



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:08 AM UTC

PDB ID : 4V93 / pdb_00004v93
EMDB ID : EMD-2627
Title : Fitted coordinates for Lumbricus terrestris hemoglobin cryo-EM complex (EMD-2627)
Authors : Chen, W.T.; Chen, Y.C.; Liou, H.H.; Chao, C.Y.
Deposited on : 2014-04-16
Resolution : 8.10 Å(reported)
Based on initial model : 2GTL

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 ⓘ 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.dev132
MolProbity : 4-5-2 with Phenix2.0
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

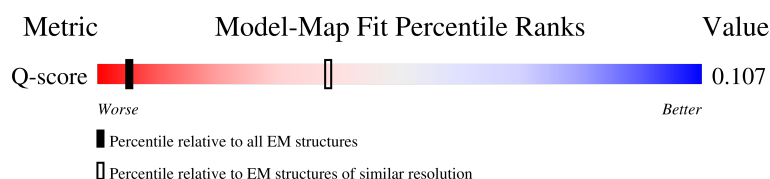
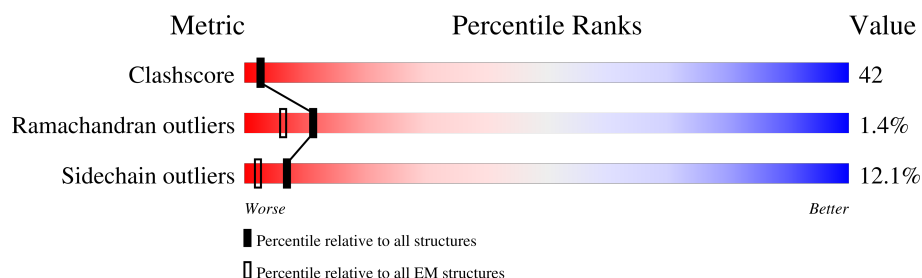
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

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 $\leq 5\%$. 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	A0	149	34% 60% 33% 7%
1	A5	149	34% 58% 34% 8%
1	AC	149	34% 58% 34% 8%
1	AH	149	34% 58% 34% 7%

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Mol	Chain	Length	Quality of chain
1	AM	149	
1	AR	149	
1	AW	149	
1	Ab	149	
1	Ag	149	
1	Al	149	
1	Aq	149	
1	Av	149	
2	A1	140	
2	A6	140	
2	AD	140	
2	AI	140	
2	AN	140	
2	AS	140	
2	AX	140	
2	Ac	140	
2	Ah	140	
2	Am	140	
2	Ar	140	
2	Aw	140	
3	A2	147	
3	A3	147	
3	A7	147	
3	AA	147	
3	AE	147	

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Mol	Chain	Length	Quality of chain
3	AF	147	
3	AJ	147	
3	AK	147	
3	AO	147	
3	AP	147	
3	AT	147	
3	AU	147	
3	AY	147	
3	AZ	147	
3	Ad	147	
3	Ae	147	
3	Ai	147	
3	Aj	147	
3	An	147	
3	Ao	147	
3	As	147	
3	At	147	
3	Ax	147	
3	Ay	147	
4	A4	145	
4	AB	145	
4	AG	145	
4	AL	145	
4	AQ	145	
4	AV	145	

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Mol	Chain	Length	Quality of chain
4	Aa	145	
4	Af	145	
4	Ak	145	
4	Ap	145	
4	Au	145	
4	Az	145	
4	B2	145	
4	B3	145	
4	B7	145	
4	BA	145	
4	BE	145	
4	BF	145	
4	BJ	145	
4	BK	145	
4	BO	145	
4	BP	145	
4	BT	145	
4	BU	145	
4	BY	145	
4	BZ	145	
4	Bd	145	
4	Be	145	
4	Bi	145	
4	Bj	145	
4	Bn	145	

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Mol	Chain	Length	Quality of chain
4	Bo	145	
4	Bs	145	
4	Bt	145	
4	Bx	145	
4	By	145	
5	B0	158	
5	B5	158	
5	BC	158	
5	BH	158	
5	BM	158	
5	BR	158	
5	BW	158	
5	Bb	158	
5	Bg	158	
5	Bl	158	
5	Bq	158	
5	Bv	158	
5	C4	158	
5	CB	158	
5	CG	158	
5	CL	158	
5	CQ	158	
5	CV	158	
5	Ca	158	
5	Cf	158	

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Mol	Chain	Length	Quality of chain
5	Ck	158	
5	Cp	158	
5	Cu	158	
5	Cz	158	
6	B1	151	
6	B6	151	
6	BD	151	
6	BI	151	
6	BN	151	
6	BS	151	
6	BX	151	
6	Bc	151	
6	Bh	151	
6	Bm	151	
6	Br	151	
6	Bw	151	
7	B4	170	
7	BB	170	
7	BG	170	
7	BL	170	
7	BQ	170	
7	BV	170	
7	Ba	170	
7	Bf	170	
7	Bk	170	

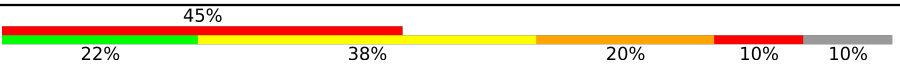
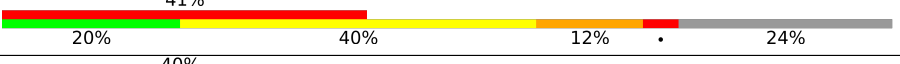
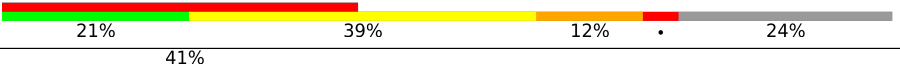
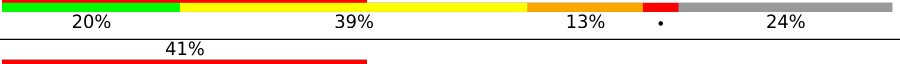
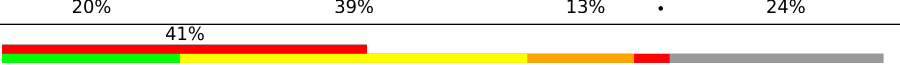
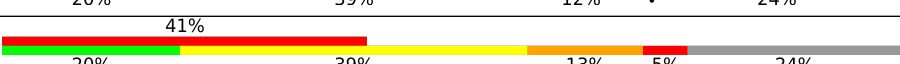
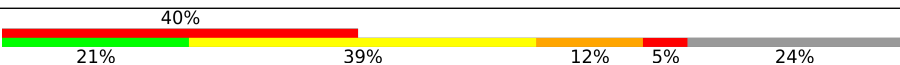
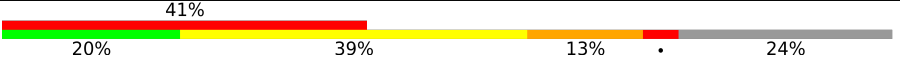
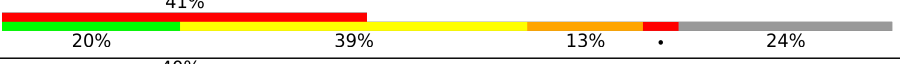
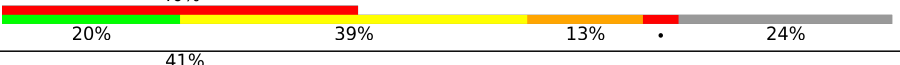
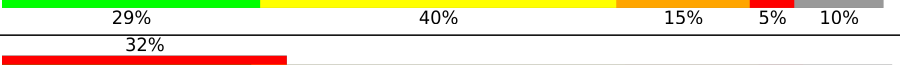
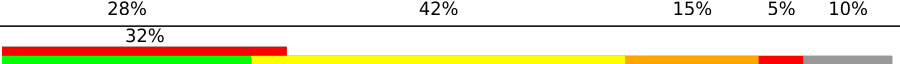
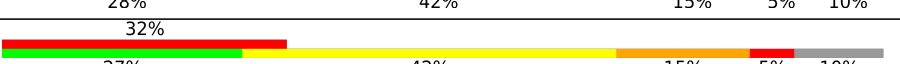
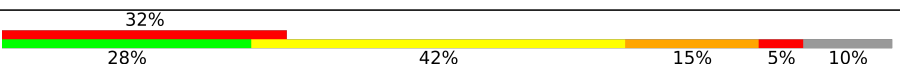
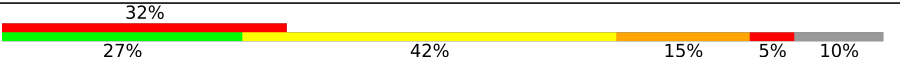
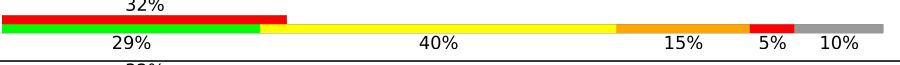
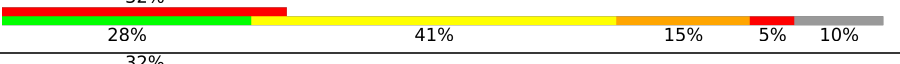
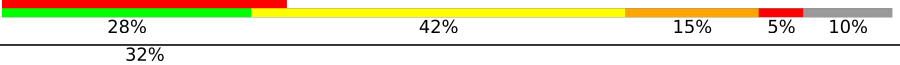
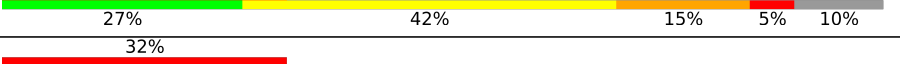
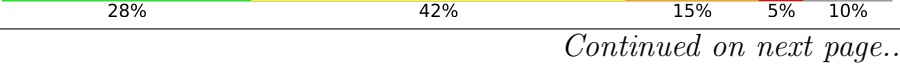
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Mol	Chain	Length	Quality of chain
7	Bp	170	
7	Bu	170	
7	Bz	170	
7	C3	170	
7	CA	170	
7	CF	170	
7	CK	170	
7	CP	170	
7	CU	170	
7	CZ	170	
7	Ce	170	
7	Cj	170	
7	Co	170	
7	Ct	170	
7	Cy	170	
8	C0	240	
8	C5	240	
8	CC	240	
8	CH	240	
8	CM	240	
8	CR	240	
8	CW	240	
8	Cb	240	
8	Cg	240	
8	Cl	240	

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Mol	Chain	Length	Quality of chain
8	Cq	240	
8	Cv	240	
9	C1	288	
9	C6	288	
9	CD	288	
9	CI	288	
9	CN	288	
9	CS	288	
9	CX	288	
9	Cc	288	
9	Ch	288	
9	Cm	288	
9	Cr	288	
9	Cw	288	
10	C2	240	
10	C7	240	
10	CE	240	
10	CJ	240	
10	CO	240	
10	CT	240	
10	CY	240	
10	Cd	240	
10	Ci	240	
10	Cn	240	
10	Cs	240	

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Mol	Chain	Length	Quality of chain
10	C _x	240	32% 27% 42% 15% 5% 10%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 231000 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 EXTRACELLULAR GLOBIN-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	A5	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	AC	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	AH	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	AM	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	AR	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	AW	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	Ab	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	Ag	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	Al	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	Aq	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		
1	Av	149	Total	C	N	O	S	0	0
			1191	758	212	218	3		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A0	49	GLU	ASP	conflict	UNP P11069
A5	49	GLU	ASP	conflict	UNP P11069
AC	49	GLU	ASP	conflict	UNP P11069
AH	49	GLU	ASP	conflict	UNP P11069
AM	49	GLU	ASP	conflict	UNP P11069
AR	49	GLU	ASP	conflict	UNP P11069

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Chain	Residue	Modelled	Actual	Comment	Reference
AW	49	GLU	ASP	conflict	UNP P11069
Ab	49	GLU	ASP	conflict	UNP P11069
Ag	49	GLU	ASP	conflict	UNP P11069
Al	49	GLU	ASP	conflict	UNP P11069
Aq	49	GLU	ASP	conflict	UNP P11069
Av	49	GLU	ASP	conflict	UNP P11069

- Molecule 2 is a protein called HEMOGLOBIN CHAIN D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A1	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	A6	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	AD	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	AI	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	AN	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	AS	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	AX	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	Ac	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	Ah	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	Am	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	Ar	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
2	Aw	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		

- Molecule 3 is a protein called EXTRACELLULAR GLOBIN-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A2	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	A3	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	A7	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AA	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AE	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AF	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AJ	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AK	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AO	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AP	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AT	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AU	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AY	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	AZ	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	Ad	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	Ae	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	Ai	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	Aj	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	An	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	Ao	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	As	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	At	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
3	Ax	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ay	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	78	LYS	ASP	conflict	UNP P13579
A3	78	LYS	ASP	conflict	UNP P13579
A7	78	LYS	ASP	conflict	UNP P13579
AA	78	LYS	ASP	conflict	UNP P13579
AE	78	LYS	ASP	conflict	UNP P13579
AF	78	LYS	ASP	conflict	UNP P13579
AJ	78	LYS	ASP	conflict	UNP P13579
AK	78	LYS	ASP	conflict	UNP P13579
AO	78	LYS	ASP	conflict	UNP P13579
AP	78	LYS	ASP	conflict	UNP P13579
AT	78	LYS	ASP	conflict	UNP P13579
AU	78	LYS	ASP	conflict	UNP P13579
AY	78	LYS	ASP	conflict	UNP P13579
AZ	78	LYS	ASP	conflict	UNP P13579
Ad	78	LYS	ASP	conflict	UNP P13579
Ae	78	LYS	ASP	conflict	UNP P13579
Ai	78	LYS	ASP	conflict	UNP P13579
Aj	78	LYS	ASP	conflict	UNP P13579
An	78	LYS	ASP	conflict	UNP P13579
Ao	78	LYS	ASP	conflict	UNP P13579
As	78	LYS	ASP	conflict	UNP P13579
At	78	LYS	ASP	conflict	UNP P13579
Ax	78	LYS	ASP	conflict	UNP P13579
Ay	78	LYS	ASP	conflict	UNP P13579

- Molecule 4 is a protein called EXTRACELLULAR GLOBIN-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A4	145	Total	C	N	O	S	0	0
			1148	720	212	213	3		
4	AB	145	Total	C	N	O	S	0	0
			1148	720	212	213	3		
4	AG	145	Total	C	N	O	S	0	0
			1148	720	212	213	3		
4	AL	145	Total	C	N	O	S	0	0
			1148	720	212	213	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	AQ	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	AV	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Aa	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Af	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Ak	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Ap	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Au	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Az	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	B2	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	B3	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	B7	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BA	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BE	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BF	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BJ	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BK	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BO	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BP	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BT	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BU	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	BY	145	Total 1148	C 720	N 212	O 213	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	BZ	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Bd	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Be	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Bi	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Bj	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Bn	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Bo	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Bs	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Bt	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	Bx	145	Total 1148	C 720	N 212	O 213	S 3	0	0
4	By	145	Total 1148	C 720	N 212	O 213	S 3	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A4	66	ASP	GLU	conflict	UNP P02218
AB	66	ASP	GLU	conflict	UNP P02218
AG	66	ASP	GLU	conflict	UNP P02218
AL	66	ASP	GLU	conflict	UNP P02218
AQ	66	ASP	GLU	conflict	UNP P02218
AV	66	ASP	GLU	conflict	UNP P02218
Aa	66	ASP	GLU	conflict	UNP P02218
Af	66	ASP	GLU	conflict	UNP P02218
Ak	66	ASP	GLU	conflict	UNP P02218
Ap	66	ASP	GLU	conflict	UNP P02218
Au	66	ASP	GLU	conflict	UNP P02218
Az	66	ASP	GLU	conflict	UNP P02218
B2	66	ASP	GLU	conflict	UNP P02218
B3	66	ASP	GLU	conflict	UNP P02218
B7	66	ASP	GLU	conflict	UNP P02218
BA	66	ASP	GLU	conflict	UNP P02218
BE	66	ASP	GLU	conflict	UNP P02218

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Chain	Residue	Modelled	Actual	Comment	Reference
BF	66	ASP	GLU	conflict	UNP P02218
BJ	66	ASP	GLU	conflict	UNP P02218
BK	66	ASP	GLU	conflict	UNP P02218
BO	66	ASP	GLU	conflict	UNP P02218
BP	66	ASP	GLU	conflict	UNP P02218
BT	66	ASP	GLU	conflict	UNP P02218
BU	66	ASP	GLU	conflict	UNP P02218
BY	66	ASP	GLU	conflict	UNP P02218
BZ	66	ASP	GLU	conflict	UNP P02218
Bd	66	ASP	GLU	conflict	UNP P02218
Be	66	ASP	GLU	conflict	UNP P02218
Bi	66	ASP	GLU	conflict	UNP P02218
Bj	66	ASP	GLU	conflict	UNP P02218
Bn	66	ASP	GLU	conflict	UNP P02218
Bo	66	ASP	GLU	conflict	UNP P02218
Bs	66	ASP	GLU	conflict	UNP P02218
Bt	66	ASP	GLU	conflict	UNP P02218
Bx	66	ASP	GLU	conflict	UNP P02218
By	66	ASP	GLU	conflict	UNP P02218

- Molecule 5 is a protein called HEMOGLOBIN CHAIN D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B0	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	B5	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	BC	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	BH	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	BM	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	BR	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	BW	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Bb	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Bg	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Bl	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Bq	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Bv	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	C4	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	CB	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	CG	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	CL	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	CQ	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	CV	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Ca	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Cf	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Ck	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Cp	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Cu	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		
5	Cz	140	Total	C	N	O	S	0	0
			1129	725	198	202	4		

- Molecule 6 is a protein called EXTRACELLULAR GLOBIN-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B1	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	B6	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	BD	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	BI	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	BN	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	BS	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	BX	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	Bc	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	Bh	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	Bm	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	Br	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		
6	Bw	147	Total	C	N	O	S	0	0
			1209	769	222	214	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	78	LYS	ASP	conflict	UNP P13579
B6	78	LYS	ASP	conflict	UNP P13579
BD	78	LYS	ASP	conflict	UNP P13579
BI	78	LYS	ASP	conflict	UNP P13579
BN	78	LYS	ASP	conflict	UNP P13579
BS	78	LYS	ASP	conflict	UNP P13579
BX	78	LYS	ASP	conflict	UNP P13579
Bc	78	LYS	ASP	conflict	UNP P13579
Bh	78	LYS	ASP	conflict	UNP P13579
Bm	78	LYS	ASP	conflict	UNP P13579
Br	78	LYS	ASP	conflict	UNP P13579
Bw	78	LYS	ASP	conflict	UNP P13579

- Molecule 7 is a protein called EXTRACELLULAR GLOBIN-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B4	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	BB	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	BG	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	BL	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	BQ	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	BV	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Ba	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Bf	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Bk	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Bp	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Bu	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Bz	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	C3	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	CA	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	CF	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	CK	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	CP	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	CU	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	CZ	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Ce	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Cj	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Co	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Ct	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		
7	Cy	149	Total	C	N	O	S	0	0
			1190	758	212	217	3		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B4	49	GLU	ASP	conflict	UNP P11069
BB	49	GLU	ASP	conflict	UNP P11069
BG	49	GLU	ASP	conflict	UNP P11069
BL	49	GLU	ASP	conflict	UNP P11069
BQ	49	GLU	ASP	conflict	UNP P11069
BV	49	GLU	ASP	conflict	UNP P11069
Ba	49	GLU	ASP	conflict	UNP P11069
Bf	49	GLU	ASP	conflict	UNP P11069
Bk	49	GLU	ASP	conflict	UNP P11069
Bp	49	GLU	ASP	conflict	UNP P11069
Bu	49	GLU	ASP	conflict	UNP P11069
Bz	49	GLU	ASP	conflict	UNP P11069
C3	49	GLU	ASP	conflict	UNP P11069
CA	49	GLU	ASP	conflict	UNP P11069
CF	49	GLU	ASP	conflict	UNP P11069
CK	49	GLU	ASP	conflict	UNP P11069
CP	49	GLU	ASP	conflict	UNP P11069
CU	49	GLU	ASP	conflict	UNP P11069
CZ	49	GLU	ASP	conflict	UNP P11069
Ce	49	GLU	ASP	conflict	UNP P11069
Cj	49	GLU	ASP	conflict	UNP P11069
Co	49	GLU	ASP	conflict	UNP P11069
Ct	49	GLU	ASP	conflict	UNP P11069
Cy	49	GLU	ASP	conflict	UNP P11069

- Molecule 8 is a protein called HEMOGLOBIN LINKER CHAIN L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C0	217	Total 1751	C 1089	N 308	O 344	S 10	0	0
8	C5	217	Total 1751	C 1089	N 308	O 344	S 10	0	0
8	CC	217	Total 1751	C 1089	N 308	O 344	S 10	0	0
8	CH	217	Total 1751	C 1089	N 308	O 344	S 10	0	0
8	CM	217	Total 1751	C 1089	N 308	O 344	S 10	0	0
8	CR	217	Total 1751	C 1089	N 308	O 344	S 10	0	0
8	CW	217	Total 1751	C 1089	N 308	O 344	S 10	0	0
8	Cb	217	Total 1751	C 1089	N 308	O 344	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	Cg	217	Total	C	N	O	S	0	0
			1751	1089	308	344	10		
8	Cl	217	Total	C	N	O	S	0	0
			1751	1089	308	344	10		
8	Cq	217	Total	C	N	O	S	0	0
			1751	1089	308	344	10		
8	Cv	217	Total	C	N	O	S	0	0
			1751	1089	308	344	10		

- Molecule 9 is a protein called EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C1	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	C6	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	CD	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	CI	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	CN	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	CS	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	CX	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	Cc	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	Ch	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	Cm	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	Cr	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		
9	Cw	220	Total	C	N	O	S	0	0
			1755	1080	324	341	10		

- Molecule 10 is a protein called EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C2	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	C7	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	CE	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	CJ	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	CO	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	CT	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	CY	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	Cd	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	Ci	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	Cn	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	Cs	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		
10	Cx	215	Total	C	N	O	S	0	0
			1715	1055	299	350	11		

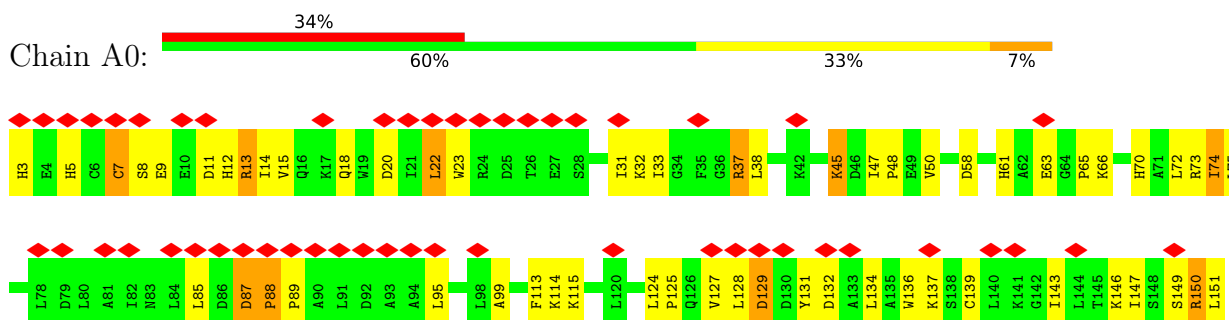
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	113	CYS	VAL	conflict	UNP Q2I742
C7	113	CYS	VAL	conflict	UNP Q2I742
CE	113	CYS	VAL	conflict	UNP Q2I742
CJ	113	CYS	VAL	conflict	UNP Q2I742
CO	113	CYS	VAL	conflict	UNP Q2I742
CT	113	CYS	VAL	conflict	UNP Q2I742
CY	113	CYS	VAL	conflict	UNP Q2I742
Cd	113	CYS	VAL	conflict	UNP Q2I742
Ci	113	CYS	VAL	conflict	UNP Q2I742
Cn	113	CYS	VAL	conflict	UNP Q2I742
Cs	113	CYS	VAL	conflict	UNP Q2I742
Cx	113	CYS	VAL	conflict	UNP Q2I742

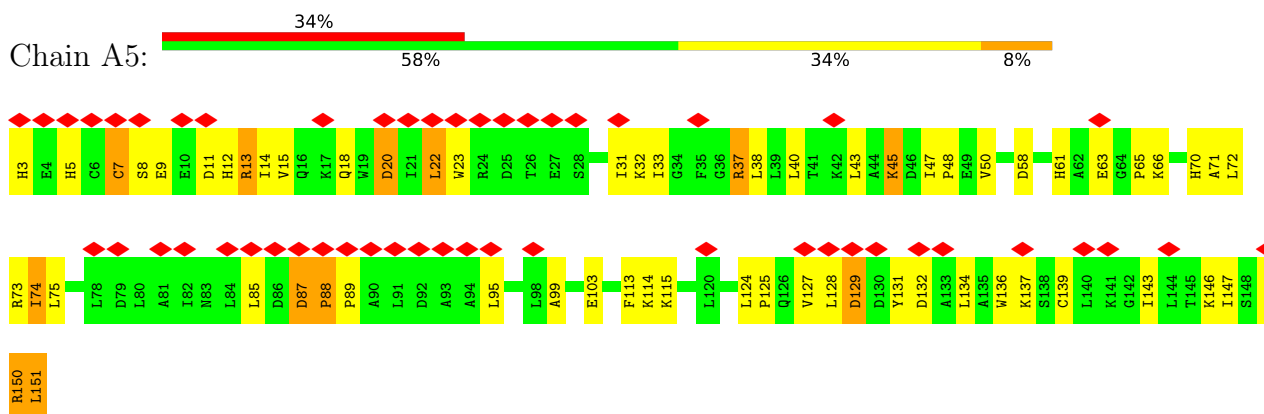
3 Residue-property plots

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.

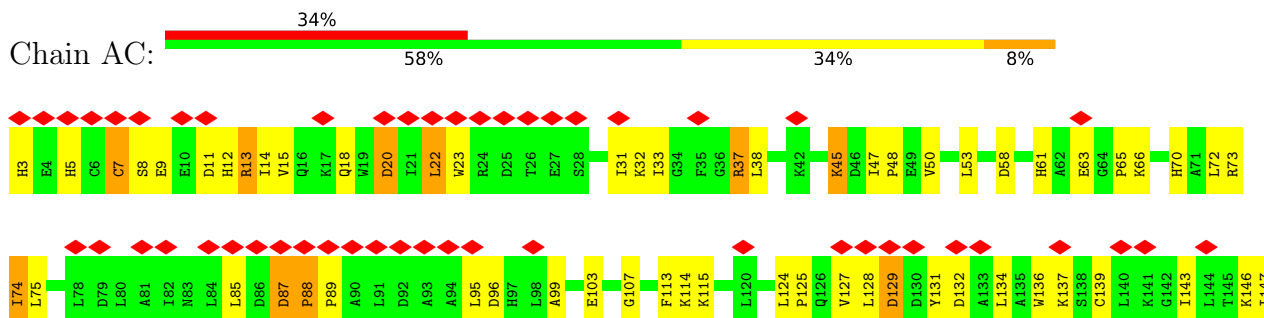
• Molecule 1: EXTRACELLULAR GLOBIN-3



• Molecule 1: EXTRACELLULAR GLOBIN-3

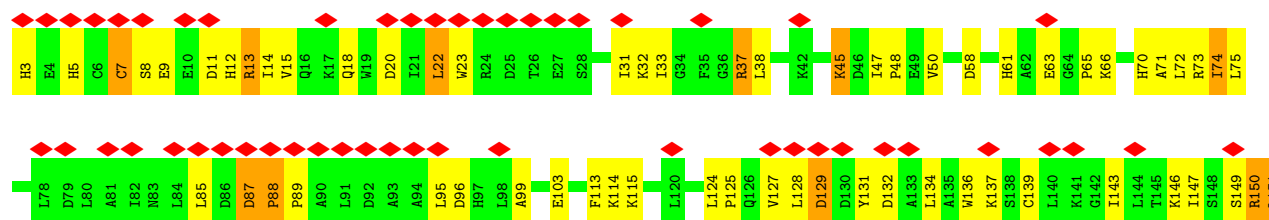


• Molecule 1: EXTRACELLULAR GLOBIN-3

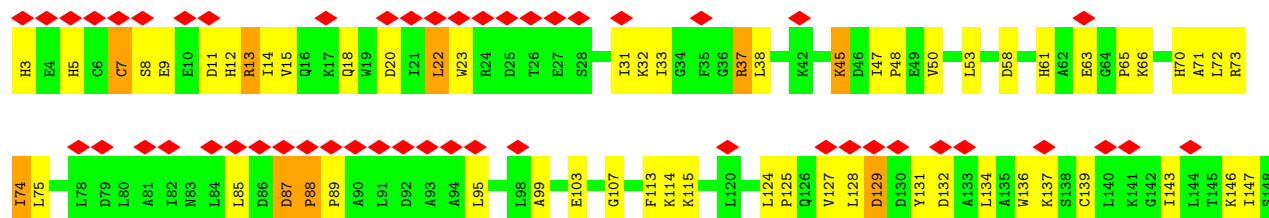




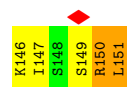
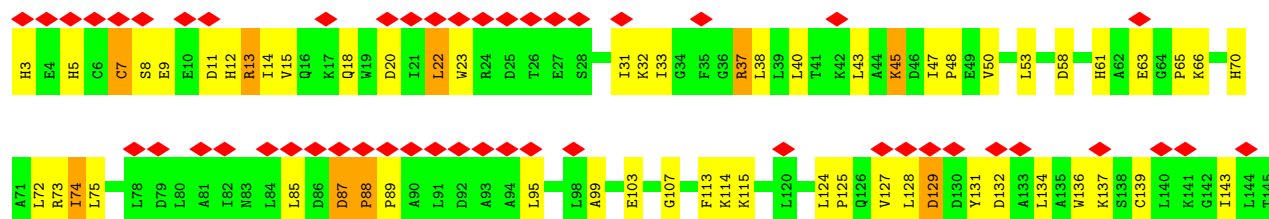
• Molecule 1: EXTRACELLULAR GLOBIN-3



