wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:03 PM BST

PDB ID	:	4UUD
EMDB ID:	:	EMD-2701
Title	:	Human dynamin 1 K44A superconstricted polymer stabilized with GTP
Authors	:	Sundborger, A.C.; Fang, S.; Heymann, J.A.; Ray, P.; Chappie, J.S.; Hinshaw, J.E.
Deposited on	:	2014-07-25
Resolution	:	12.50 Å(reported)
Based on PDB ID	:	3ZYC,3SNH,1DYN

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

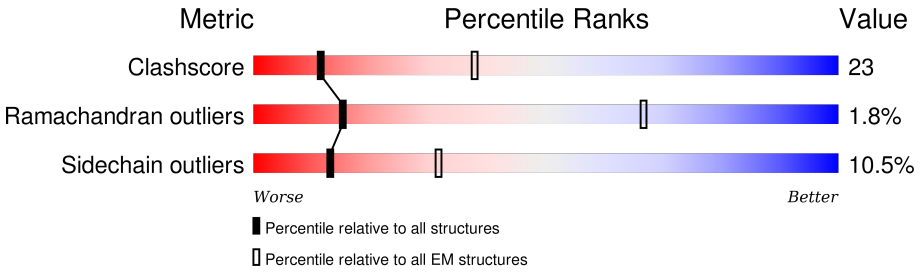
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 12.50 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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	864	24% 13% 62%
1	D	864	25% 11% 61%
1	G	864	24% 13% 62%
1	K	864	25% 11% 61%
2	B	864	9% 9% 76%
2	C	864	7% 87%
2	E	864	7% 10% 76%
2	F	864	7% 87%
2	H	864	7% 87%

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Mol	Chain	Length	Quality of chain
2	I	864	8% 10% 76%
2	J	864	7% 10% 76%
2	L	864	7% 87%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20992 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 DYNAMIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	329	Total 2567	C 1615	N 453	O 489	S 10	0	0
1	D	337	Total 2643	C 1664	N 466	O 503	S 10	0	0
1	G	329	Total 2567	C 1615	N 453	O 489	S 10	0	0
1	K	337	Total 2643	C 1664	N 466	O 503	S 10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	744	ASN	ASP	VARIANT	UNP Q05193
D	744	ASN	ASP	VARIANT	UNP Q05193
G	744	ASN	ASP	VARIANT	UNP Q05193
K	744	ASN	ASP	VARIANT	UNP Q05193

- Molecule 2 is a protein called DYNAMIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	204	Total 1697	C 1079	N 297	O 307	S 14	0	0
2	C	113	Total 946	C 609	N 158	O 175	S 4	0	0
2	E	204	Total 1697	C 1079	N 297	O 307	S 14	0	0
2	F	113	Total 946	C 609	N 158	O 175	S 4	0	0
2	H	113	Total 946	C 609	N 158	O 175	S 4	0	0
2	I	204	Total 1697	C 1079	N 297	O 307	S 14	0	0
2	J	204	Total 1697	C 1079	N 297	O 307	S 14	0	0

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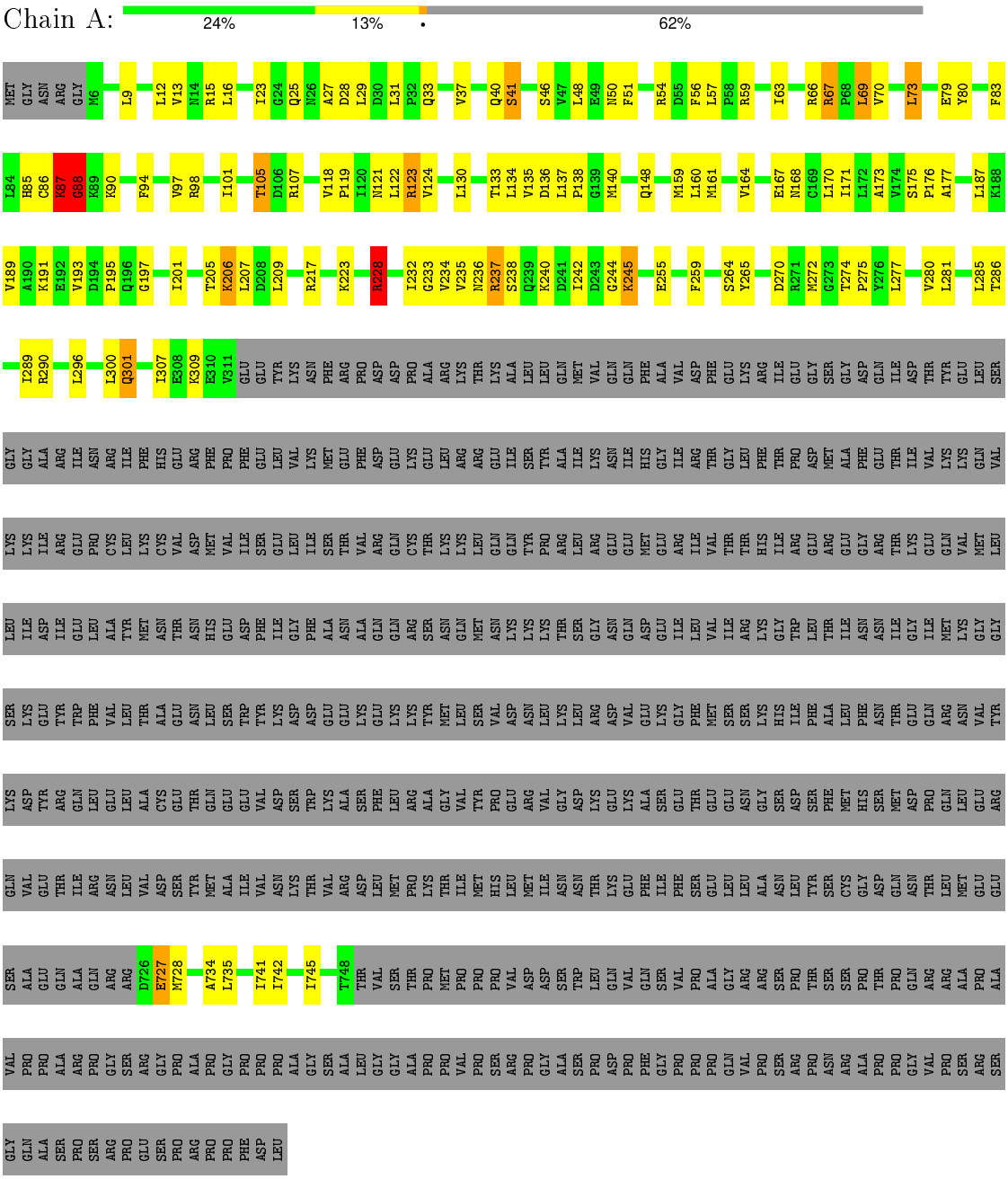
Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	113	Total	C	N	O	S	0	0
			946	609	158	175	4		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

