



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:34 PM UTC

PDB ID : 9F4B / pdb_00009f4b
EMDB ID : EMD-50187
Title : Pre-assembled baseplate cup of Klebsiella phage KP1 variant vB_Kpn_Lilla1
Authors : Orlova, E.V.; Isupov, M.N.
Deposited on : 2024-04-26
Resolution : 3.36 Å(reported)

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

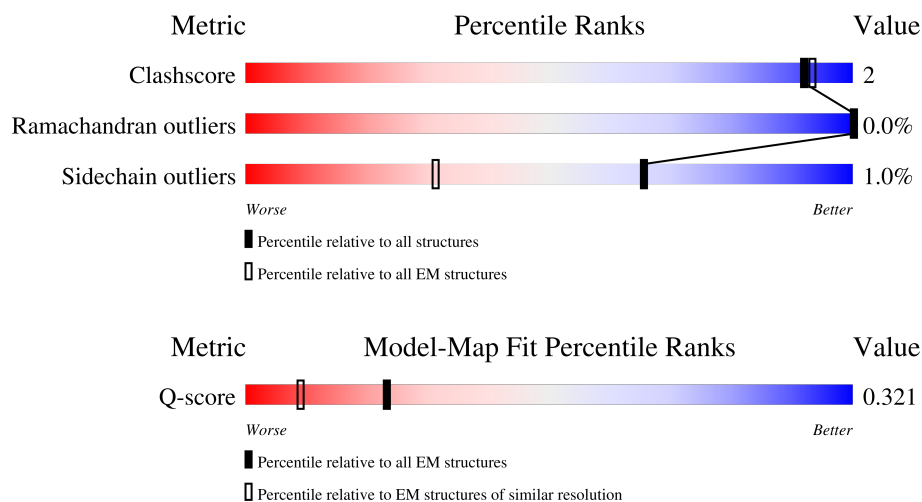
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.36 Å.

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



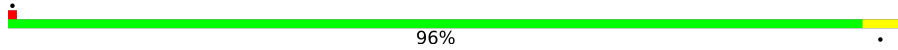
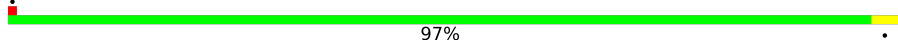
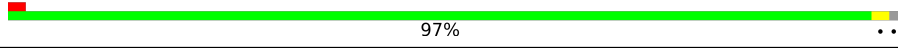
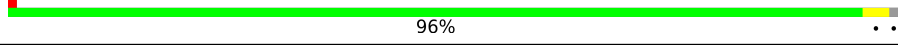
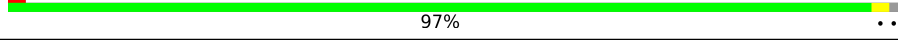
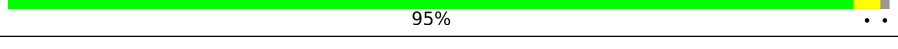
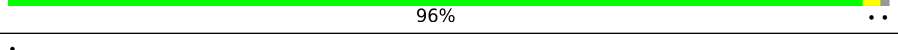
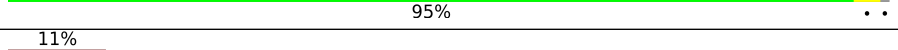
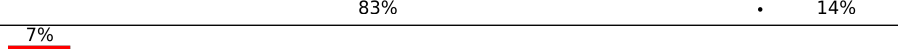
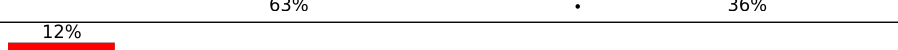
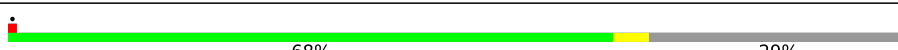
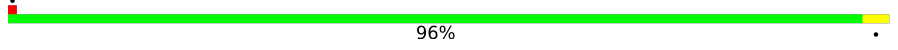
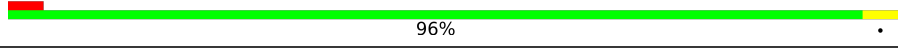
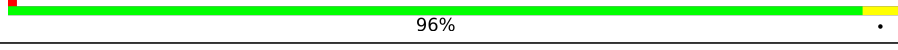
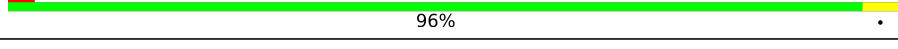
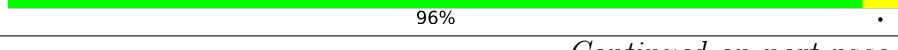
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14332 (2.86 - 3.86)

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

Mol	Chain	Length	Quality of chain
1	AM	655	97%
1	AN	655	96%
1	AO	655	96%
1	AP	655	96%

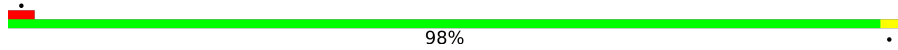
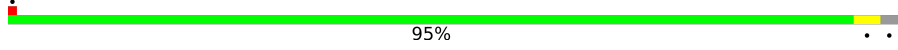
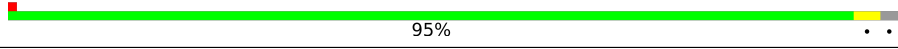
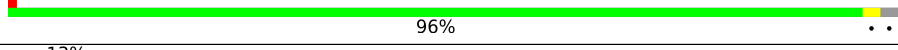
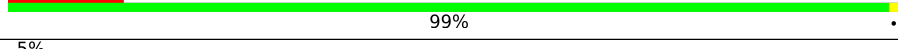
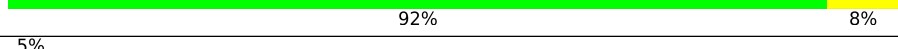
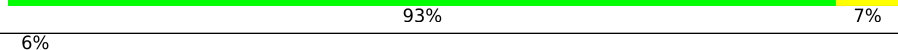
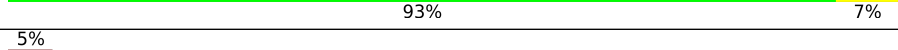
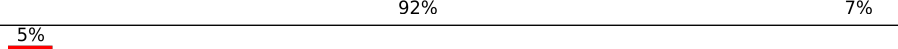
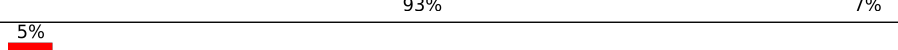
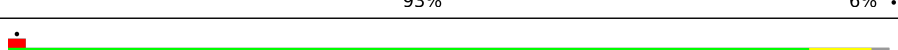
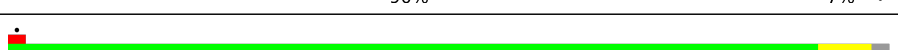
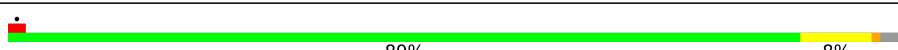
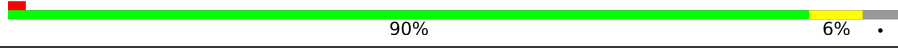
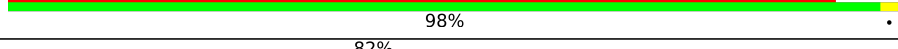
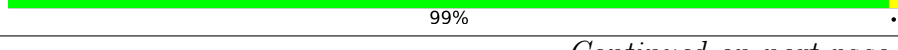
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Mol	Chain	Length	Quality of chain
1	AQ	655	
1	AR	655	
1	AS	655	
1	AT	655	
1	AU	655	
1	AV	655	
1	AW	655	
1	AX	655	
2	BK	350	
2	BL	350	
2	BM	350	
2	BN	350	
2	BO	350	
2	BP	350	
3	BQ	308	
3	BR	308	
3	BS	308	
3	BT	308	
3	BU	308	
3	BV	308	
4	AG	212	
4	AH	212	
4	AI	212	
4	AJ	212	
4	AK	212	

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Mol	Chain	Length	Quality of chain
4	AL	212	
5	BB	576	
5	BC	576	
5	BD	576	
6	BA	97	
7	A0	1032	
7	A1	1032	
7	A2	1032	
7	A3	1032	
7	AY	1032	
7	AZ	1032	
8	A4	341	
8	A5	341	
8	A6	341	
8	A7	341	
8	A8	341	
8	A9	341	
8	Aa	341	
8	Ab	341	
8	Ac	341	
8	Ad	341	
8	Ae	341	
8	Af	341	
9	LA	303	
9	LB	303	

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Mol	Chain	Length	Quality of chain
9	LC	303	90%
9	LD	303	93%
9	LE	303	84%
9	LF	303	90%
9	LG	303	93%
9	LH	303	81%
9	LI	303	90%
9	LJ	303	93%
9	LK	303	82%
9	LL	303	91%
9	LM	303	93%
9	LN	303	83%
9	LO	303	90%
9	LP	303	93%
9	LQ	303	82%
9	LR	303	91%
10	FA	607	26%
10	FB	607	23%
10	FC	607	24%
10	FJ	607	25%
10	FK	607	30%
10	FL	607	26%
10	FS	607	26%
10	FT	607	24%
10	FU	607	23%

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Mol	Chain	Length	Quality of chain
10	Fb	607	25% 95% 5%
10	Fc	607	30% 96% .
10	Fd	607	25% 96% .
10	Fk	607	27% 95% 5%
10	Fl	607	24% 96% .
10	Fm	607	25% 97% .
10	Ft	607	24% 95% 5%
10	Fu	607	30% 97% .
10	Fv	607	25% 96% .
11	FD	223	56% 98% .
11	FE	223	58% 99% .
11	FF	223	52% 96% .
11	FM	223	57% 98% .
11	FN	223	55% 99% .
11	FO	223	59% 96% .
11	FV	223	57% 98% .
11	FW	223	61% 99% .
11	FX	223	50% 96% .
11	Fe	223	56% 98% .
11	Ff	223	55% 99% .
11	Fg	223	55% 96% .
11	Fn	223	57% 98% .
11	Fo	223	60% 99% .
11	Fp	223	52% 96% .
11	Fw	223	56% 98% .

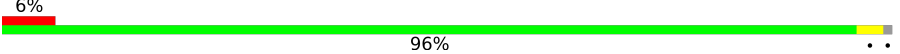
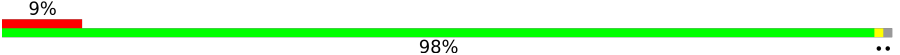
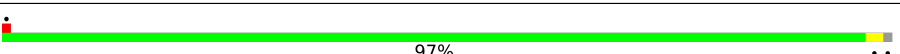
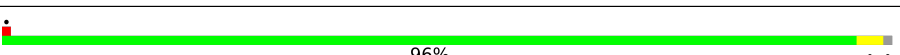
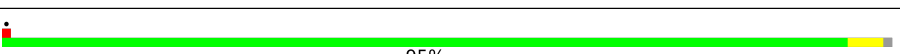
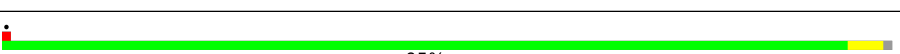
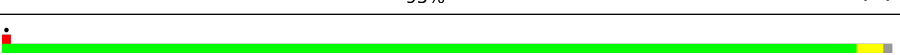
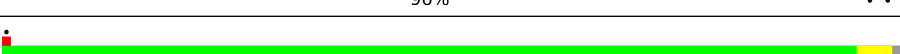
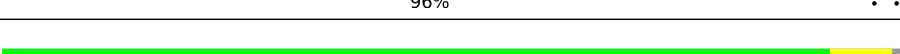
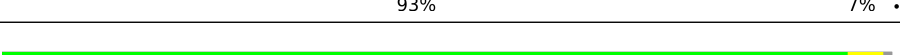
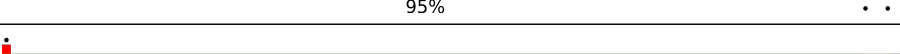
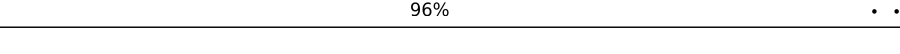
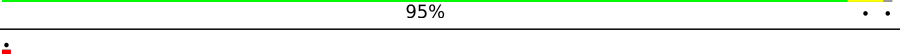
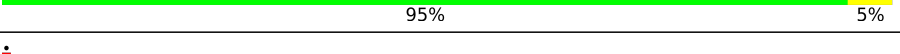
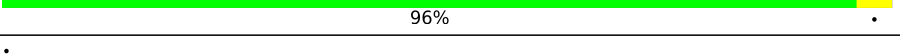
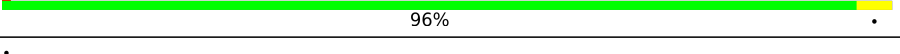
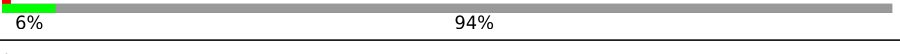
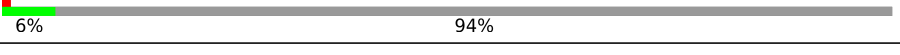
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Mol	Chain	Length	Quality of chain
11	Fx	223	59% 99% .
11	Fy	223	56% 96% .
12	F1	448	59% 96% .
12	F2	448	55% 96% .
12	FG	448	48% 97% .
12	FH	448	50% 95% .
12	FI	448	52% 95% .
12	FP	448	52% 97% .
12	FQ	448	59% 96% .
12	FR	448	57% 95% .
12	FY	448	48% 97% .
12	FZ	448	49% 95% .
12	Fa	448	50% 96% .
12	Fh	448	53% 97% .
12	Fi	448	59% 96% .
12	Fj	448	57% 96% .
12	Fq	448	48% 97% .
12	Fr	448	50% 95% .
12	Fs	448	53% 96% .
12	Fz	448	52% 97% .
13	B1	163	. 96% ..
13	B2	163	. 98% ..
13	B3	163	6% 98% ..
13	B4	163	6% 97% ..
13	B5	163	8% 98% ..

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Mol	Chain	Length	Quality of chain
13	B6	163	
13	B7	163	
13	B8	163	
13	BW	163	
13	BX	163	
13	BY	163	
13	BZ	163	
14	AA	136	
14	AB	136	
14	AC	136	
14	AD	136	
14	AE	136	
14	AF	136	
15	BE	380	
15	BF	380	
15	BG	380	
16	BH	577	
16	BI	577	
16	BJ	577	

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 440315 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
1	AT	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
1	AV	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
1	AX	646	Total	C	N	O	S	0	0
			5125	3252	853	1009	11		
1	AS	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
1	AU	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
1	AW	648	Total	C	N	O	S	0	0
			5145	3265	856	1013	11		
1	AN	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AP	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AR	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AM	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AO	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		
1	AQ	654	Total	C	N	O	S	0	0
			5191	3296	863	1021	11		

- Molecule 2 is a protein called Baseplate tail tube cap.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BL	225	Total	C	N	O	S	0	0
			1790	1131	311	342	6		
2	BN	225	Total	C	N	O	S	0	0
			1790	1131	311	342	6		
2	BP	225	Total	C	N	O	S	0	0
			1790	1131	311	342	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BK	301	Total	C	N	O	S	0	0
			2323	1455	399	461	8		
2	BM	301	Total	C	N	O	S	0	0
			2323	1455	399	461	8		
2	BO	301	Total	C	N	O	S	0	0
			2323	1455	399	461	8		

- Molecule 3 is a protein called Baseplate subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BQ	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BR	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BS	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BT	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BU	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		
3	BV	220	Total	C	N	O	S	0	0
			1719	1092	284	328	15		

- Molecule 4 is a protein called Baseplate wedge subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AH	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AJ	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AL	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AG	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AI	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		
4	AK	212	Total	C	N	O	S	0	0
			1747	1123	279	340	5		

- Molecule 5 is a protein called Baseplate central spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BB	564	Total	C	N	O	S	0	0
			4354	2709	753	871	21		
5	BC	564	Total	C	N	O	S	0	0
			4354	2709	753	871	21		
5	BD	564	Total	C	N	O	S	0	0
			4354	2709	753	871	21		

- Molecule 6 is a protein called Phospholipase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BA	97	Total	C	N	O	S	0	0
			706	440	122	140	4		

- Molecule 7 is a protein called Baseplate wedge protein gp7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AY	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	A2	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	AZ	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	A0	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	A1	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		
7	A3	1031	Total	C	N	O	S	0	0
			8438	5377	1416	1617	28		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	530	ALA	SER	conflict	UNP A0A2K9V5T9
AY	532	HIS	ASN	conflict	UNP A0A2K9V5T9
AY	536	ILE	VAL	conflict	UNP A0A2K9V5T9
A2	530	ALA	SER	conflict	UNP A0A2K9V5T9
A2	532	HIS	ASN	conflict	UNP A0A2K9V5T9
A2	536	ILE	VAL	conflict	UNP A0A2K9V5T9
AZ	530	ALA	SER	conflict	UNP A0A2K9V5T9
AZ	532	HIS	ASN	conflict	UNP A0A2K9V5T9
AZ	536	ILE	VAL	conflict	UNP A0A2K9V5T9
A0	530	ALA	SER	conflict	UNP A0A2K9V5T9
A0	532	HIS	ASN	conflict	UNP A0A2K9V5T9

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Chain	Residue	Modelled	Actual	Comment	Reference
A0	536	ILE	VAL	conflict	UNP A0A2K9V5T9
A1	530	ALA	SER	conflict	UNP A0A2K9V5T9
A1	532	HIS	ASN	conflict	UNP A0A2K9V5T9
A1	536	ILE	VAL	conflict	UNP A0A2K9V5T9
A3	530	ALA	SER	conflict	UNP A0A2K9V5T9
A3	532	HIS	ASN	conflict	UNP A0A2K9V5T9
A3	536	ILE	VAL	conflict	UNP A0A2K9V5T9

- Molecule 8 is a protein called Baseplate wedge subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ad	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Ac	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Ab	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Aa	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Ae	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	Af	329	Total	C	N	O	S	0	0
			2633	1674	438	504	17		
8	A4	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A5	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A6	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A7	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A8	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		
8	A9	334	Total	C	N	O	S	0	0
			2669	1693	446	513	17		

- Molecule 9 is a protein called Baseplate wedge tail fiber connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LA	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LB	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	LC	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LD	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LE	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LF	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LG	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LH	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LI	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LJ	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LK	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LL	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LM	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LN	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LO	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LP	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LQ	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		
9	LR	303	Total	C	N	O	S	0	0
			2270	1412	386	461	11		

- Molecule 10 is a protein called Baseplate wedge protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	FA	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FB	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FC	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	FJ	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FK	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FL	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FS	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FT	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	FU	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fb	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fc	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fd	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fk	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fl	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fm	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Ft	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fu	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		
10	Fv	607	Total	C	N	O	S	0	0
			4696	2948	795	937	16		

- Molecule 11 is a protein called Baseplate wedge subunit and tail pin.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	FD	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FE	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FF	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FM	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	FN	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FO	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FV	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FW	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	FX	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fe	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Ff	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fg	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fn	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fo	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fp	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fw	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fx	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		
11	Fy	222	Total	C	N	O	S	0	0
			1722	1092	290	336	4		

- Molecule 12 is a protein called Gp12 short tail fibers.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	FG	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	FI	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	FH	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	FP	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	FR	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	FQ	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	FY	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	Fa	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	FZ	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	Fh	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	Fj	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	Fi	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	Fq	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	Fs	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	Fr	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		
12	Fz	446	Total	C	N	O	S	0	0
			3371	2097	598	668	8		
12	F2	447	Total	C	N	O	S	0	0
			3376	2100	599	669	8		
12	F1	446	Total	C	N	O	S	0	0
			3362	2092	597	665	8		

- Molecule 13 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BW	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	BX	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	BY	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	BZ	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B1	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B2	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	B3	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B4	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B5	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B6	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B7	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		
13	B8	162	Total	C	N	O	S	0	0
			1305	825	222	253	5		

- Molecule 14 is a protein called IraD/Gp25-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AA	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AB	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AC	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AD	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AE	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		
14	AF	135	Total	C	N	O	S	0	0
			1069	662	189	214	4		

- Molecule 15 is a protein called Putative baseplate hub subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BE	379	Total	C	N	O	S	0	0
			3055	1945	511	583	16		
15	BF	379	Total	C	N	O	S	0	0
			3055	1945	511	583	16		
15	BG	379	Total	C	N	O	S	0	0
			3055	1945	511	583	16		

- Molecule 16 is a protein called Baseplate hub subunit tail length determinator.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BH	33	Total	C	N	O	S	0	0
			242	147	43	50	2		
16	BI	33	Total	C	N	O	S	0	0
			242	147	43	50	2		
16	BJ	33	Total	C	N	O	S	0	0
			242	147	43	50	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BH	87	VAL	ALA	conflict	UNP A0A2K9V5Z4
BH	530	THR	ALA	conflict	UNP A0A2K9V5Z4
BH	555	TYR	HIS	conflict	UNP A0A2K9V5Z4
BH	559	THR	MET	conflict	UNP A0A2K9V5Z4
BI	87	VAL	ALA	conflict	UNP A0A2K9V5Z4
BI	530	THR	ALA	conflict	UNP A0A2K9V5Z4
BI	555	TYR	HIS	conflict	UNP A0A2K9V5Z4
BI	559	THR	MET	conflict	UNP A0A2K9V5Z4
BJ	87	VAL	ALA	conflict	UNP A0A2K9V5Z4
BJ	530	THR	ALA	conflict	UNP A0A2K9V5Z4
BJ	555	TYR	HIS	conflict	UNP A0A2K9V5Z4
BJ	559	THR	MET	conflict	UNP A0A2K9V5Z4

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
17	BB	1	Total	Cl	0
			1	1	

- Molecule 18 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	FA	1	Total	K	0
			1	1	
18	FJ	1	Total	K	0
			1	1	
18	FS	1	Total	K	0
			1	1	
18	Fb	1	Total	K	0
			1	1	
18	Fk	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
18	Ft	1	Total	K	0
			1	1	

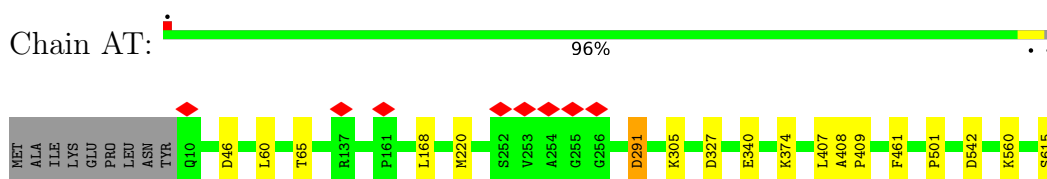
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	FB	1	Total	Zn	0
			1	1	
19	FK	1	Total	Zn	0
			1	1	
19	FT	1	Total	Zn	0
			1	1	
19	Fc	1	Total	Zn	0
			1	1	
19	Fl	1	Total	Zn	0
			1	1	
19	FG	1	Total	Zn	0
			1	1	

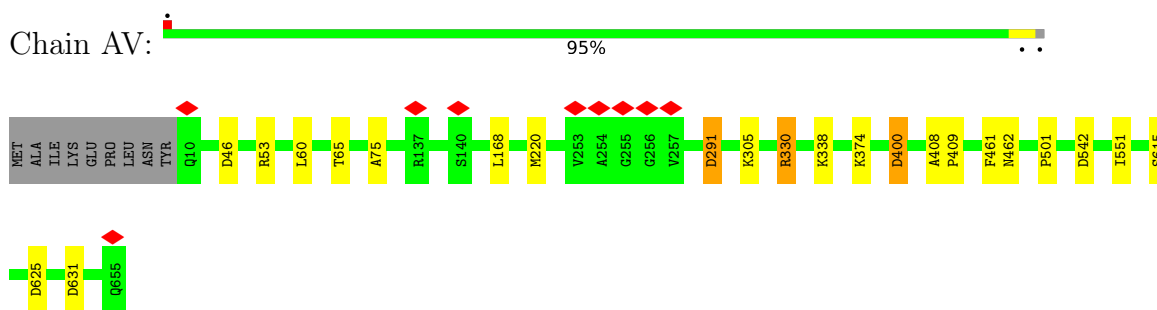
3 Residue-property plots [i](#)

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.

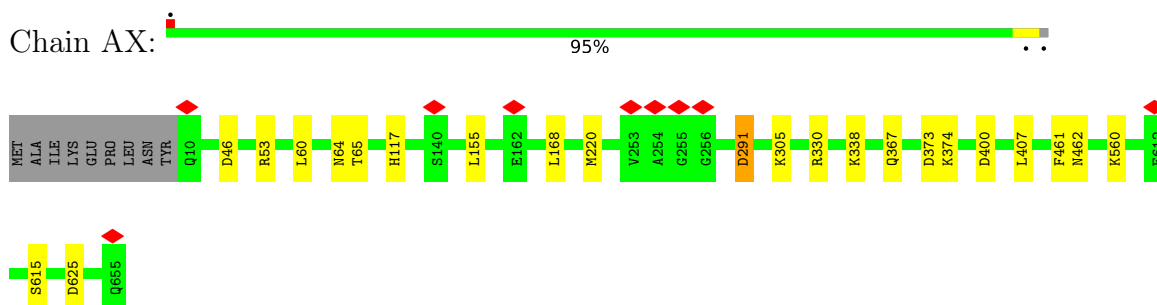
- Molecule 1: Baseplate wedge protein gp6



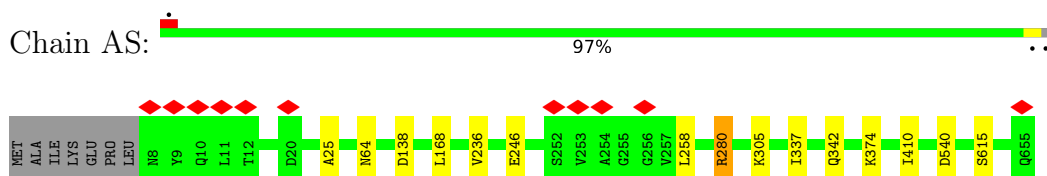
- Molecule 1: Baseplate wedge protein gp6



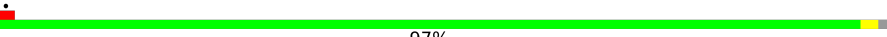
- Molecule 1: Baseplate wedge protein gp6

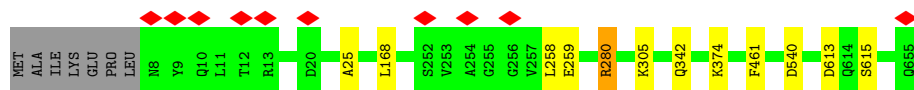


- Molecule 1: Baseplate wedge protein gp6

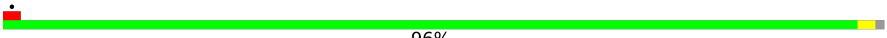


- Molecule 1: Baseplate wedge protein gp6

Chain AU:  97%

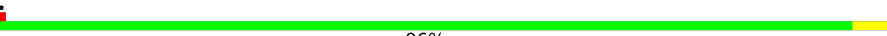


- Molecule 1: Baseplate wedge protein gp6

Chain AW:  96%

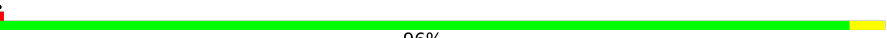


- Molecule 1: Baseplate wedge protein gp6

Chain AN:  96%

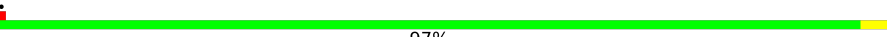


- Molecule 1: Baseplate wedge protein gp6

Chain AP:  96%

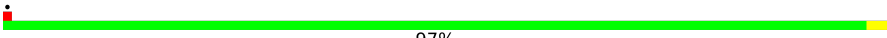


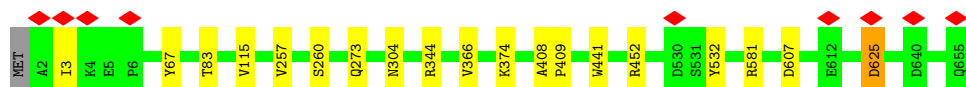
- Molecule 1: Baseplate wedge protein gp6

Chain AR:  97%

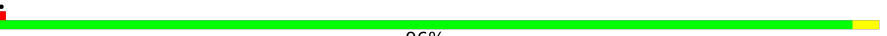


- Molecule 1: Baseplate wedge protein gp6

Chain AM:  97%



- Molecule 1: Baseplate wedge protein gp6

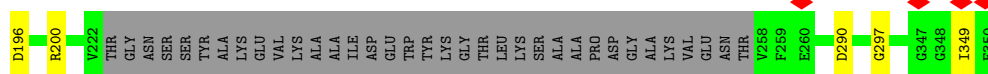
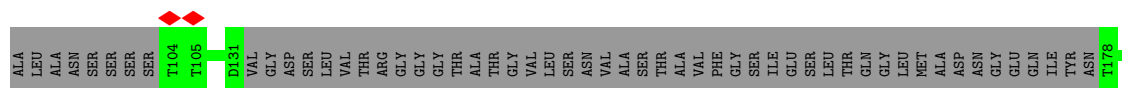
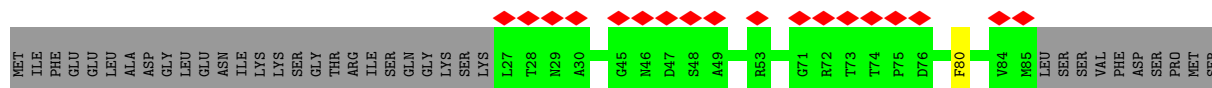
Chain AO:  96%



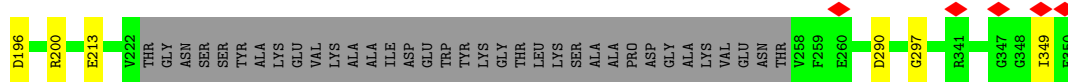
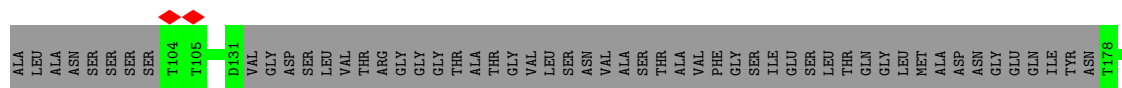
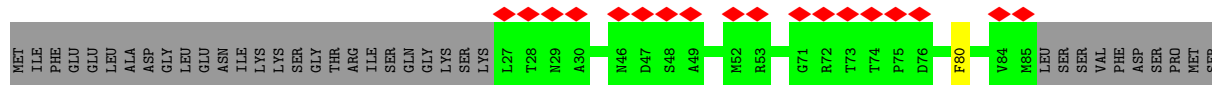
- Molecule 1: Baseplate wedge protein gp6



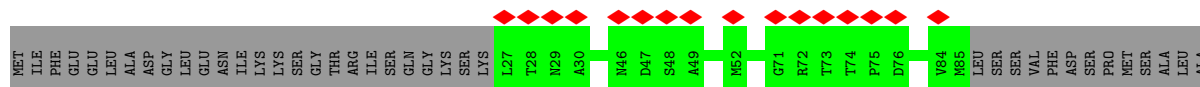
- Molecule 2: Baseplate tail tube cap

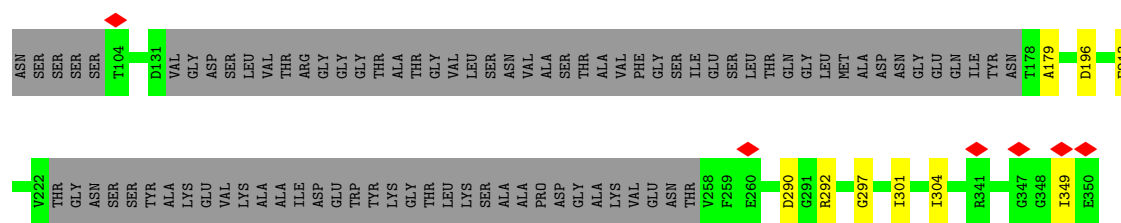


- Molecule 2: Baseplate tail tube cap

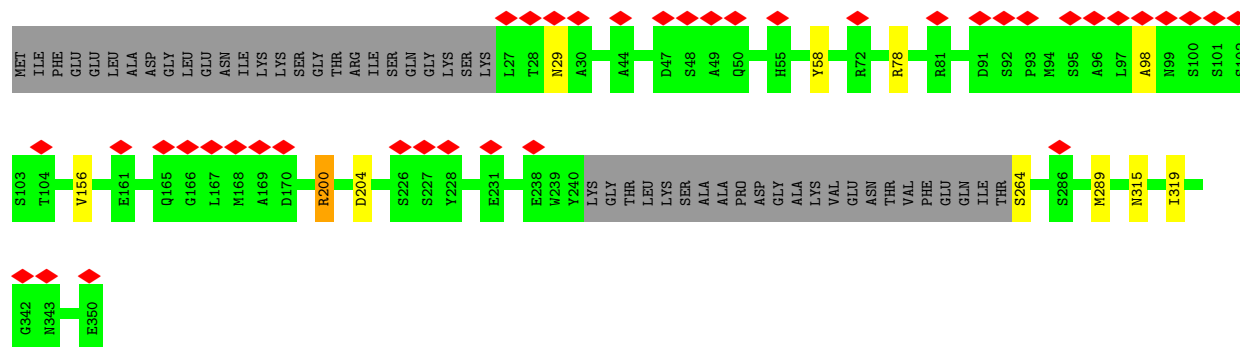
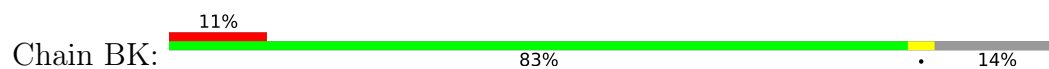


- Molecule 2: Baseplate tail tube cap

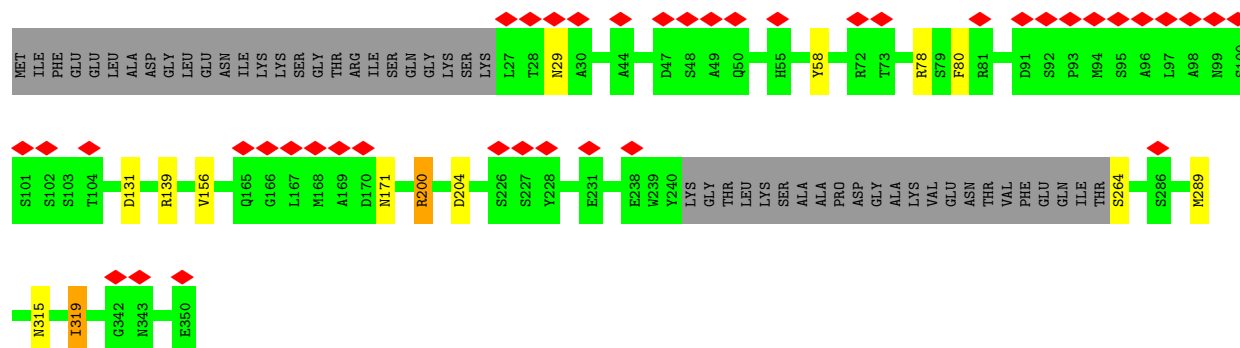
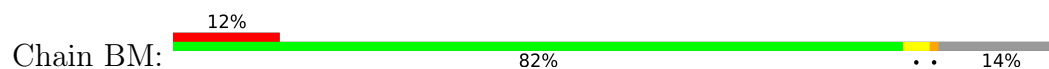




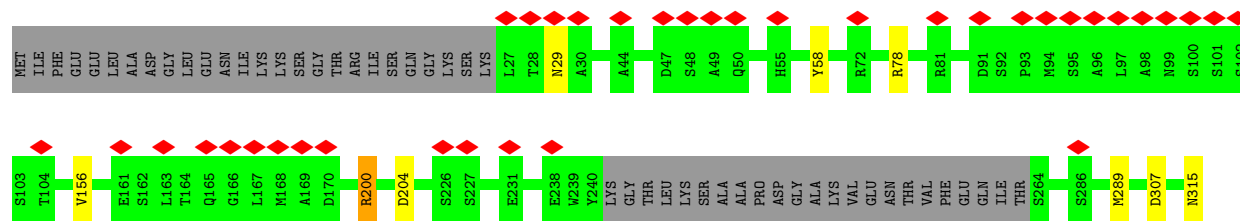
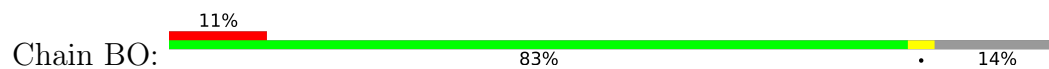
• Molecule 2: Baseplate tail tube cap

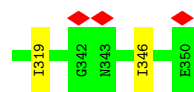


• Molecule 2: Baseplate tail tube cap

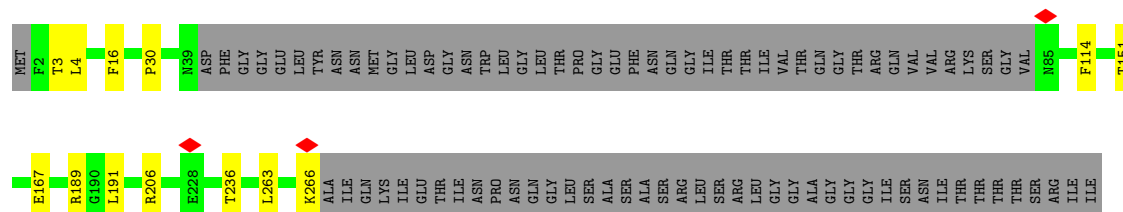


• Molecule 2: Baseplate tail tube cap

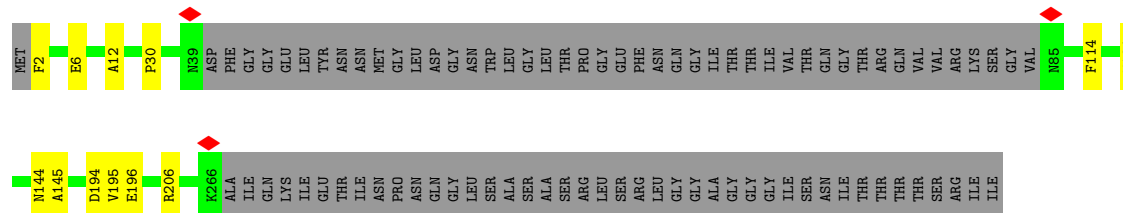




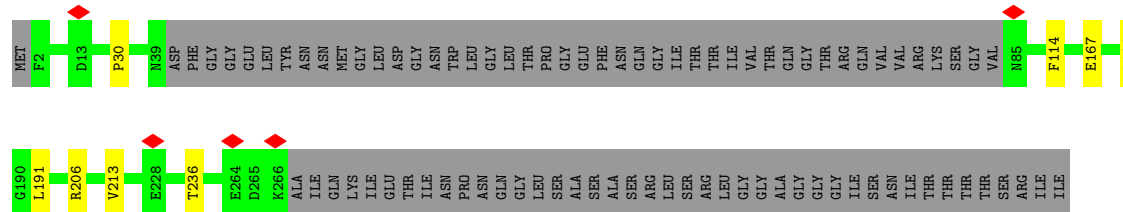
- Molecule 3: Baseplate subunit



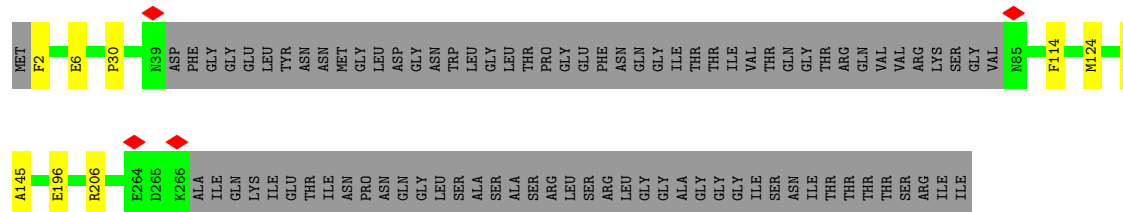
- Molecule 3: Baseplate subunit



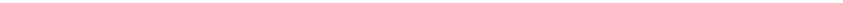
- Molecule 3: Baseplate subunit

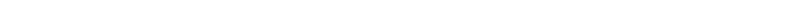


- Molecule 3: Baseplate subunit

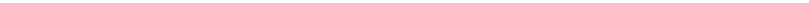


- Molecule 3: Baseplate subunit

- Chain BV: 

- Chain AH:  96%

Component	Count
M1	1
D10	1
T15	1
L75	1
V80	1
Y81	2
D82	2
F97	1
Q100	2
D104	1
S204	2
Q205	2
T206	2
I208	2
E210	2
V211	2
L212	2

- Chain A.J:  96%

M1 T15 L45 D82 F97 Q100 D104 S204 Q205 T206 T207 I208 G209 E210 V211 L212

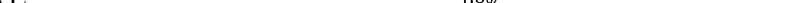
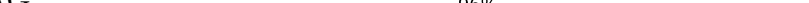
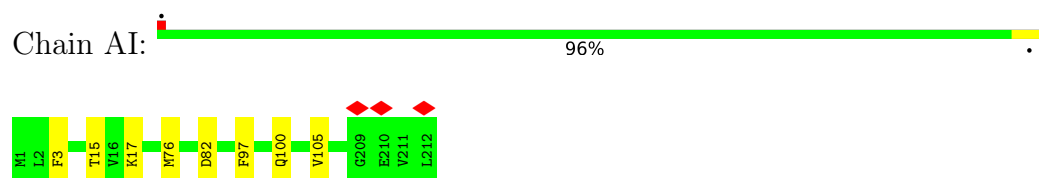
- Chain AL: 

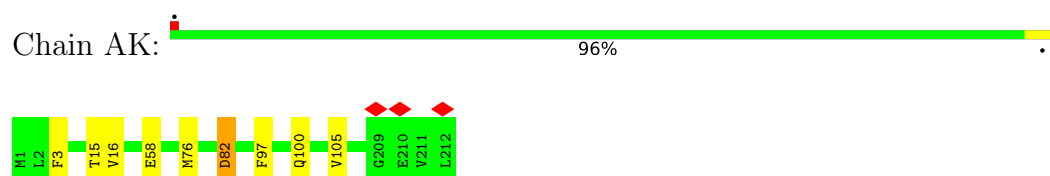
Diagram illustrating the 128-bit key schedule for the proposed algorithm. The key schedule consists of 12 rounds, each with a 128-bit key. The keys are labeled M1, T15, D82, F97, Q100, S204, Q205, T206, G209, E210, V211, and L212. The keys are arranged in a sequence, with the first five keys (M1 to Q100) being yellow and the last seven keys (S204 to L212) being green. Red diamonds are placed above the keys S204, Q205, T206, G209, E210, V211, and L212.

- Chain AG:  96%

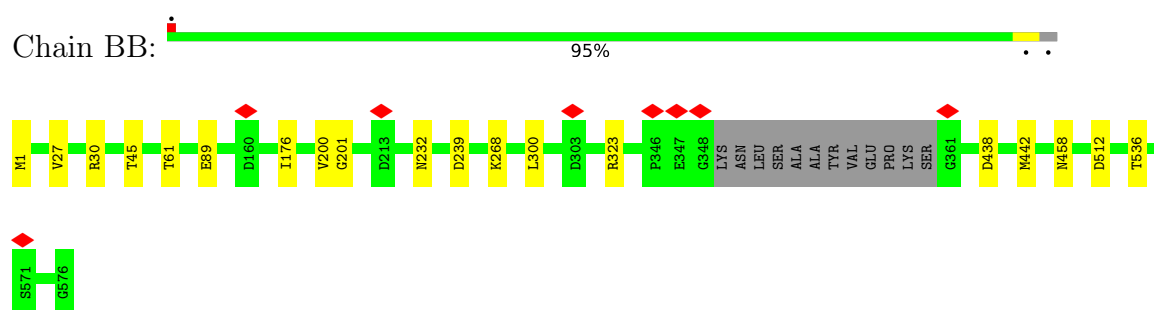
- Molecule 4: Baseplate wedge subunit



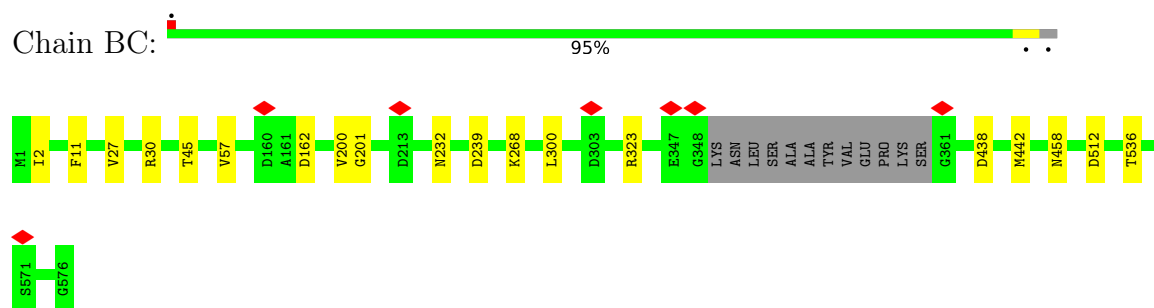
- Molecule 4: Baseplate wedge subunit



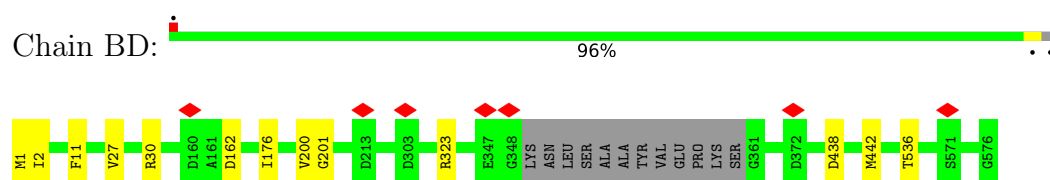
- Molecule 5: Baseplate central spike protein



- Molecule 5: Baseplate central spike protein

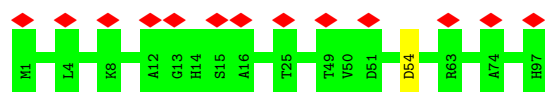


- Molecule 5: Baseplate central spike protein

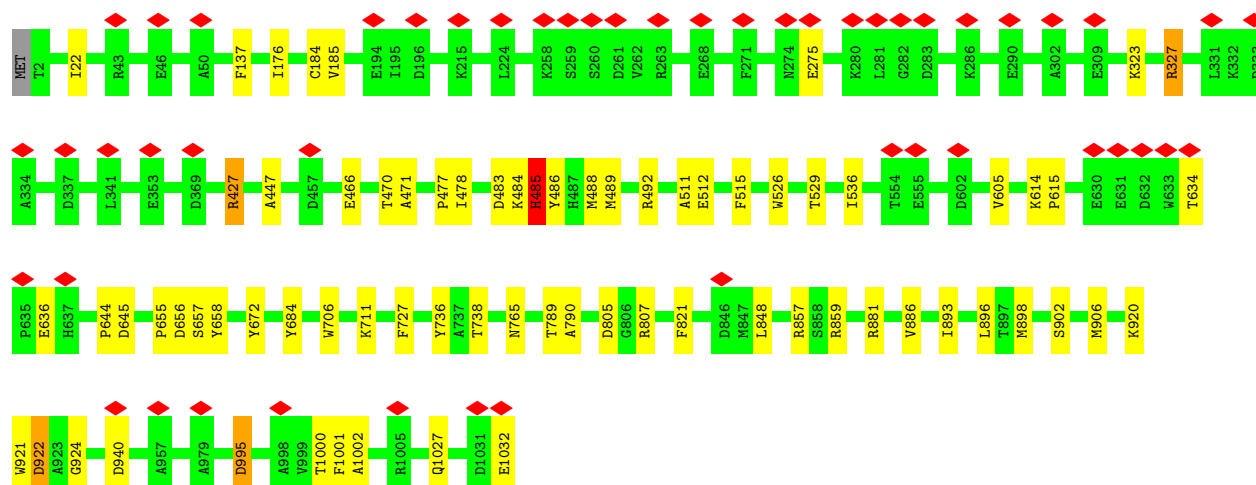


- Molecule 6: Phospholipase

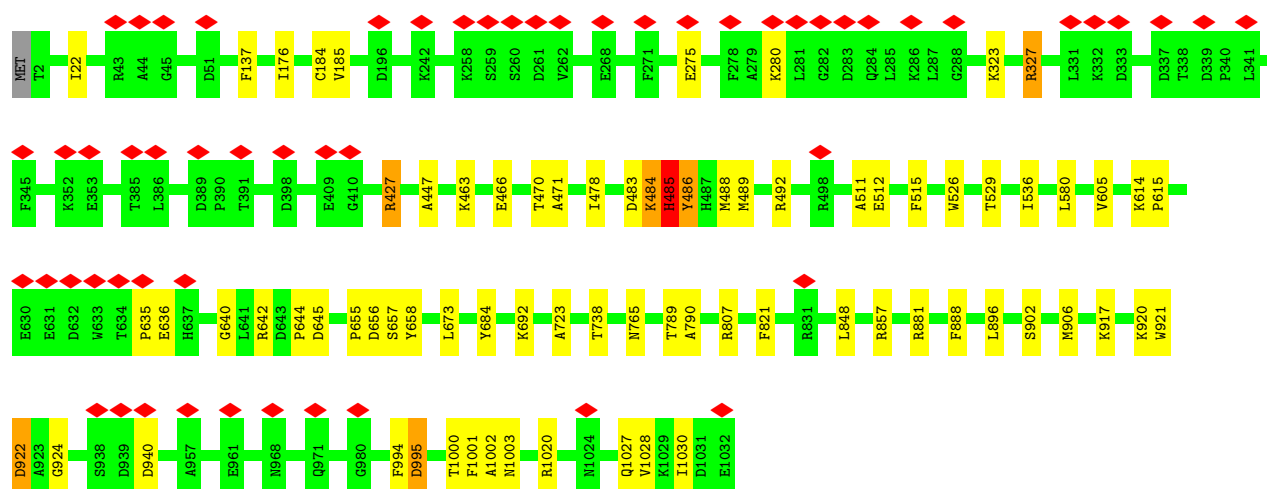




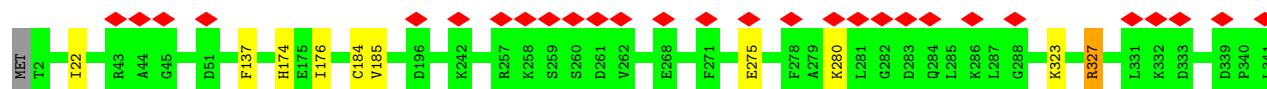
• Molecule 7: Baseplate wedge protein gp7

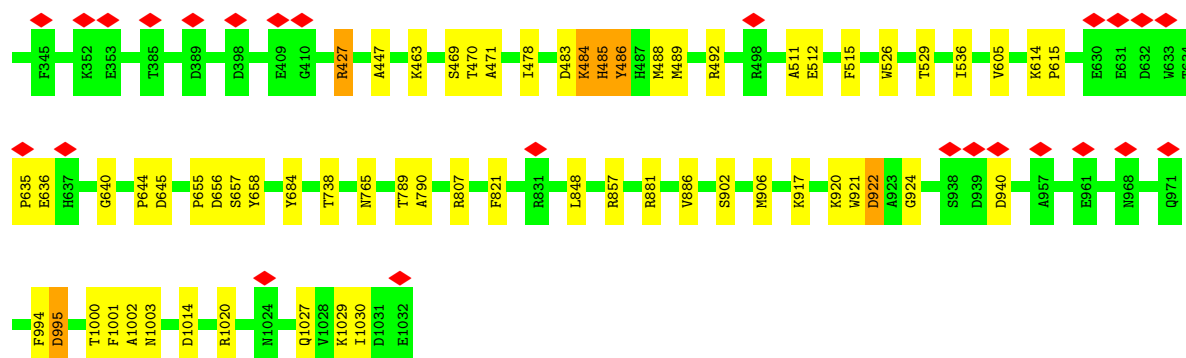


• Molecule 7: Baseplate wedge protein gp7

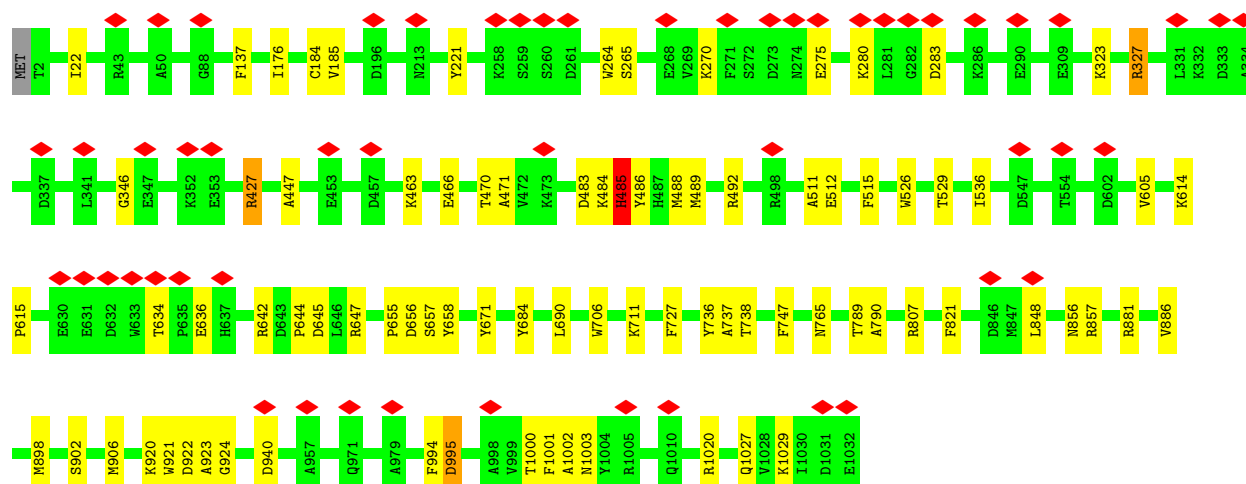


• Molecule 7: Baseplate wedge protein gp7

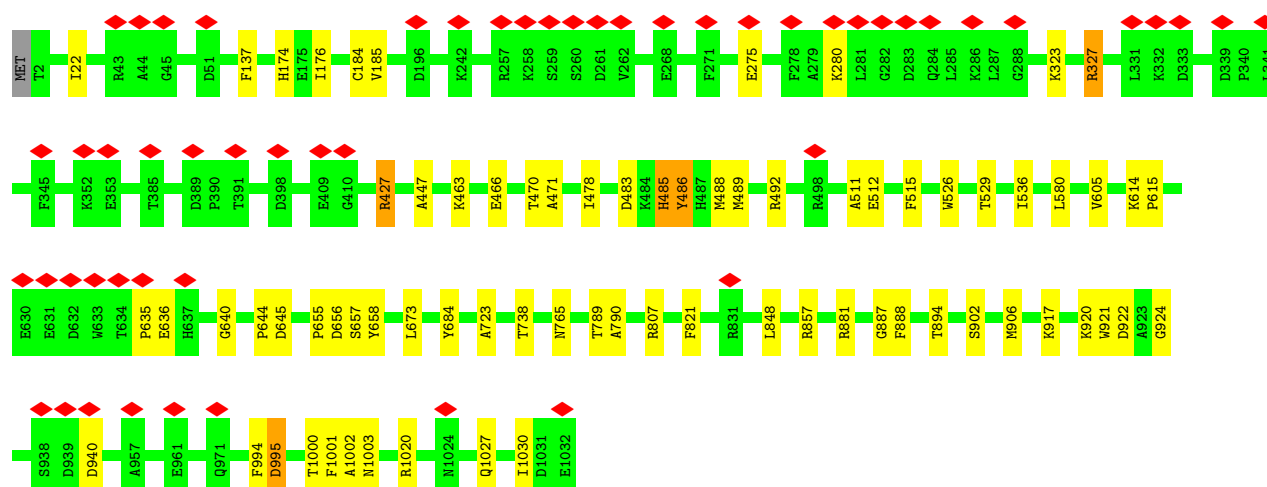




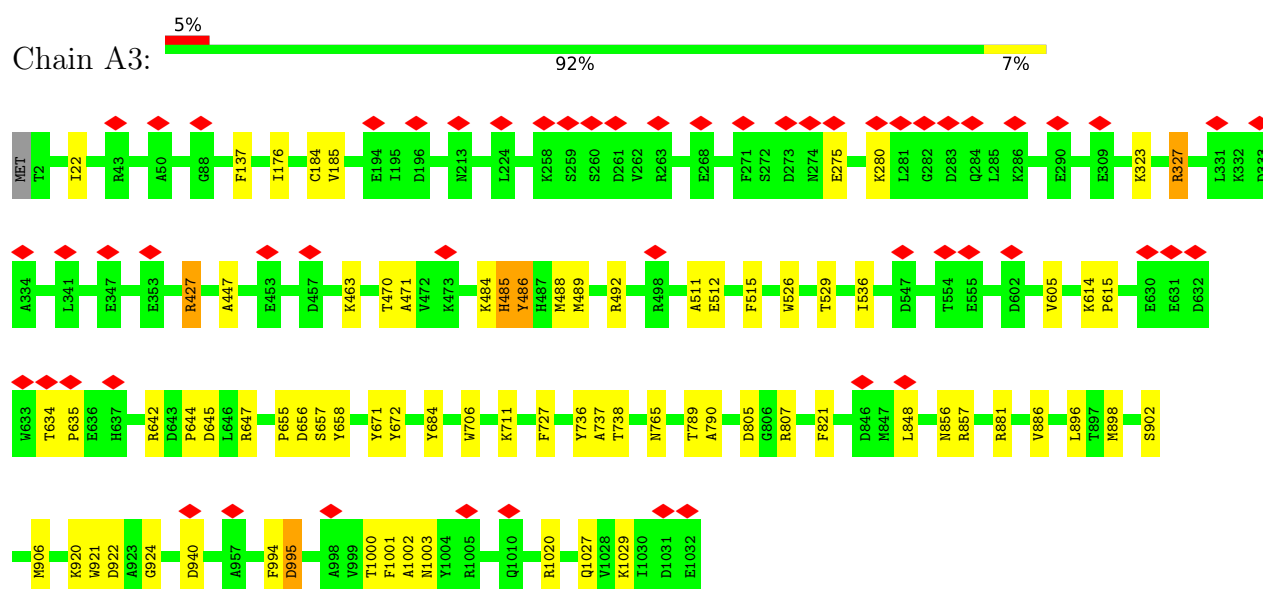
• Molecule 7: Baseplate wedge protein gp7



