Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 01:27 pm GMT

PDB ID	:	4V93
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

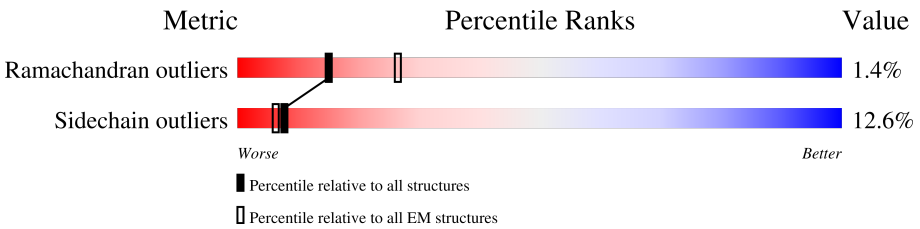
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A0	149	34% 93% 7% •
1	A5	149	34% 93% 7% •
1	AC	149	34% 93% 7% •
1	AH	149	34% 93% 7% •
1	AM	149	34% 93% 7% •
1	AR	149	34% 93% 7% •
1	AW	149	34% 93% 7% •
1	Ab	149	34% 93% 7% •
1	Ag	149	34% 93% 7% •

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Mol	Chain	Length	Quality of chain
1	Al	149	34% 93% 7% •
1	Aq	149	34% 93% 7% •
1	Av	149	34% 93% 7% •
2	A1	140	24% 89% 11%
2	A6	140	24% 89% 11%
2	AD	140	24% 89% 11%
2	AI	140	24% 89% 11%
2	AN	140	24% 89% 11%
2	AS	140	24% 89% 11%
2	AX	140	24% 89% 11%
2	Ac	140	24% 89% 11%
2	Ah	140	24% 89% 11%
2	Am	140	24% 89% 11%
2	Ar	140	24% 89% 11%
2	Aw	140	24% 89% 11%
3	A2	147	31% 86% 12% •
3	A3	147	20% 88% 10% ••
3	A7	147	31% 86% 12% •
3	AA	147	20% 88% 10% ••
3	AE	147	31% 86% 12% •
3	AF	147	20% 88% 10% ••
3	AJ	147	31% 86% 12% •
3	AK	147	20% 88% 10% ••
3	AO	147	31% 86% 12% •
3	AP	147	20% 88% 10% ••

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Mol	Chain	Length	Quality of chain
3	AT	147	31% 86% 12%
3	AU	147	20% 88% 10%
3	AY	147	31% 86% 12%
3	AZ	147	20% 88% 10%
3	Ad	147	31% 86% 12%
3	Ae	147	20% 88% 10%
3	Ai	147	31% 86% 12%
3	Aj	147	20% 88% 10%
3	An	147	31% 86% 12%
3	Ao	147	20% 88% 10%
3	As	147	31% 86% 12%
3	At	147	20% 88% 10%
3	Ax	147	31% 86% 12%
3	Ay	147	20% 88% 10%
4	A4	145	23% 90% 10%
4	AB	145	24% 90% 10%
4	AG	145	24% 90% 10%
4	AL	145	23% 90% 10%
4	AQ	145	24% 90% 10%
4	AV	145	24% 90% 10%
4	Aa	145	23% 90% 10%
4	Af	145	24% 90% 10%
4	Ak	145	24% 90% 10%
4	Ap	145	23% 90% 10%
4	Au	145	24% 90% 10%

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Mol	Chain	Length	Quality of chain
4	Az	145	24% 90% 10%
4	B2	145	36% 91% 8%
4	B3	145	41% 90% 8%
4	B7	145	36% 91% 8%
4	BA	145	41% 90% 8%
4	BE	145	36% 91% 8%
4	BF	145	41% 90% 8%
4	BJ	145	36% 91% 8%
4	BK	145	41% 90% 8%
4	BO	145	36% 91% 8%
4	BP	145	41% 90% 8%
4	BT	145	36% 91% 8%
4	BU	145	41% 90% 8%
4	BY	145	36% 91% 8%
4	BZ	145	41% 90% 8%
4	Bd	145	36% 91% 8%
4	Be	145	41% 90% 8%
4	Bi	145	36% 91% 8%
4	Bj	145	41% 90% 8%
4	Bn	145	36% 91% 8%
4	Bo	145	41% 90% 8%
4	Bs	145	36% 91% 8%
4	Bt	145	41% 90% 8%
4	Bx	145	36% 91% 8%
4	By	145	41% 90% 8%

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Mol	Chain	Length	Quality of chain
5	B0	158	14% 80% 8% • 11%
5	B5	158	13% 80% 8% • 11%
5	BC	158	14% 80% 8% • 11%
5	BH	158	14% 80% 8% • 11%
5	BM	158	13% 80% 8% • 11%
5	BR	158	14% 80% 8% • 11%
5	BW	158	14% 80% 8% • 11%
5	Bb	158	13% 80% 8% • 11%
5	Bg	158	14% 80% 8% • 11%
5	Bl	158	14% 80% 8% • 11%
5	Bq	158	13% 80% 8% • 11%
5	Bv	158	14% 80% 8% • 11%
5	C4	158	20% 82% 7% 11%
5	CB	158	20% 82% 7% 11%
5	CG	158	20% 82% 7% 11%
5	CL	158	20% 82% 7% 11%
5	CQ	158	20% 82% 7% 11%
5	CV	158	20% 82% 7% 11%
5	Ca	158	20% 82% 7% 11%
5	Cf	158	20% 82% 7% 11%
5	Ck	158	20% 82% 7% 11%
5	Cp	158	20% 82% 7% 11%
5	Cu	158	20% 82% 7% 11%
5	Cz	158	20% 82% 7% 11%
6	B1	151	39% 85% 10% • •

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Mol	Chain	Length	Quality of chain
6	B6	151	38% 85% 10%
6	BD	151	38% 85% 10%
6	BI	151	39% 85% 10%
6	BN	151	38% 85% 10%
6	BS	151	38% 85% 10%
6	BX	151	39% 85% 10%
6	Bc	151	38% 85% 10%
6	Bh	151	38% 85% 10%
6	Bm	151	39% 85% 10%
6	Br	151	38% 85% 10%
6	Bw	151	38% 85% 10%
7	B4	170	20% 81% 6% 12%
7	BB	170	20% 81% 6% 12%
7	BG	170	21% 81% 6% 12%
7	BL	170	20% 81% 6% 12%
7	BQ	170	20% 81% 6% 12%
7	BV	170	21% 81% 6% 12%
7	Ba	170	20% 81% 6% 12%
7	Bf	170	20% 81% 6% 12%
7	Bk	170	21% 81% 6% 12%
7	Bp	170	20% 81% 6% 12%
7	Bu	170	20% 81% 6% 12%
7	Bz	170	21% 81% 6% 12%
7	C3	170	26% 81% 5% 12%
7	CA	170	26% 81% 5% 12%

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Mol	Chain	Length	Quality of chain
7	CF	170	26% 81% 5% 12%
7	CK	170	26% 81% 5% 12%
7	CP	170	26% 81% 5% 12%
7	CU	170	26% 81% 5% 12%
7	CZ	170	26% 81% 5% 12%
7	Ce	170	26% 81% 5% 12%
7	Cj	170	26% 81% 5% 12%
7	Co	170	26% 81% 5% 12%
7	Ct	170	26% 81% 5% 12%
7	Cy	170	26% 81% 5% 12%
8	C0	240	45% 64% 19% 6% 10%
8	C5	240	45% 64% 19% 6% 10%
8	CC	240	45% 64% 19% 6% 10%
8	CH	240	45% 64% 19% 6% 10%
8	CM	240	45% 64% 19% 6% 10%
8	CR	240	45% 64% 19% 6% 10%
8	CW	240	45% 64% 19% 6% 10%
8	Cb	240	45% 64% 19% 6% 10%
8	Cg	240	45% 64% 19% 6% 10%
8	Cl	240	45% 64% 19% 6% 10%
8	Cq	240	45% 64% 19% 6% 10%
8	Cv	240	45% 64% 19% 6% 10%
9	C1	288	41% 59% 15% 24%
9	C6	288	40% 59% 15% 24%
9	CD	288	41% 59% 15% 24%

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Mol	Chain	Length	Quality of chain
9	CI	288	41% 59% 15% 24%
9	CN	288	40% 59% 15% 24%
9	CS	288	41% 59% 15% 24%
9	CX	288	41% 59% 15% 24%
9	Cc	288	40% 59% 15% 24%
9	Ch	288	41% 59% 15% 24%
9	Cm	288	41% 59% 15% 24%
9	Cr	288	40% 59% 15% 24%
9	Cw	288	41% 59% 15% 24%
10	C2	240	32% 69% 16% 10%
10	C7	240	32% 70% 16% 10%
10	CE	240	32% 70% 16% 10%
10	CJ	240	32% 69% 16% 10%
10	CO	240	32% 70% 16% 10%
10	CT	240	32% 70% 16% 10%
10	CY	240	32% 69% 16% 10%
10	Cd	240	32% 70% 16% 10%
10	Ci	240	32% 70% 16% 10%
10	Cn	240	32% 69% 16% 10%
10	Cs	240	32% 70% 16% 10%
10	Cx	240	32% 70% 16% 10%

2 Entry composition (i)

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

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

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

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

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

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

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
			Total	C	N	O	S		
4	A4	145	1148	720	212	213	3	0	0
			Total	C	N	O	S		
4	AB	145	1148	720	212	213	3	0	0
			Total	C	N	O	S		
4	AG	145	1148	720	212	213	3	0	0
			Total	C	N	O	S		
4	AL	145	1148	720	212	213	3	0	0

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BZ	145	1148	720	212	213	3	0	0
4	Bd	145	1148	720	212	213	3	0	0
4	Be	145	1148	720	212	213	3	0	0
4	Bi	145	1148	720	212	213	3	0	0
4	Bj	145	1148	720	212	213	3	0	0
4	Bn	145	1148	720	212	213	3	0	0
4	Bo	145	1148	720	212	213	3	0	0
4	Bs	145	1148	720	212	213	3	0	0
4	Bt	145	1148	720	212	213	3	0	0
4	Bx	145	1148	720	212	213	3	0	0
4	By	145	1148	720	212	213	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
			Total	C	N	O	S		
5	B0	140	1129	725	198	202	4	0	0
5	B5	140	1129	725	198	202	4	0	0
5	BC	140	1129	725	198	202	4	0	0
5	BH	140	1129	725	198	202	4	0	0
5	BM	140	1129	725	198	202	4	0	0
5	BR	140	1129	725	198	202	4	0	0
5	BW	140	1129	725	198	202	4	0	0
5	Bb	140	1129	725	198	202	4	0	0
5	Bg	140	1129	725	198	202	4	0	0
5	Bl	140	1129	725	198	202	4	0	0

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

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

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

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

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
			Total	C	N	O	S		
7	B4	149	1190	758	212	217	3	0	0
			Total	C	N	O	S		
7	BB	149	1190	758	212	217	3	0	0
			Total	C	N	O	S		
7	BG	149	1190	758	212	217	3	0	0
			Total	C	N	O	S		
7	BL	149	1190	758	212	217	3	0	0

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

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
			Total	C	N	O	S		
8	C0	217	1751	1089	308	344	10	0	0
8	C5	217	1751	1089	308	344	10	0	0
8	CC	217	1751	1089	308	344	10	0	0
8	CH	217	1751	1089	308	344	10	0	0
8	CM	217	1751	1089	308	344	10	0	0
8	CR	217	1751	1089	308	344	10	0	0
8	CW	217	1751	1089	308	344	10	0	0
8	Cb	217	1751	1089	308	344	10	0	0

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

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

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

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

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

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

There are 12 discrepancies between the modelled and reference sequences:

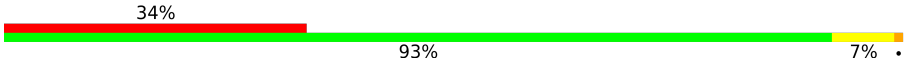
Chain	Residue	Modelled	Actual	Comment	Reference
C2	113	CYS	VAL	conflict	UNP Q2I742
C7	113	CYS	VAL	conflict	UNP Q2I742
CE	113	CYS	VAL	conflict	UNP Q2I742
CJ	113	CYS	VAL	conflict	UNP Q2I742
CO	113	CYS	VAL	conflict	UNP Q2I742
CT	113	CYS	VAL	conflict	UNP Q2I742
CY	113	CYS	VAL	conflict	UNP Q2I742
Cd	113	CYS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

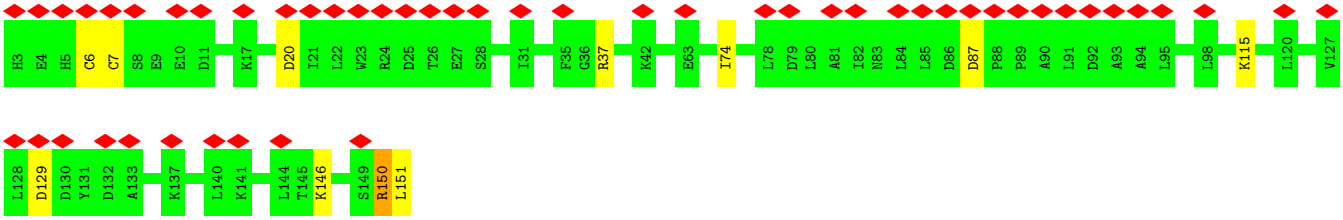
3 Residue-property plots (i)

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

- Molecule 1: EXTRACELLULAR GLOBIN-3

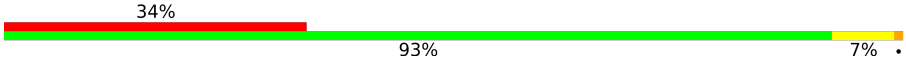
Chain A0:

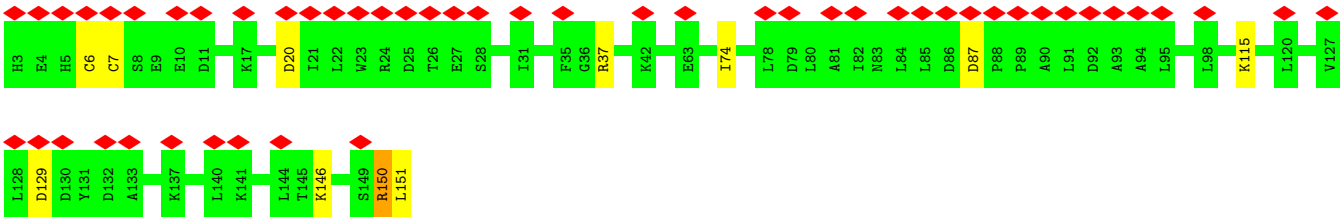




- Molecule 1: EXTRACELLULAR GLOBIN-3

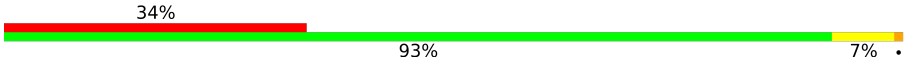
Chain A5:

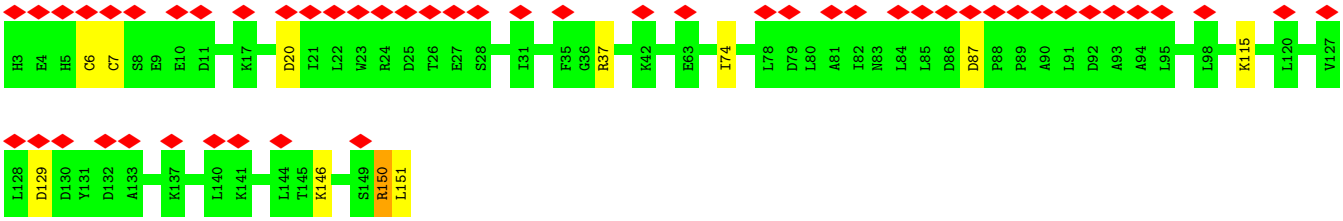




- Molecule 1: EXTRACELLULAR GLOBIN-3

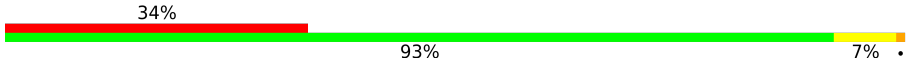
Chain AC:

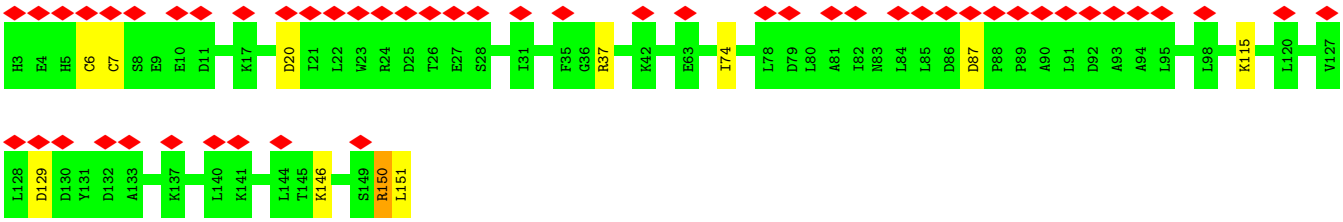




- Molecule 1: EXTRACELLULAR GLOBIN-3

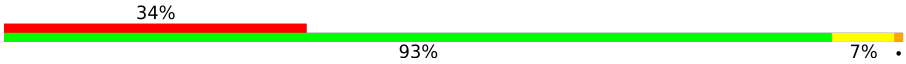
Chain AH:

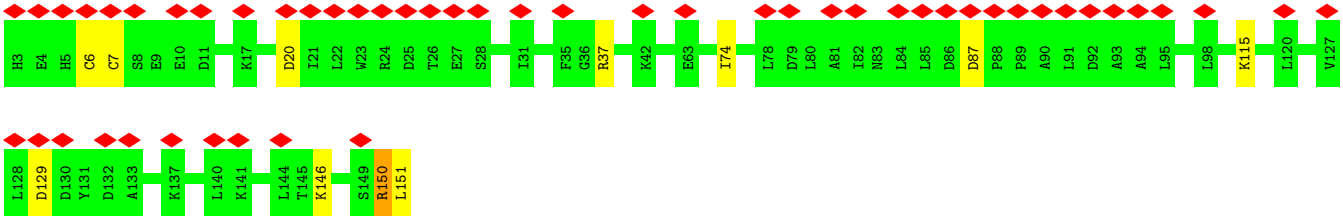




• Molecule 1: EXTRACELLULAR GLOBIN-3

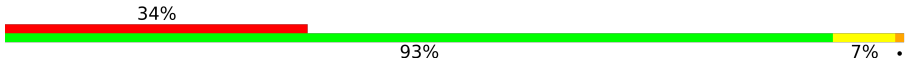
Chain AM:

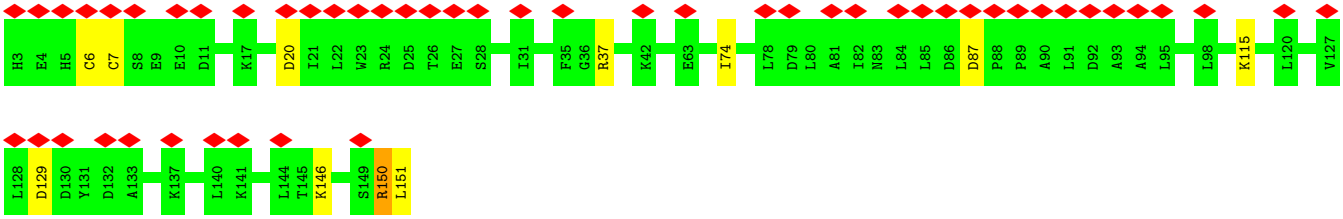




• Molecule 1: EXTRACELLULAR GLOBIN-3

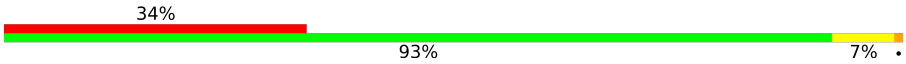
Chain AR:

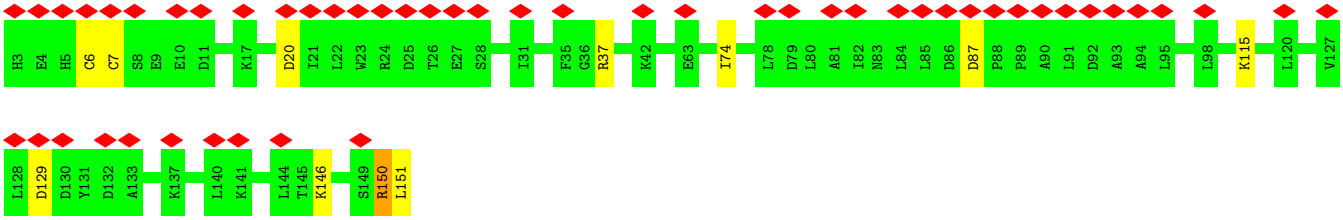




• Molecule 1: EXTRACELLULAR GLOBIN-3

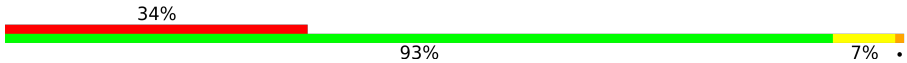
Chain AW:

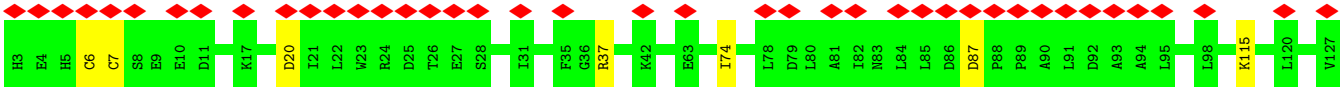


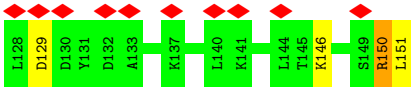


• Molecule 1: EXTRACELLULAR GLOBIN-3

Chain Ab:

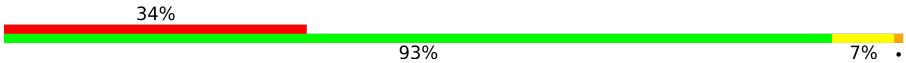


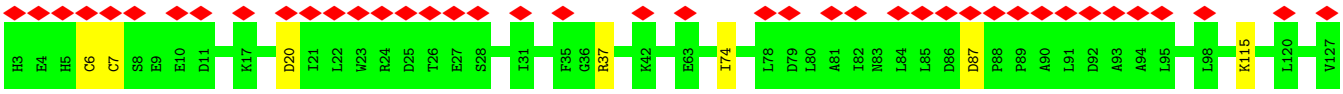


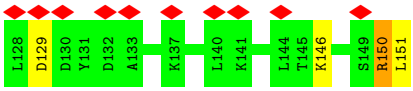


• Molecule 1: EXTRACELLULAR GLOBIN-3

Chain Ag:

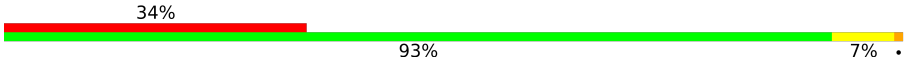


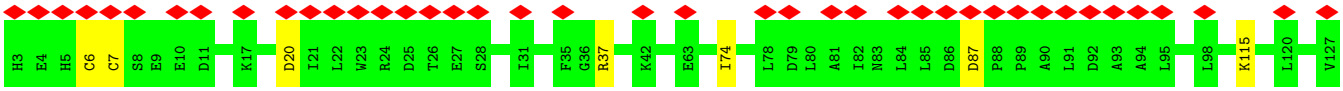


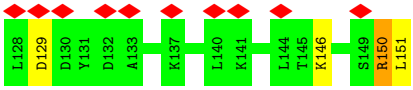


• Molecule 1: EXTRACELLULAR GLOBIN-3

Chain Al:

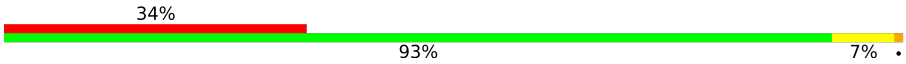


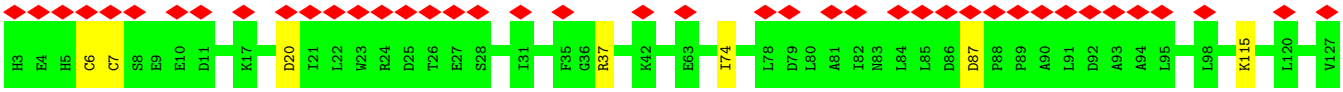


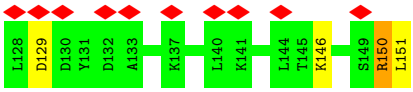


• Molecule 1: EXTRACELLULAR GLOBIN-3

Chain Aq:

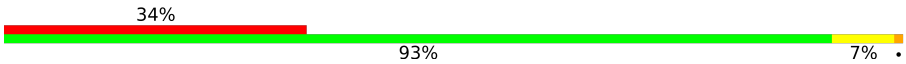


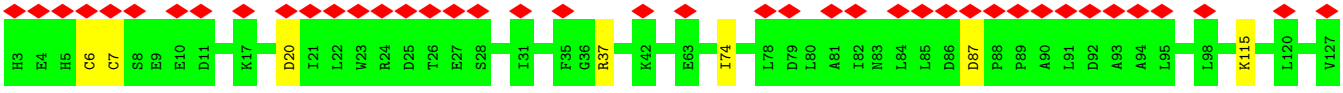


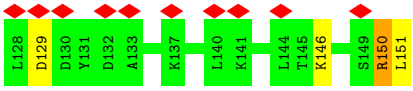


• Molecule 1: EXTRACELLULAR GLOBIN-3

Chain Av:

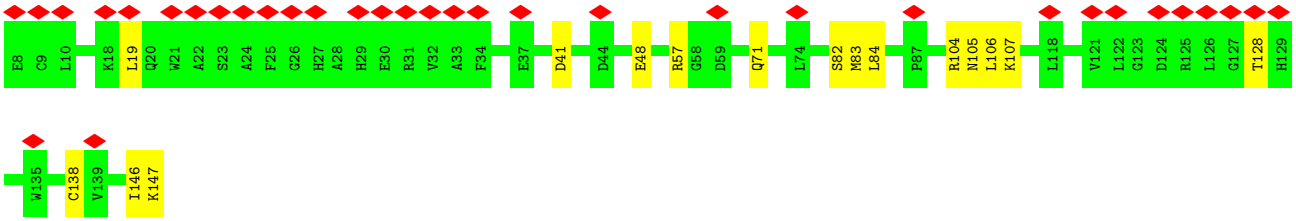






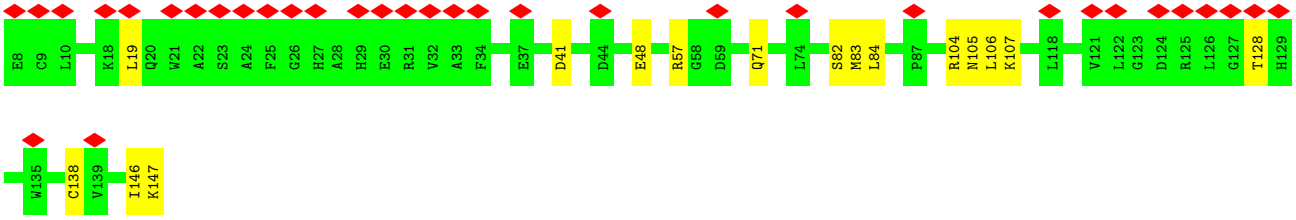
• Molecule 2: HEMOGLOBIN CHAIN D1

Chain A1:



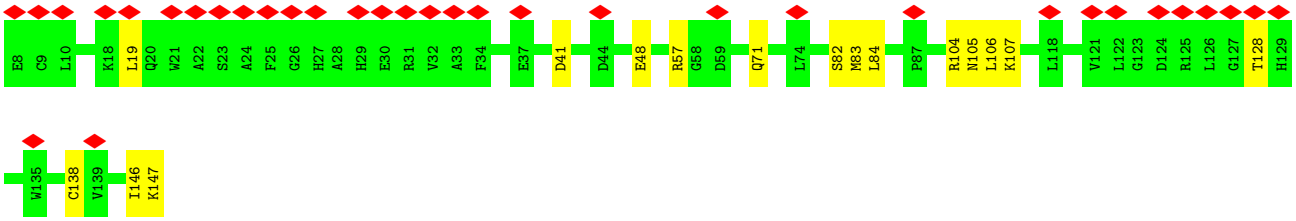
- Molecule 2: HEMOGLOBIN CHAIN D1

Chain A6:



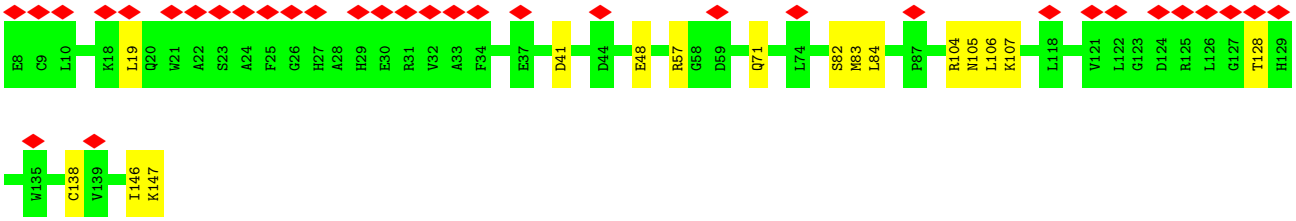
- Molecule 2: HEMOGLOBIN CHAIN D1

Chain AD:



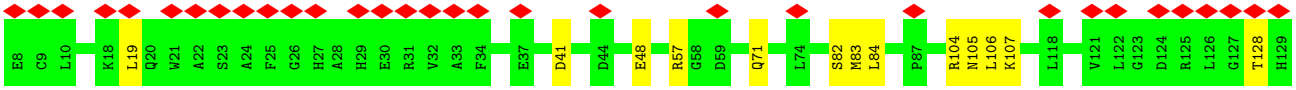
- Molecule 2: HEMOGLOBIN CHAIN D1

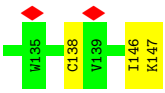
Chain AI:



- Molecule 2: HEMOGLOBIN CHAIN D1

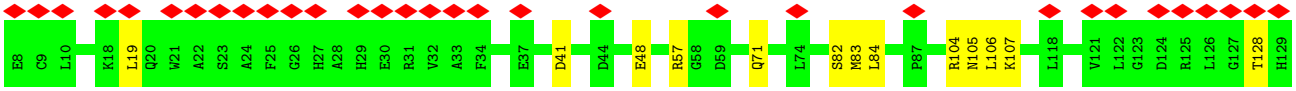
Chain AN:

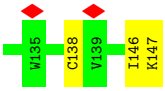




• Molecule 2: HEMOGLOBIN CHAIN D1

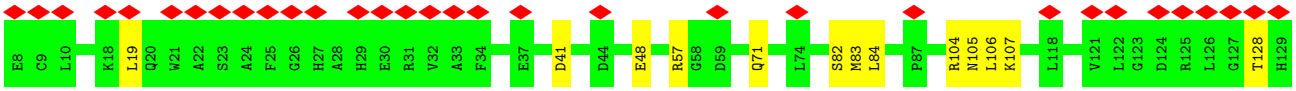
Chain AS:

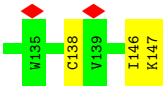




• Molecule 2: HEMOGLOBIN CHAIN D1

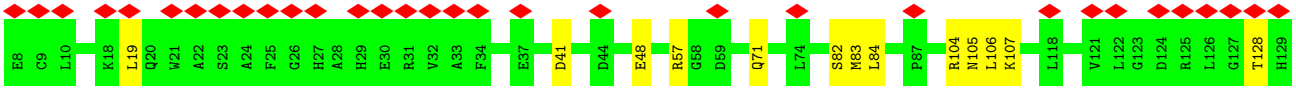
Chain AX:

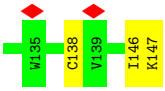




• Molecule 2: HEMOGLOBIN CHAIN D1

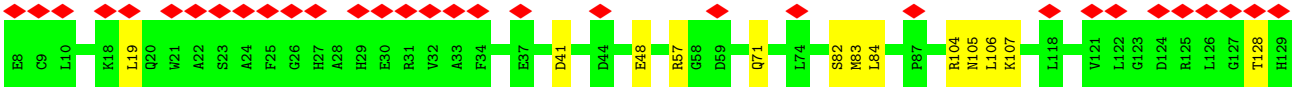
Chain Ac:

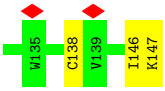




• Molecule 2: HEMOGLOBIN CHAIN D1

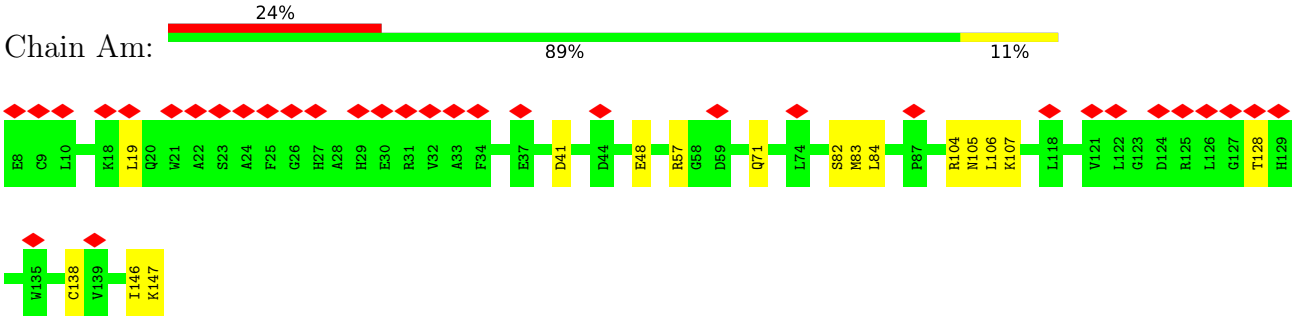
Chain Ah:





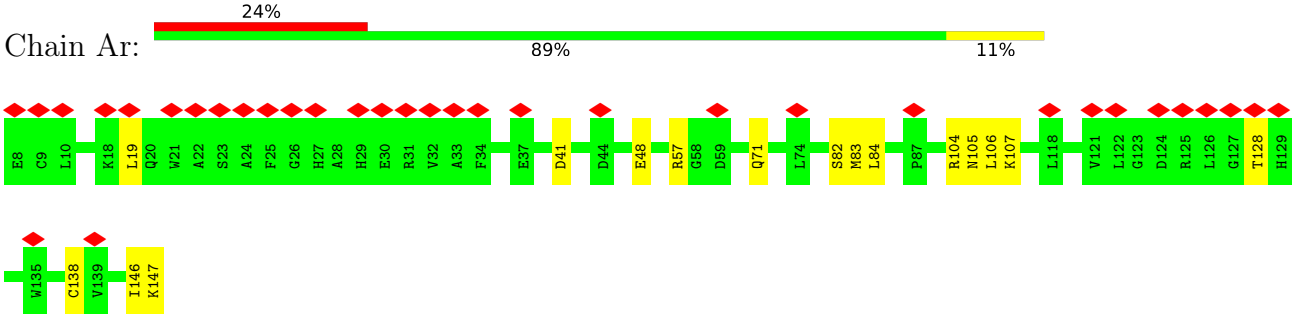
• Molecule 2: HEMOGLOBIN CHAIN D1

Chain Am:



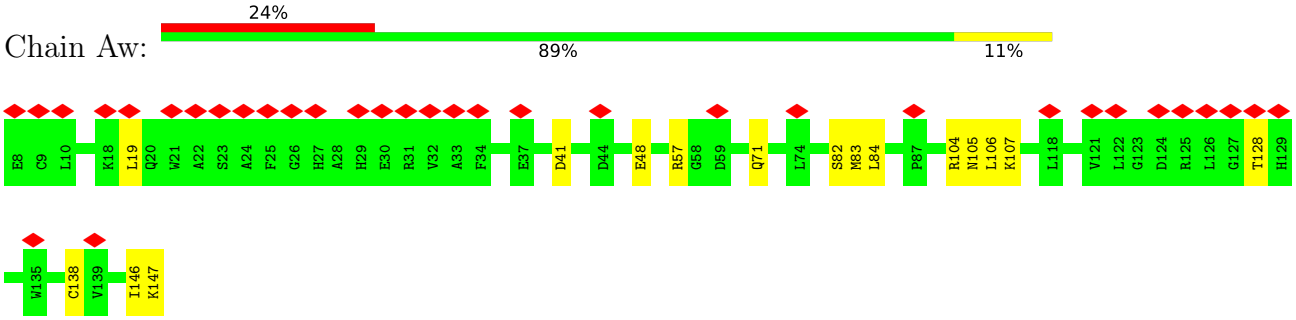
- Molecule 2: HEMOGLOBIN CHAIN D1

Chain Ar:



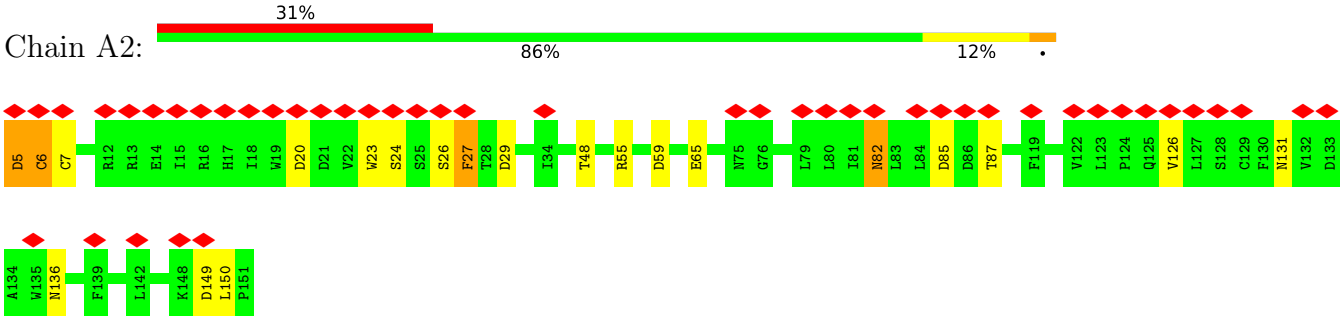
- Molecule 2: HEMOGLOBIN CHAIN D1

Chain Aw:



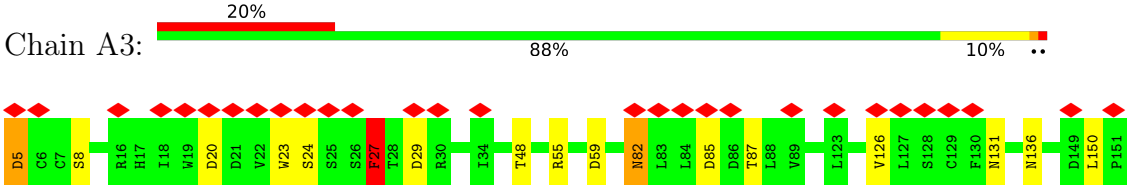
- Molecule 3: EXTRACELLULAR GLOBIN-4

Chain A2:



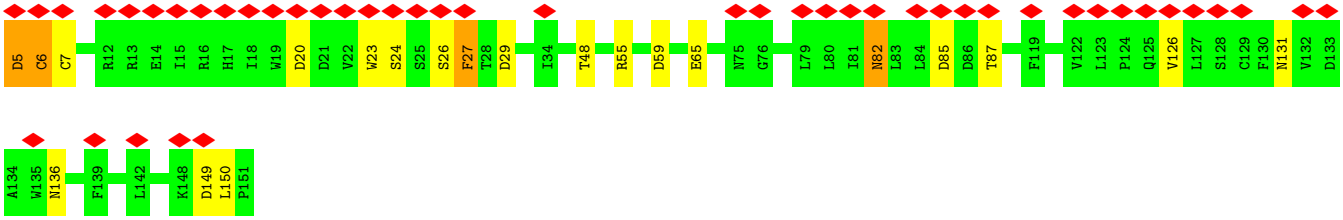
- Molecule 3: EXTRACELLULAR GLOBIN-4

Chain A3:



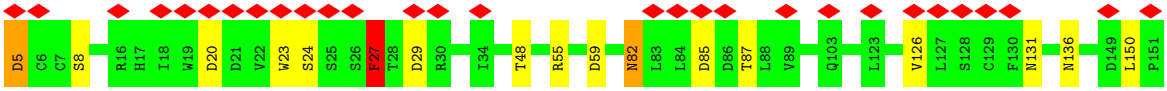
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain A7:



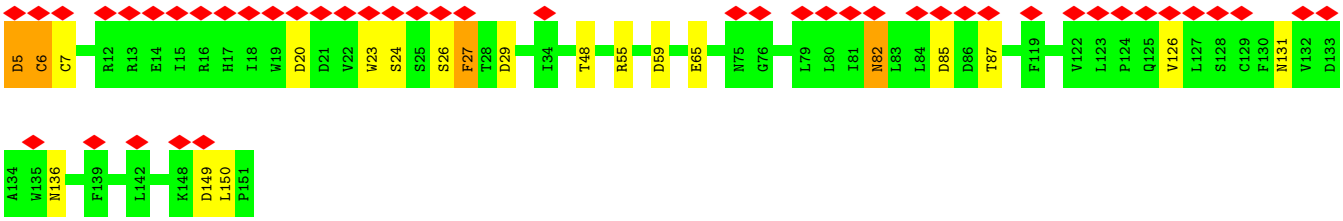
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain AA:



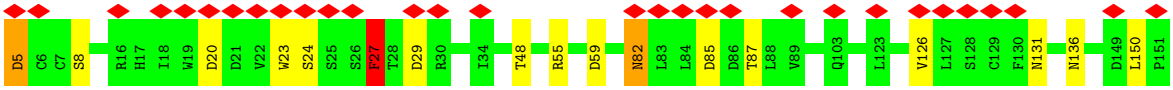
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain AE:



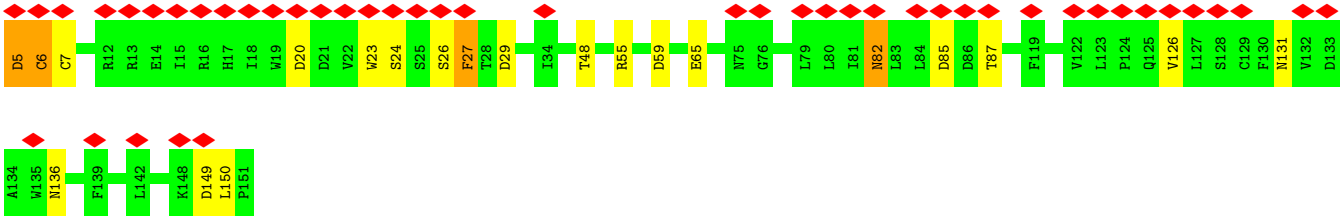
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain AF:



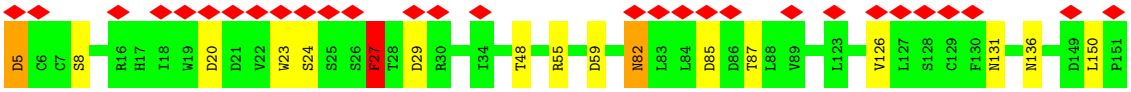
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain AJ:



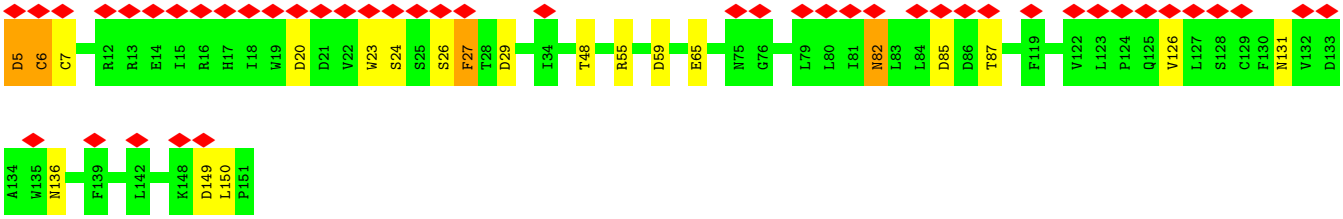
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain AK:



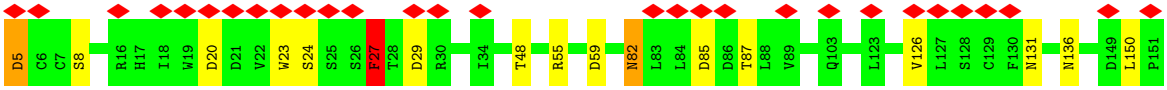
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain AO:



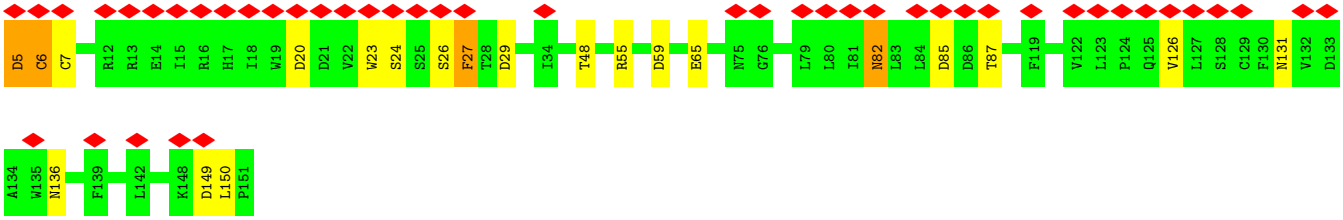
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain AP:



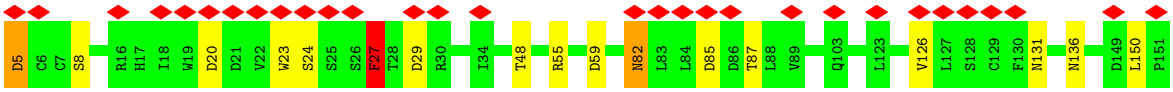
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain AT:



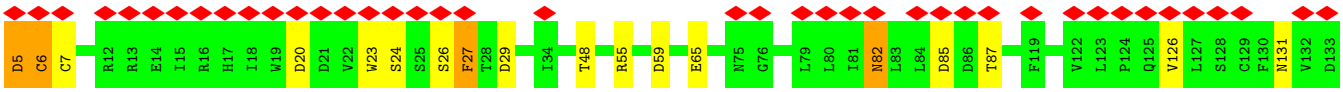
• Molecule 3: EXTRACELLULAR GLOBIN-4

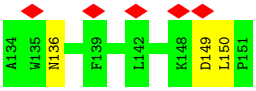
Chain AU:



• Molecule 3: EXTRACELLULAR GLOBIN-4

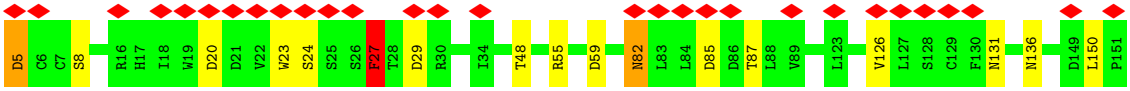
Chain AY:





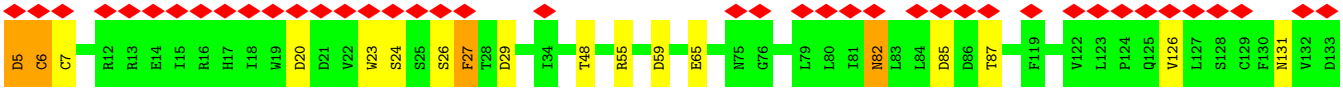
• Molecule 3: EXTRACELLULAR GLOBIN-4

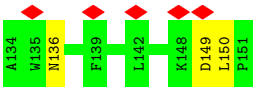
Chain AZ:



• Molecule 3: EXTRACELLULAR GLOBIN-4

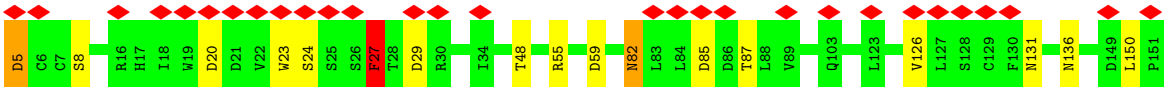
Chain Ad:





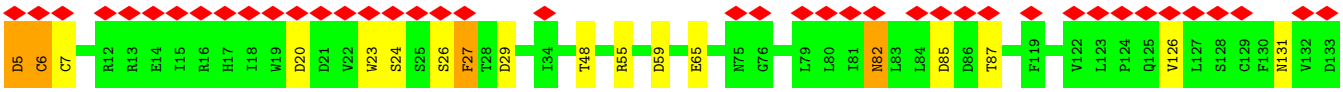
• Molecule 3: EXTRACELLULAR GLOBIN-4

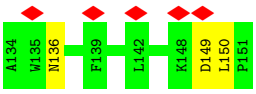
Chain Ae:



• Molecule 3: EXTRACELLULAR GLOBIN-4

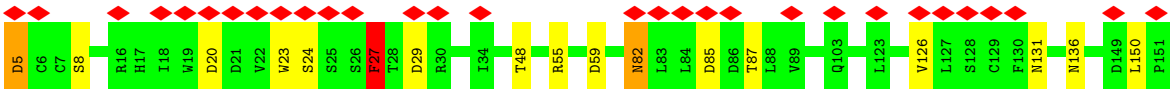
Chain Ai:





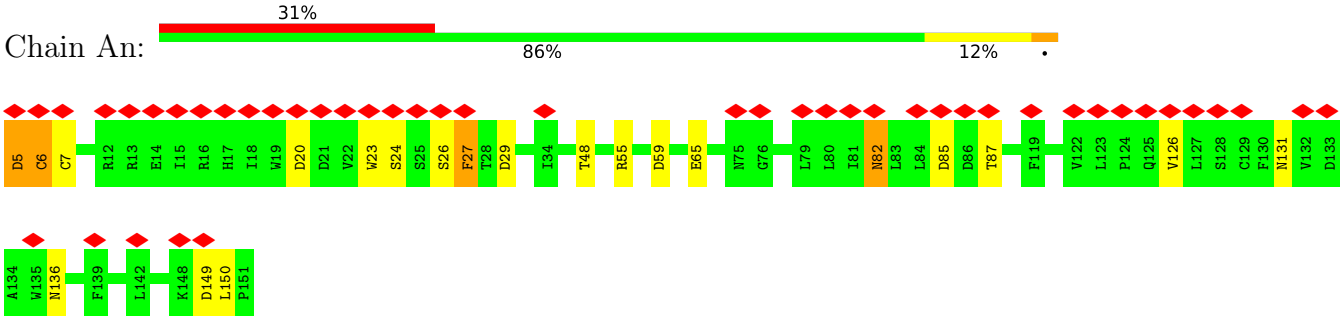
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain Aj:



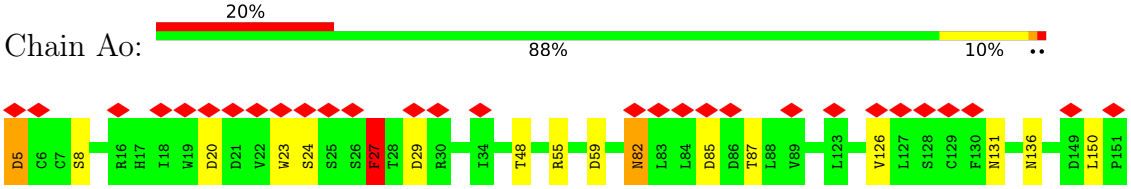
• Molecule 3: EXTRACELLULAR GLOBIN-4

Chain An:



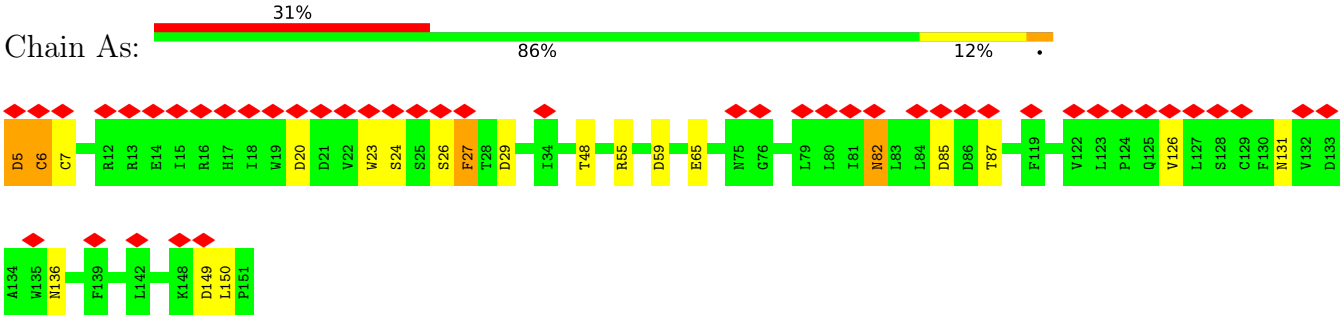
- Molecule 3: EXTRACELLULAR GLOBIN-4

Chain Ao:



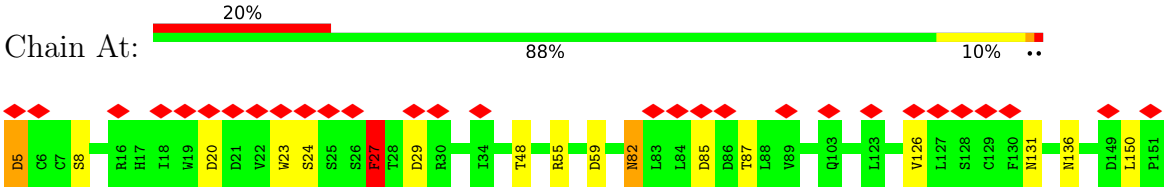
- Molecule 3: EXTRACELLULAR GLOBIN-4

Chain As:



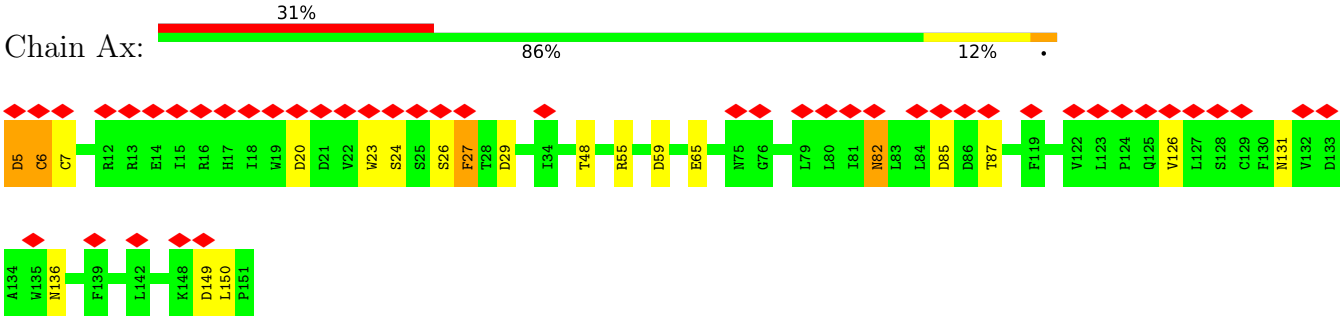
- Molecule 3: EXTRACELLULAR GLOBIN-4

Chain At:



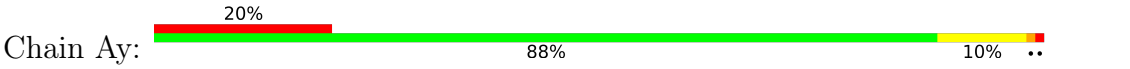
- Molecule 3: EXTRACELLULAR GLOBIN-4

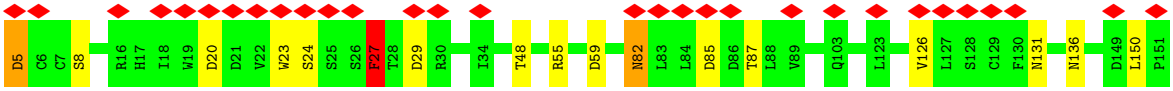
Chain Ax:



- Molecule 3: EXTRACELLULAR GLOBIN-4

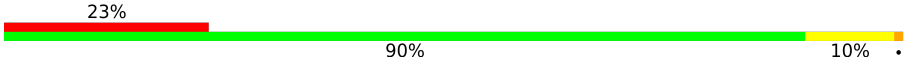
Chain Ay:

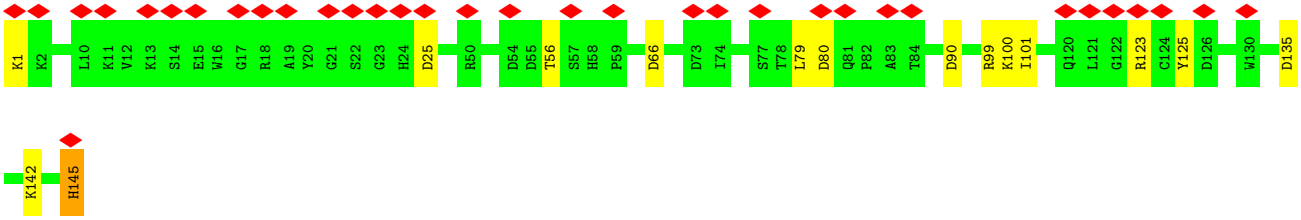




• Molecule 4: EXTRACELLULAR GLOBIN-2

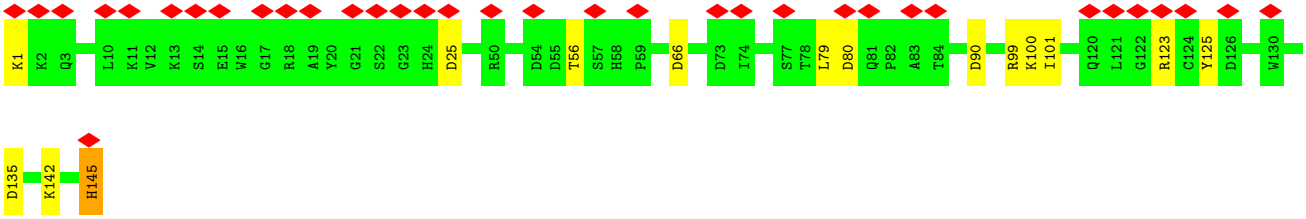
Chain A4:





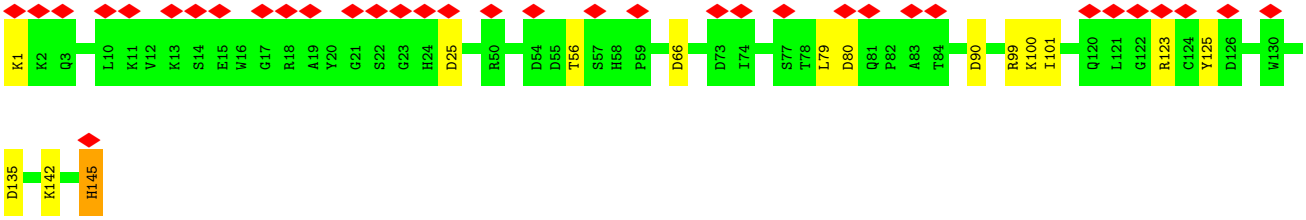
• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain AB:



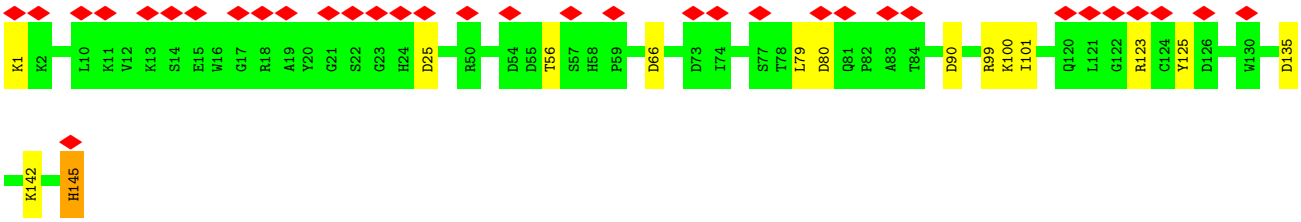
• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain AG:



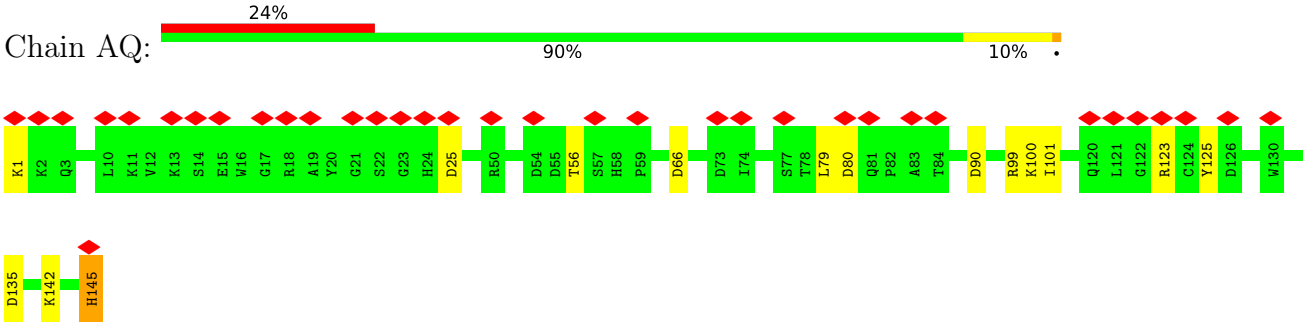
• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain AL:



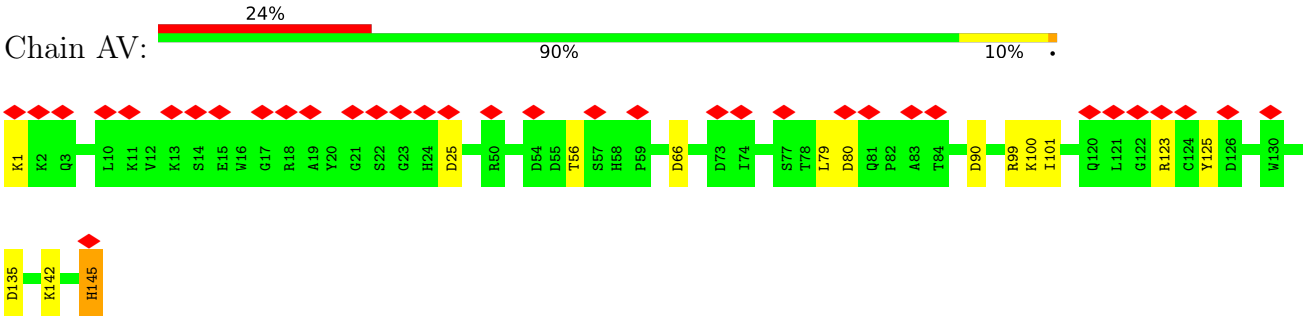
• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain AQ:



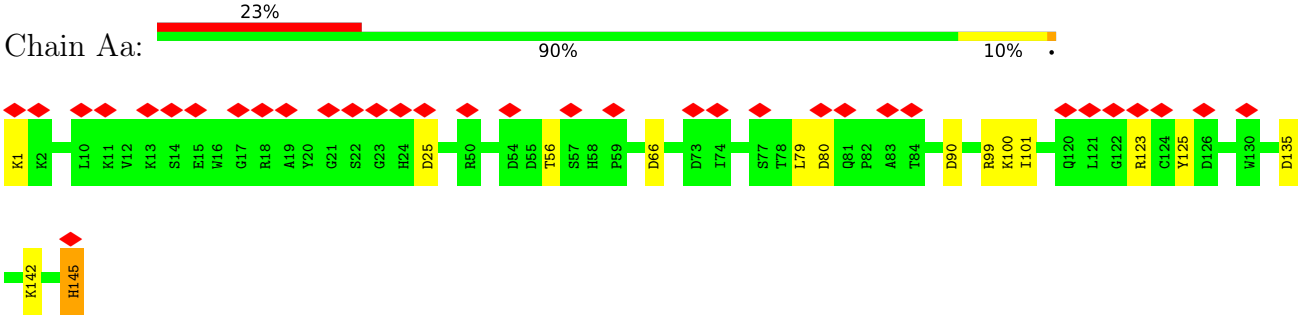
- Molecule 4: EXTRACELLULAR GLOBIN-2

Chain AV:



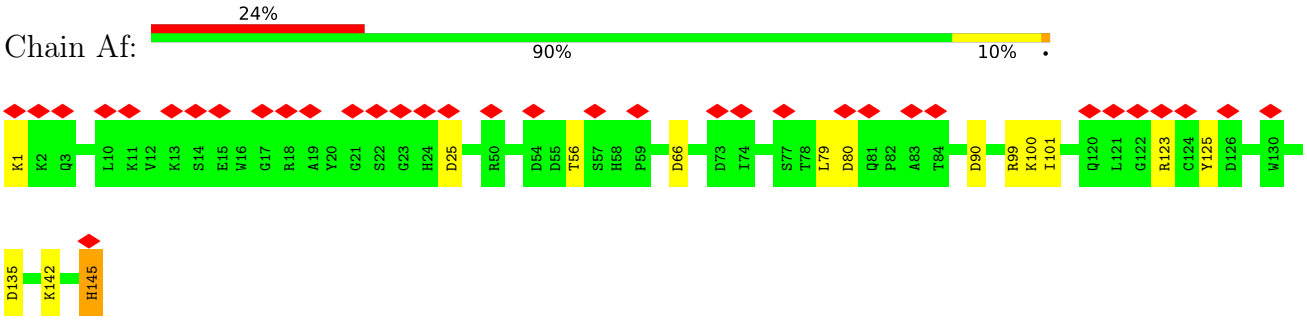
- Molecule 4: EXTRACELLULAR GLOBIN-2

Chain Aa:



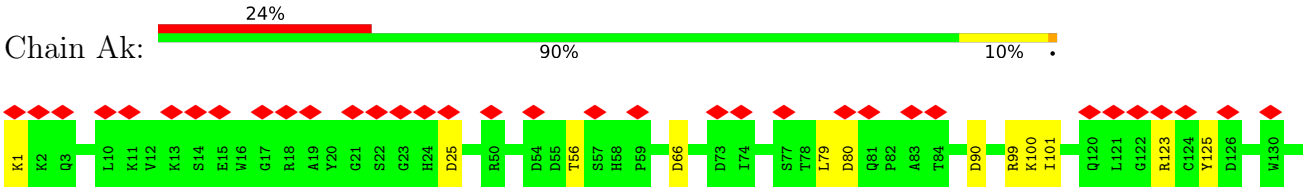
- Molecule 4: EXTRACELLULAR GLOBIN-2

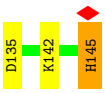
Chain Af:



- Molecule 4: EXTRACELLULAR GLOBIN-2

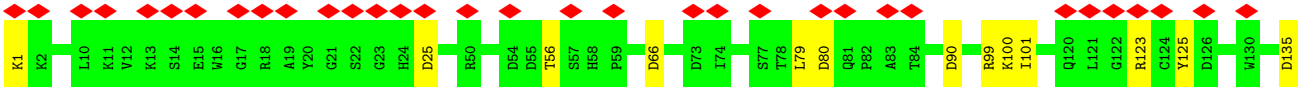
Chain Ak:





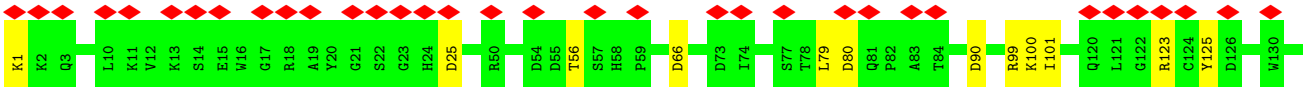
• Molecule 4: EXTRACELLULAR GLOBIN-2

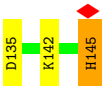
Chain Ap:



• Molecule 4: EXTRACELLULAR GLOBIN-2

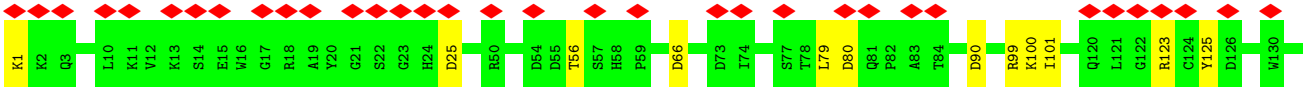
Chain Au:

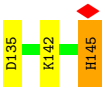




• Molecule 4: EXTRACELLULAR GLOBIN-2

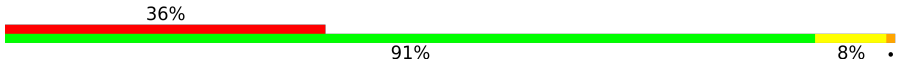
Chain Az:

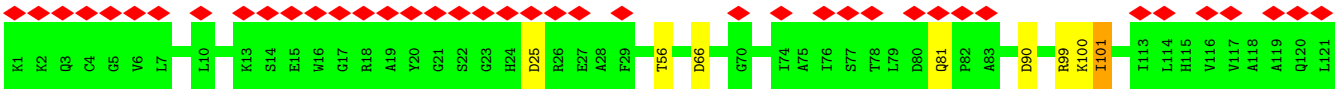


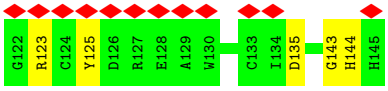


• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain B2:

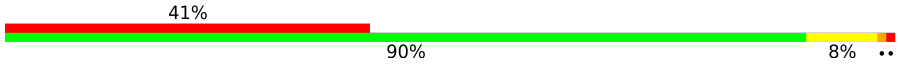


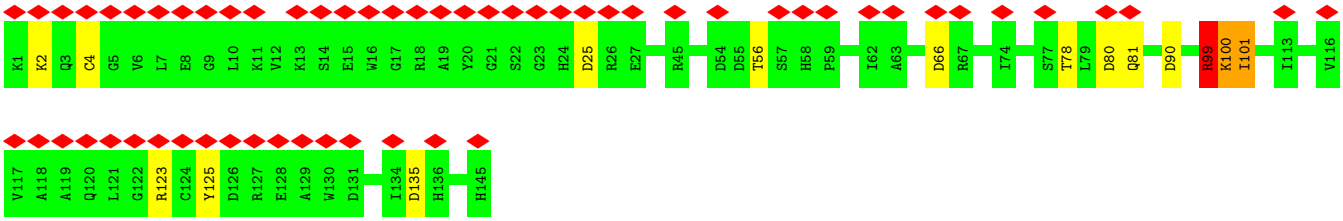




• Molecule 4: EXTRACELLULAR GLOBIN-2

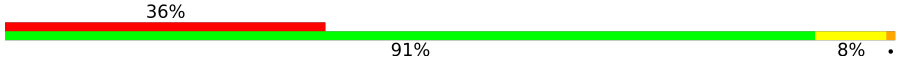
Chain B3:

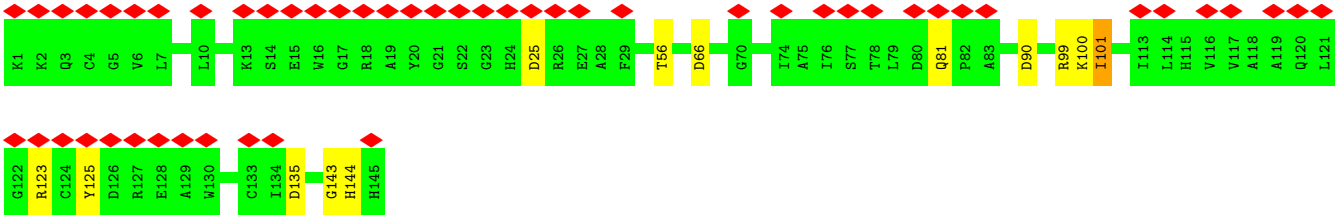




- Molecule 4: EXTRACELLULAR GLOBIN-2

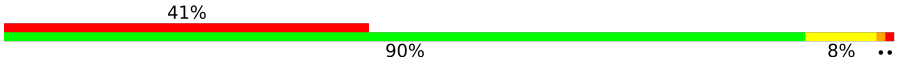
Chain B7:

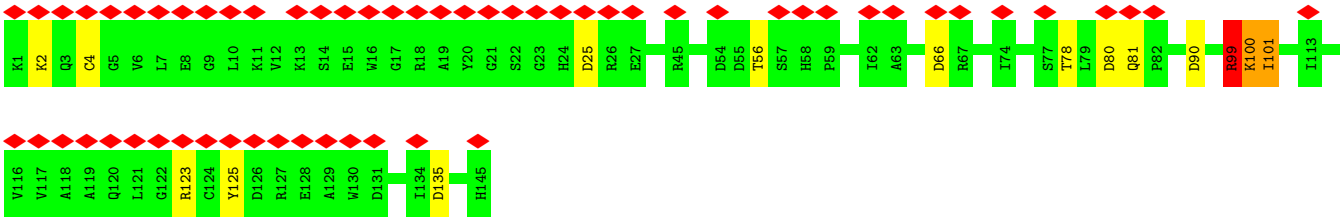




- Molecule 4: EXTRACELLULAR GLOBIN-2

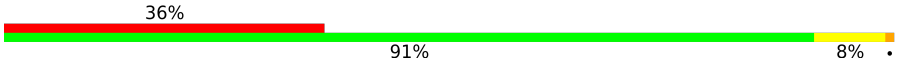
Chain BA:

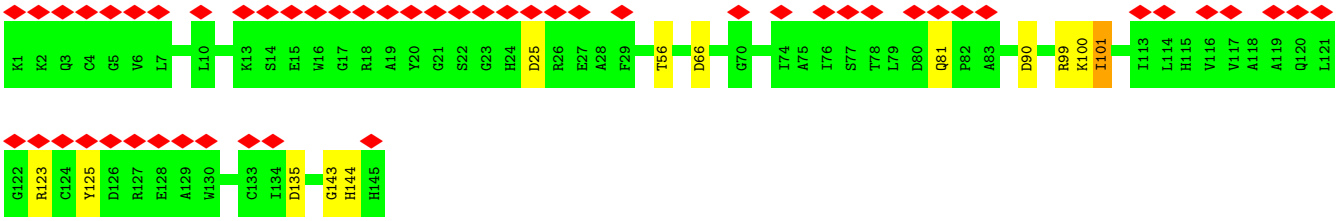




- Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BE:





- Molecule 4: EXTRACELLULAR GLOBIN-2

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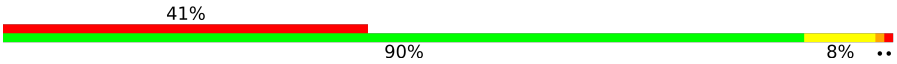
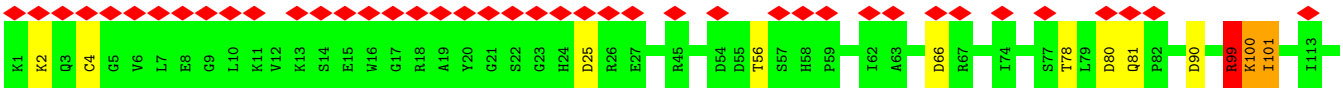
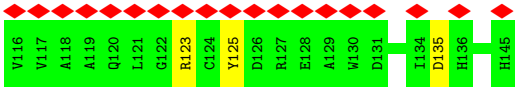
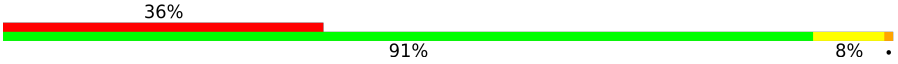


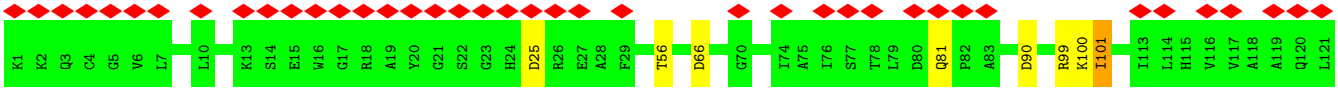


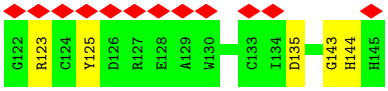


• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BJ:

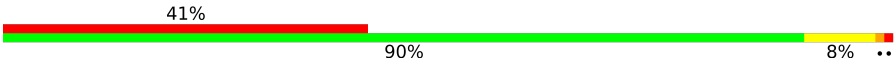


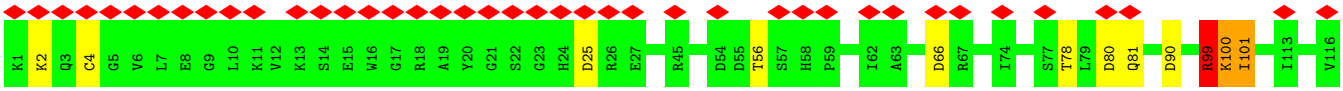


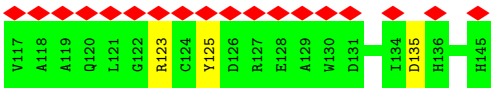


• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BK:

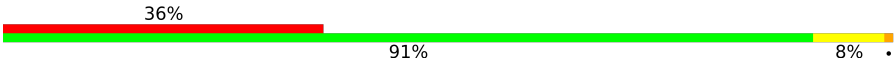


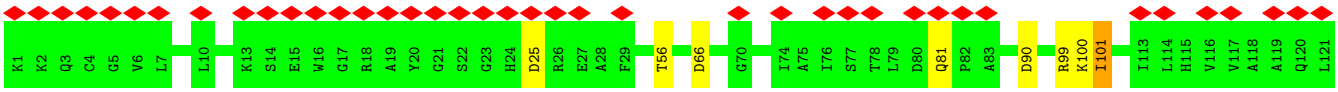


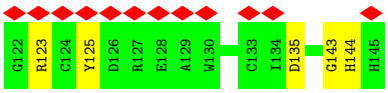


• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BO:

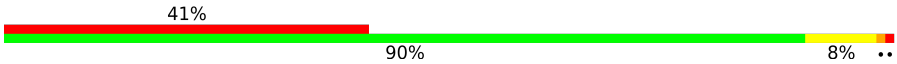


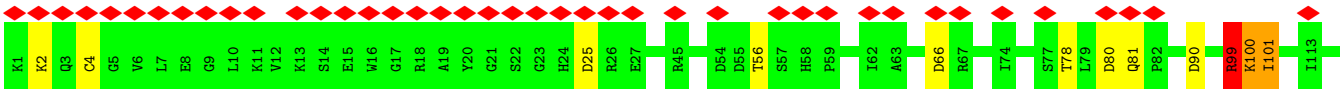


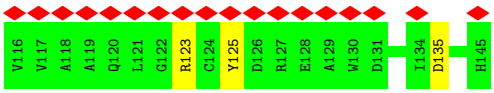


• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BP:







• Molecule 4: EXTRACELLULAR GLOBIN-2

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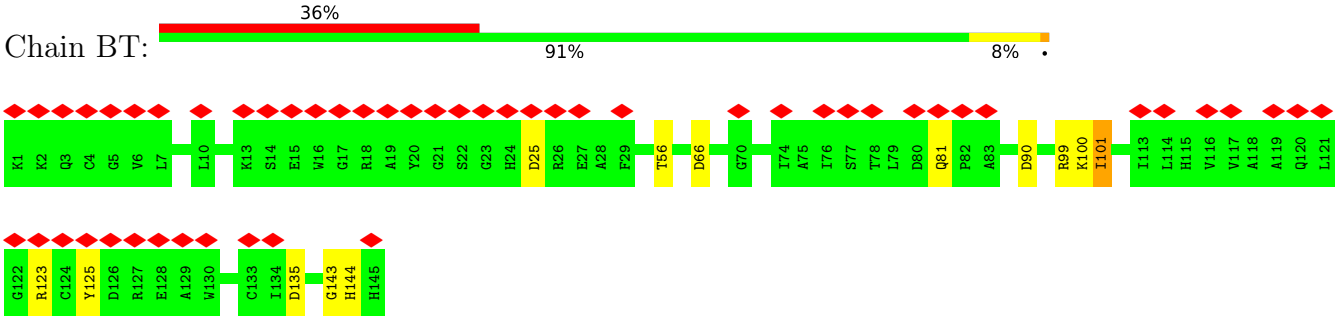
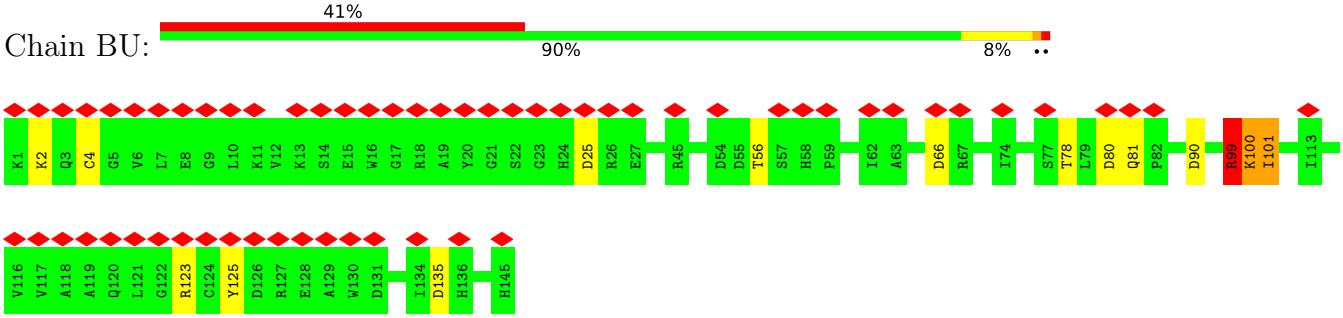


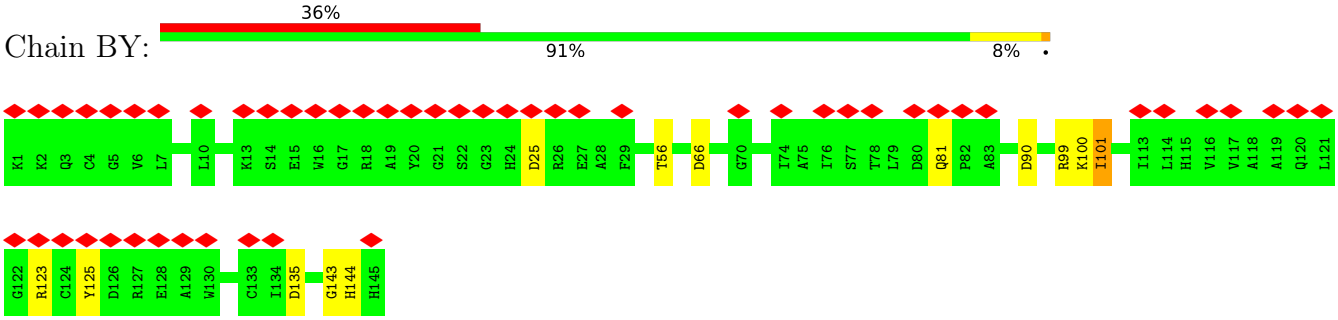
• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BU:



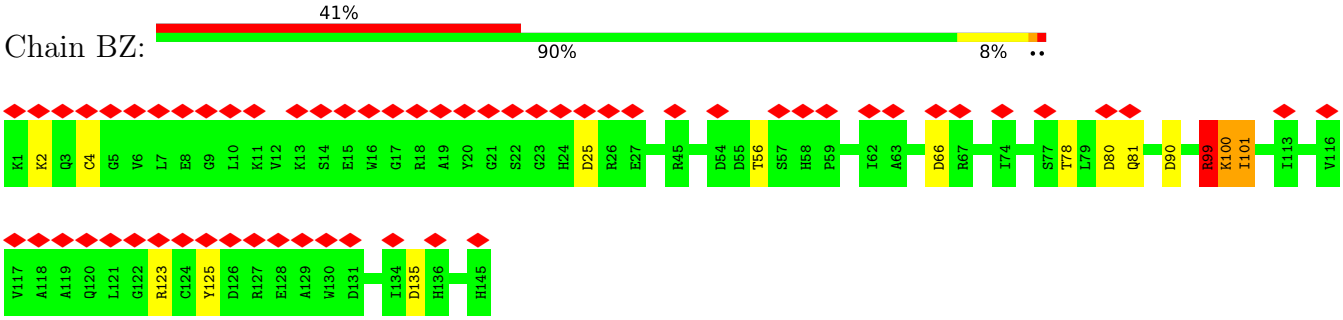
• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain BY:



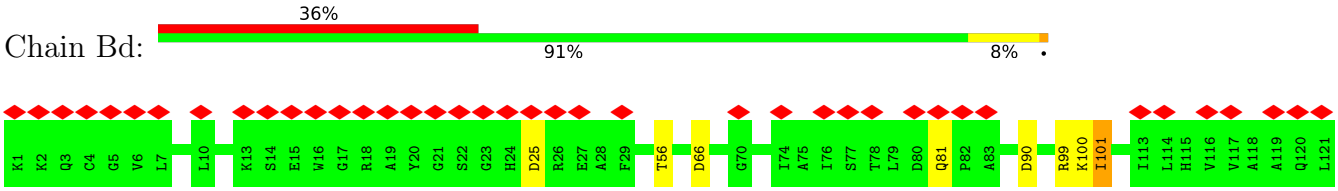
• Molecule 4: EXTRACELLULAR GLOBIN-2

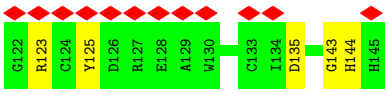
Chain BZ:



• Molecule 4: EXTRACELLULAR GLOBIN-2

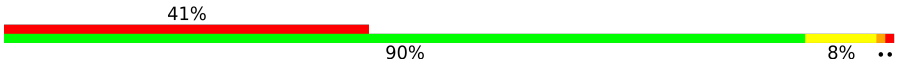
Chain Bd:

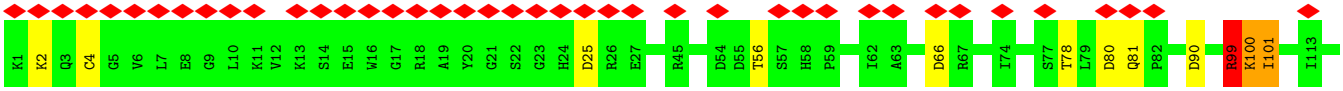




• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain Be:





• Molecule 4: EXTRACELLULAR GLOBIN-2

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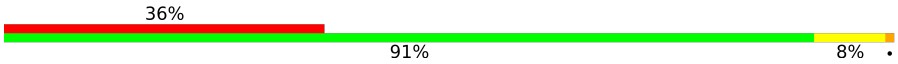
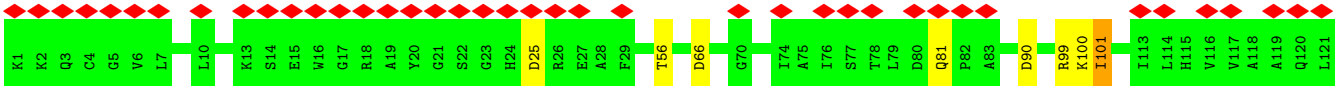
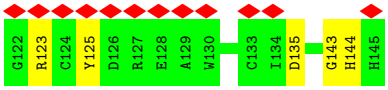
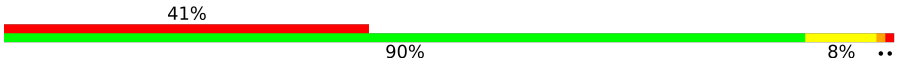


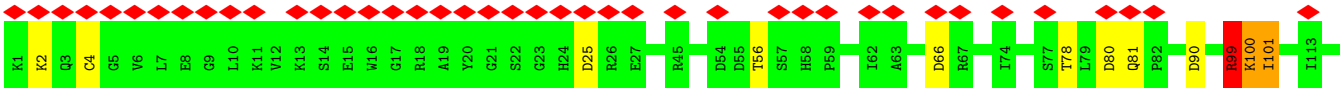


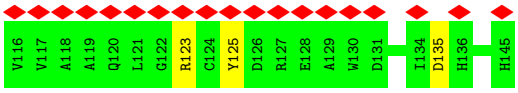


• Molecule 4: EXTRACELLULAR GLOBIN-2

Chain Bj:







• Molecule 4: EXTRACELLULAR GLOBIN-2

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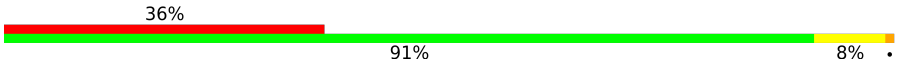

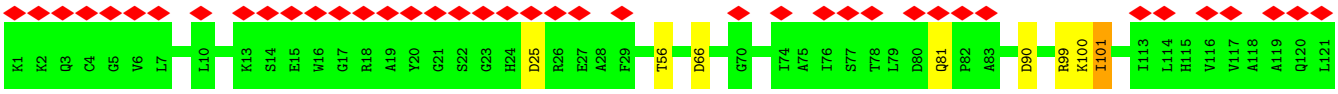

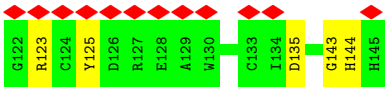

• Molecule 4: EXTRACELLULAR GLOBIN-2

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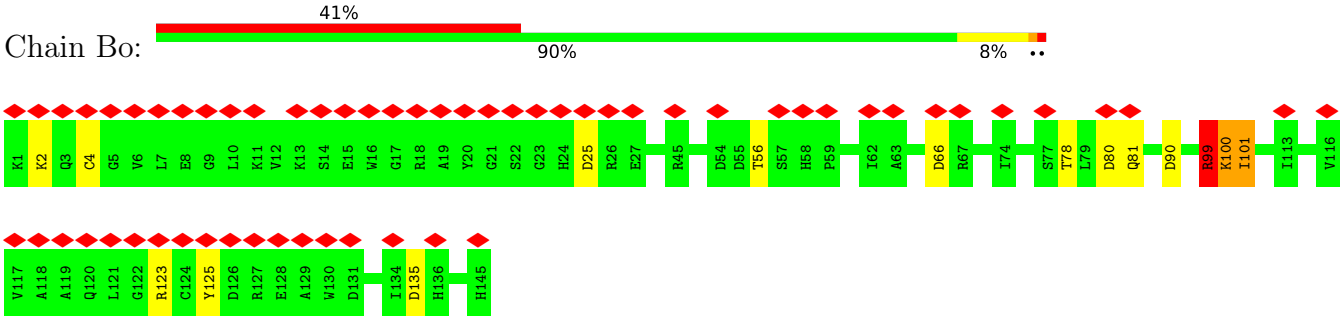
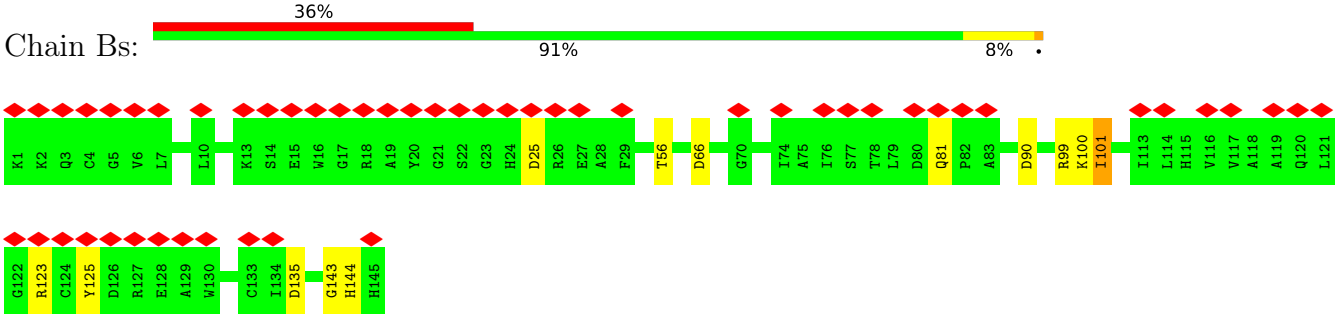


- Molecule 4: EXTRACELLULAR GLOBIN-2

Chain Bs:



- Molecule 4: EXTRACELLULAR GLOBIN-2

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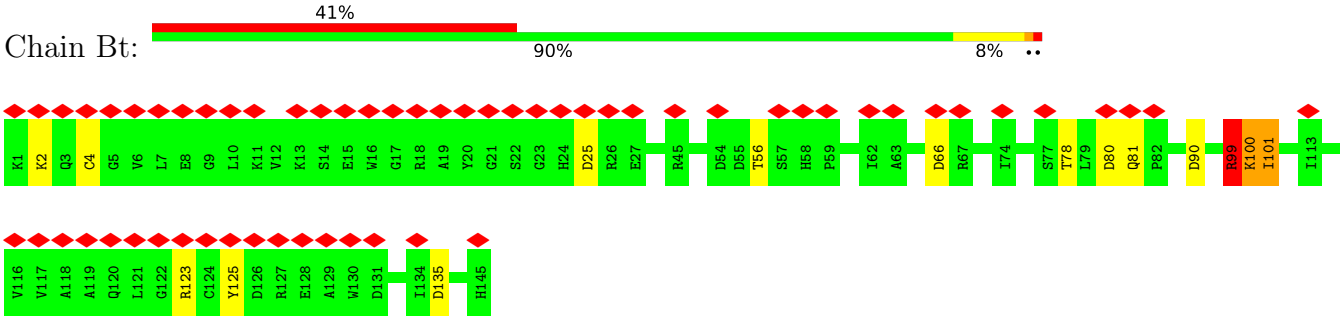
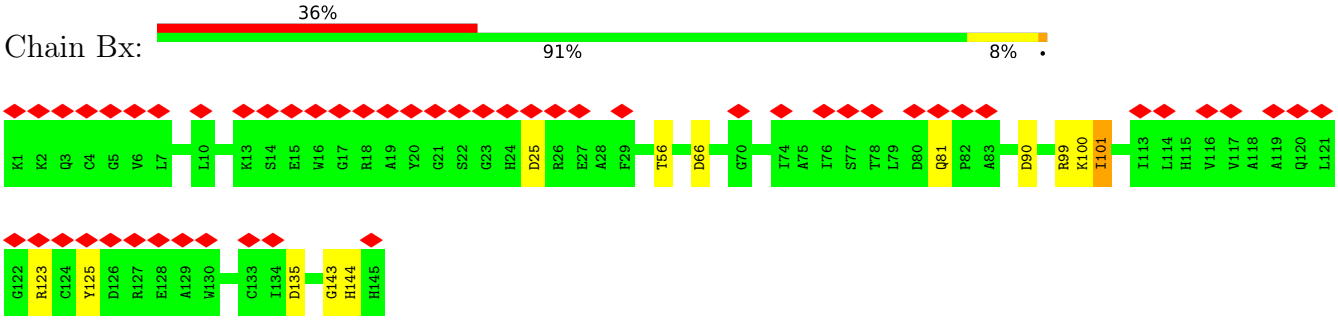


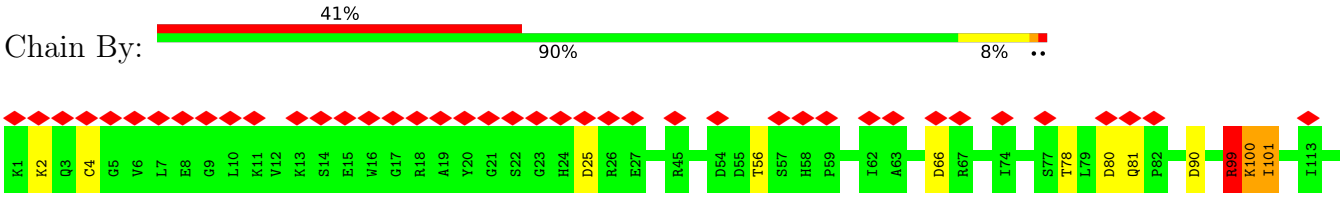
- Molecule 4: EXTRACELLULAR GLOBIN-2

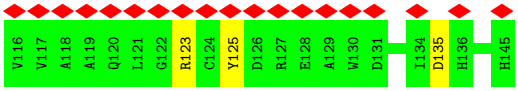
Chain Bx:



- Molecule 4: EXTRACELLULAR GLOBIN-2

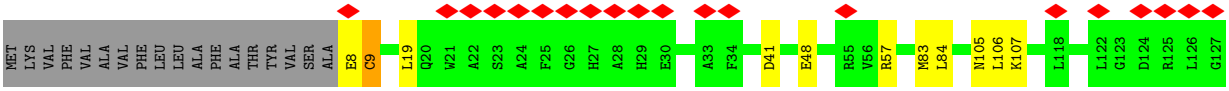
Chain By:

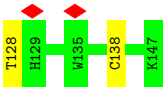




• Molecule 5: HEMOGLOBIN CHAIN D1

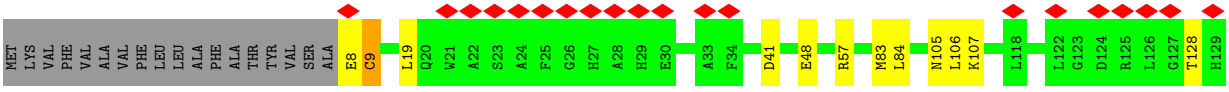
Chain B0:

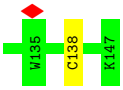




• Molecule 5: HEMOGLOBIN CHAIN D1

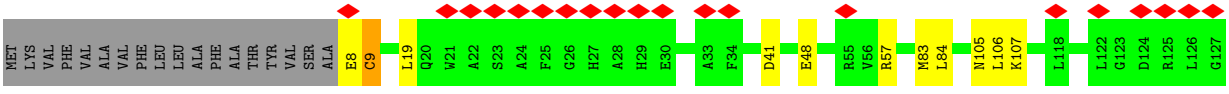
Chain B5:

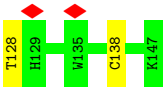




• Molecule 5: HEMOGLOBIN CHAIN D1

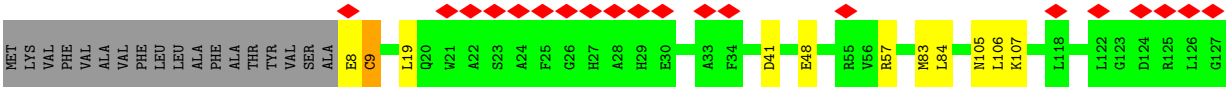
Chain BC:

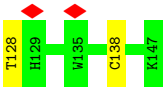




• Molecule 5: HEMOGLOBIN CHAIN D1

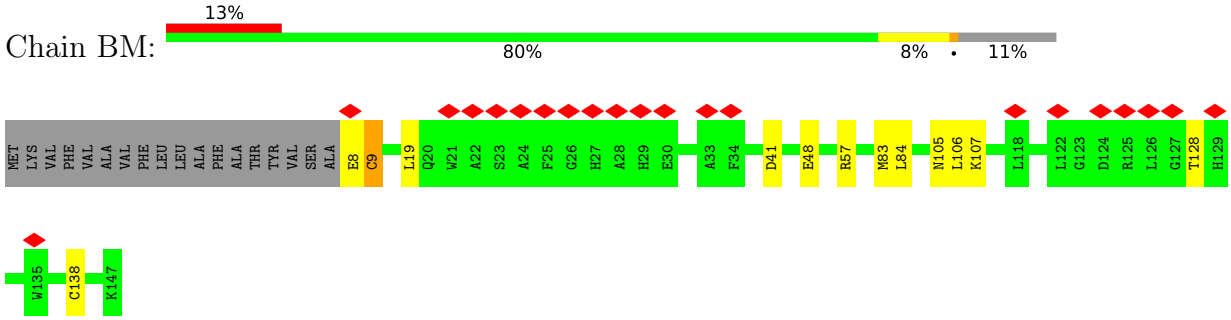
Chain BH:





• Molecule 5: HEMOGLOBIN CHAIN D1

Chain BM:



- Molecule 5: HEMOGLOBIN CHAIN D1

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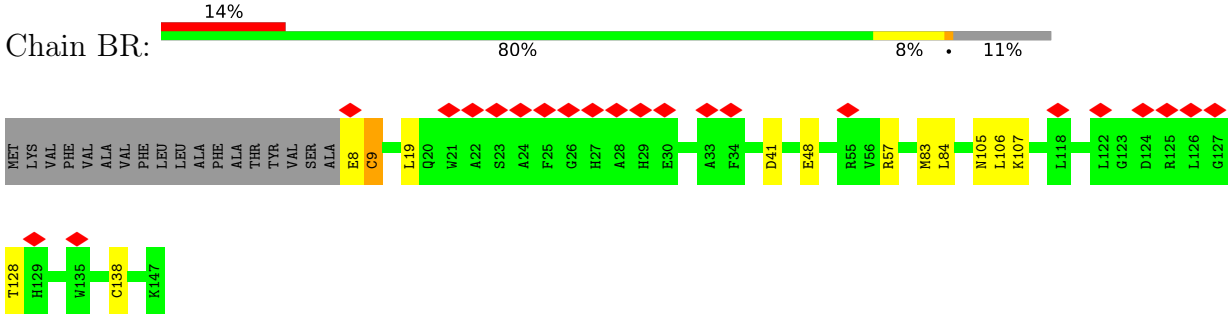

- Molecule 5: HEMOGLOBIN CHAIN D1

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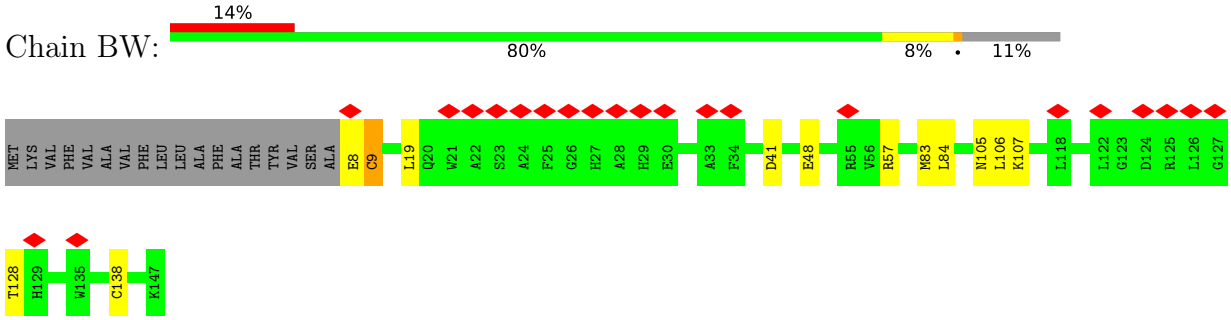
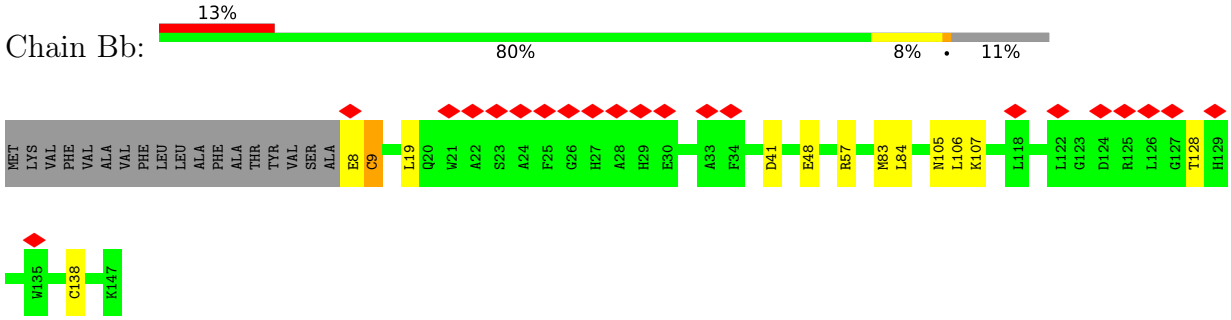


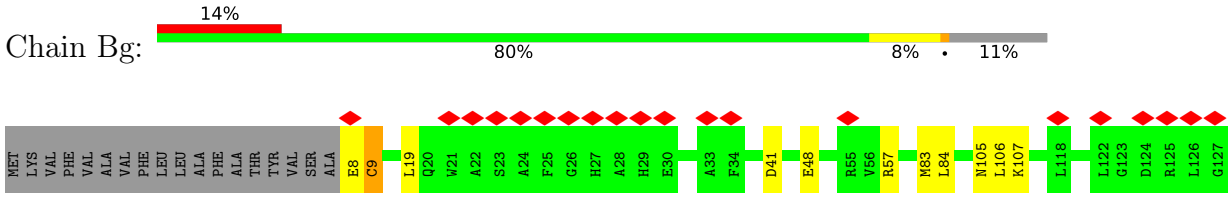
- Molecule 5: HEMOGLOBIN CHAIN D1

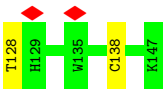
Chain Bb:



- Molecule 5: HEMOGLOBIN CHAIN D1

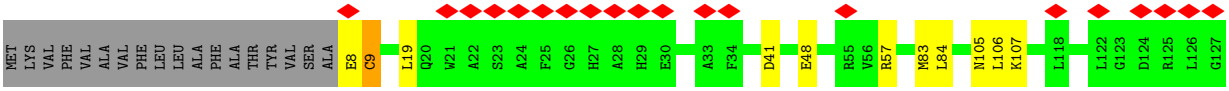
Chain Bg:

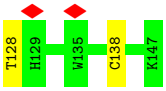




• Molecule 5: HEMOGLOBIN CHAIN D1

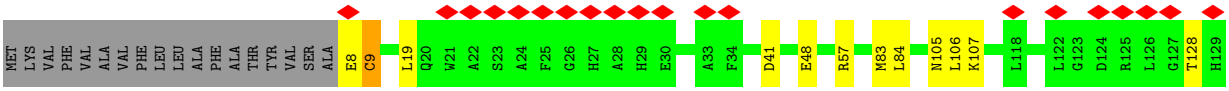
Chain Bl:

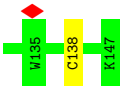




• Molecule 5: HEMOGLOBIN CHAIN D1

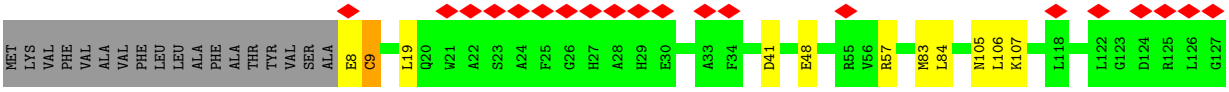
Chain Bq:

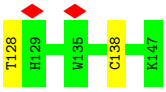




• Molecule 5: HEMOGLOBIN CHAIN D1

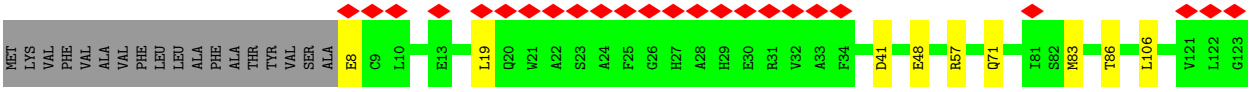
Chain Bv:

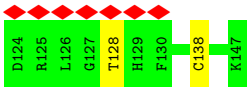




• Molecule 5: HEMOGLOBIN CHAIN D1

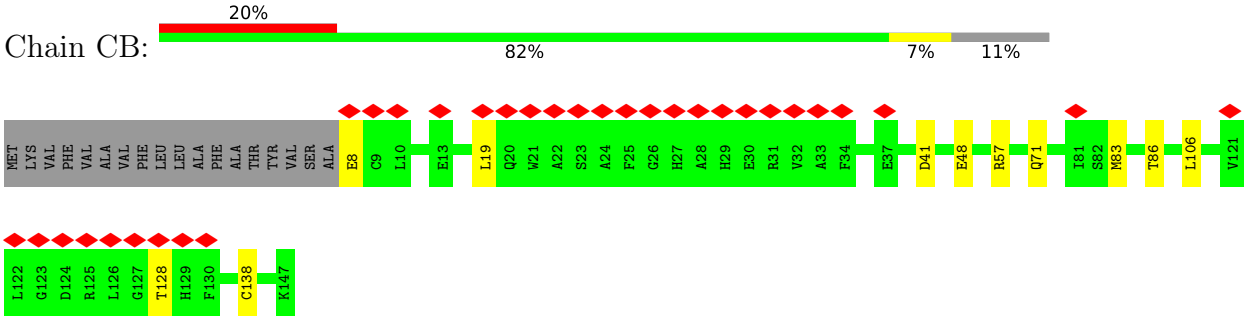
Chain C4:





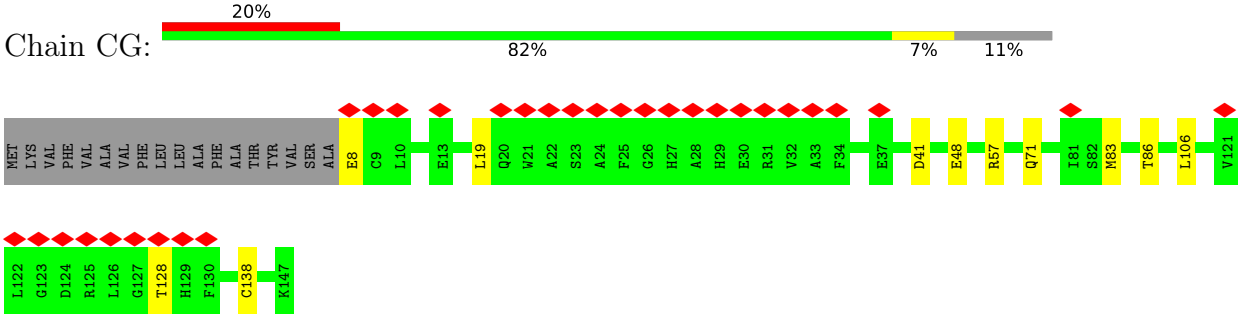
• Molecule 5: HEMOGLOBIN CHAIN D1

Chain CB:



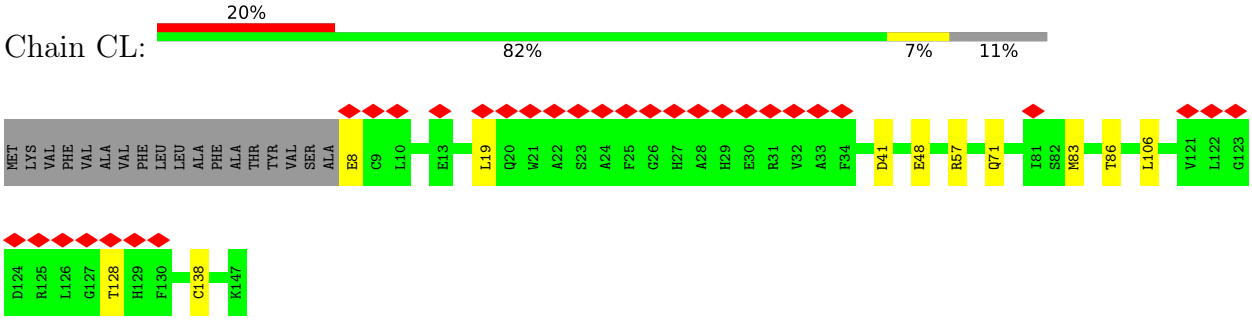
• Molecule 5: HEMOGLOBIN CHAIN D1

Chain CG:



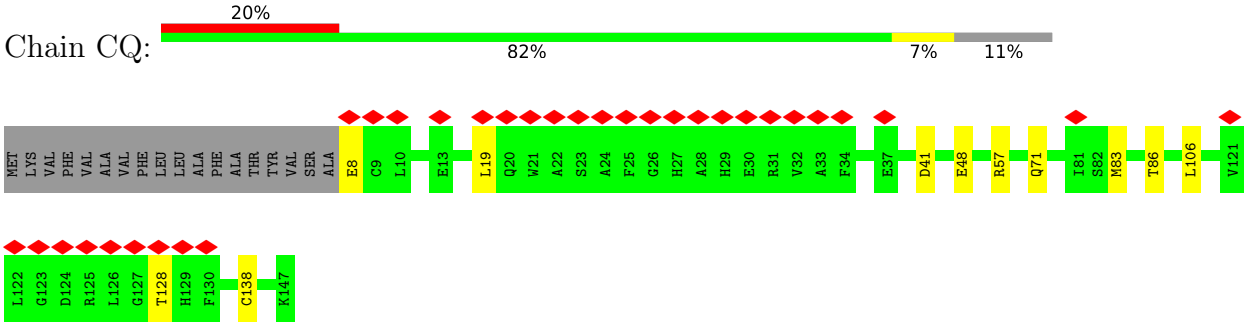
• Molecule 5: HEMOGLOBIN CHAIN D1

Chain CL:



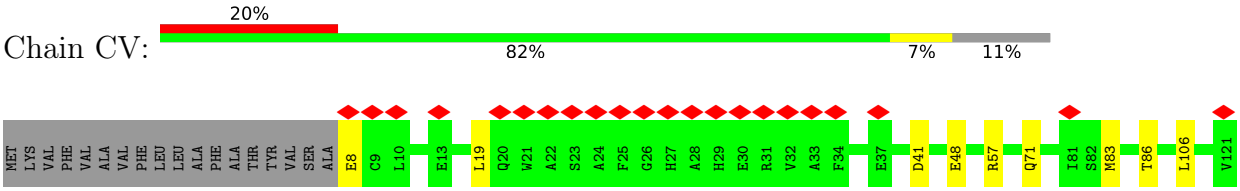
• Molecule 5: HEMOGLOBIN CHAIN D1

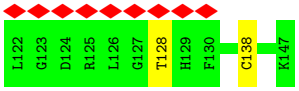
Chain CQ:



• Molecule 5: HEMOGLOBIN CHAIN D1

Chain CV:



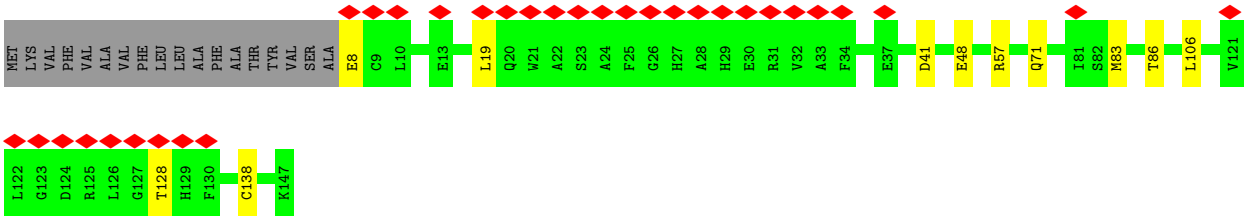


• Molecule 5: HEMOGLOBIN CHAIN D1

Chain Ca:

• Molecule 5: HEMOGLOBIN CHAIN D1

Chain Cf:

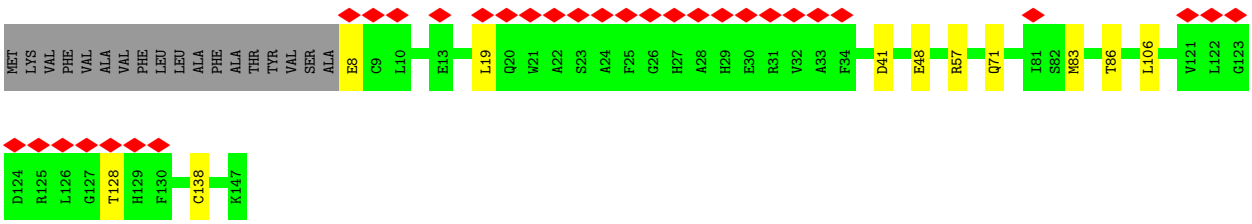


• Molecule 5: HEMOGLOBIN CHAIN D1

Chain Ck:

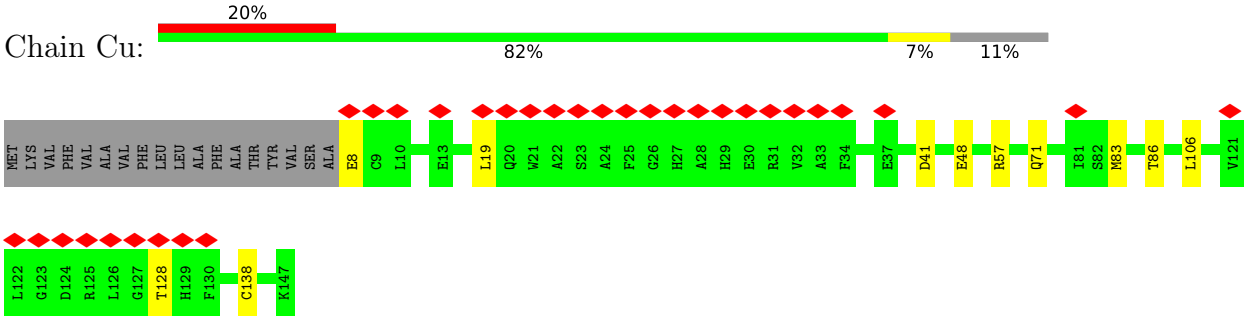
• Molecule 5: HEMOGLOBIN CHAIN D1

Chain Cp:



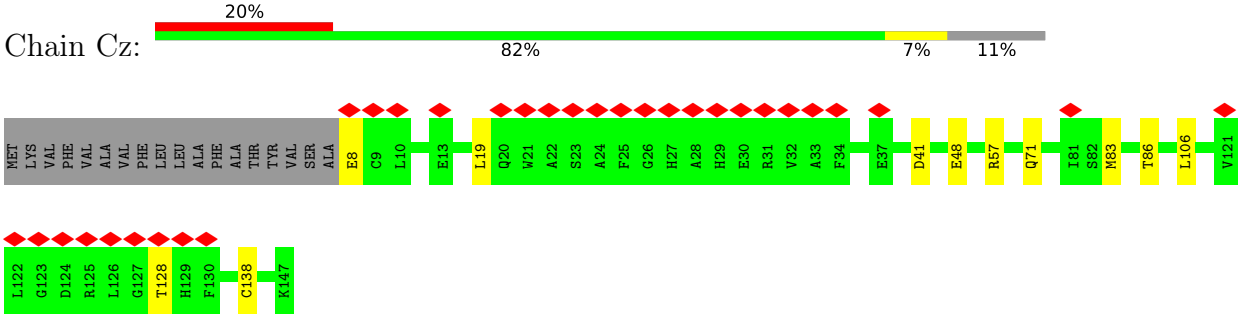
• Molecule 5: HEMOGLOBIN CHAIN D1

Chain Cu:



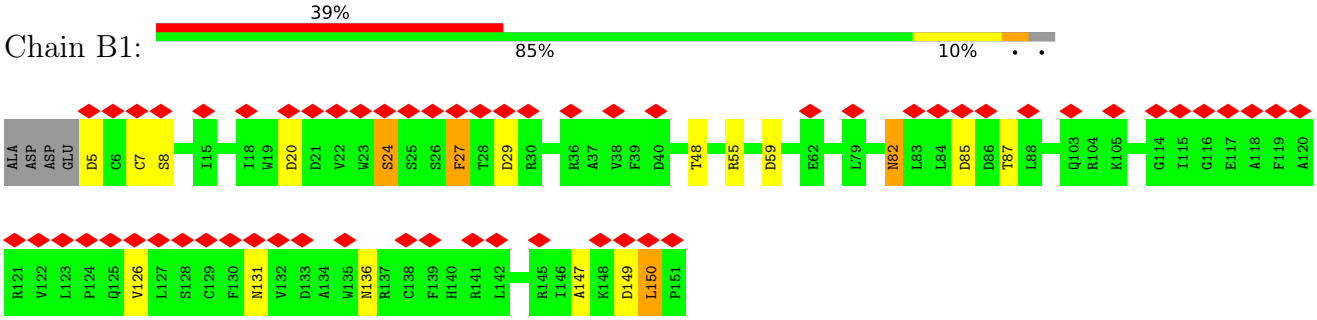
- Molecule 5: HEMOGLOBIN CHAIN D1

Chain Cz:



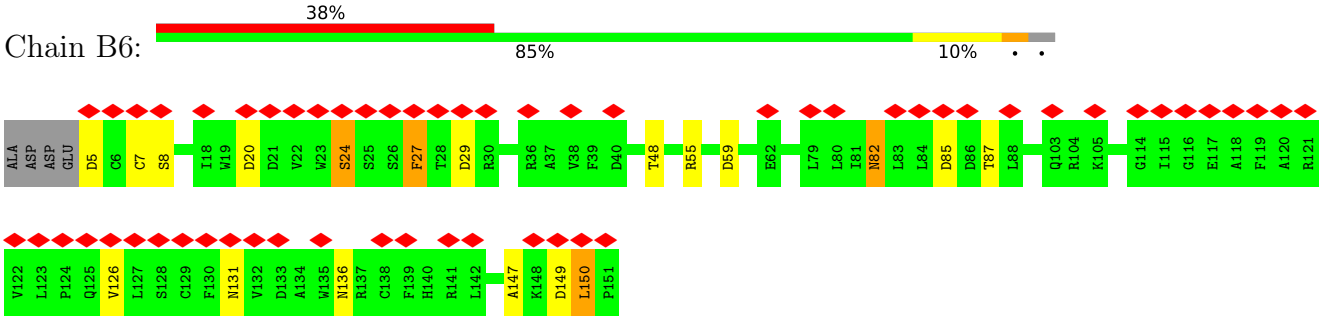
- Molecule 6: EXTRACELLULAR GLOBIN-4

Chain B1:



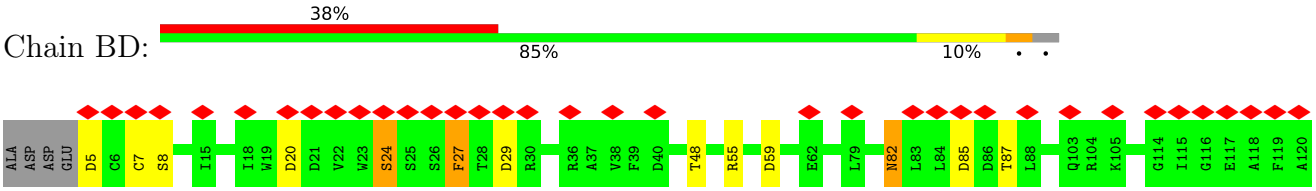
- Molecule 6: EXTRACELLULAR GLOBIN-4

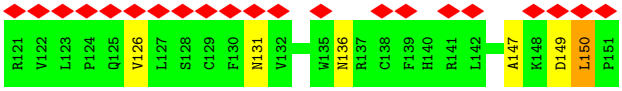
Chain B6:



- Molecule 6: EXTRACELLULAR GLOBIN-4

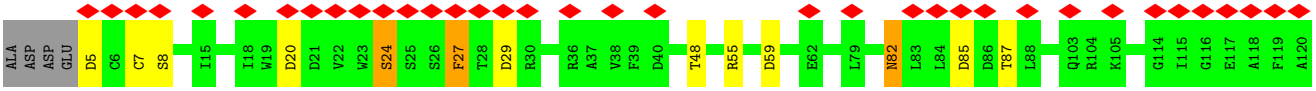
Chain BD:

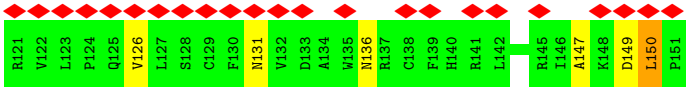




• Molecule 6: EXTRACELLULAR GLOBIN-4

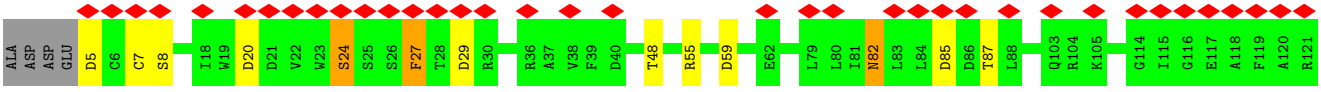
Chain BI:

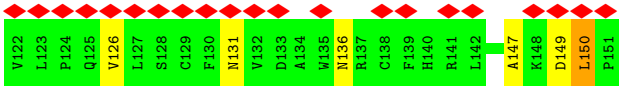




• Molecule 6: EXTRACELLULAR GLOBIN-4

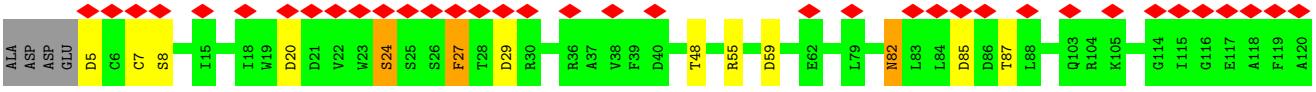
Chain BN:

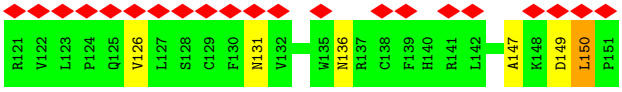




• Molecule 6: EXTRACELLULAR GLOBIN-4

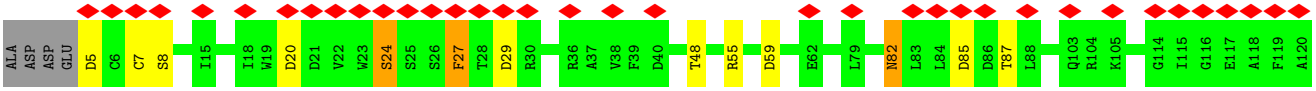
Chain BS:

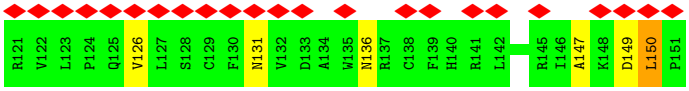




• Molecule 6: EXTRACELLULAR GLOBIN-4

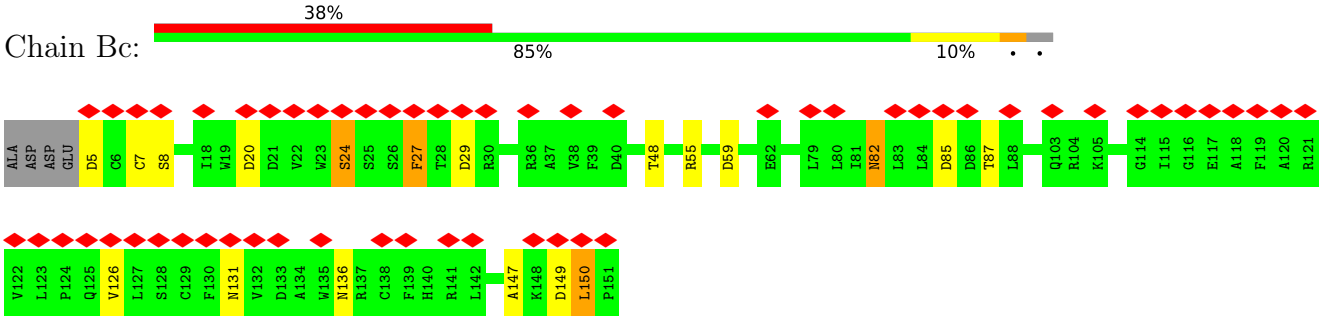
Chain BX:





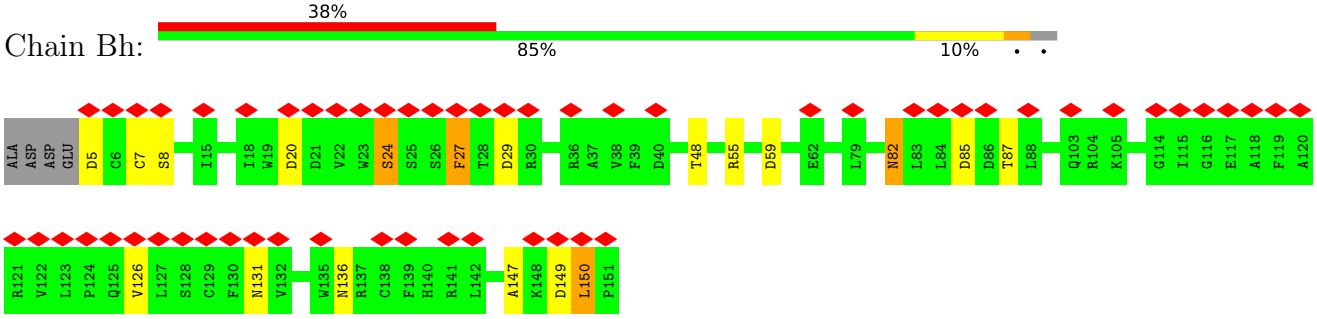
• Molecule 6: EXTRACELLULAR GLOBIN-4

Chain Bc:



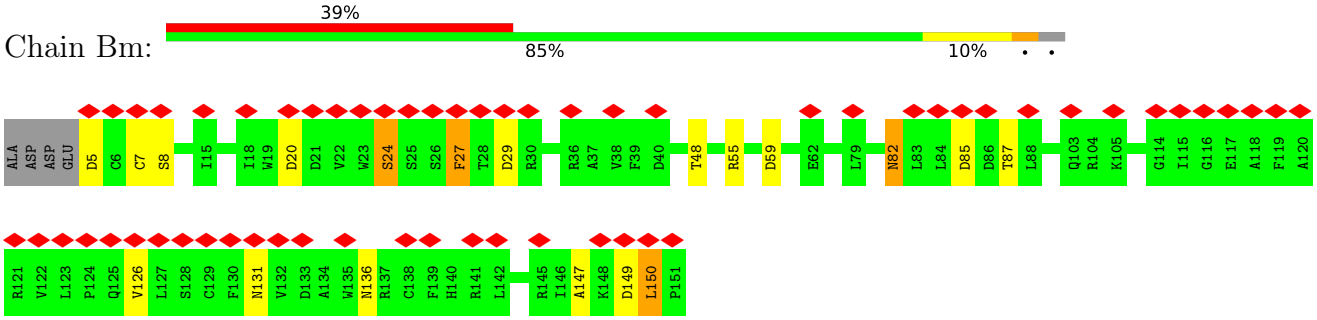
- Molecule 6: EXTRACELLULAR GLOBIN-4

Chain Bh:



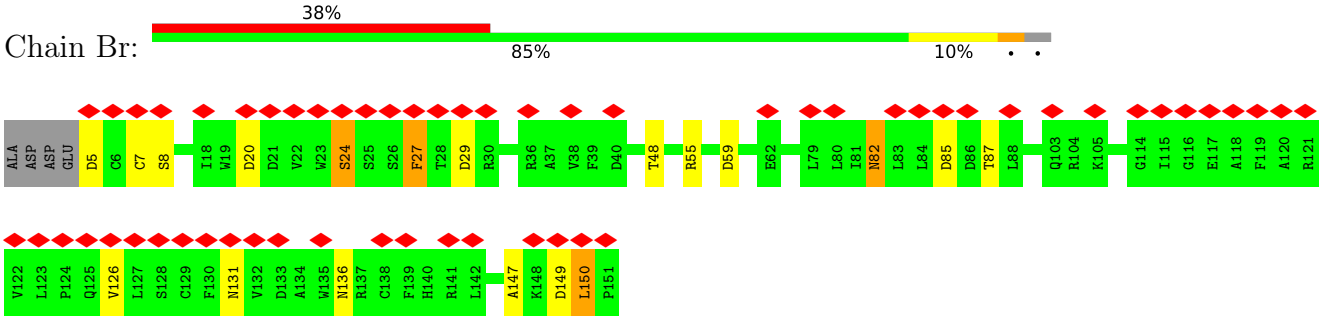
- Molecule 6: EXTRACELLULAR GLOBIN-4

Chain Bm:



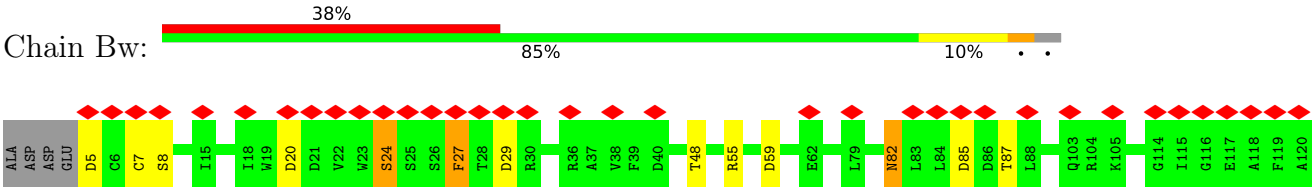
- Molecule 6: EXTRACELLULAR GLOBIN-4

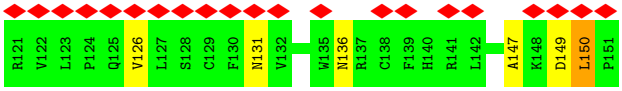
Chain Br:



- Molecule 6: EXTRACELLULAR GLOBIN-4

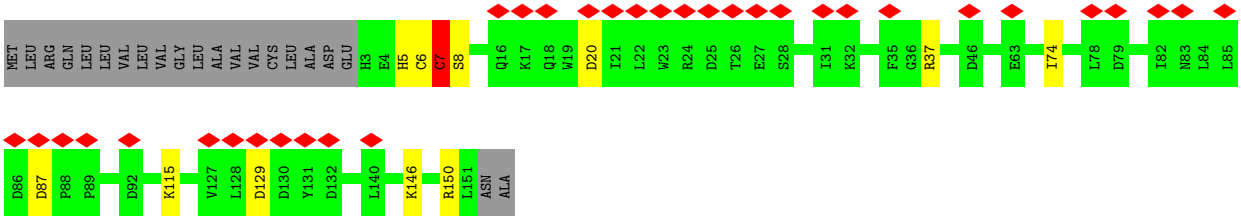
Chain Bw:





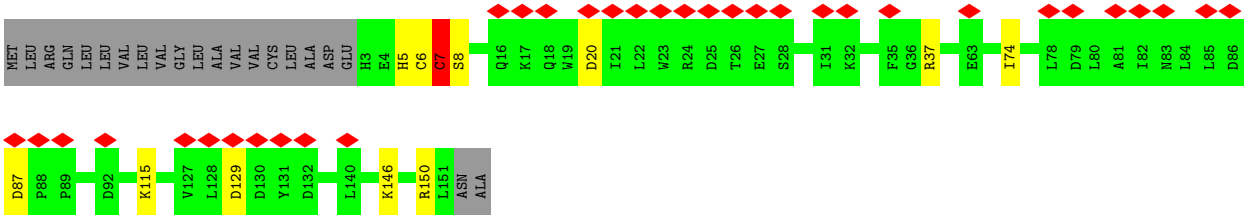
• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain B4:



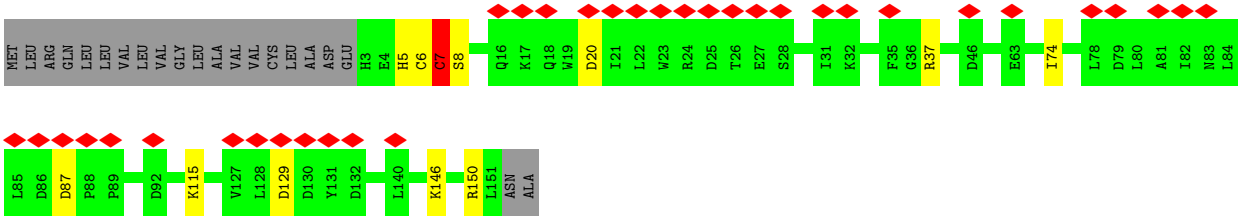
• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain BB:



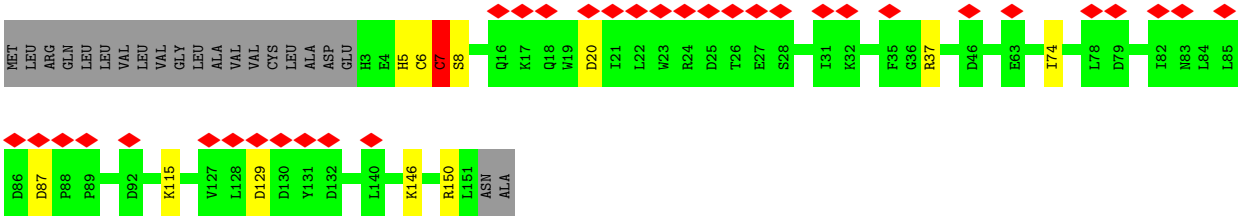
• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain BG:



• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain BL:

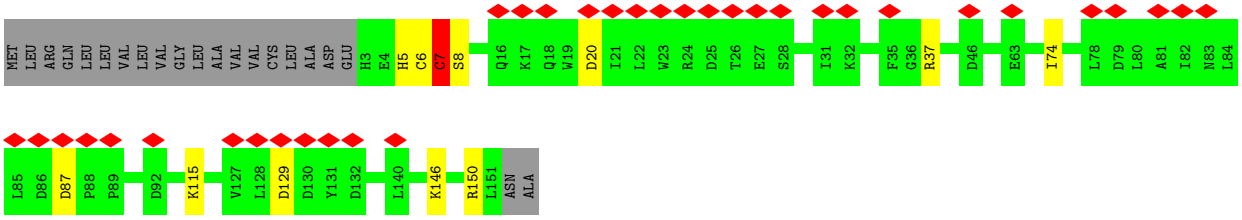


• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain BQ:

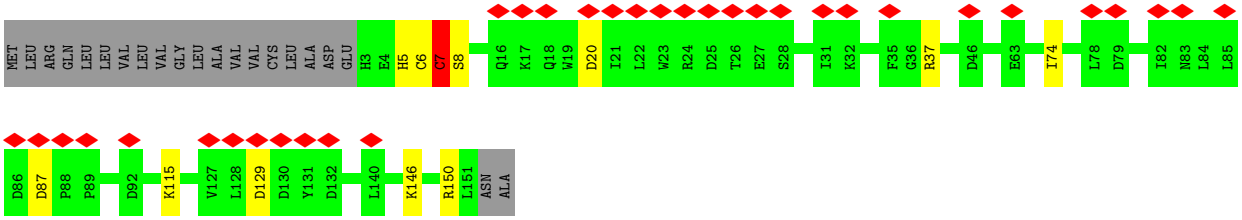
- Molecule 7: EXTRACELLULAR GLOBIN-3

Chain BV:



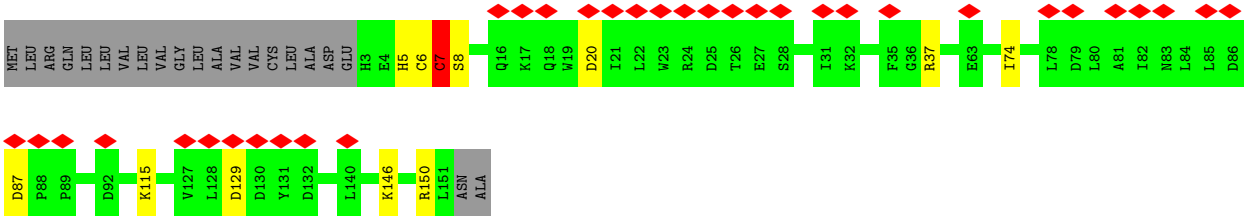
- Molecule 7: EXTRACELLULAR GLOBIN-3

Chain Ba:



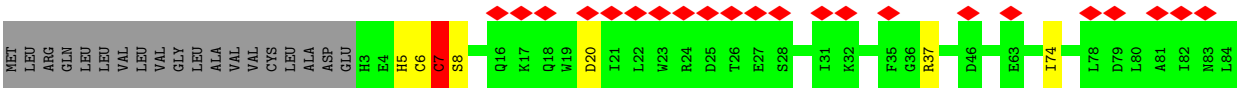
- Molecule 7: EXTRACELLULAR GLOBIN-3

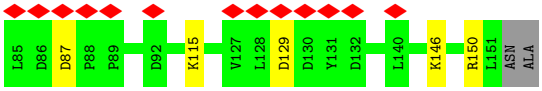
Chain Bf:



- Molecule 7: EXTRACELLULAR GLOBIN-3

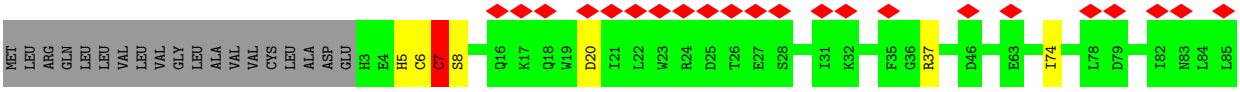
Chain Bk:

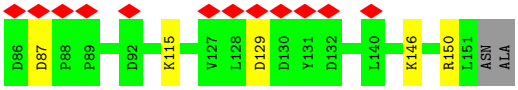




• Molecule 7: EXTRACELLULAR GLOBIN-3

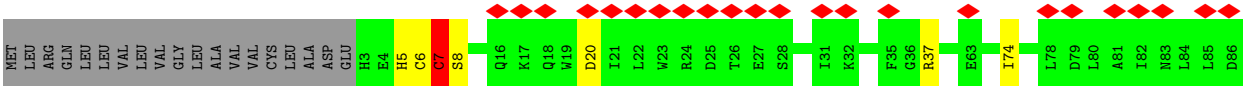
Chain Bp:

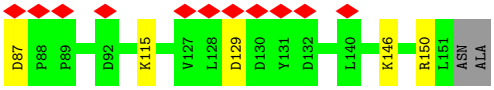




• Molecule 7: EXTRACELLULAR GLOBIN-3

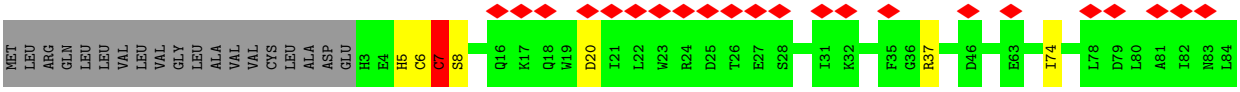
Chain Bu:

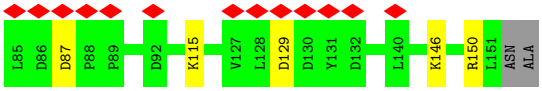




• Molecule 7: EXTRACELLULAR GLOBIN-3

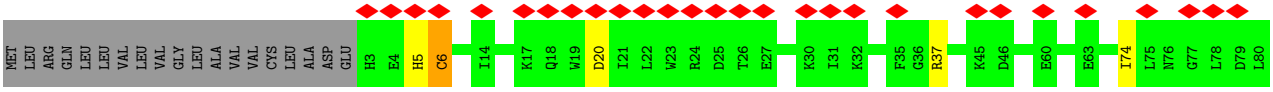
Chain Bz:

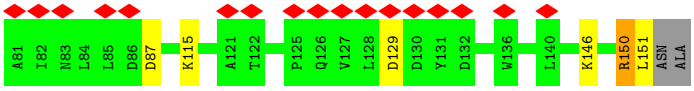




• Molecule 7: EXTRACELLULAR GLOBIN-3

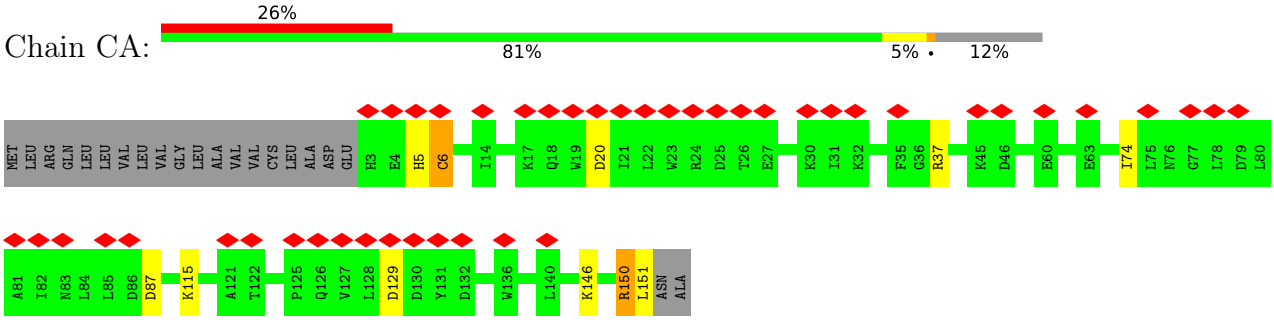
Chain C3:





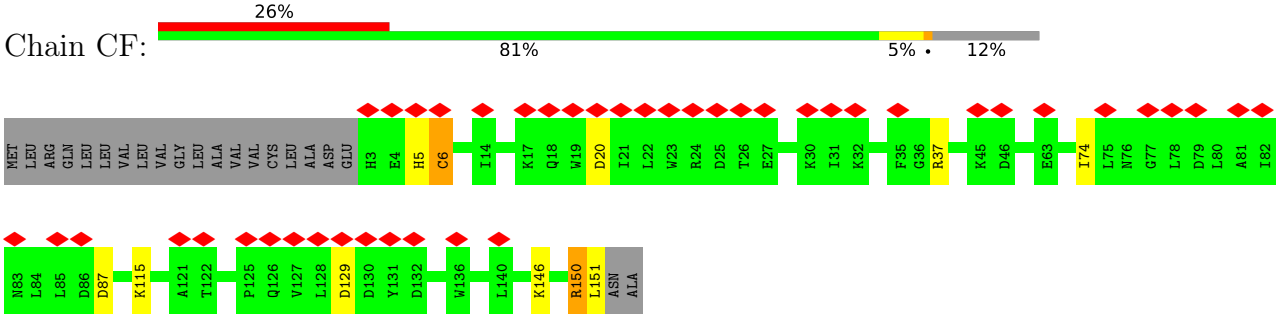
• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain CA:



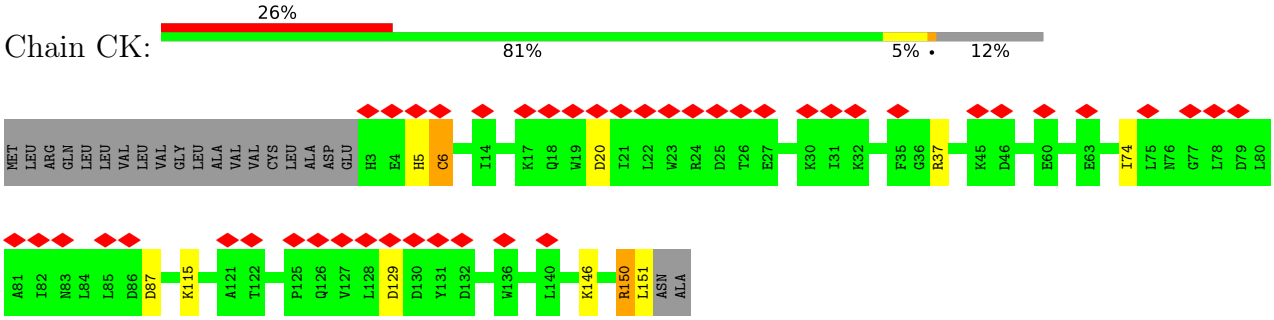
• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain CF:



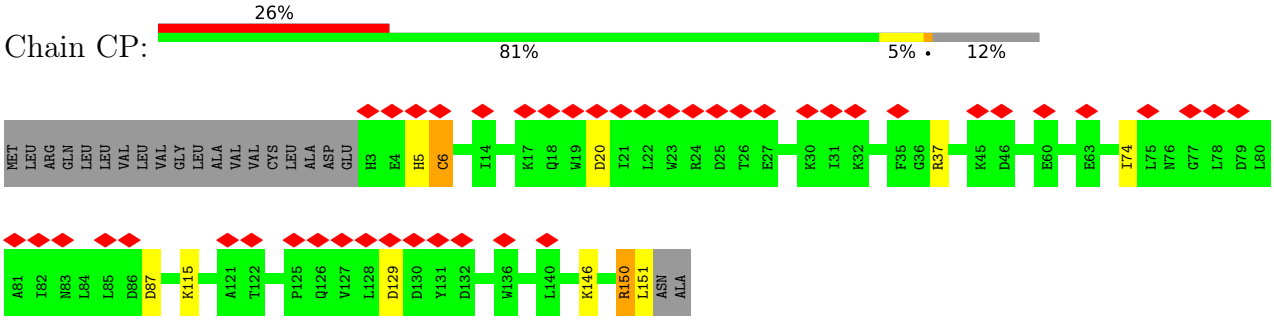
• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain CK:



• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain CP:



• Molecule 7: EXTRACELLULAR GLOBIN-3

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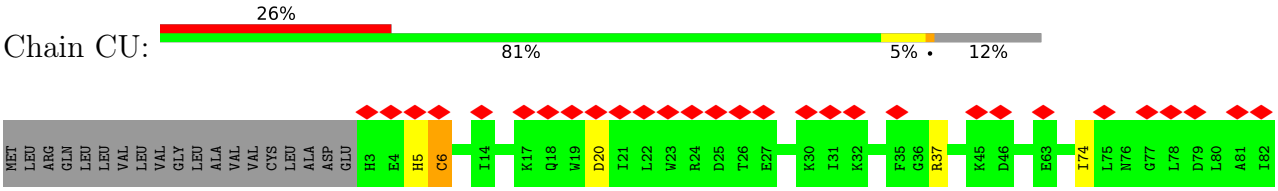
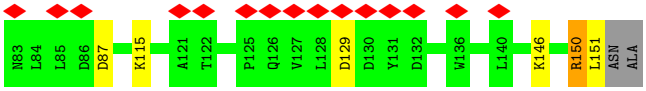
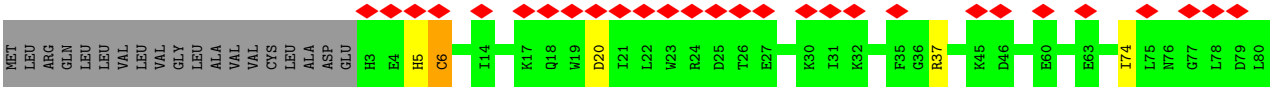
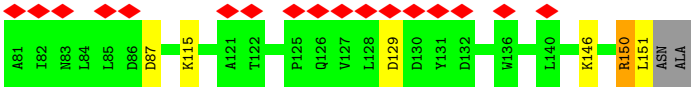




• Molecule 7: EXTRACELLULAR GLOBIN-3

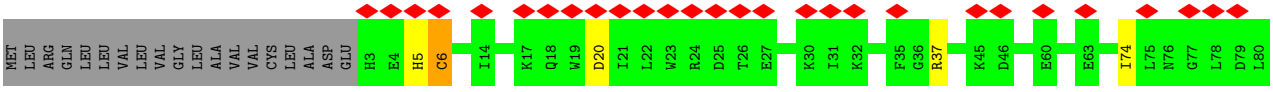
Chain CZ:

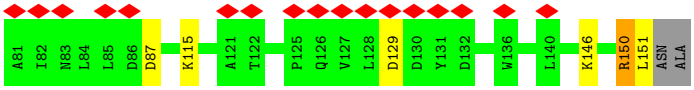




• Molecule 7: EXTRACELLULAR GLOBIN-3

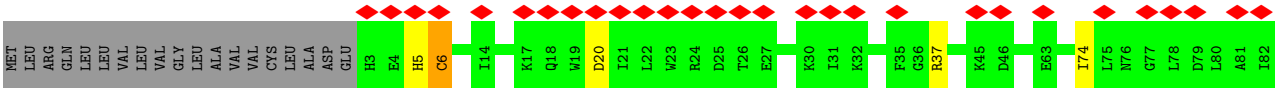
Chain Ce:

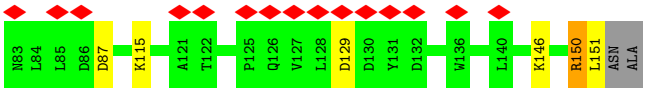




• Molecule 7: EXTRACELLULAR GLOBIN-3

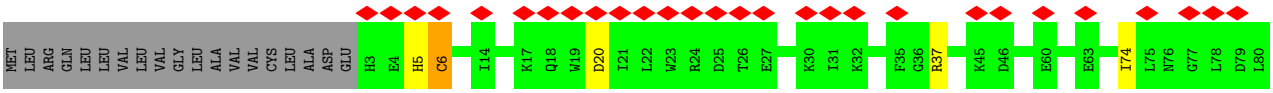
Chain Cj:

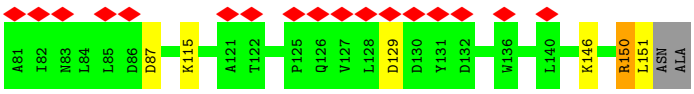




• Molecule 7: EXTRACELLULAR GLOBIN-3

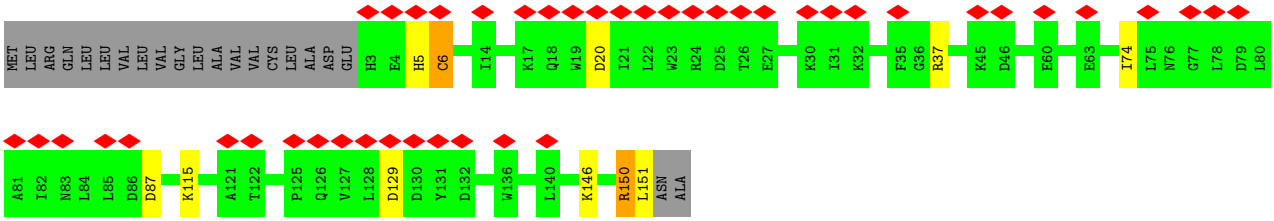
Chain Co:





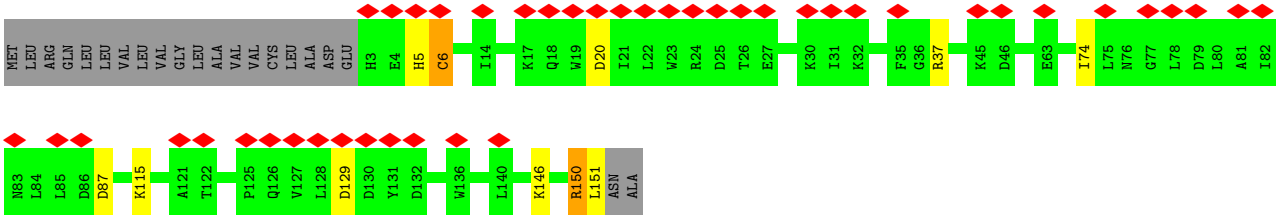
• Molecule 7: EXTRACELLULAR GLOBIN-3

Chain Ct:



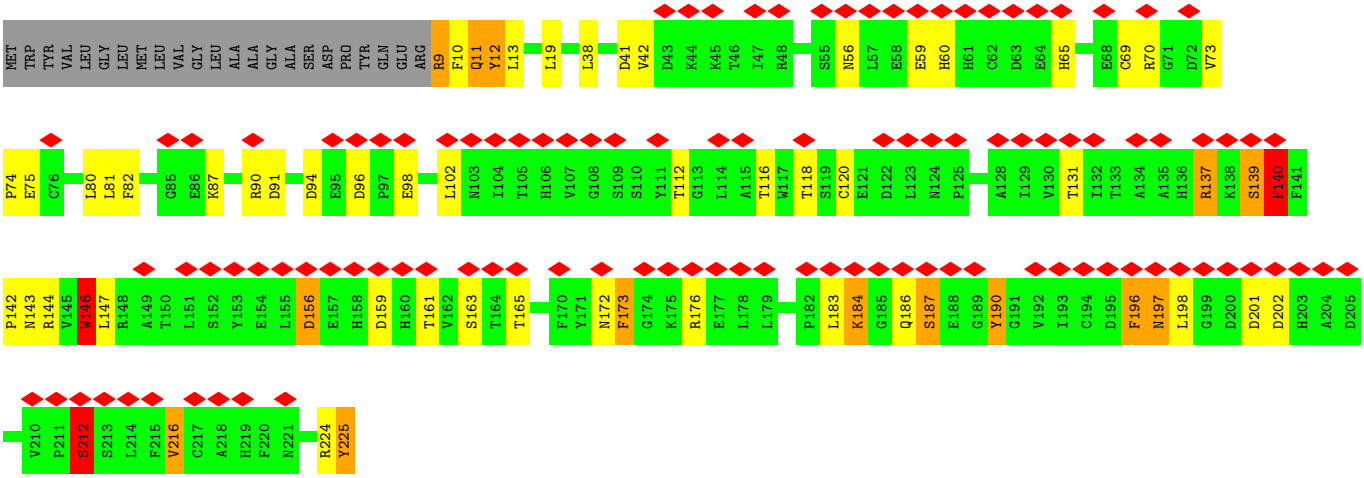
- Molecule 7: EXTRACELLULAR GLOBIN-3

Chain Cy:



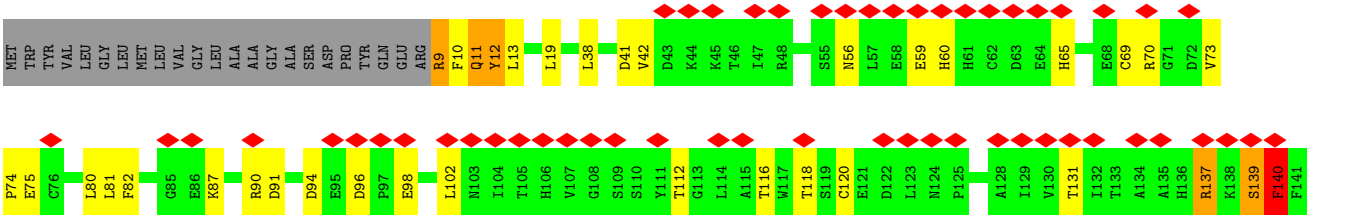
- Molecule 8: HEMOGLOBIN LINKER CHAIN L1

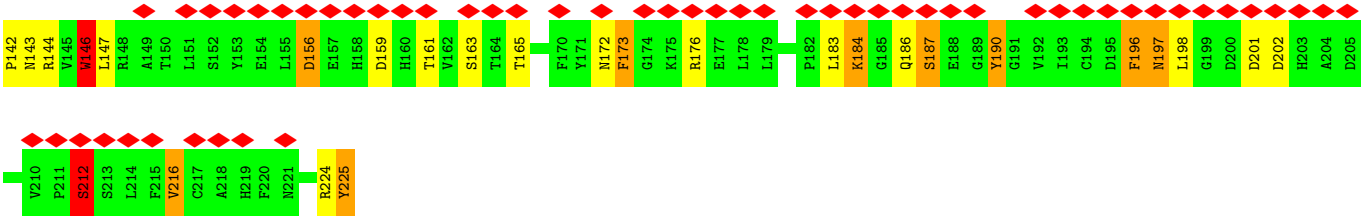
Chain C0:



- Molecule 8: HEMOGLOBIN LINKER CHAIN L1

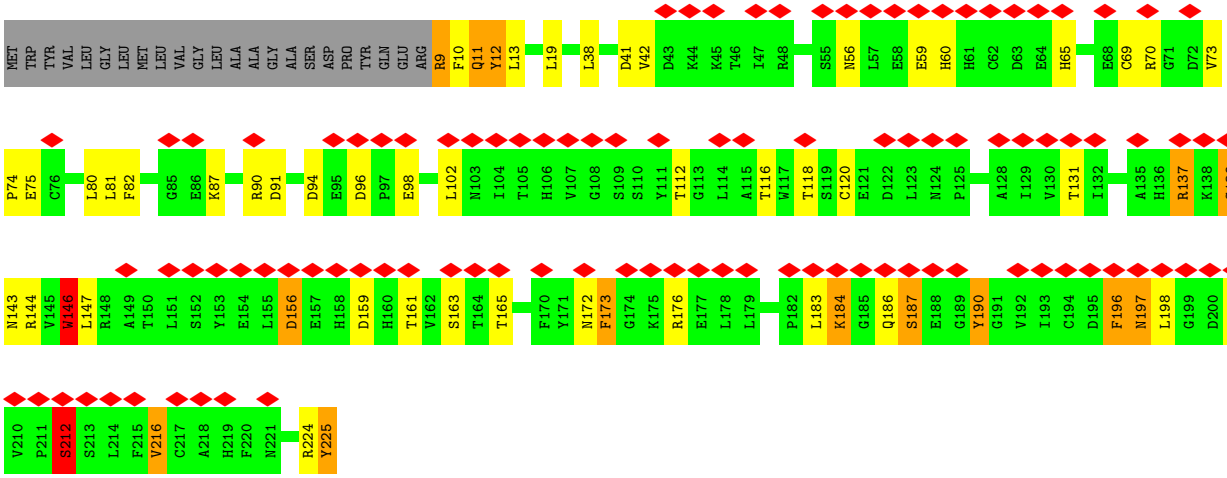
Chain C5:





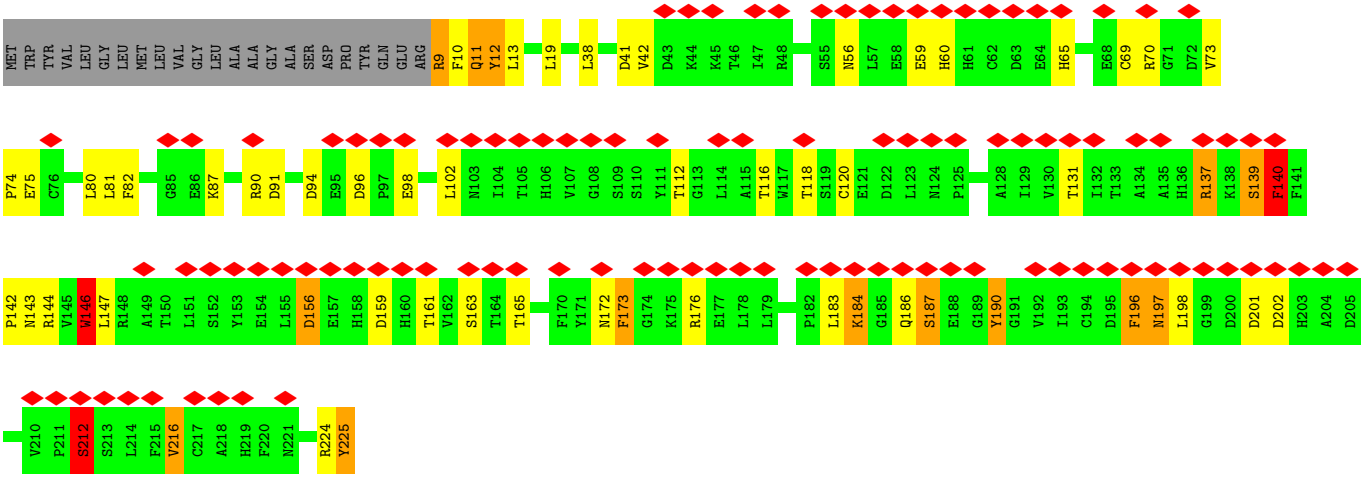
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

Chain CC:



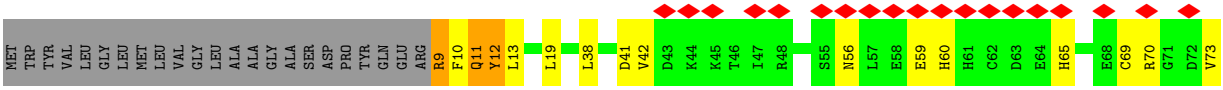
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

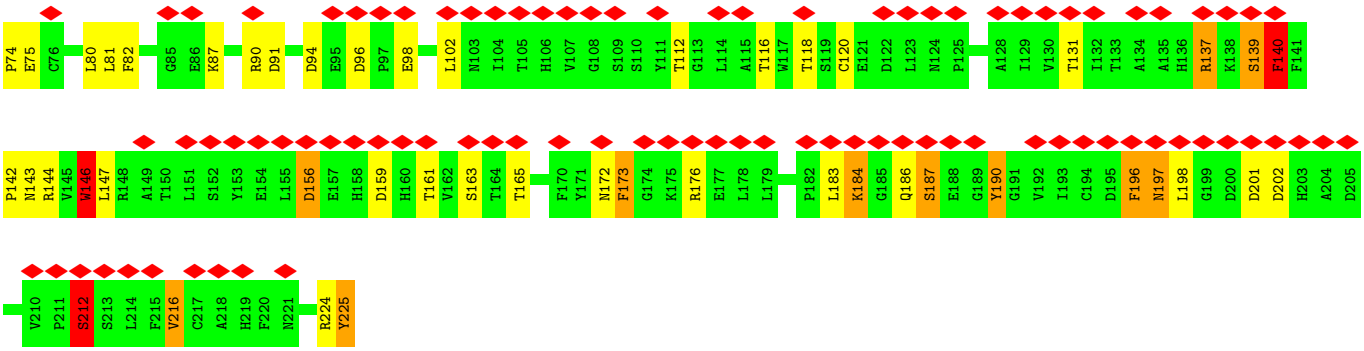
Chain CH:



• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

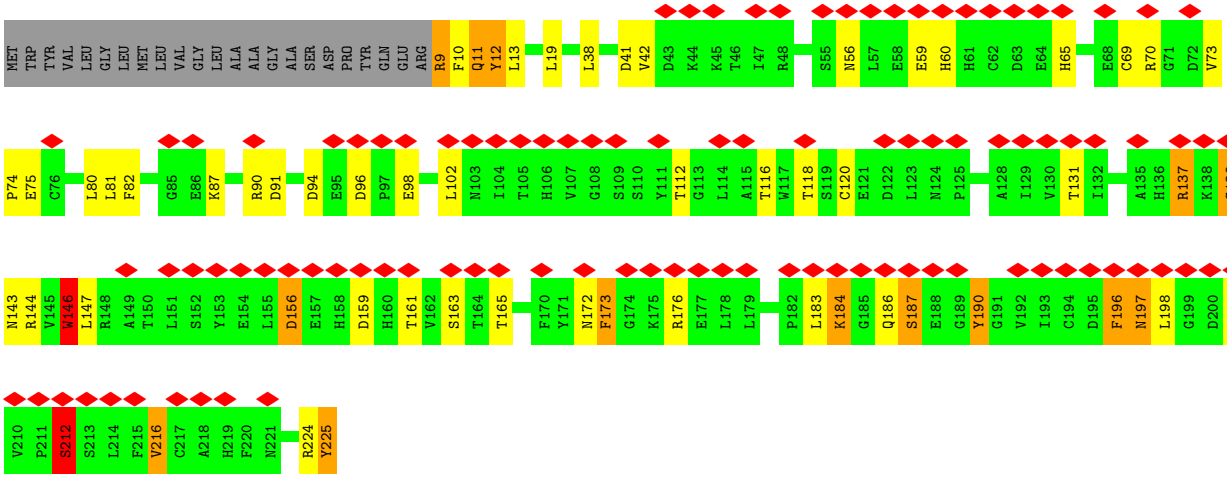
Chain CM:





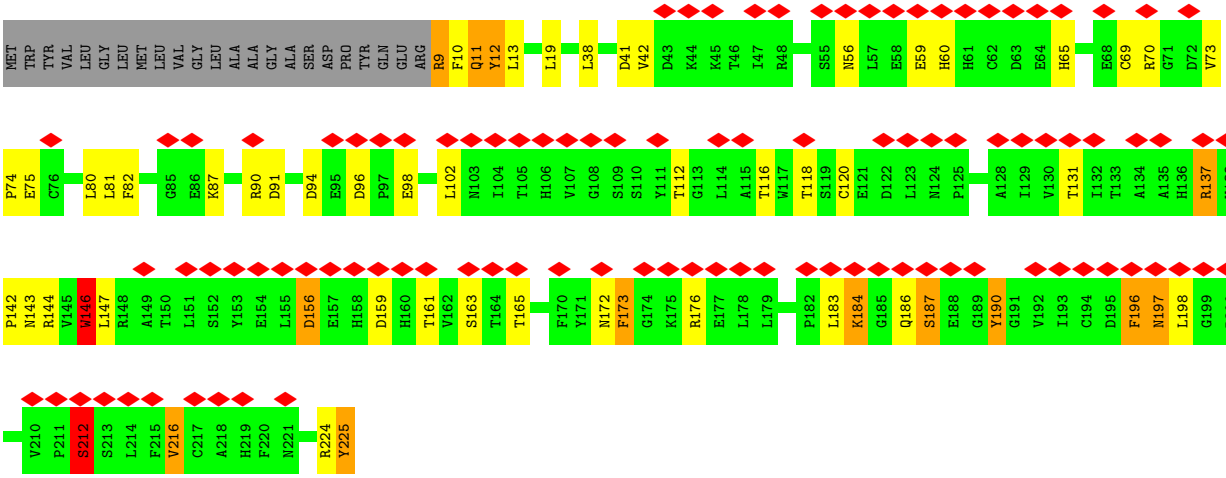
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

Chain CR:



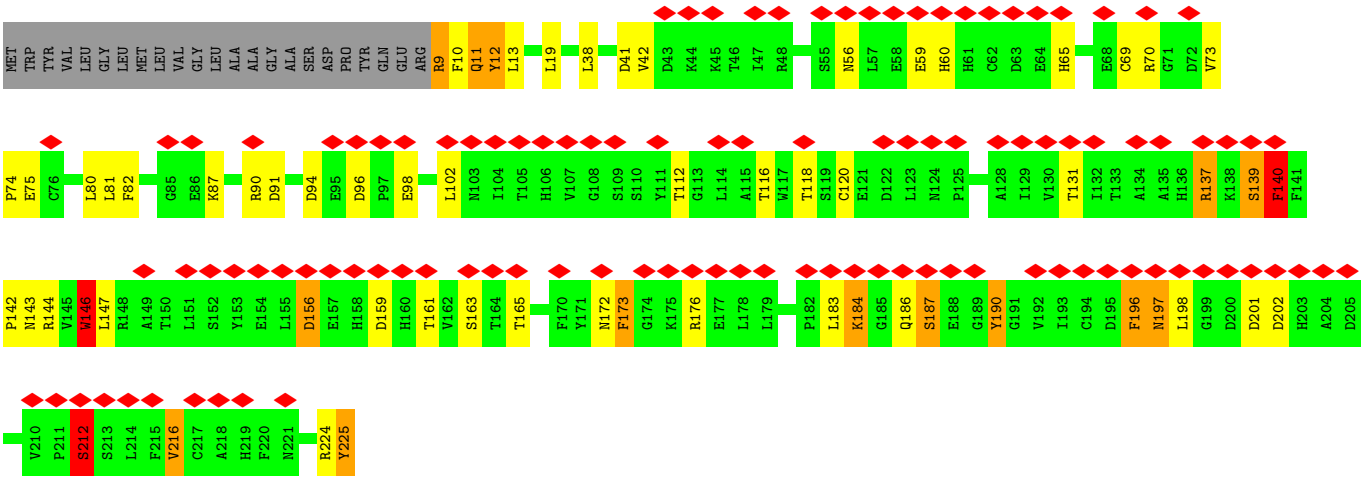
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

Chain CW:



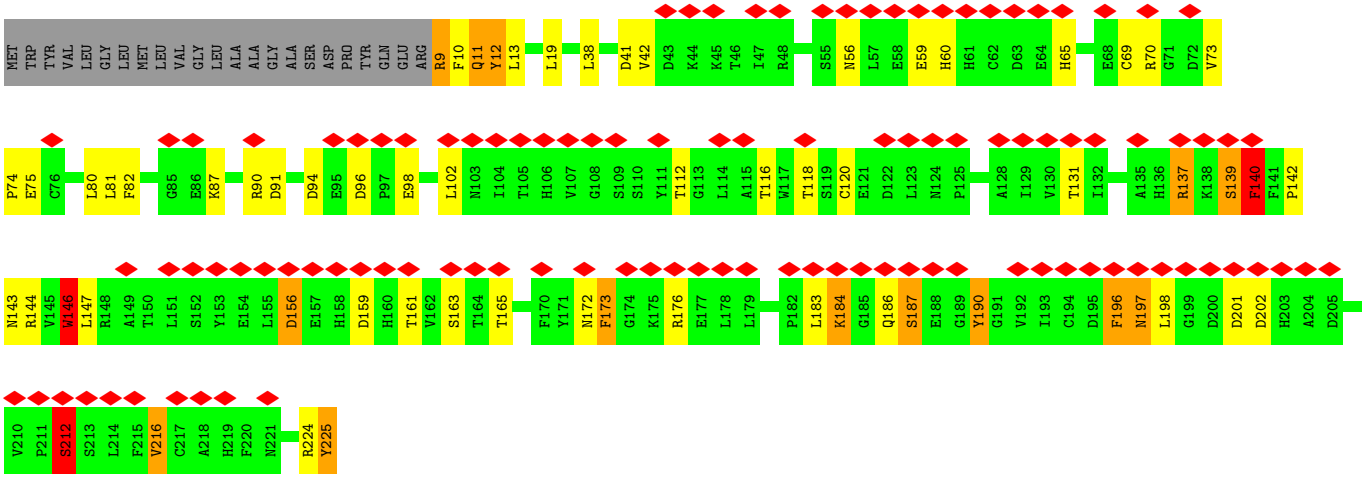
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

Chain Cb:



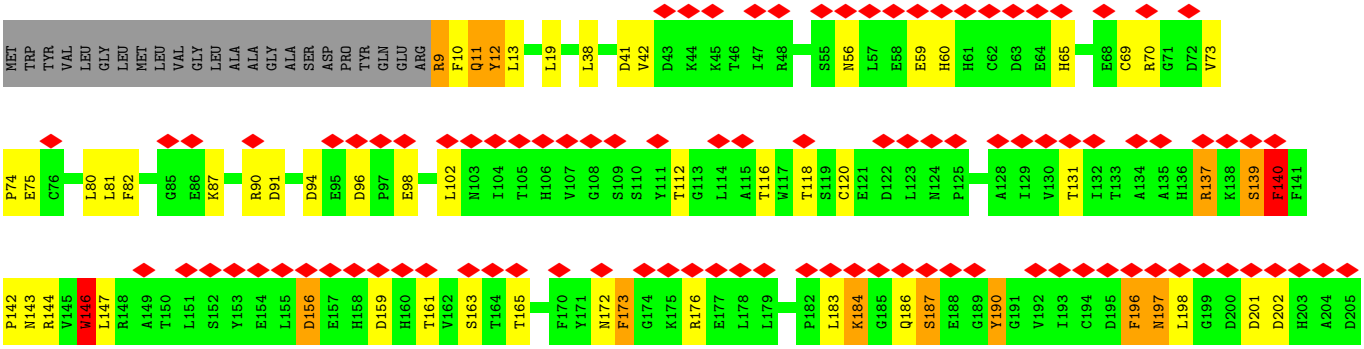
- Molecule 8: HEMOGLOBIN LINKER CHAIN L1

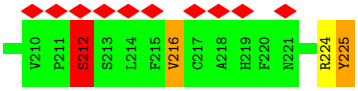
Chain Cg:



- Molecule 8: HEMOGLOBIN LINKER CHAIN L1

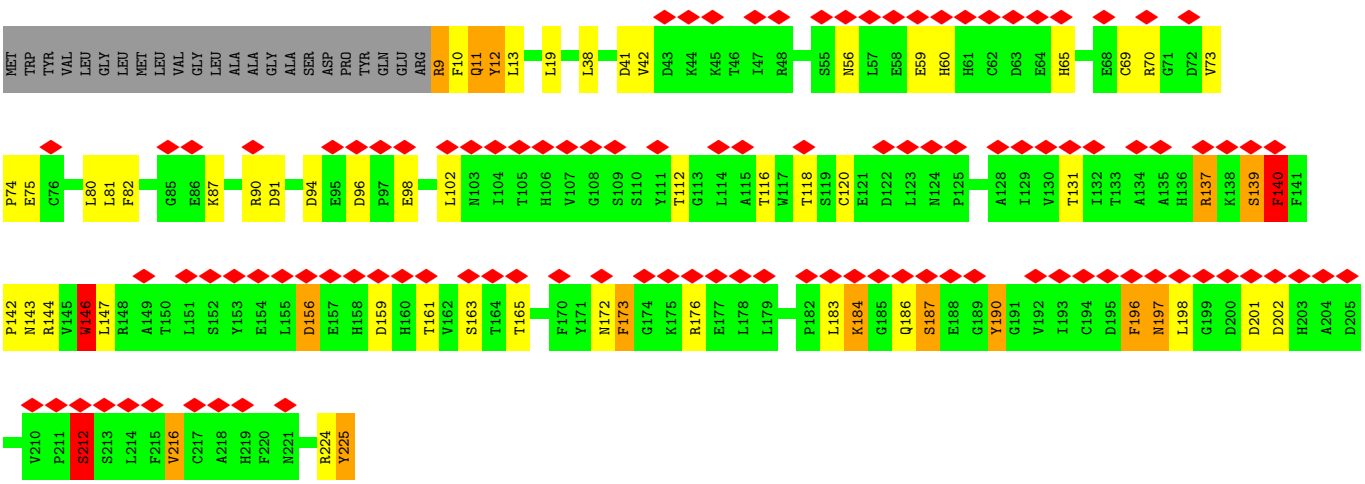
Chain Cl:





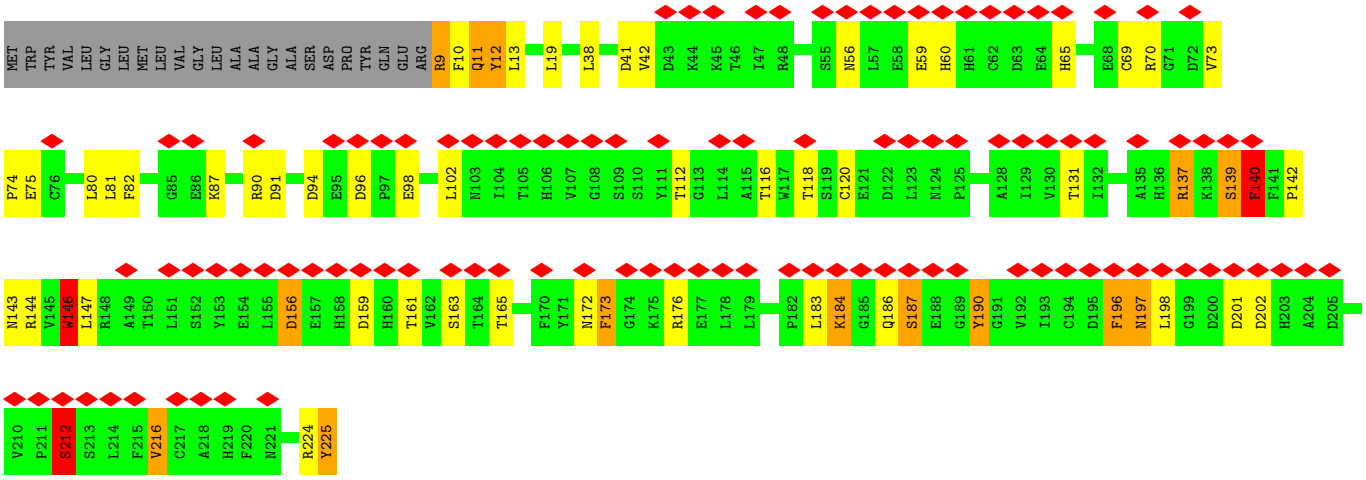
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

Chain Cq:



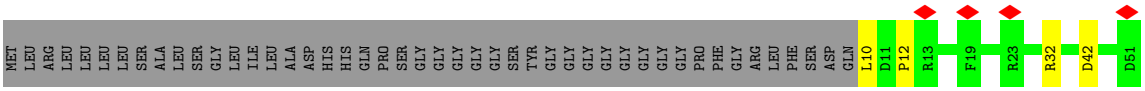
• Molecule 8: HEMOGLOBIN LINKER CHAIN L1

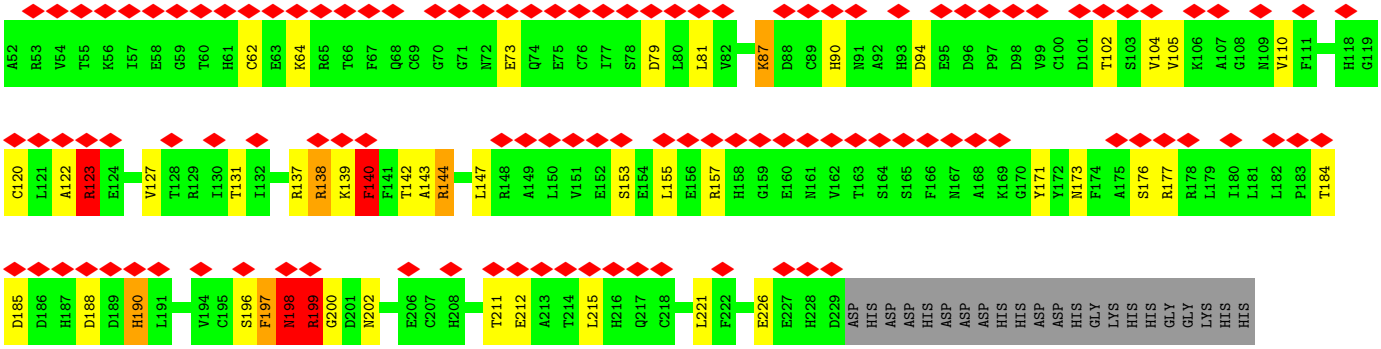
Chain Cv:



• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

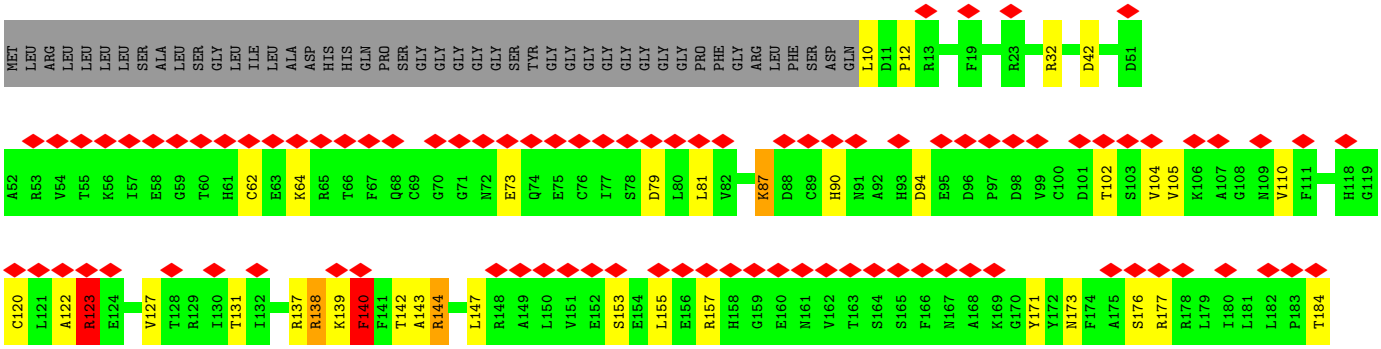
Chain C1:





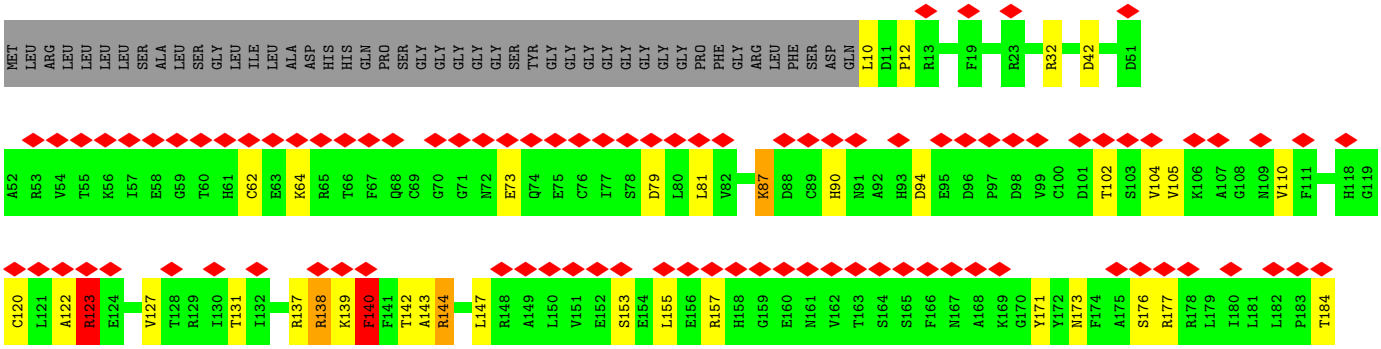
• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

Chain C6:



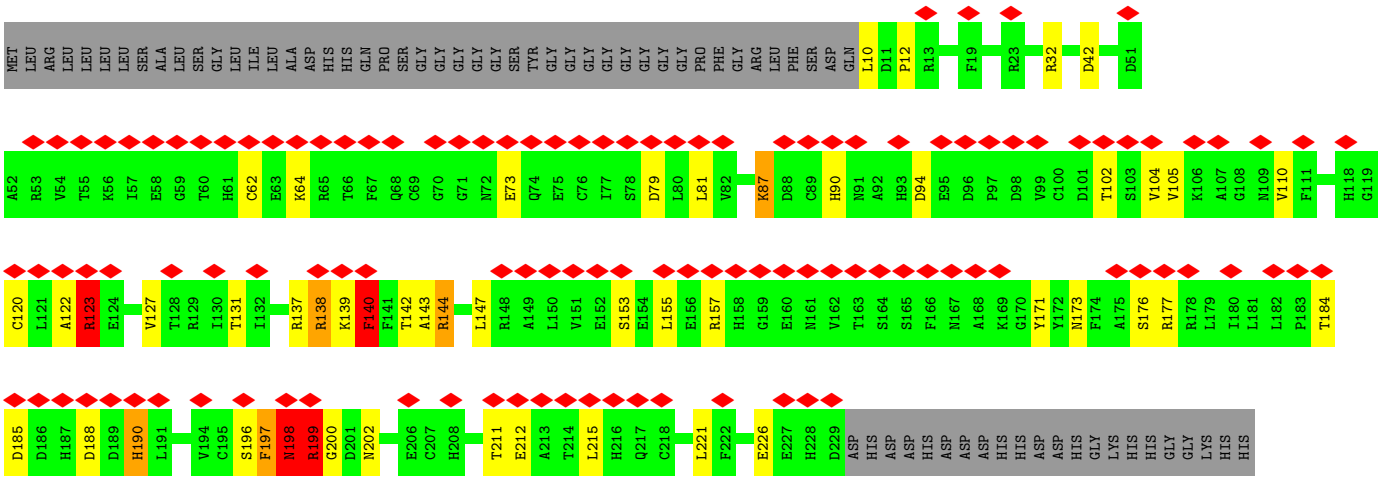
• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

Chain CD:



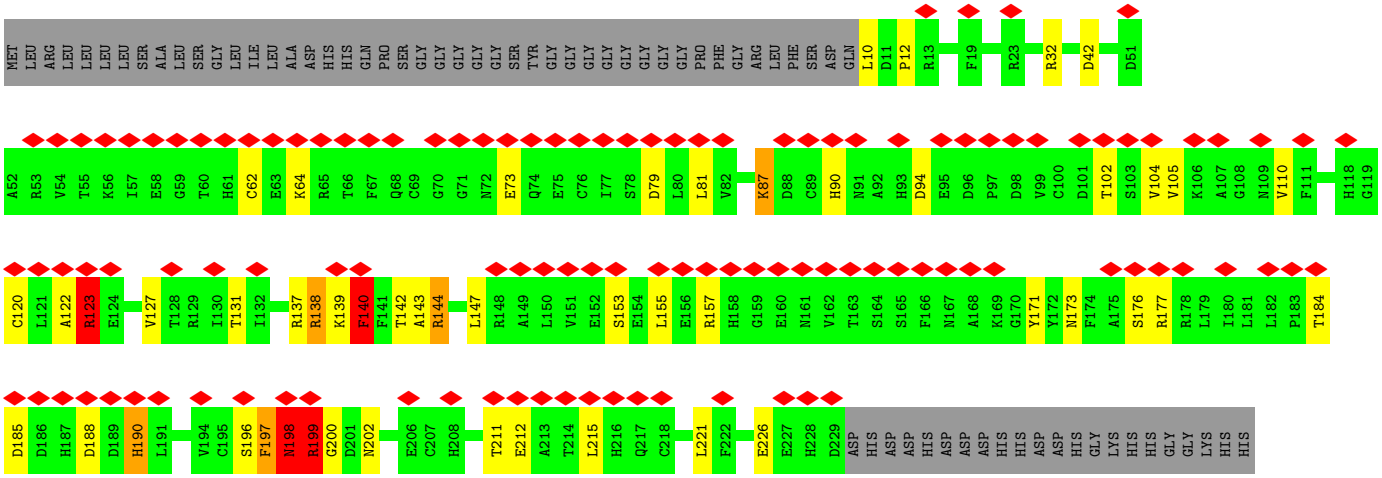
• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

Chain CI:



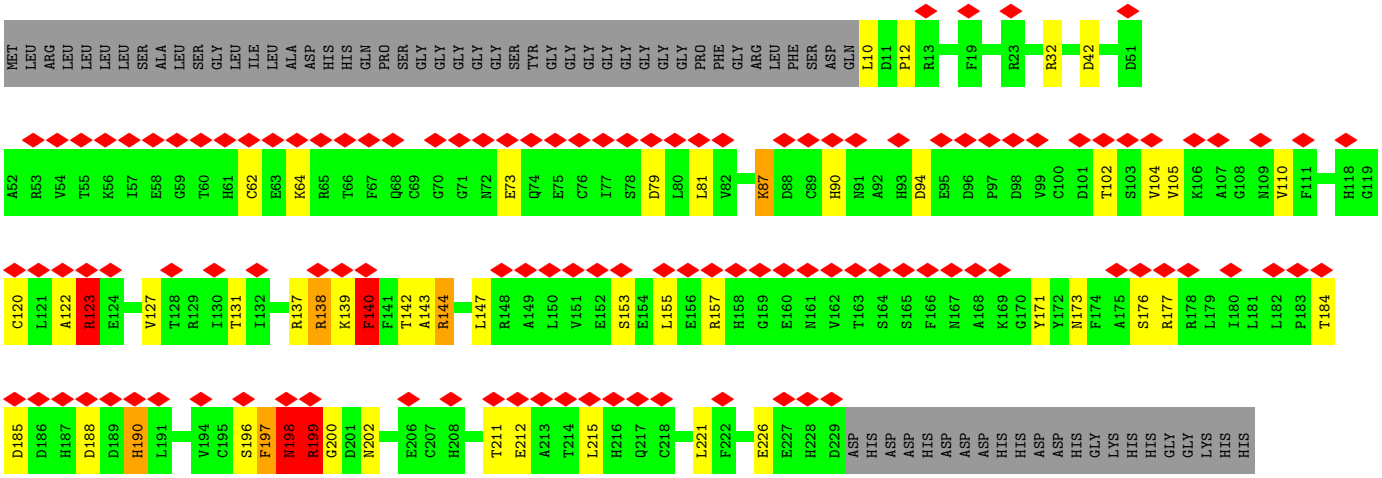
- Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

Chain CN:



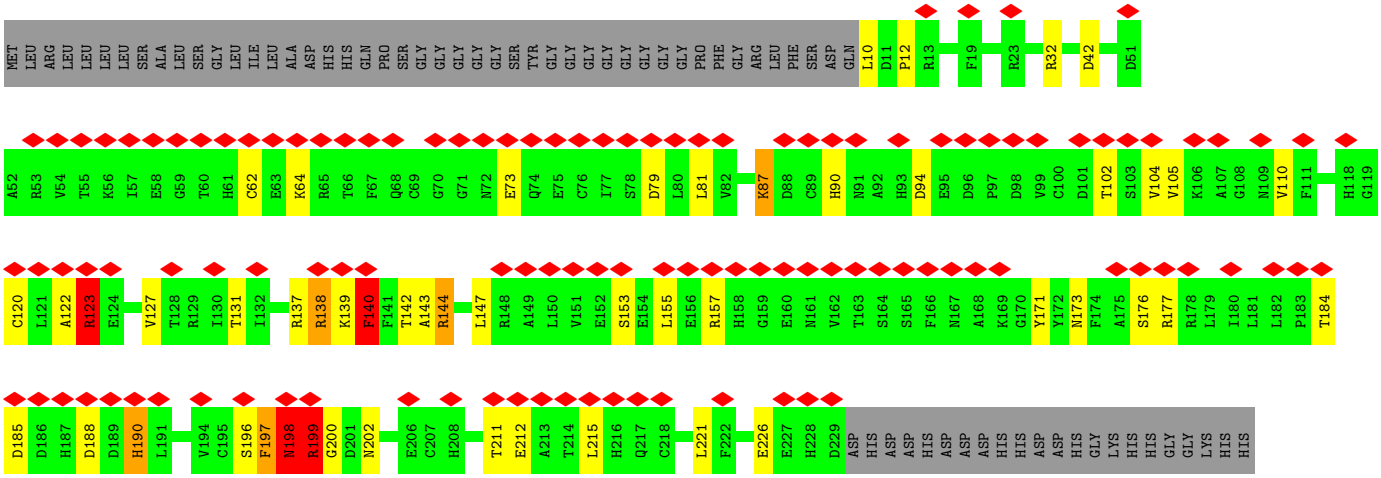
- Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

Chain CS:



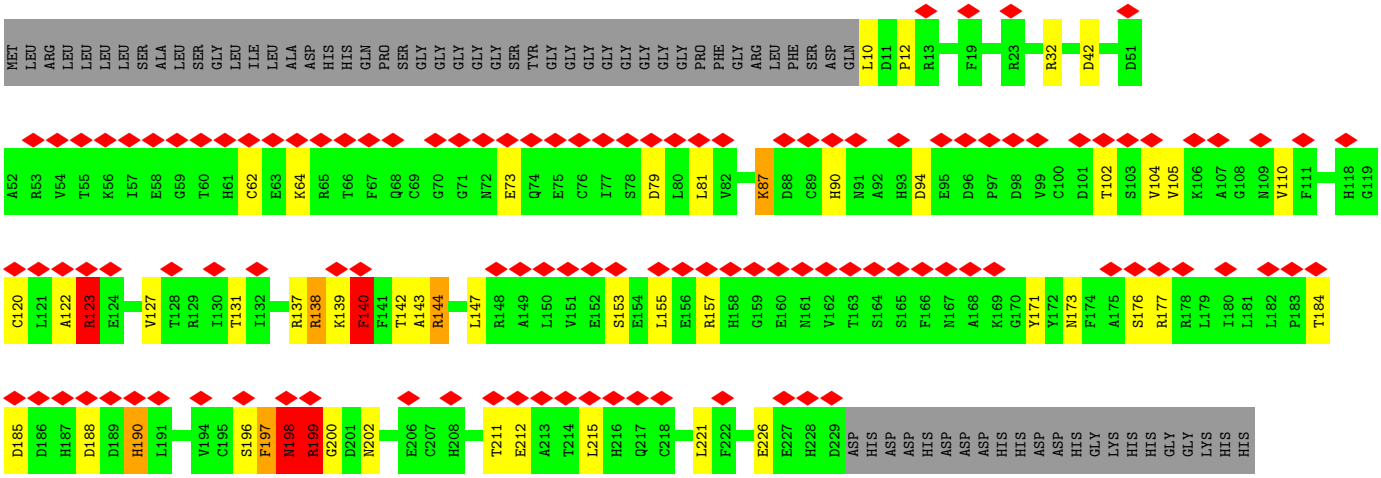
• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

Chain CX: 41% 59% 15% • • 24%



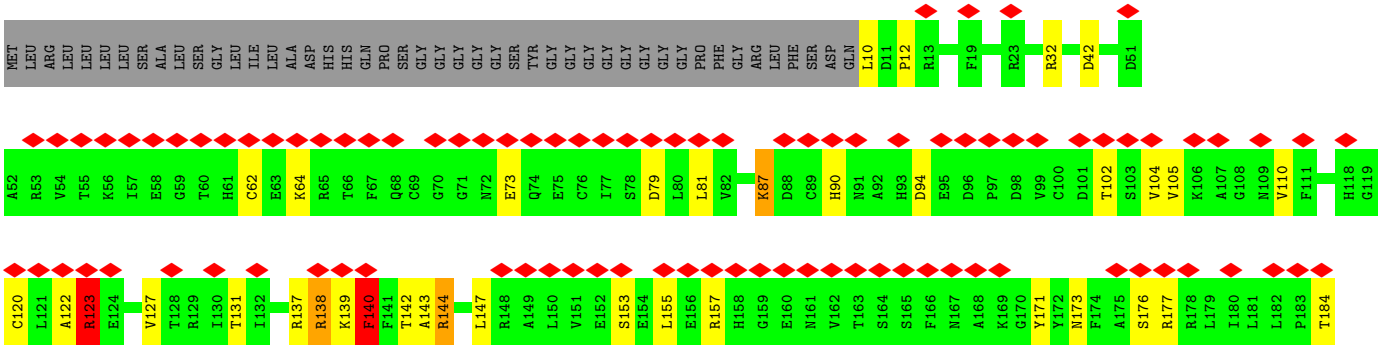
• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

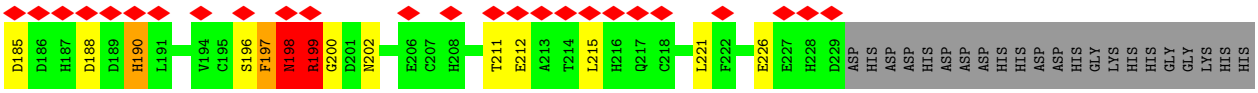
Chain Cc: 40% 59% 15% • • 24%



• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

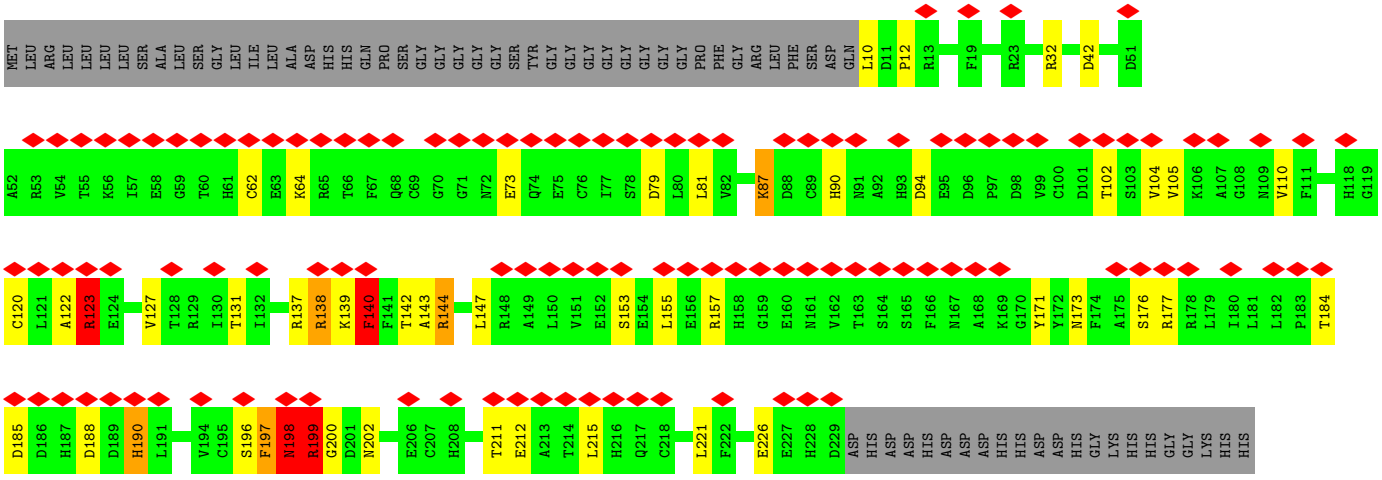
Chain Ch: 41% 59% 15% • • 24%





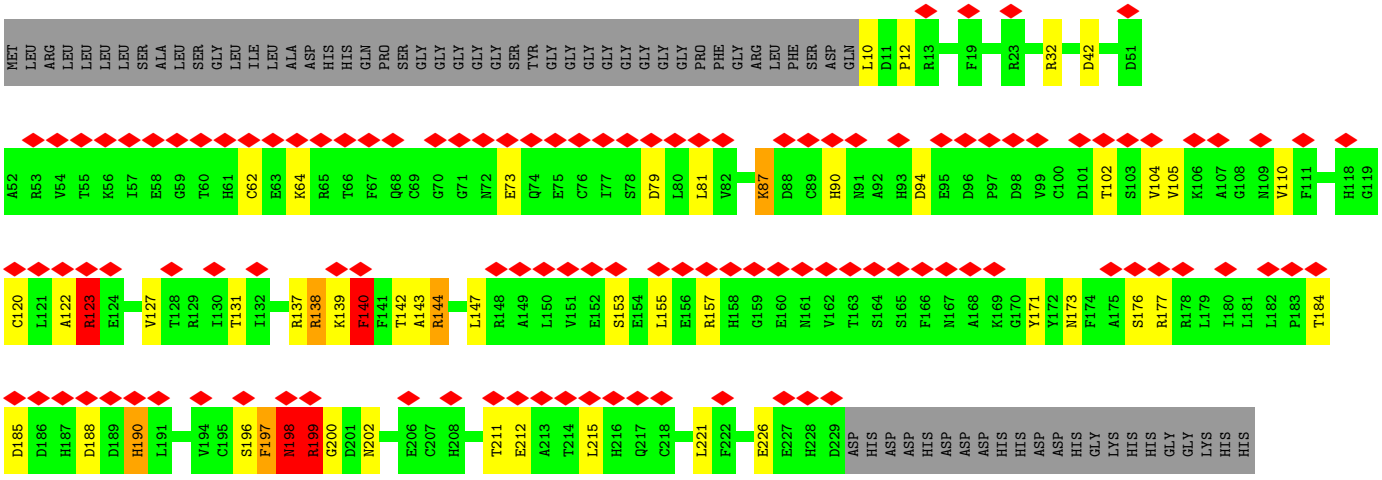
• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

Chain Cm:



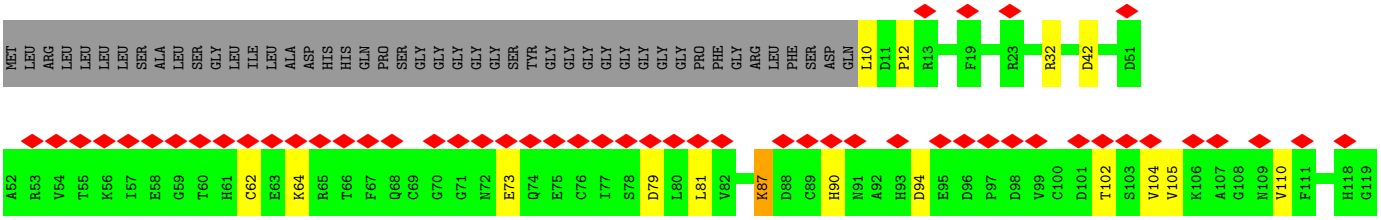
• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

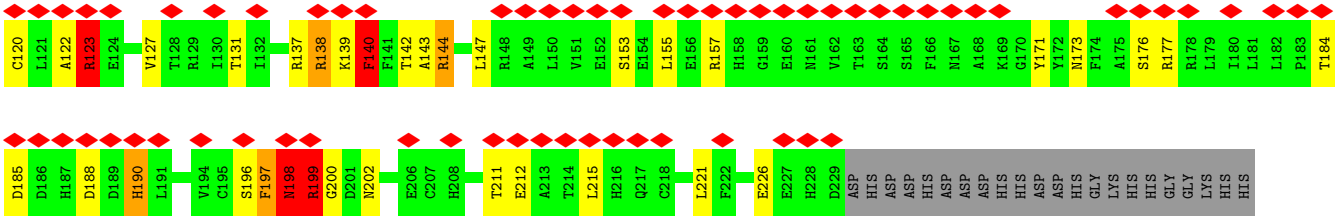
Chain Cr:



• Molecule 9: EXTRACELLULAR HEMOGLOBIN LINKER L2 SUBUNIT

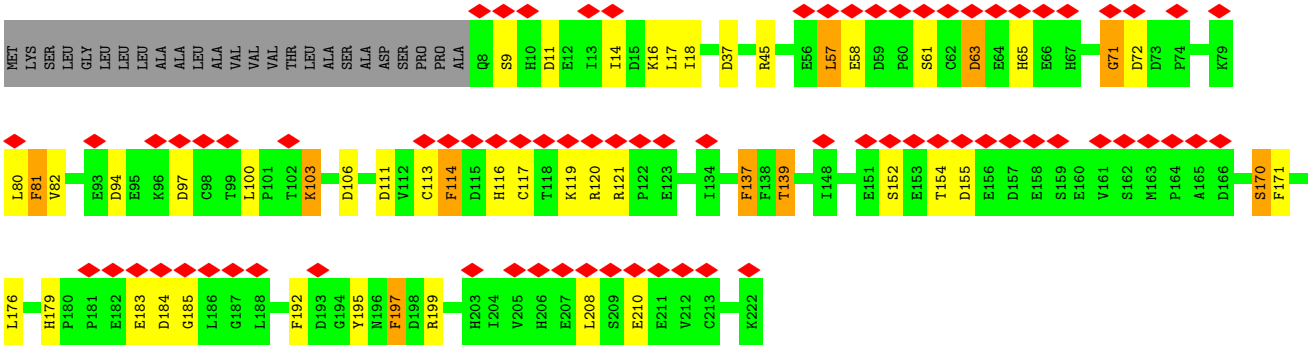
Chain Cw:





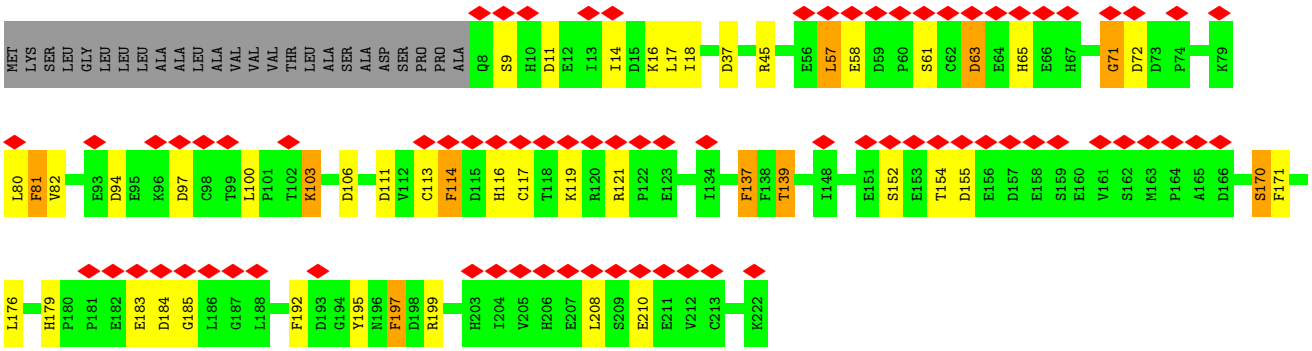
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain C2:



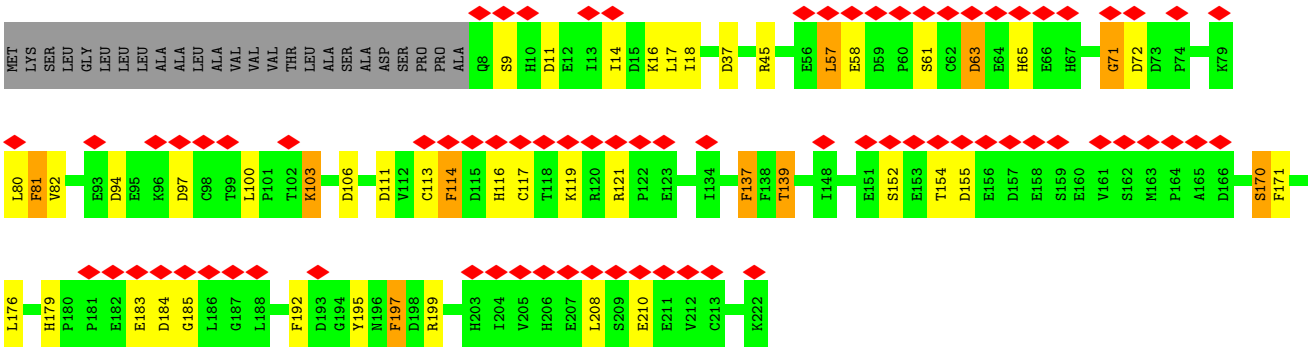
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain C7:



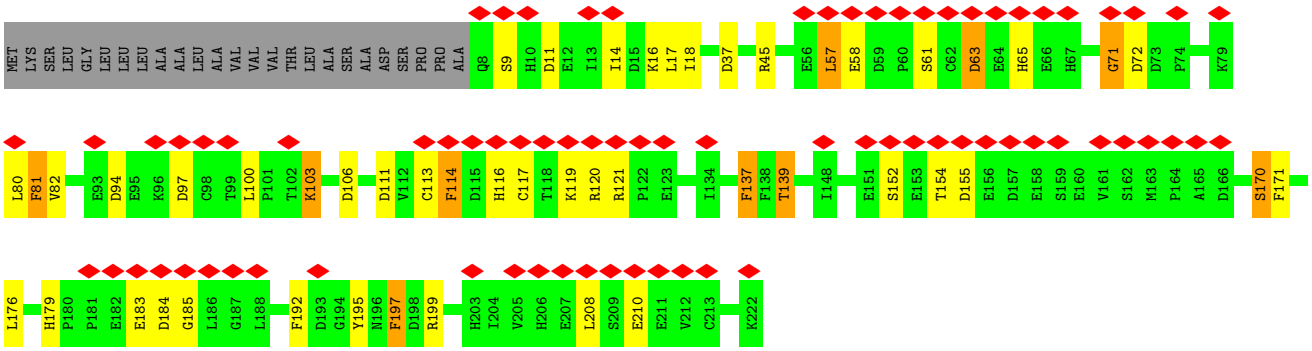
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain CE:



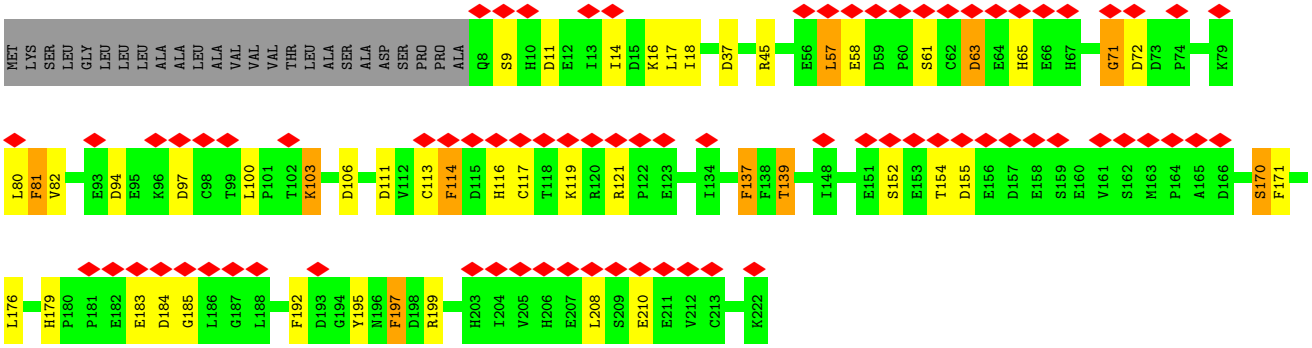
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain CJ:



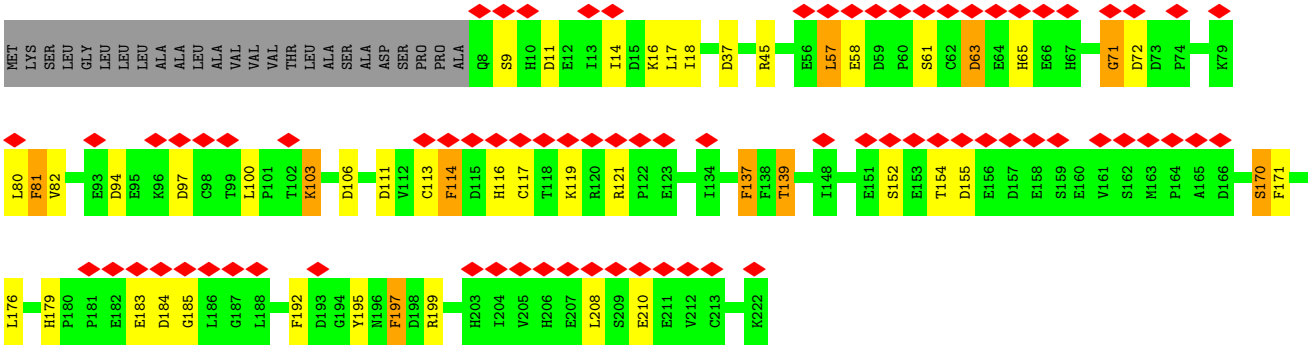
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain CO:



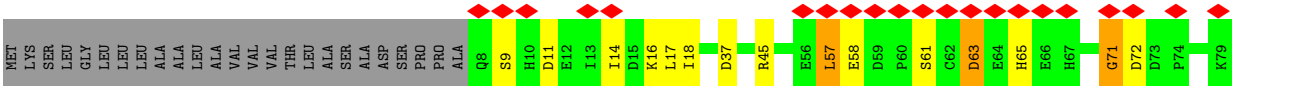
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

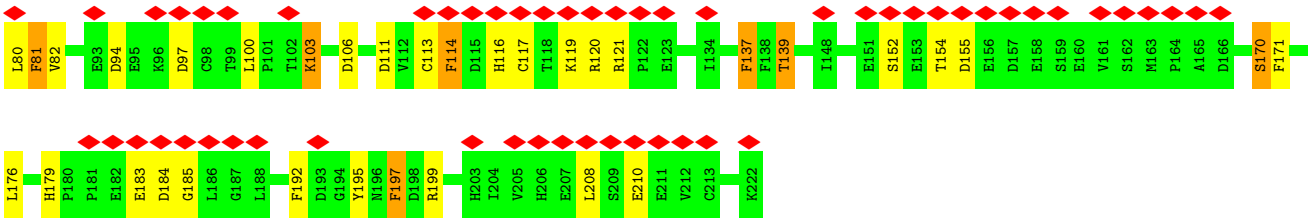
Chain CT:



• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

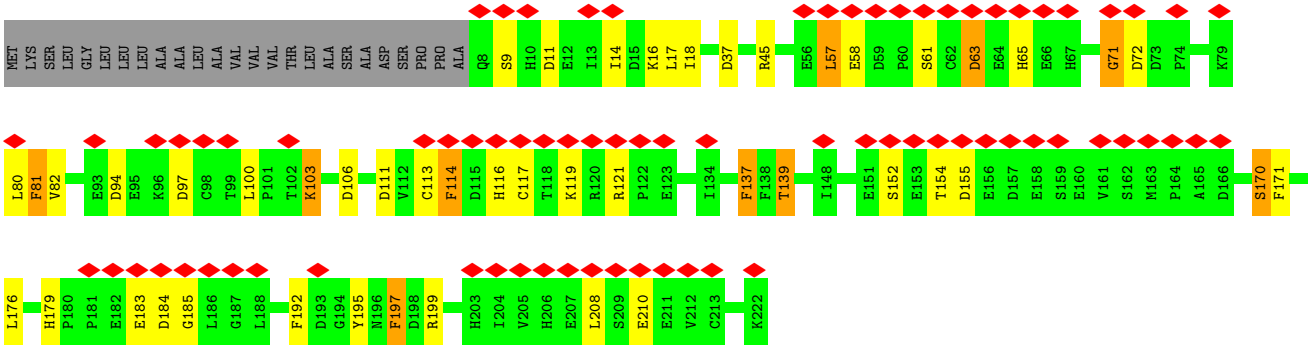
Chain CY:





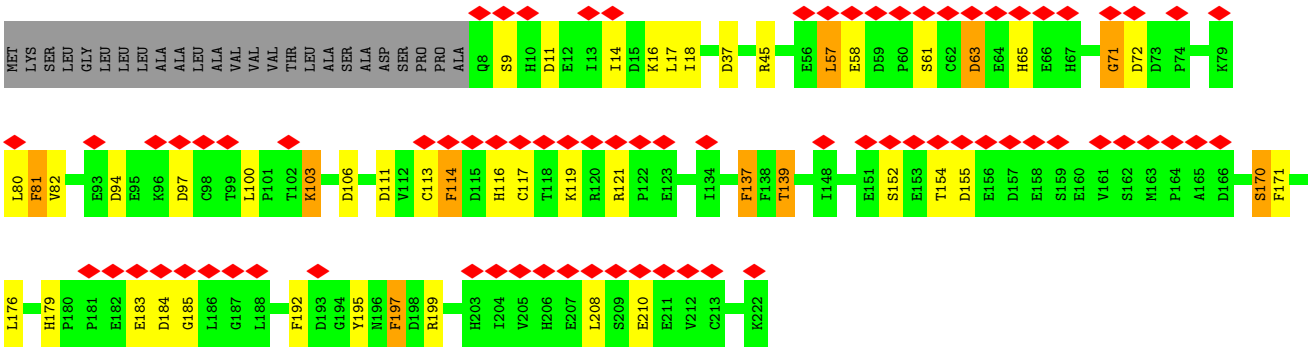
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain Cd:



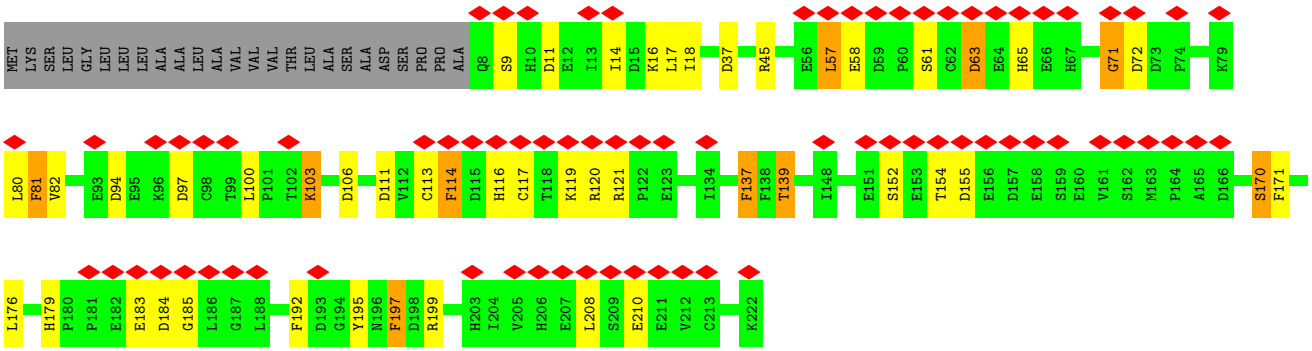
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain Ci:



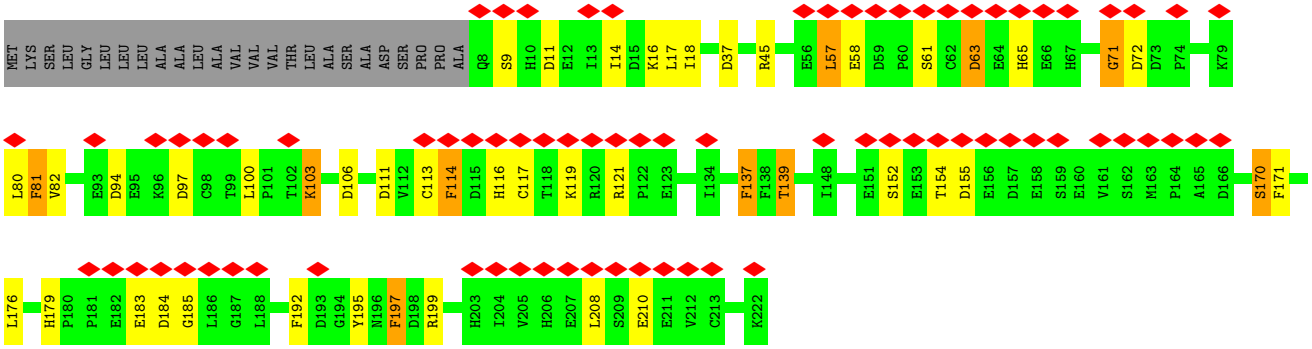
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain Cn:



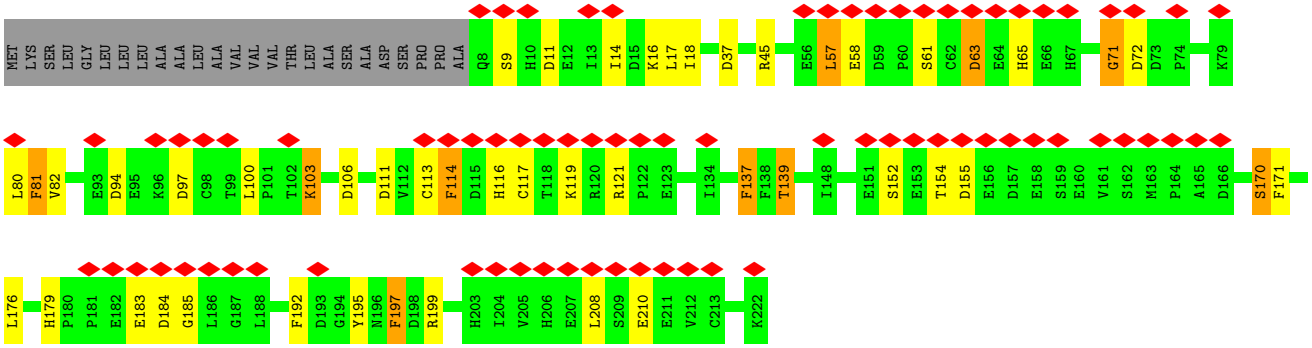
• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain Cs:



• Molecule 10: EXTRACELLULAR HEMOGLOBIN LINKER L3 SUBUNIT

Chain Cx:



4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	520.0, 520.0, 520.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.48	0/1216	0.70	1/1641 (0.1%)
1	A5	0.48	0/1216	0.70	1/1641 (0.1%)
1	AC	0.48	0/1216	0.70	1/1641 (0.1%)
1	AH	0.48	0/1216	0.70	1/1641 (0.1%)
1	AM	0.48	0/1216	0.70	1/1641 (0.1%)
1	AR	0.48	0/1216	0.70	1/1641 (0.1%)
1	AW	0.48	0/1216	0.70	1/1641 (0.1%)
1	Ab	0.48	0/1216	0.70	1/1641 (0.1%)
1	Ag	0.48	0/1216	0.70	1/1641 (0.1%)
1	Al	0.48	0/1216	0.70	1/1641 (0.1%)
1	Aq	0.48	0/1216	0.70	1/1641 (0.1%)
1	Av	0.48	0/1216	0.70	1/1641 (0.1%)
2	A1	0.55	0/1159	0.70	1/1568 (0.1%)
2	A6	0.55	0/1159	0.70	1/1568 (0.1%)
2	AD	0.55	0/1159	0.70	1/1568 (0.1%)
2	AI	0.55	0/1159	0.70	1/1568 (0.1%)
2	AN	0.55	0/1159	0.70	1/1568 (0.1%)
2	AS	0.55	0/1159	0.70	1/1568 (0.1%)
2	AX	0.55	0/1159	0.70	1/1568 (0.1%)
2	Ac	0.55	0/1159	0.70	1/1568 (0.1%)
2	Ah	0.55	0/1159	0.70	1/1568 (0.1%)
2	Am	0.55	0/1159	0.70	1/1568 (0.1%)
2	Ar	0.55	0/1159	0.70	1/1568 (0.1%)
2	Aw	0.55	0/1159	0.70	1/1568 (0.1%)
3	A2	0.51	0/1237	0.85	5/1670 (0.3%)
3	A3	0.56	0/1237	0.91	4/1670 (0.2%)
3	A7	0.51	0/1237	0.85	5/1670 (0.3%)
3	AA	0.56	0/1237	0.91	4/1670 (0.2%)
3	AE	0.51	0/1237	0.85	5/1670 (0.3%)
3	AF	0.56	0/1237	0.91	4/1670 (0.2%)
3	AJ	0.51	0/1237	0.85	5/1670 (0.3%)
3	AK	0.56	0/1237	0.91	4/1670 (0.2%)
3	AO	0.51	0/1237	0.85	5/1670 (0.3%)
3	AP	0.56	0/1237	0.91	4/1670 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	AT	0.51	0/1237	0.85	5/1670 (0.3%)
3	AU	0.56	0/1237	0.91	4/1670 (0.2%)
3	AY	0.51	0/1237	0.85	5/1670 (0.3%)
3	AZ	0.56	0/1237	0.91	4/1670 (0.2%)
3	Ad	0.51	0/1237	0.85	5/1670 (0.3%)
3	Ae	0.56	0/1237	0.91	4/1670 (0.2%)
3	Ai	0.51	0/1237	0.85	5/1670 (0.3%)
3	Aj	0.56	0/1237	0.91	4/1670 (0.2%)
3	An	0.51	0/1237	0.85	5/1670 (0.3%)
3	Ao	0.56	0/1237	0.91	4/1670 (0.2%)
3	As	0.51	0/1237	0.85	5/1670 (0.3%)
3	At	0.56	0/1237	0.91	4/1670 (0.2%)
3	Ax	0.51	0/1237	0.85	5/1670 (0.3%)
3	Ay	0.56	0/1237	0.91	4/1670 (0.2%)
4	A4	0.60	0/1176	0.75	2/1587 (0.1%)
4	AB	0.59	0/1176	0.75	2/1587 (0.1%)
4	AG	0.60	0/1176	0.74	2/1587 (0.1%)
4	AL	0.60	0/1176	0.75	2/1587 (0.1%)
4	AQ	0.59	0/1176	0.75	2/1587 (0.1%)
4	AV	0.60	0/1176	0.74	2/1587 (0.1%)
4	Aa	0.60	0/1176	0.75	2/1587 (0.1%)
4	Af	0.59	0/1176	0.75	2/1587 (0.1%)
4	Ak	0.60	0/1176	0.74	2/1587 (0.1%)
4	Ap	0.60	0/1176	0.75	2/1587 (0.1%)
4	Au	0.59	0/1176	0.75	2/1587 (0.1%)
4	Az	0.60	0/1176	0.74	2/1587 (0.1%)
4	B2	0.56	0/1176	0.80	2/1587 (0.1%)
4	B3	0.60	0/1176	0.81	5/1587 (0.3%)
4	B7	0.56	0/1176	0.80	2/1587 (0.1%)
4	BA	0.60	0/1176	0.81	5/1587 (0.3%)
4	BE	0.56	0/1176	0.80	2/1587 (0.1%)
4	BF	0.60	0/1176	0.81	5/1587 (0.3%)
4	BJ	0.56	0/1176	0.80	2/1587 (0.1%)
4	BK	0.60	0/1176	0.81	5/1587 (0.3%)
4	BO	0.56	0/1176	0.80	2/1587 (0.1%)
4	BP	0.60	0/1176	0.81	5/1587 (0.3%)
4	BT	0.56	0/1176	0.80	2/1587 (0.1%)
4	BU	0.60	0/1176	0.81	5/1587 (0.3%)
4	BY	0.56	0/1176	0.80	2/1587 (0.1%)
4	BZ	0.60	0/1176	0.81	5/1587 (0.3%)
4	Bd	0.56	0/1176	0.80	2/1587 (0.1%)
4	Be	0.60	0/1176	0.81	5/1587 (0.3%)
4	Bi	0.56	0/1176	0.80	2/1587 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	Bj	0.60	0/1176	0.81	5/1587 (0.3%)
4	Bn	0.56	0/1176	0.80	2/1587 (0.1%)
4	Bo	0.60	0/1176	0.81	5/1587 (0.3%)
4	Bs	0.56	0/1176	0.80	2/1587 (0.1%)
4	Bt	0.60	0/1176	0.81	5/1587 (0.3%)
4	Bx	0.56	0/1176	0.80	2/1587 (0.1%)
4	By	0.60	0/1176	0.81	5/1587 (0.3%)
5	B0	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	B5	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	BC	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	BH	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	BM	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	BR	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	BW	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	Bb	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	Bg	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	Bl	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	Bq	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	Bv	0.58	1/1159 (0.1%)	0.74	1/1568 (0.1%)
5	C4	0.55	0/1159	0.73	0/1568
5	CB	0.55	0/1159	0.73	0/1568
5	CG	0.55	0/1159	0.73	0/1568
5	CL	0.55	0/1159	0.73	0/1568
5	CQ	0.55	0/1159	0.73	0/1568
5	CV	0.55	0/1159	0.73	0/1568
5	Ca	0.55	0/1159	0.73	0/1568
5	Cf	0.55	0/1159	0.73	0/1568
5	Ck	0.55	0/1159	0.73	0/1568
5	Cp	0.55	0/1159	0.73	0/1568
5	Cu	0.55	0/1159	0.73	0/1568
5	Cz	0.55	0/1159	0.73	0/1568
6	B1	0.53	0/1237	0.81	6/1670 (0.4%)
6	B6	0.53	0/1237	0.81	6/1670 (0.4%)
6	BD	0.53	0/1237	0.81	6/1670 (0.4%)
6	BI	0.53	0/1237	0.81	6/1670 (0.4%)
6	BN	0.53	0/1237	0.81	6/1670 (0.4%)
6	BS	0.53	0/1237	0.81	6/1670 (0.4%)
6	BX	0.53	0/1237	0.81	6/1670 (0.4%)
6	Bc	0.53	0/1237	0.81	6/1670 (0.4%)
6	Bh	0.53	0/1237	0.81	6/1670 (0.4%)
6	Bm	0.53	0/1237	0.81	6/1670 (0.4%)
6	Br	0.53	0/1237	0.81	6/1670 (0.4%)
6	Bw	0.53	0/1237	0.81	6/1670 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	B4	0.46	0/1215	0.67	1/1641 (0.1%)
7	BB	0.46	0/1215	0.67	1/1641 (0.1%)
7	BG	0.46	0/1215	0.67	1/1641 (0.1%)
7	BL	0.46	0/1215	0.67	1/1641 (0.1%)
7	BQ	0.46	0/1215	0.67	1/1641 (0.1%)
7	BV	0.46	0/1215	0.67	1/1641 (0.1%)
7	Ba	0.46	0/1215	0.67	1/1641 (0.1%)
7	Bf	0.46	0/1215	0.67	1/1641 (0.1%)
7	Bk	0.46	0/1215	0.67	1/1641 (0.1%)
7	Bp	0.46	0/1215	0.67	1/1641 (0.1%)
7	Bu	0.46	0/1215	0.67	1/1641 (0.1%)
7	Bz	0.46	0/1215	0.67	1/1641 (0.1%)
7	C3	0.46	0/1215	0.66	1/1641 (0.1%)
7	CA	0.46	0/1215	0.66	1/1641 (0.1%)
7	CF	0.46	0/1215	0.66	1/1641 (0.1%)
7	CK	0.46	0/1215	0.66	1/1641 (0.1%)
7	CP	0.46	0/1215	0.66	1/1641 (0.1%)
7	CU	0.46	0/1215	0.66	1/1641 (0.1%)
7	CZ	0.46	0/1215	0.66	1/1641 (0.1%)
7	Ce	0.46	0/1215	0.66	1/1641 (0.1%)
7	Cj	0.46	0/1215	0.66	1/1641 (0.1%)
7	Co	0.46	0/1215	0.66	1/1641 (0.1%)
7	Ct	0.46	0/1215	0.66	1/1641 (0.1%)
7	Cy	0.46	0/1215	0.66	1/1641 (0.1%)
8	C0	0.91	0/1789	1.51	30/2418 (1.2%)
8	C5	0.91	0/1789	1.51	30/2418 (1.2%)
8	CC	0.91	0/1789	1.51	30/2418 (1.2%)
8	CH	0.91	0/1789	1.51	30/2418 (1.2%)
8	CM	0.91	0/1789	1.51	30/2418 (1.2%)
8	CR	0.91	0/1789	1.51	30/2418 (1.2%)
8	CW	0.91	0/1789	1.51	30/2418 (1.2%)
8	Cb	0.91	0/1789	1.51	30/2418 (1.2%)
8	Cg	0.91	0/1789	1.51	30/2418 (1.2%)
8	Cl	0.91	0/1789	1.51	30/2418 (1.2%)
8	Cq	0.91	0/1789	1.51	30/2418 (1.2%)
8	Cv	0.91	0/1789	1.51	30/2418 (1.2%)
9	C1	0.84	0/1786	1.26	17/2412 (0.7%)
9	C6	0.84	0/1786	1.26	17/2412 (0.7%)
9	CD	0.84	0/1786	1.26	17/2412 (0.7%)
9	CI	0.84	0/1786	1.26	17/2412 (0.7%)
9	CN	0.84	0/1786	1.26	17/2412 (0.7%)
9	CS	0.84	0/1786	1.26	17/2412 (0.7%)
9	CX	0.84	0/1786	1.26	17/2412 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	Cc	0.84	0/1786	1.26	17/2412 (0.7%)
9	Ch	0.84	0/1786	1.26	17/2412 (0.7%)
9	Cm	0.84	0/1786	1.26	17/2412 (0.7%)
9	Cr	0.84	0/1786	1.26	17/2412 (0.7%)
9	Cw	0.84	0/1786	1.26	17/2412 (0.7%)
10	C2	0.88	1/1752 (0.1%)	1.77	16/2362 (0.7%)
10	C7	0.88	1/1752 (0.1%)	1.77	15/2362 (0.6%)
10	CE	0.88	1/1752 (0.1%)	1.77	15/2362 (0.6%)
10	CJ	0.88	1/1752 (0.1%)	1.77	16/2362 (0.7%)
10	CO	0.88	1/1752 (0.1%)	1.77	15/2362 (0.6%)
10	CT	0.88	1/1752 (0.1%)	1.77	15/2362 (0.6%)
10	CY	0.88	1/1752 (0.1%)	1.77	16/2362 (0.7%)
10	Cd	0.88	1/1752 (0.1%)	1.77	15/2362 (0.6%)
10	Ci	0.88	1/1752 (0.1%)	1.77	15/2362 (0.6%)
10	Cn	0.88	1/1752 (0.1%)	1.77	16/2362 (0.7%)
10	Cs	0.88	1/1752 (0.1%)	1.77	15/2362 (0.6%)
10	Cx	0.88	1/1752 (0.1%)	1.77	15/2362 (0.6%)
All	All	0.65	24/236268 (0.0%)	1.03	1096/319080 (0.3%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C7	57	LEU	C-N	12.30	1.62	1.34
10	CO	57	LEU	C-N	12.30	1.62	1.34
10	Cd	57	LEU	C-N	12.30	1.62	1.34
10	Cs	57	LEU	C-N	12.30	1.62	1.34
10	C2	57	LEU	C-N	12.29	1.62	1.34
10	CJ	57	LEU	C-N	12.29	1.62	1.34
10	CY	57	LEU	C-N	12.29	1.62	1.34
10	Cn	57	LEU	C-N	12.29	1.62	1.34
10	CE	57	LEU	C-N	12.26	1.62	1.34
10	CT	57	LEU	C-N	12.26	1.62	1.34
10	Ci	57	LEU	C-N	12.26	1.62	1.34
10	Cx	57	LEU	C-N	12.26	1.62	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B0	8	GLU	CG-CD	6.70	1.62	1.51
5	BH	8	GLU	CG-CD	6.70	1.62	1.51
5	BW	8	GLU	CG-CD	6.70	1.62	1.51
5	Bl	8	GLU	CG-CD	6.70	1.62	1.51
5	BC	8	GLU	CG-CD	6.66	1.61	1.51
5	BR	8	GLU	CG-CD	6.66	1.61	1.51
5	Bg	8	GLU	CG-CD	6.66	1.61	1.51
5	Bv	8	GLU	CG-CD	6.66	1.61	1.51
5	B5	8	GLU	CG-CD	6.65	1.61	1.51
5	BM	8	GLU	CG-CD	6.65	1.61	1.51
5	Bb	8	GLU	CG-CD	6.65	1.61	1.51
5	Bq	8	GLU	CG-CD	6.65	1.61	1.51