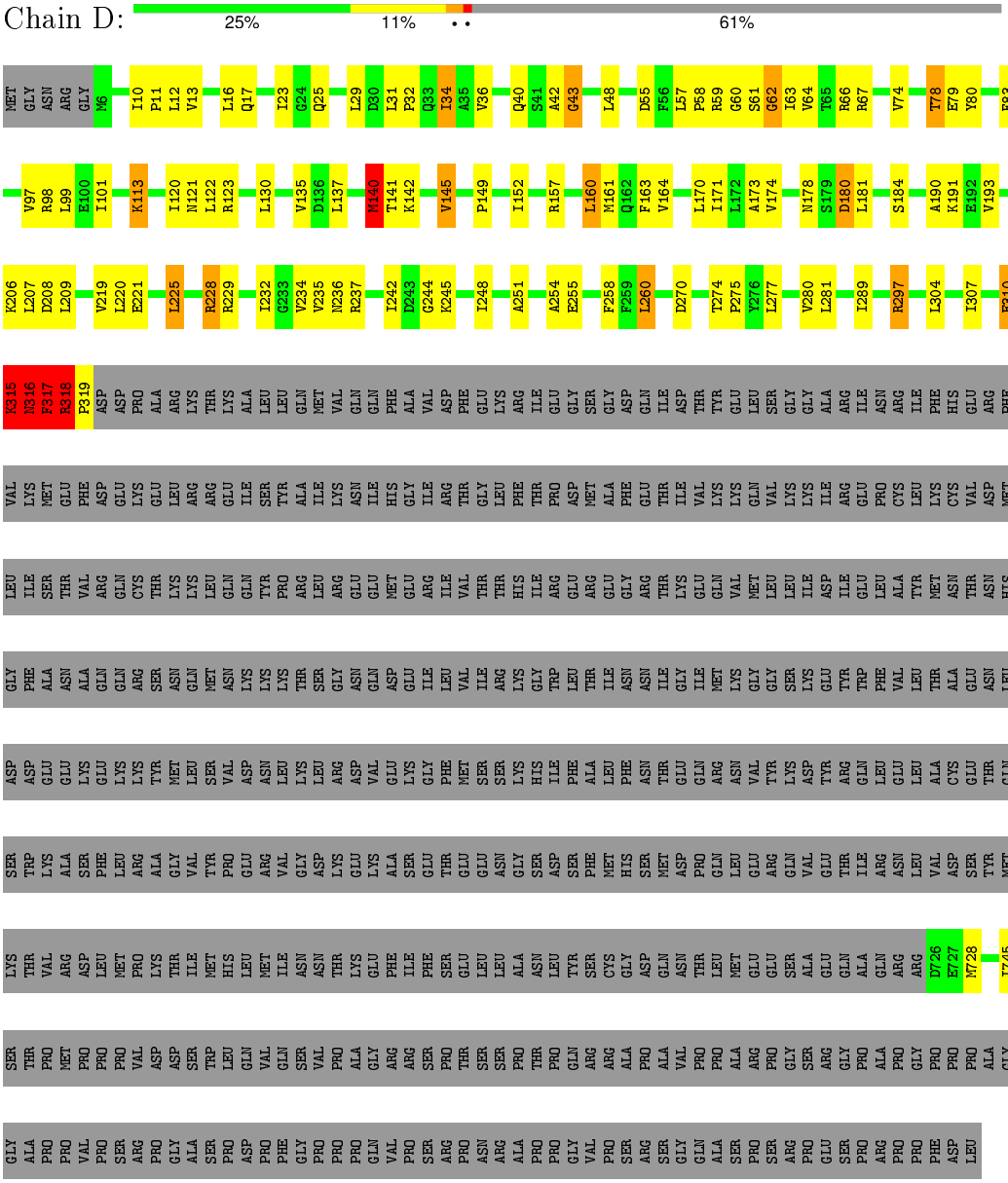
- Molecule 1: DYNAMIN-1

Chain A:



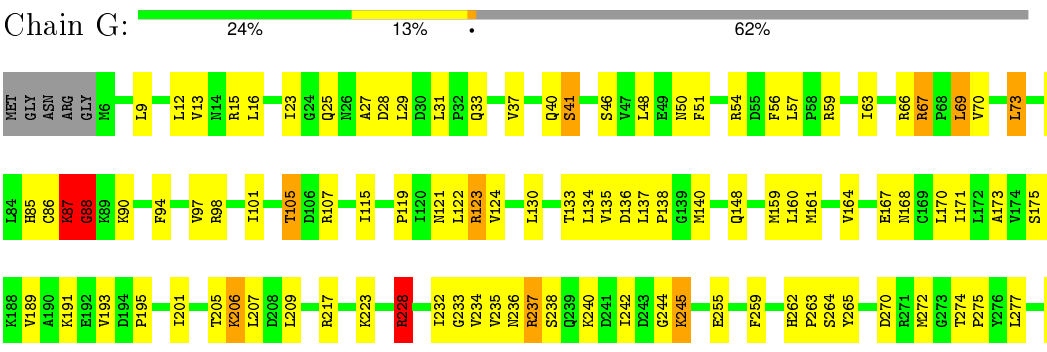
- Molecule 1: DYNAMIN-1

Chain D:



- Molecule 1: DYNAMIN-1

Chain G:



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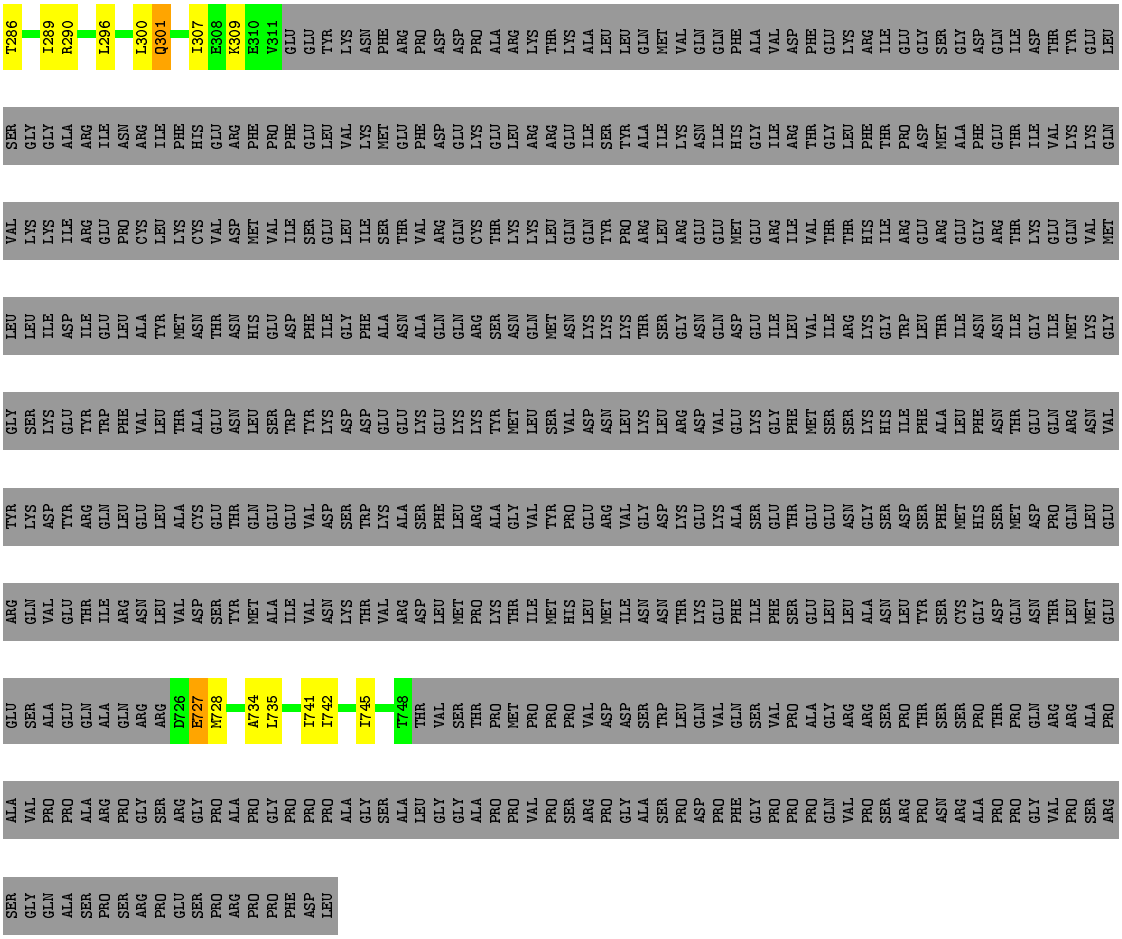
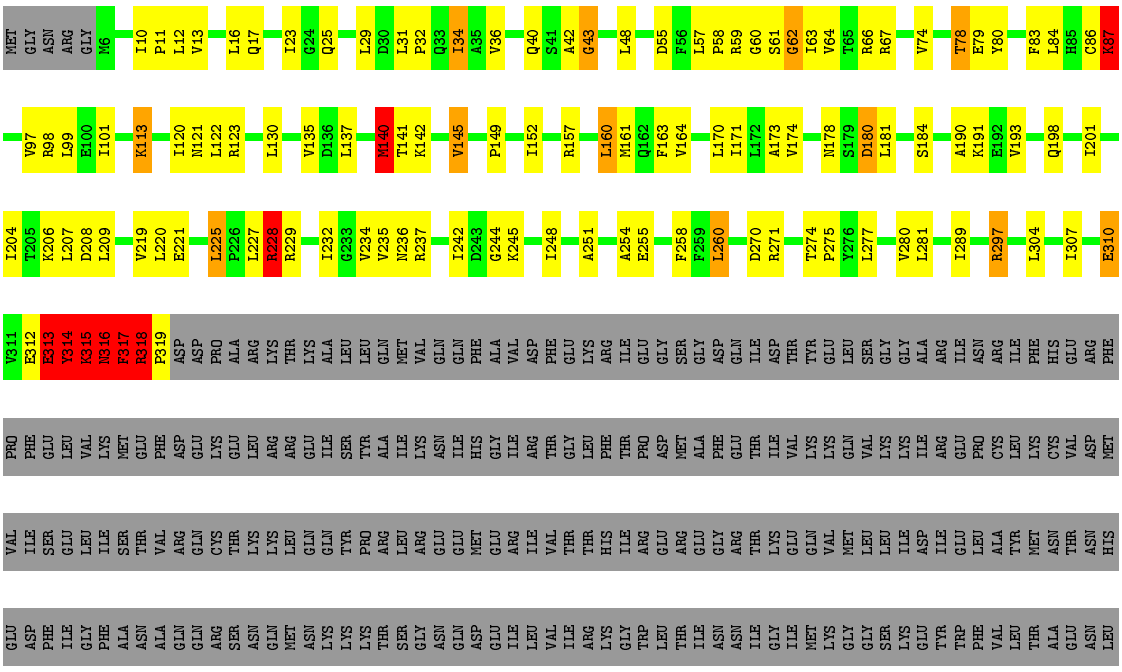
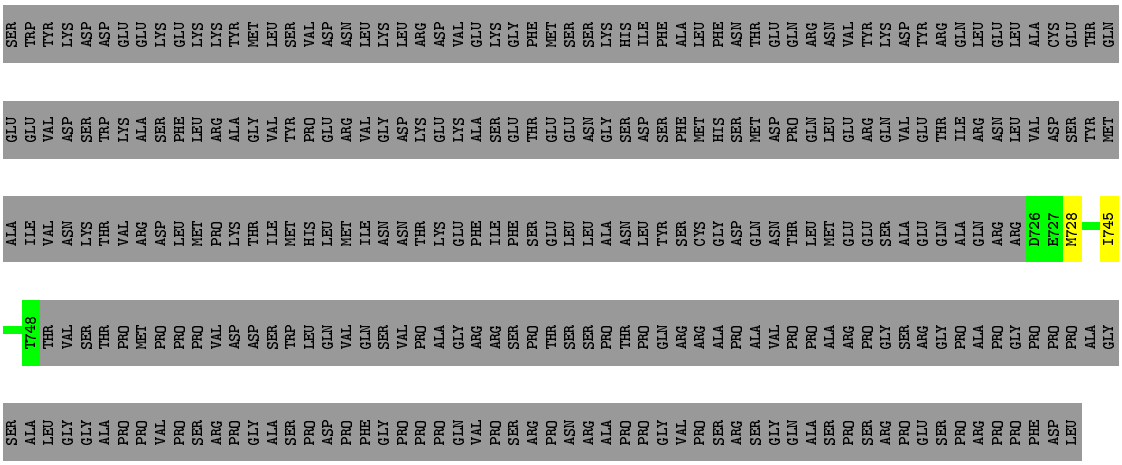


- Molecule 1: DYNAMIN-1

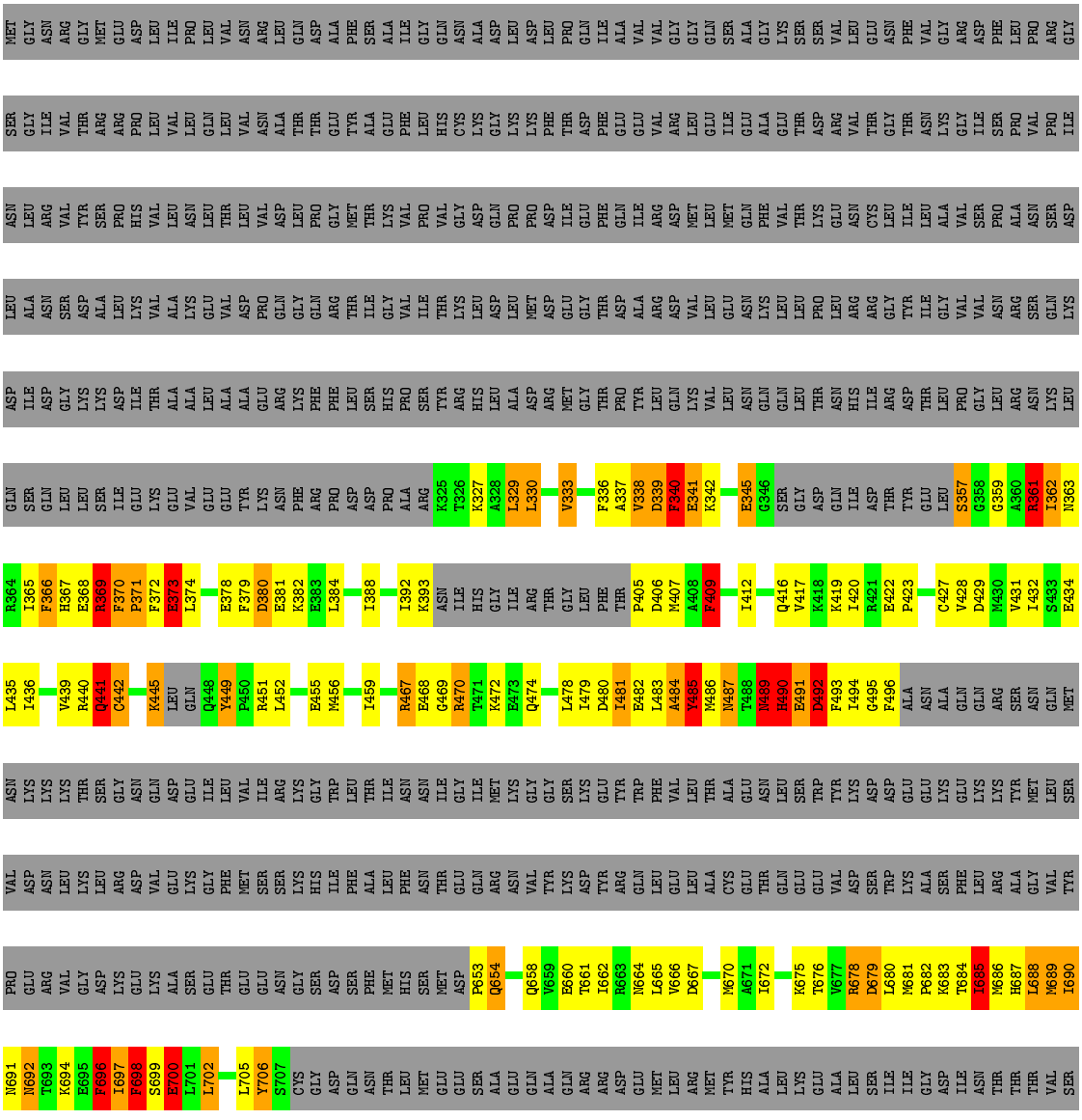
Chain K:

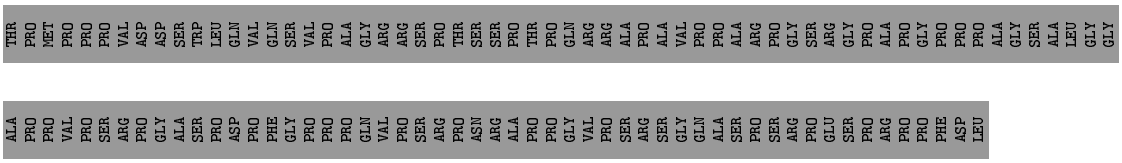




- Molecule 2: DYNAMIN-1

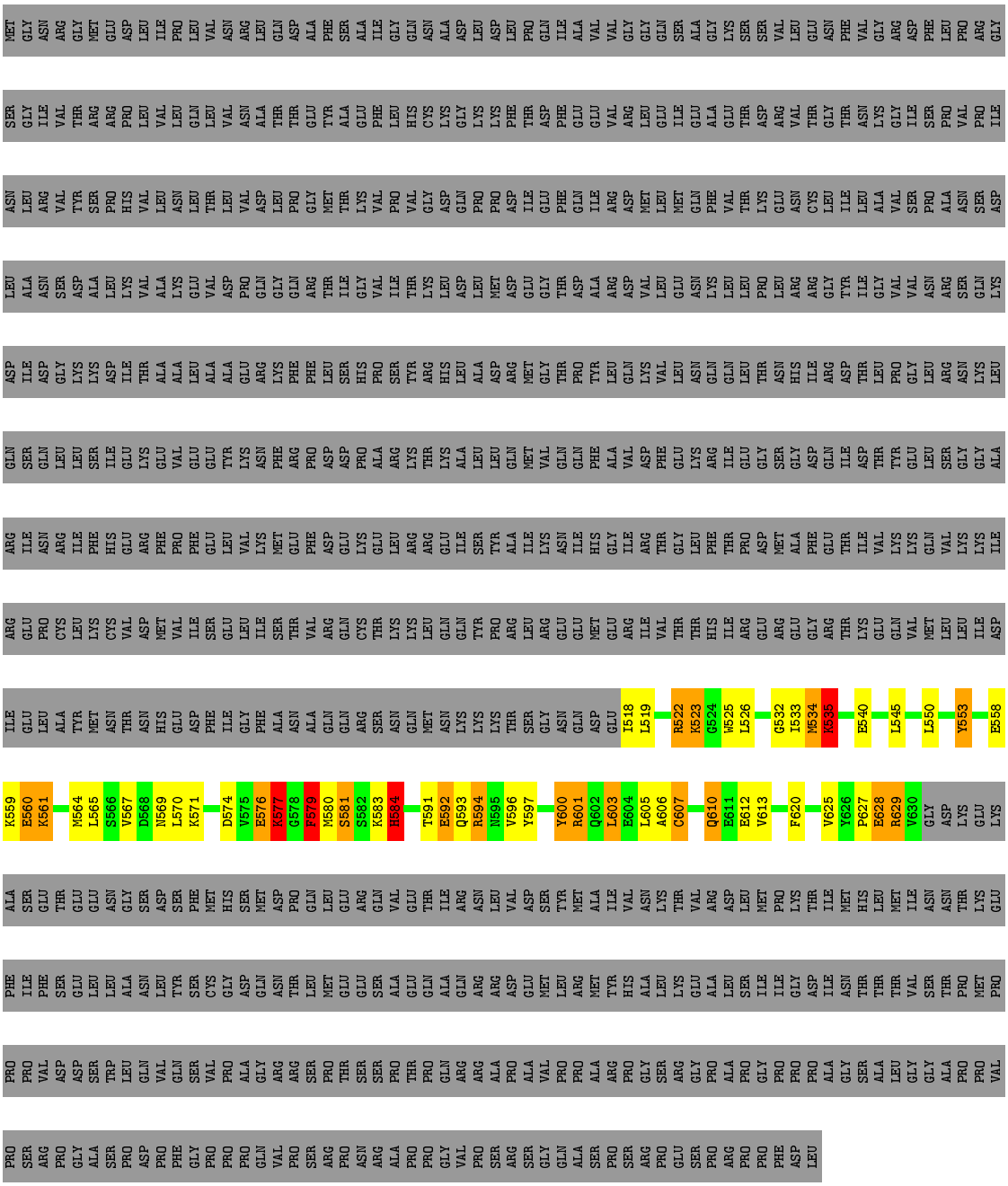
Chain B:





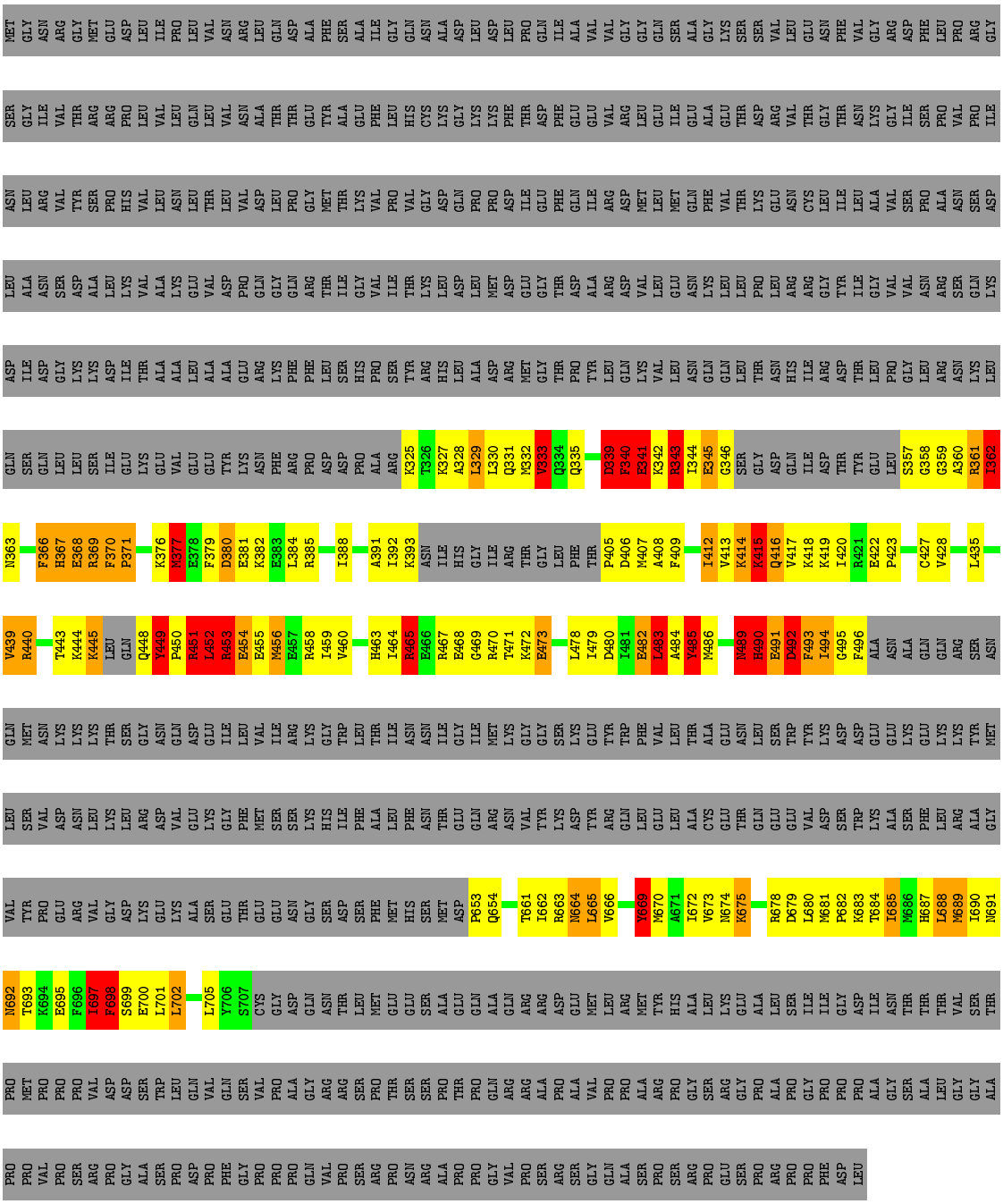
- Molecule 2: DYNAMIN-1

Chain C: 7% 87%



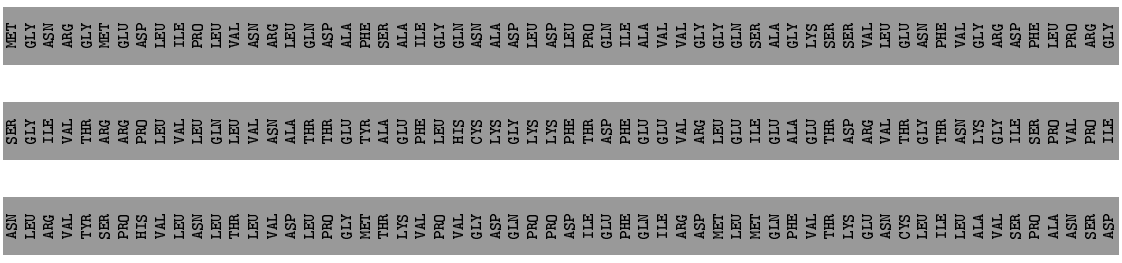
- Molecule 2: DYNAMIN-1

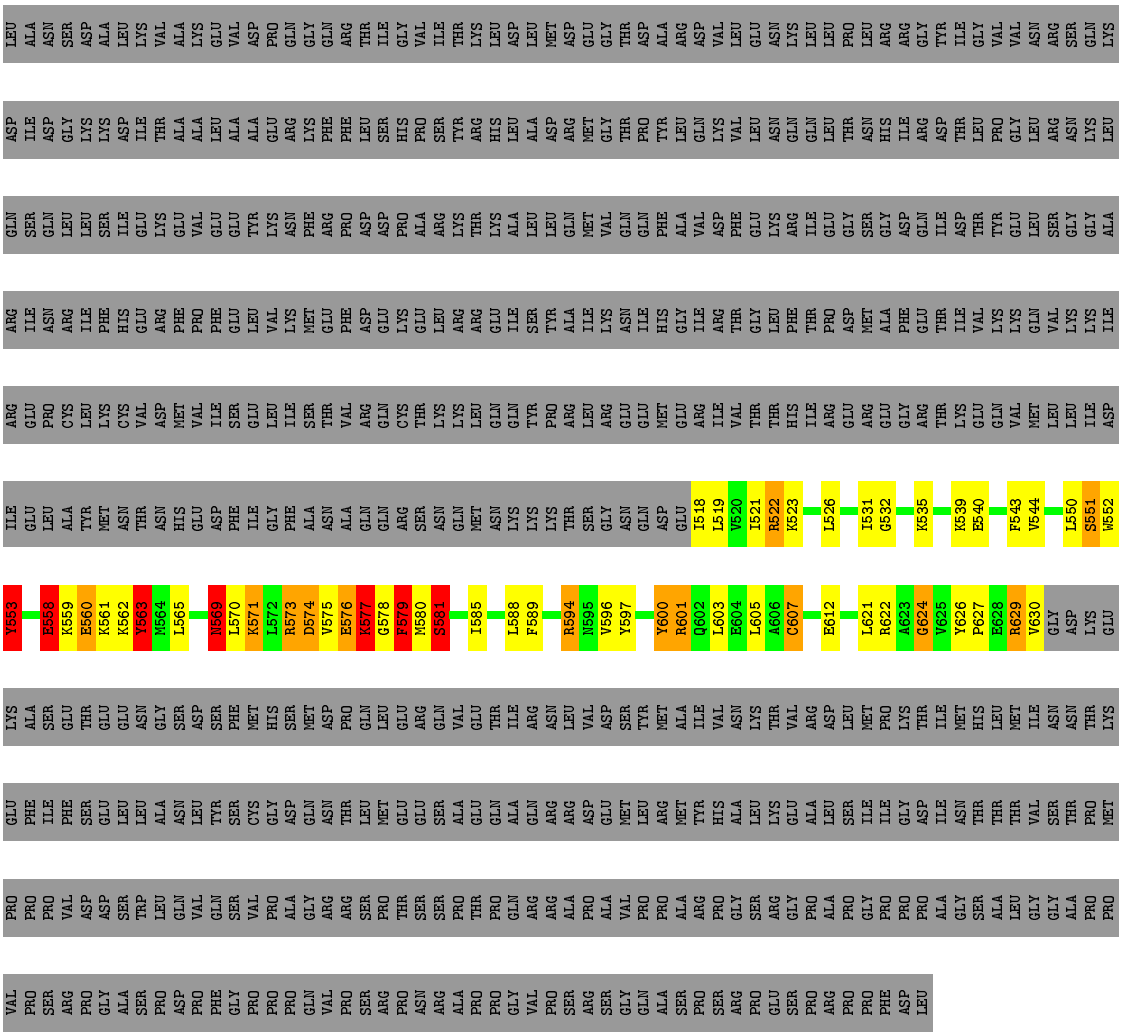
Chain E: 7% 10% 76%