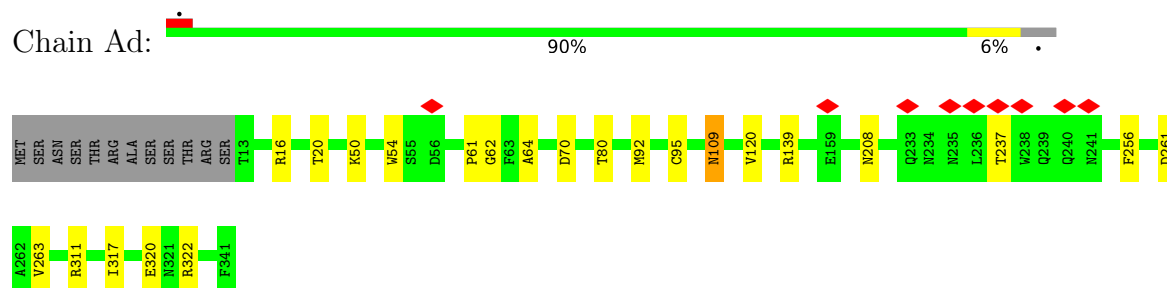
• Molecule 7: Baseplate wedge protein gp7



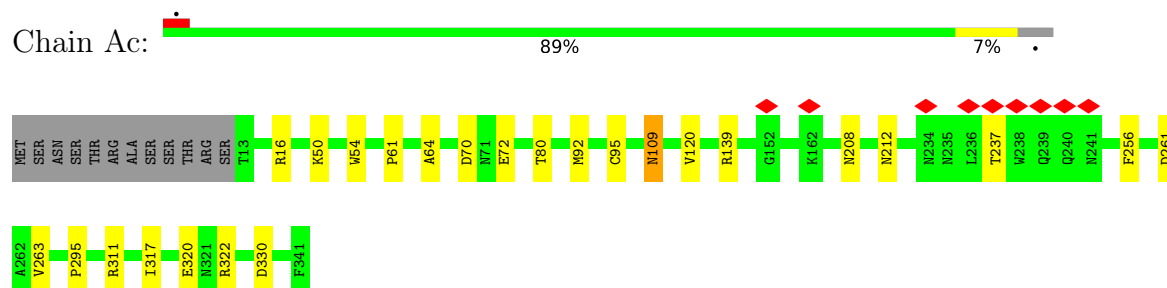
• Molecule 7: Baseplate wedge protein gp7



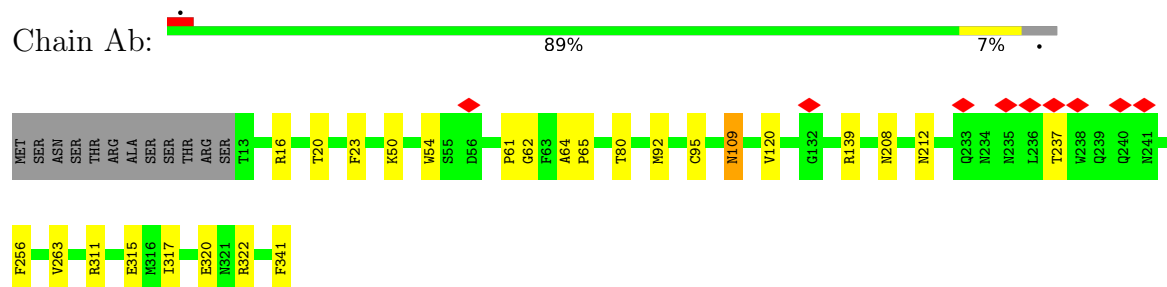
- Molecule 8: Baseplate wedge subunit



- Molecule 8: Baseplate wedge subunit

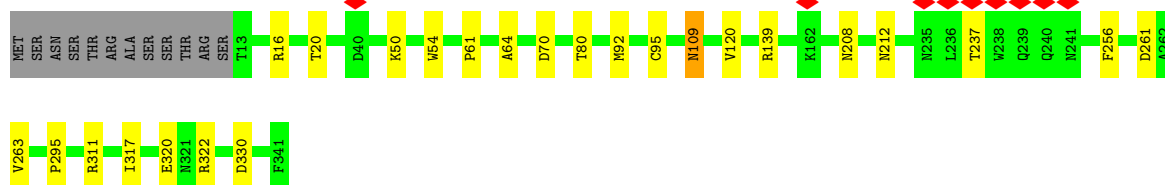


- Molecule 8: Baseplate wedge subunit



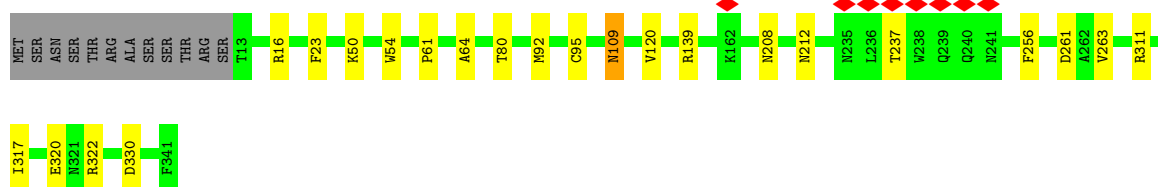
- Molecule 8: Baseplate wedge subunit

Chain Aa:  89% 7% .



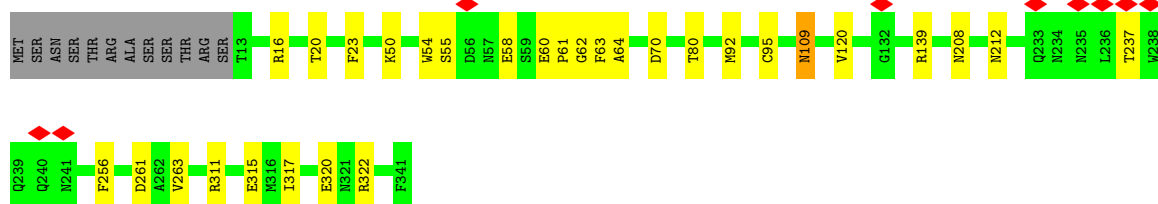
- Molecule 8: Baseplate wedge subunit

Chain Ae:  90% 6% .



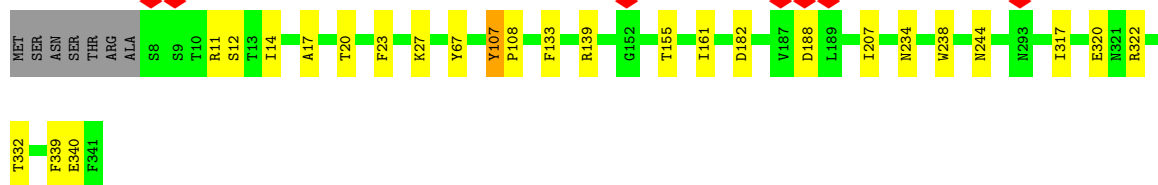
- Molecule 8: Baseplate wedge subunit

Chain Af:  88% 9% .



- Molecule 8: Baseplate wedge subunit

Chain A4:  90% 7% .



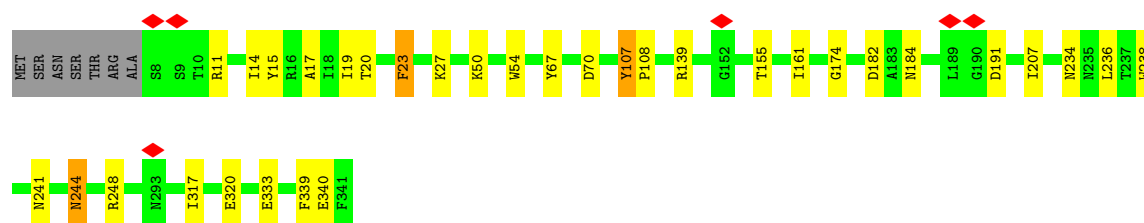
- Molecule 8: Baseplate wedge subunit

Chain A5:  91% 6% .



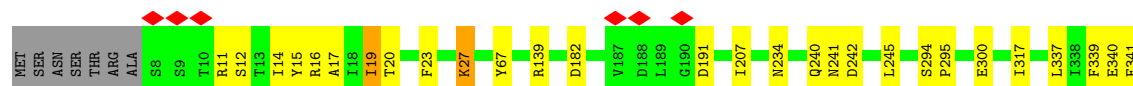
- Molecule 8: Baseplate wedge subunit

Chain A6:  88% 9% ..



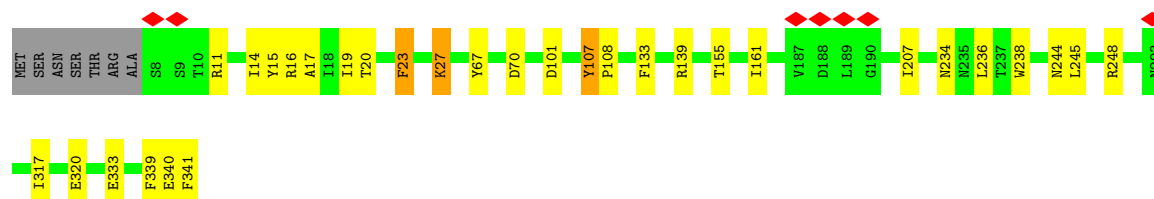
- Molecule 8: Baseplate wedge subunit

Chain A7:  90% 8% ..



- Molecule 8: Baseplate wedge subunit

Chain A8:  89% 8% ..

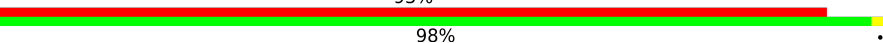


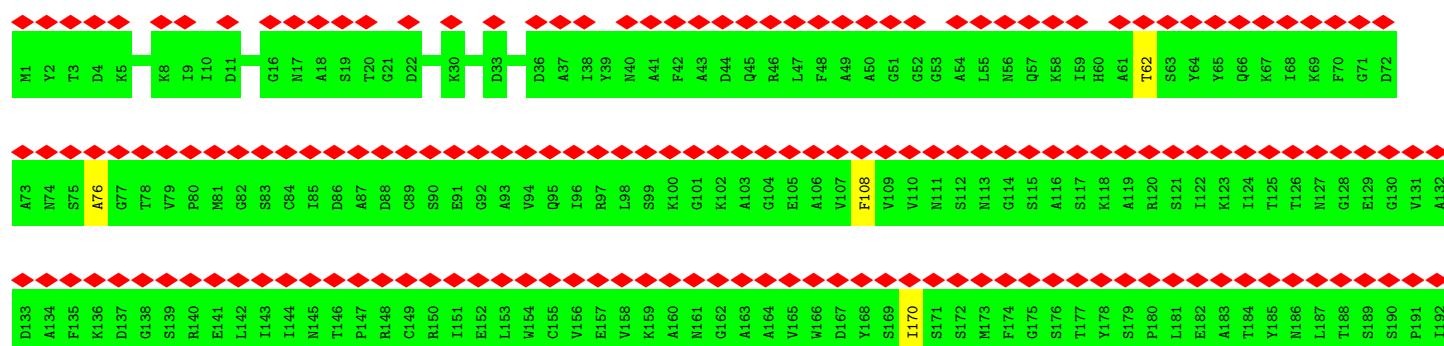
- Molecule 8: Baseplate wedge subunit

Chain A9:  91% 6% ..



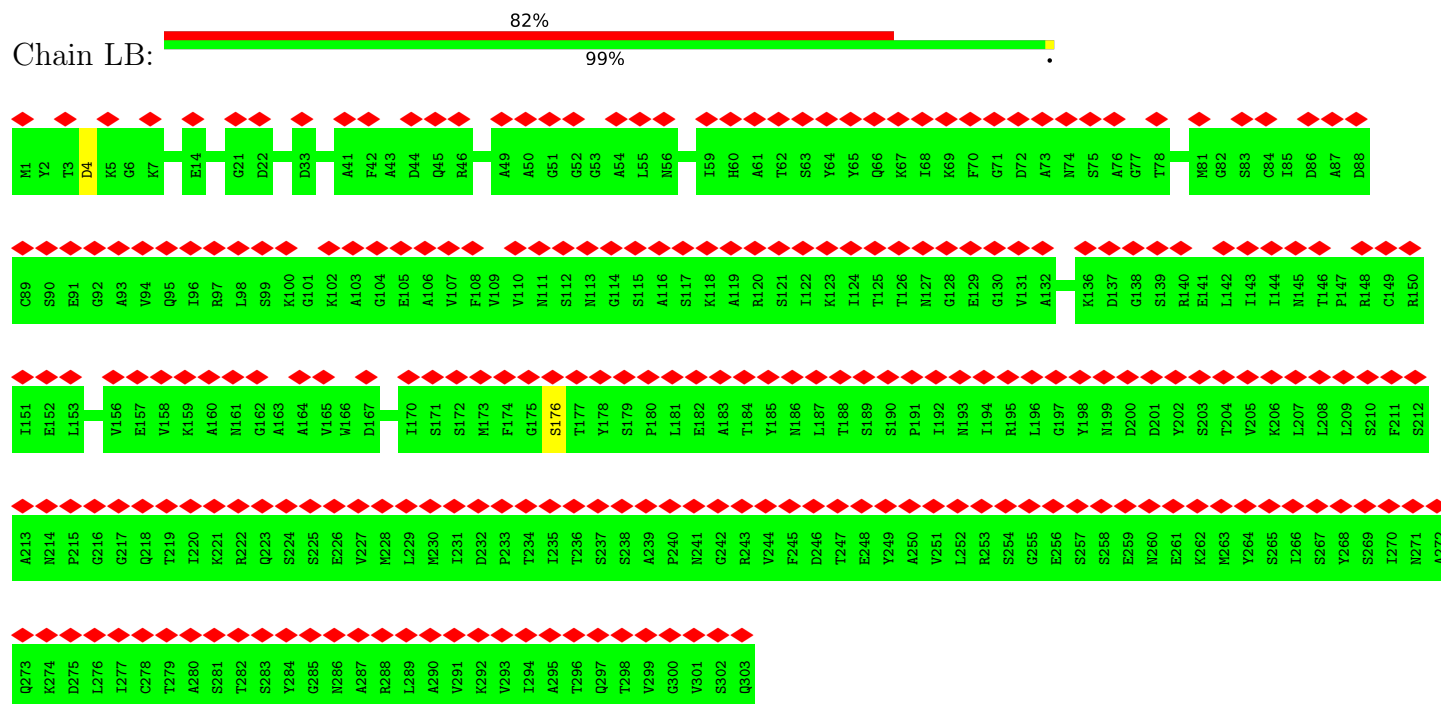
- Molecule 9: Baseplate wedge tail fiber connector

Chain LA:  93% 98% ..

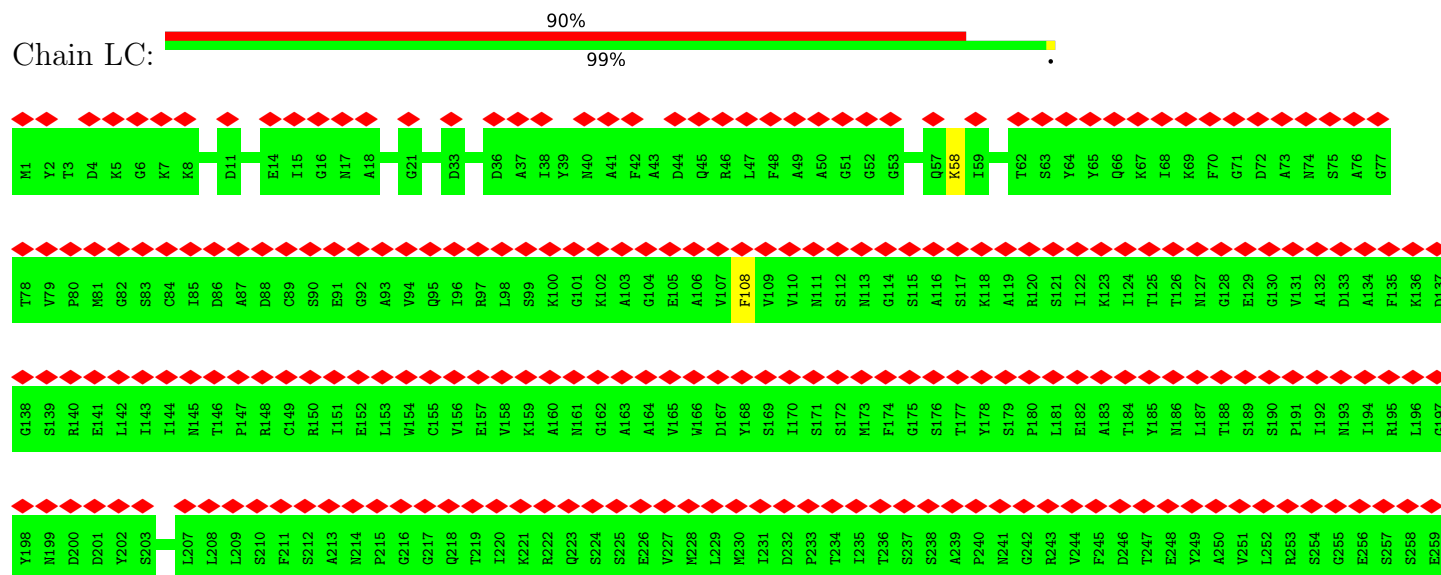


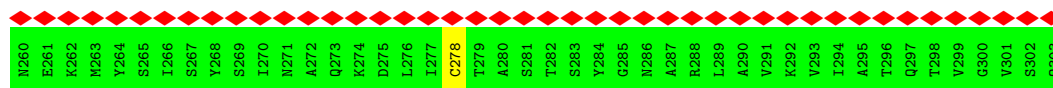


• Molecule 9: Baseplate wedge tail fiber connector

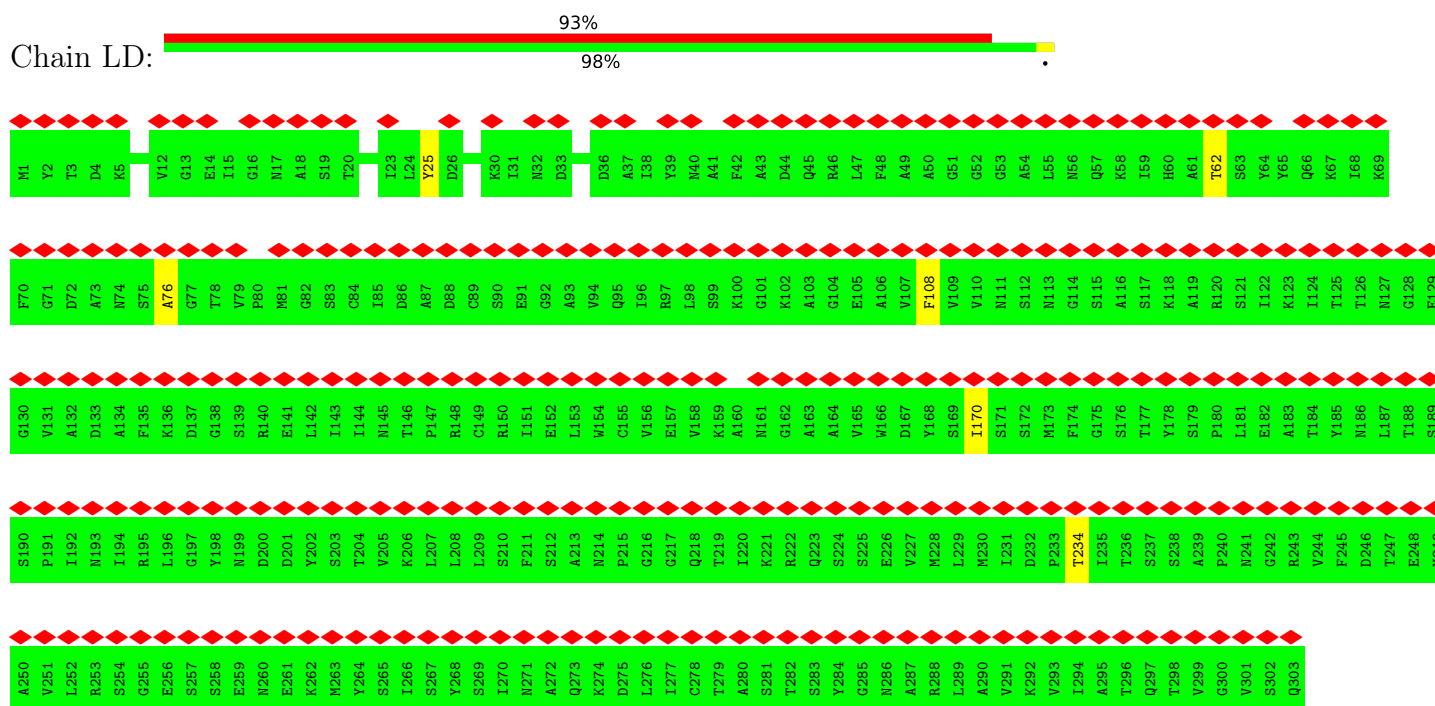


• Molecule 9: Baseplate wedge tail fiber connector

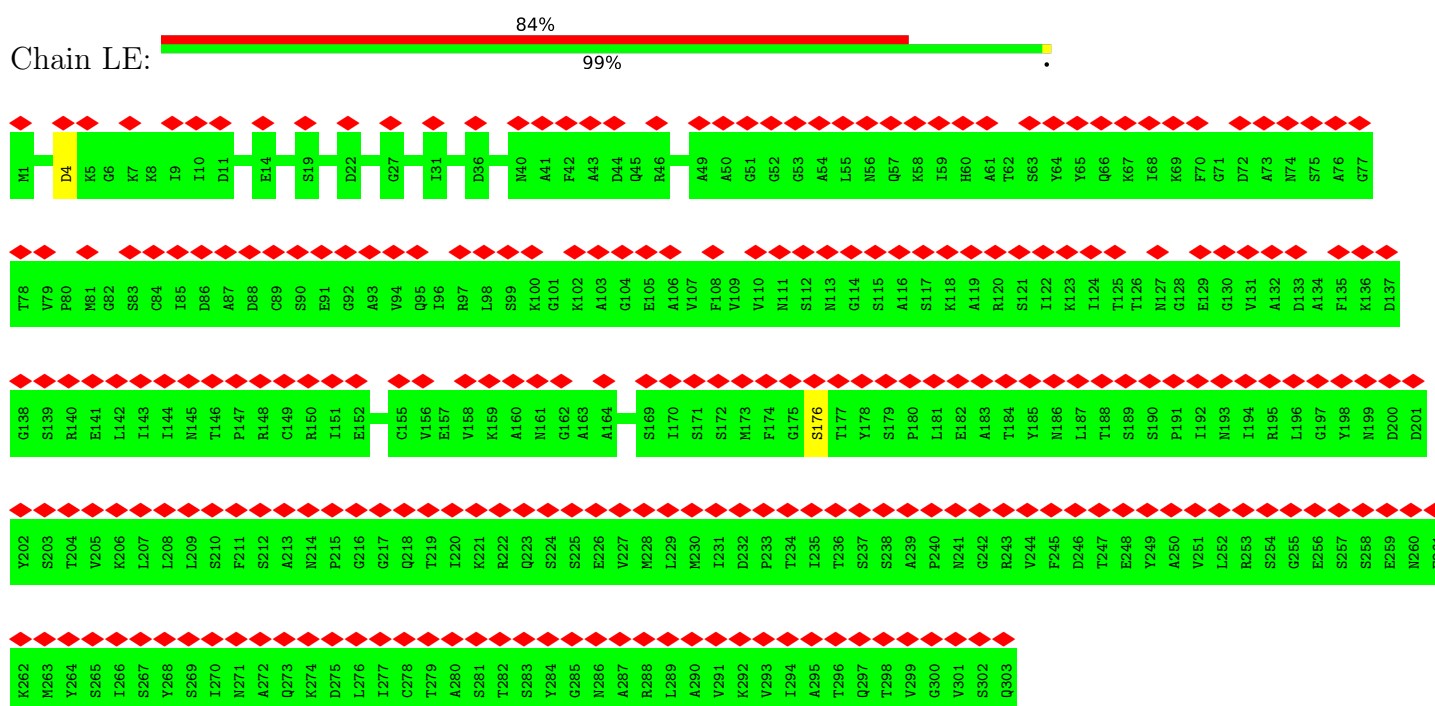




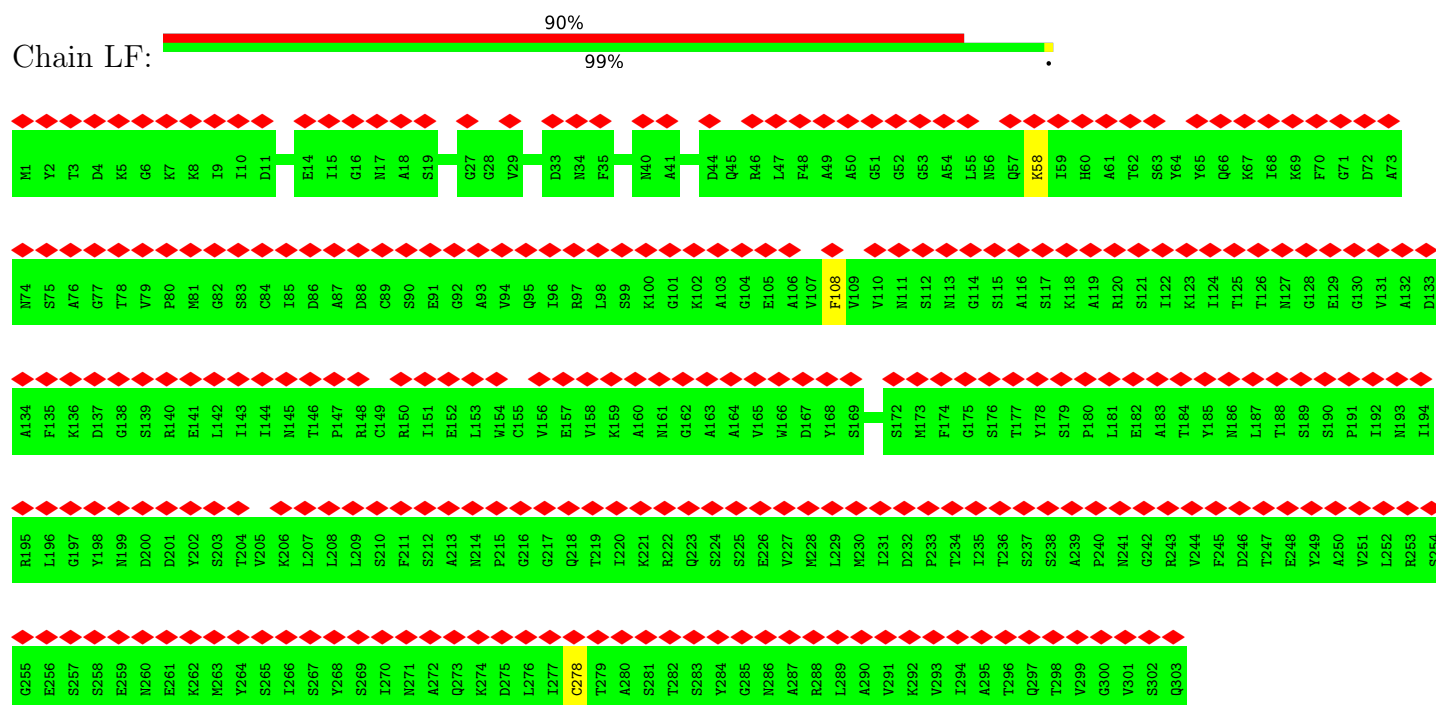
• Molecule 9: Baseplate wedge tail fiber connector



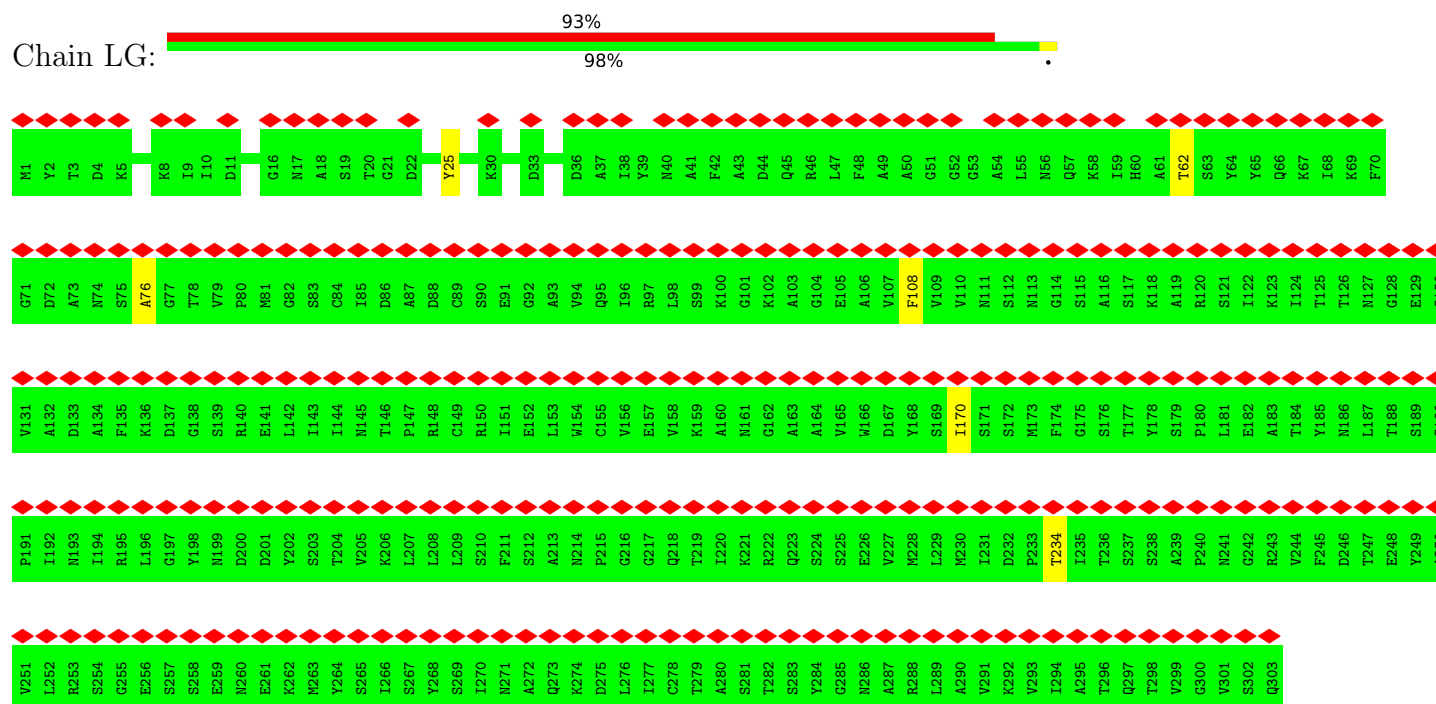
• Molecule 9: Baseplate wedge tail fiber connector



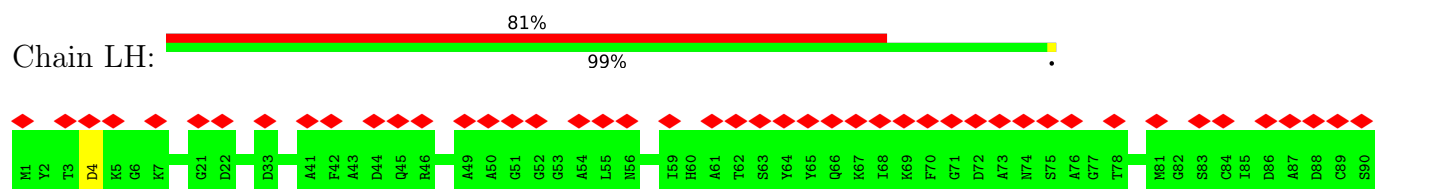
• Molecule 9: Baseplate wedge tail fiber connector

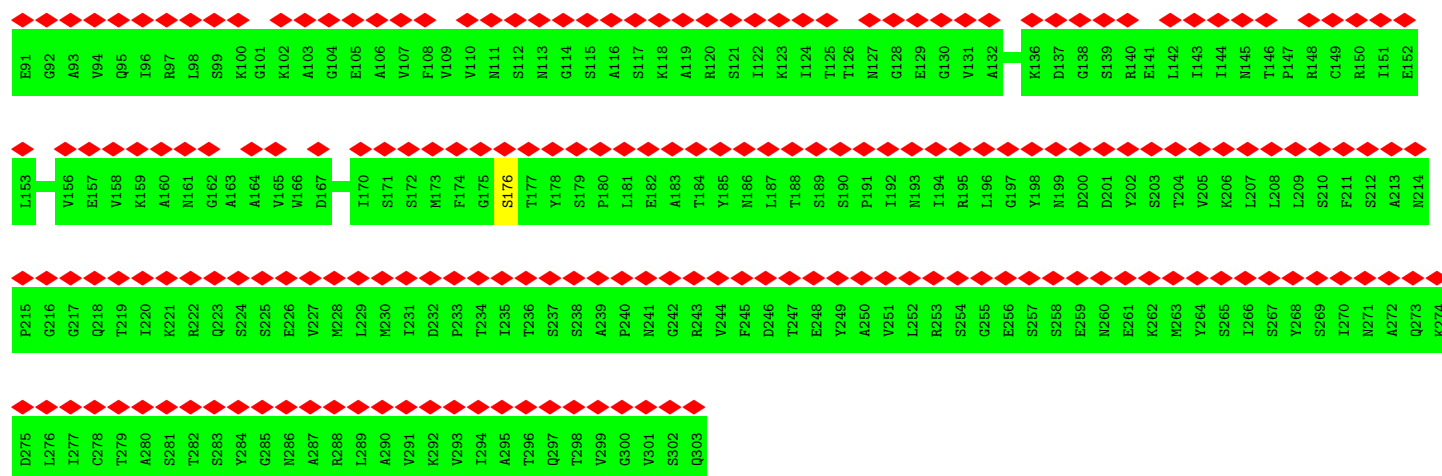


• Molecule 9: Baseplate wedge tail fiber connector

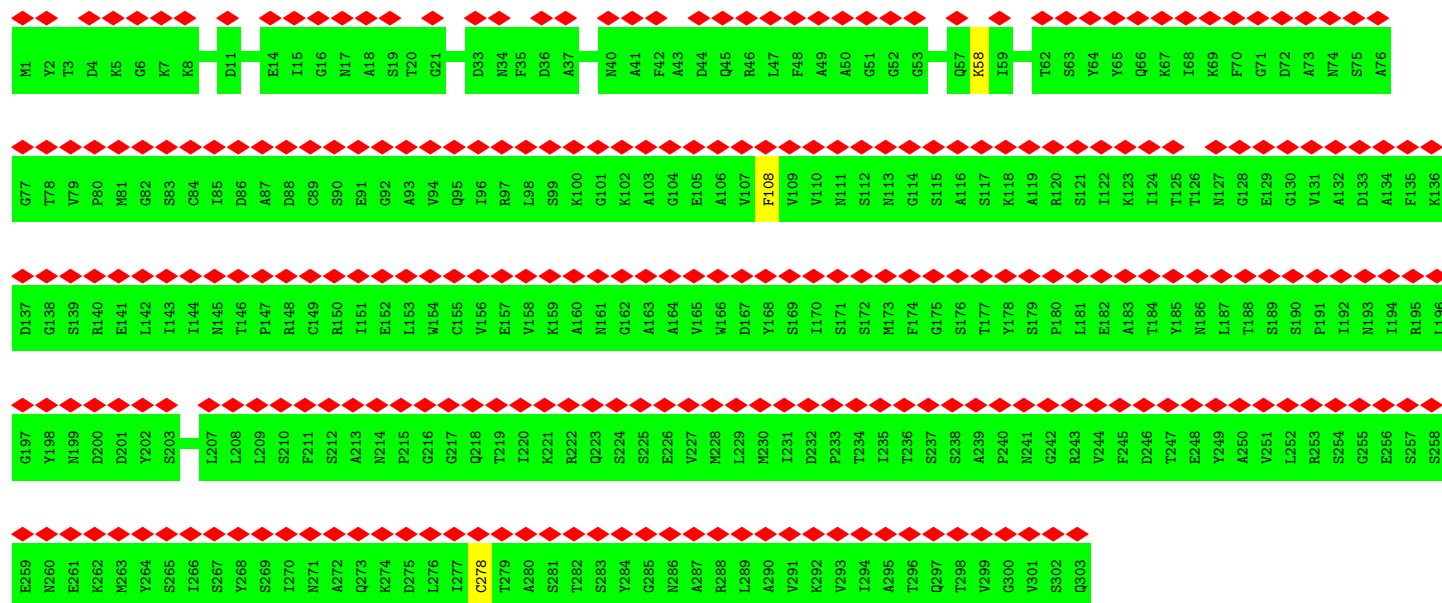
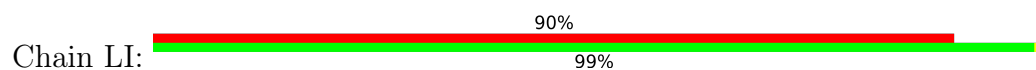


• Molecule 9: Baseplate wedge tail fiber connector



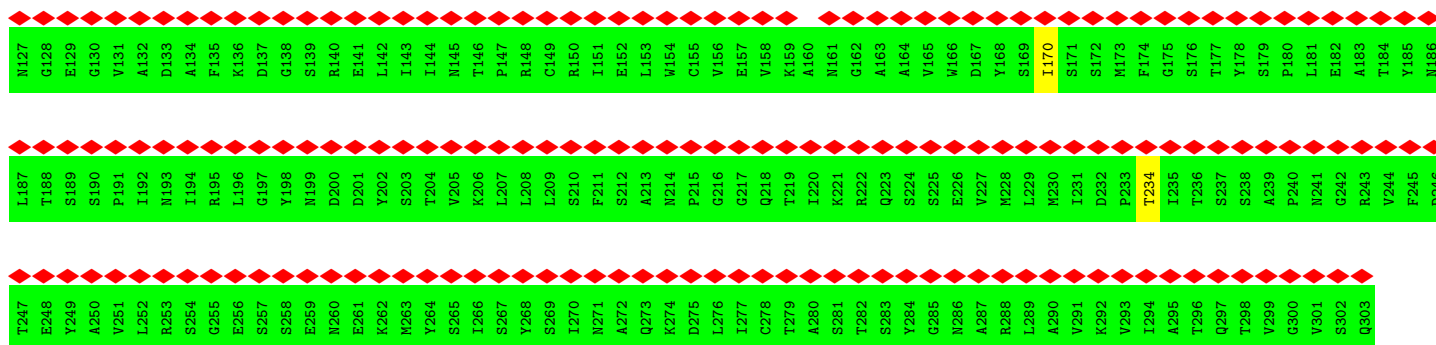


• Molecule 9: Baseplate wedge tail fiber connector

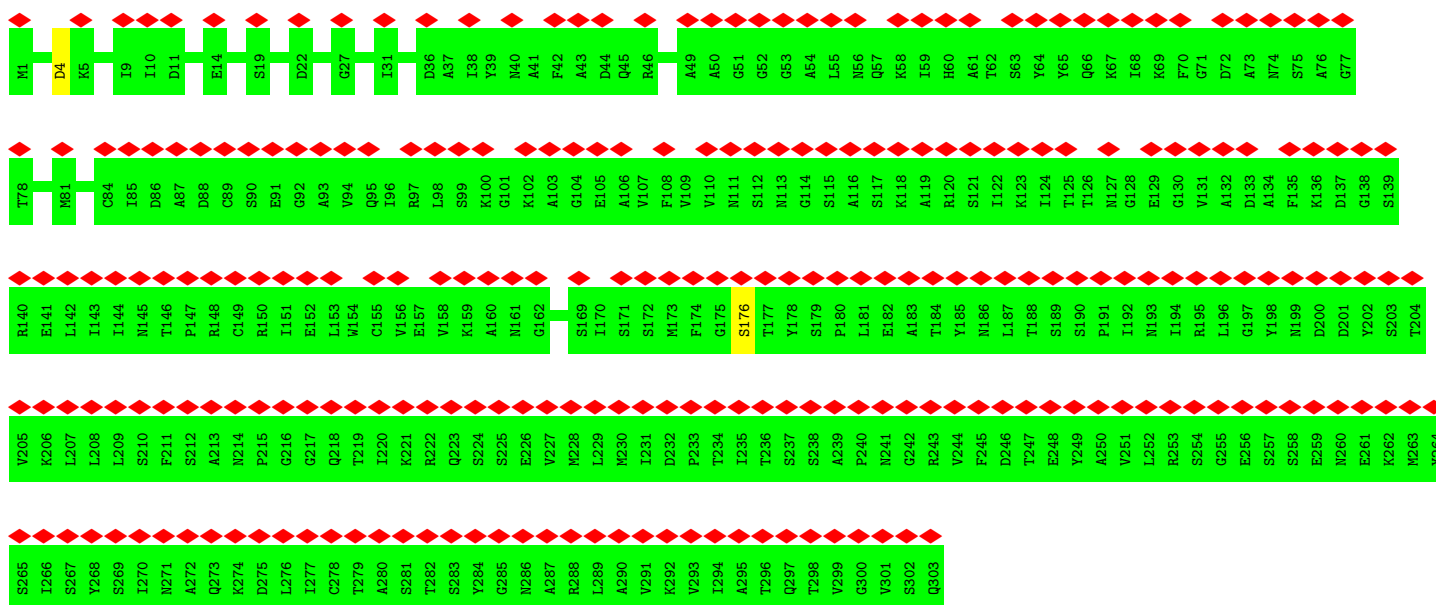
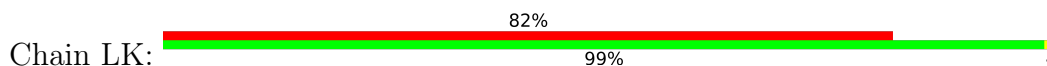


• Molecule 9: Baseplate wedge tail fiber connector

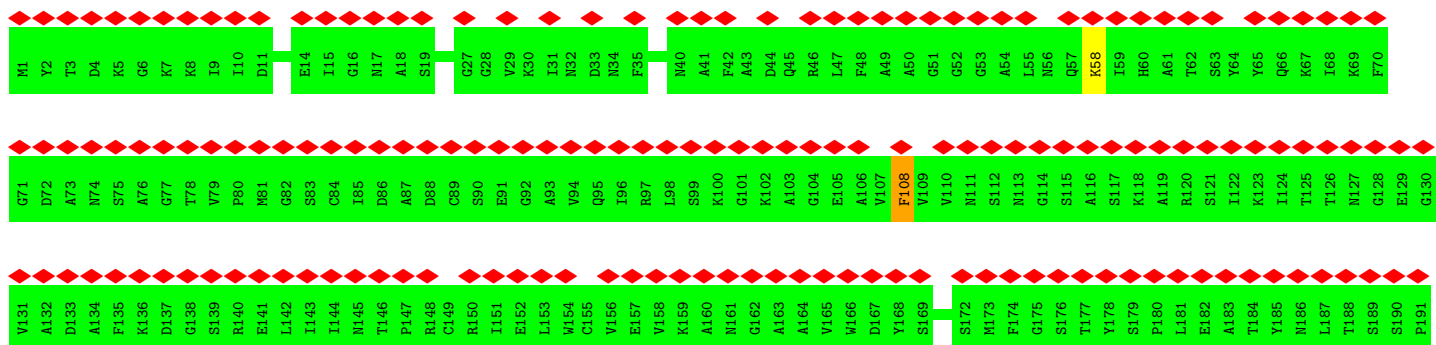


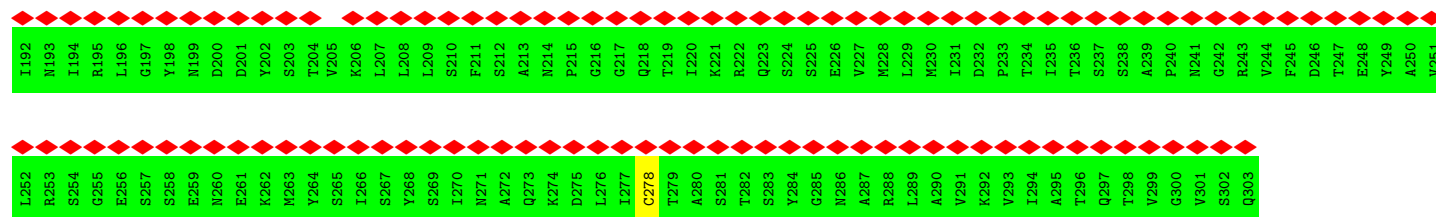


• Molecule 9: Baseplate wedge tail fiber connector

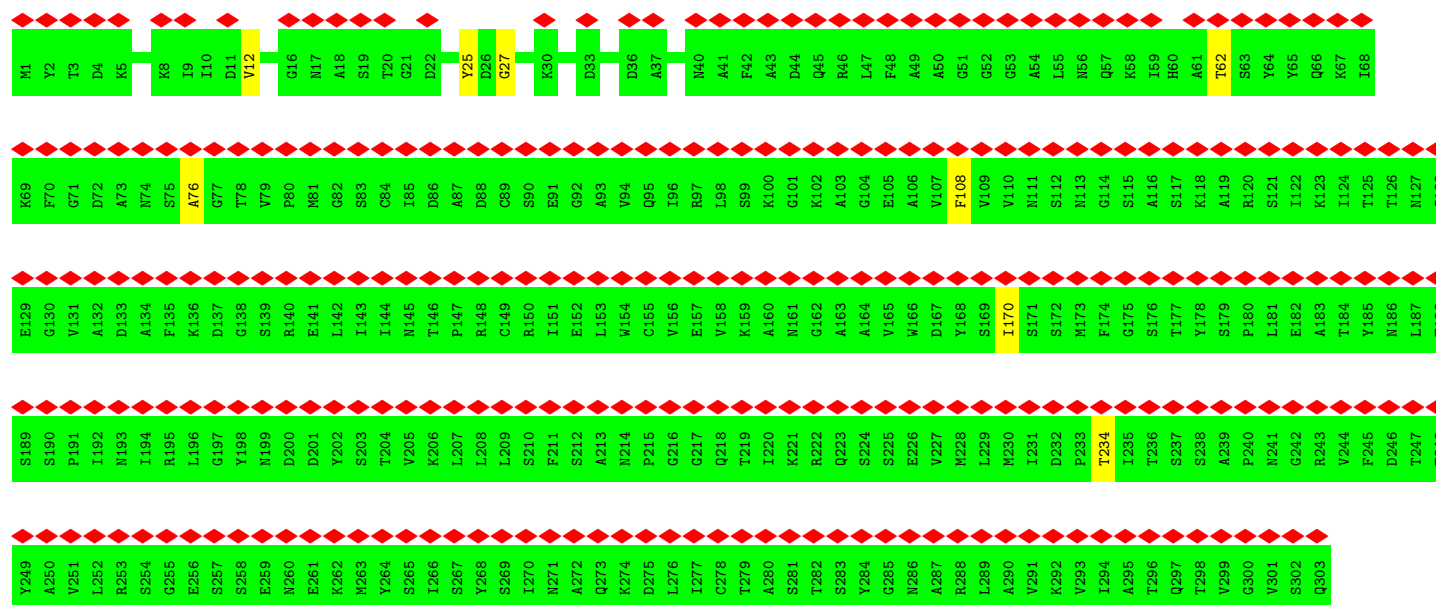


• Molecule 9: Baseplate wedge tail fiber connector

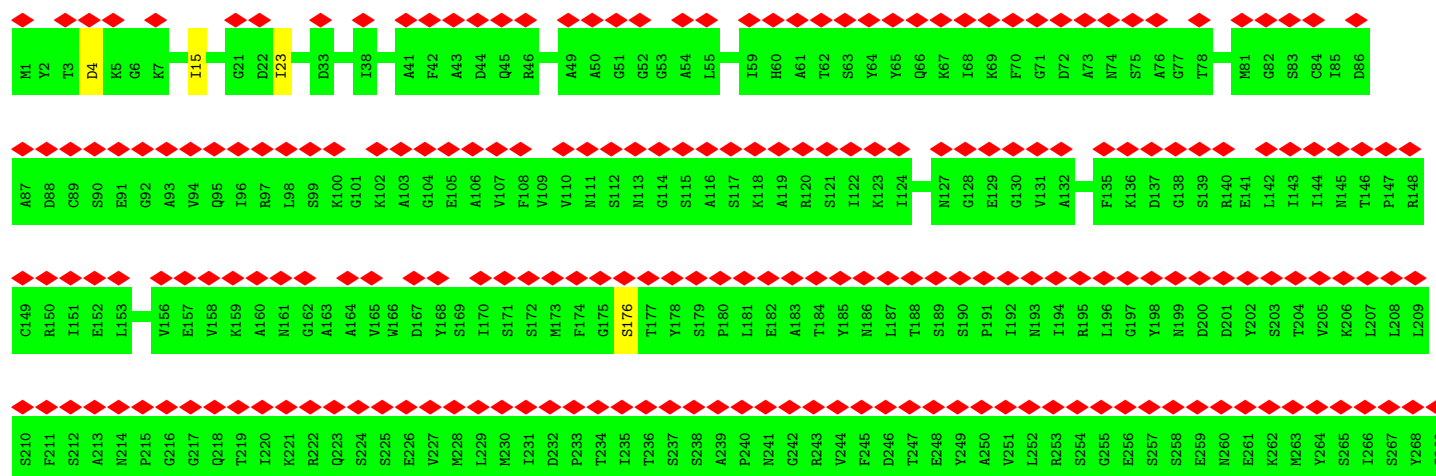
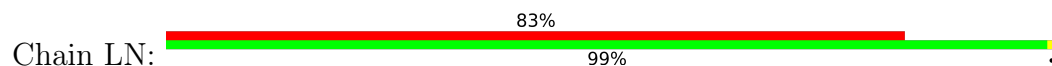