All (1096) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	CE	57	LEU	O-C-N	-59.80	27.02	122.70
10	CT	57	LEU	O-C-N	-59.80	27.02	122.70
10	Ci	57	LEU	O-C-N	-59.80	27.02	122.70
10	Cx	57	LEU	O-C-N	-59.80	27.02	122.70
10	C7	57	LEU	O-C-N	-59.79	27.03	122.70
10	CO	57	LEU	O-C-N	-59.79	27.03	122.70
10	Cd	57	LEU	O-C-N	-59.79	27.03	122.70
10	Cs	57	LEU	O-C-N	-59.79	27.03	122.70
10	C2	57	LEU	O-C-N	-59.78	27.06	122.70
10	CJ	57	LEU	O-C-N	-59.78	27.06	122.70
10	CY	57	LEU	O-C-N	-59.78	27.06	122.70
10	Cn	57	LEU	O-C-N	-59.78	27.06	122.70
8	C0	190	TYR	CB-CG-CD2	-18.04	110.17	121.00
8	CH	190	TYR	CB-CG-CD2	-18.04	110.17	121.00
8	CW	190	TYR	CB-CG-CD2	-18.04	110.17	121.00
8	Cl	190	TYR	CB-CG-CD2	-18.04	110.17	121.00
8	CC	190	TYR	CB-CG-CD2	-18.04	110.17	121.00
8	CR	190	TYR	CB-CG-CD2	-18.04	110.17	121.00
8	Cg	190	TYR	CB-CG-CD2	-18.04	110.17	121.00
8	Cv	190	TYR	CB-CG-CD2	-18.04	110.17	121.00
8	C5	190	TYR	CB-CG-CD2	-18.02	110.19	121.00
8	CM	190	TYR	CB-CG-CD2	-18.02	110.19	121.00
8	Cb	190	TYR	CB-CG-CD2	-18.02	110.19	121.00
8	Cq	190	TYR	CB-CG-CD2	-18.02	110.19	121.00
3	AF	27	PHE	CB-CG-CD1	14.18	130.73	120.80
3	AU	27	PHE	CB-CG-CD1	14.18	130.73	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Aj	27	PHE	CB-CG-CD1	14.18	130.73	120.80
3	Ay	27	PHE	CB-CG-CD1	14.18	130.73	120.80
3	AA	27	PHE	CB-CG-CD1	14.13	130.69	120.80
3	AP	27	PHE	CB-CG-CD1	14.13	130.69	120.80
3	Ae	27	PHE	CB-CG-CD1	14.13	130.69	120.80
3	At	27	PHE	CB-CG-CD1	14.13	130.69	120.80
3	A3	27	PHE	CB-CG-CD1	14.12	130.68	120.80
3	AK	27	PHE	CB-CG-CD1	14.12	130.68	120.80
3	AZ	27	PHE	CB-CG-CD1	14.12	130.68	120.80
3	Ao	27	PHE	CB-CG-CD1	14.12	130.68	120.80
3	A3	27	PHE	CB-CG-CD2	-13.70	111.21	120.80
3	AK	27	PHE	CB-CG-CD2	-13.70	111.21	120.80
3	AZ	27	PHE	CB-CG-CD2	-13.70	111.21	120.80
3	Ao	27	PHE	CB-CG-CD2	-13.70	111.21	120.80
3	AF	27	PHE	CB-CG-CD2	-13.68	111.22	120.80
3	AU	27	PHE	CB-CG-CD2	-13.68	111.22	120.80
3	Aj	27	PHE	CB-CG-CD2	-13.68	111.22	120.80
3	Ay	27	PHE	CB-CG-CD2	-13.68	111.22	120.80
3	AA	27	PHE	CB-CG-CD2	-13.65	111.25	120.80
3	AP	27	PHE	CB-CG-CD2	-13.65	111.25	120.80
3	Ae	27	PHE	CB-CG-CD2	-13.65	111.25	120.80
3	At	27	PHE	CB-CG-CD2	-13.65	111.25	120.80
8	C0	190	TYR	CB-CG-CD1	12.34	128.40	121.00
8	CH	190	TYR	CB-CG-CD1	12.34	128.40	121.00
8	CW	190	TYR	CB-CG-CD1	12.34	128.40	121.00
8	Cl	190	TYR	CB-CG-CD1	12.34	128.40	121.00
8	CC	190	TYR	CB-CG-CD1	12.32	128.39	121.00
8	CR	190	TYR	CB-CG-CD1	12.32	128.39	121.00
8	Cg	190	TYR	CB-CG-CD1	12.32	128.39	121.00
8	Cv	190	TYR	CB-CG-CD1	12.32	128.39	121.00
8	C5	190	TYR	CB-CG-CD1	12.27	128.36	121.00
8	CM	190	TYR	CB-CG-CD1	12.27	128.36	121.00
8	Cb	190	TYR	CB-CG-CD1	12.27	128.36	121.00
8	Cq	190	TYR	CB-CG-CD1	12.27	128.36	121.00
8	CC	225	TYR	CB-CG-CD1	-12.04	113.78	121.00
8	CR	225	TYR	CB-CG-CD1	-12.04	113.78	121.00
8	Cg	225	TYR	CB-CG-CD1	-12.04	113.78	121.00
8	Cv	225	TYR	CB-CG-CD1	-12.04	113.78	121.00
8	C0	225	TYR	CB-CG-CD1	-12.00	113.80	121.00
8	CH	225	TYR	CB-CG-CD1	-12.00	113.80	121.00
8	CW	225	TYR	CB-CG-CD1	-12.00	113.80	121.00
8	Cl	225	TYR	CB-CG-CD1	-12.00	113.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C5	225	TYR	CB-CG-CD1	-11.98	113.81	121.00
8	CM	225	TYR	CB-CG-CD1	-11.98	113.81	121.00
8	Cb	225	TYR	CB-CG-CD1	-11.98	113.81	121.00
8	Cq	225	TYR	CB-CG-CD1	-11.98	113.81	121.00
3	A2	27	PHE	CB-CG-CD2	-11.37	112.84	120.80
3	AJ	27	PHE	CB-CG-CD2	-11.37	112.84	120.80
3	AY	27	PHE	CB-CG-CD2	-11.37	112.84	120.80
3	An	27	PHE	CB-CG-CD2	-11.37	112.84	120.80
3	AE	27	PHE	CB-CG-CD2	-11.33	112.87	120.80
3	AT	27	PHE	CB-CG-CD2	-11.33	112.87	120.80
3	Ai	27	PHE	CB-CG-CD2	-11.33	112.87	120.80
3	Ax	27	PHE	CB-CG-CD2	-11.33	112.87	120.80
3	A7	27	PHE	CB-CG-CD2	-11.32	112.88	120.80
3	AO	27	PHE	CB-CG-CD2	-11.32	112.88	120.80
3	Ad	27	PHE	CB-CG-CD2	-11.32	112.88	120.80
3	As	27	PHE	CB-CG-CD2	-11.32	112.88	120.80
8	CC	41	ASP	CB-CG-OD2	-10.77	108.61	118.30
8	CR	41	ASP	CB-CG-OD2	-10.77	108.61	118.30
8	Cg	41	ASP	CB-CG-OD2	-10.77	108.61	118.30
8	Cv	41	ASP	CB-CG-OD2	-10.77	108.61	118.30
8	C5	41	ASP	CB-CG-OD2	-10.74	108.63	118.30
8	CM	41	ASP	CB-CG-OD2	-10.74	108.63	118.30
8	Cb	41	ASP	CB-CG-OD2	-10.74	108.63	118.30
8	Cq	41	ASP	CB-CG-OD2	-10.74	108.63	118.30
8	C0	41	ASP	CB-CG-OD2	-10.70	108.67	118.30
8	CH	41	ASP	CB-CG-OD2	-10.70	108.67	118.30
8	CW	41	ASP	CB-CG-OD2	-10.70	108.67	118.30
8	Cl	41	ASP	CB-CG-OD2	-10.70	108.67	118.30
8	C5	156	ASP	CB-CG-OD1	10.61	127.85	118.30
8	CM	156	ASP	CB-CG-OD1	10.61	127.85	118.30
8	Cb	156	ASP	CB-CG-OD1	10.61	127.85	118.30
8	Cq	156	ASP	CB-CG-OD1	10.61	127.85	118.30
8	CC	156	ASP	CB-CG-OD1	10.60	127.84	118.30
8	CR	156	ASP	CB-CG-OD1	10.60	127.84	118.30
8	Cg	156	ASP	CB-CG-OD1	10.60	127.84	118.30
8	Cv	156	ASP	CB-CG-OD1	10.60	127.84	118.30
8	C0	156	ASP	CB-CG-OD1	10.60	127.84	118.30
8	CH	156	ASP	CB-CG-OD1	10.60	127.84	118.30
8	CW	156	ASP	CB-CG-OD1	10.60	127.84	118.30
8	Cl	156	ASP	CB-CG-OD1	10.60	127.84	118.30
8	C5	140	PHE	CB-CG-CD2	-10.50	113.45	120.80
8	CM	140	PHE	CB-CG-CD2	-10.50	113.45	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	Cb	140	PHE	CB-CG-CD2	-10.50	113.45	120.80
8	Cq	140	PHE	CB-CG-CD2	-10.50	113.45	120.80
8	C0	140	PHE	CB-CG-CD2	-10.50	113.45	120.80
8	CH	140	PHE	CB-CG-CD2	-10.50	113.45	120.80
8	CW	140	PHE	CB-CG-CD2	-10.50	113.45	120.80
8	Cl	140	PHE	CB-CG-CD2	-10.50	113.45	120.80
8	CC	140	PHE	CB-CG-CD2	-10.46	113.47	120.80
8	CR	140	PHE	CB-CG-CD2	-10.46	113.47	120.80
8	Cg	140	PHE	CB-CG-CD2	-10.46	113.47	120.80
8	Cv	140	PHE	CB-CG-CD2	-10.46	113.47	120.80
3	A7	27	PHE	CB-CG-CD1	10.43	128.10	120.80
3	AO	27	PHE	CB-CG-CD1	10.43	128.10	120.80
3	Ad	27	PHE	CB-CG-CD1	10.43	128.10	120.80
3	As	27	PHE	CB-CG-CD1	10.43	128.10	120.80
3	A2	27	PHE	CB-CG-CD1	10.40	128.08	120.80
3	AJ	27	PHE	CB-CG-CD1	10.40	128.08	120.80
3	AY	27	PHE	CB-CG-CD1	10.40	128.08	120.80
3	An	27	PHE	CB-CG-CD1	10.40	128.08	120.80
3	AE	27	PHE	CB-CG-CD1	10.36	128.05	120.80
3	AT	27	PHE	CB-CG-CD1	10.36	128.05	120.80
3	Ai	27	PHE	CB-CG-CD1	10.36	128.05	120.80
3	Ax	27	PHE	CB-CG-CD1	10.36	128.05	120.80
10	CE	195	TYR	CB-CG-CD1	-9.70	115.18	121.00
10	CT	195	TYR	CB-CG-CD1	-9.70	115.18	121.00
10	Ci	195	TYR	CB-CG-CD1	-9.70	115.18	121.00
10	Cx	195	TYR	CB-CG-CD1	-9.70	115.18	121.00
10	C7	195	TYR	CB-CG-CD1	-9.69	115.19	121.00
10	CO	195	TYR	CB-CG-CD1	-9.69	115.19	121.00
10	Cd	195	TYR	CB-CG-CD1	-9.69	115.19	121.00
10	Cs	195	TYR	CB-CG-CD1	-9.69	115.19	121.00
10	C2	195	TYR	CB-CG-CD1	-9.67	115.20	121.00
10	CJ	195	TYR	CB-CG-CD1	-9.67	115.20	121.00
10	CY	195	TYR	CB-CG-CD1	-9.67	115.20	121.00
10	Cn	195	TYR	CB-CG-CD1	-9.67	115.20	121.00
10	CE	81	PHE	CB-CG-CD2	-9.41	114.21	120.80
10	CT	81	PHE	CB-CG-CD2	-9.41	114.21	120.80
10	Ci	81	PHE	CB-CG-CD2	-9.41	114.21	120.80
10	Cx	81	PHE	CB-CG-CD2	-9.41	114.21	120.80
10	C7	81	PHE	CB-CG-CD2	-9.37	114.24	120.80
10	CO	81	PHE	CB-CG-CD2	-9.37	114.24	120.80
10	Cd	81	PHE	CB-CG-CD2	-9.37	114.24	120.80
10	Cs	81	PHE	CB-CG-CD2	-9.37	114.24	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C2	81	PHE	CB-CG-CD2	-9.37	114.24	120.80
10	CJ	81	PHE	CB-CG-CD2	-9.37	114.24	120.80
10	CY	81	PHE	CB-CG-CD2	-9.37	114.24	120.80
10	Cn	81	PHE	CB-CG-CD2	-9.37	114.24	120.80
8	C5	201	ASP	CB-CA-C	-9.29	91.81	110.40
8	CM	201	ASP	CB-CA-C	-9.29	91.81	110.40
8	Cb	201	ASP	CB-CA-C	-9.29	91.81	110.40
8	Cq	201	ASP	CB-CA-C	-9.29	91.81	110.40
8	CC	201	ASP	CB-CA-C	-9.28	91.84	110.40
8	CR	201	ASP	CB-CA-C	-9.28	91.84	110.40
8	Cg	201	ASP	CB-CA-C	-9.28	91.84	110.40
8	Cv	201	ASP	CB-CA-C	-9.28	91.84	110.40
8	C0	201	ASP	CB-CA-C	-9.27	91.85	110.40
8	CH	201	ASP	CB-CA-C	-9.27	91.85	110.40
8	CW	201	ASP	CB-CA-C	-9.27	91.85	110.40
8	Cl	201	ASP	CB-CA-C	-9.27	91.85	110.40
1	A0	150	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	AH	150	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	AW	150	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	Al	150	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	AC	150	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	AR	150	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	Ag	150	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	Av	150	ARG	NE-CZ-NH2	-8.90	115.85	120.30
8	CC	41	ASP	CB-CG-OD1	8.88	126.30	118.30
8	CR	41	ASP	CB-CG-OD1	8.88	126.30	118.30
8	Cg	41	ASP	CB-CG-OD1	8.88	126.30	118.30
8	Cv	41	ASP	CB-CG-OD1	8.88	126.30	118.30
1	A5	150	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	AM	150	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	Ab	150	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	Aq	150	ARG	NE-CZ-NH2	-8.86	115.87	120.30
8	C5	41	ASP	CB-CG-OD1	8.86	126.27	118.30
8	CM	41	ASP	CB-CG-OD1	8.86	126.27	118.30
8	Cb	41	ASP	CB-CG-OD1	8.86	126.27	118.30
8	Cq	41	ASP	CB-CG-OD1	8.86	126.27	118.30
4	BE	99	ARG	NE-CZ-NH2	-8.82	115.89	120.30
4	BT	99	ARG	NE-CZ-NH2	-8.82	115.89	120.30
4	Bi	99	ARG	NE-CZ-NH2	-8.82	115.89	120.30
4	Bx	99	ARG	NE-CZ-NH2	-8.82	115.89	120.30
8	C0	41	ASP	CB-CG-OD1	8.81	126.23	118.30
8	CH	41	ASP	CB-CG-OD1	8.81	126.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	CW	41	ASP	CB-CG-OD1	8.81	126.23	118.30
8	Cl	41	ASP	CB-CG-OD1	8.81	126.23	118.30
4	B7	99	ARG	NE-CZ-NH2	-8.79	115.90	120.30
4	BO	99	ARG	NE-CZ-NH2	-8.79	115.90	120.30
4	Bd	99	ARG	NE-CZ-NH2	-8.79	115.90	120.30
4	Bs	99	ARG	NE-CZ-NH2	-8.79	115.90	120.30
4	B2	99	ARG	NE-CZ-NH2	-8.76	115.92	120.30
4	BJ	99	ARG	NE-CZ-NH2	-8.76	115.92	120.30
4	BY	99	ARG	NE-CZ-NH2	-8.76	115.92	120.30
4	Bn	99	ARG	NE-CZ-NH2	-8.76	115.92	120.30
4	B2	101	ILE	CB-CA-C	-8.70	94.20	111.60
4	BJ	101	ILE	CB-CA-C	-8.70	94.20	111.60
4	BY	101	ILE	CB-CA-C	-8.70	94.20	111.60
4	Bn	101	ILE	CB-CA-C	-8.70	94.20	111.60
4	B7	101	ILE	CB-CA-C	-8.70	94.20	111.60
4	BO	101	ILE	CB-CA-C	-8.70	94.20	111.60
4	Bd	101	ILE	CB-CA-C	-8.70	94.20	111.60
4	Bs	101	ILE	CB-CA-C	-8.70	94.20	111.60
4	BE	101	ILE	CB-CA-C	-8.70	94.21	111.60
4	BT	101	ILE	CB-CA-C	-8.70	94.21	111.60
4	Bi	101	ILE	CB-CA-C	-8.70	94.21	111.60
4	Bx	101	ILE	CB-CA-C	-8.70	94.21	111.60
10	C7	197	PHE	CA-CB-CG	-8.69	93.04	113.90
10	CO	197	PHE	CA-CB-CG	-8.69	93.04	113.90
10	Cd	197	PHE	CA-CB-CG	-8.69	93.04	113.90
10	Cs	197	PHE	CA-CB-CG	-8.69	93.04	113.90
10	CE	197	PHE	CA-CB-CG	-8.68	93.07	113.90
10	CT	197	PHE	CA-CB-CG	-8.68	93.07	113.90
10	Ci	197	PHE	CA-CB-CG	-8.68	93.07	113.90
10	Cx	197	PHE	CA-CB-CG	-8.68	93.07	113.90
10	C2	197	PHE	CA-CB-CG	-8.67	93.09	113.90
10	CJ	197	PHE	CA-CB-CG	-8.67	93.09	113.90
10	CY	197	PHE	CA-CB-CG	-8.67	93.09	113.90
10	Cn	197	PHE	CA-CB-CG	-8.67	93.09	113.90
8	C0	156	ASP	CB-CG-OD2	-8.57	110.58	118.30
8	CH	156	ASP	CB-CG-OD2	-8.57	110.58	118.30
8	CW	156	ASP	CB-CG-OD2	-8.57	110.58	118.30
8	Cl	156	ASP	CB-CG-OD2	-8.57	110.58	118.30
8	C5	156	ASP	CB-CG-OD2	-8.57	110.59	118.30
8	CM	156	ASP	CB-CG-OD2	-8.57	110.59	118.30
8	Cb	156	ASP	CB-CG-OD2	-8.57	110.59	118.30
8	Cq	156	ASP	CB-CG-OD2	-8.57	110.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	CC	156	ASP	CB-CG-OD2	-8.57	110.59	118.30
8	CR	156	ASP	CB-CG-OD2	-8.57	110.59	118.30
8	Cg	156	ASP	CB-CG-OD2	-8.57	110.59	118.30
8	Cv	156	ASP	CB-CG-OD2	-8.57	110.59	118.30
8	C0	140	PHE	CB-CG-CD1	8.22	126.56	120.80
8	CH	140	PHE	CB-CG-CD1	8.22	126.56	120.80
8	CW	140	PHE	CB-CG-CD1	8.22	126.56	120.80
8	Cl	140	PHE	CB-CG-CD1	8.22	126.56	120.80
8	C5	140	PHE	CB-CG-CD1	8.19	126.53	120.80
8	CM	140	PHE	CB-CG-CD1	8.19	126.53	120.80
8	Cb	140	PHE	CB-CG-CD1	8.19	126.53	120.80
8	Cq	140	PHE	CB-CG-CD1	8.19	126.53	120.80
8	C0	11	GLN	C-N-CA	8.17	142.12	121.70
8	CC	140	PHE	CB-CG-CD1	8.17	126.52	120.80
8	CH	11	GLN	C-N-CA	8.17	142.12	121.70
8	CR	140	PHE	CB-CG-CD1	8.17	126.52	120.80
8	CW	11	GLN	C-N-CA	8.17	142.12	121.70
8	Cg	140	PHE	CB-CG-CD1	8.17	126.52	120.80
8	Cl	11	GLN	C-N-CA	8.17	142.12	121.70
8	Cv	140	PHE	CB-CG-CD1	8.17	126.52	120.80
8	C5	11	GLN	C-N-CA	8.17	142.11	121.70
8	CM	11	GLN	C-N-CA	8.17	142.11	121.70
8	Cb	11	GLN	C-N-CA	8.17	142.11	121.70
8	Cq	11	GLN	C-N-CA	8.17	142.11	121.70
8	CC	11	GLN	C-N-CA	8.16	142.11	121.70
8	CR	11	GLN	C-N-CA	8.16	142.11	121.70
8	Cg	11	GLN	C-N-CA	8.16	142.11	121.70
8	Cv	11	GLN	C-N-CA	8.16	142.11	121.70
10	CE	195	TYR	CA-CB-CG	-8.13	97.95	113.40
10	CT	195	TYR	CA-CB-CG	-8.13	97.95	113.40
10	Ci	195	TYR	CA-CB-CG	-8.13	97.95	113.40
10	Cx	195	TYR	CA-CB-CG	-8.13	97.95	113.40
10	C7	195	TYR	CA-CB-CG	-8.13	97.95	113.40
10	CO	195	TYR	CA-CB-CG	-8.13	97.95	113.40
10	Cd	195	TYR	CA-CB-CG	-8.13	97.95	113.40
10	Cs	195	TYR	CA-CB-CG	-8.13	97.95	113.40
10	C2	195	TYR	CA-CB-CG	-8.12	97.96	113.40
10	CJ	195	TYR	CA-CB-CG	-8.12	97.96	113.40
10	CY	195	TYR	CA-CB-CG	-8.12	97.96	113.40
10	Cn	195	TYR	CA-CB-CG	-8.12	97.96	113.40
10	C2	57	LEU	C-N-CA	-8.08	101.51	121.70
10	CJ	57	LEU	C-N-CA	-8.08	101.51	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	CY	57	LEU	C-N-CA	-8.08	101.51	121.70
10	Cn	57	LEU	C-N-CA	-8.08	101.51	121.70
10	C7	57	LEU	C-N-CA	-8.07	101.51	121.70
10	CO	57	LEU	C-N-CA	-8.07	101.51	121.70
10	Cd	57	LEU	C-N-CA	-8.07	101.51	121.70
10	Cs	57	LEU	C-N-CA	-8.07	101.51	121.70
10	CE	57	LEU	C-N-CA	-8.06	101.54	121.70
10	CT	57	LEU	C-N-CA	-8.06	101.54	121.70
10	Ci	57	LEU	C-N-CA	-8.06	101.54	121.70
10	Cx	57	LEU	C-N-CA	-8.06	101.54	121.70
6	BD	27	PHE	CA-CB-CG	-7.99	94.72	113.90
6	BS	27	PHE	CA-CB-CG	-7.99	94.72	113.90
6	Bh	27	PHE	CA-CB-CG	-7.99	94.72	113.90
6	Bw	27	PHE	CA-CB-CG	-7.99	94.72	113.90
6	B1	27	PHE	CA-CB-CG	-7.99	94.73	113.90
6	B6	27	PHE	CA-CB-CG	-7.99	94.73	113.90
6	BI	27	PHE	CA-CB-CG	-7.99	94.73	113.90
6	BN	27	PHE	CA-CB-CG	-7.99	94.73	113.90
6	BX	27	PHE	CA-CB-CG	-7.99	94.73	113.90
6	Bc	27	PHE	CA-CB-CG	-7.99	94.73	113.90
6	Bm	27	PHE	CA-CB-CG	-7.99	94.73	113.90
6	Br	27	PHE	CA-CB-CG	-7.99	94.73	113.90
9	C1	197	PHE	CB-CG-CD2	-7.92	115.25	120.80
9	CI	197	PHE	CB-CG-CD2	-7.92	115.25	120.80
9	CX	197	PHE	CB-CG-CD2	-7.92	115.25	120.80
9	Cm	197	PHE	CB-CG-CD2	-7.92	115.25	120.80
9	CD	197	PHE	CB-CG-CD2	-7.92	115.25	120.80
9	CS	197	PHE	CB-CG-CD2	-7.92	115.25	120.80
9	Ch	197	PHE	CB-CG-CD2	-7.92	115.25	120.80
9	Cw	197	PHE	CB-CG-CD2	-7.92	115.25	120.80
9	C6	197	PHE	CB-CG-CD2	-7.90	115.27	120.80
9	CN	197	PHE	CB-CG-CD2	-7.90	115.27	120.80
9	Cc	197	PHE	CB-CG-CD2	-7.90	115.27	120.80
9	Cr	197	PHE	CB-CG-CD2	-7.90	115.27	120.80
6	BD	149	ASP	CB-CA-C	-7.72	94.96	110.40
6	BS	149	ASP	CB-CA-C	-7.72	94.96	110.40
6	Bh	149	ASP	CB-CA-C	-7.72	94.96	110.40
6	Bw	149	ASP	CB-CA-C	-7.72	94.96	110.40
6	B1	149	ASP	CB-CA-C	-7.72	94.96	110.40
6	BI	149	ASP	CB-CA-C	-7.72	94.96	110.40
6	BX	149	ASP	CB-CA-C	-7.72	94.96	110.40
6	Bm	149	ASP	CB-CA-C	-7.72	94.96	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B6	149	ASP	CB-CA-C	-7.71	94.97	110.40
6	BN	149	ASP	CB-CA-C	-7.71	94.97	110.40
6	Bc	149	ASP	CB-CA-C	-7.71	94.97	110.40
6	Br	149	ASP	CB-CA-C	-7.71	94.97	110.40
3	A7	27	PHE	CB-CA-C	-7.35	95.70	110.40
3	AO	27	PHE	CB-CA-C	-7.35	95.70	110.40
3	Ad	27	PHE	CB-CA-C	-7.35	95.70	110.40
3	As	27	PHE	CB-CA-C	-7.35	95.70	110.40
3	AE	27	PHE	CB-CA-C	-7.33	95.73	110.40
3	AT	27	PHE	CB-CA-C	-7.33	95.73	110.40
3	Ai	27	PHE	CB-CA-C	-7.33	95.73	110.40
3	Ax	27	PHE	CB-CA-C	-7.33	95.73	110.40
3	A2	27	PHE	CB-CA-C	-7.32	95.76	110.40
3	AJ	27	PHE	CB-CA-C	-7.32	95.76	110.40
3	AY	27	PHE	CB-CA-C	-7.32	95.76	110.40
3	An	27	PHE	CB-CA-C	-7.32	95.76	110.40
8	C5	156	ASP	CB-CA-C	-7.28	95.83	110.40
8	CM	156	ASP	CB-CA-C	-7.28	95.83	110.40
8	Cb	156	ASP	CB-CA-C	-7.28	95.83	110.40
8	Cq	156	ASP	CB-CA-C	-7.28	95.83	110.40
10	C7	57	LEU	CA-C-N	-7.28	101.18	117.20
8	CC	156	ASP	CB-CA-C	-7.28	95.84	110.40
10	CO	57	LEU	CA-C-N	-7.28	101.18	117.20
8	CR	156	ASP	CB-CA-C	-7.28	95.84	110.40
10	Cd	57	LEU	CA-C-N	-7.28	101.18	117.20
8	Cg	156	ASP	CB-CA-C	-7.28	95.84	110.40
10	Cs	57	LEU	CA-C-N	-7.28	101.18	117.20
8	Cv	156	ASP	CB-CA-C	-7.28	95.84	110.40
8	C0	156	ASP	CB-CA-C	-7.27	95.86	110.40
8	CH	156	ASP	CB-CA-C	-7.27	95.86	110.40
8	CW	156	ASP	CB-CA-C	-7.27	95.86	110.40
8	Cl	156	ASP	CB-CA-C	-7.27	95.86	110.40
10	C2	57	LEU	CA-C-N	-7.26	101.22	117.20
10	CJ	57	LEU	CA-C-N	-7.26	101.22	117.20
10	CY	57	LEU	CA-C-N	-7.26	101.22	117.20
10	Cn	57	LEU	CA-C-N	-7.26	101.22	117.20
10	CE	57	LEU	CA-C-N	-7.26	101.24	117.20
10	CT	57	LEU	CA-C-N	-7.26	101.24	117.20
10	Ci	57	LEU	CA-C-N	-7.26	101.24	117.20
10	Cx	57	LEU	CA-C-N	-7.26	101.24	117.20
3	A7	5	ASP	C-N-CA	-7.13	103.88	121.70
3	AO	5	ASP	C-N-CA	-7.13	103.88	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Ad	5	ASP	C-N-CA	-7.13	103.88	121.70
3	As	5	ASP	C-N-CA	-7.13	103.88	121.70
3	A2	5	ASP	C-N-CA	-7.12	103.90	121.70
3	AJ	5	ASP	C-N-CA	-7.12	103.90	121.70
3	AY	5	ASP	C-N-CA	-7.12	103.90	121.70
3	An	5	ASP	C-N-CA	-7.12	103.90	121.70
3	AE	5	ASP	C-N-CA	-7.11	103.92	121.70
3	AT	5	ASP	C-N-CA	-7.11	103.92	121.70
3	Ai	5	ASP	C-N-CA	-7.11	103.92	121.70
3	Ax	5	ASP	C-N-CA	-7.11	103.92	121.70
10	C2	137	PHE	CB-CG-CD2	-7.08	115.84	120.80
10	CJ	137	PHE	CB-CG-CD2	-7.08	115.84	120.80
10	CY	137	PHE	CB-CG-CD2	-7.08	115.84	120.80
10	Cn	137	PHE	CB-CG-CD2	-7.08	115.84	120.80
10	C7	137	PHE	CB-CG-CD2	-7.04	115.87	120.80
10	CO	137	PHE	CB-CG-CD2	-7.04	115.87	120.80
10	Cd	137	PHE	CB-CG-CD2	-7.04	115.87	120.80
10	Cs	137	PHE	CB-CG-CD2	-7.04	115.87	120.80
10	CE	137	PHE	CB-CG-CD2	-7.02	115.89	120.80
10	CT	137	PHE	CB-CG-CD2	-7.02	115.89	120.80
10	Ci	137	PHE	CB-CG-CD2	-7.02	115.89	120.80
10	Cx	137	PHE	CB-CG-CD2	-7.02	115.89	120.80
10	CE	170	SER	CA-C-N	-7.00	101.80	117.20
10	CT	170	SER	CA-C-N	-7.00	101.80	117.20
10	Ci	170	SER	CA-C-N	-7.00	101.80	117.20
10	Cx	170	SER	CA-C-N	-7.00	101.80	117.20
10	C2	170	SER	CA-C-N	-6.99	101.83	117.20
10	CJ	170	SER	CA-C-N	-6.99	101.83	117.20
10	CY	170	SER	CA-C-N	-6.99	101.83	117.20
10	Cn	170	SER	CA-C-N	-6.99	101.83	117.20
10	C7	170	SER	CA-C-N	-6.98	101.83	117.20
10	CO	170	SER	CA-C-N	-6.98	101.83	117.20
10	Cd	170	SER	CA-C-N	-6.98	101.83	117.20
10	Cs	170	SER	CA-C-N	-6.98	101.83	117.20
8	C0	12	TYR	N-CA-CB	-6.96	98.07	110.60
8	CH	12	TYR	N-CA-CB	-6.96	98.07	110.60
8	CW	12	TYR	N-CA-CB	-6.96	98.07	110.60
8	Cl	12	TYR	N-CA-CB	-6.96	98.07	110.60
8	C5	12	TYR	N-CA-CB	-6.95	98.09	110.60
8	CM	12	TYR	N-CA-CB	-6.95	98.09	110.60
8	Cb	12	TYR	N-CA-CB	-6.95	98.09	110.60
8	Cq	12	TYR	N-CA-CB	-6.95	98.09	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	CC	12	TYR	N-CA-CB	-6.95	98.09	110.60
8	CR	12	TYR	N-CA-CB	-6.95	98.09	110.60
8	Cg	12	TYR	N-CA-CB	-6.95	98.09	110.60
8	Cv	12	TYR	N-CA-CB	-6.95	98.09	110.60
2	AD	105	ASN	CB-CA-C	-6.84	96.71	110.40
2	AS	105	ASN	CB-CA-C	-6.84	96.71	110.40
2	Ah	105	ASN	CB-CA-C	-6.84	96.71	110.40
2	Aw	105	ASN	CB-CA-C	-6.84	96.71	110.40
2	A1	105	ASN	CB-CA-C	-6.83	96.73	110.40
2	AI	105	ASN	CB-CA-C	-6.83	96.73	110.40
2	AX	105	ASN	CB-CA-C	-6.83	96.73	110.40
2	Am	105	ASN	CB-CA-C	-6.83	96.73	110.40
2	A6	105	ASN	CB-CA-C	-6.83	96.75	110.40
2	AN	105	ASN	CB-CA-C	-6.83	96.75	110.40
2	Ac	105	ASN	CB-CA-C	-6.83	96.75	110.40
2	Ar	105	ASN	CB-CA-C	-6.83	96.75	110.40
8	C0	190	TYR	CB-CA-C	-6.76	96.88	110.40
8	CH	190	TYR	CB-CA-C	-6.76	96.88	110.40
8	CW	190	TYR	CB-CA-C	-6.76	96.88	110.40
8	Cl	190	TYR	CB-CA-C	-6.76	96.88	110.40
8	CC	225	TYR	CB-CG-CD2	6.76	125.05	121.00
8	CR	225	TYR	CB-CG-CD2	6.76	125.05	121.00
8	Cg	225	TYR	CB-CG-CD2	6.76	125.05	121.00
8	Cv	225	TYR	CB-CG-CD2	6.76	125.05	121.00
8	C5	190	TYR	CB-CA-C	-6.75	96.91	110.40
8	CM	190	TYR	CB-CA-C	-6.75	96.91	110.40
8	Cb	190	TYR	CB-CA-C	-6.75	96.91	110.40
8	Cq	190	TYR	CB-CA-C	-6.75	96.91	110.40
8	CC	190	TYR	CB-CA-C	-6.74	96.92	110.40
8	CR	190	TYR	CB-CA-C	-6.74	96.92	110.40
8	Cg	190	TYR	CB-CA-C	-6.74	96.92	110.40
8	Cv	190	TYR	CB-CA-C	-6.74	96.92	110.40
8	C0	225	TYR	CB-CG-CD2	6.69	125.01	121.00
8	CH	225	TYR	CB-CG-CD2	6.69	125.01	121.00
8	CW	225	TYR	CB-CG-CD2	6.69	125.01	121.00
8	Cl	225	TYR	CB-CG-CD2	6.69	125.01	121.00
8	C5	225	TYR	CB-CG-CD2	6.66	125.00	121.00
8	CM	225	TYR	CB-CG-CD2	6.66	125.00	121.00
8	Cb	225	TYR	CB-CG-CD2	6.66	125.00	121.00
8	Cq	225	TYR	CB-CG-CD2	6.66	125.00	121.00
4	BF	100	LYS	CA-CB-CG	6.63	127.99	113.40
4	BU	100	LYS	CA-CB-CG	6.63	127.99	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Bj	100	LYS	CA-CB-CG	6.63	127.99	113.40
4	By	100	LYS	CA-CB-CG	6.63	127.99	113.40
8	C5	140	PHE	N-CA-CB	6.63	122.53	110.60
8	CM	140	PHE	N-CA-CB	6.63	122.53	110.60
8	Cb	140	PHE	N-CA-CB	6.63	122.53	110.60
8	Cq	140	PHE	N-CA-CB	6.63	122.53	110.60
8	C0	140	PHE	N-CA-CB	6.63	122.53	110.60
8	CH	140	PHE	N-CA-CB	6.63	122.53	110.60
8	CW	140	PHE	N-CA-CB	6.63	122.53	110.60
8	Cl	140	PHE	N-CA-CB	6.63	122.53	110.60
4	B3	100	LYS	CA-CB-CG	6.62	127.96	113.40
4	BA	100	LYS	CA-CB-CG	6.62	127.96	113.40
4	BK	100	LYS	CA-CB-CG	6.62	127.96	113.40
4	BP	100	LYS	CA-CB-CG	6.62	127.96	113.40
4	BZ	100	LYS	CA-CB-CG	6.62	127.96	113.40
4	Be	100	LYS	CA-CB-CG	6.62	127.96	113.40
4	Bo	100	LYS	CA-CB-CG	6.62	127.96	113.40
4	Bt	100	LYS	CA-CB-CG	6.62	127.96	113.40
8	CC	140	PHE	N-CA-CB	6.60	122.48	110.60
8	CR	140	PHE	N-CA-CB	6.60	122.48	110.60
8	Cg	140	PHE	N-CA-CB	6.60	122.48	110.60
8	Cv	140	PHE	N-CA-CB	6.60	122.48	110.60
8	C5	75	GLU	CB-CG-CD	-6.50	96.66	114.20
8	CM	75	GLU	CB-CG-CD	-6.50	96.66	114.20
8	Cb	75	GLU	CB-CG-CD	-6.50	96.66	114.20
8	Cq	75	GLU	CB-CG-CD	-6.50	96.66	114.20
8	C0	75	GLU	CB-CG-CD	-6.48	96.69	114.20
8	CH	75	GLU	CB-CG-CD	-6.48	96.69	114.20
8	CW	75	GLU	CB-CG-CD	-6.48	96.69	114.20
8	Cl	75	GLU	CB-CG-CD	-6.48	96.69	114.20
8	CC	75	GLU	CB-CG-CD	-6.47	96.73	114.20
8	CR	75	GLU	CB-CG-CD	-6.47	96.73	114.20
8	Cg	75	GLU	CB-CG-CD	-6.47	96.73	114.20
8	Cv	75	GLU	CB-CG-CD	-6.47	96.73	114.20
9	C6	140	PHE	CB-CA-C	-6.39	97.62	110.40
9	CN	140	PHE	CB-CA-C	-6.39	97.62	110.40
9	Cc	140	PHE	CB-CA-C	-6.39	97.62	110.40
9	Cr	140	PHE	CB-CA-C	-6.39	97.62	110.40
9	C1	140	PHE	CB-CA-C	-6.38	97.64	110.40
9	CD	140	PHE	CB-CA-C	-6.38	97.64	110.40
9	CI	140	PHE	CB-CA-C	-6.38	97.64	110.40
9	CS	140	PHE	CB-CA-C	-6.38	97.64	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CX	140	PHE	CB-CA-C	-6.38	97.64	110.40
9	Ch	140	PHE	CB-CA-C	-6.38	97.64	110.40
9	Cm	140	PHE	CB-CA-C	-6.38	97.64	110.40
9	Cw	140	PHE	CB-CA-C	-6.38	97.64	110.40
10	CE	195	TYR	CB-CA-C	-6.34	97.72	110.40
10	CT	195	TYR	CB-CA-C	-6.34	97.72	110.40
10	Ci	195	TYR	CB-CA-C	-6.34	97.72	110.40
10	Cx	195	TYR	CB-CA-C	-6.34	97.72	110.40
10	C2	195	TYR	CB-CA-C	-6.33	97.73	110.40
10	C7	195	TYR	CB-CA-C	-6.33	97.73	110.40
10	CJ	195	TYR	CB-CA-C	-6.33	97.73	110.40
10	CO	195	TYR	CB-CA-C	-6.33	97.73	110.40
10	CY	195	TYR	CB-CA-C	-6.33	97.73	110.40
10	Cd	195	TYR	CB-CA-C	-6.33	97.73	110.40
10	Cn	195	TYR	CB-CA-C	-6.33	97.73	110.40
10	Cs	195	TYR	CB-CA-C	-6.33	97.73	110.40
8	C0	225	TYR	CA-CB-CG	-6.28	101.47	113.40
8	CH	225	TYR	CA-CB-CG	-6.28	101.47	113.40
8	CW	225	TYR	CA-CB-CG	-6.28	101.47	113.40
8	Cl	225	TYR	CA-CB-CG	-6.28	101.47	113.40
9	C6	199	ARG	NE-CZ-NH2	-6.26	117.17	120.30
8	CC	225	TYR	CA-CB-CG	-6.26	101.50	113.40
9	CN	199	ARG	NE-CZ-NH2	-6.26	117.17	120.30
8	CR	225	TYR	CA-CB-CG	-6.26	101.50	113.40
9	Cc	199	ARG	NE-CZ-NH2	-6.26	117.17	120.30
8	Cg	225	TYR	CA-CB-CG	-6.26	101.50	113.40
9	Cr	199	ARG	NE-CZ-NH2	-6.26	117.17	120.30
8	Cv	225	TYR	CA-CB-CG	-6.26	101.50	113.40
8	C5	225	TYR	CA-CB-CG	-6.26	101.50	113.40
8	CM	225	TYR	CA-CB-CG	-6.26	101.50	113.40
8	Cb	225	TYR	CA-CB-CG	-6.26	101.50	113.40
8	Cq	225	TYR	CA-CB-CG	-6.26	101.50	113.40
9	CD	196	SER	C-N-CA	6.24	137.31	121.70
9	CS	196	SER	C-N-CA	6.24	137.31	121.70
9	Ch	196	SER	C-N-CA	6.24	137.31	121.70
9	Cw	196	SER	C-N-CA	6.24	137.31	121.70
9	C1	199	ARG	NE-CZ-NH2	-6.24	117.18	120.30
9	CI	199	ARG	NE-CZ-NH2	-6.24	117.18	120.30
9	CX	199	ARG	NE-CZ-NH2	-6.24	117.18	120.30
9	Cm	199	ARG	NE-CZ-NH2	-6.24	117.18	120.30
9	C6	196	SER	C-N-CA	6.22	137.26	121.70
9	CN	196	SER	C-N-CA	6.22	137.26	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Cc	196	SER	C-N-CA	6.22	137.26	121.70
9	Cr	196	SER	C-N-CA	6.22	137.26	121.70
8	C0	186	GLN	C-N-CA	6.22	137.25	121.70
8	C0	225	TYR	N-CA-CB	6.22	121.80	110.60
8	CH	186	GLN	C-N-CA	6.22	137.25	121.70
8	CH	225	TYR	N-CA-CB	6.22	121.80	110.60
8	CW	186	GLN	C-N-CA	6.22	137.25	121.70
8	CW	225	TYR	N-CA-CB	6.22	121.80	110.60
8	Cl	186	GLN	C-N-CA	6.22	137.25	121.70
8	Cl	225	TYR	N-CA-CB	6.22	121.80	110.60
9	C1	196	SER	C-N-CA	6.22	137.25	121.70
9	CI	196	SER	C-N-CA	6.22	137.25	121.70
9	CX	196	SER	C-N-CA	6.22	137.25	121.70
9	Cm	196	SER	C-N-CA	6.22	137.25	121.70
8	CC	186	GLN	C-N-CA	6.22	137.25	121.70
8	CR	186	GLN	C-N-CA	6.22	137.25	121.70
8	Cg	186	GLN	C-N-CA	6.22	137.25	121.70
8	Cv	186	GLN	C-N-CA	6.22	137.25	121.70
8	C5	186	GLN	C-N-CA	6.21	137.22	121.70
8	CC	225	TYR	N-CA-CB	6.21	121.77	110.60
8	CM	186	GLN	C-N-CA	6.21	137.22	121.70
8	CR	225	TYR	N-CA-CB	6.21	121.77	110.60
8	Cb	186	GLN	C-N-CA	6.21	137.22	121.70
8	Cg	225	TYR	N-CA-CB	6.21	121.77	110.60
8	Cq	186	GLN	C-N-CA	6.21	137.22	121.70
8	Cv	225	TYR	N-CA-CB	6.21	121.77	110.60
8	C0	146	TRP	N-CA-C	-6.20	94.26	111.00
8	CC	146	TRP	N-CA-C	-6.20	94.26	111.00
8	CH	146	TRP	N-CA-C	-6.20	94.26	111.00
8	CR	146	TRP	N-CA-C	-6.20	94.26	111.00
8	CW	146	TRP	N-CA-C	-6.20	94.26	111.00
8	Cg	146	TRP	N-CA-C	-6.20	94.26	111.00
8	Cl	146	TRP	N-CA-C	-6.20	94.26	111.00
8	Cv	146	TRP	N-CA-C	-6.20	94.26	111.00
9	C1	144	ARG	CB-CA-C	-6.20	98.00	110.40
9	CI	144	ARG	CB-CA-C	-6.20	98.00	110.40
9	CX	144	ARG	CB-CA-C	-6.20	98.00	110.40
9	Cm	144	ARG	CB-CA-C	-6.20	98.00	110.40
8	C5	225	TYR	N-CA-CB	6.20	121.75	110.60
8	CM	225	TYR	N-CA-CB	6.20	121.75	110.60
8	Cb	225	TYR	N-CA-CB	6.20	121.75	110.60
8	Cq	225	TYR	N-CA-CB	6.20	121.75	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C6	144	ARG	CB-CA-C	-6.19	98.02	110.40
9	CN	144	ARG	CB-CA-C	-6.19	98.02	110.40
9	Cc	144	ARG	CB-CA-C	-6.19	98.02	110.40
9	Cr	144	ARG	CB-CA-C	-6.19	98.02	110.40
8	C5	146	TRP	N-CA-C	-6.19	94.29	111.00
8	CM	146	TRP	N-CA-C	-6.19	94.29	111.00
8	Cb	146	TRP	N-CA-C	-6.19	94.29	111.00
8	Cq	146	TRP	N-CA-C	-6.19	94.29	111.00
10	C7	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	CE	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	CO	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	CT	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	Cd	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	Ci	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	Cs	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	Cx	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	C2	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	CJ	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	CY	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
10	Cn	195	TYR	CD1-CE1-CZ	-6.18	114.23	119.80
9	CD	199	ARG	NE-CZ-NH2	-6.18	117.21	120.30
9	CS	199	ARG	NE-CZ-NH2	-6.18	117.21	120.30
9	Ch	199	ARG	NE-CZ-NH2	-6.18	117.21	120.30
9	Cw	199	ARG	NE-CZ-NH2	-6.18	117.21	120.30
9	CD	144	ARG	CB-CA-C	-6.18	98.05	110.40
9	CS	144	ARG	CB-CA-C	-6.18	98.05	110.40
9	Ch	144	ARG	CB-CA-C	-6.18	98.05	110.40
9	Cw	144	ARG	CB-CA-C	-6.18	98.05	110.40
9	CD	199	ARG	CG-CD-NE	-6.17	98.85	111.80
9	CS	199	ARG	CG-CD-NE	-6.17	98.85	111.80
9	Ch	199	ARG	CG-CD-NE	-6.17	98.85	111.80
9	Cw	199	ARG	CG-CD-NE	-6.17	98.85	111.80
9	C6	199	ARG	CG-CD-NE	-6.16	98.88	111.80
9	CN	199	ARG	CG-CD-NE	-6.16	98.88	111.80
9	Cc	199	ARG	CG-CD-NE	-6.16	98.88	111.80
9	Cr	199	ARG	CG-CD-NE	-6.16	98.88	111.80
9	C1	199	ARG	CG-CD-NE	-6.14	98.90	111.80
9	CI	199	ARG	CG-CD-NE	-6.14	98.90	111.80
9	CX	199	ARG	CG-CD-NE	-6.14	98.90	111.80
9	Cm	199	ARG	CG-CD-NE	-6.14	98.90	111.80
8	CC	173	PHE	CA-CB-CG	-6.11	99.23	113.90
8	CR	173	PHE	CA-CB-CG	-6.11	99.23	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Cg	173	PHE	CA-CB-CG	-6.11	99.23	113.90
8	Cv	173	PHE	CA-CB-CG	-6.11	99.23	113.90
8	C5	173	PHE	CA-CB-CG	-6.10	99.25	113.90
8	CM	173	PHE	CA-CB-CG	-6.10	99.25	113.90
8	Cb	173	PHE	CA-CB-CG	-6.10	99.25	113.90
8	Cq	173	PHE	CA-CB-CG	-6.10	99.25	113.90
8	C0	173	PHE	CA-CB-CG	-6.09	99.29	113.90
8	CH	173	PHE	CA-CB-CG	-6.09	99.29	113.90
8	CW	173	PHE	CA-CB-CG	-6.09	99.29	113.90
8	Cl	173	PHE	CA-CB-CG	-6.09	99.29	113.90
8	C0	9	ARG	CD-NE-CZ	-6.06	115.11	123.60
8	CH	9	ARG	CD-NE-CZ	-6.06	115.11	123.60
8	CW	9	ARG	CD-NE-CZ	-6.06	115.11	123.60
8	Cl	9	ARG	CD-NE-CZ	-6.06	115.11	123.60
8	CC	9	ARG	CD-NE-CZ	-6.06	115.12	123.60
8	CR	9	ARG	CD-NE-CZ	-6.06	115.12	123.60
8	Cg	9	ARG	CD-NE-CZ	-6.06	115.12	123.60
8	Cv	9	ARG	CD-NE-CZ	-6.06	115.12	123.60
8	C5	9	ARG	CD-NE-CZ	-6.04	115.14	123.60
8	CM	9	ARG	CD-NE-CZ	-6.04	115.14	123.60
8	Cb	9	ARG	CD-NE-CZ	-6.04	115.14	123.60
8	Cq	9	ARG	CD-NE-CZ	-6.04	115.14	123.60
6	B1	27	PHE	CB-CG-CD1	-5.98	116.61	120.80
6	BI	27	PHE	CB-CG-CD1	-5.98	116.61	120.80
6	BX	27	PHE	CB-CG-CD1	-5.98	116.61	120.80
6	Bm	27	PHE	CB-CG-CD1	-5.98	116.61	120.80
9	C1	42	ASP	CB-CA-C	-5.98	98.44	110.40
9	CI	42	ASP	CB-CA-C	-5.98	98.44	110.40
9	CX	42	ASP	CB-CA-C	-5.98	98.44	110.40
9	Cm	42	ASP	CB-CA-C	-5.98	98.44	110.40
9	C6	42	ASP	CB-CA-C	-5.97	98.46	110.40
9	CN	42	ASP	CB-CA-C	-5.97	98.46	110.40
9	Cc	42	ASP	CB-CA-C	-5.97	98.46	110.40
9	Cr	42	ASP	CB-CA-C	-5.97	98.46	110.40
9	CD	42	ASP	CB-CA-C	-5.96	98.47	110.40
9	CS	42	ASP	CB-CA-C	-5.96	98.47	110.40
9	Ch	42	ASP	CB-CA-C	-5.96	98.47	110.40
9	Cw	42	ASP	CB-CA-C	-5.96	98.47	110.40
6	B6	27	PHE	CB-CG-CD1	-5.92	116.65	120.80
6	BN	27	PHE	CB-CG-CD1	-5.92	116.65	120.80
6	Bc	27	PHE	CB-CG-CD1	-5.92	116.65	120.80
6	Br	27	PHE	CB-CG-CD1	-5.92	116.65	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C1	42	ASP	N-CA-CB	5.92	121.25	110.60
9	CI	42	ASP	N-CA-CB	5.92	121.25	110.60
9	CX	42	ASP	N-CA-CB	5.92	121.25	110.60
9	Cm	42	ASP	N-CA-CB	5.92	121.25	110.60
6	BD	27	PHE	CB-CG-CD1	-5.92	116.66	120.80
6	BS	27	PHE	CB-CG-CD1	-5.92	116.66	120.80
6	Bh	27	PHE	CB-CG-CD1	-5.92	116.66	120.80
6	Bw	27	PHE	CB-CG-CD1	-5.92	116.66	120.80
9	C6	42	ASP	N-CA-CB	5.91	121.24	110.60
9	CN	42	ASP	N-CA-CB	5.91	121.24	110.60
9	Cc	42	ASP	N-CA-CB	5.91	121.24	110.60
9	Cr	42	ASP	N-CA-CB	5.91	121.24	110.60
9	CD	42	ASP	N-CA-CB	5.91	121.24	110.60
9	CS	42	ASP	N-CA-CB	5.91	121.24	110.60
9	Ch	42	ASP	N-CA-CB	5.91	121.24	110.60
9	Cw	42	ASP	N-CA-CB	5.91	121.24	110.60
8	CC	212	SER	CB-CA-C	-5.90	98.89	110.10
8	CR	212	SER	CB-CA-C	-5.90	98.89	110.10
8	Cg	212	SER	CB-CA-C	-5.90	98.89	110.10
8	Cv	212	SER	CB-CA-C	-5.90	98.89	110.10
9	CD	185	ASP	CA-CB-CG	-5.90	100.43	113.40
9	CS	185	ASP	CA-CB-CG	-5.90	100.43	113.40
9	Ch	185	ASP	CA-CB-CG	-5.90	100.43	113.40
9	Cw	185	ASP	CA-CB-CG	-5.90	100.43	113.40
8	C5	212	SER	CB-CA-C	-5.89	98.92	110.10
8	CM	212	SER	CB-CA-C	-5.89	98.92	110.10
8	Cb	212	SER	CB-CA-C	-5.89	98.92	110.10
8	Cq	212	SER	CB-CA-C	-5.89	98.92	110.10
9	C1	185	ASP	CA-CB-CG	-5.88	100.45	113.40
9	CI	185	ASP	CA-CB-CG	-5.88	100.45	113.40
9	CX	185	ASP	CA-CB-CG	-5.88	100.45	113.40
9	Cm	185	ASP	CA-CB-CG	-5.88	100.45	113.40
8	C0	212	SER	CB-CA-C	-5.88	98.92	110.10
8	CH	212	SER	CB-CA-C	-5.88	98.92	110.10
8	CW	212	SER	CB-CA-C	-5.88	98.92	110.10
8	Cl	212	SER	CB-CA-C	-5.88	98.92	110.10
9	C6	185	ASP	CA-CB-CG	-5.88	100.47	113.40
9	CN	185	ASP	CA-CB-CG	-5.88	100.47	113.40
9	Cc	185	ASP	CA-CB-CG	-5.88	100.47	113.40
9	Cr	185	ASP	CA-CB-CG	-5.88	100.47	113.40
8	C0	140	PHE	CB-CA-C	-5.85	98.71	110.40
8	CH	140	PHE	CB-CA-C	-5.85	98.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	CW	140	PHE	CB-CA-C	-5.85	98.71	110.40
8	Cl	140	PHE	CB-CA-C	-5.85	98.71	110.40
8	C5	140	PHE	CB-CA-C	-5.84	98.72	110.40
8	CC	140	PHE	CB-CA-C	-5.84	98.72	110.40
8	CM	140	PHE	CB-CA-C	-5.84	98.72	110.40
8	CR	140	PHE	CB-CA-C	-5.84	98.72	110.40
8	Cb	140	PHE	CB-CA-C	-5.84	98.72	110.40
8	Cg	140	PHE	CB-CA-C	-5.84	98.72	110.40
8	Cq	140	PHE	CB-CA-C	-5.84	98.72	110.40
8	Cv	140	PHE	CB-CA-C	-5.84	98.72	110.40
8	C5	187	SER	N-CA-CB	5.84	119.26	110.50
8	CM	187	SER	N-CA-CB	5.84	119.26	110.50
8	Cb	187	SER	N-CA-CB	5.84	119.26	110.50
8	Cq	187	SER	N-CA-CB	5.84	119.26	110.50
8	C0	187	SER	N-CA-CB	5.83	119.25	110.50
8	CH	187	SER	N-CA-CB	5.83	119.25	110.50
8	CW	187	SER	N-CA-CB	5.83	119.25	110.50
8	Cl	187	SER	N-CA-CB	5.83	119.25	110.50
8	CC	187	SER	N-CA-CB	5.83	119.25	110.50
8	CR	187	SER	N-CA-CB	5.83	119.25	110.50
8	Cg	187	SER	N-CA-CB	5.83	119.25	110.50
8	Cv	187	SER	N-CA-CB	5.83	119.25	110.50
4	AG	79	LEU	CB-CA-C	-5.74	99.29	110.20
4	AV	79	LEU	CB-CA-C	-5.74	99.29	110.20
4	Ak	79	LEU	CB-CA-C	-5.74	99.29	110.20
4	Az	79	LEU	CB-CA-C	-5.74	99.29	110.20
4	A4	79	LEU	CB-CA-C	-5.74	99.29	110.20
4	AL	79	LEU	CB-CA-C	-5.74	99.29	110.20
4	Aa	79	LEU	CB-CA-C	-5.74	99.29	110.20
4	Ap	79	LEU	CB-CA-C	-5.74	99.29	110.20
8	C0	196	PHE	N-CA-CB	-5.74	100.27	110.60
8	CH	196	PHE	N-CA-CB	-5.74	100.27	110.60
8	CW	196	PHE	N-CA-CB	-5.74	100.27	110.60
8	Cl	196	PHE	N-CA-CB	-5.74	100.27	110.60
4	AB	79	LEU	CB-CA-C	-5.73	99.31	110.20
4	AQ	79	LEU	CB-CA-C	-5.73	99.31	110.20
4	Af	79	LEU	CB-CA-C	-5.73	99.31	110.20
4	Au	79	LEU	CB-CA-C	-5.73	99.31	110.20
8	C5	196	PHE	N-CA-CB	-5.73	100.29	110.60
8	CM	196	PHE	N-CA-CB	-5.73	100.29	110.60
8	Cb	196	PHE	N-CA-CB	-5.73	100.29	110.60
8	Cq	196	PHE	N-CA-CB	-5.73	100.29	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B6	150	LEU	CA-CB-CG	-5.72	102.13	115.30
6	BN	150	LEU	CA-CB-CG	-5.72	102.13	115.30
6	Bc	150	LEU	CA-CB-CG	-5.72	102.13	115.30
6	Br	150	LEU	CA-CB-CG	-5.72	102.13	115.30
6	B1	150	LEU	CA-CB-CG	-5.72	102.15	115.30
6	BD	150	LEU	CA-CB-CG	-5.72	102.14	115.30
6	BI	150	LEU	CA-CB-CG	-5.72	102.15	115.30
6	BS	150	LEU	CA-CB-CG	-5.72	102.14	115.30
6	BX	150	LEU	CA-CB-CG	-5.72	102.15	115.30
6	Bh	150	LEU	CA-CB-CG	-5.72	102.14	115.30
6	Bm	150	LEU	CA-CB-CG	-5.72	102.15	115.30
6	Bw	150	LEU	CA-CB-CG	-5.72	102.14	115.30
8	CC	196	PHE	N-CA-CB	-5.71	100.33	110.60
8	CR	196	PHE	N-CA-CB	-5.71	100.33	110.60
8	Cg	196	PHE	N-CA-CB	-5.71	100.33	110.60
8	Cv	196	PHE	N-CA-CB	-5.71	100.33	110.60
4	B3	4	CYS	CB-CA-C	-5.70	98.99	110.40
4	BK	4	CYS	CB-CA-C	-5.70	98.99	110.40
4	BZ	4	CYS	CB-CA-C	-5.70	98.99	110.40
4	Bo	4	CYS	CB-CA-C	-5.70	98.99	110.40
4	BF	4	CYS	CB-CA-C	-5.68	99.04	110.40
4	BU	4	CYS	CB-CA-C	-5.68	99.04	110.40
4	Bj	4	CYS	CB-CA-C	-5.68	99.04	110.40
4	By	4	CYS	CB-CA-C	-5.68	99.04	110.40
4	BA	4	CYS	CB-CA-C	-5.67	99.06	110.40
4	BP	4	CYS	CB-CA-C	-5.67	99.06	110.40
4	Be	4	CYS	CB-CA-C	-5.67	99.06	110.40
4	Bt	4	CYS	CB-CA-C	-5.67	99.06	110.40
4	BA	101	ILE	CB-CA-C	-5.57	100.46	111.60
4	BF	101	ILE	CB-CA-C	-5.57	100.46	111.60
4	BP	101	ILE	CB-CA-C	-5.57	100.46	111.60
4	BU	101	ILE	CB-CA-C	-5.57	100.46	111.60
4	Be	101	ILE	CB-CA-C	-5.57	100.46	111.60
4	Bj	101	ILE	CB-CA-C	-5.57	100.46	111.60
4	Bt	101	ILE	CB-CA-C	-5.57	100.46	111.60
4	By	101	ILE	CB-CA-C	-5.57	100.46	111.60
4	B3	101	ILE	CB-CA-C	-5.57	100.47	111.60
4	BK	101	ILE	CB-CA-C	-5.57	100.47	111.60
4	BZ	101	ILE	CB-CA-C	-5.57	100.47	111.60
4	Bo	101	ILE	CB-CA-C	-5.57	100.47	111.60
9	C1	226	GLU	CB-CG-CD	-5.51	99.31	114.20
9	CI	226	GLU	CB-CG-CD	-5.51	99.31	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	CX	226	GLU	CB-CG-CD	-5.51	99.31	114.20
9	Cm	226	GLU	CB-CG-CD	-5.51	99.31	114.20
9	CD	226	GLU	CB-CG-CD	-5.51	99.32	114.20
9	CS	226	GLU	CB-CG-CD	-5.51	99.32	114.20
9	Ch	226	GLU	CB-CG-CD	-5.51	99.32	114.20
9	Cw	226	GLU	CB-CG-CD	-5.51	99.32	114.20
10	C2	171	PHE	CA-CB-CG	-5.51	100.68	113.90
10	CE	171	PHE	CA-CB-CG	-5.51	100.68	113.90
10	CJ	171	PHE	CA-CB-CG	-5.51	100.68	113.90
10	CT	171	PHE	CA-CB-CG	-5.51	100.68	113.90
10	CY	171	PHE	CA-CB-CG	-5.51	100.68	113.90
10	Ci	171	PHE	CA-CB-CG	-5.51	100.68	113.90
10	Cn	171	PHE	CA-CB-CG	-5.51	100.68	113.90
10	Cx	171	PHE	CA-CB-CG	-5.51	100.68	113.90
9	C6	226	GLU	CB-CG-CD	-5.51	99.33	114.20
9	CN	226	GLU	CB-CG-CD	-5.51	99.33	114.20
9	Cc	226	GLU	CB-CG-CD	-5.51	99.33	114.20
9	Cr	226	GLU	CB-CG-CD	-5.51	99.33	114.20
4	BA	99	ARG	C-N-CA	-5.50	107.95	121.70
4	BP	99	ARG	C-N-CA	-5.50	107.95	121.70
4	Be	99	ARG	C-N-CA	-5.50	107.95	121.70
4	Bt	99	ARG	C-N-CA	-5.50	107.95	121.70
4	B3	99	ARG	C-N-CA	-5.50	107.96	121.70
4	BK	99	ARG	C-N-CA	-5.50	107.96	121.70
4	BZ	99	ARG	C-N-CA	-5.50	107.96	121.70
4	Bo	99	ARG	C-N-CA	-5.50	107.96	121.70
10	C7	171	PHE	CA-CB-CG	-5.49	100.72	113.90
10	CO	171	PHE	CA-CB-CG	-5.49	100.72	113.90
10	Cd	171	PHE	CA-CB-CG	-5.49	100.72	113.90
10	Cs	171	PHE	CA-CB-CG	-5.49	100.72	113.90
4	BF	99	ARG	C-N-CA	-5.49	107.98	121.70
4	BU	99	ARG	C-N-CA	-5.49	107.98	121.70
4	Bj	99	ARG	C-N-CA	-5.49	107.98	121.70
4	By	99	ARG	C-N-CA	-5.49	107.98	121.70
9	C6	184	THR	CA-CB-CG2	-5.49	104.72	112.40
9	CN	184	THR	CA-CB-CG2	-5.49	104.72	112.40
9	Cc	184	THR	CA-CB-CG2	-5.49	104.72	112.40
9	Cr	184	THR	CA-CB-CG2	-5.49	104.72	112.40
9	C1	184	THR	CA-CB-CG2	-5.49	104.72	112.40
9	CI	184	THR	CA-CB-CG2	-5.49	104.72	112.40
9	CX	184	THR	CA-CB-CG2	-5.49	104.72	112.40
9	Cm	184	THR	CA-CB-CG2	-5.49	104.72	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B1	27	PHE	CB-CG-CD2	5.48	124.64	120.80
6	BI	27	PHE	CB-CG-CD2	5.48	124.64	120.80
6	BX	27	PHE	CB-CG-CD2	5.48	124.64	120.80
6	Bm	27	PHE	CB-CG-CD2	5.48	124.64	120.80
9	C1	79	ASP	CA-CB-CG	-5.47	101.36	113.40
9	CI	79	ASP	CA-CB-CG	-5.47	101.36	113.40
9	CX	79	ASP	CA-CB-CG	-5.47	101.36	113.40
9	Cm	79	ASP	CA-CB-CG	-5.47	101.36	113.40
9	CD	79	ASP	CA-CB-CG	-5.47	101.36	113.40
9	CD	184	THR	CA-CB-CG2	-5.47	104.74	112.40
9	CS	79	ASP	CA-CB-CG	-5.47	101.36	113.40
9	CS	184	THR	CA-CB-CG2	-5.47	104.74	112.40
9	Ch	79	ASP	CA-CB-CG	-5.47	101.36	113.40
9	Ch	184	THR	CA-CB-CG2	-5.47	104.74	112.40
9	Cw	79	ASP	CA-CB-CG	-5.47	101.36	113.40
9	Cw	184	THR	CA-CB-CG2	-5.47	104.74	112.40
9	C6	79	ASP	CA-CB-CG	-5.47	101.38	113.40
9	CN	79	ASP	CA-CB-CG	-5.47	101.38	113.40
9	Cc	79	ASP	CA-CB-CG	-5.47	101.38	113.40
9	Cr	79	ASP	CA-CB-CG	-5.47	101.38	113.40
6	B6	27	PHE	CB-CG-CD2	5.46	124.62	120.80
6	BN	27	PHE	CB-CG-CD2	5.46	124.62	120.80
6	Bc	27	PHE	CB-CG-CD2	5.46	124.62	120.80
6	Br	27	PHE	CB-CG-CD2	5.46	124.62	120.80
6	BD	27	PHE	CB-CG-CD2	5.44	124.61	120.80
6	BS	27	PHE	CB-CG-CD2	5.44	124.61	120.80
6	Bh	27	PHE	CB-CG-CD2	5.44	124.61	120.80
6	Bw	27	PHE	CB-CG-CD2	5.44	124.61	120.80
7	CF	150	ARG	CD-NE-CZ	-5.40	116.05	123.60
7	CU	150	ARG	CD-NE-CZ	-5.40	116.05	123.60
7	Cj	150	ARG	CD-NE-CZ	-5.40	116.05	123.60
7	Cy	150	ARG	CD-NE-CZ	-5.40	116.05	123.60
4	B3	100	LYS	CB-CA-C	5.38	121.16	110.40
4	BK	100	LYS	CB-CA-C	5.38	121.16	110.40
4	BZ	100	LYS	CB-CA-C	5.38	121.16	110.40
4	Bo	100	LYS	CB-CA-C	5.38	121.16	110.40
7	CA	150	ARG	CD-NE-CZ	-5.37	116.08	123.60
7	CP	150	ARG	CD-NE-CZ	-5.37	116.08	123.60
7	Ce	150	ARG	CD-NE-CZ	-5.37	116.08	123.60
7	Ct	150	ARG	CD-NE-CZ	-5.37	116.08	123.60
4	BF	100	LYS	CB-CA-C	5.37	121.14	110.40
4	BU	100	LYS	CB-CA-C	5.37	121.14	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Bj	100	LYS	CB-CA-C	5.37	121.14	110.40
4	By	100	LYS	CB-CA-C	5.37	121.14	110.40
4	BA	100	LYS	CB-CA-C	5.36	121.12	110.40
4	BP	100	LYS	CB-CA-C	5.36	121.12	110.40
4	Be	100	LYS	CB-CA-C	5.36	121.12	110.40
4	Bt	100	LYS	CB-CA-C	5.36	121.12	110.40
7	C3	150	ARG	CD-NE-CZ	-5.36	116.10	123.60
7	CK	150	ARG	CD-NE-CZ	-5.36	116.10	123.60
7	CZ	150	ARG	CD-NE-CZ	-5.36	116.10	123.60
7	Co	150	ARG	CD-NE-CZ	-5.36	116.10	123.60
9	C1	87	LYS	CB-CA-C	-5.33	99.75	110.40
9	CI	87	LYS	CB-CA-C	-5.33	99.75	110.40
9	CX	87	LYS	CB-CA-C	-5.33	99.75	110.40
9	Cm	87	LYS	CB-CA-C	-5.33	99.75	110.40
9	C6	87	LYS	CB-CA-C	-5.32	99.77	110.40
9	CD	87	LYS	CB-CA-C	-5.32	99.77	110.40
9	CN	87	LYS	CB-CA-C	-5.32	99.77	110.40
9	CS	87	LYS	CB-CA-C	-5.32	99.77	110.40
9	Cc	87	LYS	CB-CA-C	-5.32	99.77	110.40
9	Ch	87	LYS	CB-CA-C	-5.32	99.77	110.40
9	Cr	87	LYS	CB-CA-C	-5.32	99.77	110.40
9	Cw	87	LYS	CB-CA-C	-5.32	99.77	110.40
10	C7	63	ASP	N-CA-CB	5.32	120.17	110.60
10	CO	63	ASP	N-CA-CB	5.32	120.17	110.60
10	Cd	63	ASP	N-CA-CB	5.32	120.17	110.60
10	Cs	63	ASP	N-CA-CB	5.32	120.17	110.60
7	BB	7	CYS	N-CA-C	-5.30	96.70	111.00
7	BQ	7	CYS	N-CA-C	-5.30	96.70	111.00
7	Bf	7	CYS	N-CA-C	-5.30	96.70	111.00
7	Bu	7	CYS	N-CA-C	-5.30	96.70	111.00
9	C1	143	ALA	CB-CA-C	-5.30	102.16	110.10
9	CI	143	ALA	CB-CA-C	-5.30	102.16	110.10
9	CX	143	ALA	CB-CA-C	-5.30	102.16	110.10
9	Cm	143	ALA	CB-CA-C	-5.30	102.16	110.10
7	B4	7	CYS	N-CA-C	-5.29	96.71	111.00
7	BL	7	CYS	N-CA-C	-5.29	96.71	111.00
7	Ba	7	CYS	N-CA-C	-5.29	96.71	111.00
7	Bp	7	CYS	N-CA-C	-5.29	96.71	111.00
9	C1	123	ARG	CB-CA-C	-5.29	99.81	110.40
10	CE	63	ASP	N-CA-CB	5.29	120.13	110.60
9	CI	123	ARG	CB-CA-C	-5.29	99.81	110.40
10	CT	63	ASP	N-CA-CB	5.29	120.13	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CX	123	ARG	CB-CA-C	-5.29	99.81	110.40
10	Ci	63	ASP	N-CA-CB	5.29	120.13	110.60
9	Cm	123	ARG	CB-CA-C	-5.29	99.81	110.40
10	Cx	63	ASP	N-CA-CB	5.29	120.13	110.60
10	C2	63	ASP	N-CA-CB	5.29	120.12	110.60
10	CJ	63	ASP	N-CA-CB	5.29	120.12	110.60
10	CY	63	ASP	N-CA-CB	5.29	120.12	110.60
10	Cn	63	ASP	N-CA-CB	5.29	120.12	110.60
7	BG	7	CYS	N-CA-C	-5.29	96.73	111.00
7	BV	7	CYS	N-CA-C	-5.29	96.73	111.00
7	Bk	7	CYS	N-CA-C	-5.29	96.73	111.00
7	Bz	7	CYS	N-CA-C	-5.29	96.73	111.00
9	CD	123	ARG	CB-CA-C	-5.29	99.83	110.40
9	CS	123	ARG	CB-CA-C	-5.29	99.83	110.40
9	Ch	123	ARG	CB-CA-C	-5.29	99.83	110.40
9	Cw	123	ARG	CB-CA-C	-5.29	99.83	110.40
9	C6	123	ARG	CB-CA-C	-5.28	99.83	110.40
9	CN	123	ARG	CB-CA-C	-5.28	99.83	110.40
9	Cc	123	ARG	CB-CA-C	-5.28	99.83	110.40
9	Cr	123	ARG	CB-CA-C	-5.28	99.83	110.40
9	C6	143	ALA	CB-CA-C	-5.28	102.18	110.10
9	CN	143	ALA	CB-CA-C	-5.28	102.18	110.10
9	Cc	143	ALA	CB-CA-C	-5.28	102.18	110.10
9	Cr	143	ALA	CB-CA-C	-5.28	102.18	110.10
10	C7	210	GLU	CA-CB-CG	-5.28	101.79	113.40
10	CO	210	GLU	CA-CB-CG	-5.28	101.79	113.40
10	Cd	210	GLU	CA-CB-CG	-5.28	101.79	113.40
10	Cs	210	GLU	CA-CB-CG	-5.28	101.79	113.40
9	CD	143	ALA	CB-CA-C	-5.27	102.19	110.10
9	CS	143	ALA	CB-CA-C	-5.27	102.19	110.10
9	Ch	143	ALA	CB-CA-C	-5.27	102.19	110.10
9	Cw	143	ALA	CB-CA-C	-5.27	102.19	110.10
10	CE	210	GLU	CA-CB-CG	-5.26	101.82	113.40
10	CT	210	GLU	CA-CB-CG	-5.26	101.82	113.40
10	Ci	210	GLU	CA-CB-CG	-5.26	101.82	113.40
10	Cx	210	GLU	CA-CB-CG	-5.26	101.82	113.40
3	AF	5	ASP	CB-CG-OD1	5.25	123.03	118.30
3	AU	5	ASP	CB-CG-OD1	5.25	123.03	118.30
3	Aj	5	ASP	CB-CG-OD1	5.25	123.03	118.30
3	Ay	5	ASP	CB-CG-OD1	5.25	123.03	118.30
3	AA	5	ASP	CB-CG-OD1	5.25	123.02	118.30
3	AP	5	ASP	CB-CG-OD1	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Ae	5	ASP	CB-CG-OD1	5.25	123.02	118.30
3	At	5	ASP	CB-CG-OD1	5.25	123.02	118.30
10	C2	210	GLU	CA-CB-CG	-5.25	101.86	113.40
10	CJ	210	GLU	CA-CB-CG	-5.25	101.86	113.40
10	CY	210	GLU	CA-CB-CG	-5.25	101.86	113.40
10	Cn	210	GLU	CA-CB-CG	-5.25	101.86	113.40
8	C5	65	HIS	C-N-CA	5.24	134.79	121.70
8	CM	65	HIS	C-N-CA	5.24	134.79	121.70
8	Cb	65	HIS	C-N-CA	5.24	134.79	121.70
8	Cq	65	HIS	C-N-CA	5.24	134.79	121.70
8	CC	65	HIS	C-N-CA	5.23	134.78	121.70
8	CR	65	HIS	C-N-CA	5.23	134.78	121.70
8	Cg	65	HIS	C-N-CA	5.23	134.78	121.70
8	Cv	65	HIS	C-N-CA	5.23	134.78	121.70
3	A3	5	ASP	CB-CG-OD1	5.23	123.01	118.30
3	AK	5	ASP	CB-CG-OD1	5.23	123.01	118.30
3	AZ	5	ASP	CB-CG-OD1	5.23	123.01	118.30
3	Ao	5	ASP	CB-CG-OD1	5.23	123.01	118.30
8	C0	161	THR	CA-CB-CG2	-5.22	105.09	112.40
8	C5	161	THR	CA-CB-CG2	-5.22	105.09	112.40
8	CH	161	THR	CA-CB-CG2	-5.22	105.09	112.40
8	CM	161	THR	CA-CB-CG2	-5.22	105.09	112.40
8	CW	161	THR	CA-CB-CG2	-5.22	105.09	112.40
8	Cb	161	THR	CA-CB-CG2	-5.22	105.09	112.40
8	Cl	161	THR	CA-CB-CG2	-5.22	105.09	112.40
8	Cq	161	THR	CA-CB-CG2	-5.22	105.09	112.40
3	A7	6	CYS	N-CA-CB	5.22	119.99	110.60
3	AO	6	CYS	N-CA-CB	5.22	119.99	110.60
3	Ad	6	CYS	N-CA-CB	5.22	119.99	110.60
3	As	6	CYS	N-CA-CB	5.22	119.99	110.60
8	C0	65	HIS	C-N-CA	5.22	134.75	121.70
8	CH	65	HIS	C-N-CA	5.22	134.75	121.70
8	CW	65	HIS	C-N-CA	5.22	134.75	121.70
8	Cl	65	HIS	C-N-CA	5.22	134.75	121.70
3	AE	6	CYS	N-CA-CB	5.21	119.98	110.60
3	AT	6	CYS	N-CA-CB	5.21	119.98	110.60
3	Ai	6	CYS	N-CA-CB	5.21	119.98	110.60
3	Ax	6	CYS	N-CA-CB	5.21	119.98	110.60
3	A2	6	CYS	N-CA-CB	5.21	119.97	110.60
3	AJ	6	CYS	N-CA-CB	5.21	119.97	110.60
3	AY	6	CYS	N-CA-CB	5.21	119.97	110.60
3	An	6	CYS	N-CA-CB	5.21	119.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B0	8	GLU	CB-CG-CD	-5.20	100.15	114.20
5	BH	8	GLU	CB-CG-CD	-5.20	100.15	114.20
5	BW	8	GLU	CB-CG-CD	-5.20	100.15	114.20
5	Bl	8	GLU	CB-CG-CD	-5.20	100.15	114.20
8	CC	161	THR	CA-CB-CG2	-5.20	105.12	112.40
8	CR	161	THR	CA-CB-CG2	-5.20	105.12	112.40
8	Cg	161	THR	CA-CB-CG2	-5.20	105.12	112.40
8	Cv	161	THR	CA-CB-CG2	-5.20	105.12	112.40
5	B5	8	GLU	CB-CG-CD	-5.20	100.17	114.20
5	BM	8	GLU	CB-CG-CD	-5.20	100.17	114.20
5	Bb	8	GLU	CB-CG-CD	-5.20	100.17	114.20
5	Bq	8	GLU	CB-CG-CD	-5.20	100.17	114.20
5	BC	8	GLU	CB-CG-CD	-5.19	100.19	114.20
5	BR	8	GLU	CB-CG-CD	-5.19	100.19	114.20
5	Bg	8	GLU	CB-CG-CD	-5.19	100.19	114.20
5	Bv	8	GLU	CB-CG-CD	-5.19	100.19	114.20
8	CC	202	ASP	CA-CB-CG	-5.19	101.98	113.40
8	CR	202	ASP	CA-CB-CG	-5.19	101.98	113.40
8	Cg	202	ASP	CA-CB-CG	-5.19	101.98	113.40
8	Cv	202	ASP	CA-CB-CG	-5.19	101.98	113.40
8	C0	202	ASP	CA-CB-CG	-5.18	102.00	113.40
8	CH	202	ASP	CA-CB-CG	-5.18	102.00	113.40
8	CW	202	ASP	CA-CB-CG	-5.18	102.00	113.40
8	Cl	202	ASP	CA-CB-CG	-5.18	102.00	113.40
8	C5	202	ASP	CA-CB-CG	-5.18	102.01	113.40
8	CM	202	ASP	CA-CB-CG	-5.18	102.01	113.40
8	Cb	202	ASP	CA-CB-CG	-5.18	102.01	113.40
8	Cq	202	ASP	CA-CB-CG	-5.18	102.01	113.40
6	BD	27	PHE	C-N-CA	-5.16	108.79	121.70
6	BS	27	PHE	C-N-CA	-5.16	108.79	121.70
6	Bh	27	PHE	C-N-CA	-5.16	108.79	121.70
6	Bw	27	PHE	C-N-CA	-5.16	108.79	121.70
6	B1	27	PHE	C-N-CA	-5.16	108.81	121.70
6	B6	27	PHE	C-N-CA	-5.16	108.81	121.70
6	BI	27	PHE	C-N-CA	-5.16	108.81	121.70
6	BN	27	PHE	C-N-CA	-5.16	108.81	121.70
6	BX	27	PHE	C-N-CA	-5.16	108.81	121.70
6	Bc	27	PHE	C-N-CA	-5.16	108.81	121.70
6	Bm	27	PHE	C-N-CA	-5.16	108.81	121.70
6	Br	27	PHE	C-N-CA	-5.16	108.81	121.70
4	AG	145	HIS	N-CA-C	-5.12	97.18	111.00
4	AV	145	HIS	N-CA-C	-5.12	97.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Ak	145	HIS	N-CA-C	-5.12	97.18	111.00
4	Az	145	HIS	N-CA-C	-5.12	97.18	111.00
9	CD	185	ASP	CA-C-N	-5.11	105.96	117.20
9	CS	185	ASP	CA-C-N	-5.11	105.96	117.20
9	Ch	185	ASP	CA-C-N	-5.11	105.96	117.20
9	Cw	185	ASP	CA-C-N	-5.11	105.96	117.20
4	AB	145	HIS	N-CA-C	-5.11	97.21	111.00
4	AQ	145	HIS	N-CA-C	-5.11	97.21	111.00
4	Af	145	HIS	N-CA-C	-5.11	97.21	111.00
4	Au	145	HIS	N-CA-C	-5.11	97.21	111.00
4	A4	145	HIS	N-CA-C	-5.10	97.22	111.00
4	AL	145	HIS	N-CA-C	-5.10	97.22	111.00
4	Aa	145	HIS	N-CA-C	-5.10	97.22	111.00
4	Ap	145	HIS	N-CA-C	-5.10	97.22	111.00
9	C1	185	ASP	CA-C-N	-5.10	105.97	117.20
9	CI	185	ASP	CA-C-N	-5.10	105.97	117.20
9	CX	185	ASP	CA-C-N	-5.10	105.97	117.20
9	Cm	185	ASP	CA-C-N	-5.10	105.97	117.20
9	C6	185	ASP	CA-C-N	-5.10	105.97	117.20
9	CN	185	ASP	CA-C-N	-5.10	105.97	117.20
9	Cc	185	ASP	CA-C-N	-5.10	105.97	117.20
9	Cr	185	ASP	CA-C-N	-5.10	105.97	117.20
3	AF	27	PHE	CB-CA-C	-5.08	100.24	110.40
3	AU	27	PHE	CB-CA-C	-5.08	100.24	110.40
3	Aj	27	PHE	CB-CA-C	-5.08	100.24	110.40
3	Ay	27	PHE	CB-CA-C	-5.08	100.24	110.40
9	C1	197	PHE	C-N-CA	5.08	134.39	121.70
9	CI	197	PHE	C-N-CA	5.08	134.39	121.70
9	CX	197	PHE	C-N-CA	5.08	134.39	121.70
9	Cm	197	PHE	C-N-CA	5.08	134.39	121.70
10	C2	120	ARG	NE-CZ-NH2	-5.07	117.76	120.30
10	CJ	120	ARG	NE-CZ-NH2	-5.07	117.76	120.30
10	CY	120	ARG	NE-CZ-NH2	-5.07	117.76	120.30
10	Cn	120	ARG	NE-CZ-NH2	-5.07	117.76	120.30
3	A3	27	PHE	CB-CA-C	-5.07	100.26	110.40
3	AK	27	PHE	CB-CA-C	-5.07	100.26	110.40
3	AZ	27	PHE	CB-CA-C	-5.07	100.26	110.40
3	Ao	27	PHE	CB-CA-C	-5.07	100.26	110.40
3	AA	27	PHE	CB-CA-C	-5.07	100.27	110.40
3	AP	27	PHE	CB-CA-C	-5.07	100.27	110.40
3	Ae	27	PHE	CB-CA-C	-5.07	100.27	110.40
3	At	27	PHE	CB-CA-C	-5.07	100.27	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	CD	197	PHE	C-N-CA	5.06	134.35	121.70
9	CS	197	PHE	C-N-CA	5.06	134.35	121.70
9	Ch	197	PHE	C-N-CA	5.06	134.35	121.70
9	Cw	197	PHE	C-N-CA	5.06	134.35	121.70
9	C6	197	PHE	C-N-CA	5.05	134.33	121.70
9	CN	197	PHE	C-N-CA	5.05	134.33	121.70
9	Cc	197	PHE	C-N-CA	5.05	134.33	121.70
9	Cr	197	PHE	C-N-CA	5.05	134.33	121.70
10	CE	81	PHE	CD1-CG-CD2	5.05	124.86	118.30
10	CT	81	PHE	CD1-CG-CD2	5.05	124.86	118.30
10	Ci	81	PHE	CD1-CG-CD2	5.05	124.86	118.30
10	Cx	81	PHE	CD1-CG-CD2	5.05	124.86	118.30
10	C7	81	PHE	CD1-CG-CD2	5.03	124.84	118.30
10	CO	81	PHE	CD1-CG-CD2	5.03	124.84	118.30
10	Cd	81	PHE	CD1-CG-CD2	5.03	124.84	118.30
10	Cs	81	PHE	CD1-CG-CD2	5.03	124.84	118.30
10	C2	81	PHE	CD1-CG-CD2	5.02	124.83	118.30
10	CJ	81	PHE	CD1-CG-CD2	5.02	124.83	118.30
10	CY	81	PHE	CD1-CG-CD2	5.02	124.83	118.30
10	Cn	81	PHE	CD1-CG-CD2	5.02	124.83	118.30

There are no chirality outliers.

