Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 11:43 pm GMT

PDB ID	:	5IV5
EMDB ID	:	EMD-3374
Title	:	Cryo-electron microscopy structure of the hexagonal pre-attachment T4 baseplate-tail tube complex
Authors	:	Taylor, N.M.I.; Guerrero-Ferreira, R.C.; Goldie, K.N.; Stahlberg, H.; Leiman, P.G.
Deposited on	:	2016-03-19
Resolution	:	4.11 Å(reported)
Based on initial models	:	1N7Z, 1K28, 1S2E, 4KU0, 1EL6, 2FKK, 3H2T, 1OCY, 4HRZ, 1H6W

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:

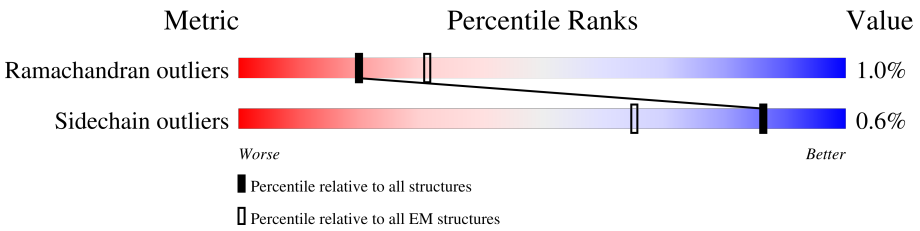
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.11 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	A	660	99%
1	B	660	5% 96%
1	BH	660	99%
1	BI	660	5% 96%
1	EA	660	99%
1	EB	660	5% 96%
1	GD	660	99%
1	GE	660	5% 96%
1	X	660	99%

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Mol	Chain	Length	Quality of chain
1	Y	660	5% 96%
1	u	660	99%
1	v	660	5% 96%
2	BJ	1032	5% 92% 5%
2	C	1032	6% 92% 5%
2	EC	1032	6% 92% 5%
2	GF	1032	5% 92% 5%
2	Z	1032	5% 92% 5%
2	w	1032	5% 92% 5%
3	CA	334	97%
3	CB	334	98%
3	D	334	97%
3	E	334	98%
3	ED	334	97%
3	EE	334	98%
3	GG	334	97%
3	GH	334	98%
3	a	334	97%
3	b	334	98%
3	x	334	97%
3	y	334	98%
4	AA	288	98% 99%
4	AB	288	99% 99%
4	CC	288	99% 99%
4	CD	288	99% 99%

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Mol	Chain	Length	Quality of chain
4	CE	288	99% / 99%
4	EF	288	99% / 99%
4	EG	288	99% / 99%
4	EH	288	99% / 99%
4	F	288	99% / 99%
4	G	288	99% / 99%
4	GI	288	99% / 99%
4	GJ	288	98% / 99%
4	H	288	99% / 99%
4	HA	288	99% / 99%
4	c	288	99% / 99%
4	d	288	99% / 99%
4	e	288	99% / 99%
4	z	288	99% / 99%
5	AC	602	18% / 96%
5	AD	602	15% / 95% / 5%
5	AE	602	17% / 95% / 5%
5	CF	602	17% / 96%
5	CG	602	16% / 95% / 5%
5	CH	602	17% / 95% / 5%
5	EI	602	17% / 96%
5	EJ	602	16% / 95% / 5%
5	FA	602	17% / 95% / 5%
5	HB	602	17% / 96%
5	HC	602	16% / 95% / 5%

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Mol	Chain	Length	Quality of chain
5	HD	602	17% 95% 5%
5	I	602	17% 96% .
5	J	602	17% 95% 5%
5	K	602	18% 95% 5%
5	f	602	18% 96% .
5	g	602	17% 95% 5%
5	h	602	18% 95% 5%
6	AF	219	52% 98% .
6	AG	219	59% 98% .
6	AH	219	55% 98% .
6	CI	219	53% 98% .
6	CJ	219	59% 98% .
6	DA	219	55% 98% .
6	FB	219	53% 98% .
6	FC	219	59% 98% .
6	FD	219	52% 98% .
6	HE	219	52% 98% .
6	HF	219	61% 98% .
6	HG	219	55% 98% .
6	L	219	54% 98% .
6	M	219	61% 98% .
6	N	219	54% 98% .
6	i	219	52% 98% .
6	j	219	60% 98% .
6	k	219	53% 98% .

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Mol	Chain	Length	Quality of chain
7	AI	527	32% 98%
7	AJ	527	38% 98%
7	BA	527	34% 98%
7	DB	527	32% 98%
7	DC	527	38% 98%
7	DD	527	33% 98%
7	FE	527	31% 98%
7	FF	527	37% 98%
7	FG	527	32% 98%
7	HH	527	31% 98%
7	HI	527	38% 98%
7	HJ	527	34% 98%
7	O	527	32% 98%
7	P	527	37% 98%
7	Q	527	33% 98%
7	l	527	31% 98%
7	m	527	36% 98%
7	n	527	34% 98%
8	BB	163	55% 99%
8	BC	163	90% 99%
8	DE	163	53% 99%
8	DF	163	91% 99%
8	FH	163	55% 99%
8	FI	163	91% 99%
8	IA	163	55% 99%

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Mol	Chain	Length	Quality of chain
8	IB	163	91% 99%
8	R	163	53% 99%
8	S	163	93% 99%
8	o	163	56% 99%
8	p	163	92% 99%
9	BD	132	6% 95% 5%
9	DG	132	6% 95% 5%
9	FJ	132	8% 95% 5%
9	IC	132	7% 95% 5%
9	T	132	6% 95% 5%
9	q	132	6% 95% 5%
10	BE	364	44% 55%
10	DH	364	44% 55%
10	GA	364	44% 55%
10	ID	364	44% 55%
10	U	364	44% 55%
10	r	364	44% 55%
11	BF	196	96%
11	DI	196	96%
11	GB	196	96%
11	IE	196	96%
11	V	196	96%
11	s	196	96%
12	BG	320	11% 58% 40%
12	DJ	320	11% 58% 40%

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Mol	Chain	Length	Quality of chain
12	GC	320	11% 58% • 40%
12	IF	320	11% 58% • 40%
12	W	320	10% 58% • 40%
12	t	320	10% 58% • 40%
13	YA	575	34% 88% 8% •
13	YB	575	33% 88% 8% •
13	YC	575	33% 88% 8% •
14	YD	391	15% 83% 10% 7%
14	YE	391	15% 83% 10% 7%
14	YF	391	15% 83% 10% 7%
15	ZA	97	33% 96% • •

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 549576 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 Baseplate wedge protein gp6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	658	5235	3308	867	1050	10	0	0
1	B	648	5157	3259	854	1034	10	0	0
1	X	658	5235	3308	867	1050	10	0	0
1	Y	648	5157	3259	854	1034	10	0	0
1	u	658	5235	3308	867	1050	10	0	0
1	v	648	5157	3259	854	1034	10	0	0
1	BH	658	5235	3308	867	1050	10	0	0
1	BI	648	5157	3259	854	1034	10	0	0
1	EA	658	5235	3308	867	1050	10	0	0
1	EB	648	5157	3259	854	1034	10	0	0
1	GD	658	5235	3308	867	1050	10	0	0
1	GE	648	5157	3259	854	1034	10	0	0

- Molecule 2 is a protein called Baseplate wedge protein gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1004	8199	5247	1347	1578	27	0	0
2	Z	1004	8199	5247	1347	1578	27	0	0
2	w	1004	8199	5247	1347	1578	27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BJ	1004	8199	5247	1347	1578	27	0	0
2	EC	1004	8199	5247	1347	1578	27	0	0
2	GF	1004	8199	5247	1347	1578	27	0	0

- Molecule 3 is a protein called Baseplate wedge protein gp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	328	2631	1677	430	507	17	0	0
3	E	332	2658	1692	434	515	17	0	0
3	a	328	2631	1677	430	507	17	0	0
3	b	332	2658	1692	434	515	17	0	0
3	x	328	2631	1677	430	507	17	0	0
3	y	332	2658	1692	434	515	17	0	0
3	CA	328	2631	1677	430	507	17	0	0
3	CB	332	2658	1692	434	515	17	0	0
3	ED	328	2631	1677	430	507	17	0	0
3	EE	332	2658	1692	434	515	17	0	0
3	GG	328	2631	1677	430	507	17	0	0
3	GH	332	2658	1692	434	515	17	0	0

- Molecule 4 is a protein called Baseplate wedge protein gp9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	288	2175	1354	366	446	9	0	0
4	G	288	2175	1354	366	446	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	288	2175	1354	366	446	9	0	0
4	c	288	2175	1354	366	446	9	0	0
4	d	288	2175	1354	366	446	9	0	0
4	e	288	2175	1354	366	446	9	0	0
4	z	288	2175	1354	366	446	9	0	0
4	AA	288	2175	1354	366	446	9	0	0
4	AB	288	2175	1354	366	446	9	0	0
4	CC	288	2175	1354	366	446	9	0	0
4	CD	288	2175	1354	366	446	9	0	0
4	CE	288	2175	1354	366	446	9	0	0
4	EF	288	2175	1354	366	446	9	0	0
4	EG	288	2175	1354	366	446	9	0	0
4	EH	288	2175	1354	366	446	9	0	0
4	GI	288	2175	1354	366	446	9	0	0
4	GJ	288	2175	1354	366	446	9	0	0
4	HA	288	2175	1354	366	446	9	0	0

- Molecule 5 is a protein called Baseplate wedge protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	602	4675	2933	779	953	10	0	0
5	J	602	4675	2933	779	953	10	0	0
5	K	602	4675	2933	779	953	10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	602	4675	2933	779	953	10	0	0
5	g	602	4675	2933	779	953	10	0	0
5	h	602	4675	2933	779	953	10	0	0
5	AC	602	4675	2933	779	953	10	0	0
5	AD	602	4675	2933	779	953	10	0	0
5	AE	602	4675	2933	779	953	10	0	0
5	CF	602	4675	2933	779	953	10	0	0
5	CG	602	4675	2933	779	953	10	0	0
5	CH	602	4675	2933	779	953	10	0	0
5	EI	602	4675	2933	779	953	10	0	0
5	EJ	602	4675	2933	779	953	10	0	0
5	FA	602	4675	2933	779	953	10	0	0
5	HB	602	4675	2933	779	953	10	0	0
5	HC	602	4675	2933	779	953	10	0	0
5	HD	602	4675	2933	779	953	10	0	0

- Molecule 6 is a protein called Baseplate wedge protein gp11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	218	1665	1056	273	334	2	0	0
6	M	218	1665	1056	273	334	2	0	0
6	N	218	1665	1056	273	334	2	0	0
6	i	218	1665	1056	273	334	2	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	j	218	1665	1056	273	334	2	0	0
6	k	218	1665	1056	273	334	2	0	0
6	AF	218	1665	1056	273	334	2	0	0
6	AG	218	1665	1056	273	334	2	0	0
6	AH	218	1665	1056	273	334	2	0	0
6	CI	218	1665	1056	273	334	2	0	0
6	CJ	218	1665	1056	273	334	2	0	0
6	DA	218	1665	1056	273	334	2	0	0
6	FB	218	1665	1056	273	334	2	0	0
6	FC	218	1665	1056	273	334	2	0	0
6	FD	218	1665	1056	273	334	2	0	0
6	HE	218	1665	1056	273	334	2	0	0
6	HF	218	1665	1056	273	334	2	0	0
6	HG	218	1665	1056	273	334	2	0	0

- Molecule 7 is a protein called Short tail fiber protein gp12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	O	526	3945	2429	702	803	11	0	0
7	P	526	3945	2429	702	803	11	0	0
7	Q	526	3945	2429	702	803	11	0	0
7	l	526	3945	2429	702	803	11	0	0
7	m	526	3945	2429	702	803	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	n	526	3945	2429	702	803	11	0	0
7	AI	526	3945	2429	702	803	11	0	0
7	AJ	526	3945	2429	702	803	11	0	0
7	BA	526	3945	2429	702	803	11	0	0
7	DB	526	3945	2429	702	803	11	0	0
7	DC	526	3945	2429	702	803	11	0	0
7	DD	526	3945	2429	702	803	11	0	0
7	FE	526	3945	2429	702	803	11	0	0
7	FF	526	3945	2429	702	803	11	0	0
7	FG	526	3945	2429	702	803	11	0	0
7	HH	526	3945	2429	702	803	11	0	0
7	HI	526	3945	2429	702	803	11	0	0
7	HJ	526	3945	2429	702	803	11	0	0

- Molecule 8 is a protein called Tail tube protein gp19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	R	162	1296	823	218	252	3	0	0
8	S	162	1296	823	218	252	3	0	0
8	o	162	1296	823	218	252	3	0	0
8	p	162	1296	823	218	252	3	0	0
8	BB	162	1296	823	218	252	3	0	0
8	BC	162	1296	823	218	252	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	DE	162	1296	823	218	252	3	0	0
8	DF	162	1296	823	218	252	3	0	0
8	FH	162	1296	823	218	252	3	0	0
8	FI	162	1296	823	218	252	3	0	0
8	IA	162	1296	823	218	252	3	0	0
8	IB	162	1296	823	218	252	3	0	0

- Molecule 9 is a protein called Baseplate wedge protein gp25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	T	126	1011	636	169	202	4	0	0
9	q	126	1011	636	169	202	4	0	0
9	BD	126	1011	636	169	202	4	0	0
9	DG	126	1011	636	169	202	4	0	0
9	FJ	126	1011	636	169	202	4	0	0
9	IC	126	1011	636	169	202	4	0	0

- Molecule 10 is a protein called Baseplate tail-tube protein gp48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	U	165	1317	846	219	247	5	0	0
10	r	165	1317	846	219	247	5	0	0
10	BE	165	1317	846	219	247	5	0	0
10	DH	165	1317	846	219	247	5	0	0
10	GA	165	1317	846	219	247	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	ID	165	1317	846	219	247	5	0	0

- Molecule 11 is a protein called Baseplate wedge protein gp53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	V	193	1599	1035	259	299	6	0	0
11	s	193	1599	1035	259	299	6	0	0
11	BF	193	1599	1035	259	299	6	0	0
11	DI	193	1599	1035	259	299	6	0	0
11	GB	193	1599	1035	259	299	6	0	0
11	IE	193	1599	1035	259	299	6	0	0

- Molecule 12 is a protein called Baseplate tail-tube protein gp54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	W	192	1524	955	257	301	11	0	0
12	t	192	1524	955	257	301	11	0	0
12	BG	192	1524	955	257	301	11	0	0
12	DJ	192	1524	955	257	301	11	0	0
12	GC	192	1524	955	257	301	11	0	0
12	IF	192	1524	955	257	301	11	0	0

- Molecule 13 is a protein called Peptidoglycan hydrolase gp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	YA	554	25692	15942	4536	5088	126	554	0
13	YB	554	25692	15942	4536	5088	126	554	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	YC	554	25692	15942	4536	5088	126	554	0

- Molecule 14 is a protein called Baseplate hub protein gp27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	YD	364	17472	11148	2868	3354	102	364	0
14	YE	364	17472	11148	2868	3354	102	364	0
14	YF	364	17472	11148	2868	3354	102	364	0

- Molecule 15 is a protein called Uncharacterized 10.2 kDa protein in segC-Gp6 intergenic region.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	ZA	96	4254	2682	720	834	18	96	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	O	1	1	1	0
16	l	1	1	1	0
16	AI	1	1	1	0
16	DB	1	1	1	0
16	FE	1	1	1	0
16	HH	1	1	1	0

- Molecule 17 is FE (III) ION (three-letter code: FE) (formula: Fe).

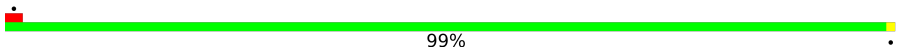
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
17	ZA	1	6	6	1

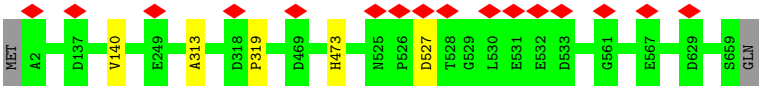
3 Residue-property plots (i)

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: Baseplate wedge protein gp6

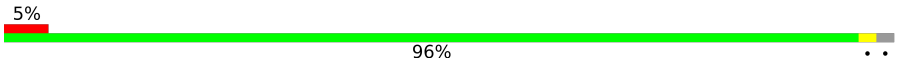
Chain A:

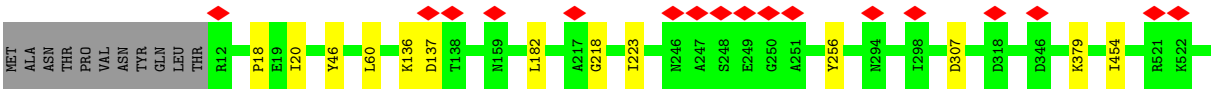


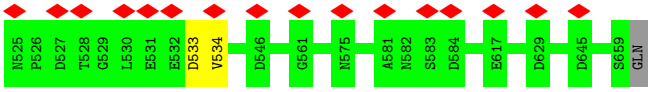


• Molecule 1: Baseplate wedge protein gp6

Chain B:

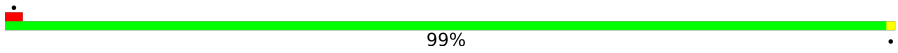


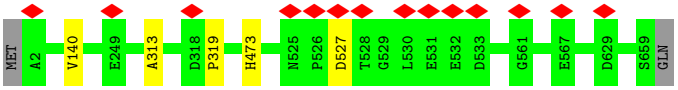




• Molecule 1: Baseplate wedge protein gp6

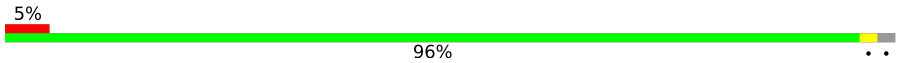
Chain X:

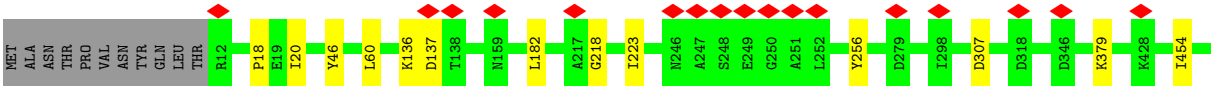


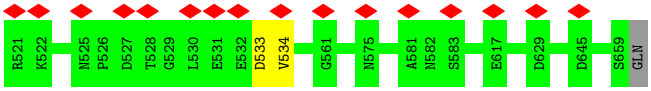


• Molecule 1: Baseplate wedge protein gp6

Chain Y:

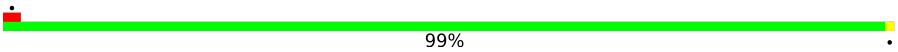


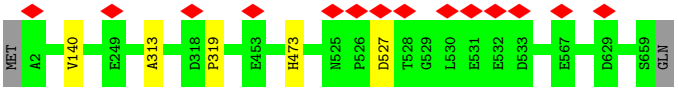




• Molecule 1: Baseplate wedge protein gp6

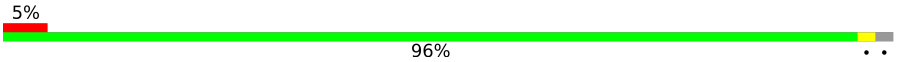
Chain u:

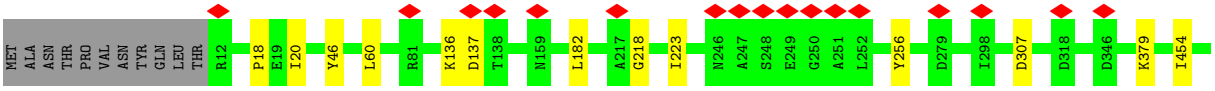


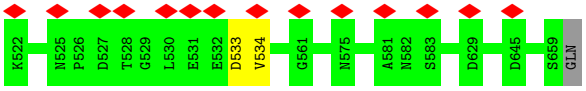


• Molecule 1: Baseplate wedge protein gp6

Chain v:

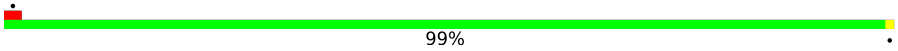


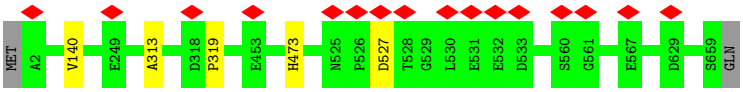




• Molecule 1: Baseplate wedge protein gp6

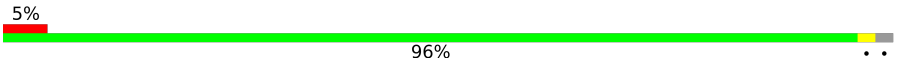
Chain BH:

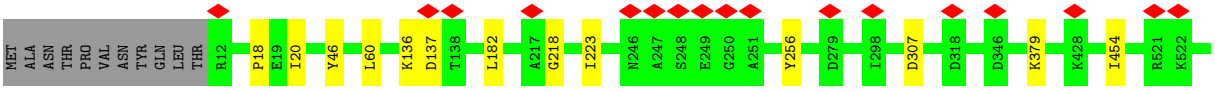


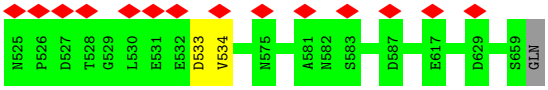


• Molecule 1: Baseplate wedge protein gp6

Chain BI:

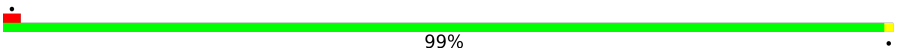


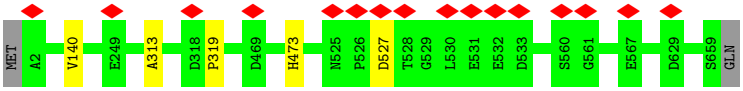




• Molecule 1: Baseplate wedge protein gp6

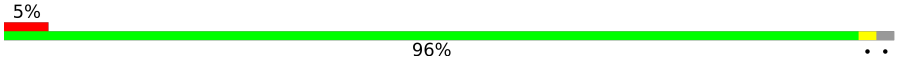
Chain EA:

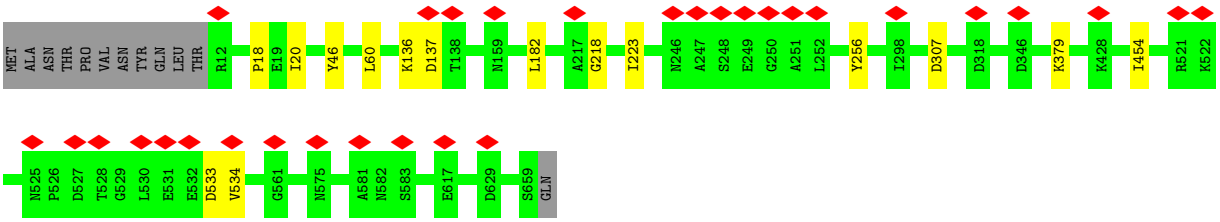




• Molecule 1: Baseplate wedge protein gp6

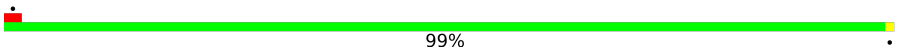
Chain EB:

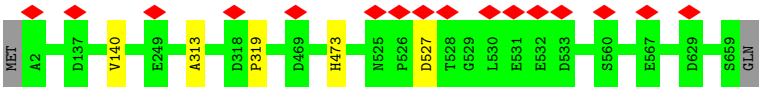




• Molecule 1: Baseplate wedge protein gp6

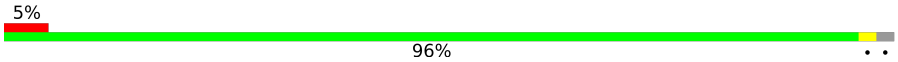
Chain GD:

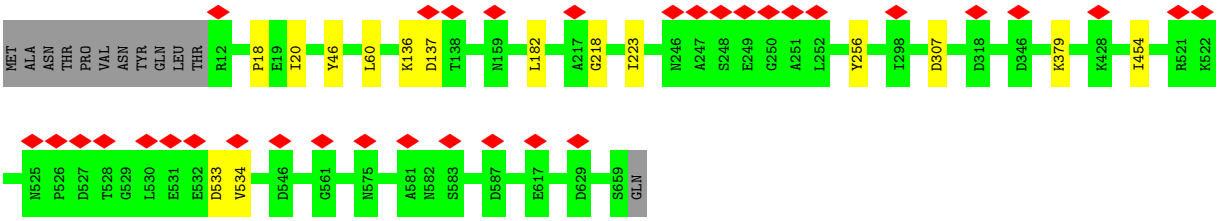




• Molecule 1: Baseplate wedge protein gp6

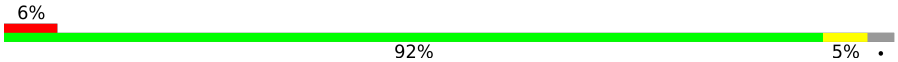
Chain GE:

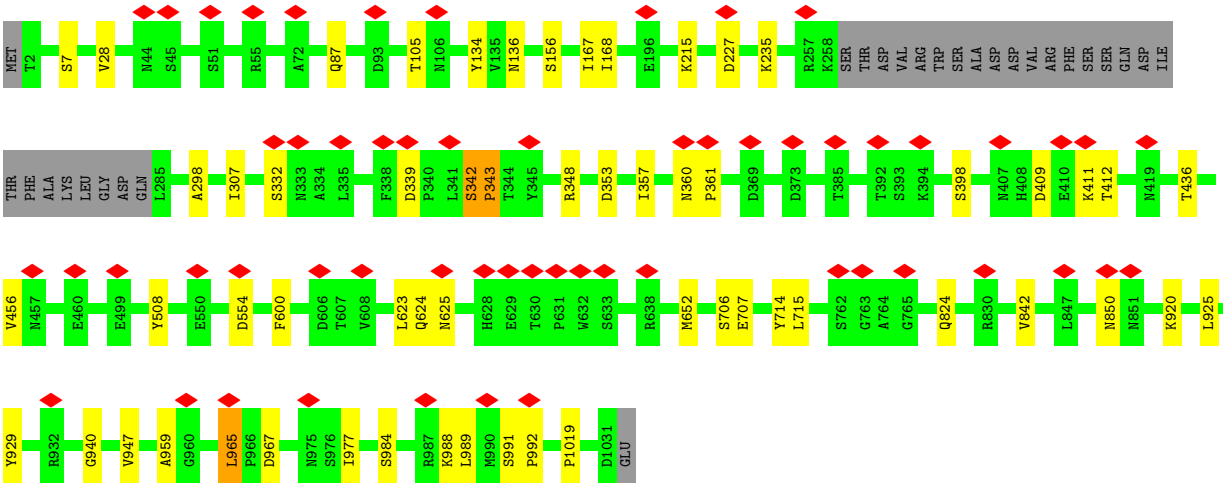




• Molecule 2: Baseplate wedge protein gp7

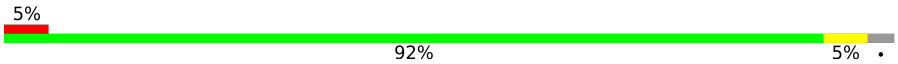
Chain C:

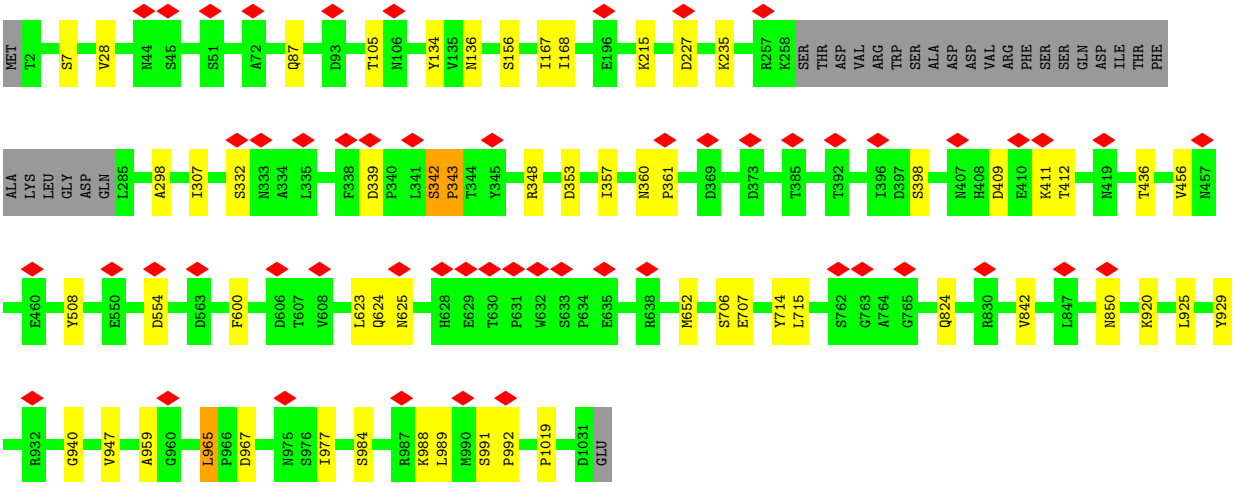




• Molecule 2: Baseplate wedge protein gp7

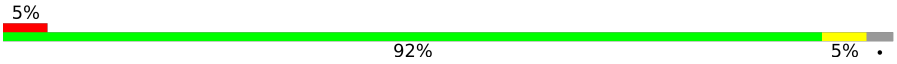
Chain Z:

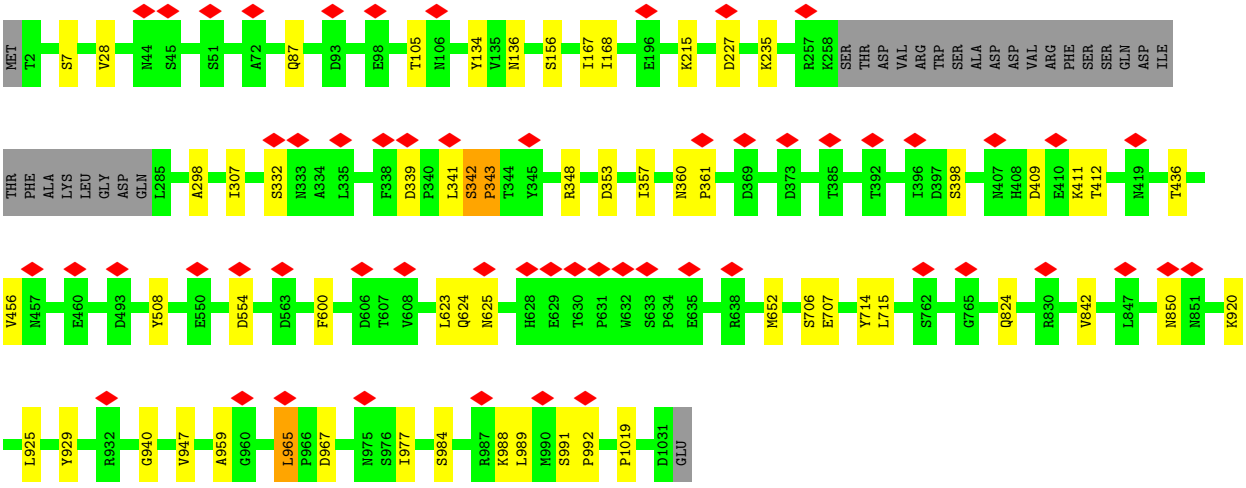




- Molecule 2: Baseplate wedge protein gp7

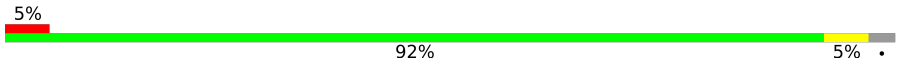
Chain w:

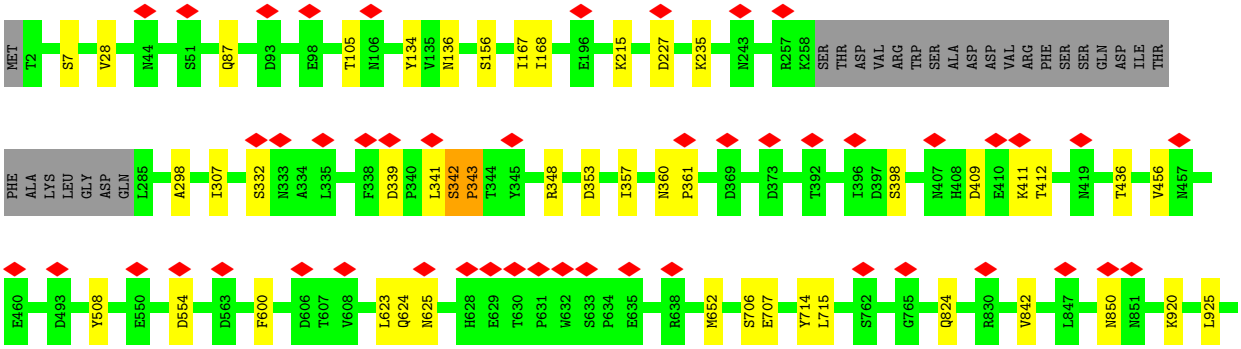


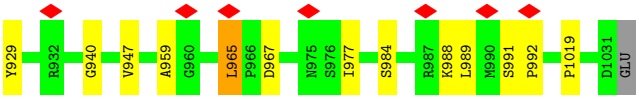


- Molecule 2: Baseplate wedge protein gp7

Chain BJ:

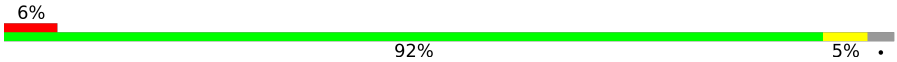


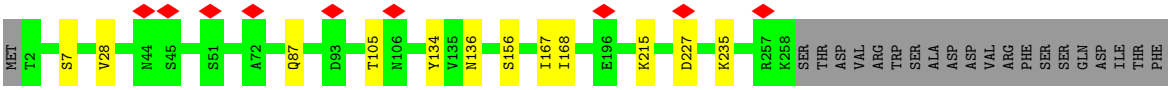


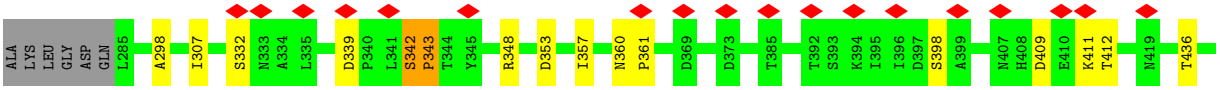


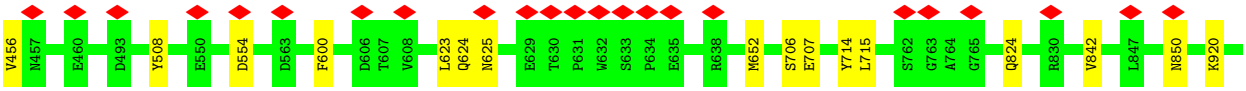
• Molecule 2: Baseplate wedge protein gp7

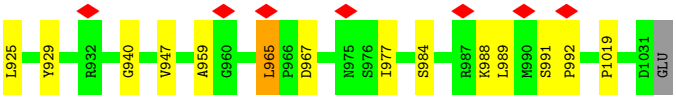
Chain EC:





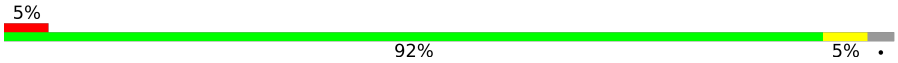


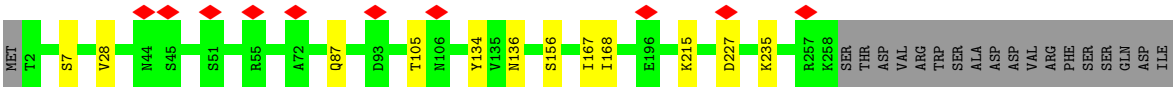


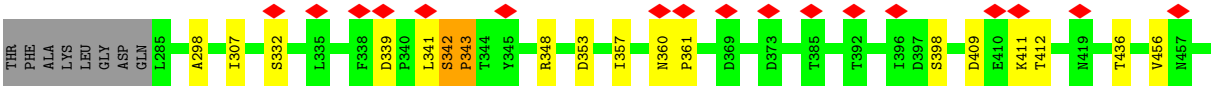


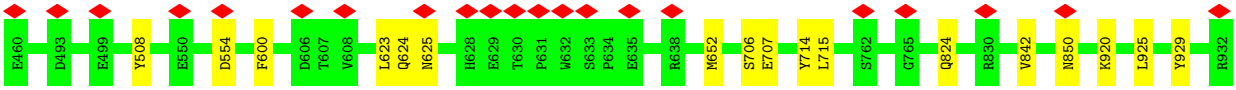
• Molecule 2: Baseplate wedge protein gp7

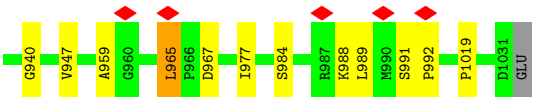
Chain GF:





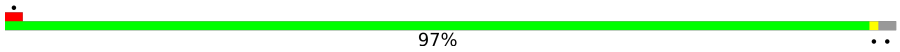


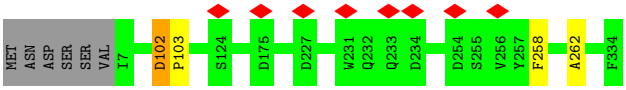




• Molecule 3: Baseplate wedge protein gp8

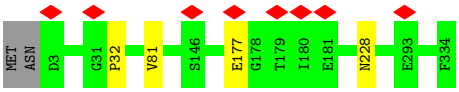
Chain D:





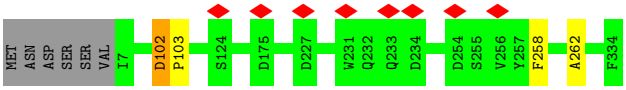
• Molecule 3: Baseplate wedge protein gp8

Chain E: 98%



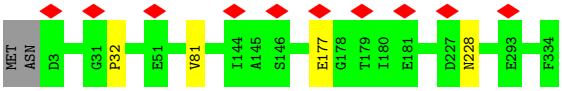
• Molecule 3: Baseplate wedge protein gp8

Chain a: 97%



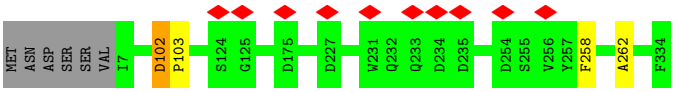
• Molecule 3: Baseplate wedge protein gp8

Chain b: 98%



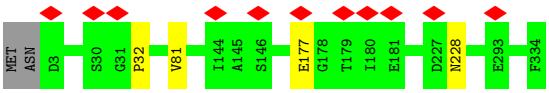
• Molecule 3: Baseplate wedge protein gp8

Chain x: 97%



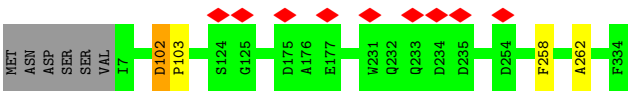
• Molecule 3: Baseplate wedge protein gp8

Chain y: 98%



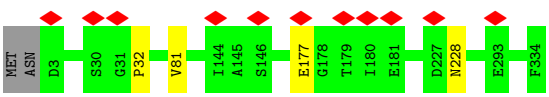
• Molecule 3: Baseplate wedge protein gp8

Chain CA: 97%



• Molecule 3: Baseplate wedge protein gp8

Chain CB: 98%



• Molecule 3: Baseplate wedge protein gp8

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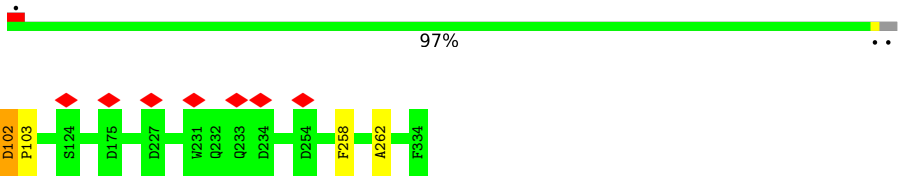

• Molecule 3: Baseplate wedge protein gp8

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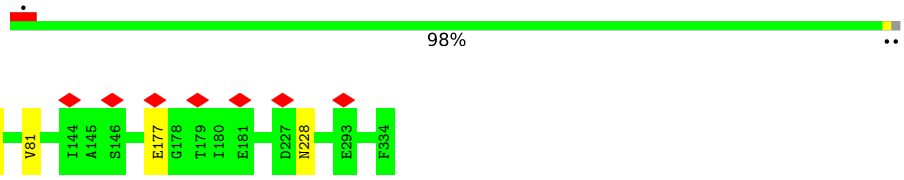

• Molecule 3: Baseplate wedge protein gp8

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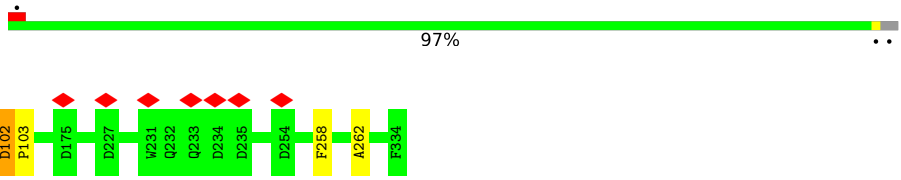

• Molecule 3: Baseplate wedge protein gp8

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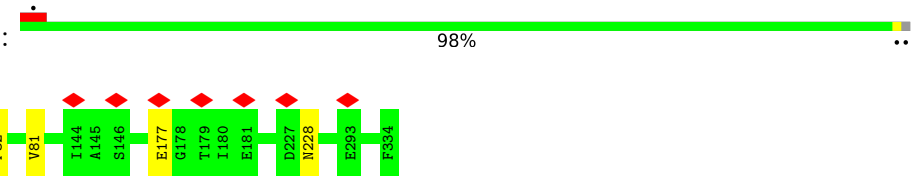
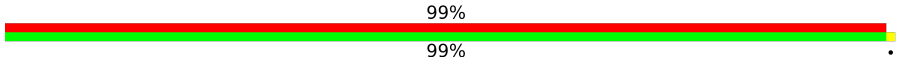
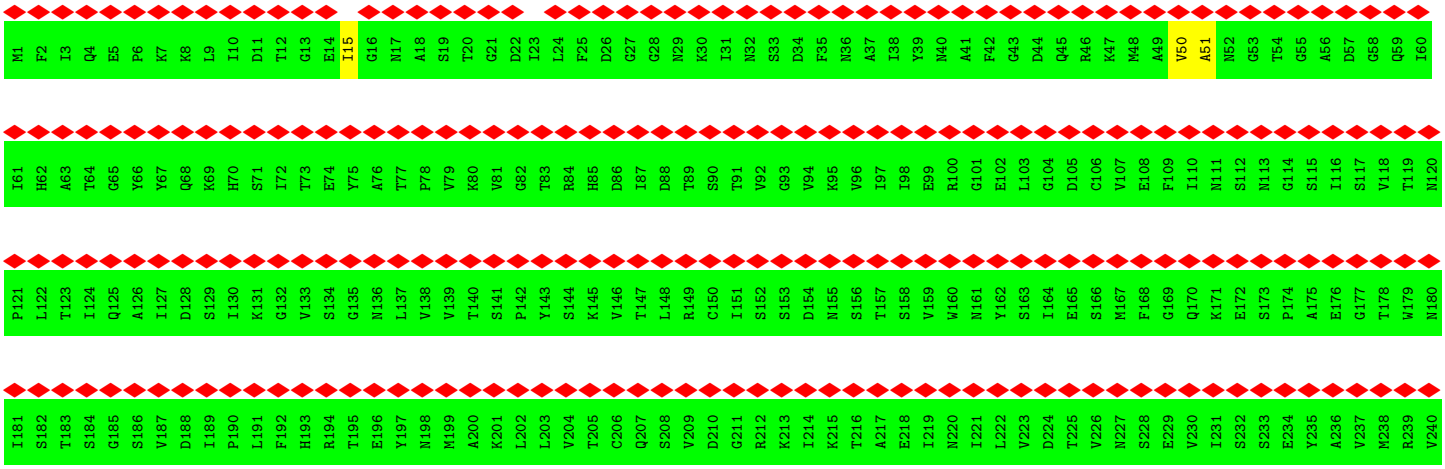


• Molecule 4: Baseplate wedge protein gp9

Chain F:





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- Molecule 4: Baseplate wedge protein gp9

Chain G: 99% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 K30 I31 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60

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- Molecule 4: Baseplate wedge protein gp9

Chain H: 99% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 K30 I31 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60

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I181 S182 T183 S184 G185 S186 V187 D188 I189 P190 L191 F192 H193 R194 T195 E196 Y197 N198 M199 A200 K201 L202 L203 V204 T205 C206 Q207 S208 V209 D210 G211 R212 K213 I214 K215 T216 A217 E218 I219 N220 I221 L222 V223 D224 T225 V226 N227 S228 E229 V230 I231 S232 S233 E234 Y235 A236 V237 M238 R239 V240

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- Molecule 4: Baseplate wedge protein gp9

Chain c: 99% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 K30 I31 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60

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- Molecule 4: Baseplate wedge protein gp9

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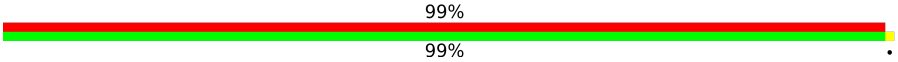

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- Molecule 4: Baseplate wedge protein gp9

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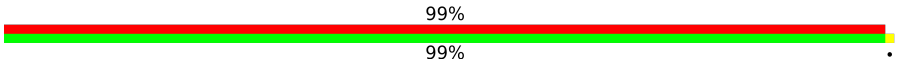

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- Molecule 4: Baseplate wedge protein gp9

Chain z: 99% 99%

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- Molecule 4: Baseplate wedge protein gp9

Chain AA: 98% 99%

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- Molecule 4: Baseplate wedge protein gp9

Chain AB: 99% 99%

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N242 E243 T244 E245 E246 D247 E248 I249 A250 N251 I252 A253 F254 S255 I256 K257 E258 N259 Y260 V261 T262 A263 T264 I265 S266 S267 S268 T269 V270 G271 M272 R273 A274 A275 V276 K277 V278 I279 A280 T281 Q282 K283 I284 G285 V286 A287 Q288

- Molecule 4: Baseplate wedge protein gp9

Chain CC: 99% 99%

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- Molecule 4: Baseplate wedge protein gp9

Chain CD: 99% 99%

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- Molecule 4: Baseplate wedge protein gp9

Chain CE: 99% 99%

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I61 H62 A63 T64 G65 Y66 Y67 Q68 K69 H70 S71 I72 T73 E74 Y75 A76 T77 P78 V79 K80 V81 G82 T83 R84 H85 D86 I87 D88 T89 S90 T91 V92 G93 V94 K95 V96 I97 I98 E99 R100 G101 E102 L103 G104 D105 C106 V107 E108 F109 I110 N111 S112 N113 G114 S115 I116 S117 V118 T119 N120

P121 L122 T123 I124 Q125 A126 I127 D128 S129 I130 K131 G132 V133 S134 G135 N136 L137 V138 V139 T140 S141 P142 Y143 S144 K145 V146 T147 L148 R149 C150 I151 S152 S153 D154 N155 S156 T157 S158 V159 W160 N161 Y162 S163 I164 E165 S166 M167 F168 G169 Q170 K171 E172 S173 P174 A175 E176 G177 T178 W179 N180

I181 S182 T183 S184 G185 S186 V187 D188 I189 P190 L191 F192 H193 R194 T195 E196 Y197 N198 M199 A200 K201 L202 L203 V204 T205 C206 Q207 S208 V209 D210 G211 R212 K213 I214 K215 T216 A217 E218 I219 N220 I221 L222 V223 D224 T225 V226 N227 S228 E229 V230 I231 S232 S233 E234 Y235 A236 V237 M238 R239 V240

G241 N242 E243 T244 E245 E246 D247 E248 I249 A250 N251 I252 A253 F254 S255 I256 K257 E258 N259 Y260 V261 T262 A263 T264 I265 S266 S267 S268 T269 V270 G271 M272 R273 A274 A275 V276 K277 V278 I279 A280 T281 Q282 K283 I284 G285 V286 A287 Q288

- Molecule 4: Baseplate wedge protein gp9

Chain EF: 99% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 K30 I31 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60

I61 H62 A63 T64 G65 Y66 Y67 Q68 K69 H70 S71 I72 T73 E74 Y75 A76 T77 P78 V79 K80 V81 G82 T83 R84 H85 D86 I87 D88 T89 S90 T91 V92 G93 V94 K95 V96 I97 I98 E99 R100 G101 E102 L103 G104 D105 C106 V107 E108 F109 I110 N111 S112 N113 G114 S115 I116 S117 V118 T119 N120

P121 L122 T123 I124 Q125 A126 I127 D128 S129 I130 K131 G132 V133 S134 G135 N136 L137 V138 V139 T140 S141 P142 Y143 S144 K145 V146 T147 L148 R149 C150 I151 S152 S153 D154 N155 S156 T157 S158 V159 W160 N161 Y162 S163 I164 E165 S166 M167 F168 G169 Q170 K171 E172 S173 P174 A175 E176 G177 T178 W179 N180

I181 S182 T183 S184 G185 S186 V187 D188 I189 P190 L191 F192 H193 R194 T195 E196 Y197 N198 M199 A200 K201 L202 L203 V204 T205 C206 Q207 S208 V209 D210 G211 R212 K213 I214 K215 T216 A217 E218 I219 N220 I221 L222 V223 D224 T225 V226 N227 S228 E229 V230 I231 S232 S233 E234 Y235 A236 V237 M238 R239 V240

G241 N242 E243 T244 E245 E246 D247 E248 I249 A250 N251 I252 A253 F254 S255 I256 K257 E258 N259 Y260 V261 T262 A263 T264 I265 S266 S267 S268 T269 V270 G271 M272 R273 A274 A275 V276 K277 V278 I279 A280 T281 Q282 K283 I284 G285 V286 A287 Q288

- Molecule 4: Baseplate wedge protein gp9

Chain EG: 99% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 K30 I31 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60

I61 H62 A63 T64 G65 Y66 Y67 Q68 K69 H70 S71 I72 T73 E74 Y75 A76 T77 P78 V79 K80 V81 G82 T83 R84 H85 D86 I87 D88 T89 S90 T91 V92 G93 V94 K95 V96 I97 I98 E99 R100 G101 E102 L103 G104 D105 C106 V107 E108 F109 I110 N111 S112 N113 G114 S115 I116 S117 V118 T119 N120

P121 L122 T123 I124 Q125 A126 I127 D128 S129 I130 K131 G132 V133 S134 G135 N136 L137 V138 V139 T140 S141 P142 Y143 S144 K145 V146 T147 L148 R149 C150 I151 S152 S153 D154 N155 S156 T157 S158 V159 W160 N161 Y162 S163 I164 E165 S166 M167 F168 G169 Q170 K171 E172 S173 P174 A175 E176 G177 T178 W179 N180

I181 S182 T183 S184 G185 S186 V187 D188 I189 P190 L191 F192 H193 R194 T195 E196 Y197 N198 M199 A200 K201 L202 L203 V204 T205 C206 Q207 S208 V209 D210 G211 R212 K213 I214 K215 T216 A217 E218 I219 N220 I221 L222 V223 D224 T225 V226 N227 S228 E229 V230 I231 S232 S233 E234 Y235 A236 V237 M238 R239 V240

G241 N242 E243 T244 E245 E246 D247 E248 I249 A250 N251 I252 A253 F254 S255 I256 K257 E258 N259 Y260 V261 T262 A263 T264 I265 S266 S267 S268 T269 V270 G271 M272 R273 A274 A275 V276 K277 V278 I279 A280 T281 Q282 K283 I284 G285 V286 A287 Q288

- Molecule 4: Baseplate wedge protein gp9

Chain EH: 99% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 K30 I31 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60

I61 H62 A63 T64 G65 Y66 Y67 Q68 K69 H70 S71 I72 T73 E74 Y75 A76 T77 P78 V79 K80 V81 G82 T83 R84 H85 D86 I87 D88 T89 S90 T91 V92 G93 V94 K95 V96 I97 I98 E99 R100 G101 E102 L103 G104 D105 C106 V107 E108 F109 I110 N111 S112 N113 G114 S115 I116 S117 V118 T119 N120

P121 L122 T123 I124 Q125 A126 I127 D128 S129 I130 K131 G132 V133 S134 G135 N136 L137 V138 V139 T140 S141 P142 Y143 S144 K145 V146 T147 L148 R149 C150 I151 S152 S153 D154 N155 S156 T157 S158 V159 W160 N161 Y162 S163 I164 E165 S166 M167 F168 G169 Q170 K171 E172 S173 P174 A175 E176 G177 T178 W179 N180

I181 S182 T183 S184 G185 S186 V187 D188 I189 P190 L191 F192 H193 R194 T195 E196 Y197 N198 M199 A200 K201 L202 L203 V204 T205 C206 Q207 S208 V209 D210 G211 R212 K213 I214 K215 T216 A217 E218 I219 N220 I221 L222 V223 D224 T225 V226 N227 S228 E229 V230 I231 S232 S233 E234 Y235 A236 V237 M238 R239 V240

G241 N242 E243 T244 E245 E246 D247 E248 I249 A250 N251 I252 A253 F254 S255 I256 K257 E258 N259 Y260 V261 T262 A263 T264 I265 S266 S267 S268 T269 V270 G271 M272 R273 A274 A275 V276 K277 V278 I279 A280 T281 Q282 K283 I284 G285 V286 A287 Q288

- Molecule 4: Baseplate wedge protein gp9

Chain GI: 99% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 K30 I31 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60

I61 H62 A63 T64 G65 Y66 Y67 Q68 K69 H70 S71 I72 T73 E74 Y75 A76 T77 P78 V79 K80 V81 G82 T83 R84 H85 D86 I87 D88 T89 S90 T91 V92 G93 V94 K95 V96 I97 I98 E99 R100 G101 E102 L103 G104 D105 C106 V107 E108 F109 I110 N111 S112 N113 G114 S115 I116 S117 V118 T119 N120

P121 L122 T123 I124 Q125 A126 I127 D128 S129 I130 K131 G132 V133 S134 G135 N136 L137 V138 V139 T140 S141 P142 Y143 S144 K145 V146 T147 L148 R149 C150 I151 S152 S153 D154 N155 S156 T157 S158 V159 W160 N161 Y162 S163 I164 E165 S166 M167 F168 G169 Q170 K171 E172 S173 P174 A175 E176 G177 T178 W179 N180

I181 S182 T183 S184 G185 S186 V187 D188 I189 P190 L191 F192 H193 R194 T195 E196 Y197 N198 M199 A200 K201 L202 L203 V204 T205 C206 Q207 S208 V209 D210 G211 R212 K213 I214 K215 T216 A217 E218 I219 N220 I221 L222 V223 D224 T225 V226 N227 S228 E229 V230 I231 S232 S233 E234 Y235 A236 V237 M238 R239 V240

G241 N242 E243 T244 E245 E246 D247 E248 I249 A250 N251 I252 A253 F254 S255 I256 K257 E258 N259 Y260 V261 T262 A263 T264 I265 S266 S267 S268 T269 V270 G271 M272 R273 A274 A275 V276 K277 V278 I279 A280 T281 Q282 K283 I284 G285 V286 A287 Q288

- Molecule 4: Baseplate wedge protein gp9

Chain GJ: 98% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60 I61

H62 A63 T64 G65 Y66 Y67 Q68 K69 H70 S71 I72 T73 E74 Y75 A76 T77 P78 V79 K80 V81 G82 T83 R84 H85 D86 I87 D88 T89 S90 T91 V92 G93 V94 K95 V96 I97 I98 E99 R100 G101 E102 L103 G104 D105 C106 V107 E108 F109 I110 N111 S112 N113 G114 S115 I116 S117 V118 T119 N120 P121