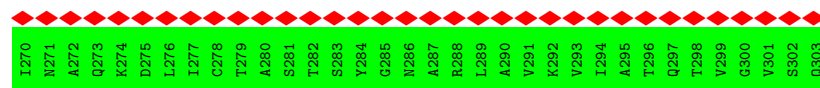


• Molecule 9: Baseplate wedge tail fiber connector

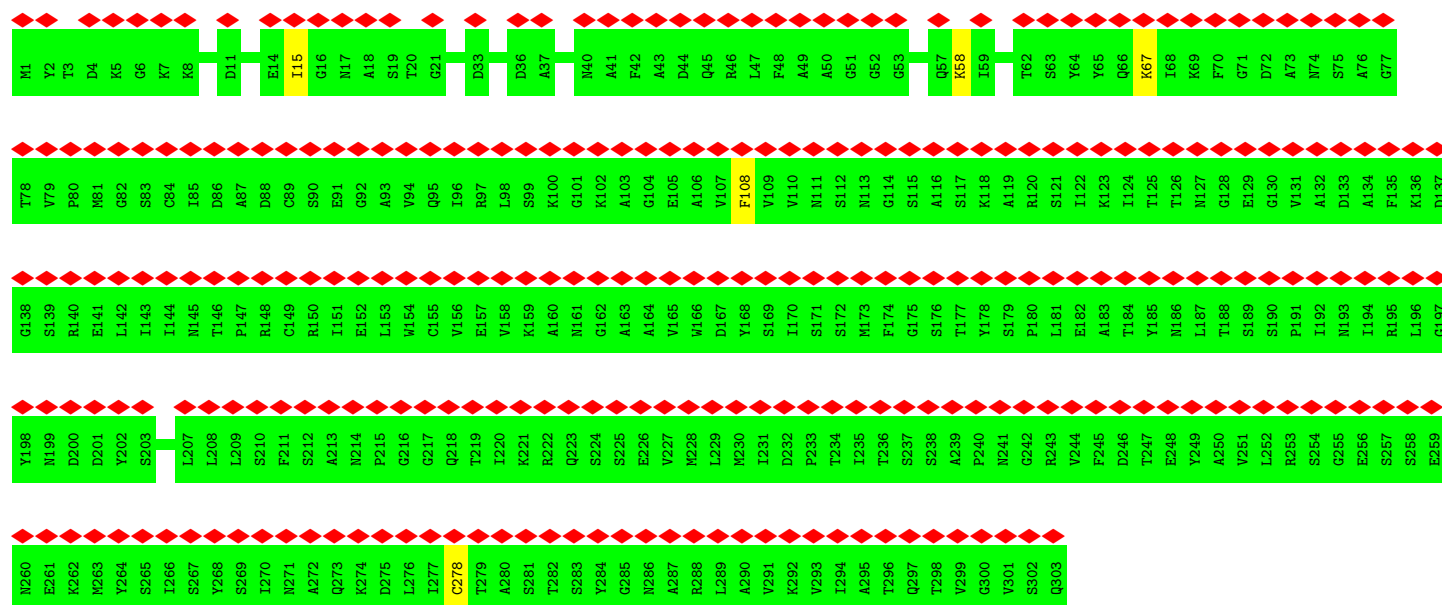


• Molecule 9: Baseplate wedge tail fiber connector

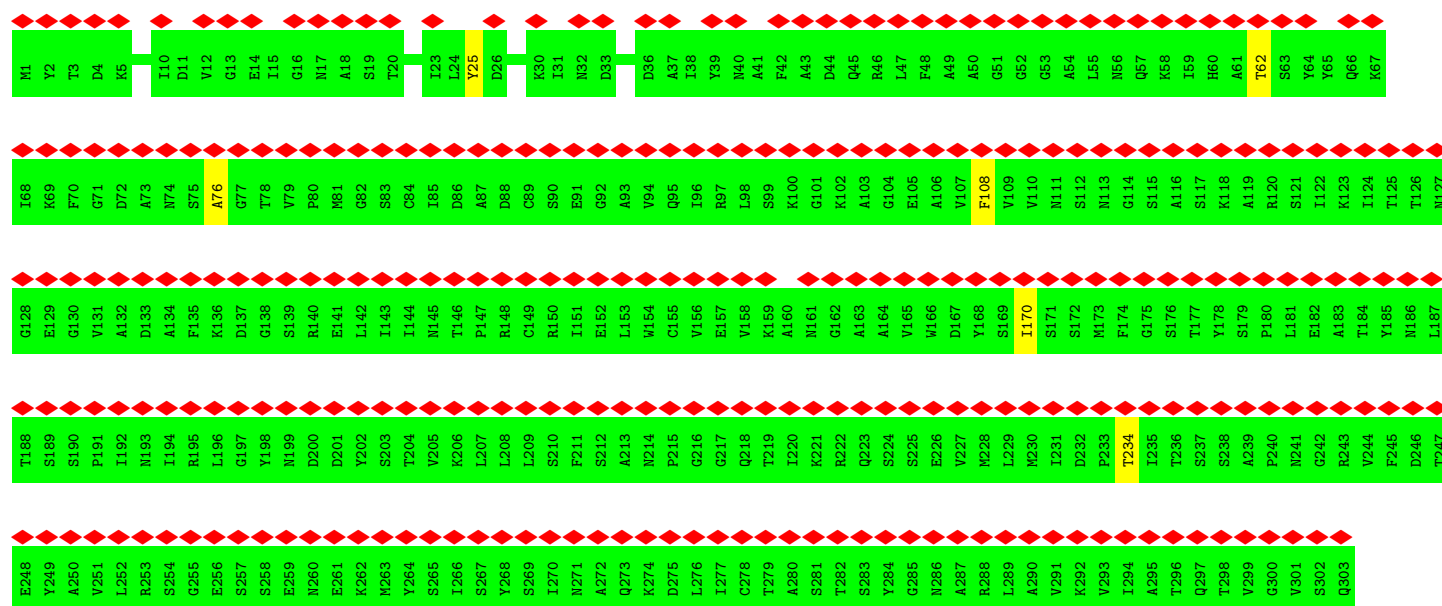




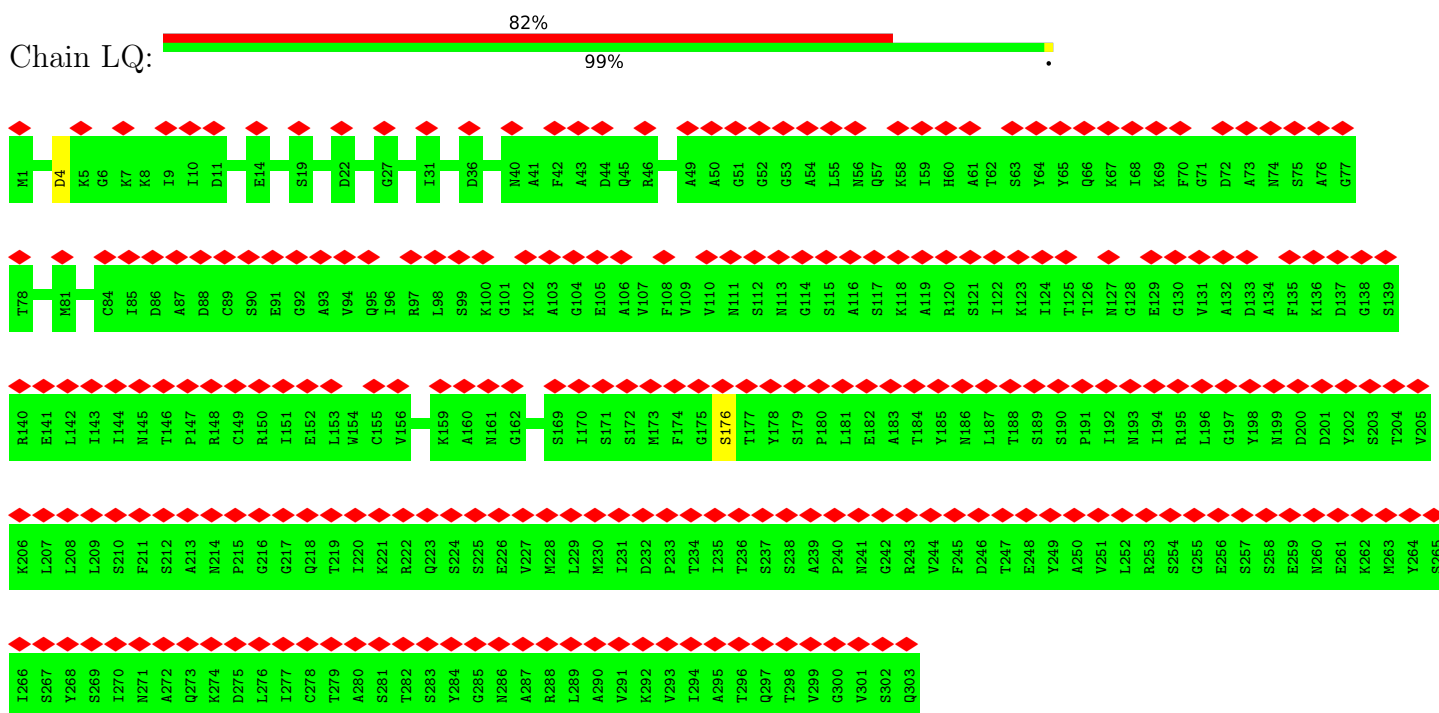
• Molecule 9: Baseplate wedge tail fiber connector



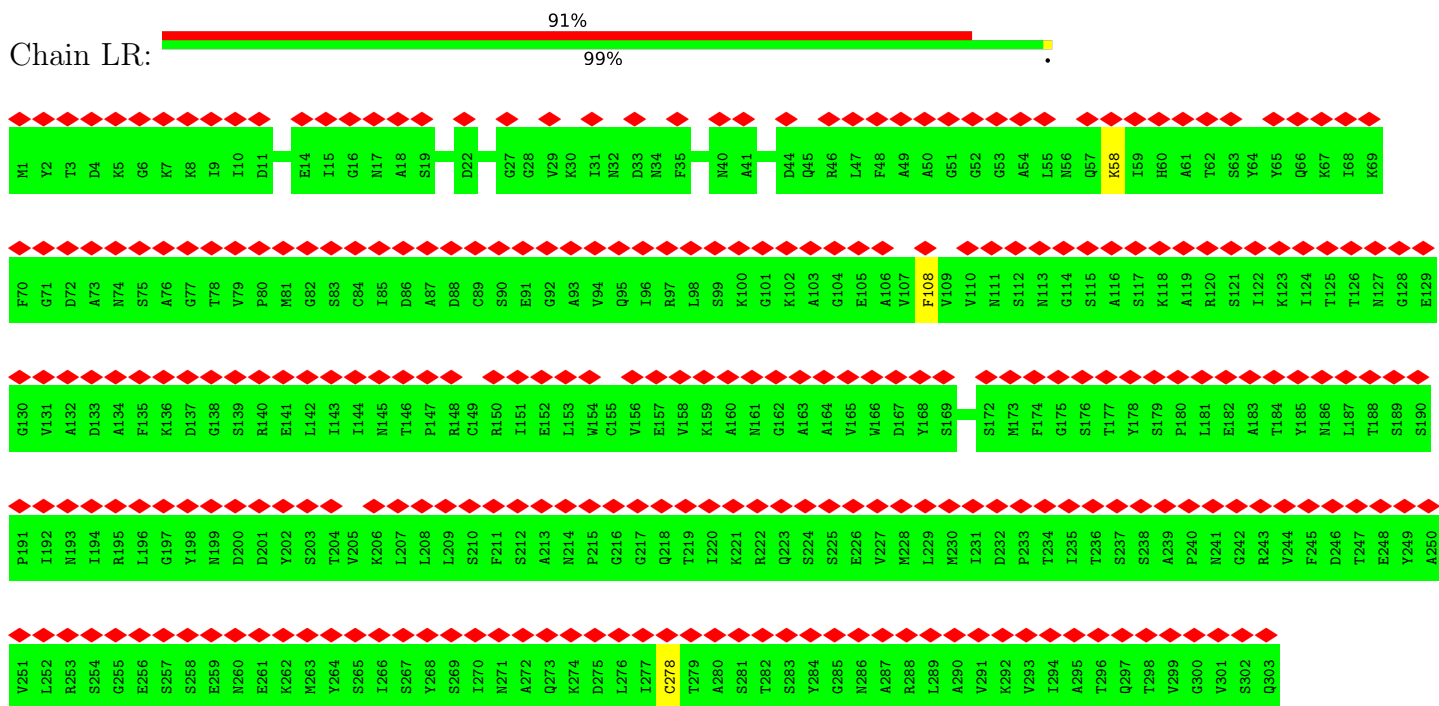
• Molecule 9: Baseplate wedge tail fiber connector



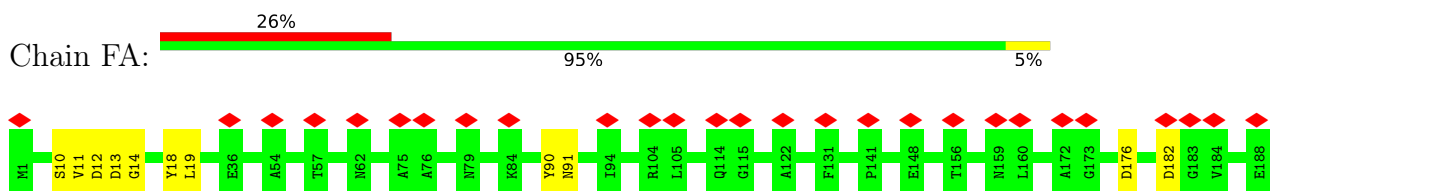
• Molecule 9: Baseplate wedge tail fiber connector

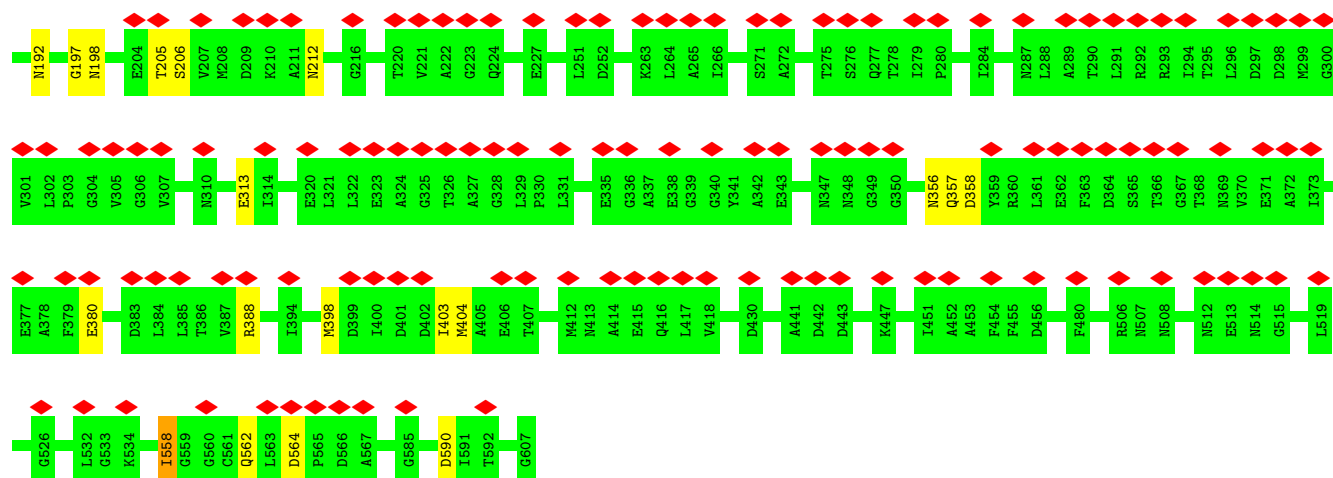


• Molecule 9: Baseplate wedge tail fiber connector

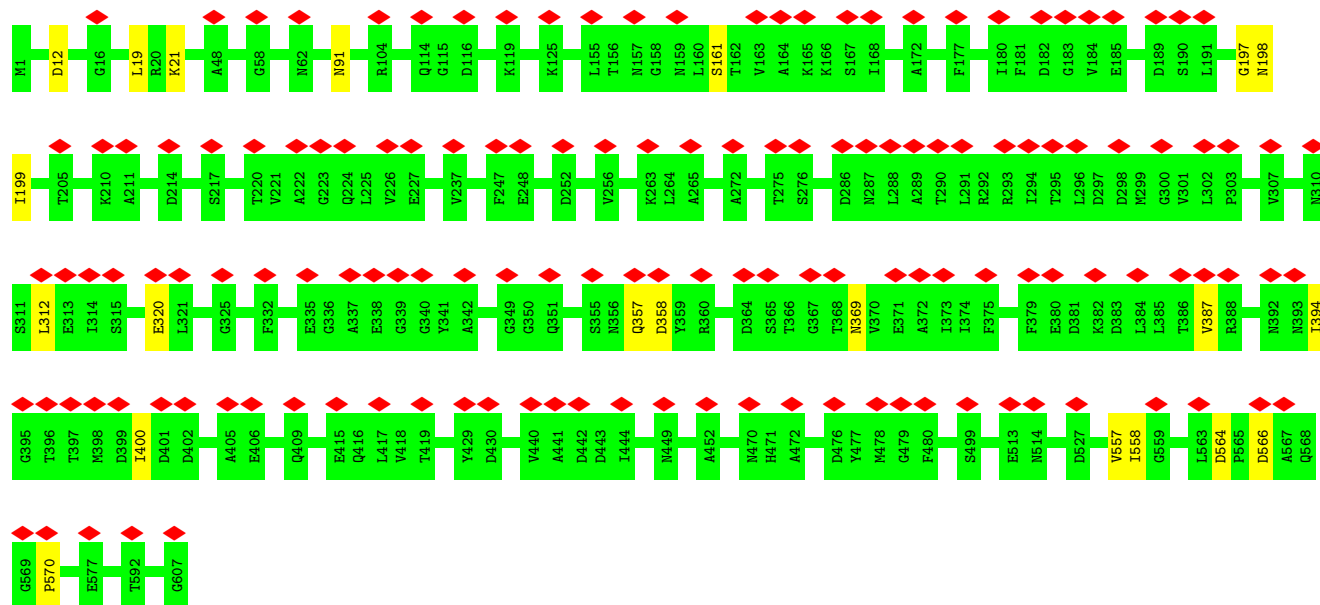


• Molecule 10: Baseplate wedge protein gp10

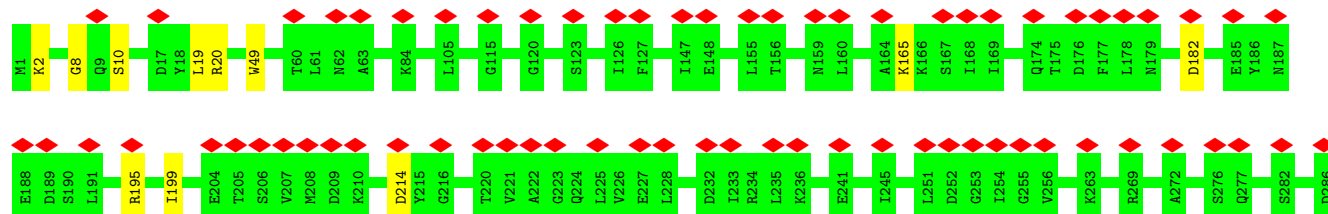


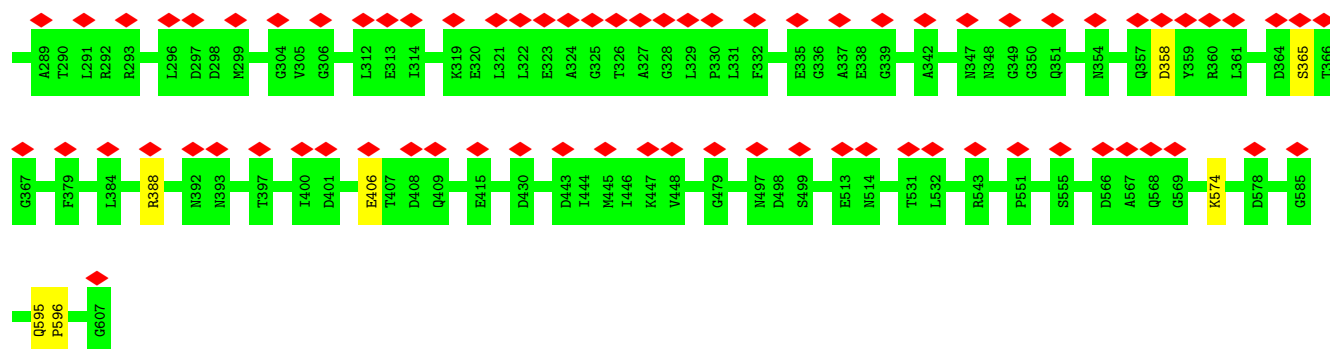


- Molecule 10: Baseplate wedge protein gp10

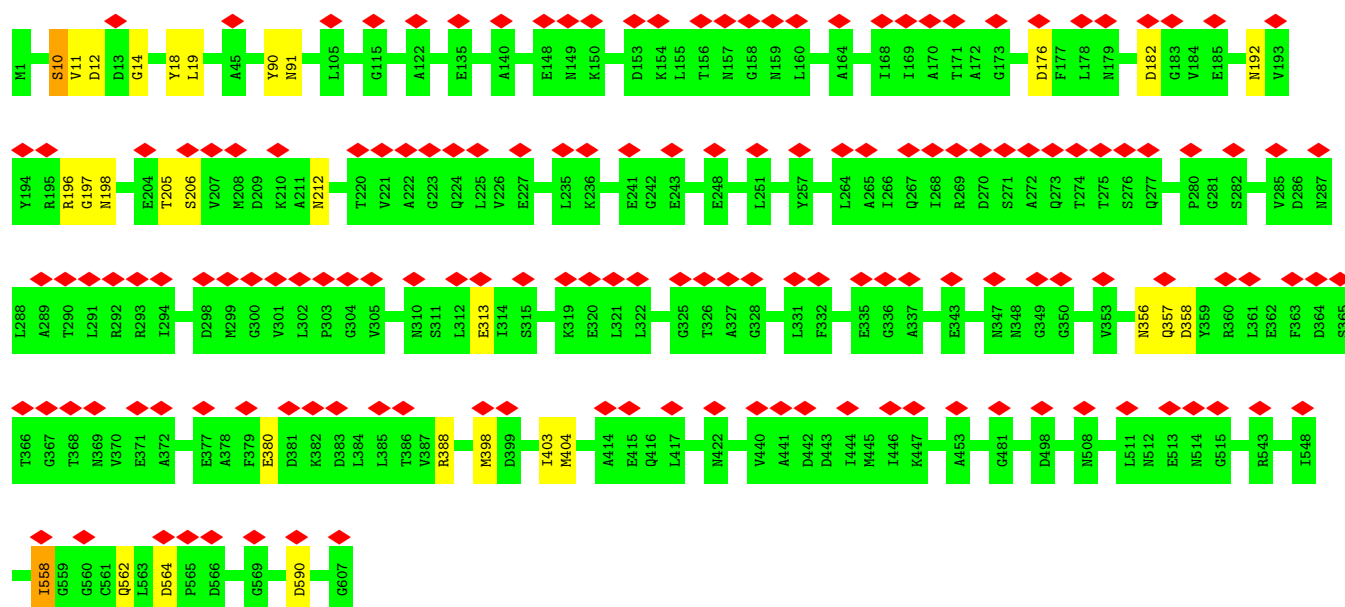


- Molecule 10: Baseplate wedge protein gp10

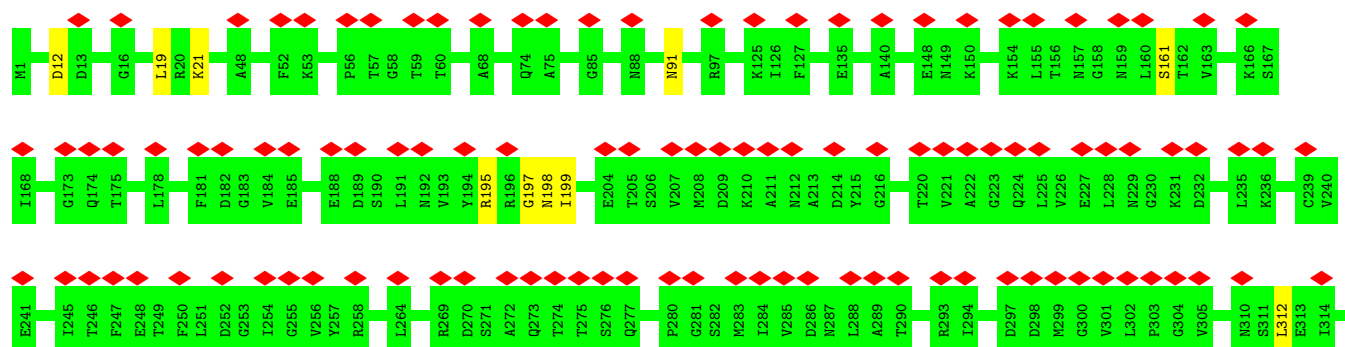


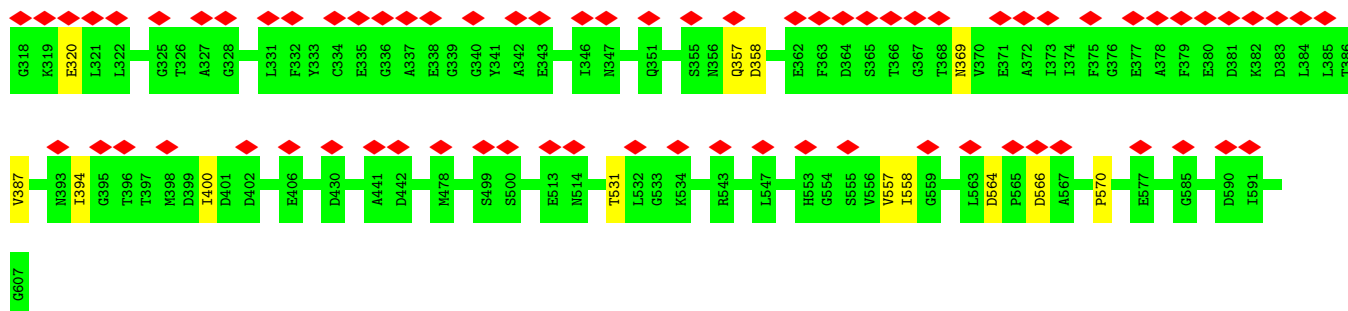


• Molecule 10: Baseplate wedge protein gp10

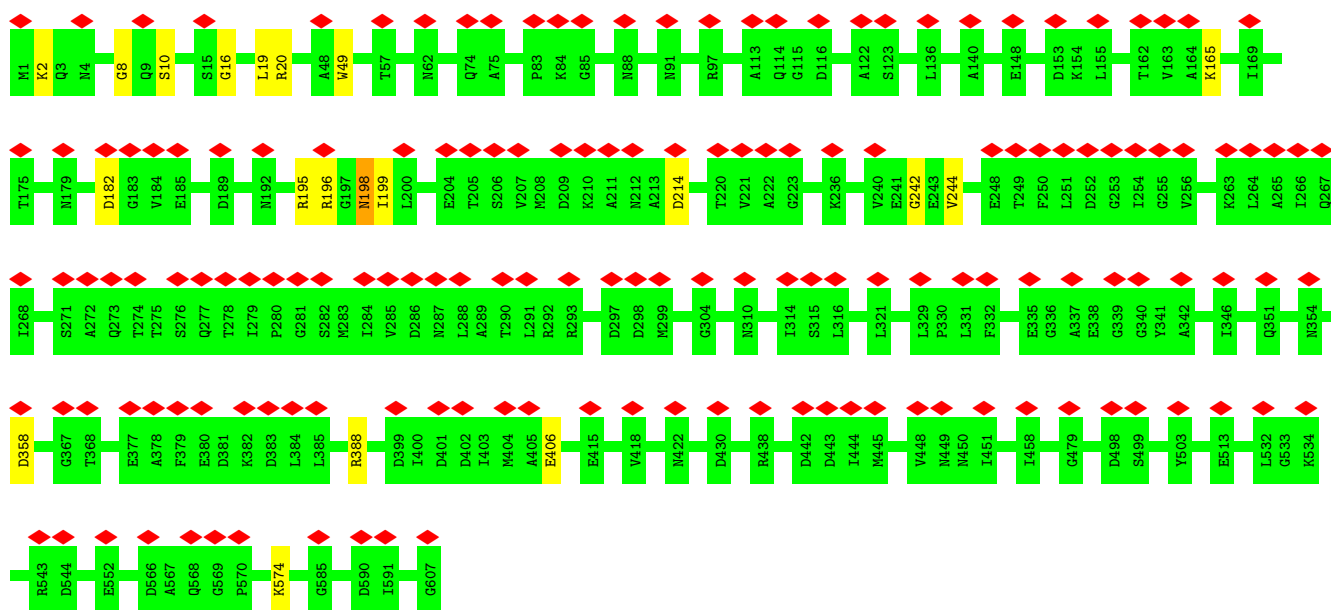


• Molecule 10: Baseplate wedge protein gp10

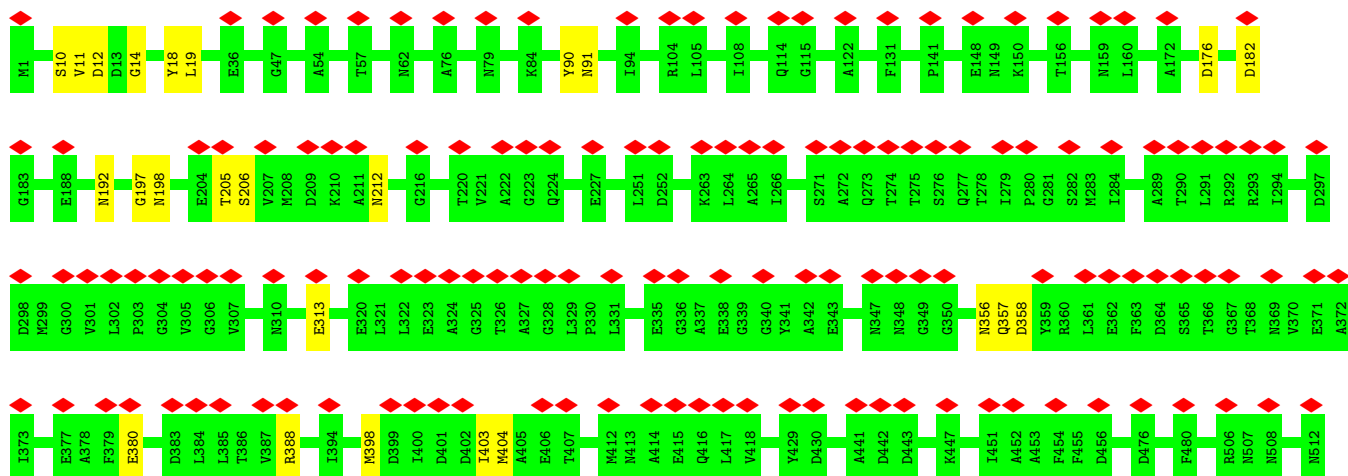


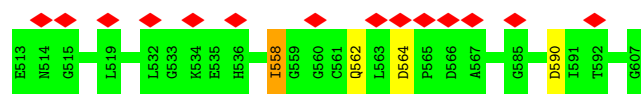


• Molecule 10: Baseplate wedge protein gp10

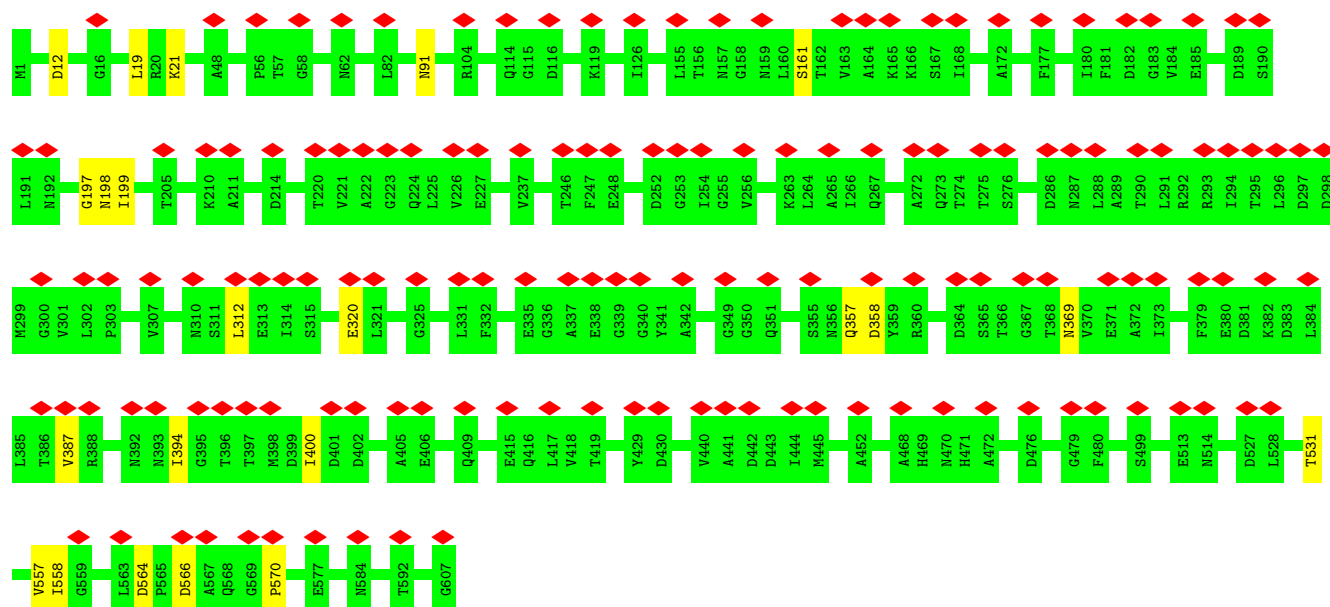


• Molecule 10: Baseplate wedge protein gp10

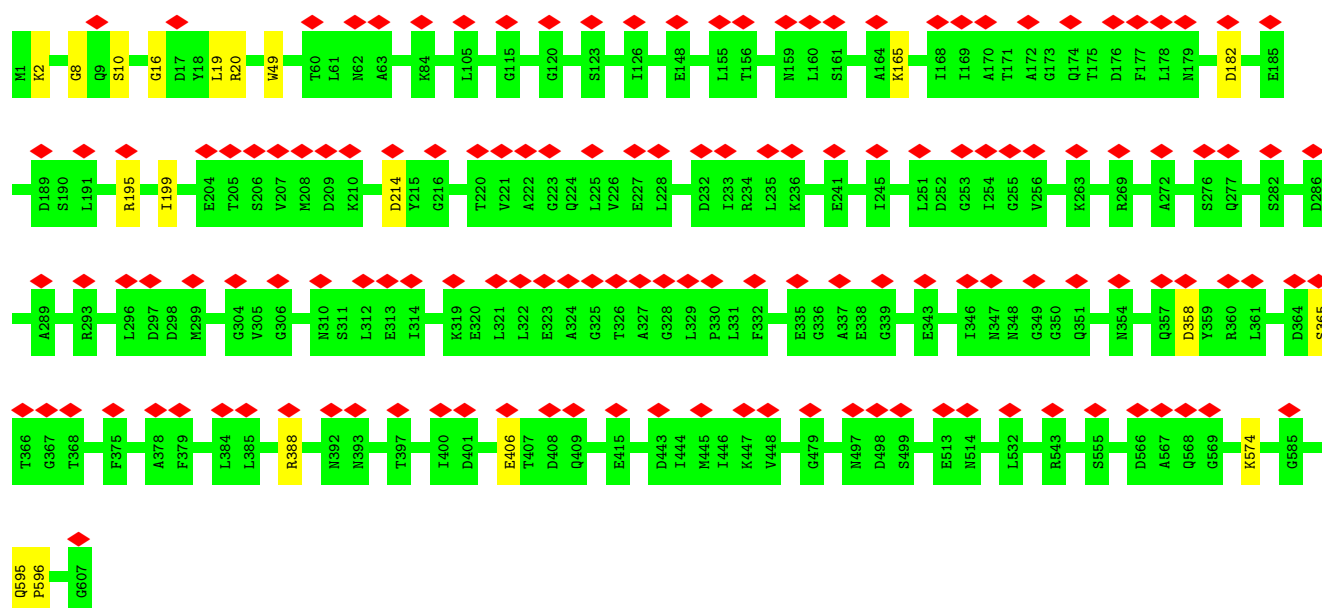




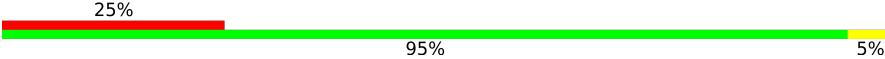
• Molecule 10: Baseplate wedge protein gp10

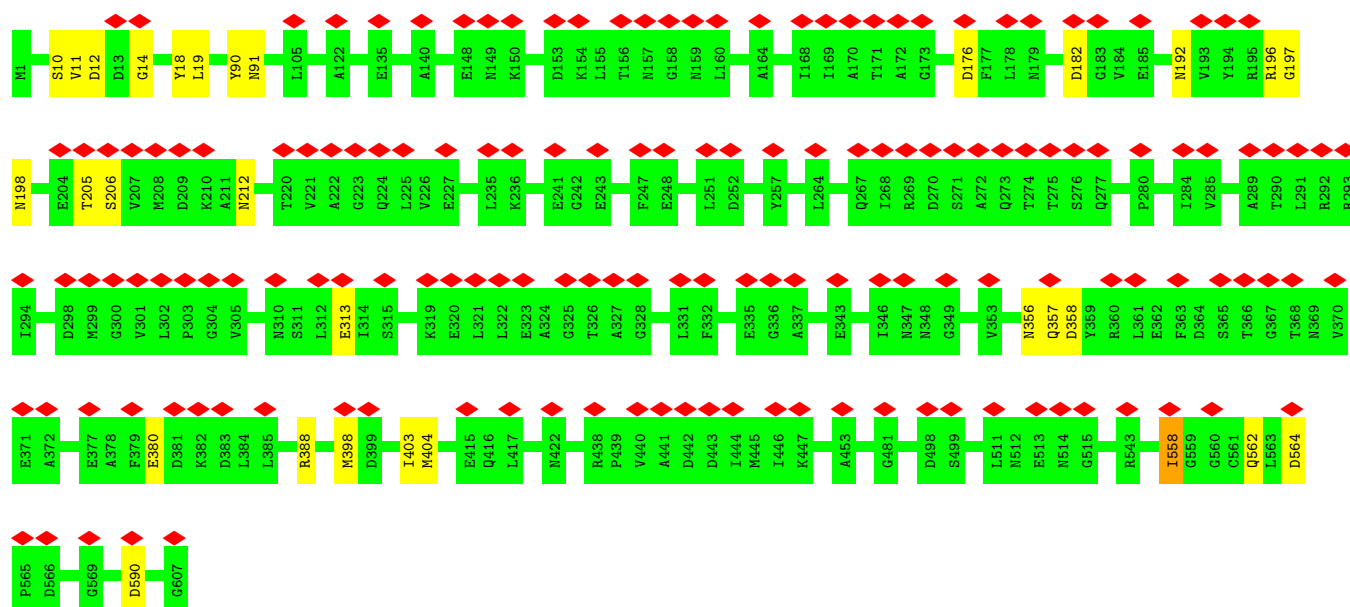


• Molecule 10: Baseplate wedge protein gp10

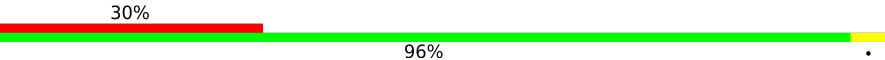


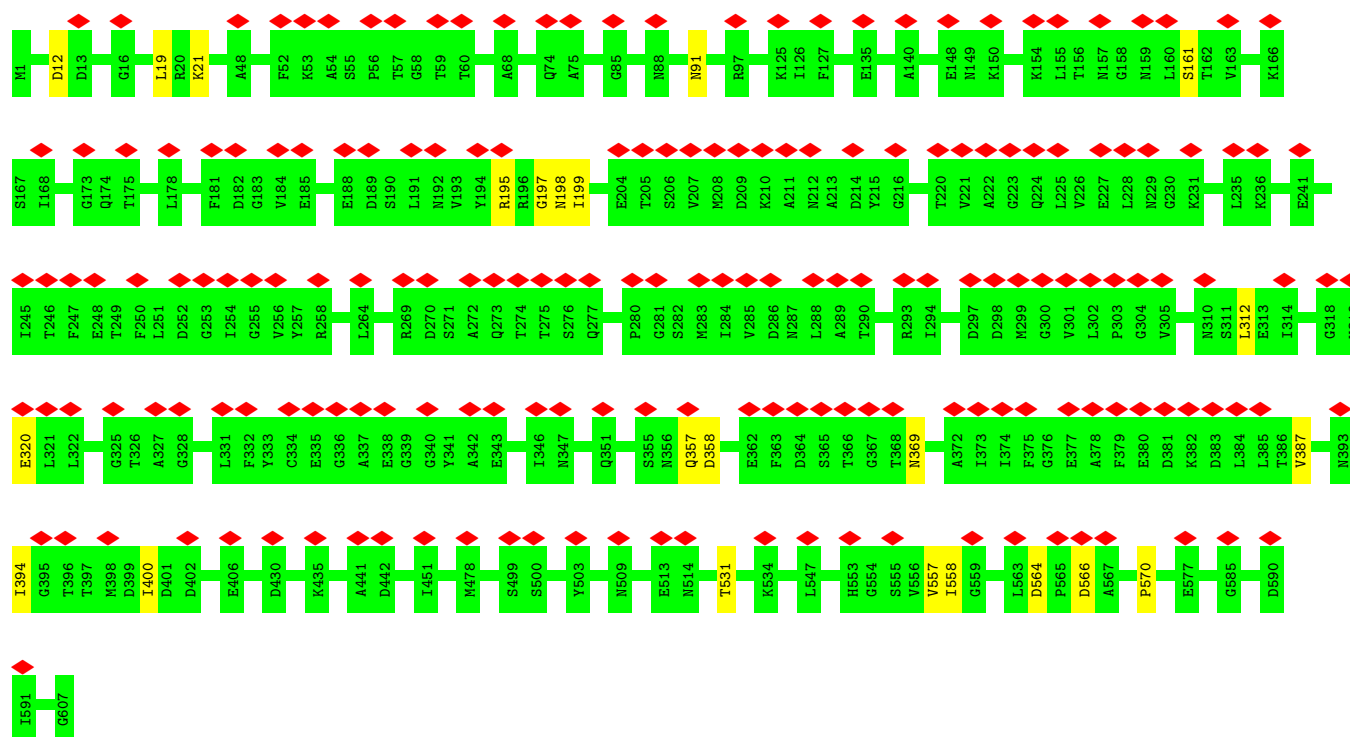
• Molecule 10: Baseplate wedge protein gp10

Chain Fb: 

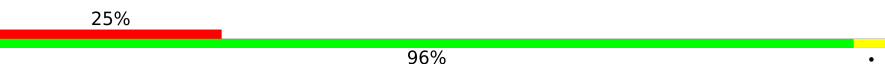


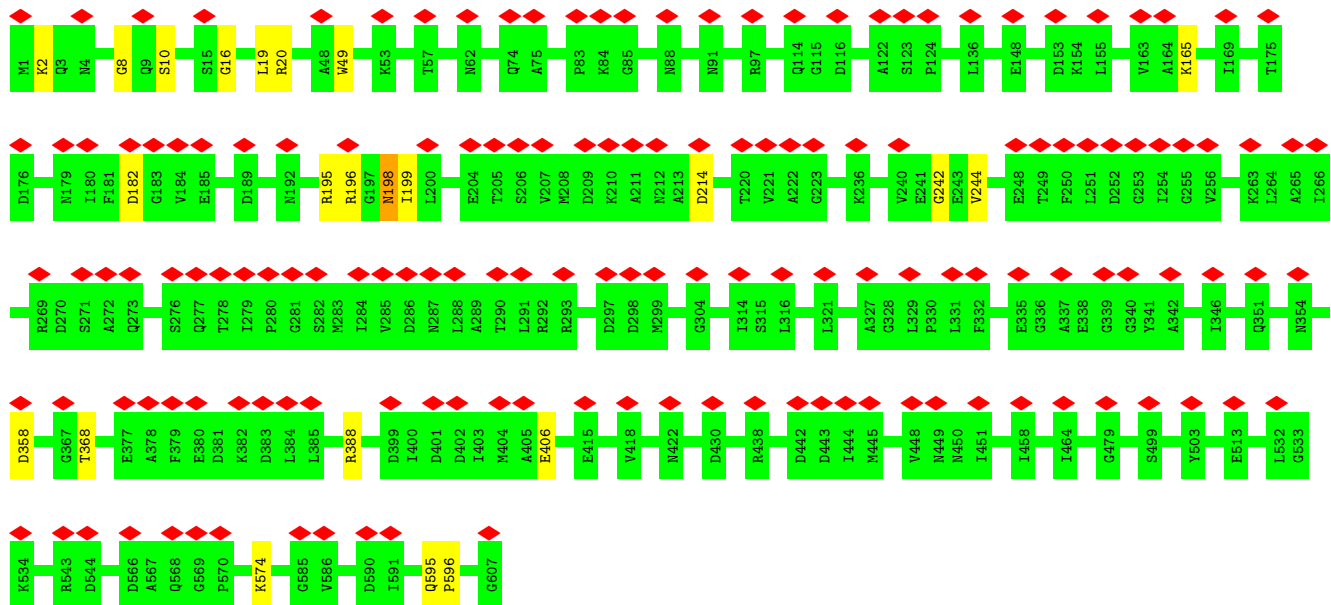
• Molecule 10: Baseplate wedge protein gp10

Chain Fc: 



• Molecule 10: Baseplate wedge protein gp10

Chain Fd: 

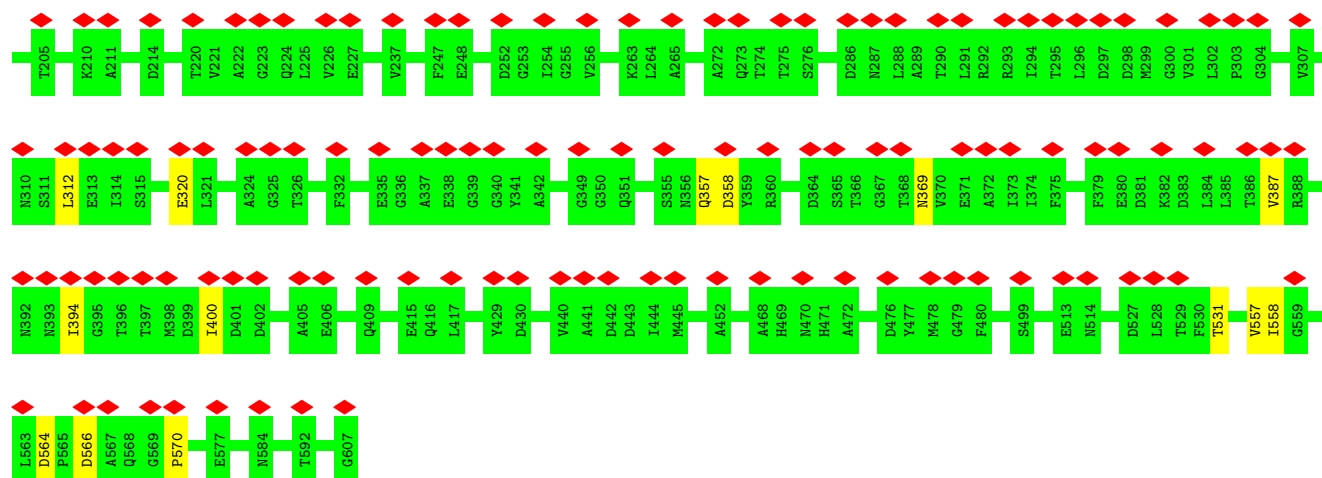


• Molecule 10: Baseplate wedge protein gp10

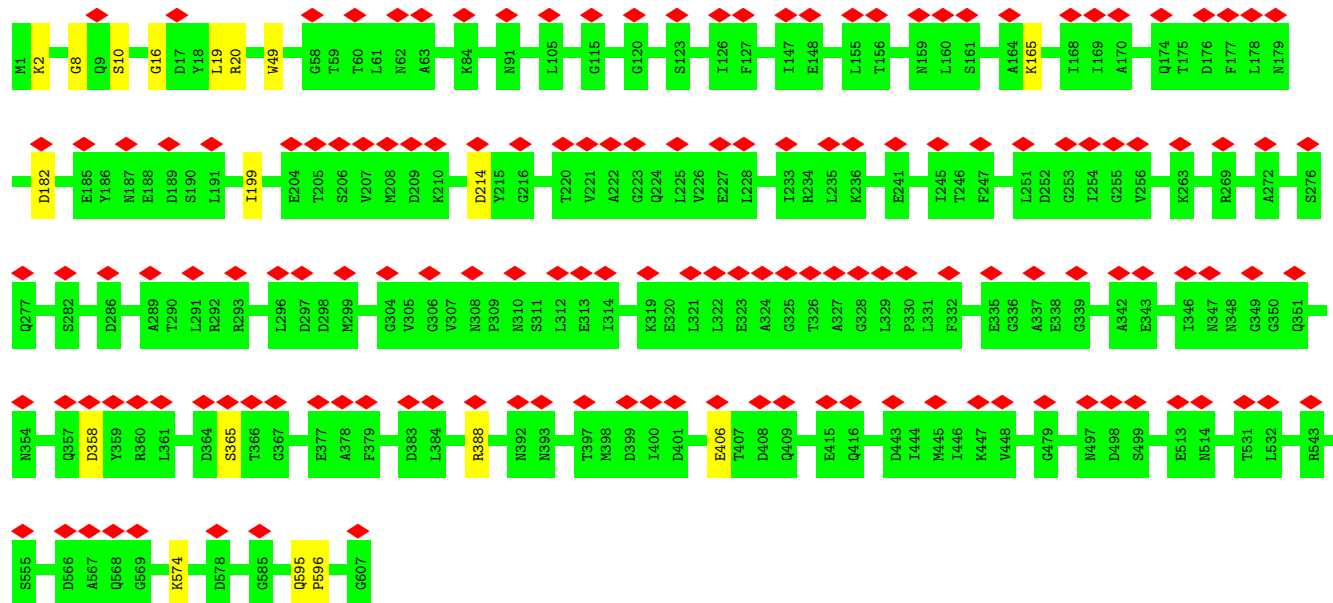


• Molecule 10: Baseplate wedge protein gp10

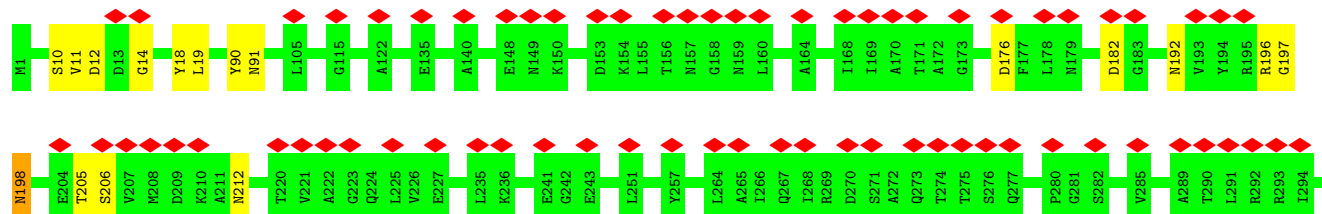


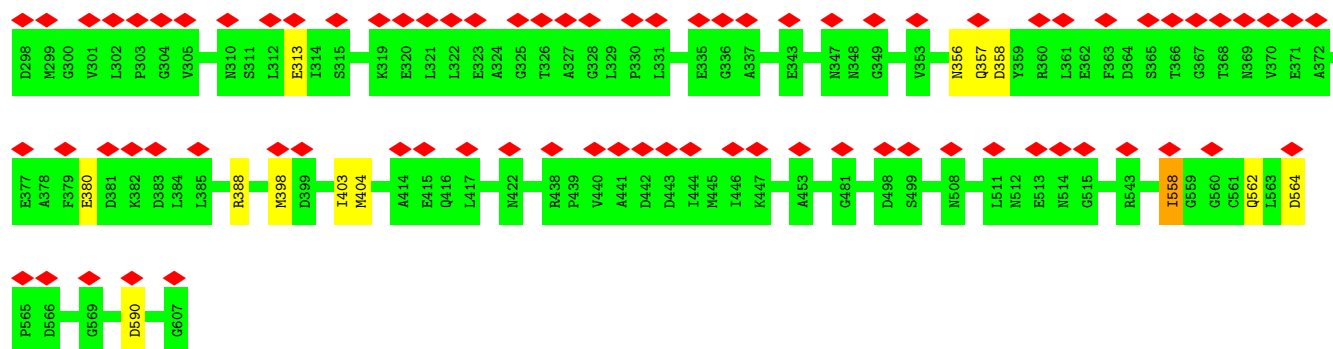


• Molecule 10: Baseplate wedge protein gp10

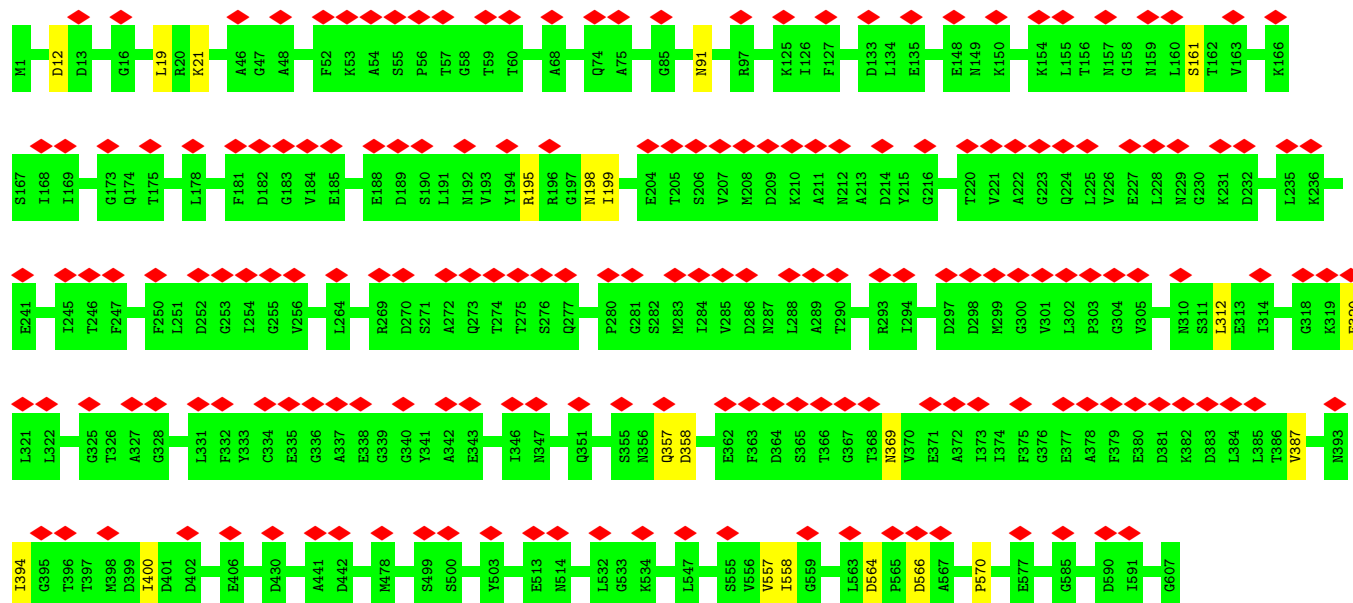


• Molecule 10: Baseplate wedge protein gp10

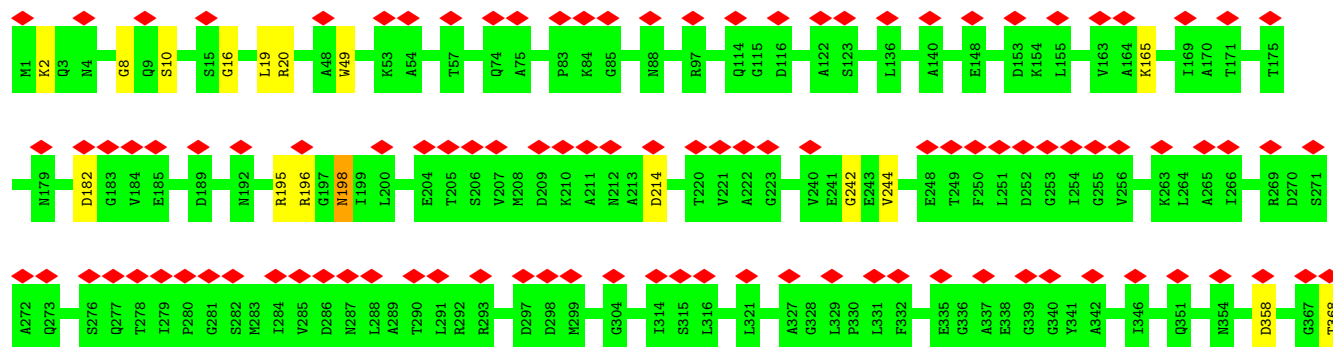


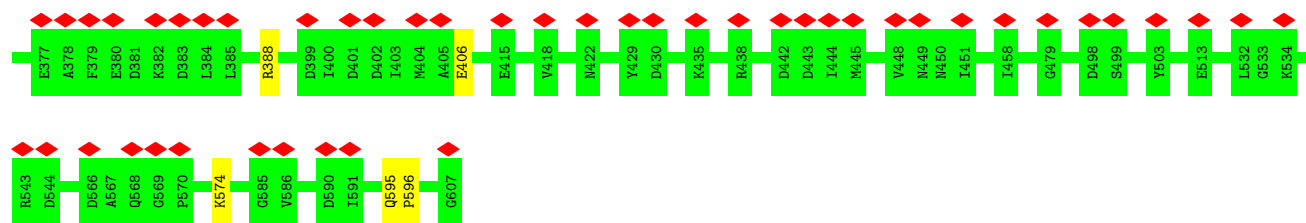


• Molecule 10: Baseplate wedge protein gp10



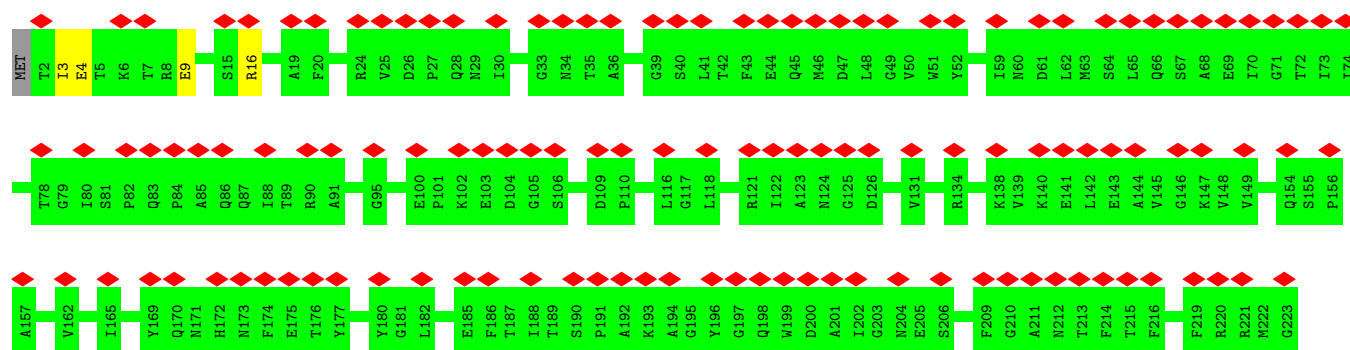
• Molecule 10: Baseplate wedge protein gp10