• Molecule 1: EXTRACELLULAR GLOBIN-3

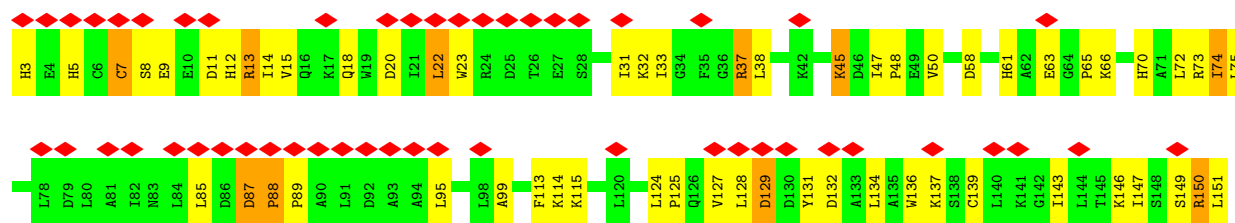


• Molecule 1: EXTRACELLULAR GLOBIN-3

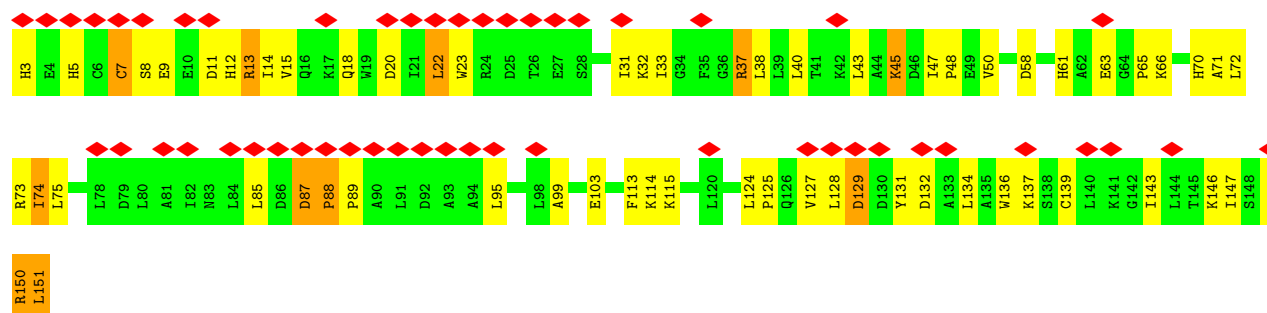


• Molecule 1: EXTRACELLULAR GLOBIN-3

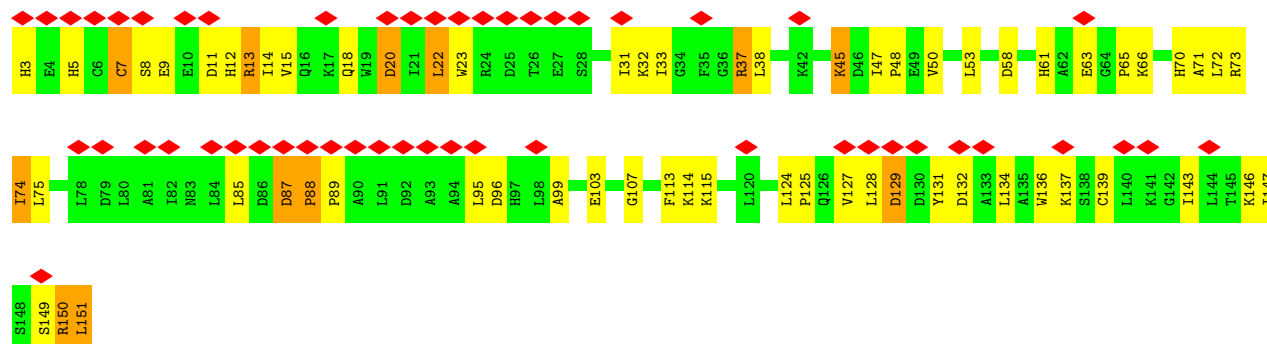




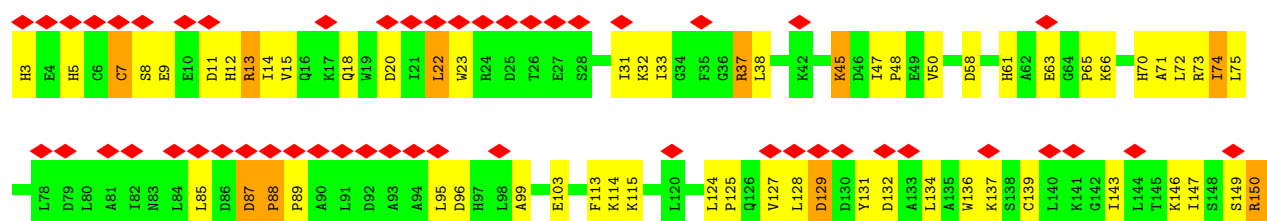
• Molecule 1: EXTRACELLULAR GLOBIN-3



• Molecule 1: EXTRACELLULAR GLOBIN-3

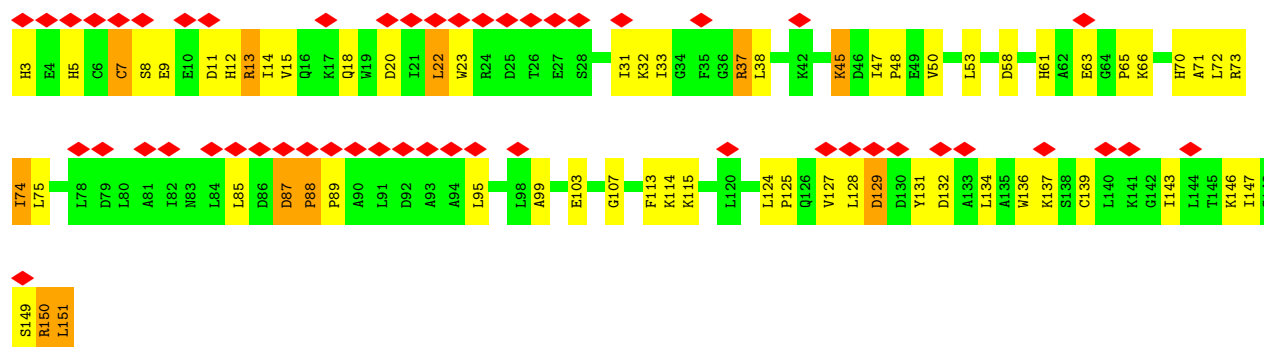


• Molecule 1: EXTRACELLULAR GLOBIN-3

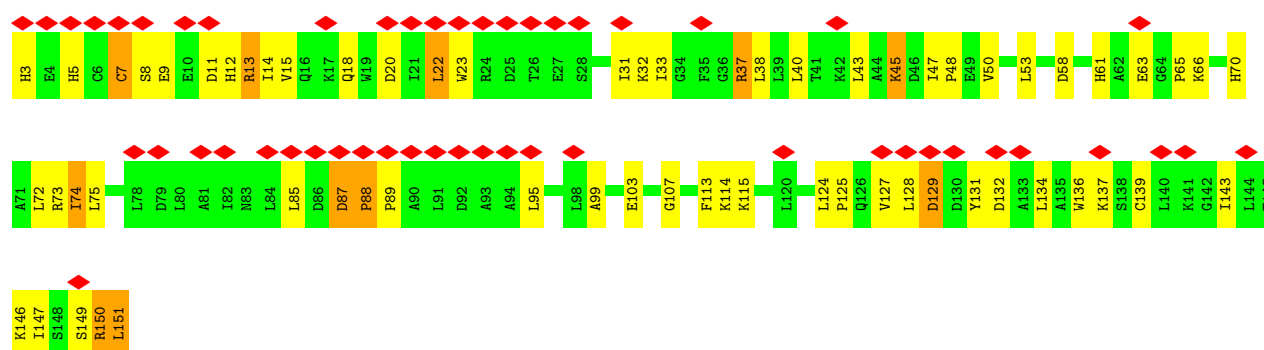


• Molecule 1: EXTRACELLULAR GLOBIN-3

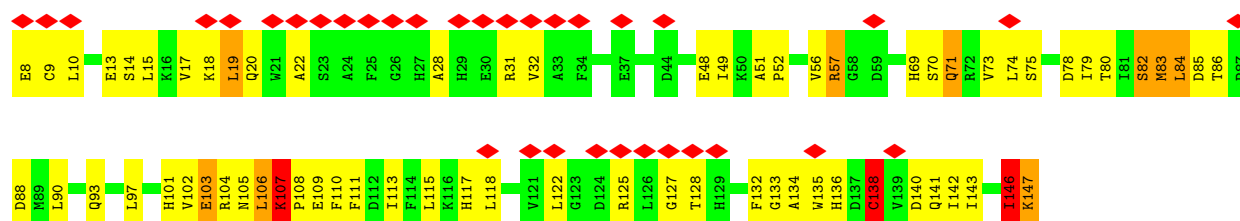




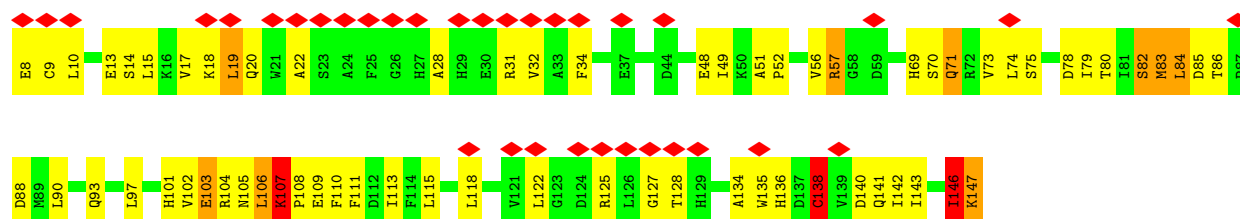
• Molecule 1: EXTRACELLULAR GLOBIN-3



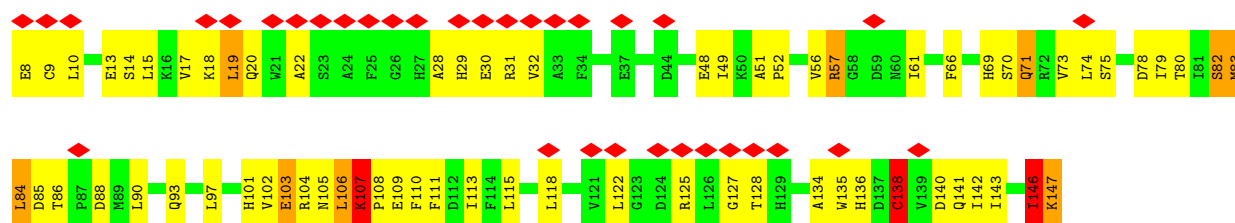
• Molecule 2: HEMOGLOBIN CHAIN D1



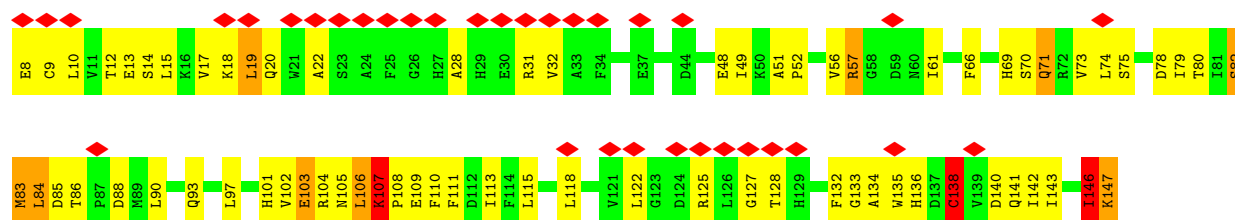
• Molecule 2: HEMOGLOBIN CHAIN D1



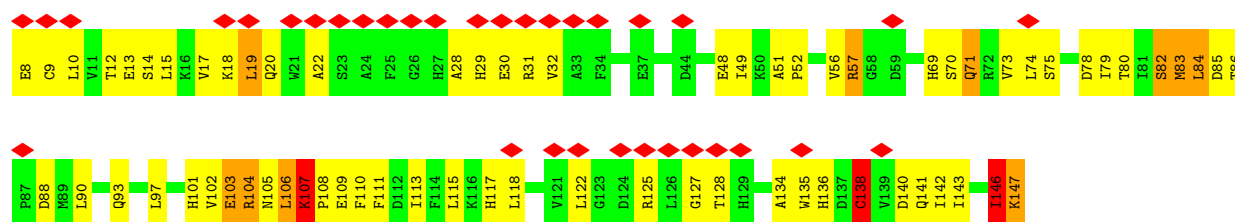
• Molecule 2: HEMOGLOBIN CHAIN D1



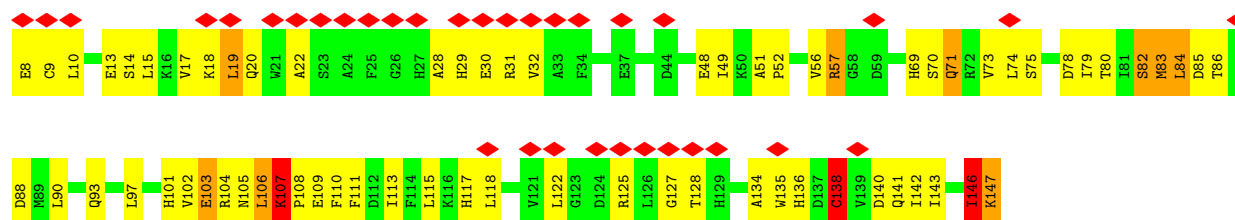
• Molecule 2: HEMOGLOBIN CHAIN D1



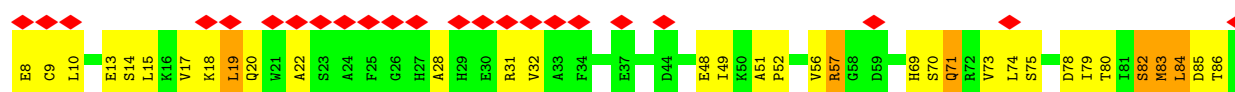
• Molecule 2: HEMOGLOBIN CHAIN D1

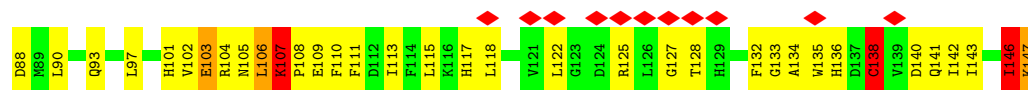


• Molecule 2: HEMOGLOBIN CHAIN D1

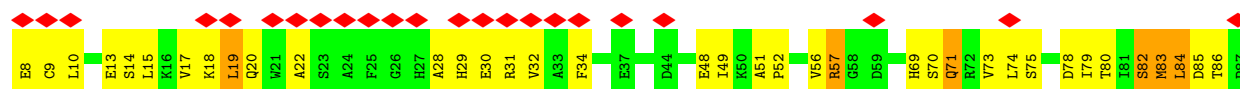


• Molecule 2: HEMOGLOBIN CHAIN D1

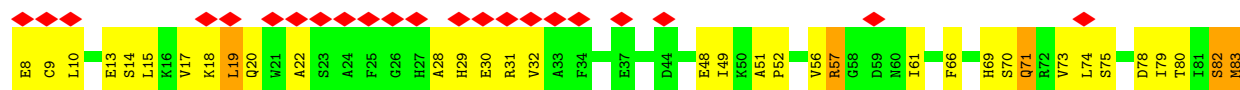




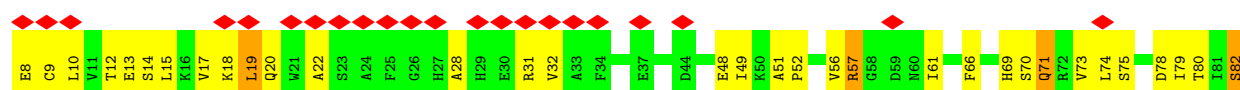
• Molecule 2: HEMOGLOBIN CHAIN D1



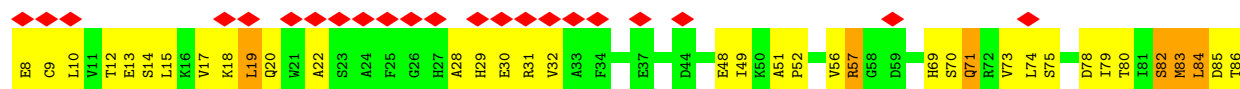
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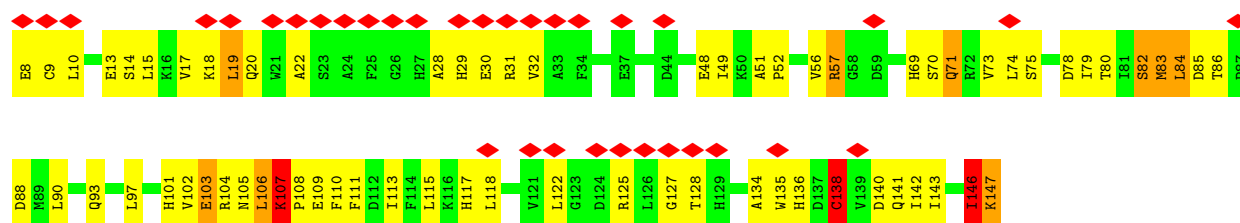


• Molecule 2: HEMOGLOBIN CHAIN D1

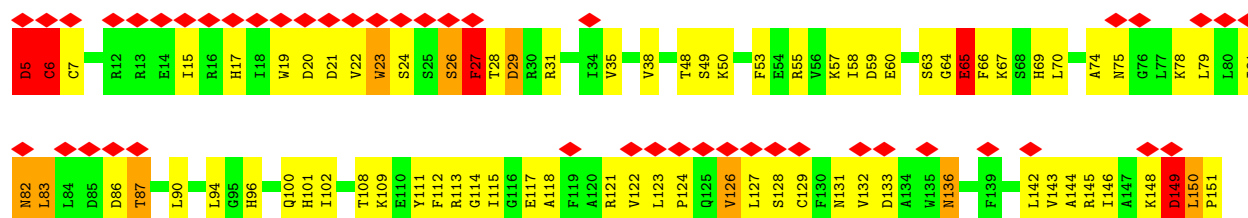


• Molecule 2: HEMOGLOBIN CHAIN D1

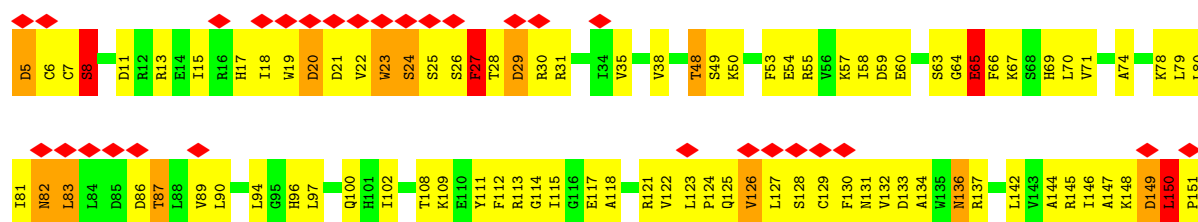




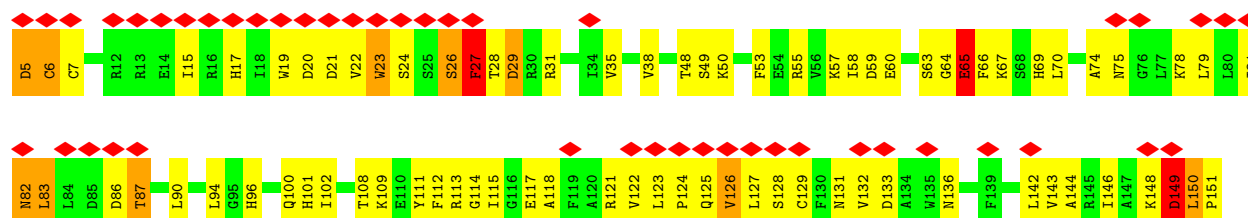
• Molecule 3: EXTRACELLULAR GLOBIN-4



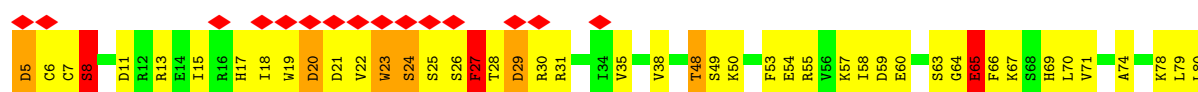
• Molecule 3: EXTRACELLULAR GLOBIN-4

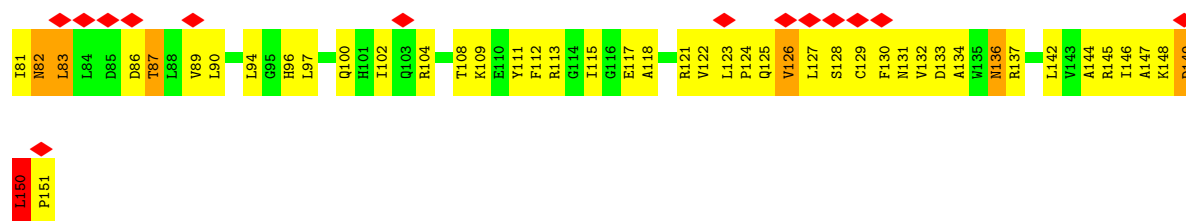


• Molecule 3: EXTRACELLULAR GLOBIN-4

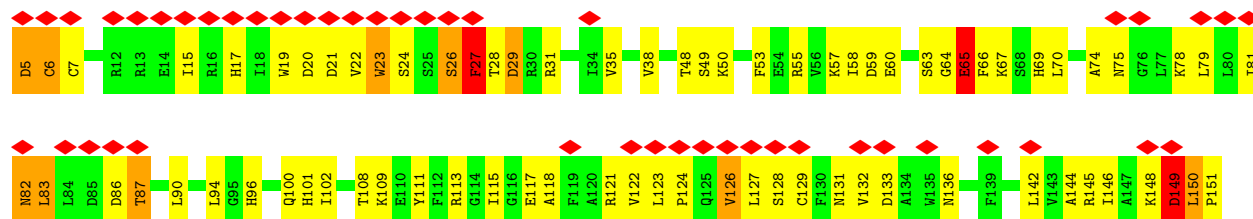


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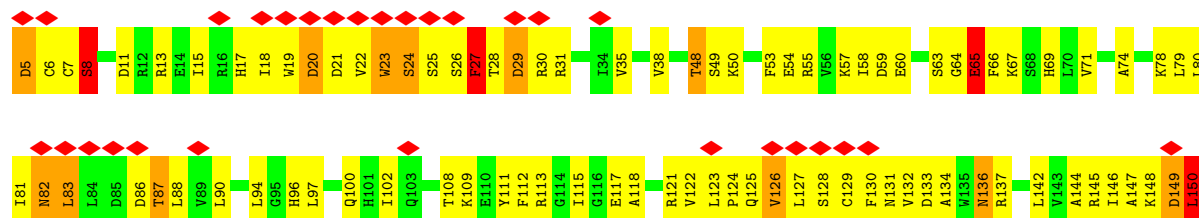
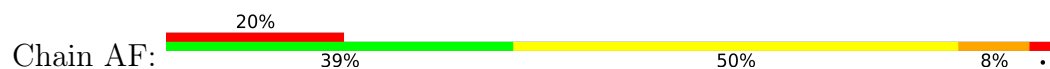




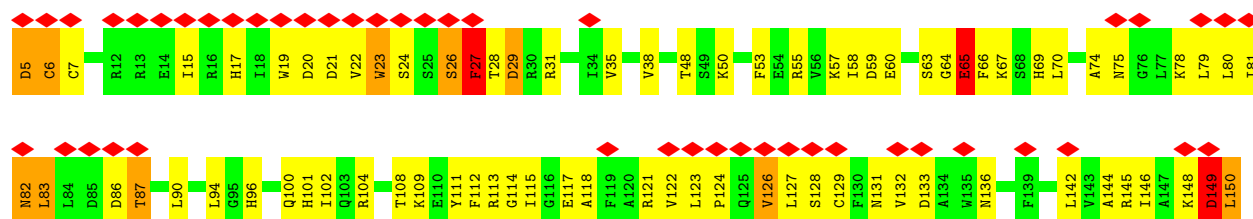
- Molecule 3: EXTRACELLULAR GLOBIN-4



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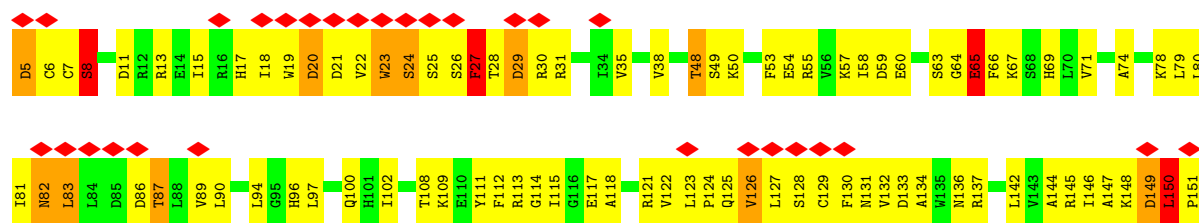


- Molecule 3: EXTRACELLULAR GLOBIN-4

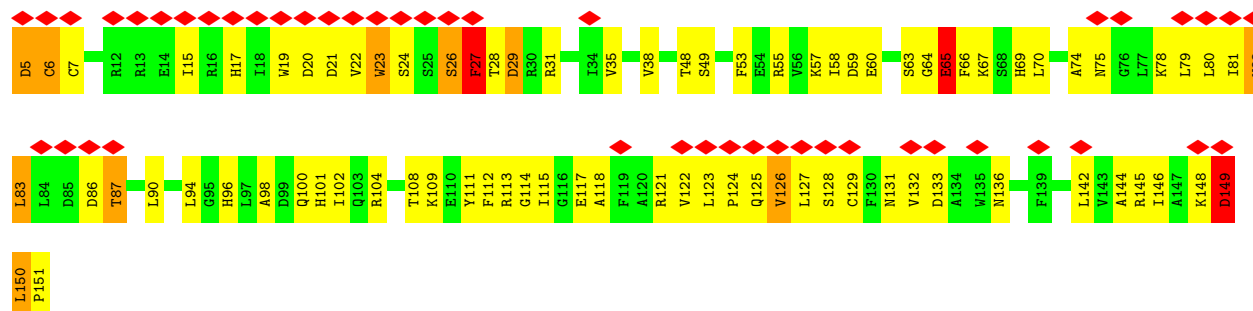


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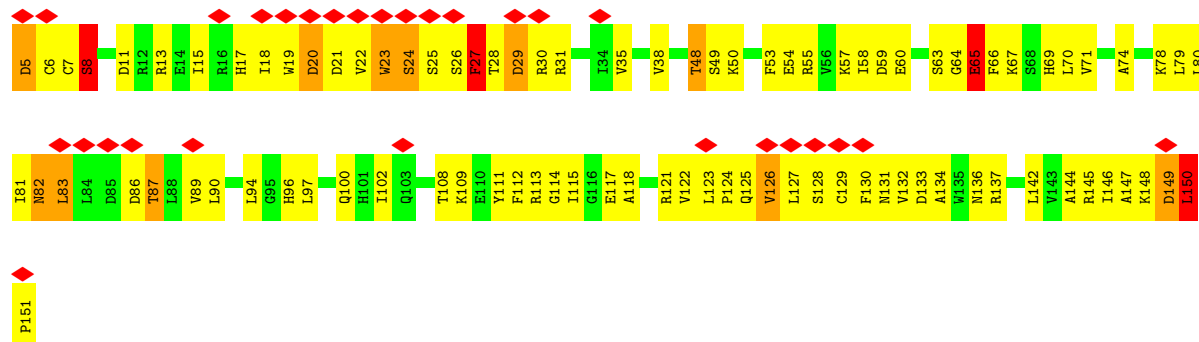




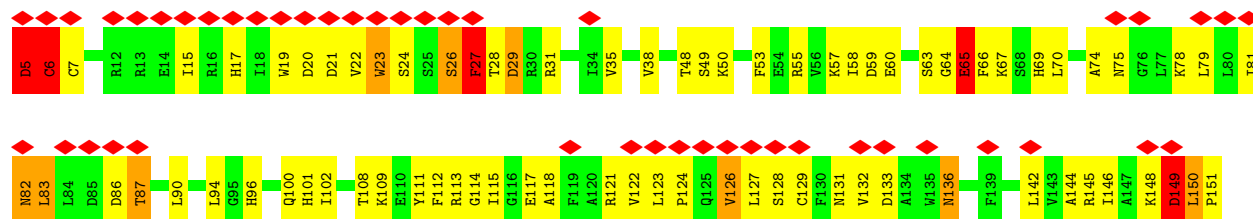
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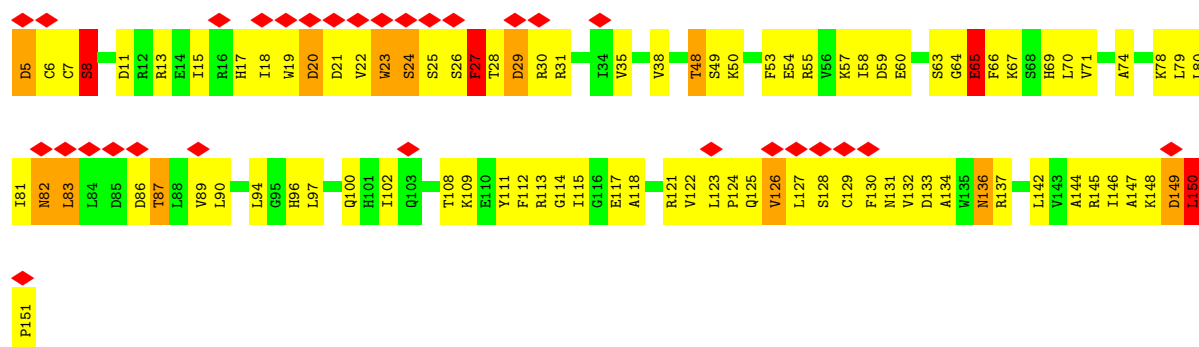


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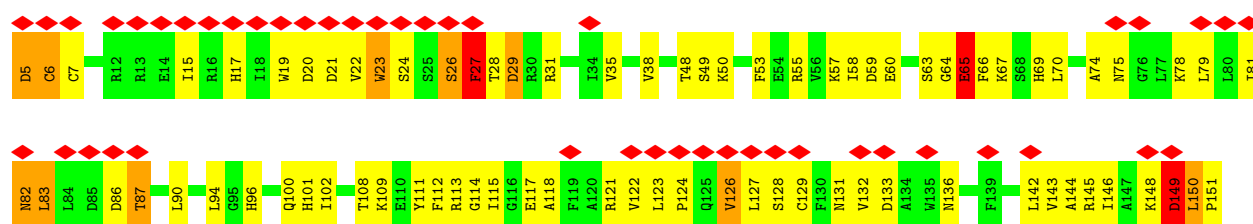


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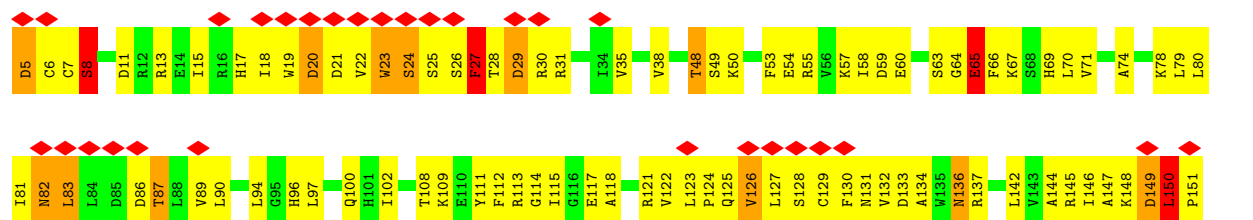




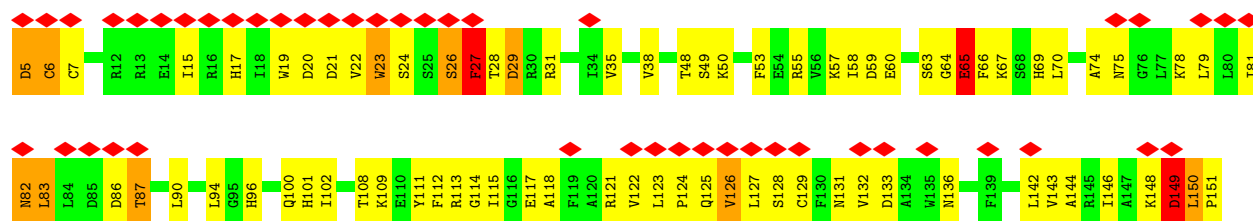
• Molecule 3: EXTRACELLULAR GLOBIN-4



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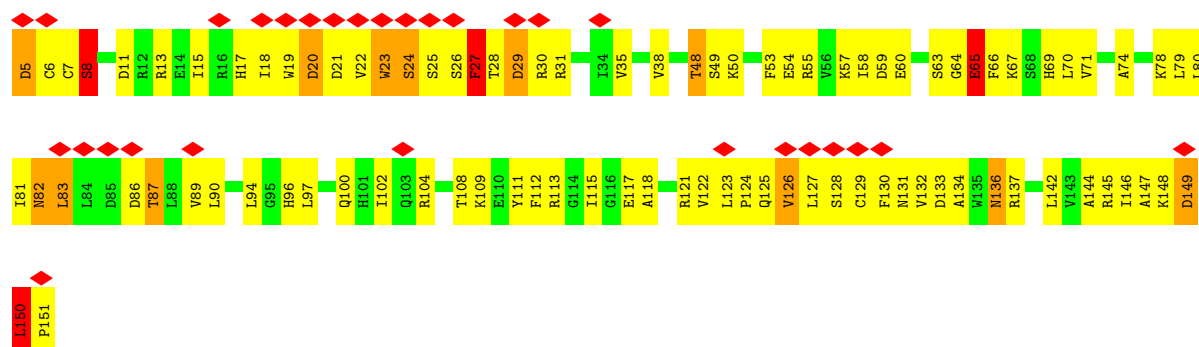


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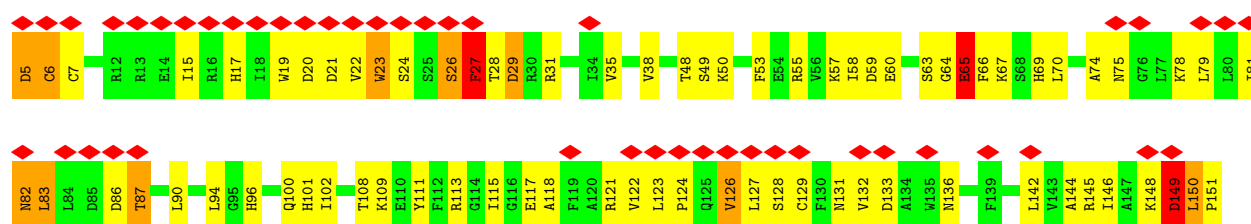


• Molecule 3: EXTRACELLULAR GLOBIN-4

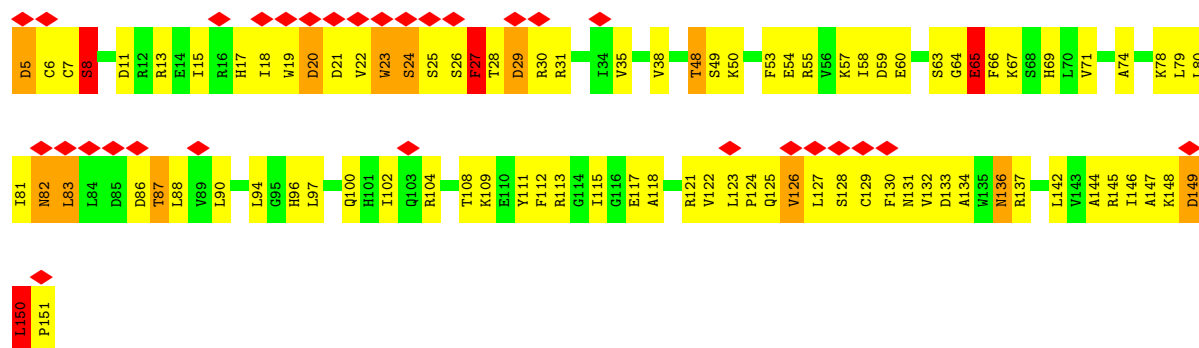




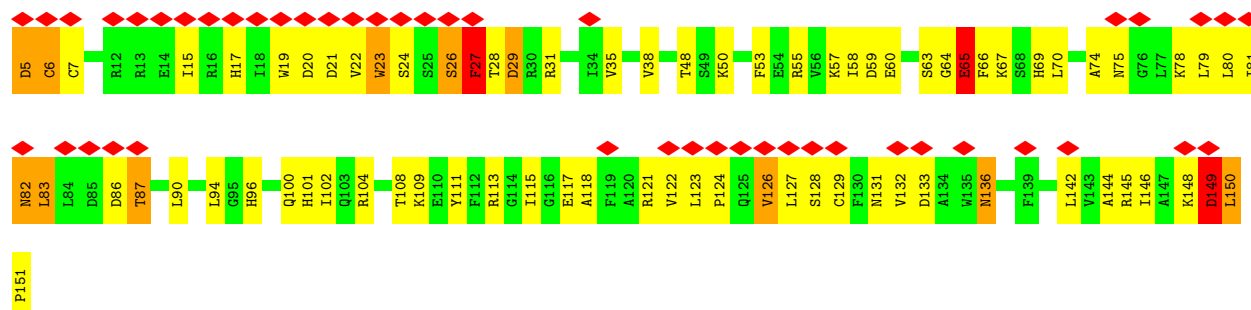
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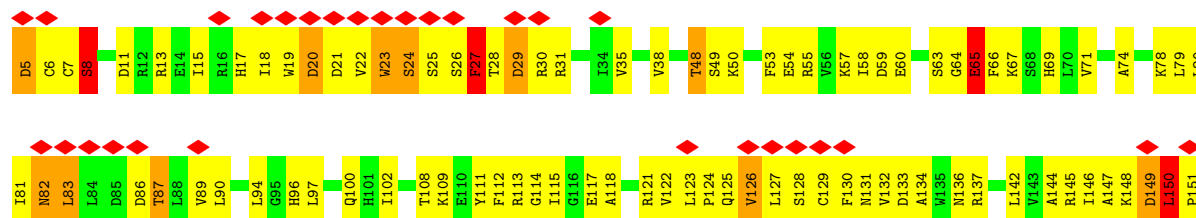
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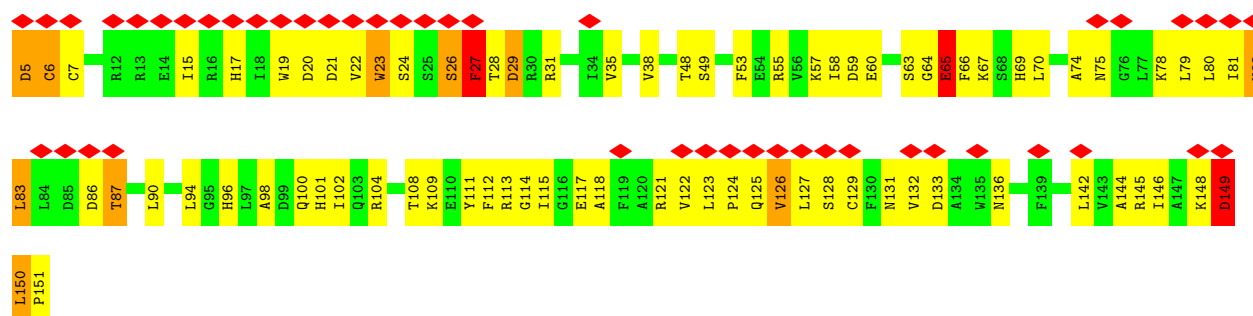
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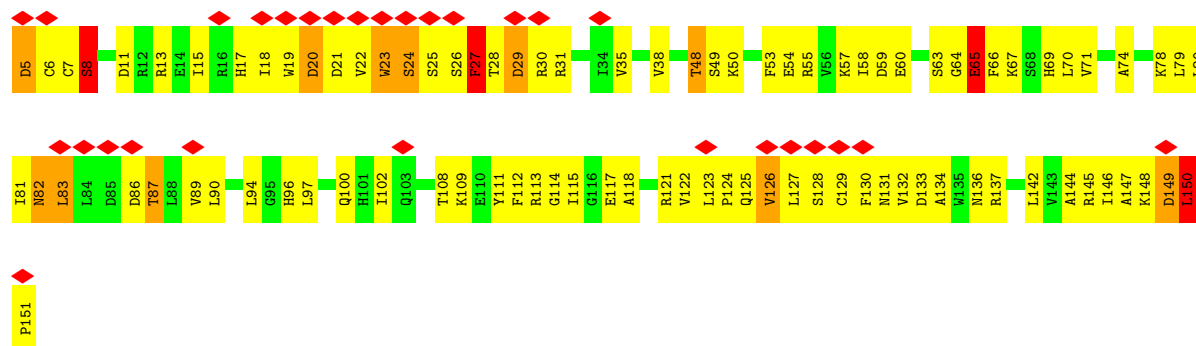
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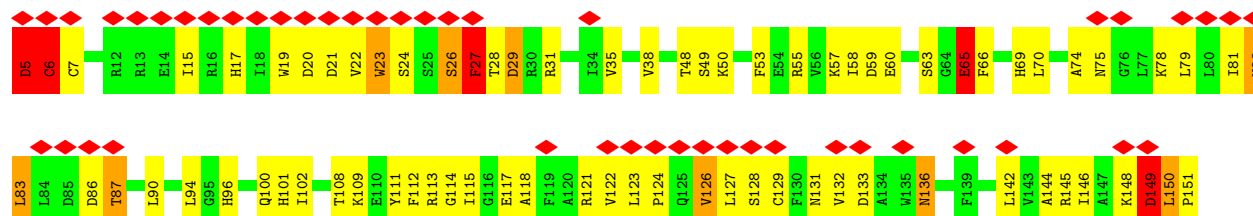
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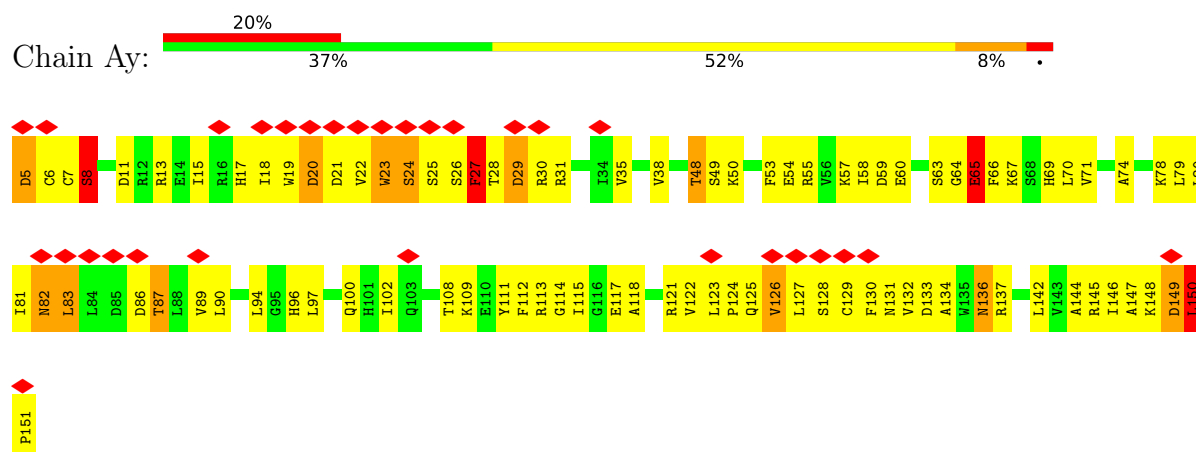
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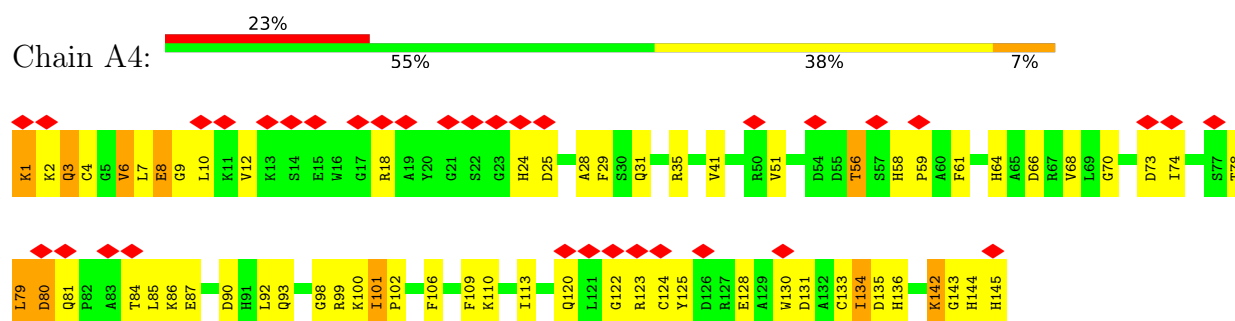
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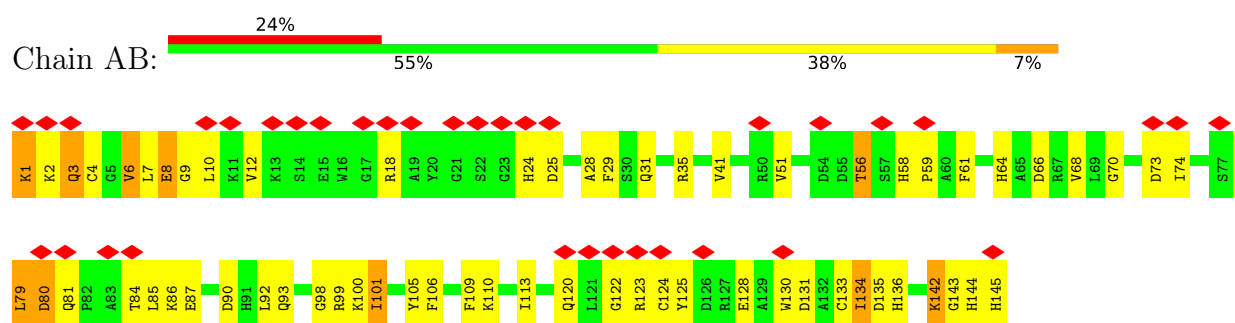
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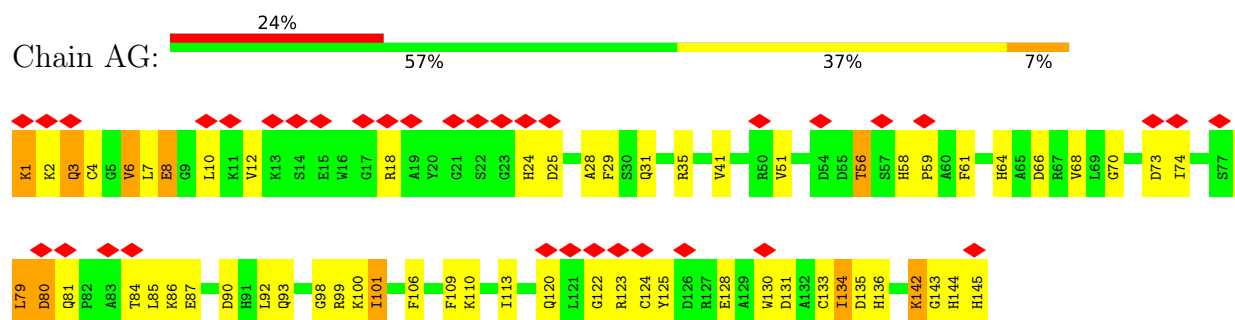
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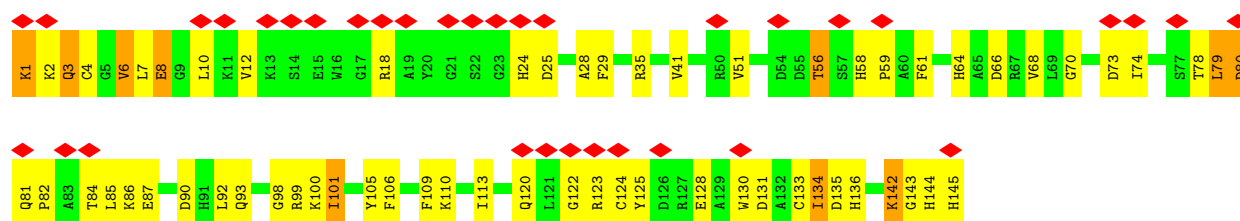
- Molecule 4: EXTRACELLULAR GLOBIN-2