L122 T123 I124 Q125 A126 I127 D128 S129 I130 K131 G132 V133 S134 G135 N136 L137 V138 V139 T140 S141 P142 Y143 S144 K145 V146 T147 L148 R149 C150 I151 S152 S153 D154 N155 S156 T157 S158 V159 W160 N161 Y162 S163 I164 E165 S166 M167 F168 G169 Q170 K171 E172 S173 P174 A175 E176 G177 T178 W179 N180 I181

S182 T183 S184 G185 S186 V187 D188 I189 P190 L191 F192 H193 R194 T195 E196 Y197 N198 M199 A200 K201 L202 L203 V204 T205 C206 Q207 S208 V209 D210 G211 R212 K213 I214 K215 T216 A217 E218 I219 N220 I221 L222 V223 D224 T225 V226 N227 S228 E229 V230 I231 S232 S233 E234 Y235 A236 V237 M238 R239 V240 G241

N242 E243 T244 E245 E246 D247 E248 I249 A250 N251 I252 A253 F254 S255 I256 K257 E258 N259 Y260 V261 T262 A263 T264 I265 S266 S267 S268 T269 V270 G271 M272 R273 A274 A275 V276 K277 V278 I279 A280 T281 Q282 K283 I284 G285 V286 A287 Q288

- Molecule 4: Baseplate wedge protein gp9

Chain HA: 99% 99%

M1 F2 I3 Q4 E5 P6 K7 K8 L9 I10 D11 T12 G13 E14 I15 G16 N17 A18 S19 T20 G21 D22 I23 L24 F25 D26 G27 G28 N29 K30 I31 N32 S33 D34 F35 N36 A37 I38 Y39 N40 A41 F42 G43 D44 Q45 R46 K47 M48 A49 V50 A51 N52 G53 T54 G55 A56 D57 G58 Q59 I60

I61 H62 A63 T64 G65 Y66 Y67 Q68 K69 H70 S71 I72 T73 E74 Y75 A76 T77 P78 V79 K80 V81 G82 T83 R84 H85 D86 I87 D88 T89 S90 T91 V92 G93 V94 K95 V96 I97 T98 E99 R100 G101 E102 L103 G104 D105 C106 V107 E108 F109 I110 N111 S112 N113 G114 S115 I116 S117 V118 T119 N120

P121 L122 T123 I124 Q125 A126 I127 D128 S129 I130 K131 G132 V133 S134 G135 N136 L137 V138 V139 T140 S141 P142 Y143 S144 K145 V146 T147 L148 R149 C150 I151 S152 S153 D154 N155 S156 T157 S158 V159 W160 N161 Y162 S163 I164 E165 S166 M167 F168 G169 Q170 K171 E172 S173 P174 A175 E176 G177 T178 W179 N180

I181 S182 T183 S184 G185 S186 V187 D188 I189 P190 L191 F192 H193 R194 T195 E196 Y197 N198 M199 A200 K201 L202 L203 V204 T205 C206 Q207 S208 V209 D210 G211 R212 K213 I214 K215 T216 A217 E218 I219 N220 I221 L222 V223 D224 T225 V226 N227 S228 E229 V230 I231 S232 S233 E234 Y235 A236 V237 M238 R239 V240

G241 N242 E243 T244 E245 E246 D247 E248 I249 A250 N251 I252 A253 F254 S255 I256 K257 E258 N259 Y260 V261 T262 A263 T264 I265 S266 S267 S268 T269 V270 G271 M272 R273 A274 A275 V276 K277 V278 I279 A280 T281 Q282 K283 I284 G285 V286 A287 Q288

- Molecule 5: Baseplate wedge protein gp10

Chain I: 17% 96%

M1 N9 V10 V11 D12 I24 D39 G40 D41 T61 K83 G84 T85 V86 A100 T101 W102 N103 V104 A112 S120 A121 N127 V128 R129 D132 L133 E134 T155 S156 S157 D158 I159 V171 Q172 L178 D179 V180 R196 G203 D204 E208 D211

E217 N218 E219 F228 D249 S252 L266 D267 S268 K269 L270 T271 S272 K273 T274 S275 L276 E277 G278 D284 T287 M288 F293 S294 A295 L298 I299 P300 N305 P306 N307 E310 N314 G315 I316 L317 Q318 A321 V324 G325 M326 P327 L328 F329 H330 C331

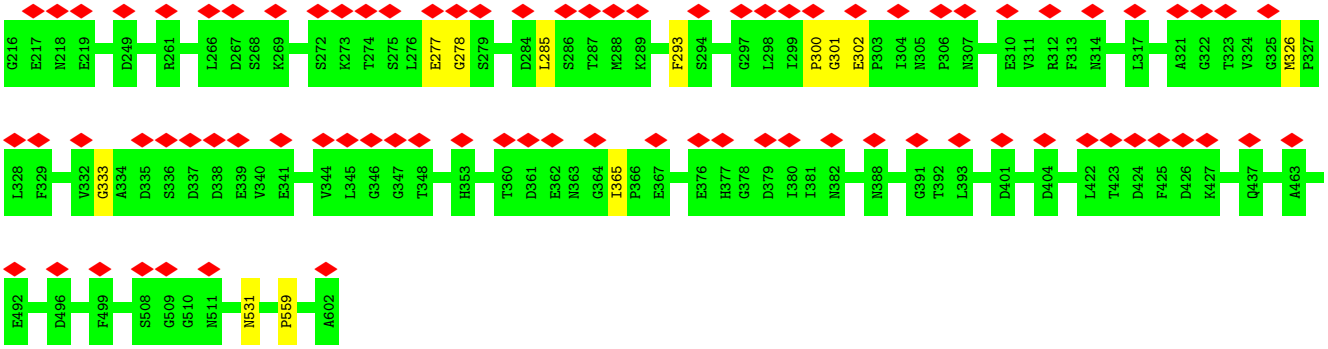
V332 G333 A334 D335 S336 D337 D338 E339 V340 E341 Q351 S352 H353 D361 E362 N363 G364 I365 P366 E387 F371 E376 N388 G391 T392 L393 L394 L406 K427 D493 I494 S495 D496 D507 S508 G509 E546 C555 Q556 Y557 D558 P559 D560 E561 S562 T581

A602

- Molecule 5: Baseplate wedge protein gp10

Chain J: 17% 95% 5%

M1 I24 D41 T61 A62 S74 G84 T85 V86 N90 A100 T101 W102 N103 V104 A112 G119 S120 R129 Q150 I151 D152 K153 I154 T155 S156 S157 D158 I159 R164 V171 Q174 V180 F181 R182 R196 D204 E208 G213 S214 P215



• Molecule 5: Baseplate wedge protein gp10

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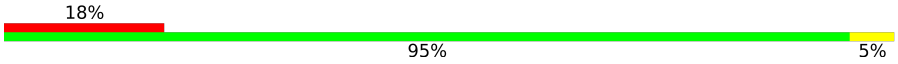
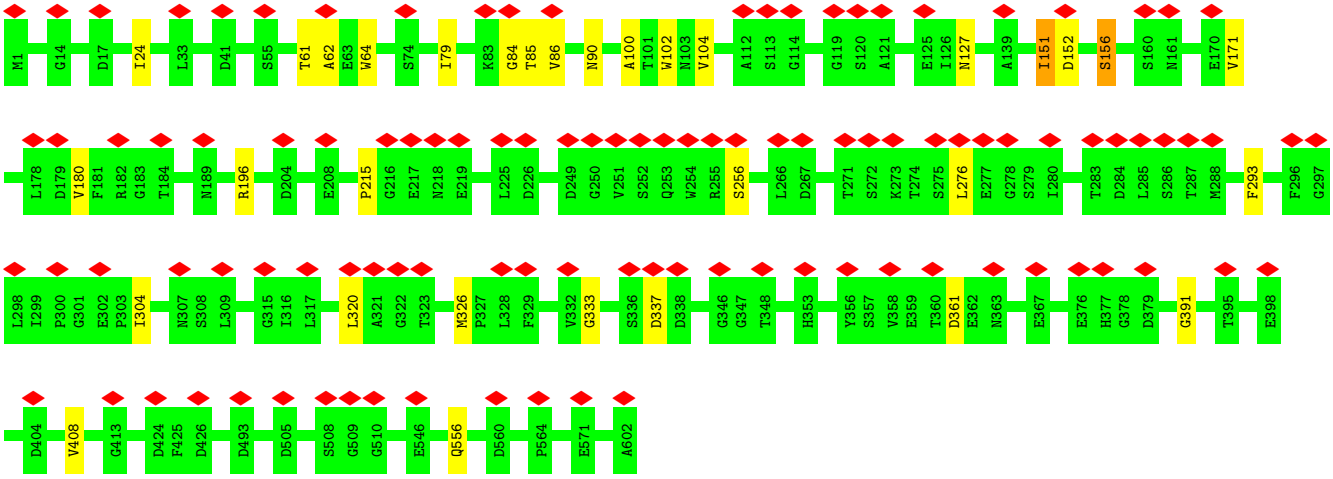
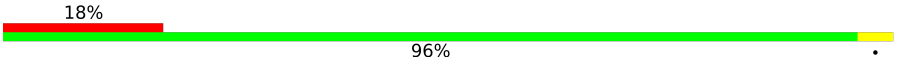
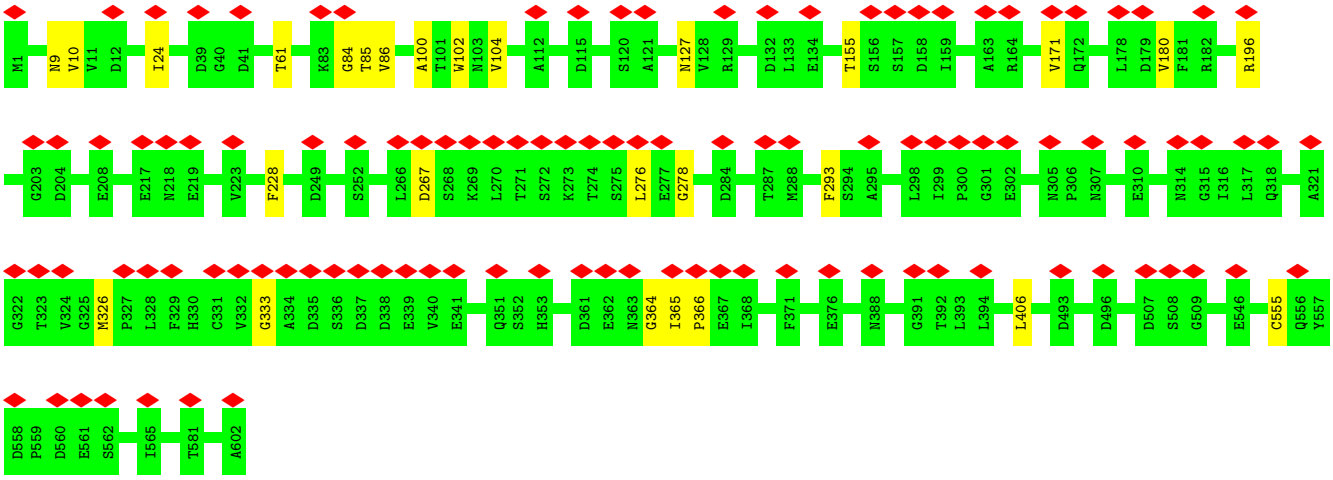




• Molecule 5: Baseplate wedge protein gp10

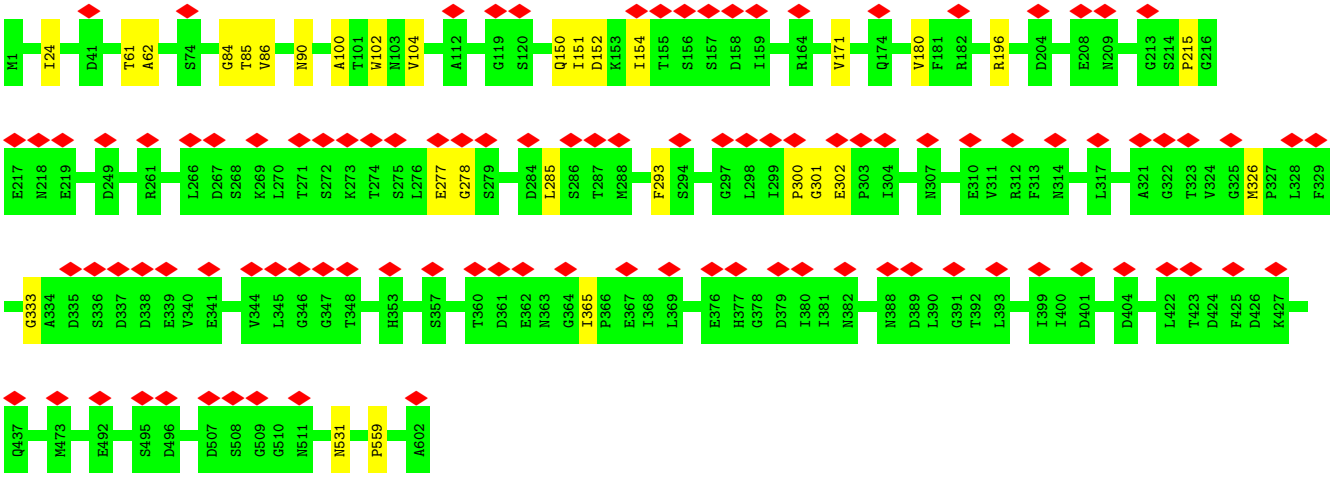
Chain f:





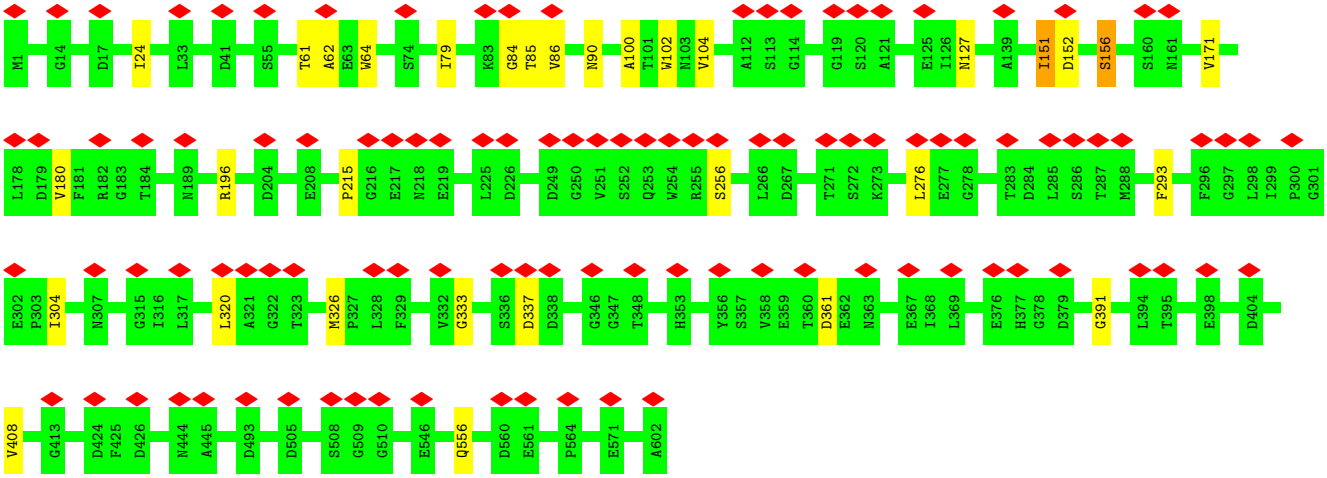
• Molecule 5: Baseplate wedge protein gp10

Chain g: 17% 95% 5%



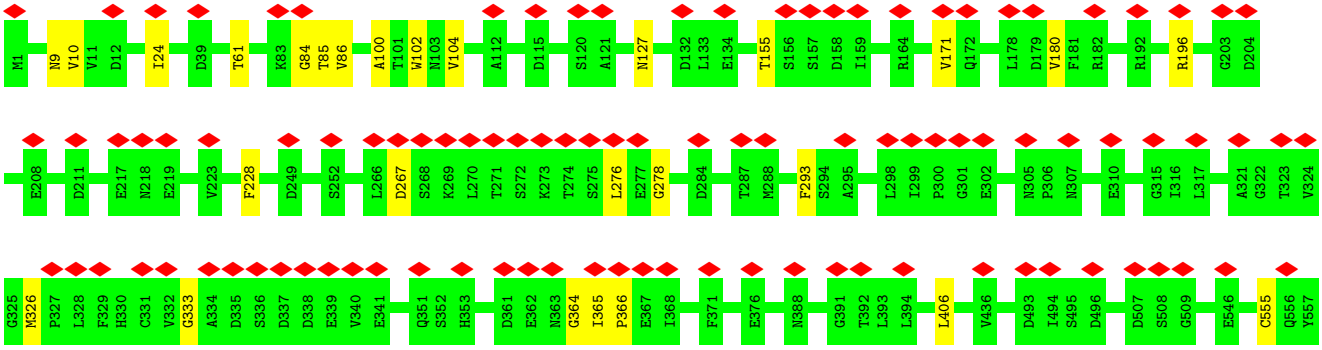
- Molecule 5: Baseplate wedge protein gp10

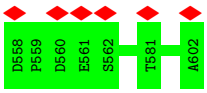
Chain h: 18% 95% 5%



- Molecule 5: Baseplate wedge protein gp10

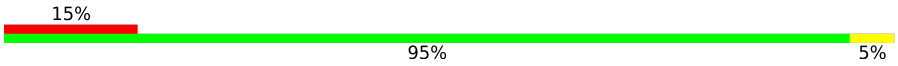
Chain AC: 18% 96%

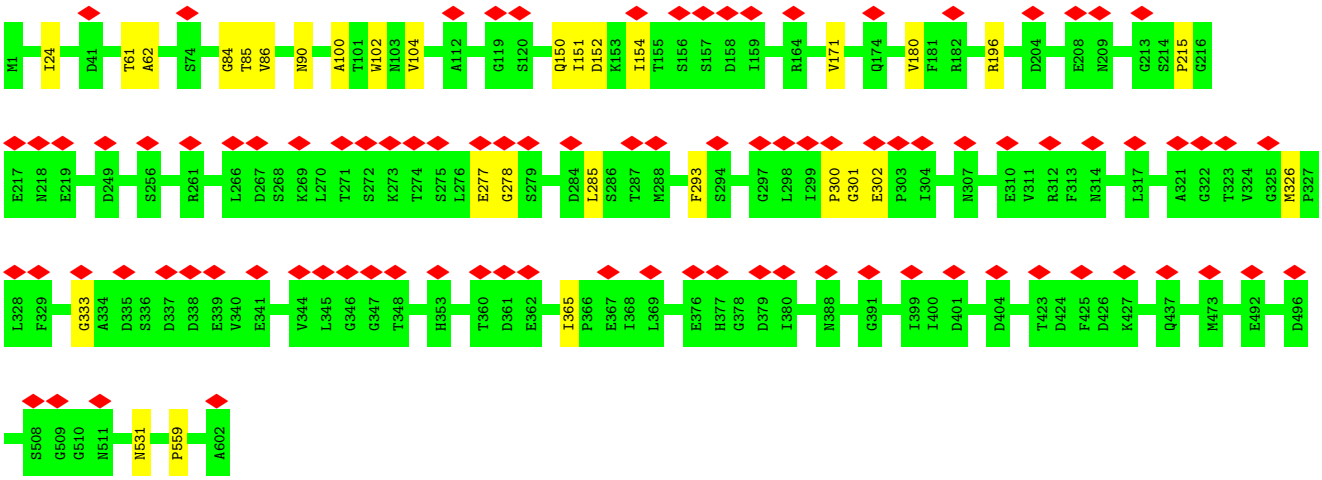




• Molecule 5: Baseplate wedge protein gp10

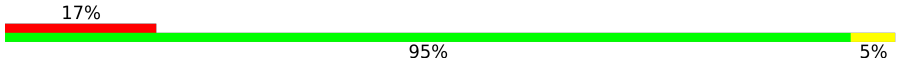
Chain AD:

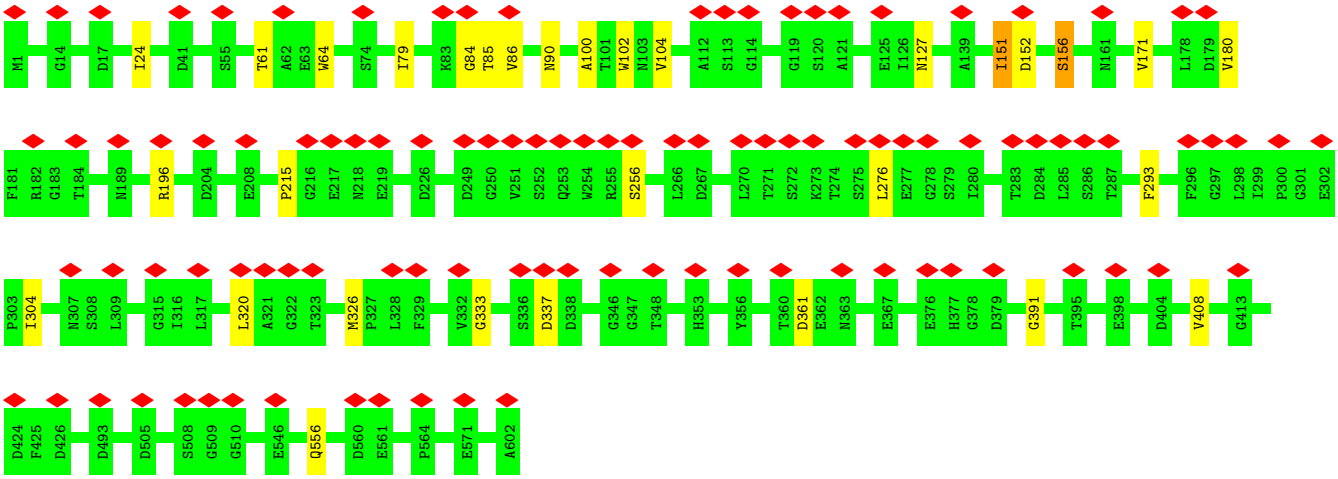




• Molecule 5: Baseplate wedge protein gp10

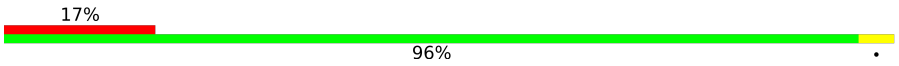
Chain AE:

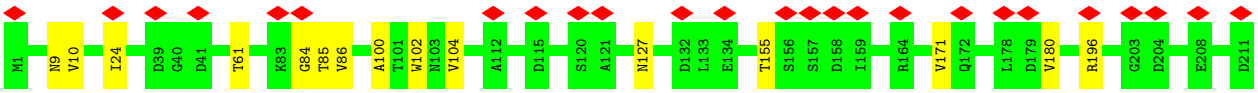


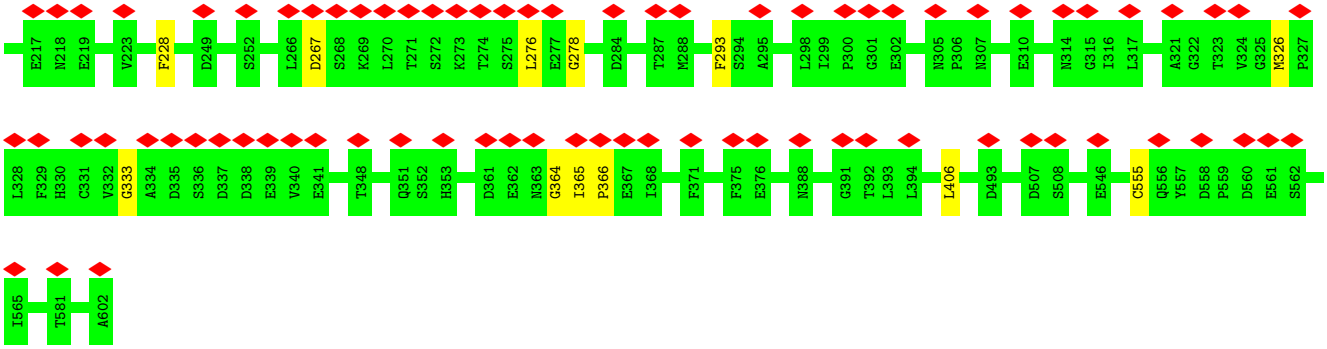


• Molecule 5: Baseplate wedge protein gp10

Chain CF:

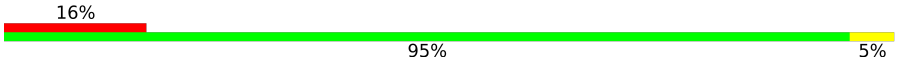


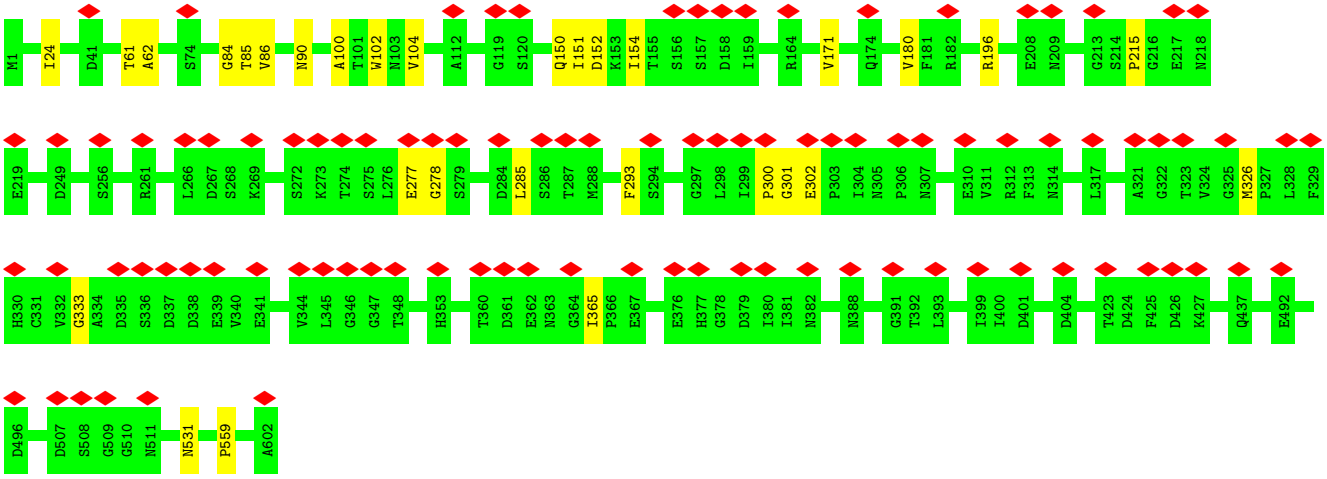




• Molecule 5: Baseplate wedge protein gp10

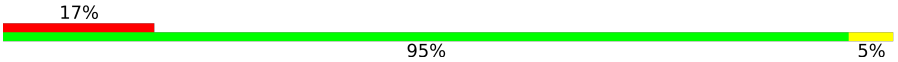
Chain CG:

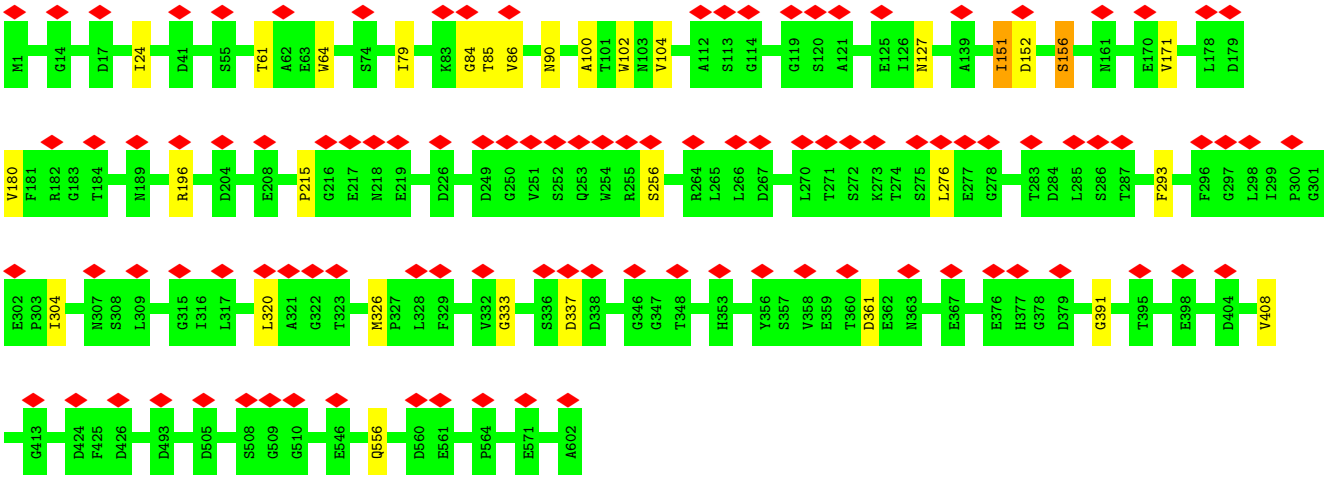




• Molecule 5: Baseplate wedge protein gp10

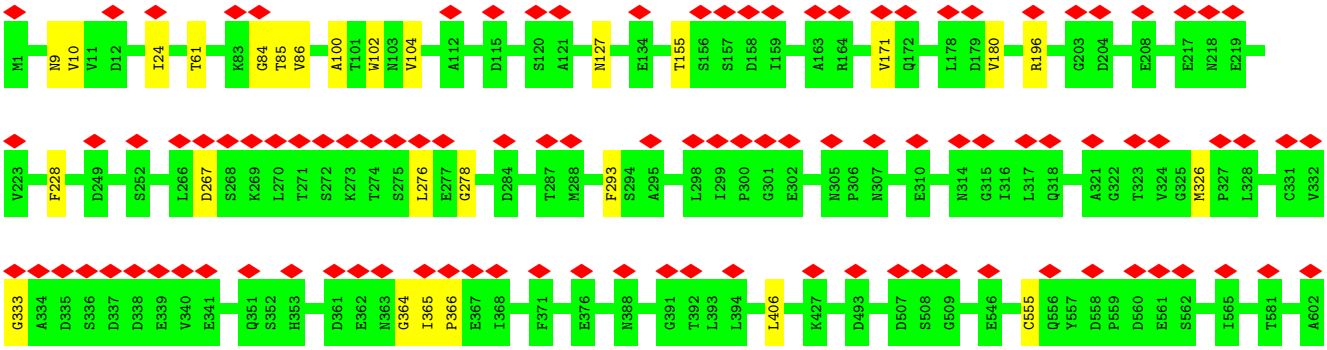
Chain CH:





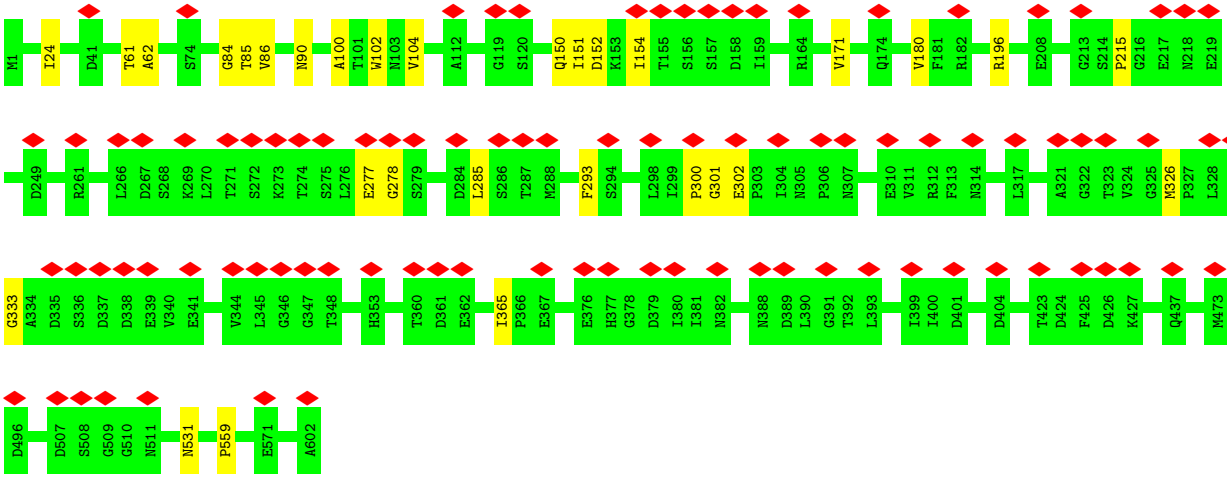
• Molecule 5: Baseplate wedge protein gp10

Chain EI: 17% 96%



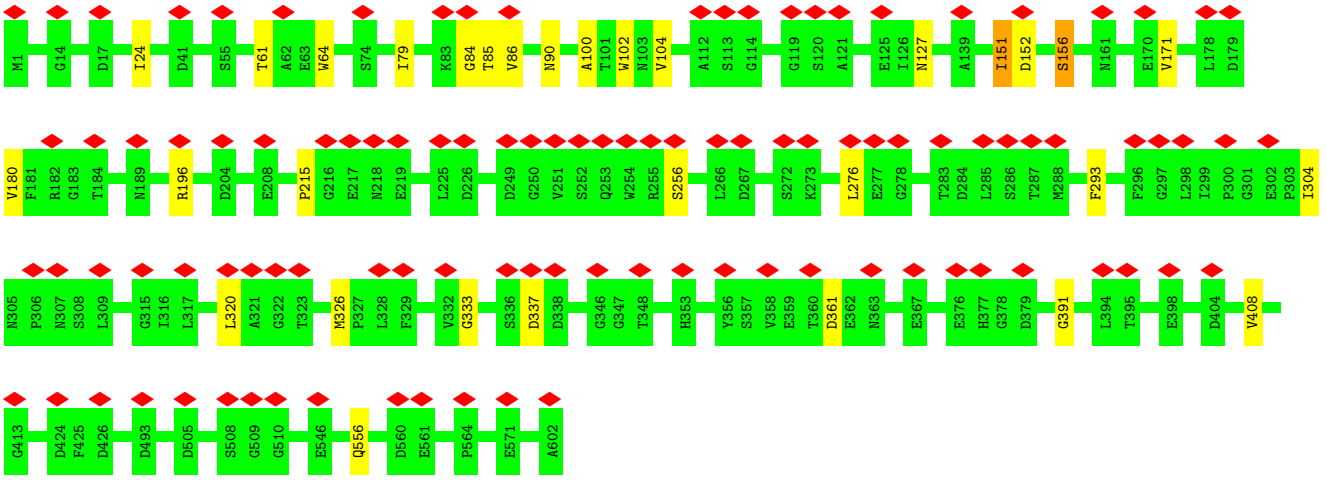
- Molecule 5: Baseplate wedge protein gp10

Chain EJ: 16% 95% 5%



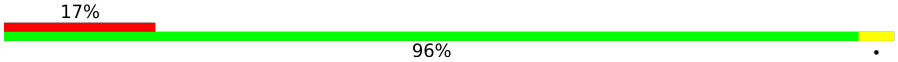
- Molecule 5: Baseplate wedge protein gp10

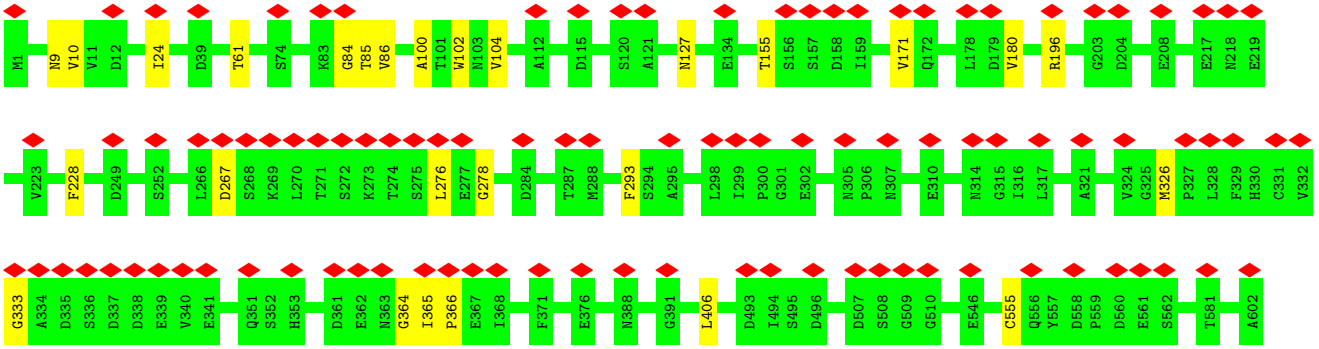
Chain FA: 17% 95% 5%



- Molecule 5: Baseplate wedge protein gp10

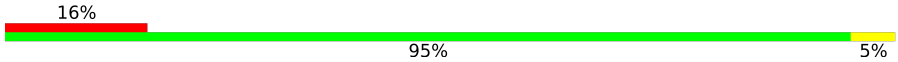
Chain HB:

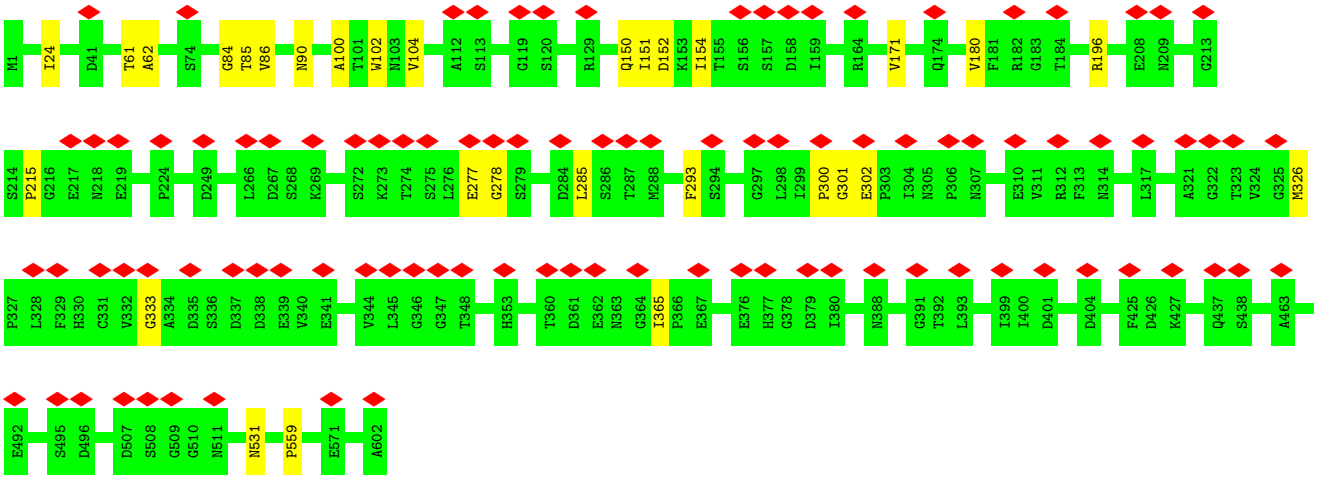




- Molecule 5: Baseplate wedge protein gp10

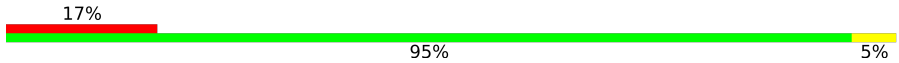
Chain HC:

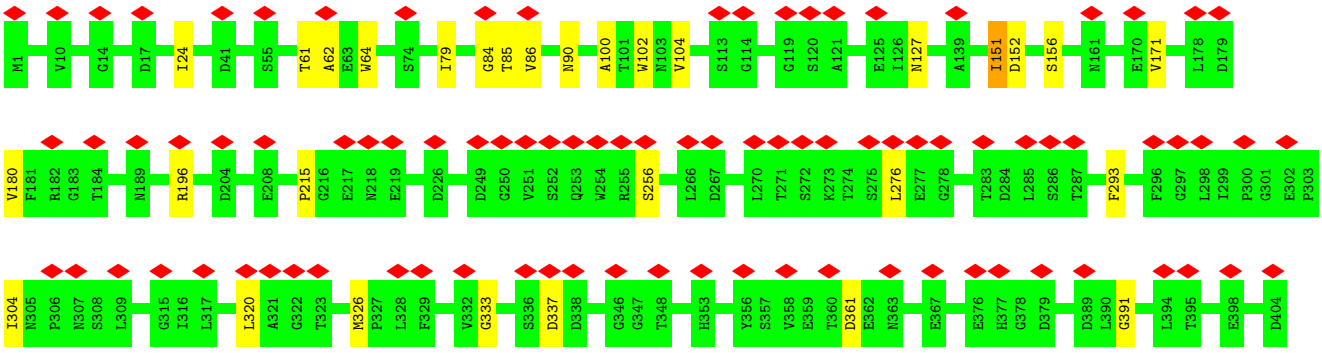


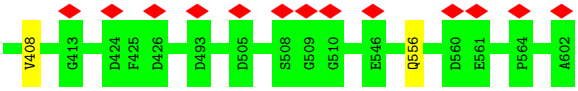


- Molecule 5: Baseplate wedge protein gp10

Chain HD:

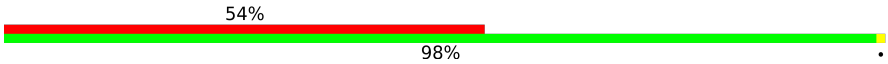


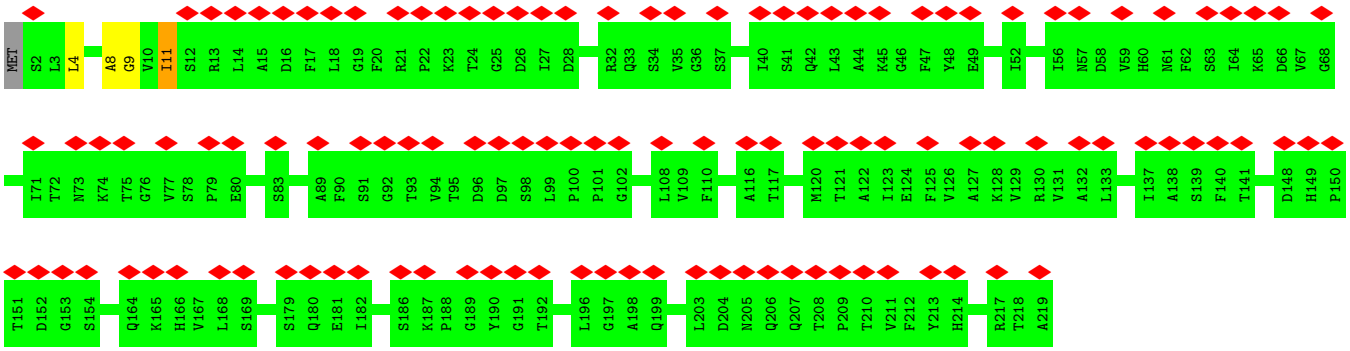




• Molecule 6: Baseplate wedge protein gp11

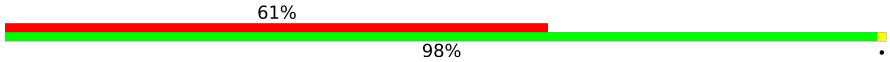
Chain L:

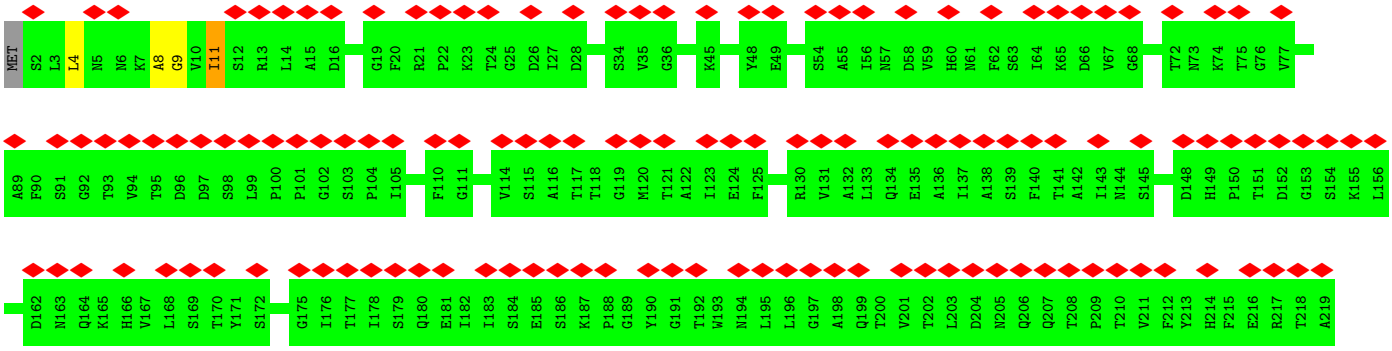




• Molecule 6: Baseplate wedge protein gp11

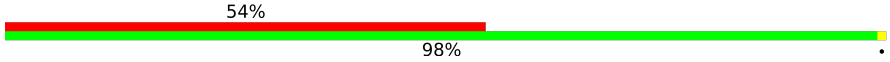
Chain M:

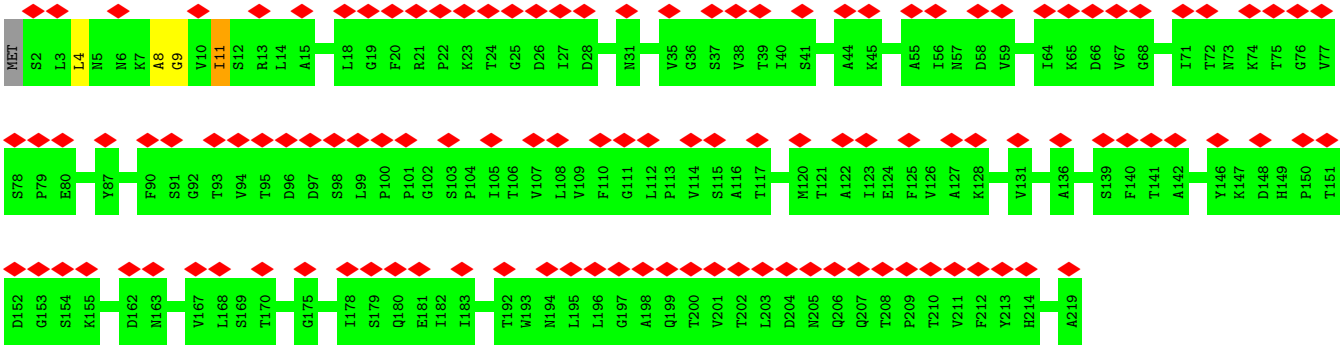




• Molecule 6: Baseplate wedge protein gp11

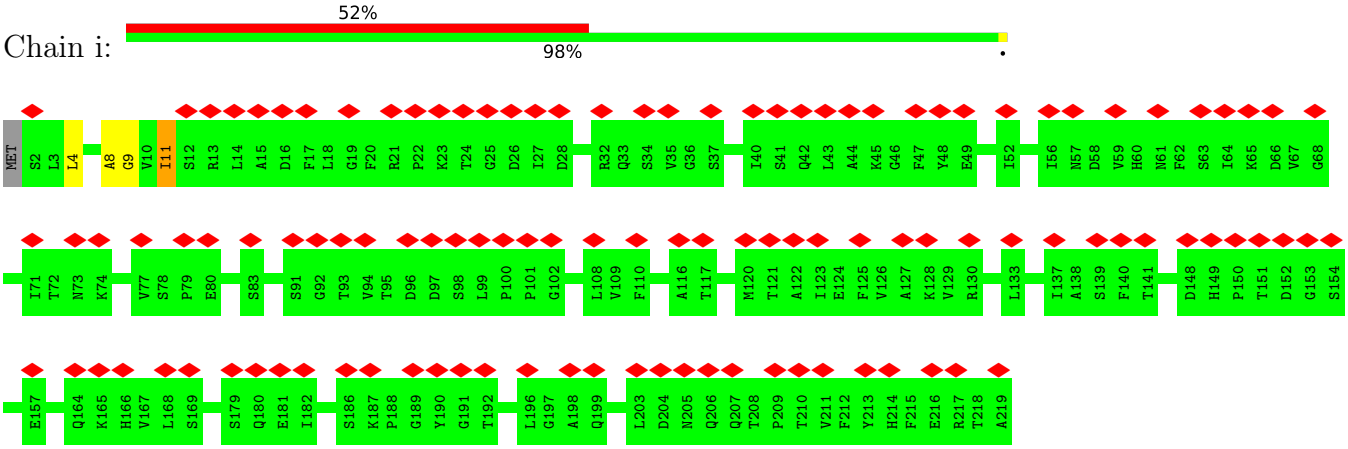
Chain N:





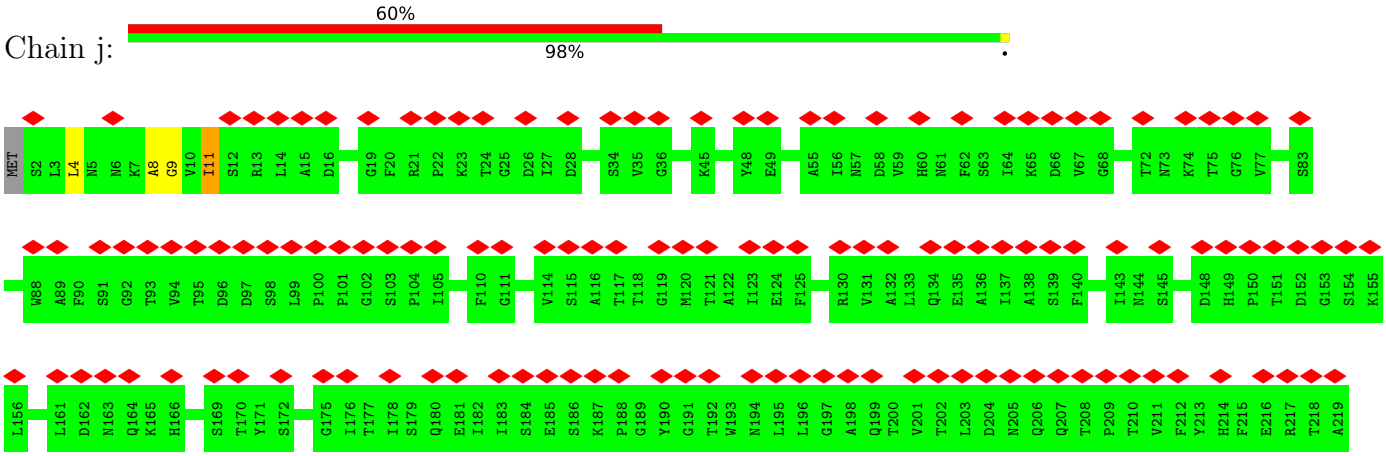
• Molecule 6: Baseplate wedge protein gp11

Chain i:



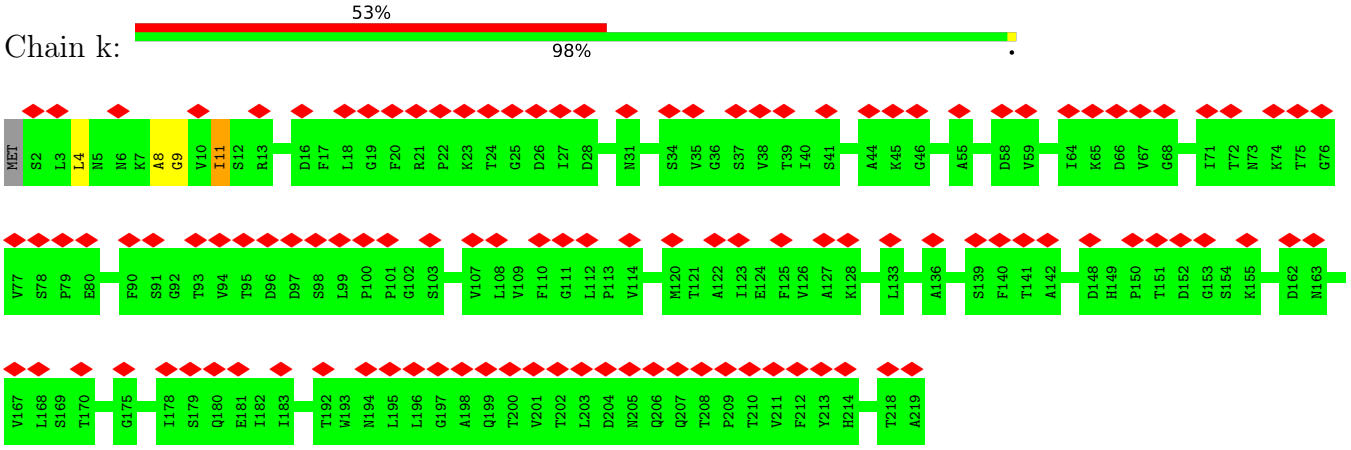
- Molecule 6: Baseplate wedge protein gp11

Chain j:



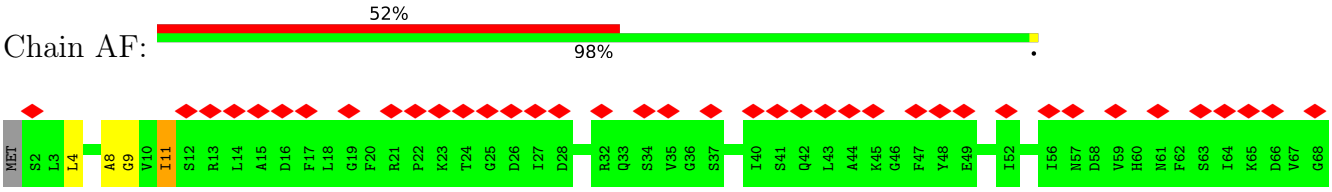
- Molecule 6: Baseplate wedge protein gp11

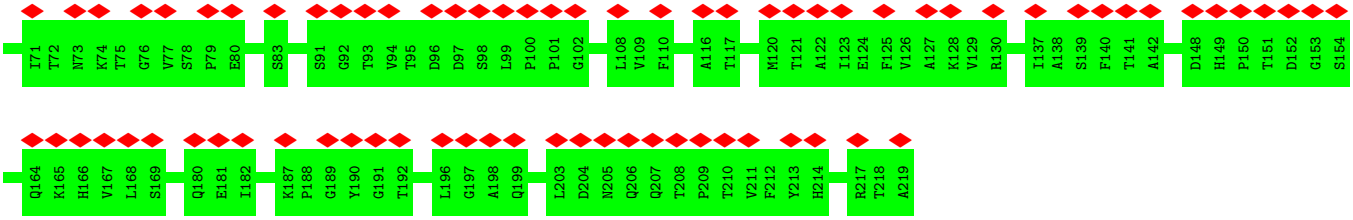
Chain k:



- Molecule 6: Baseplate wedge protein gp11

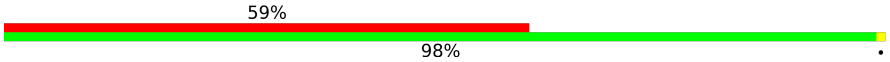
Chain AF:

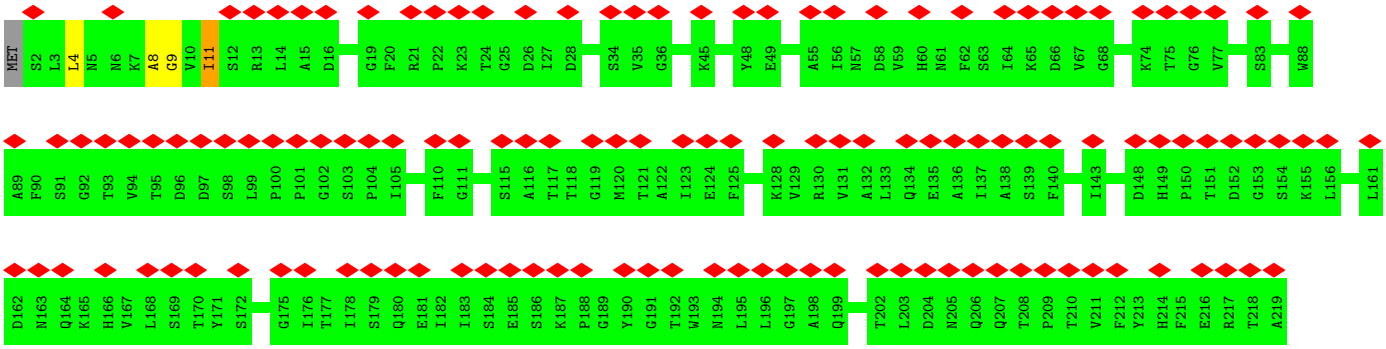




• Molecule 6: Baseplate wedge protein gp11

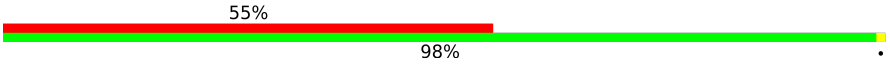
Chain AG:

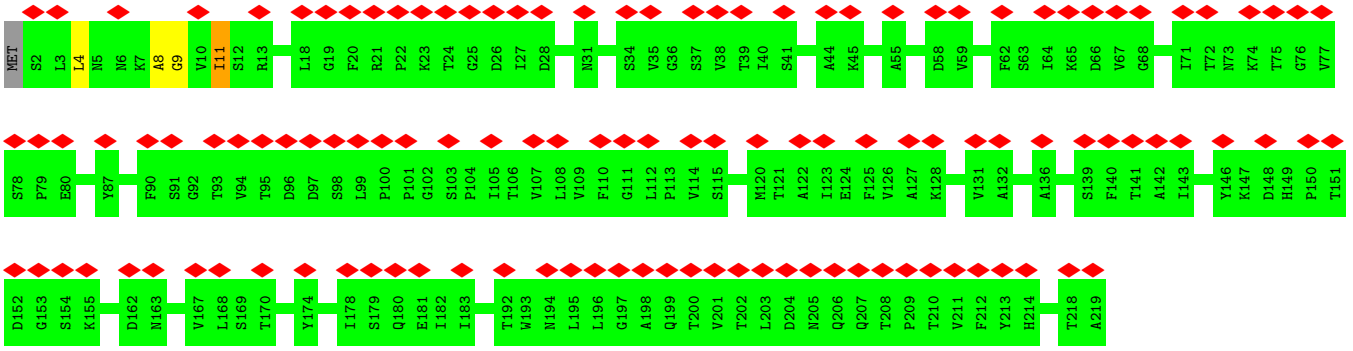




• Molecule 6: Baseplate wedge protein gp11

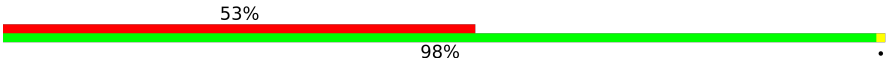
Chain AH:

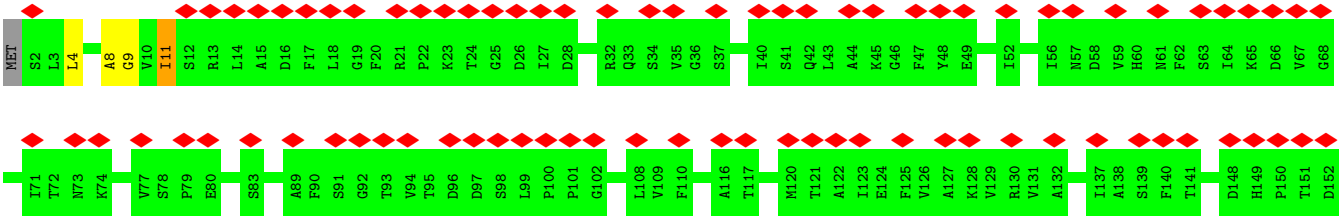


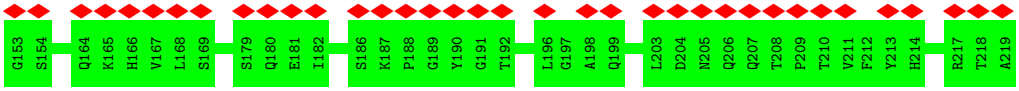


• Molecule 6: Baseplate wedge protein gp11

Chain CI:

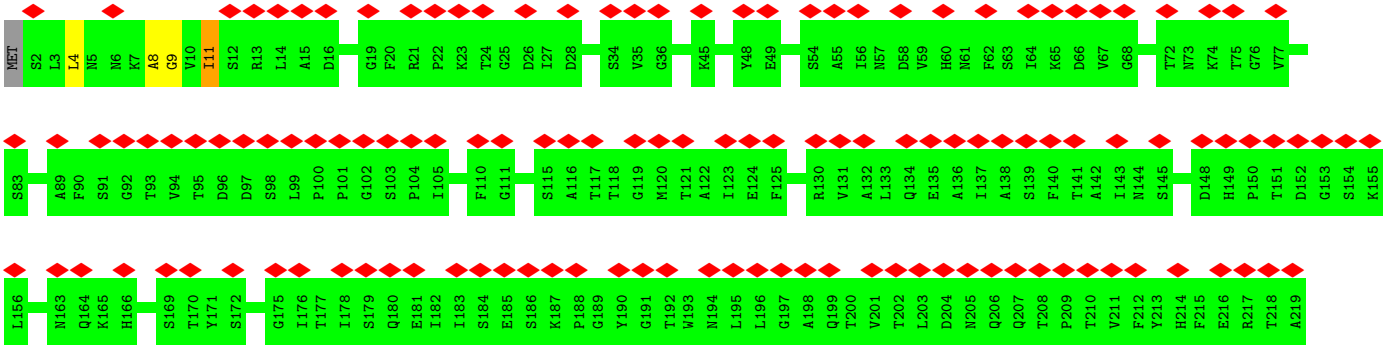






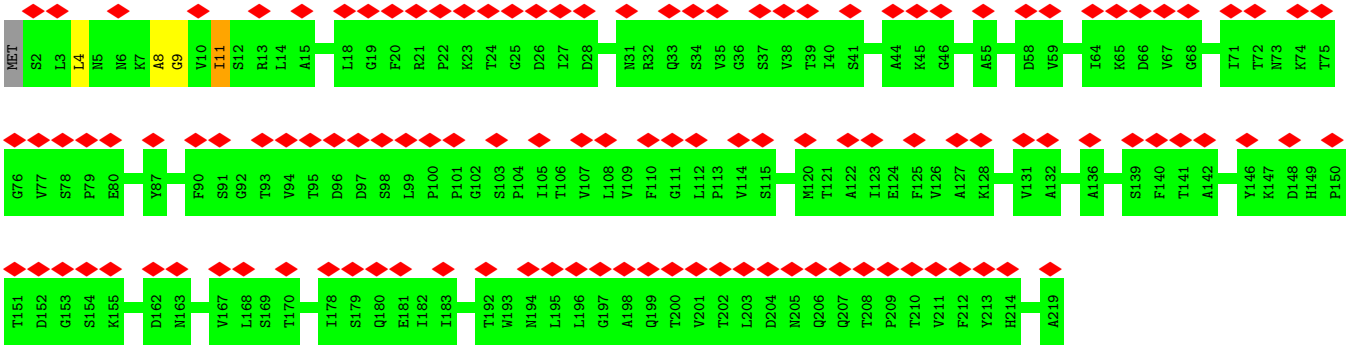
• Molecule 6: Baseplate wedge protein gp11

Chain CJ: 59% 98%



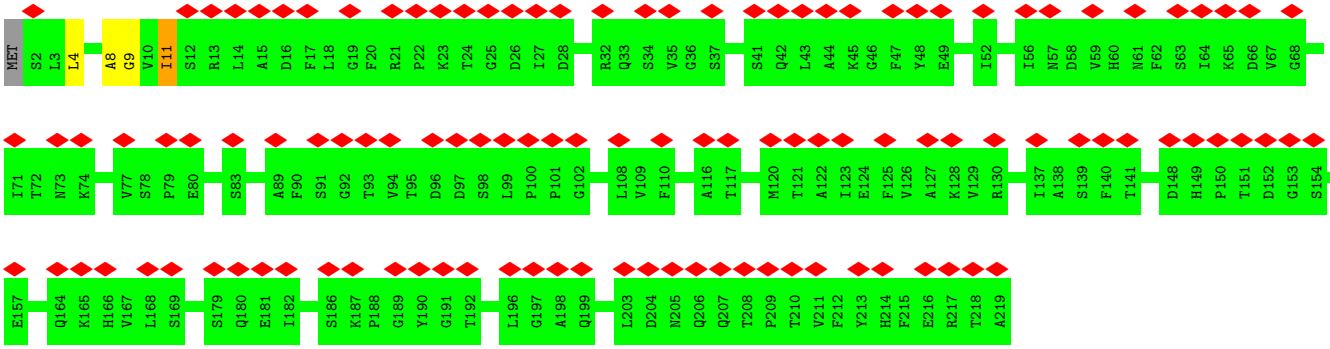
• Molecule 6: Baseplate wedge protein gp11

Chain DA: 55% 98%



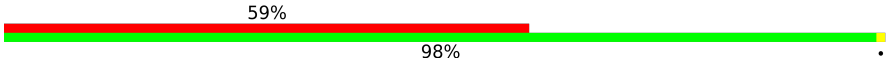
• Molecule 6: Baseplate wedge protein gp11

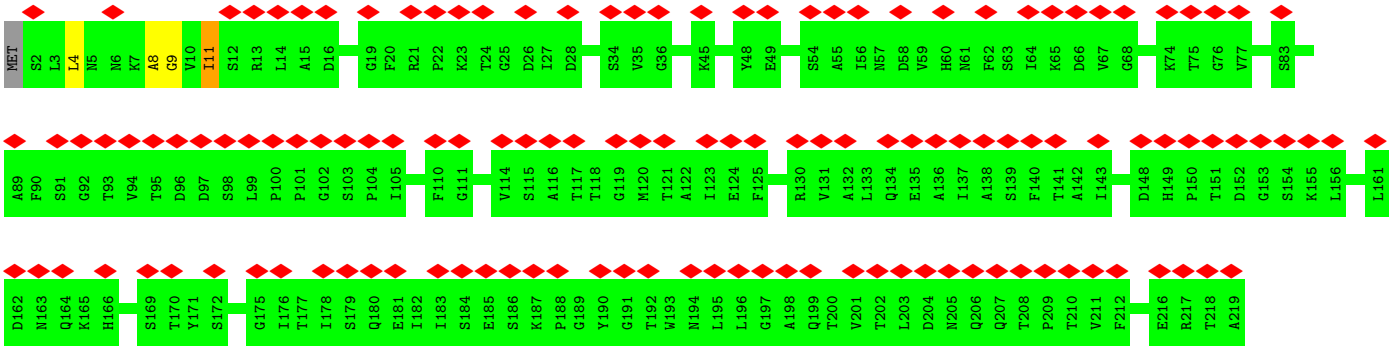
Chain FB: 53% 98%



• Molecule 6: Baseplate wedge protein gp11

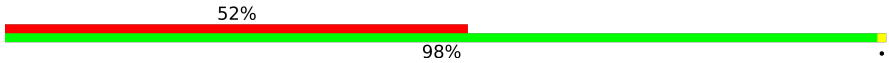
Chain FC:

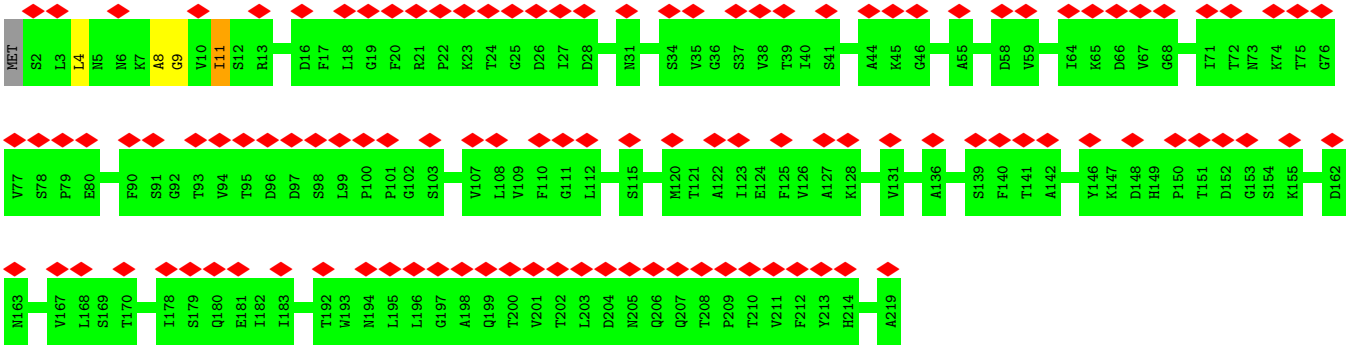




- Molecule 6: Baseplate wedge protein gp11

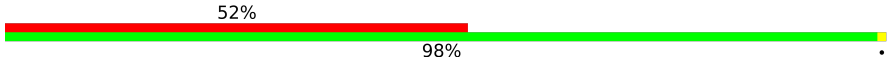
Chain FD:

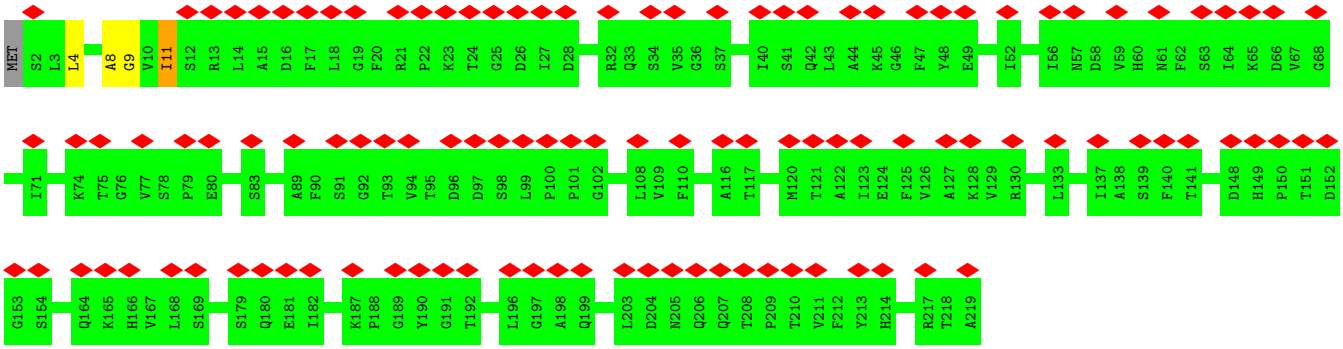




- Molecule 6: Baseplate wedge protein gp11

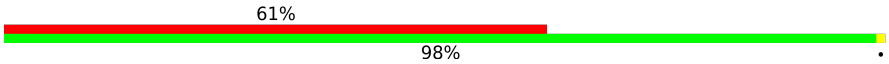
Chain HE:

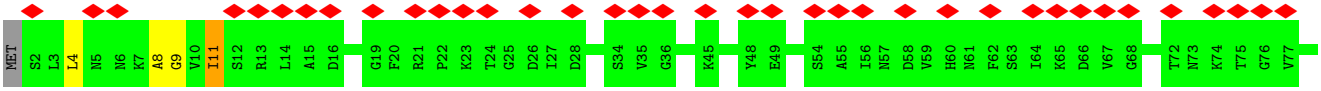


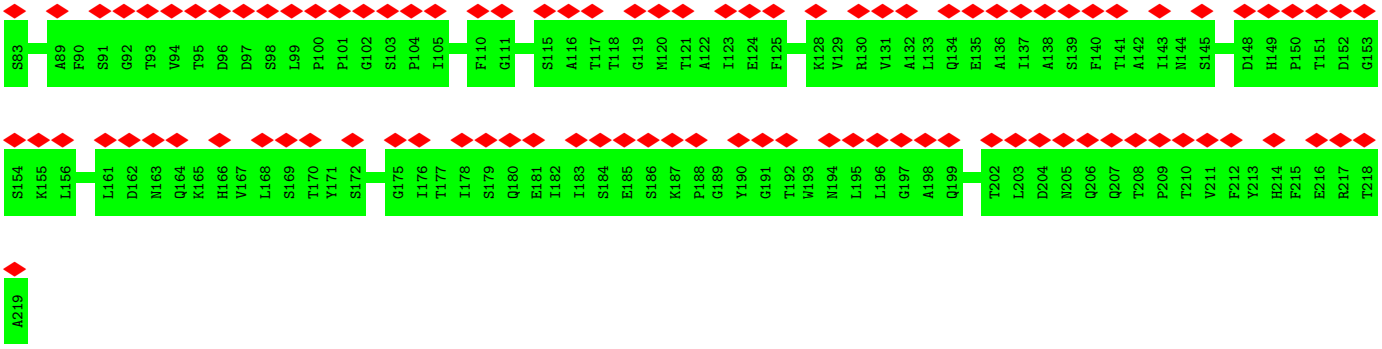


- Molecule 6: Baseplate wedge protein gp11

Chain HF:

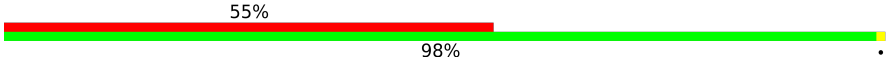


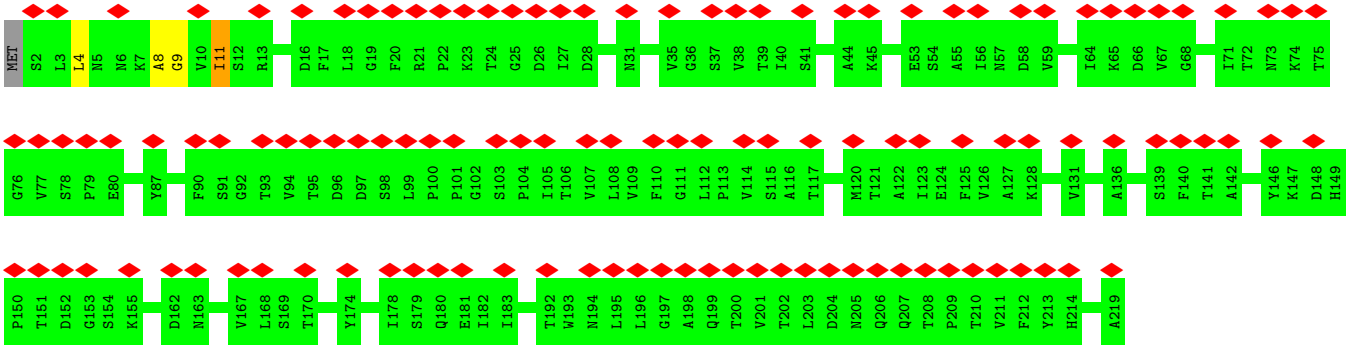




• Molecule 6: Baseplate wedge protein gp11

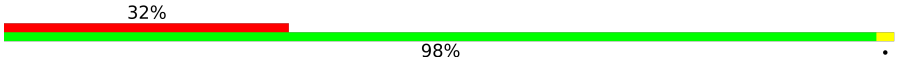
Chain HG:

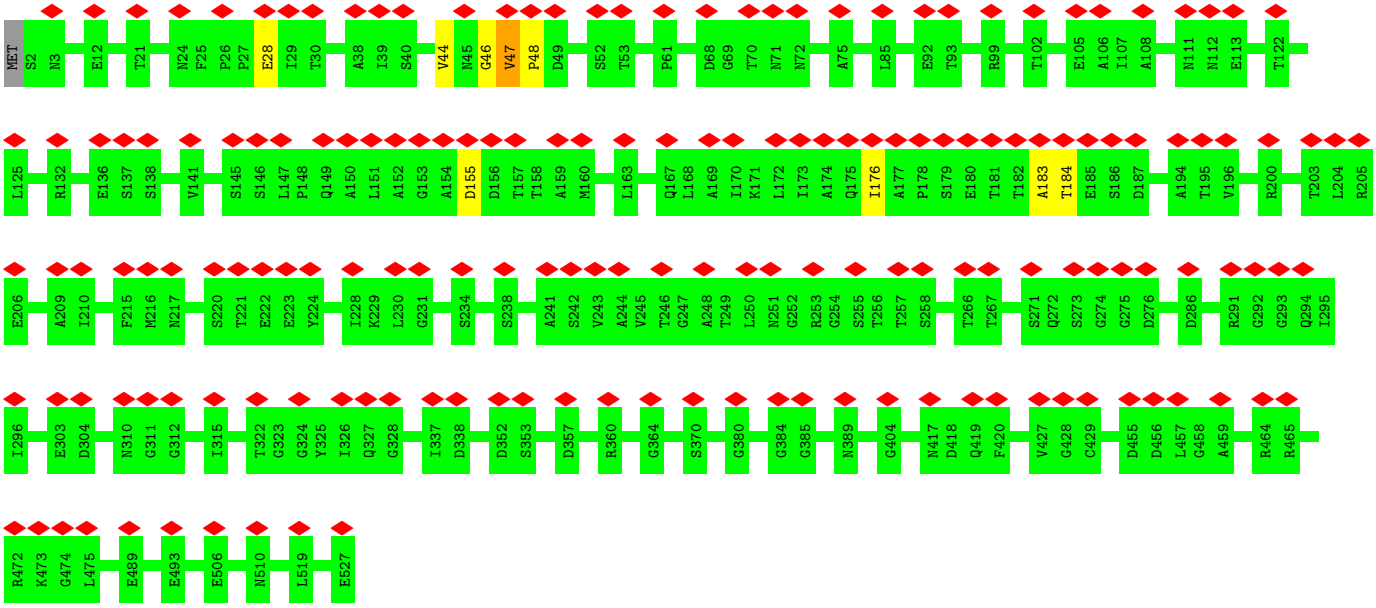




• Molecule 7: Short tail fiber protein gp12

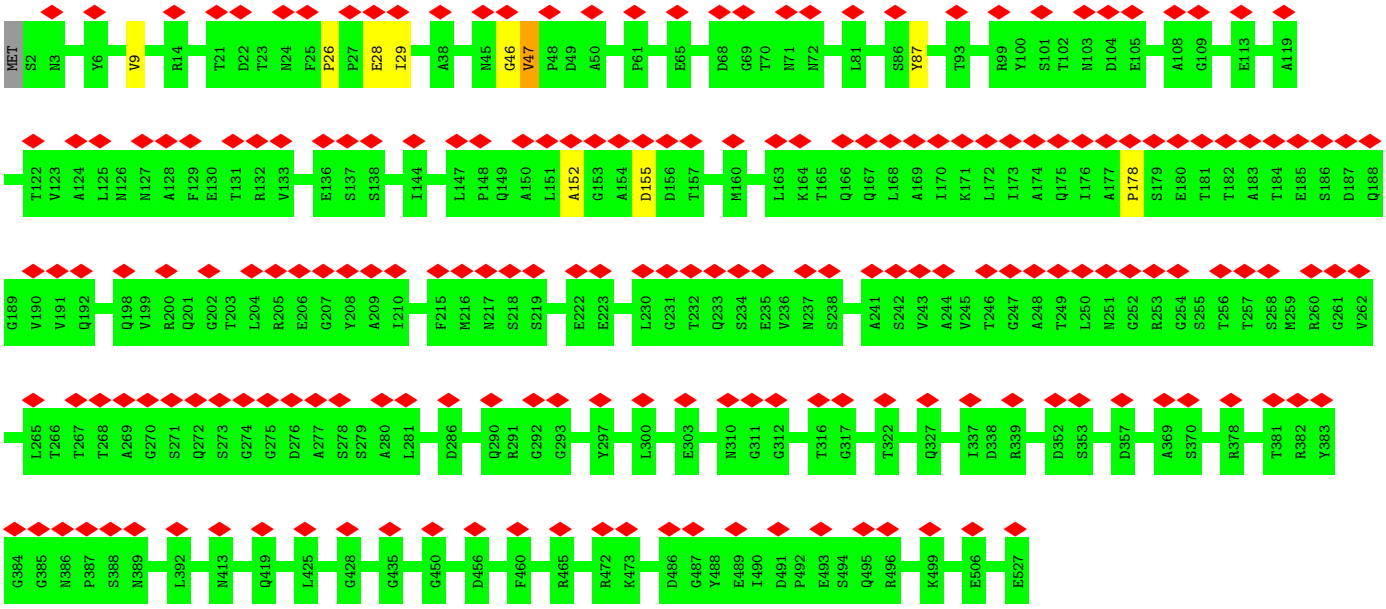
Chain O:





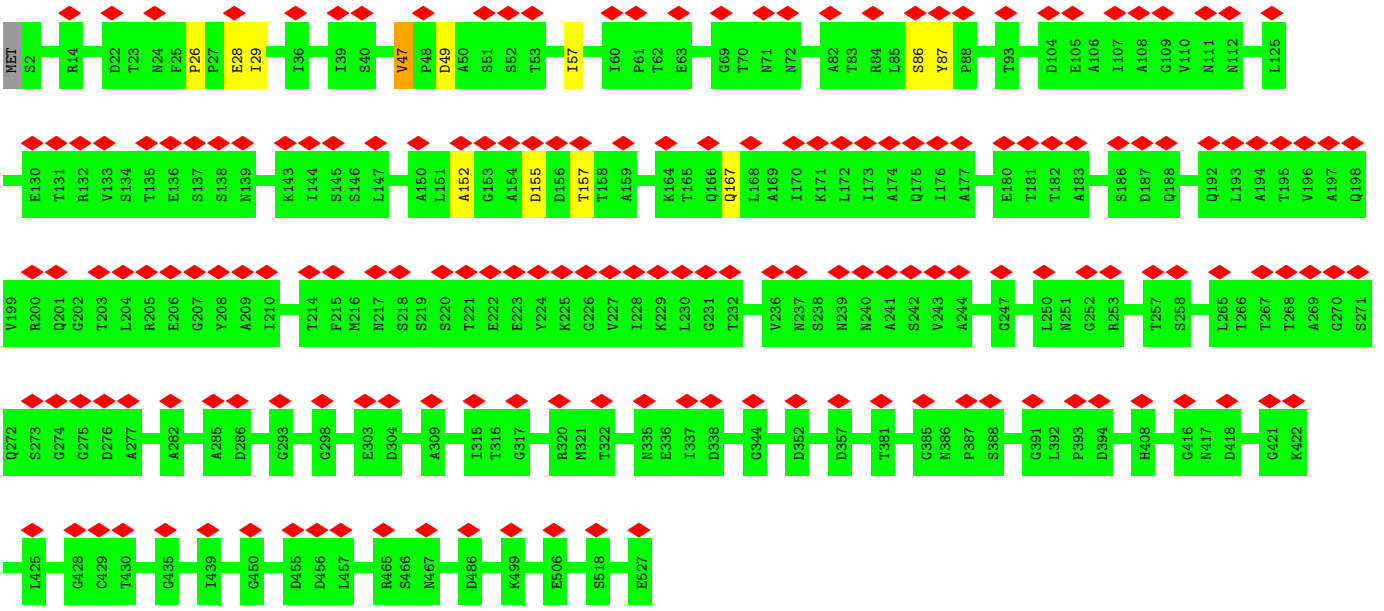
• Molecule 7: Short tail fiber protein gp12

Chain P: 37% 98%



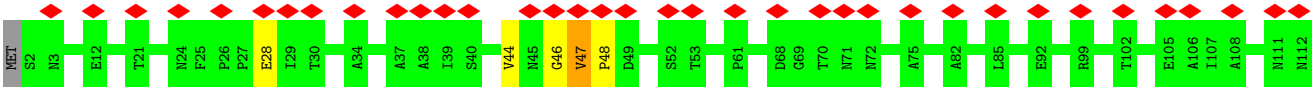
- Molecule 7: Short tail fiber protein gp12

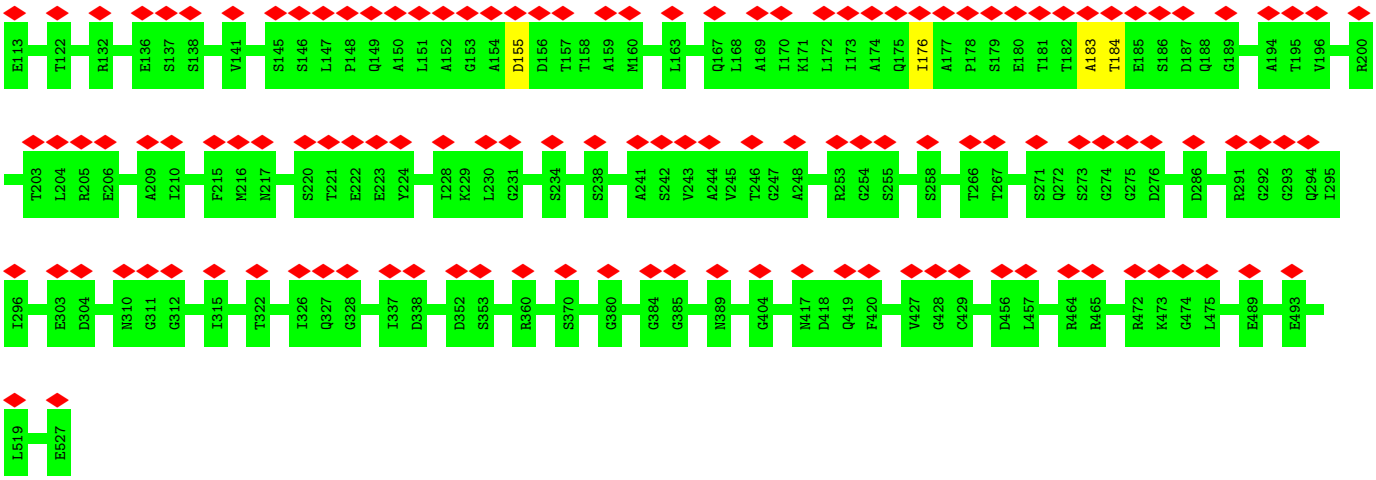
Chain Q: 33% 98%



- Molecule 7: Short tail fiber protein gp12

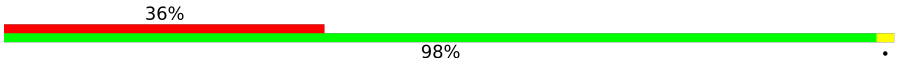
Chain l: 31% 98%

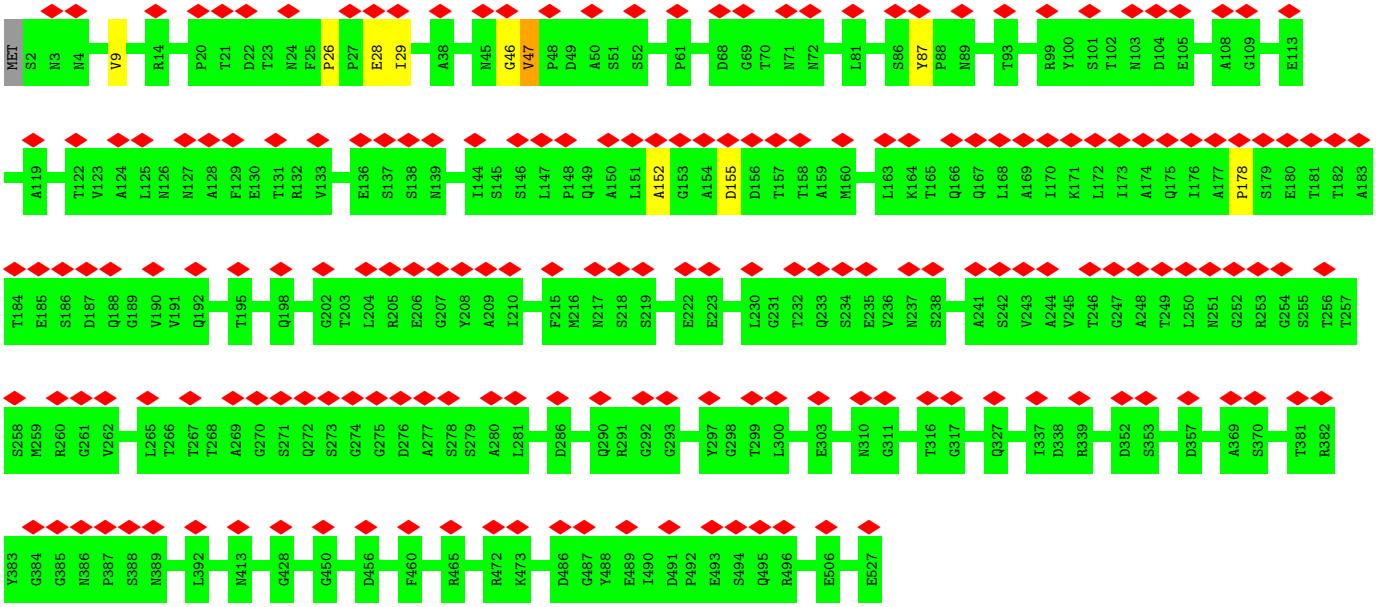




- Molecule 7: Short tail fiber protein gp12

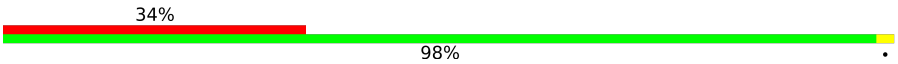
Chain m:

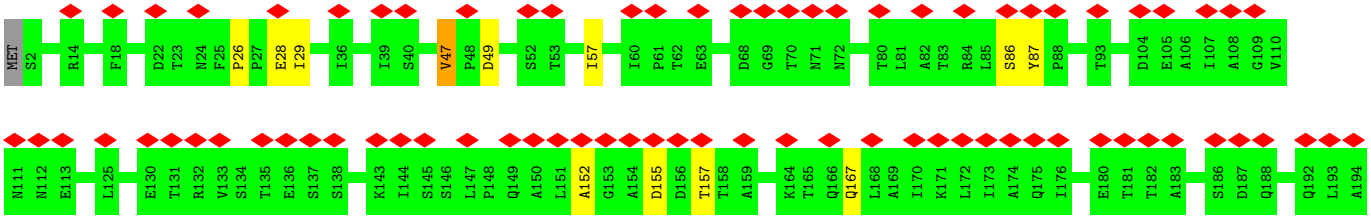


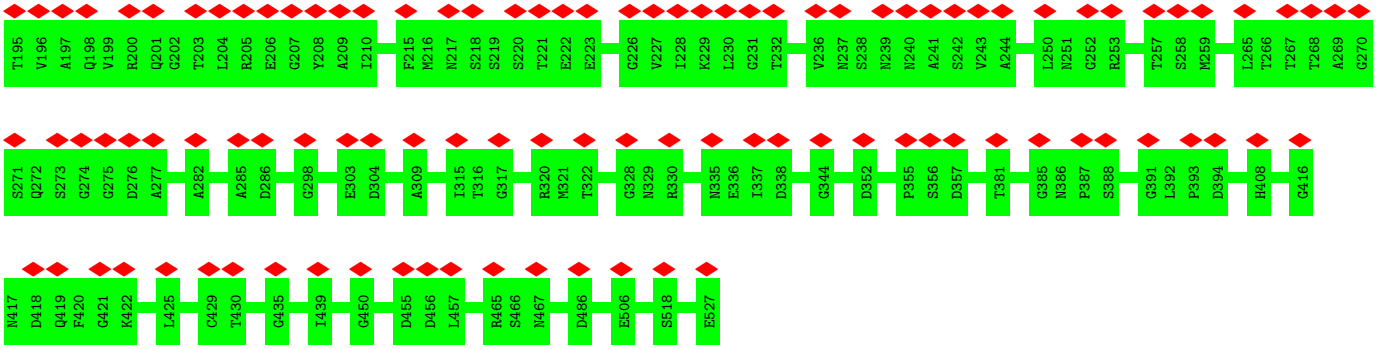


- Molecule 7: Short tail fiber protein gp12

Chain n:

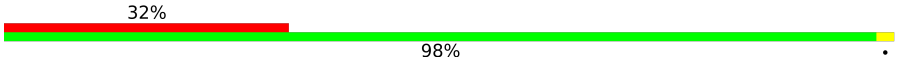


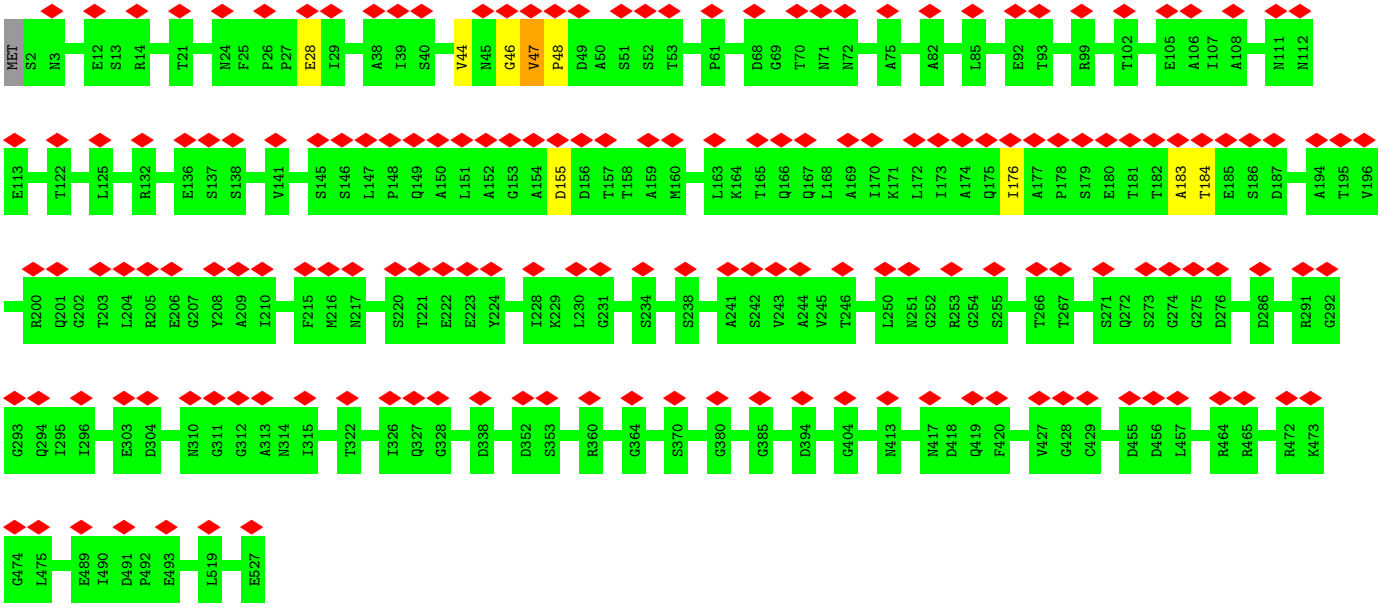




• Molecule 7: Short tail fiber protein gp12

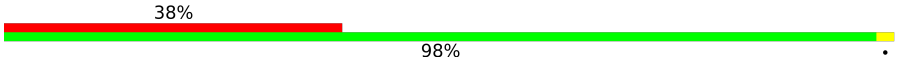
Chain AI:

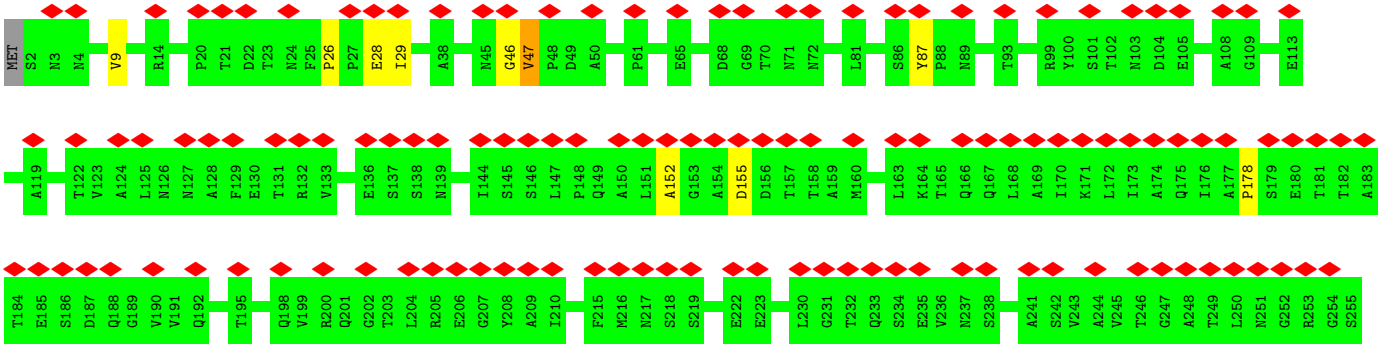


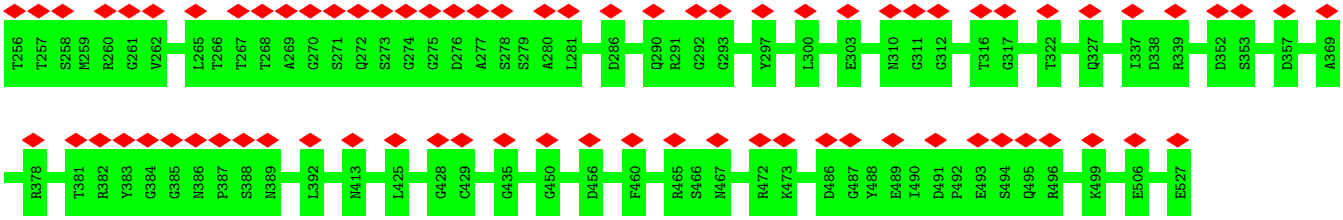


• Molecule 7: Short tail fiber protein gp12

Chain AJ:

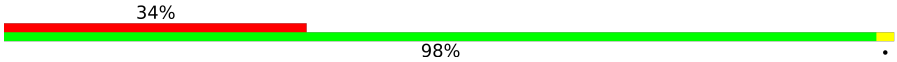


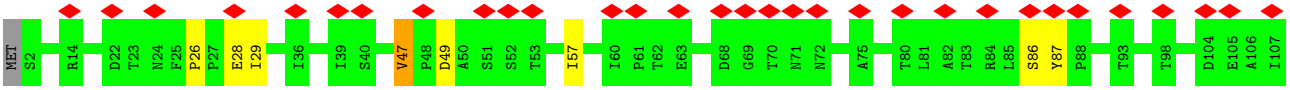


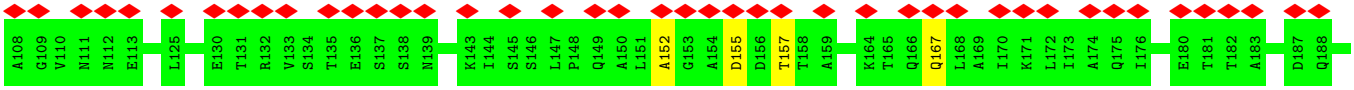


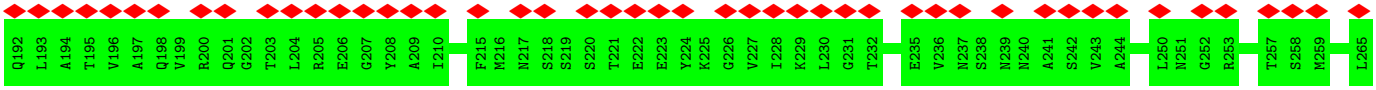
• Molecule 7: Short tail fiber protein gp12

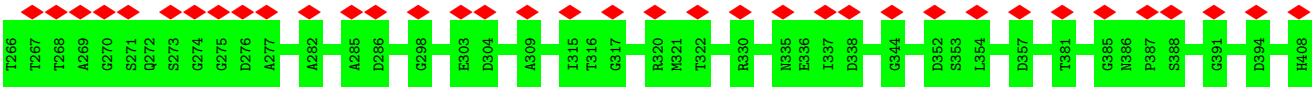
Chain BA:

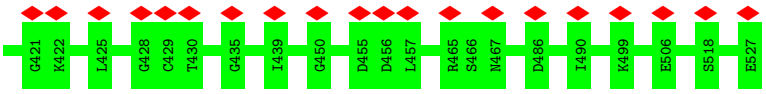






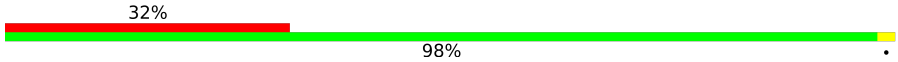


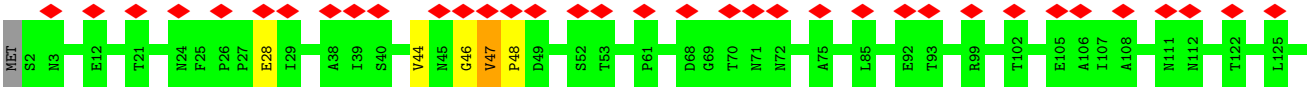


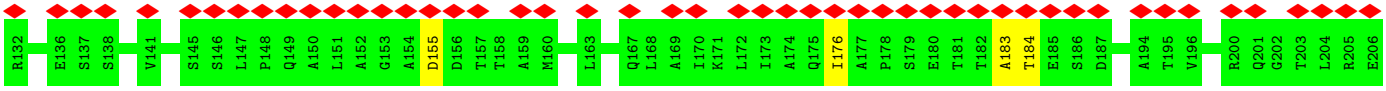


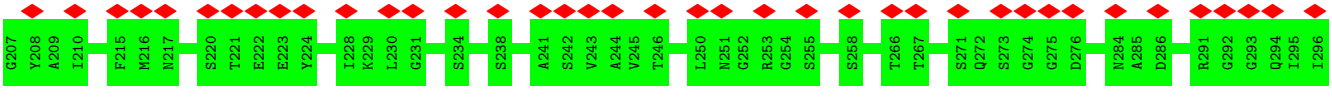
• Molecule 7: Short tail fiber protein gp12

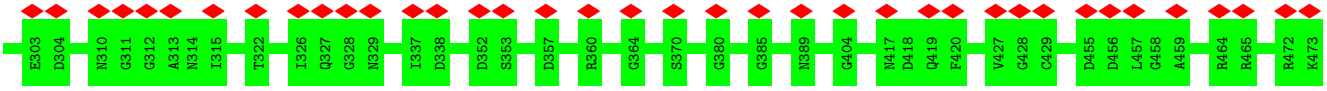
Chain DB:

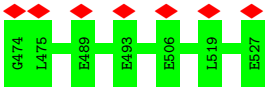






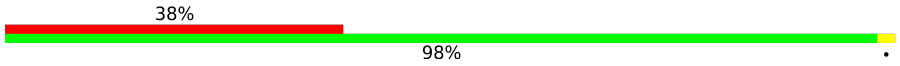


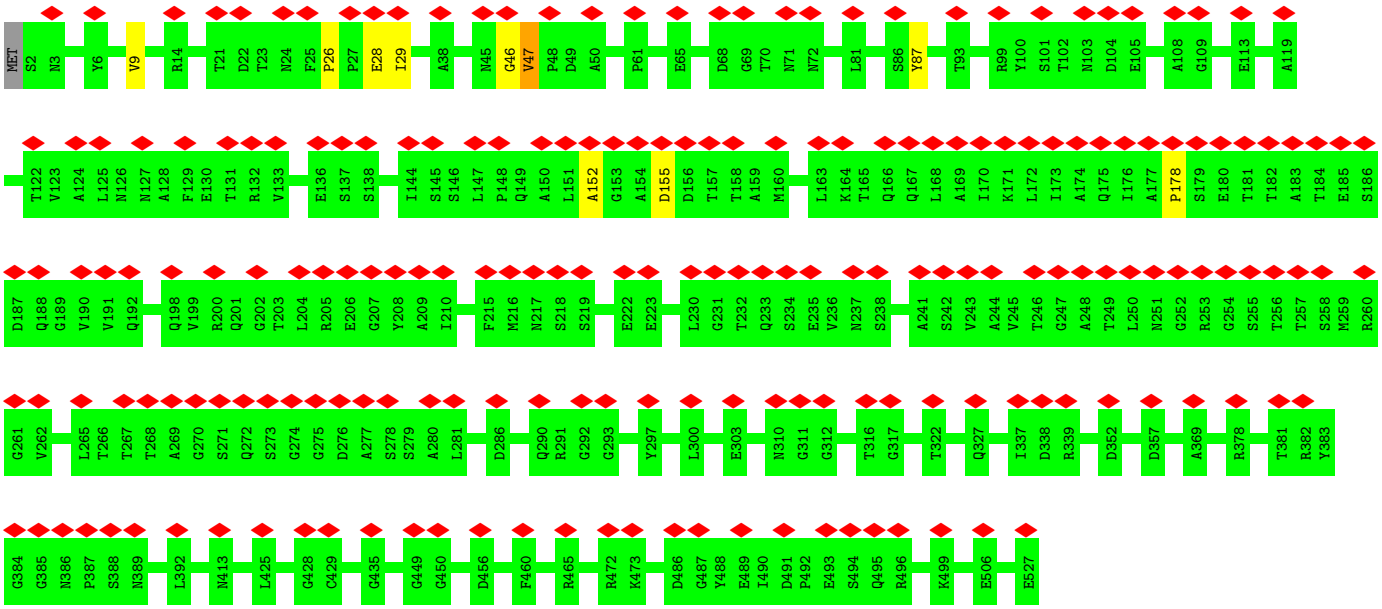




• Molecule 7: Short tail fiber protein gp12

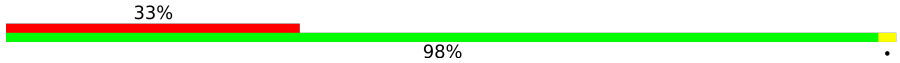
Chain DC:

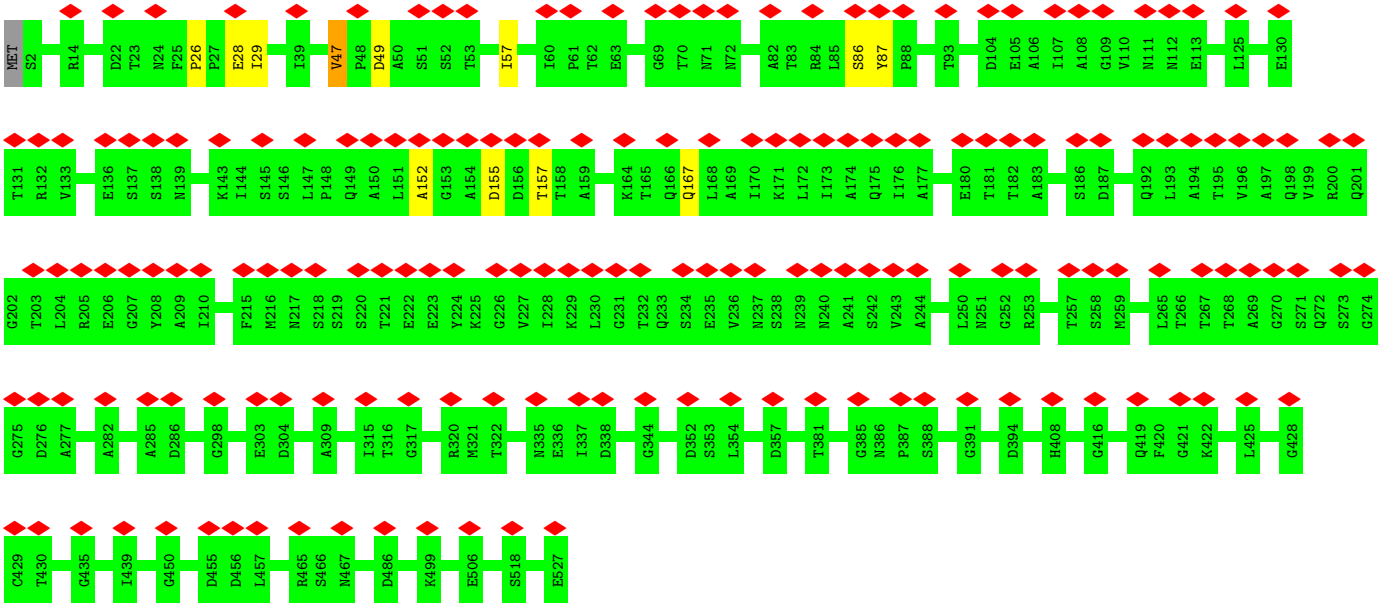




• Molecule 7: Short tail fiber protein gp12

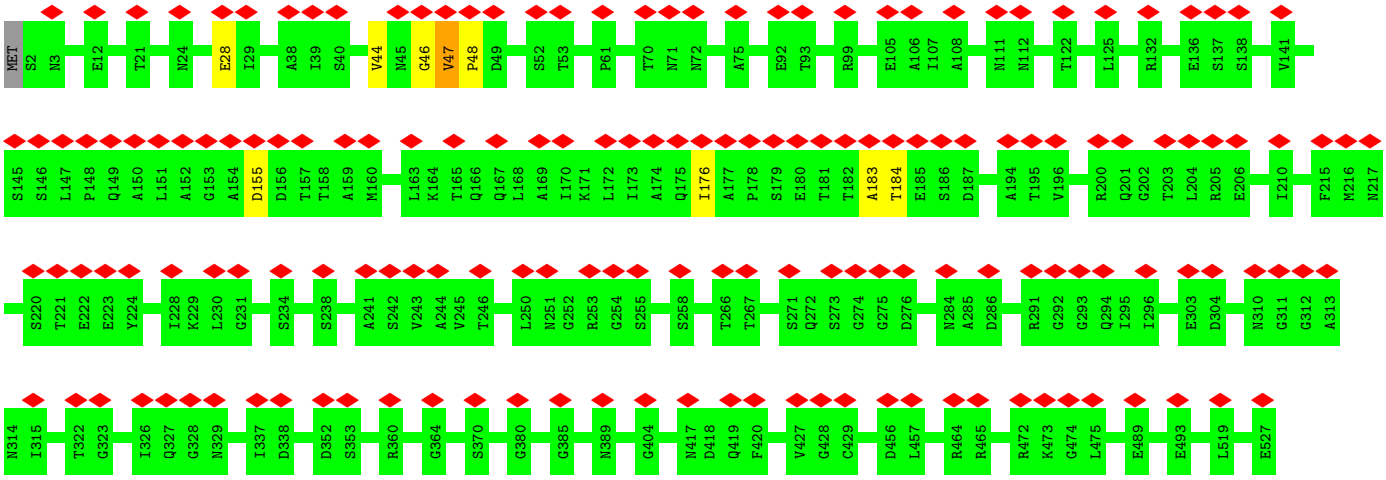
Chain DD:





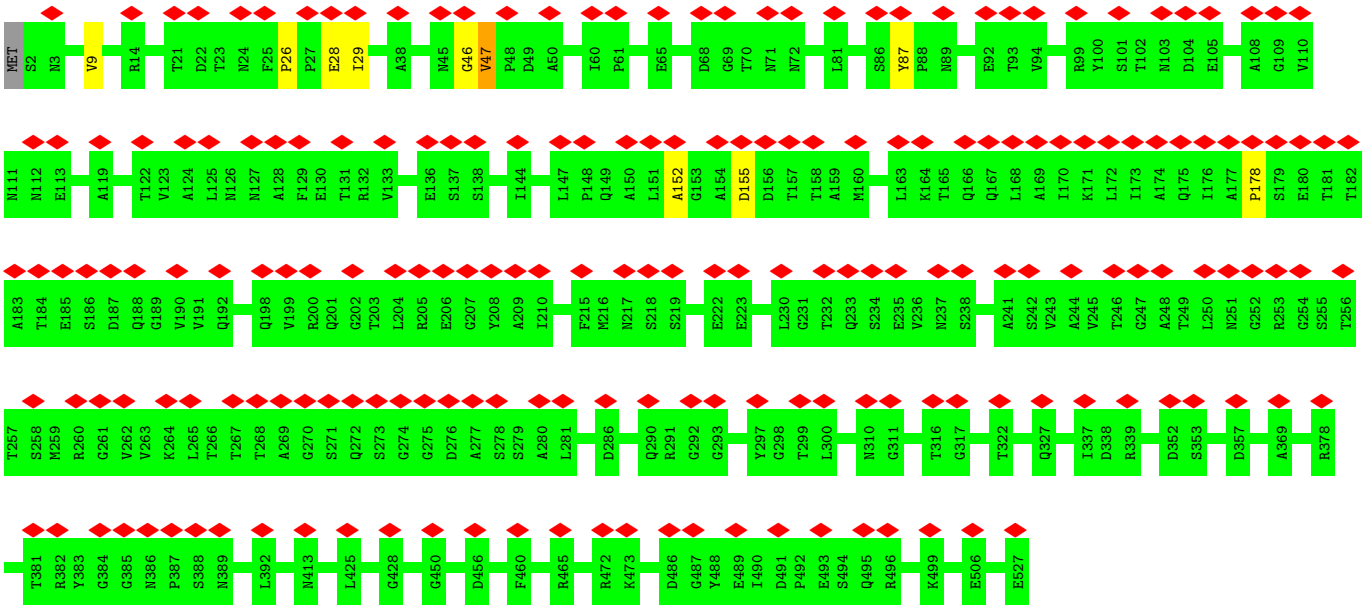
• Molecule 7: Short tail fiber protein gp12

Chain FE: 31% 98%



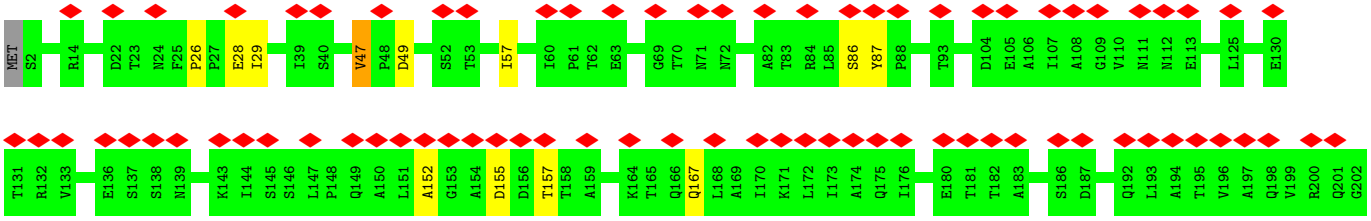
- Molecule 7: Short tail fiber protein gp12

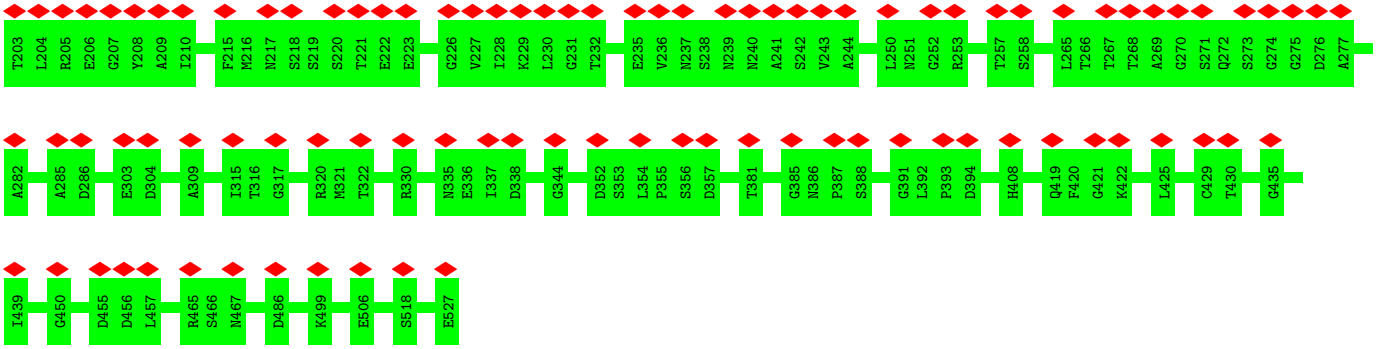
Chain FF: 37% 98%



- Molecule 7: Short tail fiber protein gp12

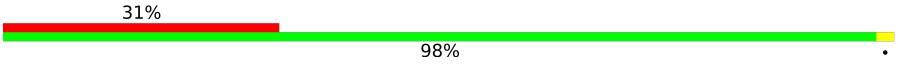
Chain FG: 32% 98%

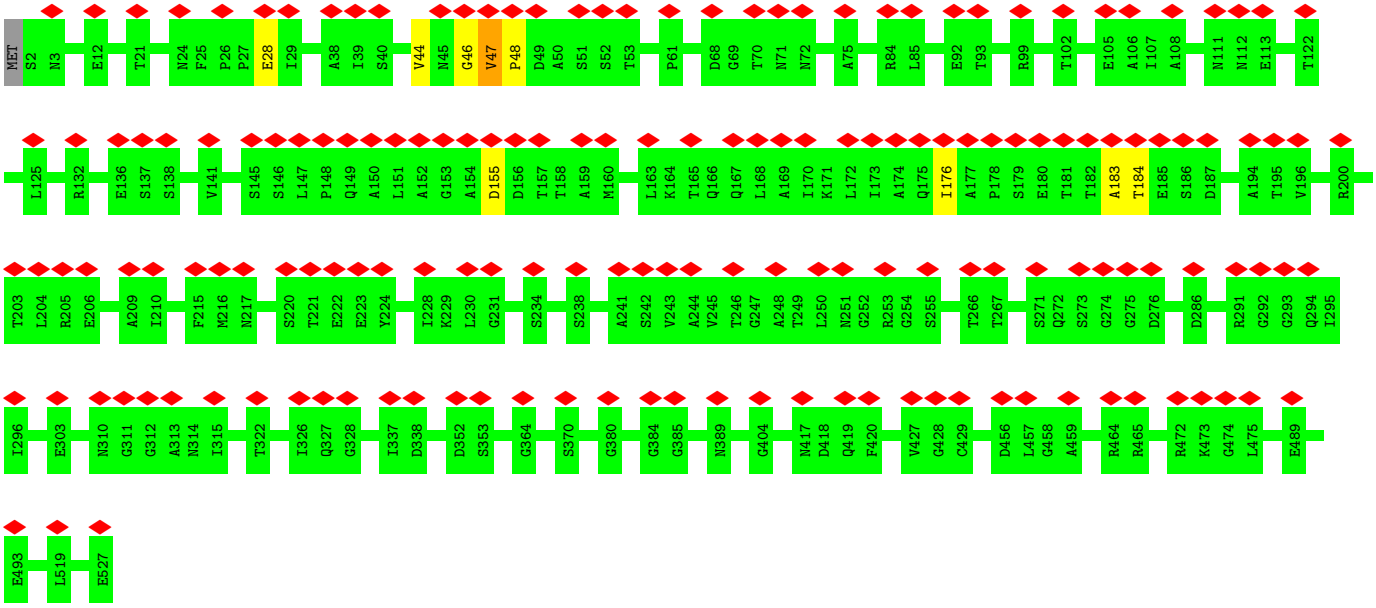




- Molecule 7: Short tail fiber protein gp12

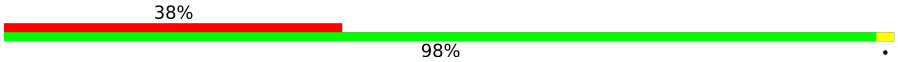
Chain HH:

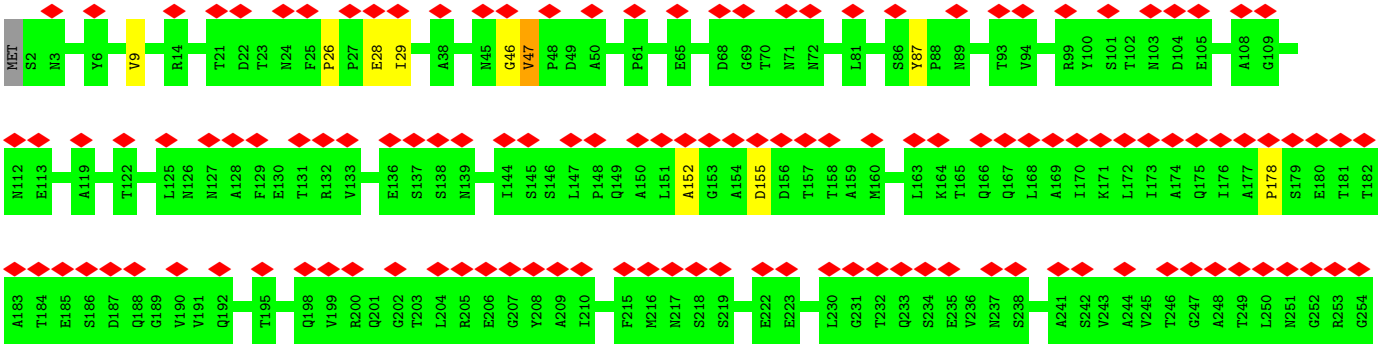


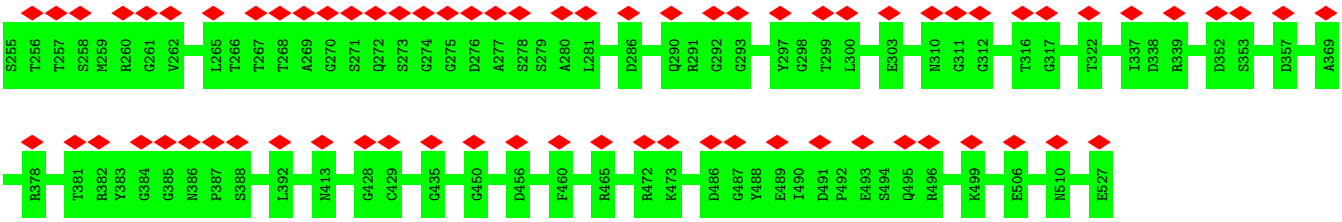


- Molecule 7: Short tail fiber protein gp12

Chain HI:

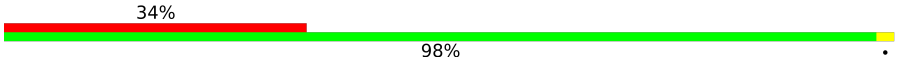


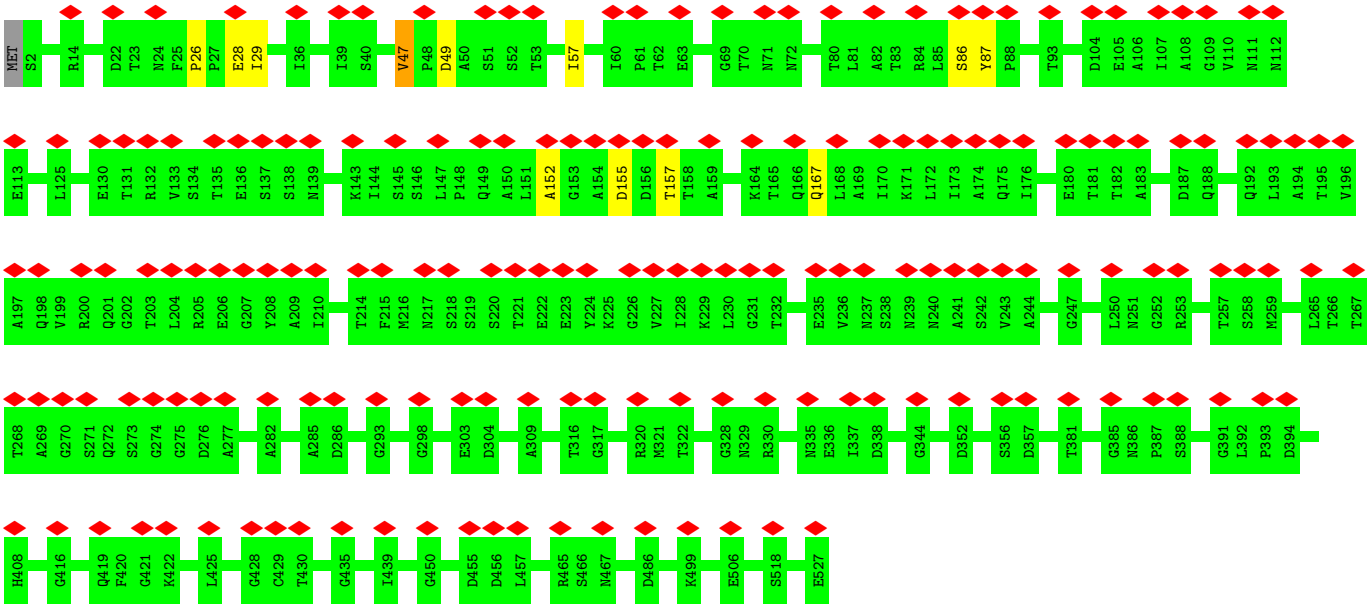




• Molecule 7: Short tail fiber protein gp12

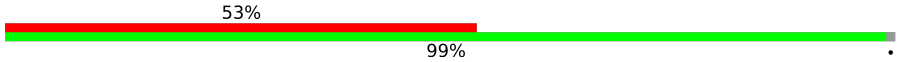
Chain HJ:

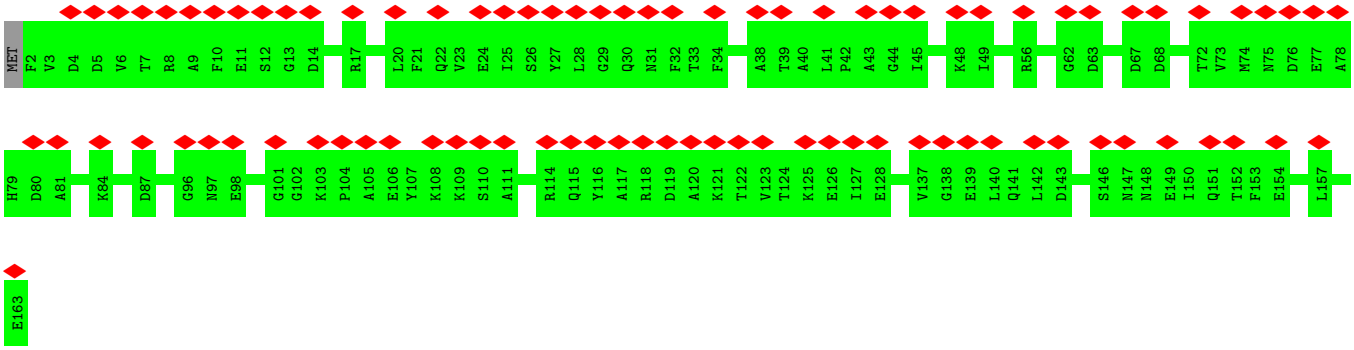




• Molecule 8: Tail tube protein gp19

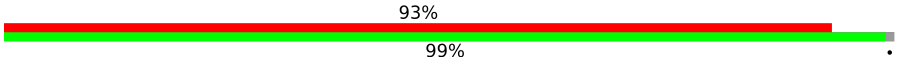
Chain R:

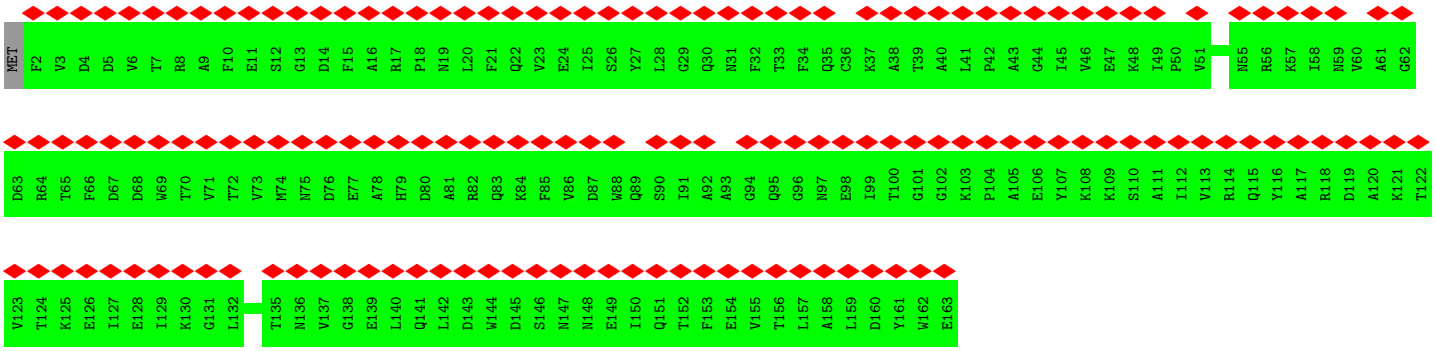




• Molecule 8: Tail tube protein gp19

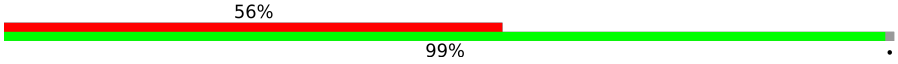
Chain S:

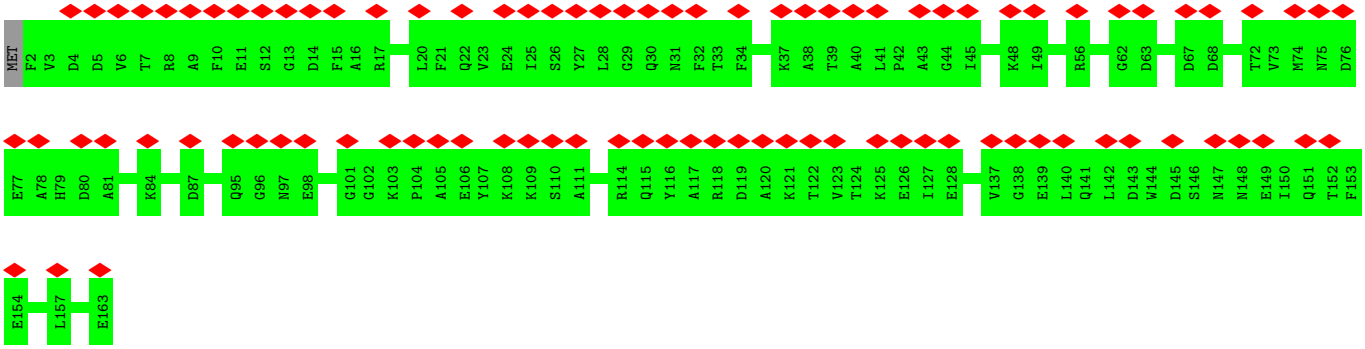




- Molecule 8: Tail tube protein gp19

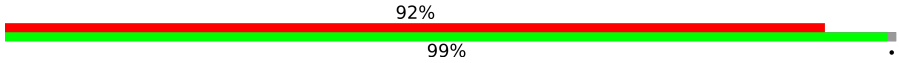
Chain o:

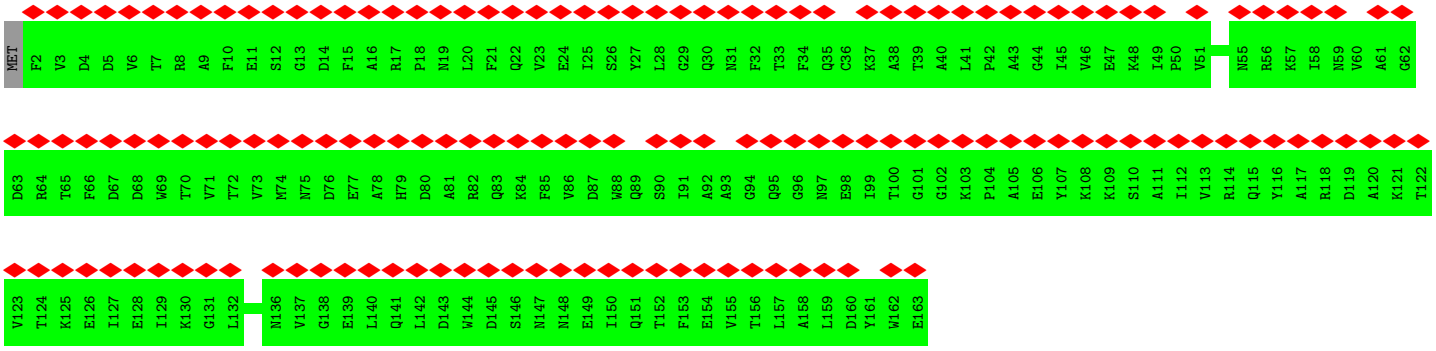




- Molecule 8: Tail tube protein gp19

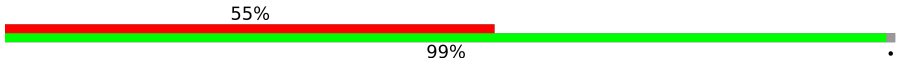
Chain p:

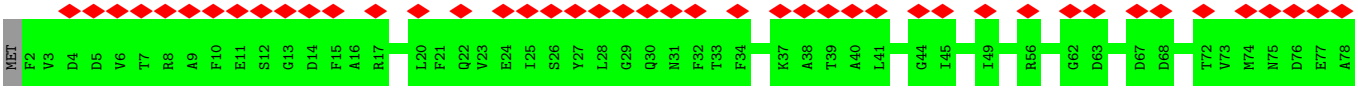


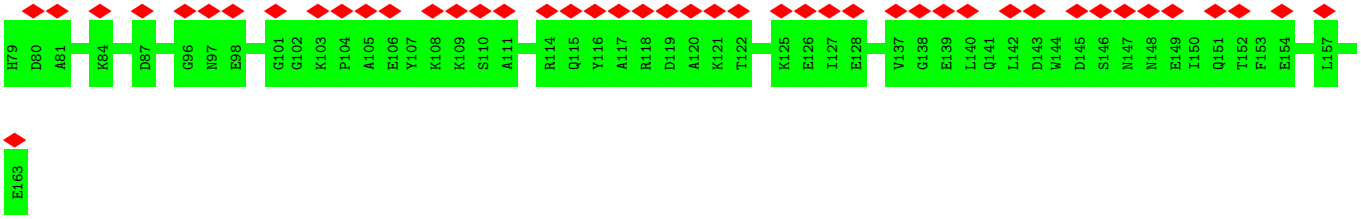


- Molecule 8: Tail tube protein gp19

Chain BB:

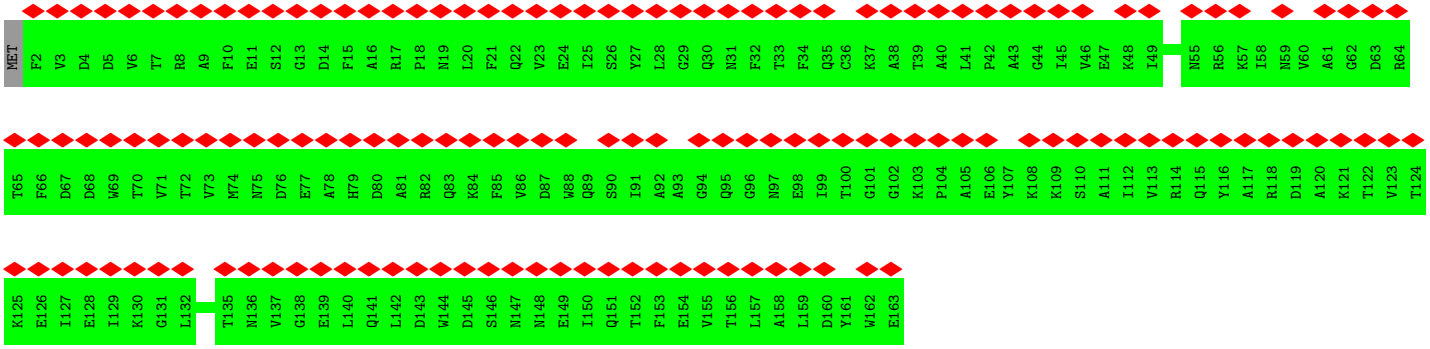






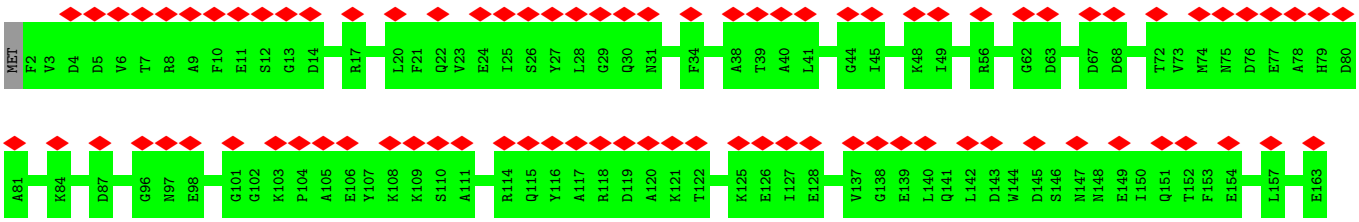
• Molecule 8: Tail tube protein gp19

Chain BC: 90% 99%



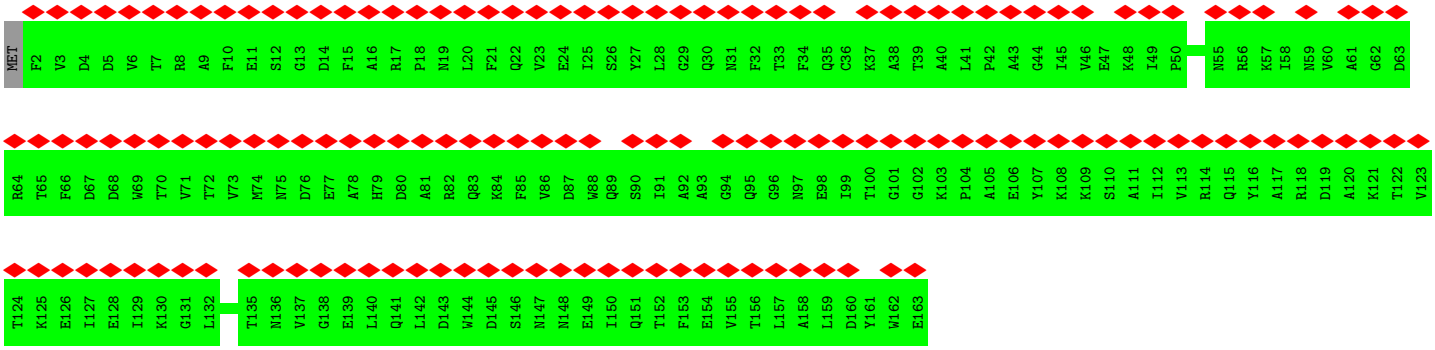
• Molecule 8: Tail tube protein gp19

Chain DE: 53% 99%



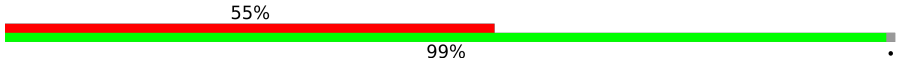
• Molecule 8: Tail tube protein gp19

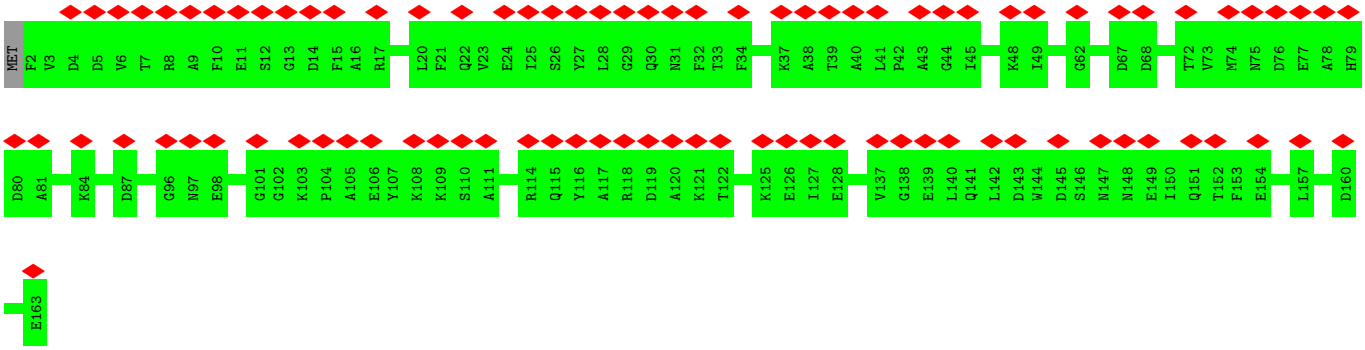
Chain DF: 91% 99%



• Molecule 8: Tail tube protein gp19

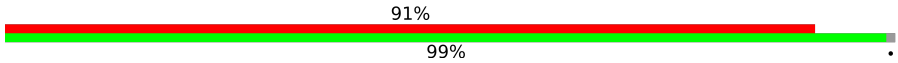
Chain FH:

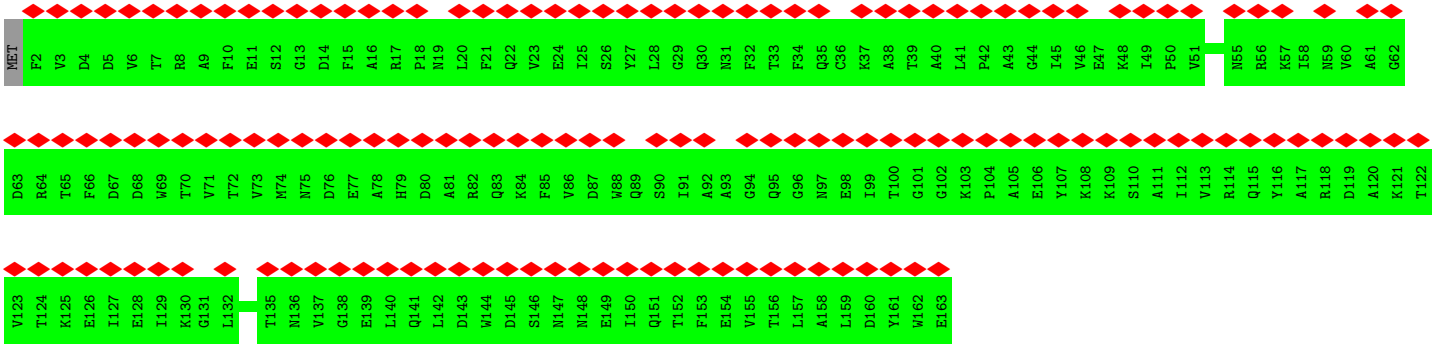




- Molecule 8: Tail tube protein gp19

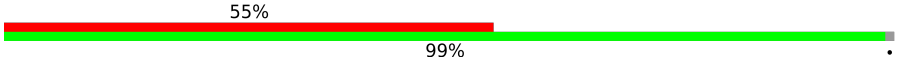
Chain FI:

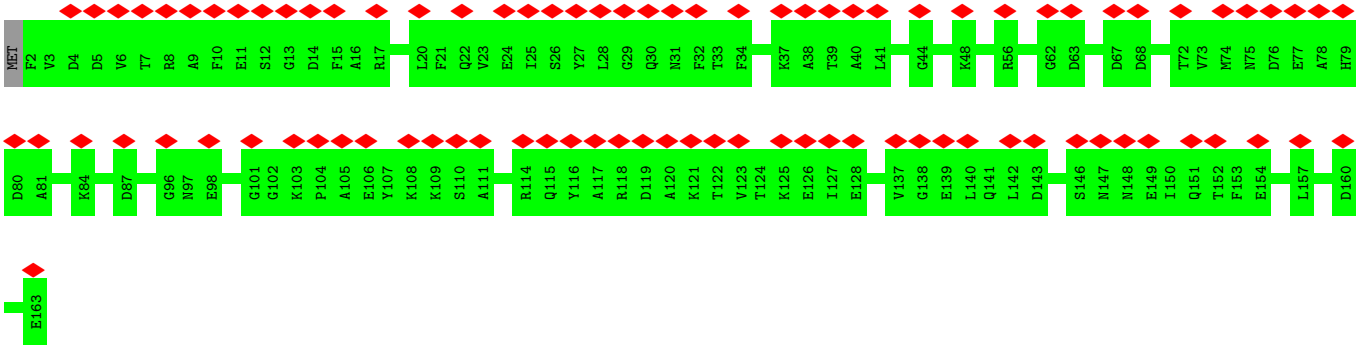




- Molecule 8: Tail tube protein gp19

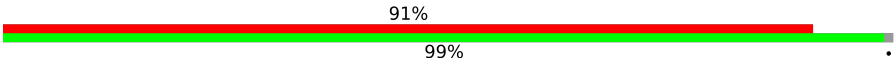
Chain IA:

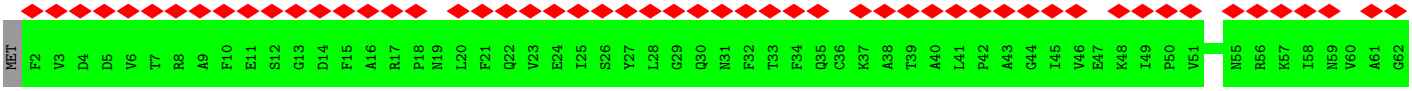


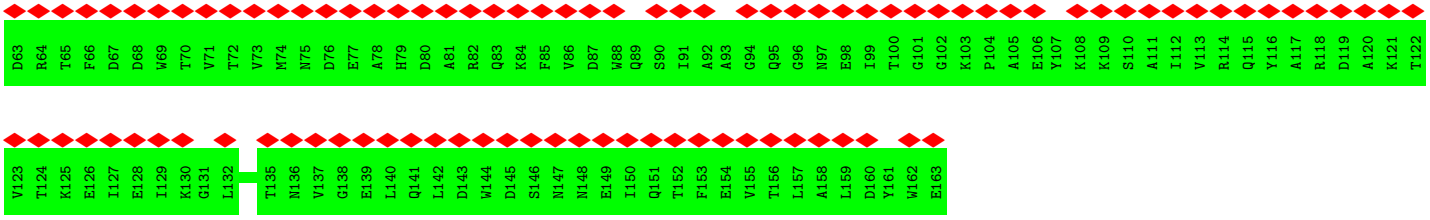


- Molecule 8: Tail tube protein gp19

Chain IB:

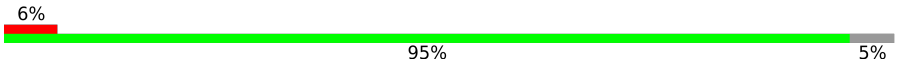


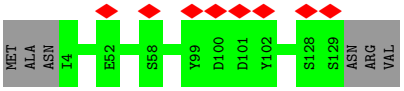




• Molecule 9: Baseplate wedge protein gp25

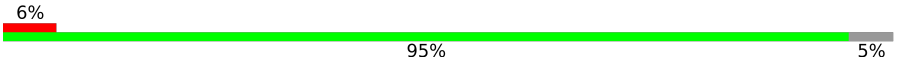
Chain T:

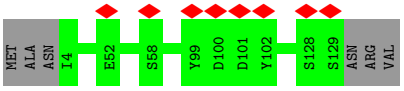




• Molecule 9: Baseplate wedge protein gp25

Chain q:





• Molecule 9: Baseplate wedge protein gp25

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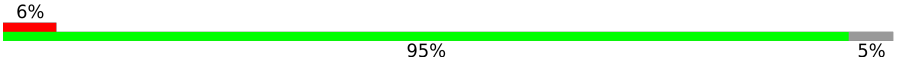
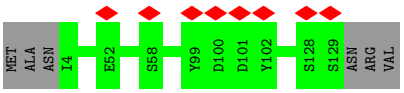
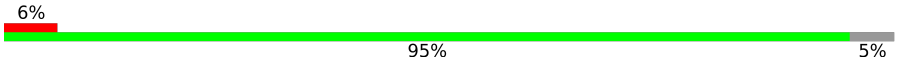
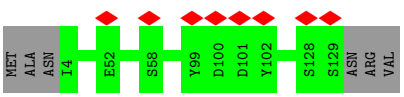




• Molecule 9: Baseplate wedge protein gp25

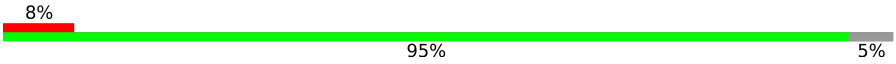
Chain DG:

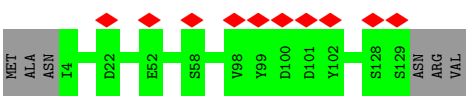




• Molecule 9: Baseplate wedge protein gp25

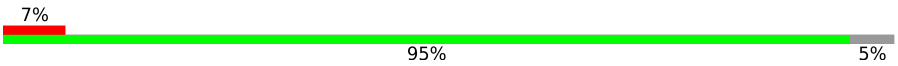
Chain FJ:

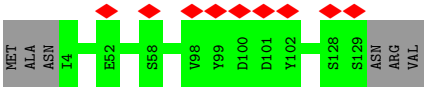




• Molecule 9: Baseplate wedge protein gp25

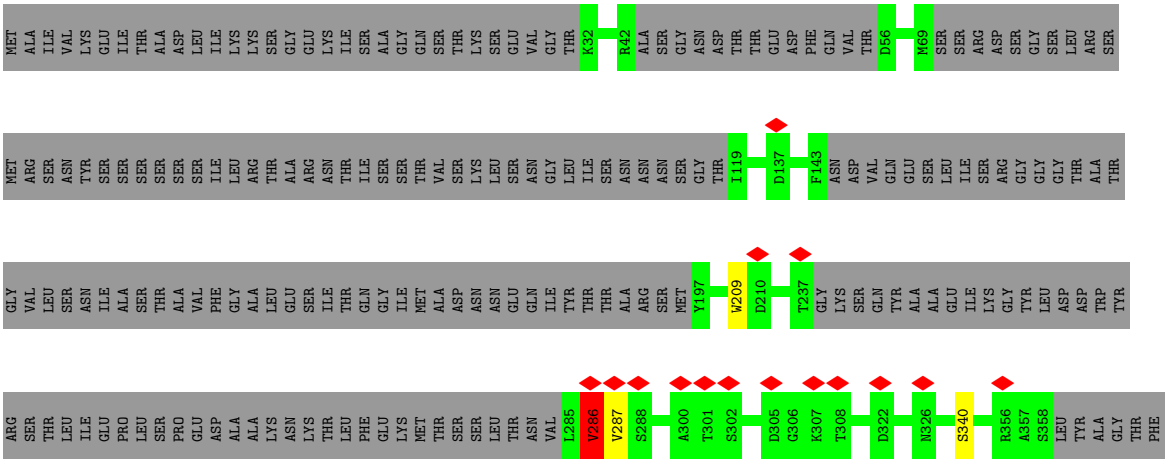
Chain IC:





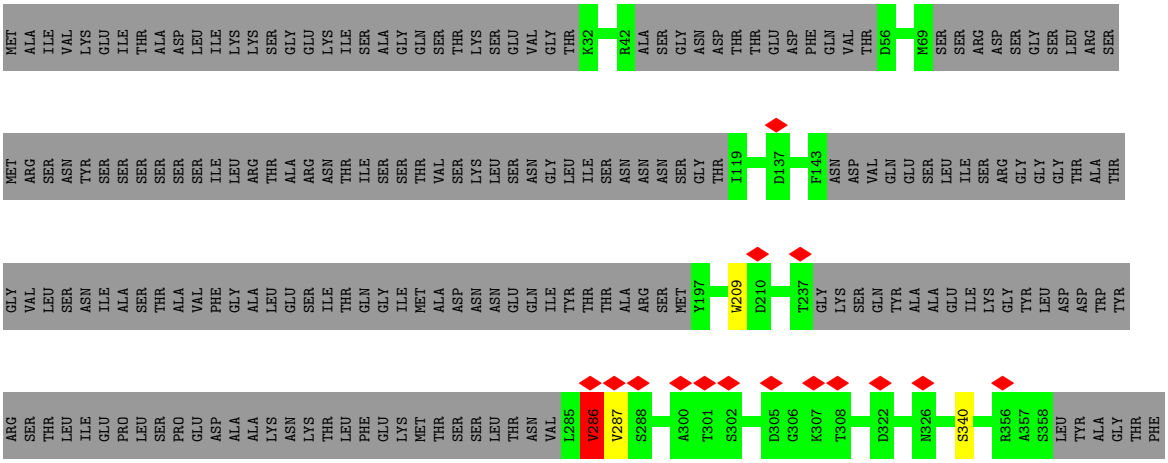
• Molecule 10: Baseplate tail-tube protein gp48

Chain U:



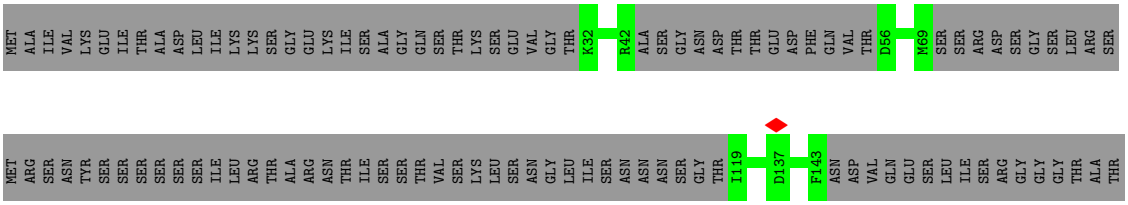
• Molecule 10: Baseplate tail-tube protein gp48

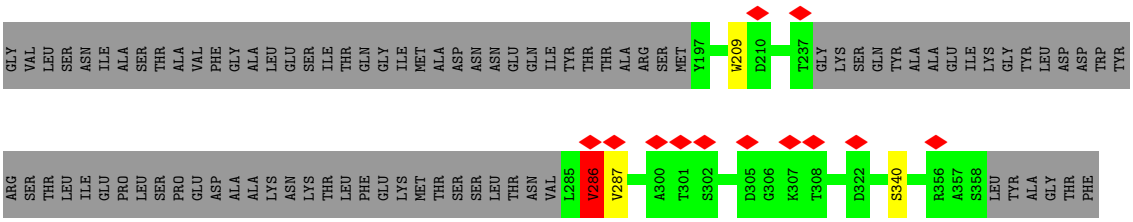
Chain r:



• Molecule 10: Baseplate tail-tube protein gp48

Chain BE:





• Molecule 10: Baseplate tail-tube protein gp48

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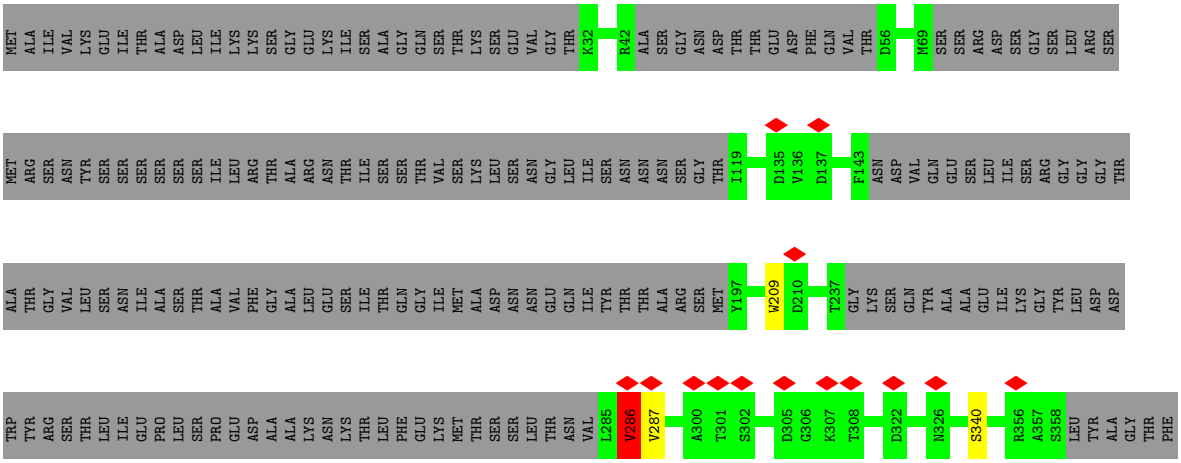

• Molecule 10: Baseplate tail-tube protein gp48

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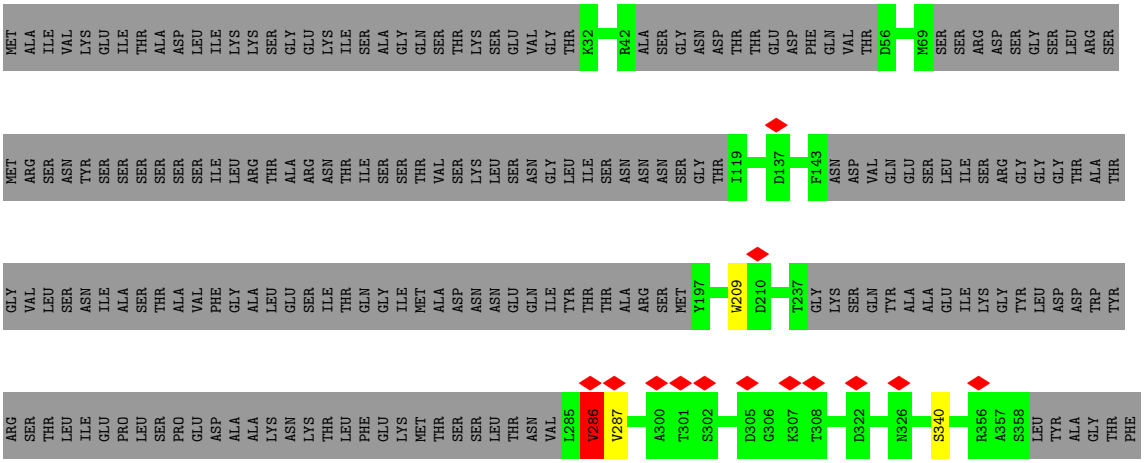

• Molecule 10: Baseplate tail-tube protein gp48

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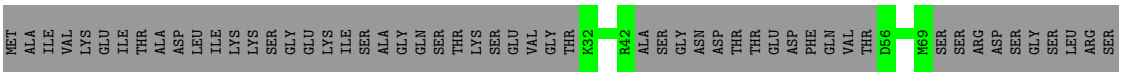
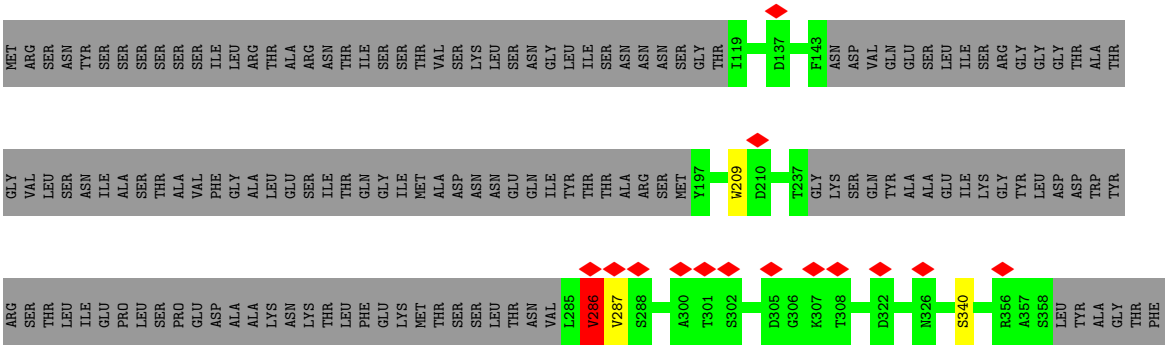
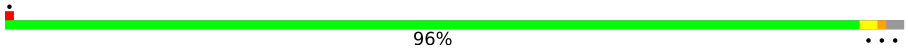
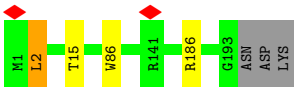




- Molecule 11: Baseplate wedge protein gp53

Chain V:





- Molecule 11: Baseplate wedge protein gp53

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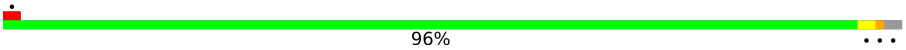

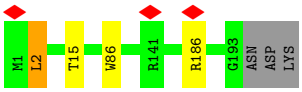

- Molecule 11: Baseplate wedge protein gp53

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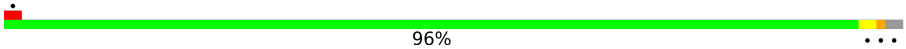
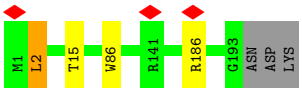
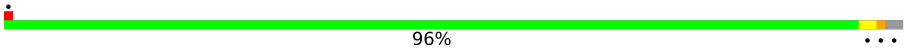
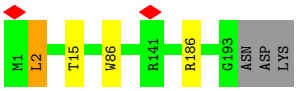




- Molecule 11: Baseplate wedge protein gp53

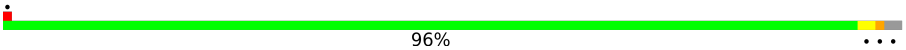
Chain DI:

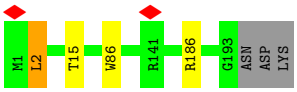




- Molecule 11: Baseplate wedge protein gp53

Chain GB:





- Molecule 11: Baseplate wedge protein gp53

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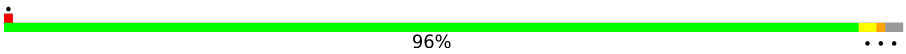
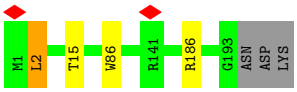
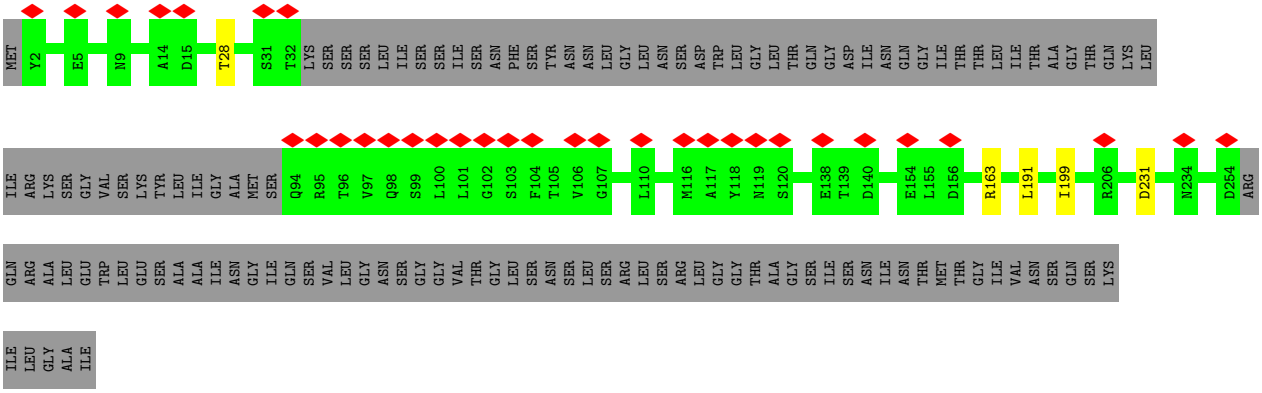




• Molecule 12: Baseplate tail-tube protein gp54

Chain W:



• Molecule 12: Baseplate tail-tube protein gp54

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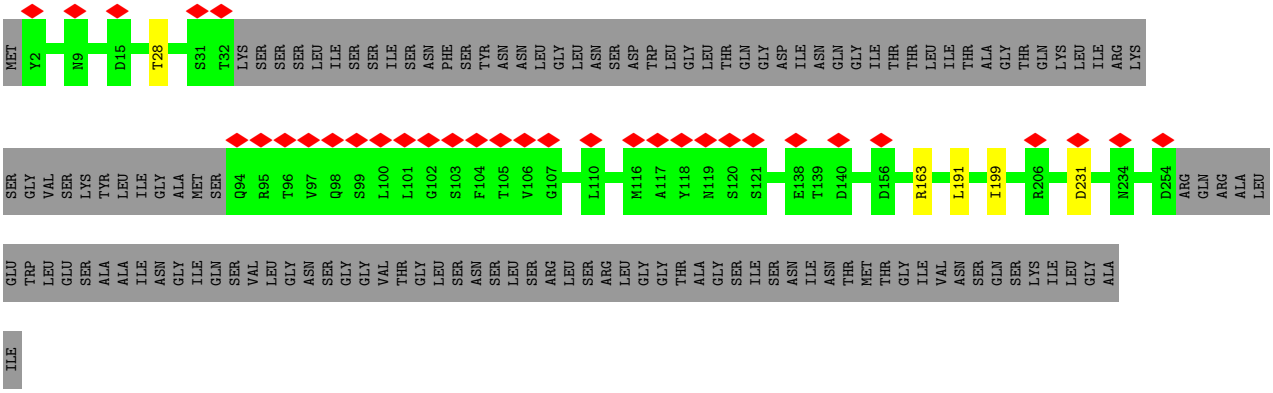
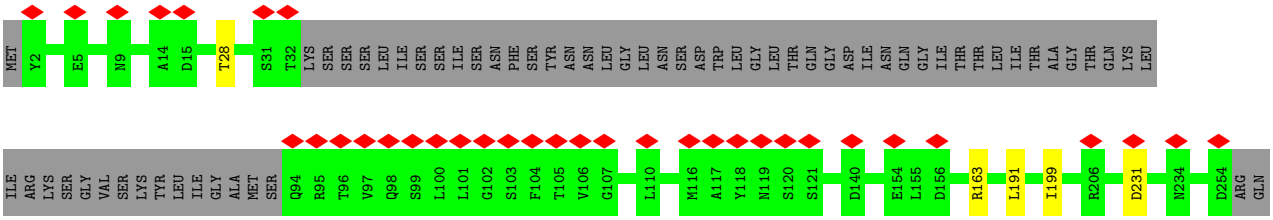
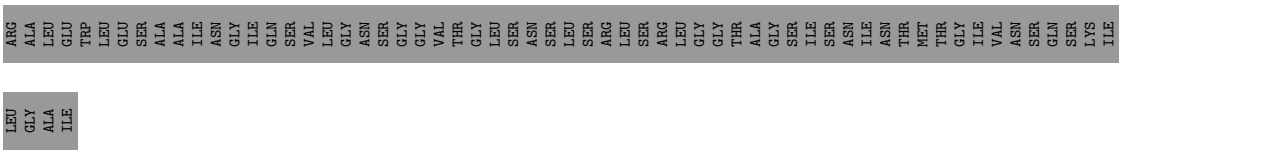


• Molecule 12: Baseplate tail-tube protein gp54

Chain BG:





• Molecule 12: Baseplate tail-tube protein gp54

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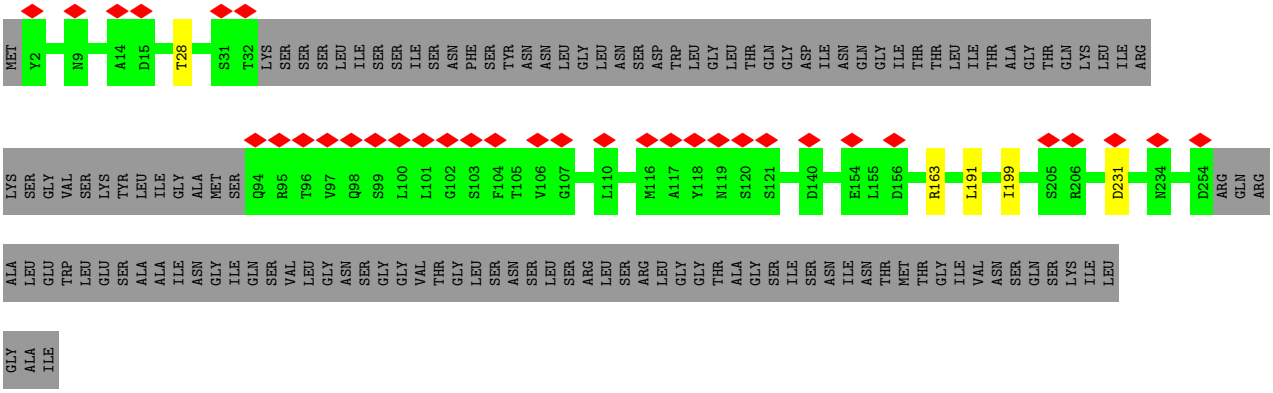