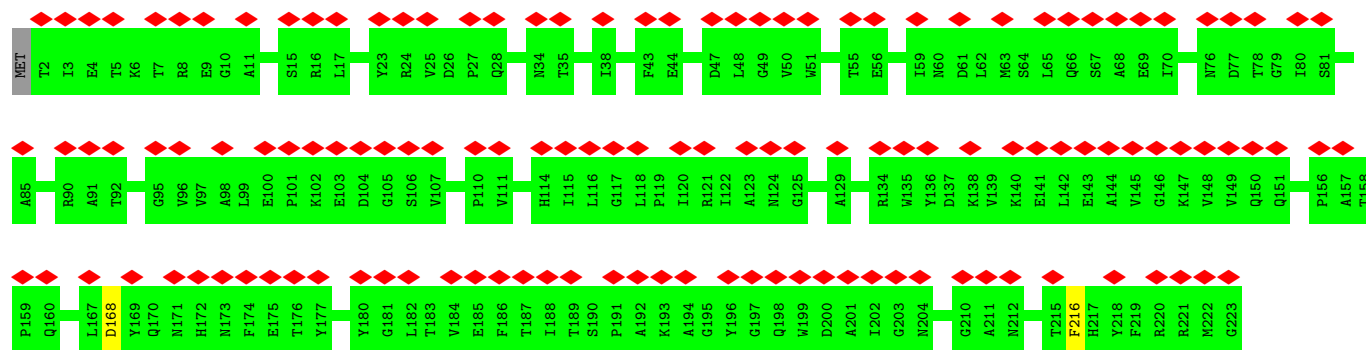
- Molecule 11: Baseplate wedge subunit and tail pin

Chain FD: 56% 98%



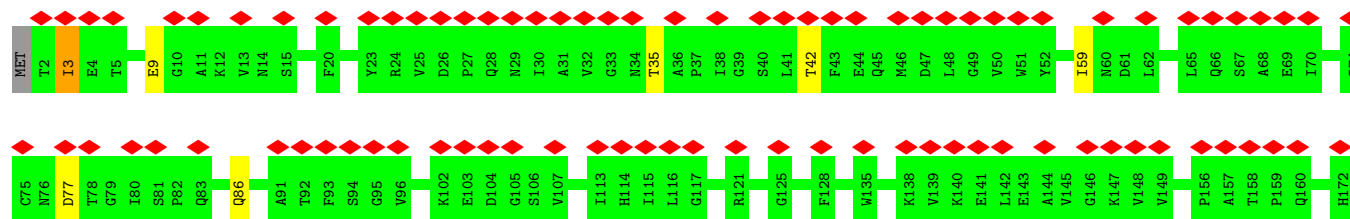
- Molecule 11: Baseplate wedge subunit and tail pin

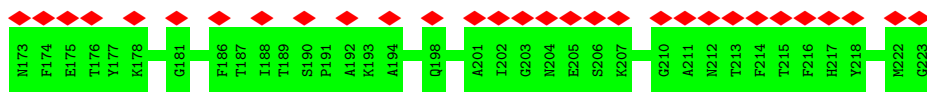
Chain FE: 58% 99%



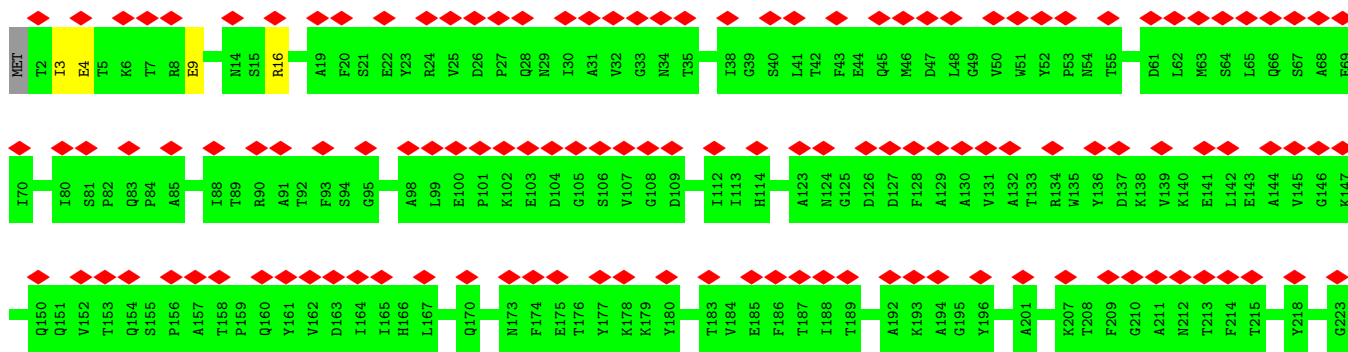
- Molecule 11: Baseplate wedge subunit and tail pin

Chain FF: 52% 96%

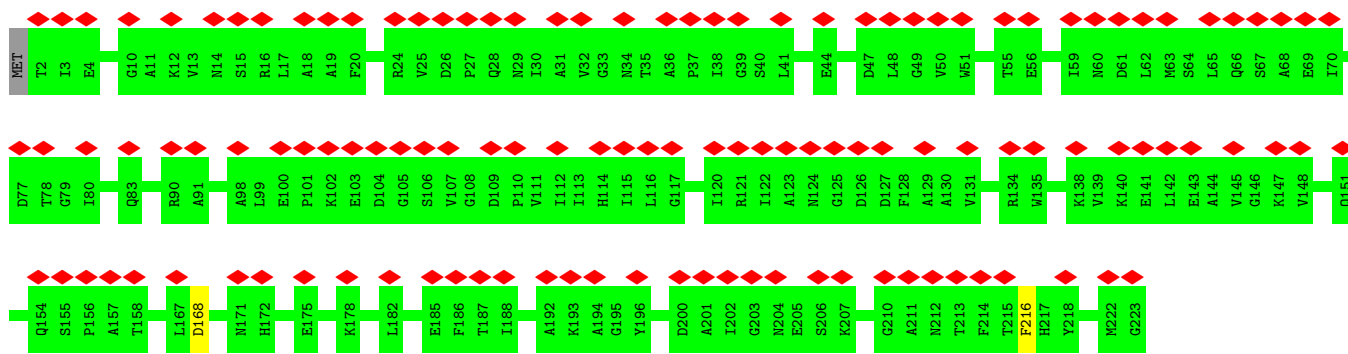




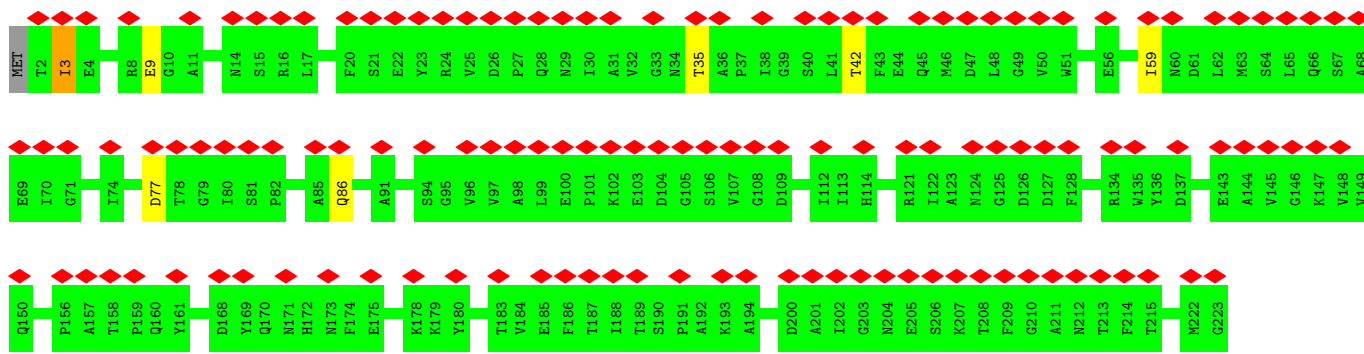
- Molecule 11: Baseplate wedge subunit and tail pin



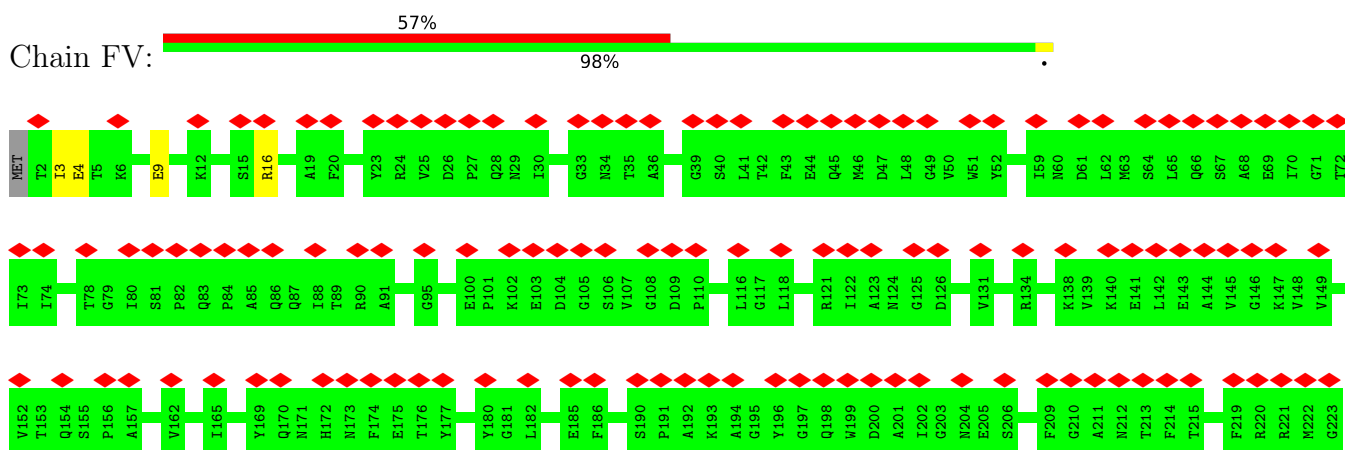
- Molecule 11: Baseplate wedge subunit and tail pin



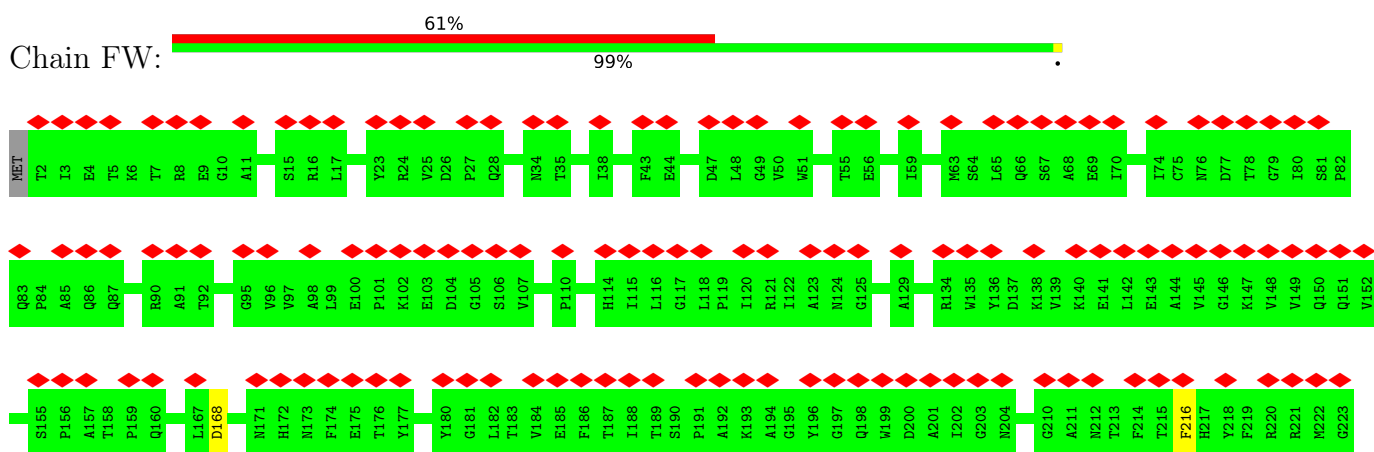
- Molecule 11: Baseplate wedge subunit and tail pin



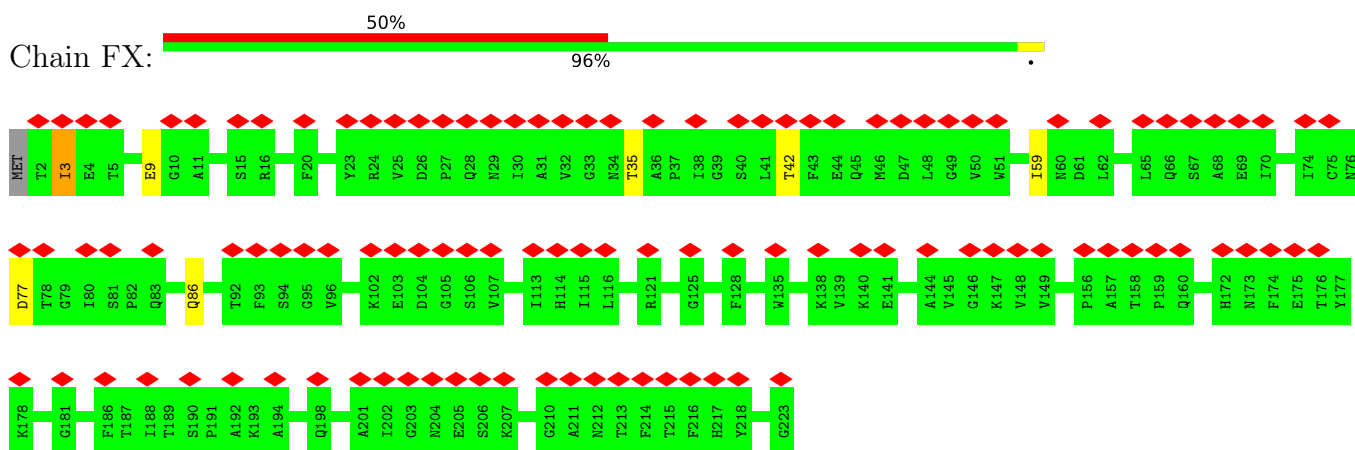
- Molecule 11: Baseplate wedge subunit and tail pin



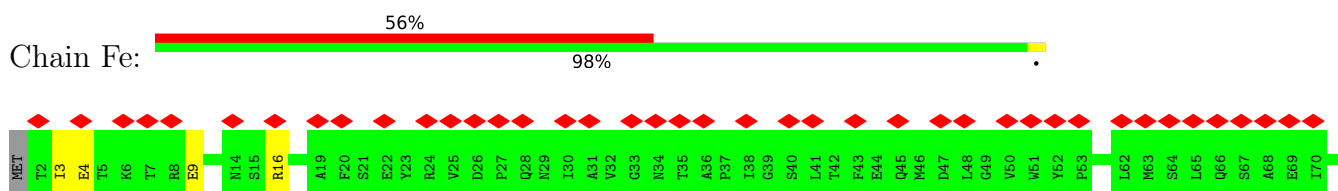
- Molecule 11: Baseplate wedge subunit and tail pin

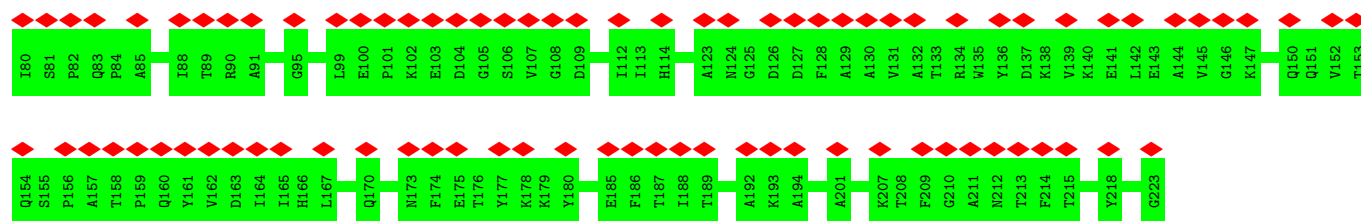


- Molecule 11: Baseplate wedge subunit and tail pin

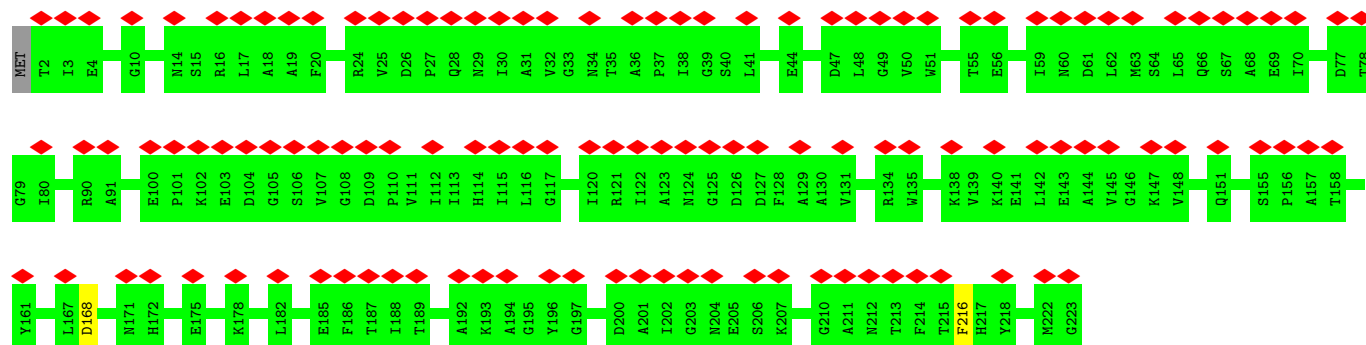


- Molecule 11: Baseplate wedge subunit and tail pin

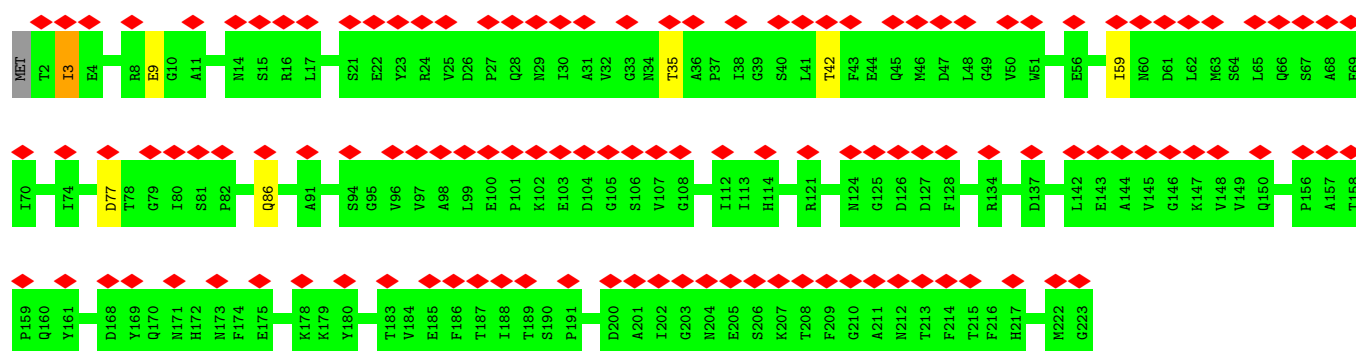




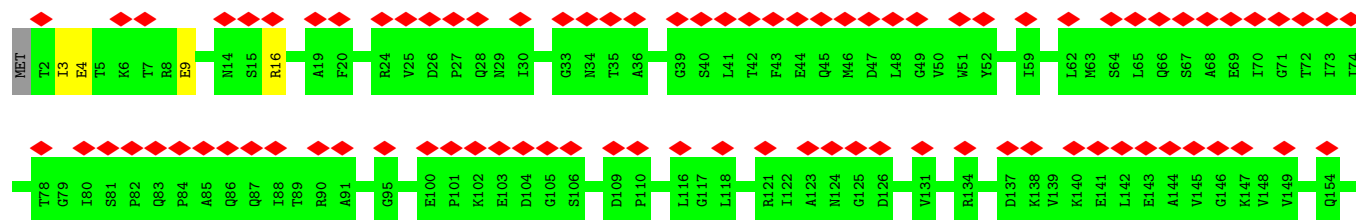
- Molecule 11: Baseplate wedge subunit and tail pin

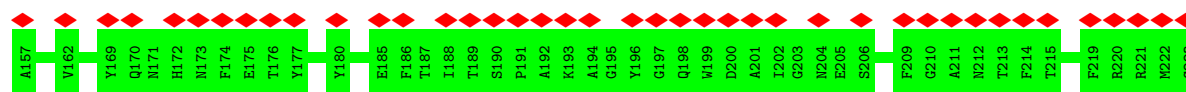


- Molecule 11: Baseplate wedge subunit and tail pin



- Molecule 11: Baseplate wedge subunit and tail pin

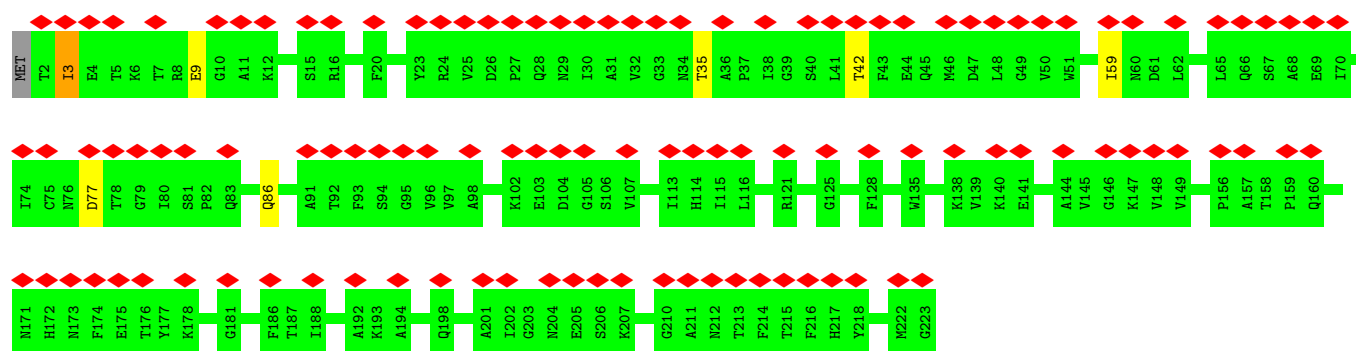




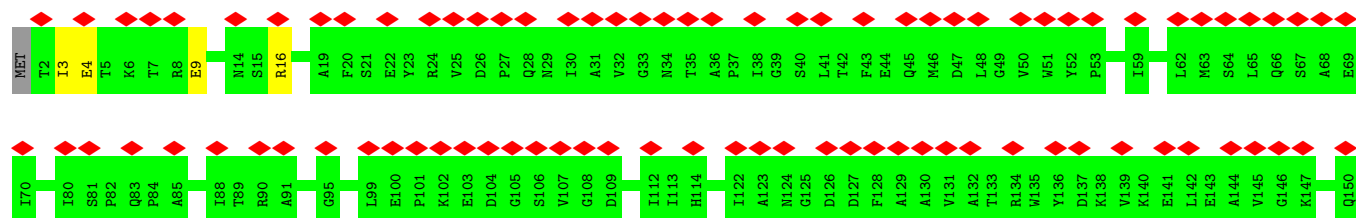
- Molecule 11: Baseplate wedge subunit and tail pin

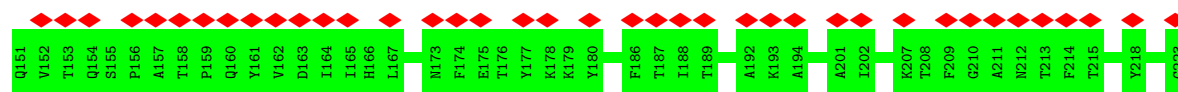


- Molecule 11: Baseplate wedge subunit and tail pin



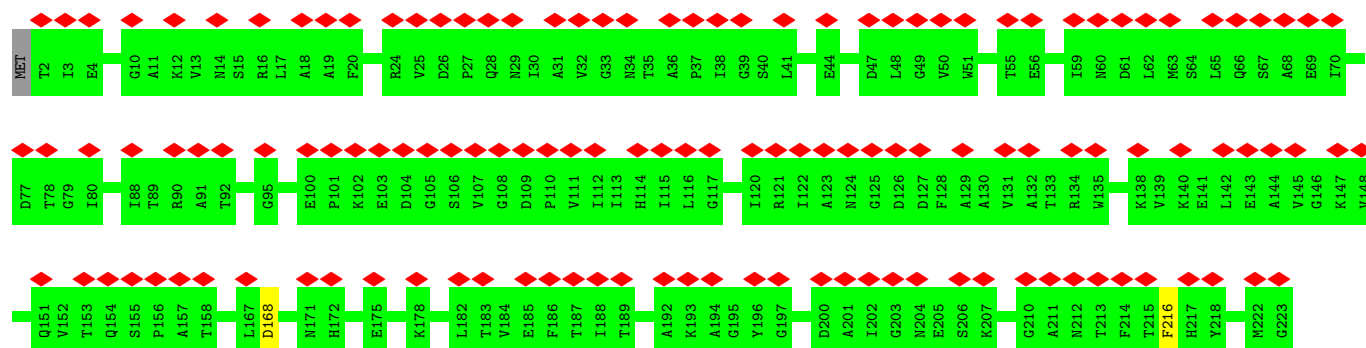
- Molecule 11: Baseplate wedge subunit and tail pin





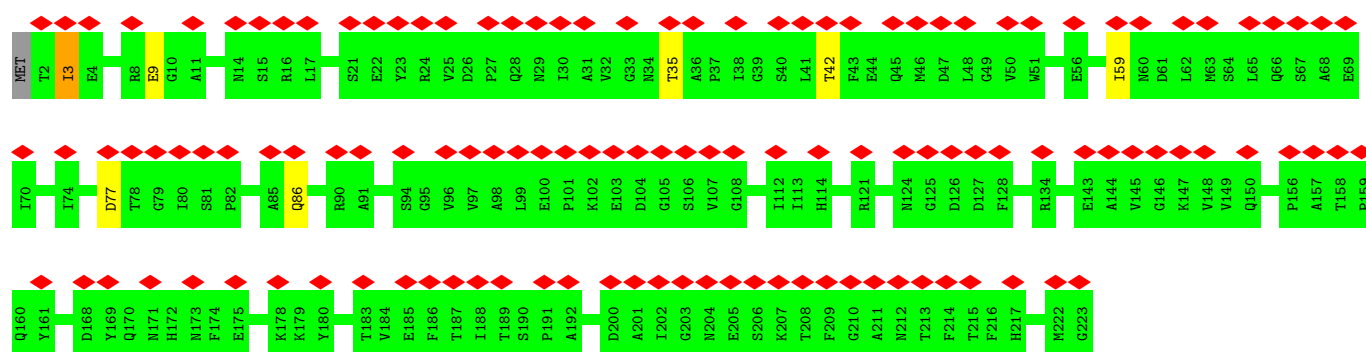
- Molecule 11: Baseplate wedge subunit and tail pin

Chain Fx: 59% 99%



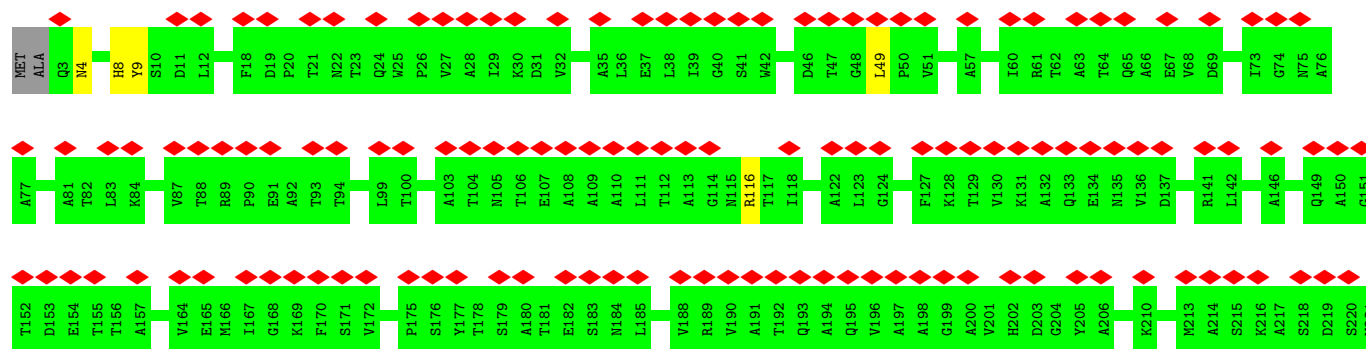
- Molecule 11: Baseplate wedge subunit and tail pin