All (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
1	A5	150	ARG	Sidechain
3	A7	23	TRP	Peptide
3	AA	23	TRP	Peptide
3	AA	27	PHE	Peptide
4	AB	142	LYS	Peptide
1	AC	150	ARG	Sidechain
3	AE	23	TRP	Peptide
3	AF	23	TRP	Peptide
3	AF	27	PHE	Peptide
4	AG	142	LYS	Peptide
1	AH	150	ARG	Sidechain
3	AJ	23	TRP	Peptide

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Mol	Chain	Res	Type	Group
3	AK	23	TRP	Peptide
3	AK	27	PHE	Peptide
4	AL	142	LYS	Peptide
1	AM	150	ARG	Sidechain
3	AO	23	TRP	Peptide
3	AP	23	TRP	Peptide
3	AP	27	PHE	Peptide
4	AQ	142	LYS	Peptide
1	AR	150	ARG	Sidechain
3	AT	23	TRP	Peptide
3	AU	23	TRP	Peptide
3	AU	27	PHE	Peptide
4	AV	142	LYS	Peptide
1	AW	150	ARG	Sidechain
3	AY	23	TRP	Peptide
3	AZ	23	TRP	Peptide
3	AZ	27	PHE	Peptide
4	Aa	142	LYS	Peptide
1	Ab	150	ARG	Sidechain
3	Ad	23	TRP	Peptide
3	Ae	23	TRP	Peptide
3	Ae	27	PHE	Peptide
4	Af	142	LYS	Peptide
1	Ag	150	ARG	Sidechain
3	Ai	23	TRP	Peptide
3	Aj	23	TRP	Peptide
3	Aj	27	PHE	Peptide
4	Ak	142	LYS	Peptide
1	Al	150	ARG	Sidechain
3	An	23	TRP	Peptide
3	Ao	23	TRP	Peptide
3	Ao	27	PHE	Peptide
4	Ap	142	LYS	Peptide
1	Aq	150	ARG	Sidechain
3	As	23	TRP	Peptide
3	At	23	TRP	Peptide
3	At	27	PHE	Peptide
4	Au	142	LYS	Peptide
1	Av	150	ARG	Sidechain
3	Ax	23	TRP	Peptide
3	Ay	23	TRP	Peptide
3	Ay	27	PHE	Peptide

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Mol	Chain	Res	Type	Group
4	Az	142	LYS	Peptide
5	B0	83	MET	Peptide
5	B0	9	CYS	Peptide
6	B1	147	ALA	Peptide
4	B2	143	GLY	Peptide
4	B2	144	HIS	Peptide
4	B3	78	THR	Peptide
4	B3	99	ARG	Sidechain
7	B4	150	ARG	Peptide
7	B4	6	CYS	Peptide
7	B4	7	CYS	Peptide
5	B5	83	MET	Peptide
5	B5	9	CYS	Peptide
6	B6	147	ALA	Peptide
4	B7	143	GLY	Peptide
4	B7	144	HIS	Peptide
4	BA	78	THR	Peptide
4	BA	99	ARG	Sidechain
7	BB	150	ARG	Peptide
7	BB	6	CYS	Peptide
7	BB	7	CYS	Peptide
5	BC	83	MET	Peptide
5	BC	9	CYS	Peptide
6	BD	147	ALA	Peptide
4	BE	143	GLY	Peptide
4	BE	144	HIS	Peptide
4	BF	78	THR	Peptide
4	BF	99	ARG	Sidechain
7	BG	150	ARG	Peptide
7	BG	6	CYS	Peptide
7	BG	7	CYS	Peptide
5	BH	83	MET	Peptide
5	BH	9	CYS	Peptide
6	BI	147	ALA	Peptide
4	BJ	143	GLY	Peptide
4	BJ	144	HIS	Peptide
4	BK	78	THR	Peptide
4	BK	99	ARG	Sidechain
7	BL	150	ARG	Peptide
7	BL	6	CYS	Peptide
7	BL	7	CYS	Peptide
5	BM	83	MET	Peptide

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Mol	Chain	Res	Type	Group
5	BM	9	CYS	Peptide
6	BN	147	ALA	Peptide
4	BO	143	GLY	Peptide
4	BO	144	HIS	Peptide
4	BP	78	THR	Peptide
4	BP	99	ARG	Sidechain
7	BQ	150	ARG	Peptide
7	BQ	6	CYS	Peptide
7	BQ	7	CYS	Peptide
5	BR	83	MET	Peptide
5	BR	9	CYS	Peptide
6	BS	147	ALA	Peptide
4	BT	143	GLY	Peptide
4	BT	144	HIS	Peptide
4	BU	78	THR	Peptide
4	BU	99	ARG	Sidechain
7	BV	150	ARG	Peptide
7	BV	6	CYS	Peptide
7	BV	7	CYS	Peptide
5	BW	83	MET	Peptide
5	BW	9	CYS	Peptide
6	BX	147	ALA	Peptide
4	BY	143	GLY	Peptide
4	BY	144	HIS	Peptide
4	BZ	78	THR	Peptide
4	BZ	99	ARG	Sidechain
7	Ba	150	ARG	Peptide
7	Ba	6	CYS	Peptide
7	Ba	7	CYS	Peptide
5	Bb	83	MET	Peptide
5	Bb	9	CYS	Peptide
6	Bc	147	ALA	Peptide
4	Bd	143	GLY	Peptide
4	Bd	144	HIS	Peptide
4	Be	78	THR	Peptide
4	Be	99	ARG	Sidechain
7	Bf	150	ARG	Peptide
7	Bf	6	CYS	Peptide
7	Bf	7	CYS	Peptide
5	Bg	83	MET	Peptide
5	Bg	9	CYS	Peptide
6	Bh	147	ALA	Peptide

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Mol	Chain	Res	Type	Group
4	Bi	143	GLY	Peptide
4	Bi	144	HIS	Peptide
4	Bj	78	THR	Peptide
4	Bj	99	ARG	Sidechain
7	Bk	150	ARG	Peptide
7	Bk	6	CYS	Peptide
7	Bk	7	CYS	Peptide
5	Bl	83	MET	Peptide
5	Bl	9	CYS	Peptide
6	Bm	147	ALA	Peptide
4	Bn	143	GLY	Peptide
4	Bn	144	HIS	Peptide
4	Bo	78	THR	Peptide
4	Bo	99	ARG	Sidechain
7	Bp	150	ARG	Peptide
7	Bp	6	CYS	Peptide
7	Bp	7	CYS	Peptide
5	Bq	83	MET	Peptide
5	Bq	9	CYS	Peptide
6	Br	147	ALA	Peptide
4	Bs	143	GLY	Peptide
4	Bs	144	HIS	Peptide
4	Bt	78	THR	Peptide
4	Bt	99	ARG	Sidechain
7	Bu	150	ARG	Peptide
7	Bu	6	CYS	Peptide
7	Bu	7	CYS	Peptide
5	Bv	83	MET	Peptide
5	Bv	9	CYS	Peptide
6	Bw	147	ALA	Peptide
4	Bx	143	GLY	Peptide
4	Bx	144	HIS	Peptide
4	By	78	THR	Peptide
4	By	99	ARG	Sidechain
7	Bz	150	ARG	Peptide
7	Bz	6	CYS	Peptide
7	Bz	7	CYS	Peptide
8	C0	120	CYS	Peptide
8	C0	137	ARG	Peptide
8	C0	139	SER	Peptide
8	C0	140	PHE	Peptide
8	C0	142	PRO	Peptide

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Mol	Chain	Res	Type	Group
8	C0	146	TRP	Peptide
8	C0	184	LYS	Peptide
8	C0	196	PHE	Peptide
8	C0	197	ASN	Peptide
8	C0	212	SER	Peptide
8	C0	224	ARG	Peptide
8	C0	74	PRO	Peptide
9	C1	122	ALA	Peptide
9	C1	123	ARG	Sidechain
9	C1	138	ARG	Sidechain
9	C1	140	PHE	Peptide
9	C1	142	THR	Peptide
9	C1	177	ARG	Sidechain
9	C1	190	HIS	Peptide
9	C1	198	ASN	Peptide
9	C1	199	ARG	Sidechain
9	C1	200	GLY	Peptide
10	C2	103	LYS	Peptide
10	C2	116	HIS	Peptide
10	C2	139	THR	Peptide
10	C2	170	SER	Mainchain
10	C2	185	GLY	Peptide
10	C2	192	PHE	Peptide
10	C2	57	LEU	Mainchain
10	C2	71	GLY	Peptide
7	C3	150	ARG	Sidechain
7	C3	6	CYS	Peptide
5	C4	83	MET	Peptide
8	C5	120	CYS	Peptide
8	C5	137	ARG	Peptide
8	C5	139	SER	Peptide
8	C5	140	PHE	Peptide
8	C5	142	PRO	Peptide
8	C5	146	TRP	Peptide
8	C5	184	LYS	Peptide
8	C5	196	PHE	Peptide
8	C5	197	ASN	Peptide
8	C5	212	SER	Peptide
8	C5	224	ARG	Peptide
8	C5	74	PRO	Peptide
9	C6	122	ALA	Peptide
9	C6	123	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	C6	138	ARG	Sidechain
9	C6	140	PHE	Peptide
9	C6	142	THR	Peptide
9	C6	177	ARG	Sidechain
9	C6	190	HIS	Peptide
9	C6	198	ASN	Peptide
9	C6	199	ARG	Sidechain
9	C6	200	GLY	Peptide
10	C7	103	LYS	Peptide
10	C7	116	HIS	Peptide
10	C7	139	THR	Peptide
10	C7	170	SER	Mainchain
10	C7	185	GLY	Peptide
10	C7	192	PHE	Peptide
10	C7	57	LEU	Mainchain
10	C7	71	GLY	Peptide
7	CA	150	ARG	Sidechain
7	CA	6	CYS	Peptide
5	CB	83	MET	Peptide
8	CC	120	CYS	Peptide
8	CC	137	ARG	Peptide
8	CC	139	SER	Peptide
8	CC	140	PHE	Peptide
8	CC	142	PRO	Peptide
8	CC	146	TRP	Peptide
8	CC	184	LYS	Peptide
8	CC	196	PHE	Peptide
8	CC	197	ASN	Peptide
8	CC	212	SER	Peptide
8	CC	224	ARG	Peptide
8	CC	74	PRO	Peptide
9	CD	122	ALA	Peptide
9	CD	123	ARG	Sidechain
9	CD	138	ARG	Sidechain
9	CD	140	PHE	Peptide
9	CD	142	THR	Peptide
9	CD	177	ARG	Sidechain
9	CD	190	HIS	Peptide
9	CD	198	ASN	Peptide
9	CD	199	ARG	Sidechain
9	CD	200	GLY	Peptide
10	CE	103	LYS	Peptide

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Mol	Chain	Res	Type	Group
10	CE	116	HIS	Peptide
10	CE	139	THR	Peptide
10	CE	170	SER	Mainchain
10	CE	185	GLY	Peptide
10	CE	192	PHE	Peptide
10	CE	57	LEU	Mainchain
10	CE	71	GLY	Peptide
7	CF	150	ARG	Sidechain
7	CF	6	CYS	Peptide
5	CG	83	MET	Peptide
8	CH	120	CYS	Peptide
8	CH	137	ARG	Peptide
8	CH	139	SER	Peptide
8	CH	140	PHE	Peptide
8	CH	142	PRO	Peptide
8	CH	146	TRP	Peptide
8	CH	184	LYS	Peptide
8	CH	196	PHE	Peptide
8	CH	197	ASN	Peptide
8	CH	212	SER	Peptide
8	CH	224	ARG	Peptide
8	CH	74	PRO	Peptide
9	CI	122	ALA	Peptide
9	CI	123	ARG	Sidechain
9	CI	138	ARG	Sidechain
9	CI	140	PHE	Peptide
9	CI	142	THR	Peptide
9	CI	177	ARG	Sidechain
9	CI	190	HIS	Peptide
9	CI	198	ASN	Peptide
9	CI	199	ARG	Sidechain
9	CI	200	GLY	Peptide
10	CJ	103	LYS	Peptide
10	CJ	116	HIS	Peptide
10	CJ	139	THR	Peptide
10	CJ	170	SER	Mainchain
10	CJ	185	GLY	Peptide
10	CJ	192	PHE	Peptide
10	CJ	57	LEU	Mainchain
10	CJ	71	GLY	Peptide
7	CK	150	ARG	Sidechain
7	CK	6	CYS	Peptide

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Mol	Chain	Res	Type	Group
5	CL	83	MET	Peptide
8	CM	120	CYS	Peptide
8	CM	137	ARG	Peptide
8	CM	139	SER	Peptide
8	CM	140	PHE	Peptide
8	CM	142	PRO	Peptide
8	CM	146	TRP	Peptide
8	CM	184	LYS	Peptide
8	CM	196	PHE	Peptide
8	CM	197	ASN	Peptide
8	CM	212	SER	Peptide
8	CM	224	ARG	Peptide
8	CM	74	PRO	Peptide
9	CN	122	ALA	Peptide
9	CN	123	ARG	Sidechain
9	CN	138	ARG	Sidechain
9	CN	140	PHE	Peptide
9	CN	142	THR	Peptide
9	CN	177	ARG	Sidechain
9	CN	190	HIS	Peptide
9	CN	198	ASN	Peptide
9	CN	199	ARG	Sidechain
9	CN	200	GLY	Peptide
10	CO	103	LYS	Peptide
10	CO	116	HIS	Peptide
10	CO	139	THR	Peptide
10	CO	170	SER	Mainchain
10	CO	185	GLY	Peptide
10	CO	192	PHE	Peptide
10	CO	57	LEU	Mainchain
10	CO	71	GLY	Peptide
7	CP	150	ARG	Sidechain
7	CP	6	CYS	Peptide
5	CQ	83	MET	Peptide
8	CR	120	CYS	Peptide
8	CR	137	ARG	Peptide
8	CR	139	SER	Peptide
8	CR	140	PHE	Peptide
8	CR	142	PRO	Peptide
8	CR	146	TRP	Peptide
8	CR	184	LYS	Peptide
8	CR	196	PHE	Peptide

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Mol	Chain	Res	Type	Group
8	CR	197	ASN	Peptide
8	CR	212	SER	Peptide
8	CR	224	ARG	Peptide
8	CR	74	PRO	Peptide
9	CS	122	ALA	Peptide
9	CS	123	ARG	Sidechain
9	CS	138	ARG	Sidechain
9	CS	140	PHE	Peptide
9	CS	142	THR	Peptide
9	CS	177	ARG	Sidechain
9	CS	190	HIS	Peptide
9	CS	198	ASN	Peptide
9	CS	199	ARG	Sidechain
9	CS	200	GLY	Peptide
10	CT	103	LYS	Peptide
10	CT	116	HIS	Peptide
10	CT	139	THR	Peptide
10	CT	170	SER	Mainchain
10	CT	185	GLY	Peptide
10	CT	192	PHE	Peptide
10	CT	57	LEU	Mainchain
10	CT	71	GLY	Peptide
7	CU	150	ARG	Sidechain
7	CU	6	CYS	Peptide
5	CV	83	MET	Peptide
8	CW	120	CYS	Peptide
8	CW	137	ARG	Peptide
8	CW	139	SER	Peptide
8	CW	140	PHE	Peptide
8	CW	142	PRO	Peptide
8	CW	146	TRP	Peptide
8	CW	184	LYS	Peptide
8	CW	196	PHE	Peptide
8	CW	197	ASN	Peptide
8	CW	212	SER	Peptide
8	CW	224	ARG	Peptide
8	CW	74	PRO	Peptide
9	CX	122	ALA	Peptide
9	CX	123	ARG	Sidechain
9	CX	138	ARG	Sidechain
9	CX	140	PHE	Peptide
9	CX	142	THR	Peptide

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Mol	Chain	Res	Type	Group
9	CX	177	ARG	Sidechain
9	CX	190	HIS	Peptide
9	CX	198	ASN	Peptide
9	CX	199	ARG	Sidechain
9	CX	200	GLY	Peptide
10	CY	103	LYS	Peptide
10	CY	116	HIS	Peptide
10	CY	139	THR	Peptide
10	CY	170	SER	Mainchain
10	CY	185	GLY	Peptide
10	CY	192	PHE	Peptide
10	CY	57	LEU	Mainchain
10	CY	71	GLY	Peptide
7	CZ	150	ARG	Sidechain
7	CZ	6	CYS	Peptide
5	Ca	83	MET	Peptide
8	Cb	120	CYS	Peptide
8	Cb	137	ARG	Peptide
8	Cb	139	SER	Peptide
8	Cb	140	PHE	Peptide
8	Cb	142	PRO	Peptide
8	Cb	146	TRP	Peptide
8	Cb	184	LYS	Peptide
8	Cb	196	PHE	Peptide
8	Cb	197	ASN	Peptide
8	Cb	212	SER	Peptide
8	Cb	224	ARG	Peptide
8	Cb	74	PRO	Peptide
9	Cc	122	ALA	Peptide
9	Cc	123	ARG	Sidechain
9	Cc	138	ARG	Sidechain
9	Cc	140	PHE	Peptide
9	Cc	142	THR	Peptide
9	Cc	177	ARG	Sidechain
9	Cc	190	HIS	Peptide
9	Cc	198	ASN	Peptide
9	Cc	199	ARG	Sidechain
9	Cc	200	GLY	Peptide
10	Cd	103	LYS	Peptide
10	Cd	116	HIS	Peptide
10	Cd	139	THR	Peptide
10	Cd	170	SER	Mainchain

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Mol	Chain	Res	Type	Group
10	Cd	185	GLY	Peptide
10	Cd	192	PHE	Peptide
10	Cd	57	LEU	Mainchain
10	Cd	71	GLY	Peptide
7	Ce	150	ARG	Sidechain
7	Ce	6	CYS	Peptide
5	Cf	83	MET	Peptide
8	Cg	120	CYS	Peptide
8	Cg	137	ARG	Peptide
8	Cg	139	SER	Peptide
8	Cg	140	PHE	Peptide
8	Cg	142	PRO	Peptide
8	Cg	146	TRP	Peptide
8	Cg	184	LYS	Peptide
8	Cg	196	PHE	Peptide
8	Cg	197	ASN	Peptide
8	Cg	212	SER	Peptide
8	Cg	224	ARG	Peptide
8	Cg	74	PRO	Peptide
9	Ch	122	ALA	Peptide
9	Ch	123	ARG	Sidechain
9	Ch	138	ARG	Sidechain
9	Ch	140	PHE	Peptide
9	Ch	142	THR	Peptide
9	Ch	177	ARG	Sidechain
9	Ch	190	HIS	Peptide
9	Ch	198	ASN	Peptide
9	Ch	199	ARG	Sidechain
9	Ch	200	GLY	Peptide
10	Ci	103	LYS	Peptide
10	Ci	116	HIS	Peptide
10	Ci	139	THR	Peptide
10	Ci	170	SER	Mainchain
10	Ci	185	GLY	Peptide
10	Ci	192	PHE	Peptide
10	Ci	57	LEU	Mainchain
10	Ci	71	GLY	Peptide
7	Cj	150	ARG	Sidechain
7	Cj	6	CYS	Peptide
5	Ck	83	MET	Peptide
8	Cl	120	CYS	Peptide
8	Cl	137	ARG	Peptide

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Mol	Chain	Res	Type	Group
8	Cl	139	SER	Peptide
8	Cl	140	PHE	Peptide
8	Cl	142	PRO	Peptide
8	Cl	146	TRP	Peptide
8	Cl	184	LYS	Peptide
8	Cl	196	PHE	Peptide
8	Cl	197	ASN	Peptide
8	Cl	212	SER	Peptide
8	Cl	224	ARG	Peptide
8	Cl	74	PRO	Peptide
9	Cm	122	ALA	Peptide
9	Cm	123	ARG	Sidechain
9	Cm	138	ARG	Sidechain
9	Cm	140	PHE	Peptide
9	Cm	142	THR	Peptide
9	Cm	177	ARG	Sidechain
9	Cm	190	HIS	Peptide
9	Cm	198	ASN	Peptide
9	Cm	199	ARG	Sidechain
9	Cm	200	GLY	Peptide
10	Cn	103	LYS	Peptide
10	Cn	116	HIS	Peptide
10	Cn	139	THR	Peptide
10	Cn	170	SER	Mainchain
10	Cn	185	GLY	Peptide
10	Cn	192	PHE	Peptide
10	Cn	57	LEU	Mainchain
10	Cn	71	GLY	Peptide
7	Co	150	ARG	Sidechain
7	Co	6	CYS	Peptide
5	Cp	83	MET	Peptide
8	Cq	120	CYS	Peptide
8	Cq	137	ARG	Peptide
8	Cq	139	SER	Peptide
8	Cq	140	PHE	Peptide
8	Cq	142	PRO	Peptide
8	Cq	146	TRP	Peptide
8	Cq	184	LYS	Peptide
8	Cq	196	PHE	Peptide
8	Cq	197	ASN	Peptide
8	Cq	212	SER	Peptide
8	Cq	224	ARG	Peptide

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Mol	Chain	Res	Type	Group
8	Cq	74	PRO	Peptide
9	Cr	122	ALA	Peptide
9	Cr	123	ARG	Sidechain
9	Cr	138	ARG	Sidechain
9	Cr	140	PHE	Peptide
9	Cr	142	THR	Peptide
9	Cr	177	ARG	Sidechain
9	Cr	190	HIS	Peptide
9	Cr	198	ASN	Peptide
9	Cr	199	ARG	Sidechain
9	Cr	200	GLY	Peptide
10	Cs	103	LYS	Peptide
10	Cs	116	HIS	Peptide
10	Cs	139	THR	Peptide
10	Cs	170	SER	Mainchain
10	Cs	185	GLY	Peptide
10	Cs	192	PHE	Peptide
10	Cs	57	LEU	Mainchain
10	Cs	71	GLY	Peptide
7	Ct	150	ARG	Sidechain
7	Ct	6	CYS	Peptide
5	Cu	83	MET	Peptide
8	Cv	120	CYS	Peptide
8	Cv	137	ARG	Peptide
8	Cv	139	SER	Peptide
8	Cv	140	PHE	Peptide
8	Cv	142	PRO	Peptide
8	Cv	146	TRP	Peptide
8	Cv	184	LYS	Peptide
8	Cv	196	PHE	Peptide
8	Cv	197	ASN	Peptide
8	Cv	212	SER	Peptide
8	Cv	224	ARG	Peptide
8	Cv	74	PRO	Peptide
9	Cw	122	ALA	Peptide
9	Cw	123	ARG	Sidechain
9	Cw	138	ARG	Sidechain
9	Cw	140	PHE	Peptide
9	Cw	142	THR	Peptide
9	Cw	177	ARG	Sidechain
9	Cw	190	HIS	Peptide
9	Cw	198	ASN	Peptide

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Mol	Chain	Res	Type	Group
9	Cw	199	ARG	Sidechain
9	Cw	200	GLY	Peptide
10	Cx	103	LYS	Peptide
10	Cx	116	HIS	Peptide
10	Cx	139	THR	Peptide
10	Cx	170	SER	Mainchain
10	Cx	185	GLY	Peptide
10	Cx	192	PHE	Peptide
10	Cx	57	LEU	Mainchain
10	Cx	71	GLY	Peptide
7	Cy	150	ARG	Sidechain
7	Cy	6	CYS	Peptide
5	Cz	83	MET	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	22 63
1	A5	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	22 63
1	AC	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	22 63
1	AH	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	22 63
1	AM	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	22 63
1	AR	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	22 63
1	AW	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	22 63
1	Ab	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	22 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ag	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	22	63
1	Al	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	22	63
1	Aq	147/149 (99%)	124 (84%)	22 (15%)	1 (1%)	22	63
1	Av	147/149 (99%)	125 (85%)	21 (14%)	1 (1%)	22	63
2	A1	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	A6	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	AD	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	AI	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	AN	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	AS	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	AX	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	Ac	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	Ah	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	Am	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	Ar	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
2	Aw	138/140 (99%)	118 (86%)	19 (14%)	1 (1%)	22	63
3	A2	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	A3	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	A7	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AA	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AE	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AF	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AJ	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AK	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AO	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AP	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AT	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AU	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AY	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	AZ	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	Ad	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Ae	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	Ai	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	Aj	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	An	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	Ao	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	As	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	At	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	Ax	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
3	Ay	145/147 (99%)	123 (85%)	18 (12%)	4 (3%)	5	30
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	22	63
5	B5	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	BC	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	BH	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	BM	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	BR	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	BW	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Bb	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Bg	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Bl	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Bq	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Bv	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	C4	138/158 (87%)	119 (86%)	18 (13%)	1 (1%)	22	63
5	CB	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	CG	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	CL	138/158 (87%)	119 (86%)	18 (13%)	1 (1%)	22	63
5	CQ	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	CV	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Ca	138/158 (87%)	119 (86%)	18 (13%)	1 (1%)	22	63
5	Cf	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Ck	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Cp	138/158 (87%)	119 (86%)	18 (13%)	1 (1%)	22	63
5	Cu	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
5	Cz	138/158 (87%)	118 (86%)	19 (14%)	1 (1%)	22	63
6	B1	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	B6	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	BD	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	BI	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	BN	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	BS	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	BX	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	Bc	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	Bh	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	Bm	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	Br	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
6	Bw	145/151 (96%)	119 (82%)	21 (14%)	5 (3%)	3	26
7	B4	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	BB	147/170 (86%)	125 (85%)	20 (14%)	2 (1%)	11	46
7	BG	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	BL	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	BQ	147/170 (86%)	125 (85%)	20 (14%)	2 (1%)	11	46
7	BV	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	Ba	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	Bf	147/170 (86%)	125 (85%)	20 (14%)	2 (1%)	11	46
7	Bk	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	Bp	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	Bu	147/170 (86%)	125 (85%)	20 (14%)	2 (1%)	11	46
7	Bz	147/170 (86%)	124 (84%)	21 (14%)	2 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	C3	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	CA	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	CF	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	CK	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	CP	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	CU	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	CZ	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	Ce	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	Cj	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	Co	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	Ct	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
7	Cy	147/170 (86%)	125 (85%)	21 (14%)	1 (1%)	22	63
8	C0	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	C5	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	CC	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	CH	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	CM	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	CR	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	CW	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	Cb	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	Cg	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	Cl	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	Cq	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
8	Cv	211/240 (88%)	190 (90%)	17 (8%)	4 (2%)	8	38
9	C1	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	C6	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	CD	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	CI	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	CN	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	CS	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	CX	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Cc	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	Ch	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	Cm	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	Cr	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
9	Cw	216/288 (75%)	201 (93%)	13 (6%)	2 (1%)	17	57
10	C2	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	C7	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	CE	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	CJ	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	CO	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	CT	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	CY	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	Cd	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	Ci	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	Cn	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	Cs	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
10	Cx	213/240 (89%)	184 (86%)	23 (11%)	6 (3%)	5	30
All	All	28308/31116 (91%)	24544 (87%)	3380 (12%)	384 (1%)	15	46

All (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
3	AA	87	THR
3	AE	29	ASP
3	AE	87	THR
3	AF	87	THR
3	AJ	29	ASP
3	AJ	87	THR
3	AK	87	THR
3	AO	29	ASP
3	AO	87	THR

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Mol	Chain	Res	Type
3	AP	87	THR
3	AT	29	ASP
3	AT	87	THR
3	AU	87	THR
3	AY	29	ASP
3	AY	87	THR
3	AZ	87	THR
3	Ad	29	ASP
3	Ad	87	THR
3	Ae	87	THR
3	Ai	29	ASP
3	Ai	87	THR
3	Aj	87	THR
3	An	29	ASP
3	An	87	THR
3	Ao	87	THR
3	As	29	ASP
3	As	87	THR
3	At	87	THR
3	Ax	29	ASP
3	Ax	87	THR
3	Ay	87	THR
6	B1	87	THR
7	B4	7	CYS
6	B6	87	THR
7	BB	7	CYS
6	BD	87	THR
7	BG	7	CYS
6	BI	87	THR
7	BL	7	CYS
6	BN	87	THR
7	BQ	7	CYS
6	BS	87	THR
7	BV	7	CYS
6	BX	87	THR
7	Ba	7	CYS
6	Bc	87	THR
7	Bf	7	CYS
6	Bh	87	THR
7	Bk	7	CYS
6	Bm	87	THR
7	Bp	7	CYS

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Mol	Chain	Res	Type
6	Br	87	THR
7	Bu	7	CYS
6	Bw	87	THR
7	Bz	7	CYS
8	C0	212	SER
10	C2	58	GLU
8	C5	212	SER
10	C7	58	GLU
8	CC	212	SER
10	CE	58	GLU
8	CH	212	SER
10	CJ	58	GLU
8	CM	212	SER
10	CO	58	GLU
8	CR	212	SER
10	CT	58	GLU
8	CW	212	SER
10	CY	58	GLU
8	Cb	212	SER
10	Cd	58	GLU
8	Cg	212	SER
10	Ci	58	GLU
8	Cl	212	SER
10	Cn	58	GLU
8	Cq	212	SER
10	Cs	58	GLU
8	Cv	212	SER
10	Cx	58	GLU
3	A3	29	ASP
3	AA	29	ASP
3	AF	29	ASP
3	AK	29	ASP
3	AP	29	ASP
3	AU	29	ASP
3	AZ	29	ASP
3	Ae	29	ASP
3	Aj	29	ASP
3	Ao	29	ASP
3	At	29	ASP
3	Ay	29	ASP
6	B1	24	SER
6	B1	29	ASP

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Mol	Chain	Res	Type
6	B6	24	SER
6	B6	29	ASP
6	BD	24	SER
6	BD	29	ASP
6	BI	24	SER
6	BI	29	ASP
6	BN	24	SER
6	BN	29	ASP
6	BS	24	SER
6	BS	29	ASP
6	BX	24	SER
6	BX	29	ASP
6	Bc	24	SER
6	Bc	29	ASP
6	Bh	24	SER
6	Bh	29	ASP
6	Bm	24	SER
6	Bm	29	ASP
6	Br	24	SER
6	Br	29	ASP
6	Bw	24	SER
6	Bw	29	ASP
8	C0	184	LYS
10	C2	94	ASP
8	C5	184	LYS
10	C7	94	ASP
8	CC	184	LYS
10	CE	94	ASP
8	CH	184	LYS
10	CJ	94	ASP
8	CM	184	LYS
10	CO	94	ASP
8	CR	184	LYS
10	CT	94	ASP
8	CW	184	LYS
10	CY	94	ASP
8	Cb	184	LYS
10	Cd	94	ASP
8	Cg	184	LYS
10	Ci	94	ASP
8	Cl	184	LYS
10	Cn	94	ASP

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Mol	Chain	Res	Type
8	Cq	184	LYS
10	Cs	94	ASP
8	Cv	184	LYS
10	Cx	94	ASP
1	A0	87	ASP
1	A5	87	ASP
1	AC	87	ASP
1	AH	87	ASP
1	AM	87	ASP
1	AR	87	ASP
1	AW	87	ASP
1	Ab	87	ASP
1	Ag	87	ASP
1	Al	87	ASP
1	Aq	87	ASP
1	Av	87	ASP
9	C1	198	ASN
10	C2	114	PHE
9	C6	198	ASN
10	C7	114	PHE
9	CD	198	ASN
10	CE	114	PHE
9	CI	198	ASN
10	CJ	114	PHE
9	CN	198	ASN
10	CO	114	PHE
9	CS	198	ASN
10	CT	114	PHE
9	CX	198	ASN
10	CY	114	PHE
9	Cc	198	ASN
10	Cd	114	PHE
9	Ch	198	ASN
10	Ci	114	PHE
9	Cm	198	ASN
10	Cn	114	PHE
9	Cr	198	ASN
10	Cs	114	PHE
9	Cw	198	ASN
10	Cx	114	PHE
3	A2	20	ASP
3	A7	20	ASP

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Mol	Chain	Res	Type
3	AE	20	ASP
3	AJ	20	ASP
3	AO	20	ASP
3	AT	20	ASP
3	AY	20	ASP
3	Ad	20	ASP
3	Ai	20	ASP
3	An	20	ASP
3	As	20	ASP
3	Ax	20	ASP
5	B0	57	ARG
6	B1	20	ASP
7	B4	87	ASP
5	B5	57	ARG
7	BB	87	ASP
5	BC	57	ARG
6	BD	20	ASP
7	BG	87	ASP
5	BH	57	ARG
6	BI	20	ASP
7	BL	87	ASP
5	BM	57	ARG
7	BQ	87	ASP
5	BR	57	ARG
6	BS	20	ASP
7	BV	87	ASP
5	BW	57	ARG
6	BX	20	ASP
7	Ba	87	ASP
5	Bb	57	ARG
7	Bf	87	ASP
5	Bg	57	ARG
6	Bh	20	ASP
7	Bk	87	ASP
5	Bl	57	ARG
6	Bm	20	ASP
7	Bp	87	ASP
5	Bq	57	ARG
7	Bu	87	ASP
5	Bv	57	ARG
6	Bw	20	ASP
7	Bz	87	ASP

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Mol	Chain	Res	Type
10	C2	113	CYS
10	C2	121	ARG
7	C3	87	ASP
10	C7	113	CYS
10	C7	121	ARG
7	CA	87	ASP
10	CE	113	CYS
10	CE	121	ARG
7	CF	87	ASP
10	CJ	113	CYS
10	CJ	121	ARG
7	CK	87	ASP
10	CO	113	CYS
10	CO	121	ARG
7	CP	87	ASP
10	CT	113	CYS
10	CT	121	ARG
7	CU	87	ASP
10	CY	113	CYS
10	CY	121	ARG
7	CZ	87	ASP
10	Cd	113	CYS
10	Cd	121	ARG
7	Ce	87	ASP
10	Ci	113	CYS
10	Ci	121	ARG
7	Cj	87	ASP
10	Cn	113	CYS
10	Cn	121	ARG
7	Co	87	ASP
10	Cs	113	CYS
10	Cs	121	ARG
7	Ct	87	ASP
10	Cx	113	CYS
10	Cx	121	ARG
7	Cy	87	ASP
2	A1	57	ARG
3	A3	20	ASP
3	A3	82	ASN
2	A6	57	ARG
3	AA	20	ASP
3	AA	82	ASN

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Mol	Chain	Res	Type
2	AD	57	ARG
3	AF	20	ASP
3	AF	82	ASN
2	AI	57	ARG
3	AK	20	ASP
3	AK	82	ASN
2	AN	57	ARG
3	AP	20	ASP
3	AP	82	ASN
2	AS	57	ARG
3	AU	20	ASP
3	AU	82	ASN
2	AX	57	ARG
3	AZ	20	ASP
3	AZ	82	ASN
2	Ac	57	ARG
3	Ae	20	ASP
3	Ae	82	ASN
2	Ah	57	ARG
3	Aj	20	ASP
3	Aj	82	ASN
2	Am	57	ARG
3	Ao	20	ASP
3	Ao	82	ASN
2	Ar	57	ARG
3	At	20	ASP
3	At	82	ASN
2	Aw	57	ARG
3	Ay	20	ASP
3	Ay	82	ASN
6	B6	20	ASP
6	BD	82	ASN
6	BN	20	ASP
6	BS	82	ASN
6	Bc	20	ASP
6	Bh	82	ASN
6	Br	20	ASP
6	Bw	82	ASN
8	C0	12	TYR
5	C4	57	ARG
8	C5	12	TYR
5	CB	57	ARG

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Mol	Chain	Res	Type
8	CC	12	TYR
5	CG	57	ARG
8	CH	12	TYR
5	CL	57	ARG
8	CM	12	TYR
5	CQ	57	ARG
8	CR	12	TYR
5	CV	57	ARG
8	CW	12	TYR
5	Ca	57	ARG
8	Cb	12	TYR
5	Cf	57	ARG
8	Cg	12	TYR
5	Ck	57	ARG
8	Cl	12	TYR
5	Cp	57	ARG
8	Cq	12	TYR
5	Cu	57	ARG
8	Cv	12	TYR
5	Cz	57	ARG
3	A2	82	ASN
3	A7	82	ASN
3	AE	82	ASN
3	AJ	82	ASN
3	AO	82	ASN
3	AT	82	ASN
3	AY	82	ASN
3	Ad	82	ASN
3	Ai	82	ASN
3	An	82	ASN
3	As	82	ASN
3	Ax	82	ASN
6	B1	82	ASN
6	B6	82	ASN
6	BI	82	ASN
6	BN	82	ASN
6	BX	82	ASN
6	Bc	82	ASN
6	Bm	82	ASN
6	Br	82	ASN
9	C1	12	PRO
9	C6	12	PRO

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Mol	Chain	Res	Type
9	CD	12	PRO
9	CI	12	PRO
9	CN	12	PRO
9	CS	12	PRO
9	CX	12	PRO
9	Cc	12	PRO
9	Ch	12	PRO
9	Cm	12	PRO
9	Cr	12	PRO
9	Cw	12	PRO
10	C2	71	GLY
10	C7	71	GLY
10	CE	71	GLY
10	CJ	71	GLY
10	CO	71	GLY
10	CT	71	GLY
10	CY	71	GLY
10	Cd	71	GLY
10	Ci	71	GLY
10	Cn	71	GLY
10	Cs	71	GLY
10	Cx	71	GLY
8	C0	216	VAL
8	C5	216	VAL
8	CC	216	VAL
8	CH	216	VAL
8	CM	216	VAL
8	CR	216	VAL
8	CW	216	VAL
8	Cb	216	VAL
8	Cg	216	VAL
8	Cl	216	VAL
8	Cq	216	VAL
8	Cv	216	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A0	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	A5	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	AC	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	AH	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	AM	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	AR	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	AW	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	Ab	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	Ag	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	Al	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	Aq	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	Av	128/128 (100%)	119 (93%)	9 (7%)	15	40
2	A1	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	A6	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	AD	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	AI	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	AN	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	AS	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	AX	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	Ac	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	Ah	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	Am	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	Ar	121/121 (100%)	107 (88%)	14 (12%)	5	21
2	Aw	121/121 (100%)	107 (88%)	14 (12%)	5	21
3	A2	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	A3	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	A7	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	AA	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	AE	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	AF	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	AJ	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	AK	131/131 (100%)	118 (90%)	13 (10%)	8	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AO	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	AP	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	AT	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	AU	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	AY	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	AZ	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	Ad	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	Ae	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	Ai	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	Aj	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	An	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	Ao	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	As	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	At	131/131 (100%)	118 (90%)	13 (10%)	8	26
3	Ax	131/131 (100%)	114 (87%)	17 (13%)	4	18
3	Ay	131/131 (100%)	118 (90%)	13 (10%)	8	26
4	A4	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	AB	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	AG	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	AL	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	AQ	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	AV	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Aa	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Af	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Ak	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Ap	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Au	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Az	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	B2	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	B3	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	B7	117/117 (100%)	107 (92%)	10 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	BA	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	BE	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	BF	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	BJ	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	BK	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	BO	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	BP	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	BT	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	BU	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	BY	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	BZ	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Bd	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	Be	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Bi	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	Bj	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Bn	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	Bo	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Bs	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	Bt	117/117 (100%)	104 (89%)	13 (11%)	6	22
4	Bx	117/117 (100%)	107 (92%)	10 (8%)	10	33
4	By	117/117 (100%)	104 (89%)	13 (11%)	6	22
5	B0	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	B5	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	BC	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	BH	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	BM	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	BR	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	BW	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	Bb	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	Bg	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	Bl	121/135 (90%)	111 (92%)	10 (8%)	11	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Bq	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	Bv	121/135 (90%)	111 (92%)	10 (8%)	11	34
5	C4	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	CB	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	CG	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	CL	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	CQ	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	CV	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	Ca	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	Cf	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	Ck	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	Cp	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	Cu	121/135 (90%)	112 (93%)	9 (7%)	13	38
5	Cz	121/135 (90%)	112 (93%)	9 (7%)	13	38
6	B1	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	B6	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	BD	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	BI	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	BN	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	BS	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	BX	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	Bc	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	Bh	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	Bm	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	Br	131/134 (98%)	117 (89%)	14 (11%)	6	23
6	Bw	131/134 (98%)	117 (89%)	14 (11%)	6	23
7	B4	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	BB	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	BG	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	BL	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	BQ	128/145 (88%)	120 (94%)	8 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BV	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	Ba	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	Bf	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	Bk	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	Bp	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	Bu	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	Bz	128/145 (88%)	120 (94%)	8 (6%)	18	43
7	C3	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	CA	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	CF	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	CK	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	CP	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	CU	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	CZ	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	Ce	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	Cj	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	Co	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	Ct	128/145 (88%)	119 (93%)	9 (7%)	15	40
7	Cy	128/145 (88%)	119 (93%)	9 (7%)	15	40
8	C0	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	C5	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	CC	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	CH	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	CM	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	CR	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	CW	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	Cb	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	Cg	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	Cl	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	Cq	195/212 (92%)	147 (75%)	48 (25%)	0	3
8	Cv	195/212 (92%)	147 (75%)	48 (25%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	C1	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	C6	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	CD	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	CI	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	CN	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	CS	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	CX	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	Cc	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	Ch	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	Cm	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	Cr	193/241 (80%)	154 (80%)	39 (20%)	1	7
9	Cw	193/241 (80%)	154 (80%)	39 (20%)	1	7
10	C2	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	C7	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	CE	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	CJ	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	CO	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	CT	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	CY	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	Cd	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	Ci	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	Cn	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	Cs	193/211 (92%)	158 (82%)	35 (18%)	1	10
10	Cx	193/211 (92%)	158 (82%)	35 (18%)	1	10
All	All	24864/26640 (93%)	21732 (87%)	3132 (13%)	8	19

All (3132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	6	CYS
1	A0	7	CYS
1	A0	20	ASP
1	A0	37	ARG
1	A0	74	ILE

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Mol	Chain	Res	Type
1	A0	115	LYS
1	A0	129	ASP
1	A0	146	LYS
1	A0	151	LEU
2	A1	19	LEU
2	A1	41	ASP
2	A1	48	GLU
2	A1	71	GLN
2	A1	82	SER
2	A1	83	MET
2	A1	84	LEU
2	A1	104	ARG
2	A1	106	LEU
2	A1	107	LYS
2	A1	128	THR
2	A1	138	CYS
2	A1	146	ILE
2	A1	147	LYS
3	A2	5	ASP
3	A2	6	CYS
3	A2	7	CYS
3	A2	24	SER
3	A2	26	SER
3	A2	27	PHE
3	A2	48	THR
3	A2	55	ARG
3	A2	59	ASP
3	A2	65	GLU
3	A2	82	ASN
3	A2	85	ASP
3	A2	126	VAL
3	A2	131	ASN
3	A2	136	ASN
3	A2	149	ASP
3	A2	150	LEU
3	A3	5	ASP
3	A3	8	SER
3	A3	24	SER
3	A3	27	PHE
3	A3	48	THR
3	A3	55	ARG
3	A3	59	ASP

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Mol	Chain	Res	Type
3	A3	82	ASN
3	A3	85	ASP
3	A3	126	VAL
3	A3	131	ASN
3	A3	136	ASN
3	A3	150	LEU
4	A4	1	LYS
4	A4	25	ASP
4	A4	56	THR
4	A4	66	ASP
4	A4	80	ASP
4	A4	90	ASP
4	A4	99	ARG
4	A4	100	LYS
4	A4	101	ILE
4	A4	123	ARG
4	A4	125	TYR
4	A4	135	ASP
4	A4	145	HIS
1	A5	6	CYS
1	A5	7	CYS
1	A5	20	ASP
1	A5	37	ARG
1	A5	74	ILE
1	A5	115	LYS
1	A5	129	ASP
1	A5	146	LYS
1	A5	151	LEU
2	A6	19	LEU
2	A6	41	ASP
2	A6	48	GLU
2	A6	71	GLN
2	A6	82	SER
2	A6	83	MET
2	A6	84	LEU
2	A6	104	ARG
2	A6	106	LEU
2	A6	107	LYS
2	A6	128	THR
2	A6	138	CYS
2	A6	146	ILE
2	A6	147	LYS

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Mol	Chain	Res	Type
3	A7	5	ASP
3	A7	6	CYS
3	A7	7	CYS
3	A7	24	SER
3	A7	26	SER
3	A7	27	PHE
3	A7	48	THR
3	A7	55	ARG
3	A7	59	ASP
3	A7	65	GLU
3	A7	82	ASN
3	A7	85	ASP
3	A7	126	VAL
3	A7	131	ASN
3	A7	136	ASN
3	A7	149	ASP
3	A7	150	LEU
3	AA	5	ASP
3	AA	8	SER
3	AA	24	SER
3	AA	27	PHE
3	AA	48	THR
3	AA	55	ARG
3	AA	59	ASP
3	AA	82	ASN
3	AA	85	ASP
3	AA	126	VAL
3	AA	131	ASN
3	AA	136	ASN
3	AA	150	LEU
4	AB	1	LYS
4	AB	25	ASP
4	AB	56	THR
4	AB	66	ASP
4	AB	80	ASP
4	AB	90	ASP
4	AB	99	ARG
4	AB	100	LYS
4	AB	101	ILE
4	AB	123	ARG
4	AB	125	TYR
4	AB	135	ASP

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Mol	Chain	Res	Type
4	AB	145	HIS
1	AC	6	CYS
1	AC	7	CYS
1	AC	20	ASP
1	AC	37	ARG
1	AC	74	ILE
1	AC	115	LYS
1	AC	129	ASP
1	AC	146	LYS
1	AC	151	LEU
2	AD	19	LEU
2	AD	41	ASP
2	AD	48	GLU
2	AD	71	GLN
2	AD	82	SER
2	AD	83	MET
2	AD	84	LEU
2	AD	104	ARG
2	AD	106	LEU
2	AD	107	LYS
2	AD	128	THR
2	AD	138	CYS
2	AD	146	ILE
2	AD	147	LYS
3	AE	5	ASP
3	AE	6	CYS
3	AE	7	CYS
3	AE	24	SER
3	AE	26	SER
3	AE	27	PHE
3	AE	48	THR
3	AE	55	ARG
3	AE	59	ASP
3	AE	65	GLU
3	AE	82	ASN
3	AE	85	ASP
3	AE	126	VAL
3	AE	131	ASN
3	AE	136	ASN
3	AE	149	ASP
3	AE	150	LEU
3	AF	5	ASP

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Mol	Chain	Res	Type
3	AF	8	SER
3	AF	24	SER
3	AF	27	PHE
3	AF	48	THR
3	AF	55	ARG
3	AF	59	ASP
3	AF	82	ASN
3	AF	85	ASP
3	AF	126	VAL
3	AF	131	ASN
3	AF	136	ASN
3	AF	150	LEU
4	AG	1	LYS
4	AG	25	ASP
4	AG	56	THR
4	AG	66	ASP
4	AG	80	ASP
4	AG	90	ASP
4	AG	99	ARG
4	AG	100	LYS
4	AG	101	ILE
4	AG	123	ARG
4	AG	125	TYR
4	AG	135	ASP
4	AG	145	HIS
1	AH	6	CYS
1	AH	7	CYS
1	AH	20	ASP
1	AH	37	ARG
1	AH	74	ILE
1	AH	115	LYS
1	AH	129	ASP
1	AH	146	LYS
1	AH	151	LEU
2	AI	19	LEU
2	AI	41	ASP
2	AI	48	GLU
2	AI	71	GLN
2	AI	82	SER
2	AI	83	MET
2	AI	84	LEU
2	AI	104	ARG

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Mol	Chain	Res	Type
2	AI	106	LEU
2	AI	107	LYS
2	AI	128	THR
2	AI	138	CYS
2	AI	146	ILE
2	AI	147	LYS
3	AJ	5	ASP
3	AJ	6	CYS
3	AJ	7	CYS
3	AJ	24	SER
3	AJ	26	SER
3	AJ	27	PHE
3	AJ	48	THR
3	AJ	55	ARG
3	AJ	59	ASP
3	AJ	65	GLU
3	AJ	82	ASN
3	AJ	85	ASP
3	AJ	126	VAL
3	AJ	131	ASN
3	AJ	136	ASN
3	AJ	149	ASP
3	AJ	150	LEU
3	AK	5	ASP
3	AK	8	SER
3	AK	24	SER
3	AK	27	PHE
3	AK	48	THR
3	AK	55	ARG
3	AK	59	ASP
3	AK	82	ASN
3	AK	85	ASP
3	AK	126	VAL
3	AK	131	ASN
3	AK	136	ASN
3	AK	150	LEU
4	AL	1	LYS
4	AL	25	ASP
4	AL	56	THR
4	AL	66	ASP
4	AL	80	ASP
4	AL	90	ASP

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Mol	Chain	Res	Type
4	AL	99	ARG
4	AL	100	LYS
4	AL	101	ILE
4	AL	123	ARG
4	AL	125	TYR
4	AL	135	ASP
4	AL	145	HIS
1	AM	6	CYS
1	AM	7	CYS
1	AM	20	ASP
1	AM	37	ARG
1	AM	74	ILE
1	AM	115	LYS
1	AM	129	ASP
1	AM	146	LYS
1	AM	151	LEU
2	AN	19	LEU
2	AN	41	ASP
2	AN	48	GLU
2	AN	71	GLN
2	AN	82	SER
2	AN	83	MET
2	AN	84	LEU
2	AN	104	ARG
2	AN	106	LEU
2	AN	107	LYS
2	AN	128	THR
2	AN	138	CYS
2	AN	146	ILE
2	AN	147	LYS
3	AO	5	ASP
3	AO	6	CYS
3	AO	7	CYS
3	AO	24	SER
3	AO	26	SER
3	AO	27	PHE
3	AO	48	THR
3	AO	55	ARG
3	AO	59	ASP
3	AO	65	GLU
3	AO	82	ASN
3	AO	85	ASP

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Mol	Chain	Res	Type
3	AO	126	VAL
3	AO	131	ASN
3	AO	136	ASN
3	AO	149	ASP
3	AO	150	LEU
3	AP	5	ASP
3	AP	8	SER
3	AP	24	SER
3	AP	27	PHE
3	AP	48	THR
3	AP	55	ARG
3	AP	59	ASP
3	AP	82	ASN
3	AP	85	ASP
3	AP	126	VAL
3	AP	131	ASN
3	AP	136	ASN
3	AP	150	LEU
4	AQ	1	LYS
4	AQ	25	ASP
4	AQ	56	THR
4	AQ	66	ASP
4	AQ	80	ASP
4	AQ	90	ASP
4	AQ	99	ARG
4	AQ	100	LYS
4	AQ	101	ILE
4	AQ	123	ARG
4	AQ	125	TYR
4	AQ	135	ASP
4	AQ	145	HIS
1	AR	6	CYS
1	AR	7	CYS
1	AR	20	ASP
1	AR	37	ARG
1	AR	74	ILE
1	AR	115	LYS
1	AR	129	ASP
1	AR	146	LYS
1	AR	151	LEU
2	AS	19	LEU
2	AS	41	ASP

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Mol	Chain	Res	Type
2	AS	48	GLU
2	AS	71	GLN
2	AS	82	SER
2	AS	83	MET
2	AS	84	LEU
2	AS	104	ARG
2	AS	106	LEU
2	AS	107	LYS
2	AS	128	THR
2	AS	138	CYS
2	AS	146	ILE
2	AS	147	LYS
3	AT	5	ASP
3	AT	6	CYS
3	AT	7	CYS
3	AT	24	SER
3	AT	26	SER
3	AT	27	PHE
3	AT	48	THR
3	AT	55	ARG
3	AT	59	ASP
3	AT	65	GLU
3	AT	82	ASN
3	AT	85	ASP
3	AT	126	VAL
3	AT	131	ASN
3	AT	136	ASN
3	AT	149	ASP
3	AT	150	LEU
3	AU	5	ASP
3	AU	8	SER
3	AU	24	SER
3	AU	27	PHE
3	AU	48	THR
3	AU	55	ARG
3	AU	59	ASP
3	AU	82	ASN
3	AU	85	ASP
3	AU	126	VAL
3	AU	131	ASN
3	AU	136	ASN
3	AU	150	LEU

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Mol	Chain	Res	Type
4	AV	1	LYS
4	AV	25	ASP
4	AV	56	THR
4	AV	66	ASP
4	AV	80	ASP
4	AV	90	ASP
4	AV	99	ARG
4	AV	100	LYS
4	AV	101	ILE
4	AV	123	ARG
4	AV	125	TYR
4	AV	135	ASP
4	AV	145	HIS
1	AW	6	CYS
1	AW	7	CYS
1	AW	20	ASP
1	AW	37	ARG
1	AW	74	ILE
1	AW	115	LYS
1	AW	129	ASP
1	AW	146	LYS
1	AW	151	LEU
2	AX	19	LEU
2	AX	41	ASP
2	AX	48	GLU
2	AX	71	GLN
2	AX	82	SER
2	AX	83	MET
2	AX	84	LEU
2	AX	104	ARG
2	AX	106	LEU
2	AX	107	LYS
2	AX	128	THR
2	AX	138	CYS
2	AX	146	ILE
2	AX	147	LYS
3	AY	5	ASP
3	AY	6	CYS
3	AY	7	CYS
3	AY	24	SER
3	AY	26	SER
3	AY	27	PHE

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Mol	Chain	Res	Type
3	AY	48	THR
3	AY	55	ARG
3	AY	59	ASP
3	AY	65	GLU
3	AY	82	ASN
3	AY	85	ASP
3	AY	126	VAL
3	AY	131	ASN
3	AY	136	ASN
3	AY	149	ASP
3	AY	150	LEU
3	AZ	5	ASP
3	AZ	8	SER
3	AZ	24	SER
3	AZ	27	PHE
3	AZ	48	THR
3	AZ	55	ARG
3	AZ	59	ASP
3	AZ	82	ASN
3	AZ	85	ASP
3	AZ	126	VAL
3	AZ	131	ASN
3	AZ	136	ASN
3	AZ	150	LEU
4	Aa	1	LYS
4	Aa	25	ASP
4	Aa	56	THR
4	Aa	66	ASP
4	Aa	80	ASP
4	Aa	90	ASP
4	Aa	99	ARG
4	Aa	100	LYS
4	Aa	101	ILE
4	Aa	123	ARG
4	Aa	125	TYR
4	Aa	135	ASP
4	Aa	145	HIS
1	Ab	6	CYS
1	Ab	7	CYS
1	Ab	20	ASP
1	Ab	37	ARG
1	Ab	74	ILE

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Mol	Chain	Res	Type
1	Ab	115	LYS
1	Ab	129	ASP
1	Ab	146	LYS
1	Ab	151	LEU
2	Ac	19	LEU
2	Ac	41	ASP
2	Ac	48	GLU
2	Ac	71	GLN
2	Ac	82	SER
2	Ac	83	MET
2	Ac	84	LEU
2	Ac	104	ARG
2	Ac	106	LEU
2	Ac	107	LYS
2	Ac	128	THR
2	Ac	138	CYS
2	Ac	146	ILE
2	Ac	147	LYS
3	Ad	5	ASP
3	Ad	6	CYS
3	Ad	7	CYS
3	Ad	24	SER
3	Ad	26	SER
3	Ad	27	PHE
3	Ad	48	THR
3	Ad	55	ARG
3	Ad	59	ASP
3	Ad	65	GLU
3	Ad	82	ASN
3	Ad	85	ASP
3	Ad	126	VAL
3	Ad	131	ASN
3	Ad	136	ASN
3	Ad	149	ASP
3	Ad	150	LEU
3	Ae	5	ASP
3	Ae	8	SER
3	Ae	24	SER
3	Ae	27	PHE
3	Ae	48	THR
3	Ae	55	ARG
3	Ae	59	ASP

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Mol	Chain	Res	Type
3	Ae	82	ASN
3	Ae	85	ASP
3	Ae	126	VAL
3	Ae	131	ASN
3	Ae	136	ASN
3	Ae	150	LEU
4	Af	1	LYS
4	Af	25	ASP
4	Af	56	THR
4	Af	66	ASP
4	Af	80	ASP
4	Af	90	ASP
4	Af	99	ARG
4	Af	100	LYS
4	Af	101	ILE
4	Af	123	ARG
4	Af	125	TYR
4	Af	135	ASP
4	Af	145	HIS
1	Ag	6	CYS
1	Ag	7	CYS
1	Ag	20	ASP
1	Ag	37	ARG
1	Ag	74	ILE
1	Ag	115	LYS
1	Ag	129	ASP
1	Ag	146	LYS
1	Ag	151	LEU
2	Ah	19	LEU
2	Ah	41	ASP
2	Ah	48	GLU
2	Ah	71	GLN
2	Ah	82	SER
2	Ah	83	MET
2	Ah	84	LEU
2	Ah	104	ARG
2	Ah	106	LEU
2	Ah	107	LYS
2	Ah	128	THR
2	Ah	138	CYS
2	Ah	146	ILE
2	Ah	147	LYS