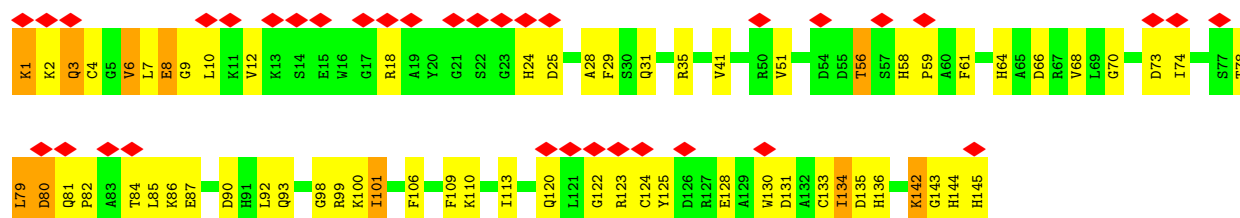
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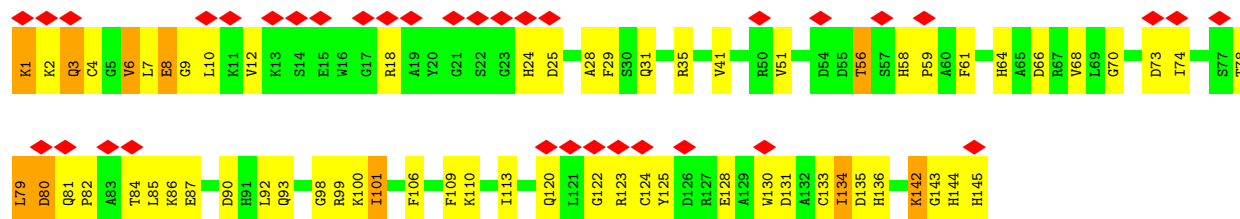
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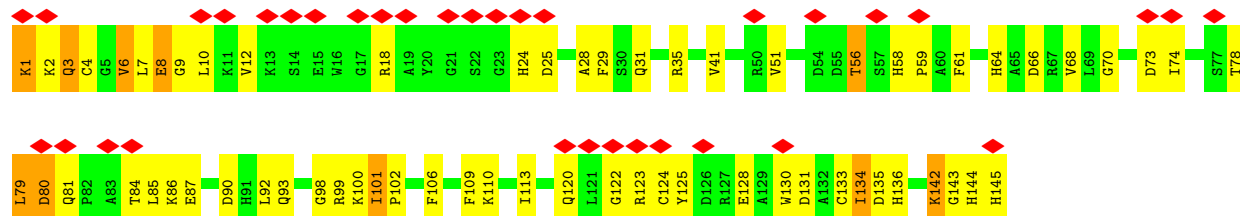
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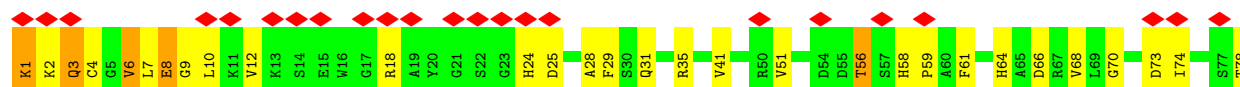
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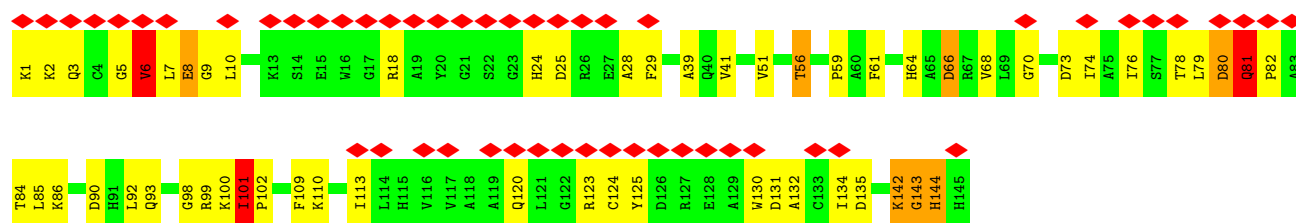
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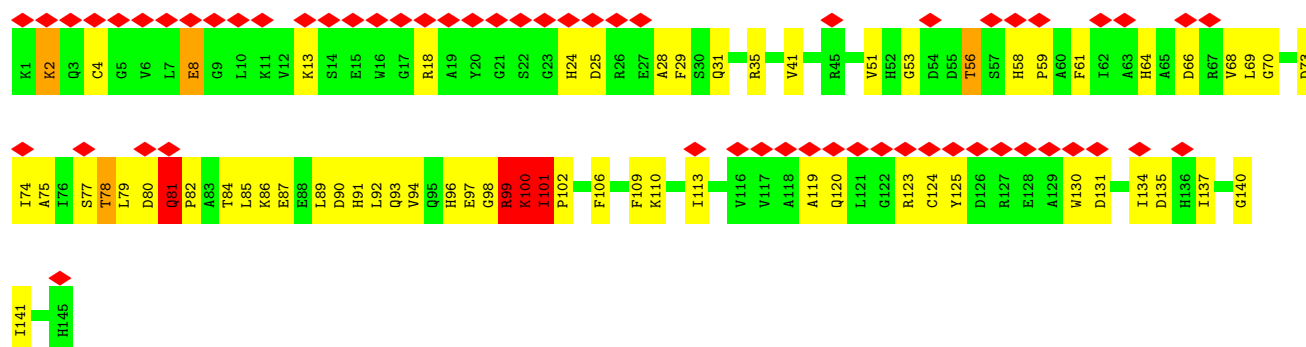
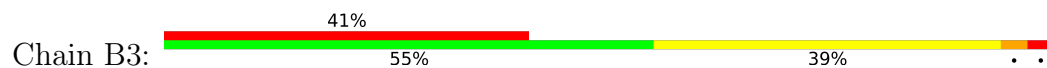
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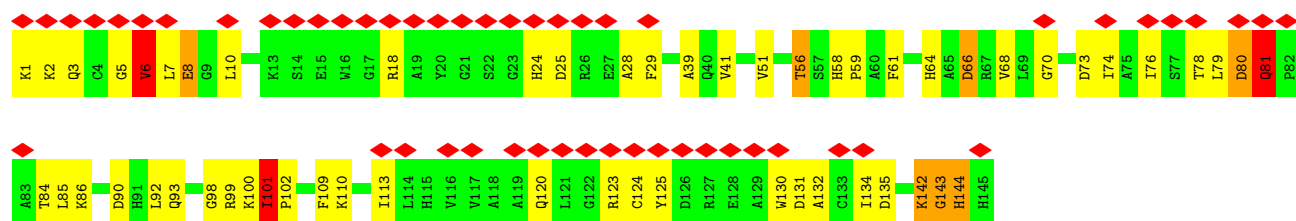
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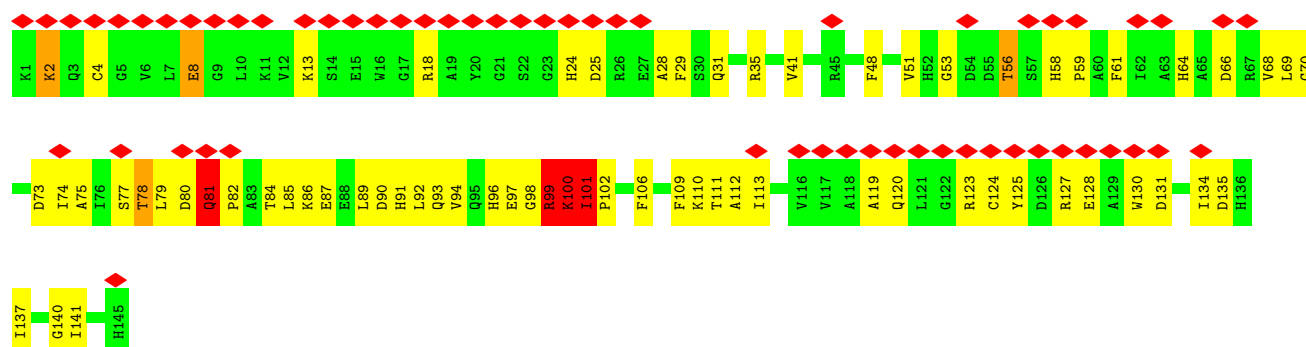
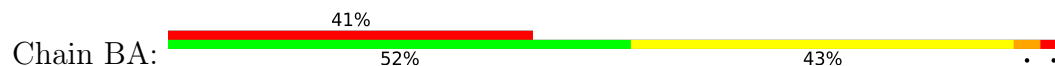
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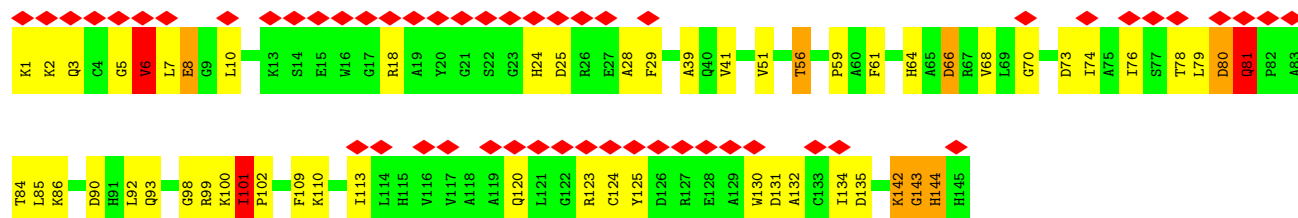


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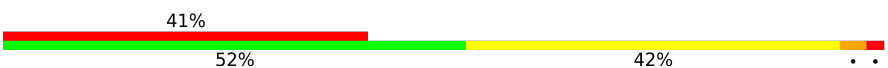


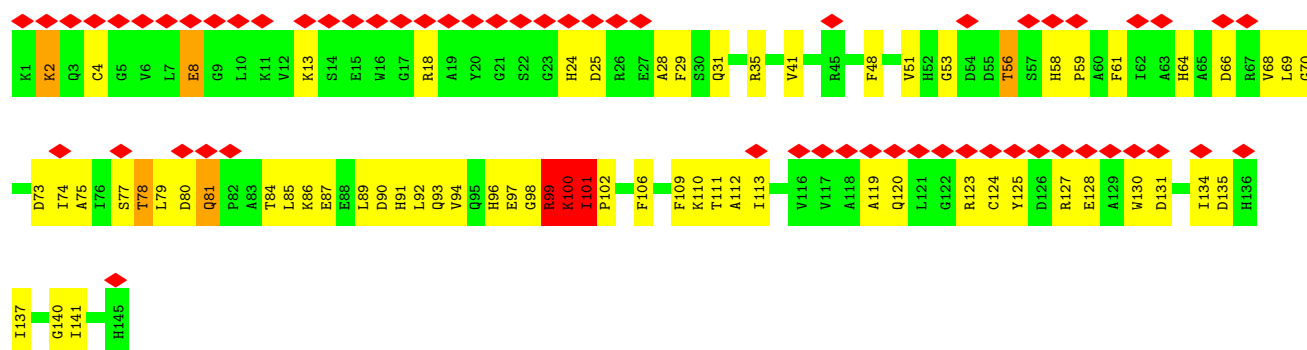
- Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BE: 



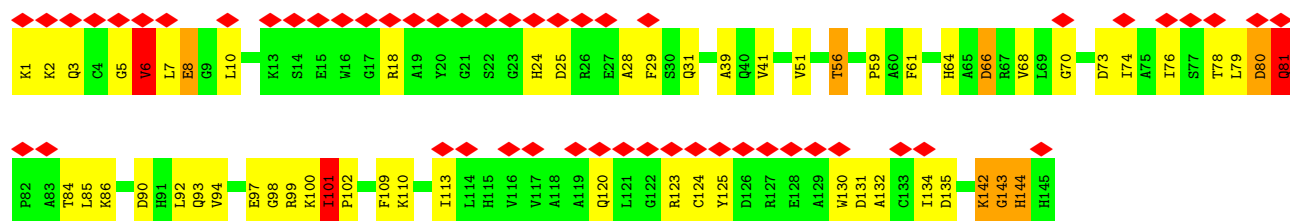
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Chain BF: 



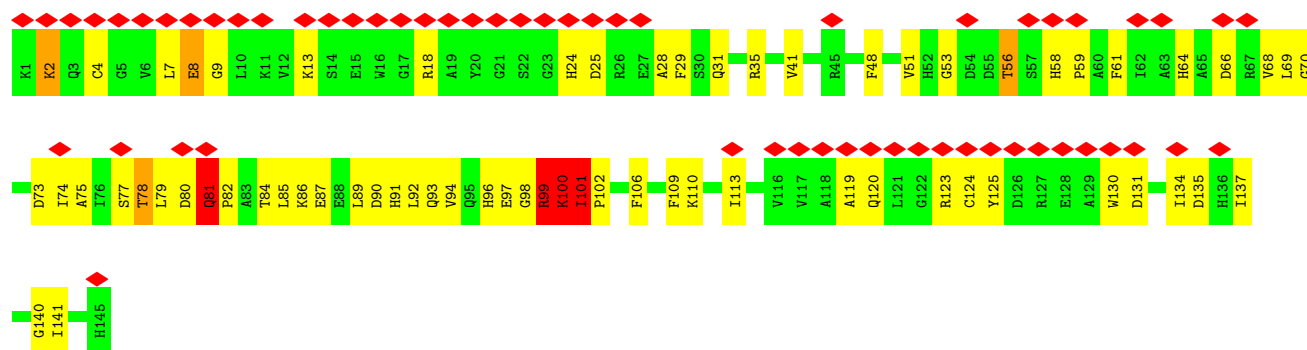
- Molecule 4: EXTRACELLULAR GLOBIN-2

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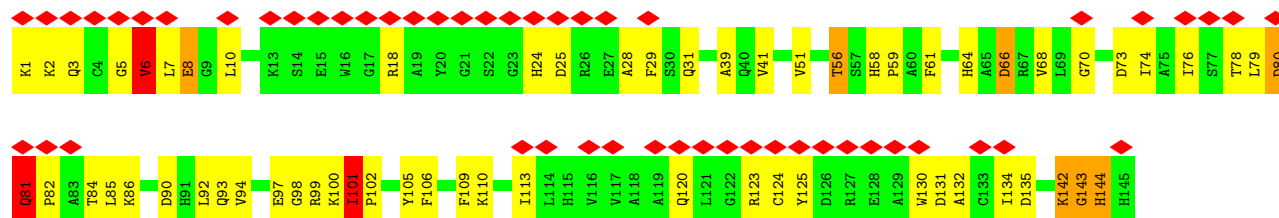
- Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BK: 



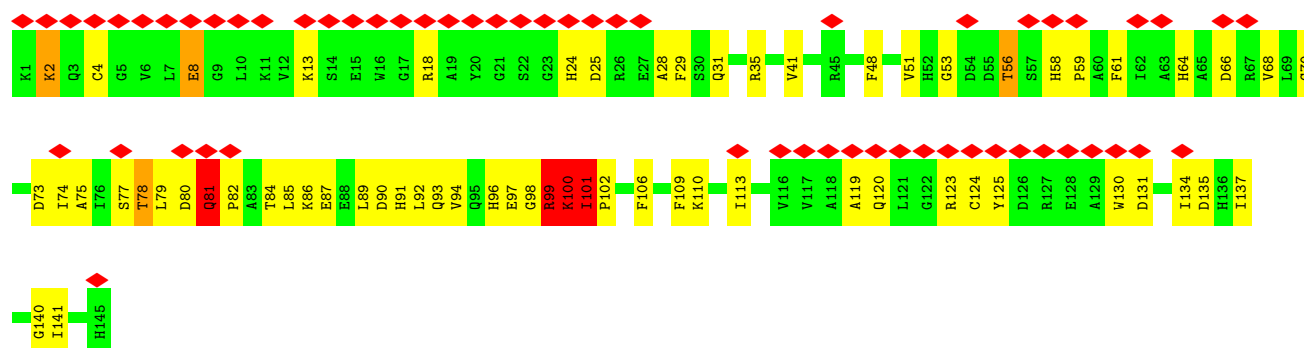
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Chain BO: 



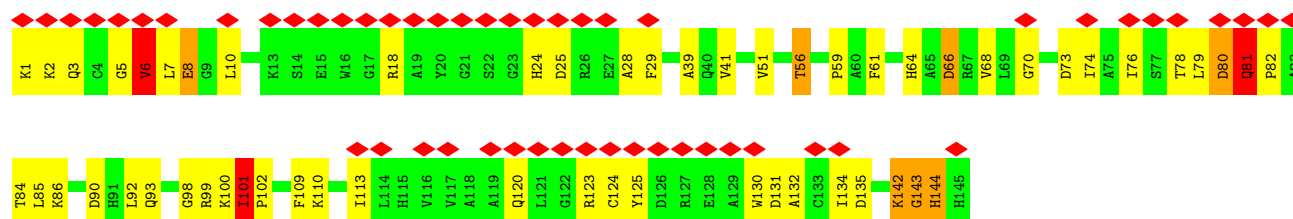
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Chain BP: 



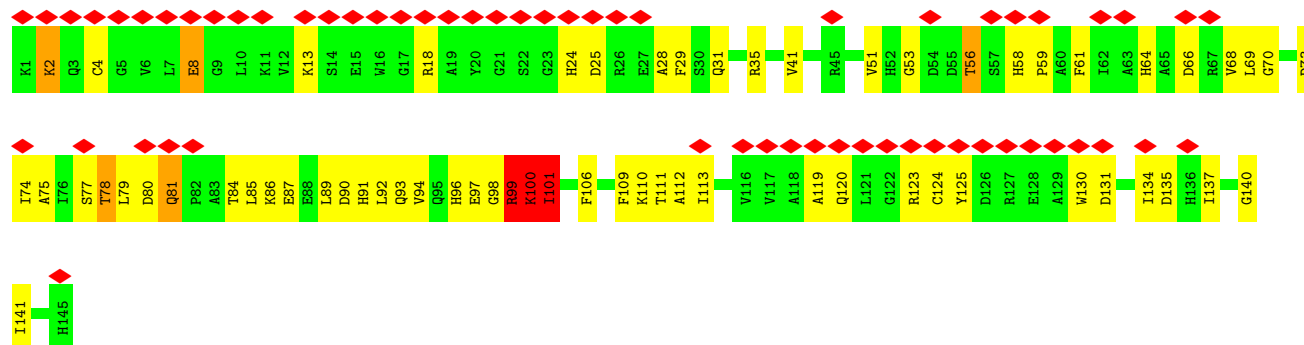
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Chain BT: 



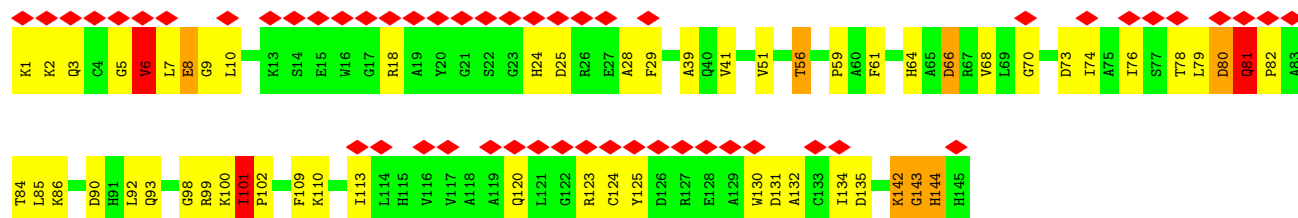
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Chain BU: 



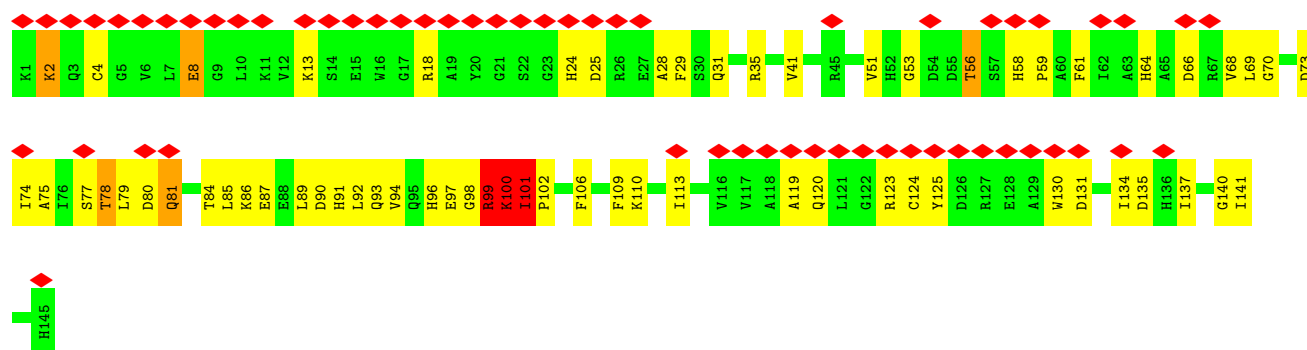
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Chain BY: 



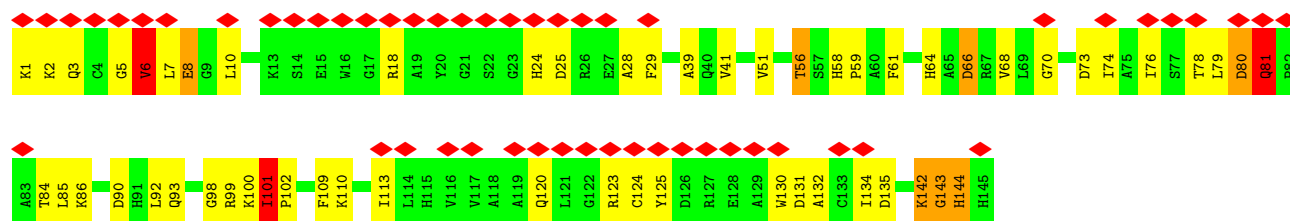
- Molecule 4: EXTRACELLULAR GLOBIN-2

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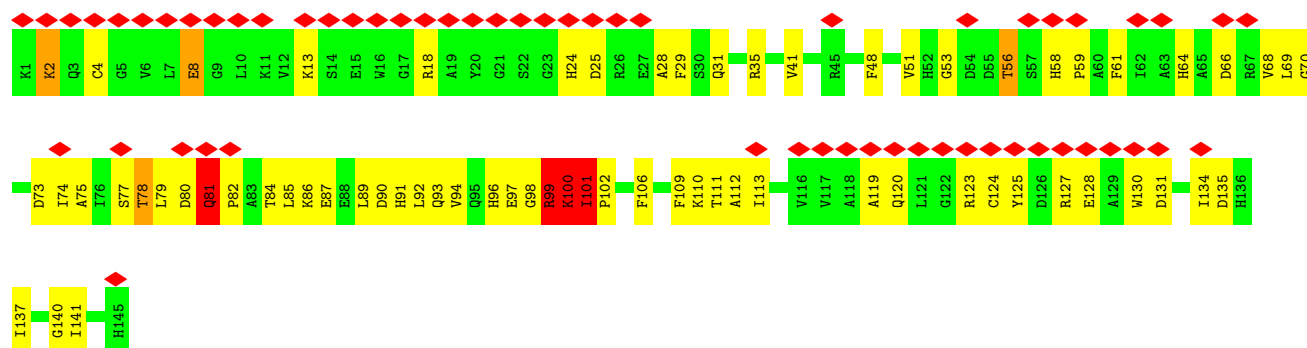
- Molecule 4: EXTRACELLULAR GLOBIN-2

Chain Bd: 

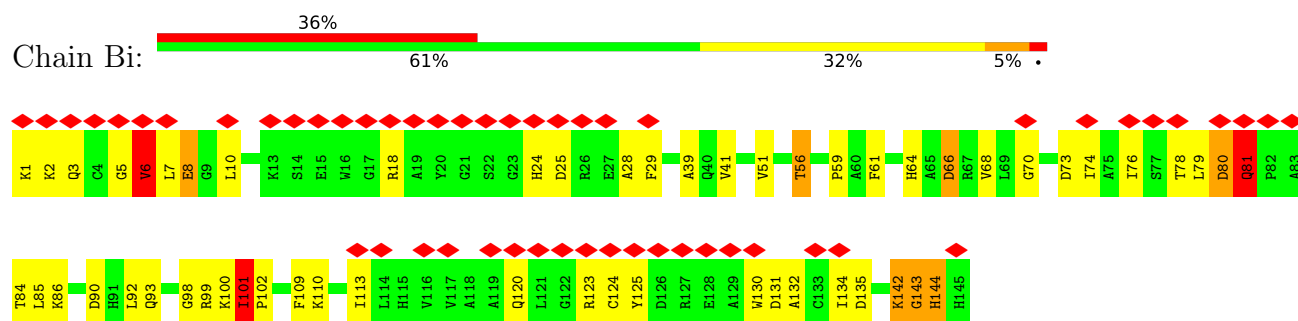


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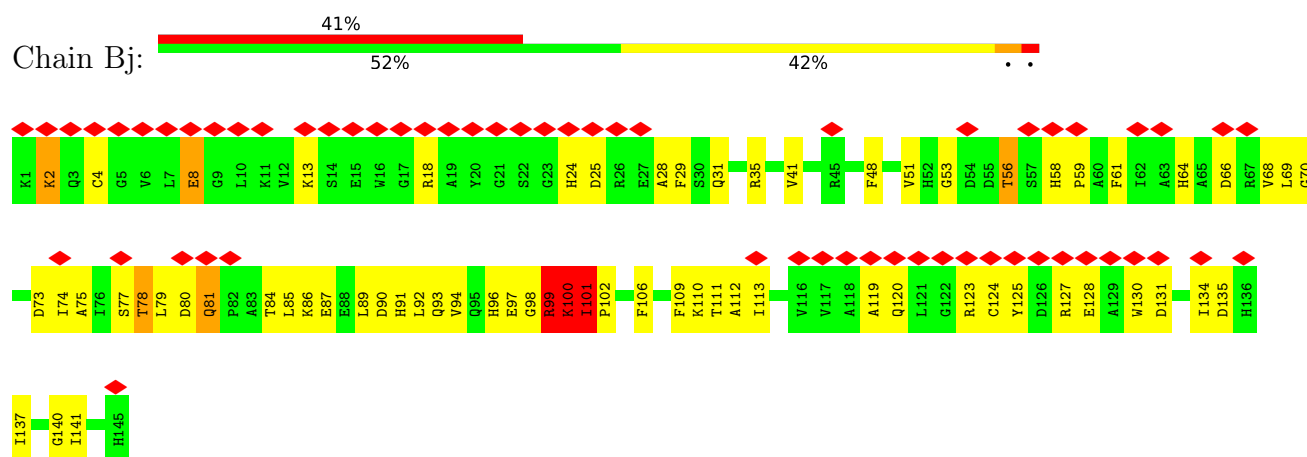
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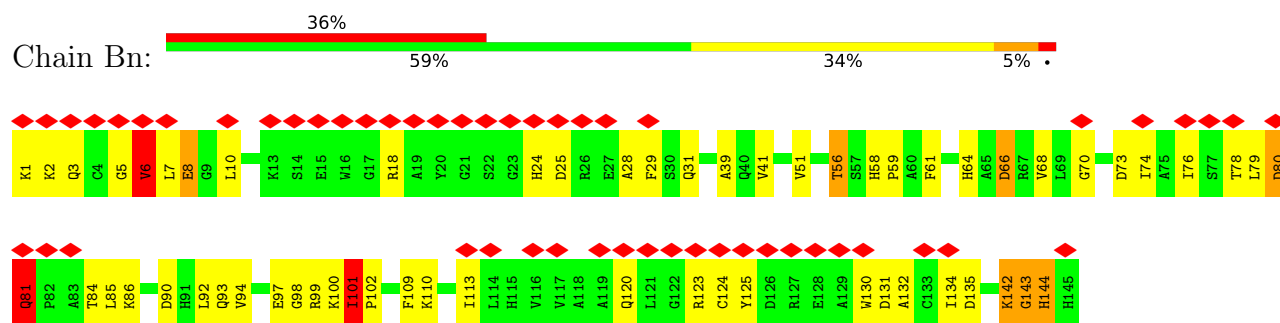
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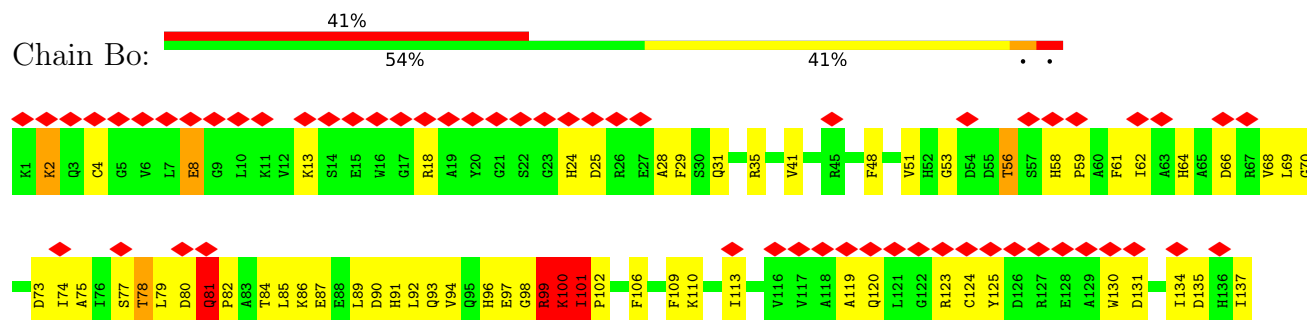
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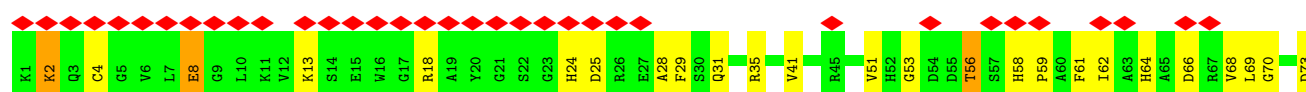


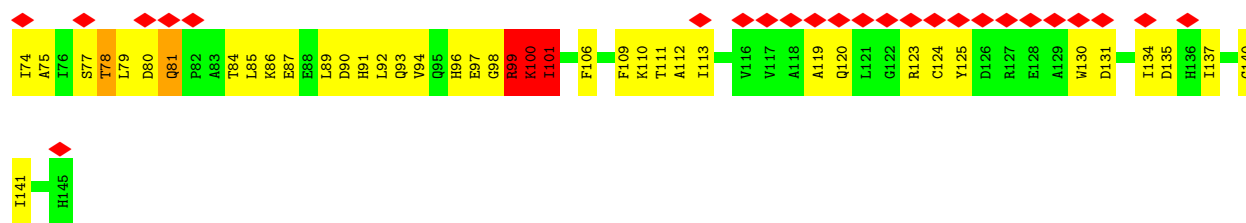
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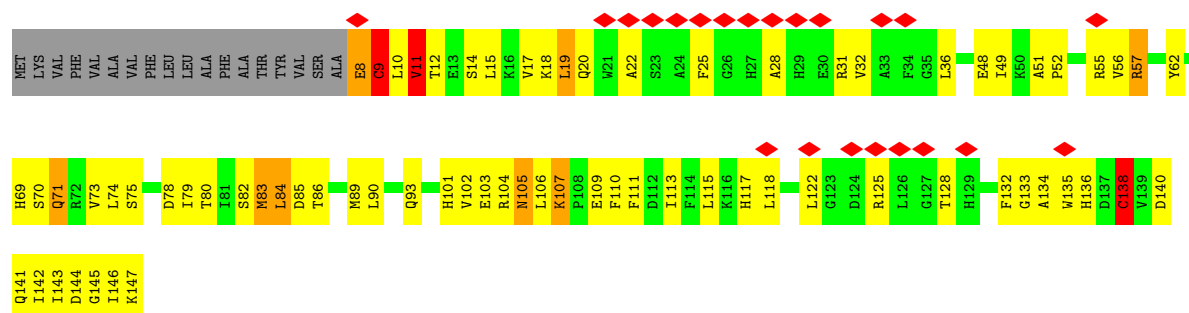
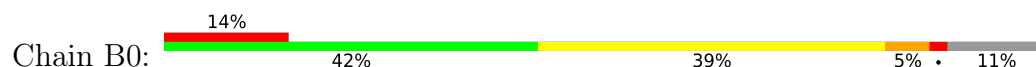
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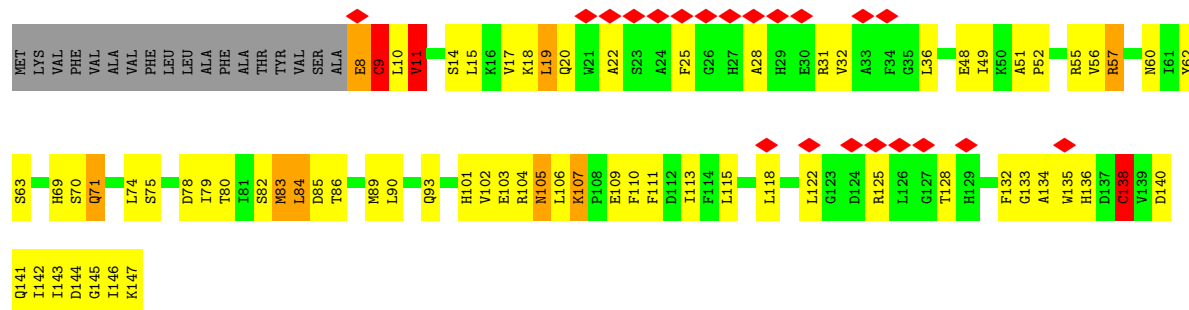
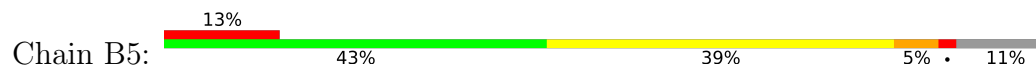




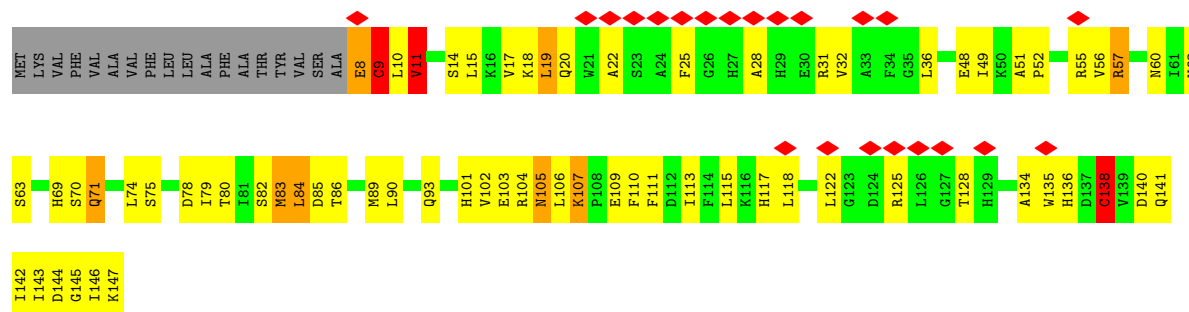
- Molecule 5: HEMOGLOBIN CHAIN D1



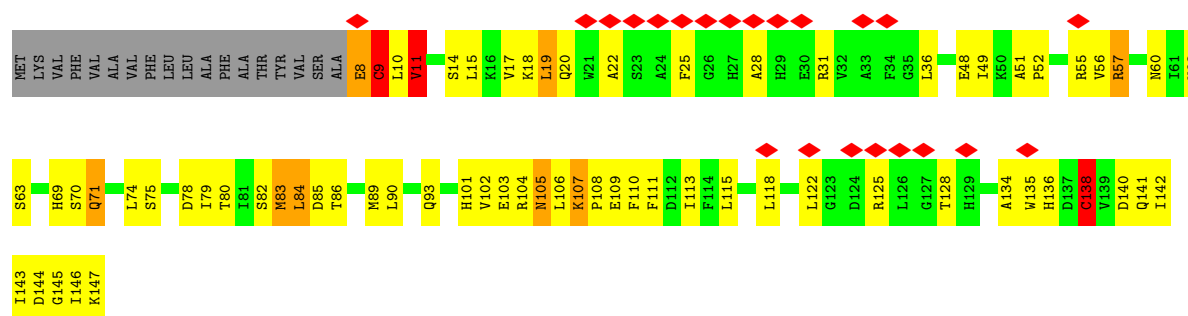
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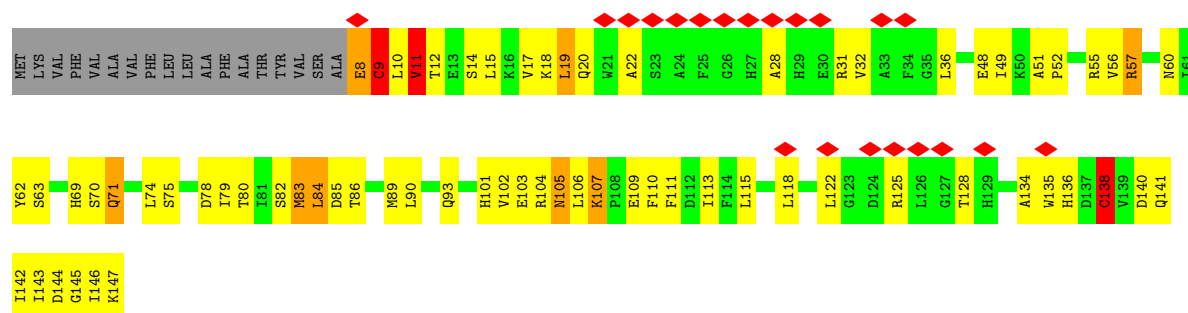
- Molecule 5: HEMOGLOBIN CHAIN D1