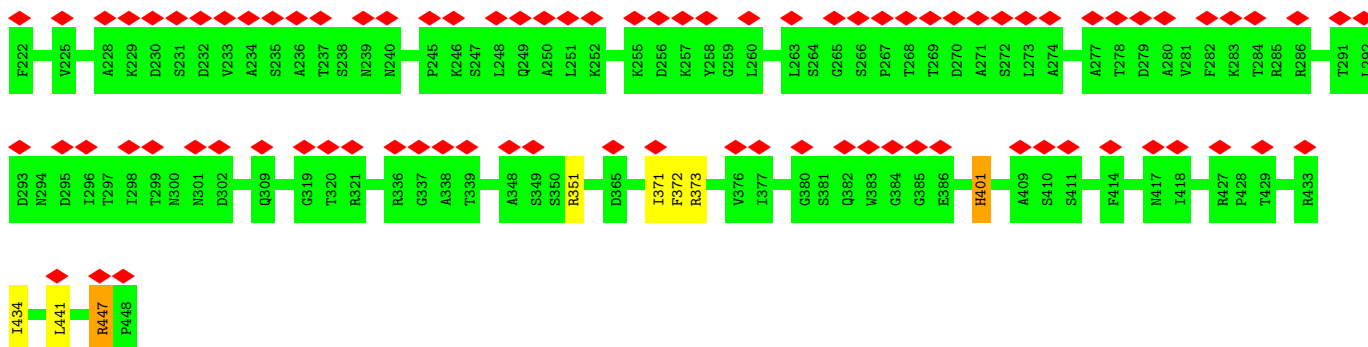
Chain Fy: 56% 96%



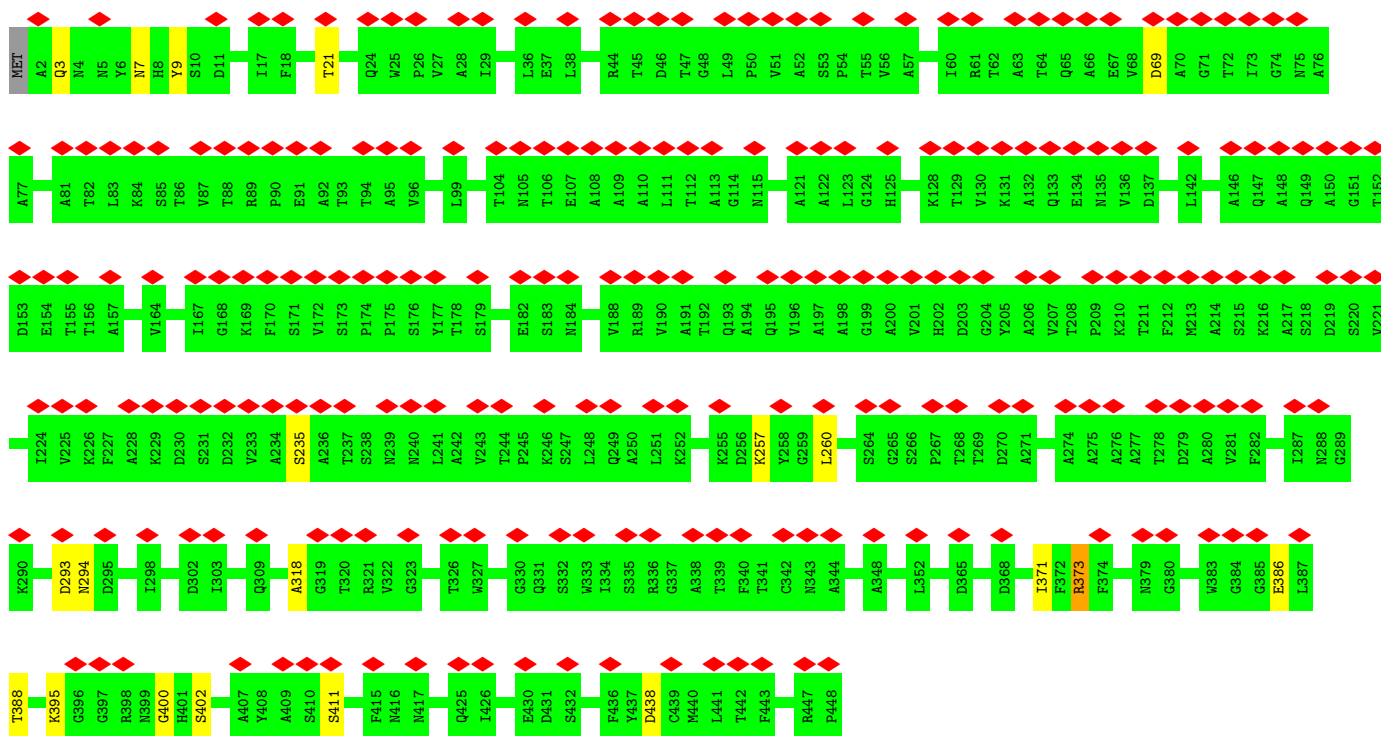
- Molecule 12: Gp12 short tail fibers

Chain FG: 48% 97%

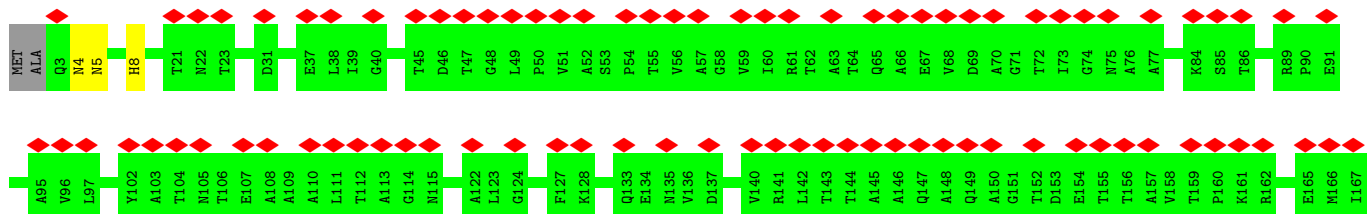


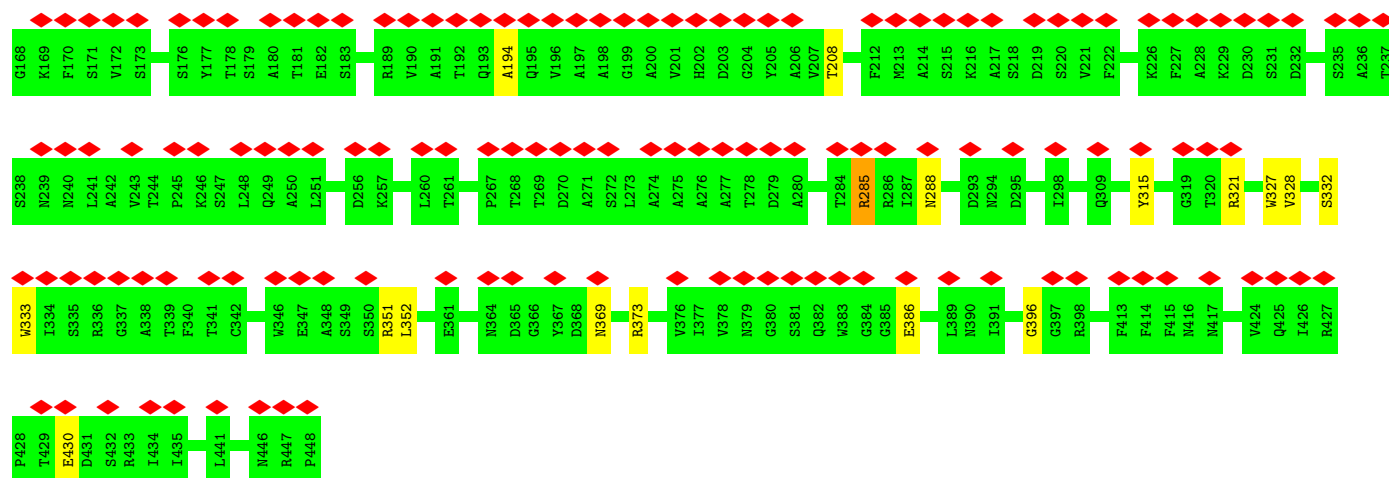


- Molecule 12: Gp12 short tail fibers



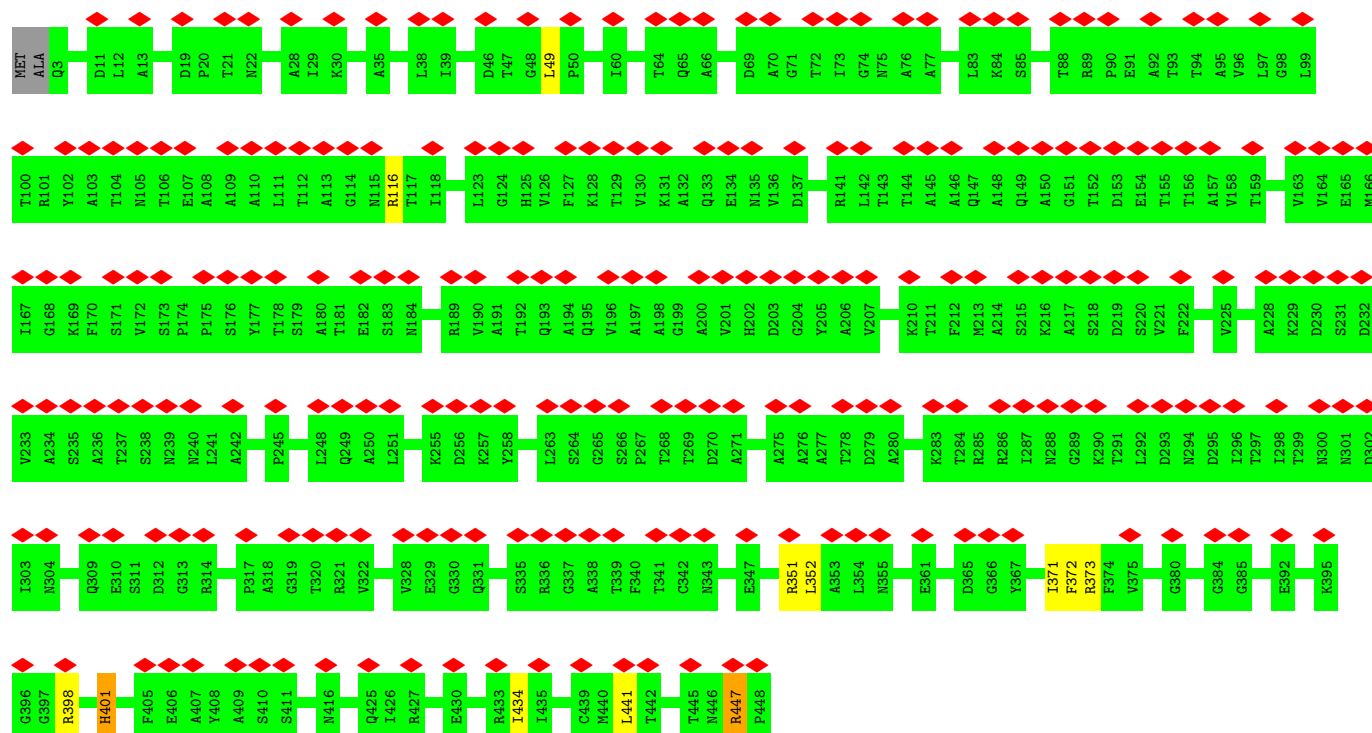
- Molecule 12: Gp12 short tail fibers





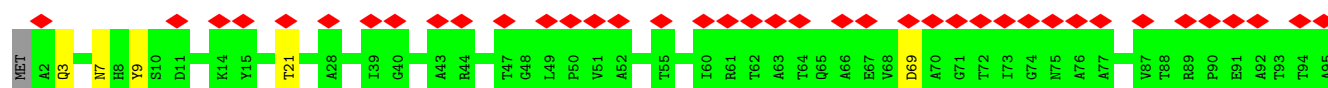
• Molecule 12: Gp12 short tail fibers

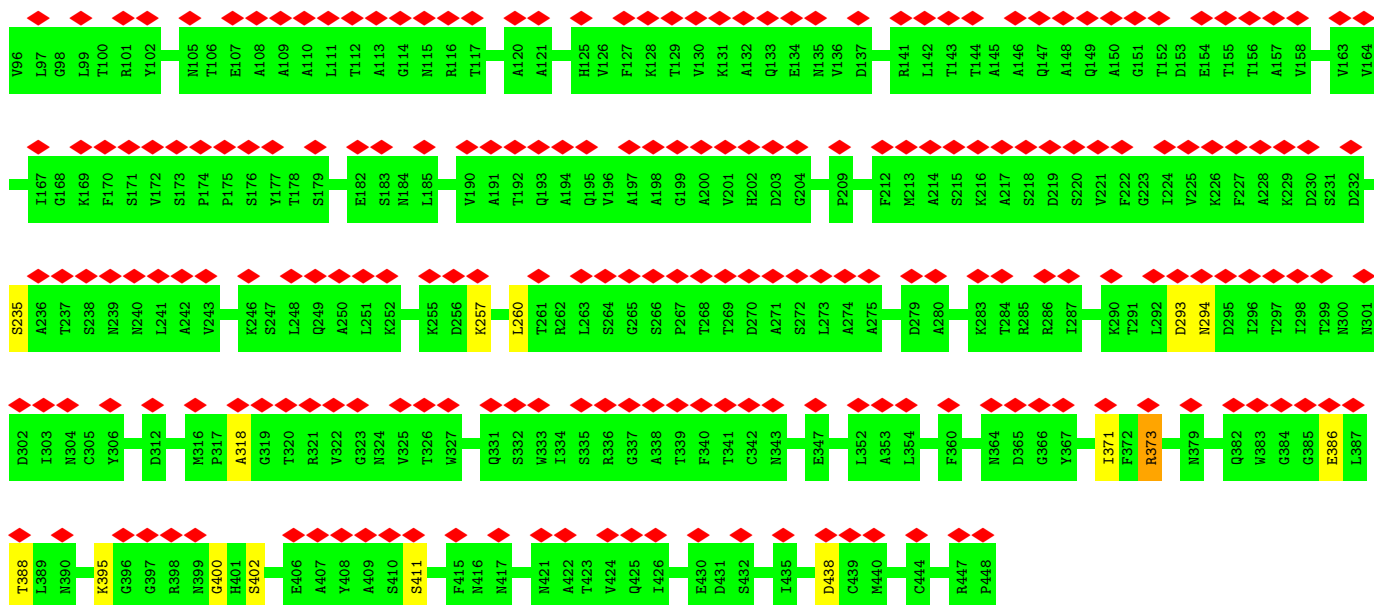
Chain FP: 52% 97%



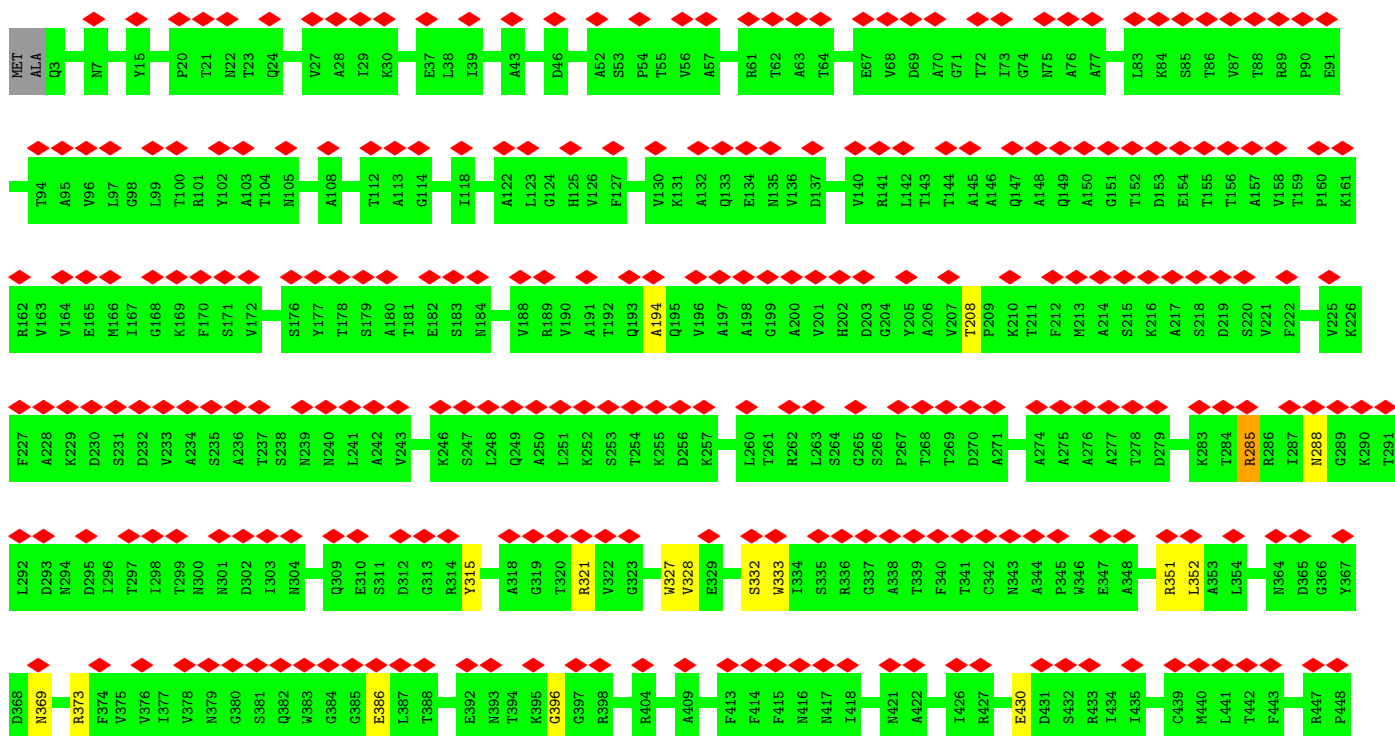
• Molecule 12: Gp12 short tail fibers

Chain FR: 57% 95%



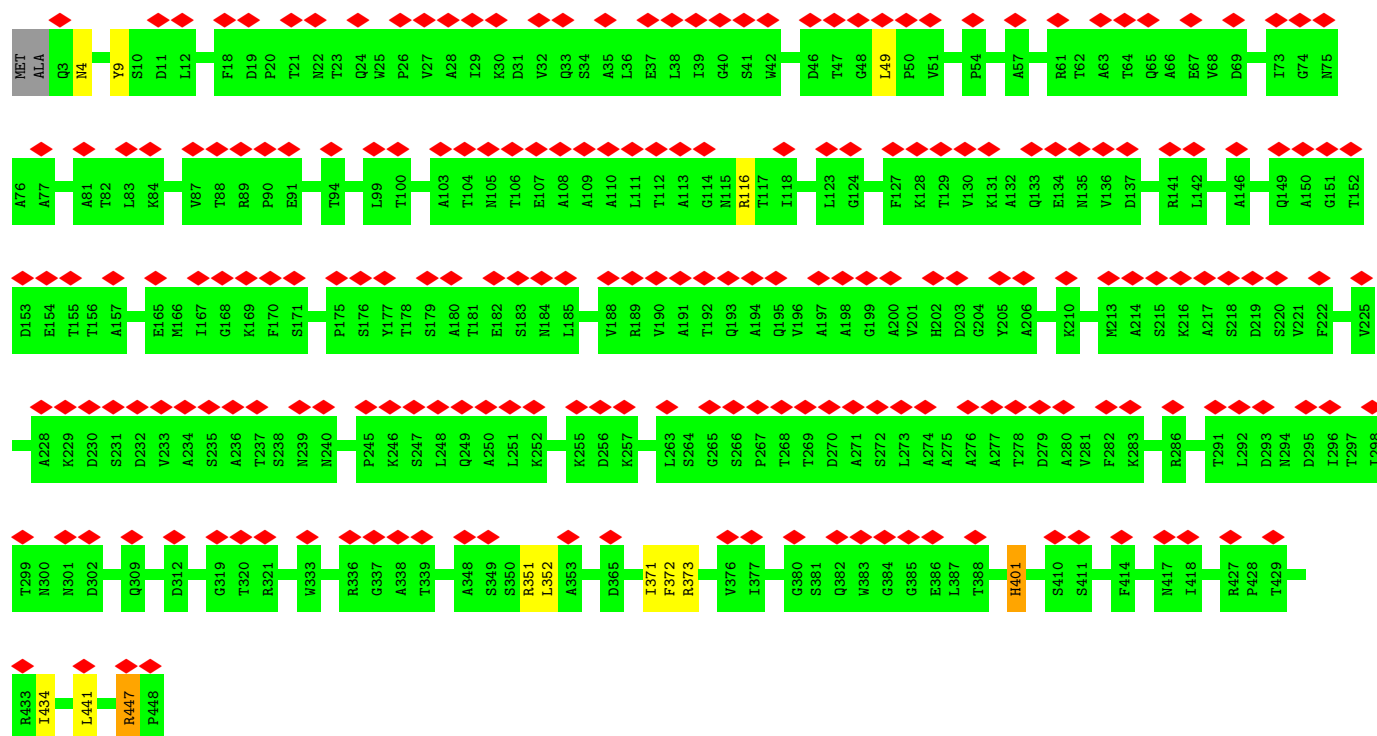


• Molecule 12: Gp12 short tail fibers



• Molecule 12: Gp12 short tail fibers



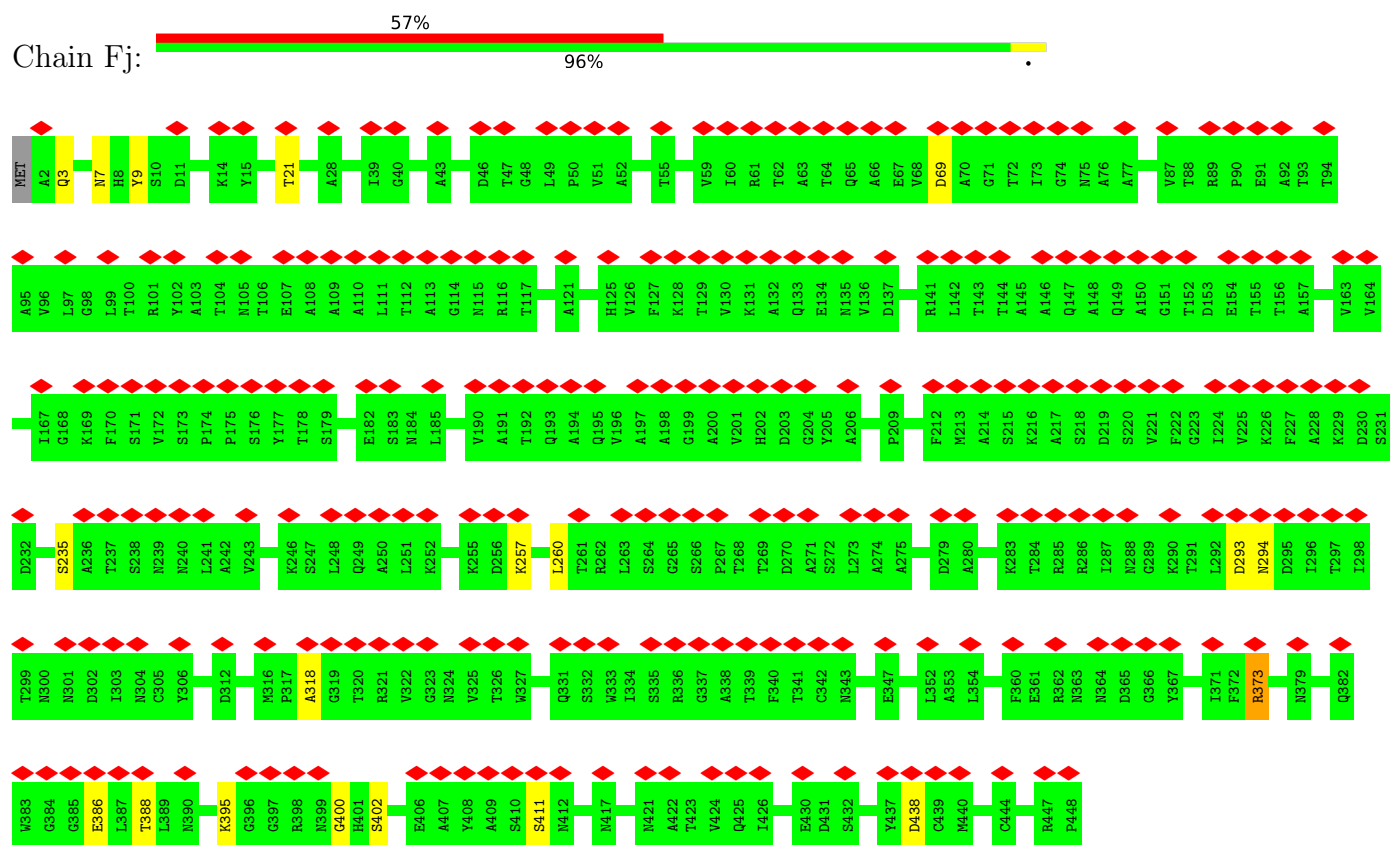


• Molecule 12: Gp12 short tail fibers

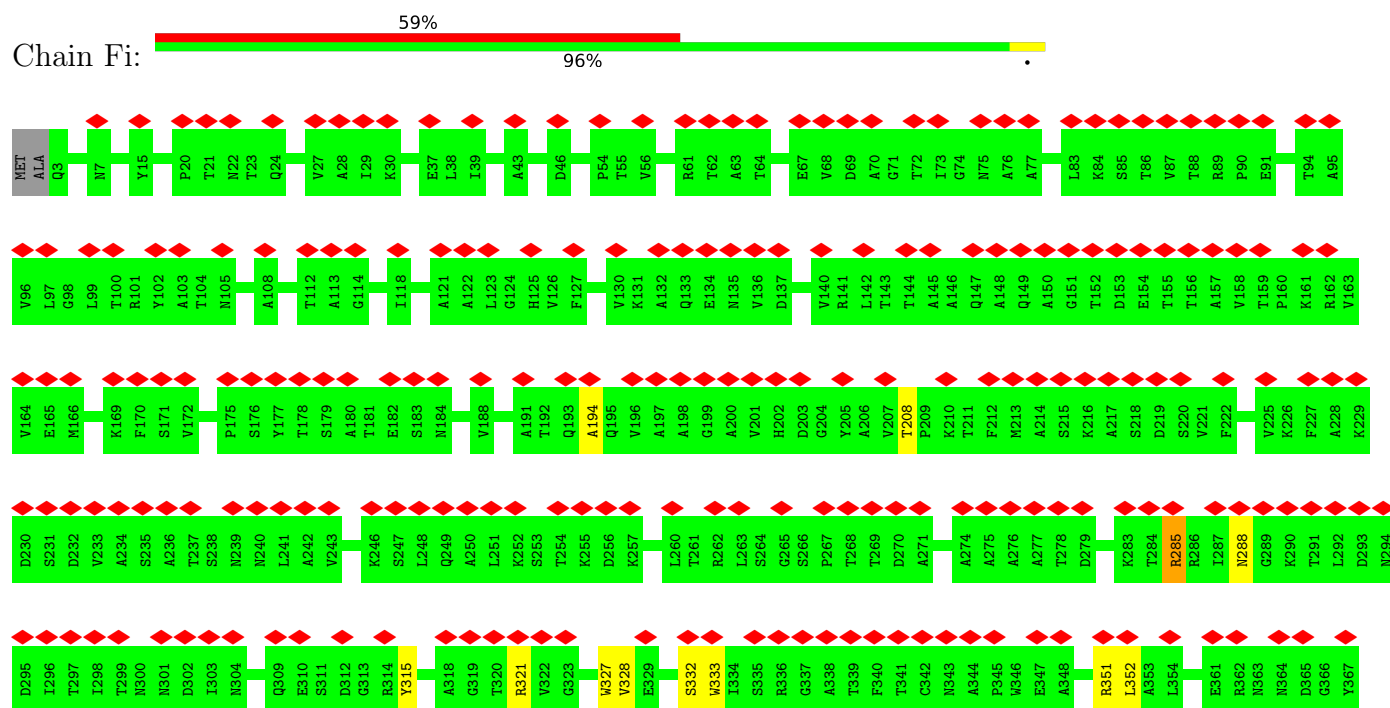


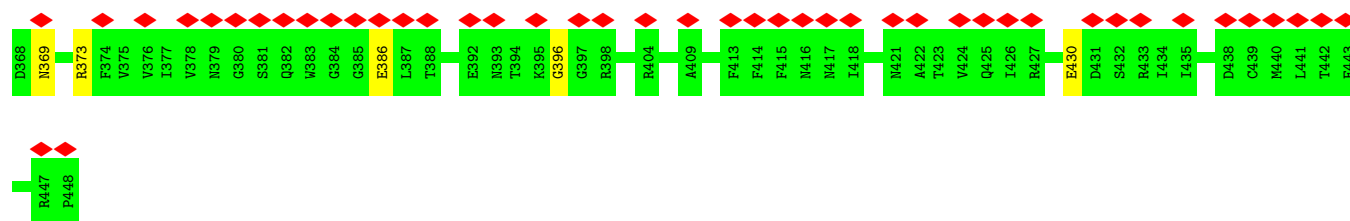
• Molecule 12: Gp12 short tail fibers

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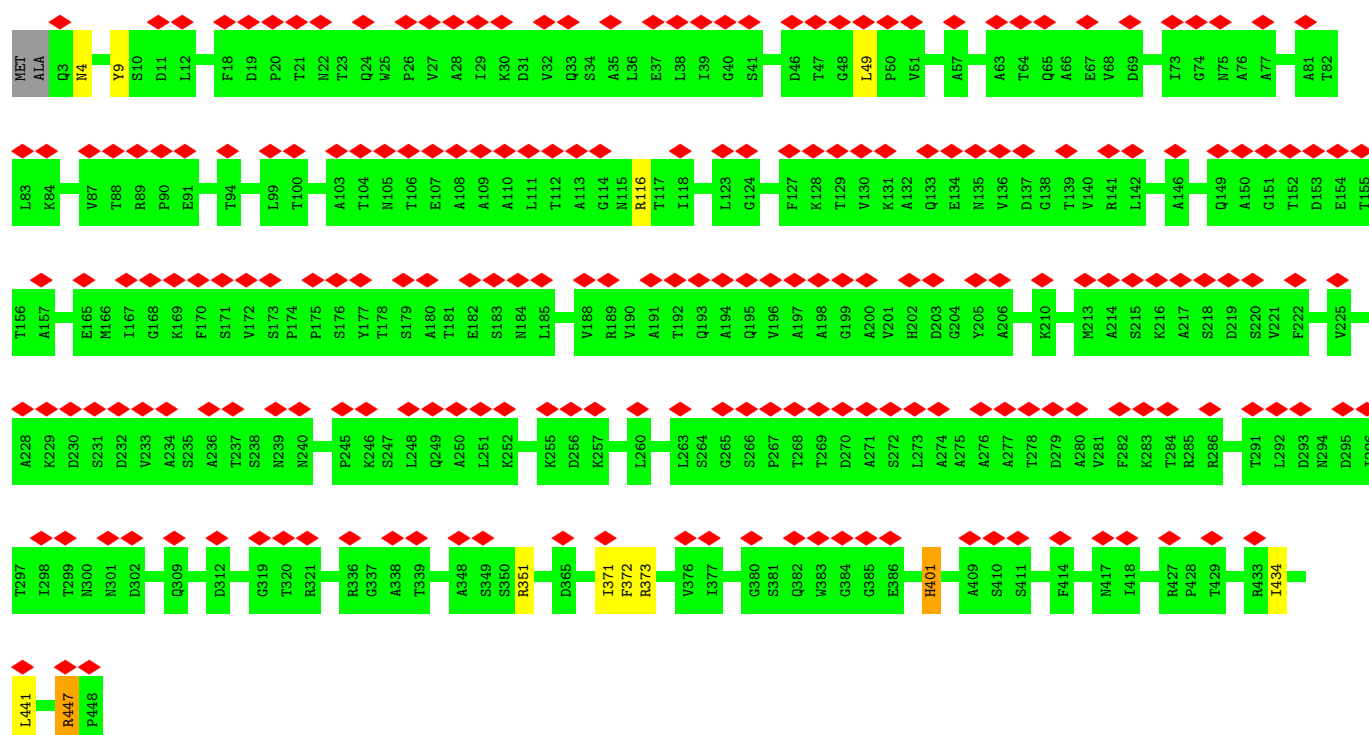


- Molecule 12: Gp12 short tail fibers

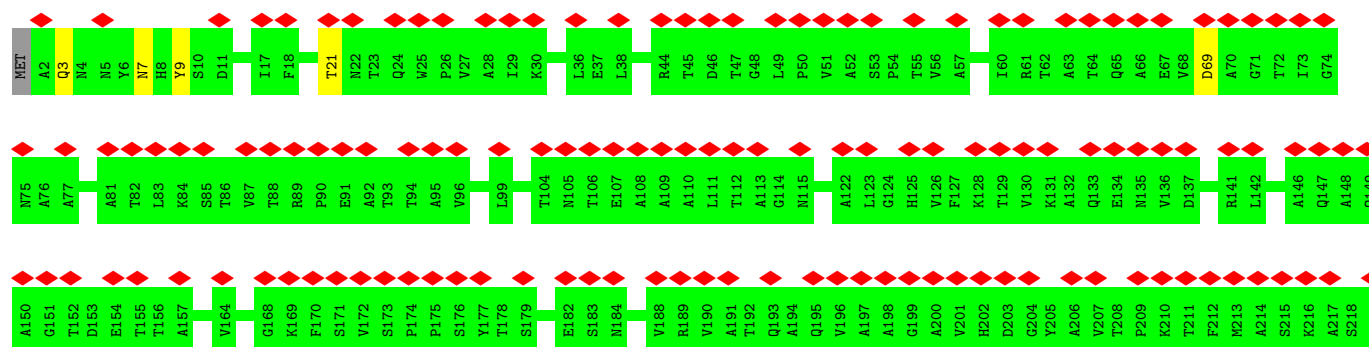


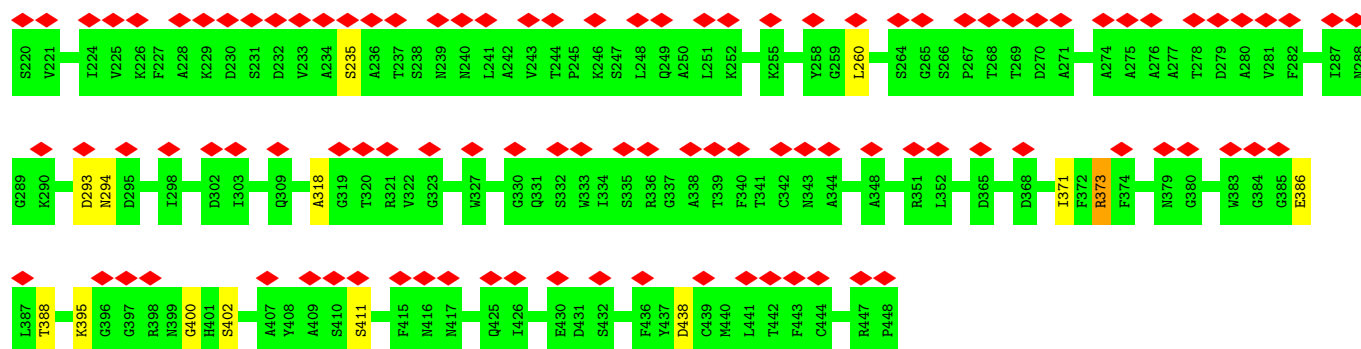


• Molecule 12: Gp12 short tail fibers

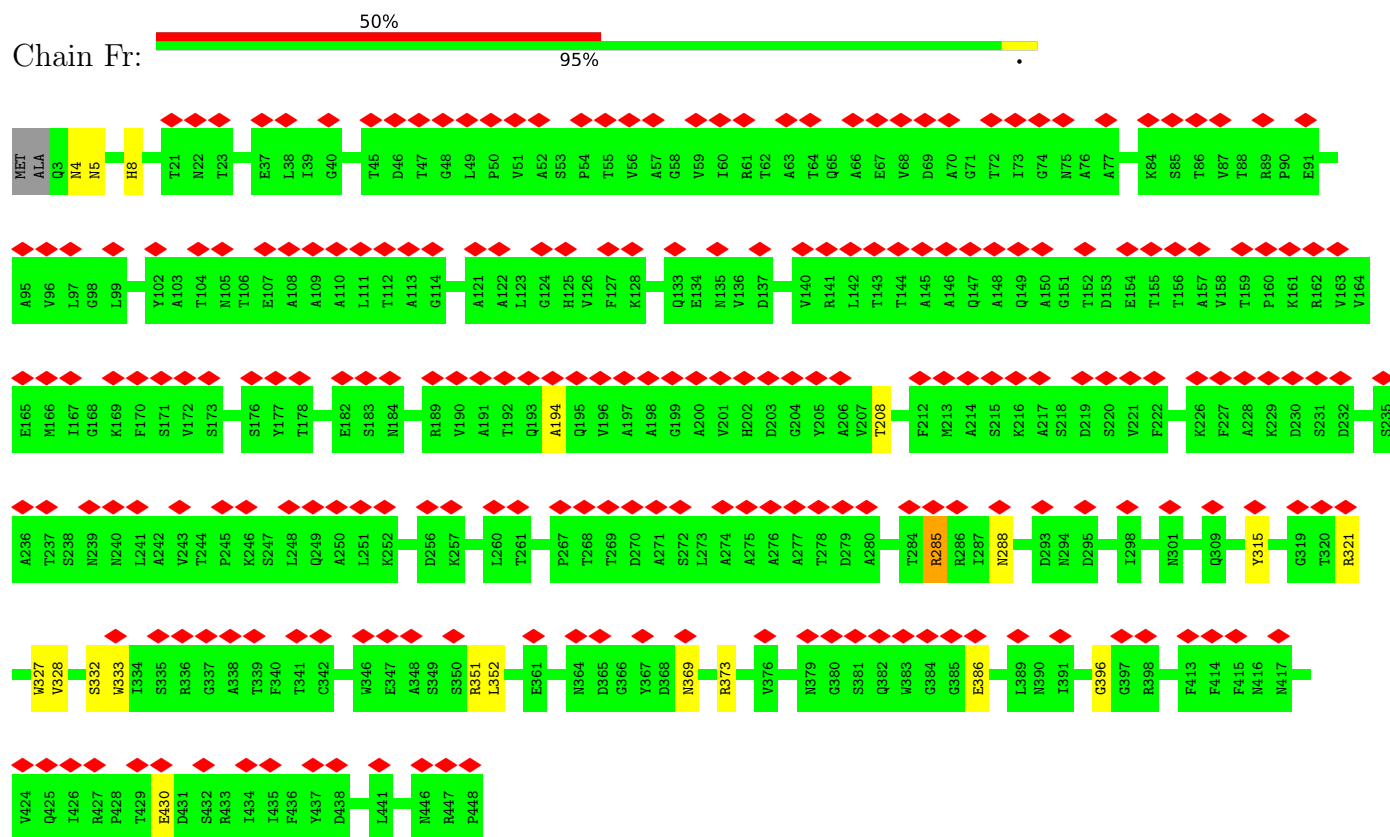


• Molecule 12: Gp12 short tail fibers

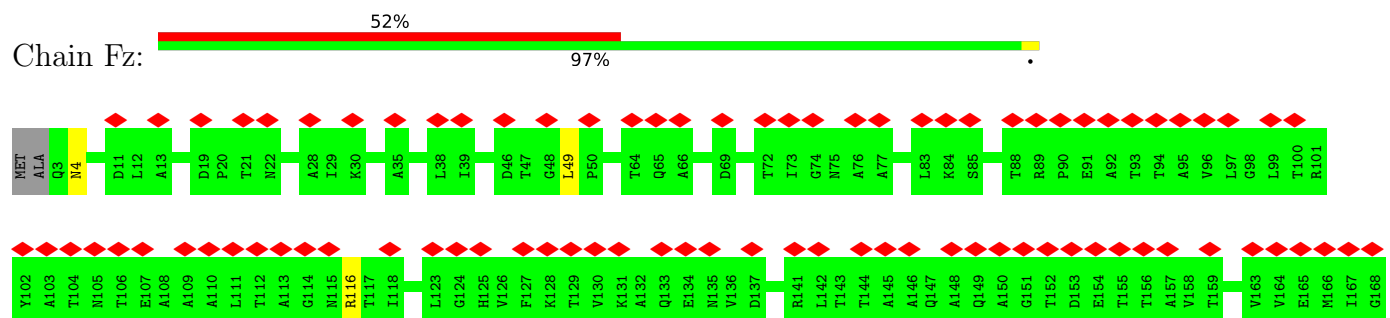


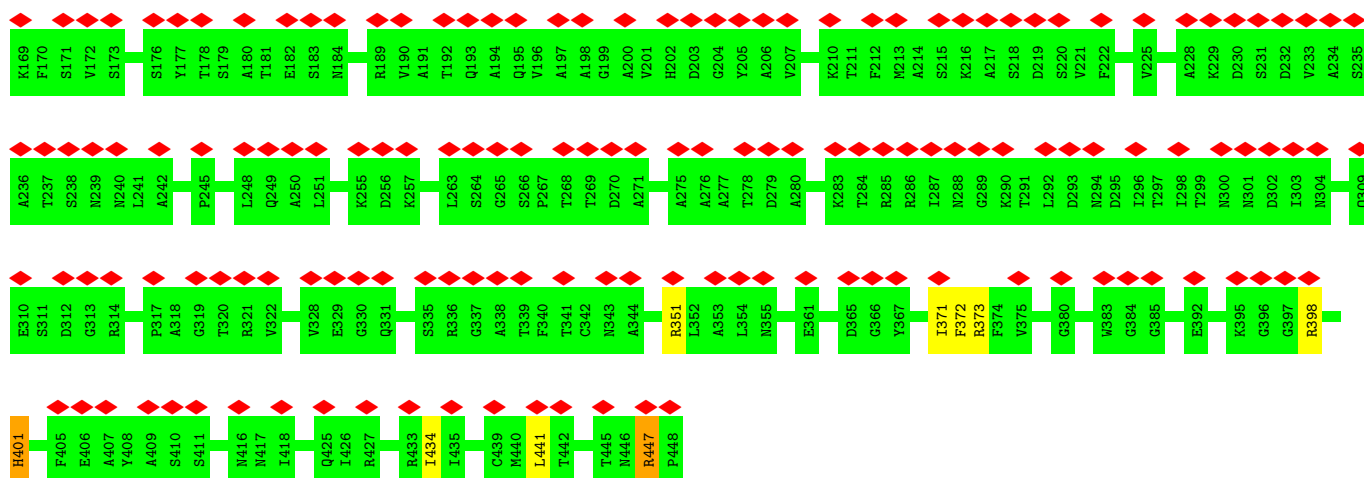


• Molecule 12: Gp12 short tail fibers

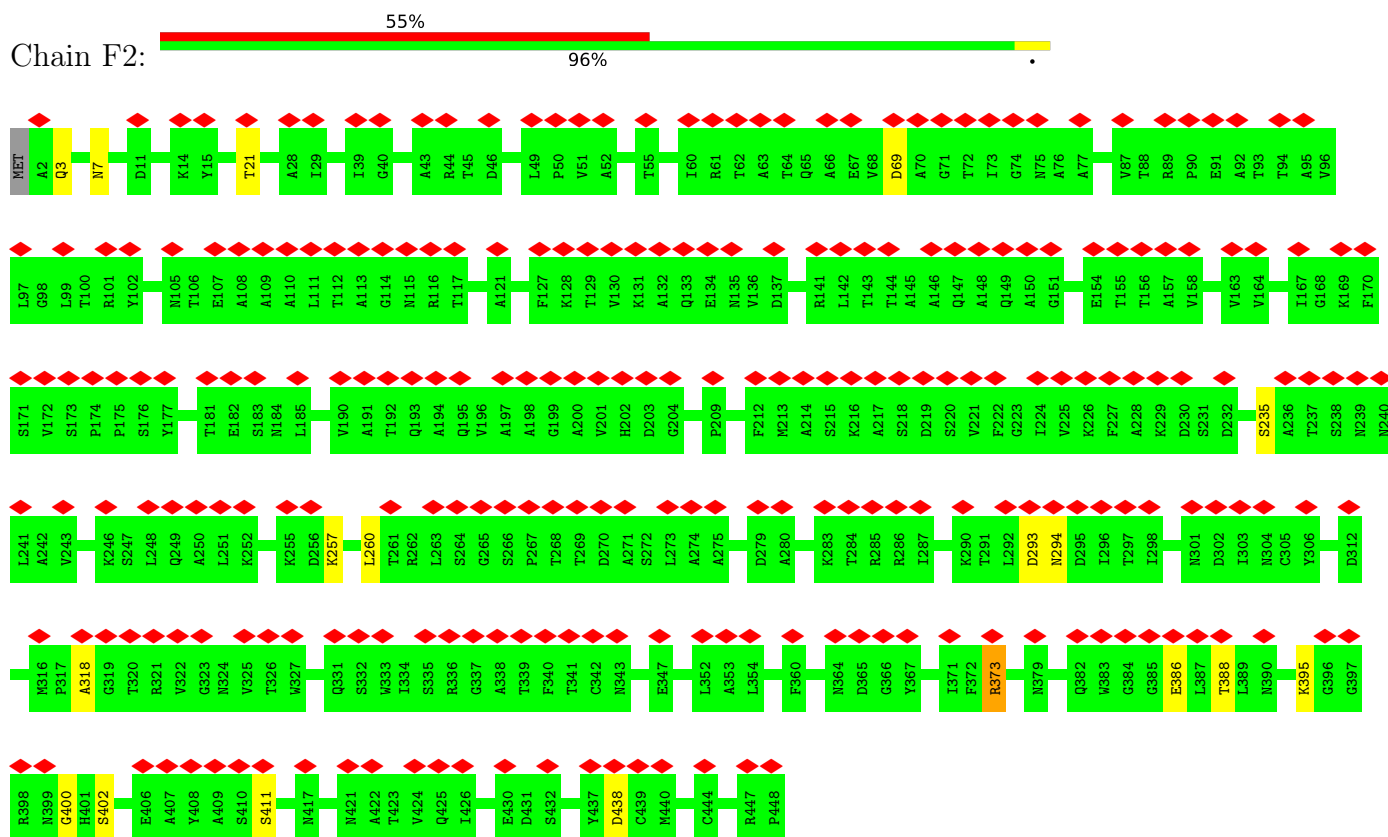


• Molecule 12: Gp12 short tail fibers

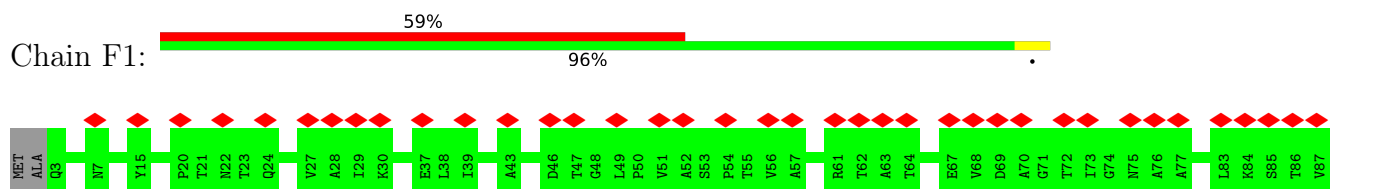




• Molecule 12: Gp12 short tail fibers



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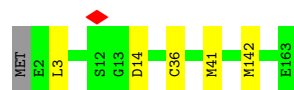




- Molecule 13: Tail tube protein



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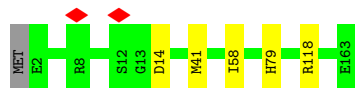


- Molecule 13: Tail tube protein

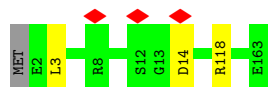




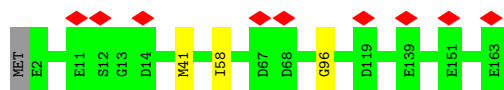
- Molecule 13: Tail tube protein



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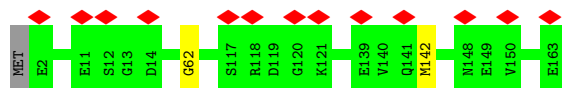
- Molecule 13: Tail tube protein



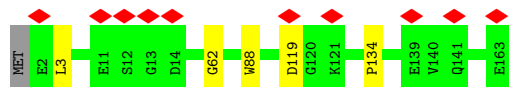
- Molecule 13: Tail tube protein



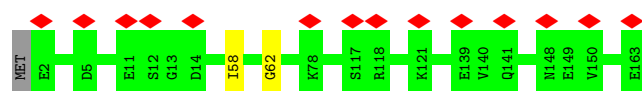
- Molecule 13: Tail tube protein



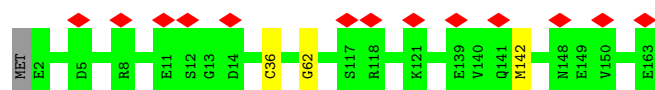
- Molecule 13: Tail tube protein



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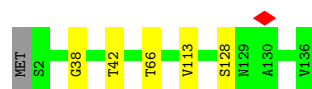
- Molecule 13: Tail tube protein



- Molecule 14: IraD/Gp25-like domain-containing protein



- Molecule 14: IraD/Gp25-like domain-containing protein



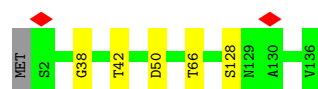
- Molecule 14: IraD/Gp25-like domain-containing protein



- Molecule 14: IraD/Gp25-like domain-containing protein



- Molecule 14: IraD/Gp25-like domain-containing protein



- Molecule 16: Baseplate hub subunit tail length determinator

- Molecule 16: Baseplate hub subunit tail length determinator



Gln Pro Ile Gln V545 N546 K551 N552 Y555 V556 Y557 S577	ASP	GLU	ALA	ILE	MET	THR
	LEU	ARG	LYS	GLY	LEU	GLU
	LYS	LEU	MET	SER	ILE	ASP
	VAL	ILE	ARG	GLY	ASP	ASN
	GLU	ILE	ALA	LYS	LEU	LYS
	LEU	THR	TYR	ASP	LYS	LYS
	ASP	ALA	VAL	VAL	VAL	PHE
	GLN	ALA	ASP	ILE	HIS	ASP
	LEU	ASN	ARG	ASP	PHE	ASP
	LYS	ASN	GLN	LYS	ASN	LEU
LEU	ALA	GLU	LEU	TYR	LYS	
LEU	GLU	ARG	GLY	TRP	PHE	
ASP	ALA	GLU	GLY	THR	GLY	
SER	LEU	ASP	ILE	LEU	GLU	
ILE	LYS	GLU	MET	PHE	ILE	
SER	ARG	GLN	LEU	GLY	LYS	
GLU	THR	PRO	GLY	LYS	SER	
PRO	LYS	GLU	MET	ASN	VAL	
ALA	ALA	TRP	SER	PHE	LYS	
PRO	TYR	LYS	LYS	VAL	SER	
THR	VAL	ARG	LEU	GLY	GLY	
ALA	GLU	LYS	ALA	PHE	PHE	
GLU	LYS	LEU	ALA	ASN	GLY	
ILE	THR	SER	MET	LYN	LYS	
PRO	ALA	LYS	LEU	ALA	ILE	
ALA	SER	PHE	ARG	LYS	SER	
ALA	ASP	GLN	ALA	GLU	LEU	
GLU	SER	LYS	LEU	TRP	THR	
GLN	THR	PHE	GLY	GLY	ASP	
PRO	ARG	THR	PHE	PRO	LYS	
GLU	LEU	GLY	ASN	LEU	ILE	
VAL	ASP	GLN	ASP	LEU	SER	
LYS	SER	ILE	SER	THR	SER	
GLN	ALA	ALA	ALA	ALA	MET	
ALA	ALA	LYS	ALA	GLU	VAL	
ALA	THR	LEU	LEU	ILE	ALA	
ASP	THR	SER	ASP	VAL	LEU	
SER	ARG	GLY	ARG	LYS	GLN	
ARG	TYR	GLU	PHE	SER	ALA	
GLU	LYS	LYS	GLN	PHE	MET	
THR	GLU	GLU	THR	VAL	LYS	
ALA	LEU	GLN	VAL	LYS	ALA	
ARG	LEU	TYR	ALA	ASP	ALA	
GLU	SER	PRO	ALA	GLY	VAL	
SER	PRO	GLU	LEU	LEU	GLY	
ASN	THR	VAL	PRO	ALA	GLY	
THR	THR	VAL	ASP	GLU	VAL	
GLN	SER	LYS	GLU	ASP	ILE	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	34528	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	83505	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.317	Depositor
Minimum map value	-1.951	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	691.416, 691.416, 691.416	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AM	0.56	0/5307	1.00	3/7218 (0.0%)
1	AN	0.57	0/5307	1.02	3/7218 (0.0%)
1	AO	0.56	0/5307	1.01	6/7218 (0.1%)
1	AP	0.57	0/5307	1.02	3/7218 (0.0%)
1	AQ	0.56	0/5307	1.02	4/7218 (0.1%)
1	AR	0.57	0/5307	1.01	3/7218 (0.0%)
1	AS	0.57	0/5260	1.03	4/7154 (0.1%)
1	AT	0.56	0/5239	1.03	5/7125 (0.1%)
1	AU	0.57	0/5260	1.03	5/7154 (0.1%)
1	AV	0.57	0/5239	1.04	8/7125 (0.1%)
1	AW	0.57	0/5260	1.02	3/7154 (0.0%)
1	AX	0.56	0/5239	1.04	5/7125 (0.1%)
2	BK	0.62	0/2370	1.15	3/3220 (0.1%)
2	BL	0.62	0/1828	1.07	1/2480 (0.0%)
2	BM	0.62	0/2370	1.15	5/3220 (0.2%)
2	BN	0.61	0/1828	1.07	1/2480 (0.0%)
2	BO	0.62	0/2370	1.14	6/3220 (0.2%)
2	BP	0.62	0/1828	1.08	3/2480 (0.1%)
3	BQ	0.56	0/1757	1.02	2/2383 (0.1%)
3	BR	0.57	0/1757	1.07	3/2383 (0.1%)
3	BS	0.56	0/1757	1.03	2/2383 (0.1%)
3	BT	0.57	0/1757	1.06	0/2383
3	BU	0.57	0/1757	1.04	2/2383 (0.1%)
3	BV	0.56	0/1757	1.04	2/2383 (0.1%)
4	AG	0.54	0/1794	0.99	2/2435 (0.1%)
4	AH	0.54	0/1794	0.99	1/2435 (0.0%)
4	AI	0.54	0/1794	1.00	0/2435
4	AJ	0.55	0/1794	0.97	0/2435
4	AK	0.54	0/1794	0.99	1/2435 (0.0%)
4	AL	0.54	0/1794	0.98	0/2435
5	BB	0.60	0/4441	1.08	5/6025 (0.1%)
5	BC	0.59	0/4441	1.07	7/6025 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	BD	0.59	0/4441	1.07	4/6025 (0.1%)
6	BA	0.75	0/721	1.15	1/982 (0.1%)
7	A0	0.65	0/8656	1.09	9/11738 (0.1%)
7	A1	0.65	0/8656	1.09	9/11738 (0.1%)
7	A2	0.65	0/8656	1.09	9/11738 (0.1%)
7	A3	0.65	0/8656	1.09	9/11738 (0.1%)
7	AY	0.65	0/8656	1.09	9/11738 (0.1%)
7	AZ	0.65	0/8656	1.09	9/11738 (0.1%)
8	A4	0.58	0/2743	1.06	3/3730 (0.1%)
8	A5	0.59	0/2743	1.06	4/3730 (0.1%)
8	A6	0.58	0/2743	1.06	5/3730 (0.1%)
8	A7	0.59	0/2743	1.05	4/3730 (0.1%)
8	A8	0.58	0/2743	1.05	4/3730 (0.1%)
8	A9	0.58	0/2743	1.03	1/3730 (0.0%)
8	Aa	0.67	0/2707	1.13	3/3682 (0.1%)
8	Ab	0.67	0/2707	1.13	3/3682 (0.1%)
8	Ac	0.67	0/2707	1.13	3/3682 (0.1%)
8	Ad	0.67	0/2707	1.13	3/3682 (0.1%)
8	Ae	0.67	0/2707	1.13	3/3682 (0.1%)
8	Af	0.67	0/2707	1.14	3/3682 (0.1%)
9	LA	0.73	0/2304	1.07	3/3114 (0.1%)
9	LB	0.72	0/2304	1.07	0/3114
9	LC	0.71	0/2304	1.03	0/3114
9	LD	0.73	0/2304	1.07	3/3114 (0.1%)
9	LE	0.72	0/2304	1.07	0/3114
9	LF	0.71	0/2304	1.03	0/3114
9	LG	0.73	0/2304	1.07	3/3114 (0.1%)
9	LH	0.72	0/2304	1.07	0/3114
9	LI	0.71	0/2304	1.03	0/3114
9	LJ	0.73	0/2304	1.07	3/3114 (0.1%)
9	LK	0.72	0/2304	1.07	0/3114
9	LL	0.71	0/2304	1.03	1/3114 (0.0%)
9	LM	0.73	0/2304	1.07	3/3114 (0.1%)
9	LN	0.72	0/2304	1.07	0/3114
9	LO	0.71	0/2304	1.03	0/3114
9	LP	0.73	0/2304	1.07	3/3114 (0.1%)
9	LQ	0.72	0/2304	1.07	0/3114
9	LR	0.71	0/2304	1.03	0/3114
10	FA	0.56	0/4789	0.99	3/6512 (0.0%)
10	FB	0.58	0/4789	0.98	6/6512 (0.1%)
10	FC	0.57	0/4789	0.99	2/6512 (0.0%)
10	FJ	0.56	0/4789	0.99	3/6512 (0.0%)
10	FK	0.58	0/4789	0.98	6/6512 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	FL	0.57	0/4789	0.99	2/6512 (0.0%)
10	FS	0.56	0/4789	0.99	3/6512 (0.0%)
10	FT	0.58	0/4789	0.98	6/6512 (0.1%)
10	FU	0.57	0/4789	0.99	2/6512 (0.0%)
10	Fb	0.56	0/4789	0.99	3/6512 (0.0%)
10	Fc	0.58	0/4789	0.98	6/6512 (0.1%)
10	Fd	0.57	0/4789	0.99	2/6512 (0.0%)
10	Fk	0.56	0/4789	0.99	3/6512 (0.0%)
10	Fl	0.58	0/4789	0.98	6/6512 (0.1%)
10	Fm	0.57	0/4789	0.99	2/6512 (0.0%)
10	Ft	0.56	0/4789	0.99	3/6512 (0.0%)
10	Fu	0.58	0/4789	0.98	6/6512 (0.1%)
10	Fv	0.57	0/4789	0.99	2/6512 (0.0%)
11	FD	0.62	0/1761	0.98	1/2397 (0.0%)
11	FE	0.60	0/1761	1.00	1/2397 (0.0%)
11	FF	0.61	0/1761	1.00	2/2397 (0.1%)
11	FM	0.62	0/1761	0.98	1/2397 (0.0%)
11	FN	0.60	0/1761	1.00	1/2397 (0.0%)
11	FO	0.61	0/1761	1.00	2/2397 (0.1%)
11	FV	0.62	0/1761	0.98	1/2397 (0.0%)
11	FW	0.60	0/1761	1.00	1/2397 (0.0%)
11	FX	0.61	0/1761	1.00	2/2397 (0.1%)
11	Fe	0.62	0/1761	0.98	1/2397 (0.0%)
11	Ff	0.60	0/1761	1.00	1/2397 (0.0%)
11	Fg	0.61	0/1761	1.00	2/2397 (0.1%)
11	Fn	0.62	0/1761	0.98	1/2397 (0.0%)
11	Fo	0.60	0/1761	1.00	1/2397 (0.0%)
11	Fp	0.61	0/1761	1.00	2/2397 (0.1%)
11	Fw	0.62	0/1761	0.98	1/2397 (0.0%)
11	Fx	0.60	0/1761	1.00	1/2397 (0.0%)
11	Fy	0.61	0/1761	1.00	2/2397 (0.1%)
12	F1	0.62	0/3426	1.04	0/4675
12	F2	0.61	0/3440	1.06	4/4694 (0.1%)
12	FG	0.61	0/3435	1.05	1/4687 (0.0%)
12	FH	0.62	0/3426	1.04	0/4675
12	FI	0.61	0/3440	1.06	4/4694 (0.1%)
12	FP	0.61	0/3435	1.05	1/4687 (0.0%)
12	FQ	0.62	0/3426	1.04	0/4675
12	FR	0.61	0/3440	1.06	4/4694 (0.1%)
12	FY	0.61	0/3435	1.05	1/4687 (0.0%)
12	FZ	0.62	0/3426	1.04	0/4675
12	Fa	0.61	0/3440	1.06	4/4694 (0.1%)
12	Fh	0.61	0/3435	1.05	1/4687 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	Fi	0.62	0/3426	1.04	0/4675
12	Fj	0.61	0/3440	1.06	4/4694 (0.1%)
12	Fq	0.61	0/3435	1.05	1/4687 (0.0%)
12	Fr	0.62	0/3426	1.04	0/4675
12	Fs	0.61	0/3440	1.06	4/4694 (0.1%)
12	Fz	0.61	0/3435	1.05	1/4687 (0.0%)
13	B1	0.55	0/1339	0.99	1/1821 (0.1%)
13	B2	0.55	0/1339	0.99	1/1821 (0.1%)
13	B3	0.60	0/1339	1.03	0/1821
13	B4	0.60	0/1339	1.04	1/1821 (0.1%)
13	B5	0.59	0/1339	1.05	0/1821
13	B6	0.60	0/1339	1.05	1/1821 (0.1%)
13	B7	0.59	0/1339	1.03	0/1821
13	B8	0.60	0/1339	1.07	2/1821 (0.1%)
13	BW	0.55	0/1339	0.98	1/1821 (0.1%)
13	BX	0.56	0/1339	1.00	3/1821 (0.2%)
13	BY	0.55	0/1339	0.99	1/1821 (0.1%)
13	BZ	0.55	0/1339	1.02	3/1821 (0.2%)
14	AA	0.56	0/1084	1.10	1/1470 (0.1%)
14	AB	0.56	0/1084	1.11	1/1470 (0.1%)
14	AC	0.57	0/1084	1.11	1/1470 (0.1%)
14	AD	0.56	0/1084	1.14	0/1470
14	AE	0.56	0/1084	1.11	2/1470 (0.1%)
14	AF	0.57	0/1084	1.12	1/1470 (0.1%)
15	BE	0.58	0/3125	1.05	2/4232 (0.0%)
15	BF	0.58	0/3125	1.04	1/4232 (0.0%)
15	BG	0.58	0/3125	1.06	3/4232 (0.1%)
16	BH	0.66	0/246	1.14	0/334
16	BI	0.66	0/246	1.12	0/334
16	BJ	0.63	0/246	1.10	0/334
All	All	0.61	0/449782	1.04	361/611230 (0.1%)

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
2	BM	0	1
7	A0	0	2
7	A1	0	2
7	A2	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	A3	0	2
7	AY	0	2
7	AZ	0	3
8	A6	0	1
10	FA	0	2
10	FC	0	1
10	FJ	0	2
10	FL	0	1
10	FS	0	2
10	FU	0	1
10	Fb	0	2
10	Fd	0	1
10	Fk	0	2
10	Fm	0	1
10	Ft	0	2
10	Fv	0	1
11	FF	0	1
11	FO	0	1
11	FX	0	1
11	Fg	0	1
11	Fp	0	1
11	Fy	0	1
12	F1	0	1
12	FH	0	1
12	FQ	0	1
12	FZ	0	1
12	Fi	0	1
12	Fr	0	1
15	BE	0	1
15	BF	0	1
15	BG	0	1
All	All	0	49

There are no bond length outliers.