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Mol	Chain	Res	Type
3	Ai	5	ASP
3	Ai	6	CYS
3	Ai	7	CYS
3	Ai	24	SER
3	Ai	26	SER
3	Ai	27	PHE
3	Ai	48	THR
3	Ai	55	ARG
3	Ai	59	ASP
3	Ai	65	GLU
3	Ai	82	ASN
3	Ai	85	ASP
3	Ai	126	VAL
3	Ai	131	ASN
3	Ai	136	ASN
3	Ai	149	ASP
3	Ai	150	LEU
3	Aj	5	ASP
3	Aj	8	SER
3	Aj	24	SER
3	Aj	27	PHE
3	Aj	48	THR
3	Aj	55	ARG
3	Aj	59	ASP
3	Aj	82	ASN
3	Aj	85	ASP
3	Aj	126	VAL
3	Aj	131	ASN
3	Aj	136	ASN
3	Aj	150	LEU
4	Ak	1	LYS
4	Ak	25	ASP
4	Ak	56	THR
4	Ak	66	ASP
4	Ak	80	ASP
4	Ak	90	ASP
4	Ak	99	ARG
4	Ak	100	LYS
4	Ak	101	ILE
4	Ak	123	ARG
4	Ak	125	TYR
4	Ak	135	ASP

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Mol	Chain	Res	Type
4	Ak	145	HIS
1	Al	6	CYS
1	Al	7	CYS
1	Al	20	ASP
1	Al	37	ARG
1	Al	74	ILE
1	Al	115	LYS
1	Al	129	ASP
1	Al	146	LYS
1	Al	151	LEU
2	Am	19	LEU
2	Am	41	ASP
2	Am	48	GLU
2	Am	71	GLN
2	Am	82	SER
2	Am	83	MET
2	Am	84	LEU
2	Am	104	ARG
2	Am	106	LEU
2	Am	107	LYS
2	Am	128	THR
2	Am	138	CYS
2	Am	146	ILE
2	Am	147	LYS
3	An	5	ASP
3	An	6	CYS
3	An	7	CYS
3	An	24	SER
3	An	26	SER
3	An	27	PHE
3	An	48	THR
3	An	55	ARG
3	An	59	ASP
3	An	65	GLU
3	An	82	ASN
3	An	85	ASP
3	An	126	VAL
3	An	131	ASN
3	An	136	ASN
3	An	149	ASP
3	An	150	LEU
3	Ao	5	ASP

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Mol	Chain	Res	Type
3	Ao	8	SER
3	Ao	24	SER
3	Ao	27	PHE
3	Ao	48	THR
3	Ao	55	ARG
3	Ao	59	ASP
3	Ao	82	ASN
3	Ao	85	ASP
3	Ao	126	VAL
3	Ao	131	ASN
3	Ao	136	ASN
3	Ao	150	LEU
4	Ap	1	LYS
4	Ap	25	ASP
4	Ap	56	THR
4	Ap	66	ASP
4	Ap	80	ASP
4	Ap	90	ASP
4	Ap	99	ARG
4	Ap	100	LYS
4	Ap	101	ILE
4	Ap	123	ARG
4	Ap	125	TYR
4	Ap	135	ASP
4	Ap	145	HIS
1	Aq	6	CYS
1	Aq	7	CYS
1	Aq	20	ASP
1	Aq	37	ARG
1	Aq	74	ILE
1	Aq	115	LYS
1	Aq	129	ASP
1	Aq	146	LYS
1	Aq	151	LEU
2	Ar	19	LEU
2	Ar	41	ASP
2	Ar	48	GLU
2	Ar	71	GLN
2	Ar	82	SER
2	Ar	83	MET
2	Ar	84	LEU
2	Ar	104	ARG

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Mol	Chain	Res	Type
2	Ar	106	LEU
2	Ar	107	LYS
2	Ar	128	THR
2	Ar	138	CYS
2	Ar	146	ILE
2	Ar	147	LYS
3	As	5	ASP
3	As	6	CYS
3	As	7	CYS
3	As	24	SER
3	As	26	SER
3	As	27	PHE
3	As	48	THR
3	As	55	ARG
3	As	59	ASP
3	As	65	GLU
3	As	82	ASN
3	As	85	ASP
3	As	126	VAL
3	As	131	ASN
3	As	136	ASN
3	As	149	ASP
3	As	150	LEU
3	At	5	ASP
3	At	8	SER
3	At	24	SER
3	At	27	PHE
3	At	48	THR
3	At	55	ARG
3	At	59	ASP
3	At	82	ASN
3	At	85	ASP
3	At	126	VAL
3	At	131	ASN
3	At	136	ASN
3	At	150	LEU
4	Au	1	LYS
4	Au	25	ASP
4	Au	56	THR
4	Au	66	ASP
4	Au	80	ASP
4	Au	90	ASP

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Mol	Chain	Res	Type
4	Au	99	ARG
4	Au	100	LYS
4	Au	101	ILE
4	Au	123	ARG
4	Au	125	TYR
4	Au	135	ASP
4	Au	145	HIS
1	Av	6	CYS
1	Av	7	CYS
1	Av	20	ASP
1	Av	37	ARG
1	Av	74	ILE
1	Av	115	LYS
1	Av	129	ASP
1	Av	146	LYS
1	Av	151	LEU
2	Aw	19	LEU
2	Aw	41	ASP
2	Aw	48	GLU
2	Aw	71	GLN
2	Aw	82	SER
2	Aw	83	MET
2	Aw	84	LEU
2	Aw	104	ARG
2	Aw	106	LEU
2	Aw	107	LYS
2	Aw	128	THR
2	Aw	138	CYS
2	Aw	146	ILE
2	Aw	147	LYS
3	Ax	5	ASP
3	Ax	6	CYS
3	Ax	7	CYS
3	Ax	24	SER
3	Ax	26	SER
3	Ax	27	PHE
3	Ax	48	THR
3	Ax	55	ARG
3	Ax	59	ASP
3	Ax	65	GLU
3	Ax	82	ASN
3	Ax	85	ASP

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Mol	Chain	Res	Type
3	Ax	126	VAL
3	Ax	131	ASN
3	Ax	136	ASN
3	Ax	149	ASP
3	Ax	150	LEU
3	Ay	5	ASP
3	Ay	8	SER
3	Ay	24	SER
3	Ay	27	PHE
3	Ay	48	THR
3	Ay	55	ARG
3	Ay	59	ASP
3	Ay	82	ASN
3	Ay	85	ASP
3	Ay	126	VAL
3	Ay	131	ASN
3	Ay	136	ASN
3	Ay	150	LEU
4	Az	1	LYS
4	Az	25	ASP
4	Az	56	THR
4	Az	66	ASP
4	Az	80	ASP
4	Az	90	ASP
4	Az	99	ARG
4	Az	100	LYS
4	Az	101	ILE
4	Az	123	ARG
4	Az	125	TYR
4	Az	135	ASP
4	Az	145	HIS
5	B0	9	CYS
5	B0	19	LEU
5	B0	41	ASP
5	B0	48	GLU
5	B0	84	LEU
5	B0	105	ASN
5	B0	106	LEU
5	B0	107	LYS
5	B0	128	THR
5	B0	138	CYS
6	B1	5	ASP

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Mol	Chain	Res	Type
6	B1	7	CYS
6	B1	8	SER
6	B1	24	SER
6	B1	27	PHE
6	B1	48	THR
6	B1	55	ARG
6	B1	59	ASP
6	B1	82	ASN
6	B1	85	ASP
6	B1	126	VAL
6	B1	131	ASN
6	B1	136	ASN
6	B1	150	LEU
4	B2	25	ASP
4	B2	56	THR
4	B2	66	ASP
4	B2	81	GLN
4	B2	90	ASP
4	B2	100	LYS
4	B2	101	ILE
4	B2	123	ARG
4	B2	125	TYR
4	B2	135	ASP
4	B3	2	LYS
4	B3	25	ASP
4	B3	56	THR
4	B3	66	ASP
4	B3	80	ASP
4	B3	81	GLN
4	B3	90	ASP
4	B3	99	ARG
4	B3	100	LYS
4	B3	101	ILE
4	B3	123	ARG
4	B3	125	TYR
4	B3	135	ASP
7	B4	5	HIS
7	B4	8	SER
7	B4	20	ASP
7	B4	37	ARG
7	B4	74	ILE
7	B4	115	LYS

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Mol	Chain	Res	Type
7	B4	129	ASP
7	B4	146	LYS
5	B5	9	CYS
5	B5	19	LEU
5	B5	41	ASP
5	B5	48	GLU
5	B5	84	LEU
5	B5	105	ASN
5	B5	106	LEU
5	B5	107	LYS
5	B5	128	THR
5	B5	138	CYS
6	B6	5	ASP
6	B6	7	CYS
6	B6	8	SER
6	B6	24	SER
6	B6	27	PHE
6	B6	48	THR
6	B6	55	ARG
6	B6	59	ASP
6	B6	82	ASN
6	B6	85	ASP
6	B6	126	VAL
6	B6	131	ASN
6	B6	136	ASN
6	B6	150	LEU
4	B7	25	ASP
4	B7	56	THR
4	B7	66	ASP
4	B7	81	GLN
4	B7	90	ASP
4	B7	100	LYS
4	B7	101	ILE
4	B7	123	ARG
4	B7	125	TYR
4	B7	135	ASP
4	BA	2	LYS
4	BA	25	ASP
4	BA	56	THR
4	BA	66	ASP
4	BA	80	ASP
4	BA	81	GLN

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Mol	Chain	Res	Type
4	BA	90	ASP
4	BA	99	ARG
4	BA	100	LYS
4	BA	101	ILE
4	BA	123	ARG
4	BA	125	TYR
4	BA	135	ASP
7	BB	5	HIS
7	BB	8	SER
7	BB	20	ASP
7	BB	37	ARG
7	BB	74	ILE
7	BB	115	LYS
7	BB	129	ASP
7	BB	146	LYS
5	BC	9	CYS
5	BC	19	LEU
5	BC	41	ASP
5	BC	48	GLU
5	BC	84	LEU
5	BC	105	ASN
5	BC	106	LEU
5	BC	107	LYS
5	BC	128	THR
5	BC	138	CYS
6	BD	5	ASP
6	BD	7	CYS
6	BD	8	SER
6	BD	24	SER
6	BD	27	PHE
6	BD	48	THR
6	BD	55	ARG
6	BD	59	ASP
6	BD	82	ASN
6	BD	85	ASP
6	BD	126	VAL
6	BD	131	ASN
6	BD	136	ASN
6	BD	150	LEU
4	BE	25	ASP
4	BE	56	THR
4	BE	66	ASP

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Mol	Chain	Res	Type
4	BE	81	GLN
4	BE	90	ASP
4	BE	100	LYS
4	BE	101	ILE
4	BE	123	ARG
4	BE	125	TYR
4	BE	135	ASP
4	BF	2	LYS
4	BF	25	ASP
4	BF	56	THR
4	BF	66	ASP
4	BF	80	ASP
4	BF	81	GLN
4	BF	90	ASP
4	BF	99	ARG
4	BF	100	LYS
4	BF	101	ILE
4	BF	123	ARG
4	BF	125	TYR
4	BF	135	ASP
7	BG	5	HIS
7	BG	8	SER
7	BG	20	ASP
7	BG	37	ARG
7	BG	74	ILE
7	BG	115	LYS
7	BG	129	ASP
7	BG	146	LYS
5	BH	9	CYS
5	BH	19	LEU
5	BH	41	ASP
5	BH	48	GLU
5	BH	84	LEU
5	BH	105	ASN
5	BH	106	LEU
5	BH	107	LYS
5	BH	128	THR
5	BH	138	CYS
6	BI	5	ASP
6	BI	7	CYS
6	BI	8	SER
6	BI	24	SER

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Mol	Chain	Res	Type
6	BI	27	PHE
6	BI	48	THR
6	BI	55	ARG
6	BI	59	ASP
6	BI	82	ASN
6	BI	85	ASP
6	BI	126	VAL
6	BI	131	ASN
6	BI	136	ASN
6	BI	150	LEU
4	BJ	25	ASP
4	BJ	56	THR
4	BJ	66	ASP
4	BJ	81	GLN
4	BJ	90	ASP
4	BJ	100	LYS
4	BJ	101	ILE
4	BJ	123	ARG
4	BJ	125	TYR
4	BJ	135	ASP
4	BK	2	LYS
4	BK	25	ASP
4	BK	56	THR
4	BK	66	ASP
4	BK	80	ASP
4	BK	81	GLN
4	BK	90	ASP
4	BK	99	ARG
4	BK	100	LYS
4	BK	101	ILE
4	BK	123	ARG
4	BK	125	TYR
4	BK	135	ASP
7	BL	5	HIS
7	BL	8	SER
7	BL	20	ASP
7	BL	37	ARG
7	BL	74	ILE
7	BL	115	LYS
7	BL	129	ASP
7	BL	146	LYS
5	BM	9	CYS

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Mol	Chain	Res	Type
5	BM	19	LEU
5	BM	41	ASP
5	BM	48	GLU
5	BM	84	LEU
5	BM	105	ASN
5	BM	106	LEU
5	BM	107	LYS
5	BM	128	THR
5	BM	138	CYS
6	BN	5	ASP
6	BN	7	CYS
6	BN	8	SER
6	BN	24	SER
6	BN	27	PHE
6	BN	48	THR
6	BN	55	ARG
6	BN	59	ASP
6	BN	82	ASN
6	BN	85	ASP
6	BN	126	VAL
6	BN	131	ASN
6	BN	136	ASN
6	BN	150	LEU
4	BO	25	ASP
4	BO	56	THR
4	BO	66	ASP
4	BO	81	GLN
4	BO	90	ASP
4	BO	100	LYS
4	BO	101	ILE
4	BO	123	ARG
4	BO	125	TYR
4	BO	135	ASP
4	BP	2	LYS
4	BP	25	ASP
4	BP	56	THR
4	BP	66	ASP
4	BP	80	ASP
4	BP	81	GLN
4	BP	90	ASP
4	BP	99	ARG
4	BP	100	LYS

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Mol	Chain	Res	Type
4	BP	101	ILE
4	BP	123	ARG
4	BP	125	TYR
4	BP	135	ASP
7	BQ	5	HIS
7	BQ	8	SER
7	BQ	20	ASP
7	BQ	37	ARG
7	BQ	74	ILE
7	BQ	115	LYS
7	BQ	129	ASP
7	BQ	146	LYS
5	BR	9	CYS
5	BR	19	LEU
5	BR	41	ASP
5	BR	48	GLU
5	BR	84	LEU
5	BR	105	ASN
5	BR	106	LEU
5	BR	107	LYS
5	BR	128	THR
5	BR	138	CYS
6	BS	5	ASP
6	BS	7	CYS
6	BS	8	SER
6	BS	24	SER
6	BS	27	PHE
6	BS	48	THR
6	BS	55	ARG
6	BS	59	ASP
6	BS	82	ASN
6	BS	85	ASP
6	BS	126	VAL
6	BS	131	ASN
6	BS	136	ASN
6	BS	150	LEU
4	BT	25	ASP
4	BT	56	THR
4	BT	66	ASP
4	BT	81	GLN
4	BT	90	ASP
4	BT	100	LYS

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Mol	Chain	Res	Type
4	BT	101	ILE
4	BT	123	ARG
4	BT	125	TYR
4	BT	135	ASP
4	BU	2	LYS
4	BU	25	ASP
4	BU	56	THR
4	BU	66	ASP
4	BU	80	ASP
4	BU	81	GLN
4	BU	90	ASP
4	BU	99	ARG
4	BU	100	LYS
4	BU	101	ILE
4	BU	123	ARG
4	BU	125	TYR
4	BU	135	ASP
7	BV	5	HIS
7	BV	8	SER
7	BV	20	ASP
7	BV	37	ARG
7	BV	74	ILE
7	BV	115	LYS
7	BV	129	ASP
7	BV	146	LYS
5	BW	9	CYS
5	BW	19	LEU
5	BW	41	ASP
5	BW	48	GLU
5	BW	84	LEU
5	BW	105	ASN
5	BW	106	LEU
5	BW	107	LYS
5	BW	128	THR
5	BW	138	CYS
6	BX	5	ASP
6	BX	7	CYS
6	BX	8	SER
6	BX	24	SER
6	BX	27	PHE
6	BX	48	THR
6	BX	55	ARG

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Mol	Chain	Res	Type
6	BX	59	ASP
6	BX	82	ASN
6	BX	85	ASP
6	BX	126	VAL
6	BX	131	ASN
6	BX	136	ASN
6	BX	150	LEU
4	BY	25	ASP
4	BY	56	THR
4	BY	66	ASP
4	BY	81	GLN
4	BY	90	ASP
4	BY	100	LYS
4	BY	101	ILE
4	BY	123	ARG
4	BY	125	TYR
4	BY	135	ASP
4	BZ	2	LYS
4	BZ	25	ASP
4	BZ	56	THR
4	BZ	66	ASP
4	BZ	80	ASP
4	BZ	81	GLN
4	BZ	90	ASP
4	BZ	99	ARG
4	BZ	100	LYS
4	BZ	101	ILE
4	BZ	123	ARG
4	BZ	125	TYR
4	BZ	135	ASP
7	Ba	5	HIS
7	Ba	8	SER
7	Ba	20	ASP
7	Ba	37	ARG
7	Ba	74	ILE
7	Ba	115	LYS
7	Ba	129	ASP
7	Ba	146	LYS
5	Bb	9	CYS
5	Bb	19	LEU
5	Bb	41	ASP
5	Bb	48	GLU

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Mol	Chain	Res	Type
5	Bb	84	LEU
5	Bb	105	ASN
5	Bb	106	LEU
5	Bb	107	LYS
5	Bb	128	THR
5	Bb	138	CYS
6	Bc	5	ASP
6	Bc	7	CYS
6	Bc	8	SER
6	Bc	24	SER
6	Bc	27	PHE
6	Bc	48	THR
6	Bc	55	ARG
6	Bc	59	ASP
6	Bc	82	ASN
6	Bc	85	ASP
6	Bc	126	VAL
6	Bc	131	ASN
6	Bc	136	ASN
6	Bc	150	LEU
4	Bd	25	ASP
4	Bd	56	THR
4	Bd	66	ASP
4	Bd	81	GLN
4	Bd	90	ASP
4	Bd	100	LYS
4	Bd	101	ILE
4	Bd	123	ARG
4	Bd	125	TYR
4	Bd	135	ASP
4	Be	2	LYS
4	Be	25	ASP
4	Be	56	THR
4	Be	66	ASP
4	Be	80	ASP
4	Be	81	GLN
4	Be	90	ASP
4	Be	99	ARG
4	Be	100	LYS
4	Be	101	ILE
4	Be	123	ARG
4	Be	125	TYR

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Mol	Chain	Res	Type
4	Be	135	ASP
7	Bf	5	HIS
7	Bf	8	SER
7	Bf	20	ASP
7	Bf	37	ARG
7	Bf	74	ILE
7	Bf	115	LYS
7	Bf	129	ASP
7	Bf	146	LYS
5	Bg	9	CYS
5	Bg	19	LEU
5	Bg	41	ASP
5	Bg	48	GLU
5	Bg	84	LEU
5	Bg	105	ASN
5	Bg	106	LEU
5	Bg	107	LYS
5	Bg	128	THR
5	Bg	138	CYS
6	Bh	5	ASP
6	Bh	7	CYS
6	Bh	8	SER
6	Bh	24	SER
6	Bh	27	PHE
6	Bh	48	THR
6	Bh	55	ARG
6	Bh	59	ASP
6	Bh	82	ASN
6	Bh	85	ASP
6	Bh	126	VAL
6	Bh	131	ASN
6	Bh	136	ASN
6	Bh	150	LEU
4	Bi	25	ASP
4	Bi	56	THR
4	Bi	66	ASP
4	Bi	81	GLN
4	Bi	90	ASP
4	Bi	100	LYS
4	Bi	101	ILE
4	Bi	123	ARG
4	Bi	125	TYR

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Mol	Chain	Res	Type
4	Bi	135	ASP
4	Bj	2	LYS
4	Bj	25	ASP
4	Bj	56	THR
4	Bj	66	ASP
4	Bj	80	ASP
4	Bj	81	GLN
4	Bj	90	ASP
4	Bj	99	ARG
4	Bj	100	LYS
4	Bj	101	ILE
4	Bj	123	ARG
4	Bj	125	TYR
4	Bj	135	ASP
7	Bk	5	HIS
7	Bk	8	SER
7	Bk	20	ASP
7	Bk	37	ARG
7	Bk	74	ILE
7	Bk	115	LYS
7	Bk	129	ASP
7	Bk	146	LYS
5	Bl	9	CYS
5	Bl	19	LEU
5	Bl	41	ASP
5	Bl	48	GLU
5	Bl	84	LEU
5	Bl	105	ASN
5	Bl	106	LEU
5	Bl	107	LYS
5	Bl	128	THR
5	Bl	138	CYS
6	Bm	5	ASP
6	Bm	7	CYS
6	Bm	8	SER
6	Bm	24	SER
6	Bm	27	PHE
6	Bm	48	THR
6	Bm	55	ARG
6	Bm	59	ASP
6	Bm	82	ASN
6	Bm	85	ASP

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Mol	Chain	Res	Type
6	Bm	126	VAL
6	Bm	131	ASN
6	Bm	136	ASN
6	Bm	150	LEU
4	Bn	25	ASP
4	Bn	56	THR
4	Bn	66	ASP
4	Bn	81	GLN
4	Bn	90	ASP
4	Bn	100	LYS
4	Bn	101	ILE
4	Bn	123	ARG
4	Bn	125	TYR
4	Bn	135	ASP
4	Bo	2	LYS
4	Bo	25	ASP
4	Bo	56	THR
4	Bo	66	ASP
4	Bo	80	ASP
4	Bo	81	GLN
4	Bo	90	ASP
4	Bo	99	ARG
4	Bo	100	LYS
4	Bo	101	ILE
4	Bo	123	ARG
4	Bo	125	TYR
4	Bo	135	ASP
7	Bp	5	HIS
7	Bp	8	SER
7	Bp	20	ASP
7	Bp	37	ARG
7	Bp	74	ILE
7	Bp	115	LYS
7	Bp	129	ASP
7	Bp	146	LYS
5	Bq	9	CYS
5	Bq	19	LEU
5	Bq	41	ASP
5	Bq	48	GLU
5	Bq	84	LEU
5	Bq	105	ASN
5	Bq	106	LEU

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Mol	Chain	Res	Type
5	Bq	107	LYS
5	Bq	128	THR
5	Bq	138	CYS
6	Br	5	ASP
6	Br	7	CYS
6	Br	8	SER
6	Br	24	SER
6	Br	27	PHE
6	Br	48	THR
6	Br	55	ARG
6	Br	59	ASP
6	Br	82	ASN
6	Br	85	ASP
6	Br	126	VAL
6	Br	131	ASN
6	Br	136	ASN
6	Br	150	LEU
4	Bs	25	ASP
4	Bs	56	THR
4	Bs	66	ASP
4	Bs	81	GLN
4	Bs	90	ASP
4	Bs	100	LYS
4	Bs	101	ILE
4	Bs	123	ARG
4	Bs	125	TYR
4	Bs	135	ASP
4	Bt	2	LYS
4	Bt	25	ASP
4	Bt	56	THR
4	Bt	66	ASP
4	Bt	80	ASP
4	Bt	81	GLN
4	Bt	90	ASP
4	Bt	99	ARG
4	Bt	100	LYS
4	Bt	101	ILE
4	Bt	123	ARG
4	Bt	125	TYR
4	Bt	135	ASP
7	Bu	5	HIS
7	Bu	8	SER

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Mol	Chain	Res	Type
7	Bu	20	ASP
7	Bu	37	ARG
7	Bu	74	ILE
7	Bu	115	LYS
7	Bu	129	ASP
7	Bu	146	LYS
5	Bv	9	CYS
5	Bv	19	LEU
5	Bv	41	ASP
5	Bv	48	GLU
5	Bv	84	LEU
5	Bv	105	ASN
5	Bv	106	LEU
5	Bv	107	LYS
5	Bv	128	THR
5	Bv	138	CYS
6	Bw	5	ASP
6	Bw	7	CYS
6	Bw	8	SER
6	Bw	24	SER
6	Bw	27	PHE
6	Bw	48	THR
6	Bw	55	ARG
6	Bw	59	ASP
6	Bw	82	ASN
6	Bw	85	ASP
6	Bw	126	VAL
6	Bw	131	ASN
6	Bw	136	ASN
6	Bw	150	LEU
4	Bx	25	ASP
4	Bx	56	THR
4	Bx	66	ASP
4	Bx	81	GLN
4	Bx	90	ASP
4	Bx	100	LYS
4	Bx	101	ILE
4	Bx	123	ARG
4	Bx	125	TYR
4	Bx	135	ASP
4	By	2	LYS
4	By	25	ASP

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Mol	Chain	Res	Type
4	By	56	THR
4	By	66	ASP
4	By	80	ASP
4	By	81	GLN
4	By	90	ASP
4	By	99	ARG
4	By	100	LYS
4	By	101	ILE
4	By	123	ARG
4	By	125	TYR
4	By	135	ASP
7	Bz	5	HIS
7	Bz	8	SER
7	Bz	20	ASP
7	Bz	37	ARG
7	Bz	74	ILE
7	Bz	115	LYS
7	Bz	129	ASP
7	Bz	146	LYS
8	C0	9	ARG
8	C0	10	PHE
8	C0	11	GLN
8	C0	13	LEU
8	C0	19	LEU
8	C0	38	LEU
8	C0	42	VAL
8	C0	56	ASN
8	C0	59	GLU
8	C0	60	HIS
8	C0	69	CYS
8	C0	70	ARG
8	C0	73	VAL
8	C0	80	LEU
8	C0	81	LEU
8	C0	82	PHE
8	C0	87	LYS
8	C0	90	ARG
8	C0	91	ASP
8	C0	94	ASP
8	C0	96	ASP
8	C0	98	GLU
8	C0	102	LEU

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Mol	Chain	Res	Type
8	C0	112	THR
8	C0	116	THR
8	C0	118	THR
8	C0	131	THR
8	C0	137	ARG
8	C0	139	SER
8	C0	140	PHE
8	C0	143	ASN
8	C0	144	ARG
8	C0	146	TRP
8	C0	147	LEU
8	C0	156	ASP
8	C0	159	ASP
8	C0	163	SER
8	C0	165	THR
8	C0	172	ASN
8	C0	173	PHE
8	C0	176	ARG
8	C0	183	LEU
8	C0	187	SER
8	C0	190	TYR
8	C0	197	ASN
8	C0	198	LEU
8	C0	216	VAL
8	C0	225	TYR
9	C1	10	LEU
9	C1	32	ARG
9	C1	62	CYS
9	C1	64	LYS
9	C1	73	GLU
9	C1	81	LEU
9	C1	87	LYS
9	C1	90	HIS
9	C1	94	ASP
9	C1	102	THR
9	C1	104	VAL
9	C1	105	VAL
9	C1	110	VAL
9	C1	120	CYS
9	C1	123	ARG
9	C1	127	VAL
9	C1	131	THR

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Mol	Chain	Res	Type
9	C1	137	ARG
9	C1	138	ARG
9	C1	139	LYS
9	C1	140	PHE
9	C1	144	ARG
9	C1	147	LEU
9	C1	153	SER
9	C1	155	LEU
9	C1	157	ARG
9	C1	171	TYR
9	C1	173	ASN
9	C1	176	SER
9	C1	188	ASP
9	C1	190	HIS
9	C1	197	PHE
9	C1	198	ASN
9	C1	199	ARG
9	C1	202	ASN
9	C1	211	THR
9	C1	212	GLU
9	C1	215	LEU
9	C1	221	LEU
10	C2	9	SER
10	C2	11	ASP
10	C2	14	ILE
10	C2	16	LYS
10	C2	17	LEU
10	C2	18	ILE
10	C2	37	ASP
10	C2	45	ARG
10	C2	61	SER
10	C2	63	ASP
10	C2	65	HIS
10	C2	72	ASP
10	C2	80	LEU
10	C2	81	PHE
10	C2	82	VAL
10	C2	97	ASP
10	C2	100	LEU
10	C2	103	LYS
10	C2	106	ASP
10	C2	111	ASP

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Mol	Chain	Res	Type
10	C2	114	PHE
10	C2	117	CYS
10	C2	119	LYS
10	C2	137	PHE
10	C2	139	THR
10	C2	152	SER
10	C2	154	THR
10	C2	155	ASP
10	C2	176	LEU
10	C2	179	HIS
10	C2	183	GLU
10	C2	184	ASP
10	C2	197	PHE
10	C2	199	ARG
10	C2	208	LEU
7	C3	5	HIS
7	C3	6	CYS
7	C3	20	ASP
7	C3	37	ARG
7	C3	74	ILE
7	C3	115	LYS
7	C3	129	ASP
7	C3	146	LYS
7	C3	151	LEU
5	C4	8	GLU
5	C4	19	LEU
5	C4	41	ASP
5	C4	48	GLU
5	C4	71	GLN
5	C4	86	THR
5	C4	106	LEU
5	C4	128	THR
5	C4	138	CYS
8	C5	9	ARG
8	C5	10	PHE
8	C5	11	GLN
8	C5	13	LEU
8	C5	19	LEU
8	C5	38	LEU
8	C5	42	VAL
8	C5	56	ASN
8	C5	59	GLU

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Mol	Chain	Res	Type
8	C5	60	HIS
8	C5	69	CYS
8	C5	70	ARG
8	C5	73	VAL
8	C5	80	LEU
8	C5	81	LEU
8	C5	82	PHE
8	C5	87	LYS
8	C5	90	ARG
8	C5	91	ASP
8	C5	94	ASP
8	C5	96	ASP
8	C5	98	GLU
8	C5	102	LEU
8	C5	112	THR
8	C5	116	THR
8	C5	118	THR
8	C5	131	THR
8	C5	137	ARG
8	C5	139	SER
8	C5	140	PHE
8	C5	143	ASN
8	C5	144	ARG
8	C5	146	TRP
8	C5	147	LEU
8	C5	156	ASP
8	C5	159	ASP
8	C5	163	SER
8	C5	165	THR
8	C5	172	ASN
8	C5	173	PHE
8	C5	176	ARG
8	C5	183	LEU
8	C5	187	SER
8	C5	190	TYR
8	C5	197	ASN
8	C5	198	LEU
8	C5	216	VAL
8	C5	225	TYR
9	C6	10	LEU
9	C6	32	ARG
9	C6	62	CYS

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Mol	Chain	Res	Type
9	C6	64	LYS
9	C6	73	GLU
9	C6	81	LEU
9	C6	87	LYS
9	C6	90	HIS
9	C6	94	ASP
9	C6	102	THR
9	C6	104	VAL
9	C6	105	VAL
9	C6	110	VAL
9	C6	120	CYS
9	C6	123	ARG
9	C6	127	VAL
9	C6	131	THR
9	C6	137	ARG
9	C6	138	ARG
9	C6	139	LYS
9	C6	140	PHE
9	C6	144	ARG
9	C6	147	LEU
9	C6	153	SER
9	C6	155	LEU
9	C6	157	ARG
9	C6	171	TYR
9	C6	173	ASN
9	C6	176	SER
9	C6	188	ASP
9	C6	190	HIS
9	C6	197	PHE
9	C6	198	ASN
9	C6	199	ARG
9	C6	202	ASN
9	C6	211	THR
9	C6	212	GLU
9	C6	215	LEU
9	C6	221	LEU
10	C7	9	SER
10	C7	11	ASP
10	C7	14	ILE
10	C7	16	LYS
10	C7	17	LEU
10	C7	18	ILE

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Mol	Chain	Res	Type
10	C7	37	ASP
10	C7	45	ARG
10	C7	61	SER
10	C7	63	ASP
10	C7	65	HIS
10	C7	72	ASP
10	C7	80	LEU
10	C7	81	PHE
10	C7	82	VAL
10	C7	97	ASP
10	C7	100	LEU
10	C7	103	LYS
10	C7	106	ASP
10	C7	111	ASP
10	C7	114	PHE
10	C7	117	CYS
10	C7	119	LYS
10	C7	137	PHE
10	C7	139	THR
10	C7	152	SER
10	C7	154	THR
10	C7	155	ASP
10	C7	176	LEU
10	C7	179	HIS
10	C7	183	GLU
10	C7	184	ASP
10	C7	197	PHE
10	C7	199	ARG
10	C7	208	LEU
7	CA	5	HIS
7	CA	6	CYS
7	CA	20	ASP
7	CA	37	ARG
7	CA	74	ILE
7	CA	115	LYS
7	CA	129	ASP
7	CA	146	LYS
7	CA	151	LEU
5	CB	8	GLU
5	CB	19	LEU
5	CB	41	ASP
5	CB	48	GLU

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Mol	Chain	Res	Type
5	CB	71	GLN
5	CB	86	THR
5	CB	106	LEU
5	CB	128	THR
5	CB	138	CYS
8	CC	9	ARG
8	CC	10	PHE
8	CC	11	GLN
8	CC	13	LEU
8	CC	19	LEU
8	CC	38	LEU
8	CC	42	VAL
8	CC	56	ASN
8	CC	59	GLU
8	CC	60	HIS
8	CC	69	CYS
8	CC	70	ARG
8	CC	73	VAL
8	CC	80	LEU
8	CC	81	LEU
8	CC	82	PHE
8	CC	87	LYS
8	CC	90	ARG
8	CC	91	ASP
8	CC	94	ASP
8	CC	96	ASP
8	CC	98	GLU
8	CC	102	LEU
8	CC	112	THR
8	CC	116	THR
8	CC	118	THR
8	CC	131	THR
8	CC	137	ARG
8	CC	139	SER
8	CC	140	PHE
8	CC	143	ASN
8	CC	144	ARG
8	CC	146	TRP
8	CC	147	LEU
8	CC	156	ASP
8	CC	159	ASP
8	CC	163	SER

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Mol	Chain	Res	Type
8	CC	165	THR
8	CC	172	ASN
8	CC	173	PHE
8	CC	176	ARG
8	CC	183	LEU
8	CC	187	SER
8	CC	190	TYR
8	CC	197	ASN
8	CC	198	LEU
8	CC	216	VAL
8	CC	225	TYR
9	CD	10	LEU
9	CD	32	ARG
9	CD	62	CYS
9	CD	64	LYS
9	CD	73	GLU
9	CD	81	LEU
9	CD	87	LYS
9	CD	90	HIS
9	CD	94	ASP
9	CD	102	THR
9	CD	104	VAL
9	CD	105	VAL
9	CD	110	VAL
9	CD	120	CYS
9	CD	123	ARG
9	CD	127	VAL
9	CD	131	THR
9	CD	137	ARG
9	CD	138	ARG
9	CD	139	LYS
9	CD	140	PHE
9	CD	144	ARG
9	CD	147	LEU
9	CD	153	SER
9	CD	155	LEU
9	CD	157	ARG
9	CD	171	TYR
9	CD	173	ASN
9	CD	176	SER
9	CD	188	ASP
9	CD	190	HIS

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Mol	Chain	Res	Type
9	CD	197	PHE
9	CD	198	ASN
9	CD	199	ARG
9	CD	202	ASN
9	CD	211	THR
9	CD	212	GLU
9	CD	215	LEU
9	CD	221	LEU
10	CE	9	SER
10	CE	11	ASP
10	CE	14	ILE
10	CE	16	LYS
10	CE	17	LEU
10	CE	18	ILE
10	CE	37	ASP
10	CE	45	ARG
10	CE	61	SER
10	CE	63	ASP
10	CE	65	HIS
10	CE	72	ASP
10	CE	80	LEU
10	CE	81	PHE
10	CE	82	VAL
10	CE	97	ASP
10	CE	100	LEU
10	CE	103	LYS
10	CE	106	ASP
10	CE	111	ASP
10	CE	114	PHE
10	CE	117	CYS
10	CE	119	LYS
10	CE	137	PHE
10	CE	139	THR
10	CE	152	SER
10	CE	154	THR
10	CE	155	ASP
10	CE	176	LEU
10	CE	179	HIS
10	CE	183	GLU
10	CE	184	ASP
10	CE	197	PHE
10	CE	199	ARG

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Mol	Chain	Res	Type
10	CE	208	LEU
7	CF	5	HIS
7	CF	6	CYS
7	CF	20	ASP
7	CF	37	ARG
7	CF	74	ILE
7	CF	115	LYS
7	CF	129	ASP
7	CF	146	LYS
7	CF	151	LEU
5	CG	8	GLU
5	CG	19	LEU
5	CG	41	ASP
5	CG	48	GLU
5	CG	71	GLN
5	CG	86	THR
5	CG	106	LEU
5	CG	128	THR
5	CG	138	CYS
8	CH	9	ARG
8	CH	10	PHE
8	CH	11	GLN
8	CH	13	LEU
8	CH	19	LEU
8	CH	38	LEU
8	CH	42	VAL
8	CH	56	ASN
8	CH	59	GLU
8	CH	60	HIS
8	CH	69	CYS
8	CH	70	ARG
8	CH	73	VAL
8	CH	80	LEU
8	CH	81	LEU
8	CH	82	PHE
8	CH	87	LYS
8	CH	90	ARG
8	CH	91	ASP
8	CH	94	ASP
8	CH	96	ASP
8	CH	98	GLU
8	CH	102	LEU

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Mol	Chain	Res	Type
8	CH	112	THR
8	CH	116	THR
8	CH	118	THR
8	CH	131	THR
8	CH	137	ARG
8	CH	139	SER
8	CH	140	PHE
8	CH	143	ASN
8	CH	144	ARG
8	CH	146	TRP
8	CH	147	LEU
8	CH	156	ASP
8	CH	159	ASP
8	CH	163	SER
8	CH	165	THR
8	CH	172	ASN
8	CH	173	PHE
8	CH	176	ARG
8	CH	183	LEU
8	CH	187	SER
8	CH	190	TYR
8	CH	197	ASN
8	CH	198	LEU
8	CH	216	VAL
8	CH	225	TYR
9	CI	10	LEU
9	CI	32	ARG
9	CI	62	CYS
9	CI	64	LYS
9	CI	73	GLU
9	CI	81	LEU
9	CI	87	LYS
9	CI	90	HIS
9	CI	94	ASP
9	CI	102	THR
9	CI	104	VAL
9	CI	105	VAL
9	CI	110	VAL
9	CI	120	CYS
9	CI	123	ARG
9	CI	127	VAL
9	CI	131	THR

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Mol	Chain	Res	Type
9	CI	137	ARG
9	CI	138	ARG
9	CI	139	LYS
9	CI	140	PHE
9	CI	144	ARG
9	CI	147	LEU
9	CI	153	SER
9	CI	155	LEU
9	CI	157	ARG
9	CI	171	TYR
9	CI	173	ASN
9	CI	176	SER
9	CI	188	ASP
9	CI	190	HIS
9	CI	197	PHE
9	CI	198	ASN
9	CI	199	ARG
9	CI	202	ASN
9	CI	211	THR
9	CI	212	GLU
9	CI	215	LEU
9	CI	221	LEU
10	CJ	9	SER
10	CJ	11	ASP
10	CJ	14	ILE
10	CJ	16	LYS
10	CJ	17	LEU
10	CJ	18	ILE
10	CJ	37	ASP
10	CJ	45	ARG
10	CJ	61	SER
10	CJ	63	ASP
10	CJ	65	HIS
10	CJ	72	ASP
10	CJ	80	LEU
10	CJ	81	PHE
10	CJ	82	VAL
10	CJ	97	ASP
10	CJ	100	LEU
10	CJ	103	LYS
10	CJ	106	ASP
10	CJ	111	ASP

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Mol	Chain	Res	Type
10	CJ	114	PHE
10	CJ	117	CYS
10	CJ	119	LYS
10	CJ	137	PHE
10	CJ	139	THR
10	CJ	152	SER
10	CJ	154	THR
10	CJ	155	ASP
10	CJ	176	LEU
10	CJ	179	HIS
10	CJ	183	GLU
10	CJ	184	ASP
10	CJ	197	PHE
10	CJ	199	ARG
10	CJ	208	LEU
7	CK	5	HIS
7	CK	6	CYS
7	CK	20	ASP
7	CK	37	ARG
7	CK	74	ILE
7	CK	115	LYS
7	CK	129	ASP
7	CK	146	LYS
7	CK	151	LEU
5	CL	8	GLU
5	CL	19	LEU
5	CL	41	ASP
5	CL	48	GLU
5	CL	71	GLN
5	CL	86	THR
5	CL	106	LEU
5	CL	128	THR
5	CL	138	CYS
8	CM	9	ARG
8	CM	10	PHE
8	CM	11	GLN
8	CM	13	LEU
8	CM	19	LEU
8	CM	38	LEU
8	CM	42	VAL
8	CM	56	ASN
8	CM	59	GLU

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Mol	Chain	Res	Type
8	CM	60	HIS
8	CM	69	CYS
8	CM	70	ARG
8	CM	73	VAL
8	CM	80	LEU
8	CM	81	LEU
8	CM	82	PHE
8	CM	87	LYS
8	CM	90	ARG
8	CM	91	ASP
8	CM	94	ASP
8	CM	96	ASP
8	CM	98	GLU
8	CM	102	LEU
8	CM	112	THR
8	CM	116	THR
8	CM	118	THR
8	CM	131	THR
8	CM	137	ARG
8	CM	139	SER
8	CM	140	PHE
8	CM	143	ASN
8	CM	144	ARG
8	CM	146	TRP
8	CM	147	LEU
8	CM	156	ASP
8	CM	159	ASP
8	CM	163	SER
8	CM	165	THR
8	CM	172	ASN
8	CM	173	PHE
8	CM	176	ARG
8	CM	183	LEU
8	CM	187	SER
8	CM	190	TYR
8	CM	197	ASN
8	CM	198	LEU
8	CM	216	VAL
8	CM	225	TYR
9	CN	10	LEU
9	CN	32	ARG
9	CN	62	CYS

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Mol	Chain	Res	Type
9	CN	64	LYS
9	CN	73	GLU
9	CN	81	LEU
9	CN	87	LYS
9	CN	90	HIS
9	CN	94	ASP
9	CN	102	THR
9	CN	104	VAL
9	CN	105	VAL
9	CN	110	VAL
9	CN	120	CYS
9	CN	123	ARG
9	CN	127	VAL
9	CN	131	THR
9	CN	137	ARG
9	CN	138	ARG
9	CN	139	LYS
9	CN	140	PHE
9	CN	144	ARG
9	CN	147	LEU
9	CN	153	SER
9	CN	155	LEU
9	CN	157	ARG
9	CN	171	TYR
9	CN	173	ASN
9	CN	176	SER
9	CN	188	ASP
9	CN	190	HIS
9	CN	197	PHE
9	CN	198	ASN
9	CN	199	ARG
9	CN	202	ASN
9	CN	211	THR
9	CN	212	GLU
9	CN	215	LEU
9	CN	221	LEU
10	CO	9	SER
10	CO	11	ASP
10	CO	14	ILE
10	CO	16	LYS
10	CO	17	LEU
10	CO	18	ILE

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Mol	Chain	Res	Type
10	CO	37	ASP
10	CO	45	ARG
10	CO	61	SER
10	CO	63	ASP
10	CO	65	HIS
10	CO	72	ASP
10	CO	80	LEU
10	CO	81	PHE
10	CO	82	VAL
10	CO	97	ASP
10	CO	100	LEU
10	CO	103	LYS
10	CO	106	ASP
10	CO	111	ASP
10	CO	114	PHE
10	CO	117	CYS
10	CO	119	LYS
10	CO	137	PHE
10	CO	139	THR
10	CO	152	SER
10	CO	154	THR
10	CO	155	ASP
10	CO	176	LEU
10	CO	179	HIS
10	CO	183	GLU
10	CO	184	ASP
10	CO	197	PHE
10	CO	199	ARG
10	CO	208	LEU
7	CP	5	HIS
7	CP	6	CYS
7	CP	20	ASP
7	CP	37	ARG
7	CP	74	ILE
7	CP	115	LYS
7	CP	129	ASP
7	CP	146	LYS
7	CP	151	LEU
5	CQ	8	GLU
5	CQ	19	LEU
5	CQ	41	ASP
5	CQ	48	GLU

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Mol	Chain	Res	Type
5	CQ	71	GLN
5	CQ	86	THR
5	CQ	106	LEU
5	CQ	128	THR
5	CQ	138	CYS
8	CR	9	ARG
8	CR	10	PHE
8	CR	11	GLN
8	CR	13	LEU
8	CR	19	LEU
8	CR	38	LEU
8	CR	42	VAL
8	CR	56	ASN
8	CR	59	GLU
8	CR	60	HIS
8	CR	69	CYS
8	CR	70	ARG
8	CR	73	VAL
8	CR	80	LEU
8	CR	81	LEU
8	CR	82	PHE
8	CR	87	LYS
8	CR	90	ARG
8	CR	91	ASP
8	CR	94	ASP
8	CR	96	ASP
8	CR	98	GLU
8	CR	102	LEU
8	CR	112	THR
8	CR	116	THR
8	CR	118	THR
8	CR	131	THR
8	CR	137	ARG
8	CR	139	SER
8	CR	140	PHE
8	CR	143	ASN
8	CR	144	ARG
8	CR	146	TRP
8	CR	147	LEU
8	CR	156	ASP
8	CR	159	ASP
8	CR	163	SER

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Mol	Chain	Res	Type
8	CR	165	THR
8	CR	172	ASN
8	CR	173	PHE
8	CR	176	ARG
8	CR	183	LEU
8	CR	187	SER
8	CR	190	TYR
8	CR	197	ASN
8	CR	198	LEU
8	CR	216	VAL
8	CR	225	TYR
9	CS	10	LEU
9	CS	32	ARG
9	CS	62	CYS
9	CS	64	LYS
9	CS	73	GLU
9	CS	81	LEU
9	CS	87	LYS
9	CS	90	HIS
9	CS	94	ASP
9	CS	102	THR
9	CS	104	VAL
9	CS	105	VAL
9	CS	110	VAL
9	CS	120	CYS
9	CS	123	ARG
9	CS	127	VAL
9	CS	131	THR
9	CS	137	ARG
9	CS	138	ARG
9	CS	139	LYS
9	CS	140	PHE
9	CS	144	ARG
9	CS	147	LEU
9	CS	153	SER
9	CS	155	LEU
9	CS	157	ARG
9	CS	171	TYR
9	CS	173	ASN
9	CS	176	SER
9	CS	188	ASP
9	CS	190	HIS

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Mol	Chain	Res	Type
9	CS	197	PHE
9	CS	198	ASN
9	CS	199	ARG
9	CS	202	ASN
9	CS	211	THR
9	CS	212	GLU
9	CS	215	LEU
9	CS	221	LEU
10	CT	9	SER
10	CT	11	ASP
10	CT	14	ILE
10	CT	16	LYS
10	CT	17	LEU
10	CT	18	ILE
10	CT	37	ASP
10	CT	45	ARG
10	CT	61	SER
10	CT	63	ASP
10	CT	65	HIS
10	CT	72	ASP
10	CT	80	LEU
10	CT	81	PHE
10	CT	82	VAL
10	CT	97	ASP
10	CT	100	LEU
10	CT	103	LYS
10	CT	106	ASP
10	CT	111	ASP
10	CT	114	PHE
10	CT	117	CYS
10	CT	119	LYS
10	CT	137	PHE
10	CT	139	THR
10	CT	152	SER
10	CT	154	THR
10	CT	155	ASP
10	CT	176	LEU
10	CT	179	HIS
10	CT	183	GLU
10	CT	184	ASP
10	CT	197	PHE
10	CT	199	ARG

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Mol	Chain	Res	Type
10	CT	208	LEU
7	CU	5	HIS
7	CU	6	CYS
7	CU	20	ASP
7	CU	37	ARG
7	CU	74	ILE
7	CU	115	LYS
7	CU	129	ASP
7	CU	146	LYS
7	CU	151	LEU
5	CV	8	GLU
5	CV	19	LEU
5	CV	41	ASP
5	CV	48	GLU
5	CV	71	GLN
5	CV	86	THR
5	CV	106	LEU
5	CV	128	THR
5	CV	138	CYS
8	CW	9	ARG
8	CW	10	PHE
8	CW	11	GLN
8	CW	13	LEU
8	CW	19	LEU
8	CW	38	LEU
8	CW	42	VAL
8	CW	56	ASN
8	CW	59	GLU
8	CW	60	HIS
8	CW	69	CYS
8	CW	70	ARG
8	CW	73	VAL
8	CW	80	LEU
8	CW	81	LEU
8	CW	82	PHE
8	CW	87	LYS
8	CW	90	ARG
8	CW	91	ASP
8	CW	94	ASP
8	CW	96	ASP
8	CW	98	GLU
8	CW	102	LEU

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Mol	Chain	Res	Type
8	CW	112	THR
8	CW	116	THR
8	CW	118	THR
8	CW	131	THR
8	CW	137	ARG
8	CW	139	SER
8	CW	140	PHE
8	CW	143	ASN
8	CW	144	ARG
8	CW	146	TRP
8	CW	147	LEU
8	CW	156	ASP
8	CW	159	ASP
8	CW	163	SER
8	CW	165	THR
8	CW	172	ASN
8	CW	173	PHE
8	CW	176	ARG
8	CW	183	LEU
8	CW	187	SER
8	CW	190	TYR
8	CW	197	ASN
8	CW	198	LEU
8	CW	216	VAL
8	CW	225	TYR
9	CX	10	LEU
9	CX	32	ARG
9	CX	62	CYS
9	CX	64	LYS
9	CX	73	GLU
9	CX	81	LEU
9	CX	87	LYS
9	CX	90	HIS
9	CX	94	ASP
9	CX	102	THR
9	CX	104	VAL
9	CX	105	VAL
9	CX	110	VAL
9	CX	120	CYS
9	CX	123	ARG
9	CX	127	VAL
9	CX	131	THR

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Mol	Chain	Res	Type
9	CX	137	ARG
9	CX	138	ARG
9	CX	139	LYS
9	CX	140	PHE
9	CX	144	ARG
9	CX	147	LEU
9	CX	153	SER
9	CX	155	LEU
9	CX	157	ARG
9	CX	171	TYR
9	CX	173	ASN
9	CX	176	SER
9	CX	188	ASP
9	CX	190	HIS
9	CX	197	PHE
9	CX	198	ASN
9	CX	199	ARG
9	CX	202	ASN
9	CX	211	THR
9	CX	212	GLU
9	CX	215	LEU
9	CX	221	LEU
10	CY	9	SER
10	CY	11	ASP
10	CY	14	ILE
10	CY	16	LYS
10	CY	17	LEU
10	CY	18	ILE
10	CY	37	ASP
10	CY	45	ARG
10	CY	61	SER
10	CY	63	ASP
10	CY	65	HIS
10	CY	72	ASP
10	CY	80	LEU
10	CY	81	PHE
10	CY	82	VAL
10	CY	97	ASP
10	CY	100	LEU
10	CY	103	LYS
10	CY	106	ASP
10	CY	111	ASP

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Mol	Chain	Res	Type
10	CY	114	PHE
10	CY	117	CYS
10	CY	119	LYS
10	CY	137	PHE
10	CY	139	THR
10	CY	152	SER
10	CY	154	THR
10	CY	155	ASP
10	CY	176	LEU
10	CY	179	HIS
10	CY	183	GLU
10	CY	184	ASP
10	CY	197	PHE
10	CY	199	ARG
10	CY	208	LEU
7	CZ	5	HIS
7	CZ	6	CYS
7	CZ	20	ASP
7	CZ	37	ARG
7	CZ	74	ILE
7	CZ	115	LYS
7	CZ	129	ASP
7	CZ	146	LYS
7	CZ	151	LEU
5	Ca	8	GLU
5	Ca	19	LEU
5	Ca	41	ASP
5	Ca	48	GLU
5	Ca	71	GLN
5	Ca	86	THR
5	Ca	106	LEU
5	Ca	128	THR
5	Ca	138	CYS
8	Cb	9	ARG
8	Cb	10	PHE
8	Cb	11	GLN
8	Cb	13	LEU
8	Cb	19	LEU
8	Cb	38	LEU
8	Cb	42	VAL
8	Cb	56	ASN
8	Cb	59	GLU

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Mol	Chain	Res	Type
8	Cb	60	HIS
8	Cb	69	CYS
8	Cb	70	ARG
8	Cb	73	VAL
8	Cb	80	LEU
8	Cb	81	LEU
8	Cb	82	PHE
8	Cb	87	LYS
8	Cb	90	ARG
8	Cb	91	ASP
8	Cb	94	ASP
8	Cb	96	ASP
8	Cb	98	GLU
8	Cb	102	LEU
8	Cb	112	THR
8	Cb	116	THR
8	Cb	118	THR
8	Cb	131	THR
8	Cb	137	ARG
8	Cb	139	SER
8	Cb	140	PHE
8	Cb	143	ASN
8	Cb	144	ARG
8	Cb	146	TRP
8	Cb	147	LEU
8	Cb	156	ASP
8	Cb	159	ASP
8	Cb	163	SER
8	Cb	165	THR
8	Cb	172	ASN
8	Cb	173	PHE
8	Cb	176	ARG
8	Cb	183	LEU
8	Cb	187	SER
8	Cb	190	TYR
8	Cb	197	ASN
8	Cb	198	LEU
8	Cb	216	VAL
8	Cb	225	TYR
9	Cc	10	LEU
9	Cc	32	ARG
9	Cc	62	CYS

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Mol	Chain	Res	Type
9	Cc	64	LYS
9	Cc	73	GLU
9	Cc	81	LEU
9	Cc	87	LYS
9	Cc	90	HIS
9	Cc	94	ASP
9	Cc	102	THR
9	Cc	104	VAL
9	Cc	105	VAL
9	Cc	110	VAL
9	Cc	120	CYS
9	Cc	123	ARG
9	Cc	127	VAL
9	Cc	131	THR
9	Cc	137	ARG
9	Cc	138	ARG
9	Cc	139	LYS
9	Cc	140	PHE
9	Cc	144	ARG
9	Cc	147	LEU
9	Cc	153	SER
9	Cc	155	LEU
9	Cc	157	ARG
9	Cc	171	TYR
9	Cc	173	ASN
9	Cc	176	SER
9	Cc	188	ASP
9	Cc	190	HIS
9	Cc	197	PHE
9	Cc	198	ASN
9	Cc	199	ARG
9	Cc	202	ASN
9	Cc	211	THR
9	Cc	212	GLU
9	Cc	215	LEU
9	Cc	221	LEU
10	Cd	9	SER
10	Cd	11	ASP
10	Cd	14	ILE
10	Cd	16	LYS
10	Cd	17	LEU
10	Cd	18	ILE

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Mol	Chain	Res	Type
10	Cd	37	ASP
10	Cd	45	ARG
10	Cd	61	SER
10	Cd	63	ASP
10	Cd	65	HIS
10	Cd	72	ASP
10	Cd	80	LEU
10	Cd	81	PHE
10	Cd	82	VAL
10	Cd	97	ASP
10	Cd	100	LEU
10	Cd	103	LYS
10	Cd	106	ASP
10	Cd	111	ASP
10	Cd	114	PHE
10	Cd	117	CYS
10	Cd	119	LYS
10	Cd	137	PHE
10	Cd	139	THR
10	Cd	152	SER
10	Cd	154	THR
10	Cd	155	ASP
10	Cd	176	LEU
10	Cd	179	HIS
10	Cd	183	GLU
10	Cd	184	ASP
10	Cd	197	PHE
10	Cd	199	ARG
10	Cd	208	LEU
7	Ce	5	HIS
7	Ce	6	CYS
7	Ce	20	ASP
7	Ce	37	ARG
7	Ce	74	ILE
7	Ce	115	LYS
7	Ce	129	ASP
7	Ce	146	LYS
7	Ce	151	LEU
5	Cf	8	GLU
5	Cf	19	LEU
5	Cf	41	ASP
5	Cf	48	GLU

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Mol	Chain	Res	Type
5	Cf	71	GLN
5	Cf	86	THR
5	Cf	106	LEU
5	Cf	128	THR
5	Cf	138	CYS
8	Cg	9	ARG
8	Cg	10	PHE
8	Cg	11	GLN
8	Cg	13	LEU
8	Cg	19	LEU
8	Cg	38	LEU
8	Cg	42	VAL
8	Cg	56	ASN
8	Cg	59	GLU
8	Cg	60	HIS
8	Cg	69	CYS
8	Cg	70	ARG
8	Cg	73	VAL
8	Cg	80	LEU
8	Cg	81	LEU
8	Cg	82	PHE
8	Cg	87	LYS
8	Cg	90	ARG
8	Cg	91	ASP
8	Cg	94	ASP
8	Cg	96	ASP
8	Cg	98	GLU
8	Cg	102	LEU
8	Cg	112	THR
8	Cg	116	THR
8	Cg	118	THR
8	Cg	131	THR
8	Cg	137	ARG
8	Cg	139	SER
8	Cg	140	PHE
8	Cg	143	ASN
8	Cg	144	ARG
8	Cg	146	TRP
8	Cg	147	LEU
8	Cg	156	ASP
8	Cg	159	ASP
8	Cg	163	SER

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Mol	Chain	Res	Type
8	Cg	165	THR
8	Cg	172	ASN
8	Cg	173	PHE
8	Cg	176	ARG
8	Cg	183	LEU
8	Cg	187	SER
8	Cg	190	TYR
8	Cg	197	ASN
8	Cg	198	LEU
8	Cg	216	VAL
8	Cg	225	TYR
9	Ch	10	LEU
9	Ch	32	ARG
9	Ch	62	CYS
9	Ch	64	LYS
9	Ch	73	GLU
9	Ch	81	LEU
9	Ch	87	LYS
9	Ch	90	HIS
9	Ch	94	ASP
9	Ch	102	THR
9	Ch	104	VAL
9	Ch	105	VAL
9	Ch	110	VAL
9	Ch	120	CYS
9	Ch	123	ARG
9	Ch	127	VAL
9	Ch	131	THR
9	Ch	137	ARG
9	Ch	138	ARG
9	Ch	139	LYS
9	Ch	140	PHE
9	Ch	144	ARG
9	Ch	147	LEU
9	Ch	153	SER
9	Ch	155	LEU
9	Ch	157	ARG
9	Ch	171	TYR
9	Ch	173	ASN
9	Ch	176	SER
9	Ch	188	ASP
9	Ch	190	HIS

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Mol	Chain	Res	Type
9	Ch	197	PHE
9	Ch	198	ASN
9	Ch	199	ARG
9	Ch	202	ASN
9	Ch	211	THR
9	Ch	212	GLU
9	Ch	215	LEU
9	Ch	221	LEU
10	Ci	9	SER
10	Ci	11	ASP
10	Ci	14	ILE
10	Ci	16	LYS
10	Ci	17	LEU
10	Ci	18	ILE
10	Ci	37	ASP
10	Ci	45	ARG
10	Ci	61	SER
10	Ci	63	ASP
10	Ci	65	HIS
10	Ci	72	ASP
10	Ci	80	LEU
10	Ci	81	PHE
10	Ci	82	VAL
10	Ci	97	ASP
10	Ci	100	LEU
10	Ci	103	LYS
10	Ci	106	ASP
10	Ci	111	ASP
10	Ci	114	PHE
10	Ci	117	CYS
10	Ci	119	LYS
10	Ci	137	PHE
10	Ci	139	THR
10	Ci	152	SER
10	Ci	154	THR
10	Ci	155	ASP
10	Ci	176	LEU
10	Ci	179	HIS
10	Ci	183	GLU
10	Ci	184	ASP
10	Ci	197	PHE
10	Ci	199	ARG

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Mol	Chain	Res	Type
10	Ci	208	LEU
7	Cj	5	HIS
7	Cj	6	CYS
7	Cj	20	ASP
7	Cj	37	ARG
7	Cj	74	ILE
7	Cj	115	LYS
7	Cj	129	ASP
7	Cj	146	LYS
7	Cj	151	LEU
5	Ck	8	GLU
5	Ck	19	LEU
5	Ck	41	ASP
5	Ck	48	GLU
5	Ck	71	GLN
5	Ck	86	THR
5	Ck	106	LEU
5	Ck	128	THR
5	Ck	138	CYS
8	Cl	9	ARG
8	Cl	10	PHE
8	Cl	11	GLN
8	Cl	13	LEU
8	Cl	19	LEU
8	Cl	38	LEU
8	Cl	42	VAL
8	Cl	56	ASN
8	Cl	59	GLU
8	Cl	60	HIS
8	Cl	69	CYS
8	Cl	70	ARG
8	Cl	73	VAL
8	Cl	80	LEU
8	Cl	81	LEU
8	Cl	82	PHE
8	Cl	87	LYS
8	Cl	90	ARG
8	Cl	91	ASP
8	Cl	94	ASP
8	Cl	96	ASP
8	Cl	98	GLU
8	Cl	102	LEU

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Mol	Chain	Res	Type
8	Cl	112	THR
8	Cl	116	THR
8	Cl	118	THR
8	Cl	131	THR
8	Cl	137	ARG
8	Cl	139	SER
8	Cl	140	PHE
8	Cl	143	ASN
8	Cl	144	ARG
8	Cl	146	TRP
8	Cl	147	LEU
8	Cl	156	ASP
8	Cl	159	ASP
8	Cl	163	SER
8	Cl	165	THR
8	Cl	172	ASN
8	Cl	173	PHE
8	Cl	176	ARG
8	Cl	183	LEU
8	Cl	187	SER
8	Cl	190	TYR
8	Cl	197	ASN
8	Cl	198	LEU
8	Cl	216	VAL
8	Cl	225	TYR
9	Cm	10	LEU
9	Cm	32	ARG
9	Cm	62	CYS
9	Cm	64	LYS
9	Cm	73	GLU
9	Cm	81	LEU
9	Cm	87	LYS
9	Cm	90	HIS
9	Cm	94	ASP
9	Cm	102	THR
9	Cm	104	VAL
9	Cm	105	VAL
9	Cm	110	VAL
9	Cm	120	CYS
9	Cm	123	ARG
9	Cm	127	VAL
9	Cm	131	THR

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Mol	Chain	Res	Type
9	Cm	137	ARG
9	Cm	138	ARG
9	Cm	139	LYS
9	Cm	140	PHE
9	Cm	144	ARG
9	Cm	147	LEU
9	Cm	153	SER
9	Cm	155	LEU
9	Cm	157	ARG
9	Cm	171	TYR
9	Cm	173	ASN
9	Cm	176	SER
9	Cm	188	ASP
9	Cm	190	HIS
9	Cm	197	PHE
9	Cm	198	ASN
9	Cm	199	ARG
9	Cm	202	ASN
9	Cm	211	THR
9	Cm	212	GLU
9	Cm	215	LEU
9	Cm	221	LEU
10	Cn	9	SER
10	Cn	11	ASP
10	Cn	14	ILE
10	Cn	16	LYS
10	Cn	17	LEU
10	Cn	18	ILE
10	Cn	37	ASP
10	Cn	45	ARG
10	Cn	61	SER
10	Cn	63	ASP
10	Cn	65	HIS
10	Cn	72	ASP
10	Cn	80	LEU
10	Cn	81	PHE
10	Cn	82	VAL
10	Cn	97	ASP
10	Cn	100	LEU
10	Cn	103	LYS
10	Cn	106	ASP
10	Cn	111	ASP