- Molecule 2: DYNAMIN-1

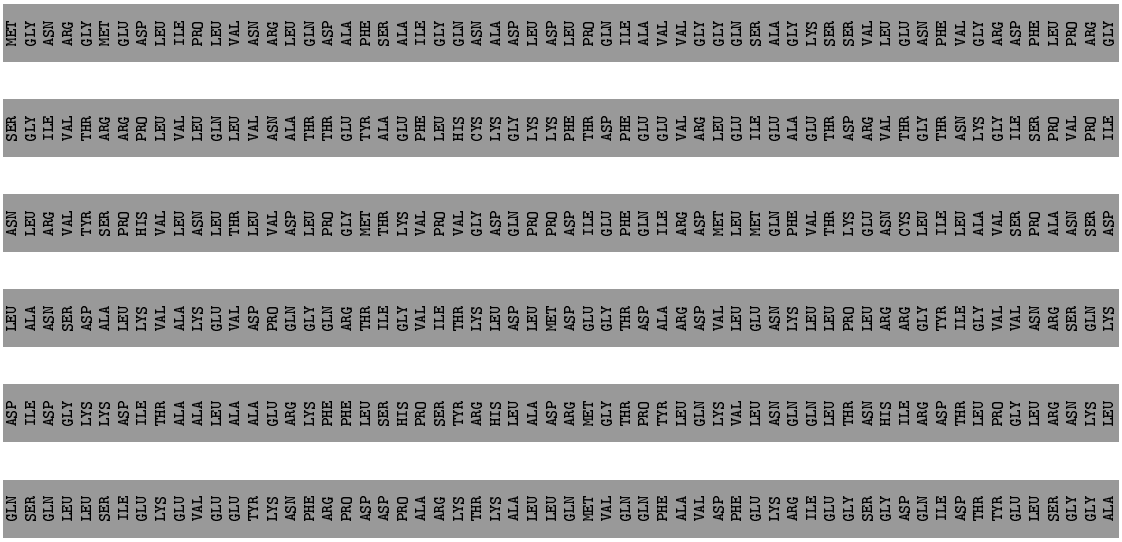
Chain F: 7% 87%

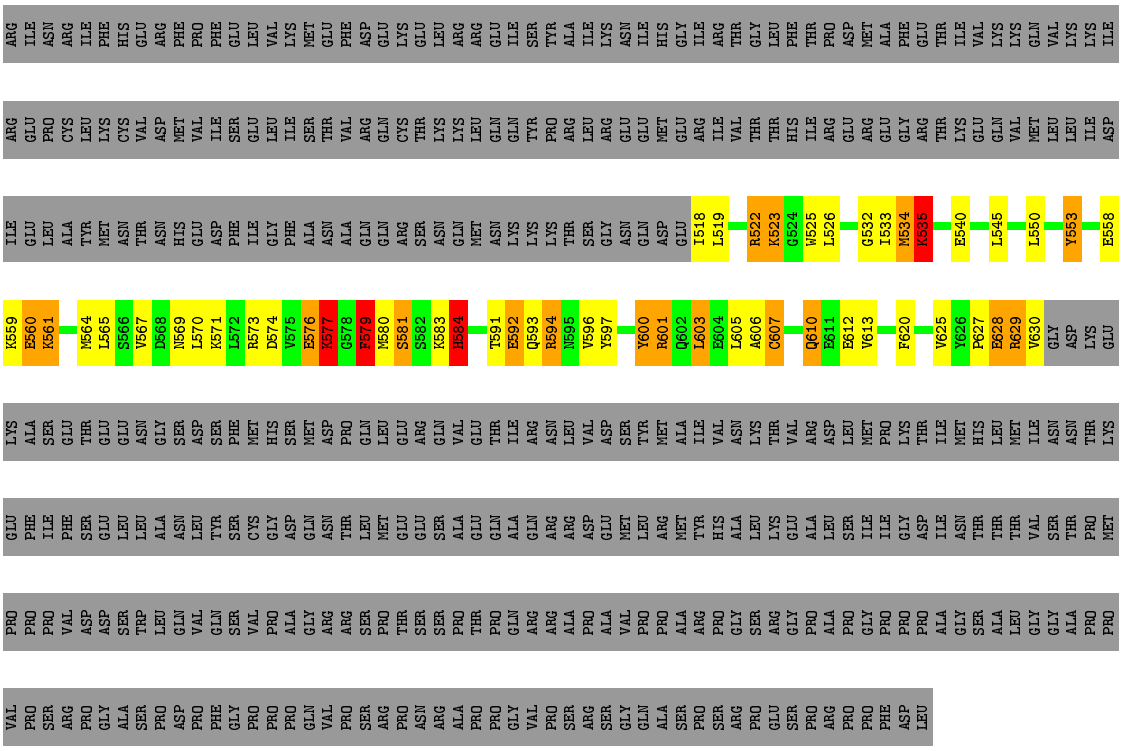




- Molecule 2: DYNAMIN-1

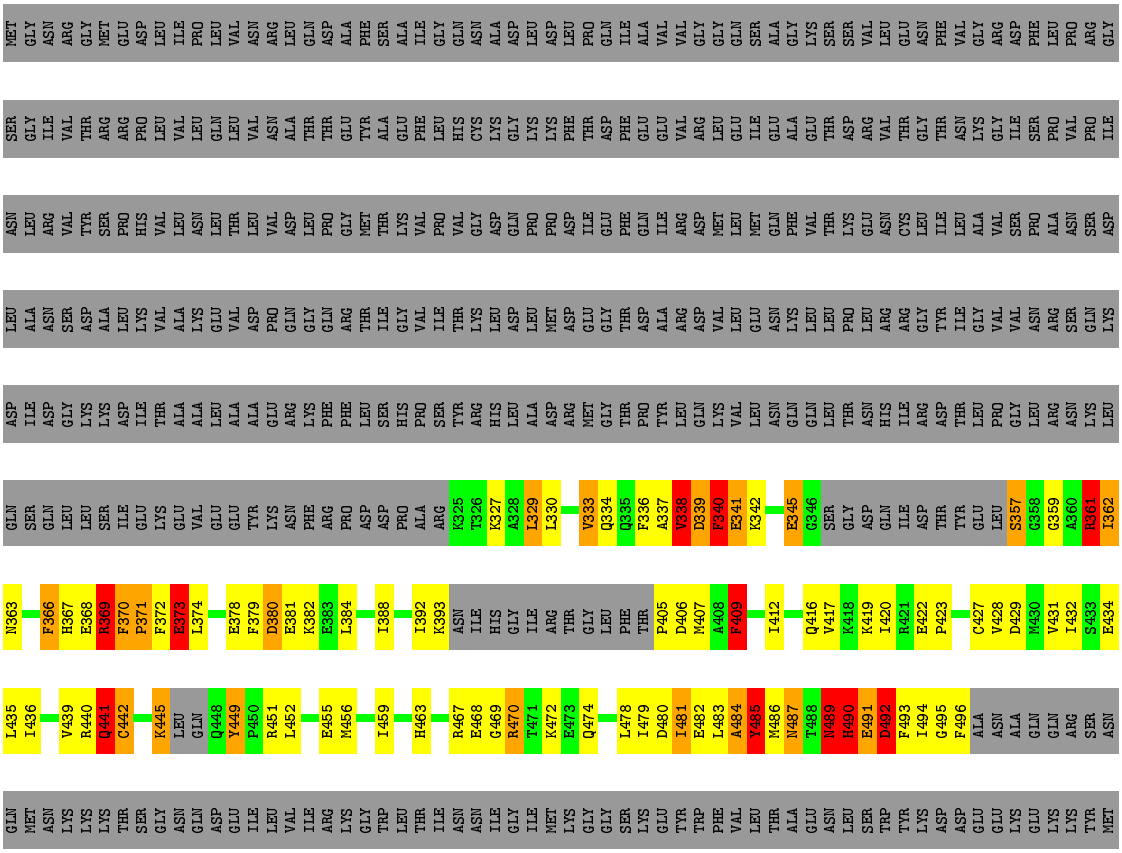
Chain H: 7% 87%