All (361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BM	200	ARG	NE-CZ-NH1	-8.21	113.29	121.50
15	BG	326	ASP	CA-CB-CG	7.91	120.51	112.60
2	BK	200	ARG	NE-CZ-NH1	-7.66	113.84	121.50
2	BO	200	ARG	NE-CZ-NH1	-7.59	113.91	121.50
10	Fu	357	GLN	CB-CG-CD	7.27	124.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	FT	357	GLN	CB-CG-CD	7.25	124.93	112.60
10	FK	357	GLN	CB-CG-CD	7.25	124.93	112.60
10	Fl	357	GLN	CB-CG-CD	7.25	124.93	112.60
10	FB	357	GLN	CB-CG-CD	7.25	124.92	112.60
10	Fc	357	GLN	CB-CG-CD	7.24	124.90	112.60
1	AS	280	ARG	CG-CD-NE	-6.95	96.70	112.00
8	Aa	256	PHE	CA-CB-CG	6.88	120.68	113.80
8	Ad	256	PHE	CA-CB-CG	6.86	120.66	113.80
1	AV	461	PHE	N-CA-C	6.86	118.41	111.07
8	Ac	256	PHE	CA-CB-CG	6.86	120.66	113.80
8	Ab	256	PHE	CA-CB-CG	6.85	120.65	113.80
8	Af	256	PHE	CA-CB-CG	6.85	120.65	113.80
8	Ae	256	PHE	CA-CB-CG	6.83	120.64	113.80
8	A6	339	PHE	CA-CB-CG	6.81	120.61	113.80
10	Fl	198	ASN	OD1-CG-ND2	-6.79	115.81	122.60
10	FT	198	ASN	OD1-CG-ND2	-6.77	115.83	122.60
7	AZ	275	GLU	CB-CG-CD	6.75	124.08	112.60
7	A2	275	GLU	CB-CG-CD	6.75	124.08	112.60
7	A0	275	GLU	CB-CG-CD	6.75	124.08	112.60
10	FB	198	ASN	OD1-CG-ND2	-6.75	115.85	122.60
10	Fc	198	ASN	OD1-CG-ND2	-6.75	115.85	122.60
7	AY	275	GLU	CB-CG-CD	6.75	124.07	112.60
8	A4	339	PHE	CA-CB-CG	6.74	120.54	113.80
7	A3	275	GLU	CB-CG-CD	6.74	124.06	112.60
10	FK	198	ASN	OD1-CG-ND2	-6.74	115.86	122.60
1	AT	461	PHE	N-CA-C	6.74	118.28	111.07
10	Fu	198	ASN	OD1-CG-ND2	-6.72	115.88	122.60
7	A1	275	GLU	CB-CG-CD	6.71	124.00	112.60
7	A3	492	ARG	NE-CZ-NH2	6.70	125.23	119.20
7	AY	492	ARG	NE-CZ-NH2	6.69	125.22	119.20
7	A0	492	ARG	NE-CZ-NH2	6.69	125.22	119.20
7	A2	492	ARG	NE-CZ-NH2	6.68	125.22	119.20
7	A1	492	ARG	NE-CZ-NH2	6.68	125.21	119.20
7	AZ	492	ARG	NE-CZ-NH2	6.68	125.21	119.20
2	BM	200	ARG	NE-CZ-NH2	6.61	125.15	119.20
2	BO	200	ARG	NE-CZ-NH2	6.54	125.09	119.20
8	Af	109	ASN	CA-CB-CG	6.48	119.08	112.60
1	AU	280	ARG	CG-CD-NE	-6.47	97.77	112.00
8	Ac	109	ASN	CA-CB-CG	6.45	119.05	112.60
8	Ad	109	ASN	CA-CB-CG	6.44	119.04	112.60
8	Aa	109	ASN	CA-CB-CG	6.43	119.03	112.60
8	Ae	109	ASN	CA-CB-CG	6.42	119.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	Ab	109	ASN	CA-CB-CG	6.40	119.00	112.60
8	A8	339	PHE	CA-CB-CG	6.38	120.18	113.80
3	BS	236	THR	CA-C-N	6.36	129.26	120.49
3	BS	236	THR	C-N-CA	6.36	129.26	120.49
8	A7	339	PHE	CA-CB-CG	6.24	120.04	113.80
2	BK	200	ARG	NE-CZ-NH2	6.24	124.81	119.20
10	Fb	358	ASP	CA-CB-CG	6.22	118.82	112.60
3	BR	194	ASP	CA-CB-CG	6.21	118.81	112.60
10	Fk	358	ASP	CA-CB-CG	6.21	118.81	112.60
1	AW	461	PHE	N-CA-C	6.21	117.71	111.07
10	FS	358	ASP	CA-CB-CG	6.21	118.81	112.60
14	AB	128	SER	N-CA-C	6.20	117.92	111.03
2	BL	196	ASP	CA-CB-CG	6.20	118.80	112.60
10	FA	358	ASP	CA-CB-CG	6.20	118.80	112.60
10	FJ	358	ASP	CA-CB-CG	6.19	118.79	112.60
10	Ft	358	ASP	CA-CB-CG	6.18	118.78	112.60
3	BQ	236	THR	CA-C-N	6.14	128.96	120.49
3	BQ	236	THR	C-N-CA	6.14	128.96	120.49
2	BN	196	ASP	CA-CB-CG	6.12	118.72	112.60
8	A6	23	PHE	CA-CB-CG	6.10	119.90	113.80
14	AE	128	SER	N-CA-C	6.09	117.79	111.03
12	Fa	7	ASN	CA-CB-CG	6.08	118.67	112.60
12	Fs	7	ASN	CA-CB-CG	6.07	118.67	112.60
12	FR	7	ASN	CA-CB-CG	6.07	118.67	112.60
12	FI	7	ASN	CA-CB-CG	6.06	118.66	112.60
12	Fj	7	ASN	CA-CB-CG	6.06	118.66	112.60
1	AX	117	HIS	CA-CB-CG	6.05	119.85	113.80
12	F2	7	ASN	CA-CB-CG	6.04	118.64	112.60
1	AV	625	ASP	CA-CB-CG	6.03	118.63	112.60
8	A5	339	PHE	CA-CB-CG	6.01	119.81	113.80
1	AM	374	LYS	CB-CA-C	5.94	115.42	111.20
1	AR	456	ASP	CA-CB-CG	5.93	118.53	112.60
1	AQ	374	LYS	CB-CA-C	5.93	115.41	111.20
12	Fs	438	ASP	CA-CB-CG	5.91	118.51	112.60
2	BK	204	ASP	CA-CB-CG	5.90	118.50	112.60
1	AX	461	PHE	N-CA-C	5.90	118.49	111.71
8	A6	244	ASN	CB-CA-C	5.90	119.11	111.50
12	FR	438	ASP	CA-CB-CG	5.89	118.49	112.60
12	Fj	438	ASP	CA-CB-CG	5.89	118.49	112.60
1	AX	625	ASP	CA-CB-CG	5.88	118.48	112.60
12	FI	438	ASP	CA-CB-CG	5.88	118.48	112.60
12	Fa	438	ASP	CA-CB-CG	5.87	118.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Fp	9	GLU	CB-CG-CD	5.86	122.56	112.60
11	FO	9	GLU	CB-CG-CD	5.85	122.55	112.60
11	FF	9	GLU	CB-CG-CD	5.85	122.55	112.60
11	Fy	9	GLU	CB-CG-CD	5.85	122.54	112.60
11	Fg	9	GLU	CB-CG-CD	5.84	122.52	112.60
12	F2	438	ASP	CA-CB-CG	5.84	118.44	112.60
11	FX	9	GLU	CB-CG-CD	5.83	122.52	112.60
3	BU	236	THR	CA-C-N	5.82	128.30	120.50
3	BU	236	THR	C-N-CA	5.82	128.30	120.50
7	A2	327	ARG	NE-CZ-NH2	5.81	124.43	119.20
7	AZ	327	ARG	NE-CZ-NH2	5.81	124.43	119.20
8	A8	19	ILE	N-CA-CB	-5.80	106.48	112.28
1	AN	246	GLU	CB-CG-CD	5.79	122.45	112.60
7	A0	327	ARG	NE-CZ-NH2	5.79	124.41	119.20
7	A3	327	ARG	NE-CZ-NH2	5.79	124.41	119.20
5	BC	30	ARG	NE-CZ-NH2	5.79	124.41	119.20
7	AY	327	ARG	NE-CZ-NH2	5.79	124.41	119.20
7	A1	327	ARG	NE-CZ-NH2	5.79	124.41	119.20
8	A8	23	PHE	CA-CB-CG	5.76	119.56	113.80
14	AA	128	SER	N-CA-C	5.76	117.42	111.03
13	BX	14	ASP	CA-CB-CG	5.72	118.32	112.60
1	AO	625	ASP	CA-CB-CG	5.72	118.32	112.60
8	A9	339	PHE	CA-CB-CG	5.72	119.52	113.80
1	AV	291	ASP	CA-CB-CG	5.70	118.30	112.60
10	FK	564	ASP	CA-CB-CG	5.68	118.28	112.60
13	B1	14	ASP	CA-CB-CG	5.67	118.27	112.60
13	B8	36	CYS	CA-C-N	5.67	128.20	120.54
13	B8	36	CYS	C-N-CA	5.67	128.20	120.54
2	BO	204	ASP	CA-CB-CG	5.67	118.27	112.60
10	Fu	564	ASP	CA-CB-CG	5.67	118.27	112.60
8	A6	19	ILE	N-CA-CB	-5.66	106.62	112.28
10	FB	564	ASP	CA-CB-CG	5.66	118.26	112.60
10	F1	564	ASP	CA-CB-CG	5.65	118.25	112.60
8	A5	191	ASP	CA-CB-CG	5.65	118.25	112.60
10	Fc	564	ASP	CA-CB-CG	5.64	118.24	112.60
5	BB	30	ARG	NE-CZ-NH2	5.64	124.28	119.20
10	FT	564	ASP	CA-CB-CG	5.64	118.24	112.60
5	BB	438	ASP	CA-CB-CG	5.64	118.24	112.60
10	Ft	590	ASP	CA-CB-CG	5.63	118.23	112.60
1	AT	625	ASP	CA-CB-CG	5.62	118.22	112.60
10	Fb	590	ASP	CA-CB-CG	5.62	118.22	112.60
10	Fu	566	ASP	CA-CB-CG	5.61	118.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	AC	100	ASP	CA-CB-CG	5.61	118.21	112.60
10	FA	590	ASP	CA-CB-CG	5.60	118.20	112.60
10	FK	566	ASP	CA-CB-CG	5.60	118.20	112.60
10	FS	590	ASP	CA-CB-CG	5.60	118.20	112.60
10	FT	566	ASP	CA-CB-CG	5.59	118.19	112.60
10	FB	566	ASP	CA-CB-CG	5.59	118.19	112.60
10	Fc	566	ASP	CA-CB-CG	5.57	118.17	112.60
1	AS	280	ARG	NE-CZ-NH1	-5.57	115.93	121.50
10	Fc	570	PRO	N-CA-C	5.57	123.94	112.47
10	Fl	570	PRO	N-CA-C	5.56	123.93	112.47
13	BY	14	ASP	CA-CB-CG	5.56	118.16	112.60
10	FK	570	PRO	N-CA-C	5.56	123.93	112.47
10	FJ	590	ASP	CA-CB-CG	5.56	118.16	112.60
10	FB	570	PRO	N-CA-C	5.55	123.91	112.47
10	FT	570	PRO	N-CA-C	5.55	123.91	112.47
15	BG	239	ASN	CA-CB-CG	5.55	118.15	112.60
5	BC	11	PHE	CA-CB-CG	5.55	119.35	113.80
7	A2	137	PHE	CA-CB-CG	5.55	119.35	113.80
1	AR	246	GLU	CB-CG-CD	5.54	122.02	112.60
1	AM	625	ASP	CA-CB-CG	5.54	118.14	112.60
10	Fl	566	ASP	CA-CB-CG	5.54	118.14	112.60
8	A7	191	ASP	CA-CB-CG	5.54	118.14	112.60
10	Fk	590	ASP	CA-CB-CG	5.54	118.14	112.60
9	LM	108	PHE	CA-CB-CG	5.53	119.33	113.80
10	Fu	570	PRO	N-CA-C	5.53	123.86	112.47
1	AN	456	ASP	CA-CB-CG	5.52	118.12	112.60
7	AY	137	PHE	CA-CB-CG	5.51	119.31	113.80
7	A0	137	PHE	CA-CB-CG	5.51	119.31	113.80
9	LP	108	PHE	CA-CB-CG	5.51	119.31	113.80
2	BP	179	ALA	CA-C-N	5.51	129.08	120.82
2	BP	179	ALA	C-N-CA	5.51	129.08	120.82
4	AK	82	ASP	CA-CB-CG	5.51	118.11	112.60
9	LG	108	PHE	CA-CB-CG	5.50	119.30	113.80
1	AM	607	ASP	CA-CB-CG	5.50	118.10	112.60
7	A1	137	PHE	CA-CB-CG	5.50	119.30	113.80
9	LA	108	PHE	CA-CB-CG	5.49	119.29	113.80
9	LJ	108	PHE	CA-CB-CG	5.49	119.29	113.80
5	BC	438	ASP	CA-CB-CG	5.49	118.08	112.60
7	A3	137	PHE	CA-CB-CG	5.49	119.29	113.80
13	BZ	14	ASP	CA-CB-CG	5.48	118.08	112.60
9	LD	108	PHE	CA-CB-CG	5.47	119.27	113.80
13	B2	14	ASP	CA-CB-CG	5.46	118.06	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	AZ	137	PHE	CA-CB-CG	5.46	119.26	113.80
10	FL	182	ASP	CA-CB-CG	5.45	118.05	112.60
10	FC	182	ASP	CA-CB-CG	5.44	118.04	112.60
15	BF	239	ASN	CA-CB-CG	5.44	118.04	112.60
8	A7	300	GLU	CB-CG-CD	5.44	121.85	112.60
10	Fv	182	ASP	CA-CB-CG	5.44	118.04	112.60
1	AP	246	GLU	CB-CG-CD	5.44	121.85	112.60
8	A4	107	TYR	CB-CA-C	5.43	117.48	109.22
10	FU	182	ASP	CA-CB-CG	5.43	118.03	112.60
10	Fm	182	ASP	CA-CB-CG	5.43	118.03	112.60
15	BE	239	ASN	CA-CB-CG	5.43	118.03	112.60
1	AV	400	ASP	CA-CB-CG	5.42	118.03	112.60
2	BP	196	ASP	CA-CB-CG	5.42	118.02	112.60
2	BM	204	ASP	CA-CB-CG	5.42	118.02	112.60
15	BE	303	ASP	CA-CB-CG	5.41	118.01	112.60
10	Fd	182	ASP	CA-CB-CG	5.41	118.01	112.60
5	BD	438	ASP	CA-CB-CG	5.41	118.01	112.60
1	AP	456	ASP	CA-CB-CG	5.40	118.00	112.60
13	BZ	36	CYS	CA-C-N	5.40	127.77	120.38
13	BZ	36	CYS	C-N-CA	5.40	127.77	120.38
2	BM	200	ARG	CG-CD-NE	-5.39	100.13	112.00
1	AU	461	PHE	N-CA-C	5.39	116.85	110.97
1	AQ	625	ASP	CA-CB-CG	5.38	117.98	112.60
8	A7	19	ILE	N-CA-CB	-5.38	106.90	112.28
8	A8	107	TYR	CB-CA-C	5.38	117.39	109.22
1	AQ	291	ASP	CA-CB-CG	5.35	117.95	112.60
8	A5	19	ILE	N-CA-CB	-5.35	106.87	112.06
1	AS	540	ASP	CA-CB-CG	5.35	117.95	112.60
1	AQ	607	ASP	CA-CB-CG	5.35	117.95	112.60
8	Ab	139	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	AO	374	LYS	CB-CA-C	5.34	114.99	111.20
1	AX	291	ASP	CA-CB-CG	5.32	117.92	112.60
13	BW	14	ASP	CA-CB-CG	5.32	117.92	112.60
1	AX	64	ASN	CA-CB-CG	-5.32	107.28	112.60
8	Ad	139	ARG	NE-CZ-NH2	5.32	123.98	119.20
8	A5	101	ASP	CA-CB-CG	5.31	117.91	112.60
8	Af	139	ARG	NE-CZ-NH2	5.31	123.98	119.20
13	BX	36	CYS	CA-C-N	5.30	127.64	120.38
13	BX	36	CYS	C-N-CA	5.30	127.64	120.38
8	Ae	139	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	AS	138	ASP	CA-CB-CG	5.29	117.89	112.60
1	AV	551	ILE	CA-C-N	5.28	128.12	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AV	551	ILE	C-N-CA	5.28	128.12	121.36
1	AU	540	ASP	CA-CB-CG	5.28	117.88	112.60
2	BM	131	ASP	CA-CB-CG	5.28	117.88	112.60
5	BB	512	ASP	CA-CB-CG	5.28	117.88	112.60
8	Ac	139	ARG	NE-CZ-NH2	5.28	123.95	119.20
6	BA	54	ASP	CA-CB-CG	5.27	117.87	112.60
8	Aa	139	ARG	NE-CZ-NH2	5.27	123.94	119.20
8	A4	188	ASP	CA-CB-CG	5.27	117.87	112.60
9	LG	76	ALA	CA-C-N	5.26	125.10	120.10
9	LG	76	ALA	C-N-CA	5.26	125.10	120.10
5	BB	239	ASP	CA-CB-CG	5.25	117.85	112.60
5	BC	239	ASP	CA-CB-CG	5.25	117.85	112.60
13	B6	119	ASP	CA-CB-CG	5.25	117.85	112.60
1	AW	540	ASP	CA-CB-CG	5.24	117.84	112.60
9	LD	76	ALA	CA-C-N	5.24	125.08	120.10
9	LD	76	ALA	C-N-CA	5.24	125.08	120.10
5	BC	162	ASP	CA-CB-CG	5.24	117.84	112.60
4	AG	82	ASP	CA-CB-CG	5.22	117.82	112.60
7	A0	656	ASP	CA-CB-CG	5.22	117.82	112.60
7	A1	656	ASP	CA-CB-CG	5.22	117.82	112.60
7	A3	656	ASP	CA-CB-CG	5.22	117.82	112.60
9	LA	76	ALA	CA-C-N	5.22	125.06	120.10
9	LA	76	ALA	C-N-CA	5.22	125.06	120.10
11	Fy	77	ASP	CA-CB-CG	5.21	117.81	112.60
1	AO	374	LYS	O-C-N	-5.21	119.13	121.53
5	BD	11	PHE	CA-CB-CG	5.21	119.01	113.80
1	AP	142	ASP	CA-CB-CG	5.20	117.80	112.60
7	AY	656	ASP	CA-CB-CG	5.20	117.80	112.60
12	Fz	401	HIS	CA-CB-CG	5.20	119.00	113.80
12	FY	401	HIS	CA-CB-CG	5.20	119.00	113.80
9	LM	76	ALA	CA-C-N	5.20	125.03	120.10
9	LM	76	ALA	C-N-CA	5.20	125.03	120.10
2	BO	307	ASP	CA-CB-CG	5.19	117.79	112.60
1	AO	607	ASP	CA-CB-CG	5.19	117.79	112.60
10	Fl	358	ASP	CA-CB-CG	5.19	117.79	112.60
12	FG	401	HIS	CA-CB-CG	5.19	118.99	113.80
1	AO	291	ASP	CA-CB-CG	5.19	117.79	112.60
7	AZ	656	ASP	CA-CB-CG	5.19	117.79	112.60
3	BR	195	VAL	CA-C-N	5.18	128.58	120.75
3	BR	195	VAL	C-N-CA	5.18	128.58	120.75
7	A2	485	HIS	CA-CB-CG	-5.18	108.62	113.80
11	FF	77	ASP	CA-CB-CG	5.18	117.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Fh	401	HIS	CA-CB-CG	5.18	118.98	113.80
7	A2	656	ASP	CA-CB-CG	5.18	117.78	112.60
10	FK	358	ASP	CA-CB-CG	5.18	117.78	112.60
7	A3	485	HIS	CA-CB-CG	-5.18	108.62	113.80
11	FX	77	ASP	CA-CB-CG	5.18	117.78	112.60
11	Fp	77	ASP	CA-CB-CG	5.17	117.78	112.60
10	Fu	358	ASP	CA-CB-CG	5.17	117.77	112.60
11	Fg	77	ASP	CA-CB-CG	5.17	117.77	112.60
10	FT	358	ASP	CA-CB-CG	5.17	117.77	112.60
10	Fc	358	ASP	CA-CB-CG	5.17	117.77	112.60
12	Fq	401	HIS	CA-CB-CG	5.17	118.97	113.80
9	LP	76	ALA	CA-C-N	5.17	125.01	120.10
9	LP	76	ALA	C-N-CA	5.17	125.01	120.10
7	A1	485	HIS	CA-CB-CG	-5.16	108.64	113.80
7	A3	486	TYR	CB-CA-C	5.16	117.96	110.79
10	FB	358	ASP	CA-CB-CG	5.16	117.76	112.60
11	FO	77	ASP	CA-CB-CG	5.16	117.76	112.60
1	AT	327	ASP	CA-CB-CG	5.16	117.76	112.60
11	FN	216	PHE	CA-CB-CG	5.16	118.96	113.80
12	FP	401	HIS	CA-CB-CG	5.16	118.96	113.80
1	AT	291	ASP	CA-CB-CG	5.15	117.75	112.60
7	AY	485	HIS	CA-CB-CG	-5.15	108.65	113.80
7	A0	485	HIS	CA-CB-CG	-5.14	108.66	113.80
11	Fo	216	PHE	CA-CB-CG	5.14	118.94	113.80
1	AT	542	ASP	CA-CB-CG	5.14	117.74	112.60
7	AZ	485	HIS	CA-CB-CG	-5.14	108.66	113.80
5	BD	162	ASP	CA-CB-CG	5.14	117.74	112.60
7	AZ	486	TYR	CB-CA-C	5.14	117.93	110.79
7	AY	486	TYR	CB-CA-C	5.13	117.93	110.79
7	A2	486	TYR	CB-CA-C	5.13	117.93	110.79
9	LJ	76	ALA	CA-C-N	5.13	124.97	120.10
9	LJ	76	ALA	C-N-CA	5.13	124.97	120.10
11	FW	216	PHE	CA-CB-CG	5.13	118.93	113.80
4	AH	10	ASP	CA-CB-CG	5.13	117.73	112.60
11	FE	216	PHE	CA-CB-CG	5.12	118.92	113.80
7	A0	486	TYR	CB-CA-C	5.12	117.90	110.79
7	A1	486	TYR	CB-CA-C	5.12	117.90	110.79
14	AE	50	ASP	CA-CB-CG	5.11	117.71	112.60
13	B4	119	ASP	CA-CB-CG	5.11	117.71	112.60
11	Fn	9	GLU	CB-CG-CD	5.11	121.29	112.60
12	FR	69	ASP	CA-CB-CG	5.11	117.71	112.60
1	AU	613	ASP	CA-CB-CG	5.11	117.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BV	236	THR	CA-C-N	5.11	127.53	120.49
3	BV	236	THR	C-N-CA	5.11	127.53	120.49
10	FL	358	ASP	CA-CB-CG	5.11	117.70	112.60
11	Fx	216	PHE	CA-CB-CG	5.11	118.91	113.80
11	FV	9	GLU	CB-CG-CD	5.10	121.27	112.60
10	Fm	358	ASP	CA-CB-CG	5.10	117.70	112.60
11	FD	9	GLU	CB-CG-CD	5.10	121.26	112.60
12	FR	21	THR	N-CA-C	5.10	117.22	111.11
11	Fe	9	GLU	CB-CG-CD	5.09	121.26	112.60
10	FU	358	ASP	CA-CB-CG	5.09	117.69	112.60
11	FM	9	GLU	CB-CG-CD	5.09	121.26	112.60
10	Fv	358	ASP	CA-CB-CG	5.09	117.69	112.60
10	FC	358	ASP	CA-CB-CG	5.09	117.69	112.60
11	Fw	9	GLU	CB-CG-CD	5.09	121.25	112.60
11	Ff	216	PHE	CA-CB-CG	5.08	118.88	113.80
7	A3	655	PRO	CA-C-N	5.08	127.34	120.38
7	A3	655	PRO	C-N-CA	5.08	127.34	120.38
1	AV	631	ASP	CA-CB-CG	5.08	117.68	112.60
5	BD	30	ARG	NE-CZ-NH2	5.07	123.77	119.20
12	Fs	69	ASP	CA-CB-CG	5.07	117.67	112.60
12	Fa	21	THR	N-CA-C	5.07	117.19	111.11
1	AU	280	ARG	NE-CZ-NH1	-5.07	116.44	121.50
7	A0	655	PRO	CA-C-N	5.07	127.32	120.38
7	A0	655	PRO	C-N-CA	5.07	127.32	120.38
12	Fs	21	THR	N-CA-C	5.06	117.19	111.11
10	Fd	358	ASP	CA-CB-CG	5.06	117.66	112.60
12	FI	69	ASP	CA-CB-CG	5.06	117.66	112.60
7	AY	655	PRO	CA-C-N	5.06	127.31	120.38
7	AY	655	PRO	C-N-CA	5.06	127.31	120.38
1	AR	607	ASP	CA-CB-CG	5.05	117.65	112.60
7	A2	655	PRO	CA-C-N	5.05	127.30	120.38
7	A2	655	PRO	C-N-CA	5.05	127.30	120.38
12	Fa	69	ASP	CA-CB-CG	5.05	117.65	112.60
12	F2	69	ASP	CA-CB-CG	5.05	117.65	112.60
7	A1	655	PRO	CA-C-N	5.05	127.29	120.38
7	A1	655	PRO	C-N-CA	5.05	127.29	120.38
12	FI	21	THR	N-CA-C	5.05	117.17	111.11
12	F2	21	THR	N-CA-C	5.04	117.16	111.11
5	BB	458	ASN	CA-CB-CG	5.04	117.64	112.60
10	FS	182	ASP	CA-CB-CG	5.04	117.64	112.60
10	Fb	182	ASP	CA-CB-CG	5.04	117.64	112.60
10	FA	182	ASP	CA-CB-CG	5.03	117.63	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	BG	329	ASP	CA-CB-CG	5.03	117.63	112.60
12	Fj	21	THR	N-CA-C	5.03	117.15	111.11
1	AV	542	ASP	CA-CB-CG	5.03	117.63	112.60
5	BC	512	ASP	CA-CB-CG	5.03	117.63	112.60
2	BO	346	ILE	CA-C-N	5.02	125.11	120.34
2	BO	346	ILE	C-N-CA	5.02	125.11	120.34
7	AZ	655	PRO	CA-C-N	5.02	127.26	120.38
7	AZ	655	PRO	C-N-CA	5.02	127.26	120.38
8	A6	107	TYR	CB-CA-C	5.02	116.85	109.22
10	FJ	182	ASP	CA-CB-CG	5.02	117.62	112.60
14	AF	50	ASP	CA-CB-CG	5.02	117.62	112.60
12	Fj	69	ASP	CA-CB-CG	5.02	117.62	112.60
4	AG	187	ARG	NE-CZ-NH2	5.02	123.71	119.20
1	AN	607	ASP	CA-CB-CG	5.01	117.61	112.60
10	Fk	182	ASP	CA-CB-CG	5.01	117.61	112.60
1	AO	20	ASP	CA-CB-CG	5.01	117.61	112.60
10	Ft	182	ASP	CA-CB-CG	5.01	117.61	112.60
5	BC	458	ASN	CA-CB-CG	5.01	117.61	112.60
1	AW	138	ASP	CA-CB-CG	5.01	117.61	112.60
9	LL	108	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A0	427	ARG	Sidechain
7	A0	447	ALA	Peptide
7	A1	427	ARG	Sidechain
7	A1	447	ALA	Peptide
7	A2	427	ARG	Sidechain
7	A2	447	ALA	Peptide
7	A2	484	LYS	Peptide
7	A3	427	ARG	Sidechain
7	A3	447	ALA	Peptide
8	A6	184	ASN	Peptide
7	AY	427	ARG	Sidechain
7	AY	447	ALA	Peptide
7	AZ	427	ARG	Sidechain
7	AZ	447	ALA	Peptide
7	AZ	484	LYS	Peptide
15	BE	86	TYR	Sidechain
15	BF	86	TYR	Sidechain