• Molecule 12: Baseplate tail-tube protein gp54

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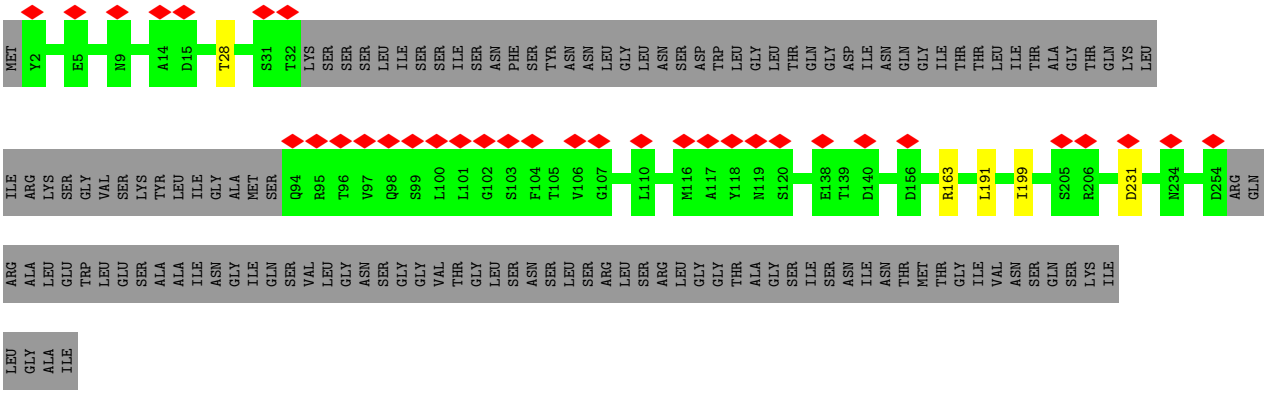
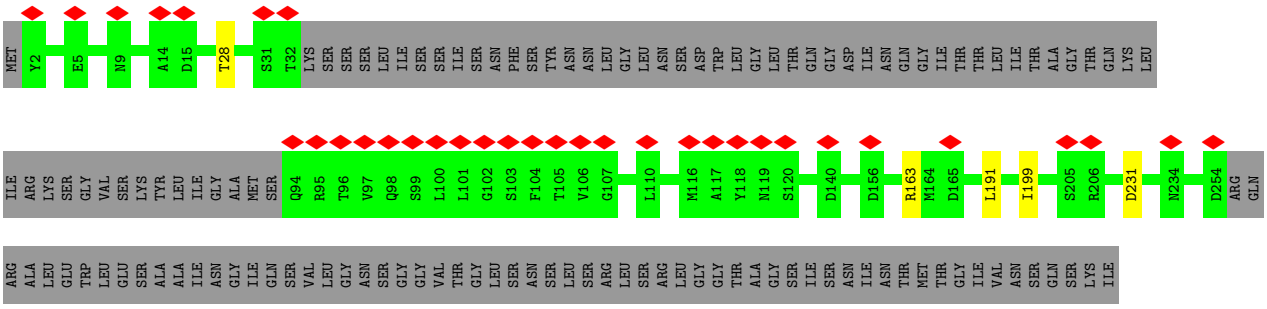


• Molecule 12: Baseplate tail-tube protein gp54

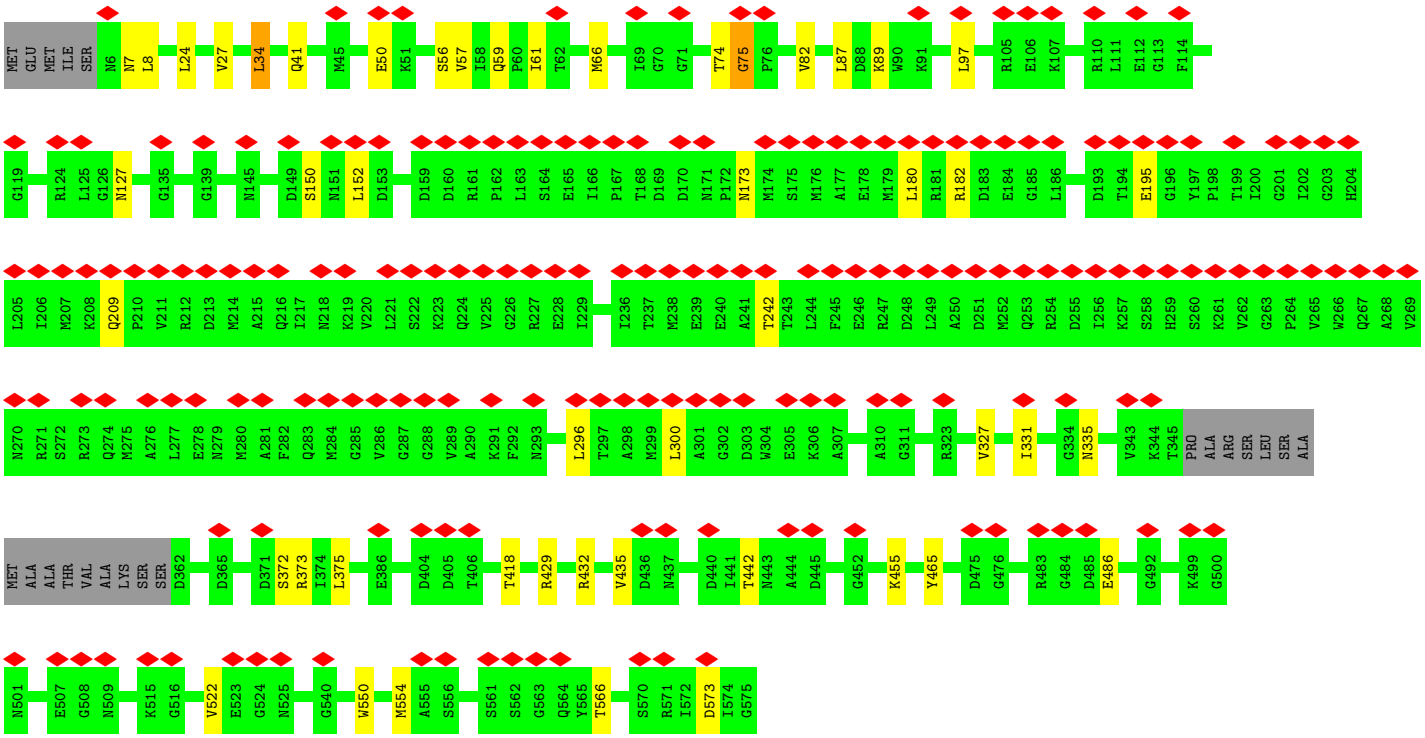
Chain IF:



LEU GLY ALA ILE

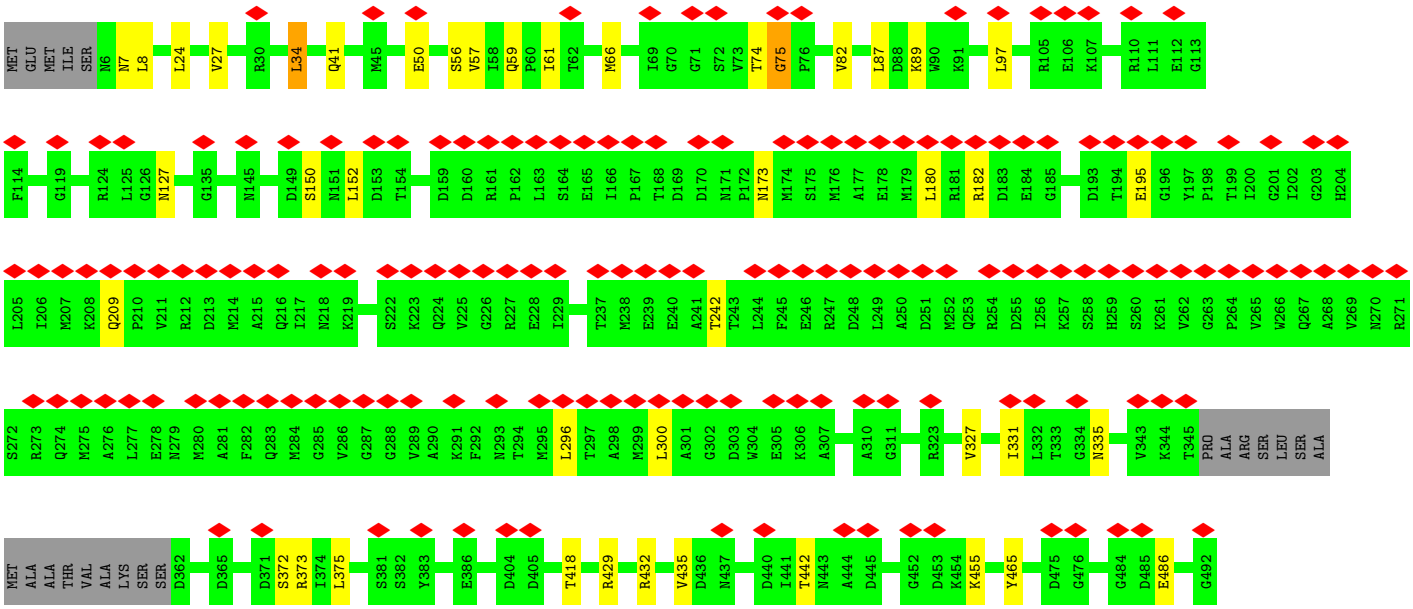
- Molecule 13: Peptidoglycan hydrolase gp5

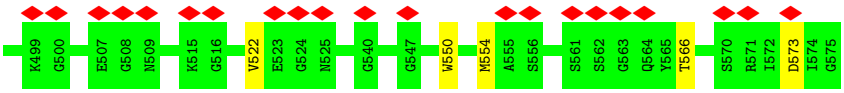
Chain YA:



- Molecule 13: Peptidoglycan hydrolase gp5

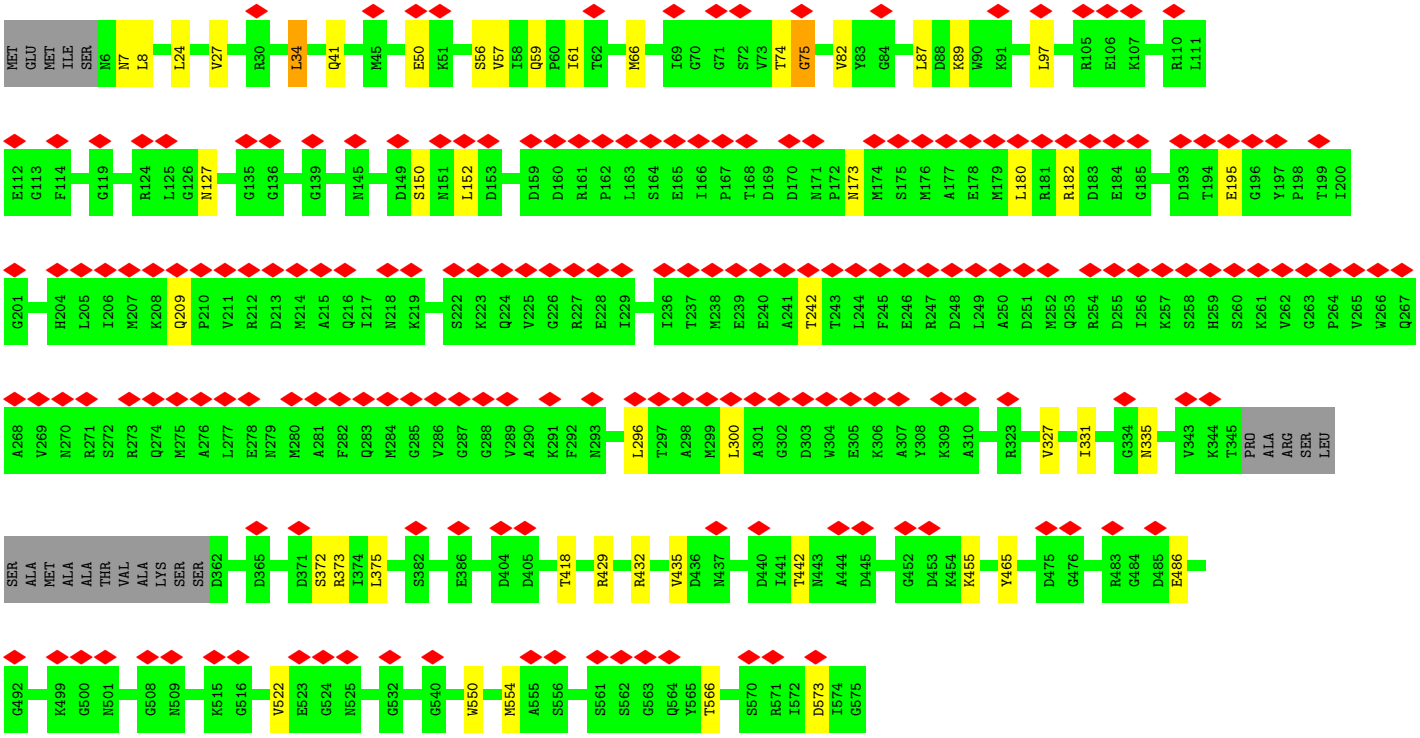
Chain YB:





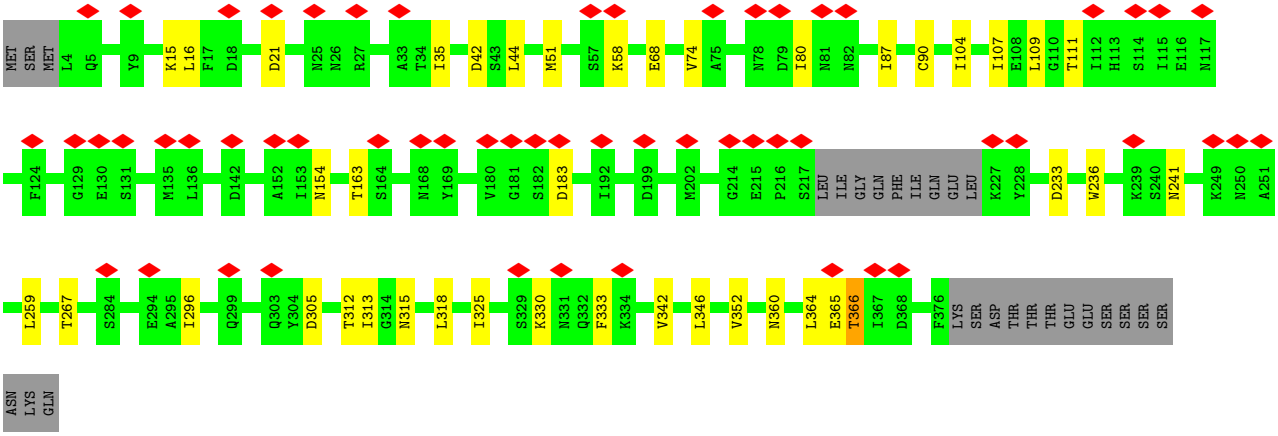
• Molecule 13: Peptidoglycan hydrolase gp5

Chain YC:



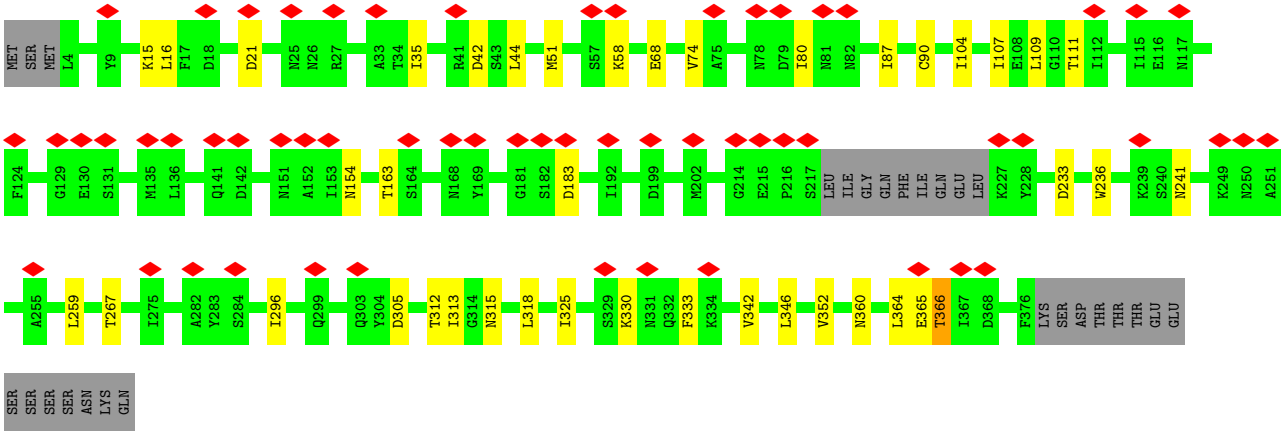
• Molecule 14: Baseplate hub protein gp27

Chain YD:



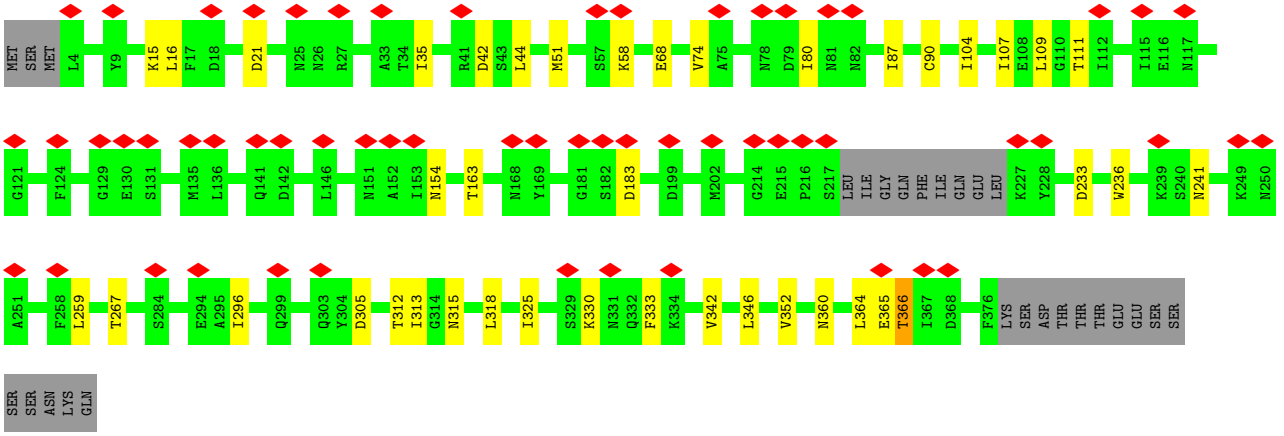
• Molecule 14: Baseplate hub protein gp27

Chain YE:



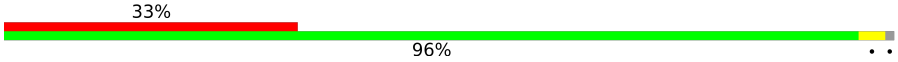
• Molecule 14: Baseplate hub protein gp27

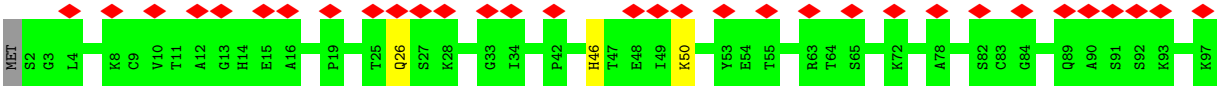
Chain YF:



• Molecule 15: Uncharacterized 10.2 kDa protein in segC-Gp6 intergenic region

Chain ZA:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	37913	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37700	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0263	Depositor
Map size (Å)	636.48, 636.48, 636.48	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.326, 1.326, 1.326	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	A	0.75	0/5337	0.66	1/7256 (0.0%)
1	B	0.71	1/5257 (0.0%)	0.66	1/7144 (0.0%)
1	BH	0.75	0/5337	0.66	1/7256 (0.0%)
1	BI	0.71	1/5257 (0.0%)	0.65	1/7144 (0.0%)
1	EA	0.75	0/5337	0.66	1/7256 (0.0%)
1	EB	0.71	1/5257 (0.0%)	0.65	1/7144 (0.0%)
1	GD	0.75	0/5337	0.66	1/7256 (0.0%)
1	GE	0.71	1/5257 (0.0%)	0.65	1/7144 (0.0%)
1	X	0.75	0/5337	0.66	1/7256 (0.0%)
1	Y	0.71	1/5257 (0.0%)	0.66	1/7144 (0.0%)
1	u	0.75	0/5337	0.66	1/7256 (0.0%)
1	v	0.71	1/5257 (0.0%)	0.65	1/7144 (0.0%)
2	BJ	0.65	2/8405 (0.0%)	0.73	2/11412 (0.0%)
2	C	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
2	EC	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
2	GF	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
2	Z	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
2	w	0.65	2/8405 (0.0%)	0.74	2/11412 (0.0%)
3	CA	0.70	1/2709 (0.0%)	0.57	0/3694
3	CB	0.68	1/2736 (0.0%)	0.62	0/3731
3	D	0.70	1/2709 (0.0%)	0.57	0/3694
3	E	0.68	1/2736 (0.0%)	0.62	0/3731
3	ED	0.70	1/2709 (0.0%)	0.57	0/3694
3	EE	0.68	1/2736 (0.0%)	0.62	0/3731
3	GG	0.70	1/2709 (0.0%)	0.57	0/3694
3	GH	0.68	1/2736 (0.0%)	0.62	0/3731
3	a	0.70	1/2709 (0.0%)	0.57	0/3694
3	b	0.68	1/2736 (0.0%)	0.62	0/3731
3	x	0.70	1/2709 (0.0%)	0.57	0/3694
3	y	0.68	1/2736 (0.0%)	0.62	0/3731
4	AA	0.28	0/2205	0.48	0/2988
4	AB	0.28	0/2205	0.48	0/2988

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	CC	0.28	0/2205	0.48	0/2988
4	CD	0.28	0/2205	0.48	0/2988
4	CE	0.28	0/2205	0.48	0/2988
4	EF	0.28	0/2205	0.48	0/2988
4	EG	0.28	0/2205	0.48	0/2988
4	EH	0.28	0/2205	0.48	0/2988
4	F	0.28	0/2205	0.48	0/2988
4	G	0.28	0/2205	0.48	0/2988
4	GI	0.28	0/2205	0.48	0/2988
4	GJ	0.28	0/2205	0.48	0/2988
4	H	0.28	0/2205	0.48	0/2988
4	HA	0.28	0/2205	0.48	0/2988
4	c	0.28	0/2205	0.48	0/2988
4	d	0.28	0/2205	0.48	0/2988
4	e	0.28	0/2205	0.48	0/2988
4	z	0.28	0/2205	0.48	0/2988
5	AC	0.48	0/4778	0.68	2/6513 (0.0%)
5	AD	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	AE	0.50	0/4778	0.70	3/6513 (0.0%)
5	CF	0.48	0/4778	0.68	2/6513 (0.0%)
5	CG	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	CH	0.50	0/4778	0.70	3/6513 (0.0%)
5	EI	0.48	0/4778	0.68	2/6513 (0.0%)
5	EJ	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	FA	0.50	0/4778	0.70	3/6513 (0.0%)
5	HB	0.48	0/4778	0.68	2/6513 (0.0%)
5	HC	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	HD	0.50	0/4778	0.70	4/6513 (0.1%)
5	I	0.48	0/4778	0.68	2/6513 (0.0%)
5	J	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	K	0.50	0/4778	0.70	4/6513 (0.1%)
5	f	0.48	0/4778	0.68	2/6513 (0.0%)
5	g	0.49	1/4778 (0.0%)	0.69	5/6513 (0.1%)
5	h	0.50	0/4778	0.70	4/6513 (0.1%)
6	AF	0.34	0/1700	0.51	0/2318
6	AG	0.34	0/1700	0.51	0/2318
6	AH	0.34	0/1700	0.51	0/2318
6	CI	0.34	0/1700	0.51	0/2318
6	CJ	0.34	0/1700	0.51	0/2318
6	DA	0.34	0/1700	0.51	0/2318
6	FB	0.34	0/1700	0.51	0/2318
6	FC	0.34	0/1700	0.51	0/2318
6	FD	0.34	0/1700	0.51	0/2318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	HE	0.34	0/1700	0.51	0/2318
6	HF	0.34	0/1700	0.51	0/2318
6	HG	0.34	0/1700	0.51	0/2318
6	L	0.34	0/1700	0.51	0/2318
6	M	0.34	0/1700	0.51	0/2318
6	N	0.34	0/1700	0.51	0/2318
6	i	0.34	0/1700	0.51	0/2318
6	j	0.34	0/1700	0.51	0/2318
6	k	0.34	0/1700	0.51	0/2318
7	AI	0.39	0/4016	0.61	0/5464
7	AJ	0.39	1/4016 (0.0%)	0.61	0/5464
7	BA	0.40	1/4016 (0.0%)	0.60	0/5464
7	DB	0.39	0/4016	0.61	0/5464
7	DC	0.39	1/4016 (0.0%)	0.60	0/5464
7	DD	0.40	1/4016 (0.0%)	0.60	0/5464
7	FE	0.39	0/4016	0.61	0/5464
7	FF	0.39	1/4016 (0.0%)	0.60	0/5464
7	FG	0.40	1/4016 (0.0%)	0.60	0/5464
7	HH	0.39	0/4016	0.61	0/5464
7	HI	0.39	1/4016 (0.0%)	0.60	0/5464
7	HJ	0.40	1/4016 (0.0%)	0.60	0/5464
7	O	0.39	0/4016	0.61	0/5464
7	P	0.39	1/4016 (0.0%)	0.60	0/5464
7	Q	0.40	1/4016 (0.0%)	0.60	0/5464
7	l	0.39	0/4016	0.61	0/5464
7	m	0.39	1/4016 (0.0%)	0.61	0/5464
7	n	0.40	1/4016 (0.0%)	0.60	0/5464
8	BB	0.45	0/1325	0.58	0/1797
8	BC	0.45	0/1325	0.58	0/1797
8	DE	0.44	0/1325	0.58	0/1797
8	DF	0.45	0/1325	0.58	0/1797
8	FH	0.44	0/1325	0.58	0/1797
8	FI	0.44	0/1325	0.58	0/1797
8	IA	0.44	0/1325	0.58	0/1797
8	IB	0.45	0/1325	0.58	0/1797
8	R	0.44	0/1325	0.58	0/1797
8	S	0.45	0/1325	0.58	0/1797
8	o	0.44	0/1325	0.58	0/1797
8	p	0.44	0/1325	0.58	0/1797
9	BD	0.55	0/1027	0.59	0/1392
9	DG	0.55	0/1027	0.59	0/1392
9	FJ	0.55	0/1027	0.59	0/1392
9	IC	0.55	0/1027	0.59	0/1392

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	T	0.55	0/1027	0.59	0/1392
9	q	0.55	0/1027	0.59	0/1392
10	BE	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	DH	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	GA	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	ID	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	U	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
10	r	0.77	1/1346 (0.1%)	0.72	2/1821 (0.1%)
11	BF	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	DI	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	GB	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	IE	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	V	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
11	s	0.77	1/1643 (0.1%)	0.76	3/2228 (0.1%)
12	BG	0.62	1/1557 (0.1%)	0.68	3/2118 (0.1%)
12	DJ	0.62	1/1557 (0.1%)	0.68	4/2118 (0.2%)
12	GC	0.62	1/1557 (0.1%)	0.68	3/2118 (0.1%)
12	IF	0.63	1/1557 (0.1%)	0.68	3/2118 (0.1%)
12	W	0.62	1/1557 (0.1%)	0.68	3/2118 (0.1%)
12	t	0.62	1/1557 (0.1%)	0.68	3/2118 (0.1%)
13	YA	0.49	0/26166	0.60	24/35454 (0.1%)
13	YB	0.49	0/26166	0.60	24/35454 (0.1%)
13	YC	0.49	0/26166	0.60	24/35454 (0.1%)
14	YD	0.61	0/17880	0.64	6/24252 (0.0%)
14	YE	0.61	0/17880	0.64	6/24252 (0.0%)
14	YF	0.61	0/17880	0.64	6/24252 (0.0%)
15	ZA	0.33	0/4344	0.54	0/5904
All	All	0.55	66/561066 (0.0%)	0.63	226/762456 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	8
1	BH	0	1
1	BI	0	8
1	EA	0	1
1	EB	0	8
1	GD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	GE	0	8
1	X	0	1
1	Y	0	8
1	u	0	1
1	v	0	8
2	BJ	0	38
2	C	0	38
2	EC	0	38
2	GF	0	38
2	Z	0	38
2	w	0	38
3	CA	0	2
3	CB	0	3
3	D	0	2
3	E	0	3
3	ED	0	2
3	EE	0	3
3	GG	0	2
3	GH	0	3
3	a	0	2
3	b	0	3
3	x	0	2
3	y	0	3
5	AC	0	17
5	AD	0	13
5	AE	0	16
5	CF	0	17
5	CG	0	13
5	CH	0	16
5	EI	0	17
5	EJ	0	13
5	FA	0	16
5	HB	0	17
5	HC	0	13
5	HD	0	16
5	I	0	17
5	J	0	13
5	K	0	16
5	f	0	17
5	g	0	13
5	h	0	16
6	AF	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	AG	0	3
6	AH	0	3
6	CI	0	3
6	CJ	0	3
6	DA	0	3
6	FB	0	3
6	FC	0	3
6	FD	0	3
6	HE	0	3
6	HF	0	3
6	HG	0	3
6	L	0	3
6	M	0	3
6	N	0	3
6	i	0	3
6	j	0	3
6	k	0	3
7	AI	0	4
7	AJ	0	6
7	BA	0	5
7	DB	0	4
7	DC	0	6
7	DD	0	5
7	FE	0	4
7	FF	0	6
7	FG	0	5
7	HH	0	4
7	HI	0	6
7	HJ	0	5
7	O	0	4
7	P	0	6
7	Q	0	5
7	l	0	4
7	m	0	6
7	n	0	5
10	BE	0	1
10	DH	0	1
10	GA	0	1
10	ID	0	1
10	U	0	1
10	r	0	1
11	BF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	DI	0	1
11	GB	0	1
11	IE	0	1
11	V	0	1
11	s	0	1
13	YA	0	7
13	YB	0	7
13	YC	0	7
14	YD	0	6
14	YE	0	6
14	YF	0	6
All	All	0	783

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CA	258	PHE	C-N	-20.87	0.94	1.34
3	ED	258	PHE	C-N	-20.85	0.94	1.34
3	GG	258	PHE	C-N	-20.84	0.94	1.34
3	x	258	PHE	C-N	-20.84	0.94	1.34
3	a	258	PHE	C-N	-20.82	0.94	1.34
3	D	258	PHE	C-N	-20.82	0.94	1.34
1	v	307	ASP	C-N	-12.66	1.10	1.34
1	GE	307	ASP	C-N	-12.65	1.10	1.34
1	Y	307	ASP	C-N	-12.65	1.10	1.34
1	B	307	ASP	C-N	-12.64	1.10	1.34
1	EB	307	ASP	C-N	-12.60	1.10	1.34
1	BI	307	ASP	C-N	-12.60	1.10	1.34
2	w	652	MET	C-N	-10.23	1.10	1.34
2	C	652	MET	C-N	-10.23	1.10	1.34
2	EC	652	MET	C-N	-10.22	1.10	1.34
2	Z	652	MET	C-N	-10.22	1.10	1.34
2	GF	652	MET	C-N	-10.22	1.10	1.34
2	BJ	652	MET	C-N	-10.21	1.10	1.34
7	Q	26	PRO	C-N	-8.32	1.18	1.34
7	FG	26	PRO	C-N	-8.30	1.18	1.34
7	n	26	PRO	C-N	-8.29	1.18	1.34
7	HJ	26	PRO	C-N	-8.28	1.18	1.34
7	DD	26	PRO	C-N	-8.28	1.18	1.34
7	BA	26	PRO	C-N	-8.25	1.18	1.34
11	BF	86	TRP	CB-CG	-7.02	1.37	1.50
11	V	86	TRP	CB-CG	-6.99	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	s	86	TRP	CB-CG	-6.97	1.37	1.50
11	IE	86	TRP	CB-CG	-6.96	1.37	1.50
11	GB	86	TRP	CB-CG	-6.96	1.37	1.50
11	DI	86	TRP	CB-CG	-6.95	1.37	1.50
5	g	531	ASN	C-N	-6.59	1.18	1.34
5	J	531	ASN	C-N	-6.59	1.19	1.34
5	AD	531	ASN	C-N	-6.58	1.19	1.34
5	HC	531	ASN	C-N	-6.58	1.19	1.34
5	CG	531	ASN	C-N	-6.56	1.19	1.34
5	EJ	531	ASN	C-N	-6.53	1.19	1.34
7	DC	26	PRO	C-N	-6.14	1.22	1.34
7	AJ	26	PRO	C-N	-6.13	1.22	1.34
7	HI	26	PRO	C-N	-6.13	1.22	1.34
7	FF	26	PRO	C-N	-6.13	1.22	1.34
7	P	26	PRO	C-N	-6.11	1.22	1.34
7	m	26	PRO	C-N	-6.09	1.22	1.34
10	BE	209	TRP	CB-CG	-5.86	1.39	1.50
10	GA	209	TRP	CB-CG	-5.84	1.39	1.50
10	U	209	TRP	CB-CG	-5.83	1.39	1.50
10	r	209	TRP	CB-CG	-5.82	1.39	1.50
10	DH	209	TRP	CB-CG	-5.80	1.39	1.50
10	ID	209	TRP	CB-CG	-5.80	1.39	1.50
2	GF	714	TYR	CD2-CE2	-5.74	1.30	1.39
2	BJ	714	TYR	CD2-CE2	-5.74	1.30	1.39
2	Z	714	TYR	CD2-CE2	-5.72	1.30	1.39
2	EC	714	TYR	CD2-CE2	-5.72	1.30	1.39
2	C	714	TYR	CD2-CE2	-5.70	1.30	1.39
2	w	714	TYR	CD2-CE2	-5.64	1.30	1.39
12	IF	28	THR	C-N	-5.60	1.21	1.34
12	GC	28	THR	C-N	-5.56	1.21	1.34
12	BG	28	THR	C-N	-5.55	1.21	1.34
12	W	28	THR	C-N	-5.54	1.21	1.34
12	DJ	28	THR	C-N	-5.54	1.21	1.34
12	t	28	THR	C-N	-5.54	1.21	1.34
3	b	81	VAL	C-N	-5.37	1.21	1.34
3	GH	81	VAL	C-N	-5.36	1.21	1.34
3	CB	81	VAL	C-N	-5.35	1.21	1.34
3	E	81	VAL	C-N	-5.34	1.21	1.34
3	y	81	VAL	C-N	-5.33	1.21	1.34
3	EE	81	VAL	C-N	-5.31	1.21	1.34

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	BF	186	ARG	NE-CZ-NH1	-11.68	114.46	120.30
11	s	186	ARG	NE-CZ-NH1	-11.58	114.51	120.30
11	GB	186	ARG	NE-CZ-NH1	-11.56	114.52	120.30
11	V	186	ARG	NE-CZ-NH1	-11.54	114.53	120.30
11	DI	186	ARG	NE-CZ-NH1	-11.50	114.55	120.30
11	IE	186	ARG	NE-CZ-NH1	-11.49	114.55	120.30
13	YB	75[A]	GLY	C-N-CD	-9.24	100.28	120.60
13	YB	75[B]	GLY	C-N-CD	-9.24	100.28	120.60
13	YB	75[C]	GLY	C-N-CD	-9.24	100.28	120.60
13	YB	75[D]	GLY	C-N-CD	-9.24	100.28	120.60
13	YB	75[E]	GLY	C-N-CD	-9.24	100.28	120.60
13	YB	75[F]	GLY	C-N-CD	-9.24	100.28	120.60
13	YA	75[A]	GLY	C-N-CD	-9.23	100.30	120.60
13	YA	75[B]	GLY	C-N-CD	-9.23	100.30	120.60
13	YA	75[C]	GLY	C-N-CD	-9.23	100.30	120.60
13	YA	75[D]	GLY	C-N-CD	-9.23	100.30	120.60
13	YA	75[E]	GLY	C-N-CD	-9.23	100.30	120.60
13	YA	75[F]	GLY	C-N-CD	-9.23	100.30	120.60
13	YC	75[A]	GLY	C-N-CD	-9.21	100.33	120.60
13	YC	75[B]	GLY	C-N-CD	-9.21	100.33	120.60
13	YC	75[C]	GLY	C-N-CD	-9.21	100.33	120.60
13	YC	75[D]	GLY	C-N-CD	-9.21	100.33	120.60
13	YC	75[E]	GLY	C-N-CD	-9.21	100.33	120.60
13	YC	75[F]	GLY	C-N-CD	-9.21	100.33	120.60
11	GB	186	ARG	NE-CZ-NH2	8.27	124.43	120.30
11	BF	186	ARG	NE-CZ-NH2	8.22	124.41	120.30
11	V	186	ARG	NE-CZ-NH2	8.18	124.39	120.30
11	IE	186	ARG	NE-CZ-NH2	8.13	124.37	120.30
11	DI	186	ARG	NE-CZ-NH2	8.11	124.36	120.30
11	s	186	ARG	NE-CZ-NH2	8.08	124.34	120.30
12	BG	231	ASP	CB-CG-OD1	6.48	124.13	118.30
12	W	231	ASP	CB-CG-OD1	6.42	124.08	118.30
12	GC	231	ASP	CB-CG-OD1	6.42	124.08	118.30
5	CG	285	LEU	CB-CG-CD1	-6.42	100.09	111.00
12	IF	231	ASP	CB-CG-OD1	6.41	124.07	118.30
12	t	231	ASP	CB-CG-OD1	6.41	124.07	118.30
12	DJ	231	ASP	CB-CG-OD1	6.41	124.07	118.30
5	g	285	LEU	CB-CG-CD1	-6.40	100.12	111.00
5	EJ	285	LEU	CB-CG-CD1	-6.39	100.14	111.00
5	h	326	MET	CG-SD-CE	-6.37	90.00	100.20
5	K	326	MET	CG-SD-CE	-6.37	90.01	100.20
5	AD	285	LEU	CB-CG-CD1	-6.37	100.17	111.00
5	HC	285	LEU	CB-CG-CD1	-6.37	100.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	285	LEU	CB-CG-CD1	-6.37	100.17	111.00
5	AE	326	MET	CG-SD-CE	-6.36	90.02	100.20
5	FA	326	MET	CG-SD-CE	-6.35	90.04	100.20
5	HD	326	MET	CG-SD-CE	-6.35	90.04	100.20
5	CH	326	MET	CG-SD-CE	-6.35	90.05	100.20
10	GA	286	VAL	CB-CA-C	6.11	123.00	111.40
10	BE	286	VAL	CB-CA-C	6.10	122.99	111.40
5	EJ	326	MET	CG-SD-CE	-6.10	90.44	100.20
10	r	286	VAL	CB-CA-C	6.10	122.98	111.40
10	U	286	VAL	CB-CA-C	6.09	122.98	111.40
5	HC	326	MET	CG-SD-CE	-6.09	90.45	100.20
5	AD	326	MET	CG-SD-CE	-6.09	90.46	100.20
5	CG	326	MET	CG-SD-CE	-6.09	90.46	100.20
5	J	326	MET	CG-SD-CE	-6.08	90.47	100.20
5	g	326	MET	CG-SD-CE	-6.08	90.47	100.20
10	DH	286	VAL	CB-CA-C	6.08	122.94	111.40
10	ID	286	VAL	CB-CA-C	6.06	122.92	111.40
5	J	301	GLY	N-CA-C	-6.04	98.01	113.10
5	AD	301	GLY	N-CA-C	-6.04	98.00	113.10
13	YA	34[A]	LEU	CA-CB-CG	6.04	129.19	115.30
13	YA	34[B]	LEU	CA-CB-CG	6.04	129.19	115.30
13	YA	34[C]	LEU	CA-CB-CG	6.04	129.19	115.30
13	YA	34[D]	LEU	CA-CB-CG	6.04	129.19	115.30
13	YA	34[E]	LEU	CA-CB-CG	6.04	129.19	115.30
13	YA	34[F]	LEU	CA-CB-CG	6.04	129.19	115.30
5	g	301	GLY	N-CA-C	-6.04	98.01	113.10
5	HC	301	GLY	N-CA-C	-6.03	98.03	113.10
5	EJ	301	GLY	N-CA-C	-6.02	98.04	113.10
5	CG	301	GLY	N-CA-C	-6.02	98.04	113.10
13	YB	34[A]	LEU	CA-CB-CG	6.02	129.14	115.30
13	YB	34[B]	LEU	CA-CB-CG	6.02	129.14	115.30
13	YB	34[C]	LEU	CA-CB-CG	6.02	129.14	115.30
13	YB	34[D]	LEU	CA-CB-CG	6.02	129.14	115.30
13	YB	34[E]	LEU	CA-CB-CG	6.02	129.14	115.30
13	YB	34[F]	LEU	CA-CB-CG	6.02	129.14	115.30
13	YC	34[A]	LEU	CA-CB-CG	6.01	129.12	115.30
13	YC	34[B]	LEU	CA-CB-CG	6.01	129.12	115.30
13	YC	34[C]	LEU	CA-CB-CG	6.01	129.12	115.30
13	YC	34[D]	LEU	CA-CB-CG	6.01	129.12	115.30
13	YC	34[E]	LEU	CA-CB-CG	6.01	129.12	115.30
13	YC	34[F]	LEU	CA-CB-CG	6.01	129.12	115.30
10	U	287	VAL	CG1-CB-CG2	-5.99	101.32	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	ID	287	VAL	CG1-CB-CG2	-5.98	101.34	110.90
10	r	287	VAL	CG1-CB-CG2	-5.97	101.35	110.90
10	BE	287	VAL	CG1-CB-CG2	-5.97	101.35	110.90
10	GA	287	VAL	CG1-CB-CG2	-5.97	101.35	110.90
10	DH	287	VAL	CG1-CB-CG2	-5.96	101.36	110.90
1	GE	60	LEU	CA-CB-CG	-5.96	101.59	115.30
1	BI	60	LEU	CA-CB-CG	-5.94	101.63	115.30
1	v	60	LEU	CA-CB-CG	-5.94	101.64	115.30
1	EB	60	LEU	CA-CB-CG	-5.94	101.64	115.30
1	B	60	LEU	CA-CB-CG	-5.93	101.67	115.30
1	Y	60	LEU	CA-CB-CG	-5.92	101.69	115.30
2	EC	715	LEU	CA-CB-CG	5.76	128.54	115.30
2	BJ	715	LEU	CA-CB-CG	5.75	128.54	115.30
5	AC	326	MET	CG-SD-CE	-5.75	91.00	100.20
2	w	715	LEU	CA-CB-CG	5.75	128.51	115.30
2	C	715	LEU	CA-CB-CG	5.74	128.50	115.30
5	EI	326	MET	CG-SD-CE	-5.74	91.02	100.20
2	Z	715	LEU	CA-CB-CG	5.73	128.49	115.30
2	GF	715	LEU	CA-CB-CG	5.73	128.47	115.30
5	f	326	MET	CG-SD-CE	-5.72	91.04	100.20
5	HB	326	MET	CG-SD-CE	-5.72	91.04	100.20
5	CF	326	MET	CG-SD-CE	-5.72	91.05	100.20
2	w	965	LEU	CA-CB-CG	5.72	128.46	115.30
5	I	326	MET	CG-SD-CE	-5.72	91.05	100.20
5	AD	365	ILE	C-N-CD	5.71	140.40	128.40
5	EJ	365	ILE	C-N-CD	5.71	140.40	128.40
5	g	365	ILE	C-N-CD	5.70	140.38	128.40
5	HC	365	ILE	C-N-CD	5.70	140.37	128.40
5	J	365	ILE	C-N-CD	5.70	140.37	128.40
5	CG	365	ILE	C-N-CD	5.70	140.37	128.40
2	C	965	LEU	CA-CB-CG	5.70	128.41	115.30
2	EC	965	LEU	CA-CB-CG	5.69	128.39	115.30
2	Z	965	LEU	CA-CB-CG	5.69	128.38	115.30
2	GF	965	LEU	CA-CB-CG	5.69	128.38	115.30
2	BJ	965	LEU	CA-CB-CG	5.68	128.37	115.30
5	HD	337	ASP	CB-CG-OD1	5.48	123.23	118.30
12	t	191	LEU	CA-CB-CG	-5.46	102.75	115.30
5	K	337	ASP	CB-CG-OD1	5.45	123.21	118.30
12	IF	191	LEU	CA-CB-CG	-5.45	102.76	115.30
5	h	337	ASP	CB-CG-OD1	5.45	123.21	118.30
12	W	191	LEU	CA-CB-CG	-5.44	102.79	115.30
5	I	406	LEU	CA-CB-CG	-5.43	102.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	GC	191	LEU	CA-CB-CG	-5.43	102.80	115.30
12	DJ	191	LEU	CA-CB-CG	-5.43	102.81	115.30
14	YF	259[A]	LEU	CA-CB-CG	-5.43	102.81	115.30
14	YF	259[B]	LEU	CA-CB-CG	-5.43	102.81	115.30
14	YF	259[C]	LEU	CA-CB-CG	-5.43	102.81	115.30
14	YF	259[D]	LEU	CA-CB-CG	-5.43	102.81	115.30
14	YF	259[E]	LEU	CA-CB-CG	-5.43	102.81	115.30
14	YF	259[F]	LEU	CA-CB-CG	-5.43	102.81	115.30
5	EI	406	LEU	CA-CB-CG	-5.43	102.81	115.30
5	CF	406	LEU	CA-CB-CG	-5.43	102.82	115.30
5	CH	337	ASP	CB-CG-OD1	5.42	123.18	118.30
5	AC	406	LEU	CA-CB-CG	-5.42	102.83	115.30
14	YD	259[A]	LEU	CA-CB-CG	-5.42	102.84	115.30
14	YD	259[B]	LEU	CA-CB-CG	-5.42	102.84	115.30
14	YD	259[C]	LEU	CA-CB-CG	-5.42	102.84	115.30
14	YD	259[D]	LEU	CA-CB-CG	-5.42	102.84	115.30
14	YD	259[E]	LEU	CA-CB-CG	-5.42	102.84	115.30
14	YD	259[F]	LEU	CA-CB-CG	-5.42	102.84	115.30
14	YE	259[A]	LEU	CA-CB-CG	-5.42	102.83	115.30
14	YE	259[B]	LEU	CA-CB-CG	-5.42	102.83	115.30
14	YE	259[C]	LEU	CA-CB-CG	-5.42	102.83	115.30
14	YE	259[D]	LEU	CA-CB-CG	-5.42	102.83	115.30
14	YE	259[E]	LEU	CA-CB-CG	-5.42	102.83	115.30
14	YE	259[F]	LEU	CA-CB-CG	-5.42	102.83	115.30
5	HB	406	LEU	CA-CB-CG	-5.42	102.84	115.30
1	GD	527	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	527	ASP	CB-CG-OD1	5.41	123.17	118.30
12	BG	191	LEU	CA-CB-CG	-5.41	102.87	115.30
1	u	527	ASP	CB-CG-OD1	5.40	123.16	118.30
5	AE	337	ASP	CB-CG-OD1	5.40	123.16	118.30
1	BH	527	ASP	CB-CG-OD1	5.40	123.16	118.30
5	f	406	LEU	CA-CB-CG	-5.40	102.88	115.30
5	FA	337	ASP	CB-CG-OD1	5.39	123.16	118.30
1	X	527	ASP	CB-CG-OD1	5.38	123.15	118.30
1	EA	527	ASP	CB-CG-OD1	5.38	123.14	118.30
5	AD	62	ALA	N-CA-C	5.34	125.41	111.00
5	g	62	ALA	N-CA-C	5.33	125.40	111.00
5	EJ	62	ALA	N-CA-C	5.33	125.40	111.00
5	CG	62	ALA	N-CA-C	5.33	125.40	111.00
11	V	2	LEU	CB-CG-CD1	-5.33	101.94	111.00
12	DJ	163	ARG	NE-CZ-NH2	5.32	122.96	120.30
5	HC	62	ALA	N-CA-C	5.32	125.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	DI	2	LEU	CB-CG-CD1	-5.32	101.96	111.00
5	J	62	ALA	N-CA-C	5.31	125.35	111.00
11	BF	2	LEU	CB-CG-CD1	-5.31	101.97	111.00
11	IE	2	LEU	CB-CG-CD1	-5.31	101.98	111.00
11	s	2	LEU	CB-CG-CD1	-5.30	101.99	111.00
11	GB	2	LEU	CB-CG-CD1	-5.29	102.00	111.00
13	YB	75[A]	GLY	C-N-CA	5.27	144.15	122.00
13	YB	75[B]	GLY	C-N-CA	5.27	144.15	122.00
13	YB	75[C]	GLY	C-N-CA	5.27	144.15	122.00
13	YB	75[D]	GLY	C-N-CA	5.27	144.15	122.00
13	YB	75[E]	GLY	C-N-CA	5.27	144.15	122.00
13	YB	75[F]	GLY	C-N-CA	5.27	144.15	122.00
13	YA	75[A]	GLY	C-N-CA	5.27	144.14	122.00
13	YA	75[B]	GLY	C-N-CA	5.27	144.14	122.00
13	YA	75[C]	GLY	C-N-CA	5.27	144.14	122.00
13	YA	75[D]	GLY	C-N-CA	5.27	144.14	122.00
13	YA	75[E]	GLY	C-N-CA	5.27	144.14	122.00
13	YA	75[F]	GLY	C-N-CA	5.27	144.14	122.00
13	YC	75[A]	GLY	C-N-CA	5.26	144.11	122.00
13	YC	75[B]	GLY	C-N-CA	5.26	144.11	122.00
13	YC	75[C]	GLY	C-N-CA	5.26	144.11	122.00
13	YC	75[D]	GLY	C-N-CA	5.26	144.11	122.00
13	YC	75[E]	GLY	C-N-CA	5.26	144.11	122.00
13	YC	75[F]	GLY	C-N-CA	5.26	144.11	122.00
12	IF	163	ARG	NE-CZ-NH2	5.25	122.93	120.30
12	t	163	ARG	NE-CZ-NH2	5.23	122.91	120.30
12	W	163	ARG	NE-CZ-NH2	5.17	122.89	120.30
12	BG	163	ARG	NE-CZ-NH2	5.15	122.88	120.30
13	YA	8[A]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YA	8[B]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YA	8[C]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YA	8[D]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YA	8[E]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YA	8[F]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YC	8[A]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YC	8[B]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YC	8[C]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YC	8[D]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YC	8[E]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YC	8[F]	LEU	CA-CB-CG	-5.15	103.46	115.30
13	YB	8[A]	LEU	CA-CB-CG	-5.14	103.47	115.30
13	YB	8[B]	LEU	CA-CB-CG	-5.14	103.47	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	YB	8[C]	LEU	CA-CB-CG	-5.14	103.47	115.30
13	YB	8[D]	LEU	CA-CB-CG	-5.14	103.47	115.30
13	YB	8[E]	LEU	CA-CB-CG	-5.14	103.47	115.30
13	YB	8[F]	LEU	CA-CB-CG	-5.14	103.47	115.30
12	GC	163	ARG	NE-CZ-NH2	5.11	122.86	120.30
5	AE	556	GLN	N-CA-CB	5.07	119.72	110.60
5	HD	556	GLN	N-CA-CB	5.07	119.72	110.60
5	CH	556	GLN	N-CA-CB	5.06	119.72	110.60
5	K	556	GLN	N-CA-CB	5.06	119.70	110.60
5	h	556	GLN	N-CA-CB	5.05	119.69	110.60
5	FA	556	GLN	N-CA-CB	5.04	119.66	110.60
12	DJ	163	ARG	NE-CZ-NH1	-5.03	117.78	120.30
5	h	62	ALA	N-CA-C	5.02	124.55	111.00
5	K	62	ALA	N-CA-C	5.01	124.53	111.00
5	HD	62	ALA	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (783) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ALA	Peptide
5	AC	100	ALA	Peptide
5	AC	102	TRP	Peptide
5	AC	127	ASN	Peptide
5	AC	155	THR	Peptide
5	AC	196	ARG	Peptide
5	AC	267	ASP	Peptide
5	AC	276	LEU	Peptide
5	AC	278	GLY	Peptide
5	AC	293	PHE	Peptide
5	AC	333	GLY	Peptide
5	AC	364	GLY	Peptide
5	AC	365	ILE	Peptide
5	AC	366	PRO	Peptide
5	AC	555	CYS	Peptide
5	AC	61	THR	Peptide
5	AC	84	GLY	Peptide
5	AC	9	ASN	Peptide
5	AD	100	ALA	Peptide
5	AD	102	TRP	Peptide
5	AD	150	GLN	Peptide
5	AD	152	ASP	Peptide

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Mol	Chain	Res	Type	Group
5	AD	196	ARG	Peptide
5	AD	215	PRO	Peptide
5	AD	278	GLY	Peptide
5	AD	293	PHE	Peptide
5	AD	300	PRO	Peptide
5	AD	302	GLU	Peptide
5	AD	333	GLY	Peptide
5	AD	61	THR	Peptide
5	AD	84	GLY	Peptide
5	AE	100	ALA	Peptide
5	AE	102	TRP	Peptide
5	AE	127	ASN	Peptide
5	AE	151	ILE	Peptide
5	AE	156	SER	Peptide
5	AE	196	ARG	Peptide
5	AE	215	PRO	Peptide
5	AE	256	SER	Peptide
5	AE	276	LEU	Peptide
5	AE	293	PHE	Peptide
5	AE	320	LEU	Peptide
5	AE	333	GLY	Peptide
5	AE	361	ASP	Peptide
5	AE	391	GLY	Peptide
5	AE	61	THR	Peptide
5	AE	84	GLY	Peptide
6	AF	11	ILE	Peptide
6	AF	8	ALA	Peptide
6	AF	9	GLY	Peptide
6	AG	11	ILE	Peptide
6	AG	8	ALA	Peptide
6	AG	9	GLY	Peptide
6	AH	11	ILE	Peptide
6	AH	8	ALA	Peptide
6	AH	9	GLY	Peptide
7	AI	28	GLU	Peptide
7	AI	44	VAL	Peptide
7	AI	46	GLY	Peptide
7	AI	47	VAL	Peptide
7	AJ	152	ALA	Peptide
7	AJ	178	PRO	Peptide
7	AJ	28	GLU	Peptide
7	AJ	46	GLY	Peptide