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Mol	Chain	Res	Type
10	Cn	114	PHE
10	Cn	117	CYS
10	Cn	119	LYS
10	Cn	137	PHE
10	Cn	139	THR
10	Cn	152	SER
10	Cn	154	THR
10	Cn	155	ASP
10	Cn	176	LEU
10	Cn	179	HIS
10	Cn	183	GLU
10	Cn	184	ASP
10	Cn	197	PHE
10	Cn	199	ARG
10	Cn	208	LEU
7	Co	5	HIS
7	Co	6	CYS
7	Co	20	ASP
7	Co	37	ARG
7	Co	74	ILE
7	Co	115	LYS
7	Co	129	ASP
7	Co	146	LYS
7	Co	151	LEU
5	Cp	8	GLU
5	Cp	19	LEU
5	Cp	41	ASP
5	Cp	48	GLU
5	Cp	71	GLN
5	Cp	86	THR
5	Cp	106	LEU
5	Cp	128	THR
5	Cp	138	CYS
8	Cq	9	ARG
8	Cq	10	PHE
8	Cq	11	GLN
8	Cq	13	LEU
8	Cq	19	LEU
8	Cq	38	LEU
8	Cq	42	VAL
8	Cq	56	ASN
8	Cq	59	GLU

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Mol	Chain	Res	Type
8	Cq	60	HIS
8	Cq	69	CYS
8	Cq	70	ARG
8	Cq	73	VAL
8	Cq	80	LEU
8	Cq	81	LEU
8	Cq	82	PHE
8	Cq	87	LYS
8	Cq	90	ARG
8	Cq	91	ASP
8	Cq	94	ASP
8	Cq	96	ASP
8	Cq	98	GLU
8	Cq	102	LEU
8	Cq	112	THR
8	Cq	116	THR
8	Cq	118	THR
8	Cq	131	THR
8	Cq	137	ARG
8	Cq	139	SER
8	Cq	140	PHE
8	Cq	143	ASN
8	Cq	144	ARG
8	Cq	146	TRP
8	Cq	147	LEU
8	Cq	156	ASP
8	Cq	159	ASP
8	Cq	163	SER
8	Cq	165	THR
8	Cq	172	ASN
8	Cq	173	PHE
8	Cq	176	ARG
8	Cq	183	LEU
8	Cq	187	SER
8	Cq	190	TYR
8	Cq	197	ASN
8	Cq	198	LEU
8	Cq	216	VAL
8	Cq	225	TYR
9	Cr	10	LEU
9	Cr	32	ARG
9	Cr	62	CYS

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Mol	Chain	Res	Type
9	Cr	64	LYS
9	Cr	73	GLU
9	Cr	81	LEU
9	Cr	87	LYS
9	Cr	90	HIS
9	Cr	94	ASP
9	Cr	102	THR
9	Cr	104	VAL
9	Cr	105	VAL
9	Cr	110	VAL
9	Cr	120	CYS
9	Cr	123	ARG
9	Cr	127	VAL
9	Cr	131	THR
9	Cr	137	ARG
9	Cr	138	ARG
9	Cr	139	LYS
9	Cr	140	PHE
9	Cr	144	ARG
9	Cr	147	LEU
9	Cr	153	SER
9	Cr	155	LEU
9	Cr	157	ARG
9	Cr	171	TYR
9	Cr	173	ASN
9	Cr	176	SER
9	Cr	188	ASP
9	Cr	190	HIS
9	Cr	197	PHE
9	Cr	198	ASN
9	Cr	199	ARG
9	Cr	202	ASN
9	Cr	211	THR
9	Cr	212	GLU
9	Cr	215	LEU
9	Cr	221	LEU
10	Cs	9	SER
10	Cs	11	ASP
10	Cs	14	ILE
10	Cs	16	LYS
10	Cs	17	LEU
10	Cs	18	ILE

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Mol	Chain	Res	Type
10	Cs	37	ASP
10	Cs	45	ARG
10	Cs	61	SER
10	Cs	63	ASP
10	Cs	65	HIS
10	Cs	72	ASP
10	Cs	80	LEU
10	Cs	81	PHE
10	Cs	82	VAL
10	Cs	97	ASP
10	Cs	100	LEU
10	Cs	103	LYS
10	Cs	106	ASP
10	Cs	111	ASP
10	Cs	114	PHE
10	Cs	117	CYS
10	Cs	119	LYS
10	Cs	137	PHE
10	Cs	139	THR
10	Cs	152	SER
10	Cs	154	THR
10	Cs	155	ASP
10	Cs	176	LEU
10	Cs	179	HIS
10	Cs	183	GLU
10	Cs	184	ASP
10	Cs	197	PHE
10	Cs	199	ARG
10	Cs	208	LEU
7	Ct	5	HIS
7	Ct	6	CYS
7	Ct	20	ASP
7	Ct	37	ARG
7	Ct	74	ILE
7	Ct	115	LYS
7	Ct	129	ASP
7	Ct	146	LYS
7	Ct	151	LEU
5	Cu	8	GLU
5	Cu	19	LEU
5	Cu	41	ASP
5	Cu	48	GLU

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Mol	Chain	Res	Type
5	Cu	71	GLN
5	Cu	86	THR
5	Cu	106	LEU
5	Cu	128	THR
5	Cu	138	CYS
8	Cv	9	ARG
8	Cv	10	PHE
8	Cv	11	GLN
8	Cv	13	LEU
8	Cv	19	LEU
8	Cv	38	LEU
8	Cv	42	VAL
8	Cv	56	ASN
8	Cv	59	GLU
8	Cv	60	HIS
8	Cv	69	CYS
8	Cv	70	ARG
8	Cv	73	VAL
8	Cv	80	LEU
8	Cv	81	LEU
8	Cv	82	PHE
8	Cv	87	LYS
8	Cv	90	ARG
8	Cv	91	ASP
8	Cv	94	ASP
8	Cv	96	ASP
8	Cv	98	GLU
8	Cv	102	LEU
8	Cv	112	THR
8	Cv	116	THR
8	Cv	118	THR
8	Cv	131	THR
8	Cv	137	ARG
8	Cv	139	SER
8	Cv	140	PHE
8	Cv	143	ASN
8	Cv	144	ARG
8	Cv	146	TRP
8	Cv	147	LEU
8	Cv	156	ASP
8	Cv	159	ASP
8	Cv	163	SER

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Mol	Chain	Res	Type
8	Cv	165	THR
8	Cv	172	ASN
8	Cv	173	PHE
8	Cv	176	ARG
8	Cv	183	LEU
8	Cv	187	SER
8	Cv	190	TYR
8	Cv	197	ASN
8	Cv	198	LEU
8	Cv	216	VAL
8	Cv	225	TYR
9	Cw	10	LEU
9	Cw	32	ARG
9	Cw	62	CYS
9	Cw	64	LYS
9	Cw	73	GLU
9	Cw	81	LEU
9	Cw	87	LYS
9	Cw	90	HIS
9	Cw	94	ASP
9	Cw	102	THR
9	Cw	104	VAL
9	Cw	105	VAL
9	Cw	110	VAL
9	Cw	120	CYS
9	Cw	123	ARG
9	Cw	127	VAL
9	Cw	131	THR
9	Cw	137	ARG
9	Cw	138	ARG
9	Cw	139	LYS
9	Cw	140	PHE
9	Cw	144	ARG
9	Cw	147	LEU
9	Cw	153	SER
9	Cw	155	LEU
9	Cw	157	ARG
9	Cw	171	TYR
9	Cw	173	ASN
9	Cw	176	SER
9	Cw	188	ASP
9	Cw	190	HIS

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Mol	Chain	Res	Type
9	Cw	197	PHE
9	Cw	198	ASN
9	Cw	199	ARG
9	Cw	202	ASN
9	Cw	211	THR
9	Cw	212	GLU
9	Cw	215	LEU
9	Cw	221	LEU
10	Cx	9	SER
10	Cx	11	ASP
10	Cx	14	ILE
10	Cx	16	LYS
10	Cx	17	LEU
10	Cx	18	ILE
10	Cx	37	ASP
10	Cx	45	ARG
10	Cx	61	SER
10	Cx	63	ASP
10	Cx	65	HIS
10	Cx	72	ASP
10	Cx	80	LEU
10	Cx	81	PHE
10	Cx	82	VAL
10	Cx	97	ASP
10	Cx	100	LEU
10	Cx	103	LYS
10	Cx	106	ASP
10	Cx	111	ASP
10	Cx	114	PHE
10	Cx	117	CYS
10	Cx	119	LYS
10	Cx	137	PHE
10	Cx	139	THR
10	Cx	152	SER
10	Cx	154	THR
10	Cx	155	ASP
10	Cx	176	LEU
10	Cx	179	HIS
10	Cx	183	GLU
10	Cx	184	ASP
10	Cx	197	PHE
10	Cx	199	ARG

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Mol	Chain	Res	Type
10	Cx	208	LEU
7	Cy	5	HIS
7	Cy	6	CYS
7	Cy	20	ASP
7	Cy	37	ARG
7	Cy	74	ILE
7	Cy	115	LYS
7	Cy	129	ASP
7	Cy	146	LYS
7	Cy	151	LEU
5	Cz	8	GLU
5	Cz	19	LEU
5	Cz	41	ASP
5	Cz	48	GLU
5	Cz	71	GLN
5	Cz	86	THR
5	Cz	106	LEU
5	Cz	128	THR
5	Cz	138	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (662) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	12	HIS
1	A0	16	GLN
1	A0	18	GLN
1	A0	126	GLN
2	A1	20	GLN
2	A1	46	HIS
2	A1	117	HIS
3	A2	131	ASN
3	A2	136	ASN
3	A3	17	HIS
3	A3	131	ASN
3	A3	136	ASN
4	A4	52	HIS
4	A4	144	HIS
1	A5	12	HIS
1	A5	16	GLN
1	A5	18	GLN
1	A5	126	GLN
2	A6	20	GLN

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Mol	Chain	Res	Type
2	A6	46	HIS
2	A6	117	HIS
3	A7	131	ASN
3	A7	136	ASN
3	AA	17	HIS
3	AA	131	ASN
3	AA	136	ASN
4	AB	31	GLN
4	AB	52	HIS
4	AB	144	HIS
1	AC	12	HIS
1	AC	16	GLN
1	AC	18	GLN
1	AC	126	GLN
2	AD	20	GLN
2	AD	46	HIS
2	AD	117	HIS
3	AE	131	ASN
3	AE	136	ASN
3	AF	17	HIS
3	AF	131	ASN
3	AF	136	ASN
4	AG	52	HIS
4	AG	144	HIS
1	AH	12	HIS
1	AH	16	GLN
1	AH	18	GLN
1	AH	126	GLN
2	AI	20	GLN
2	AI	46	HIS
2	AI	117	HIS
3	AJ	131	ASN
3	AJ	136	ASN
3	AK	17	HIS
3	AK	131	ASN
3	AK	136	ASN
4	AL	52	HIS
4	AL	144	HIS
1	AM	12	HIS
1	AM	16	GLN
1	AM	18	GLN
1	AM	126	GLN

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Mol	Chain	Res	Type
2	AN	20	GLN
2	AN	46	HIS
2	AN	117	HIS
3	AO	131	ASN
3	AO	136	ASN
3	AP	17	HIS
3	AP	131	ASN
3	AP	136	ASN
4	AQ	31	GLN
4	AQ	52	HIS
4	AQ	144	HIS
1	AR	12	HIS
1	AR	16	GLN
1	AR	18	GLN
1	AR	126	GLN
2	AS	20	GLN
2	AS	46	HIS
2	AS	117	HIS
3	AT	131	ASN
3	AT	136	ASN
3	AU	17	HIS
3	AU	131	ASN
3	AU	136	ASN
4	AV	52	HIS
4	AV	144	HIS
1	AW	12	HIS
1	AW	16	GLN
1	AW	18	GLN
1	AW	126	GLN
2	AX	20	GLN
2	AX	46	HIS
2	AX	117	HIS
3	AY	131	ASN
3	AY	136	ASN
3	AZ	17	HIS
3	AZ	131	ASN
3	AZ	136	ASN
4	Aa	52	HIS
4	Aa	144	HIS
1	Ab	12	HIS
1	Ab	16	GLN
1	Ab	18	GLN

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Mol	Chain	Res	Type
1	Ab	126	GLN
2	Ac	20	GLN
2	Ac	46	HIS
2	Ac	117	HIS
3	Ad	131	ASN
3	Ad	136	ASN
3	Ae	17	HIS
3	Ae	131	ASN
3	Ae	136	ASN
4	Af	31	GLN
4	Af	52	HIS
4	Af	144	HIS
1	Ag	12	HIS
1	Ag	16	GLN
1	Ag	18	GLN
1	Ag	126	GLN
2	Ah	20	GLN
2	Ah	46	HIS
2	Ah	117	HIS
3	Ai	131	ASN
3	Ai	136	ASN
3	Aj	17	HIS
3	Aj	131	ASN
3	Aj	136	ASN
4	Ak	52	HIS
4	Ak	144	HIS
1	Al	12	HIS
1	Al	16	GLN
1	Al	18	GLN
1	Al	126	GLN
2	Am	20	GLN
2	Am	46	HIS
2	Am	117	HIS
3	An	131	ASN
3	An	136	ASN
3	Ao	17	HIS
3	Ao	131	ASN
3	Ao	136	ASN
4	Ap	52	HIS
4	Ap	144	HIS
1	Aq	12	HIS
1	Aq	16	GLN

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Mol	Chain	Res	Type
1	Aq	18	GLN
1	Aq	126	GLN
2	Ar	20	GLN
2	Ar	46	HIS
2	Ar	117	HIS
3	As	131	ASN
3	As	136	ASN
3	At	17	HIS
3	At	131	ASN
3	At	136	ASN
4	Au	52	HIS
4	Au	144	HIS
1	Av	12	HIS
1	Av	16	GLN
1	Av	18	GLN
1	Av	126	GLN
2	Aw	20	GLN
2	Aw	46	HIS
2	Aw	117	HIS
3	Ax	131	ASN
3	Ax	136	ASN
3	Ay	17	HIS
3	Ay	131	ASN
3	Ay	136	ASN
4	Az	52	HIS
4	Az	144	HIS
5	B0	20	GLN
5	B0	46	HIS
5	B0	101	HIS
5	B0	117	HIS
6	B1	82	ASN
6	B1	96	HIS
6	B1	131	ASN
6	B1	136	ASN
4	B2	120	GLN
4	B3	31	GLN
4	B3	81	GLN
4	B3	96	HIS
7	B4	3	HIS
7	B4	12	HIS
7	B4	16	GLN
7	B4	18	GLN

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Mol	Chain	Res	Type
7	B4	126	GLN
5	B5	20	GLN
5	B5	46	HIS
5	B5	101	HIS
5	B5	117	HIS
6	B6	82	ASN
6	B6	96	HIS
6	B6	131	ASN
6	B6	136	ASN
4	B7	52	HIS
4	B7	120	GLN
4	BA	81	GLN
4	BA	96	HIS
7	BB	3	HIS
7	BB	12	HIS
7	BB	16	GLN
7	BB	18	GLN
7	BB	126	GLN
5	BC	20	GLN
5	BC	46	HIS
5	BC	101	HIS
5	BC	117	HIS
6	BD	82	ASN
6	BD	96	HIS
6	BD	131	ASN
6	BD	136	ASN
4	BE	31	GLN
4	BE	120	GLN
4	BF	52	HIS
4	BF	81	GLN
4	BF	96	HIS
7	BG	3	HIS
7	BG	12	HIS
7	BG	16	GLN
7	BG	18	GLN
7	BG	126	GLN
5	BH	20	GLN
5	BH	46	HIS
5	BH	101	HIS
5	BH	117	HIS
6	BI	82	ASN
6	BI	96	HIS

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Mol	Chain	Res	Type
6	BI	131	ASN
6	BI	136	ASN
4	BJ	52	HIS
4	BJ	120	GLN
4	BK	81	GLN
4	BK	96	HIS
7	BL	3	HIS
7	BL	12	HIS
7	BL	16	GLN
7	BL	18	GLN
7	BL	126	GLN
5	BM	20	GLN
5	BM	46	HIS
5	BM	101	HIS
5	BM	117	HIS
6	BN	82	ASN
6	BN	96	HIS
6	BN	131	ASN
6	BN	136	ASN
4	BO	31	GLN
4	BO	52	HIS
4	BO	120	GLN
4	BP	81	GLN
4	BP	96	HIS
7	BQ	3	HIS
7	BQ	12	HIS
7	BQ	16	GLN
7	BQ	18	GLN
7	BQ	126	GLN
5	BR	20	GLN
5	BR	46	HIS
5	BR	101	HIS
5	BR	117	HIS
6	BS	82	ASN
6	BS	96	HIS
6	BS	131	ASN
6	BS	136	ASN
4	BT	52	HIS
4	BT	120	GLN
4	BU	31	GLN
4	BU	52	HIS
4	BU	81	GLN

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Mol	Chain	Res	Type
4	BU	96	HIS
7	BV	3	HIS
7	BV	12	HIS
7	BV	16	GLN
7	BV	18	GLN
7	BV	126	GLN
5	BW	20	GLN
5	BW	46	HIS
5	BW	101	HIS
5	BW	117	HIS
6	BX	82	ASN
6	BX	96	HIS
6	BX	131	ASN
6	BX	136	ASN
4	BY	120	GLN
4	BZ	81	GLN
4	BZ	96	HIS
7	Ba	3	HIS
7	Ba	12	HIS
7	Ba	16	GLN
7	Ba	18	GLN
7	Ba	126	GLN
5	Bb	20	GLN
5	Bb	46	HIS
5	Bb	101	HIS
5	Bb	117	HIS
6	Bc	82	ASN
6	Bc	96	HIS
6	Bc	131	ASN
6	Bc	136	ASN
4	Bd	52	HIS
4	Bd	120	GLN
4	Be	81	GLN
4	Be	96	HIS
7	Bf	3	HIS
7	Bf	12	HIS
7	Bf	16	GLN
7	Bf	18	GLN
7	Bf	126	GLN
5	Bg	20	GLN
5	Bg	46	HIS
5	Bg	101	HIS

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Mol	Chain	Res	Type
5	Bg	117	HIS
6	Bh	82	ASN
6	Bh	96	HIS
6	Bh	131	ASN
6	Bh	136	ASN
4	Bi	31	GLN
4	Bi	120	GLN
4	Bj	52	HIS
4	Bj	81	GLN
4	Bj	96	HIS
7	Bk	3	HIS
7	Bk	12	HIS
7	Bk	16	GLN
7	Bk	18	GLN
7	Bk	126	GLN
5	Bl	20	GLN
5	Bl	46	HIS
5	Bl	101	HIS
5	Bl	117	HIS
6	Bm	82	ASN
6	Bm	96	HIS
6	Bm	131	ASN
6	Bm	136	ASN
4	Bn	52	HIS
4	Bn	120	GLN
4	Bo	81	GLN
4	Bo	96	HIS
7	Bp	3	HIS
7	Bp	12	HIS
7	Bp	16	GLN
7	Bp	18	GLN
7	Bp	126	GLN
5	Bq	20	GLN
5	Bq	46	HIS
5	Bq	101	HIS
5	Bq	117	HIS
6	Br	82	ASN
6	Br	96	HIS
6	Br	131	ASN
6	Br	136	ASN
4	Bs	31	GLN
4	Bs	52	HIS

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Mol	Chain	Res	Type
4	Bs	120	GLN
4	Bt	81	GLN
4	Bt	96	HIS
7	Bu	3	HIS
7	Bu	12	HIS
7	Bu	16	GLN
7	Bu	18	GLN
7	Bu	126	GLN
5	Bv	20	GLN
5	Bv	46	HIS
5	Bv	101	HIS
5	Bv	117	HIS
6	Bw	82	ASN
6	Bw	96	HIS
6	Bw	131	ASN
6	Bw	136	ASN
4	Bx	52	HIS
4	Bx	120	GLN
4	By	31	GLN
4	By	52	HIS
4	By	81	GLN
4	By	96	HIS
7	Bz	3	HIS
7	Bz	12	HIS
7	Bz	16	GLN
7	Bz	18	GLN
7	Bz	126	GLN
8	C0	11	GLN
8	C0	18	ASN
8	C0	20	HIS
8	C0	49	GLN
8	C0	172	ASN
8	C0	186	GLN
9	C1	17	ASN
9	C1	74	GLN
9	C1	118	HIS
9	C1	173	ASN
9	C1	217	GLN
10	C2	10	HIS
10	C2	75	GLN
10	C2	116	HIS
7	C3	12	HIS

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Mol	Chain	Res	Type
7	C3	16	GLN
7	C3	18	GLN
7	C3	83	ASN
7	C3	126	GLN
5	C4	20	GLN
5	C4	46	HIS
5	C4	96	HIS
5	C4	117	HIS
5	C4	141	GLN
8	C5	11	GLN
8	C5	18	ASN
8	C5	20	HIS
8	C5	49	GLN
8	C5	172	ASN
8	C5	186	GLN
9	C6	74	GLN
9	C6	118	HIS
9	C6	173	ASN
9	C6	217	GLN
10	C7	10	HIS
10	C7	75	GLN
10	C7	116	HIS
7	CA	12	HIS
7	CA	16	GLN
7	CA	18	GLN
7	CA	83	ASN
7	CA	126	GLN
5	CB	20	GLN
5	CB	46	HIS
5	CB	96	HIS
5	CB	117	HIS
5	CB	141	GLN
8	CC	11	GLN
8	CC	18	ASN
8	CC	20	HIS
8	CC	49	GLN
8	CC	172	ASN
8	CC	186	GLN
9	CD	74	GLN
9	CD	118	HIS
9	CD	173	ASN
9	CD	217	GLN

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Mol	Chain	Res	Type
10	CE	10	HIS
10	CE	75	GLN
10	CE	116	HIS
7	CF	12	HIS
7	CF	16	GLN
7	CF	18	GLN
7	CF	83	ASN
7	CF	126	GLN
5	CG	20	GLN
5	CG	46	HIS
5	CG	96	HIS
5	CG	117	HIS
5	CG	141	GLN
8	CH	11	GLN
8	CH	18	ASN
8	CH	20	HIS
8	CH	49	GLN
8	CH	172	ASN
8	CH	186	GLN
9	CI	17	ASN
9	CI	74	GLN
9	CI	118	HIS
9	CI	173	ASN
9	CI	217	GLN
10	CJ	10	HIS
10	CJ	75	GLN
10	CJ	116	HIS
7	CK	12	HIS
7	CK	16	GLN
7	CK	18	GLN
7	CK	83	ASN
7	CK	126	GLN
5	CL	20	GLN
5	CL	46	HIS
5	CL	96	HIS
5	CL	117	HIS
5	CL	141	GLN
8	CM	11	GLN
8	CM	18	ASN
8	CM	20	HIS
8	CM	49	GLN
8	CM	172	ASN

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Mol	Chain	Res	Type
8	CM	186	GLN
9	CN	17	ASN
9	CN	74	GLN
9	CN	118	HIS
9	CN	173	ASN
9	CN	217	GLN
10	CO	10	HIS
10	CO	75	GLN
10	CO	116	HIS
7	CP	12	HIS
7	CP	16	GLN
7	CP	18	GLN
7	CP	83	ASN
7	CP	126	GLN
5	CQ	20	GLN
5	CQ	46	HIS
5	CQ	96	HIS
5	CQ	117	HIS
5	CQ	141	GLN
8	CR	11	GLN
8	CR	18	ASN
8	CR	20	HIS
8	CR	49	GLN
8	CR	172	ASN
8	CR	186	GLN
9	CS	74	GLN
9	CS	118	HIS
9	CS	173	ASN
9	CS	217	GLN
10	CT	10	HIS
10	CT	75	GLN
10	CT	116	HIS
7	CU	12	HIS
7	CU	16	GLN
7	CU	18	GLN
7	CU	83	ASN
7	CU	126	GLN
5	CV	20	GLN
5	CV	46	HIS
5	CV	96	HIS
5	CV	117	HIS
5	CV	141	GLN

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Mol	Chain	Res	Type
8	CW	11	GLN
8	CW	20	HIS
8	CW	49	GLN
8	CW	172	ASN
8	CW	186	GLN
9	CX	74	GLN
9	CX	118	HIS
9	CX	173	ASN
9	CX	217	GLN
10	CY	10	HIS
10	CY	75	GLN
10	CY	116	HIS
7	CZ	12	HIS
7	CZ	16	GLN
7	CZ	18	GLN
7	CZ	83	ASN
7	CZ	126	GLN
5	Ca	20	GLN
5	Ca	46	HIS
5	Ca	96	HIS
5	Ca	117	HIS
5	Ca	141	GLN
8	Cb	11	GLN
8	Cb	18	ASN
8	Cb	20	HIS
8	Cb	49	GLN
8	Cb	172	ASN
8	Cb	186	GLN
9	Cc	74	GLN
9	Cc	118	HIS
9	Cc	173	ASN
9	Cc	217	GLN
10	Cd	10	HIS
10	Cd	75	GLN
10	Cd	116	HIS
7	Ce	12	HIS
7	Ce	16	GLN
7	Ce	18	GLN
7	Ce	83	ASN
7	Ce	126	GLN
5	Cf	20	GLN
5	Cf	46	HIS

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Mol	Chain	Res	Type
5	Cf	96	HIS
5	Cf	117	HIS
5	Cf	141	GLN
8	Cg	11	GLN
8	Cg	18	ASN
8	Cg	20	HIS
8	Cg	49	GLN
8	Cg	172	ASN
8	Cg	186	GLN
9	Ch	74	GLN
9	Ch	118	HIS
9	Ch	173	ASN
9	Ch	217	GLN
10	Ci	10	HIS
10	Ci	75	GLN
10	Ci	116	HIS
7	Cj	12	HIS
7	Cj	16	GLN
7	Cj	18	GLN
7	Cj	83	ASN
7	Cj	126	GLN
5	Ck	20	GLN
5	Ck	46	HIS
5	Ck	96	HIS
5	Ck	117	HIS
5	Ck	141	GLN
8	Cl	11	GLN
8	Cl	18	ASN
8	Cl	20	HIS
8	Cl	49	GLN
8	Cl	172	ASN
8	Cl	186	GLN
9	Cm	17	ASN
9	Cm	74	GLN
9	Cm	118	HIS
9	Cm	173	ASN
9	Cm	217	GLN
10	Cn	10	HIS
10	Cn	75	GLN
10	Cn	116	HIS
7	Co	12	HIS
7	Co	16	GLN

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Mol	Chain	Res	Type
7	Co	18	GLN
7	Co	83	ASN
7	Co	126	GLN
5	Cp	20	GLN
5	Cp	46	HIS
5	Cp	96	HIS
5	Cp	117	HIS
5	Cp	141	GLN
8	Cq	11	GLN
8	Cq	18	ASN
8	Cq	20	HIS
8	Cq	49	GLN
8	Cq	172	ASN
8	Cq	186	GLN
9	Cr	17	ASN
9	Cr	74	GLN
9	Cr	118	HIS
9	Cr	173	ASN
9	Cr	217	GLN
10	Cs	10	HIS
10	Cs	75	GLN
10	Cs	116	HIS
7	Ct	12	HIS
7	Ct	16	GLN
7	Ct	18	GLN
7	Ct	83	ASN
7	Ct	126	GLN
5	Cu	20	GLN
5	Cu	46	HIS
5	Cu	96	HIS
5	Cu	117	HIS
5	Cu	141	GLN
8	Cv	11	GLN
8	Cv	18	ASN
8	Cv	20	HIS
8	Cv	49	GLN
8	Cv	172	ASN
8	Cv	186	GLN
9	Cw	74	GLN
9	Cw	118	HIS
9	Cw	173	ASN
9	Cw	217	GLN

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Mol	Chain	Res	Type
10	Cx	10	HIS
10	Cx	75	GLN
10	Cx	116	HIS
7	Cy	12	HIS
7	Cy	16	GLN
7	Cy	18	GLN
7	Cy	83	ASN
7	Cy	126	GLN
5	Cz	20	GLN
5	Cz	46	HIS
5	Cz	96	HIS
5	Cz	117	HIS
5	Cz	141	GLN

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 monosaccharides 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
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

All 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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	57:LEU	C	58:GLU	N	4.76
1	CR	57:LEU	C	58:GLU	N	4.76
1	CW	57:LEU	C	58:GLU	N	4.76
1	Cb	57:LEU	C	58:GLU	N	4.76
1	Cg	57:LEU	C	58:GLU	N	4.76
1	Cl	57:LEU	C	58:GLU	N	4.76
1	Cq	57:LEU	C	58:GLU	N	4.76
1	Cv	57:LEU	C	58:GLU	N	4.76
1	C1	58:GLU	C	59:GLY	N	4.75
1	C6	58:GLU	C	59:GLY	N	4.75
1	CD	58:GLU	C	59:GLY	N	4.75
1	CI	58:GLU	C	59:GLY	N	4.75
1	CN	58:GLU	C	59:GLY	N	4.75
1	CS	58:GLU	C	59:GLY	N	4.75
1	CX	58:GLU	C	59:GLY	N	4.75
1	Cc	58:GLU	C	59:GLY	N	4.75
1	Ch	58:GLU	C	59:GLY	N	4.75
1	Cm	58:GLU	C	59:GLY	N	4.75
1	Cr	58:GLU	C	59:GLY	N	4.75
1	Cw	58:GLU	C	59:GLY	N	4.75
1	C0	43:ASP	C	44:LYS	N	3.32
1	C5	43:ASP	C	44:LYS	N	3.32
1	CC	43:ASP	C	44:LYS	N	3.32
1	CH	43:ASP	C	44:LYS	N	3.32
1	CM	43:ASP	C	44:LYS	N	3.32
1	CR	43:ASP	C	44:LYS	N	3.32
1	CW	43:ASP	C	44:LYS	N	3.32
1	Cb	43:ASP	C	44:LYS	N	3.32
1	Cg	43:ASP	C	44:LYS	N	3.32
1	Cl	43:ASP	C	44:LYS	N	3.32
1	Cq	43:ASP	C	44:LYS	N	3.32
1	Cv	43:ASP	C	44:LYS	N	3.32
1	C2	57:LEU	C	58:GLU	N	1.62
1	C7	57:LEU	C	58:GLU	N	1.62
1	CE	57:LEU	C	58:GLU	N	1.62
1	CJ	57:LEU	C	58:GLU	N	1.62
1	CO	57:LEU	C	58:GLU	N	1.62
1	CT	57:LEU	C	58:GLU	N	1.62
1	CY	57:LEU	C	58:GLU	N	1.62
1	Cd	57:LEU	C	58:GLU	N	1.62
1	Ci	57:LEU	C	58:GLU	N	1.62
1	Cn	57:LEU	C	58:GLU	N	1.62

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Cs	57:LEU	C	58:GLU	N	1.62
1	Cx	57:LEU	C	58:GLU	N	1.62

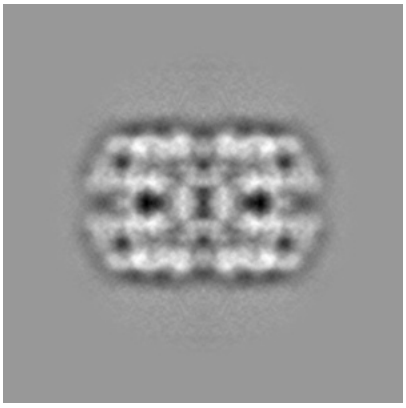
6 Map visualisation (i)

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.

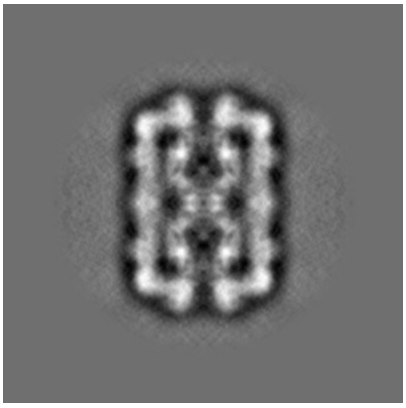
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

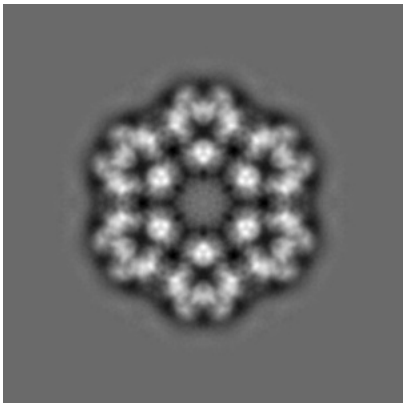
6.1.1 Primary map



X



Y

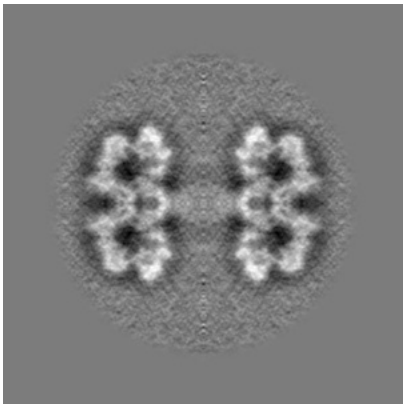


Z

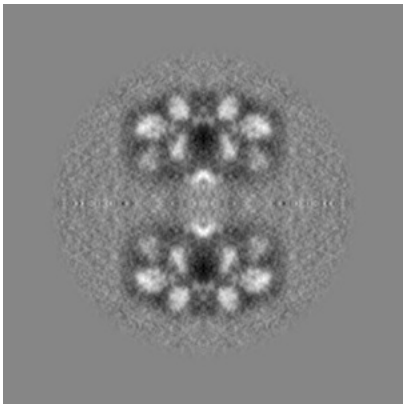
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

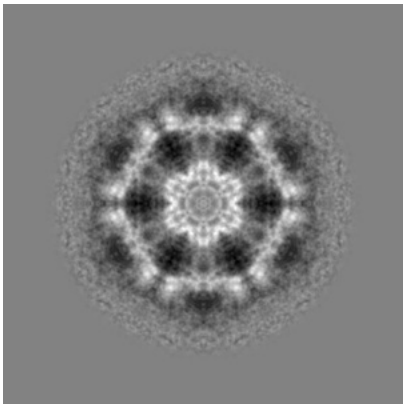
6.2.1 Primary map



X Index: 200



Y Index: 200

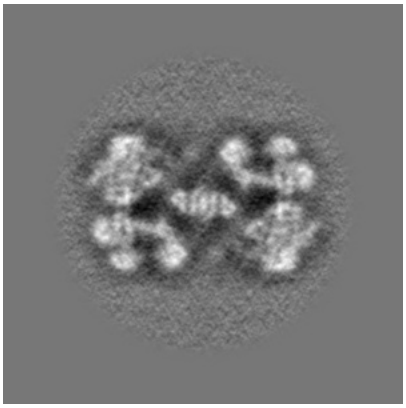


Z Index: 200

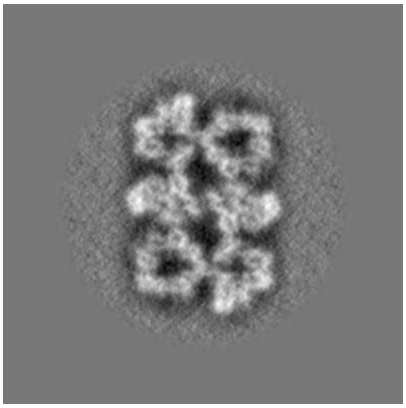
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

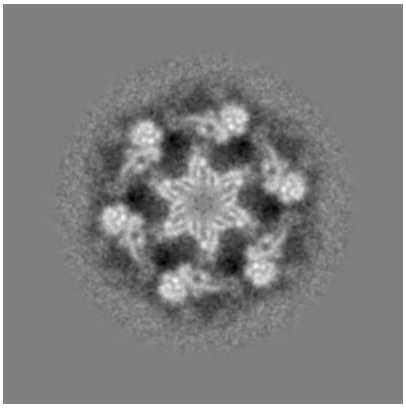
6.3.1 Primary map



X Index: 173



Y Index: 151

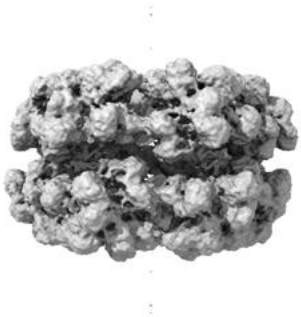


Z Index: 205

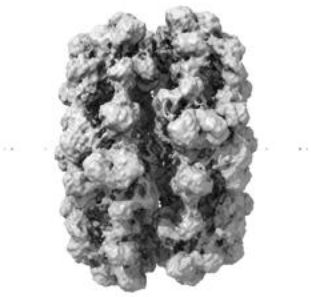
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

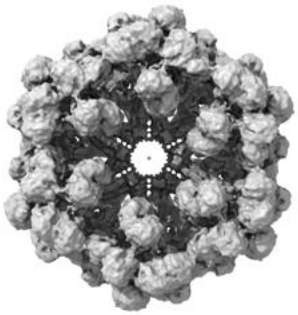
6.4.1 Primary map



X



Y



Z

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.

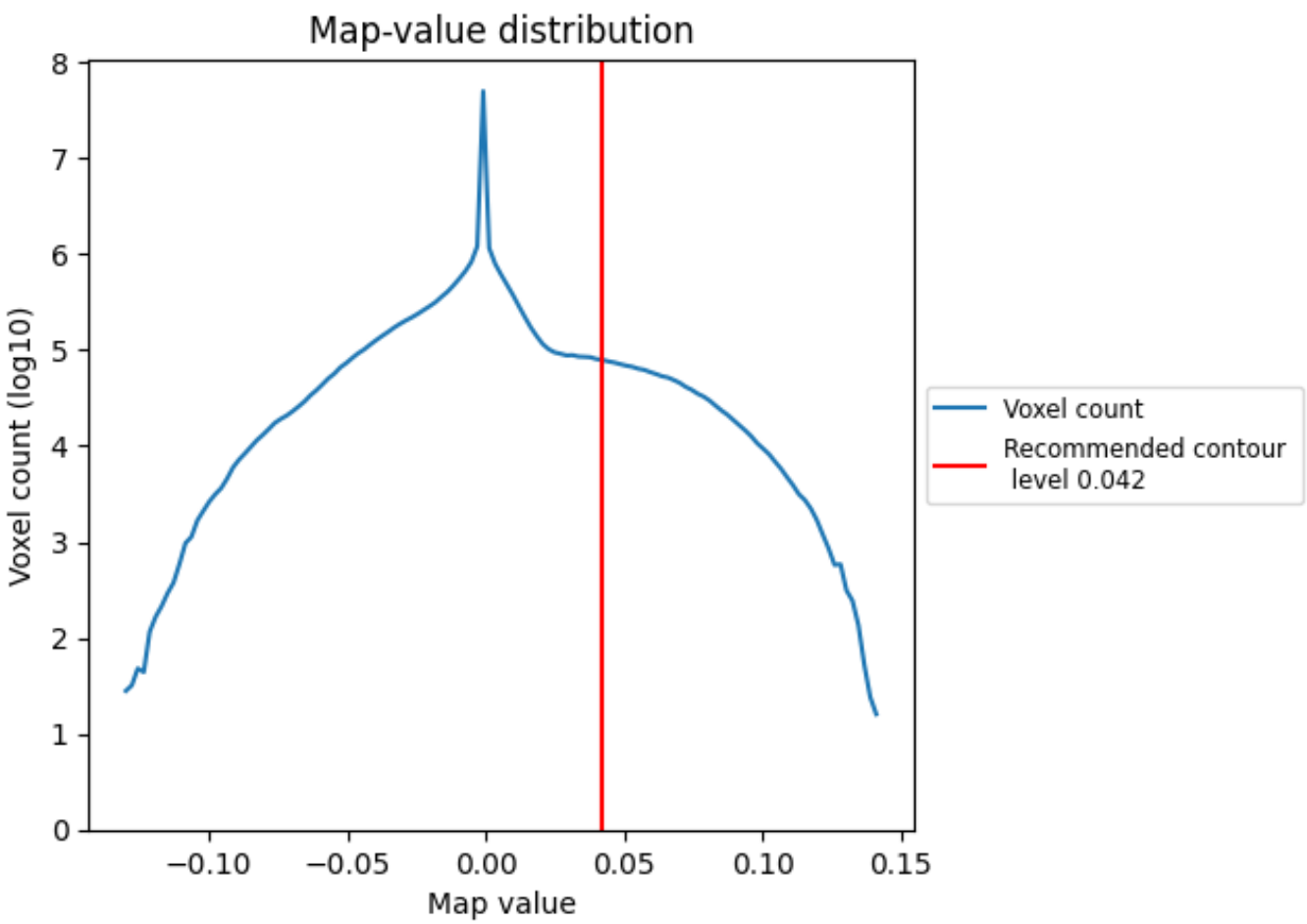
6.5 Mask visualisation (i)

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

7 Map analysis (i)

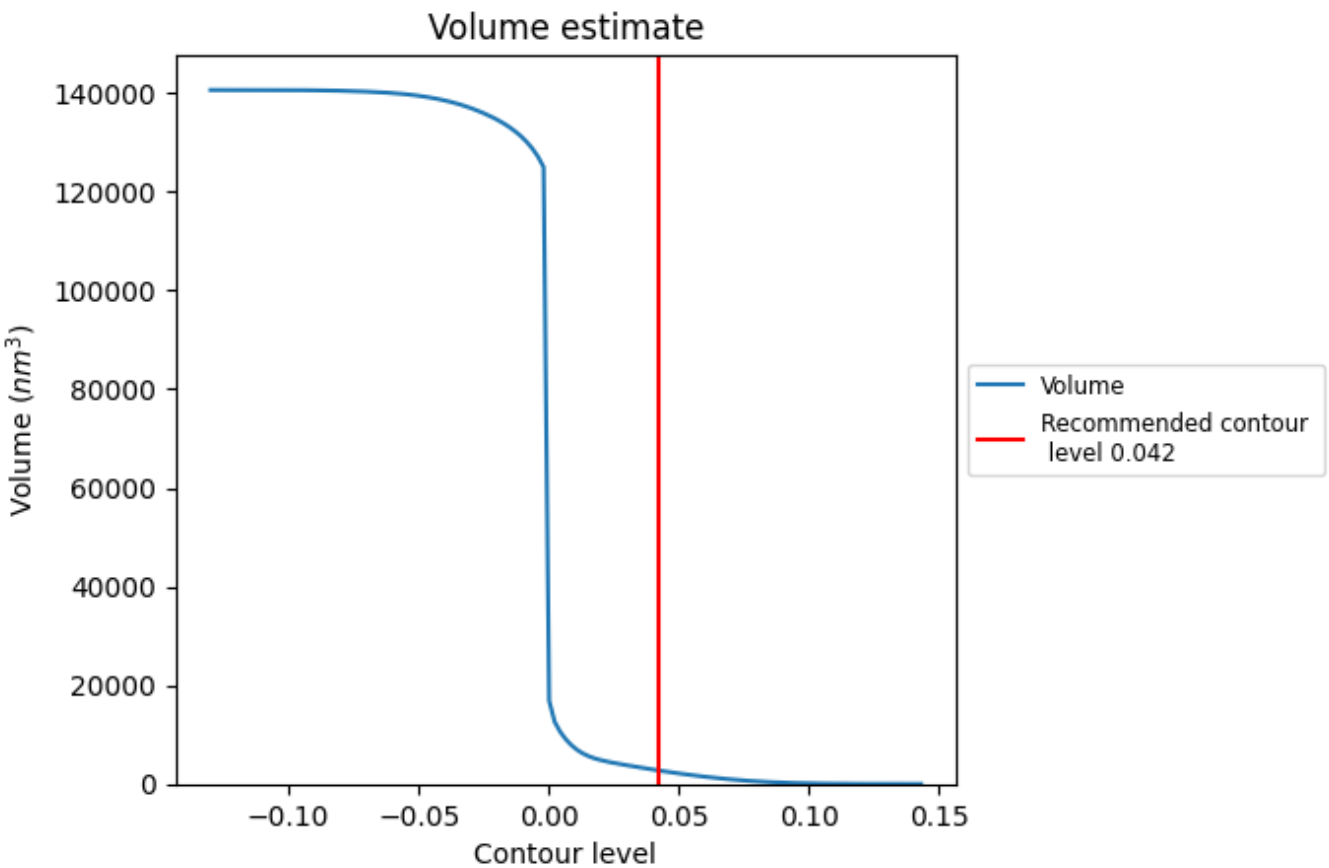
This section contains the results of statistical analysis of the map.

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.

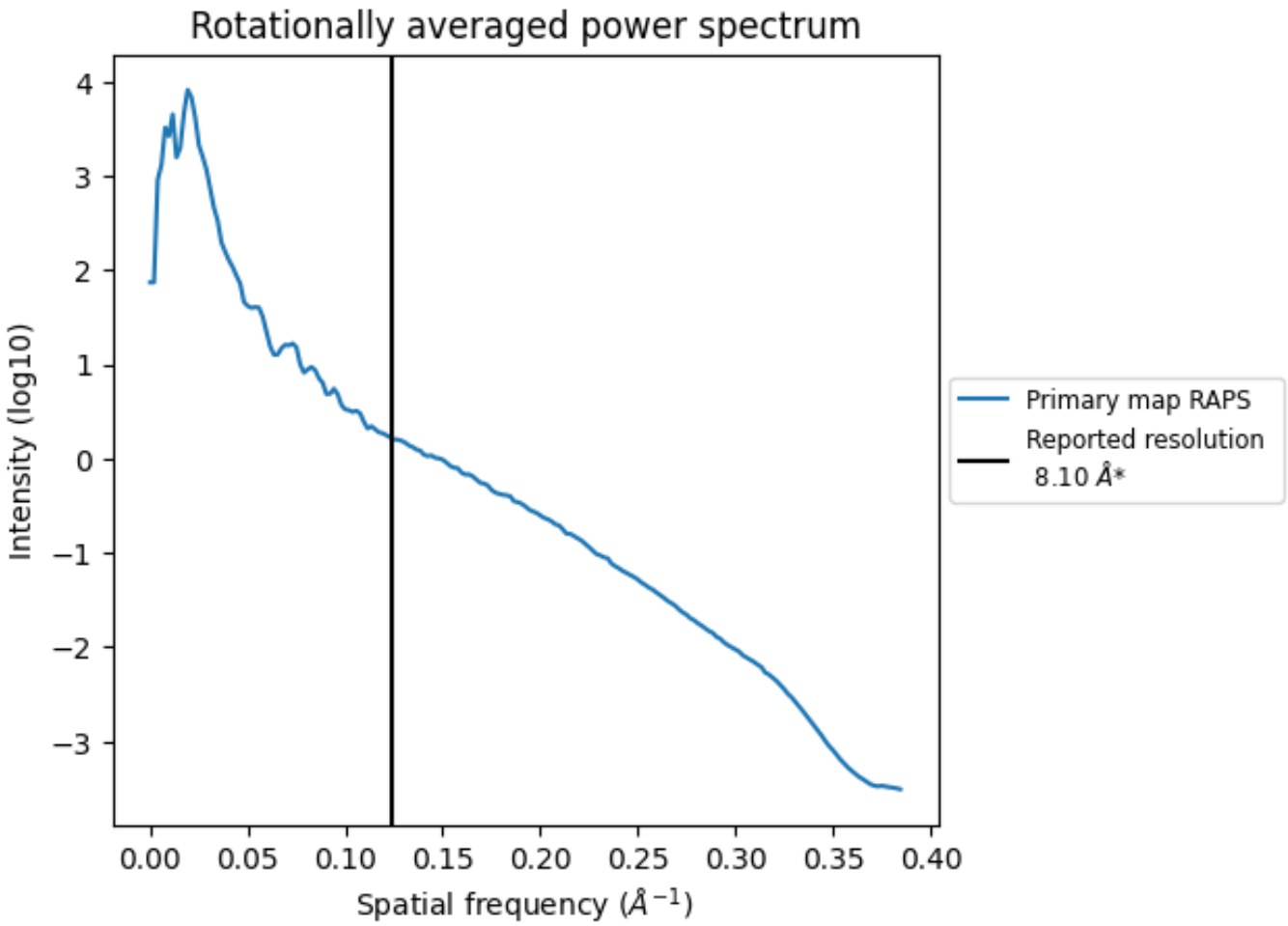
7.2 Volume estimate (i)



The volume at the recommended contour level is 2748 nm^3; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.123 Å^{-1}

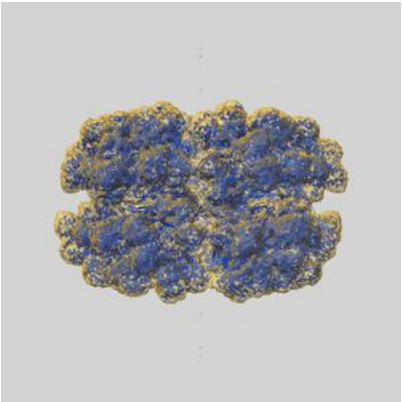
8 Fourier-Shell correlation (i)

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

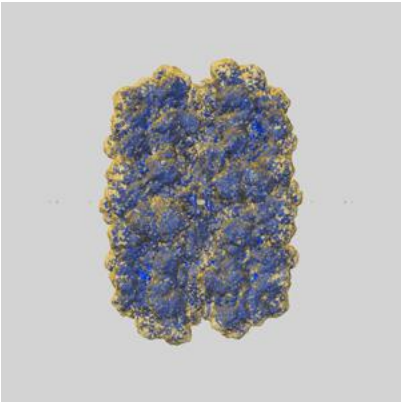
9 Map-model fit (i)

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 23.

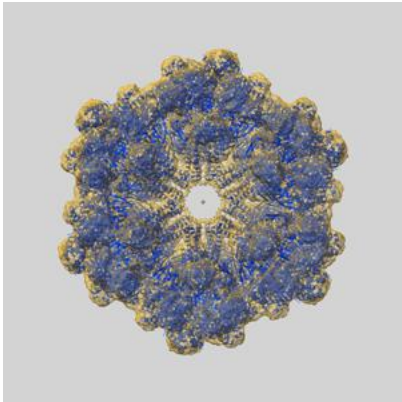
9.1 Map-model overlay (i)



X



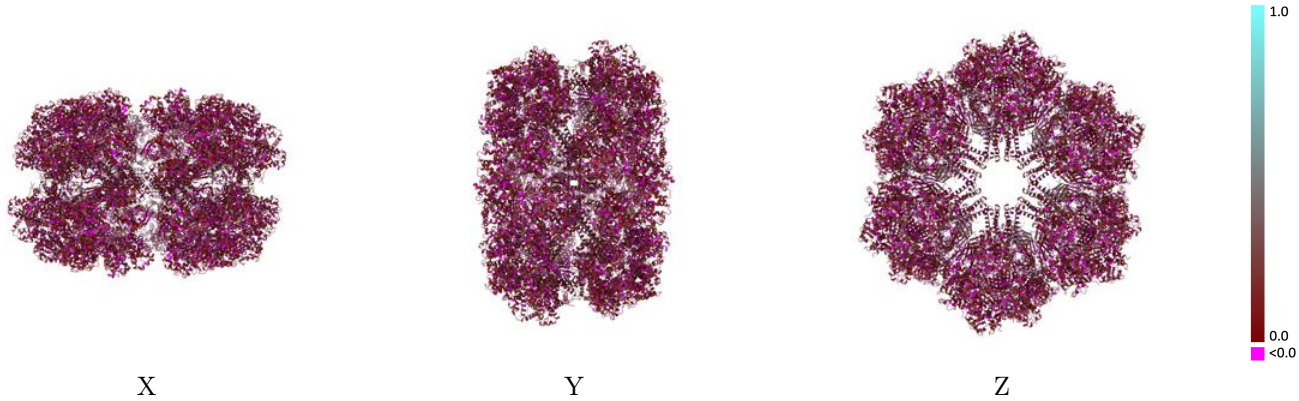
Y



Z

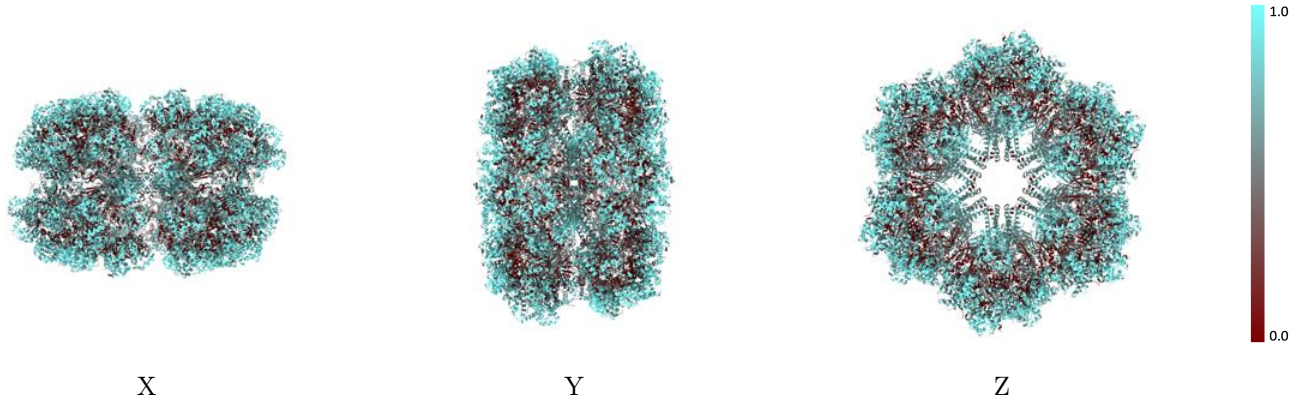
The images above show the 3D surface view of the map at the recommended contour level 0.042 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



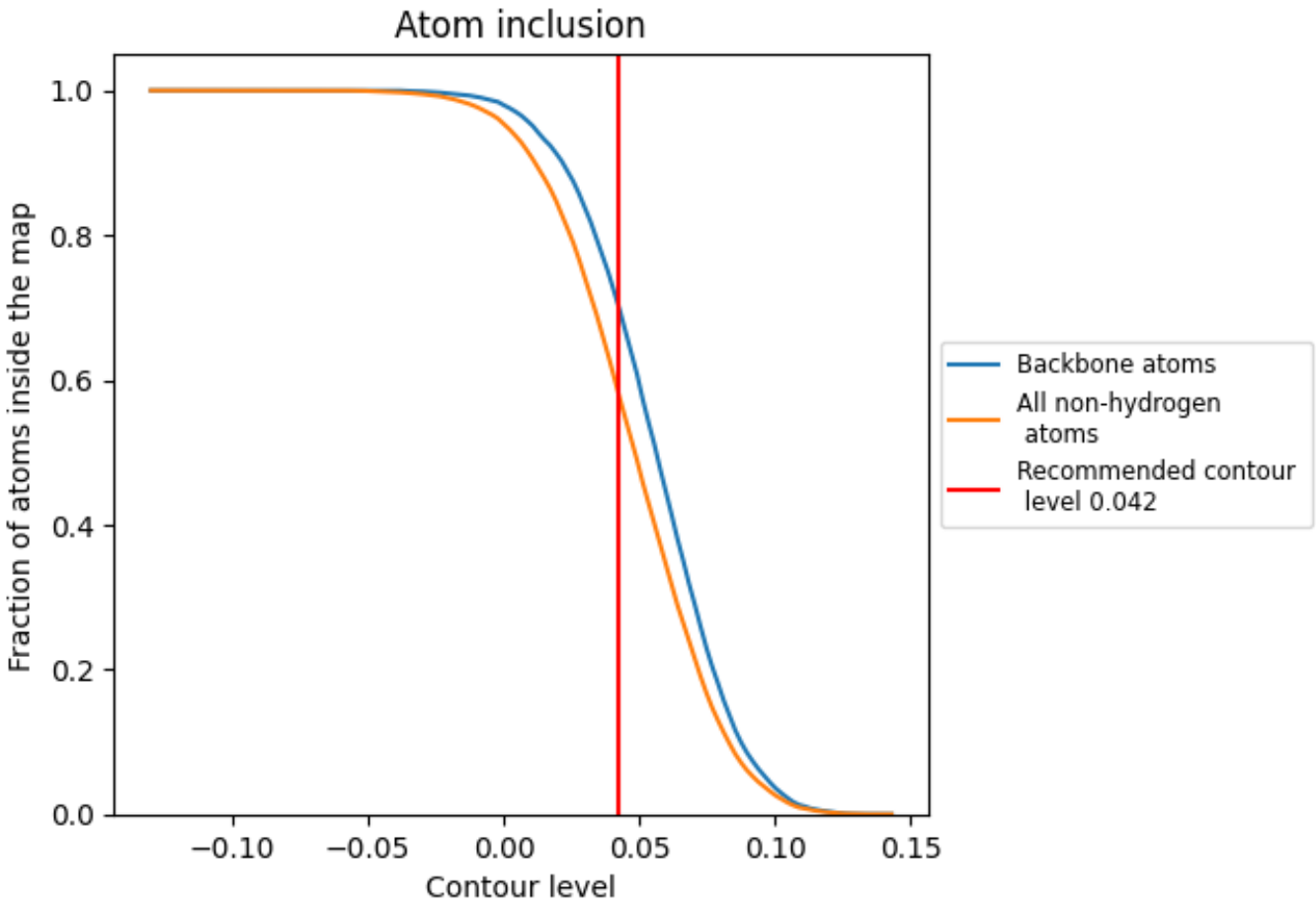
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	0.5867	0.1070
A0	0.5473	0.1090
A1	0.6724	0.1140
A2	0.6221	0.1040
A3	0.7115	0.1110
A4	0.6601	0.1230
A5	0.5448	0.1080
A6	0.6715	0.1130
A7	0.6213	0.1070
AA	0.7132	0.1160
AB	0.6610	0.1270
AC	0.5465	0.1110
AD	0.6697	0.1140
AE	0.6187	0.1050
AF	0.7081	0.1140
AG	0.6619	0.1260
AH	0.5473	0.1090
AI	0.6724	0.1140
AJ	0.6221	0.1050
AK	0.7115	0.1140
AL	0.6601	0.1250
AM	0.5448	0.1080
AN	0.6715	0.1120
AO	0.6213	0.1060
AP	0.7132	0.1140
AQ	0.6610	0.1260
AR	0.5465	0.1090
AS	0.6697	0.1120
AT	0.6187	0.1060
AU	0.7081	0.1150
AV	0.6619	0.1270
AW	0.5473	0.1120
AX	0.6724	0.1170
AY	0.6221	0.1040
AZ	0.7115	0.1150

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Chain	Atom inclusion	Q-score
Aa	0.6601	0.1250
Ab	0.5448	0.1120
Ac	0.6715	0.1160
Ad	0.6213	0.1050
Ae	0.7132	0.1130
Af	0.6610	0.1250
Ag	0.5465	0.1070
Ah	0.6697	0.1110
Ai	0.6187	0.1070
Aj	0.7081	0.1120
Ak	0.6619	0.1230
Al	0.5473	0.1080
Am	0.6724	0.1150
An	0.6221	0.1040
Ao	0.7115	0.1120
Ap	0.6601	0.1210
Aq	0.5448	0.1060
Ar	0.6715	0.1150
As	0.6213	0.1050
At	0.7132	0.1110
Au	0.6601	0.1220
Av	0.5465	0.1070
Aw	0.6697	0.1140
Ax	0.6187	0.1060
Ay	0.7081	0.1100
Az	0.6619	0.1240
B0	0.7282	0.1310
B1	0.5447	0.0870
B2	0.6059	0.1130
B3	0.5240	0.0950
B4	0.6596	0.1200
B5	0.7255	0.1300
B6	0.5430	0.0850
B7	0.6077	0.1150
BA	0.5231	0.0900
BB	0.6604	0.1230
BC	0.7264	0.1250
BD	0.5455	0.0830
BE	0.6085	0.1150
BF	0.5196	0.0920
BG	0.6570	0.1230
BH	0.7282	0.1280

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Chain	Atom inclusion	Q-score
BI	0.5447	0.0850
BJ	0.6059	0.1170
BK	0.5240	0.0980
BL	0.6596	0.1240
BM	0.7255	0.1290
BN	0.5430	0.0810
BO	0.6077	0.1160
BP	0.5231	0.0950
BQ	0.6604	0.1270
BR	0.7264	0.1290
BS	0.5455	0.0830
BT	0.6085	0.1140
BU	0.5196	0.0930
BV	0.6570	0.1230
BW	0.7282	0.1290
BX	0.5447	0.0840
BY	0.6059	0.1120
BZ	0.5240	0.0940
Ba	0.6596	0.1220
Bb	0.7255	0.1280
Bc	0.5430	0.0820
Bd	0.6077	0.1120
Be	0.5231	0.0910
Bf	0.6604	0.1180
Bg	0.7264	0.1280
Bh	0.5455	0.0830
Bi	0.6085	0.1170
Bj	0.5196	0.0880
Bk	0.6570	0.1190
Bl	0.7282	0.1310
Bm	0.5447	0.0820
Bn	0.6059	0.1170
Bo	0.5240	0.0900
Bp	0.6596	0.1220
Bq	0.7255	0.1290
Br	0.5430	0.0810
Bs	0.6077	0.1160
Bt	0.5231	0.0880
Bu	0.6604	0.1220
Bv	0.7264	0.1300
Bw	0.5455	0.0840
Bx	0.6085	0.1140

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Chain	Atom inclusion	Q-score
By	0.5196	0.0900
Bz	0.6570	0.1200
C0	0.4218	0.0950
C1	0.4210	0.0940
C2	0.5453	0.1010
C3	0.6288	0.0980
C4	0.7012	0.1200
C5	0.4194	0.0960
C6	0.4233	0.0950
C7	0.5459	0.1040
CA	0.6323	0.0990
CB	0.7012	0.1150
CC	0.4200	0.0980
CD	0.4227	0.0990
CE	0.5441	0.1020
CF	0.6305	0.0990
CG	0.7057	0.1160
CH	0.4218	0.0960
CI	0.4210	0.0990
CJ	0.5453	0.1040
CK	0.6288	0.0980
CL	0.7012	0.1130
CM	0.4194	0.0960
CN	0.4233	0.0990
CO	0.5459	0.1050
CP	0.6323	0.0970
CQ	0.7012	0.1140
CR	0.4200	0.0970
CS	0.4227	0.0980
CT	0.5441	0.1040
CU	0.6305	0.0950
CV	0.7057	0.1170
CW	0.4218	0.0960
CX	0.4210	0.0970
CY	0.5453	0.1030
CZ	0.6288	0.0960
Ca	0.7012	0.1190
Cb	0.4194	0.0970
Cc	0.4233	0.0970
Cd	0.5459	0.1020
Ce	0.6323	0.1020
Cf	0.7012	0.1190

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Chain	Atom inclusion	Q-score
Cg	0.4200	0.0960
Ch	0.4227	0.0970
Ci	0.5441	0.1040
Cj	0.6305	0.1010
Ck	0.7057	0.1180
Cl	0.4218	0.0940
Cm	0.4210	0.0960
Cn	0.5453	0.1050
Co	0.6288	0.0980
Cp	0.7012	0.1170
Cq	0.4194	0.0940
Cr	0.4233	0.0960
Cs	0.5459	0.1030
Ct	0.6323	0.0970
Cu	0.7012	0.1170
Cv	0.4200	0.0960
Cw	0.4227	0.0950
Cx	0.5441	0.1030
Cy	0.6305	0.0960
Cz	0.7057	0.1190