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Mol	Chain	Res	Type	Group
15	BG	86	TYR	Sidechain
2	BM	264	SER	Peptide
12	F1	321	ARG	Peptide
10	FA	10	SER	Peptide
10	FA	356	ASN	Peptide
10	FC	10	SER	Peptide
11	FF	3	ILE	Peptide
12	FH	321	ARG	Peptide
10	FJ	10	SER	Peptide
10	FJ	356	ASN	Peptide
10	FL	10	SER	Peptide
11	FO	3	ILE	Peptide
12	FQ	321	ARG	Peptide
10	FS	10	SER	Peptide
10	FS	356	ASN	Peptide
10	FU	10	SER	Peptide
11	FX	3	ILE	Peptide
12	FZ	321	ARG	Peptide
10	Fb	10	SER	Peptide
10	Fb	356	ASN	Peptide
10	Fd	10	SER	Peptide
11	Fg	3	ILE	Peptide
12	Fi	321	ARG	Peptide
10	Fk	10	SER	Peptide
10	Fk	356	ASN	Peptide
10	Fm	10	SER	Peptide
11	Fp	3	ILE	Peptide
12	Fr	321	ARG	Peptide
10	Ft	10	SER	Peptide
10	Ft	356	ASN	Peptide
10	Fv	10	SER	Peptide
11	Fy	3	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AM	5191	0	5061	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AN	5191	0	5061	22	0
1	AO	5191	0	5061	14	0
1	AP	5191	0	5061	17	0
1	AQ	5191	0	5061	14	0
1	AR	5191	0	5061	21	0
1	AS	5145	0	5008	12	0
1	AT	5125	0	4993	10	0
1	AU	5145	0	5008	4	0
1	AV	5125	0	4993	14	0
1	AW	5145	0	5008	11	0
1	AX	5125	0	4993	13	0
2	BK	2323	0	2255	6	0
2	BL	1790	0	1747	3	0
2	BM	2323	0	2255	5	0
2	BN	1790	0	1747	4	0
2	BO	2323	0	2255	5	0
2	BP	1790	0	1747	2	0
3	BQ	1719	0	1662	8	0
3	BR	1719	0	1662	8	0
3	BS	1719	0	1662	3	0
3	BT	1719	0	1662	8	0
3	BU	1719	0	1662	5	0
3	BV	1719	0	1662	4	0
4	AG	1747	0	1652	12	0
4	AH	1747	0	1652	20	0
4	AI	1747	0	1652	14	0
4	AJ	1747	0	1652	15	0
4	AK	1747	0	1652	14	0
4	AL	1747	0	1652	11	0
5	BB	4354	0	4218	6	0
5	BC	4354	0	4218	3	0
5	BD	4354	0	4218	3	0
6	BA	706	0	700	0	0
7	A0	8438	0	8098	119	0
7	A1	8438	0	8098	108	0
7	A2	8438	0	8098	109	0
7	A3	8438	0	8098	111	0
7	AY	8438	0	8098	117	0
7	AZ	8438	0	8098	105	0
8	A4	2669	0	2557	44	0
8	A5	2669	0	2557	45	0
8	A6	2669	0	2557	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A7	2669	0	2557	38	0
8	A8	2669	0	2557	37	0
8	A9	2669	0	2557	40	0
8	Aa	2633	0	2518	26	0
8	Ab	2633	0	2518	30	0
8	Ac	2633	0	2518	30	0
8	Ad	2633	0	2518	27	0
8	Ae	2633	0	2518	31	0
8	Af	2633	0	2518	40	0
9	LA	2270	0	2236	2	0
9	LB	2270	0	2236	2	0
9	LC	2270	0	2236	2	0
9	LD	2270	0	2236	3	0
9	LE	2270	0	2236	2	0
9	LF	2270	0	2236	2	0
9	LG	2270	0	2236	3	0
9	LH	2270	0	2236	2	0
9	LI	2270	0	2236	2	0
9	LJ	2270	0	2236	3	0
9	LK	2270	0	2236	2	0
9	LL	2270	0	2236	2	0
9	LM	2270	0	2236	7	0
9	LN	2270	0	2236	4	0
9	LO	2270	0	2236	4	0
9	LP	2270	0	2236	3	0
9	LQ	2270	0	2236	2	0
9	LR	2270	0	2236	2	0
10	FA	4696	0	4547	29	0
10	FB	4696	0	4548	16	0
10	FC	4696	0	4547	19	0
10	FJ	4696	0	4548	32	0
10	FK	4696	0	4548	15	0
10	FL	4696	0	4547	21	0
10	FS	4696	0	4547	35	0
10	FT	4696	0	4548	14	0
10	FU	4696	0	4547	17	0
10	Fb	4696	0	4548	33	0
10	Fc	4696	0	4548	15	0
10	Fd	4696	0	4547	27	0
10	Fk	4696	0	4548	37	0
10	Fl	4696	0	4548	15	0
10	Fm	4696	0	4547	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Ft	4696	0	4548	34	0
10	Fu	4696	0	4548	14	0
10	Fv	4696	0	4547	25	0
11	FD	1722	0	1676	1	0
11	FE	1722	0	1676	0	0
11	FF	1722	0	1676	2	0
11	FM	1722	0	1676	1	0
11	FN	1722	0	1676	0	0
11	FO	1722	0	1676	2	0
11	FV	1722	0	1676	1	0
11	FW	1722	0	1676	0	0
11	FX	1722	0	1676	2	0
11	Fe	1722	0	1676	1	0
11	Ff	1722	0	1676	0	0
11	Fg	1722	0	1676	2	0
11	Fh	1722	0	1676	1	0
11	Fo	1722	0	1676	0	0
11	Fp	1722	0	1676	2	0
11	Fw	1722	0	1676	1	0
11	Fx	1722	0	1676	0	0
11	Fy	1722	0	1676	2	0
12	F1	3362	0	3297	15	0
12	F2	3376	0	3317	10	0
12	FG	3371	0	3312	11	0
12	FH	3362	0	3297	20	0
12	FI	3376	0	3317	16	0
12	FP	3371	0	3312	10	0
12	FQ	3362	0	3297	14	0
12	FR	3376	0	3317	11	0
12	FY	3371	0	3312	11	0
12	FZ	3362	0	3297	17	0
12	Fa	3376	0	3317	13	0
12	Fh	3371	0	3312	9	0
12	Fi	3362	0	3297	14	0
12	Fj	3376	0	3317	10	0
12	Fq	3371	0	3312	10	0
12	Fr	3362	0	3297	20	0
12	Fs	3376	0	3317	16	0
12	Fz	3371	0	3312	10	0
13	B1	1305	0	1235	4	0
13	B2	1305	0	1235	2	0
13	B3	1305	0	1235	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B4	1305	0	1235	3	0
13	B5	1305	0	1235	2	0
13	B6	1305	0	1235	3	0
13	B7	1305	0	1235	2	0
13	B8	1305	0	1235	2	0
13	BW	1305	0	1235	3	0
13	BX	1305	0	1235	3	0
13	BY	1305	0	1235	5	0
13	BZ	1305	0	1235	6	0
14	AA	1069	0	1069	2	0
14	AB	1069	0	1069	2	0
14	AC	1069	0	1069	7	0
14	AD	1069	0	1069	5	0
14	AE	1069	0	1069	2	0
14	AF	1069	0	1069	4	0
15	BE	3055	0	2962	10	0
15	BF	3055	0	2962	8	0
15	BG	3055	0	2962	7	0
16	BH	242	0	239	0	0
16	BI	242	0	239	0	0
16	BJ	242	0	239	0	0
17	BB	1	0	0	0	0
18	FA	1	0	0	0	0
18	FJ	1	0	0	0	0
18	FS	1	0	0	0	0
18	Fb	1	0	0	0	0
18	Fk	1	0	0	0	0
18	Ft	1	0	0	0	0
19	FB	1	0	0	0	0
19	FG	1	0	0	0	0
19	FK	1	0	0	0	0
19	FT	1	0	0	0	0
19	Fc	1	0	0	0	0
19	Fl	1	0	0	0	0
All	All	440315	0	427316	1308	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (1308) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:906:MET:HE1	8:A9:27:LYS:CD	1.54	1.37
7:AZ:469:SER:OG	8:Af:62:GLY:HA3	1.14	1.28
7:AY:483:ASP:OD1	8:Ac:72:GLU:HG2	1.30	1.27
7:A2:906:MET:HE1	8:A5:27:LYS:CD	1.63	1.26
7:A2:1028:VAL:CG2	8:A5:14:ILE:HG22	1.67	1.24
7:AZ:469:SER:OG	8:Af:62:GLY:CA	1.84	1.22
1:AP:2:ALA:CB	7:A0:636:GLU:HB2	1.68	1.21
7:AZ:906:MET:HE1	8:A7:27:LYS:CD	1.68	1.21
1:AR:2:ALA:CB	7:AY:636:GLU:HB2	1.73	1.17
1:AR:2:ALA:HB2	7:AY:636:GLU:HB2	1.24	1.17
4:AH:97:PHE:CE2	7:A3:644:PRO:HG2	1.79	1.15
4:AK:97:PHE:CZ	7:A1:644:PRO:HG2	1.83	1.14
1:AP:2:ALA:HB2	7:A0:636:GLU:CB	1.77	1.14
7:A0:1001:PHE:CE1	10:F1:19:LEU:HD23	1.84	1.13
4:AG:97:PHE:CZ	7:A2:644:PRO:HG2	1.85	1.12
7:A2:906:MET:HE1	8:A5:27:LYS:HD3	1.24	1.11
4:AI:97:PHE:CZ	7:AZ:644:PRO:HG2	1.85	1.11
7:A3:1001:PHE:CE1	10:FT:19:LEU:HD23	1.85	1.10
7:A1:906:MET:HE1	8:A9:27:LYS:HD2	1.22	1.09
8:Aa:16:ARG:HD3	8:A7:67:TYR:CE1	1.88	1.09
4:AL:97:PHE:CE2	7:AY:644:PRO:HG2	1.88	1.08
4:AJ:97:PHE:CE2	7:A0:644:PRO:HG2	1.88	1.08
7:AY:920:LYS:O	10:FC:19:LEU:HD23	1.52	1.08
7:AZ:906:MET:HE1	8:A7:27:LYS:HD3	1.31	1.08
7:A1:906:MET:HE1	8:A9:27:LYS:HD3	1.28	1.08
7:AY:1001:PHE:CE1	10:FB:19:LEU:HD23	1.88	1.07
7:AZ:469:SER:CB	8:Af:62:GLY:HA3	1.85	1.07
7:A1:906:MET:SD	8:A9:27:LYS:HE3	1.94	1.07
7:A1:1001:PHE:CE1	10:Fu:19:LEU:HD23	1.90	1.07
8:Ac:16:ARG:HD3	8:A9:67:TYR:CE1	1.89	1.07
7:A2:1028:VAL:HG23	8:A5:14:ILE:HG22	1.31	1.06
7:AY:906:MET:HE1	8:A4:27:LYS:HD2	1.33	1.06
7:A2:1001:PHE:CE1	10:FK:19:LEU:HD23	1.91	1.06
8:Ac:61:PRO:O	8:A9:11:ARG:HB3	1.55	1.06
7:A1:906:MET:CE	8:A9:27:LYS:HD2	1.87	1.04
4:AJ:97:PHE:CZ	7:A0:644:PRO:HG2	1.91	1.04
7:AZ:1001:PHE:CE1	10:Fc:19:LEU:HD23	1.91	1.04
8:Ae:16:ARG:HD3	8:A5:67:TYR:CE1	1.93	1.04
7:A1:906:MET:SD	8:A9:27:LYS:CE	2.46	1.03
7:A1:920:LYS:O	10:Fv:19:LEU:HD23	1.58	1.03
4:AK:97:PHE:CE2	7:A1:644:PRO:HG2	1.92	1.03
7:A1:906:MET:CE	8:A9:27:LYS:CD	2.35	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AH:97:PHE:CZ	7:A3:644:PRO:HG2	1.93	1.03
8:Aa:16:ARG:HD3	8:A7:67:TYR:CD1	1.94	1.02
7:AZ:920:LYS:O	10:Fd:19:LEU:HD23	1.59	1.02
8:Ab:61:PRO:O	8:A8:11:ARG:HB3	1.60	1.02
7:A2:906:MET:CE	8:A5:27:LYS:CD	2.38	1.01
7:A2:920:LYS:O	10:FL:19:LEU:HD23	1.60	1.01
1:AR:2:ALA:HB2	7:AY:636:GLU:CB	1.90	1.01
4:AG:97:PHE:CE2	7:A2:644:PRO:HG2	1.95	1.00
7:A2:906:MET:HE1	8:A5:27:LYS:HD2	1.39	1.00
4:AI:97:PHE:CE2	7:AZ:644:PRO:HG2	1.98	0.99
7:AY:483:ASP:CG	8:Ac:72:GLU:HG2	1.88	0.98
7:AZ:906:MET:HE1	8:A7:27:LYS:HD2	1.40	0.98
7:AY:1001:PHE:CZ	10:FB:19:LEU:CD2	2.45	0.97
7:A0:920:LYS:O	10:Fm:19:LEU:HD23	1.64	0.97
7:A2:906:MET:SD	8:A5:27:LYS:HE3	2.04	0.97
7:A3:1001:PHE:CZ	10:FT:19:LEU:CD2	2.49	0.96
8:Ac:16:ARG:HD3	8:A9:67:TYR:CD1	2.00	0.96
4:AL:97:PHE:CZ	7:AY:644:PRO:HG2	2.00	0.96
7:A2:906:MET:CE	8:A5:27:LYS:HD2	1.93	0.96
7:A3:920:LYS:O	10:FU:19:LEU:HD23	1.66	0.95
8:Ab:16:ARG:HD3	8:A8:67:TYR:CE1	2.01	0.95
7:A0:1001:PHE:CZ	10:Fl:19:LEU:CD2	2.50	0.95
7:A2:906:MET:SD	8:A5:27:LYS:CE	2.55	0.94
7:AZ:469:SER:OG	8:Af:62:GLY:C	2.11	0.94
4:AH:100:GLN:NE2	7:A3:647:ARG:NH1	2.16	0.93
7:AZ:906:MET:CE	8:A7:27:LYS:CD	2.46	0.93
8:Ae:16:ARG:HD3	8:A5:67:TYR:CD1	2.03	0.93
7:A0:765:ASN:OD1	8:A8:207:ILE:CD1	2.17	0.92
7:A0:484:LYS:NZ	8:A7:182:ASP:OD1	2.03	0.92
7:AY:906:MET:SD	8:A4:27:LYS:NZ	2.43	0.92
7:A1:1001:PHE:CZ	10:Fu:19:LEU:CD2	2.52	0.92
7:A0:1001:PHE:CE1	10:Fl:19:LEU:CD2	2.52	0.91
1:AP:2:ALA:HB2	7:A0:636:GLU:HB2	0.92	0.91
7:AZ:1001:PHE:CZ	10:Fc:19:LEU:CD2	2.53	0.91
8:Ad:16:ARG:HD3	8:A4:67:TYR:CE1	2.06	0.91
1:AQ:3:ILE:HD11	7:A1:635:PRO:HA	1.51	0.91
7:A1:483:ASP:OD2	8:A8:139:ARG:NH2	2.04	0.90
7:A2:1028:VAL:HG22	8:A5:14:ILE:HG22	1.49	0.90
7:A2:1001:PHE:CZ	10:FK:19:LEU:CD2	2.54	0.90
7:AZ:906:MET:CE	8:A7:27:LYS:HD2	2.00	0.90
7:A3:1001:PHE:CE1	10:FT:19:LEU:CD2	2.56	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AY:906:MET:CE	8:A4:27:LYS:HD2	2.02	0.88
4:AH:97:PHE:CE2	7:A3:644:PRO:CG	2.57	0.87
4:AH:100:GLN:NE2	7:A3:647:ARG:HH11	1.72	0.87
1:AN:2:ALA:HB2	7:A3:634:THR:O	1.75	0.86
1:AQ:3:ILE:HD13	7:A1:636:GLU:H	1.40	0.86
7:A0:902:SER:HB3	8:A8:340:GLU:O	1.76	0.86
7:AZ:469:SER:HG	8:Af:62:GLY:C	1.82	0.85
7:AZ:906:MET:SD	8:A7:27:LYS:CE	2.65	0.84
8:Af:16:ARG:HD3	8:A6:67:TYR:CE1	2.12	0.84
7:AZ:906:MET:SD	8:A7:27:LYS:HE3	2.18	0.84
1:AO:205:LEU:CD2	1:AO:276:ILE:HG22	2.08	0.84
7:A0:906:MET:HE1	8:A8:27:LYS:HD3	1.59	0.84
7:AY:466:GLU:O	8:A9:11:ARG:NH2	2.11	0.83
7:A1:1001:PHE:CE1	10:Fu:19:LEU:CD2	2.61	0.83
1:AM:3:ILE:CD1	7:A2:635:PRO:HA	2.09	0.83
7:A1:765:ASN:OD1	8:A9:207:ILE:HD12	1.79	0.83
8:Af:60:GLU:HG3	8:Af:62:GLY:H	1.44	0.82
7:A2:906:MET:CE	8:A5:27:LYS:HD3	2.05	0.82
1:AP:2:ALA:N	7:A0:636:GLU:OE1	2.12	0.82
8:Ab:16:ARG:HD3	8:A8:67:TYR:CD1	2.15	0.82
7:AZ:1001:PHE:CE1	10:Fc:19:LEU:CD2	2.62	0.82
10:Ft:205:THR:HG22	10:Ft:206:SER:H	1.46	0.81
1:AR:153:ILE:HD12	1:AM:441:TRP:HD1	1.44	0.81
7:A2:1001:PHE:CE1	10:FK:19:LEU:CD2	2.62	0.81
10:Fb:205:THR:HG22	10:Fb:206:SER:H	1.46	0.81
10:FS:205:THR:HG22	10:FS:206:SER:H	1.45	0.81
7:A0:1002:ALA:H	10:Fk:19:LEU:HD23	1.44	0.81
10:FJ:205:THR:HG22	10:FJ:206:SER:H	1.46	0.81
7:AZ:469:SER:OG	8:Af:62:GLY:O	1.99	0.81
10:Fk:205:THR:HG22	10:Fk:206:SER:H	1.46	0.81
7:AZ:765:ASN:OD1	8:A7:207:ILE:HD12	1.80	0.80
4:AJ:97:PHE:CE2	7:A0:644:PRO:CG	2.65	0.80
10:FA:205:THR:HG22	10:FA:206:SER:H	1.46	0.80
7:AY:906:MET:HE1	8:A4:27:LYS:CD	2.11	0.80
7:A3:902:SER:HB3	8:A6:340:GLU:O	1.82	0.80
8:Af:317:ILE:HG23	8:A6:23:PHE:CG	2.18	0.79
7:A0:922:ASP:OD1	7:A0:922:ASP:O	2.00	0.79
1:AT:560:LYS:NZ	7:A3:805:ASP:OD1	2.16	0.79
4:AK:97:PHE:CE2	7:A1:644:PRO:CG	2.65	0.79
8:Ae:64:ALA:HB2	8:A5:14:ILE:HD11	1.65	0.79
7:AZ:484:LYS:NZ	8:A6:182:ASP:OD1	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ad:61:PRO:O	8:A4:11:ARG:HB3	1.83	0.78
7:A2:1028:VAL:CG2	8:A5:14:ILE:CG2	2.57	0.78
7:AY:1001:PHE:CZ	10:FB:19:LEU:HD23	2.16	0.78
1:AW:615:SER:HB2	7:AY:614:LYS:HE2	1.64	0.78
7:AY:484:LYS:NZ	8:A9:182:ASP:OD1	2.12	0.78
8:Ae:64:ALA:HB2	8:A5:14:ILE:CD1	2.14	0.78
8:Ab:320:GLU:HG3	8:A8:17:ALA:HB2	1.67	0.77
7:A2:922:ASP:OD1	7:A2:922:ASP:O	2.01	0.77
4:AH:100:GLN:HE21	7:A3:647:ARG:NH1	1.80	0.77
4:AI:100:GLN:OE1	7:AZ:645:ASP:OD2	2.03	0.77
7:AY:483:ASP:OD2	8:Ac:72:GLU:CD	2.28	0.76
7:AY:1001:PHE:CE1	10:FB:19:LEU:CD2	2.64	0.76
4:AJ:82:ASP:OD2	7:A0:684:TYR:OH	2.03	0.76
8:Ac:80:THR:HA	8:Ac:311:ARG:NH1	2.01	0.76
7:AZ:995:ASP:HB3	10:Fd:8:GLY:H	1.51	0.76
4:AL:97:PHE:CE2	7:AY:644:PRO:CG	2.68	0.76
7:A1:995:ASP:HB3	10:Fv:8:GLY:H	1.51	0.76
8:Ab:80:THR:HA	8:Ab:311:ARG:NH1	2.01	0.76
4:AL:100:GLN:OE1	7:AY:645:ASP:OD2	2.03	0.76
7:AZ:515:PHE:HD1	7:AZ:526:TRP:HB2	1.51	0.76
1:AR:2:ALA:N	7:AY:636:GLU:OE1	2.19	0.76
5:BB:1:MET:HE2	15:BE:271:ASN:HB3	1.67	0.76
7:A0:515:PHE:HD1	7:A0:526:TRP:HB2	1.51	0.76
7:A3:765:ASN:OD1	8:A6:207:ILE:CD1	2.34	0.76
8:Ad:80:THR:HA	8:Ad:311:ARG:NH1	2.01	0.75
7:A2:995:ASP:HB3	10:FL:8:GLY:H	1.51	0.75
1:AN:153:ILE:HD12	1:AO:441:TRP:HD1	1.49	0.75
7:AY:483:ASP:OD1	8:Ac:72:GLU:CG	2.25	0.75
7:AZ:483:ASP:OD2	8:A6:139:ARG:NH2	2.19	0.75
7:A3:484:LYS:NZ	8:A5:182:ASP:OD1	2.15	0.75
4:AG:97:PHE:CE2	7:A2:644:PRO:CG	2.68	0.75
7:A1:922:ASP:OD1	7:A1:922:ASP:O	2.03	0.75
8:Aa:80:THR:HA	8:Aa:311:ARG:NH1	2.01	0.75
7:A3:515:PHE:HD1	7:A3:526:TRP:HB2	1.51	0.75
7:A0:995:ASP:HB3	10:Fm:8:GLY:H	1.49	0.75
7:A1:515:PHE:HD1	7:A1:526:TRP:HB2	1.51	0.75
7:A2:765:ASN:OD1	8:A5:207:ILE:HD12	1.86	0.75
8:Ae:80:THR:HA	8:Ae:311:ARG:NH1	2.01	0.75
8:Af:80:THR:HA	8:Af:311:ARG:NH1	2.01	0.75
8:Aa:16:ARG:CD	8:A7:67:TYR:CE1	2.68	0.74
7:A0:922:ASP:OD1	10:Fk:12:ASP:HA	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AI:97:PHE:CE2	7:AZ:644:PRO:CG	2.70	0.74
7:A3:922:ASP:OD1	10:FS:11:VAL:O	2.05	0.74
7:A2:515:PHE:HD1	7:A2:526:TRP:HB2	1.51	0.74
1:AO:3:ILE:HG21	7:AZ:636:GLU:O	1.88	0.74
7:AY:515:PHE:HD1	7:AY:526:TRP:HB2	1.51	0.74
7:A2:906:MET:SD	8:A5:27:LYS:CD	2.76	0.74
7:A3:924:GLY:N	10:FS:12:ASP:OD1	2.16	0.74
7:A0:765:ASN:OD1	8:A8:207:ILE:HD12	1.88	0.74
8:Ad:70:ASP:OD1	8:A4:20:THR:OG1	2.05	0.73
1:AR:2:ALA:HA	7:AY:634:THR:O	1.87	0.73
7:A3:765:ASN:OD1	8:A6:207:ILE:HD12	1.88	0.73
7:AZ:512:GLU:HA	7:AZ:515:PHE:CE2	2.24	0.73
7:A1:512:GLU:HA	7:A1:515:PHE:CE2	2.24	0.73
7:AY:512:GLU:HA	7:AY:515:PHE:CE2	2.24	0.73
8:Ab:317:ILE:HG23	8:A8:23:PHE:CG	2.24	0.73
7:A0:1001:PHE:CZ	10:Fl:19:LEU:HD22	2.23	0.72
4:AH:82:ASP:OD2	7:A3:684:TYR:OH	2.06	0.72
4:AJ:100:GLN:NE2	7:A0:645:ASP:OD2	2.21	0.72
7:A3:512:GLU:HA	7:A3:515:PHE:CE2	2.24	0.72
13:BY:118:ARG:NH1	13:B8:62:GLY:O	2.21	0.72
7:A0:512:GLU:HA	7:A0:515:PHE:CE2	2.24	0.72
13:B2:118:ARG:NH1	13:B7:62:GLY:O	2.23	0.72
7:A1:906:MET:SD	8:A9:27:LYS:NZ	2.61	0.72
8:Af:16:ARG:HD3	8:A6:67:TYR:CD1	2.25	0.72
8:Ae:317:ILE:HG23	8:A5:23:PHE:CG	2.24	0.71
1:AU:615:SER:HB2	7:A0:614:LYS:HE2	1.71	0.71
7:A2:515:PHE:CZ	7:A2:536:ILE:HD11	2.25	0.71
7:A0:515:PHE:CZ	7:A0:536:ILE:HD11	2.25	0.71
7:A3:515:PHE:CZ	7:A3:536:ILE:HD11	2.25	0.71
7:AY:515:PHE:CZ	7:AY:536:ILE:HD11	2.25	0.71
7:A2:512:GLU:HA	7:A2:515:PHE:CE2	2.24	0.71
7:A1:515:PHE:CZ	7:A1:536:ILE:HD11	2.25	0.71
7:A2:485:HIS:CD2	8:A4:244:ASN:ND2	2.58	0.71
7:A1:922:ASP:OD1	10:Ft:12:ASP:HA	1.91	0.70
7:AY:658:TYR:OH	14:AF:38:GLY:HA3	1.91	0.70
1:AQ:3:ILE:CD1	7:A1:635:PRO:HA	2.19	0.70
7:AZ:515:PHE:CZ	7:AZ:536:ILE:HD11	2.25	0.70
7:A0:1027:GLN:HE21	8:Ab:322:ARG:HH12	1.39	0.70
7:A2:995:ASP:OD1	7:A2:995:ASP:O	2.10	0.70
7:A3:995:ASP:OD1	7:A3:995:ASP:O	2.10	0.70
8:Af:70:ASP:OD1	8:A6:20:THR:OG1	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AZ:995:ASP:OD1	7:AZ:995:ASP:O	2.10	0.70
1:AX:560:LYS:NZ	7:AY:805:ASP:OD1	2.25	0.70
7:A0:185:VAL:O	10:Fk:562:GLN:NE2	2.24	0.70
8:Ae:16:ARG:CD	8:A5:67:TYR:CE1	2.74	0.70
1:AN:2:ALA:HB2	7:A3:635:PRO:HA	1.73	0.70
4:AG:100:GLN:OE1	7:A2:645:ASP:OD2	2.10	0.69
8:Ac:16:ARG:CD	8:A9:67:TYR:CE1	2.71	0.69
7:A3:922:ASP:OD1	10:FS:12:ASP:HA	1.93	0.69
7:A3:1002:ALA:H	10:FS:19:LEU:HD23	1.57	0.69
4:AH:100:GLN:OE1	7:A3:645:ASP:OD1	2.09	0.69
7:A3:1001:PHE:CZ	10:FT:19:LEU:HD22	2.27	0.69
1:AQ:3:ILE:HD13	7:A1:636:GLU:N	2.07	0.69
13:B1:118:ARG:NH1	13:B5:62:GLY:O	2.26	0.69
7:AY:995:ASP:OD1	7:AY:995:ASP:O	2.10	0.69
4:AK:100:GLN:OE1	7:A1:645:ASP:OD2	2.11	0.69
7:AY:176:ILE:HD12	8:A9:234:ASN:HA	1.75	0.69
7:AY:478:ILE:HG21	8:A9:161:ILE:HD11	1.75	0.69
7:A0:940:ASP:O	10:Fl:21:LYS:HE2	1.93	0.69
8:Ad:317:ILE:HG23	8:A4:23:PHE:CD2	2.26	0.69
7:A0:1003:ASN:OD1	10:Fk:18:TYR:HB3	1.91	0.69
8:Aa:317:ILE:HG23	8:A7:23:PHE:CG	2.28	0.69
7:A0:995:ASP:OD1	7:A0:995:ASP:O	2.10	0.69
7:A3:427:ARG:HH22	7:A3:489:MET:HE1	1.58	0.69
8:Ab:315:GLU:OE2	8:A8:244:ASN:ND2	2.23	0.69
4:AI:105:VAL:HG23	7:AZ:640:GLY:O	1.93	0.69
7:A2:1028:VAL:HG23	8:A5:14:ILE:CG2	2.18	0.69
7:A0:1001:PHE:HA	10:Fk:19:LEU:CD2	2.23	0.69
8:Ac:263:VAL:HG21	10:Ft:14:GLY:O	1.93	0.69
7:AZ:427:ARG:HH22	7:AZ:489:MET:HE1	1.58	0.68
7:A3:924:GLY:H	10:FS:12:ASP:CG	2.01	0.68
8:Ad:16:ARG:HD3	8:A4:67:TYR:CD1	2.28	0.68
12:FR:373:ARG:HD3	12:FR:388:THR:HB	1.75	0.68
12:Fa:373:ARG:HD3	12:Fa:388:THR:HB	1.75	0.68
7:A2:1002:ALA:H	10:FJ:19:LEU:HD23	1.58	0.68
7:AZ:1002:ALA:H	10:Fb:19:LEU:HD23	1.58	0.68
7:A0:765:ASN:OD1	8:A8:207:ILE:HD13	1.90	0.68
7:A1:995:ASP:OD1	7:A1:995:ASP:O	2.10	0.68
7:AY:902:SER:HB3	8:A4:340:GLU:O	1.93	0.68
12:Fj:373:ARG:HD3	12:Fj:388:THR:HB	1.75	0.68
7:A3:922:ASP:OD1	10:FS:11:VAL:C	2.37	0.68
7:A3:995:ASP:HB3	10:FU:8:GLY:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:427:ARG:HH22	7:A2:489:MET:HE1	1.58	0.68
8:Ab:341:PHE:CE2	8:A8:27:LYS:HD2	2.27	0.68
8:Af:317:ILE:HG23	8:A6:23:PHE:CD2	2.29	0.68
1:AO:3:ILE:CD1	7:AZ:635:PRO:HA	2.22	0.68
1:AR:2:ALA:HB3	7:AY:636:GLU:HB2	1.72	0.68
7:A3:1027:GLN:HE21	8:Af:322:ARG:HH12	1.40	0.68
8:Aa:263:VAL:HG21	10:Fb:14:GLY:O	1.94	0.68
12:F5:373:ARG:HD3	12:F5:388:THR:HB	1.75	0.68
1:AR:2:ALA:HB2	7:AY:636:GLU:CG	2.24	0.67
7:A1:1002:ALA:H	10:Ft:19:LEU:HD23	1.57	0.67
8:Af:55:SER:HB3	8:Af:63:PHE:CE1	2.30	0.67
7:AY:995:ASP:HB3	10:FC:8:GLY:H	1.58	0.67
12:FI:373:ARG:HD3	12:FI:388:THR:HB	1.75	0.67
7:A3:658:TYR:OH	14:AC:38:GLY:HA3	1.94	0.67
7:AY:427:ARG:HH22	7:AY:489:MET:HE1	1.58	0.67
8:Ad:263:VAL:HG21	10:FA:14:GLY:O	1.94	0.67
7:AY:1000:THR:OG1	10:FB:12:ASP:OD1	2.07	0.67
7:A1:427:ARG:HH22	7:A1:489:MET:HE1	1.58	0.67
7:AY:483:ASP:CG	8:Ac:72:GLU:CG	2.66	0.67
7:A0:427:ARG:HH22	7:A0:489:MET:HE1	1.58	0.67
7:A0:924:GLY:H	10:Fk:12:ASP:CG	2.02	0.67
7:A0:1002:ALA:O	10:Fk:19:LEU:HB3	1.95	0.67
12:F2:373:ARG:HD3	12:F2:388:THR:HB	1.75	0.67
1:AS:236:VAL:HG21	7:A2:692:LYS:CG	2.24	0.67
10:Fv:198:ASN:ND2	12:FH:8:HIS:NE2	2.42	0.67
7:AZ:1027:GLN:HE21	8:Aa:322:ARG:HH12	1.42	0.67
7:A0:658:TYR:OH	14:AD:38:GLY:HA3	1.95	0.66
8:Af:58:GLU:HA	8:Af:63:PHE:CG	2.29	0.66
7:A0:176:ILE:HD12	8:A7:234:ASN:HA	1.76	0.66
7:A1:1001:PHE:CZ	10:Fu:19:LEU:HD22	2.30	0.66
8:Ab:61:PRO:C	8:A8:11:ARG:HB3	2.19	0.66
7:A1:765:ASN:OD1	8:A9:207:ILE:CD1	2.42	0.66
7:A1:1027:GLN:HE21	8:Ac:322:ARG:HH12	1.43	0.66
8:Ad:317:ILE:HG23	8:A4:23:PHE:CG	2.30	0.66
1:AM:3:ILE:HG21	7:A2:636:GLU:O	1.95	0.66
7:AY:920:LYS:NZ	10:FA:18:TYR:CE1	2.63	0.66
7:A3:1000:THR:OG1	10:FT:12:ASP:OD1	2.09	0.66
7:AY:1001:PHE:CZ	10:FB:19:LEU:HD22	2.29	0.66
15:BF:375:LYS:H	15:BF:375:LYS:HD3	1.59	0.66
7:A3:906:MET:SD	8:A6:27:LYS:HD3	2.36	0.66
8:Ac:317:ILE:HG23	8:A9:23:PHE:CG	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Ft:398:MET:HE2	10:Ft:403:ILE:HG22	1.78	0.66
1:AV:330:ARG:HG2	1:AV:330:ARG:HH21	1.61	0.65
4:AK:105:VAL:HG23	7:A1:640:GLY:O	1.95	0.65
7:AZ:1001:PHE:CZ	10:Fc:19:LEU:HD22	2.31	0.65
7:A1:906:MET:CE	8:A9:27:LYS:HD3	2.15	0.65
8:Ae:263:VAL:HG21	10:FJ:14:GLY:O	1.95	0.65
8:Af:61:PRO:O	8:A6:11:ARG:HG3	1.95	0.65
7:A1:657:SER:OG	14:AE:42:THR:HA	1.97	0.65
10:FA:398:MET:HE2	10:FA:403:ILE:HG22	1.78	0.65
1:AS:236:VAL:HG21	7:A2:692:LYS:HG3	1.79	0.65
10:FJ:398:MET:HE2	10:FJ:403:ILE:HG22	1.79	0.65
10:Fk:398:MET:HE2	10:Fk:403:ILE:HG22	1.79	0.65
7:A2:940:ASP:O	10:FK:21:LYS:HE2	1.97	0.65
7:A0:1001:PHE:HA	10:Fk:19:LEU:HD21	1.79	0.65
7:AZ:940:ASP:O	10:Fc:21:LYS:HE2	1.98	0.64
7:AY:922:ASP:CG	7:AY:922:ASP:O	2.40	0.64
10:Fb:398:MET:HE2	10:Fb:403:ILE:HG22	1.79	0.64
7:AY:920:LYS:O	10:FC:19:LEU:CD2	2.39	0.64
10:FS:398:MET:HE2	10:FS:403:ILE:HG22	1.79	0.64
7:A3:185:VAL:O	10:FS:562:GLN:NE2	2.30	0.64
7:A2:1001:PHE:CZ	10:FK:19:LEU:HD22	2.31	0.64
7:A1:940:ASP:O	10:Fu:21:LYS:HE2	1.98	0.64
7:A2:484:LYS:NZ	8:A4:182:ASP:OD1	2.24	0.63
7:A2:1027:GLN:HE21	8:Ae:322:ARG:HH12	1.45	0.63
7:A2:185:VAL:O	10:FJ:562:GLN:NE2	2.30	0.63
7:A2:765:ASN:OD1	8:A5:207:ILE:CD1	2.45	0.63
4:AL:82:ASP:OD2	7:AY:684:TYR:OH	2.15	0.63
7:A3:906:MET:SD	8:A6:27:LYS:NZ	2.71	0.63
7:AZ:185:VAL:O	10:Fb:562:GLN:NE2	2.32	0.63
7:AZ:512:GLU:HA	7:AZ:515:PHE:CD2	2.34	0.62
7:A0:906:MET:CE	8:A8:27:LYS:HD3	2.28	0.62
7:A3:940:ASP:O	10:FT:21:LYS:HE2	1.99	0.62
4:AJ:100:GLN:OE1	7:A0:645:ASP:OD2	2.17	0.62
7:A1:512:GLU:HA	7:A1:515:PHE:CD2	2.35	0.62
7:A1:185:VAL:O	10:Ft:562:GLN:NE2	2.32	0.62
7:A3:512:GLU:HA	7:A3:515:PHE:CD2	2.35	0.62
7:A3:922:ASP:OD1	10:FS:12:ASP:CA	2.46	0.62
7:AY:512:GLU:HA	7:AY:515:PHE:CD2	2.35	0.62
7:A0:924:GLY:N	10:Fk:12:ASP:OD1	2.23	0.62
7:A1:902:SER:HB3	8:A9:340:GLU:O	1.99	0.62
8:Ad:61:PRO:C	8:A4:11:ARG:HB3	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Ae:64:ALA:CB	8:A5:14:ILE:HD11	2.29	0.62
4:AJ:100:GLN:NE2	7:A0:647:ARG:NH1	2.48	0.62
4:AK:97:PHE:CE2	7:A1:644:PRO:CB	2.82	0.62
4:AH:100:GLN:NE2	7:A3:645:ASP:OD1	2.33	0.61
10:Fd:195:ARG:HD3	12:Fs:9:TYR:CE1	2.35	0.61
7:AZ:469:SER:HB3	8:Af:62:GLY:HA3	1.79	0.61
7:A0:512:GLU:HA	7:A0:515:PHE:CD2	2.35	0.61
4:AJ:100:GLN:CD	7:A0:645:ASP:OD2	2.43	0.61
7:AZ:922:ASP:O	7:AZ:922:ASP:CG	2.43	0.61
10:FA:205:THR:HG22	10:FA:206:SER:N	2.15	0.61
1:AP:16:ASN:ND2	7:A0:706:TRP:CE3	2.68	0.61
7:A3:1001:PHE:HA	10:FS:19:LEU:CD2	2.29	0.61
8:Af:58:GLU:HA	8:Af:63:PHE:CD1	2.34	0.61
4:AG:105:VAL:HG23	7:A2:640:GLY:O	2.01	0.61
7:AZ:906:MET:CE	8:A7:27:LYS:HD3	2.16	0.61
7:A1:924:GLY:N	10:Ft:12:ASP:OD1	2.25	0.61
4:AG:97:PHE:CE2	7:A2:644:PRO:CB	2.84	0.61
10:FJ:205:THR:HG22	10:FJ:206:SER:N	2.15	0.61
7:A2:512:GLU:HA	7:A2:515:PHE:CD2	2.35	0.60
7:AZ:765:ASN:OD1	8:A7:207:ILE:CD1	2.48	0.60
8:Ab:263:VAL:HG21	10:Fk:14:GLY:O	2.02	0.60
7:A0:280:LYS:HB2	9:LM:25:TYR:CD2	2.35	0.60
10:FL:198:ASN:ND2	12:FZ:8:HIS:NE2	2.48	0.60
7:A0:995:ASP:CB	10:Fm:8:GLY:H	2.15	0.60
10:FB:557:VAL:HG12	10:FC:574:LYS:HG2	1.84	0.60
7:AZ:924:GLY:N	10:Fb:12:ASP:OD1	2.25	0.60
7:A0:922:ASP:OD1	10:Fk:12:ASP:CA	2.49	0.60
7:A3:906:MET:HE1	8:A6:27:LYS:HD3	1.84	0.60
8:Ae:317:ILE:C	8:A5:20:THR:CG2	2.74	0.60
10:Fl:557:VAL:HG12	10:Fm:574:LYS:HG2	1.84	0.60
7:A2:657:SER:OG	14:AB:42:THR:HA	2.02	0.60
10:FS:205:THR:HG22	10:FS:206:SER:N	2.15	0.60
2:BL:200:ARG:NH1	3:BT:196:GLU:OE1	2.34	0.59
1:AP:370:THR:HB	7:A0:886:VAL:O	2.02	0.59
7:AY:898:MET:HE3	8:A4:320:GLU:OE1	2.02	0.59
7:A2:488:MET:HE3	7:A2:511:ALA:HA	1.84	0.59
7:AZ:1000:THR:OG1	10:Fc:12:ASP:OD1	2.15	0.59
7:A3:488:MET:HE3	7:A3:511:ALA:HA	1.84	0.59
4:AI:97:PHE:CE2	7:AZ:644:PRO:CB	2.84	0.59
7:AZ:174:HIS:ND1	8:A6:236:LEU:HD11	2.17	0.59
8:Af:315:GLU:OE2	8:A6:244:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Ft:192:ASN:OD1	10:Fv:165:LYS:NZ	2.35	0.59
7:A1:921:TRP:O	7:A1:922:ASP:HB3	2.02	0.59
10:FT:557:VAL:HG12	10:FU:574:LYS:HG2	1.84	0.59
7:A1:488:MET:HE3	7:A1:511:ALA:HA	1.84	0.59
10:Fc:557:VAL:HG12	10:Fd:574:LYS:HG2	1.84	0.59
15:BE:375:LYS:HD3	15:BE:375:LYS:H	1.66	0.59
1:AV:220:MET:SD	7:A0:727:PHE:CE2	2.96	0.59
10:Fb:205:THR:HG22	10:Fb:206:SER:N	2.15	0.59
12:FQ:373:ARG:HD2	12:FQ:386:GLU:HG2	1.84	0.59
7:A0:898:MET:HE3	8:A8:320:GLU:OE1	2.03	0.59
10:FK:557:VAL:HG12	10:FL:574:LYS:HG2	1.84	0.59
7:A2:921:TRP:O	7:A2:922:ASP:HB3	2.02	0.59
7:A3:921:TRP:O	7:A3:922:ASP:HB3	2.02	0.59
12:FZ:373:ARG:HD2	12:FZ:386:GLU:HG2	1.84	0.59
7:A2:922:ASP:OD2	10:FJ:10:SER:O	2.20	0.58
7:A1:789:THR:HG21	7:A1:821:PHE:CD1	2.38	0.58
12:F1:373:ARG:HD2	12:F1:386:GLU:HG2	1.85	0.58
4:AH:100:GLN:HE22	7:A3:647:ARG:HH11	1.49	0.58
7:AZ:789:THR:HG21	7:AZ:821:PHE:CD1	2.38	0.58
10:Fk:205:THR:HG22	10:Fk:206:SER:N	2.15	0.58
12:FH:373:ARG:HD2	12:FH:386:GLU:HG2	1.84	0.58
7:A2:1000:THR:OG1	10:FK:12:ASP:OD1	2.15	0.58
7:A0:789:THR:HG21	7:A0:821:PHE:CD1	2.38	0.58
1:AM:3:ILE:HD13	7:A2:635:PRO:HA	1.85	0.58
7:AY:765:ASN:OD1	8:A4:207:ILE:CD1	2.51	0.58
7:AZ:488:MET:HE3	7:AZ:511:ALA:HA	1.84	0.58
7:A0:921:TRP:O	7:A0:922:ASP:HB3	2.02	0.58
7:A1:614:LYS:HB3	7:A1:615:PRO:HD3	1.85	0.58
4:AJ:104:ASP:OD2	7:A0:642:ARG:HD3	2.02	0.58
7:AY:614:LYS:HB3	7:AY:615:PRO:HD3	1.85	0.58
7:A2:922:ASP:O	7:A2:922:ASP:CG	2.47	0.58
7:A2:1028:VAL:HG22	8:A5:14:ILE:CG2	2.30	0.58
7:A3:1003:ASN:OD1	10:FS:18:TYR:HB3	2.02	0.58
8:A7:19:ILE:O	8:A7:19:ILE:HG23	2.02	0.58
10:Fu:557:VAL:HG12	10:Fv:574:LYS:HG2	1.84	0.58
7:AY:488:MET:HE3	7:AY:511:ALA:HA	1.84	0.58
7:A2:485:HIS:HD2	8:A4:244:ASN:ND2	2.01	0.58
7:A2:789:THR:HG21	7:A2:821:PHE:CD1	2.38	0.58
7:A2:924:GLY:H	10:FJ:12:ASP:CG	2.09	0.58
7:AZ:906:MET:SD	8:A7:27:LYS:CD	2.91	0.58
8:Ae:64:ALA:CA	8:A5:14:ILE:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A0:488:MET:HE3	7:A0:511:ALA:HA	1.84	0.58
7:A0:614:LYS:HB3	7:A0:615:PRO:HD3	1.85	0.58
7:A3:789:THR:HG21	7:A3:821:PHE:CD1	2.38	0.58
1:AW:342:GLN:HE22	1:AQ:344:ARG:NE	2.01	0.58
7:AY:789:THR:HG21	7:AY:821:PHE:CD1	2.38	0.58
4:AH:100:GLN:HE22	7:A3:645:ASP:CG	2.11	0.58
7:A1:924:GLY:H	10:Ft:12:ASP:CG	2.10	0.58
8:Ae:317:ILE:C	8:A5:20:THR:HG22	2.28	0.58
12:Fi:373:ARG:HD2	12:Fi:386:GLU:HG2	1.84	0.58
1:AT:220:MET:SD	7:A3:727:PHE:CE2	2.97	0.58
7:AZ:921:TRP:O	7:AZ:922:ASP:HB3	2.03	0.58
7:A3:614:LYS:HB3	7:A3:615:PRO:HD3	1.85	0.58
8:Ae:92:MET:HA	8:Ae:92:MET:HE2	1.86	0.58
1:AX:330:ARG:HG2	1:AX:330:ARG:HH21	1.69	0.57
5:BC:200:VAL:HG22	5:BC:201:GLY:N	2.19	0.57
5:BD:200:VAL:HG22	5:BD:201:GLY:N	2.19	0.57
8:Ac:320:GLU:HG3	8:A9:17:ALA:HB2	1.86	0.57
8:Ab:16:ARG:HD3	8:A8:67:TYR:HE1	1.66	0.57
8:Af:320:GLU:HG3	8:A6:17:ALA:HB2	1.85	0.57
12:Fr:373:ARG:HD2	12:Fr:386:GLU:HG2	1.84	0.57
7:AZ:614:LYS:HB3	7:AZ:615:PRO:HD3	1.85	0.57
7:AY:921:TRP:O	7:AY:922:ASP:HB3	2.04	0.57
7:A0:466:GLU:O	8:A7:11:ARG:NH2	2.37	0.57
8:Aa:92:MET:HA	8:Aa:92:MET:HE2	1.86	0.57
10:Fb:192:ASN:OD1	10:Fd:165:LYS:NZ	2.35	0.57
7:A2:614:LYS:HB3	7:A2:615:PRO:HD3	1.85	0.57
8:Ad:62:GLY:C	8:A4:14:ILE:HD12	2.30	0.57
8:Ad:92:MET:HE2	8:Ad:92:MET:HA	1.86	0.57
8:Ab:92:MET:HA	8:Ab:92:MET:HE2	1.86	0.57
4:AH:97:PHE:CE2	7:A3:644:PRO:CB	2.86	0.57
7:A2:1003:ASN:OD1	10:FJ:18:TYR:HB3	2.04	0.57
8:Ac:92:MET:HE2	8:Ac:92:MET:HA	1.87	0.57
8:Af:92:MET:HA	8:Af:92:MET:HE2	1.86	0.57
10:FJ:196:ARG:HH11	12:FY:4:ASN:HB3	1.68	0.57
10:Fv:195:ARG:HD3	12:FI:9:TYR:CE1	2.40	0.57
1:AO:205:LEU:HD22	1:AO:276:ILE:HG22	1.85	0.57
7:AY:893:ILE:HG22	8:A4:332:THR:O	2.03	0.57
7:A2:902:SER:HB3	8:A5:340:GLU:O	2.05	0.57
8:Ae:64:ALA:CB	8:A5:14:ILE:CD1	2.83	0.57
7:AZ:1027:GLN:NE2	8:Aa:322:ARG:HH12	2.03	0.57
10:FS:192:ASN:OD1	10:FU:165:LYS:NZ	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AU:25:ALA:HB1	4:AI:3:PHE:HB2	1.86	0.57
7:A2:478:ILE:HG21	8:A4:161:ILE:HD11	1.87	0.57
7:A2:658:TYR:OH	14:AB:38:GLY:HA3	2.05	0.57
7:AZ:924:GLY:H	10:Fb:12:ASP:CG	2.10	0.57
7:A0:1027:GLN:NE2	8:Ab:322:ARG:HH12	2.01	0.57
7:A1:906:MET:SD	8:A9:27:LYS:CD	2.88	0.57
7:AZ:657:SER:OG	14:AA:42:THR:HA	2.04	0.57
7:AZ:1002:ALA:O	10:Fb:19:LEU:HB3	2.05	0.57
1:AN:2:ALA:CB	7:A3:635:PRO:HA	2.35	0.56
10:Ft:205:THR:HG22	10:Ft:206:SER:N	2.15	0.56
1:AS:25:ALA:HB1	4:AG:3:PHE:HB2	1.87	0.56
7:AZ:658:TYR:OH	14:AA:38:GLY:HA3	2.05	0.56
7:A1:1027:GLN:NE2	8:Ac:322:ARG:HH12	2.03	0.56
7:A3:176:ILE:HD12	8:A5:234:ASN:HA	1.86	0.56
10:FJ:192:ASN:OD1	10:FL:165:LYS:NZ	2.35	0.56
10:Fk:192:ASN:OD1	10:Fm:165:LYS:NZ	2.35	0.56
7:AZ:995:ASP:CB	10:Fd:8:GLY:H	2.19	0.56
7:A0:1001:PHE:CD1	10:Fl:19:LEU:HD23	2.39	0.56
7:A1:1003:ASN:OD1	10:Ft:18:TYR:HB3	2.05	0.56
10:Ft:196:ARG:HH11	12:FG:4:ASN:HB3	1.70	0.56
3:BT:124:MET:HE2	3:BT:124:MET:HA	1.87	0.56
7:AZ:176:ILE:HD12	8:A6:234:ASN:HA	1.87	0.56
7:A1:658:TYR:OH	14:AE:38:GLY:HA3	2.06	0.56
10:FA:192:ASN:OD1	10:FC:165:LYS:NZ	2.35	0.56
7:A0:1001:PHE:CD2	10:Fk:19:LEU:HD11	2.41	0.56
7:A2:1001:PHE:HA	10:FJ:19:LEU:CD2	2.35	0.56
7:AZ:1001:PHE:HA	10:Fb:19:LEU:CD2	2.36	0.56
7:AY:477:PRO:HA	8:A9:162:LYS:HG2	1.87	0.56
7:A0:1000:THR:OG1	10:Fl:12:ASP:OD1	2.14	0.56
7:A1:1002:ALA:O	10:Ft:19:LEU:HB3	2.06	0.56
7:A3:1027:GLN:NE2	8:Af:322:ARG:HH12	2.02	0.56
8:Ac:261:ASP:OD2	10:Ft:18:TYR:OH	2.20	0.56
8:Ad:20:THR:HG22	8:A4:317:ILE:O	2.06	0.56
8:Aa:261:ASP:OD2	10:Fb:18:TYR:OH	2.21	0.56
1:AN:153:ILE:HD12	1:AO:441:TRP:CD1	2.38	0.55
7:A2:924:GLY:N	10:FJ:12:ASP:OD1	2.24	0.55
7:A2:995:ASP:CB	10:FL:8:GLY:H	2.18	0.55
7:A1:1001:PHE:HA	10:Ft:19:LEU:CD2	2.36	0.55
7:A2:1002:ALA:O	10:FJ:19:LEU:HB3	2.05	0.55
7:AZ:1003:ASN:OD1	10:Fb:18:TYR:HB3	2.05	0.55
1:AW:25:ALA:HB1	4:AK:3:PHE:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:61:LEU:HD13	7:AY:672:TYR:CD1	2.41	0.55
8:Ad:261:ASP:OD2	10:FA:18:TYR:OH	2.22	0.55
7:A1:995:ASP:CB	10:Fv:8:GLY:H	2.19	0.55
7:A1:1000:THR:OG1	10:Fu:12:ASP:OD1	2.15	0.55
1:AS:615:SER:HB2	7:A3:614:LYS:HE2	1.88	0.55
4:AL:100:GLN:CD	7:AY:645:ASP:OD2	2.48	0.55
7:AZ:902:SER:HB3	8:A7:340:GLU:O	2.07	0.55
8:Af:263:VAL:HG21	10:FS:14:GLY:O	2.06	0.55
1:AQ:3:ILE:HG21	7:A1:636:GLU:O	2.07	0.55
5:BB:200:VAL:HG22	5:BB:201:GLY:N	2.21	0.55
15:BE:153:ALA:HB1	15:BE:184:ILE:HD11	1.89	0.55
15:BF:153:ALA:HB1	15:BF:184:ILE:HD11	1.88	0.55
4:AJ:97:PHE:CE2	7:A0:644:PRO:CB	2.90	0.55
7:AY:1002:ALA:H	10:FA:19:LEU:HD23	1.71	0.55
8:Af:20:THR:OG1	8:A6:70:ASP:OD1	2.20	0.54
12:F2:402:SER:HB3	12:F1:396:GLY:HA3	1.90	0.54
1:AV:220:MET:SD	7:A0:727:PHE:HE2	2.30	0.54
8:Ad:61:PRO:O	8:A4:12:SER:O	2.25	0.54
9:LH:4:ASP:O	9:LI:58:LYS:NZ	2.29	0.54
10:Fk:205:THR:CG2	10:Fk:206:SER:H	2.19	0.54
12:Fi:402:SER:HB3	12:FH:396:GLY:HA3	1.90	0.54
12:Fj:402:SER:HB3	12:Fi:396:GLY:HA3	1.90	0.54
12:Fa:402:SER:HB3	12:FZ:396:GLY:HA3	1.90	0.54
1:AV:46:ASP:OD2	14:AD:87:ARG:NH2	2.38	0.54
7:AZ:483:ASP:OD1	8:A6:248:ARG:NH2	2.38	0.54
8:Aa:70:ASP:OD1	8:A7:20:THR:OG1	2.18	0.54
10:Fd:198:ASN:ND2	12:Fr:8:HIS:NE2	2.44	0.54
1:AR:16:ASN:OD1	7:AY:711:LYS:CE	2.56	0.54
7:A3:1002:ALA:O	10:FS:19:LEU:HB3	2.07	0.54
10:FJ:205:THR:CG2	10:FJ:206:SER:H	2.19	0.54
12:FP:372:PHE:CD1	12:FP:434:ILE:HD11	2.43	0.54
1:AX:374:LYS:HE3	7:AY:857:ARG:O	2.07	0.54
7:AZ:1014:ASP:OD2	8:A7:15:TYR:OH	2.19	0.54
12:Fz:402:SER:HB3	12:Fr:396:GLY:HA3	1.90	0.54
12:Fz:372:PHE:CD1	12:Fz:434:ILE:HD11	2.43	0.54
1:AT:220:MET:SD	7:A3:727:PHE:HE2	2.30	0.54
4:AH:100:GLN:CD	7:A3:645:ASP:OD1	2.51	0.54
10:Ft:205:THR:CG2	10:Ft:206:SER:H	2.19	0.54
12:FG:372:PHE:CD1	12:FG:434:ILE:HD11	2.43	0.54
12:Fq:372:PHE:CD1	12:Fq:434:ILE:HD11	2.43	0.54
7:A0:994:PHE:O	10:Fm:16:GLY:HA3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:483:ASP:OD1	8:A8:248:ARG:NH2	2.36	0.54
7:A3:1001:PHE:HA	10:FS:19:LEU:HD21	1.88	0.54
10:FA:205:THR:CG2	10:FA:206:SER:H	2.19	0.54
7:A1:920:LYS:O	10:Fv:19:LEU:CD2	2.46	0.54
8:A5:19:ILE:HG23	8:A5:19:ILE:O	2.08	0.54
12:Fh:372:PHE:CD1	12:Fh:434:ILE:HD11	2.43	0.54
1:AN:370:THR:HB	7:A3:886:VAL:O	2.07	0.54
7:AY:921:TRP:CE3	10:FC:19:LEU:HD11	2.43	0.54
7:AY:1027:GLN:HE21	8:Ad:322:ARG:HH12	1.56	0.53
12:FR:402:SER:HB3	12:FQ:396:GLY:HA3	1.90	0.53
7:A2:1027:GLN:NE2	8:Ae:322:ARG:HH12	2.06	0.53
2:BM:315:ASN:HD21	3:BS:189:ARG:CZ	2.22	0.53
7:AY:921:TRP:CE3	10:FC:19:LEU:CD1	2.91	0.53
7:A1:922:ASP:OD1	10:Ft:12:ASP:CA	2.56	0.53
8:Ad:317:ILE:CG2	8:A4:23:PHE:CD2	2.91	0.53
1:AP:2:ALA:HA	7:A0:634:THR:O	2.08	0.53
12:FY:372:PHE:CD1	12:FY:434:ILE:HD11	2.43	0.53
7:A2:920:LYS:O	10:FL:19:LEU:CD2	2.47	0.53
7:AZ:922:ASP:OD1	10:Fb:14:GLY:N	2.41	0.53
1:AS:374:LYS:HE3	7:A2:857:ARG:O	2.09	0.53
9:LN:4:ASP:O	9:LO:58:LYS:NZ	2.29	0.53
1:AT:46:ASP:OD2	14:AC:87:ARG:NH2	2.38	0.53
2:BP:349:ILE:HD12	14:AD:75:ARG:HG2	1.90	0.53
4:AK:82:ASP:OD2	7:A1:684:TYR:OH	2.23	0.53
7:AZ:906:MET:SD	8:A7:27:LYS:NZ	2.82	0.53
7:A3:1027:GLN:HE21	8:Af:322:ARG:NH1	2.06	0.53
8:Ae:261:ASP:OD2	10:FJ:18:TYR:OH	2.23	0.53
12:FQ:373:ARG:NE	12:FQ:386:GLU:OE2	2.43	0.53
7:A0:1027:GLN:HE21	8:Ab:322:ARG:NH1	2.05	0.52
1:AO:205:LEU:HD23	1:AO:276:ILE:HG22	1.90	0.52
8:Ad:16:ARG:HD3	8:A4:67:TYR:HE1	1.70	0.52
12:FH:373:ARG:NE	12:FH:386:GLU:OE2	2.43	0.52
7:A2:995:ASP:O	7:A2:995:ASP:CG	2.53	0.52
12:F1:373:ARG:NE	12:F1:386:GLU:OE2	2.43	0.52
1:AX:615:SER:HB2	7:A2:614:LYS:HE2	1.91	0.52
7:A3:1001:PHE:CD2	10:FS:19:LEU:HD11	2.45	0.52
10:FL:195:ARG:HD3	12:Fa:9:TYR:CE1	2.43	0.52
1:AV:65:THR:HA	1:AP:68:ILE:CD1	2.40	0.52
7:A0:995:ASP:O	7:A0:995:ASP:CG	2.53	0.52
7:A1:995:ASP:O	7:A1:995:ASP:CG	2.53	0.52
9:LK:4:ASP:O	9:LL:58:LYS:NZ	2.29	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:FZ:373:ARG:NE	12:FZ:386:GLU:OE2	2.43	0.52
7:A0:922:ASP:C	10:Fk:11:VAL:O	2.53	0.52
1:AT:374:LYS:HE3	7:A3:857:ARG:O	2.10	0.52
1:AR:370:THR:HB	7:AY:886:VAL:O	2.09	0.52
15:BE:328:LYS:NZ	15:BG:99:GLY:O	2.39	0.52
1:AT:65:THR:HA	1:AN:68:ILE:CD1	2.40	0.52
7:AZ:995:ASP:O	7:AZ:995:ASP:CG	2.53	0.52
7:A0:922:ASP:OD1	7:A0:922:ASP:C	2.53	0.52
7:AY:924:GLY:N	10:FA:12:ASP:OD1	2.23	0.52
7:A1:174:HIS:ND1	8:A8:236:LEU:HD11	2.24	0.52
1:AW:374:LYS:HE3	7:A1:857:ARG:O	2.10	0.52
4:AG:104:ASP:OD2	7:A2:642:ARG:HD3	2.09	0.52
8:Ae:317:ILE:HG23	8:A5:23:PHE:HB2	1.92	0.51
12:Fr:373:ARG:NE	12:Fr:386:GLU:OE2	2.43	0.51
7:A3:906:MET:CE	8:A6:27:LYS:HD3	2.40	0.51
7:A3:995:ASP:O	7:A3:995:ASP:CG	2.53	0.51
1:AS:342:GLN:HE22	1:AM:344:ARG:NE	2.09	0.51
7:A0:922:ASP:OD1	10:Fk:11:VAL:O	2.28	0.51
7:A1:1001:PHE:HA	10:Ft:19:LEU:HD21	1.92	0.51
7:AY:995:ASP:O	7:AY:995:ASP:CG	2.53	0.51
7:A0:483:ASP:CG	8:A7:139:ARG:HH22	2.18	0.51
7:AY:185:VAL:O	10:FA:562:GLN:NE2	2.43	0.51
7:AY:922:ASP:O	7:AY:922:ASP:OD1	2.28	0.51
7:A3:898:MET:HE3	8:A6:320:GLU:OE1	2.09	0.51
10:Fv:195:ARG:O	10:Fv:198:ASN:OD1	2.29	0.51
12:Fi:373:ARG:NE	12:Fi:386:GLU:OE2	2.42	0.51
10:Ft:398:MET:HE1	10:Fu:400:ILE:HB	1.93	0.51
7:A0:515:PHE:CD1	7:A0:526:TRP:HB2	2.40	0.51
10:FA:398:MET:HE1	10:FB:400:ILE:HB	1.93	0.51
3:BR:124:MET:HA	3:BR:124:MET:HE2	1.93	0.51
4:AI:82:ASP:OD2	7:AZ:684:TYR:OH	2.26	0.51
7:AZ:1027:GLN:HE21	8:Aa:322:ARG:NH1	2.07	0.51
8:Ad:20:THR:HG22	8:A4:317:ILE:C	2.36	0.51
8:Ae:320:GLU:HG3	8:A5:17:ALA:HB2	1.92	0.51
9:LQ:4:ASP:O	9:LR:58:LYS:NZ	2.29	0.51
3:BT:206:ARG:NH1	13:BZ:93:HIS:CD2	2.79	0.51
7:A2:920:LYS:NZ	10:FJ:18:TYR:CE1	2.79	0.51
7:AZ:920:LYS:NZ	10:Fb:18:TYR:CE1	2.79	0.51
1:AO:3:ILE:HD13	7:AZ:635:PRO:HA	1.93	0.51
3:BR:206:ARG:NH1	13:BW:93:HIS:CD2	2.79	0.51
7:A2:486:TYR:HB3	8:A4:238:TRP:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A0:657:SER:OG	14:AD:42:THR:HA	2.11	0.51
7:A1:922:ASP:OD1	10:Ft:11:VAL:O	2.29	0.51
10:Fk:398:MET:HE1	10:Fl:400:ILE:HB	1.93	0.51
7:A2:483:ASP:OD2	8:A4:139:ARG:NH2	2.44	0.50
8:Ae:317:ILE:HG23	8:A5:23:PHE:CD2	2.45	0.50
7:A3:789:THR:O	7:A3:790:ALA:HB3	2.12	0.50
1:AS:64:ASN:HD21	7:A2:673:LEU:CD2	2.24	0.50
8:Ad:320:GLU:HG3	8:A4:17:ALA:HB2	1.94	0.50
1:AU:342:GLN:HE22	1:AO:344:ARG:NE	2.09	0.50
7:A2:848:LEU:HD23	7:A2:848:LEU:H	1.77	0.50
7:A0:221:TYR:CD2	10:Fk:571:GLY:HA3	2.46	0.50
7:A3:848:LEU:H	7:A3:848:LEU:HD23	1.77	0.50
8:Ab:317:ILE:HG23	8:A8:23:PHE:CD2	2.46	0.50
15:BG:153:ALA:HB1	15:BG:184:ILE:HD11	1.94	0.50
7:A1:920:LYS:NZ	10:Ft:18:TYR:CE1	2.79	0.50
7:A1:1027:GLN:HE21	8:Ac:322:ARG:NH1	2.08	0.50
8:Af:261:ASP:OD2	10:FS:18:TYR:OH	2.28	0.50
9:LE:4:ASP:O	9:LF:58:LYS:NZ	2.29	0.50
7:A2:1001:PHE:HA	10:FJ:19:LEU:HD21	1.93	0.50
7:AZ:478:ILE:HG21	8:A6:161:ILE:HD11	1.93	0.50
7:AY:789:THR:O	7:AY:790:ALA:HB3	2.12	0.50
7:A2:789:THR:O	7:A2:790:ALA:HB3	2.12	0.50
7:AZ:789:THR:O	7:AZ:790:ALA:HB3	2.12	0.50
1:AX:46:ASP:OD2	14:AF:87:ARG:NH2	2.37	0.50
2:BL:349:ILE:HD12	14:AF:75:ARG:HG2	1.92	0.50
7:AZ:848:LEU:HD23	7:AZ:848:LEU:H	1.77	0.50
7:AZ:1001:PHE:HA	10:Fb:19:LEU:HD21	1.93	0.50
10:FJ:398:MET:HE1	10:FK:400:ILE:HB	1.93	0.50
10:Fb:196:ARG:HH11	12:Fq:4:ASN:HB3	1.74	0.50
1:AV:330:ARG:HH21	1:AV:330:ARG:CG	2.25	0.50
7:AY:1032:GLU:OE2	7:A2:463:LYS:NZ	2.41	0.50
8:Aa:317:ILE:HG23	8:A7:23:PHE:HB2	1.93	0.50
10:Fd:242:GLY:O	12:Fr:4:ASN:HB2	2.12	0.50
10:Fk:388:ARG:HH22	10:Fl:320:GLU:CD	2.20	0.50
7:AY:848:LEU:HD23	7:AY:848:LEU:H	1.77	0.49
7:A3:280:LYS:HB2	9:LG:25:TYR:CD2	2.47	0.49
10:Fb:388:ARG:HH22	10:Fc:320:GLU:CD	2.20	0.49
10:Ft:388:ARG:HH22	10:Fu:320:GLU:CD	2.20	0.49
4:AH:104:ASP:OD2	7:A3:642:ARG:HD3	2.12	0.49
7:AY:478:ILE:CG2	8:A9:161:ILE:HD11	2.39	0.49
7:A2:1027:GLN:HE21	8:Ae:322:ARG:NH1	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:922:ASP:OD1	7:A1:922:ASP:C	2.54	0.49
10:FS:388:ARG:HH22	10:FT:320:GLU:CD	2.20	0.49
10:Fb:398:MET:HE1	10:Fc:400:ILE:HB	1.93	0.49
13:BW:118:ARG:NH1	13:B6:62:GLY:O	2.45	0.49
7:A3:995:ASP:CB	10:FU:8:GLY:H	2.25	0.49
3:BV:12:ALA:CB	13:B1:58:ILE:HD11	2.43	0.49
7:AY:1001:PHE:CE2	10:FB:19:LEU:CD2	2.94	0.49
7:A2:906:MET:SD	8:A5:27:LYS:NZ	2.85	0.49
7:A3:920:LYS:NZ	10:FS:18:TYR:CE1	2.81	0.49
11:FF:3:ILE:HG22	11:FF:3:ILE:O	2.13	0.49
1:AN:2:ALA:HB2	7:A3:635:PRO:CA	2.42	0.49
1:AN:16:ASN:ND2	7:A3:706:TRP:CE3	2.80	0.49
4:AL:100:GLN:NE2	7:AY:645:ASP:OD2	2.45	0.49
7:A0:848:LEU:H	7:A0:848:LEU:HD23	1.77	0.49
10:FS:398:MET:HE1	10:FT:400:ILE:HB	1.93	0.49
1:AT:615:SER:HB2	7:AZ:614:LYS:HE2	1.95	0.49
4:AJ:100:GLN:NE2	7:A0:647:ARG:HH11	2.09	0.49
7:A1:789:THR:O	7:A1:790:ALA:HB3	2.12	0.49
10:Fc:195:ARG:HD3	12:Fq:9:TYR:CE1	2.48	0.49
3:BT:206:ARG:HH11	13:BZ:93:HIS:CD2	2.31	0.49
7:A0:789:THR:O	7:A0:790:ALA:HB3	2.12	0.49
7:A1:894:THR:HG23	8:A9:333:GLU:HB3	1.95	0.49
7:A3:922:ASP:OD1	7:A3:922:ASP:O	2.31	0.49
8:Ab:23:PHE:CD1	8:A8:317:ILE:HG23	2.48	0.49
11:FO:3:ILE:HG22	11:FO:3:ILE:O	2.13	0.49
1:AR:16:ASN:ND2	7:AY:706:TRP:CE3	2.79	0.49
3:BS:30:PRO:HG2	3:BS:114:PHE:CZ	2.48	0.49
7:A3:515:PHE:CD1	7:A3:526:TRP:HB2	2.40	0.49
10:FA:388:ARG:HH22	10:FB:320:GLU:CD	2.20	0.49
10:Fd:244:VAL:CG1	12:Fr:5:ASN:OD1	2.61	0.49
12:Fi:373:ARG:HD2	12:Fi:386:GLU:OE2	2.13	0.49
1:AV:501:PRO:HB3	7:A0:856:ASN:CG	2.37	0.49
1:AR:153:ILE:HD12	1:AM:441:TRP:CD1	2.35	0.49
7:AZ:1030:ILE:HB	8:A7:16:ARG:HG2	1.95	0.49
7:A1:848:LEU:HD23	7:A1:848:LEU:H	1.77	0.49
11:FX:3:ILE:O	11:FX:3:ILE:HG22	2.13	0.49
1:AV:374:LYS:HE3	7:A0:857:ARG:O	2.12	0.48
1:AX:373:ASP:O	7:AY:859:ARG:HA	2.13	0.48
3:BU:3:THR:HG22	3:BU:4:LEU:H	1.78	0.48
3:BQ:263:LEU:O	3:BQ:266:LYS:HE3	2.13	0.48
8:Ae:317:ILE:O	8:A5:20:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Af:60:GLU:HG3	8:Af:62:GLY:N	2.22	0.48
12:FZ:373:ARG:HD2	12:FZ:386:GLU:OE2	2.13	0.48
1:AV:615:SER:HB2	7:A1:614:LYS:HE2	1.96	0.48
2:BL:80:PHE:CZ	4:AL:1:MET:HE2	2.48	0.48
10:FA:11:VAL:HA	10:FC:20:ARG:HD2	1.95	0.48
10:FJ:11:VAL:HA	10:FL:20:ARG:HD2	1.96	0.48
10:Fb:11:VAL:HA	10:Fd:20:ARG:HD2	1.95	0.48
1:AX:65:THR:HA	1:AR:68:ILE:CD1	2.44	0.48
7:A1:280:LYS:HB2	9:LP:25:TYR:CD2	2.48	0.48
12:Fa:294:ASN:HA	12:FZ:285:ARG:NH1	2.29	0.48
2:BN:80:PHE:CZ	4:AH:1:MET:HE2	2.48	0.48
7:AY:765:ASN:OD1	8:A4:207:ILE:HD13	2.13	0.48
7:A2:485:HIS:CD2	8:A4:244:ASN:HD21	2.30	0.48
7:A2:515:PHE:CD1	7:A2:526:TRP:HB2	2.40	0.48
8:Af:60:GLU:HG2	8:Af:63:PHE:HB2	1.95	0.48
10:FJ:388:ARG:HH22	10:FK:320:GLU:CD	2.20	0.48
10:Fk:11:VAL:HA	10:Fm:20:ARG:HD2	1.96	0.48
11:Fy:3:ILE:O	11:Fy:3:ILE:HG22	2.13	0.48
12:F2:294:ASN:HA	12:F1:285:ARG:NH1	2.29	0.48
13:BZ:41:MET:HE1	13:B1:79:HIS:CE1	2.49	0.48
7:AY:515:PHE:CD1	7:AY:526:TRP:HB2	2.40	0.48
7:AY:921:TRP:CZ3	10:FC:19:LEU:CD1	2.96	0.48
7:AZ:280:LYS:HB2	9:LJ:25:TYR:CD2	2.49	0.48
8:A8:107:TYR:HB3	8:A8:108:PRO:HD2	1.94	0.48
10:FU:365:SER:HB2	12:FP:398:ARG:HD3	1.96	0.48
10:Ft:11:VAL:HA	10:Fv:20:ARG:HD2	1.96	0.48
10:Fv:244:VAL:CG1	12:FH:5:ASN:OD1	2.62	0.48
12:F1:373:ARG:HD2	12:F1:386:GLU:OE2	2.13	0.48
2:BK:315:ASN:HD21	3:BU:189:ARG:CZ	2.26	0.48
7:A1:478:ILE:HG21	8:A8:161:ILE:HD11	1.94	0.48
12:FH:373:ARG:HD2	12:FH:386:GLU:OE2	2.13	0.48
1:AW:614:GLN:OE1	7:AY:614:LYS:HD3	2.14	0.48
3:BU:30:PRO:HG2	3:BU:114:PHE:CZ	2.49	0.48
12:FI:294:ASN:HA	12:FH:285:ARG:NH1	2.29	0.48
12:Fj:294:ASN:HA	12:Fi:285:ARG:NH1	2.29	0.48
7:AY:940:ASP:O	10:FB:21:LYS:HE2	2.13	0.48
7:AZ:515:PHE:CD1	7:AZ:526:TRP:HB2	2.40	0.48
10:FC:365:SER:HB2	12:Fz:398:ARG:HD3	1.96	0.48
10:FS:11:VAL:HA	10:FU:20:ARG:HD2	1.96	0.48
11:Fg:3:ILE:HG22	11:Fg:3:ILE:O	2.13	0.48
12:FR:294:ASN:HA	12:FQ:285:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:FQ:373:ARG:HD2	12:FQ:386:GLU:OE2	2.13	0.48
12:Fq:294:ASN:HA	12:Fr:285:ARG:NH1	2.29	0.48
1:AP:2:ALA:HB2	7:A0:636:GLU:CG	2.39	0.48
7:A1:176:ILE:HD12	8:A8:234:ASN:HA	1.95	0.48
7:A1:486:TYR:HB3	8:A8:238:TRP:CB	2.44	0.48
8:Af:317:ILE:CG2	8:A6:23:PHE:CD2	2.96	0.48
11:Fp:3:ILE:HG22	11:Fp:3:ILE:O	2.13	0.48
12:FY:401:HIS:CE1	12:Fa:395:LYS:HE2	2.49	0.48
12:Fr:373:ARG:HD2	12:Fr:386:GLU:OE2	2.13	0.48
8:Ab:80:THR:HA	8:Ab:311:ARG:HH12	1.79	0.47
12:Fh:401:HIS:CE1	12:Fj:395:LYS:HE2	2.49	0.47
7:A2:280:LYS:HB2	9:LD:25:TYR:CD2	2.48	0.47
7:A1:738:THR:HG22	7:A1:738:THR:O	2.15	0.47
7:A3:738:THR:HG22	7:A3:738:THR:O	2.14	0.47
8:Aa:320:GLU:HG3	8:A7:17:ALA:HB2	1.95	0.47
7:A0:738:THR:HG22	7:A0:738:THR:O	2.15	0.47
10:FA:357:GLN:HE22	11:FD:3:ILE:HG12	1.80	0.47
8:Ad:61:PRO:O	8:A4:11:ARG:C	2.58	0.47
8:Ac:61:PRO:C	8:A9:11:ARG:HB3	2.35	0.47
2:BO:315:ASN:HD21	3:BQ:189:ARG:CZ	2.27	0.47
7:AY:922:ASP:OD2	10:FA:13:ASP:N	2.47	0.47
12:FP:401:HIS:CE1	12:FR:395:LYS:HE2	2.50	0.47
1:AN:43:GLU:OE2	7:A3:671:TYR:HE2	1.96	0.47
2:BN:200:ARG:NH1	3:BR:196:GLU:OE1	2.42	0.47
7:AY:738:THR:HG22	7:AY:738:THR:O	2.14	0.47
10:FS:357:GLN:HE22	11:FV:3:ILE:HG12	1.80	0.47
5:BB:1:MET:HE2	15:BE:271:ASN:CB	2.42	0.47
7:AY:657:SER:OG	14:AF:42:THR:HA	2.15	0.47
7:A2:1020:ARG:HD3	8:Ae:212:ASN:O	2.15	0.47
7:A2:1030:ILE:HB	8:A5:16:ARG:HG2	1.97	0.47
7:A0:283:ASP:O	9:LO:15:ILE:HG12	2.15	0.47
12:FG:401:HIS:CE1	12:FI:395:LYS:HE2	2.49	0.47
12:Fq:401:HIS:CE1	12:Fq:395:LYS:HE2	2.49	0.47
12:Fz:401:HIS:CE1	12:F2:395:LYS:HE2	2.49	0.47
15:BG:375:LYS:H	15:BG:375:LYS:HD3	1.79	0.47
7:A1:515:PHE:CD1	7:A1:526:TRP:HB2	2.40	0.47
3:BQ:30:PRO:HG2	3:BQ:114:PHE:CZ	2.50	0.47
8:Ab:20:THR:OG1	8:A8:70:ASP:OD1	2.28	0.47
8:Af:55:SER:HB3	8:Af:63:PHE:HE1	1.80	0.47
10:Fk:357:GLN:HE22	11:Fh:3:ILE:HG12	1.80	0.47
7:A2:738:THR:O	7:A2:738:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Ft:357:GLN:HE22	11:Fw:3:ILE:HG12	1.80	0.47
13:BZ:118:ARG:NH1	13:B4:62:GLY:O	2.46	0.47
14:AC:75:ARG:HH21	14:AC:75:ARG:HG3	1.80	0.47
3:BR:30:PRO:HG2	3:BR:114:PHE:CZ	2.51	0.46
7:A3:906:MET:SD	8:A6:27:LYS:CD	3.03	0.46
12:Fi:332:SER:HG	12:Fi:333:TRP:CD1	2.33	0.46
7:AY:906:MET:SD	8:A4:27:LYS:CD	3.04	0.46
8:Ab:62:GLY:C	8:A8:14:ILE:HD12	2.41	0.46
10:Fv:195:ARG:CZ	12:FI:9:TYR:CE1	2.99	0.46
1:AX:53:ARG:HD3	7:AY:658:TYR:CE2	2.51	0.46
7:AZ:922:ASP:OD2	10:Fb:11:VAL:C	2.58	0.46
7:A1:1030:ILE:HB	8:A9:16:ARG:HG2	1.96	0.46
8:Ac:61:PRO:O	8:A9:11:ARG:CB	2.45	0.46
10:Fb:205:THR:CG2	10:Fb:206:SER:H	2.19	0.46
10:Fb:357:GLN:HE22	11:Fe:3:ILE:HG12	1.80	0.46
1:AN:2:ALA:CB	7:A3:634:THR:O	2.55	0.46
4:AG:82:ASP:OD2	7:A2:684:TYR:OH	2.26	0.46
7:A0:485:HIS:HB2	8:A7:242:ASP:OD2	2.15	0.46
10:Fv:242:GLY:O	12:FH:4:ASN:HB2	2.15	0.46
12:FZ:332:SER:HG	12:FZ:333:TRP:CD1	2.34	0.46
12:Fr:332:SER:HG	12:Fr:333:TRP:CD1	2.34	0.46
13:BX:41:MET:HE1	13:BY:79:HIS:CE1	2.51	0.46
4:AK:97:PHE:CD2	7:A1:644:PRO:CB	2.99	0.46
8:Aa:80:THR:HA	8:Aa:311:ARG:HH12	1.79	0.46
8:A4:107:TYR:HB3	8:A4:108:PRO:HD2	1.97	0.46
12:FH:332:SER:HG	12:FH:333:TRP:CD1	2.34	0.46
1:AN:43:GLU:OE2	7:A3:671:TYR:CE2	2.68	0.46
7:A2:917:LYS:NZ	8:Ae:330:ASP:OD2	2.46	0.46
7:AZ:738:THR:O	7:AZ:738:THR:HG22	2.15	0.46
7:AZ:1029:LYS:HB2	8:A7:15:TYR:CZ	2.51	0.46
8:Ae:317:ILE:HG23	8:A5:23:PHE:CB	2.46	0.46
10:FS:205:THR:CG2	10:FS:206:SER:H	2.19	0.46
10:Fd:195:ARG:CZ	12:Fs:9:TYR:CE1	2.98	0.46
10:Fk:196:ARG:HH11	12:Fz:4:ASN:HB3	1.81	0.46
4:AL:97:PHE:CE2	7:AY:644:PRO:CB	2.98	0.46
7:AY:1001:PHE:HA	10:FA:19:LEU:CD2	2.45	0.46
7:A2:184:CYS:O	10:FJ:562:GLN:HB2	2.16	0.46
7:A2:994:PHE:O	10:FL:16:GLY:HA3	2.16	0.46
7:A0:902:SER:CB	8:A8:340:GLU:O	2.56	0.46
10:Fd:195:ARG:NE	12:Fs:9:TYR:CE1	2.84	0.46
12:FQ:332:SER:HG	12:FQ:333:TRP:CD1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AY:995:ASP:OD1	7:AY:995:ASP:C	2.59	0.46
7:AZ:323:LYS:HE2	7:AZ:323:LYS:HA	1.97	0.46
13:B3:41:MET:HB2	13:B8:142:MET:HE2	1.96	0.46
7:AZ:995:ASP:OD1	7:AZ:995:ASP:C	2.59	0.46
7:A3:995:ASP:OD1	7:A3:995:ASP:C	2.59	0.46
1:AN:340:GLU:HB3	7:A3:736:TYR:CZ	2.51	0.46
7:A1:995:ASP:OD1	7:A1:995:ASP:C	2.59	0.46
10:FJ:357:GLN:HE22	11:FM:3:ILE:HG12	1.80	0.46
10:FU:195:ARG:HD3	12:Fj:9:TYR:CE1	2.50	0.46
1:AP:43:GLU:OE2	7:A0:671:TYR:HE2	1.99	0.45
7:AY:184:CYS:O	10:FA:562:GLN:HB2	2.16	0.45
7:AY:323:LYS:HA	7:AY:323:LYS:HE2	1.97	0.45
7:AZ:1020:ARG:HD3	8:Aa:212:ASN:O	2.15	0.45
8:Ac:70:ASP:OD1	8:A9:20:THR:OG1	2.25	0.45
7:A2:323:LYS:HE2	7:A2:323:LYS:HA	1.97	0.45
7:AZ:486:TYR:HB3	8:A6:238:TRP:CB	2.46	0.45
7:A0:922:ASP:OD2	10:Fk:10:SER:O	2.33	0.45
7:A3:657:SER:OG	14:AC:42:THR:HA	2.16	0.45
10:FL:195:ARG:O	10:FL:198:ASN:OD1	2.34	0.45
7:AZ:994:PHE:O	10:Fd:16:GLY:HA3	2.16	0.45
7:A0:323:LYS:HA	7:A0:323:LYS:HE2	1.97	0.45
8:A5:19:ILE:O	8:A5:19:ILE:CG2	2.65	0.45
10:Fb:90:TYR:O	10:Fb:91:ASN:HB3	2.16	0.45
1:AN:297:THR:CG2	15:BE:125:SER:HB2	2.46	0.45
7:AY:896:LEU:HD22	8:A4:322:ARG:CZ	2.47	0.45
8:Aa:64:ALA:HA	8:A7:14:ILE:HG21	1.97	0.45
10:FA:90:TYR:O	10:FA:91:ASN:HB3	2.16	0.45
10:FL:244:VAL:CG1	12:FZ:5:ASN:OD1	2.64	0.45
13:B4:41:MET:HB2	13:B5:142:MET:HE2	1.98	0.45
1:AS:410:ILE:HD11	7:A2:888:PHE:CZ	2.51	0.45
7:AY:924:GLY:H	10:FA:12:ASP:CG	2.19	0.45
7:A2:580:LEU:HD11	8:A4:133:PHE:HZ	1.81	0.45
8:Ab:16:ARG:CD	8:A8:67:TYR:CE1	2.89	0.45
12:F1:332:SER:HG	12:F1:333:TRP:CD1	2.34	0.45
1:AQ:532:TYR:CD1	1:AQ:581:ARG:HD3	2.52	0.45
7:AY:921:TRP:CZ3	10:FC:19:LEU:HD12	2.52	0.45
7:A1:994:PHE:O	10:Fv:16:GLY:HA3	2.16	0.45
8:Af:20:THR:HG22	8:A6:317:ILE:O	2.17	0.45
1:AX:155:LEU:H	1:AX:155:LEU:HD23	1.82	0.45
7:A0:184:CYS:O	10:Fk:562:GLN:HB2	2.17	0.45
7:A0:995:ASP:OD1	7:A0:995:ASP:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A3:902:SER:CB	8:A6:340:GLU:O	2.59	0.45
8:Ad:263:VAL:HG21	10:FA:14:GLY:C	2.42	0.45
8:A6:107:TYR:HB3	8:A6:108:PRO:HD2	1.98	0.45
7:A2:995:ASP:OD1	7:A2:995:ASP:C	2.59	0.45
7:AZ:917:LYS:NZ	8:Aa:330:ASP:OD2	2.44	0.45
7:A1:1020:ARG:HD3	8:Ac:212:ASN:O	2.17	0.45
10:FL:195:ARG:CZ	12:Fa:9:TYR:CE1	3.00	0.45
1:AN:83:THR:HA	4:AH:15:THR:HG21	1.99	0.45
2:BM:156:VAL:HG11	15:BF:54:TYR:HB3	1.99	0.45
7:AY:483:ASP:CG	8:Ac:72:GLU:CD	2.84	0.45
7:AZ:184:CYS:O	10:Fb:562:GLN:HB2	2.17	0.45
7:A3:1020:ARG:HD3	8:Af:212:ASN:O	2.17	0.45
9:LB:4:ASP:O	9:LC:58:LYS:NZ	2.29	0.45
13:BW:142:MET:HE2	13:BY:41:MET:HB2	1.99	0.45
1:AO:408:ALA:HB3	1:AO:409:PRO:HD3	1.99	0.45
15:BE:287:ARG:O	15:BE:287:ARG:HD3	2.17	0.45
1:AT:501:PRO:HB3	7:A3:856:ASN:CG	2.41	0.44
1:AR:83:THR:HA	4:AL:15:THR:HG21	1.98	0.44
1:AR:340:GLU:HB3	7:AY:736:TYR:CZ	2.52	0.44
3:BQ:3:THR:HG22	3:BQ:4:LEU:H	1.83	0.44
7:AZ:1001:PHE:CD2	10:Fb:19:LEU:HD11	2.52	0.44
7:A1:184:CYS:O	10:Ft:562:GLN:HB2	2.17	0.44
8:Ac:317:ILE:HG23	8:A9:23:PHE:HB2	1.99	0.44
8:Aa:61:PRO:O	8:A7:12:SER:N	2.50	0.44
10:FS:90:TYR:O	10:FS:91:ASN:HB3	2.16	0.44
10:Fv:244:VAL:HG12	12:FH:5:ASN:OD1	2.17	0.44
13:B2:3:LEU:HD23	13:B7:58:ILE:HG22	2.00	0.44
1:AX:53:ARG:HD3	7:AY:658:TYR:CD2	2.52	0.44
7:AY:1001:PHE:CE2	10:FB:19:LEU:HD21	2.52	0.44
7:A0:265:SER:HA	9:LM:12:VAL:O	2.17	0.44
7:A1:894:THR:CG2	8:A9:333:GLU:HB3	2.47	0.44
7:A1:1001:PHE:CD2	10:Ft:19:LEU:HD11	2.52	0.44
7:A3:323:LYS:HE2	7:A3:323:LYS:HA	1.97	0.44
7:A3:486:TYR:HB3	8:A5:238:TRP:HB3	1.98	0.44
8:Ad:64:ALA:CB	8:A4:14:ILE:HG21	2.48	0.44
12:FQ:373:ARG:CD	12:FQ:386:GLU:OE2	2.66	0.44
12:Fi:351:ARG:HG2	12:Fi:352:LEU:N	2.33	0.44
1:AU:374:LYS:HE3	7:AZ:857:ARG:O	2.17	0.44
12:FQ:373:ARG:HD2	12:FQ:386:GLU:CD	2.43	0.44
12:Fi:373:ARG:CD	12:Fi:386:GLU:OE2	2.66	0.44
12:F1:373:ARG:CD	12:F1:386:GLU:OE2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:3:ILE:HD13	7:A2:636:GLU:H	1.82	0.44
2:BK:264:SER:N	2:BM:171:ASN:HD21	2.15	0.44
7:AY:485:HIS:HB2	8:A9:242:ASP:OD2	2.18	0.44
7:A2:1001:PHE:CD2	10:FJ:19:LEU:HD11	2.52	0.44
7:A1:323:LYS:HE2	7:A1:323:LYS:HA	1.97	0.44
10:Fk:90:TYR:O	10:Fk:91:ASN:HB3	2.16	0.44
10:Fu:195:ARG:HD3	12:FG:9:TYR:CE1	2.52	0.44
12:Fh:371:ILE:HD11	12:Fh:373:ARG:HH11	1.82	0.44
1:AO:532:TYR:CD1	1:AO:581:ARG:HD3	2.53	0.44
4:AG:97:PHE:CD2	7:A2:644:PRO:CB	3.01	0.44
7:AY:906:MET:SD	8:A4:27:LYS:CE	3.06	0.44
7:A0:920:LYS:C	10:Fm:19:LEU:HD23	2.39	0.44
8:Ac:64:ALA:HA	8:A9:14:ILE:HG21	1.99	0.44
10:Fd:195:ARG:CD	12:Fg:9:TYR:CE1	2.99	0.44
12:FH:373:ARG:CD	12:FH:386:GLU:OE2	2.66	0.44
12:FZ:351:ARG:HG2	12:FZ:352:LEU:N	2.33	0.44
12:FZ:373:ARG:HD2	12:FZ:386:GLU:CD	2.43	0.44
1:AN:2:ALA:HB2	7:A3:634:THR:C	2.40	0.44
2:BO:319:ILE:HD12	3:BQ:191:LEU:HD12	1.99	0.44
7:AZ:463:LYS:HE2	7:AZ:463:LYS:HB3	1.81	0.44
12:Fr:373:ARG:HD2	12:Fr:386:GLU:CD	2.43	0.44
15:BF:99:GLY:O	15:BG:328:LYS:NZ	2.40	0.44
7:AY:906:MET:SD	8:A4:27:LYS:HD2	2.57	0.44
8:Ad:50:LYS:NZ	8:Ad:54:TRP:CZ3	2.86	0.44
8:Ac:263:VAL:HG21	10:Ft:14:GLY:C	2.42	0.44
8:Ac:295:PRO:HA	8:A9:240:GLN:NE2	2.33	0.44
12:FG:351:ARG:HD3	12:FH:328:VAL:O	2.18	0.44
12:FH:373:ARG:HD2	12:FH:386:GLU:CD	2.43	0.44
12:FQ:351:ARG:HG2	12:FQ:352:LEU:N	2.33	0.44
12:Fq:401:HIS:CE1	12:Fg:395:LYS:CE	3.01	0.44
12:Fz:401:HIS:CE1	12:F2:395:LYS:CE	3.01	0.44
1:AS:236:VAL:CG2	7:A2:692:LYS:HG2	2.48	0.44
1:AW:410:ILE:HD11	7:A1:888:PHE:CZ	2.53	0.44
1:AP:340:GLU:HB3	7:A0:736:TYR:CZ	2.53	0.44
7:A3:1029:LYS:HB2	8:A6:15:TYR:CZ	2.53	0.44
8:Ab:50:LYS:NZ	8:Ab:54:TRP:CZ3	2.86	0.44
8:Ab:65:PRO:O	8:A8:16:ARG:HD3	2.18	0.44
8:Ae:50:LYS:NZ	8:Ae:54:TRP:CZ3	2.86	0.44
8:Af:80:THR:HA	8:Af:311:ARG:HH12	1.79	0.44
10:FL:196:ARG:NH2	12:Fa:9:TYR:O	2.51	0.44
12:Fq:351:ARG:HD3	12:Fr:328:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F1:373:ARG:HD2	12:F1:386:GLU:CD	2.43	0.44
14:AC:6:LYS:HE2	14:AC:6:LYS:HB3	1.84	0.44
15:BF:287:ARG:O	15:BF:287:ARG:HD3	2.17	0.44
7:AY:896:LEU:HD22	8:A4:322:ARG:NH1	2.33	0.44
7:A3:463:LYS:HB3	7:A3:463:LYS:HE2	1.81	0.44
12:FP:351:ARG:HD3	12:FQ:328:VAL:O	2.18	0.44
12:FY:371:ILE:HD11	12:FY:373:ARG:HH11	1.82	0.44
12:Fi:373:ARG:HD2	12:Fi:386:GLU:CD	2.43	0.44
12:Fr:351:ARG:HG2	12:Fr:352:LEU:N	2.33	0.44
15:BG:287:ARG:O	15:BG:287:ARG:HD3	2.17	0.44
1:AS:246:GLU:HG2	7:A2:723:ALA:O	2.18	0.43
1:AR:16:ASN:OD1	7:AY:711:LYS:HE2	2.18	0.43
10:Fd:244:VAL:HG12	12:Fr:5:ASN:OD1	2.18	0.43
10:Fv:196:ARG:NH2	12:FI:9:TYR:O	2.51	0.43
12:FI:257:LYS:HE2	12:FI:257:LYS:HB3	1.86	0.43
12:FI:318:ALA:HB2	12:FH:315:TYR:C	2.43	0.43
1:AP:83:THR:O	4:AJ:15:THR:HG21	2.19	0.43
3:BQ:3:THR:HG22	3:BQ:4:LEU:N	2.33	0.43
4:AI:105:VAL:CG2	7:AZ:640:GLY:O	2.63	0.43
7:A1:515:PHE:CE2	7:A1:536:ILE:CD1	3.01	0.43
7:A1:917:LYS:NZ	8:Ac:330:ASP:OD2	2.45	0.43
7:A3:922:ASP:OD1	10:FS:12:ASP:N	2.51	0.43
8:Ad:317:ILE:C	8:A4:20:THR:HG22	2.44	0.43
10:FJ:558:ILE:HG22	10:FK:558:ILE:HD12	2.00	0.43
10:Ft:313:GLU:OE2	10:Fv:388:ARG:NH2	2.51	0.43
12:FP:371:ILE:HD11	12:FP:373:ARG:HH11	1.82	0.43
12:FZ:373:ARG:CD	12:FZ:386:GLU:OE2	2.66	0.43
12:Fh:351:ARG:HD3	12:Fi:328:VAL:O	2.18	0.43
1:AT:408:ALA:HB3	1:AT:409:PRO:HD3	2.00	0.43
1:AX:220:MET:SD	7:AY:727:PHE:CE2	3.12	0.43
2:BM:58:TYR:CE1	3:BR:144:ASN:HB2	2.53	0.43
7:A0:270:LYS:HG2	9:LN:23:ILE:HG22	2.01	0.43
7:A0:280:LYS:HD2	9:LM:25:TYR:CE1	2.53	0.43
7:A3:184:CYS:O	10:FS:562:GLN:HB2	2.17	0.43
7:A3:921:TRP:CZ3	10:FU:19:LEU:CD1	3.02	0.43
8:Ab:341:PHE:CD2	8:A8:27:LYS:HD2	2.53	0.43
8:Aa:50:LYS:NZ	8:Aa:54:TRP:CZ3	2.86	0.43
8:Aa:61:PRO:O	8:A7:12:SER:O	2.35	0.43
10:Fb:558:ILE:HG22	10:Fc:558:ILE:HD12	2.01	0.43
10:Ft:90:TYR:O	10:Ft:91:ASN:HB3	2.17	0.43
12:FG:401:HIS:CE1	12:FI:395:LYS:CE	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Fz:351:ARG:HD3	12:F1:328:VAL:O	2.18	0.43
12:F2:318:ALA:HB2	12:F1:315:TYR:C	2.43	0.43
7:AY:478:ILE:HB	8:A9:161:ILE:CD1	2.48	0.43
7:A2:515:PHE:CE2	7:A2:536:ILE:CD1	3.01	0.43
10:FJ:90:TYR:O	10:FJ:91:ASN:HB3	2.16	0.43
10:FL:244:VAL:HG12	12:FZ:5:ASN:OD1	2.18	0.43
10:Fv:195:ARG:NE	12:FL:9:TYR:CE1	2.86	0.43
12:Fh:401:HIS:CE1	12:Fj:395:LYS:CE	3.01	0.43
13:BX:142:MET:HE2	13:B1:41:MET:HB2	1.99	0.43
3:BV:2:PHE:HA	3:BV:6:GLU:OE1	2.18	0.43
7:AY:920:LYS:C	10:FC:19:LEU:HD23	2.34	0.43
8:Ab:64:ALA:HB2	8:A8:14:ILE:HD13	2.01	0.43
12:FR:318:ALA:HB2	12:FQ:315:TYR:C	2.43	0.43
12:Fr:373:ARG:CD	12:Fr:386:GLU:OE2	2.66	0.43
1:AW:337:ILE:HG21	1:AQ:260:SER:O	2.19	0.43
1:AR:83:THR:O	4:AL:15:THR:HG21	2.19	0.43
2:BK:156:VAL:HG11	15:BE:54:TYR:HB3	2.00	0.43
7:AY:466:GLU:C	8:A9:11:ARG:NH2	2.77	0.43
7:AY:921:TRP:CZ3	10:FC:19:LEU:HD11	2.54	0.43
7:A0:515:PHE:CE2	7:A0:536:ILE:CD1	3.01	0.43
10:FS:313:GLU:OE2	10:FU:388:ARG:NH2	2.52	0.43
10:Fk:558:ILE:HG22	10:Fl:558:ILE:HD12	2.00	0.43
12:FY:351:ARG:HD3	12:FZ:328:VAL:O	2.18	0.43
12:Fq:371:ILE:HD11	12:Fq:373:ARG:HH11	1.82	0.43
12:Fz:371:ILE:HD11	12:Fz:373:ARG:HH11	1.82	0.43
2:BN:349:ILE:HD12	14:AC:75:ARG:HD3	2.00	0.43
7:AZ:536:ILE:O	7:AZ:536:ILE:HG22	2.19	0.43
8:Aa:263:VAL:HG21	10:Fb:14:GLY:C	2.43	0.43
8:Af:23:PHE:CD1	8:A6:317:ILE:HG23	2.53	0.43
8:Af:50:LYS:NZ	8:Af:54:TRP:CZ3	2.86	0.43
10:FA:558:ILE:HG22	10:FB:558:ILE:HD12	2.01	0.43
12:FY:401:HIS:CE1	12:Fa:395:LYS:CE	3.01	0.43
12:Fa:257:LYS:HB3	12:Fa:257:LYS:HE2	1.86	0.43
13:BY:27:TYR:CD1	13:BY:109:LYS:HE3	2.54	0.43
1:AM:408:ALA:HB3	1:AM:409:PRO:HD3	2.01	0.43
4:AH:97:PHE:CD2	7:A3:644:PRO:CB	3.01	0.43
4:AI:76:MET:HE3	4:AI:76:MET:HB2	1.94	0.43
7:A0:264:TRP:NE1	9:LM:27:GLY:HA3	2.34	0.43
10:FA:313:GLU:OE2	10:FC:388:ARG:NH2	2.52	0.43
11:Fy:35:THR:HA	12:F1:194:ALA:HB3	2.01	0.43
12:FG:371:ILE:HD11	12:FG:373:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:FR:257:LYS:HE2	12:FR:257:LYS:HB3	1.86	0.43
12:Fa:318:ALA:HB2	12:FZ:315:TYR:C	2.43	0.43
12:Fa:373:ARG:CG	12:Fa:386:GLU:HG2	2.49	0.43
7:AY:515:PHE:CE2	7:AY:536:ILE:CD1	3.01	0.43
7:A2:536:ILE:HG22	7:A2:536:ILE:O	2.19	0.43
7:A3:515:PHE:CE2	7:A3:536:ILE:CD1	3.01	0.43
8:Ae:23:PHE:CD1	8:A5:317:ILE:HG23	2.53	0.43
11:FX:35:THR:HA	12:FZ:194:ALA:HB3	2.01	0.43
12:FP:401:HIS:CE1	12:FR:395:LYS:CE	3.01	0.43
12:Fh:441:LEU:N	12:Fh:441:LEU:HD12	2.34	0.43
12:Fq:441:LEU:HD12	12:Fq:441:LEU:N	2.34	0.43
13:BX:3:LEU:HD23	13:B3:58:ILE:HG23	2.00	0.43
7:AZ:515:PHE:CE2	7:AZ:536:ILE:CD1	3.01	0.43
8:Ac:50:LYS:NZ	8:Ac:54:TRP:CZ3	2.86	0.43
8:Ac:317:ILE:C	8:A9:20:THR:HG22	2.44	0.43
8:Aa:20:THR:HG22	8:A7:317:ILE:C	2.43	0.43
8:Ae:263:VAL:HG21	10:FJ:14:GLY:C	2.43	0.43
10:Fk:313:GLU:OE2	10:Fm:388:ARG:NH2	2.52	0.43
11:Fg:35:THR:HA	12:Fi:194:ALA:HB3	2.01	0.43
12:FR:373:ARG:CG	12:FR:386:GLU:HG2	2.49	0.43
13:B6:3:LEU:HD12	13:B6:3:LEU:H	1.84	0.43
1:AP:297:THR:CG2	15:BF:125:SER:HB2	2.49	0.42
3:BV:30:PRO:HG2	3:BV:114:PHE:CZ	2.54	0.42
5:BB:89:GLU:OE2	15:BE:169:ARG:NH1	2.46	0.42
7:AY:920:LYS:NZ	10:FA:18:TYR:CZ	2.86	0.42
8:Ab:20:THR:HG22	8:A8:317:ILE:C	2.44	0.42
8:Ae:80:THR:HA	8:Ae:311:ARG:HH12	1.79	0.42
9:LP:62:THR:HG22	9:LR:108:PHE:CD2	2.54	0.42
10:FS:91:ASN:OD1	10:FU:49:TRP:HB2	2.19	0.42
10:Fb:313:GLU:OE2	10:Fd:388:ARG:NH2	2.52	0.42
12:FI:373:ARG:CG	12:FI:386:GLU:HG2	2.49	0.42
12:Fs:318:ALA:HB2	12:Fr:315:TYR:C	2.43	0.42
12:F1:351:ARG:HG2	12:F1:352:LEU:N	2.33	0.42
1:AV:53:ARG:HD3	7:A0:658:TYR:CD2	2.54	0.42
1:AO:368:CYS:SG	7:AZ:886:VAL:HG11	2.58	0.42
10:Fd:242:GLY:O	12:Fr:4:ASN:CB	2.67	0.42
1:AQ:83:THR:HA	4:AK:15:THR:HG21	2.01	0.42
3:BQ:16:PHE:HE2	3:BR:124:MET:HE1	1.84	0.42
7:A0:346:GLY:HA3	9:LN:15:ILE:HD13	2.01	0.42
7:A0:1020:ARG:HD3	8:Ab:212:ASN:O	2.18	0.42
8:Aa:317:ILE:HG23	8:A7:23:PHE:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:FS:197:GLY:O	10:FT:199:ILE:HG22	2.20	0.42
10:Fd:196:ARG:NH2	12:F8:9:TYR:O	2.52	0.42
12:Fr:373:ARG:HD2	12:Fr:386:GLU:CG	2.49	0.42
12:F1:373:ARG:HD2	12:F1:386:GLU:CG	2.49	0.42
14:AD:6:LYS:HB3	14:AD:6:LYS:HE2	1.68	0.42
1:AV:75:ALA:O	7:A0:690:LEU:HD23	2.19	0.42
1:AW:65:THR:HA	1:AQ:68:ILE:HD13	2.01	0.42
1:AR:2:ALA:CA	7:AY:634:THR:O	2.64	0.42
7:AY:536:ILE:HG22	7:AY:536:ILE:O	2.19	0.42
7:A2:176:ILE:HD12	8:A4:234:ASN:HA	2.00	0.42
7:A3:896:LEU:HA	7:A3:896:LEU:HD23	1.85	0.42
9:LD:62:THR:HG22	9:LF:108:PHE:CD2	2.54	0.42
9:LJ:62:THR:HG22	9:LL:108:PHE:CD2	2.54	0.42
10:FT:312:LEU:HD11	10:FT:387:VAL:CG1	2.50	0.42
10:Fb:91:ASN:OD1	10:Fd:49:TRP:HB2	2.19	0.42
10:Fu:312:LEU:HD11	10:Fu:387:VAL:CG1	2.50	0.42
11:FO:35:THR:HA	12:FQ:194:ALA:HB3	2.01	0.42
12:FQ:373:ARG:HD2	12:FQ:386:GLU:CG	2.49	0.42
1:AS:64:ASN:HD21	7:A2:673:LEU:HD21	1.84	0.42
5:BB:61:THR:HG21	5:BC:57:VAL:HG13	2.01	0.42
9:LG:62:THR:HG22	9:LI:108:PHE:CD2	2.54	0.42
10:FA:91:ASN:OD1	10:FC:49:TRP:HB2	2.19	0.42
10:FL:242:GLY:O	12:FZ:4:ASN:HB2	2.19	0.42
12:FP:447:ARG:NH1	12:FQ:327:TRP:CD1	2.88	0.42
12:Fq:447:ARG:NH1	12:Fr:327:TRP:CD1	2.88	0.42
12:Fz:441:LEU:HD12	12:Fz:441:LEU:N	2.34	0.42
2:BK:58:TYR:CE1	3:BT:144:ASN:HB2	2.55	0.42
4:AI:97:PHE:CD2	7:AZ:644:PRO:CB	3.02	0.42
7:A2:896:LEU:HD23	7:A2:896:LEU:HA	1.85	0.42
7:A1:536:ILE:HG22	7:A1:536:ILE:O	2.19	0.42
7:A1:1001:PHE:CE2	10:Fu:19:LEU:CD2	3.03	0.42
7:A3:536:ILE:O	7:A3:536:ILE:HG22	2.19	0.42
8:Ab:20:THR:HG22	8:A8:317:ILE:O	2.19	0.42
9:LA:62:THR:HG22	9:LC:108:PHE:CD2	2.54	0.42
10:FK:312:LEU:HD11	10:FK:387:VAL:CG1	2.50	0.42
10:Fb:197:GLY:O	10:Fc:199:ILE:HG22	2.20	0.42
11:Fp:35:THR:HA	12:Fr:194:ALA:HB3	2.01	0.42
12:FG:447:ARG:NH1	12:FH:327:TRP:CD1	2.88	0.42
12:Fj:318:ALA:HB2	12:Fi:315:TYR:C	2.43	0.42
13:B3:96:GLY:O	13:B4:56:ARG:NH1	2.53	0.42
1:AX:155:LEU:H	1:AX:155:LEU:CD2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BO:156:VAL:HG11	15:BG:54:TYR:HB3	2.02	0.42
3:BT:30:PRO:HG2	3:BT:114:PHE:CZ	2.55	0.42
4:AK:97:PHE:CE2	7:A1:644:PRO:HB2	2.54	0.42
7:A0:265:SER:HB3	9:LM:12:VAL:O	2.20	0.42
8:Aa:295:PRO:HA	8:A7:240:GLN:NE2	2.35	0.42
10:FA:197:GLY:O	10:FB:199:ILE:HG22	2.20	0.42
10:FB:312:LEU:HD11	10:FB:387:VAL:CG1	2.50	0.42
10:FJ:91:ASN:OD1	10:FL:49:TRP:HB2	2.20	0.42
10:FJ:313:GLU:OE2	10:FL:388:ARG:NH2	2.52	0.42
10:Fk:91:ASN:OD1	10:Fm:49:TRP:HB2	2.20	0.42
12:FH:351:ARG:HG2	12:FH:352:LEU:N	2.33	0.42
12:FH:373:ARG:HD2	12:FH:386:GLU:CG	2.49	0.42
12:FY:441:LEU:HD12	12:FY:441:LEU:N	2.34	0.42
12:Fz:447:ARG:NH1	12:F1:327:TRP:CD1	2.88	0.42
1:AN:16:ASN:OD1	7:A3:711:LYS:CE	2.67	0.42
8:Ae:317:ILE:O	8:A5:20:THR:CG2	2.67	0.42
10:FC:195:ARG:HD3	12:FR:9:TYR:CE1	2.54	0.42
10:FK:197:GLY:O	10:FL:199:ILE:HG22	2.20	0.42
10:Fl:312:LEU:HD11	10:Fl:387:VAL:CG1	2.50	0.42
12:Fj:373:ARG:CG	12:Fj:386:GLU:HG2	2.49	0.42
12:F2:373:ARG:CG	12:F2:386:GLU:HG2	2.49	0.42
1:AN:83:THR:O	4:AH:15:THR:HG21	2.20	0.42
1:AP:342:GLN:NE2	7:A0:737:ALA:HB2	2.35	0.42
1:AQ:83:THR:C	4:AK:15:THR:HG21	2.45	0.42
4:AK:76:MET:HE3	4:AK:76:MET:HB2	1.94	0.42
7:A0:1029:LYS:HB2	8:A8:15:TYR:CZ	2.55	0.42
7:A1:463:LYS:HE2	7:A1:463:LYS:HB3	1.81	0.42
8:A7:19:ILE:O	8:A7:19:ILE:CG2	2.67	0.42
10:FB:197:GLY:O	10:FC:199:ILE:HG22	2.20	0.42
10:FJ:197:GLY:O	10:FK:199:ILE:HG22	2.20	0.42
10:Fb:404:MET:HE1	10:Fd:406:GLU:HB3	2.02	0.42
10:Ft:91:ASN:OD1	10:Fv:49:TRP:HB2	2.20	0.42
10:Ft:558:ILE:HG22	10:Fu:558:ILE:HD12	2.01	0.42
4:AJ:100:GLN:HE22	7:A0:645:ASP:CG	2.26	0.42
5:BC:268:LYS:HD3	5:BC:300:LEU:HD12	2.02	0.42
7:AZ:922:ASP:OD2	10:Fb:11:VAL:O	2.38	0.42
7:A0:470:THR:HG22	7:A0:471:ALA:N	2.35	0.42
7:A0:923:ALA:HA	10:Fk:12:ASP:OD1	2.20	0.42
10:FS:558:ILE:HG22	10:FT:558:ILE:HD12	2.00	0.42
10:Fc:312:LEU:HD11	10:Fc:387:VAL:CG1	2.50	0.42
10:Ft:198:ASN:HD21	12:FG:8:HIS:CD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AS:337:ILE:HG21	1:AM:260:SER:O	2.19	0.41
1:AQ:370:THR:HG23	7:A1:887:GLY:O	2.19	0.41
3:BR:12:ALA:CB	13:BY:58:ILE:HD11	2.50	0.41
7:A2:470:THR:HG22	7:A2:471:ALA:N	2.35	0.41
7:A2:486:TYR:HB3	8:A4:238:TRP:HB3	2.02	0.41
7:AZ:470:THR:HG22	7:AZ:471:ALA:N	2.35	0.41
7:A3:807:ARG:HG2	7:A3:807:ARG:HH21	1.85	0.41
8:Ab:263:VAL:HG21	10:Fk:14:GLY:C	2.44	0.41
9:LM:62:THR:HG22	9:LO:108:PHE:CD2	2.54	0.41
10:Ft:197:GLY:O	10:Fu:199:ILE:HG22	2.20	0.41
12:FY:447:ARG:NH1	12:FZ:327:TRP:CD1	2.88	0.41
1:AV:408:ALA:HB3	1:AV:409:PRO:HD3	2.02	0.41
8:Af:55:SER:HB3	8:Af:63:PHE:CZ	2.55	0.41
10:FL:195:ARG:NE	12:Fa:9:TYR:CE1	2.88	0.41
10:Fk:404:MET:HE1	10:Fm:406:GLU:HB3	2.02	0.41
11:FF:35:THR:HA	12:FH:194:ALA:HB3	2.01	0.41
12:FG:401:HIS:H	12:FI:400:GLY:HA3	1.85	0.41
12:FG:441:LEU:N	12:FG:441:LEU:HD12	2.34	0.41
12:Fh:447:ARG:NH1	12:Fi:327:TRP:CD1	2.88	0.41
12:F2:257:LYS:HB3	12:F2:257:LYS:HE2	1.86	0.41
1:AO:526:THR:HB	1:AO:527:PRO:HD2	2.01	0.41
7:A2:807:ARG:HG2	7:A2:807:ARG:HH21	1.85	0.41
7:AZ:807:ARG:HH21	7:AZ:807:ARG:HG2	1.85	0.41
7:A0:536:ILE:O	7:A0:536:ILE:HG22	2.19	0.41
7:A3:922:ASP:OD1	7:A3:922:ASP:C	2.64	0.41
8:A9:327:ARG:HH11	8:A9:333:GLU:CD	2.28	0.41
10:FS:404:MET:HE1	10:FU:406:GLU:HB3	2.02	0.41
10:Fd:195:ARG:HD3	12:F8:9:TYR:CD1	2.55	0.41
10:Fk:197:GLY:O	10:Fl:199:ILE:HG22	2.20	0.41
10:Fm:365:SER:HB2	12:Fh:398:ARG:HD3	2.03	0.41
12:FP:401:HIS:H	12:FR:400:GLY:HA3	1.85	0.41
12:FP:441:LEU:HD12	12:FP:441:LEU:N	2.34	0.41
2:BO:319:ILE:HD12	3:BQ:191:LEU:CD1	2.50	0.41
5:BB:268:LYS:HD3	5:BB:300:LEU:HD12	2.01	0.41
5:BD:1:MET:HE2	15:BF:271:ASN:HB3	2.03	0.41
7:A0:515:PHE:CZ	7:A0:536:ILE:CD1	3.01	0.41
7:A3:994:PHE:O	10:FU:16:GLY:HA3	2.20	0.41
8:Af:20:THR:HG22	8:A6:317:ILE:C	2.44	0.41
10:FT:197:GLY:O	10:FU:199:ILE:HG22	2.20	0.41
12:Fi:373:ARG:HD2	12:Fi:386:GLU:CG	2.49	0.41
12:Fq:401:HIS:H	12:F8:400:GLY:HA3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Fz:401:HIS:H	12:F2:400:GLY:HA3	1.85	0.41
1:AR:297:THR:CG2	15:BG:125:SER:HB2	2.51	0.41
1:AO:83:THR:C	4:AI:15:THR:HG21	2.45	0.41
2:BM:319:ILE:CD1	3:BS:191:LEU:HD12	2.51	0.41
3:BT:2:PHE:HA	3:BT:6:GLU:OE1	2.19	0.41
7:A0:221:TYR:H	10:Fk:569:GLY:HA3	1.84	0.41
8:Aa:20:THR:HG22	8:A7:317:ILE:O	2.20	0.41
8:Af:64:ALA:HB2	8:A6:14:ILE:HD13	2.03	0.41
10:FC:595:GLN:HB3	10:FC:596:PRO:HD2	2.03	0.41
10:FK:195:ARG:HD3	12:FY:9:TYR:CE1	2.55	0.41
10:Fc:197:GLY:O	10:Fd:199:ILE:HG22	2.20	0.41
10:Fl:197:GLY:O	10:Fm:199:ILE:HG22	2.20	0.41
10:Fv:595:GLN:HB3	10:Fv:596:PRO:HD2	2.03	0.41
15:BE:99:GLY:O	15:BF:328:LYS:NZ	2.42	0.41
1:AW:64:ASN:HD21	7:A1:673:LEU:CD2	2.33	0.41
1:AM:83:THR:C	4:AG:15:THR:HG21	2.46	0.41
1:AM:83:THR:HA	4:AG:15:THR:HG21	2.02	0.41
2:BK:98:ALA:HB3	4:AJ:45:LEU:HB2	2.01	0.41
7:A0:921:TRP:CZ3	10:Fm:19:LEU:HD12	2.56	0.41
7:A3:921:TRP:CZ3	10:FU:19:LEU:HD12	2.55	0.41
8:Ae:61:PRO:O	8:A5:12:SER:O	2.39	0.41
12:Fz:373:ARG:CG	12:Fz:386:GLU:HG2	2.49	0.41
1:AN:342:GLN:NE2	7:A3:737:ALA:HB2	2.36	0.41
1:AP:43:GLU:OE2	7:A0:671:TYR:CE2	2.74	0.41
1:AQ:526:THR:HB	1:AQ:527:PRO:HD2	2.01	0.41
2:BN:80:PHE:CE2	4:AH:1:MET:HG2	2.55	0.41
2:BP:301:ILE:HG21	2:BP:304:ILE:HD11	2.03	0.41
3:BR:2:PHE:HA	3:BR:6:GLU:OE1	2.21	0.41
4:AH:75:LEU:HD22	4:AH:80:VAL:HG21	2.02	0.41
5:BD:200:VAL:HG22	5:BD:201:GLY:H	1.84	0.41
7:AZ:515:PHE:CZ	7:AZ:536:ILE:CD1	3.01	0.41
7:AZ:1001:PHE:CD1	10:Fc:19:LEU:HD23	2.50	0.41
7:A0:463:LYS:HE2	7:A0:463:LYS:HB3	1.81	0.41
8:A5:294:SER:HB2	8:A5:295:PRO:HD2	2.03	0.41
10:Ft:404:MET:HE1	10:Fv:406:GLU:HB3	2.02	0.41
12:FY:401:HIS:H	12:Fa:400:GLY:HA3	1.85	0.41
1:AV:53:ARG:HD3	7:A0:658:TYR:CE2	2.56	0.41
1:AW:246:GLU:HG2	7:A1:723:ALA:O	2.20	0.41
1:AP:16:ASN:OD1	7:A0:711:LYS:CE	2.69	0.41
3:BT:206:ARG:NH1	13:BZ:93:HIS:HD2	2.19	0.41
4:AI:97:PHE:CE2	7:AZ:644:PRO:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AY:470:THR:HG22	7:AY:471:ALA:N	2.35	0.41
7:A2:466:GLU:H	7:A2:466:GLU:HG2	1.77	0.41
7:A3:470:THR:HG22	7:A3:471:ALA:N	2.35	0.41
7:A3:921:TRP:CE3	10:FU:19:LEU:CD1	3.04	0.41
7:A3:922:ASP:C	10:FS:11:VAL:O	2.63	0.41
10:FJ:404:MET:HE1	10:FL:406:GLU:HB3	2.02	0.41
10:Fk:558:ILE:CG2	10:Fl:558:ILE:HD12	2.51	0.41
10:Fv:195:ARG:CD	12:FI:9:TYR:CE1	3.03	0.41
1:AX:560:LYS:HZ1	7:AY:805:ASP:CG	2.27	0.41
1:AR:16:ASN:OD1	7:AY:711:LYS:NZ	2.51	0.41
1:AQ:408:ALA:HB3	1:AQ:409:PRO:HD3	2.03	0.41
4:AK:97:PHE:CD2	7:A1:644:PRO:HB3	2.56	0.41
7:AY:515:PHE:CZ	7:AY:536:ILE:CD1	3.01	0.41
7:A0:807:ARG:HH21	7:A0:807:ARG:HG2	1.85	0.41
7:A1:580:LEU:HD11	8:A8:133:PHE:HZ	1.85	0.41
7:A1:921:TRP:CE3	10:Fv:19:LEU:CD1	3.04	0.41
8:Af:317:ILE:C	8:A6:20:THR:HG22	2.45	0.41
8:A6:174:GLY:H	8:A6:191:ASP:CG	2.29	0.41
10:Fv:242:GLY:O	12:FH:4:ASN:CB	2.69	0.41
12:Fj:257:LYS:HB3	12:Fj:257:LYS:HE2	1.86	0.41
12:Fs:371:ILE:HG21	12:Fs:373:ARG:HH21	1.86	0.41
1:AN:61:LEU:HD13	7:A3:672:TYR:CD1	2.56	0.41
1:AN:434:LYS:HE2	1:AN:479:HIS:CD2	2.56	0.41
1:AM:532:TYR:CD1	1:AM:581:ARG:HD3	2.56	0.41
2:BK:319:ILE:HD12	3:BU:191:LEU:HD12	2.02	0.41
8:Ad:62:GLY:O	8:A4:14:ILE:CD1	2.68	0.41
8:Ab:317:ILE:C	8:A8:20:THR:HG22	2.46	0.41
8:A7:294:SER:HB2	8:A7:295:PRO:HD2	2.03	0.41
9:LO:67:LYS:HE2	9:LO:67:LYS:HB2	1.95	0.41
10:Fd:595:GLN:HB3	10:Fd:596:PRO:HD2	2.03	0.41
12:Fh:401:HIS:H	12:Fj:400:GLY:HA3	1.85	0.41
1:AW:64:ASN:HD21	7:A1:673:LEU:HD21	1.86	0.40
7:A1:807:ARG:HH21	7:A1:807:ARG:HG2	1.85	0.40
8:Ad:317:ILE:O	8:A4:20:THR:HG22	2.21	0.40
8:A6:50:LYS:HE3	8:A6:54:TRP:CZ3	2.56	0.40
9:LA:170:ILE:HD12	9:LB:176:SER:HB2	2.03	0.40
9:LD:170:ILE:HD12	9:LE:176:SER:HB2	2.03	0.40
9:LP:170:ILE:HD12	9:LQ:176:SER:HB2	2.03	0.40
10:FA:91:ASN:O	10:FA:91:ASN:CG	2.64	0.40
10:FA:404:MET:HE1	10:FC:406:GLU:HB3	2.02	0.40
10:FS:558:ILE:CG2	10:FT:558:ILE:HD12	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:FU:595:GLN:HB3	10:FU:596:PRO:HD2	2.03	0.40
12:FI:371:ILE:HG21	12:FI:373:ARG:HH21	1.86	0.40
13:BZ:104:PRO:HA	13:BZ:107:TYR:CE2	2.56	0.40
13:B6:88:TRP:CE2	13:B6:134:PRO:HD3	2.56	0.40
7:AZ:920:LYS:O	10:Fd:19:LEU:CD2	2.47	0.40
7:A1:470:THR:HG22	7:A1:471:ALA:N	2.35	0.40
9:LM:170:ILE:HD12	9:LN:176:SER:HB2	2.03	0.40
10:FJ:558:ILE:CG2	10:FK:558:ILE:HD12	2.51	0.40
12:FI:294:ASN:HA	12:FH:285:ARG:HH11	1.86	0.40
12:F2:294:ASN:HA	12:F1:285:ARG:HH11	1.87	0.40
7:AY:807:ARG:HG2	7:AY:807:ARG:HH21	1.85	0.40
7:AY:1001:PHE:HA	10:FA:19:LEU:HD21	2.02	0.40
7:A1:466:GLU:H	7:A1:466:GLU:HG2	1.76	0.40
7:A1:1027:GLN:CD	8:A9:15:TYR:CE1	3.00	0.40
9:LJ:170:ILE:HD12	9:LK:176:SER:HB2	2.03	0.40
10:Fd:196:ARG:HD3	12:Fr:8:HIS:HB2	2.03	0.40
12:FR:371:ILE:HG21	12:FR:373:ARG:HH21	1.86	0.40
1:AT:340:GLU:HG2	1:AN:343:MET:HG3	2.02	0.40
1:AP:374:LYS:N	1:AP:375:PRO:HD3	2.37	0.40
3:BU:3:THR:HG22	3:BU:4:LEU:N	2.36	0.40
4:AI:100:GLN:CD	7:AZ:645:ASP:OD2	2.63	0.40
7:A1:515:PHE:CE1	7:A1:536:ILE:HD11	2.57	0.40
8:Ad:80:THR:HA	8:Ad:311:ARG:HH12	1.79	0.40
10:Fd:368:THR:HG22	10:Fd:368:THR:O	2.22	0.40
10:Fm:595:GLN:HB3	10:Fm:596:PRO:HD2	2.03	0.40
10:Fv:368:THR:O	10:Fv:368:THR:HG22	2.22	0.40
12:FP:351:ARG:HG3	12:FP:352:LEU:N	2.36	0.40
14:AC:74:LYS:HE2	14:AC:93:VAL:O	2.21	0.40
1:AV:220:MET:HE3	7:A0:747:PHE:CZ	2.57	0.40
2:BO:58:TYR:CE1	3:BV:144:ASN:HB2	2.57	0.40
4:AJ:209:GLY:C	4:AJ:210:GLU:HG3	2.46	0.40
7:A0:515:PHE:CE1	7:A0:536:ILE:HD11	2.57	0.40
7:A1:848:LEU:H	7:A1:848:LEU:CD2	2.35	0.40
9:LG:170:ILE:HD12	9:LH:176:SER:HB2	2.03	0.40
10:Fd:195:ARG:HD3	12:F5:9:TYR:CZ	2.55	0.40
12:FY:351:ARG:HG3	12:FY:352:LEU:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	AM	652/655 (100%)	624 (96%)	28 (4%)	0	100	100
1	AN	652/655 (100%)	622 (95%)	30 (5%)	0	100	100
1	AO	652/655 (100%)	630 (97%)	22 (3%)	0	100	100
1	AP	652/655 (100%)	625 (96%)	27 (4%)	0	100	100
1	AQ	652/655 (100%)	630 (97%)	21 (3%)	1 (0%)	43	70
1	AR	652/655 (100%)	624 (96%)	28 (4%)	0	100	100
1	AS	646/655 (99%)	610 (94%)	36 (6%)	0	100	100
1	AT	644/655 (98%)	623 (97%)	21 (3%)	0	100	100
1	AU	646/655 (99%)	616 (95%)	30 (5%)	0	100	100
1	AV	644/655 (98%)	616 (96%)	28 (4%)	0	100	100
1	AW	646/655 (99%)	616 (95%)	30 (5%)	0	100	100
1	AX	644/655 (98%)	614 (95%)	30 (5%)	0	100	100
2	BK	297/350 (85%)	273 (92%)	24 (8%)	0	100	100
2	BL	217/350 (62%)	200 (92%)	16 (7%)	1 (0%)	24	52
2	BM	297/350 (85%)	276 (93%)	21 (7%)	0	100	100
2	BN	217/350 (62%)	200 (92%)	16 (7%)	1 (0%)	24	52
2	BO	297/350 (85%)	275 (93%)	22 (7%)	0	100	100
2	BP	217/350 (62%)	198 (91%)	18 (8%)	1 (0%)	24	52
3	BQ	216/308 (70%)	208 (96%)	8 (4%)	0	100	100
3	BR	216/308 (70%)	207 (96%)	8 (4%)	1 (0%)	24	52
3	BS	216/308 (70%)	206 (95%)	10 (5%)	0	100	100
3	BT	216/308 (70%)	211 (98%)	4 (2%)	1 (0%)	24	52
3	BU	216/308 (70%)	207 (96%)	8 (4%)	1 (0%)	24	52
3	BV	216/308 (70%)	210 (97%)	6 (3%)	0	100	100
4	AG	210/212 (99%)	206 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AH	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
4	AI	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
4	AJ	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
4	AK	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
4	AL	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
5	BB	560/576 (97%)	533 (95%)	27 (5%)	0	100	100
5	BC	560/576 (97%)	533 (95%)	27 (5%)	0	100	100
5	BD	560/576 (97%)	529 (94%)	31 (6%)	0	100	100
6	BA	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
7	A0	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	A1	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	A2	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	A3	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	AY	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
7	AZ	1029/1032 (100%)	965 (94%)	64 (6%)	0	100	100
8	A4	332/341 (97%)	308 (93%)	24 (7%)	0	100	100
8	A5	332/341 (97%)	308 (93%)	24 (7%)	0	100	100
8	A6	332/341 (97%)	310 (93%)	22 (7%)	0	100	100
8	A7	332/341 (97%)	318 (96%)	14 (4%)	0	100	100
8	A8	332/341 (97%)	311 (94%)	21 (6%)	0	100	100
8	A9	332/341 (97%)	313 (94%)	19 (6%)	0	100	100
8	Aa	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Ab	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Ac	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Ad	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Ae	327/341 (96%)	306 (94%)	21 (6%)	0	100	100
8	Af	327/341 (96%)	307 (94%)	20 (6%)	0	100	100
9	LA	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LB	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LC	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LD	301/303 (99%)	294 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	LE	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LF	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LG	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LH	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LI	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LJ	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LK	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LL	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LM	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LN	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LO	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
9	LP	301/303 (99%)	294 (98%)	7 (2%)	0	100	100
9	LQ	301/303 (99%)	295 (98%)	6 (2%)	0	100	100
9	LR	301/303 (99%)	290 (96%)	11 (4%)	0	100	100
10	FA	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	FB	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	FC	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	FJ	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	FK	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	FL	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	FS	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	FT	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	FU	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	Fb	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	Fc	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	Fd	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	Fk	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	Fl	605/607 (100%)	577 (95%)	28 (5%)	0	100	100
10	Fm	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
10	Ft	605/607 (100%)	570 (94%)	35 (6%)	0	100	100
10	Fu	605/607 (100%)	577 (95%)	28 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	Fv	605/607 (100%)	568 (94%)	37 (6%)	0	100	100
11	FD	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	FE	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	FF	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	FM	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	FN	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	FO	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	FV	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	FW	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	FX	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fe	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	Ff	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fg	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fn	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	Fo	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	Fp	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fw	220/223 (99%)	211 (96%)	9 (4%)	0	100	100
11	Fx	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
11	Fy	220/223 (99%)	212 (96%)	8 (4%)	0	100	100
12	F1	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	F2	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	FG	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	FH	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	FI	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	FP	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	FQ	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	FR	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	FY	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	FZ	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	Fa	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	Fh	444/448 (99%)	430 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Fi	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	Fj	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	Fq	444/448 (99%)	430 (97%)	14 (3%)	0	100	100
12	Fr	444/448 (99%)	421 (95%)	23 (5%)	0	100	100
12	Fs	445/448 (99%)	428 (96%)	17 (4%)	0	100	100
12	Fz	444/448 (99%)	429 (97%)	15 (3%)	0	100	100
13	B1	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
13	B2	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
13	B3	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
13	B4	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
13	B5	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
13	B6	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
13	B7	160/163 (98%)	152 (95%)	8 (5%)	0	100	100
13	B8	160/163 (98%)	151 (94%)	9 (6%)	0	100	100
13	BW	160/163 (98%)	154 (96%)	6 (4%)	0	100	100
13	BX	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
13	BY	160/163 (98%)	153 (96%)	7 (4%)	0	100	100
13	BZ	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
14	AA	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
14	AB	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
14	AC	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
14	AD	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
14	AE	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
14	AF	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
15	BE	377/380 (99%)	363 (96%)	14 (4%)	0	100	100
15	BF	377/380 (99%)	360 (96%)	17 (4%)	0	100	100
15	BG	377/380 (99%)	362 (96%)	15 (4%)	0	100	100
16	BH	31/577 (5%)	27 (87%)	4 (13%)	0	100	100
16	BI	31/577 (5%)	30 (97%)	1 (3%)	0	100	100
16	BJ	31/577 (5%)	27 (87%)	4 (13%)	0	100	100
All	All	55991/59290 (94%)	53339 (95%)	2645 (5%)	7 (0%)	100	100