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Mol	Chain	Res	Type	Group
7	AJ	47	VAL	Peptide
7	AJ	87	TYR	Peptide
1	B	136	LYS	Peptide
1	B	137	ASP	Peptide
1	B	18	PRO	Peptide
1	B	182	LEU	Peptide
1	B	20	ILE	Peptide
1	B	218	GLY	Peptide
1	B	256	TYR	Peptide
1	B	533	ASP	Peptide
7	BA	152	ALA	Peptide
7	BA	28	GLU	Peptide
7	BA	47	VAL	Peptide
7	BA	57	ILE	Peptide
7	BA	86	SER	Peptide
10	BE	340	SER	Peptide
11	BF	2	LEU	Peptide
1	BH	313	ALA	Peptide
1	BI	136	LYS	Peptide
1	BI	137	ASP	Peptide
1	BI	18	PRO	Peptide
1	BI	182	LEU	Peptide
1	BI	20	ILE	Peptide
1	BI	218	GLY	Peptide
1	BI	256	TYR	Peptide
1	BI	533	ASP	Peptide
2	BJ	105	THR	Peptide
2	BJ	134	TYR	Peptide
2	BJ	136	ASN	Peptide
2	BJ	156	SER	Peptide
2	BJ	167	ILE	Peptide
2	BJ	215	LYS	Peptide
2	BJ	227	ASP	Peptide
2	BJ	235	LYS	Peptide
2	BJ	298	ALA	Peptide
2	BJ	332	SER	Peptide
2	BJ	339	ASP	Peptide
2	BJ	342	SER	Peptide
2	BJ	343	PRO	Peptide
2	BJ	348	ARG	Peptide
2	BJ	353	ASP	Peptide
2	BJ	398	SER	Peptide

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Mol	Chain	Res	Type	Group
2	BJ	409	ASP	Peptide
2	BJ	436	THR	Peptide
2	BJ	456	VAL	Peptide
2	BJ	508	TYR	Peptide
2	BJ	554	ASP	Peptide
2	BJ	600	PHE	Peptide
2	BJ	623	LEU	Peptide
2	BJ	624	GLN	Peptide
2	BJ	625	ASN	Peptide
2	BJ	706	SER	Peptide
2	BJ	824	GLN	Peptide
2	BJ	850	ASN	Peptide
2	BJ	920	LYS	Peptide
2	BJ	925	LEU	Peptide
2	BJ	929	TYR	Peptide
2	BJ	940	GLY	Peptide
2	BJ	965	LEU	Peptide
2	BJ	967	ASP	Peptide
2	BJ	984	SER	Peptide
2	BJ	988	LYS	Peptide
2	BJ	989	LEU	Peptide
2	BJ	991	SER	Peptide
2	C	105	THR	Peptide
2	C	134	TYR	Peptide
2	C	136	ASN	Peptide
2	C	156	SER	Peptide
2	C	167	ILE	Peptide
2	C	215	LYS	Peptide
2	C	227	ASP	Peptide
2	C	235	LYS	Peptide
2	C	298	ALA	Peptide
2	C	332	SER	Peptide
2	C	339	ASP	Peptide
2	C	342	SER	Peptide
2	C	343	PRO	Peptide
2	C	348	ARG	Peptide
2	C	353	ASP	Peptide
2	C	398	SER	Peptide
2	C	409	ASP	Peptide
2	C	436	THR	Peptide
2	C	456	VAL	Peptide
2	C	508	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	C	554	ASP	Peptide
2	C	600	PHE	Peptide
2	C	623	LEU	Peptide
2	C	624	GLN	Peptide
2	C	625	ASN	Peptide
2	C	706	SER	Peptide
2	C	824	GLN	Peptide
2	C	850	ASN	Peptide
2	C	920	LYS	Peptide
2	C	925	LEU	Peptide
2	C	929	TYR	Peptide
2	C	940	GLY	Peptide
2	C	965	LEU	Peptide
2	C	967	ASP	Peptide
2	C	984	SER	Peptide
2	C	988	LYS	Peptide
2	C	989	LEU	Peptide
2	C	991	SER	Peptide
3	CA	102	ASP	Peptide
3	CA	262	ALA	Peptide
3	CB	177	GLU	Peptide
3	CB	228	ASN	Peptide
3	CB	32	PRO	Peptide
5	CF	100	ALA	Peptide
5	CF	102	TRP	Peptide
5	CF	127	ASN	Peptide
5	CF	155	THR	Peptide
5	CF	196	ARG	Peptide
5	CF	267	ASP	Peptide
5	CF	276	LEU	Peptide
5	CF	278	GLY	Peptide
5	CF	293	PHE	Peptide
5	CF	333	GLY	Peptide
5	CF	364	GLY	Peptide
5	CF	365	ILE	Peptide
5	CF	366	PRO	Peptide
5	CF	555	CYS	Peptide
5	CF	61	THR	Peptide
5	CF	84	GLY	Peptide
5	CF	9	ASN	Peptide
5	CG	100	ALA	Peptide
5	CG	102	TRP	Peptide

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Mol	Chain	Res	Type	Group
5	CG	150	GLN	Peptide
5	CG	152	ASP	Peptide
5	CG	196	ARG	Peptide
5	CG	215	PRO	Peptide
5	CG	278	GLY	Peptide
5	CG	293	PHE	Peptide
5	CG	300	PRO	Peptide
5	CG	302	GLU	Peptide
5	CG	333	GLY	Peptide
5	CG	61	THR	Peptide
5	CG	84	GLY	Peptide
5	CH	100	ALA	Peptide
5	CH	102	TRP	Peptide
5	CH	127	ASN	Peptide
5	CH	151	ILE	Peptide
5	CH	156	SER	Peptide
5	CH	196	ARG	Peptide
5	CH	215	PRO	Peptide
5	CH	256	SER	Peptide
5	CH	276	LEU	Peptide
5	CH	293	PHE	Peptide
5	CH	320	LEU	Peptide
5	CH	333	GLY	Peptide
5	CH	361	ASP	Peptide
5	CH	391	GLY	Peptide
5	CH	61	THR	Peptide
5	CH	84	GLY	Peptide
6	CI	11	ILE	Peptide
6	CI	8	ALA	Peptide
6	CI	9	GLY	Peptide
6	CJ	11	ILE	Peptide
6	CJ	8	ALA	Peptide
6	CJ	9	GLY	Peptide
3	D	102	ASP	Peptide
3	D	262	ALA	Peptide
6	DA	11	ILE	Peptide
6	DA	8	ALA	Peptide
6	DA	9	GLY	Peptide
7	DB	28	GLU	Peptide
7	DB	44	VAL	Peptide
7	DB	46	GLY	Peptide
7	DB	47	VAL	Peptide

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Mol	Chain	Res	Type	Group
7	DC	152	ALA	Peptide
7	DC	178	PRO	Peptide
7	DC	28	GLU	Peptide
7	DC	46	GLY	Peptide
7	DC	47	VAL	Peptide
7	DC	87	TYR	Peptide
7	DD	152	ALA	Peptide
7	DD	28	GLU	Peptide
7	DD	47	VAL	Peptide
7	DD	57	ILE	Peptide
7	DD	86	SER	Peptide
10	DH	340	SER	Peptide
11	DI	2	LEU	Peptide
3	E	177	GLU	Peptide
3	E	228	ASN	Peptide
3	E	32	PRO	Peptide
1	EA	313	ALA	Peptide
1	EB	136	LYS	Peptide
1	EB	137	ASP	Peptide
1	EB	18	PRO	Peptide
1	EB	182	LEU	Peptide
1	EB	20	ILE	Peptide
1	EB	218	GLY	Peptide
1	EB	256	TYR	Peptide
1	EB	533	ASP	Peptide
2	EC	105	THR	Peptide
2	EC	134	TYR	Peptide
2	EC	136	ASN	Peptide
2	EC	156	SER	Peptide
2	EC	167	ILE	Peptide
2	EC	215	LYS	Peptide
2	EC	227	ASP	Peptide
2	EC	235	LYS	Peptide
2	EC	298	ALA	Peptide
2	EC	332	SER	Peptide
2	EC	339	ASP	Peptide
2	EC	342	SER	Peptide
2	EC	343	PRO	Peptide
2	EC	348	ARG	Peptide
2	EC	353	ASP	Peptide
2	EC	398	SER	Peptide
2	EC	409	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	EC	436	THR	Peptide
2	EC	456	VAL	Peptide
2	EC	508	TYR	Peptide
2	EC	554	ASP	Peptide
2	EC	600	PHE	Peptide
2	EC	623	LEU	Peptide
2	EC	624	GLN	Peptide
2	EC	625	ASN	Peptide
2	EC	706	SER	Peptide
2	EC	824	GLN	Peptide
2	EC	850	ASN	Peptide
2	EC	920	LYS	Peptide
2	EC	925	LEU	Peptide
2	EC	929	TYR	Peptide
2	EC	940	GLY	Peptide
2	EC	965	LEU	Peptide
2	EC	967	ASP	Peptide
2	EC	984	SER	Peptide
2	EC	988	LYS	Peptide
2	EC	989	LEU	Peptide
2	EC	991	SER	Peptide
3	ED	102	ASP	Peptide
3	ED	262	ALA	Peptide
3	EE	177	GLU	Peptide
3	EE	228	ASN	Peptide
3	EE	32	PRO	Peptide
5	EI	100	ALA	Peptide
5	EI	102	TRP	Peptide
5	EI	127	ASN	Peptide
5	EI	155	THR	Peptide
5	EI	196	ARG	Peptide
5	EI	267	ASP	Peptide
5	EI	276	LEU	Peptide
5	EI	278	GLY	Peptide
5	EI	293	PHE	Peptide
5	EI	333	GLY	Peptide
5	EI	364	GLY	Peptide
5	EI	365	ILE	Peptide
5	EI	366	PRO	Peptide
5	EI	555	CYS	Peptide
5	EI	61	THR	Peptide
5	EI	84	GLY	Peptide

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Mol	Chain	Res	Type	Group
5	EI	9	ASN	Peptide
5	EJ	100	ALA	Peptide
5	EJ	102	TRP	Peptide
5	EJ	150	GLN	Peptide
5	EJ	152	ASP	Peptide
5	EJ	196	ARG	Peptide
5	EJ	215	PRO	Peptide
5	EJ	278	GLY	Peptide
5	EJ	293	PHE	Peptide
5	EJ	300	PRO	Peptide
5	EJ	302	GLU	Peptide
5	EJ	333	GLY	Peptide
5	EJ	61	THR	Peptide
5	EJ	84	GLY	Peptide
5	FA	100	ALA	Peptide
5	FA	102	TRP	Peptide
5	FA	127	ASN	Peptide
5	FA	151	ILE	Peptide
5	FA	156	SER	Peptide
5	FA	196	ARG	Peptide
5	FA	215	PRO	Peptide
5	FA	256	SER	Peptide
5	FA	276	LEU	Peptide
5	FA	293	PHE	Peptide
5	FA	320	LEU	Peptide
5	FA	333	GLY	Peptide
5	FA	361	ASP	Peptide
5	FA	391	GLY	Peptide
5	FA	61	THR	Peptide
5	FA	84	GLY	Peptide
6	FB	11	ILE	Peptide
6	FB	8	ALA	Peptide
6	FB	9	GLY	Peptide
6	FC	11	ILE	Peptide
6	FC	8	ALA	Peptide
6	FC	9	GLY	Peptide
6	FD	11	ILE	Peptide
6	FD	8	ALA	Peptide
6	FD	9	GLY	Peptide
7	FE	28	GLU	Peptide
7	FE	44	VAL	Peptide
7	FE	46	GLY	Peptide

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Mol	Chain	Res	Type	Group
7	FE	47	VAL	Peptide
7	FF	152	ALA	Peptide
7	FF	178	PRO	Peptide
7	FF	28	GLU	Peptide
7	FF	46	GLY	Peptide
7	FF	47	VAL	Peptide
7	FF	87	TYR	Peptide
7	FG	152	ALA	Peptide
7	FG	28	GLU	Peptide
7	FG	47	VAL	Peptide
7	FG	57	ILE	Peptide
7	FG	86	SER	Peptide
10	GA	340	SER	Peptide
11	GB	2	LEU	Peptide
1	GD	313	ALA	Peptide
1	GE	136	LYS	Peptide
1	GE	137	ASP	Peptide
1	GE	18	PRO	Peptide
1	GE	182	LEU	Peptide
1	GE	20	ILE	Peptide
1	GE	218	GLY	Peptide
1	GE	256	TYR	Peptide
1	GE	533	ASP	Peptide
2	GF	105	THR	Peptide
2	GF	134	TYR	Peptide
2	GF	136	ASN	Peptide
2	GF	156	SER	Peptide
2	GF	167	ILE	Peptide
2	GF	215	LYS	Peptide
2	GF	227	ASP	Peptide
2	GF	235	LYS	Peptide
2	GF	298	ALA	Peptide
2	GF	332	SER	Peptide
2	GF	339	ASP	Peptide
2	GF	342	SER	Peptide
2	GF	343	PRO	Peptide
2	GF	348	ARG	Peptide
2	GF	353	ASP	Peptide
2	GF	398	SER	Peptide
2	GF	409	ASP	Peptide
2	GF	436	THR	Peptide
2	GF	456	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	GF	508	TYR	Peptide
2	GF	554	ASP	Peptide
2	GF	600	PHE	Peptide
2	GF	623	LEU	Peptide
2	GF	624	GLN	Peptide
2	GF	625	ASN	Peptide
2	GF	706	SER	Peptide
2	GF	824	GLN	Peptide
2	GF	850	ASN	Peptide
2	GF	920	LYS	Peptide
2	GF	925	LEU	Peptide
2	GF	929	TYR	Peptide
2	GF	940	GLY	Peptide
2	GF	965	LEU	Peptide
2	GF	967	ASP	Peptide
2	GF	984	SER	Peptide
2	GF	988	LYS	Peptide
2	GF	989	LEU	Peptide
2	GF	991	SER	Peptide
3	GG	102	ASP	Peptide
3	GG	262	ALA	Peptide
3	GH	177	GLU	Peptide
3	GH	228	ASN	Peptide
3	GH	32	PRO	Peptide
5	HB	100	ALA	Peptide
5	HB	102	TRP	Peptide
5	HB	127	ASN	Peptide
5	HB	155	THR	Peptide
5	HB	196	ARG	Peptide
5	HB	267	ASP	Peptide
5	HB	276	LEU	Peptide
5	HB	278	GLY	Peptide
5	HB	293	PHE	Peptide
5	HB	333	GLY	Peptide
5	HB	364	GLY	Peptide
5	HB	365	ILE	Peptide
5	HB	366	PRO	Peptide
5	HB	555	CYS	Peptide
5	HB	61	THR	Peptide
5	HB	84	GLY	Peptide
5	HB	9	ASN	Peptide
5	HC	100	ALA	Peptide

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Mol	Chain	Res	Type	Group
5	HC	102	TRP	Peptide
5	HC	150	GLN	Peptide
5	HC	152	ASP	Peptide
5	HC	196	ARG	Peptide
5	HC	215	PRO	Peptide
5	HC	278	GLY	Peptide
5	HC	293	PHE	Peptide
5	HC	300	PRO	Peptide
5	HC	302	GLU	Peptide
5	HC	333	GLY	Peptide
5	HC	61	THR	Peptide
5	HC	84	GLY	Peptide
5	HD	100	ALA	Peptide
5	HD	102	TRP	Peptide
5	HD	127	ASN	Peptide
5	HD	151	ILE	Peptide
5	HD	156	SER	Peptide
5	HD	196	ARG	Peptide
5	HD	215	PRO	Peptide
5	HD	256	SER	Peptide
5	HD	276	LEU	Peptide
5	HD	293	PHE	Peptide
5	HD	320	LEU	Peptide
5	HD	333	GLY	Peptide
5	HD	361	ASP	Peptide
5	HD	391	GLY	Peptide
5	HD	61	THR	Peptide
5	HD	84	GLY	Peptide
6	HE	11	ILE	Peptide
6	HE	8	ALA	Peptide
6	HE	9	GLY	Peptide
6	HF	11	ILE	Peptide
6	HF	8	ALA	Peptide
6	HF	9	GLY	Peptide
6	HG	11	ILE	Peptide
6	HG	8	ALA	Peptide
6	HG	9	GLY	Peptide
7	HH	28	GLU	Peptide
7	HH	44	VAL	Peptide
7	HH	46	GLY	Peptide
7	HH	47	VAL	Peptide
7	HI	152	ALA	Peptide

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Mol	Chain	Res	Type	Group
7	HI	178	PRO	Peptide
7	HI	28	GLU	Peptide
7	HI	46	GLY	Peptide
7	HI	47	VAL	Peptide
7	HI	87	TYR	Peptide
7	HJ	152	ALA	Peptide
7	HJ	28	GLU	Peptide
7	HJ	47	VAL	Peptide
7	HJ	57	ILE	Peptide
7	HJ	86	SER	Peptide
5	I	100	ALA	Peptide
5	I	102	TRP	Peptide
5	I	127	ASN	Peptide
5	I	155	THR	Peptide
5	I	196	ARG	Peptide
5	I	267	ASP	Peptide
5	I	276	LEU	Peptide
5	I	278	GLY	Peptide
5	I	293	PHE	Peptide
5	I	333	GLY	Peptide
5	I	364	GLY	Peptide
5	I	365	ILE	Peptide
5	I	366	PRO	Peptide
5	I	555	CYS	Peptide
5	I	61	THR	Peptide
5	I	84	GLY	Peptide
5	I	9	ASN	Peptide
10	ID	340	SER	Peptide
11	IE	2	LEU	Peptide
5	J	100	ALA	Peptide
5	J	102	TRP	Peptide
5	J	150	GLN	Peptide
5	J	152	ASP	Peptide
5	J	196	ARG	Peptide
5	J	215	PRO	Peptide
5	J	278	GLY	Peptide
5	J	293	PHE	Peptide
5	J	300	PRO	Peptide
5	J	302	GLU	Peptide
5	J	333	GLY	Peptide
5	J	61	THR	Peptide
5	J	84	GLY	Peptide

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Mol	Chain	Res	Type	Group
5	K	100	ALA	Peptide
5	K	102	TRP	Peptide
5	K	127	ASN	Peptide
5	K	151	ILE	Peptide
5	K	156	SER	Peptide
5	K	196	ARG	Peptide
5	K	215	PRO	Peptide
5	K	256	SER	Peptide
5	K	276	LEU	Peptide
5	K	293	PHE	Peptide
5	K	320	LEU	Peptide
5	K	333	GLY	Peptide
5	K	361	ASP	Peptide
5	K	391	GLY	Peptide
5	K	61	THR	Peptide
5	K	84	GLY	Peptide
6	L	11	ILE	Peptide
6	L	8	ALA	Peptide
6	L	9	GLY	Peptide
6	M	11	ILE	Peptide
6	M	8	ALA	Peptide
6	M	9	GLY	Peptide
6	N	11	ILE	Peptide
6	N	8	ALA	Peptide
6	N	9	GLY	Peptide
7	O	28	GLU	Peptide
7	O	44	VAL	Peptide
7	O	46	GLY	Peptide
7	O	47	VAL	Peptide
7	P	152	ALA	Peptide
7	P	178	PRO	Peptide
7	P	28	GLU	Peptide
7	P	46	GLY	Peptide
7	P	47	VAL	Peptide
7	P	87	TYR	Peptide
7	Q	152	ALA	Peptide
7	Q	28	GLU	Peptide
7	Q	47	VAL	Peptide
7	Q	57	ILE	Peptide
7	Q	86	SER	Peptide
10	U	340	SER	Peptide
11	V	2	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	X	313	ALA	Peptide
1	Y	136	LYS	Peptide
1	Y	137	ASP	Peptide
1	Y	18	PRO	Peptide
1	Y	182	LEU	Peptide
1	Y	20	ILE	Peptide
1	Y	218	GLY	Peptide
1	Y	256	TYR	Peptide
1	Y	533	ASP	Peptide
13	YA	74[A]	THR	Peptide
13	YA	74[B]	THR	Peptide
13	YA	74[C]	THR	Peptide
13	YA	74[D]	THR	Peptide
13	YA	74[E]	THR	Peptide
13	YA	74[F]	THR	Peptide
13	YA	75[B]	GLY	Peptide
13	YB	74[A]	THR	Peptide
13	YB	74[B]	THR	Peptide
13	YB	74[C]	THR	Peptide
13	YB	74[D]	THR	Peptide
13	YB	74[E]	THR	Peptide
13	YB	74[F]	THR	Peptide
13	YB	75[B]	GLY	Peptide
13	YC	74[A]	THR	Peptide
13	YC	74[B]	THR	Peptide
13	YC	74[C]	THR	Peptide
13	YC	74[D]	THR	Peptide
13	YC	74[E]	THR	Peptide
13	YC	74[F]	THR	Peptide
13	YC	75[B]	GLY	Peptide
14	YD	366[A]	THR	Peptide
14	YD	366[B]	THR	Peptide
14	YD	366[C]	THR	Peptide
14	YD	366[D]	THR	Peptide
14	YD	366[E]	THR	Peptide
14	YD	366[F]	THR	Peptide
14	YE	366[A]	THR	Peptide
14	YE	366[B]	THR	Peptide
14	YE	366[C]	THR	Peptide
14	YE	366[D]	THR	Peptide
14	YE	366[E]	THR	Peptide
14	YE	366[F]	THR	Peptide

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Mol	Chain	Res	Type	Group
14	YF	366[A]	THR	Peptide
14	YF	366[B]	THR	Peptide
14	YF	366[C]	THR	Peptide
14	YF	366[D]	THR	Peptide
14	YF	366[E]	THR	Peptide
14	YF	366[F]	THR	Peptide
2	Z	105	THR	Peptide
2	Z	134	TYR	Peptide
2	Z	136	ASN	Peptide
2	Z	156	SER	Peptide
2	Z	167	ILE	Peptide
2	Z	215	LYS	Peptide
2	Z	227	ASP	Peptide
2	Z	235	LYS	Peptide
2	Z	298	ALA	Peptide
2	Z	332	SER	Peptide
2	Z	339	ASP	Peptide
2	Z	342	SER	Peptide
2	Z	343	PRO	Peptide
2	Z	348	ARG	Peptide
2	Z	353	ASP	Peptide
2	Z	398	SER	Peptide
2	Z	409	ASP	Peptide
2	Z	436	THR	Peptide
2	Z	456	VAL	Peptide
2	Z	508	TYR	Peptide
2	Z	554	ASP	Peptide
2	Z	600	PHE	Peptide
2	Z	623	LEU	Peptide
2	Z	624	GLN	Peptide
2	Z	625	ASN	Peptide
2	Z	706	SER	Peptide
2	Z	824	GLN	Peptide
2	Z	850	ASN	Peptide
2	Z	920	LYS	Peptide
2	Z	925	LEU	Peptide
2	Z	929	TYR	Peptide
2	Z	940	GLY	Peptide
2	Z	965	LEU	Peptide
2	Z	967	ASP	Peptide
2	Z	984	SER	Peptide
2	Z	988	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	Z	989	LEU	Peptide
2	Z	991	SER	Peptide
3	a	102	ASP	Peptide
3	a	262	ALA	Peptide
3	b	177	GLU	Peptide
3	b	228	ASN	Peptide
3	b	32	PRO	Peptide
5	f	100	ALA	Peptide
5	f	102	TRP	Peptide
5	f	127	ASN	Peptide
5	f	155	THR	Peptide
5	f	196	ARG	Peptide
5	f	267	ASP	Peptide
5	f	276	LEU	Peptide
5	f	278	GLY	Peptide
5	f	293	PHE	Peptide
5	f	333	GLY	Peptide
5	f	364	GLY	Peptide
5	f	365	ILE	Peptide
5	f	366	PRO	Peptide
5	f	555	CYS	Peptide
5	f	61	THR	Peptide
5	f	84	GLY	Peptide
5	f	9	ASN	Peptide
5	g	100	ALA	Peptide
5	g	102	TRP	Peptide
5	g	150	GLN	Peptide
5	g	152	ASP	Peptide
5	g	196	ARG	Peptide
5	g	215	PRO	Peptide
5	g	278	GLY	Peptide
5	g	293	PHE	Peptide
5	g	300	PRO	Peptide
5	g	302	GLU	Peptide
5	g	333	GLY	Peptide
5	g	61	THR	Peptide
5	g	84	GLY	Peptide
5	h	100	ALA	Peptide
5	h	102	TRP	Peptide
5	h	127	ASN	Peptide
5	h	151	ILE	Peptide
5	h	156	SER	Peptide

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Mol	Chain	Res	Type	Group
5	h	196	ARG	Peptide
5	h	215	PRO	Peptide
5	h	256	SER	Peptide
5	h	276	LEU	Peptide
5	h	293	PHE	Peptide
5	h	320	LEU	Peptide
5	h	333	GLY	Peptide
5	h	361	ASP	Peptide
5	h	391	GLY	Peptide
5	h	61	THR	Peptide
5	h	84	GLY	Peptide
6	i	11	ILE	Peptide
6	i	8	ALA	Peptide
6	i	9	GLY	Peptide
6	j	11	ILE	Peptide
6	j	8	ALA	Peptide
6	j	9	GLY	Peptide
6	k	11	ILE	Peptide
6	k	8	ALA	Peptide
6	k	9	GLY	Peptide
7	l	28	GLU	Peptide
7	l	44	VAL	Peptide
7	l	46	GLY	Peptide
7	l	47	VAL	Peptide
7	m	152	ALA	Peptide
7	m	178	PRO	Peptide
7	m	28	GLU	Peptide
7	m	46	GLY	Peptide
7	m	47	VAL	Peptide
7	m	87	TYR	Peptide
7	n	152	ALA	Peptide
7	n	28	GLU	Peptide
7	n	47	VAL	Peptide
7	n	57	ILE	Peptide
7	n	86	SER	Peptide
10	r	340	SER	Peptide
11	s	2	LEU	Peptide
1	u	313	ALA	Peptide
1	v	136	LYS	Peptide
1	v	137	ASP	Peptide
1	v	18	PRO	Peptide
1	v	182	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	v	20	ILE	Peptide
1	v	218	GLY	Peptide
1	v	256	TYR	Peptide
1	v	533	ASP	Peptide
2	w	105	THR	Peptide
2	w	134	TYR	Peptide
2	w	136	ASN	Peptide
2	w	156	SER	Peptide
2	w	167	ILE	Peptide
2	w	215	LYS	Peptide
2	w	227	ASP	Peptide
2	w	235	LYS	Peptide
2	w	298	ALA	Peptide
2	w	332	SER	Peptide
2	w	339	ASP	Peptide
2	w	342	SER	Peptide
2	w	343	PRO	Peptide
2	w	348	ARG	Peptide
2	w	353	ASP	Peptide
2	w	398	SER	Peptide
2	w	409	ASP	Peptide
2	w	436	THR	Peptide
2	w	456	VAL	Peptide
2	w	508	TYR	Peptide
2	w	554	ASP	Peptide
2	w	600	PHE	Peptide
2	w	623	LEU	Peptide
2	w	624	GLN	Peptide
2	w	625	ASN	Peptide
2	w	706	SER	Peptide
2	w	824	GLN	Peptide
2	w	850	ASN	Peptide
2	w	920	LYS	Peptide
2	w	925	LEU	Peptide
2	w	929	TYR	Peptide
2	w	940	GLY	Peptide
2	w	965	LEU	Peptide
2	w	967	ASP	Peptide
2	w	984	SER	Peptide
2	w	988	LYS	Peptide
2	w	989	LEU	Peptide
2	w	991	SER	Peptide

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Mol	Chain	Res	Type	Group
3	x	102	ASP	Peptide
3	x	262	ALA	Peptide
3	y	177	GLU	Peptide
3	y	228	ASN	Peptide
3	y	32	PRO	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	A	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	29	67
1	B	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	19	58
1	BH	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	29	67
1	BI	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	19	58
1	EA	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	29	67
1	EB	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	19	58
1	GD	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	29	67
1	GE	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	19	58
1	X	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	29	67
1	Y	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	19	58
1	u	656/660 (99%)	616 (94%)	37 (6%)	3 (0%)	29	67
1	v	646/660 (98%)	602 (93%)	39 (6%)	5 (1%)	19	58
2	BJ	1000/1032 (97%)	836 (84%)	144 (14%)	20 (2%)	7	39
2	C	1000/1032 (97%)	836 (84%)	145 (14%)	19 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	EC	1000/1032 (97%)	836 (84%)	145 (14%)	19 (2%)	8	40
2	GF	1000/1032 (97%)	836 (84%)	144 (14%)	20 (2%)	7	39
2	Z	1000/1032 (97%)	837 (84%)	144 (14%)	19 (2%)	8	40
2	w	1000/1032 (97%)	837 (84%)	143 (14%)	20 (2%)	7	39
3	CA	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	25	64
3	CB	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	D	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	25	64
3	E	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	ED	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	25	64
3	EE	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	GG	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	25	64
3	GH	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	a	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	25	64
3	b	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
3	x	326/334 (98%)	312 (96%)	12 (4%)	2 (1%)	25	64
3	y	330/334 (99%)	310 (94%)	20 (6%)	0	100	100
4	AA	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	AB	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	CC	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	CD	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	CE	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	EF	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	EG	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	EH	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	F	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	G	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	GI	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	GJ	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	H	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	HA	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	c	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	e	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
4	z	286/288 (99%)	271 (95%)	11 (4%)	4 (1%)	11	46
5	AC	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	12	47
5	AD	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	8	41
5	AE	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	6	37
5	CF	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	12	47
5	CG	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	8	41
5	CH	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	6	37
5	EI	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	12	47
5	EJ	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	8	41
5	FA	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	6	37
5	HB	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	12	47
5	HC	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	8	41
5	HD	600/602 (100%)	530 (88%)	58 (10%)	12 (2%)	7	39
5	I	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	12	47
5	J	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	8	41
5	K	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	6	37
5	f	600/602 (100%)	549 (92%)	43 (7%)	8 (1%)	12	47
5	g	600/602 (100%)	538 (90%)	51 (8%)	11 (2%)	8	41
5	h	600/602 (100%)	530 (88%)	57 (10%)	13 (2%)	6	37
6	AF	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	AG	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	AH	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	CI	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	CJ	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	DA	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	FB	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	FC	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	FD	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	HE	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	HF	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	HG	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	L	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	M	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	N	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	i	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	j	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
6	k	216/219 (99%)	204 (94%)	10 (5%)	2 (1%)	17	55
7	AI	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	14	51
7	AJ	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	25	64
7	BA	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	12	47
7	DB	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	14	51
7	DC	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	25	64
7	DD	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	12	47
7	FE	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	14	51
7	FF	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	25	64
7	FG	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	12	47
7	HH	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	14	51
7	HI	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	25	64
7	HJ	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	12	47
7	O	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	14	51
7	P	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	25	64
7	Q	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	12	47
7	l	524/527 (99%)	495 (94%)	23 (4%)	6 (1%)	14	51
7	m	524/527 (99%)	493 (94%)	28 (5%)	3 (1%)	25	64
7	n	524/527 (99%)	496 (95%)	21 (4%)	7 (1%)	12	47
8	BB	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	BC	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	DE	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	DF	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	FH	160/163 (98%)	147 (92%)	13 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	FI	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	IA	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	IB	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	R	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	S	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	o	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
8	p	160/163 (98%)	147 (92%)	13 (8%)	0	100	100
9	BD	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	DG	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	FJ	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	IC	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	T	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
9	q	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
10	BE	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	25	64
10	DH	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	25	64
10	GA	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	25	64
10	ID	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	25	64
10	U	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	25	64
10	r	155/364 (43%)	145 (94%)	9 (6%)	1 (1%)	25	64
11	BF	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	DI	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	GB	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	IE	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	V	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
11	s	191/196 (97%)	175 (92%)	16 (8%)	0	100	100
12	BG	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	DJ	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	GC	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	IF	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	W	188/320 (59%)	178 (95%)	10 (5%)	0	100	100
12	t	188/320 (59%)	178 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	YA	3276/575 (570%)	3186 (97%)	90 (3%)	0	100	100
13	YB	3276/575 (570%)	3186 (97%)	90 (3%)	0	100	100
13	YC	3276/575 (570%)	3186 (97%)	90 (3%)	0	100	100
14	YD	2160/391 (552%)	2070 (96%)	84 (4%)	6 (0%)	41	76
14	YE	2160/391 (552%)	2070 (96%)	84 (4%)	6 (0%)	41	76
14	YF	2160/391 (552%)	2070 (96%)	84 (4%)	6 (0%)	41	76
15	ZA	564/97 (581%)	540 (96%)	24 (4%)	0	100	100
All	All	69756/58591 (119%)	64970 (93%)	4190 (6%)	596 (1%)	20	55

All (596) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	343	PRO
4	F	249	ILE
4	G	249	ILE
4	H	249	ILE
5	I	10	VAL
5	I	24	ILE
5	I	171	VAL
5	J	24	ILE
5	J	171	VAL
5	K	24	ILE
5	K	152	ASP
7	O	47	VAL
7	P	47	VAL
7	Q	47	VAL
10	U	286	VAL
2	Z	343	PRO
4	c	249	ILE
4	d	249	ILE
4	e	249	ILE
5	f	10	VAL
5	f	24	ILE
5	f	171	VAL
5	g	24	ILE
5	g	171	VAL
5	h	24	ILE
5	h	152	ASP
7	l	47	VAL
7	m	47	VAL

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Mol	Chain	Res	Type
7	n	47	VAL
10	r	286	VAL
2	w	343	PRO
4	z	249	ILE
4	AA	249	ILE
4	AB	249	ILE
5	AC	10	VAL
5	AC	24	ILE
5	AC	171	VAL
5	AD	24	ILE
5	AD	171	VAL
5	AE	24	ILE
5	AE	152	ASP
7	AI	47	VAL
7	AJ	47	VAL
7	BA	47	VAL
10	BE	286	VAL
2	BJ	343	PRO
4	CC	249	ILE
4	CD	249	ILE
4	CE	249	ILE
5	CF	10	VAL
5	CF	24	ILE
5	CF	171	VAL
5	CG	24	ILE
5	CG	171	VAL
5	CH	24	ILE
5	CH	152	ASP
7	DB	47	VAL
7	DC	47	VAL
7	DD	47	VAL
10	DH	286	VAL
2	EC	343	PRO
4	EF	249	ILE
4	EG	249	ILE
4	EH	249	ILE
5	EI	10	VAL
5	EI	24	ILE
5	EI	171	VAL
5	EJ	24	ILE
5	EJ	171	VAL
5	FA	24	ILE

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Mol	Chain	Res	Type
5	FA	152	ASP
7	FE	47	VAL
7	FF	47	VAL
7	FG	47	VAL
10	GA	286	VAL
2	GF	343	PRO
4	GI	249	ILE
4	GJ	249	ILE
4	HA	249	ILE
5	HB	10	VAL
5	HB	24	ILE
5	HB	171	VAL
5	HC	24	ILE
5	HC	171	VAL
5	HD	24	ILE
5	HD	152	ASP
7	HH	47	VAL
7	HI	47	VAL
7	HJ	47	VAL
10	ID	286	VAL
1	B	46	TYR
1	B	534	VAL
2	C	168	ILE
2	C	360	ASN
2	C	411	LYS
2	C	947	VAL
4	F	51	ALA
4	G	51	ALA
4	H	51	ALA
5	J	85	THR
5	J	151	ILE
5	J	154	ILE
5	K	85	THR
5	K	171	VAL
5	K	304	ILE
5	K	408	VAL
7	O	155	ASP
7	O	183	ALA
7	O	184	THR
7	Q	155	ASP
1	Y	46	TYR
1	Y	534	VAL

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Mol	Chain	Res	Type
2	Z	168	ILE
2	Z	360	ASN
2	Z	411	LYS
2	Z	947	VAL
4	c	51	ALA
4	d	51	ALA
4	e	51	ALA
5	g	85	THR
5	g	151	ILE
5	g	154	ILE
5	h	85	THR
5	h	171	VAL
5	h	304	ILE
5	h	408	VAL
7	l	155	ASP
7	l	183	ALA
7	l	184	THR
7	n	155	ASP
1	v	46	TYR
1	v	534	VAL
2	w	168	ILE
2	w	360	ASN
2	w	411	LYS
2	w	947	VAL
4	z	51	ALA
4	AA	51	ALA
4	AB	51	ALA
5	AD	85	THR
5	AD	151	ILE
5	AD	154	ILE
5	AE	85	THR
5	AE	171	VAL
5	AE	304	ILE
5	AE	408	VAL
7	AI	155	ASP
7	AI	183	ALA
7	AI	184	THR
7	BA	155	ASP
1	BI	46	TYR
1	BI	534	VAL
2	BJ	168	ILE
2	BJ	360	ASN

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Mol	Chain	Res	Type
2	BJ	411	LYS
2	BJ	947	VAL
4	CC	51	ALA
4	CD	51	ALA
4	CE	51	ALA
5	CG	85	THR
5	CG	151	ILE
5	CG	154	ILE
5	CH	85	THR
5	CH	171	VAL
5	CH	304	ILE
5	CH	408	VAL
7	DB	155	ASP
7	DB	183	ALA
7	DB	184	THR
7	DD	155	ASP
1	EB	46	TYR
1	EB	534	VAL
2	EC	168	ILE
2	EC	360	ASN
2	EC	411	LYS
2	EC	947	VAL
4	EF	51	ALA
4	EG	51	ALA
4	EH	51	ALA
5	EJ	85	THR
5	EJ	151	ILE
5	EJ	154	ILE
5	FA	85	THR
5	FA	171	VAL
5	FA	304	ILE
5	FA	408	VAL
7	FE	155	ASP
7	FE	183	ALA
7	FE	184	THR
7	FG	155	ASP
1	GE	46	TYR
1	GE	534	VAL
2	GF	168	ILE
2	GF	360	ASN
2	GF	411	LYS
2	GF	947	VAL

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Mol	Chain	Res	Type
4	GI	51	ALA
4	GJ	51	ALA
4	HA	51	ALA
5	HC	85	THR
5	HC	151	ILE
5	HC	154	ILE
5	HD	85	THR
5	HD	171	VAL
5	HD	304	ILE
5	HD	408	VAL
7	HH	155	ASP
7	HH	183	ALA
7	HH	184	THR
7	HJ	155	ASP
2	C	7	SER
2	C	28	VAL
2	C	307	ILE
2	C	412	THR
5	I	86	VAL
5	I	104	VAL
5	J	86	VAL
5	J	104	VAL
5	K	86	VAL
5	K	104	VAL
7	O	176	ILE
7	P	155	ASP
7	Q	167	GLN
2	Z	7	SER
2	Z	28	VAL
2	Z	307	ILE
2	Z	412	THR
5	f	86	VAL
5	f	104	VAL
5	g	86	VAL
5	g	104	VAL
5	h	86	VAL
5	h	104	VAL
7	l	176	ILE
7	m	155	ASP
7	n	167	GLN
2	w	7	SER
2	w	28	VAL

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Mol	Chain	Res	Type
2	w	307	ILE
2	w	412	THR
5	AC	86	VAL
5	AC	104	VAL
5	AD	86	VAL
5	AD	104	VAL
5	AE	86	VAL
5	AE	104	VAL
7	AI	176	ILE
7	AJ	155	ASP
7	BA	167	GLN
2	BJ	7	SER
2	BJ	28	VAL
2	BJ	307	ILE
2	BJ	412	THR
5	CF	86	VAL
5	CF	104	VAL
5	CG	86	VAL
5	CG	104	VAL
5	CH	86	VAL
5	CH	104	VAL
7	DB	176	ILE
7	DC	155	ASP
7	DD	167	GLN
2	EC	7	SER
2	EC	28	VAL
2	EC	307	ILE
2	EC	412	THR
5	EI	86	VAL
5	EI	104	VAL
5	EJ	86	VAL
5	EJ	104	VAL
5	FA	86	VAL
5	FA	104	VAL
7	FE	176	ILE
7	FF	155	ASP
7	FG	167	GLN
2	GF	7	SER
2	GF	28	VAL
2	GF	307	ILE
2	GF	412	THR
5	HB	86	VAL

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Mol	Chain	Res	Type
5	HB	104	VAL
5	HC	86	VAL
5	HC	104	VAL
5	HD	86	VAL
5	HD	104	VAL
7	HH	176	ILE
7	HI	155	ASP
7	HJ	167	GLN
14	YD	313[A]	ILE
14	YD	313[B]	ILE
14	YD	313[C]	ILE
14	YD	313[D]	ILE
14	YD	313[E]	ILE
14	YD	313[F]	ILE
14	YE	313[A]	ILE
14	YE	313[B]	ILE
14	YE	313[C]	ILE
14	YE	313[D]	ILE
14	YE	313[E]	ILE
14	YE	313[F]	ILE
14	YF	313[A]	ILE
14	YF	313[B]	ILE
14	YF	313[C]	ILE
14	YF	313[D]	ILE
14	YF	313[E]	ILE
14	YF	313[F]	ILE
2	C	707	GLU
2	C	959	ALA
2	C	977	ILE
3	D	103	PRO
4	F	15	ILE
4	G	15	ILE
4	H	15	ILE
5	I	85	THR
5	I	180	VAL
5	J	180	VAL
5	J	277	GLU
5	J	559	PRO
5	K	90	ASN
5	K	180	VAL
6	L	11	ILE
6	M	11	ILE

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Mol	Chain	Res	Type
6	N	11	ILE
2	Z	707	GLU
2	Z	959	ALA
2	Z	977	ILE
3	a	103	PRO
4	c	15	ILE
4	d	15	ILE
4	e	15	ILE
5	f	85	THR
5	f	180	VAL
5	g	180	VAL
5	g	277	GLU
5	g	559	PRO
5	h	90	ASN
5	h	180	VAL
6	i	11	ILE
6	j	11	ILE
6	k	11	ILE
2	w	707	GLU
2	w	959	ALA
2	w	977	ILE
3	x	103	PRO
4	z	15	ILE
4	AA	15	ILE
4	AB	15	ILE
5	AC	85	THR
5	AC	180	VAL
5	AD	180	VAL
5	AD	277	GLU
5	AD	559	PRO
5	AE	90	ASN
5	AE	180	VAL
6	AF	11	ILE
6	AG	11	ILE
6	AH	11	ILE
2	BJ	707	GLU
2	BJ	959	ALA
2	BJ	977	ILE
3	CA	103	PRO
4	CC	15	ILE
4	CD	15	ILE
4	CE	15	ILE

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Mol	Chain	Res	Type
5	CF	85	THR
5	CF	180	VAL
5	CG	180	VAL
5	CG	277	GLU
5	CG	559	PRO
5	CH	90	ASN
5	CH	180	VAL
6	CI	11	ILE
6	CJ	11	ILE
6	DA	11	ILE
2	EC	707	GLU
2	EC	959	ALA
2	EC	977	ILE
3	ED	103	PRO
4	EF	15	ILE
4	EG	15	ILE
4	EH	15	ILE
5	EI	85	THR
5	EI	180	VAL
5	EJ	180	VAL
5	EJ	277	GLU
5	FA	90	ASN
5	FA	180	VAL
6	FB	11	ILE
6	FC	11	ILE
6	FD	11	ILE
2	GF	707	GLU
2	GF	977	ILE
3	GG	103	PRO
4	GI	15	ILE
4	GJ	15	ILE
4	HA	15	ILE
5	HB	85	THR
5	HB	180	VAL
5	HC	180	VAL
5	HC	277	GLU
5	HC	559	PRO
5	HD	90	ASN
5	HD	180	VAL
6	HE	11	ILE
6	HF	11	ILE
6	HG	11	ILE

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Mol	Chain	Res	Type
1	A	140	VAL
1	A	473	HIS
1	B	379	LYS
2	C	87	GLN
2	C	342	SER
2	C	361	PRO
4	F	50	VAL
4	G	50	VAL
4	H	50	VAL
5	K	64	TRP
5	K	151	ILE
6	L	4	LEU
6	M	4	LEU
6	N	4	LEU
7	O	48	PRO
7	Q	49	ASP
7	Q	157	THR
1	X	140	VAL
1	X	473	HIS
1	Y	379	LYS
2	Z	87	GLN
2	Z	342	SER
2	Z	361	PRO
4	c	50	VAL
4	d	50	VAL
4	e	50	VAL
5	h	64	TRP
5	h	151	ILE
6	i	4	LEU
6	j	4	LEU
6	k	4	LEU
7	l	48	PRO
7	n	49	ASP
7	n	157	THR
1	u	140	VAL
1	u	473	HIS
1	v	379	LYS
2	w	87	GLN
2	w	342	SER
2	w	361	PRO
4	z	50	VAL
4	AA	50	VAL

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Mol	Chain	Res	Type
4	AB	50	VAL
5	AE	64	TRP
5	AE	151	ILE
6	AF	4	LEU
6	AG	4	LEU
6	AH	4	LEU
7	AI	48	PRO
7	BA	49	ASP
7	BA	157	THR
1	BH	140	VAL
1	BH	473	HIS
1	BI	379	LYS
2	BJ	87	GLN
2	BJ	342	SER
2	BJ	361	PRO
4	CC	50	VAL
4	CD	50	VAL
4	CE	50	VAL
5	CH	64	TRP
5	CH	151	ILE
6	CI	4	LEU
6	CJ	4	LEU
6	DA	4	LEU
7	DB	48	PRO
7	DD	49	ASP
7	DD	157	THR
1	EA	140	VAL
1	EA	473	HIS
1	EB	379	LYS
2	EC	87	GLN
2	EC	342	SER
2	EC	361	PRO
4	EF	50	VAL
4	EG	50	VAL
4	EH	50	VAL
5	EJ	559	PRO
5	FA	64	TRP
5	FA	151	ILE
6	FB	4	LEU
6	FC	4	LEU
6	FD	4	LEU
7	FE	48	PRO

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Mol	Chain	Res	Type
7	FG	49	ASP
7	FG	157	THR
1	GD	473	HIS
1	GE	379	LYS
2	GF	87	GLN
2	GF	342	SER
2	GF	361	PRO
2	GF	959	ALA
4	GI	50	VAL
4	GJ	50	VAL
4	HA	50	VAL
5	HD	64	TRP
5	HD	151	ILE
6	HE	4	LEU
6	HF	4	LEU
6	HG	4	LEU
7	HH	48	PRO
7	HJ	49	ASP
7	HJ	157	THR
1	B	454	ILE
3	D	102	ASP
5	I	228	PHE
5	J	90	ASN
5	K	156	SER
1	Y	454	ILE
3	a	102	ASP
5	f	228	PHE
5	g	90	ASN
5	h	156	SER
1	v	454	ILE
2	w	341	LEU
3	x	102	ASP
5	AC	228	PHE
5	AD	90	ASN
5	AE	156	SER
1	BI	454	ILE
2	BJ	341	LEU
3	CA	102	ASP
5	CF	228	PHE
5	CG	90	ASN
5	CH	156	SER
1	EB	454	ILE

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Mol	Chain	Res	Type
3	ED	102	ASP
5	EI	228	PHE
5	EJ	90	ASN
5	FA	156	SER
1	GD	140	VAL
1	GE	454	ILE
2	GF	341	LEU
2	GF	992	PRO
3	GG	102	ASP
5	HB	228	PHE
5	HC	90	ASN
2	C	992	PRO
2	Z	992	PRO
2	w	992	PRO
2	BJ	992	PRO
2	EC	992	PRO
2	C	357	ILE
2	Z	357	ILE
2	w	357	ILE
2	BJ	357	ILE
2	EC	357	ILE
2	GF	357	ILE
1	B	223	ILE
7	P	29	ILE
1	Y	223	ILE
7	m	29	ILE
1	v	223	ILE
7	AJ	29	ILE
1	BI	223	ILE
7	DC	29	ILE
1	EB	223	ILE
7	FF	29	ILE
1	GE	223	ILE
7	HI	29	ILE
2	C	842	VAL
2	C	1019	PRO
7	Q	87	TYR
2	Z	842	VAL
7	n	87	TYR
2	w	842	VAL
7	BA	87	TYR
2	BJ	842	VAL

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Mol	Chain	Res	Type
2	BJ	1019	PRO
7	DD	87	TYR
2	EC	842	VAL
7	FG	87	TYR
2	GF	842	VAL
7	HJ	87	TYR
7	Q	29	ILE
2	Z	1019	PRO
7	n	29	ILE
2	w	1019	PRO
7	BA	29	ILE
7	DD	29	ILE
2	EC	1019	PRO
7	FG	29	ILE
2	GF	1019	PRO
7	HJ	29	ILE
1	A	319	PRO
1	X	319	PRO
1	u	319	PRO
1	BH	319	PRO
1	EA	319	PRO
1	GD	319	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/578 (100%)	576 (100%)	0	100	100
1	B	567/578 (98%)	567 (100%)	0	100	100
1	BH	576/578 (100%)	576 (100%)	0	100	100
1	BI	567/578 (98%)	567 (100%)	0	100	100
1	EA	576/578 (100%)	576 (100%)	0	100	100
1	EB	567/578 (98%)	567 (100%)	0	100	100
1	GD	576/578 (100%)	576 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GE	567/578 (98%)	567 (100%)	0	100	100
1	X	576/578 (100%)	576 (100%)	0	100	100
1	Y	567/578 (98%)	567 (100%)	0	100	100
1	u	576/578 (100%)	576 (100%)	0	100	100
1	v	567/578 (98%)	567 (100%)	0	100	100
2	BJ	896/921 (97%)	896 (100%)	0	100	100
2	C	896/921 (97%)	896 (100%)	0	100	100
2	EC	896/921 (97%)	896 (100%)	0	100	100
2	GF	896/921 (97%)	896 (100%)	0	100	100
2	Z	896/921 (97%)	896 (100%)	0	100	100
2	w	896/921 (97%)	896 (100%)	0	100	100
3	CA	289/295 (98%)	289 (100%)	0	100	100
3	CB	293/295 (99%)	293 (100%)	0	100	100
3	D	289/295 (98%)	289 (100%)	0	100	100
3	E	293/295 (99%)	293 (100%)	0	100	100
3	ED	289/295 (98%)	289 (100%)	0	100	100
3	EE	293/295 (99%)	293 (100%)	0	100	100
3	GG	289/295 (98%)	289 (100%)	0	100	100
3	GH	293/295 (99%)	293 (100%)	0	100	100
3	a	289/295 (98%)	289 (100%)	0	100	100
3	b	293/295 (99%)	293 (100%)	0	100	100
3	x	289/295 (98%)	289 (100%)	0	100	100
3	y	293/295 (99%)	293 (100%)	0	100	100
4	AA	244/244 (100%)	244 (100%)	0	100	100
4	AB	244/244 (100%)	244 (100%)	0	100	100
4	CC	244/244 (100%)	244 (100%)	0	100	100
4	CD	244/244 (100%)	244 (100%)	0	100	100
4	CE	244/244 (100%)	244 (100%)	0	100	100
4	EF	244/244 (100%)	244 (100%)	0	100	100
4	EG	244/244 (100%)	244 (100%)	0	100	100
4	EH	244/244 (100%)	244 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	244/244 (100%)	244 (100%)	0	100	100
4	G	244/244 (100%)	244 (100%)	0	100	100
4	GI	244/244 (100%)	244 (100%)	0	100	100
4	GJ	244/244 (100%)	244 (100%)	0	100	100
4	H	244/244 (100%)	244 (100%)	0	100	100
4	HA	244/244 (100%)	244 (100%)	0	100	100
4	c	244/244 (100%)	244 (100%)	0	100	100
4	d	244/244 (100%)	244 (100%)	0	100	100
4	e	244/244 (100%)	244 (100%)	0	100	100
4	z	244/244 (100%)	244 (100%)	0	100	100
5	AC	519/519 (100%)	519 (100%)	0	100	100
5	AD	519/519 (100%)	519 (100%)	0	100	100
5	AE	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	CF	519/519 (100%)	519 (100%)	0	100	100
5	CG	519/519 (100%)	519 (100%)	0	100	100
5	CH	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	EI	519/519 (100%)	519 (100%)	0	100	100
5	EJ	519/519 (100%)	519 (100%)	0	100	100
5	FA	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	HB	519/519 (100%)	519 (100%)	0	100	100
5	HC	519/519 (100%)	519 (100%)	0	100	100
5	HD	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	I	519/519 (100%)	519 (100%)	0	100	100
5	J	519/519 (100%)	519 (100%)	0	100	100
5	K	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	f	519/519 (100%)	519 (100%)	0	100	100
5	g	519/519 (100%)	519 (100%)	0	100	100
5	h	519/519 (100%)	518 (100%)	1 (0%)	93	96
6	AF	187/188 (100%)	187 (100%)	0	100	100
6	AG	187/188 (100%)	187 (100%)	0	100	100
6	AH	187/188 (100%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	CI	187/188 (100%)	187 (100%)	0	100	100
6	CJ	187/188 (100%)	187 (100%)	0	100	100
6	DA	187/188 (100%)	187 (100%)	0	100	100
6	FB	187/188 (100%)	187 (100%)	0	100	100
6	FC	187/188 (100%)	187 (100%)	0	100	100
6	FD	187/188 (100%)	187 (100%)	0	100	100
6	HE	187/188 (100%)	187 (100%)	0	100	100
6	HF	187/188 (100%)	187 (100%)	0	100	100
6	HG	187/188 (100%)	187 (100%)	0	100	100
6	L	187/188 (100%)	187 (100%)	0	100	100
6	M	187/188 (100%)	187 (100%)	0	100	100
6	N	187/188 (100%)	187 (100%)	0	100	100
6	i	187/188 (100%)	187 (100%)	0	100	100
6	j	187/188 (100%)	187 (100%)	0	100	100
6	k	187/188 (100%)	187 (100%)	0	100	100
7	AI	426/427 (100%)	426 (100%)	0	100	100
7	AJ	426/427 (100%)	425 (100%)	1 (0%)	93	96
7	BA	426/427 (100%)	426 (100%)	0	100	100
7	DB	426/427 (100%)	426 (100%)	0	100	100
7	DC	426/427 (100%)	425 (100%)	1 (0%)	93	96
7	DD	426/427 (100%)	426 (100%)	0	100	100
7	FE	426/427 (100%)	426 (100%)	0	100	100
7	FF	426/427 (100%)	425 (100%)	1 (0%)	93	96
7	FG	426/427 (100%)	426 (100%)	0	100	100
7	HH	426/427 (100%)	426 (100%)	0	100	100
7	HI	426/427 (100%)	425 (100%)	1 (0%)	93	96
7	HJ	426/427 (100%)	426 (100%)	0	100	100
7	O	426/427 (100%)	426 (100%)	0	100	100
7	P	426/427 (100%)	425 (100%)	1 (0%)	93	96
7	Q	426/427 (100%)	426 (100%)	0	100	100
7	l	426/427 (100%)	426 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	m	426/427 (100%)	425 (100%)	1 (0%)	93	96
7	n	426/427 (100%)	426 (100%)	0	100	100
8	BB	136/137 (99%)	136 (100%)	0	100	100
8	BC	136/137 (99%)	136 (100%)	0	100	100
8	DE	136/137 (99%)	136 (100%)	0	100	100
8	DF	136/137 (99%)	136 (100%)	0	100	100
8	FH	136/137 (99%)	136 (100%)	0	100	100
8	FI	136/137 (99%)	136 (100%)	0	100	100
8	IA	136/137 (99%)	136 (100%)	0	100	100
8	IB	136/137 (99%)	136 (100%)	0	100	100
8	R	136/137 (99%)	136 (100%)	0	100	100
8	S	136/137 (99%)	136 (100%)	0	100	100
8	o	136/137 (99%)	136 (100%)	0	100	100
8	p	136/137 (99%)	136 (100%)	0	100	100
9	BD	118/123 (96%)	118 (100%)	0	100	100
9	DG	118/123 (96%)	118 (100%)	0	100	100
9	FJ	118/123 (96%)	118 (100%)	0	100	100
9	IC	118/123 (96%)	118 (100%)	0	100	100
9	T	118/123 (96%)	118 (100%)	0	100	100
9	q	118/123 (96%)	118 (100%)	0	100	100
10	BE	146/313 (47%)	145 (99%)	1 (1%)	84	90
10	DH	146/313 (47%)	145 (99%)	1 (1%)	84	90
10	GA	146/313 (47%)	145 (99%)	1 (1%)	84	90
10	ID	146/313 (47%)	145 (99%)	1 (1%)	84	90
10	U	146/313 (47%)	145 (99%)	1 (1%)	84	90
10	r	146/313 (47%)	145 (99%)	1 (1%)	84	90
11	BF	166/169 (98%)	165 (99%)	1 (1%)	86	92
11	DI	166/169 (98%)	165 (99%)	1 (1%)	86	92
11	GB	166/169 (98%)	165 (99%)	1 (1%)	86	92
11	IE	166/169 (98%)	165 (99%)	1 (1%)	86	92
11	V	166/169 (98%)	165 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	s	166/169 (98%)	165 (99%)	1 (1%)	86	92
12	BG	171/275 (62%)	170 (99%)	1 (1%)	86	92
12	DJ	171/275 (62%)	170 (99%)	1 (1%)	86	92
12	GC	171/275 (62%)	170 (99%)	1 (1%)	86	92
12	IF	171/275 (62%)	170 (99%)	1 (1%)	86	92
12	W	171/275 (62%)	170 (99%)	1 (1%)	86	92
12	t	171/275 (62%)	170 (99%)	1 (1%)	86	92
13	YA	2814/485 (580%)	2544 (90%)	270 (10%)	8	29
13	YB	2814/485 (580%)	2544 (90%)	270 (10%)	8	29
13	YC	2814/485 (580%)	2544 (90%)	270 (10%)	8	29
14	YD	1944/350 (555%)	1710 (88%)	234 (12%)	5	23
14	YE	1944/350 (555%)	1710 (88%)	234 (12%)	5	23
14	YF	1944/350 (555%)	1710 (88%)	234 (12%)	5	23
15	ZA	468/79 (592%)	450 (96%)	18 (4%)	33	58
All	All	60474/50314 (120%)	58914 (97%)	1560 (3%)	86	66