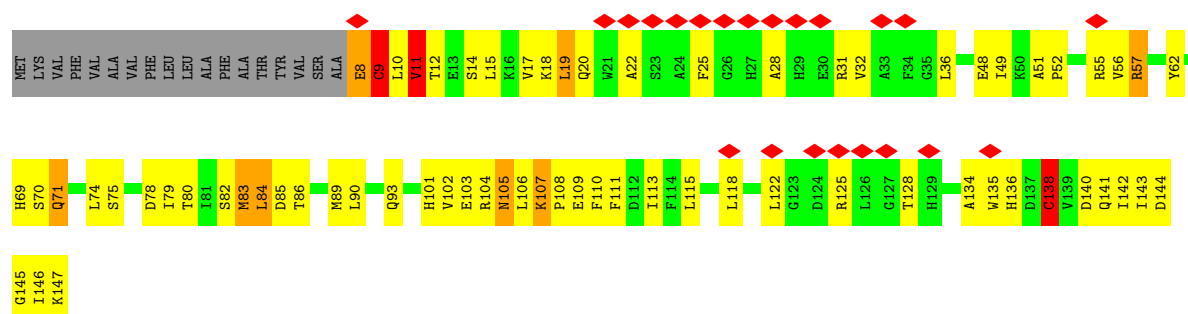
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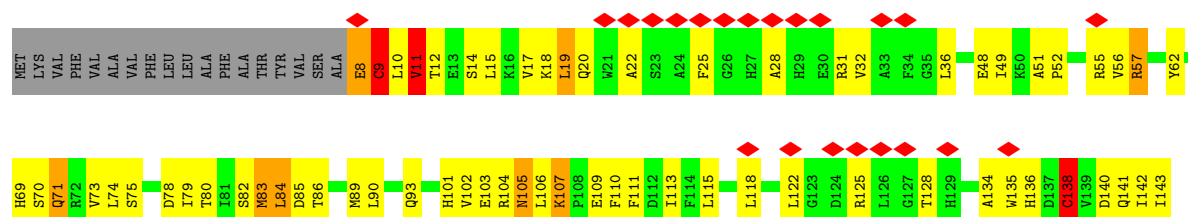
• Molecule 5: HEMOGLOBIN CHAIN D1



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• Molecule 5: HEMOGLOBIN CHAIN D1



D144
G145
I146
K147

• Molecule 5: HEMOGLOBIN CHAIN D1



MET LYS VAL PHE VAL VAL VAL PHE LEU LEU ALA ALA PHE THR TYR VAL SER ALA E8 C9 L10 L11 S14 S15 K16 V17 K18 L19 Q20 W21 A22 S23 A24 F25 G26 G27 H27 A28 H29 E30 R31 V32 A33 F34 G35 L36 E48 I49 A134 R50 A51 P52 R55 V56 R57 Y62 H69

S70 Q71 L74 S75 D78 I79 T80 I81 S82 M83 L84 D85 T86 M89 L90 Q93 H101 V102 E103 R104 N105 L106 K107 P108 E109 F110 F111 I113 F114 L115 L118 L122 G123 D124 R125 L126 G127 T128 H129 F132 G133 A134 W135 H136 D137 C138 V139 D140 Q141 I142 I143

D144
G145
I146
K147

• Molecule 5: HEMOGLOBIN CHAIN D1

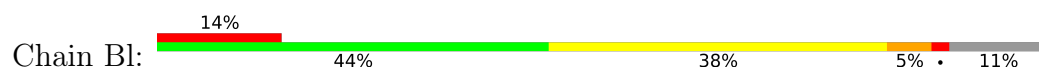


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S63 H69 Q71 L74 S75 D78 I79 T80 I81 S82 M83 L84 D85 T86 M89 L90 Q93 H101 V102 E103 R104 N105 L106 K107 P108 E109 F110 F111 I113 F114 L115 L118 L122 G123 D124 R125 L126 G127 T128 H129 A134 W135 H136 D137 C138 V139 D140 Q141

I142
I143
D144
G145
I146
K147

• Molecule 5: HEMOGLOBIN CHAIN D1



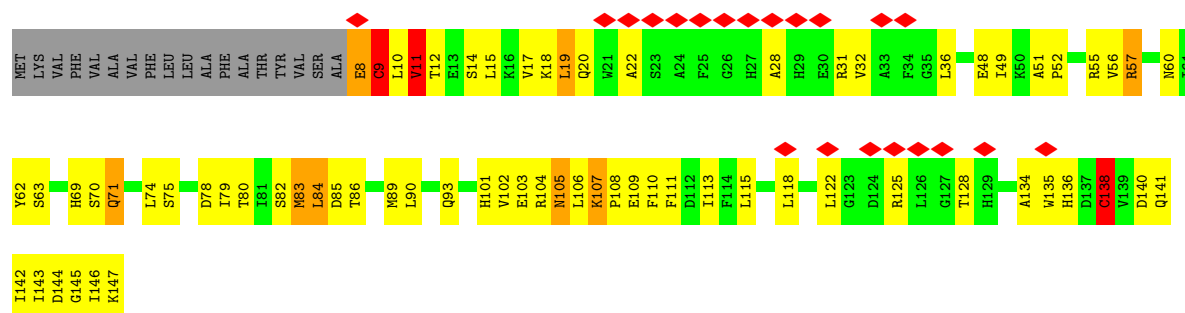
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Y62 S63 H69 Q71 L74 S75 D78 I79 T80 I81 S82 M83 L84 D85 T86 M89 L90 Q93 H101 V102 E103 R104 N105 L106 K107 P108 E109 F110 F111 I113 F114 L115 L118 L122 G123 D124 R125 L126 G127 T128 H129 A134 W135 H136 D137 C138 V139 D140 Q141

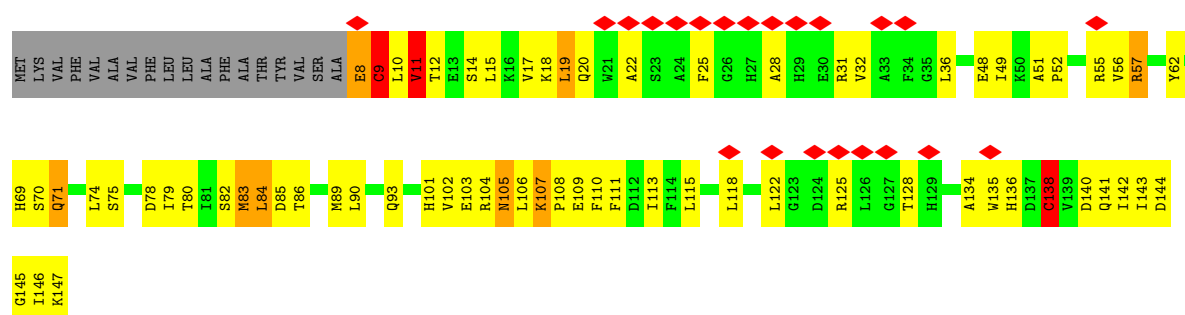
I142
I143
D144
G145
I146
K147

• Molecule 5: HEMOGLOBIN CHAIN D1

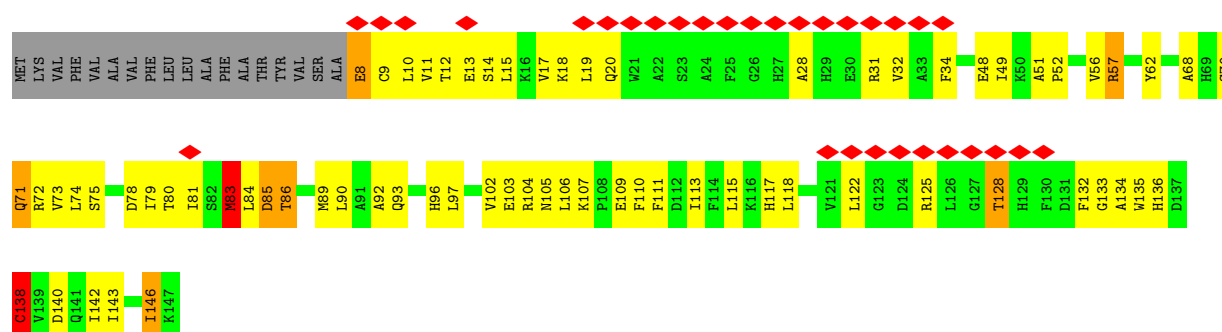




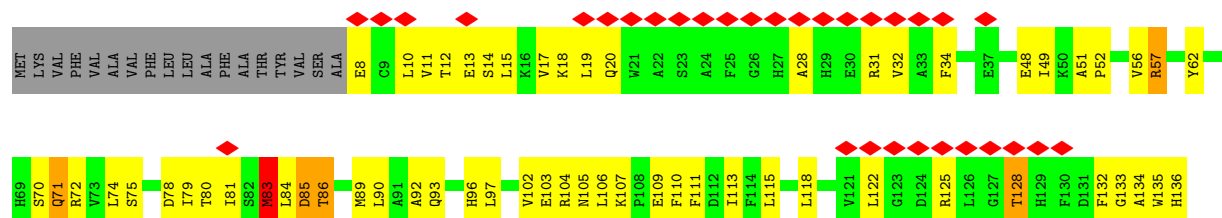
• Molecule 5: HEMOGLOBIN CHAIN D1



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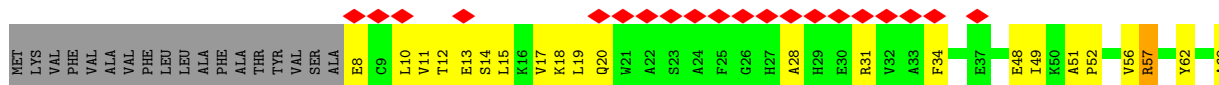


• Molecule 5: HEMOGLOBIN CHAIN D1

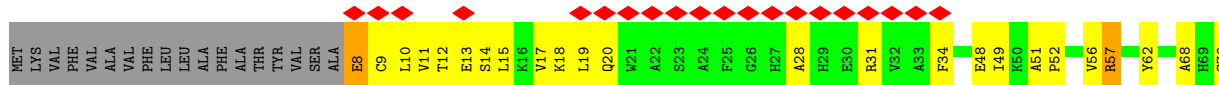




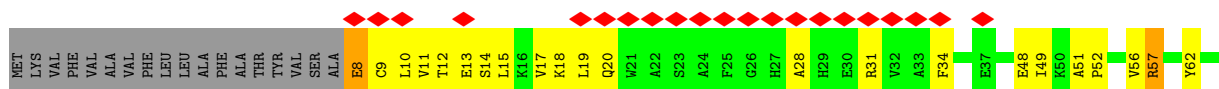
• Molecule 5: HEMOGLOBIN CHAIN D1



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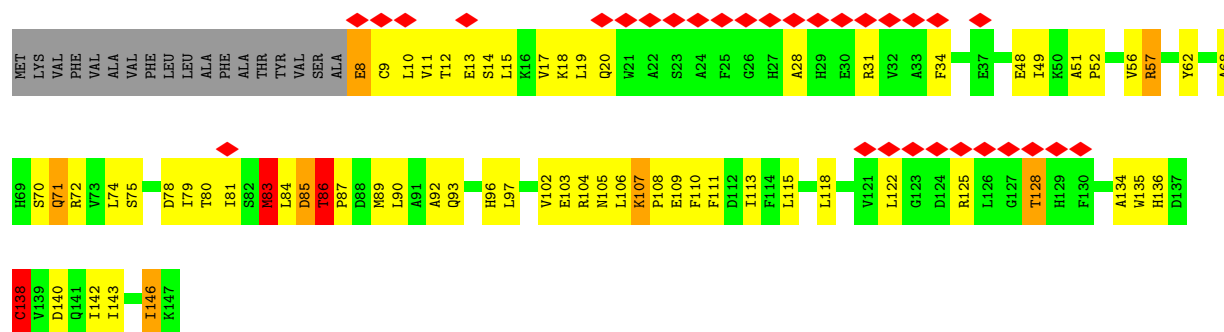


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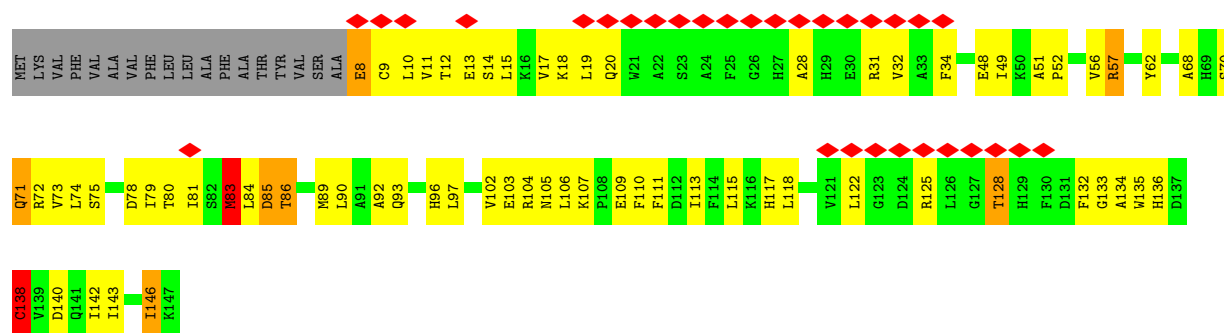


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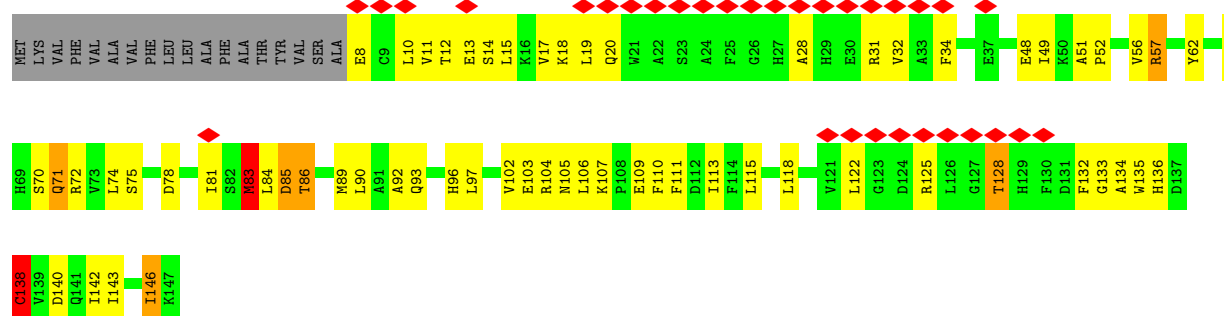




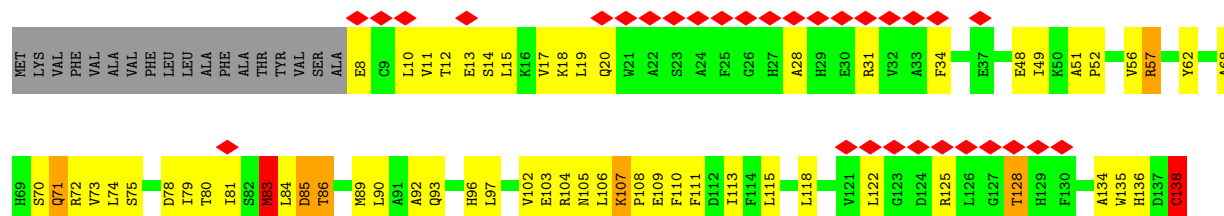
- Molecule 5: HEMOGLOBIN CHAIN D1



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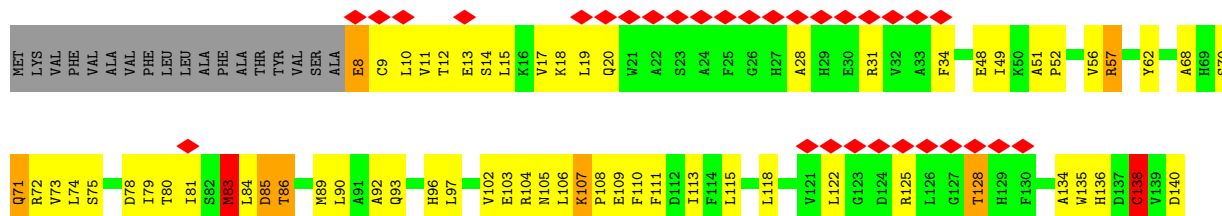


- Molecule 5: HEMOGLOBIN CHAIN D1

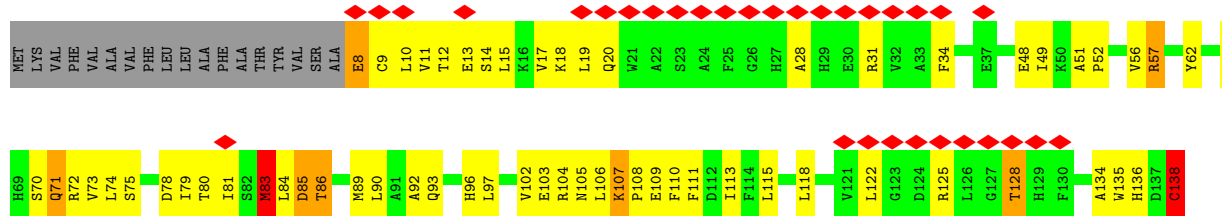




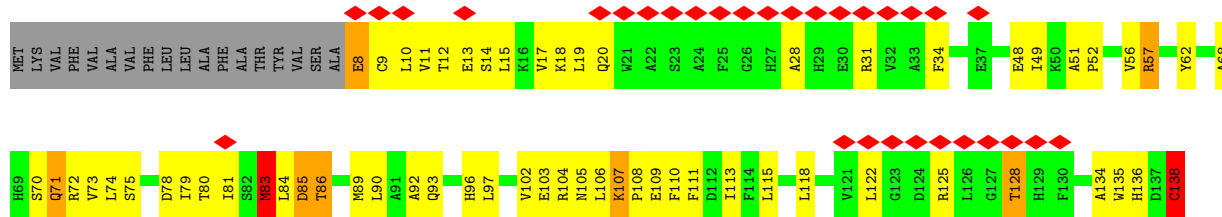
• Molecule 5: HEMOGLOBIN CHAIN D1



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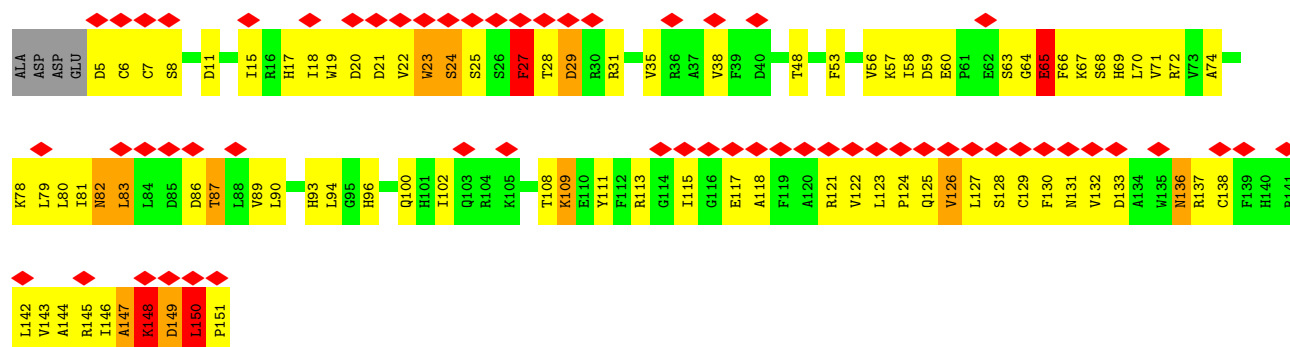


• Molecule 5: HEMOGLOBIN CHAIN D1

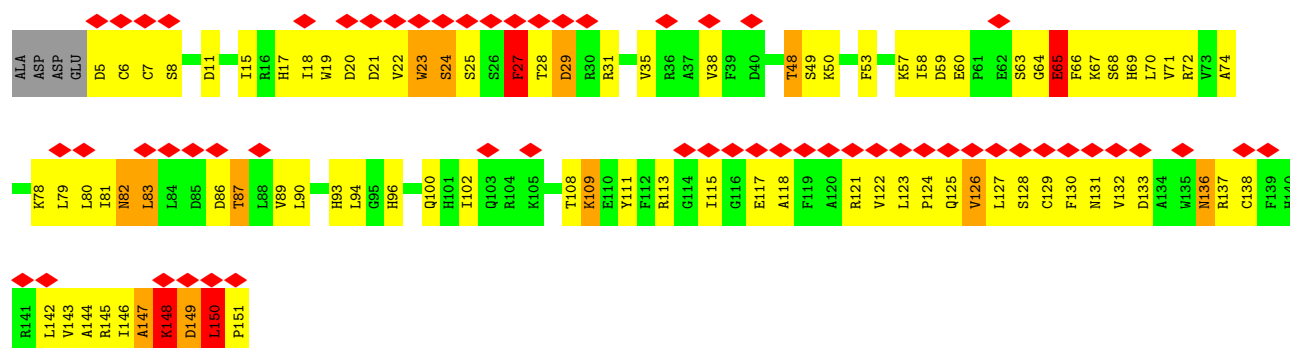


• Molecule 6: EXTRACELLULAR GLOBIN-4

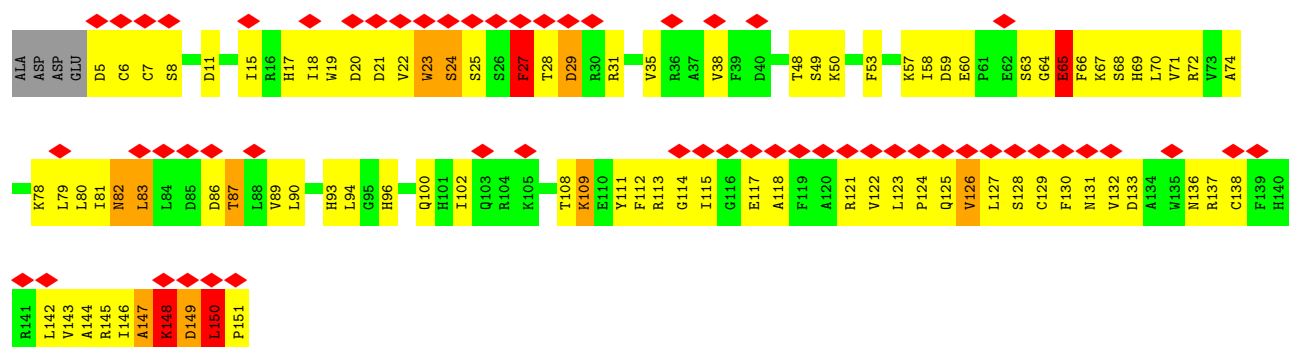




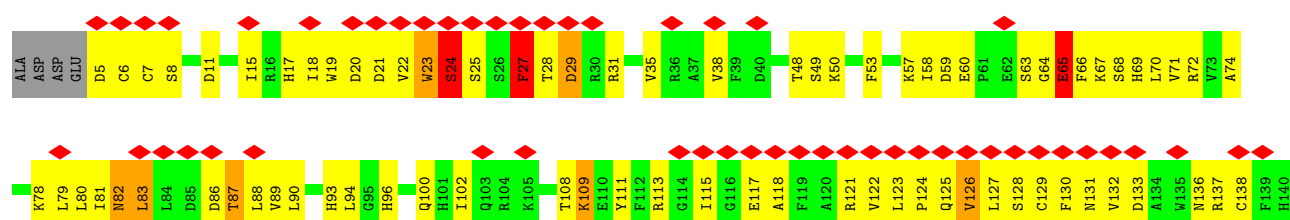
• Molecule 6: EXTRACELLULAR GLOBIN-4



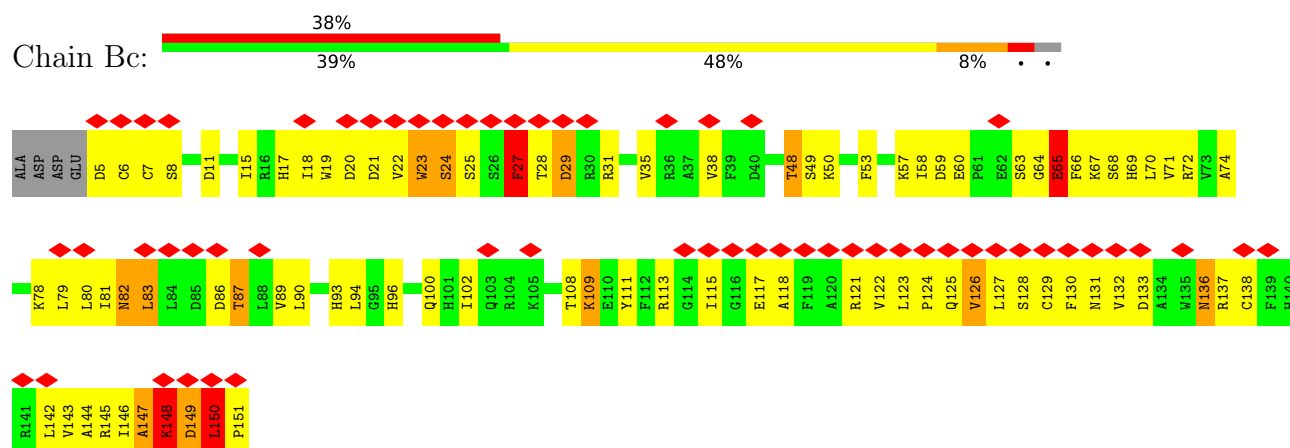
• Molecule 6: EXTRACELLULAR GLOBIN-4



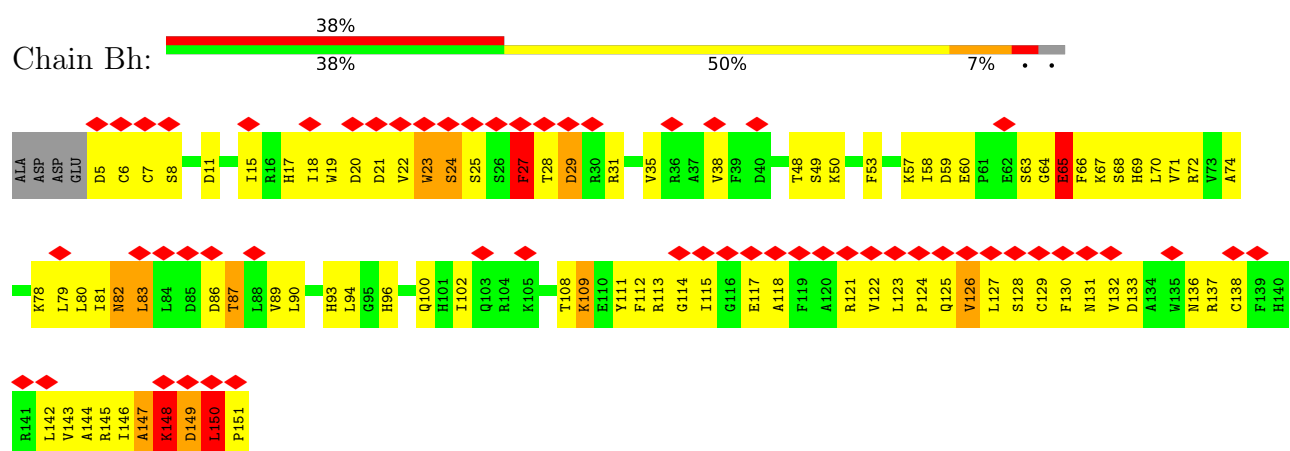
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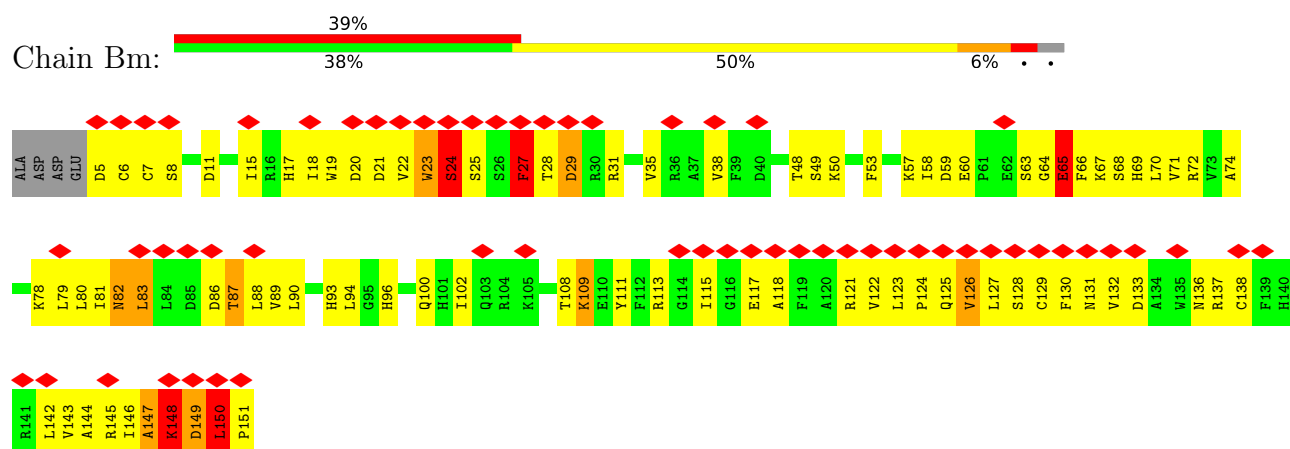




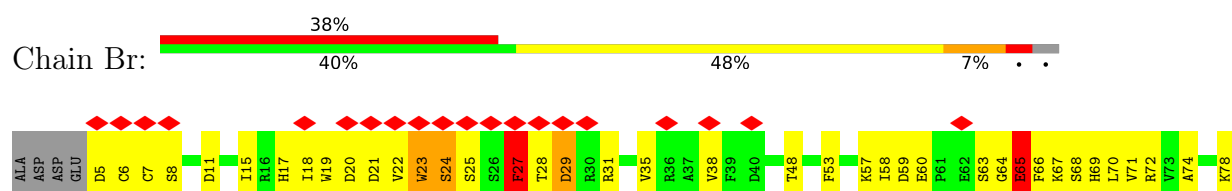
- Molecule 6: EXTRACELLULAR GLOBIN-4

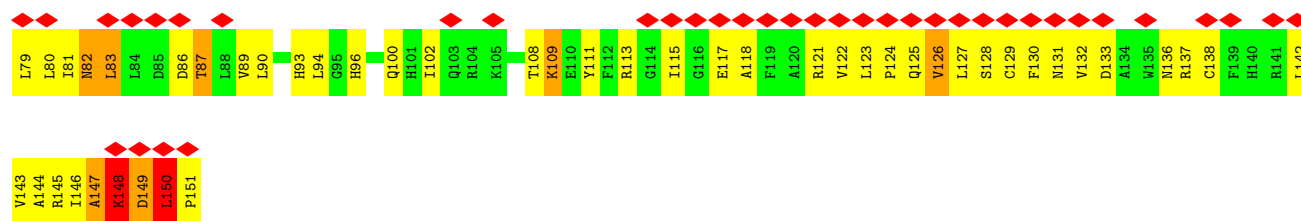


- Molecule 6: EXTRACELLULAR GLOBIN-4

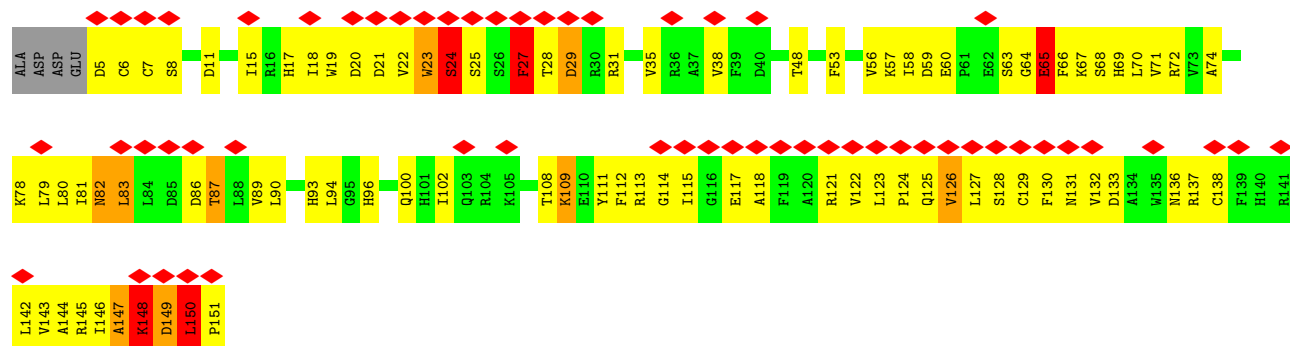


- Molecule 6: EXTRACELLULAR GLOBIN-4

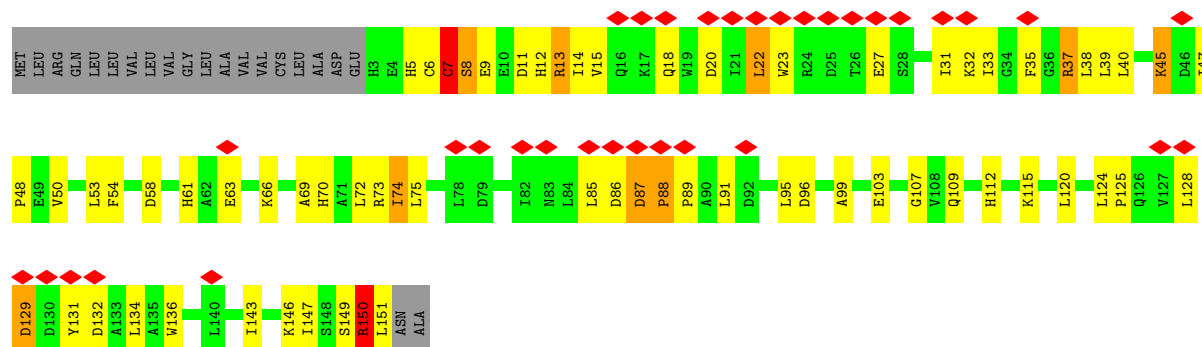




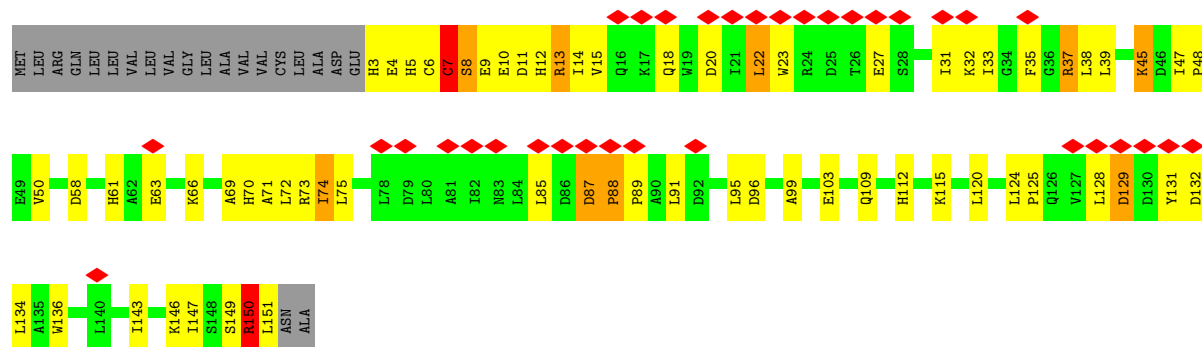
• Molecule 6: EXTRACELLULAR GLOBIN-4



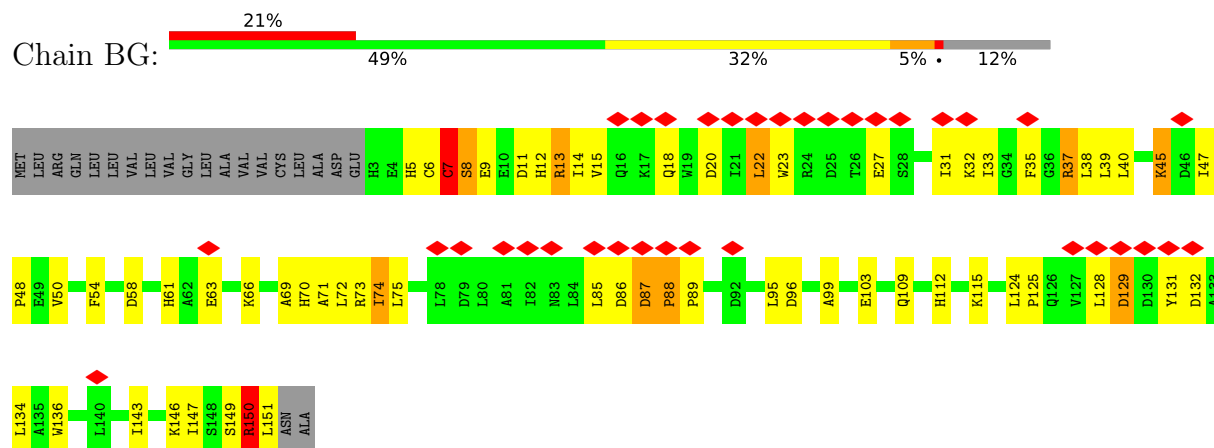
• Molecule 7: EXTRACELLULAR GLOBIN-3



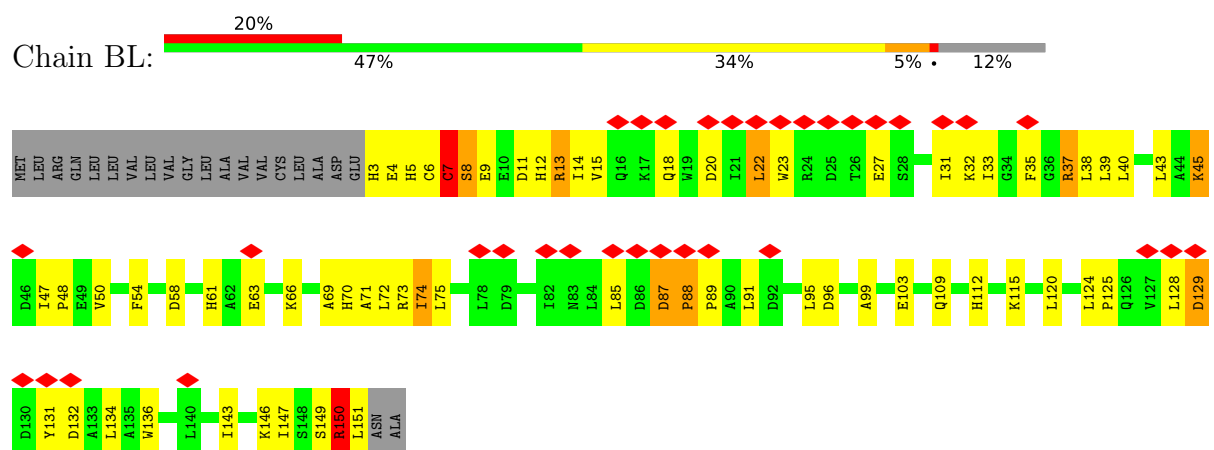
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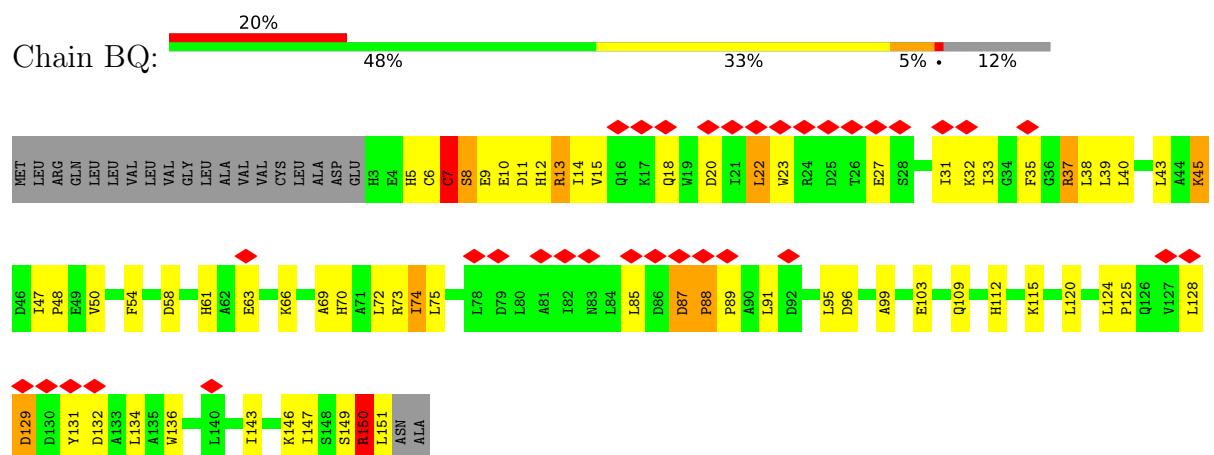
• Molecule 7: EXTRACELLULAR GLOBIN-3



