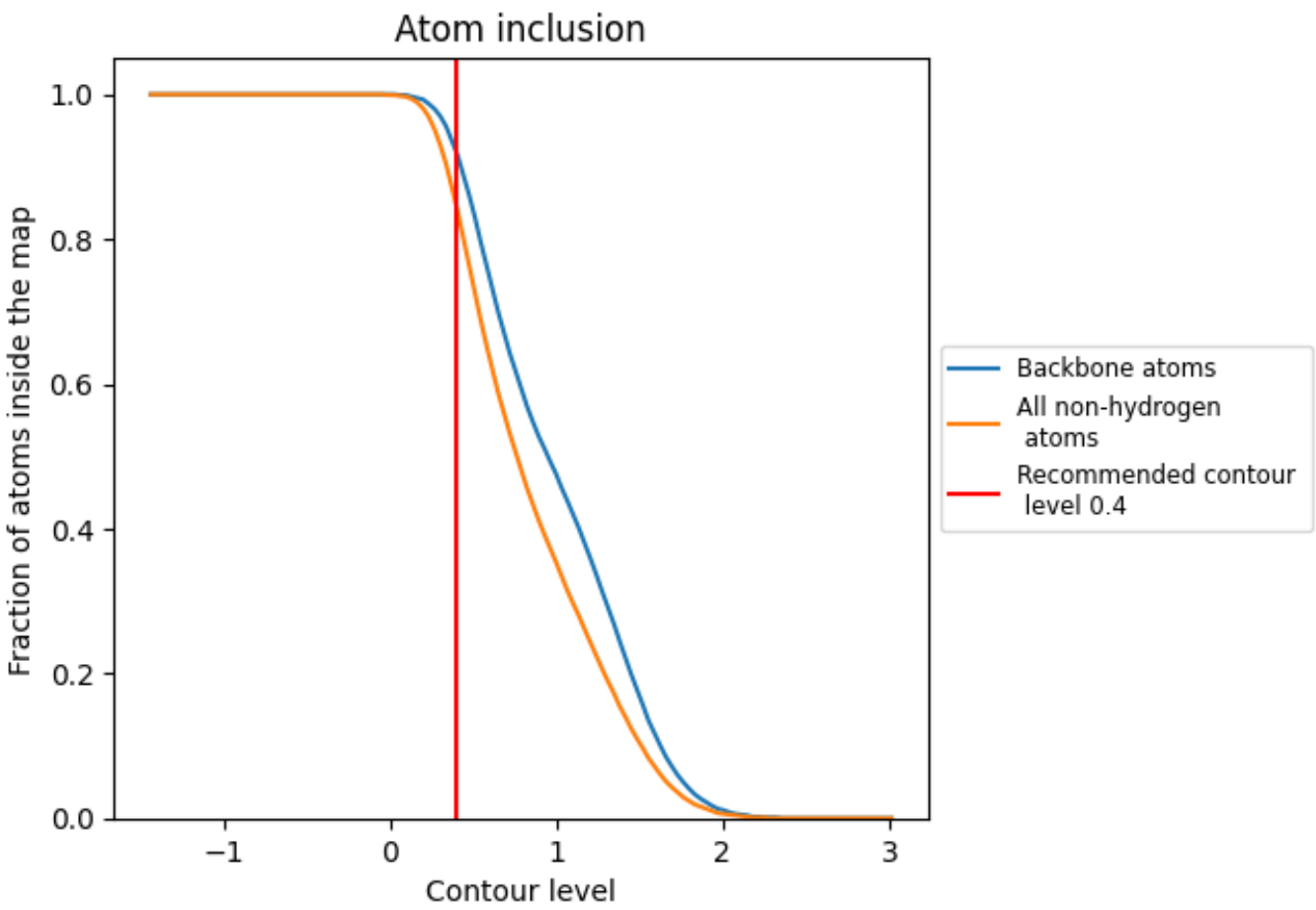
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

Chain	Atom inclusion	Q-score
All	0.8460	0.4110
1	0.7230	0.2240
2	0.5850	0.0740
3	0.5790	0.1360
4	0.5950	0.1000
5	0.7280	0.4080
6	0.5690	0.3750
7	0.6410	0.3880
9	0.7350	0.2980
A	0.9090	0.4370
B	0.9320	0.4840
C	0.9420	0.5100
D	0.9410	0.5100
E	0.9430	0.5180
F	0.9380	0.5130
G	0.9480	0.5210
H	0.9340	0.5120
I	0.9470	0.5130
J	0.9350	0.4900
K	0.9170	0.4540
M	0.9110	0.4610
N	0.7830	0.4440
O	0.9140	0.4890
P	0.9130	0.4710
Q	0.9210	0.4860
R	0.9230	0.4740
S	0.9160	0.4770
T	0.8640	0.4470
U	0.7660	0.3230
V	0.7360	0.3040
Y	0.8190	0.3670
Z	0.7240	0.3690