All (1560) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	K	79	ILE
7	P	9	VAL
10	U	286	VAL
11	V	15	THR
12	W	199	ILE
5	h	79	ILE
7	m	9	VAL
10	r	286	VAL
11	s	15	THR
12	t	199	ILE
5	AE	79	ILE
7	AJ	9	VAL
10	BE	286	VAL
11	BF	15	THR
12	BG	199	ILE
5	CH	79	ILE
7	DC	9	VAL
10	DH	286	VAL

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Mol	Chain	Res	Type
11	DI	15	THR
12	DJ	199	ILE
5	FA	79	ILE
7	FF	9	VAL
10	GA	286	VAL
11	GB	15	THR
12	GC	199	ILE
5	HD	79	ILE
7	HI	9	VAL
10	ID	286	VAL
11	IE	15	THR
12	IF	199	ILE
13	YA	7[A]	ASN
13	YA	7[B]	ASN
13	YA	7[C]	ASN
13	YA	7[D]	ASN
13	YA	7[E]	ASN
13	YA	7[F]	ASN
13	YA	24[A]	LEU
13	YA	24[B]	LEU
13	YA	24[C]	LEU
13	YA	24[D]	LEU
13	YA	24[E]	LEU
13	YA	24[F]	LEU
13	YA	27[A]	VAL
13	YA	27[B]	VAL
13	YA	27[C]	VAL
13	YA	27[D]	VAL
13	YA	27[E]	VAL
13	YA	27[F]	VAL
13	YA	34[A]	LEU
13	YA	34[B]	LEU
13	YA	34[C]	LEU
13	YA	34[D]	LEU
13	YA	34[E]	LEU
13	YA	34[F]	LEU
13	YA	41[A]	GLN
13	YA	41[B]	GLN
13	YA	41[C]	GLN
13	YA	41[D]	GLN
13	YA	41[E]	GLN
13	YA	41[F]	GLN

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Mol	Chain	Res	Type
13	YA	50[A]	GLU
13	YA	50[B]	GLU
13	YA	50[C]	GLU
13	YA	50[D]	GLU
13	YA	50[E]	GLU
13	YA	50[F]	GLU
13	YA	56[A]	SER
13	YA	56[B]	SER
13	YA	56[C]	SER
13	YA	56[D]	SER
13	YA	56[E]	SER
13	YA	56[F]	SER
13	YA	57[A]	VAL
13	YA	57[B]	VAL
13	YA	57[C]	VAL
13	YA	57[D]	VAL
13	YA	57[E]	VAL
13	YA	57[F]	VAL
13	YA	59[A]	GLN
13	YA	59[B]	GLN
13	YA	59[C]	GLN
13	YA	59[D]	GLN
13	YA	59[E]	GLN
13	YA	59[F]	GLN
13	YA	61[A]	ILE
13	YA	61[B]	ILE
13	YA	61[C]	ILE
13	YA	61[D]	ILE
13	YA	61[E]	ILE
13	YA	61[F]	ILE
13	YA	66[A]	MET
13	YA	66[B]	MET
13	YA	66[C]	MET
13	YA	66[D]	MET
13	YA	66[E]	MET
13	YA	66[F]	MET
13	YA	82[A]	VAL
13	YA	82[B]	VAL
13	YA	82[C]	VAL
13	YA	82[D]	VAL
13	YA	82[E]	VAL
13	YA	82[F]	VAL

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Mol	Chain	Res	Type
13	YA	87[A]	LEU
13	YA	87[B]	LEU
13	YA	87[C]	LEU
13	YA	87[D]	LEU
13	YA	87[E]	LEU
13	YA	87[F]	LEU
13	YA	89[A]	LYS
13	YA	89[B]	LYS
13	YA	89[C]	LYS
13	YA	89[D]	LYS
13	YA	89[E]	LYS
13	YA	89[F]	LYS
13	YA	97[A]	LEU
13	YA	97[B]	LEU
13	YA	97[C]	LEU
13	YA	97[D]	LEU
13	YA	97[E]	LEU
13	YA	97[F]	LEU
13	YA	127[A]	ASN
13	YA	127[B]	ASN
13	YA	127[C]	ASN
13	YA	127[D]	ASN
13	YA	127[E]	ASN
13	YA	127[F]	ASN
13	YA	150[A]	SER
13	YA	150[B]	SER
13	YA	150[C]	SER
13	YA	150[D]	SER
13	YA	150[E]	SER
13	YA	150[F]	SER
13	YA	152[A]	LEU
13	YA	152[B]	LEU
13	YA	152[C]	LEU
13	YA	152[D]	LEU
13	YA	152[E]	LEU
13	YA	152[F]	LEU
13	YA	173[A]	ASN
13	YA	173[B]	ASN
13	YA	173[C]	ASN
13	YA	173[D]	ASN
13	YA	173[E]	ASN
13	YA	173[F]	ASN

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Mol	Chain	Res	Type
13	YA	180[A]	LEU
13	YA	180[B]	LEU
13	YA	180[C]	LEU
13	YA	180[D]	LEU
13	YA	180[E]	LEU
13	YA	180[F]	LEU
13	YA	182[A]	ARG
13	YA	182[B]	ARG
13	YA	182[C]	ARG
13	YA	182[D]	ARG
13	YA	182[E]	ARG
13	YA	182[F]	ARG
13	YA	195[A]	GLU
13	YA	195[B]	GLU
13	YA	195[C]	GLU
13	YA	195[D]	GLU
13	YA	195[E]	GLU
13	YA	195[F]	GLU
13	YA	209[A]	GLN
13	YA	209[B]	GLN
13	YA	209[C]	GLN
13	YA	209[D]	GLN
13	YA	209[E]	GLN
13	YA	209[F]	GLN
13	YA	242[A]	THR
13	YA	242[B]	THR
13	YA	242[C]	THR
13	YA	242[D]	THR
13	YA	242[E]	THR
13	YA	242[F]	THR
13	YA	296[A]	LEU
13	YA	296[B]	LEU
13	YA	296[C]	LEU
13	YA	296[D]	LEU
13	YA	296[E]	LEU
13	YA	296[F]	LEU
13	YA	300[A]	LEU
13	YA	300[B]	LEU
13	YA	300[C]	LEU
13	YA	300[D]	LEU
13	YA	300[E]	LEU
13	YA	300[F]	LEU

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Mol	Chain	Res	Type
13	YA	327[A]	VAL
13	YA	327[B]	VAL
13	YA	327[C]	VAL
13	YA	327[D]	VAL
13	YA	327[E]	VAL
13	YA	327[F]	VAL
13	YA	331[A]	ILE
13	YA	331[B]	ILE
13	YA	331[C]	ILE
13	YA	331[D]	ILE
13	YA	331[E]	ILE
13	YA	331[F]	ILE
13	YA	335[A]	ASN
13	YA	335[B]	ASN
13	YA	335[C]	ASN
13	YA	335[D]	ASN
13	YA	335[E]	ASN
13	YA	335[F]	ASN
13	YA	372[A]	SER
13	YA	372[B]	SER
13	YA	372[C]	SER
13	YA	372[D]	SER
13	YA	372[E]	SER
13	YA	372[F]	SER
13	YA	373[A]	ARG
13	YA	373[B]	ARG
13	YA	373[C]	ARG
13	YA	373[D]	ARG
13	YA	373[E]	ARG
13	YA	373[F]	ARG
13	YA	375[A]	LEU
13	YA	375[B]	LEU
13	YA	375[C]	LEU
13	YA	375[D]	LEU
13	YA	375[E]	LEU
13	YA	375[F]	LEU
13	YA	418[A]	THR
13	YA	418[B]	THR
13	YA	418[C]	THR
13	YA	418[D]	THR
13	YA	418[E]	THR
13	YA	418[F]	THR

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Mol	Chain	Res	Type
13	YA	429[A]	ARG
13	YA	429[B]	ARG
13	YA	429[C]	ARG
13	YA	429[D]	ARG
13	YA	429[E]	ARG
13	YA	429[F]	ARG
13	YA	432[A]	ARG
13	YA	432[B]	ARG
13	YA	432[C]	ARG
13	YA	432[D]	ARG
13	YA	432[E]	ARG
13	YA	432[F]	ARG
13	YA	435[A]	VAL
13	YA	435[B]	VAL
13	YA	435[C]	VAL
13	YA	435[D]	VAL
13	YA	435[E]	VAL
13	YA	435[F]	VAL
13	YA	442[A]	THR
13	YA	442[B]	THR
13	YA	442[C]	THR
13	YA	442[D]	THR
13	YA	442[E]	THR
13	YA	442[F]	THR
13	YA	455[A]	LYS
13	YA	455[B]	LYS
13	YA	455[C]	LYS
13	YA	455[D]	LYS
13	YA	455[E]	LYS
13	YA	455[F]	LYS
13	YA	465[A]	TYR
13	YA	465[B]	TYR
13	YA	465[C]	TYR
13	YA	465[D]	TYR
13	YA	465[E]	TYR
13	YA	465[F]	TYR
13	YA	486[A]	GLU
13	YA	486[B]	GLU
13	YA	486[C]	GLU
13	YA	486[D]	GLU
13	YA	486[E]	GLU
13	YA	486[F]	GLU

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Mol	Chain	Res	Type
13	YA	522[A]	VAL
13	YA	522[B]	VAL
13	YA	522[C]	VAL
13	YA	522[D]	VAL
13	YA	522[E]	VAL
13	YA	522[F]	VAL
13	YA	550[A]	TRP
13	YA	550[B]	TRP
13	YA	550[C]	TRP
13	YA	550[D]	TRP
13	YA	550[E]	TRP
13	YA	550[F]	TRP
13	YA	554[A]	MET
13	YA	554[B]	MET
13	YA	554[C]	MET
13	YA	554[D]	MET
13	YA	554[E]	MET
13	YA	554[F]	MET
13	YA	566[A]	THR
13	YA	566[B]	THR
13	YA	566[C]	THR
13	YA	566[D]	THR
13	YA	566[E]	THR
13	YA	566[F]	THR
13	YA	573[A]	ASP
13	YA	573[B]	ASP
13	YA	573[C]	ASP
13	YA	573[D]	ASP
13	YA	573[E]	ASP
13	YA	573[F]	ASP
13	YB	7[A]	ASN
13	YB	7[B]	ASN
13	YB	7[C]	ASN
13	YB	7[D]	ASN
13	YB	7[E]	ASN
13	YB	7[F]	ASN
13	YB	24[A]	LEU
13	YB	24[B]	LEU
13	YB	24[C]	LEU
13	YB	24[D]	LEU
13	YB	24[E]	LEU
13	YB	24[F]	LEU

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Mol	Chain	Res	Type
13	YB	27[A]	VAL
13	YB	27[B]	VAL
13	YB	27[C]	VAL
13	YB	27[D]	VAL
13	YB	27[E]	VAL
13	YB	27[F]	VAL
13	YB	34[A]	LEU
13	YB	34[B]	LEU
13	YB	34[C]	LEU
13	YB	34[D]	LEU
13	YB	34[E]	LEU
13	YB	34[F]	LEU
13	YB	41[A]	GLN
13	YB	41[B]	GLN
13	YB	41[C]	GLN
13	YB	41[D]	GLN
13	YB	41[E]	GLN
13	YB	41[F]	GLN
13	YB	50[A]	GLU
13	YB	50[B]	GLU
13	YB	50[C]	GLU
13	YB	50[D]	GLU
13	YB	50[E]	GLU
13	YB	50[F]	GLU
13	YB	56[A]	SER
13	YB	56[B]	SER
13	YB	56[C]	SER
13	YB	56[D]	SER
13	YB	56[E]	SER
13	YB	56[F]	SER
13	YB	57[A]	VAL
13	YB	57[B]	VAL
13	YB	57[C]	VAL
13	YB	57[D]	VAL
13	YB	57[E]	VAL
13	YB	57[F]	VAL
13	YB	59[A]	GLN
13	YB	59[B]	GLN
13	YB	59[C]	GLN
13	YB	59[D]	GLN
13	YB	59[E]	GLN
13	YB	59[F]	GLN

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Mol	Chain	Res	Type
13	YB	61[A]	ILE
13	YB	61[B]	ILE
13	YB	61[C]	ILE
13	YB	61[D]	ILE
13	YB	61[E]	ILE
13	YB	61[F]	ILE
13	YB	66[A]	MET
13	YB	66[B]	MET
13	YB	66[C]	MET
13	YB	66[D]	MET
13	YB	66[E]	MET
13	YB	66[F]	MET
13	YB	82[A]	VAL
13	YB	82[B]	VAL
13	YB	82[C]	VAL
13	YB	82[D]	VAL
13	YB	82[E]	VAL
13	YB	82[F]	VAL
13	YB	87[A]	LEU
13	YB	87[B]	LEU
13	YB	87[C]	LEU
13	YB	87[D]	LEU
13	YB	87[E]	LEU
13	YB	87[F]	LEU
13	YB	89[A]	LYS
13	YB	89[B]	LYS
13	YB	89[C]	LYS
13	YB	89[D]	LYS
13	YB	89[E]	LYS
13	YB	89[F]	LYS
13	YB	97[A]	LEU
13	YB	97[B]	LEU
13	YB	97[C]	LEU
13	YB	97[D]	LEU
13	YB	97[E]	LEU
13	YB	97[F]	LEU
13	YB	127[A]	ASN
13	YB	127[B]	ASN
13	YB	127[C]	ASN
13	YB	127[D]	ASN
13	YB	127[E]	ASN
13	YB	127[F]	ASN

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Mol	Chain	Res	Type
13	YB	150[A]	SER
13	YB	150[B]	SER
13	YB	150[C]	SER
13	YB	150[D]	SER
13	YB	150[E]	SER
13	YB	150[F]	SER
13	YB	152[A]	LEU
13	YB	152[B]	LEU
13	YB	152[C]	LEU
13	YB	152[D]	LEU
13	YB	152[E]	LEU
13	YB	152[F]	LEU
13	YB	173[A]	ASN
13	YB	173[B]	ASN
13	YB	173[C]	ASN
13	YB	173[D]	ASN
13	YB	173[E]	ASN
13	YB	173[F]	ASN
13	YB	180[A]	LEU
13	YB	180[B]	LEU
13	YB	180[C]	LEU
13	YB	180[D]	LEU
13	YB	180[E]	LEU
13	YB	180[F]	LEU
13	YB	182[A]	ARG
13	YB	182[B]	ARG
13	YB	182[C]	ARG
13	YB	182[D]	ARG
13	YB	182[E]	ARG
13	YB	182[F]	ARG
13	YB	195[A]	GLU
13	YB	195[B]	GLU
13	YB	195[C]	GLU
13	YB	195[D]	GLU
13	YB	195[E]	GLU
13	YB	195[F]	GLU
13	YB	209[A]	GLN
13	YB	209[B]	GLN
13	YB	209[C]	GLN
13	YB	209[D]	GLN
13	YB	209[E]	GLN
13	YB	209[F]	GLN

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Mol	Chain	Res	Type
13	YB	242[A]	THR
13	YB	242[B]	THR
13	YB	242[C]	THR
13	YB	242[D]	THR
13	YB	242[E]	THR
13	YB	242[F]	THR
13	YB	296[A]	LEU
13	YB	296[B]	LEU
13	YB	296[C]	LEU
13	YB	296[D]	LEU
13	YB	296[E]	LEU
13	YB	296[F]	LEU
13	YB	300[A]	LEU
13	YB	300[B]	LEU
13	YB	300[C]	LEU
13	YB	300[D]	LEU
13	YB	300[E]	LEU
13	YB	300[F]	LEU
13	YB	327[A]	VAL
13	YB	327[B]	VAL
13	YB	327[C]	VAL
13	YB	327[D]	VAL
13	YB	327[E]	VAL
13	YB	327[F]	VAL
13	YB	331[A]	ILE
13	YB	331[B]	ILE
13	YB	331[C]	ILE
13	YB	331[D]	ILE
13	YB	331[E]	ILE
13	YB	331[F]	ILE
13	YB	335[A]	ASN
13	YB	335[B]	ASN
13	YB	335[C]	ASN
13	YB	335[D]	ASN
13	YB	335[E]	ASN
13	YB	335[F]	ASN
13	YB	372[A]	SER
13	YB	372[B]	SER
13	YB	372[C]	SER
13	YB	372[D]	SER
13	YB	372[E]	SER
13	YB	372[F]	SER

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Mol	Chain	Res	Type
13	YB	373[A]	ARG
13	YB	373[B]	ARG
13	YB	373[C]	ARG
13	YB	373[D]	ARG
13	YB	373[E]	ARG
13	YB	373[F]	ARG
13	YB	375[A]	LEU
13	YB	375[B]	LEU
13	YB	375[C]	LEU
13	YB	375[D]	LEU
13	YB	375[E]	LEU
13	YB	375[F]	LEU
13	YB	418[A]	THR
13	YB	418[B]	THR
13	YB	418[C]	THR
13	YB	418[D]	THR
13	YB	418[E]	THR
13	YB	418[F]	THR
13	YB	429[A]	ARG
13	YB	429[B]	ARG
13	YB	429[C]	ARG
13	YB	429[D]	ARG
13	YB	429[E]	ARG
13	YB	429[F]	ARG
13	YB	432[A]	ARG
13	YB	432[B]	ARG
13	YB	432[C]	ARG
13	YB	432[D]	ARG
13	YB	432[E]	ARG
13	YB	432[F]	ARG
13	YB	435[A]	VAL
13	YB	435[B]	VAL
13	YB	435[C]	VAL
13	YB	435[D]	VAL
13	YB	435[E]	VAL
13	YB	435[F]	VAL
13	YB	442[A]	THR
13	YB	442[B]	THR
13	YB	442[C]	THR
13	YB	442[D]	THR
13	YB	442[E]	THR
13	YB	442[F]	THR

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Mol	Chain	Res	Type
13	YB	455[A]	LYS
13	YB	455[B]	LYS
13	YB	455[C]	LYS
13	YB	455[D]	LYS
13	YB	455[E]	LYS
13	YB	455[F]	LYS
13	YB	465[A]	TYR
13	YB	465[B]	TYR
13	YB	465[C]	TYR
13	YB	465[D]	TYR
13	YB	465[E]	TYR
13	YB	465[F]	TYR
13	YB	486[A]	GLU
13	YB	486[B]	GLU
13	YB	486[C]	GLU
13	YB	486[D]	GLU
13	YB	486[E]	GLU
13	YB	486[F]	GLU
13	YB	522[A]	VAL
13	YB	522[B]	VAL
13	YB	522[C]	VAL
13	YB	522[D]	VAL
13	YB	522[E]	VAL
13	YB	522[F]	VAL
13	YB	550[A]	TRP
13	YB	550[B]	TRP
13	YB	550[C]	TRP
13	YB	550[D]	TRP
13	YB	550[E]	TRP
13	YB	550[F]	TRP
13	YB	554[A]	MET
13	YB	554[B]	MET
13	YB	554[C]	MET
13	YB	554[D]	MET
13	YB	554[E]	MET
13	YB	554[F]	MET
13	YB	566[A]	THR
13	YB	566[B]	THR
13	YB	566[C]	THR
13	YB	566[D]	THR
13	YB	566[E]	THR
13	YB	566[F]	THR

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Mol	Chain	Res	Type
13	YB	573[A]	ASP
13	YB	573[B]	ASP
13	YB	573[C]	ASP
13	YB	573[D]	ASP
13	YB	573[E]	ASP
13	YB	573[F]	ASP
13	YC	7[A]	ASN
13	YC	7[B]	ASN
13	YC	7[C]	ASN
13	YC	7[D]	ASN
13	YC	7[E]	ASN
13	YC	7[F]	ASN
13	YC	24[A]	LEU
13	YC	24[B]	LEU
13	YC	24[C]	LEU
13	YC	24[D]	LEU
13	YC	24[E]	LEU
13	YC	24[F]	LEU
13	YC	27[A]	VAL
13	YC	27[B]	VAL
13	YC	27[C]	VAL
13	YC	27[D]	VAL
13	YC	27[E]	VAL
13	YC	27[F]	VAL
13	YC	34[A]	LEU
13	YC	34[B]	LEU
13	YC	34[C]	LEU
13	YC	34[D]	LEU
13	YC	34[E]	LEU
13	YC	34[F]	LEU
13	YC	41[A]	GLN
13	YC	41[B]	GLN
13	YC	41[C]	GLN
13	YC	41[D]	GLN
13	YC	41[E]	GLN
13	YC	41[F]	GLN
13	YC	50[A]	GLU
13	YC	50[B]	GLU
13	YC	50[C]	GLU
13	YC	50[D]	GLU
13	YC	50[E]	GLU
13	YC	50[F]	GLU

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Mol	Chain	Res	Type
13	YC	56[A]	SER
13	YC	56[B]	SER
13	YC	56[C]	SER
13	YC	56[D]	SER
13	YC	56[E]	SER
13	YC	56[F]	SER
13	YC	57[A]	VAL
13	YC	57[B]	VAL
13	YC	57[C]	VAL
13	YC	57[D]	VAL
13	YC	57[E]	VAL
13	YC	57[F]	VAL
13	YC	59[A]	GLN
13	YC	59[B]	GLN
13	YC	59[C]	GLN
13	YC	59[D]	GLN
13	YC	59[E]	GLN
13	YC	59[F]	GLN
13	YC	61[A]	ILE
13	YC	61[B]	ILE
13	YC	61[C]	ILE
13	YC	61[D]	ILE
13	YC	61[E]	ILE
13	YC	61[F]	ILE
13	YC	66[A]	MET
13	YC	66[B]	MET
13	YC	66[C]	MET
13	YC	66[D]	MET
13	YC	66[E]	MET
13	YC	66[F]	MET
13	YC	82[A]	VAL
13	YC	82[B]	VAL
13	YC	82[C]	VAL
13	YC	82[D]	VAL
13	YC	82[E]	VAL
13	YC	82[F]	VAL
13	YC	87[A]	LEU
13	YC	87[B]	LEU
13	YC	87[C]	LEU
13	YC	87[D]	LEU
13	YC	87[E]	LEU
13	YC	87[F]	LEU

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Mol	Chain	Res	Type
13	YC	89[A]	LYS
13	YC	89[B]	LYS
13	YC	89[C]	LYS
13	YC	89[D]	LYS
13	YC	89[E]	LYS
13	YC	89[F]	LYS
13	YC	97[A]	LEU
13	YC	97[B]	LEU
13	YC	97[C]	LEU
13	YC	97[D]	LEU
13	YC	97[E]	LEU
13	YC	97[F]	LEU
13	YC	127[A]	ASN
13	YC	127[B]	ASN
13	YC	127[C]	ASN
13	YC	127[D]	ASN
13	YC	127[E]	ASN
13	YC	127[F]	ASN
13	YC	150[A]	SER
13	YC	150[B]	SER
13	YC	150[C]	SER
13	YC	150[D]	SER
13	YC	150[E]	SER
13	YC	150[F]	SER
13	YC	152[A]	LEU
13	YC	152[B]	LEU
13	YC	152[C]	LEU
13	YC	152[D]	LEU
13	YC	152[E]	LEU
13	YC	152[F]	LEU
13	YC	173[A]	ASN
13	YC	173[B]	ASN
13	YC	173[C]	ASN
13	YC	173[D]	ASN
13	YC	173[E]	ASN
13	YC	173[F]	ASN
13	YC	180[A]	LEU
13	YC	180[B]	LEU
13	YC	180[C]	LEU
13	YC	180[D]	LEU
13	YC	180[E]	LEU
13	YC	180[F]	LEU

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Mol	Chain	Res	Type
13	YC	182[A]	ARG
13	YC	182[B]	ARG
13	YC	182[C]	ARG
13	YC	182[D]	ARG
13	YC	182[E]	ARG
13	YC	182[F]	ARG
13	YC	195[A]	GLU
13	YC	195[B]	GLU
13	YC	195[C]	GLU
13	YC	195[D]	GLU
13	YC	195[E]	GLU
13	YC	195[F]	GLU
13	YC	209[A]	GLN
13	YC	209[B]	GLN
13	YC	209[C]	GLN
13	YC	209[D]	GLN
13	YC	209[E]	GLN
13	YC	209[F]	GLN
13	YC	242[A]	THR
13	YC	242[B]	THR
13	YC	242[C]	THR
13	YC	242[D]	THR
13	YC	242[E]	THR
13	YC	242[F]	THR
13	YC	296[A]	LEU
13	YC	296[B]	LEU
13	YC	296[C]	LEU
13	YC	296[D]	LEU
13	YC	296[E]	LEU
13	YC	296[F]	LEU
13	YC	300[A]	LEU
13	YC	300[B]	LEU
13	YC	300[C]	LEU
13	YC	300[D]	LEU
13	YC	300[E]	LEU
13	YC	300[F]	LEU
13	YC	327[A]	VAL
13	YC	327[B]	VAL
13	YC	327[C]	VAL
13	YC	327[D]	VAL
13	YC	327[E]	VAL
13	YC	327[F]	VAL

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Mol	Chain	Res	Type
13	YC	331[A]	ILE
13	YC	331[B]	ILE
13	YC	331[C]	ILE
13	YC	331[D]	ILE
13	YC	331[E]	ILE
13	YC	331[F]	ILE
13	YC	335[A]	ASN
13	YC	335[B]	ASN
13	YC	335[C]	ASN
13	YC	335[D]	ASN
13	YC	335[E]	ASN
13	YC	335[F]	ASN
13	YC	372[A]	SER
13	YC	372[B]	SER
13	YC	372[C]	SER
13	YC	372[D]	SER
13	YC	372[E]	SER
13	YC	372[F]	SER
13	YC	373[A]	ARG
13	YC	373[B]	ARG
13	YC	373[C]	ARG
13	YC	373[D]	ARG
13	YC	373[E]	ARG
13	YC	373[F]	ARG
13	YC	375[A]	LEU
13	YC	375[B]	LEU
13	YC	375[C]	LEU
13	YC	375[D]	LEU
13	YC	375[E]	LEU
13	YC	375[F]	LEU
13	YC	418[A]	THR
13	YC	418[B]	THR
13	YC	418[C]	THR
13	YC	418[D]	THR
13	YC	418[E]	THR
13	YC	418[F]	THR
13	YC	429[A]	ARG
13	YC	429[B]	ARG
13	YC	429[C]	ARG
13	YC	429[D]	ARG
13	YC	429[E]	ARG
13	YC	429[F]	ARG

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Mol	Chain	Res	Type
13	YC	432[A]	ARG
13	YC	432[B]	ARG
13	YC	432[C]	ARG
13	YC	432[D]	ARG
13	YC	432[E]	ARG
13	YC	432[F]	ARG
13	YC	435[A]	VAL
13	YC	435[B]	VAL
13	YC	435[C]	VAL
13	YC	435[D]	VAL
13	YC	435[E]	VAL
13	YC	435[F]	VAL
13	YC	442[A]	THR
13	YC	442[B]	THR
13	YC	442[C]	THR
13	YC	442[D]	THR
13	YC	442[E]	THR
13	YC	442[F]	THR
13	YC	455[A]	LYS
13	YC	455[B]	LYS
13	YC	455[C]	LYS
13	YC	455[D]	LYS
13	YC	455[E]	LYS
13	YC	455[F]	LYS
13	YC	465[A]	TYR
13	YC	465[B]	TYR
13	YC	465[C]	TYR
13	YC	465[D]	TYR
13	YC	465[E]	TYR
13	YC	465[F]	TYR
13	YC	486[A]	GLU
13	YC	486[B]	GLU
13	YC	486[C]	GLU
13	YC	486[D]	GLU
13	YC	486[E]	GLU
13	YC	486[F]	GLU
13	YC	522[A]	VAL
13	YC	522[B]	VAL
13	YC	522[C]	VAL
13	YC	522[D]	VAL
13	YC	522[E]	VAL
13	YC	522[F]	VAL

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Mol	Chain	Res	Type
13	YC	550[A]	TRP
13	YC	550[B]	TRP
13	YC	550[C]	TRP
13	YC	550[D]	TRP
13	YC	550[E]	TRP
13	YC	550[F]	TRP
13	YC	554[A]	MET
13	YC	554[B]	MET
13	YC	554[C]	MET
13	YC	554[D]	MET
13	YC	554[E]	MET
13	YC	554[F]	MET
13	YC	566[A]	THR
13	YC	566[B]	THR
13	YC	566[C]	THR
13	YC	566[D]	THR
13	YC	566[E]	THR
13	YC	566[F]	THR
13	YC	573[A]	ASP
13	YC	573[B]	ASP
13	YC	573[C]	ASP
13	YC	573[D]	ASP
13	YC	573[E]	ASP
13	YC	573[F]	ASP
14	YD	15[A]	LYS
14	YD	15[B]	LYS
14	YD	15[C]	LYS
14	YD	15[D]	LYS
14	YD	15[E]	LYS
14	YD	15[F]	LYS
14	YD	16[A]	LEU
14	YD	16[B]	LEU
14	YD	16[C]	LEU
14	YD	16[D]	LEU
14	YD	16[E]	LEU
14	YD	16[F]	LEU
14	YD	21[A]	ASP
14	YD	21[B]	ASP
14	YD	21[C]	ASP
14	YD	21[D]	ASP
14	YD	21[E]	ASP
14	YD	21[F]	ASP

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Mol	Chain	Res	Type
14	YD	35[A]	ILE
14	YD	35[B]	ILE
14	YD	35[C]	ILE
14	YD	35[D]	ILE
14	YD	35[E]	ILE
14	YD	35[F]	ILE
14	YD	42[A]	ASP
14	YD	42[B]	ASP
14	YD	42[C]	ASP
14	YD	42[D]	ASP
14	YD	42[E]	ASP
14	YD	42[F]	ASP
14	YD	44[A]	LEU
14	YD	44[B]	LEU
14	YD	44[C]	LEU
14	YD	44[D]	LEU
14	YD	44[E]	LEU
14	YD	44[F]	LEU
14	YD	51[A]	MET
14	YD	51[B]	MET
14	YD	51[C]	MET
14	YD	51[D]	MET
14	YD	51[E]	MET
14	YD	51[F]	MET
14	YD	58[A]	LYS
14	YD	58[B]	LYS
14	YD	58[C]	LYS
14	YD	58[D]	LYS
14	YD	58[E]	LYS
14	YD	58[F]	LYS
14	YD	68[A]	GLU
14	YD	68[B]	GLU
14	YD	68[C]	GLU
14	YD	68[D]	GLU
14	YD	68[E]	GLU
14	YD	68[F]	GLU
14	YD	74[A]	VAL
14	YD	74[B]	VAL
14	YD	74[C]	VAL
14	YD	74[D]	VAL
14	YD	74[E]	VAL
14	YD	74[F]	VAL

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Mol	Chain	Res	Type
14	YD	80[A]	ILE
14	YD	80[B]	ILE
14	YD	80[C]	ILE
14	YD	80[D]	ILE
14	YD	80[E]	ILE
14	YD	80[F]	ILE
14	YD	87[A]	ILE
14	YD	87[B]	ILE
14	YD	87[C]	ILE
14	YD	87[D]	ILE
14	YD	87[E]	ILE
14	YD	87[F]	ILE
14	YD	90[A]	CYS
14	YD	90[B]	CYS
14	YD	90[C]	CYS
14	YD	90[D]	CYS
14	YD	90[E]	CYS
14	YD	90[F]	CYS
14	YD	104[A]	ILE
14	YD	104[B]	ILE
14	YD	104[C]	ILE
14	YD	104[D]	ILE
14	YD	104[E]	ILE
14	YD	104[F]	ILE
14	YD	107[A]	ILE
14	YD	107[B]	ILE
14	YD	107[C]	ILE
14	YD	107[D]	ILE
14	YD	107[E]	ILE
14	YD	107[F]	ILE
14	YD	109[A]	LEU
14	YD	109[B]	LEU
14	YD	109[C]	LEU
14	YD	109[D]	LEU
14	YD	109[E]	LEU
14	YD	109[F]	LEU
14	YD	111[A]	THR
14	YD	111[B]	THR
14	YD	111[C]	THR
14	YD	111[D]	THR
14	YD	111[E]	THR
14	YD	111[F]	THR

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Mol	Chain	Res	Type
14	YD	154[A]	ASN
14	YD	154[B]	ASN
14	YD	154[C]	ASN
14	YD	154[D]	ASN
14	YD	154[E]	ASN
14	YD	154[F]	ASN
14	YD	163[A]	THR
14	YD	163[B]	THR
14	YD	163[C]	THR
14	YD	163[D]	THR
14	YD	163[E]	THR
14	YD	163[F]	THR
14	YD	183[A]	ASP
14	YD	183[B]	ASP
14	YD	183[C]	ASP
14	YD	183[D]	ASP
14	YD	183[E]	ASP
14	YD	183[F]	ASP
14	YD	233[A]	ASP
14	YD	233[B]	ASP
14	YD	233[C]	ASP
14	YD	233[D]	ASP
14	YD	233[E]	ASP
14	YD	233[F]	ASP
14	YD	236[A]	TRP
14	YD	236[B]	TRP
14	YD	236[C]	TRP
14	YD	236[D]	TRP
14	YD	236[E]	TRP
14	YD	236[F]	TRP
14	YD	241[A]	ASN
14	YD	241[B]	ASN
14	YD	241[C]	ASN
14	YD	241[D]	ASN
14	YD	241[E]	ASN
14	YD	241[F]	ASN
14	YD	267[A]	THR
14	YD	267[B]	THR
14	YD	267[C]	THR
14	YD	267[D]	THR
14	YD	267[E]	THR
14	YD	267[F]	THR

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Mol	Chain	Res	Type
14	YD	296[A]	ILE
14	YD	296[B]	ILE
14	YD	296[C]	ILE
14	YD	296[D]	ILE
14	YD	296[E]	ILE
14	YD	296[F]	ILE
14	YD	305[A]	ASP
14	YD	305[B]	ASP
14	YD	305[C]	ASP
14	YD	305[D]	ASP
14	YD	305[E]	ASP
14	YD	305[F]	ASP
14	YD	312[A]	THR
14	YD	312[B]	THR
14	YD	312[C]	THR
14	YD	312[D]	THR
14	YD	312[E]	THR
14	YD	312[F]	THR
14	YD	315[A]	ASN
14	YD	315[B]	ASN
14	YD	315[C]	ASN
14	YD	315[D]	ASN
14	YD	315[E]	ASN
14	YD	315[F]	ASN
14	YD	318[A]	LEU
14	YD	318[B]	LEU
14	YD	318[C]	LEU
14	YD	318[D]	LEU
14	YD	318[E]	LEU
14	YD	318[F]	LEU
14	YD	325[A]	ILE
14	YD	325[B]	ILE
14	YD	325[C]	ILE
14	YD	325[D]	ILE
14	YD	325[E]	ILE
14	YD	325[F]	ILE
14	YD	330[A]	LYS
14	YD	330[B]	LYS
14	YD	330[C]	LYS
14	YD	330[D]	LYS
14	YD	330[E]	LYS
14	YD	330[F]	LYS

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Mol	Chain	Res	Type
14	YD	333[A]	PHE
14	YD	333[B]	PHE
14	YD	333[C]	PHE
14	YD	333[D]	PHE
14	YD	333[E]	PHE
14	YD	333[F]	PHE
14	YD	342[A]	VAL
14	YD	342[B]	VAL
14	YD	342[C]	VAL
14	YD	342[D]	VAL
14	YD	342[E]	VAL
14	YD	342[F]	VAL
14	YD	346[A]	LEU
14	YD	346[B]	LEU
14	YD	346[C]	LEU
14	YD	346[D]	LEU
14	YD	346[E]	LEU
14	YD	346[F]	LEU
14	YD	352[A]	VAL
14	YD	352[B]	VAL
14	YD	352[C]	VAL
14	YD	352[D]	VAL
14	YD	352[E]	VAL
14	YD	352[F]	VAL
14	YD	360[A]	ASN
14	YD	360[B]	ASN
14	YD	360[C]	ASN
14	YD	360[D]	ASN
14	YD	360[E]	ASN
14	YD	360[F]	ASN
14	YD	364[A]	LEU
14	YD	364[B]	LEU
14	YD	364[C]	LEU
14	YD	364[D]	LEU
14	YD	364[E]	LEU
14	YD	364[F]	LEU
14	YD	365[A]	GLU
14	YD	365[B]	GLU
14	YD	365[C]	GLU
14	YD	365[D]	GLU
14	YD	365[E]	GLU
14	YD	365[F]	GLU

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Mol	Chain	Res	Type
14	YD	366[A]	THR
14	YD	366[B]	THR
14	YD	366[C]	THR
14	YD	366[D]	THR
14	YD	366[E]	THR
14	YD	366[F]	THR
14	YE	15[A]	LYS
14	YE	15[B]	LYS
14	YE	15[C]	LYS
14	YE	15[D]	LYS
14	YE	15[E]	LYS
14	YE	15[F]	LYS
14	YE	16[A]	LEU
14	YE	16[B]	LEU
14	YE	16[C]	LEU
14	YE	16[D]	LEU
14	YE	16[E]	LEU
14	YE	16[F]	LEU
14	YE	21[A]	ASP
14	YE	21[B]	ASP
14	YE	21[C]	ASP
14	YE	21[D]	ASP
14	YE	21[E]	ASP
14	YE	21[F]	ASP
14	YE	35[A]	ILE
14	YE	35[B]	ILE
14	YE	35[C]	ILE
14	YE	35[D]	ILE
14	YE	35[E]	ILE
14	YE	35[F]	ILE
14	YE	42[A]	ASP
14	YE	42[B]	ASP
14	YE	42[C]	ASP
14	YE	42[D]	ASP
14	YE	42[E]	ASP
14	YE	42[F]	ASP
14	YE	44[A]	LEU
14	YE	44[B]	LEU
14	YE	44[C]	LEU
14	YE	44[D]	LEU
14	YE	44[E]	LEU
14	YE	44[F]	LEU

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Mol	Chain	Res	Type
14	YE	51[A]	MET
14	YE	51[B]	MET
14	YE	51[C]	MET
14	YE	51[D]	MET
14	YE	51[E]	MET
14	YE	51[F]	MET
14	YE	58[A]	LYS
14	YE	58[B]	LYS
14	YE	58[C]	LYS
14	YE	58[D]	LYS
14	YE	58[E]	LYS
14	YE	58[F]	LYS
14	YE	68[A]	GLU
14	YE	68[B]	GLU
14	YE	68[C]	GLU
14	YE	68[D]	GLU
14	YE	68[E]	GLU
14	YE	68[F]	GLU
14	YE	74[A]	VAL
14	YE	74[B]	VAL
14	YE	74[C]	VAL
14	YE	74[D]	VAL
14	YE	74[E]	VAL
14	YE	74[F]	VAL
14	YE	80[A]	ILE
14	YE	80[B]	ILE
14	YE	80[C]	ILE
14	YE	80[D]	ILE
14	YE	80[E]	ILE
14	YE	80[F]	ILE
14	YE	87[A]	ILE
14	YE	87[B]	ILE
14	YE	87[C]	ILE
14	YE	87[D]	ILE
14	YE	87[E]	ILE
14	YE	87[F]	ILE
14	YE	90[A]	CYS
14	YE	90[B]	CYS
14	YE	90[C]	CYS
14	YE	90[D]	CYS
14	YE	90[E]	CYS
14	YE	90[F]	CYS

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Mol	Chain	Res	Type
14	YE	104[A]	ILE
14	YE	104[B]	ILE
14	YE	104[C]	ILE
14	YE	104[D]	ILE
14	YE	104[E]	ILE
14	YE	104[F]	ILE
14	YE	107[A]	ILE
14	YE	107[B]	ILE
14	YE	107[C]	ILE
14	YE	107[D]	ILE
14	YE	107[E]	ILE
14	YE	107[F]	ILE
14	YE	109[A]	LEU
14	YE	109[B]	LEU
14	YE	109[C]	LEU
14	YE	109[D]	LEU
14	YE	109[E]	LEU
14	YE	109[F]	LEU
14	YE	111[A]	THR
14	YE	111[B]	THR
14	YE	111[C]	THR
14	YE	111[D]	THR
14	YE	111[E]	THR
14	YE	111[F]	THR
14	YE	154[A]	ASN
14	YE	154[B]	ASN
14	YE	154[C]	ASN
14	YE	154[D]	ASN
14	YE	154[E]	ASN
14	YE	154[F]	ASN
14	YE	163[A]	THR
14	YE	163[B]	THR
14	YE	163[C]	THR
14	YE	163[D]	THR
14	YE	163[E]	THR
14	YE	163[F]	THR
14	YE	183[A]	ASP
14	YE	183[B]	ASP
14	YE	183[C]	ASP
14	YE	183[D]	ASP
14	YE	183[E]	ASP
14	YE	183[F]	ASP

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Mol	Chain	Res	Type
14	YE	233[A]	ASP
14	YE	233[B]	ASP
14	YE	233[C]	ASP
14	YE	233[D]	ASP
14	YE	233[E]	ASP
14	YE	233[F]	ASP
14	YE	236[A]	TRP
14	YE	236[B]	TRP
14	YE	236[C]	TRP
14	YE	236[D]	TRP
14	YE	236[E]	TRP
14	YE	236[F]	TRP
14	YE	241[A]	ASN
14	YE	241[B]	ASN
14	YE	241[C]	ASN
14	YE	241[D]	ASN
14	YE	241[E]	ASN
14	YE	241[F]	ASN
14	YE	267[A]	THR
14	YE	267[B]	THR
14	YE	267[C]	THR
14	YE	267[D]	THR
14	YE	267[E]	THR
14	YE	267[F]	THR
14	YE	296[A]	ILE
14	YE	296[B]	ILE
14	YE	296[C]	ILE
14	YE	296[D]	ILE
14	YE	296[E]	ILE
14	YE	296[F]	ILE
14	YE	305[A]	ASP
14	YE	305[B]	ASP
14	YE	305[C]	ASP
14	YE	305[D]	ASP
14	YE	305[E]	ASP
14	YE	305[F]	ASP
14	YE	312[A]	THR
14	YE	312[B]	THR
14	YE	312[C]	THR
14	YE	312[D]	THR
14	YE	312[E]	THR
14	YE	312[F]	THR

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Mol	Chain	Res	Type
14	YE	315[A]	ASN
14	YE	315[B]	ASN
14	YE	315[C]	ASN
14	YE	315[D]	ASN
14	YE	315[E]	ASN
14	YE	315[F]	ASN
14	YE	318[A]	LEU
14	YE	318[B]	LEU
14	YE	318[C]	LEU
14	YE	318[D]	LEU
14	YE	318[E]	LEU
14	YE	318[F]	LEU
14	YE	325[A]	ILE
14	YE	325[B]	ILE
14	YE	325[C]	ILE
14	YE	325[D]	ILE
14	YE	325[E]	ILE
14	YE	325[F]	ILE
14	YE	330[A]	LYS
14	YE	330[B]	LYS
14	YE	330[C]	LYS
14	YE	330[D]	LYS
14	YE	330[E]	LYS
14	YE	330[F]	LYS
14	YE	333[A]	PHE
14	YE	333[B]	PHE
14	YE	333[C]	PHE
14	YE	333[D]	PHE
14	YE	333[E]	PHE
14	YE	333[F]	PHE
14	YE	342[A]	VAL
14	YE	342[B]	VAL
14	YE	342[C]	VAL
14	YE	342[D]	VAL
14	YE	342[E]	VAL
14	YE	342[F]	VAL
14	YE	346[A]	LEU
14	YE	346[B]	LEU
14	YE	346[C]	LEU
14	YE	346[D]	LEU
14	YE	346[E]	LEU
14	YE	346[F]	LEU

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Mol	Chain	Res	Type
14	YE	352[A]	VAL
14	YE	352[B]	VAL
14	YE	352[C]	VAL
14	YE	352[D]	VAL
14	YE	352[E]	VAL
14	YE	352[F]	VAL
14	YE	360[A]	ASN
14	YE	360[B]	ASN
14	YE	360[C]	ASN
14	YE	360[D]	ASN
14	YE	360[E]	ASN
14	YE	360[F]	ASN
14	YE	364[A]	LEU
14	YE	364[B]	LEU
14	YE	364[C]	LEU
14	YE	364[D]	LEU
14	YE	364[E]	LEU
14	YE	364[F]	LEU
14	YE	365[A]	GLU
14	YE	365[B]	GLU
14	YE	365[C]	GLU
14	YE	365[D]	GLU
14	YE	365[E]	GLU
14	YE	365[F]	GLU
14	YE	366[A]	THR
14	YE	366[B]	THR
14	YE	366[C]	THR
14	YE	366[D]	THR
14	YE	366[E]	THR
14	YE	366[F]	THR
14	YF	15[A]	LYS
14	YF	15[B]	LYS
14	YF	15[C]	LYS
14	YF	15[D]	LYS
14	YF	15[E]	LYS
14	YF	15[F]	LYS
14	YF	16[A]	LEU
14	YF	16[B]	LEU
14	YF	16[C]	LEU
14	YF	16[D]	LEU
14	YF	16[E]	LEU
14	YF	16[F]	LEU

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Mol	Chain	Res	Type
14	YF	21[A]	ASP
14	YF	21[B]	ASP
14	YF	21[C]	ASP
14	YF	21[D]	ASP
14	YF	21[E]	ASP
14	YF	21[F]	ASP
14	YF	35[A]	ILE
14	YF	35[B]	ILE
14	YF	35[C]	ILE
14	YF	35[D]	ILE
14	YF	35[E]	ILE
14	YF	35[F]	ILE
14	YF	42[A]	ASP
14	YF	42[B]	ASP
14	YF	42[C]	ASP
14	YF	42[D]	ASP
14	YF	42[E]	ASP
14	YF	42[F]	ASP
14	YF	44[A]	LEU
14	YF	44[B]	LEU
14	YF	44[C]	LEU
14	YF	44[D]	LEU
14	YF	44[E]	LEU
14	YF	44[F]	LEU
14	YF	51[A]	MET
14	YF	51[B]	MET
14	YF	51[C]	MET
14	YF	51[D]	MET
14	YF	51[E]	MET
14	YF	51[F]	MET
14	YF	58[A]	LYS
14	YF	58[B]	LYS
14	YF	58[C]	LYS
14	YF	58[D]	LYS
14	YF	58[E]	LYS
14	YF	58[F]	LYS
14	YF	68[A]	GLU
14	YF	68[B]	GLU
14	YF	68[C]	GLU
14	YF	68[D]	GLU
14	YF	68[E]	GLU
14	YF	68[F]	GLU

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Mol	Chain	Res	Type
14	YF	74[A]	VAL
14	YF	74[B]	VAL
14	YF	74[C]	VAL
14	YF	74[D]	VAL
14	YF	74[E]	VAL
14	YF	74[F]	VAL
14	YF	80[A]	ILE
14	YF	80[B]	ILE
14	YF	80[C]	ILE
14	YF	80[D]	ILE
14	YF	80[E]	ILE
14	YF	80[F]	ILE
14	YF	87[A]	ILE
14	YF	87[B]	ILE
14	YF	87[C]	ILE
14	YF	87[D]	ILE
14	YF	87[E]	ILE
14	YF	87[F]	ILE
14	YF	90[A]	CYS
14	YF	90[B]	CYS
14	YF	90[C]	CYS
14	YF	90[D]	CYS
14	YF	90[E]	CYS
14	YF	90[F]	CYS
14	YF	104[A]	ILE
14	YF	104[B]	ILE
14	YF	104[C]	ILE
14	YF	104[D]	ILE
14	YF	104[E]	ILE
14	YF	104[F]	ILE
14	YF	107[A]	ILE
14	YF	107[B]	ILE
14	YF	107[C]	ILE
14	YF	107[D]	ILE
14	YF	107[E]	ILE
14	YF	107[F]	ILE
14	YF	109[A]	LEU
14	YF	109[B]	LEU
14	YF	109[C]	LEU
14	YF	109[D]	LEU
14	YF	109[E]	LEU
14	YF	109[F]	LEU

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Mol	Chain	Res	Type
14	YF	111[A]	THR
14	YF	111[B]	THR
14	YF	111[C]	THR
14	YF	111[D]	THR
14	YF	111[E]	THR
14	YF	111[F]	THR
14	YF	154[A]	ASN
14	YF	154[B]	ASN
14	YF	154[C]	ASN
14	YF	154[D]	ASN
14	YF	154[E]	ASN
14	YF	154[F]	ASN
14	YF	163[A]	THR
14	YF	163[B]	THR
14	YF	163[C]	THR
14	YF	163[D]	THR
14	YF	163[E]	THR
14	YF	163[F]	THR
14	YF	183[A]	ASP
14	YF	183[B]	ASP
14	YF	183[C]	ASP
14	YF	183[D]	ASP
14	YF	183[E]	ASP
14	YF	183[F]	ASP
14	YF	233[A]	ASP
14	YF	233[B]	ASP
14	YF	233[C]	ASP
14	YF	233[D]	ASP
14	YF	233[E]	ASP
14	YF	233[F]	ASP
14	YF	236[A]	TRP
14	YF	236[B]	TRP
14	YF	236[C]	TRP
14	YF	236[D]	TRP
14	YF	236[E]	TRP
14	YF	236[F]	TRP
14	YF	241[A]	ASN
14	YF	241[B]	ASN
14	YF	241[C]	ASN
14	YF	241[D]	ASN
14	YF	241[E]	ASN
14	YF	241[F]	ASN

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Mol	Chain	Res	Type
14	YF	267[A]	THR
14	YF	267[B]	THR
14	YF	267[C]	THR
14	YF	267[D]	THR
14	YF	267[E]	THR
14	YF	267[F]	THR
14	YF	296[A]	ILE
14	YF	296[B]	ILE
14	YF	296[C]	ILE
14	YF	296[D]	ILE
14	YF	296[E]	ILE
14	YF	296[F]	ILE
14	YF	305[A]	ASP
14	YF	305[B]	ASP
14	YF	305[C]	ASP
14	YF	305[D]	ASP
14	YF	305[E]	ASP
14	YF	305[F]	ASP
14	YF	312[A]	THR
14	YF	312[B]	THR
14	YF	312[C]	THR
14	YF	312[D]	THR
14	YF	312[E]	THR
14	YF	312[F]	THR
14	YF	315[A]	ASN
14	YF	315[B]	ASN
14	YF	315[C]	ASN
14	YF	315[D]	ASN
14	YF	315[E]	ASN
14	YF	315[F]	ASN
14	YF	318[A]	LEU
14	YF	318[B]	LEU
14	YF	318[C]	LEU
14	YF	318[D]	LEU
14	YF	318[E]	LEU
14	YF	318[F]	LEU
14	YF	325[A]	ILE
14	YF	325[B]	ILE
14	YF	325[C]	ILE
14	YF	325[D]	ILE
14	YF	325[E]	ILE
14	YF	325[F]	ILE

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Mol	Chain	Res	Type
14	YF	330[A]	LYS
14	YF	330[B]	LYS
14	YF	330[C]	LYS
14	YF	330[D]	LYS
14	YF	330[E]	LYS
14	YF	330[F]	LYS
14	YF	333[A]	PHE
14	YF	333[B]	PHE
14	YF	333[C]	PHE
14	YF	333[D]	PHE
14	YF	333[E]	PHE
14	YF	333[F]	PHE
14	YF	342[A]	VAL
14	YF	342[B]	VAL
14	YF	342[C]	VAL
14	YF	342[D]	VAL
14	YF	342[E]	VAL
14	YF	342[F]	VAL
14	YF	346[A]	LEU
14	YF	346[B]	LEU
14	YF	346[C]	LEU
14	YF	346[D]	LEU
14	YF	346[E]	LEU
14	YF	346[F]	LEU
14	YF	352[A]	VAL
14	YF	352[B]	VAL
14	YF	352[C]	VAL
14	YF	352[D]	VAL
14	YF	352[E]	VAL
14	YF	352[F]	VAL
14	YF	360[A]	ASN
14	YF	360[B]	ASN
14	YF	360[C]	ASN
14	YF	360[D]	ASN
14	YF	360[E]	ASN
14	YF	360[F]	ASN
14	YF	364[A]	LEU
14	YF	364[B]	LEU
14	YF	364[C]	LEU
14	YF	364[D]	LEU
14	YF	364[E]	LEU
14	YF	364[F]	LEU

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Mol	Chain	Res	Type
14	YF	365[A]	GLU
14	YF	365[B]	GLU
14	YF	365[C]	GLU
14	YF	365[D]	GLU
14	YF	365[E]	GLU
14	YF	365[F]	GLU
14	YF	366[A]	THR
14	YF	366[B]	THR
14	YF	366[C]	THR
14	YF	366[D]	THR
14	YF	366[E]	THR
14	YF	366[F]	THR
15	ZA	26[A]	GLN
15	ZA	26[B]	GLN
15	ZA	26[C]	GLN
15	ZA	26[D]	GLN
15	ZA	26[E]	GLN
15	ZA	26[F]	GLN
15	ZA	46[A]	HIS
15	ZA	46[B]	HIS
15	ZA	46[C]	HIS
15	ZA	46[D]	HIS
15	ZA	46[E]	HIS
15	ZA	46[F]	HIS
15	ZA	50[A]	LYS
15	ZA	50[B]	LYS
15	ZA	50[C]	LYS
15	ZA	50[D]	LYS
15	ZA	50[E]	LYS
15	ZA	50[F]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (602) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	159	ASN
1	A	246	ASN
1	A	255	ASN
1	A	303	ASN
1	A	434	GLN
1	A	490	ASN
1	A	644	ASN

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Mol	Chain	Res	Type
1	B	69	GLN
1	B	84	ASN
1	B	196	GLN
1	B	336	GLN
1	B	388	GLN
1	B	568	ASN
1	B	570	GLN
1	B	582	ASN
2	C	87	GLN
2	C	91	GLN
2	C	139	ASN
2	C	528	ASN
2	C	601	ASN
2	C	663	ASN
2	C	673	GLN
2	C	682	GLN
2	C	684	ASN
2	C	688	ASN
2	C	908	HIS
2	C	914	ASN
3	E	23	ASN
3	E	201	ASN
3	E	271	GLN
3	E	314	ASN
4	F	29	ASN
4	F	70	HIS
4	F	111	ASN
4	F	120	ASN
4	G	29	ASN
4	G	70	HIS
4	G	111	ASN
4	G	120	ASN
4	H	29	ASN
4	H	70	HIS
4	H	111	ASN
4	H	120	ASN
5	I	209	ASN
5	I	307	ASN
5	I	382	ASN
5	I	388	ASN
5	I	483	GLN
5	J	161	ASN