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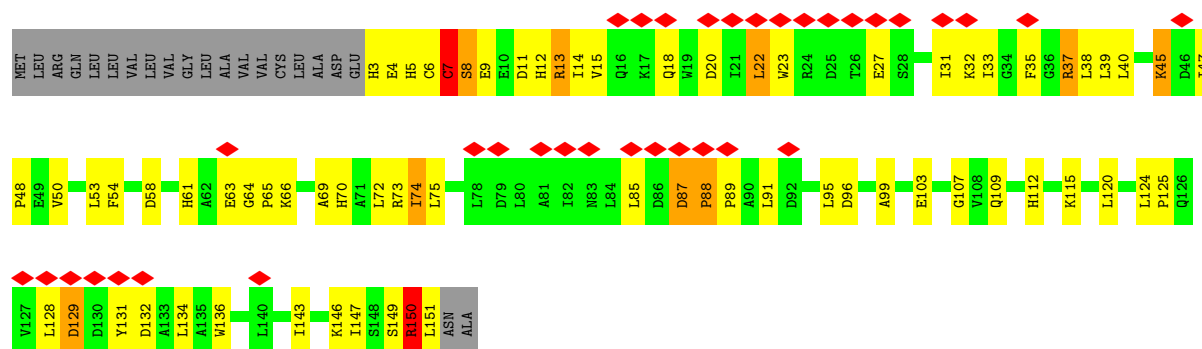


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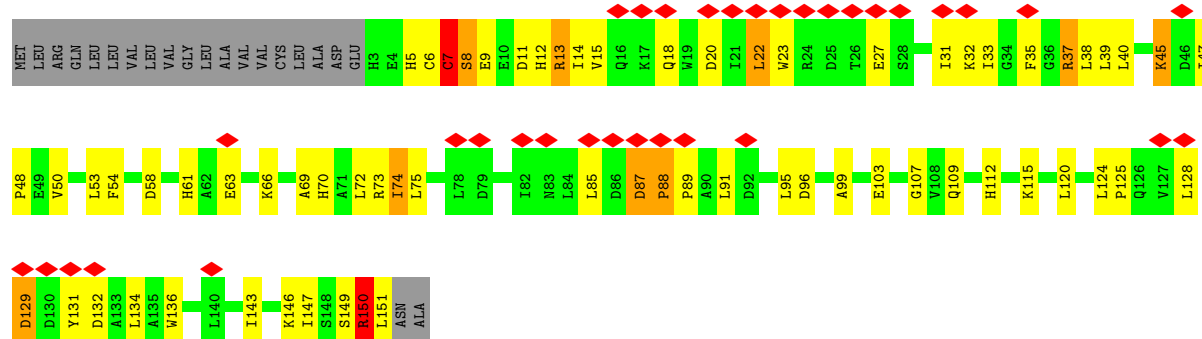


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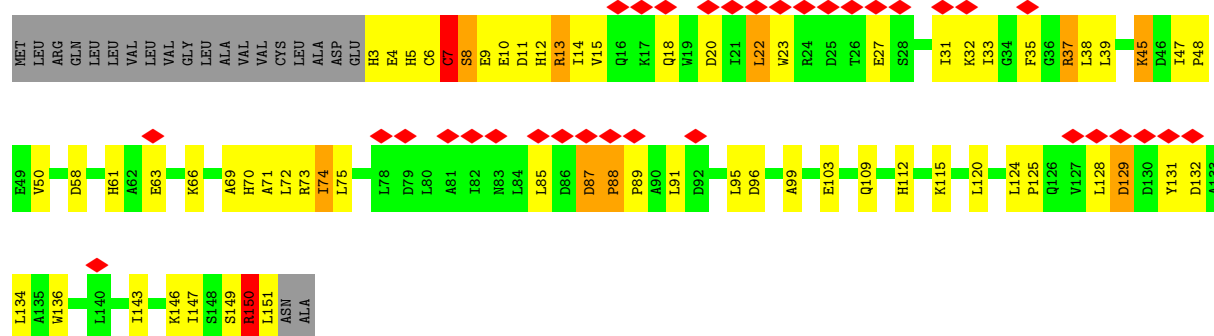




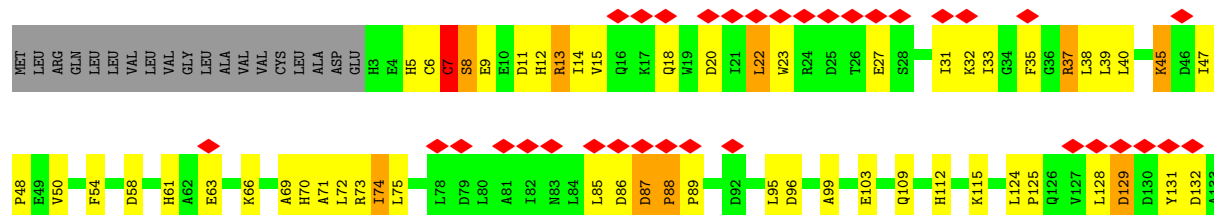
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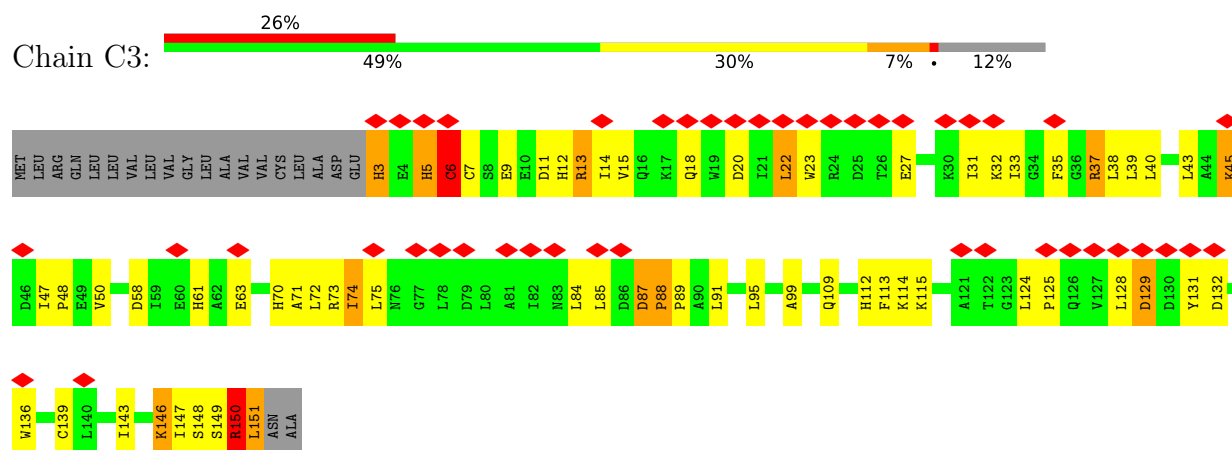


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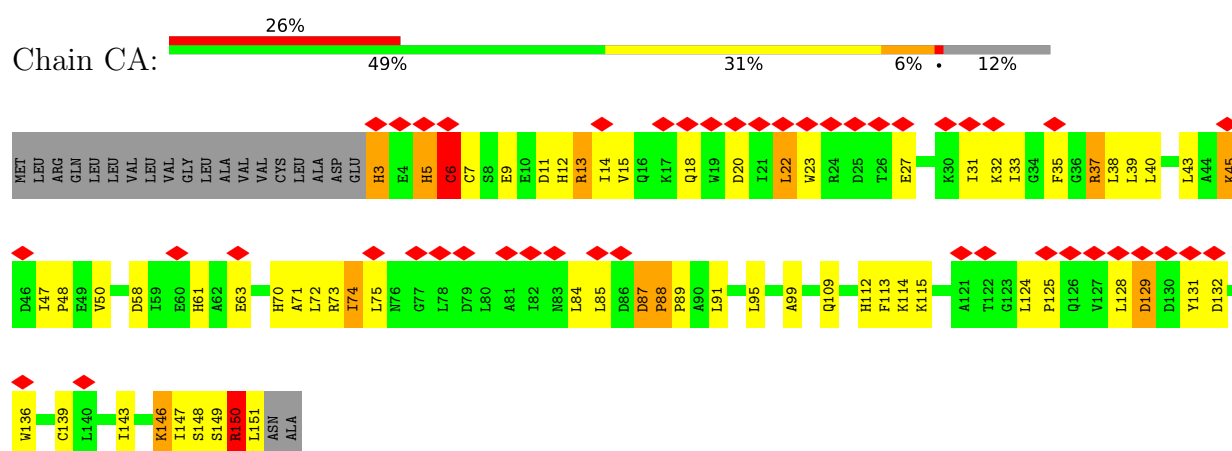


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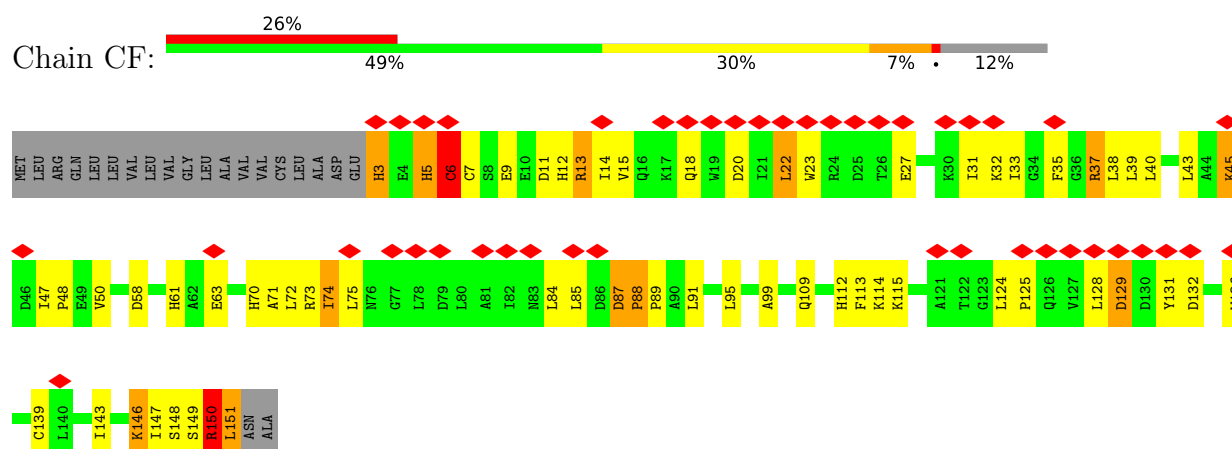




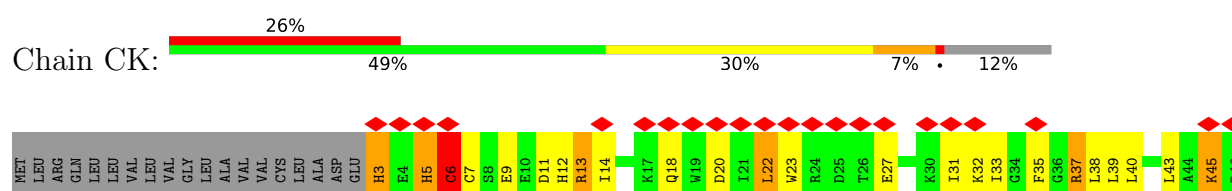
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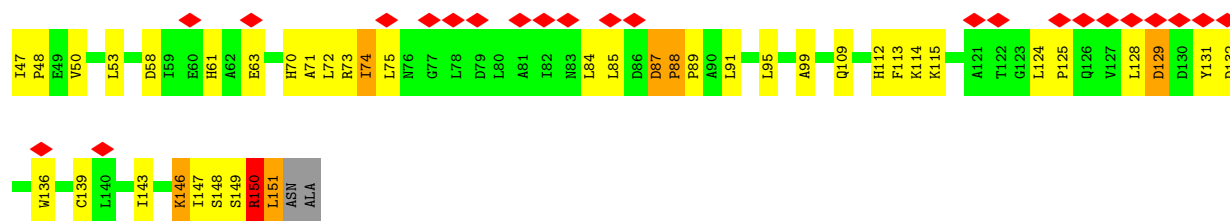


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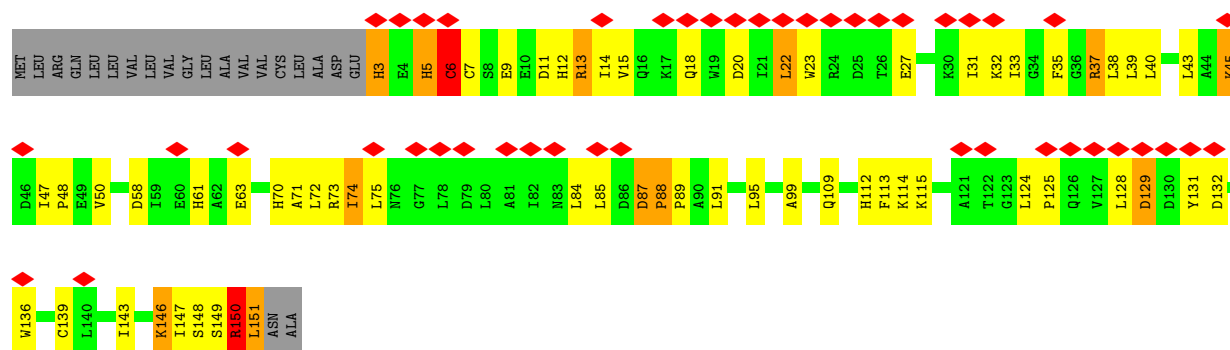


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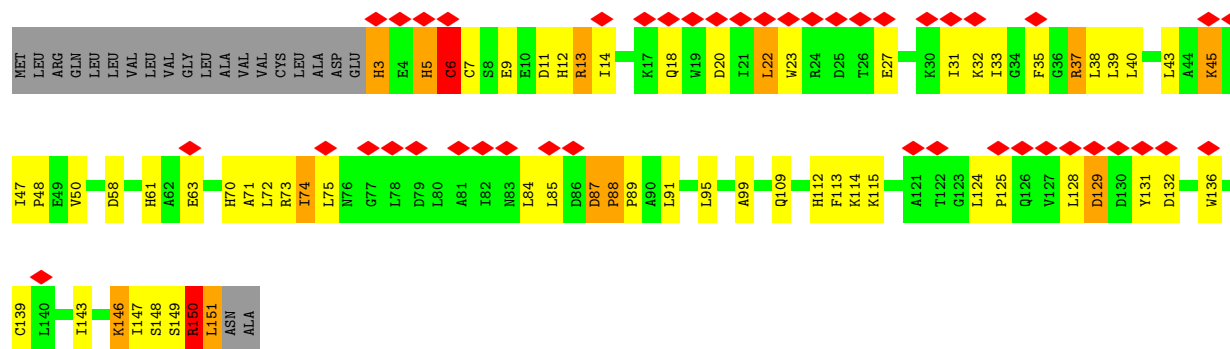




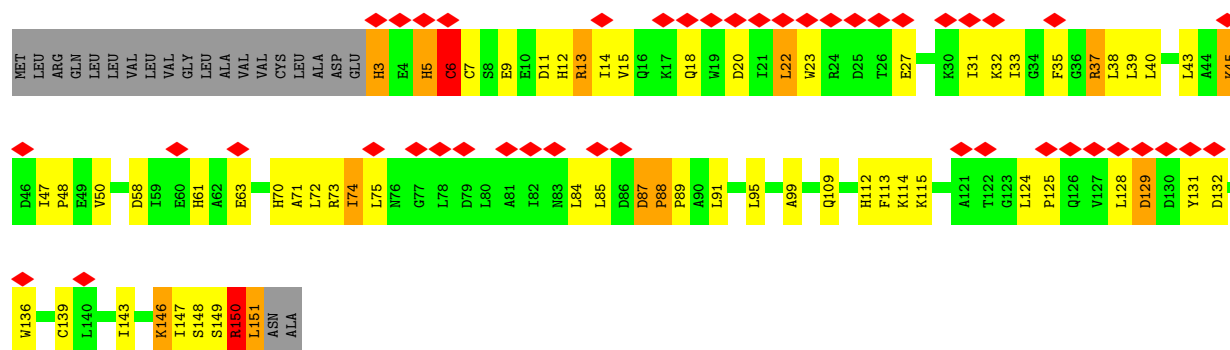
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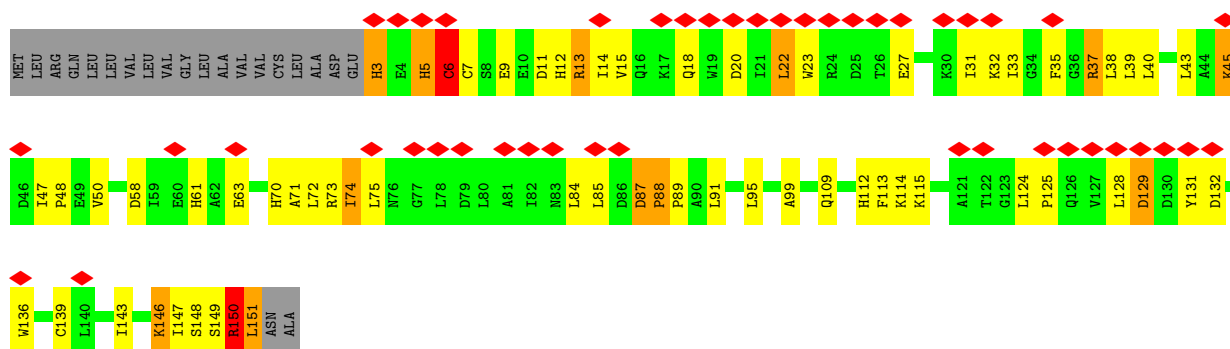
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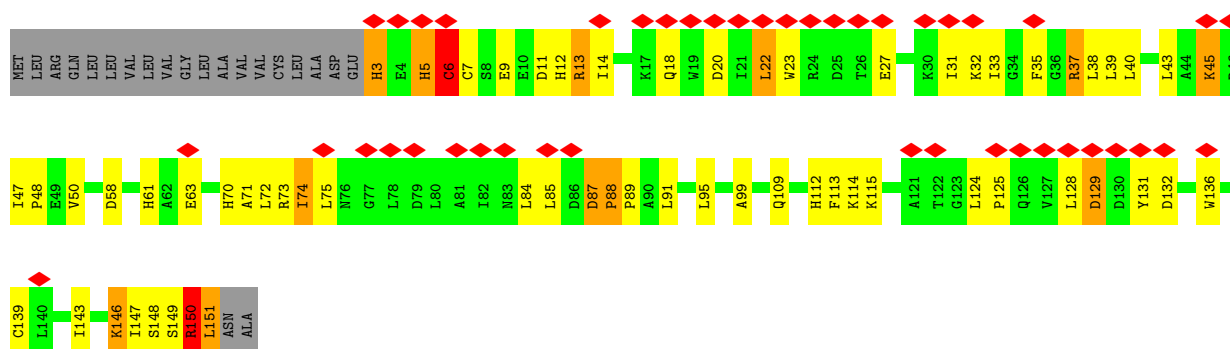
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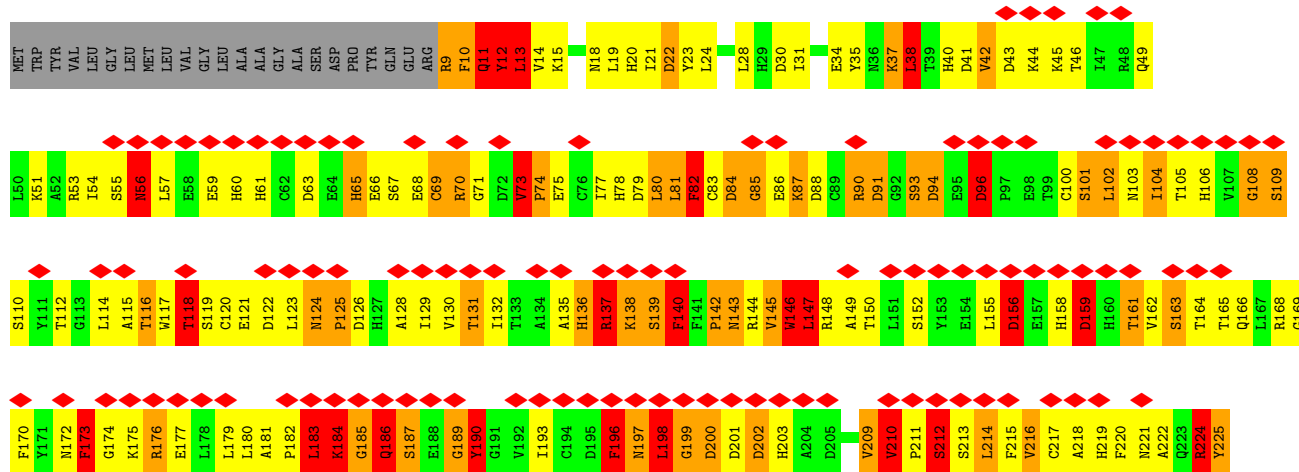
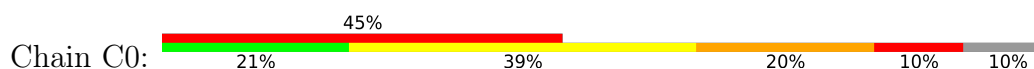
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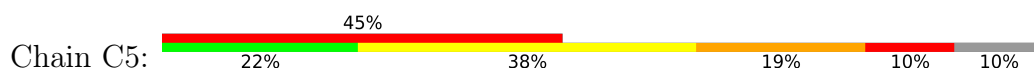
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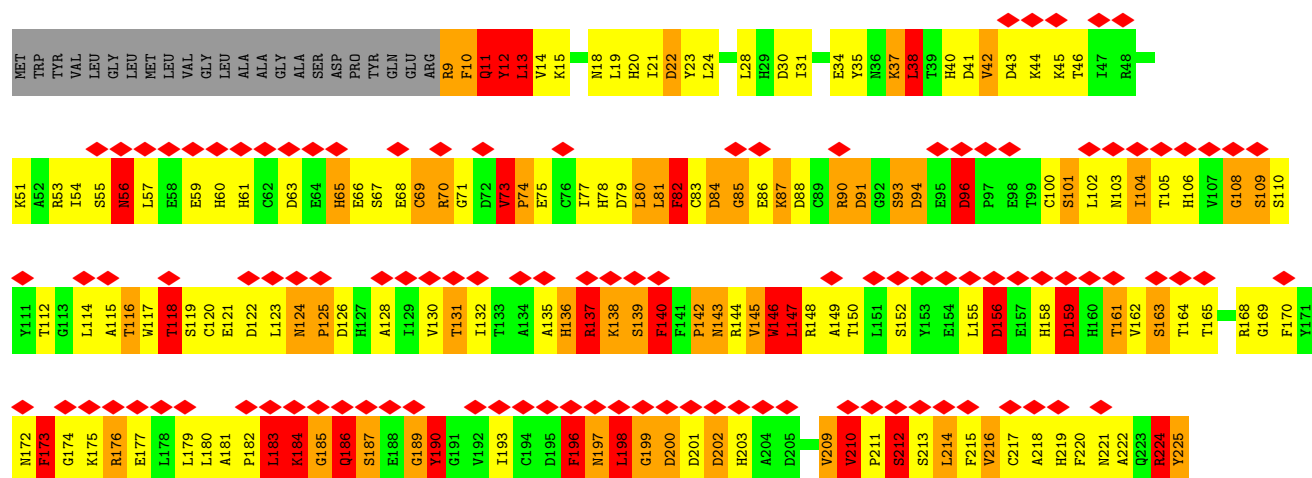


• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

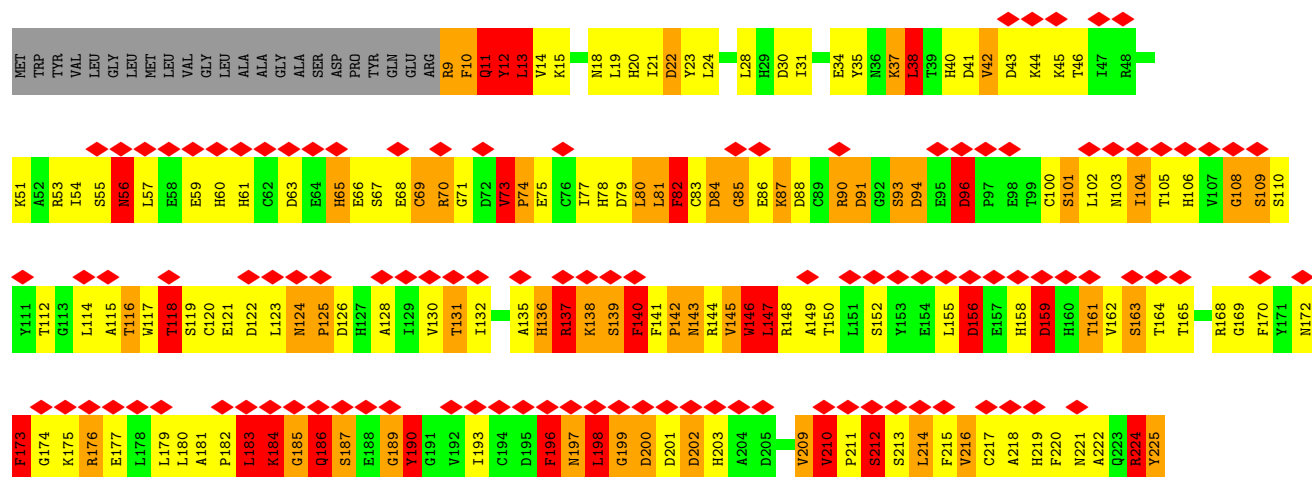
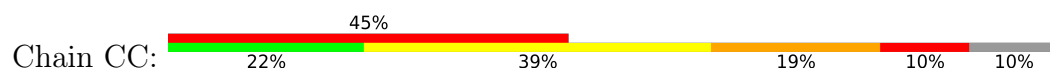


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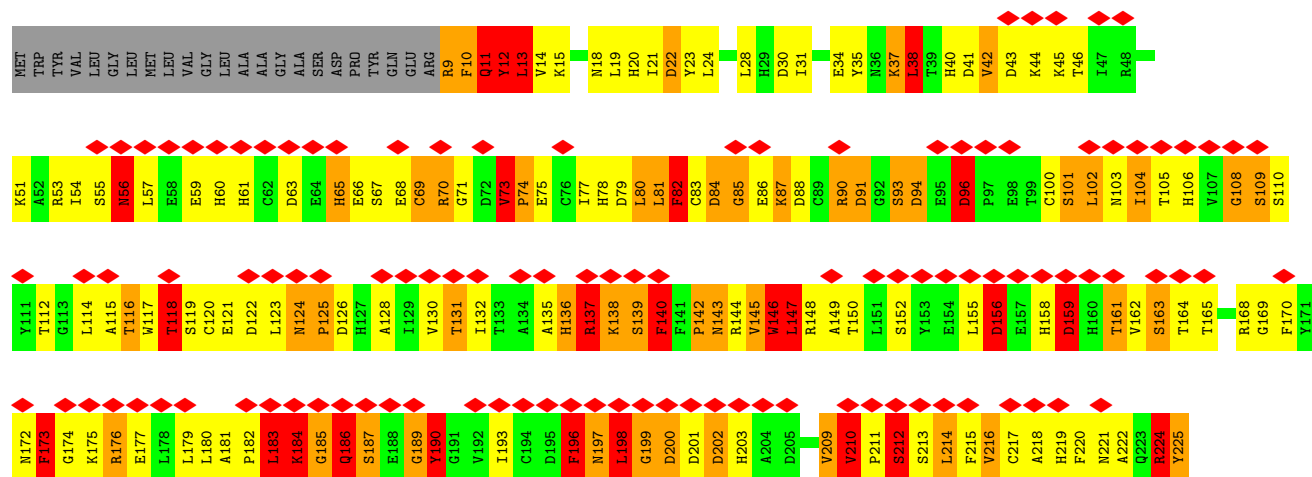
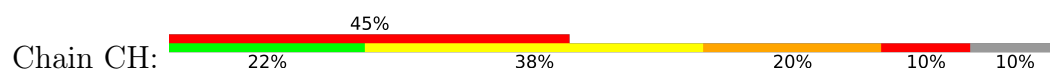




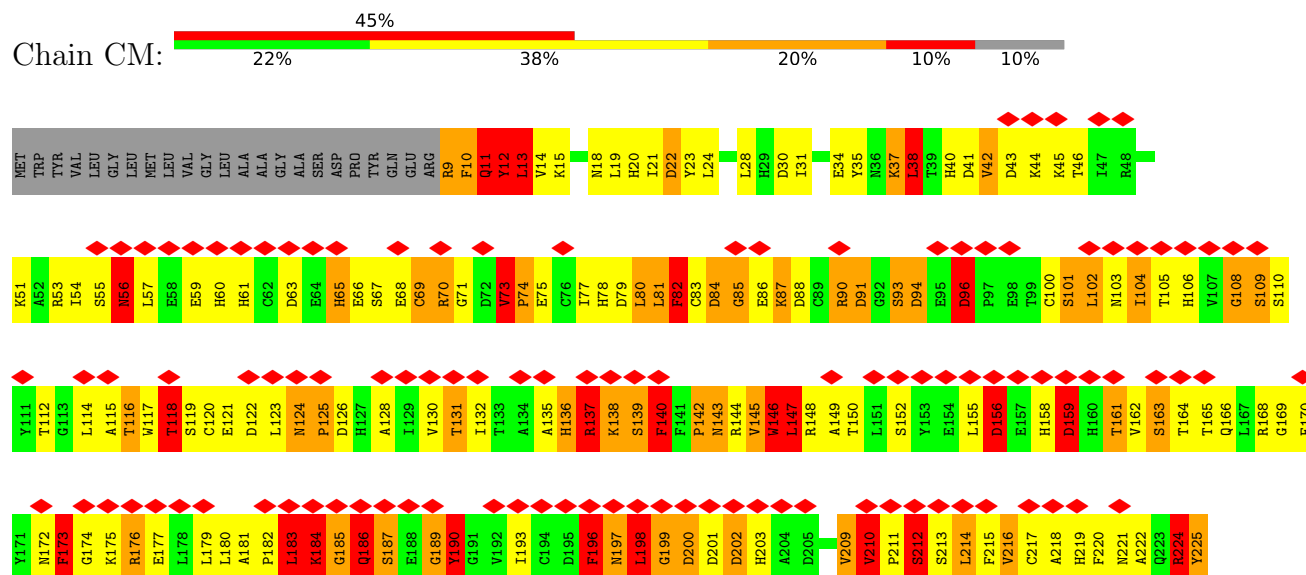
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1



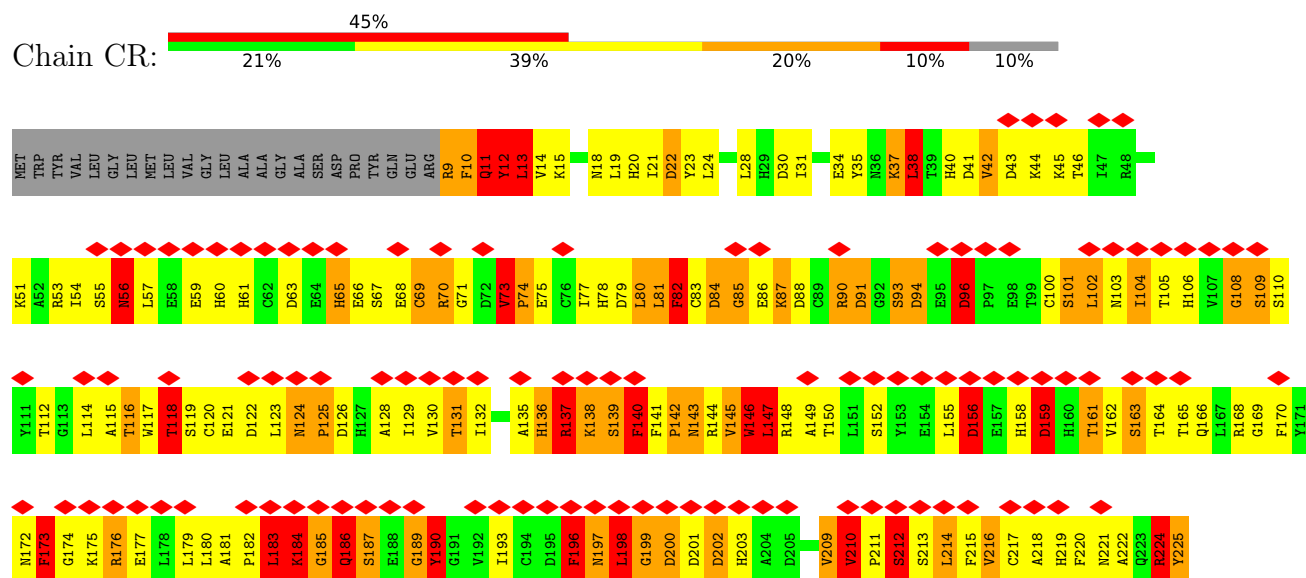
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1



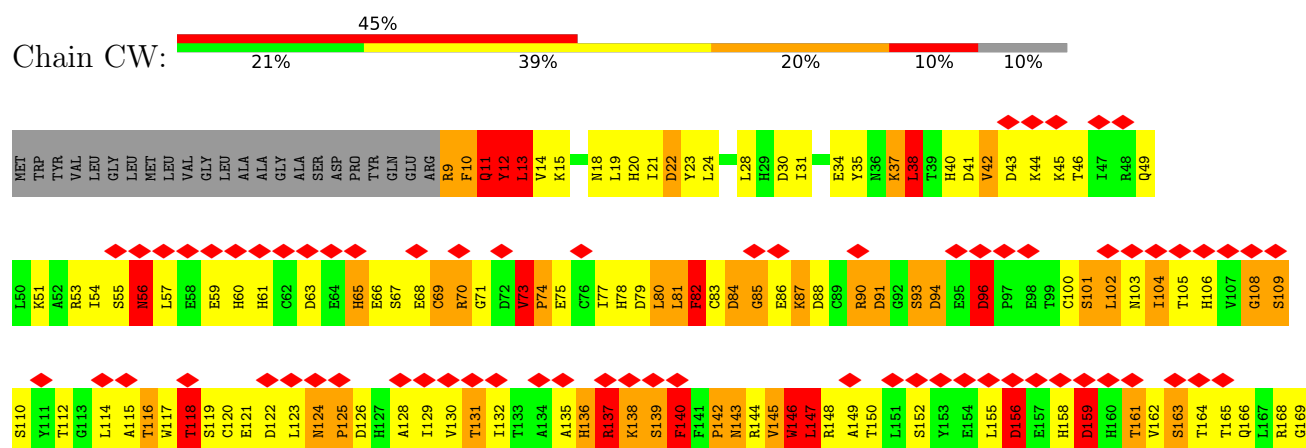
● Molecule 8: HEMOGLOBIN LINKER CHAIN L1

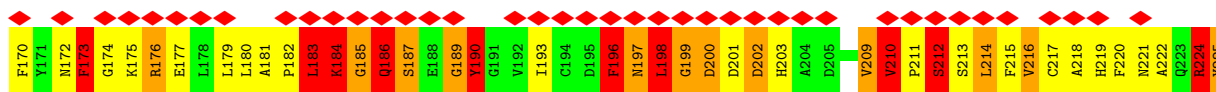


● Molecule 8: HEMOGLOBIN LINKER CHAIN L1

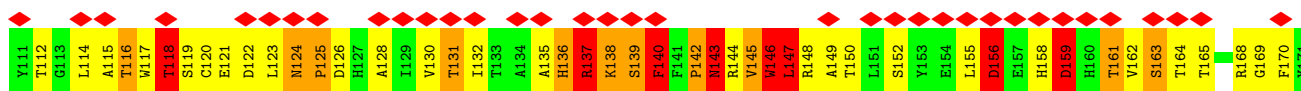
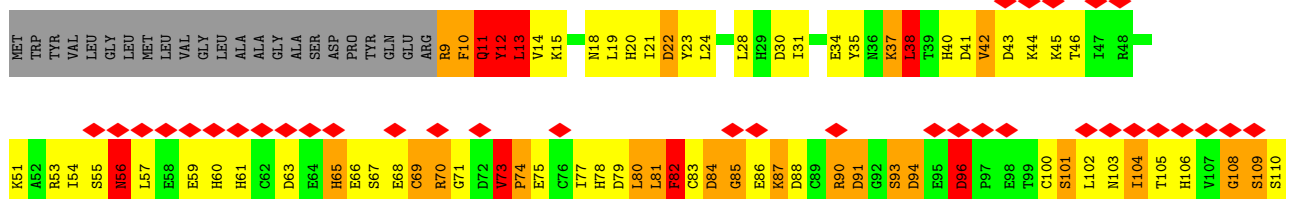
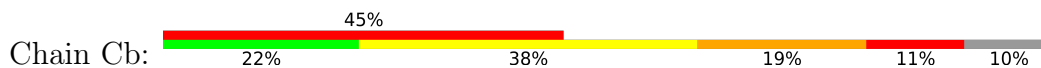