- Molecule 2: DYNAMIN-1

Chain I: 8% 10% 76%



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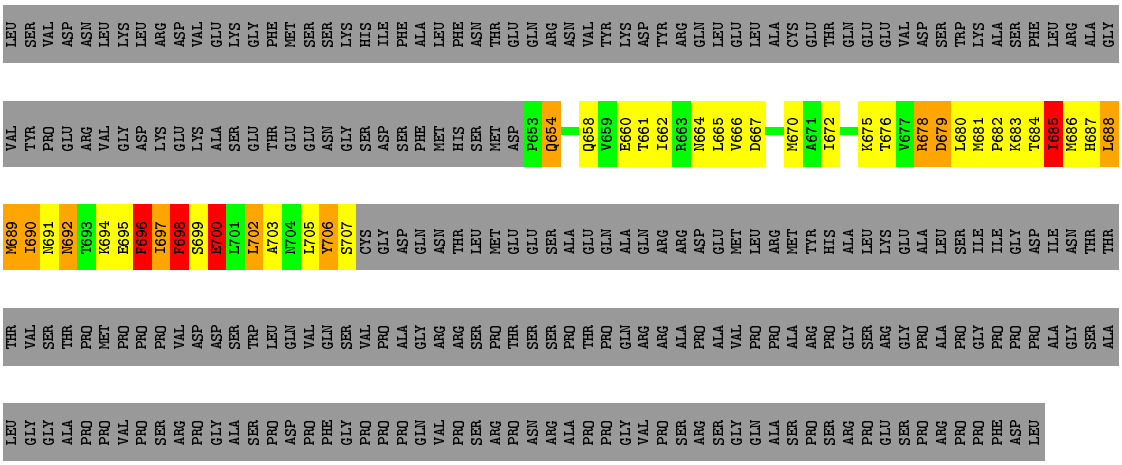
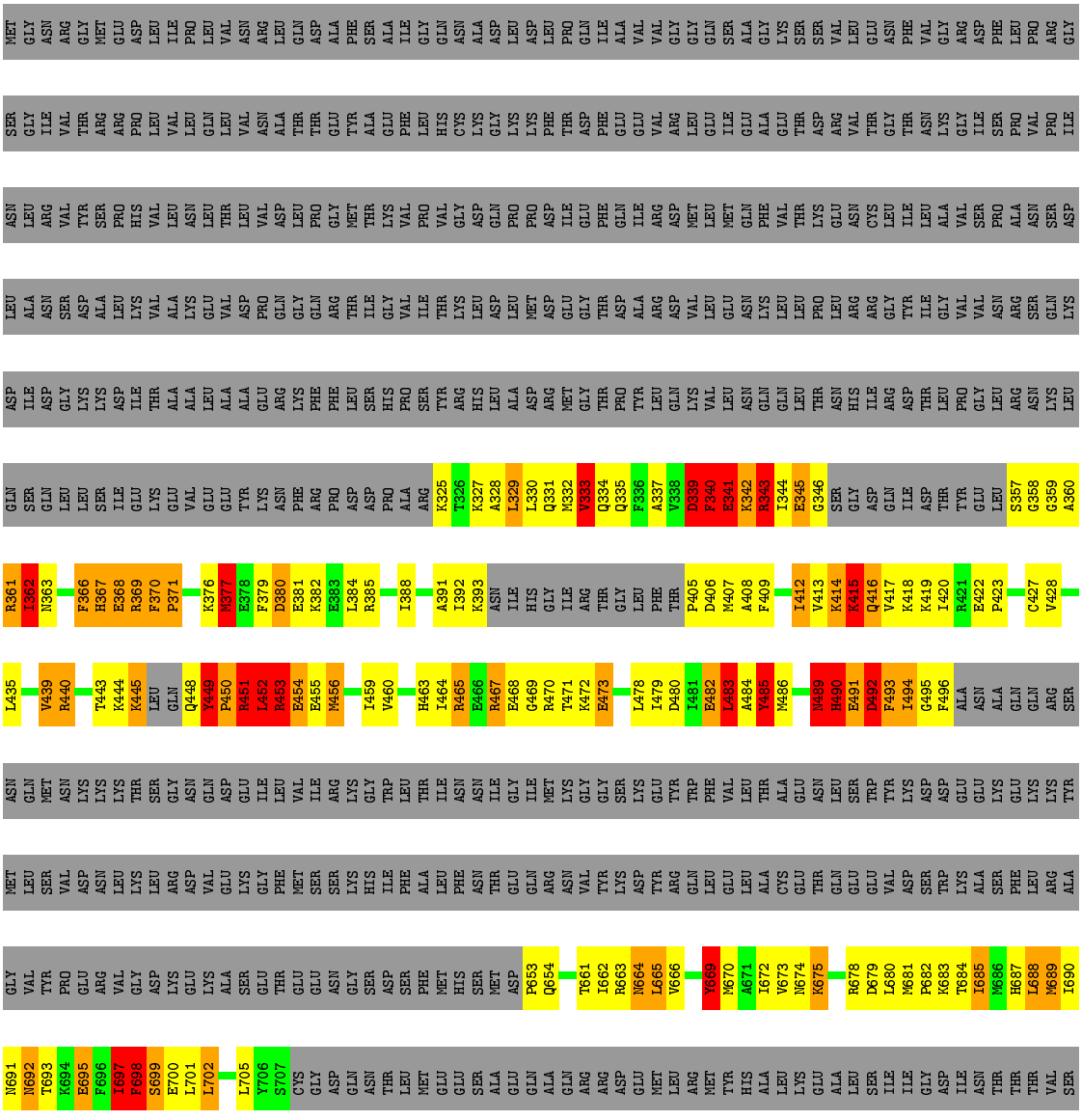
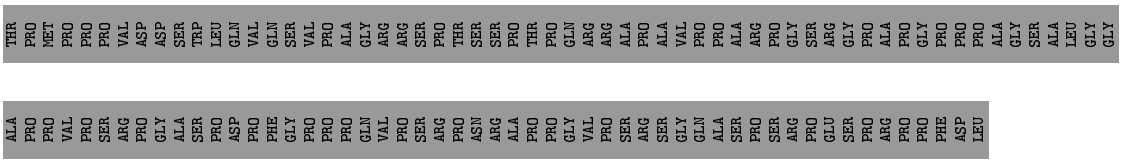