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Mol	Chain	Res	Type
5	J	198	ASN
5	J	305	ASN
5	J	382	ASN
5	J	440	GLN
5	J	504	ASN
5	J	514	HIS
5	K	127	ASN
5	K	150	GLN
5	K	198	ASN
5	K	305	ASN
5	K	318	GLN
5	K	377	HIS
5	K	410	GLN
5	K	421	ASN
5	K	440	GLN
5	K	444	ASN
5	K	483	GLN
5	K	498	ASN
5	K	504	ASN
6	L	31	ASN
6	L	164	GLN
6	M	31	ASN
6	M	164	GLN
6	M	205	ASN
6	N	31	ASN
6	N	164	GLN
7	O	24	ASN
7	O	233	GLN
7	O	389	ASN
7	O	441	GLN
7	O	520	ASN
7	P	111	ASN
7	P	166	GLN
7	P	167	GLN
7	P	233	GLN
7	P	327	GLN
7	P	329	ASN
7	P	389	ASN
7	Q	3	ASN
7	Q	139	ASN
7	Q	217	ASN
7	Q	233	GLN

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Mol	Chain	Res	Type
8	R	83	GLN
8	R	151	GLN
8	S	83	GLN
8	S	151	GLN
10	U	337	ASN
11	V	182	ASN
12	W	175	GLN
12	W	211	HIS
1	X	63	ASN
1	X	69	GLN
1	X	159	ASN
1	X	246	ASN
1	X	255	ASN
1	X	303	ASN
1	X	434	GLN
1	X	490	ASN
1	X	644	ASN
1	Y	69	GLN
1	Y	84	ASN
1	Y	196	GLN
1	Y	336	GLN
1	Y	388	GLN
1	Y	568	ASN
1	Y	570	GLN
1	Y	582	ASN
2	Z	87	GLN
2	Z	91	GLN
2	Z	139	ASN
2	Z	528	ASN
2	Z	601	ASN
2	Z	663	ASN
2	Z	673	GLN
2	Z	682	GLN
2	Z	684	ASN
2	Z	688	ASN
2	Z	908	HIS
2	Z	914	ASN
3	b	23	ASN
3	b	201	ASN
3	b	271	GLN
3	b	314	ASN
4	c	29	ASN

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Mol	Chain	Res	Type
4	c	70	HIS
4	c	111	ASN
4	c	120	ASN
4	d	29	ASN
4	d	70	HIS
4	d	111	ASN
4	d	120	ASN
4	d	155	ASN
4	e	29	ASN
4	e	70	HIS
4	e	111	ASN
4	e	120	ASN
5	f	209	ASN
5	f	307	ASN
5	f	382	ASN
5	f	388	ASN
5	f	483	GLN
5	g	161	ASN
5	g	198	ASN
5	g	305	ASN
5	g	382	ASN
5	g	440	GLN
5	g	504	ASN
5	g	514	HIS
5	g	588	ASN
5	h	127	ASN
5	h	150	GLN
5	h	198	ASN
5	h	305	ASN
5	h	318	GLN
5	h	377	HIS
5	h	410	GLN
5	h	421	ASN
5	h	440	GLN
5	h	444	ASN
5	h	483	GLN
5	h	498	ASN
5	h	504	ASN
6	i	31	ASN
6	i	164	GLN
6	j	31	ASN
6	j	205	ASN

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Mol	Chain	Res	Type
6	k	31	ASN
6	k	164	GLN
7	l	24	ASN
7	l	233	GLN
7	l	389	ASN
7	l	441	GLN
7	l	520	ASN
7	m	111	ASN
7	m	166	GLN
7	m	167	GLN
7	m	233	GLN
7	m	327	GLN
7	m	329	ASN
7	m	389	ASN
7	n	3	ASN
7	n	139	ASN
7	n	217	ASN
7	n	233	GLN
8	o	83	GLN
8	o	151	GLN
8	p	83	GLN
8	p	151	GLN
11	s	182	ASN
12	t	175	GLN
12	t	211	HIS
1	u	63	ASN
1	u	69	GLN
1	u	159	ASN
1	u	246	ASN
1	u	255	ASN
1	u	303	ASN
1	u	434	GLN
1	u	490	ASN
1	u	644	ASN
1	v	69	GLN
1	v	84	ASN
1	v	196	GLN
1	v	336	GLN
1	v	388	GLN
1	v	568	ASN
1	v	570	GLN
1	v	582	ASN

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Mol	Chain	Res	Type
2	w	87	GLN
2	w	91	GLN
2	w	139	ASN
2	w	528	ASN
2	w	601	ASN
2	w	663	ASN
2	w	673	GLN
2	w	682	GLN
2	w	684	ASN
2	w	688	ASN
2	w	908	HIS
2	w	914	ASN
3	y	23	ASN
3	y	201	ASN
3	y	271	GLN
3	y	314	ASN
4	z	29	ASN
4	z	70	HIS
4	z	111	ASN
4	z	120	ASN
4	AA	29	ASN
4	AA	70	HIS
4	AA	111	ASN
4	AA	120	ASN
4	AB	29	ASN
4	AB	70	HIS
4	AB	111	ASN
4	AB	120	ASN
5	AC	209	ASN
5	AC	307	ASN
5	AC	382	ASN
5	AC	388	ASN
5	AC	483	GLN
5	AD	161	ASN
5	AD	198	ASN
5	AD	305	ASN
5	AD	382	ASN
5	AD	440	GLN
5	AD	504	ASN
5	AD	514	HIS
5	AD	588	ASN
5	AE	127	ASN

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Mol	Chain	Res	Type
5	AE	150	GLN
5	AE	198	ASN
5	AE	305	ASN
5	AE	318	GLN
5	AE	377	HIS
5	AE	410	GLN
5	AE	421	ASN
5	AE	440	GLN
5	AE	444	ASN
5	AE	483	GLN
5	AE	498	ASN
5	AE	504	ASN
6	AF	31	ASN
6	AF	164	GLN
6	AG	31	ASN
6	AG	205	ASN
6	AH	31	ASN
6	AH	164	GLN
7	AI	24	ASN
7	AI	233	GLN
7	AI	389	ASN
7	AI	441	GLN
7	AI	520	ASN
7	AJ	111	ASN
7	AJ	166	GLN
7	AJ	167	GLN
7	AJ	233	GLN
7	AJ	327	GLN
7	AJ	329	ASN
7	AJ	389	ASN
7	BA	3	ASN
7	BA	139	ASN
7	BA	217	ASN
7	BA	233	GLN
8	BB	83	GLN
8	BB	151	GLN
8	BC	83	GLN
8	BC	151	GLN
10	BE	337	ASN
11	BF	182	ASN
12	BG	175	GLN
12	BG	211	HIS

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Mol	Chain	Res	Type
1	BH	63	ASN
1	BH	69	GLN
1	BH	159	ASN
1	BH	246	ASN
1	BH	255	ASN
1	BH	303	ASN
1	BH	434	GLN
1	BH	490	ASN
1	BH	644	ASN
1	BI	69	GLN
1	BI	84	ASN
1	BI	196	GLN
1	BI	336	GLN
1	BI	388	GLN
1	BI	568	ASN
1	BI	570	GLN
1	BI	582	ASN
2	BJ	87	GLN
2	BJ	91	GLN
2	BJ	139	ASN
2	BJ	528	ASN
2	BJ	663	ASN
2	BJ	673	GLN
2	BJ	682	GLN
2	BJ	684	ASN
2	BJ	688	ASN
2	BJ	908	HIS
2	BJ	914	ASN
3	CB	23	ASN
3	CB	201	ASN
3	CB	271	GLN
3	CB	314	ASN
4	CC	29	ASN
4	CC	70	HIS
4	CC	111	ASN
4	CC	120	ASN
4	CD	29	ASN
4	CD	70	HIS
4	CD	111	ASN
4	CD	120	ASN
4	CE	29	ASN
4	CE	70	HIS

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Mol	Chain	Res	Type
4	CE	120	ASN
5	CF	209	ASN
5	CF	307	ASN
5	CF	382	ASN
5	CF	388	ASN
5	CF	483	GLN
5	CG	161	ASN
5	CG	198	ASN
5	CG	305	ASN
5	CG	382	ASN
5	CG	440	GLN
5	CG	504	ASN
5	CG	514	HIS
5	CG	588	ASN
5	CH	127	ASN
5	CH	150	GLN
5	CH	198	ASN
5	CH	305	ASN
5	CH	318	GLN
5	CH	377	HIS
5	CH	410	GLN
5	CH	421	ASN
5	CH	440	GLN
5	CH	444	ASN
5	CH	483	GLN
5	CH	498	ASN
5	CH	504	ASN
6	CI	31	ASN
6	CI	164	GLN
6	CJ	31	ASN
6	CJ	164	GLN
6	CJ	205	ASN
6	DA	31	ASN
6	DA	164	GLN
7	DB	24	ASN
7	DB	233	GLN
7	DB	389	ASN
7	DB	441	GLN
7	DB	520	ASN
7	DC	111	ASN
7	DC	166	GLN
7	DC	167	GLN

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Mol	Chain	Res	Type
7	DC	233	GLN
7	DC	327	GLN
7	DC	329	ASN
7	DC	389	ASN
7	DD	3	ASN
7	DD	139	ASN
7	DD	217	ASN
7	DD	233	GLN
8	DE	83	GLN
8	DE	151	GLN
8	DF	83	GLN
8	DF	151	GLN
11	DI	182	ASN
12	DJ	175	GLN
12	DJ	211	HIS
1	EA	63	ASN
1	EA	69	GLN
1	EA	159	ASN
1	EA	246	ASN
1	EA	255	ASN
1	EA	303	ASN
1	EA	434	GLN
1	EA	490	ASN
1	EA	644	ASN
1	EB	69	GLN
1	EB	84	ASN
1	EB	196	GLN
1	EB	336	GLN
1	EB	388	GLN
1	EB	568	ASN
1	EB	570	GLN
1	EB	582	ASN
2	EC	87	GLN
2	EC	91	GLN
2	EC	139	ASN
2	EC	528	ASN
2	EC	663	ASN
2	EC	673	GLN
2	EC	682	GLN
2	EC	908	HIS
2	EC	914	ASN
3	EE	23	ASN

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Mol	Chain	Res	Type
3	EE	201	ASN
3	EE	271	GLN
3	EE	314	ASN
4	EF	29	ASN
4	EF	70	HIS
4	EF	111	ASN
4	EF	120	ASN
4	EG	29	ASN
4	EG	70	HIS
4	EG	111	ASN
4	EG	120	ASN
4	EG	155	ASN
4	EH	29	ASN
4	EH	70	HIS
4	EH	120	ASN
5	EI	209	ASN
5	EI	307	ASN
5	EI	382	ASN
5	EI	388	ASN
5	EI	483	GLN
5	EI	588	ASN
5	EJ	161	ASN
5	EJ	198	ASN
5	EJ	305	ASN
5	EJ	382	ASN
5	EJ	440	GLN
5	EJ	504	ASN
5	EJ	514	HIS
5	FA	127	ASN
5	FA	150	GLN
5	FA	198	ASN
5	FA	305	ASN
5	FA	318	GLN
5	FA	377	HIS
5	FA	410	GLN
5	FA	421	ASN
5	FA	440	GLN
5	FA	444	ASN
5	FA	483	GLN
5	FA	498	ASN
5	FA	504	ASN
6	FB	164	GLN

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Mol	Chain	Res	Type
6	FC	31	ASN
6	FC	164	GLN
6	FC	205	ASN
6	FD	31	ASN
6	FD	164	GLN
7	FE	24	ASN
7	FE	233	GLN
7	FE	389	ASN
7	FE	441	GLN
7	FE	520	ASN
7	FF	111	ASN
7	FF	167	GLN
7	FF	233	GLN
7	FF	327	GLN
7	FF	329	ASN
7	FF	389	ASN
7	FG	3	ASN
7	FG	139	ASN
7	FG	217	ASN
7	FG	233	GLN
8	FH	83	GLN
8	FH	151	GLN
8	FI	83	GLN
8	FI	115	GLN
8	FI	151	GLN
10	GA	337	ASN
11	GB	182	ASN
12	GC	175	GLN
12	GC	211	HIS
1	GD	63	ASN
1	GD	69	GLN
1	GD	159	ASN
1	GD	246	ASN
1	GD	255	ASN
1	GD	303	ASN
1	GD	434	GLN
1	GD	490	ASN
1	GD	644	ASN
1	GE	69	GLN
1	GE	84	ASN
1	GE	196	GLN
1	GE	336	GLN

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Mol	Chain	Res	Type
1	GE	388	GLN
1	GE	568	ASN
1	GE	570	GLN
1	GE	582	ASN
2	GF	87	GLN
2	GF	91	GLN
2	GF	139	ASN
2	GF	333	ASN
2	GF	528	ASN
2	GF	663	ASN
2	GF	673	GLN
2	GF	682	GLN
2	GF	684	ASN
2	GF	688	ASN
2	GF	908	HIS
2	GF	914	ASN
3	GH	23	ASN
3	GH	201	ASN
3	GH	271	GLN
3	GH	314	ASN
4	GI	29	ASN
4	GI	70	HIS
4	GI	111	ASN
4	GI	120	ASN
4	GJ	29	ASN
4	GJ	70	HIS
4	GJ	111	ASN
4	GJ	120	ASN
4	GJ	155	ASN
4	HA	29	ASN
4	HA	70	HIS
4	HA	111	ASN
4	HA	120	ASN
5	HB	209	ASN
5	HB	307	ASN
5	HB	388	ASN
5	HB	483	GLN
5	HB	588	ASN
5	HC	161	ASN
5	HC	198	ASN
5	HC	305	ASN
5	HC	382	ASN

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Mol	Chain	Res	Type
5	HC	440	GLN
5	HC	504	ASN
5	HC	514	HIS
5	HD	127	ASN
5	HD	150	GLN
5	HD	198	ASN
5	HD	305	ASN
5	HD	318	GLN
5	HD	377	HIS
5	HD	410	GLN
5	HD	421	ASN
5	HD	440	GLN
5	HD	444	ASN
5	HD	483	GLN
5	HD	498	ASN
5	HD	504	ASN
6	HE	31	ASN
6	HE	164	GLN
6	HF	31	ASN
6	HF	164	GLN
6	HF	205	ASN
6	HG	31	ASN
6	HG	164	GLN
7	HH	24	ASN
7	HH	233	GLN
7	HH	389	ASN
7	HH	441	GLN
7	HH	520	ASN
7	HI	111	ASN
7	HI	166	GLN
7	HI	167	GLN
7	HI	233	GLN
7	HI	327	GLN
7	HI	329	ASN
7	HI	389	ASN
7	HJ	3	ASN
7	HJ	139	ASN
7	HJ	217	ASN
7	HJ	233	GLN
8	IA	83	GLN
8	IA	151	GLN
8	IB	83	GLN

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Mol	Chain	Res	Type
8	IB	115	GLN
8	IB	151	GLN
9	IC	83	ASN
11	IE	182	ASN
12	IF	175	GLN
12	IF	211	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
13	YA	17
13	YB	17
13	YC	17
15	ZA	5
14	YD	5
14	YE	5
14	YF	5
5	CG	1
5	EJ	1
5	J	1
7	Q	1
5	g	1
7	n	1
5	AD	1
7	BA	1
7	DD	1
7	FG	1
5	HC	1
7	HJ	1
1	B	1
2	C	1
1	Y	1
2	Z	1
1	v	1
2	w	1
1	BI	1
2	BJ	1
1	EB	1
2	EC	1
1	GE	1
2	GF	1
3	D	1
3	a	1
3	x	1
3	CA	1
3	ED	1
3	GG	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	YA	76[E]:PRO	C	77[E]:VAL	N	10.44
1	YB	76[E]:PRO	C	77[E]:VAL	N	10.44
1	YC	76[E]:PRO	C	77[E]:VAL	N	10.44

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	YC	76[B]:PRO	C	77[B]:VAL	N	9.41
1	YA	76[B]:PRO	C	77[B]:VAL	N	9.40
1	YB	76[B]:PRO	C	77[B]:VAL	N	9.40
1	YA	76[C]:PRO	C	77[C]:VAL	N	9.29
1	YB	76[C]:PRO	C	77[C]:VAL	N	9.29
1	YC	76[C]:PRO	C	77[C]:VAL	N	9.29
1	YA	76[F]:PRO	C	77[F]:VAL	N	9.21
1	YB	76[F]:PRO	C	77[F]:VAL	N	9.21
1	YC	76[F]:PRO	C	77[F]:VAL	N	9.21
1	YA	76[D]:PRO	C	77[D]:VAL	N	9.00
1	YA	76[A]:PRO	C	77[A]:VAL	N	9.00
1	YB	76[D]:PRO	C	77[D]:VAL	N	9.00
1	YB	76[A]:PRO	C	77[A]:VAL	N	9.00
1	YC	76[D]:PRO	C	77[D]:VAL	N	9.00
1	YC	76[A]:PRO	C	77[A]:VAL	N	9.00
1	YA	112[B]:GLU	C	113[B]:GLY	N	3.79
1	YA	112[E]:GLU	C	113[E]:GLY	N	3.79
1	YA	112[D]:GLU	C	113[D]:GLY	N	3.79
1	YA	112[A]:GLU	C	113[A]:GLY	N	3.79
1	YB	112[B]:GLU	C	113[B]:GLY	N	3.79
1	YB	112[E]:GLU	C	113[E]:GLY	N	3.79
1	YB	112[D]:GLU	C	113[D]:GLY	N	3.79
1	YB	112[A]:GLU	C	113[A]:GLY	N	3.79
1	YC	112[E]:GLU	C	113[E]:GLY	N	3.79
1	YC	112[B]:GLU	C	113[B]:GLY	N	3.79
1	YC	112[D]:GLU	C	113[D]:GLY	N	3.79
1	YC	112[A]:GLU	C	113[A]:GLY	N	3.79
1	YA	112[F]:GLU	C	113[F]:GLY	N	3.78
1	YA	112[C]:GLU	C	113[C]:GLY	N	3.78
1	YB	112[F]:GLU	C	113[F]:GLY	N	3.78
1	YB	112[C]:GLU	C	113[C]:GLY	N	3.78
1	YC	112[F]:GLU	C	113[F]:GLY	N	3.78
1	YC	112[C]:GLU	C	113[C]:GLY	N	3.78
1	YA	574[B]:ILE	C	575[B]:GLY	N	3.02
1	YA	574[E]:ILE	C	575[E]:GLY	N	3.02
1	YA	574[C]:ILE	C	575[C]:GLY	N	3.02
1	YA	574[D]:ILE	C	575[D]:GLY	N	3.02
1	YA	574[F]:ILE	C	575[F]:GLY	N	3.02
1	YB	574[E]:ILE	C	575[E]:GLY	N	3.02
1	YB	574[B]:ILE	C	575[B]:GLY	N	3.02
1	YB	574[D]:ILE	C	575[D]:GLY	N	3.02
1	YB	574[C]:ILE	C	575[C]:GLY	N	3.02

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	YB	574[F]:ILE	C	575[F]:GLY	N	3.02
1	YC	574[E]:ILE	C	575[E]:GLY	N	3.02
1	YC	574[C]:ILE	C	575[C]:GLY	N	3.02
1	YC	574[B]:ILE	C	575[B]:GLY	N	3.02
1	YC	574[D]:ILE	C	575[D]:GLY	N	3.02
1	YC	574[F]:ILE	C	575[F]:GLY	N	3.02
1	ZA	96[B]:ILE	C	97[B]:LYS	N	2.95
1	ZA	96[E]:ILE	C	97[E]:LYS	N	2.95
1	ZA	96[C]:ILE	C	97[C]:LYS	N	2.94
1	ZA	96[F]:ILE	C	97[F]:LYS	N	2.94
1	ZA	96[D]:ILE	C	97[D]:LYS	N	2.94
1	YD	375[D]:GLU	C	376[D]:PHE	N	2.90
1	YD	375[C]:GLU	C	376[C]:PHE	N	2.90
1	YD	375[B]:GLU	C	376[B]:PHE	N	2.90
1	YD	375[E]:GLU	C	376[E]:PHE	N	2.90
1	YD	375[F]:GLU	C	376[F]:PHE	N	2.90
1	YE	375[D]:GLU	C	376[D]:PHE	N	2.90
1	YE	375[E]:GLU	C	376[E]:PHE	N	2.90
1	YE	375[B]:GLU	C	376[B]:PHE	N	2.90
1	YE	375[C]:GLU	C	376[C]:PHE	N	2.90
1	YE	375[F]:GLU	C	376[F]:PHE	N	2.90
1	YF	375[D]:GLU	C	376[D]:PHE	N	2.90
1	YF	375[C]:GLU	C	376[C]:PHE	N	2.90
1	YF	375[B]:GLU	C	376[B]:PHE	N	2.90
1	YF	375[E]:GLU	C	376[E]:PHE	N	2.90
1	YF	375[F]:GLU	C	376[F]:PHE	N	2.90
1	CG	531:ASN	C	532:LEU	N	1.19
1	EJ	531:ASN	C	532:LEU	N	1.19
1	J	531:ASN	C	532:LEU	N	1.18
1	Q	26:PRO	C	27:PRO	N	1.18
1	g	531:ASN	C	532:LEU	N	1.18
1	n	26:PRO	C	27:PRO	N	1.18
1	AD	531:ASN	C	532:LEU	N	1.18
1	BA	26:PRO	C	27:PRO	N	1.18
1	DD	26:PRO	C	27:PRO	N	1.18
1	FG	26:PRO	C	27:PRO	N	1.18
1	HC	531:ASN	C	532:LEU	N	1.18
1	HJ	26:PRO	C	27:PRO	N	1.18
1	B	307:ASP	C	308:PRO	N	1.10
1	C	652:MET	C	653:MET	N	1.10
1	Y	307:ASP	C	308:PRO	N	1.10
1	Z	652:MET	C	653:MET	N	1.10

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	307:ASP	C	308:PRO	N	1.10
1	w	652:MET	C	653:MET	N	1.10
1	BI	307:ASP	C	308:PRO	N	1.10
1	BJ	652:MET	C	653:MET	N	1.10
1	EB	307:ASP	C	308:PRO	N	1.10
1	EC	652:MET	C	653:MET	N	1.10
1	GE	307:ASP	C	308:PRO	N	1.10
1	GF	652:MET	C	653:MET	N	1.10
1	D	258:PHE	C	259:PRO	N	0.94
1	a	258:PHE	C	259:PRO	N	0.94
1	x	258:PHE	C	259:PRO	N	0.94
1	CA	258:PHE	C	259:PRO	N	0.94
1	ED	258:PHE	C	259:PRO	N	0.94
1	GG	258:PHE	C	259:PRO	N	0.94

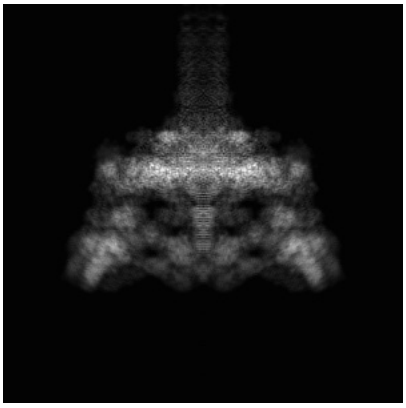
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3374. These allow visual inspection of the internal detail of the map and identification of artifacts.

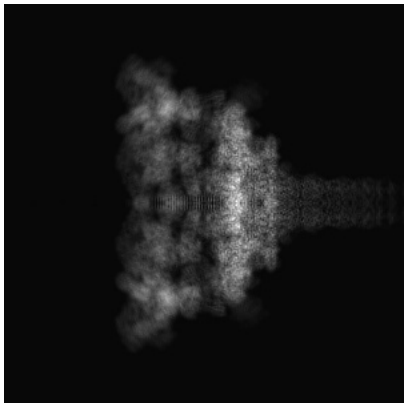
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

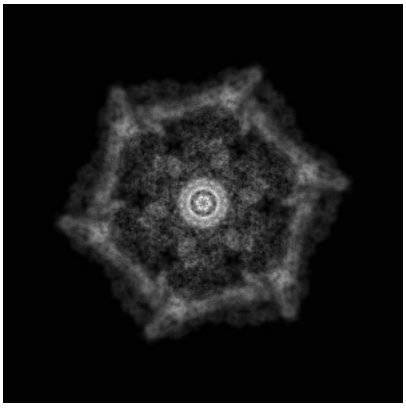
6.1.1 Primary map



X



Y

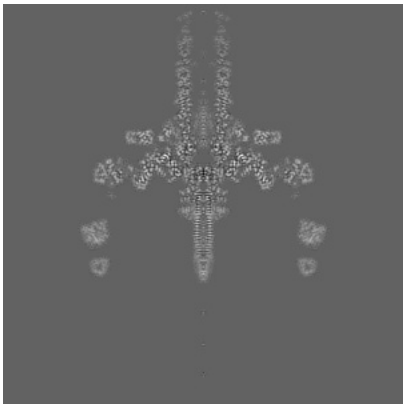


Z

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

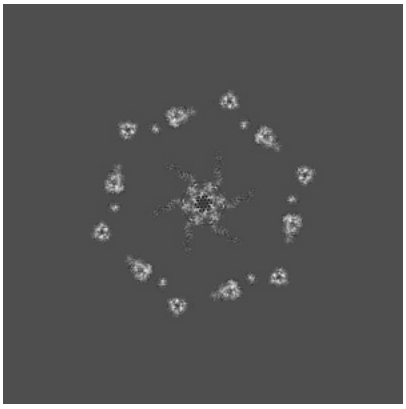
6.2 Central slices (i)

6.2.1 Primary map



X Index: 240

Y Index: 240

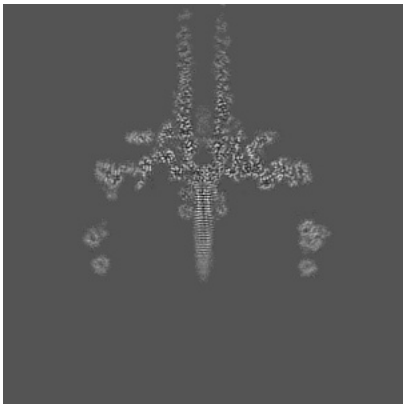


Z Index: 240

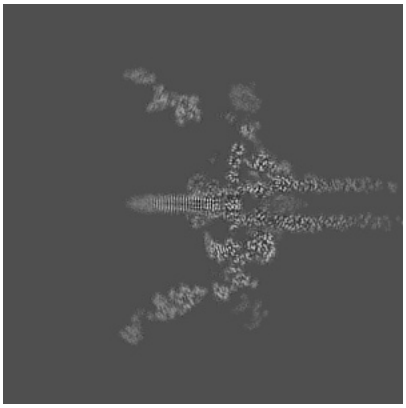
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

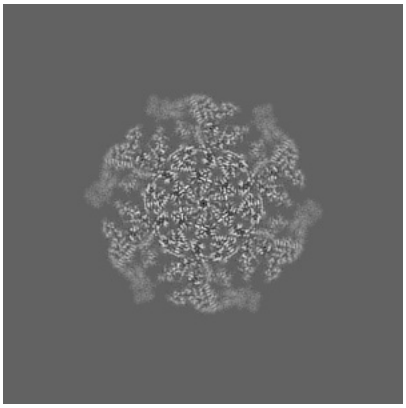
6.3.1 Primary map



X Index: 245



Y Index: 235

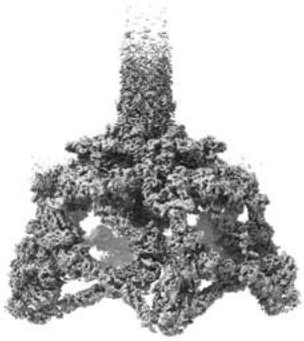


Z Index: 279

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 0.0263. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

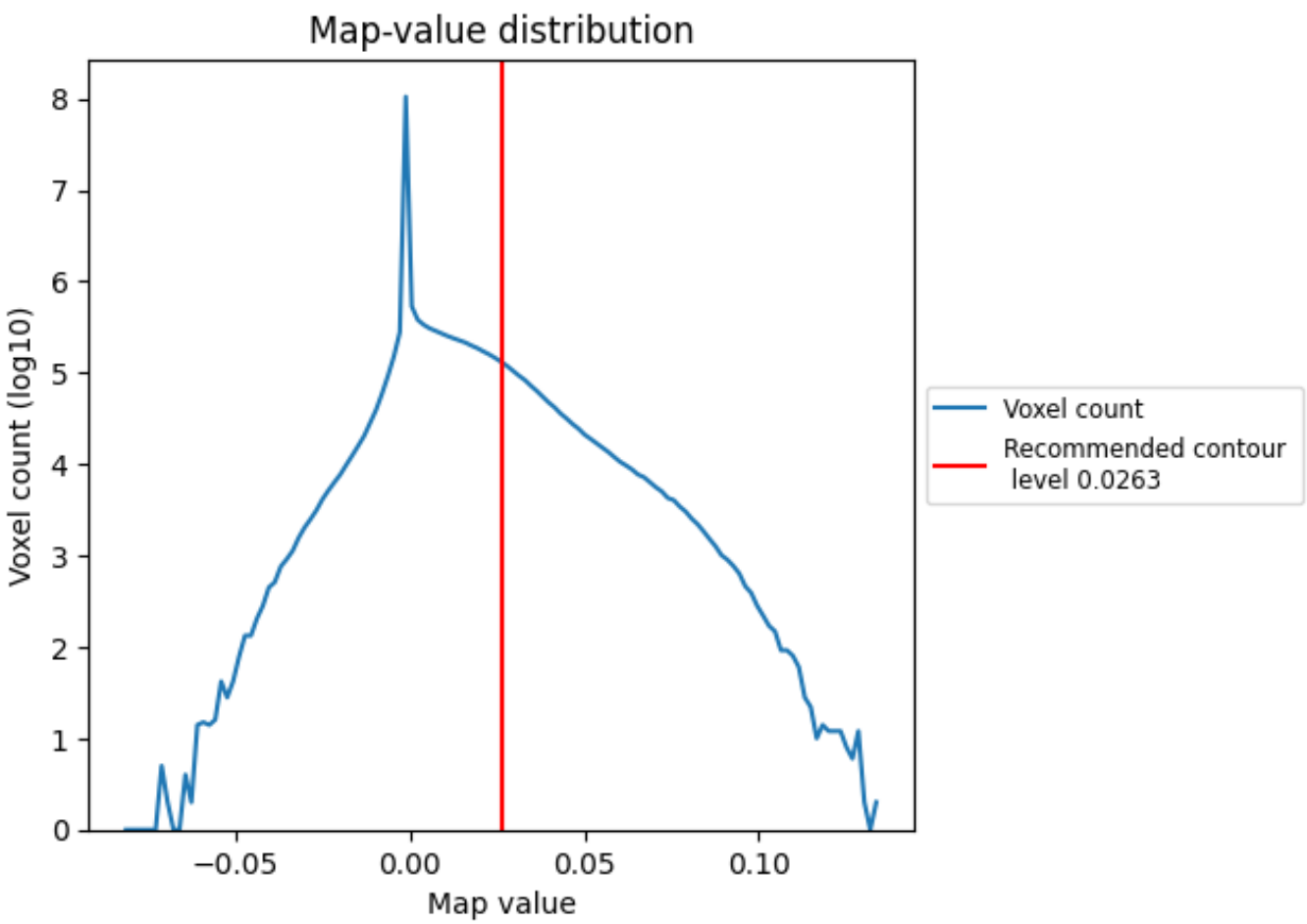
6.5 Mask visualisation (i)

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

7 Map analysis (i)

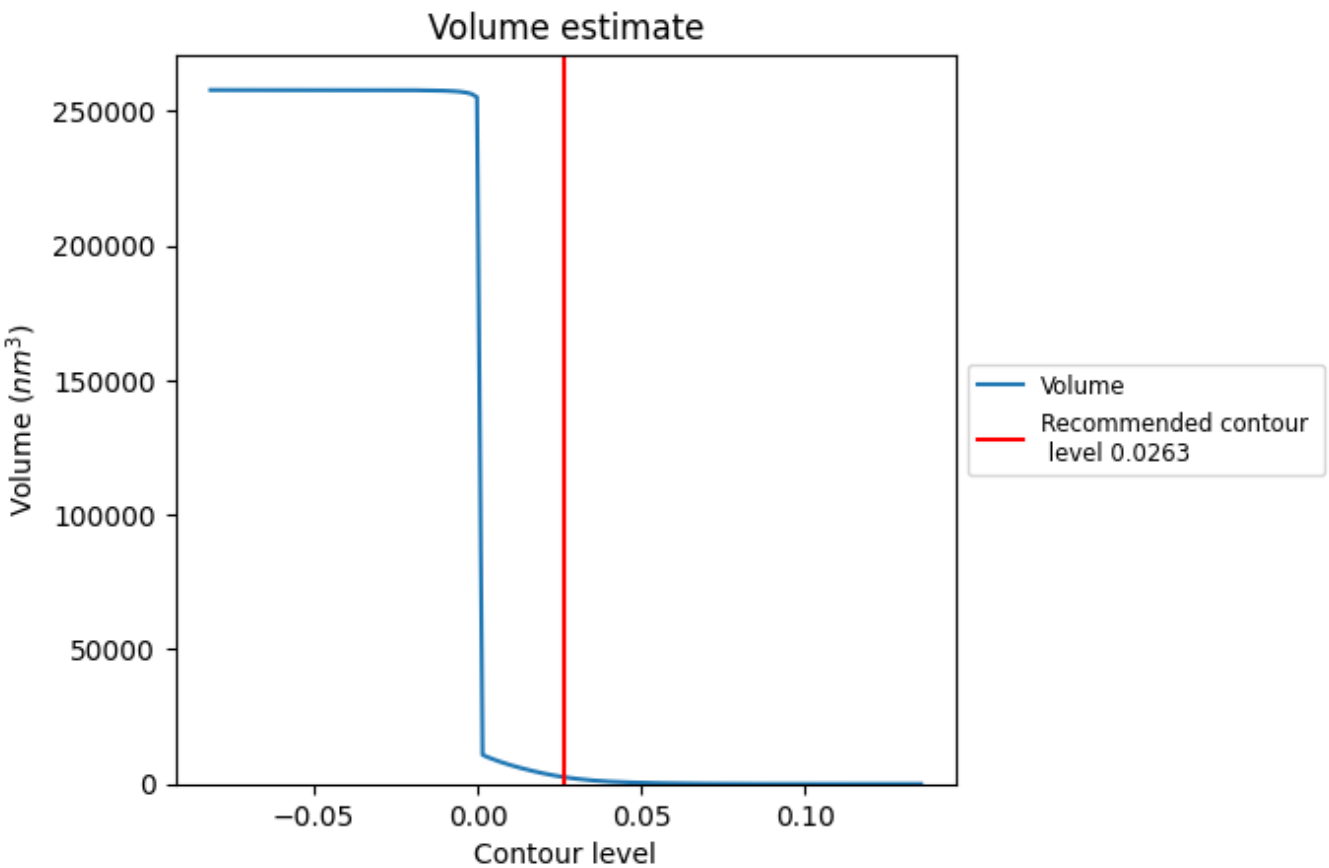
This section contains the results of statistical analysis of the map.

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.

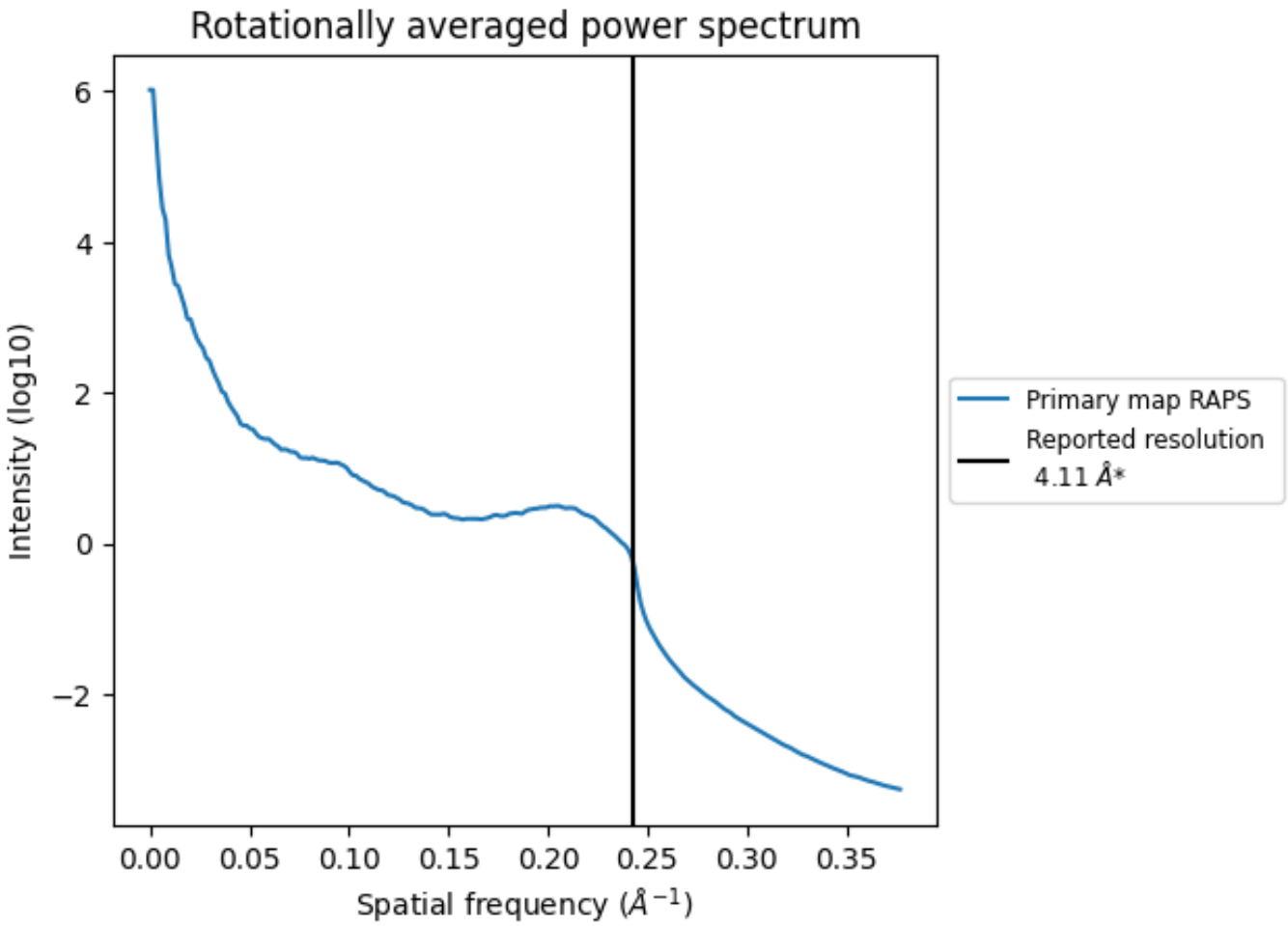
7.2 Volume estimate (i)



The volume at the recommended contour level is 2570 nm^3; this corresponds to an approximate mass of 2322 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)

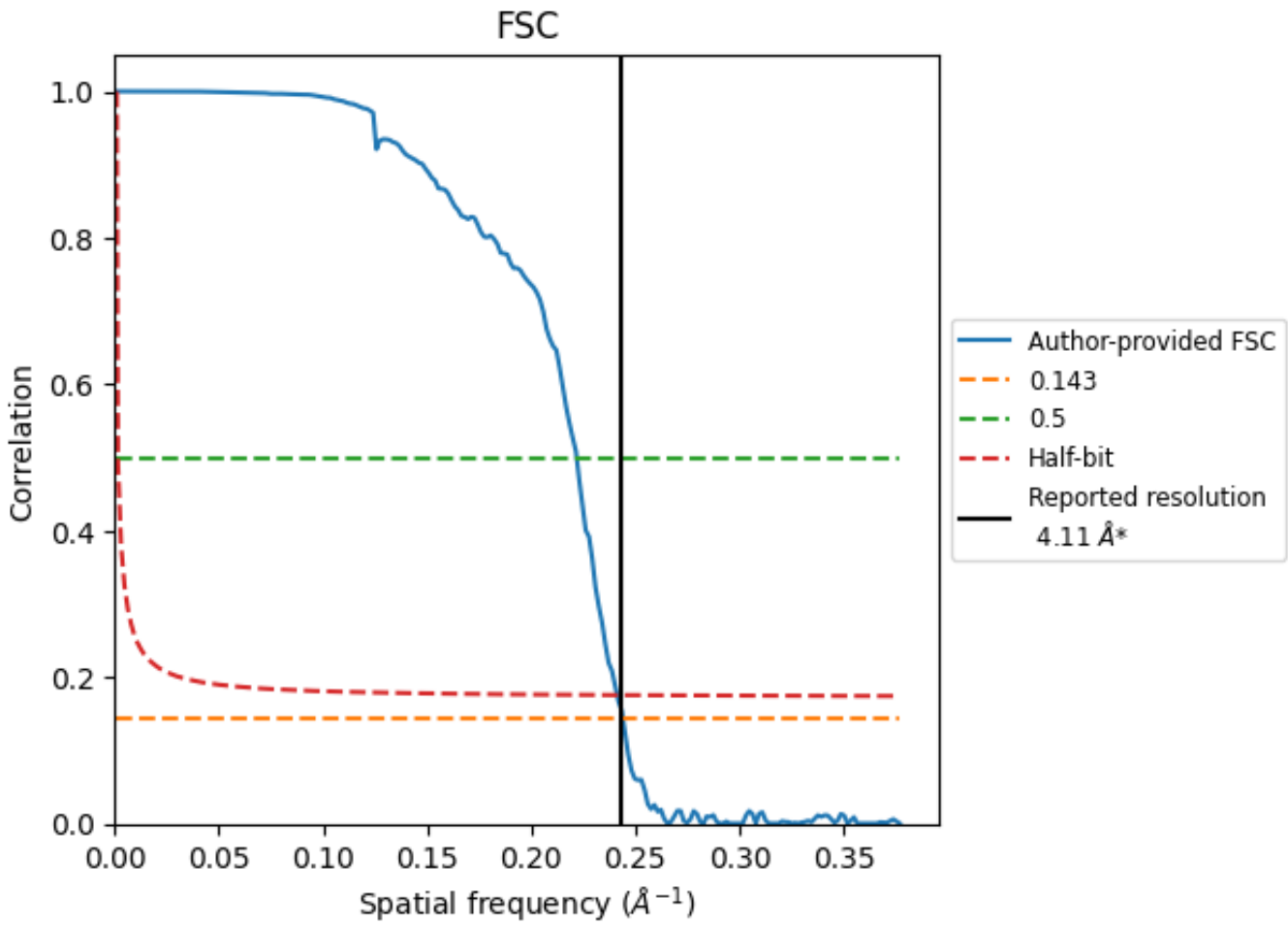


*Reported resolution corresponds to spatial frequency of 0.243 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.243 Å^{-1}

8.2 Resolution estimates (i)

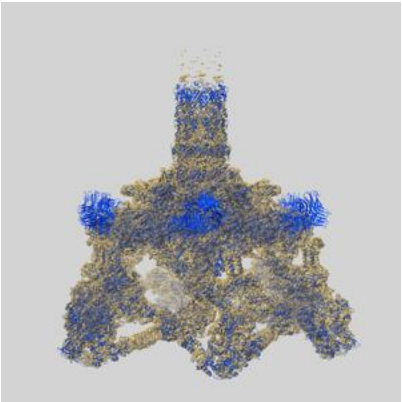
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.11	-	-
Author-provided FSC curve	4.10	4.51	4.14
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

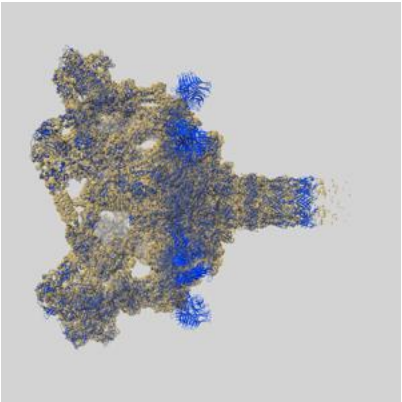
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3374 and PDB model 5IV5. Per-residue inclusion information can be found in section 3 on page 18.

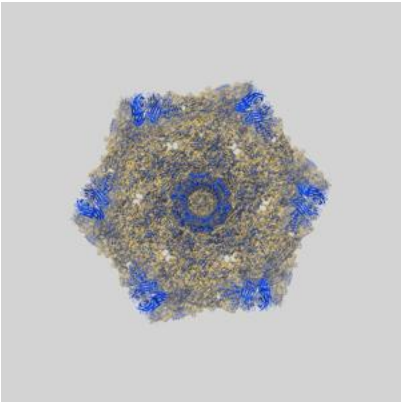
9.1 Map-model overlay (i)



X



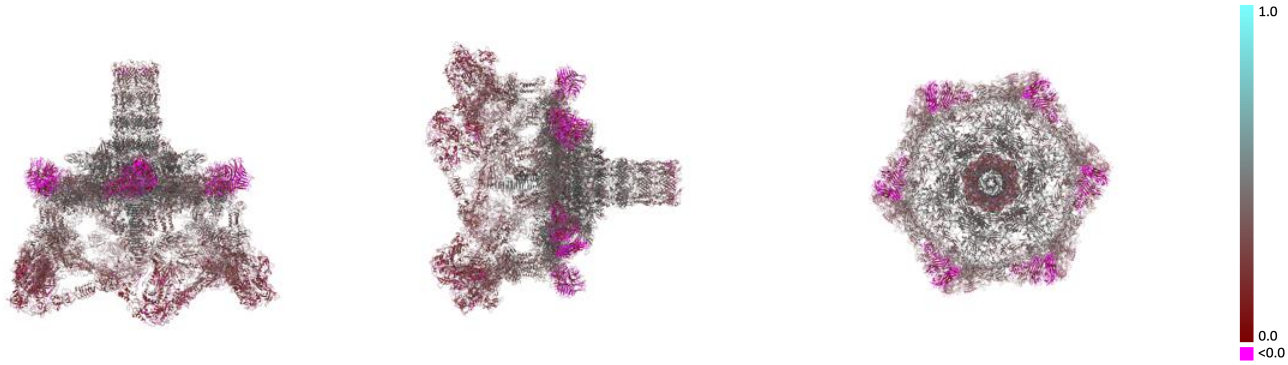
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0263 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.

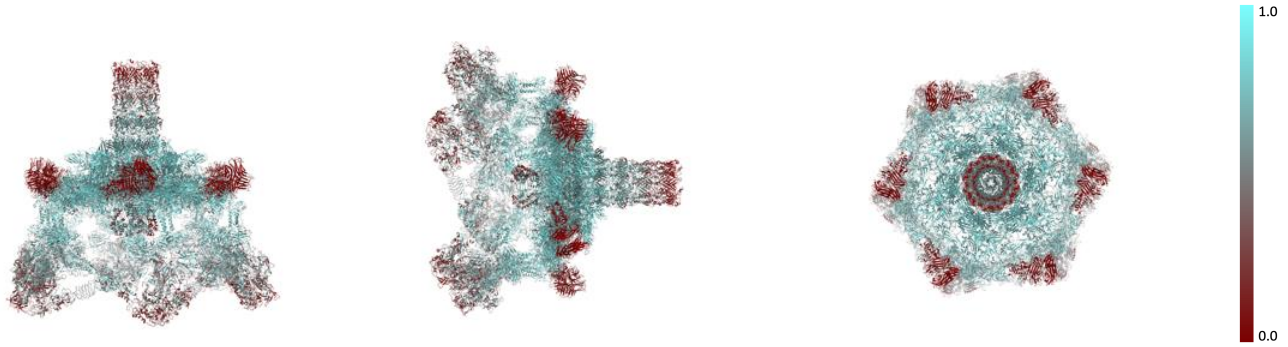
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

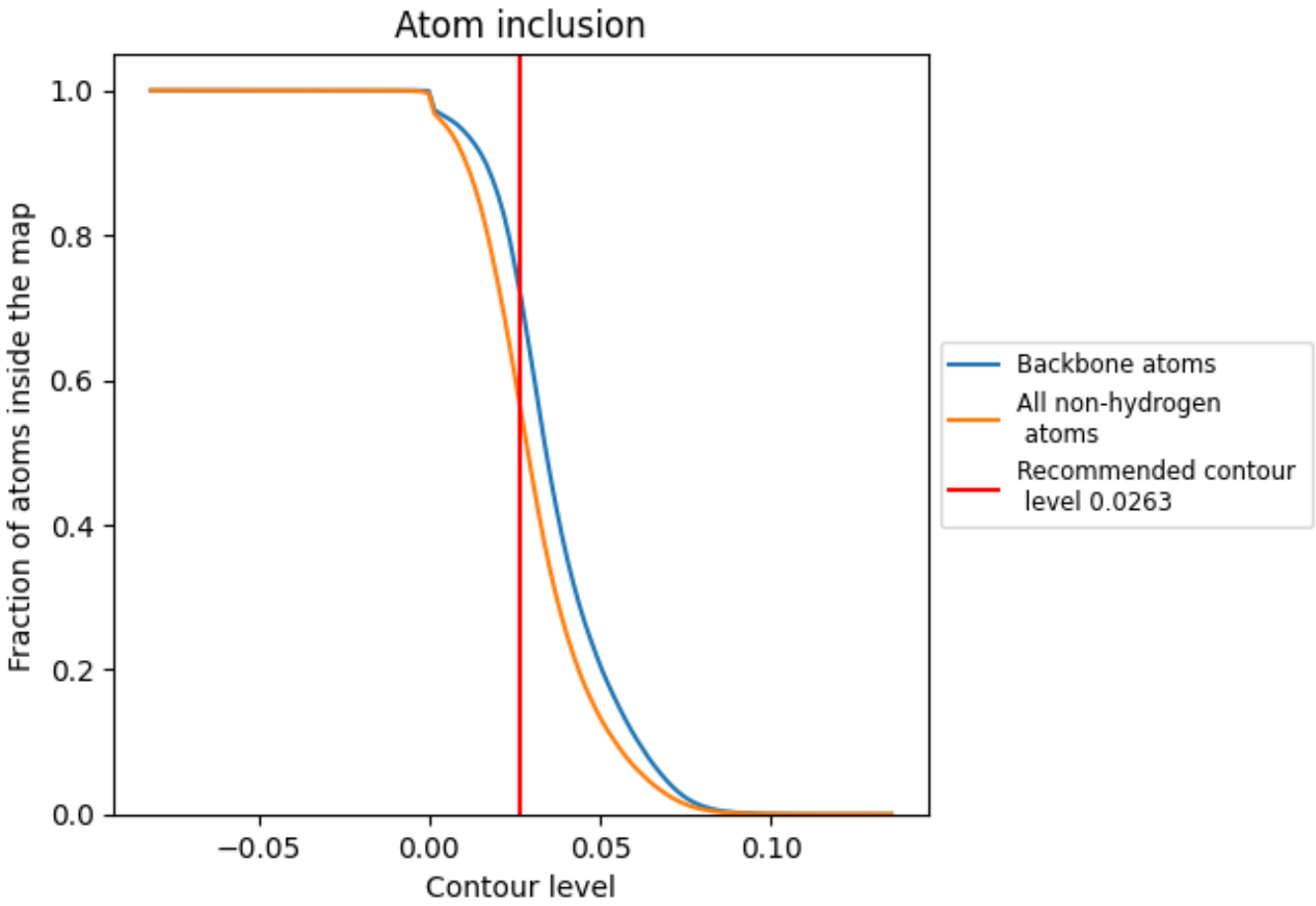
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0263).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 57% 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 (0.0263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5713	0.3120
A	0.7790	0.4270
AA	0.0242	0.0250
AB	0.0177	0.0150
AC	0.6280	0.3190
AD	0.6350	0.3060
AE	0.6306	0.3080
AF	0.3745	0.2050
AG	0.3398	0.1850
AH	0.3629	0.1880
AI	0.5257	0.2540
AJ	0.4966	0.2420
B	0.7657	0.4140
BA	0.5248	0.2550
BB	0.4163	0.3710
BC	0.1406	0.2800
BD	0.7273	0.3890
BE	0.6925	0.4360
BF	0.8081	0.4290
BG	0.5847	0.4080
BH	0.7823	0.4290
BI	0.7687	0.4160
BJ	0.7378	0.3810
C	0.7366	0.3790
CA	0.7678	0.4040
CB	0.7921	0.4170
CC	0.0088	0.0120
CD	0.0261	0.0320
CE	0.0158	0.0180
CF	0.6300	0.3180
CG	0.6345	0.3070
CH	0.6317	0.3090
CI	0.3678	0.2050
CJ	0.3331	0.1840
D	0.7658	0.4030

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Chain	Atom inclusion	Q-score
DA	0.3587	0.1910
DB	0.5265	0.2530
DC	0.5018	0.2410
DD	0.5251	0.2550
DE	0.4124	0.3720
DF	0.1445	0.2820
DG	0.7242	0.3920
DH	0.6886	0.4380
DI	0.8049	0.4290
DJ	0.5861	0.4070
E	0.7933	0.4160
EA	0.7827	0.4290
EB	0.7683	0.4150
EC	0.7372	0.3800
ED	0.7666	0.4030
EE	0.7910	0.4170
EF	0.0079	0.0130
EG	0.0233	0.0240
EH	0.0149	0.0220
EI	0.6256	0.3180
EJ	0.6335	0.3060
F	0.0079	0.0120
FA	0.6280	0.3100
FB	0.3793	0.2070
FC	0.3350	0.1850
FD	0.3787	0.1910
FE	0.5335	0.2530
FF	0.5044	0.2420
FG	0.5290	0.2540
FH	0.4069	0.3730
FI	0.1453	0.2770
FJ	0.7202	0.3910
G	0.0237	0.0320
GA	0.7026	0.4390
GB	0.8055	0.4290
GC	0.5814	0.4080
GD	0.7802	0.4280
GE	0.7681	0.4150
GF	0.7408	0.3810
GG	0.7643	0.4030
GH	0.7906	0.4170
GI	0.0102	0.0150

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Chain	Atom inclusion	Q-score
GJ	0.0251	0.0240
H	0.0144	0.0180
HA	0.0168	0.0190
HB	0.6278	0.3180
HC	0.6335	0.3070
HD	0.6339	0.3100
HE	0.3793	0.2050
HF	0.3356	0.1830
HG	0.3647	0.1890
HH	0.5234	0.2550
HI	0.4948	0.2440
HJ	0.5194	0.2540
I	0.6298	0.3170
IA	0.4085	0.3720
IB	0.1445	0.2810
IC	0.7242	0.3890
ID	0.6995	0.4410
IE	0.8030	0.4270
IF	0.5908	0.4040
J	0.6341	0.3060
K	0.6298	0.3080
L	0.3690	0.2010
M	0.3295	0.1840
N	0.3581	0.1880
O	0.5213	0.2540
P	0.4990	0.2430
Q	0.5264	0.2550
R	0.4108	0.3750
S	0.1406	0.2830
T	0.7192	0.3900
U	0.6909	0.4360
V	0.8042	0.4290
W	0.5847	0.4060
X	0.7802	0.4260
Y	0.7671	0.4120
YA	0.5394	0.4140
YB	0.5365	0.4230
YC	0.5370	0.4180
YD	0.6343	0.4410
YE	0.6340	0.4410
YF	0.6340	0.4400
Z	0.7398	0.3810

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Chain	Atom inclusion	Q-score
ZA	0.5085	0.2440
a	0.7662	0.4030
b	0.7883	0.4160
c	0.0079	0.0150
d	0.0223	0.0260
e	0.0144	0.0220
f	0.6252	0.3180
g	0.6319	0.3050
h	0.6271	0.3070
i	0.3745	0.2040
j	0.3356	0.1840
k	0.3769	0.1900
l	0.5299	0.2530
m	0.5049	0.2430
n	0.5240	0.2540
o	0.4116	0.3730
p	0.1383	0.2780
q	0.7152	0.3900
r	0.6909	0.4370
s	0.7972	0.4270
t	0.5854	0.4090
u	0.7807	0.4270
v	0.7685	0.4140
w	0.7408	0.3820
x	0.7678	0.4040
y	0.7918	0.4170
z	0.0088	0.0170