● Molecule 8: HEMOGLOBIN LINKER CHAIN L1

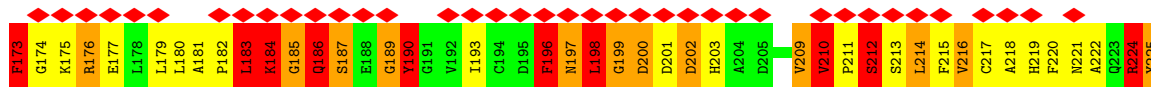
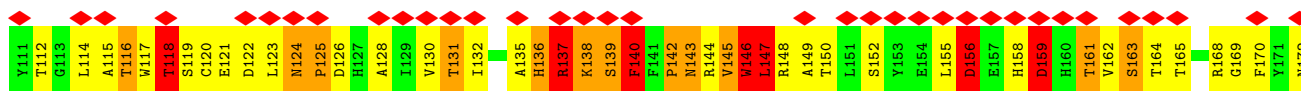
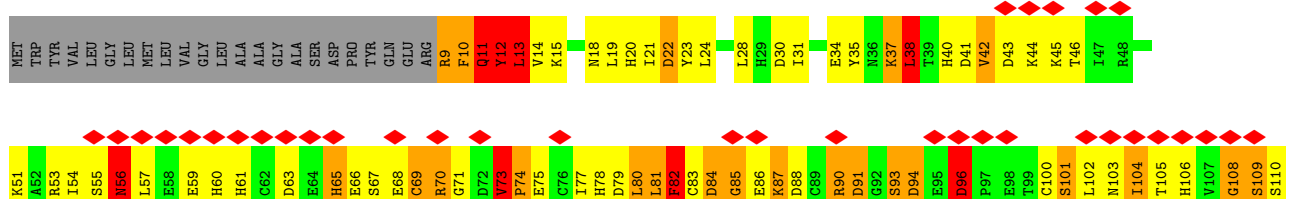
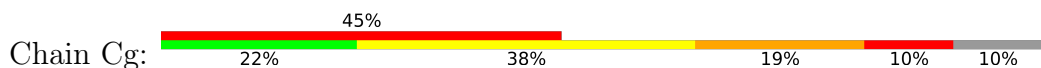




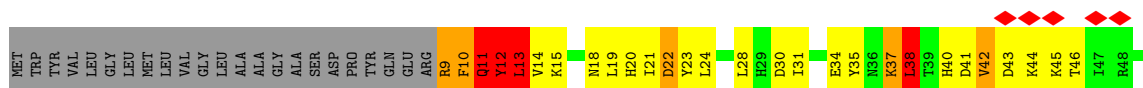
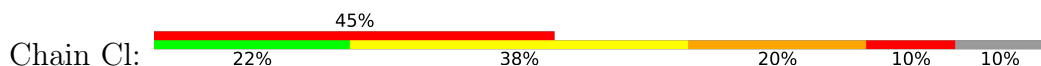
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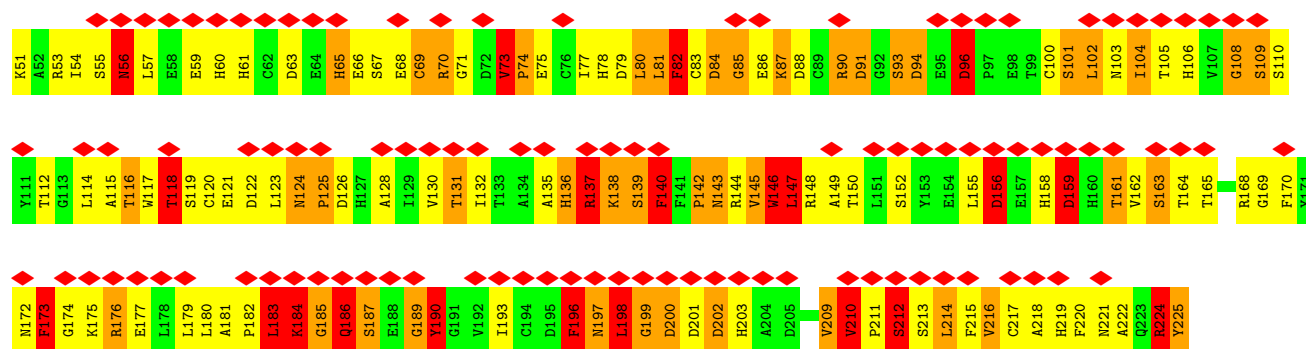


• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

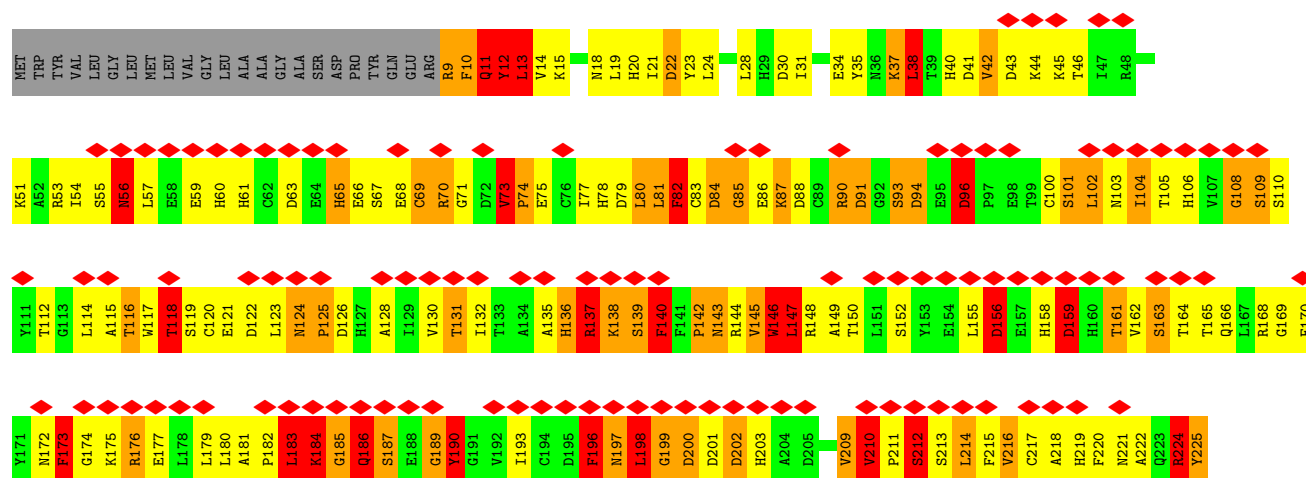
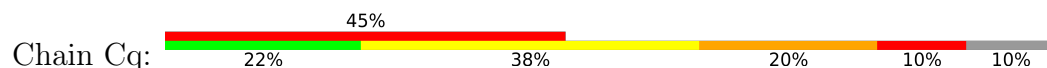


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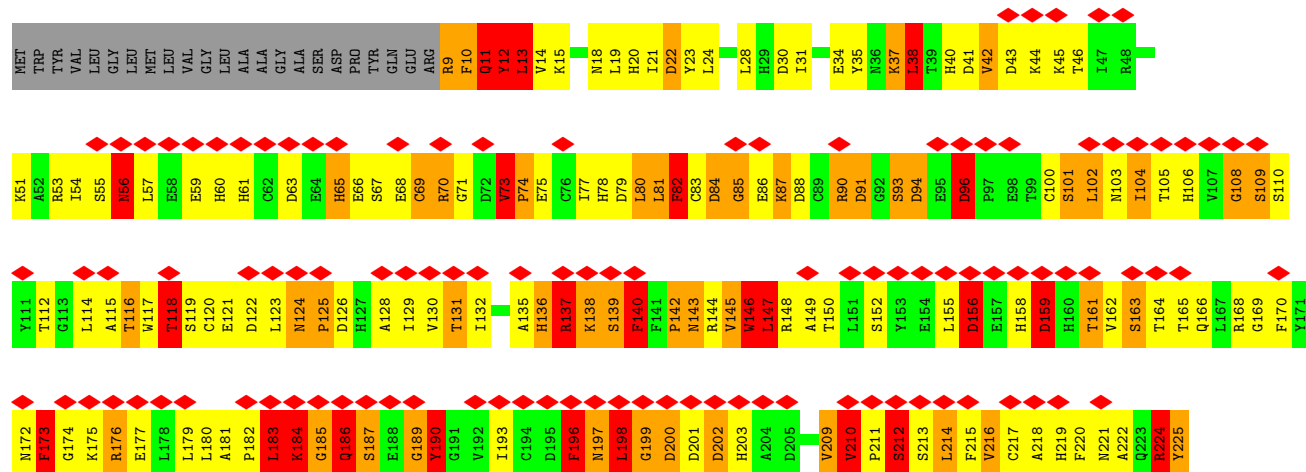
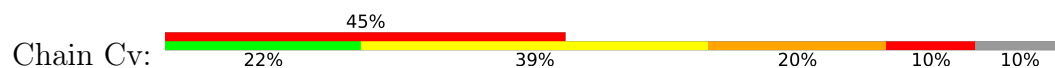




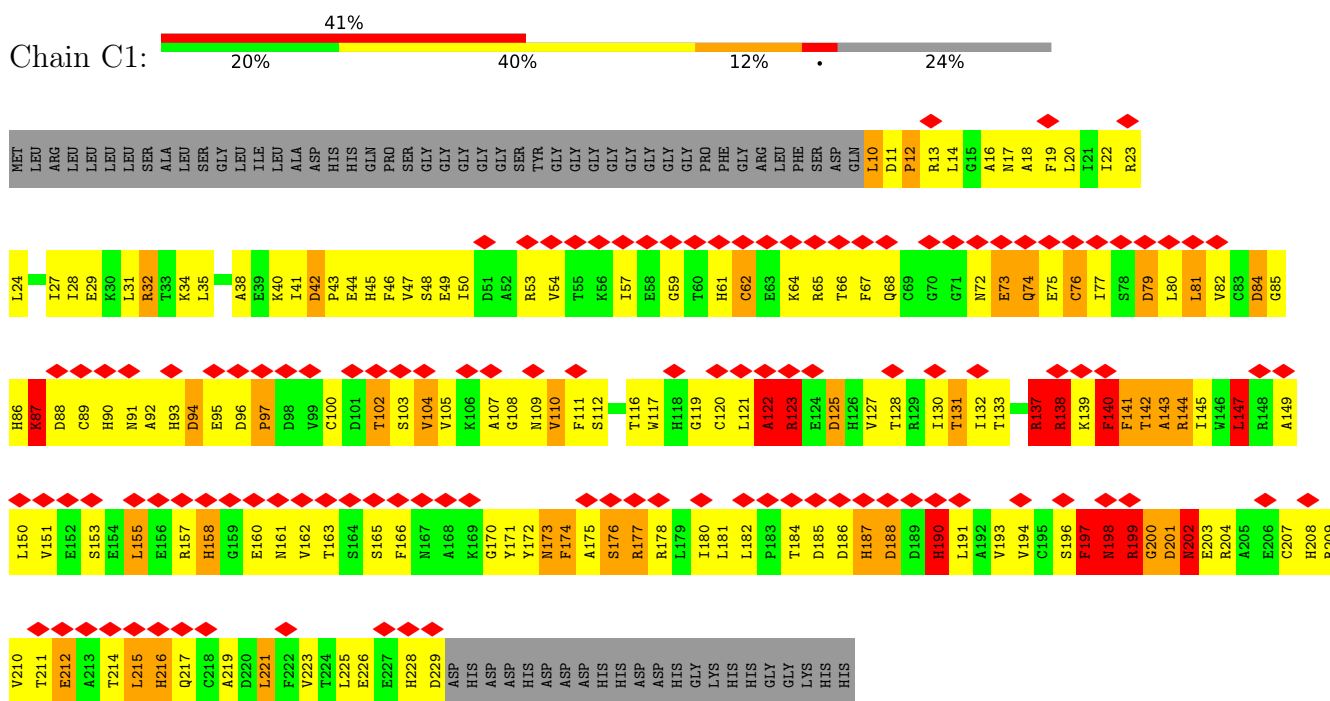
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1



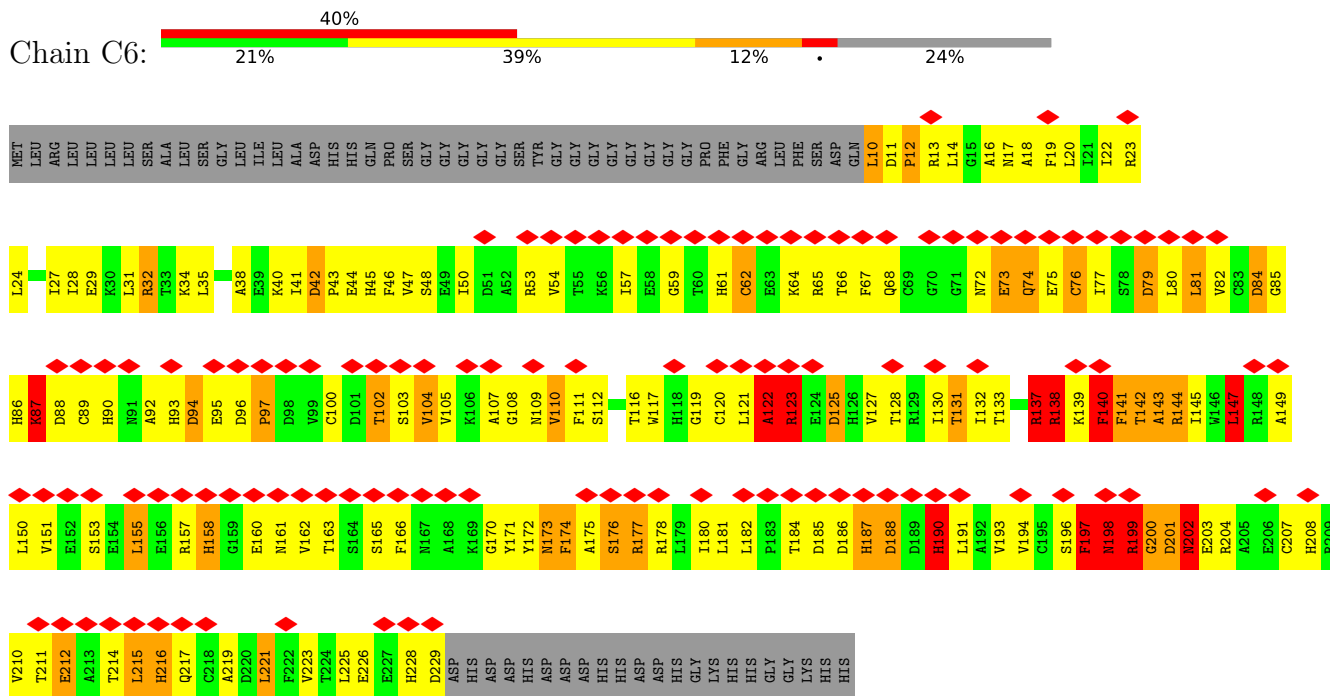
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1



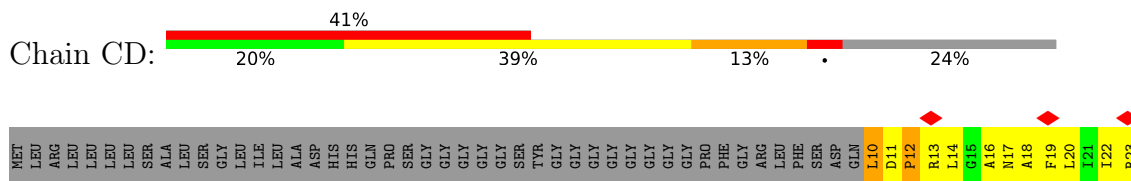
• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

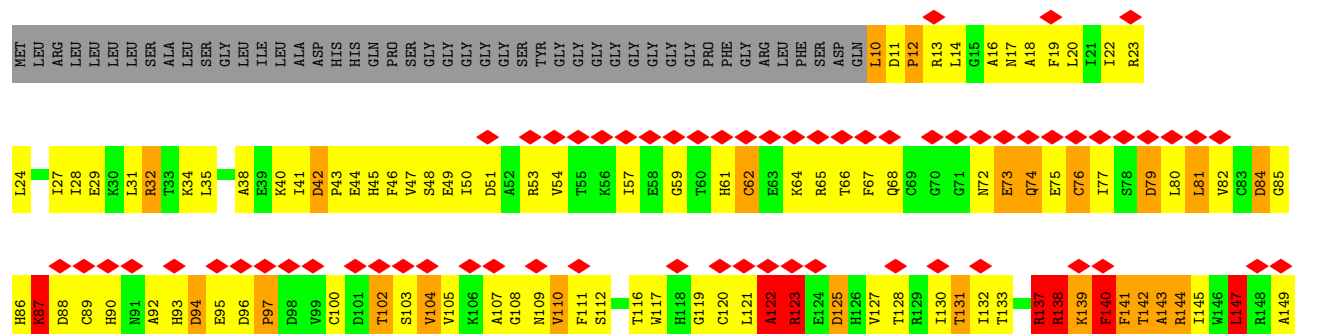


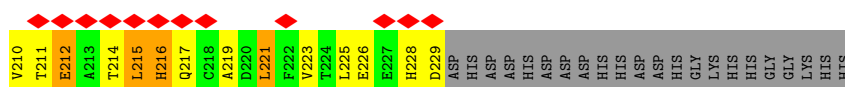
● Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT



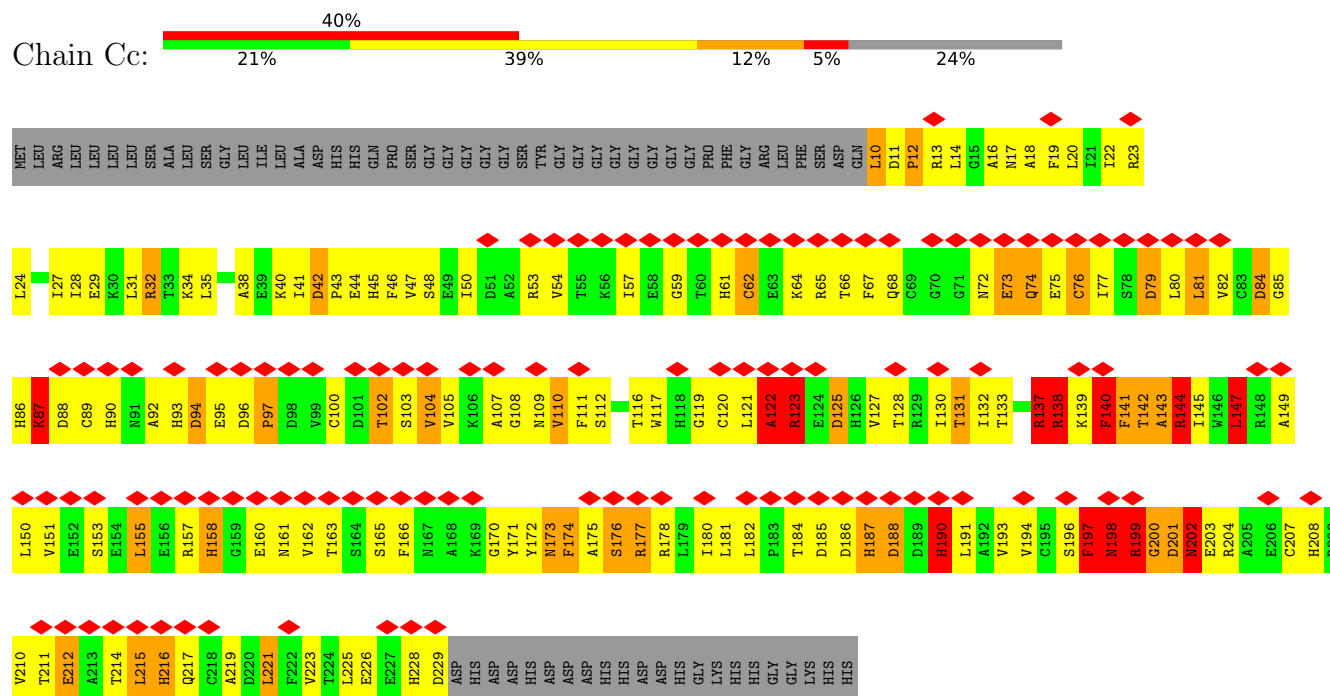
● Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT



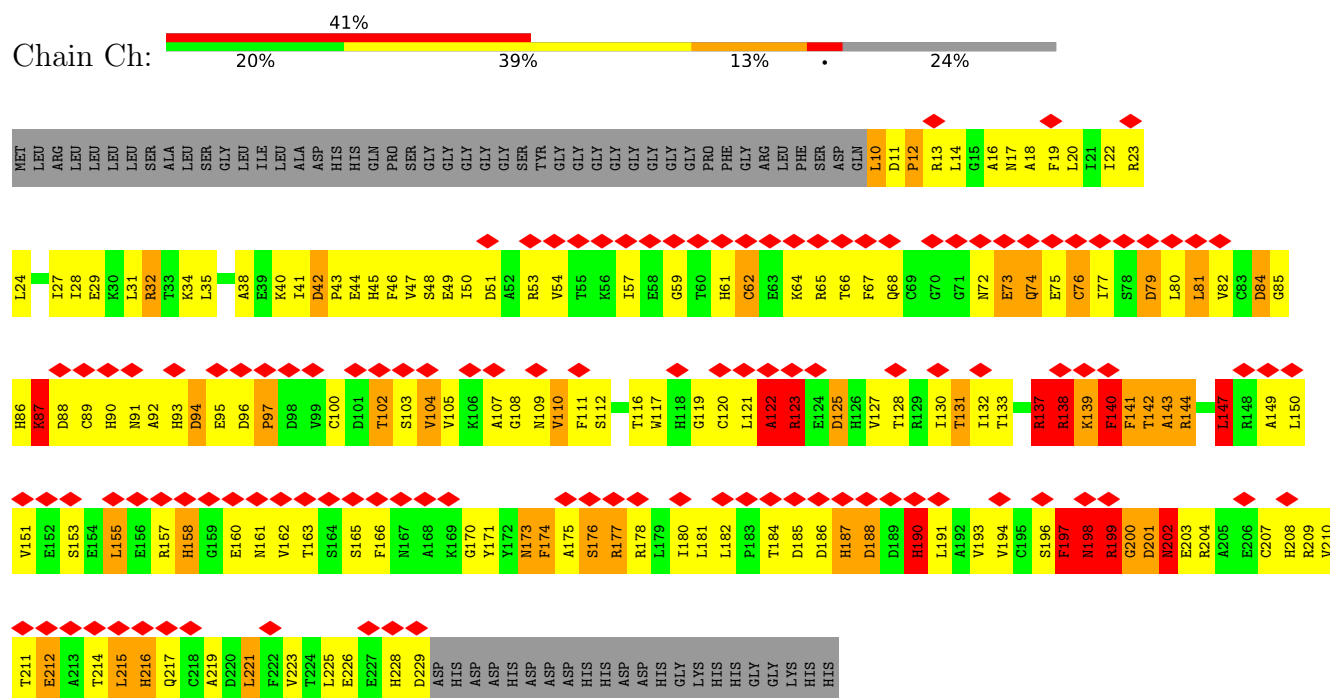




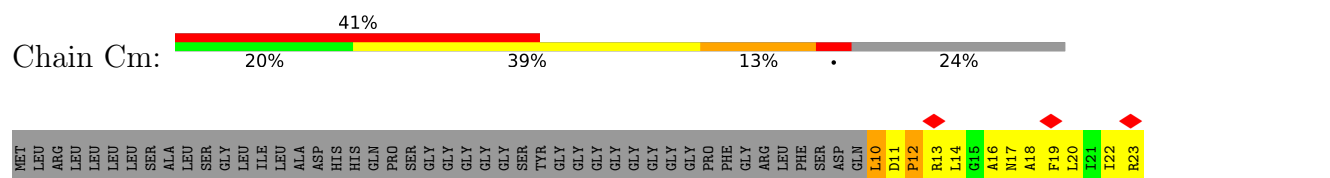
● Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

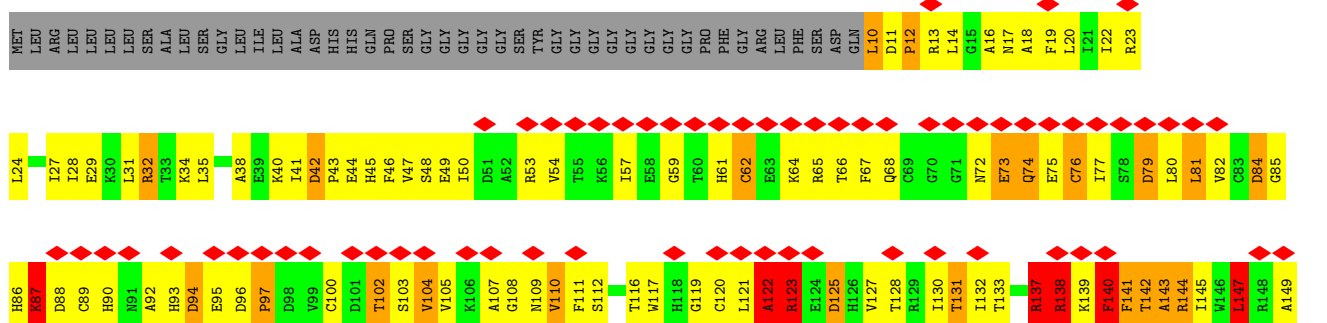


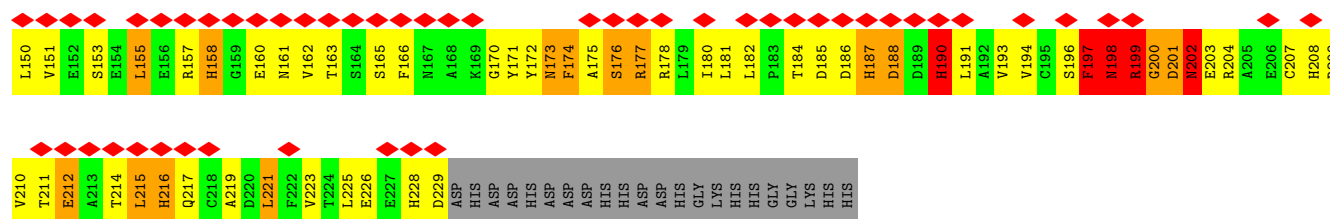
● Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT



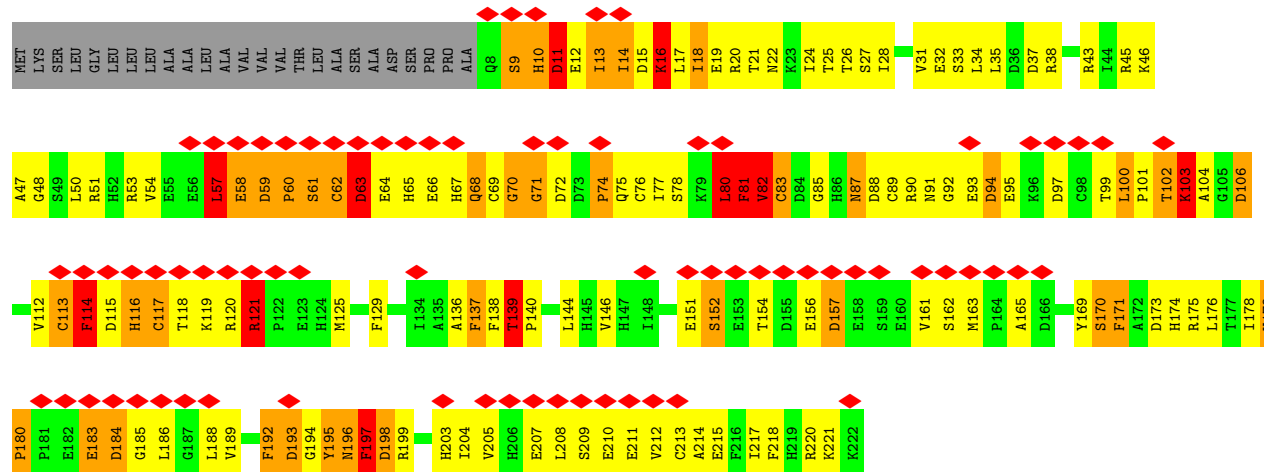
● Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT



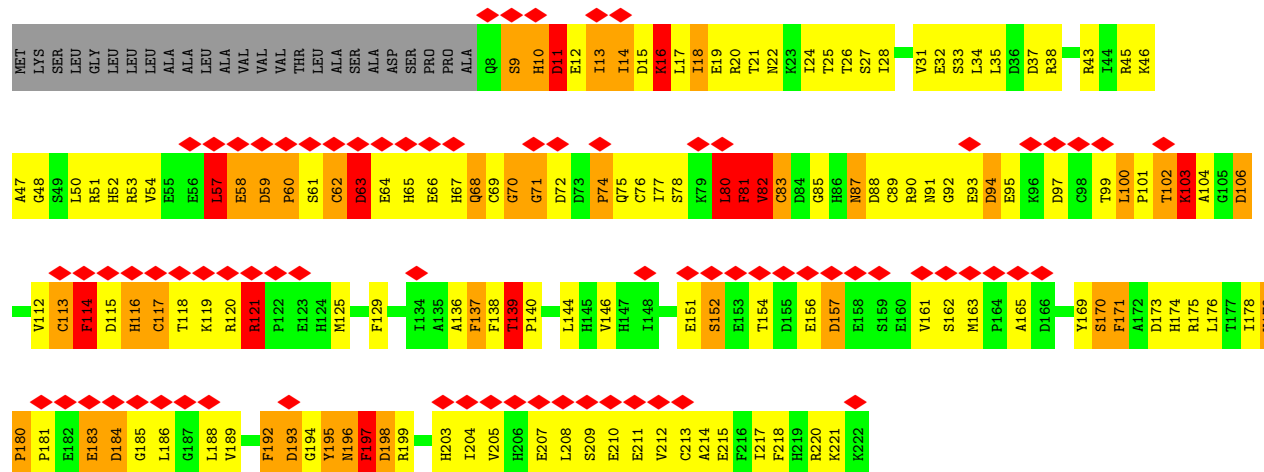




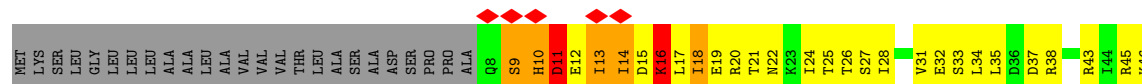
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

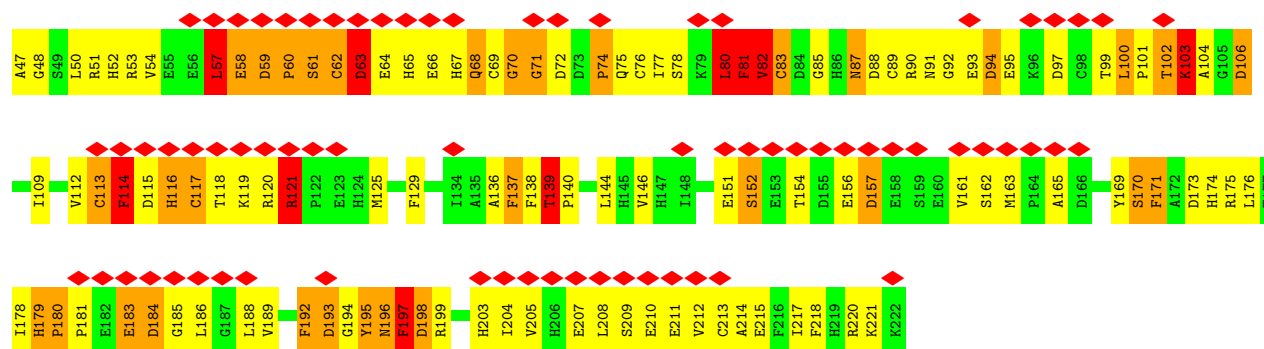


• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT



• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT



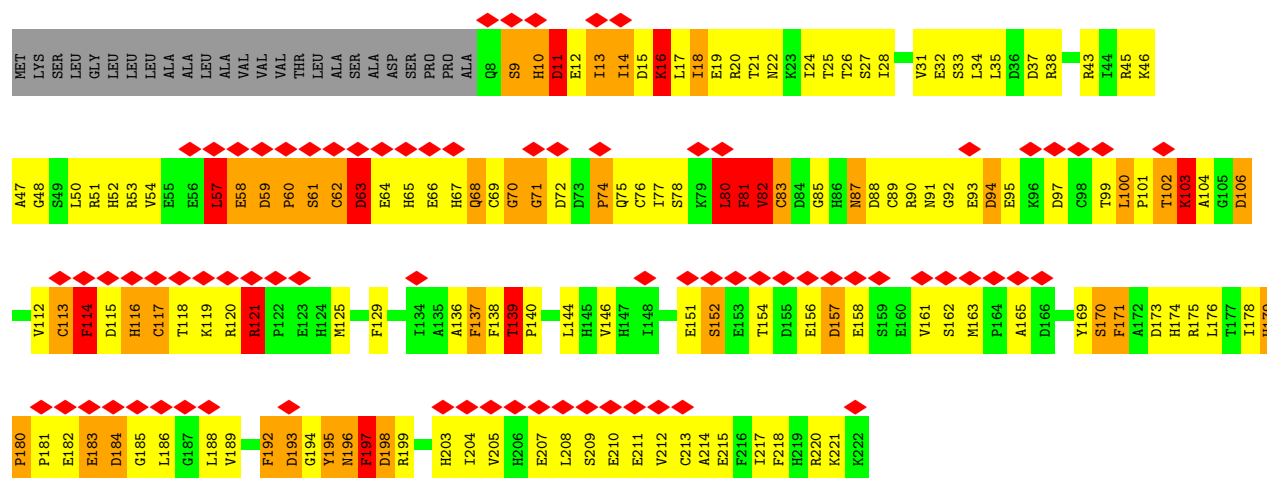


• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

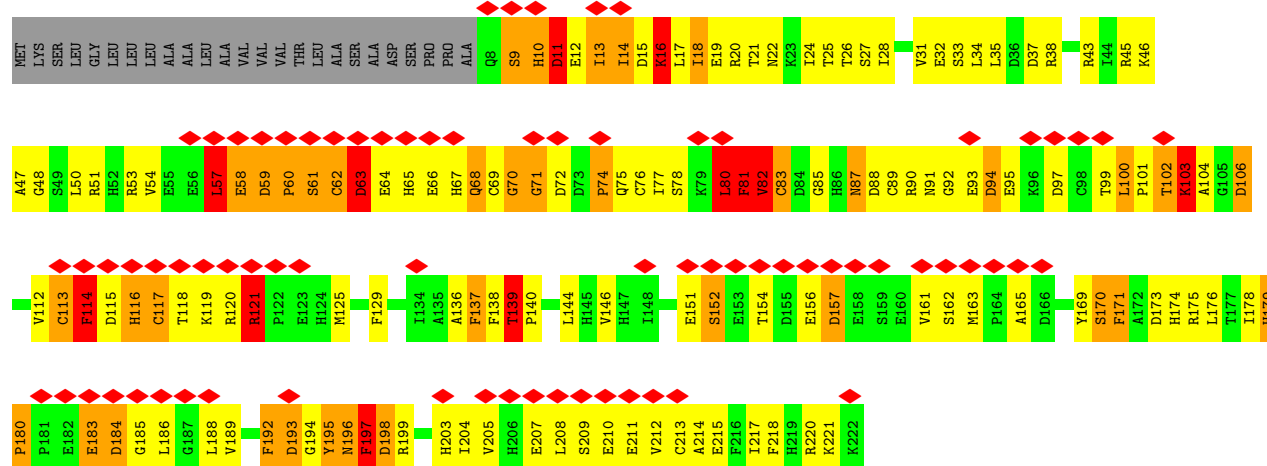


• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

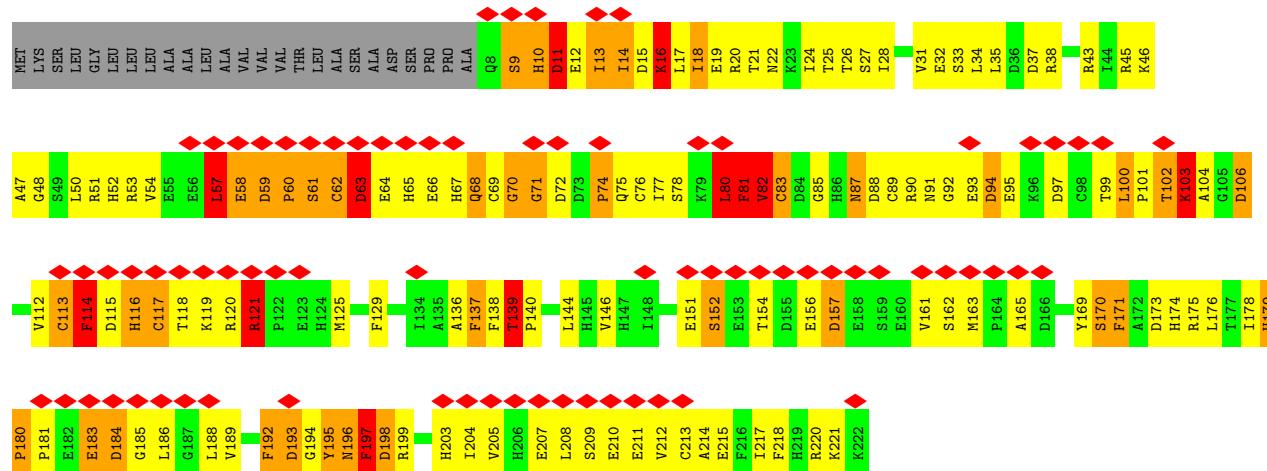




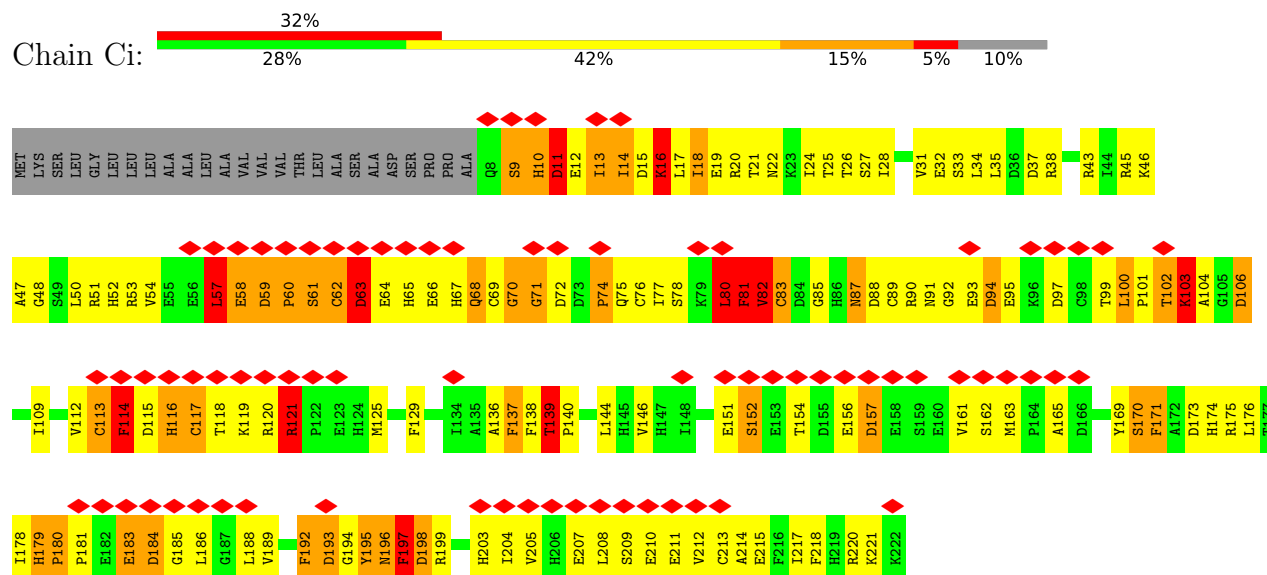
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT



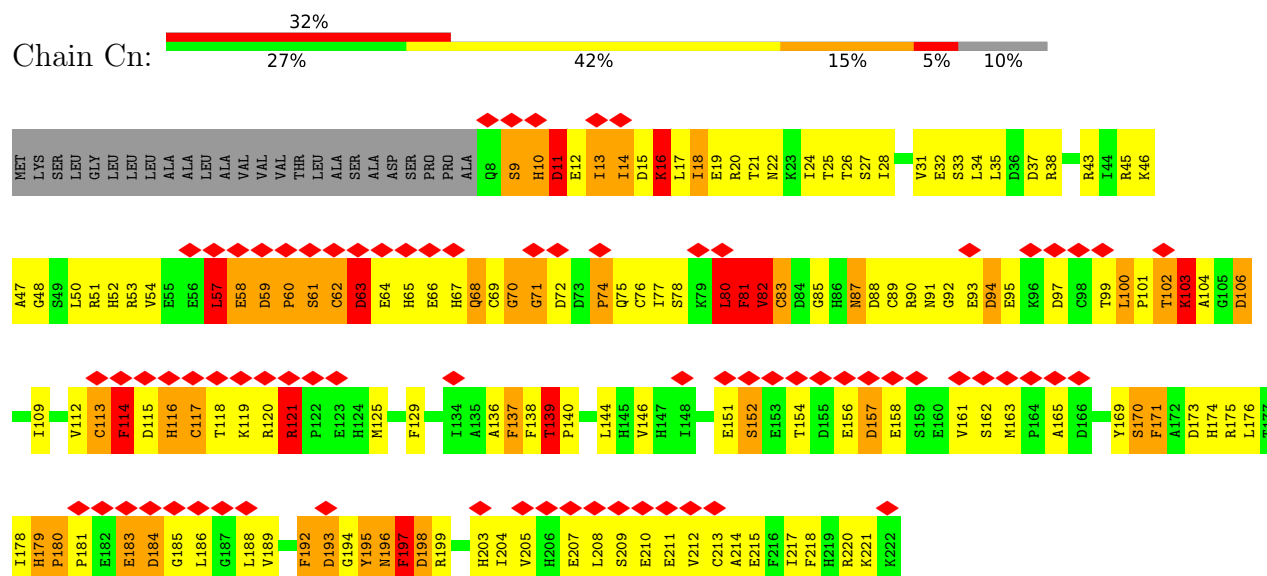
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT



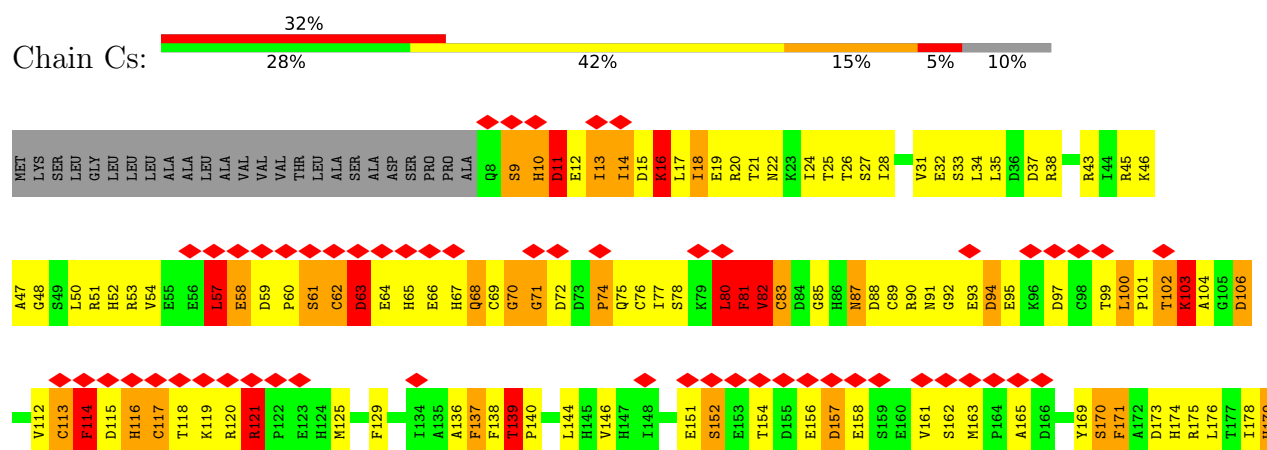
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

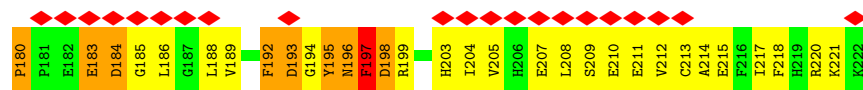


• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

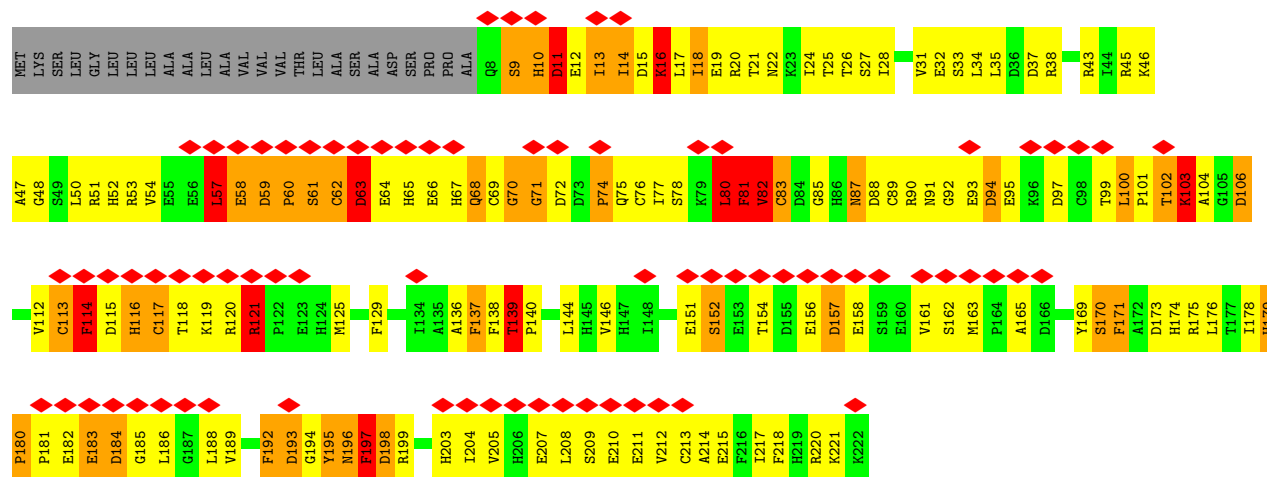


• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT





• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	4500	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	80000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.130	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.042	Depositor
Map size ($\text{\AA}$)	520.0, 520.0, 520.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A0	0.69	0/1216	1.10	9/1641 (0.5%)
1	A5	0.69	0/1216	1.10	9/1641 (0.5%)
1	AC	0.69	0/1216	1.10	9/1641 (0.5%)
1	AH	0.69	0/1216	1.10	9/1641 (0.5%)
1	AM	0.69	0/1216	1.10	9/1641 (0.5%)
1	AR	0.69	0/1216	1.10	9/1641 (0.5%)
1	AW	0.69	0/1216	1.10	9/1641 (0.5%)
1	Ab	0.69	0/1216	1.10	9/1641 (0.5%)
1	Ag	0.69	0/1216	1.10	9/1641 (0.5%)
1	Al	0.69	0/1216	1.10	9/1641 (0.5%)
1	Aq	0.69	0/1216	1.10	9/1641 (0.5%)
1	Av	0.69	0/1216	1.10	9/1641 (0.5%)
2	A1	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	A6	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	AD	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	AI	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	AN	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	AS	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	AX	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	Ac	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	Ah	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	Am	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	Ar	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
2	Aw	0.79	1/1159 (0.1%)	1.11	6/1568 (0.4%)
3	A2	0.75	0/1237	1.22	11/1670 (0.7%)
3	A3	0.82	5/1237 (0.4%)	1.19	13/1670 (0.8%)
3	A7	0.75	0/1237	1.22	11/1670 (0.7%)
3	AA	0.82	5/1237 (0.4%)	1.19	14/1670 (0.8%)
3	AE	0.75	0/1237	1.22	11/1670 (0.7%)
3	AF	0.82	5/1237 (0.4%)	1.19	13/1670 (0.8%)
3	AJ	0.75	0/1237	1.22	11/1670 (0.7%)
3	AK	0.82	5/1237 (0.4%)	1.19	13/1670 (0.8%)
3	AO	0.75	0/1237	1.22	11/1670 (0.7%)
3	AP	0.82	5/1237 (0.4%)	1.19	14/1670 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	AT	0.75	0/1237	1.22	11/1670 (0.7%)
3	AU	0.82	5/1237 (0.4%)	1.19	13/1670 (0.8%)
3	AY	0.75	0/1237	1.22	11/1670 (0.7%)
3	AZ	0.82	5/1237 (0.4%)	1.19	13/1670 (0.8%)
3	Ad	0.75	0/1237	1.22	11/1670 (0.7%)
3	Ae	0.82	5/1237 (0.4%)	1.19	14/1670 (0.8%)
3	Ai	0.75	0/1237	1.22	11/1670 (0.7%)
3	Aj	0.82	5/1237 (0.4%)	1.19	13/1670 (0.8%)
3	An	0.75	0/1237	1.22	11/1670 (0.7%)
3	Ao	0.82	5/1237 (0.4%)	1.19	13/1670 (0.8%)
3	As	0.75	0/1237	1.22	11/1670 (0.7%)
3	At	0.82	5/1237 (0.4%)	1.19	14/1670 (0.8%)
3	Ax	0.75	0/1237	1.22	11/1670 (0.7%)
3	Ay	0.82	5/1237 (0.4%)	1.19	13/1670 (0.8%)
4	A4	0.85	0/1176	1.13	7/1587 (0.4%)
4	AB	0.85	0/1176	1.13	7/1587 (0.4%)
4	AG	0.85	0/1176	1.13	7/1587 (0.4%)
4	AL	0.85	0/1176	1.13	7/1587 (0.4%)
4	AQ	0.85	0/1176	1.13	7/1587 (0.4%)
4	AV	0.85	0/1176	1.13	7/1587 (0.4%)
4	Aa	0.85	0/1176	1.13	7/1587 (0.4%)
4	Af	0.85	0/1176	1.13	7/1587 (0.4%)
4	Ak	0.85	0/1176	1.13	7/1587 (0.4%)
4	Ap	0.85	0/1176	1.13	7/1587 (0.4%)
4	Au	0.85	0/1176	1.13	7/1587 (0.4%)
4	Az	0.85	0/1176	1.13	7/1587 (0.4%)
4	B2	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	B3	0.86	0/1176	1.26	13/1587 (0.8%)
4	B7	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	BA	0.86	0/1176	1.25	13/1587 (0.8%)
4	BE	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	BF	0.86	0/1176	1.26	13/1587 (0.8%)
4	BJ	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	BK	0.86	0/1176	1.26	13/1587 (0.8%)
4	BO	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	BP	0.86	0/1176	1.25	13/1587 (0.8%)
4	BT	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	BU	0.86	0/1176	1.26	13/1587 (0.8%)
4	BY	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	BZ	0.86	0/1176	1.26	13/1587 (0.8%)
4	Bd	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	Be	0.86	0/1176	1.25	13/1587 (0.8%)
4	Bi	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	Bj	0.86	0/1176	1.26	13/1587 (0.8%)
4	Bn	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	Bo	0.86	0/1176	1.26	13/1587 (0.8%)
4	Bs	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	Bt	0.86	0/1176	1.25	13/1587 (0.8%)
4	Bx	0.81	1/1176 (0.1%)	1.22	16/1587 (1.0%)
4	By	0.86	0/1176	1.26	13/1587 (0.8%)
5	B0	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	B5	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	BC	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	BH	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	BM	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	BR	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	BW	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	Bb	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	Bg	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	Bl	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	Bq	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	Bv	0.80	1/1159 (0.1%)	1.16	16/1568 (1.0%)
5	C4	0.79	0/1159	1.15	13/1568 (0.8%)
5	CB	0.79	0/1159	1.15	12/1568 (0.8%)
5	CG	0.79	0/1159	1.15	13/1568 (0.8%)
5	CL	0.79	0/1159	1.15	13/1568 (0.8%)
5	CQ	0.79	0/1159	1.15	12/1568 (0.8%)
5	CV	0.79	0/1159	1.15	13/1568 (0.8%)
5	Ca	0.79	0/1159	1.15	13/1568 (0.8%)
5	Cf	0.79	0/1159	1.15	12/1568 (0.8%)
5	Ck	0.79	0/1159	1.15	13/1568 (0.8%)
5	Cp	0.79	0/1159	1.15	13/1568 (0.8%)
5	Cu	0.79	0/1159	1.15	12/1568 (0.8%)
5	Cz	0.79	0/1159	1.15	13/1568 (0.8%)
6	B1	0.78	3/1237 (0.2%)	1.29	12/1670 (0.7%)
6	B6	0.78	3/1237 (0.2%)	1.29	12/1670 (0.7%)
6	BD	0.78	3/1237 (0.2%)	1.30	12/1670 (0.7%)
6	BI	0.78	3/1237 (0.2%)	1.29	12/1670 (0.7%)
6	BN	0.78	3/1237 (0.2%)	1.29	12/1670 (0.7%)
6	BS	0.78	3/1237 (0.2%)	1.30	12/1670 (0.7%)
6	BX	0.78	3/1237 (0.2%)	1.29	12/1670 (0.7%)
6	Bc	0.78	3/1237 (0.2%)	1.29	12/1670 (0.7%)
6	Bh	0.78	3/1237 (0.2%)	1.30	12/1670 (0.7%)
6	Bm	0.78	3/1237 (0.2%)	1.29	12/1670 (0.7%)
6	Br	0.78	3/1237 (0.2%)	1.29	12/1670 (0.7%)
6	Bw	0.78	3/1237 (0.2%)	1.30	12/1670 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	B4	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	BB	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	BG	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	BL	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	BQ	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	BV	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	Ba	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	Bf	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	Bk	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	Bp	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	Bu	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	Bz	0.68	1/1215 (0.1%)	1.07	9/1641 (0.5%)
7	C3	0.70	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	CA	0.71	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	CF	0.70	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	CK	0.70	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	CP	0.71	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	CU	0.70	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	CZ	0.70	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	Ce	0.71	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	Cj	0.70	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	Co	0.70	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	Ct	0.71	1/1215 (0.1%)	1.09	11/1641 (0.7%)
7	Cy	0.70	1/1215 (0.1%)	1.09	11/1641 (0.7%)
8	C0	1.32	9/1789 (0.5%)	2.06	94/2418 (3.9%)
8	C5	1.32	9/1789 (0.5%)	2.06	93/2418 (3.8%)
8	CC	1.32	9/1789 (0.5%)	2.06	93/2418 (3.8%)
8	CH	1.32	9/1789 (0.5%)	2.06	94/2418 (3.9%)
8	CM	1.32	9/1789 (0.5%)	2.06	93/2418 (3.8%)
8	CR	1.32	9/1789 (0.5%)	2.06	93/2418 (3.8%)
8	CW	1.32	9/1789 (0.5%)	2.06	94/2418 (3.9%)
8	Cb	1.32	9/1789 (0.5%)	2.06	93/2418 (3.8%)
8	Cg	1.32	9/1789 (0.5%)	2.06	93/2418 (3.8%)
8	Cl	1.32	9/1789 (0.5%)	2.06	94/2418 (3.9%)
8	Cq	1.32	9/1789 (0.5%)	2.06	93/2418 (3.8%)
8	Cv	1.32	9/1789 (0.5%)	2.06	93/2418 (3.8%)
9	C1	1.23	6/1786 (0.3%)	1.84	69/2412 (2.9%)
9	C6	1.23	6/1786 (0.3%)	1.84	68/2412 (2.8%)
9	CD	1.23	6/1786 (0.3%)	1.84	68/2412 (2.8%)
9	CI	1.23	6/1786 (0.3%)	1.84	69/2412 (2.9%)
9	CN	1.23	6/1786 (0.3%)	1.84	68/2412 (2.8%)
9	CS	1.23	6/1786 (0.3%)	1.84	68/2412 (2.8%)
9	CX	1.23	6/1786 (0.3%)	1.84	69/2412 (2.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	Cc	1.23	6/1786 (0.3%)	1.84	68/2412 (2.8%)
9	Ch	1.23	6/1786 (0.3%)	1.84	68/2412 (2.8%)
9	Cm	1.23	6/1786 (0.3%)	1.84	69/2412 (2.9%)
9	Cr	1.23	6/1786 (0.3%)	1.84	68/2412 (2.8%)
9	Cw	1.23	6/1786 (0.3%)	1.84	68/2412 (2.8%)
10	C2	1.29	9/1752 (0.5%)	2.57	73/2362 (3.1%)
10	C7	1.29	9/1752 (0.5%)	2.57	74/2362 (3.1%)
10	CE	1.29	9/1752 (0.5%)	2.57	74/2362 (3.1%)
10	CJ	1.29	9/1752 (0.5%)	2.57	73/2362 (3.1%)
10	CO	1.29	9/1752 (0.5%)	2.57	74/2362 (3.1%)
10	CT	1.29	9/1752 (0.5%)	2.57	74/2362 (3.1%)
10	CY	1.29	9/1752 (0.5%)	2.57	73/2362 (3.1%)
10	Cd	1.29	9/1752 (0.5%)	2.57	74/2362 (3.1%)
10	Ci	1.29	9/1752 (0.5%)	2.57	74/2362 (3.1%)
10	Cn	1.29	9/1752 (0.5%)	2.57	73/2362 (3.1%)
10	Cs	1.29	9/1752 (0.5%)	2.57	74/2362 (3.1%)
10	Cx	1.29	9/1752 (0.5%)	2.57	74/2362 (3.1%)
All	All	0.94	444/236268 (0.2%)	1.51	4456/319080 (1.4%)

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	A0	0	1
1	A5	0	1
1	AC	0	1
1	AH	0	1
1	AM	0	1
1	AR	0	1
1	AW	0	1
1	Ab	0	1
1	Ag	0	1
1	Al	0	1
1	Aq	0	1
1	Av	0	1
3	A2	0	1
3	A3	0	2
3	A7	0	1
3	AA	0	2
3	AE	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	AF	0	2
3	AJ	0	1
3	AK	0	2
3	AO	0	1
3	AP	0	2
3	AT	0	1
3	AU	0	2
3	AY	0	1
3	AZ	0	2
3	Ad	0	1
3	Ae	0	2
3	Ai	0	1
3	Aj	0	2
3	An	0	1
3	Ao	0	2
3	As	0	1
3	At	0	2
3	Ax	0	1
3	Ay	0	2
4	A4	0	1
4	AB	0	1
4	AG	0	1
4	AL	0	1
4	AQ	0	1
4	AV	0	1
4	Aa	0	1
4	Af	0	1
4	Ak	0	1
4	Ap	0	1
4	Au	0	1
4	Az	0	1
4	B2	0	2
4	B3	0	2
4	B7	0	2
4	BA	0	2
4	BE	0	2
4	BF	0	2
4	BJ	0	2
4	BK	0	2
4	BO	0	2
4	BP	0	2
4	BT	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	BU	0	2
4	BY	0	2
4	BZ	0	2
4	Bd	0	2
4	Be	0	2
4	Bi	0	2
4	Bj	0	2
4	Bn	0	2
4	Bo	0	2
4	Bs	0	2
4	Bt	0	2
4	Bx	0	2
4	By	0	2
5	B0	0	2
5	B5	0	2
5	BC	0	2
5	BH	0	2
5	BM	0	2
5	BR	0	2
5	BW	0	2
5	Bb	0	2
5	Bg	0	2
5	Bl	0	2
5	Bq	0	2
5	Bv	0	2
5	C4	0	1
5	CB	0	1
5	CG	0	1
5	CL	0	1
5	CQ	0	1
5	CV	0	1
5	Ca	0	1
5	Cf	0	1
5	Ck	0	1
5	Cp	0	1
5	Cu	0	1
5	Cz	0	1
6	B1	0	1
6	B6	0	1
6	BD	0	1
6	BI	0	1
6	BN	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	BS	0	1
6	BX	0	1
6	Bc	0	1
6	Bh	0	1
6	Bm	0	1
6	Br	0	1
6	Bw	0	1
7	B4	0	3
7	BB	0	3
7	BG	0	3
7	BL	0	3
7	BQ	0	3
7	BV	0	3
7	Ba	0	3
7	Bf	0	3
7	Bk	0	3
7	Bp	0	3
7	Bu	0	3
7	Bz	0	3
7	C3	0	2
7	CA	0	2
7	CF	0	2
7	CK	0	2
7	CP	0	2
7	CU	0	2
7	CZ	0	2
7	Ce	0	2
7	Cj	0	2
7	Co	0	2
7	Ct	0	2
7	Cy	0	2
8	C0	0	12
8	C5	0	12
8	CC	0	12
8	CH	0	12
8	CM	0	12
8	CR	0	12
8	CW	0	12
8	Cb	0	12
8	Cg	0	12
8	Cl	0	12
8	Cq	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	Cv	0	12
9	C1	0	10
9	C6	0	10
9	CD	0	10
9	CI	0	10
9	CN	0	10
9	CS	0	10
9	CX	0	10
9	Cc	0	10
9	Ch	0	10
9	Cm	0	10
9	Cr	0	10
9	Cw	0	10
10	C2	0	8
10	C7	0	8
10	CE	0	8
10	CJ	0	8
10	CO	0	8
10	CT	0	8
10	CY	0	8
10	Cd	0	8
10	Ci	0	8
10	Cn	0	8
10	Cs	0	8
10	Cx	0	8
All	All	0	576

The worst 5 of 444 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C7	57	LEU	C-N	20.46	1.62	1.33
10	CO	57	LEU	C-N	20.46	1.62	1.33
10	Cd	57	LEU	C-N	20.46	1.62	1.33
10	Cs	57	LEU	C-N	20.46	1.62	1.33
10	C2	57	LEU	C-N	20.45	1.62	1.33

The worst 5 of 4456 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	CE	57	LEU	O-C-N	-82.07	27.02	123.04
10	CT	57	LEU	O-C-N	-82.07	27.02	123.04
10	Ci	57	LEU	O-C-N	-82.07	27.02	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Cx	57	LEU	O-C-N	-82.07	27.02	123.04
10	C7	57	LEU	O-C-N	-82.06	27.03	123.04

There are no chirality outliers.

5 of 576 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A0	150	ARG	Sidechain
3	A2	23	TRP	Peptide
3	A3	23	TRP	Peptide
3	A3	27	PHE	Peptide
4	A4	142	LYS	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	A0	1191	0	1199	49	0
1	A5	1191	0	1199	54	0
1	AC	1191	0	1199	53	0
1	AH	1191	0	1199	53	0
1	AM	1191	0	1199	52	0
1	AR	1191	0	1199	52	0
1	AW	1191	0	1199	49	0
1	Ab	1191	0	1199	52	0
1	Ag	1191	0	1199	54	0
1	Al	1191	0	1199	53	0
1	Aq	1191	0	1199	52	0
1	Av	1191	0	1199	52	0
2	A1	1129	0	1104	78	0
2	A6	1129	0	1104	78	0
2	AD	1129	0	1104	77	0
2	AI	1129	0	1104	81	0
2	AN	1129	0	1104	81	0
2	AS	1129	0	1104	78	0
2	AX	1129	0	1104	77	0
2	Ac	1129	0	1104	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ah	1129	0	1104	78	0
2	Am	1129	0	1104	81	0
2	Ar	1129	0	1104	79	0
2	Aw	1129	0	1104	77	0
3	A2	1209	0	1198	82	0
3	A3	1209	0	1198	99	0
3	A7	1209	0	1198	82	0
3	AA	1209	0	1198	96	0
3	AE	1209	0	1198	77	0
3	AF	1209	0	1198	93	0
3	AJ	1209	0	1198	80	0
3	AK	1209	0	1198	97	0
3	AO	1209	0	1198	82	0
3	AP	1209	0	1198	99	0
3	AT	1209	0	1198	81	0
3	AU	1209	0	1198	98	0
3	AY	1209	0	1198	81	0
3	AZ	1209	0	1198	98	0
3	Ad	1209	0	1198	82	0
3	Ae	1209	0	1198	95	0
3	Ai	1209	0	1198	78	0
3	Aj	1209	0	1198	94	0
3	An	1209	0	1198	80	0
3	Ao	1209	0	1198	97	0
3	As	1209	0	1198	82	0
3	At	1209	0	1198	99	0
3	Ax	1209	0	1198	80	0
3	Ay	1209	0	1198	98	0
4	A4	1148	0	1106	73	0
4	AB	1148	0	1106	74	0
4	AG	1148	0	1106	71	0
4	AL	1148	0	1106	71	0
4	AQ	1148	0	1106	74	0
4	AV	1148	0	1106	74	0
4	Aa	1148	0	1106	74	0
4	Af	1148	0	1106	75	0
4	Ak	1148	0	1106	70	0
4	Ap	1148	0	1106	74	0
4	Au	1148	0	1106	73	0
4	Az	1148	0	1106	75	0
4	B2	1148	0	1106	57	0
4	B3	1148	0	1106	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B7	1148	0	1106	55	0
4	BA	1148	0	1106	63	0
4	BE	1148	0	1106	58	0
4	BF	1148	0	1106	60	0
4	BJ	1148	0	1106	59	0
4	BK	1148	0	1106	63	0
4	BO	1148	0	1106	60	0
4	BP	1148	0	1106	59	0
4	BT	1148	0	1106	57	0
4	BU	1148	0	1106	58	0
4	BY	1148	0	1106	57	0
4	BZ	1148	0	1106	60	0
4	Bd	1148	0	1106	55	0
4	Be	1148	0	1106	63	0
4	Bi	1148	0	1106	58	0
4	Bj	1148	0	1106	60	0
4	Bn	1148	0	1106	60	0
4	Bo	1148	0	1106	63	0
4	Bs	1148	0	1106	60	0
4	Bt	1148	0	1106	60	0
4	Bx	1148	0	1106	57	0
4	By	1148	0	1106	59	0
5	B0	1129	0	1104	66	0
5	B5	1129	0	1104	65	0
5	BC	1129	0	1104	66	0
5	BH	1129	0	1104	66	0
5	BM	1129	0	1104	64	0
5	BR	1129	0	1104	63	0
5	BW	1129	0	1104	64	0
5	Bb	1129	0	1104	64	0
5	Bg	1129	0	1104	66	0
5	Bl	1129	0	1104	66	0
5	Bq	1129	0	1104	63	0
5	Bv	1129	0	1104	64	0
5	C4	1129	0	1104	74	0
5	CB	1129	0	1104	73	0
5	CG	1129	0	1104	72	0
5	CL	1129	0	1104	74	0
5	CQ	1129	0	1104	70	0
5	CV	1129	0	1104	72	0
5	Ca	1129	0	1104	75	0
5	Cf	1129	0	1104	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Ck	1129	0	1104	74	0
5	Cp	1129	0	1104	74	0
5	Cu	1129	0	1104	70	0
5	Cz	1129	0	1104	71	0
6	B1	1209	0	1198	103	0
6	B6	1209	0	1198	104	0
6	BD	1209	0	1198	105	0
6	BI	1209	0	1198	105	0
6	BN	1209	0	1198	102	0
6	BS	1209	0	1198	104	0
6	BX	1209	0	1198	102	0
6	Bc	1209	0	1198	104	0
6	Bh	1209	0	1198	107	0
6	Bm	1209	0	1198	104	0
6	Br	1209	0	1198	101	0
6	Bw	1209	0	1198	103	0
7	B4	1190	0	1199	61	0
7	BB	1190	0	1199	61	0
7	BG	1190	0	1199	59	0
7	BL	1190	0	1199	63	0
7	BQ	1190	0	1199	60	0
7	BV	1190	0	1199	61	0
7	Ba	1190	0	1199	60	0
7	Bf	1190	0	1199	61	0
7	Bk	1190	0	1199	59	0
7	Bp	1190	0	1199	62	0
7	Bu	1190	0	1199	61	0
7	Bz	1190	0	1199	61	0
7	C3	1190	0	1199	61	0
7	CA	1190	0	1199	61	0
7	CF	1190	0	1199	62	0
7	CK	1190	0	1199	62	0
7	CP	1190	0	1199	60	0
7	CU	1190	0	1199	61	0
7	CZ	1190	0	1199	61	0
7	Ce	1190	0	1199	61	0
7	Cj	1190	0	1199	61	0
7	Co	1190	0	1199	62	0
7	Ct	1190	0	1199	60	0
7	Cy	1190	0	1199	61	0
8	C0	1751	0	1643	317	0
8	C5	1751	0	1643	320	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	CC	1751	0	1643	323	0
8	CH	1751	0	1643	324	0
8	CM	1751	0	1643	326	0
8	CR	1751	0	1643	327	0
8	CW	1751	0	1643	321	0
8	Cb	1751	0	1643	322	0
8	Cg	1751	0	1643	320	0
8	Cl	1751	0	1643	325	0
8	Cq	1751	0	1643	330	0
8	Cv	1751	0	1643	325	0
9	C1	1755	0	1678	367	0
9	C6	1755	0	1678	362	0
9	CD	1755	0	1678	368	0
9	CI	1755	0	1678	367	0
9	CN	1755	0	1678	363	0
9	CS	1755	0	1678	366	0
9	CX	1755	0	1678	370	0
9	Cc	1755	0	1678	361	0
9	Ch	1755	0	1678	369	0
9	Cm	1755	0	1678	363	0
9	Cr	1755	0	1678	363	0
9	Cw	1755	0	1678	367	0
10	C2	1715	0	1587	419	0
10	C7	1715	0	1587	422	0
10	CE	1715	0	1587	427	0
10	CJ	1715	0	1587	427	0
10	CO	1715	0	1587	424	0
10	CT	1715	0	1587	428	0
10	CY	1715	0	1587	423	0
10	Cd	1715	0	1587	424	0
10	Ci	1715	0	1587	424	0
10	Cn	1715	0	1587	429	0
10	Cs	1715	0	1587	425	0
10	Cx	1715	0	1587	428	0
All	All	231000	0	224748	18966	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 42.

The worst 5 of 18966 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)
8:C5:10:PHE:CD2	10:C7:10:HIS:CD2	1.79	1.70
8:CC:10:PHE:CD2	10:CE:10:HIS:CD2	1.79	1.70
8:Cb:10:PHE:CD2	10:Cd:10:HIS:CD2	1.79	1.70
8:Cg:10:PHE:CD2	10:Ci:10:HIS:CD2	1.79	1.70
9:CD:57:ILE:HG21	10:CE:57:LEU:CD1	1.22	1.65

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	A0	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	18	56
1	A5	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	18	56
1	AC	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	18	56
1	AH	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	18	56
1	AM	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	18	56
1	AR	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	18	56
1	AW	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	18	56
1	Ab	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	18	56
1	Ag	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	18	56
1	Al	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	18	56
1	Aq	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	18	56
1	Av	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	18	56
2	A1	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	A6	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	AD	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	AI	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AN	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	AS	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	AX	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	Ac	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	Ah	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	Am	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	Ar	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
2	Aw	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	18	56
3	A2	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	A3	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	A7	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AA	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AE	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AF	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AJ	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AK	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AO	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AP	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AT	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AU	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AY	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	AZ	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	Ad	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	Ae	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	Ai	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	Aj	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	An	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	Ao	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	As	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	At	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
3	Ax	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ay	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	4	24
4	A4	143/145 (99%)	124 (87%)	19 (13%)	0	100	100
4	AB	143/145 (99%)	124 (87%)	19 (13%)	0	100	100
4	AG	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	AL	143/145 (99%)	124 (87%)	19 (13%)	0	100	100
4	AQ	143/145 (99%)	124 (87%)	19 (13%)	0	100	100
4	AV	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	Aa	143/145 (99%)	124 (87%)	19 (13%)	0	100	100
4	Af	143/145 (99%)	124 (87%)	19 (13%)	0	100	100
4	Ak	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	Ap	143/145 (99%)	124 (87%)	19 (13%)	0	100	100
4	Au	143/145 (99%)	124 (87%)	19 (13%)	0	100	100
4	Az	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	B2	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	B3	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	B7	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	BA	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	BE	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	BF	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	BJ	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	BK	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	BO	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	BP	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	BT	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	BU	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	BY	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	BZ	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	Bd	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	Be	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	Bi	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	Bj	143/145 (99%)	125 (87%)	18 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Bn	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	Bo	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	Bs	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	Bt	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
4	Bx	143/145 (99%)	128 (90%)	15 (10%)	0	100	100
4	By	143/145 (99%)	125 (87%)	18 (13%)	0	100	100
5	B0	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	B5	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	BC	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	BH	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	BM	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	BR	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	BW	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Bb	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Bg	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Bl	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Bq	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Bv	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	C4	138/158 (87%)	119 (86%)	18 (13%)	1 (1%)	18	56
5	CB	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	CG	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	CL	138/158 (87%)	119 (86%)	18 (13%)	1 (1%)	18	56
5	CQ	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	CV	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Ca	138/158 (87%)	119 (86%)	18 (13%)	1 (1%)	18	56
5	Cf	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Ck	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Cp	138/158 (87%)	119 (86%)	18 (13%)	1 (1%)	18	56
5	Cu	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
5	Cz	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	18	56
6	B1	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	B6	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	BD	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	BI	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	BN	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	BS	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	BX	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	Bc	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	Bh	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	Bm	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	Br	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
6	Bw	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	21
7	B4	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	9	40
7	BB	147/170 (86%)	125 (85%)	20 (14%)	2 (1%)	9	40
7	BG	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	9	40
7	BL	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	9	40
7	BQ	147/170 (86%)	125 (85%)	20 (14%)	2 (1%)	9	40
7	BV	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	9	40
7	Ba	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	9	40
7	Bf	147/170 (86%)	125 (85%)	20 (14%)	2 (1%)	9	40
7	Bk	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	9	40
7	Bp	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	9	40
7	Bu	147/170 (86%)	125 (85%)	20 (14%)	2 (1%)	9	40
7	Bz	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	9	40
7	C3	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	CA	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	CF	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	CK	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	CP	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	CU	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	CZ	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	Ce	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Cj	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	Co	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	Ct	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
7	Cy	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	18	56
8	C0	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	C5	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	CC	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	CH	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	CM	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	CR	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	CW	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	Cb	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	Cg	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	Cl	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	Cq	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
8	Cv	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	6	32
9	C1	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	C6	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	CD	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	CI	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	CN	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	CS	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	CX	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	Cc	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	Ch	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	Cm	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	Cr	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
9	Cw	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	14	51
10	C2	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	C7	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	CE	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CJ	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	CO	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	CT	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	CY	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	Cd	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	Ci	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	Cn	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	Cs	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
10	Cx	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	4	24
All	All	28308/31116 (91%)	24544 (87%)	3380 (12%)	384 (1%)	11	40

5 of 384 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A2	29	ASP
3	A2	87	THR
3	A3	87	THR
3	A7	29	ASP
3	A7	87	THR

5.3.2 Protein sidechains ⓘ

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	A0	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	A5	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	AC	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	AH	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	AM	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	AR	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	AW	128/128 (100%)	119 (93%)	9 (7%)	14	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ab	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	Ag	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	Al	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	Aq	128/128 (100%)	119 (93%)	9 (7%)	14	35
1	Av	128/128 (100%)	119 (93%)	9 (7%)	14	35
2	A1	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	A6	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	AD	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	AI	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	AN	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	AS	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	AX	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	Ac	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	Ah	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	Am	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	Ar	121/121 (100%)	108 (89%)	13 (11%)	6	21
2	Aw	121/121 (100%)	108 (89%)	13 (11%)	6	21
3	A2	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	A3	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	A7	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	AA	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	AE	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	AF	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	AJ	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	AK	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	AO	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	AP	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	AT	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	AU	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	AY	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	AZ	131/131 (100%)	118 (90%)	13 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ad	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	Ae	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	Ai	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	Aj	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	An	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	Ao	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	As	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	At	131/131 (100%)	118 (90%)	13 (10%)	7	24
3	Ax	131/131 (100%)	115 (88%)	16 (12%)	5	17
3	Ay	131/131 (100%)	118 (90%)	13 (10%)	7	24
4	A4	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	AB	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	AG	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	AL	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	AQ	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	AV	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Aa	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Af	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Ak	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Ap	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Au	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Az	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	B2	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	B3	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	B7	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	BA	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	BE	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	BF	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	BJ	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	BK	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	BO	117/117 (100%)	107 (92%)	10 (8%)	10	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BP	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	BT	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	BU	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	BY	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	BZ	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Bd	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	Be	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Bi	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	Bj	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Bn	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	Bo	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Bs	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	Bt	117/117 (100%)	105 (90%)	12 (10%)	7	23
4	Bx	117/117 (100%)	107 (92%)	10 (8%)	10	29
4	By	117/117 (100%)	105 (90%)	12 (10%)	7	23
5	B0	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	B5	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	BC	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	BH	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	BM	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	BR	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	BW	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	Bb	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	Bg	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	Bl	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	Bq	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	Bv	121/135 (90%)	111 (92%)	10 (8%)	10	30
5	C4	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	CB	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	CG	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	CL	121/135 (90%)	113 (93%)	8 (7%)	15	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CQ	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	CV	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	Ca	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	Cf	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	Ck	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	Cp	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	Cu	121/135 (90%)	113 (93%)	8 (7%)	15	37
5	Cz	121/135 (90%)	113 (93%)	8 (7%)	15	37
6	B1	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	B6	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	BD	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	BI	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	BN	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	BS	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	BX	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	Bc	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	Bh	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	Bm	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	Br	131/134 (98%)	116 (88%)	15 (12%)	5	18
6	Bw	131/134 (98%)	116 (88%)	15 (12%)	5	18
7	B4	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	BB	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	BG	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	BL	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	BQ	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	BV	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	Ba	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	Bf	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	Bk	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	Bp	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	Bu	128/145 (88%)	119 (93%)	9 (7%)	14	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Bz	128/145 (88%)	119 (93%)	9 (7%)	14	35
7	C3	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	CA	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	CF	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	CK	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	CP	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	CU	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	CZ	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	Ce	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	Cj	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	Co	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	Ct	128/145 (88%)	118 (92%)	10 (8%)	11	32
7	Cy	128/145 (88%)	118 (92%)	10 (8%)	11	32
8	C0	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	C5	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	CC	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	CH	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	CM	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	CR	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	CW	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	Cb	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	Cg	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	Cl	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	Cq	195/212 (92%)	147 (75%)	48 (25%)	1	4
8	Cv	195/212 (92%)	147 (75%)	48 (25%)	1	4
9	C1	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	C6	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	CD	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	CI	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	CN	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	CS	193/241 (80%)	155 (80%)	38 (20%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CX	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	Cc	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	Ch	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	Cm	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	Cr	193/241 (80%)	155 (80%)	38 (20%)	1	7
9	Cw	193/241 (80%)	155 (80%)	38 (20%)	1	7
10	C2	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	C7	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	CE	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	CJ	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	CO	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	CT	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	CY	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	Cd	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	Ci	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	Cn	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	Cs	193/211 (92%)	165 (86%)	28 (14%)	3	13
10	Cx	193/211 (92%)	165 (86%)	28 (14%)	3	13
All	All	24864/26640 (93%)	21852 (88%)	3012 (12%)	7	17

5 of 3012 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	CH	140	PHE
9	CX	155	LEU
9	CI	212	GLU
8	CH	137	ARG
5	CQ	8	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 926 such sidechains are listed below:

Mol	Chain	Res	Type
4	BU	81	GLN
10	Cs	10	HIS
4	Bo	115	HIS

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Mol	Chain	Res	Type
8	Cq	18	ASN
7	CZ	70	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	C0	2
8	C5	2
8	CC	2
8	CH	2
8	CM	2
8	CR	2
8	CW	2
8	Cb	2
8	Cg	2
8	Cl	2

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Mol	Chain	Number of breaks
8	Cq	2
8	Cv	2
9	C1	1
9	C6	1
9	CD	1
9	CI	1
9	CN	1
9	CS	1
9	CX	1
9	Cc	1
9	Ch	1
9	Cm	1
9	Cr	1
9	Cw	1
10	C2	1
10	C7	1
10	CE	1
10	CJ	1
10	CO	1
10	CT	1
10	CY	1
10	Cd	1
10	Ci	1
10	Cn	1
10	Cs	1
10	Cx	1

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C0	57:LEU	C	58:GLU	N	4.76
1	C5	57:LEU	C	58:GLU	N	4.76
1	CC	57:LEU	C	58:GLU	N	4.76
1	CH	57:LEU	C	58:GLU	N	4.76
1	CM	57:LEU	C	58:GLU	N	4.76

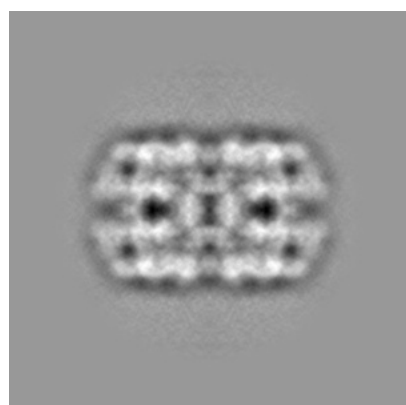
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2627. These allow visual inspection of the internal detail of the map and identification of artifacts.