• Molecule 2: DYNAMIN-1

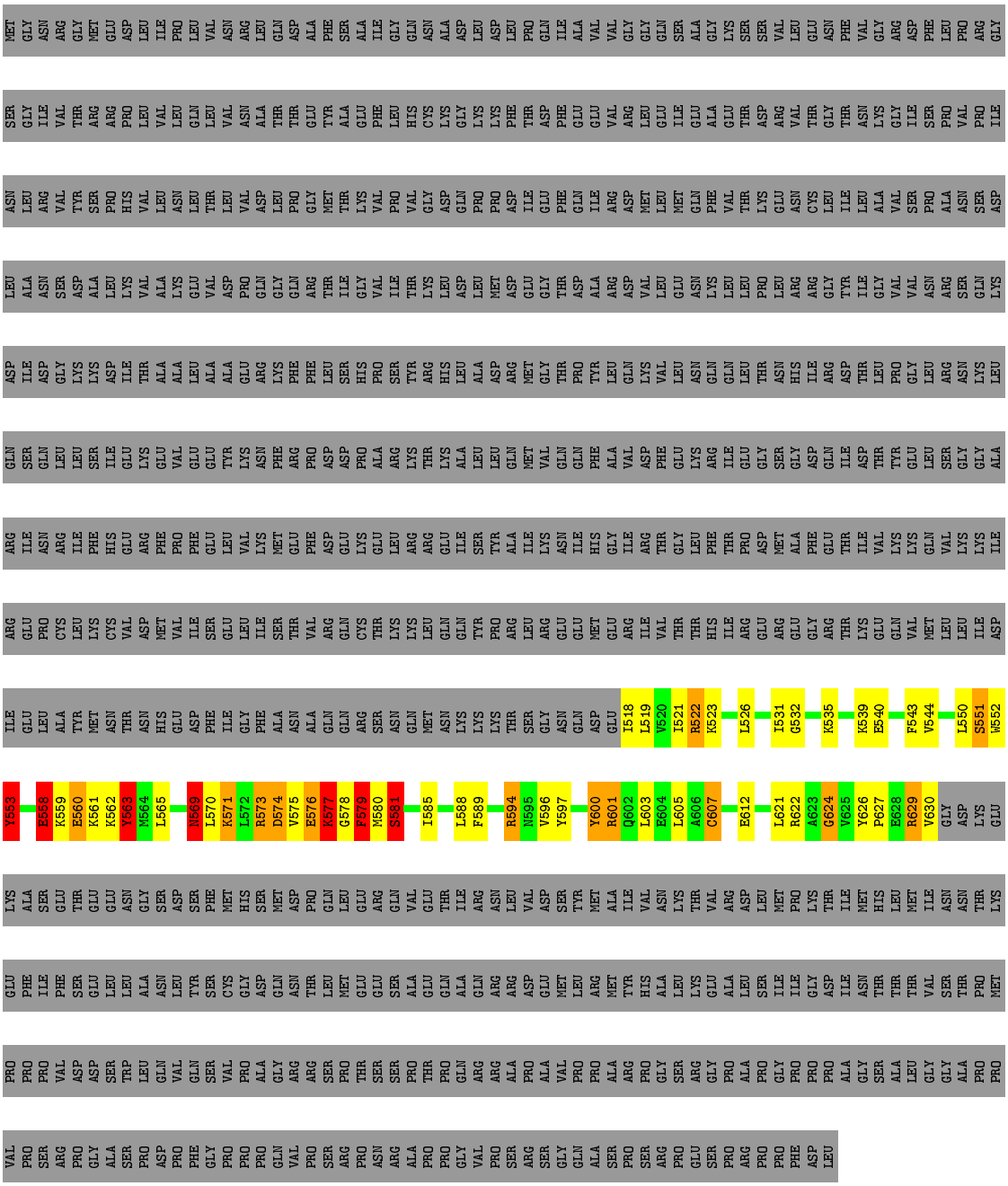
Chain J: 7% 10% 76%





- Molecule 2: DYNAMIN-1

Chain L: 7% 87%



4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL IMAGES	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK S0163 FLM	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.72	2/2604 (0.1%)	1.19	19/3524 (0.5%)
1	D	0.86	8/2683 (0.3%)	1.71	42/3630 (1.2%)
1	G	0.73	2/2604 (0.1%)	1.19	19/3524 (0.5%)
1	K	0.86	8/2683 (0.3%)	1.71	43/3630 (1.2%)
2	B	1.03	4/1718 (0.2%)	2.22	46/2293 (2.0%)
2	C	1.01	3/966 (0.3%)	1.74	34/1298 (2.6%)
2	E	1.18	6/1718 (0.3%)	2.25	67/2293 (2.9%)
2	F	1.01	4/966 (0.4%)	1.73	27/1298 (2.1%)
2	H	1.01	3/966 (0.3%)	1.74	34/1298 (2.6%)
2	I	1.03	4/1718 (0.2%)	2.22	46/2293 (2.0%)
2	J	1.18	6/1718 (0.3%)	2.25	67/2293 (2.9%)
2	L	1.02	3/966 (0.3%)	1.73	26/1298 (2.0%)
All	All	0.95	53/21310 (0.2%)	1.80	470/28672 (1.6%)

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
1	A	1	12
1	D	1	15
1	G	1	11
1	K	1	15
2	B	7	28
2	C	6	13
2	E	6	37
2	F	4	16
2	H	6	13
2	I	7	28
2	J	6	37
2	L	4	16
All	All	50	241

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	699	SER	CB-OG	-22.93	1.12	1.42
2	E	699	SER	CB-OG	-22.90	1.12	1.42
1	G	245	LYS	CA-CB	-9.85	1.32	1.53
1	A	245	LYS	CA-CB	-9.84	1.32	1.53
1	K	317	PHE	C-O	-9.47	1.05	1.23

The worst 5 of 470 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	492	ASP	CB-CG-OD2	50.51	163.76	118.30
2	I	492	ASP	CB-CG-OD2	50.42	163.68	118.30
2	I	492	ASP	CB-CG-OD1	-45.51	77.34	118.30
2	B	492	ASP	CB-CG-OD1	-45.47	77.37	118.30
1	K	318	ARG	NE-CZ-NH2	39.72	140.16	120.30

5 of 50 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	726	ASP	CA
2	B	366	PHE	CA
2	B	373	GLU	CA
2	B	441	GLN	CA
2	B	442	CYS	CA

5 of 241 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	THR	Mainchain
1	A	123	ARG	Sidechain
1	A	28	ASP	Mainchain
1	A	41	SER	Mainchain
1	A	50	ASN	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2567	0	2629	75	0
1	D	2643	0	2691	117	0
1	G	2567	0	2629	76	0
1	K	2643	0	2691	130	0
2	B	1697	0	1748	123	0
2	C	946	0	934	23	0
2	E	1697	0	1749	169	0
2	F	946	0	936	30	0
2	H	946	0	934	24	0
2	I	1697	0	1747	162	0
2	J	1697	0	1749	193	0
2	L	946	0	936	29	0
All	All	20992	0	21373	984	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 23.

The worst 5 of 984 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:454:GLU:OE1	1:K:271:ARG:NH1	1.72	1.21
1:D:317:PHE:CZ	2:E:332:MET:O	1.94	1.20
2:J:332:MET:O	1:K:317:PHE:CZ	1.94	1.18
2:J:453:ARG:N	1:K:318:ARG:HD2	1.55	1.17
1:D:318:ARG:HD2	2:E:453:ARG:N	1.55	1.14

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	325/864 (38%)	313 (96%)	10 (3%)	2 (1%)	30 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	333/864 (38%)	319 (96%)	13 (4%)	1 (0%)	46 83
1	G	325/864 (38%)	313 (96%)	10 (3%)	2 (1%)	30 74
1	K	333/864 (38%)	319 (96%)	13 (4%)	1 (0%)	46 83
2	B	194/864 (22%)	158 (81%)	28 (14%)	8 (4%)	3 35
2	C	111/864 (13%)	94 (85%)	12 (11%)	5 (4%)	3 33
2	E	194/864 (22%)	166 (86%)	23 (12%)	5 (3%)	7 45
2	F	111/864 (13%)	93 (84%)	16 (14%)	2 (2%)	11 53
2	H	111/864 (13%)	94 (85%)	12 (11%)	5 (4%)	3 33
2	I	194/864 (22%)	158 (81%)	29 (15%)	7 (4%)	4 38
2	J	194/864 (22%)	166 (86%)	23 (12%)	5 (3%)	7 45
2	L	111/864 (13%)	93 (84%)	16 (14%)	2 (2%)	11 53
All	All	2536/10368 (24%)	2286 (90%)	205 (8%)	45 (2%)	15 53

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	GLY
2	B	442	CYS
2	B	490	HIS
2	B	690	ILE
2	C	523	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	287/761 (38%)	275 (96%)	12 (4%)	36 70
1	D	295/761 (39%)	281 (95%)	14 (5%)	32 68
1	G	287/761 (38%)	275 (96%)	12 (4%)	36 70
1	K	295/761 (39%)	281 (95%)	14 (5%)	32 68
2	B	191/761 (25%)	158 (83%)	33 (17%)	2 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	102/761 (13%)	91 (89%)	11 (11%)	8 35
2	E	191/761 (25%)	151 (79%)	40 (21%)	1 10
2	F	102/761 (13%)	89 (87%)	13 (13%)	5 29
2	H	102/761 (13%)	91 (89%)	11 (11%)	8 35
2	I	191/761 (25%)	158 (83%)	33 (17%)	2 17
2	J	191/761 (25%)	151 (79%)	40 (21%)	1 10
2	L	102/761 (13%)	89 (87%)	13 (13%)	5 29
All	All	2336/9132 (26%)	2090 (90%)	246 (10%)	13 36

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	553	TYR
2	H	571	LYS
1	K	248	ILE
2	F	563	TYR
1	G	69	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	692	ASN
2	H	529	ASN
1	K	236	ASN
2	F	610	GLN
1	G	236	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.