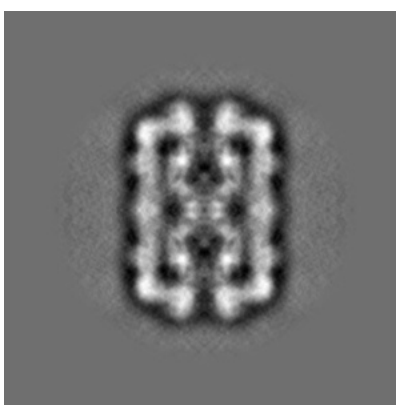
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

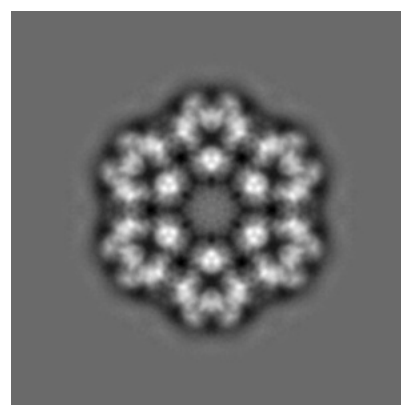
6.1.1 Primary map



X



Y

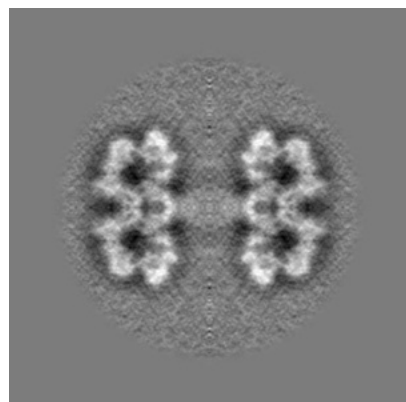


Z

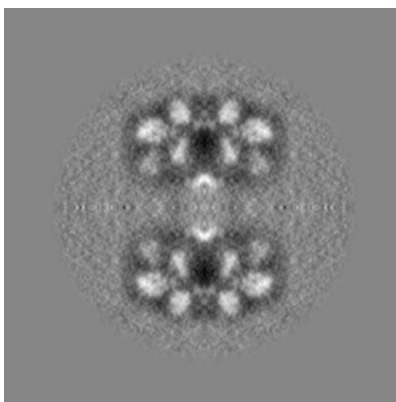
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

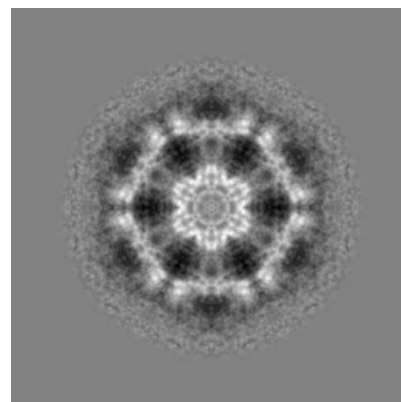
6.2.1 Primary map



X Index: 200



Y Index: 200

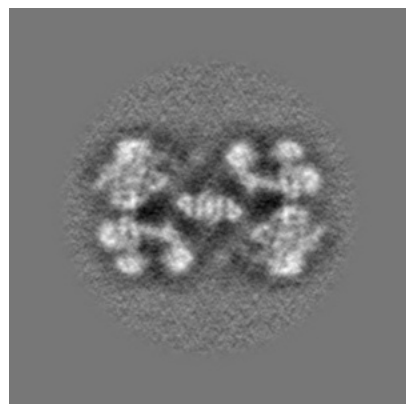


Z Index: 200

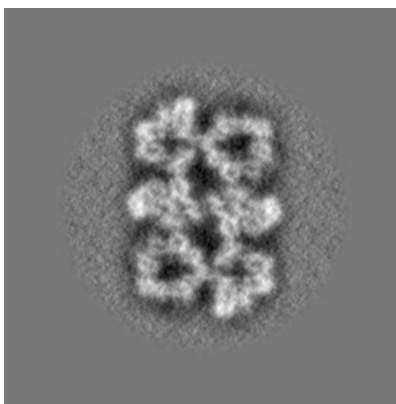
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

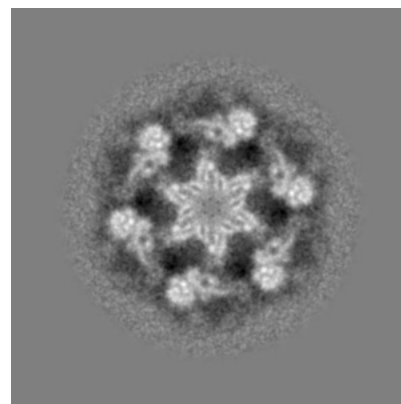
6.3.1 Primary map



X Index: 173



Y Index: 151

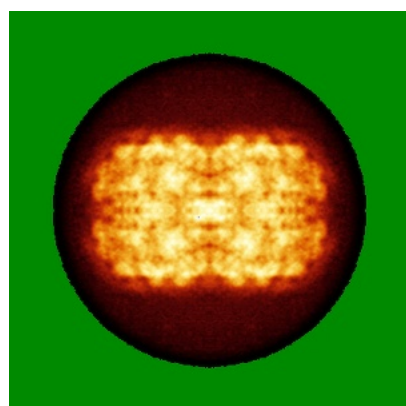


Z Index: 205

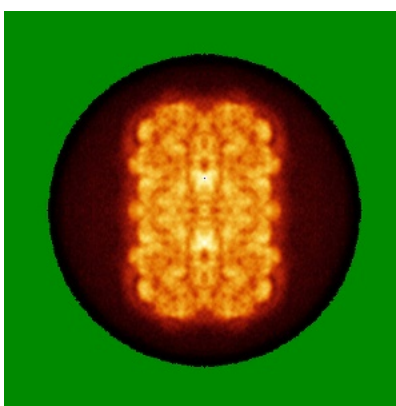
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

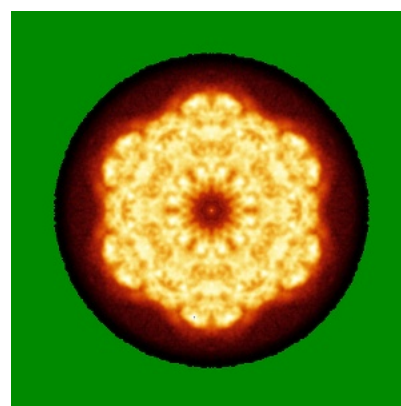
6.4.1 Primary map



X



Y

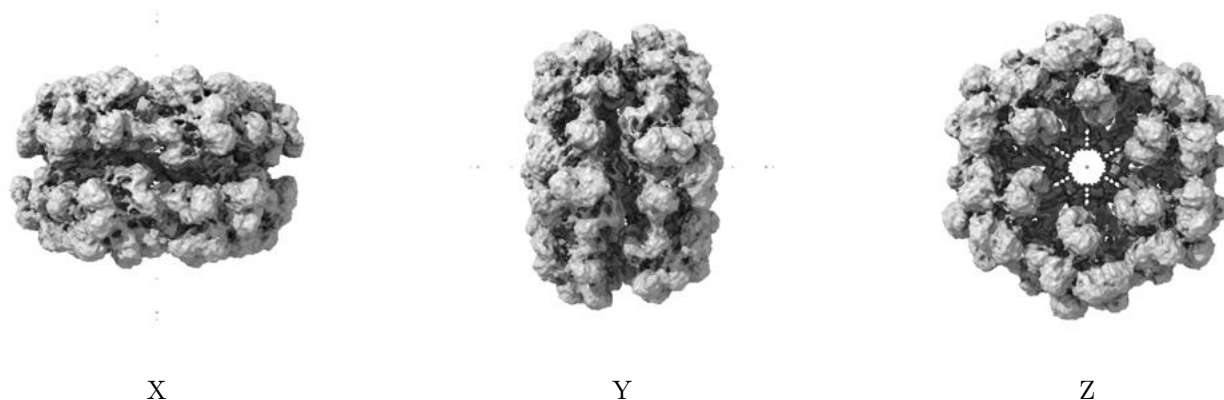


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.042. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

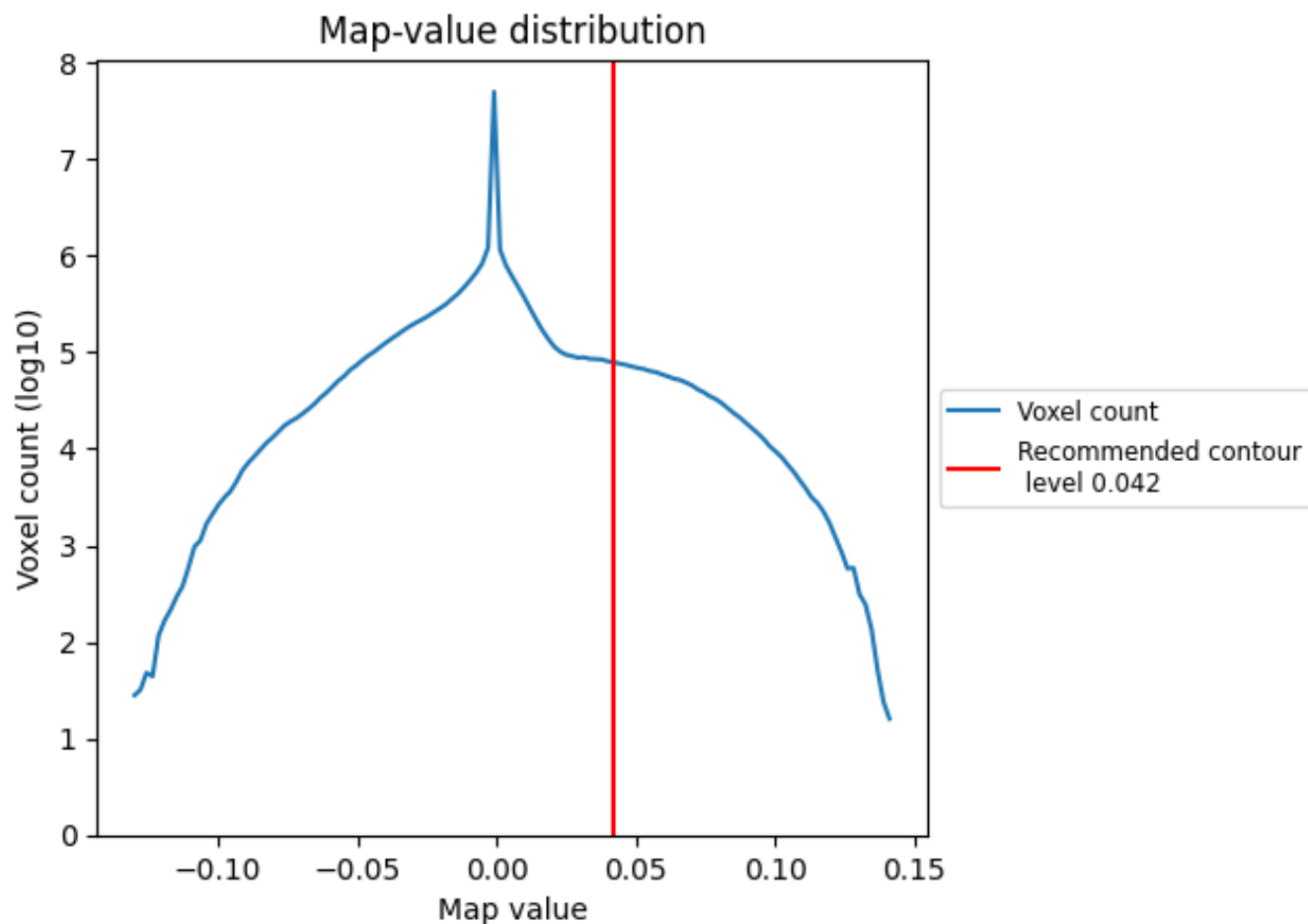
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

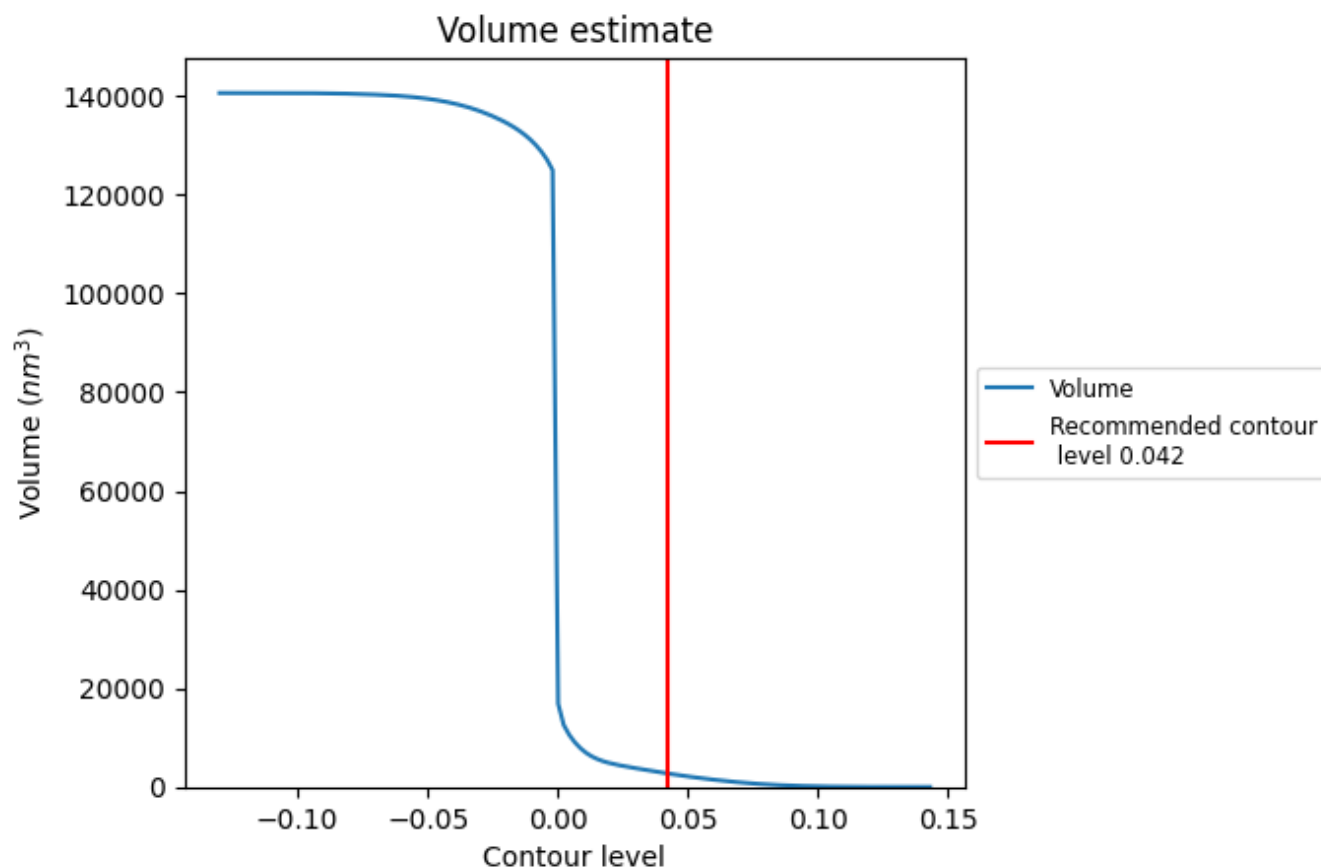
This section contains the results of statistical analysis of the map.

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.

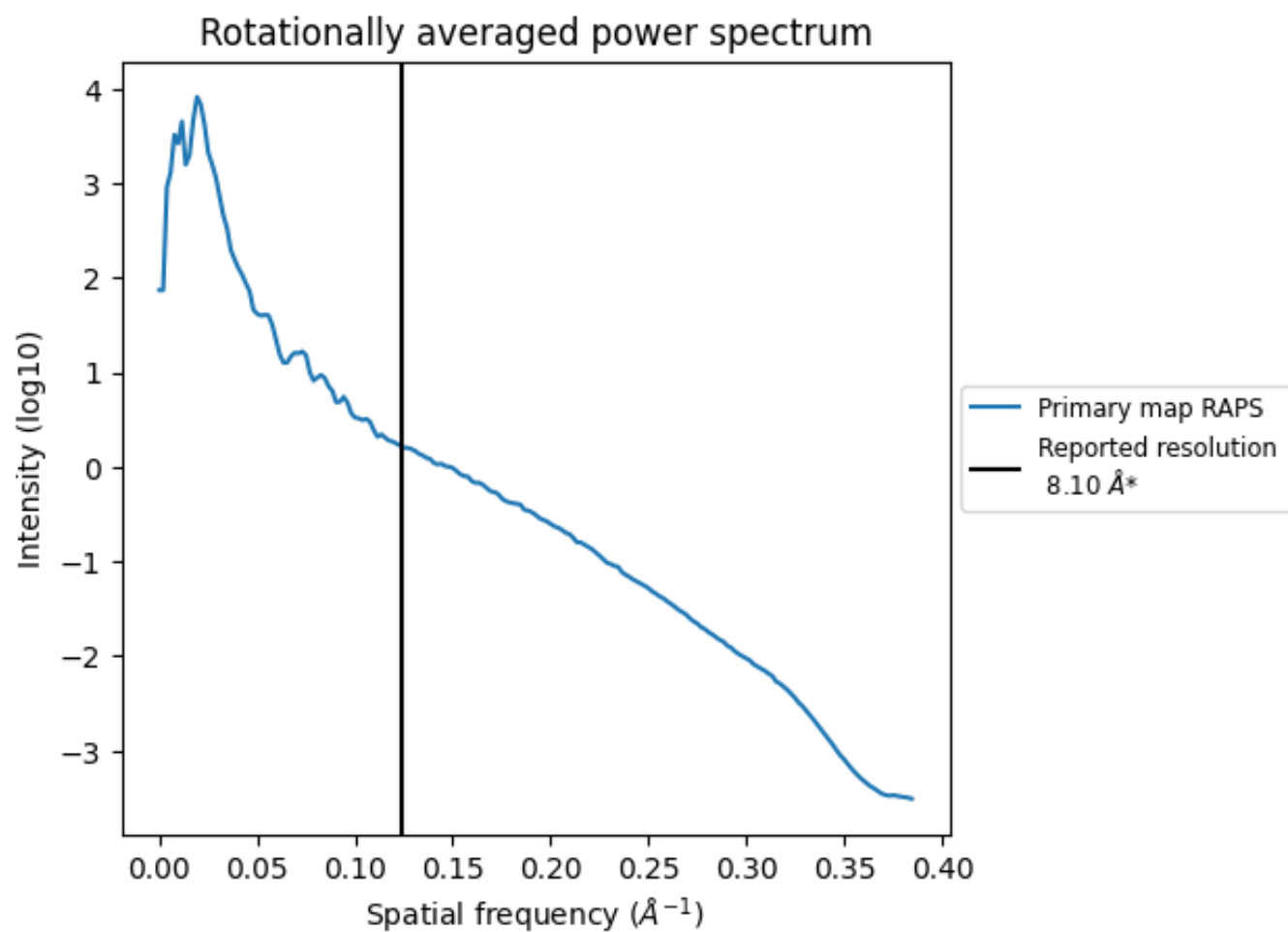
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2748 nm³; this corresponds to an approximate mass of 2483 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

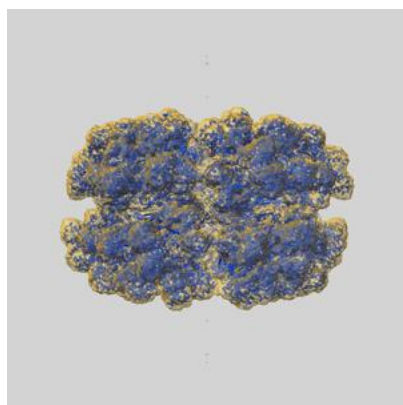
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

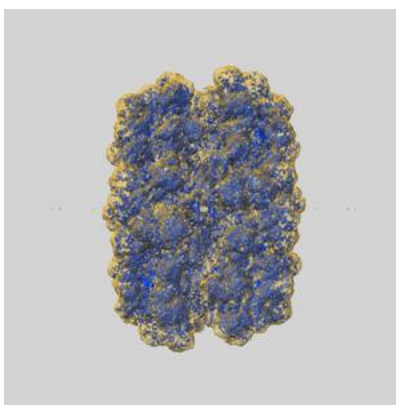
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2627 and PDB model 4V93. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

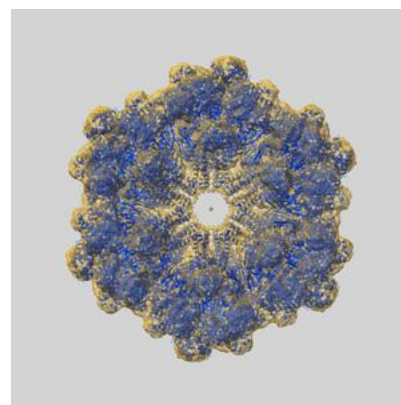
9.1 Map-model overlay [i](#)



X



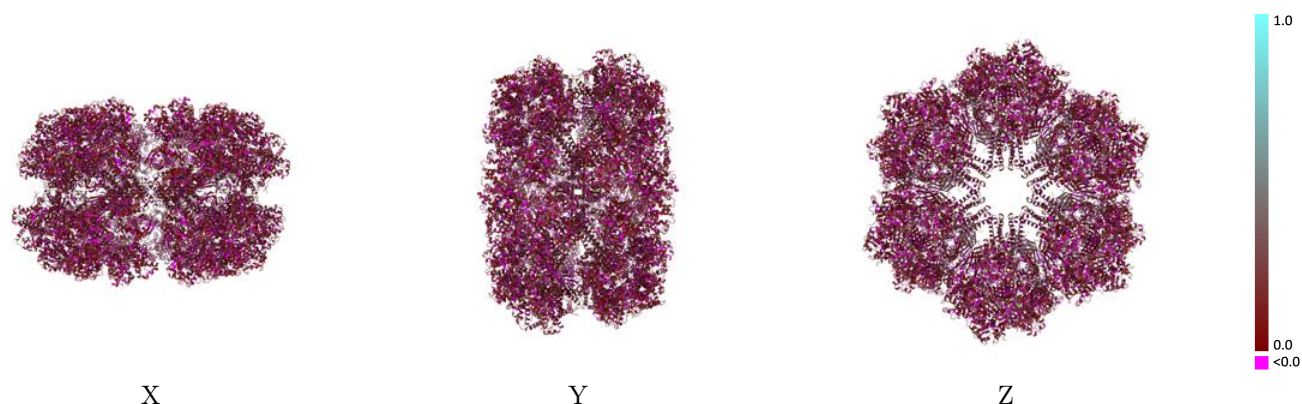
Y



Z

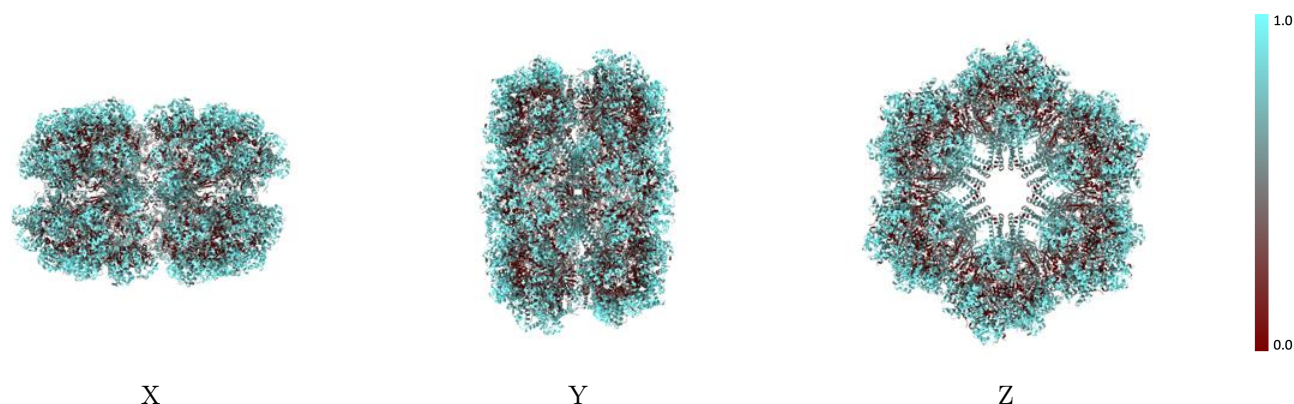
The images above show the 3D surface view of the map at the recommended contour level 0.042 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



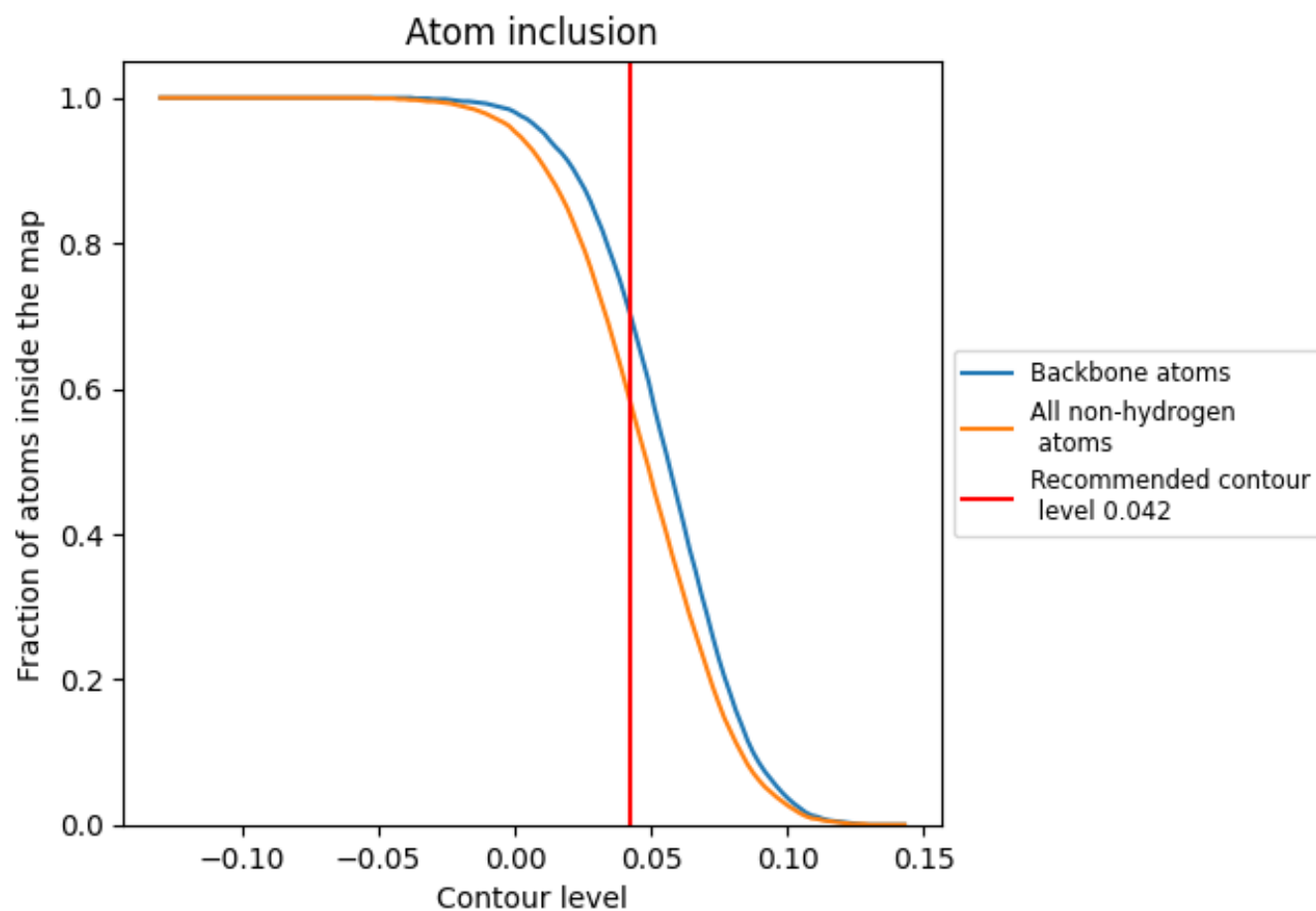
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.042).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 59% 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 (0.042) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.1070
A0	 0.5470	 0.1090
A1	 0.6720	 0.1140
A2	 0.6220	 0.1040
A3	 0.7120	 0.1110
A4	 0.6600	 0.1230
A5	 0.5450	 0.1080
A6	 0.6710	 0.1130
A7	 0.6210	 0.1070
AA	 0.7130	 0.1160
AB	 0.6610	 0.1270
AC	 0.5460	 0.1110
AD	 0.6700	 0.1140
AE	 0.6190	 0.1050
AF	 0.7080	 0.1140
AG	 0.6620	 0.1260
AH	 0.5470	 0.1090
AI	 0.6720	 0.1140
AJ	 0.6220	 0.1050
AK	 0.7120	 0.1140
AL	 0.6600	 0.1250
AM	 0.5450	 0.1080
AN	 0.6710	 0.1120
AO	 0.6210	 0.1060
AP	 0.7130	 0.1140
AQ	 0.6610	 0.1260
AR	 0.5460	 0.1090
AS	 0.6700	 0.1120
AT	 0.6190	 0.1060
AU	 0.7080	 0.1150
AV	 0.6620	 0.1270
AW	 0.5470	 0.1120
AX	 0.6720	 0.1170
AY	 0.6220	 0.1040
AZ	 0.7120	 0.1150



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Chain	Atom inclusion	Q-score
Aa	 0.6600	 0.1250
Ab	 0.5450	 0.1120
Ac	 0.6710	 0.1160
Ad	 0.6210	 0.1050
Ae	 0.7130	 0.1130
Af	 0.6610	 0.1250
Ag	 0.5460	 0.1070
Ah	 0.6700	 0.1110
Ai	 0.6190	 0.1070
Aj	 0.7080	 0.1120
Ak	 0.6620	 0.1230
Al	 0.5470	 0.1080
Am	 0.6720	 0.1150
An	 0.6220	 0.1040
Ao	 0.7120	 0.1120
Ap	 0.6600	 0.1210
Aq	 0.5450	 0.1060
Ar	 0.6710	 0.1150
As	 0.6210	 0.1050
At	 0.7130	 0.1110
Au	 0.6600	 0.1220
Av	 0.5460	 0.1070
Aw	 0.6700	 0.1140
Ax	 0.6190	 0.1060
Ay	 0.7080	 0.1100
Az	 0.6620	 0.1240
B0	 0.7280	 0.1310
B1	 0.5450	 0.0870
B2	 0.6060	 0.1130
B3	 0.5240	 0.0950
B4	 0.6600	 0.1200
B5	 0.7260	 0.1300
B6	 0.5430	 0.0850
B7	 0.6080	 0.1150
BA	 0.5230	 0.0900
BB	 0.6600	 0.1230
BC	 0.7260	 0.1250
BD	 0.5450	 0.0830
BE	 0.6090	 0.1150
BF	 0.5200	 0.0920
BG	 0.6570	 0.1230
BH	 0.7280	 0.1280

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Chain	Atom inclusion	Q-score
BI	0.5450	0.0850
BJ	0.6060	0.1170
BK	0.5240	0.0980
BL	0.6600	0.1240
BM	0.7260	0.1290
BN	0.5430	0.0810
BO	0.6080	0.1160
BP	0.5230	0.0950
BQ	0.6600	0.1270
BR	0.7260	0.1290
BS	0.5450	0.0830
BT	0.6090	0.1140
BU	0.5200	0.0930
BV	0.6570	0.1230
BW	0.7280	0.1290
BX	0.5450	0.0840
BY	0.6060	0.1120
BZ	0.5240	0.0940
Ba	0.6600	0.1220
Bb	0.7260	0.1280
Bc	0.5430	0.0820
Bd	0.6080	0.1120
Be	0.5230	0.0910
Bf	0.6600	0.1180
Bg	0.7260	0.1280
Bh	0.5450	0.0830
Bi	0.6090	0.1170
Bj	0.5200	0.0880
Bk	0.6570	0.1190
Bl	0.7280	0.1310
Bm	0.5450	0.0820
Bn	0.6060	0.1170
Bo	0.5240	0.0910
Bp	0.6600	0.1220
Bq	0.7260	0.1290
Br	0.5430	0.0810
Bs	0.6080	0.1160
Bt	0.5230	0.0880
Bu	0.6600	0.1220
Bv	0.7260	0.1300
Bw	0.5450	0.0840
Bx	0.6090	0.1140

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Chain	Atom inclusion	Q-score
By	 0.5200	 0.0900
Bz	 0.6570	 0.1200
C0	 0.4220	 0.0950
C1	 0.4210	 0.0940
C2	 0.5450	 0.1010
C3	 0.6290	 0.0980
C4	 0.7010	 0.1200
C5	 0.4190	 0.0960
C6	 0.4230	 0.0950
C7	 0.5460	 0.1040
CA	 0.6320	 0.0990
CB	 0.7010	 0.1150
CC	 0.4200	 0.0980
CD	 0.4230	 0.0990
CE	 0.5440	 0.1020
CF	 0.6300	 0.0990
CG	 0.7060	 0.1160
CH	 0.4220	 0.0960
CI	 0.4210	 0.0990
CJ	 0.5450	 0.1040
CK	 0.6290	 0.0980
CL	 0.7010	 0.1130
CM	 0.4190	 0.0960
CN	 0.4230	 0.0990
CO	 0.5460	 0.1050
CP	 0.6320	 0.0970
CQ	 0.7010	 0.1140
CR	 0.4200	 0.0970
CS	 0.4230	 0.0980
CT	 0.5440	 0.1040
CU	 0.6300	 0.0950
CV	 0.7060	 0.1170
CW	 0.4220	 0.0960
CX	 0.4210	 0.0970
CY	 0.5450	 0.1030
CZ	 0.6290	 0.0960
Ca	 0.7010	 0.1190
Cb	 0.4190	 0.0970
Cc	 0.4230	 0.0970
Cd	 0.5460	 0.1020
Ce	 0.6320	 0.1020
Cf	 0.7010	 0.1190

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Chain	Atom inclusion	Q-score
Cg	 0.4200	 0.0960
Ch	 0.4230	 0.0970
Ci	 0.5440	 0.1040
Cj	 0.6300	 0.1010
Ck	 0.7060	 0.1180
Cl	 0.4220	 0.0940
Cm	 0.4210	 0.0960
Cn	 0.5450	 0.1050
Co	 0.6290	 0.0980
Cp	 0.7010	 0.1170
Cq	 0.4190	 0.0940
Cr	 0.4230	 0.0960
Cs	 0.5460	 0.1030
Ct	 0.6320	 0.0980
Cu	 0.7010	 0.1170
Cv	 0.4200	 0.0960
Cw	 0.4230	 0.0950
Cx	 0.5440	 0.1030
Cy	 0.6300	 0.0960
Cz	 0.7060	 0.1190