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BN	297	GLY
2	BL	297	GLY
2	BP	297	GLY
3	BR	145	ALA
3	BT	145	ALA
1	AQ	245	GLY
3	BU	145	ALA

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	AM	570/571 (100%)	562 (99%)	8 (1%)	59	69
1	AN	570/571 (100%)	563 (99%)	7 (1%)	63	72
1	AO	570/571 (100%)	563 (99%)	7 (1%)	63	72
1	AP	570/571 (100%)	561 (98%)	9 (2%)	55	67
1	AQ	570/571 (100%)	561 (98%)	9 (2%)	55	67
1	AR	570/571 (100%)	563 (99%)	7 (1%)	63	72
1	AS	565/571 (99%)	561 (99%)	4 (1%)	76	77
1	AT	563/571 (99%)	558 (99%)	5 (1%)	70	75
1	AU	565/571 (99%)	560 (99%)	5 (1%)	70	75
1	AV	563/571 (99%)	555 (99%)	8 (1%)	59	69
1	AW	565/571 (99%)	562 (100%)	3 (0%)	81	80
1	AX	563/571 (99%)	554 (98%)	9 (2%)	55	67
2	BK	257/297 (86%)	253 (98%)	4 (2%)	55	67
2	BL	199/297 (67%)	198 (100%)	1 (0%)	81	80
2	BM	257/297 (86%)	250 (97%)	7 (3%)	39	60
2	BN	199/297 (67%)	197 (99%)	2 (1%)	68	74
2	BO	257/297 (86%)	253 (98%)	4 (2%)	55	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BP	199/297 (67%)	196 (98%)	3 (2%)	57	68
3	BQ	187/256 (73%)	184 (98%)	3 (2%)	55	67
3	BR	187/256 (73%)	187 (100%)	0	100	100
3	BS	187/256 (73%)	184 (98%)	3 (2%)	55	67
3	BT	187/256 (73%)	187 (100%)	0	100	100
3	BU	187/256 (73%)	183 (98%)	4 (2%)	47	64
3	BV	187/256 (73%)	185 (99%)	2 (1%)	65	73
4	AG	184/184 (100%)	184 (100%)	0	100	100
4	AH	184/184 (100%)	184 (100%)	0	100	100
4	AI	184/184 (100%)	183 (100%)	1 (0%)	81	80
4	AJ	184/184 (100%)	184 (100%)	0	100	100
4	AK	184/184 (100%)	182 (99%)	2 (1%)	65	73
4	AL	184/184 (100%)	184 (100%)	0	100	100
5	BB	474/484 (98%)	467 (98%)	7 (2%)	57	68
5	BC	474/484 (98%)	467 (98%)	7 (2%)	57	68
5	BD	474/484 (98%)	468 (99%)	6 (1%)	61	70
6	BA	80/80 (100%)	80 (100%)	0	100	100
7	A0	923/924 (100%)	916 (99%)	7 (1%)	73	76
7	A1	923/924 (100%)	916 (99%)	7 (1%)	73	76
7	A2	923/924 (100%)	915 (99%)	8 (1%)	70	75
7	A3	923/924 (100%)	916 (99%)	7 (1%)	73	76
7	AY	923/924 (100%)	915 (99%)	8 (1%)	70	75
7	AZ	923/924 (100%)	915 (99%)	8 (1%)	70	75
8	A4	293/299 (98%)	292 (100%)	1 (0%)	86	84
8	A5	293/299 (98%)	288 (98%)	5 (2%)	53	67
8	A6	293/299 (98%)	290 (99%)	3 (1%)	68	74
8	A7	293/299 (98%)	288 (98%)	5 (2%)	53	67
8	A8	293/299 (98%)	287 (98%)	6 (2%)	48	65
8	A9	293/299 (98%)	289 (99%)	4 (1%)	59	69
8	Aa	288/299 (96%)	283 (98%)	5 (2%)	53	67
8	Ab	288/299 (96%)	283 (98%)	5 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Ac	288/299 (96%)	283 (98%)	5 (2%)	53	67
8	Ad	288/299 (96%)	283 (98%)	5 (2%)	53	67
8	Ae	288/299 (96%)	283 (98%)	5 (2%)	53	67
8	Af	288/299 (96%)	283 (98%)	5 (2%)	53	67
9	LA	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LB	245/245 (100%)	245 (100%)	0	100	100
9	LC	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LD	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LE	245/245 (100%)	245 (100%)	0	100	100
9	LF	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LG	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LH	245/245 (100%)	245 (100%)	0	100	100
9	LI	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LJ	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LK	245/245 (100%)	245 (100%)	0	100	100
9	LL	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LM	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LN	245/245 (100%)	245 (100%)	0	100	100
9	LO	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LP	245/245 (100%)	244 (100%)	1 (0%)	84	82
9	LQ	245/245 (100%)	245 (100%)	0	100	100
9	LR	245/245 (100%)	244 (100%)	1 (0%)	84	82
10	FA	509/509 (100%)	503 (99%)	6 (1%)	63	72
10	FB	509/509 (100%)	505 (99%)	4 (1%)	73	76
10	FC	509/509 (100%)	507 (100%)	2 (0%)	84	82
10	FJ	509/509 (100%)	503 (99%)	6 (1%)	63	72
10	FK	509/509 (100%)	504 (99%)	5 (1%)	68	74
10	FL	509/509 (100%)	506 (99%)	3 (1%)	78	79
10	FS	509/509 (100%)	503 (99%)	6 (1%)	63	72
10	FT	509/509 (100%)	504 (99%)	5 (1%)	68	74
10	FU	509/509 (100%)	507 (100%)	2 (0%)	84	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	Fb	509/509 (100%)	503 (99%)	6 (1%)	63	72
10	Fc	509/509 (100%)	504 (99%)	5 (1%)	68	74
10	Fd	509/509 (100%)	506 (99%)	3 (1%)	78	79
10	Fk	509/509 (100%)	503 (99%)	6 (1%)	63	72
10	Fl	509/509 (100%)	504 (99%)	5 (1%)	68	74
10	Fm	509/509 (100%)	507 (100%)	2 (0%)	84	82
10	Ft	509/509 (100%)	503 (99%)	6 (1%)	63	72
10	Fu	509/509 (100%)	505 (99%)	4 (1%)	73	76
10	Fv	509/509 (100%)	506 (99%)	3 (1%)	78	79
11	FD	183/184 (100%)	181 (99%)	2 (1%)	65	73
11	FE	183/184 (100%)	182 (100%)	1 (0%)	81	80
11	FF	183/184 (100%)	180 (98%)	3 (2%)	55	67
11	FM	183/184 (100%)	181 (99%)	2 (1%)	65	73
11	FN	183/184 (100%)	182 (100%)	1 (0%)	81	80
11	FO	183/184 (100%)	180 (98%)	3 (2%)	55	67
11	FV	183/184 (100%)	181 (99%)	2 (1%)	65	73
11	FW	183/184 (100%)	182 (100%)	1 (0%)	81	80
11	FX	183/184 (100%)	180 (98%)	3 (2%)	55	67
11	Fe	183/184 (100%)	181 (99%)	2 (1%)	65	73
11	Ff	183/184 (100%)	182 (100%)	1 (0%)	81	80
11	Fg	183/184 (100%)	180 (98%)	3 (2%)	55	67
11	Fn	183/184 (100%)	181 (99%)	2 (1%)	65	73
11	Fo	183/184 (100%)	182 (100%)	1 (0%)	81	80
11	Fp	183/184 (100%)	180 (98%)	3 (2%)	55	67
11	Fw	183/184 (100%)	181 (99%)	2 (1%)	65	73
11	Fx	183/184 (100%)	182 (100%)	1 (0%)	81	80
11	Fy	183/184 (100%)	180 (98%)	3 (2%)	55	67
12	F1	357/361 (99%)	352 (99%)	5 (1%)	59	69
12	F2	360/361 (100%)	354 (98%)	6 (2%)	53	67
12	FG	360/361 (100%)	357 (99%)	3 (1%)	73	76
12	FH	357/361 (99%)	352 (99%)	5 (1%)	59	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	FI	360/361 (100%)	354 (98%)	6 (2%)	53	67
12	FP	360/361 (100%)	357 (99%)	3 (1%)	73	76
12	FQ	357/361 (99%)	352 (99%)	5 (1%)	59	69
12	FR	360/361 (100%)	354 (98%)	6 (2%)	53	67
12	FY	360/361 (100%)	357 (99%)	3 (1%)	73	76
12	FZ	357/361 (99%)	352 (99%)	5 (1%)	59	69
12	Fa	360/361 (100%)	354 (98%)	6 (2%)	53	67
12	Fh	360/361 (100%)	357 (99%)	3 (1%)	73	76
12	Fi	357/361 (99%)	352 (99%)	5 (1%)	59	69
12	Fj	360/361 (100%)	354 (98%)	6 (2%)	53	67
12	Fq	360/361 (100%)	357 (99%)	3 (1%)	73	76
12	Fr	357/361 (99%)	352 (99%)	5 (1%)	59	69
12	Fs	360/361 (100%)	354 (98%)	6 (2%)	53	67
12	Fz	360/361 (100%)	357 (99%)	3 (1%)	73	76
13	B1	138/139 (99%)	138 (100%)	0	100	100
13	B2	138/139 (99%)	138 (100%)	0	100	100
13	B3	138/139 (99%)	138 (100%)	0	100	100
13	B4	138/139 (99%)	138 (100%)	0	100	100
13	B5	138/139 (99%)	138 (100%)	0	100	100
13	B6	138/139 (99%)	138 (100%)	0	100	100
13	B7	138/139 (99%)	138 (100%)	0	100	100
13	B8	138/139 (99%)	138 (100%)	0	100	100
13	BW	138/139 (99%)	138 (100%)	0	100	100
13	BX	138/139 (99%)	138 (100%)	0	100	100
13	BY	138/139 (99%)	138 (100%)	0	100	100
13	BZ	138/139 (99%)	138 (100%)	0	100	100
14	AA	125/126 (99%)	124 (99%)	1 (1%)	73	76
14	AB	125/126 (99%)	123 (98%)	2 (2%)	55	67
14	AC	125/126 (99%)	124 (99%)	1 (1%)	73	76
14	AD	125/126 (99%)	124 (99%)	1 (1%)	73	76
14	AE	125/126 (99%)	124 (99%)	1 (1%)	73	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AF	125/126 (99%)	124 (99%)	1 (1%)	73	76
15	BE	333/334 (100%)	328 (98%)	5 (2%)	57	68
15	BF	333/334 (100%)	328 (98%)	5 (2%)	57	68
15	BG	333/334 (100%)	329 (99%)	4 (1%)	63	72
16	BH	27/497 (5%)	26 (96%)	1 (4%)	30	55
16	BI	27/497 (5%)	26 (96%)	1 (4%)	30	55
16	BJ	27/497 (5%)	27 (100%)	0	100	100
All	All	47738/50237 (95%)	47268 (99%)	470 (1%)	65	74

All (470) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AT	60	LEU
1	AT	168	LEU
1	AT	291	ASP
1	AT	305	LYS
1	AT	407	LEU
1	AV	60	LEU
1	AV	168	LEU
1	AV	291	ASP
1	AV	305	LYS
1	AV	330	ARG
1	AV	338	LYS
1	AV	400	ASP
1	AV	462	ASN
1	AX	60	LEU
1	AX	168	LEU
1	AX	291	ASP
1	AX	305	LYS
1	AX	338	LYS
1	AX	367	GLN
1	AX	400	ASP
1	AX	407	LEU
1	AX	462	ASN
1	AS	168	LEU
1	AS	258	LEU
1	AS	280	ARG
1	AS	305	LYS
1	AU	168	LEU
1	AU	258	LEU

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Mol	Chain	Res	Type
1	AU	259	GLU
1	AU	280	ARG
1	AU	305	LYS
1	AW	168	LEU
1	AW	305	LYS
1	AW	651	GLU
1	AN	9	TYR
1	AN	45	GLN
1	AN	115	VAL
1	AN	145	ASN
1	AN	183	LEU
1	AN	276	ILE
1	AN	452	ARG
1	AP	9	TYR
1	AP	45	GLN
1	AP	145	ASN
1	AP	203	VAL
1	AP	276	ILE
1	AP	366	VAL
1	AP	452	ARG
1	AP	469	LYS
1	AP	590	VAL
1	AR	30	ILE
1	AR	43	GLU
1	AR	145	ASN
1	AR	276	ILE
1	AR	366	VAL
1	AR	452	ARG
1	AR	595	ASP
1	AM	67	TYR
1	AM	115	VAL
1	AM	257	VAL
1	AM	273	GLN
1	AM	304	ASN
1	AM	366	VAL
1	AM	452	ARG
1	AM	625	ASP
1	AO	121	GLU
1	AO	257	VAL
1	AO	276	ILE
1	AO	366	VAL
1	AO	452	ARG

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Mol	Chain	Res	Type
1	AO	625	ASP
1	AO	638	GLU
1	AQ	67	TYR
1	AQ	273	GLN
1	AQ	276	ILE
1	AQ	304	ASN
1	AQ	366	VAL
1	AQ	452	ARG
1	AQ	496	ASN
1	AQ	625	ASP
1	AQ	638	GLU
2	BL	290	ASP
2	BN	213	GLU
2	BN	290	ASP
2	BP	213	GLU
2	BP	290	ASP
2	BP	292	ARG
2	BK	29	ASN
2	BK	78	ARG
2	BK	200	ARG
2	BK	289	MET
2	BM	29	ASN
2	BM	78	ARG
2	BM	80	PHE
2	BM	139	ARG
2	BM	200	ARG
2	BM	289	MET
2	BM	319	ILE
2	BO	29	ASN
2	BO	78	ARG
2	BO	200	ARG
2	BO	289	MET
3	BQ	151	THR
3	BQ	167	GLU
3	BQ	206	ARG
3	BS	167	GLU
3	BS	206	ARG
3	BS	213	VAL
3	BU	89	ILE
3	BU	167	GLU
3	BU	206	ARG
3	BU	213	VAL

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Mol	Chain	Res	Type
3	BV	165	ASP
3	BV	206	ARG
4	AI	17	LYS
4	AK	16	VAL
4	AK	58	GLU
5	BB	27	VAL
5	BB	45	THR
5	BB	176	ILE
5	BB	232	ASN
5	BB	323	ARG
5	BB	442	MET
5	BB	536	THR
5	BC	2	ILE
5	BC	27	VAL
5	BC	45	THR
5	BC	232	ASN
5	BC	323	ARG
5	BC	442	MET
5	BC	536	THR
5	BD	2	ILE
5	BD	27	VAL
5	BD	176	ILE
5	BD	323	ARG
5	BD	442	MET
5	BD	536	THR
7	AY	22	ILE
7	AY	327	ARG
7	AY	485	HIS
7	AY	529	THR
7	AY	605	VAL
7	AY	881	ARG
7	AY	922	ASP
7	AY	995	ASP
7	A2	22	ILE
7	A2	327	ARG
7	A2	485	HIS
7	A2	529	THR
7	A2	605	VAL
7	A2	881	ARG
7	A2	922	ASP
7	A2	995	ASP
7	AZ	22	ILE

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Mol	Chain	Res	Type
7	AZ	327	ARG
7	AZ	485	HIS
7	AZ	529	THR
7	AZ	605	VAL
7	AZ	881	ARG
7	AZ	922	ASP
7	AZ	995	ASP
7	A0	22	ILE
7	A0	327	ARG
7	A0	485	HIS
7	A0	529	THR
7	A0	605	VAL
7	A0	881	ARG
7	A0	995	ASP
7	A1	22	ILE
7	A1	327	ARG
7	A1	485	HIS
7	A1	529	THR
7	A1	605	VAL
7	A1	881	ARG
7	A1	995	ASP
7	A3	22	ILE
7	A3	327	ARG
7	A3	485	HIS
7	A3	529	THR
7	A3	605	VAL
7	A3	881	ARG
7	A3	995	ASP
8	Ad	95	CYS
8	Ad	109	ASN
8	Ad	120	VAL
8	Ad	208	ASN
8	Ad	237	THR
8	Ac	95	CYS
8	Ac	109	ASN
8	Ac	120	VAL
8	Ac	208	ASN
8	Ac	237	THR
8	Ab	95	CYS
8	Ab	109	ASN
8	Ab	120	VAL
8	Ab	208	ASN

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Mol	Chain	Res	Type
8	Ab	237	THR
8	Aa	95	CYS
8	Aa	109	ASN
8	Aa	120	VAL
8	Aa	208	ASN
8	Aa	237	THR
8	Ae	95	CYS
8	Ae	109	ASN
8	Ae	120	VAL
8	Ae	208	ASN
8	Ae	237	THR
8	Af	95	CYS
8	Af	109	ASN
8	Af	120	VAL
8	Af	208	ASN
8	Af	237	THR
8	A4	155	THR
8	A5	19	ILE
8	A5	27	LYS
8	A5	184	ASN
8	A5	333	GLU
8	A5	341	PHE
8	A6	155	THR
8	A6	241	ASN
8	A6	333	GLU
8	A7	27	LYS
8	A7	241	ASN
8	A7	245	LEU
8	A7	337	LEU
8	A7	341	PHE
8	A8	27	LYS
8	A8	101	ASP
8	A8	155	THR
8	A8	245	LEU
8	A8	333	GLU
8	A8	341	PHE
8	A9	27	LYS
8	A9	155	THR
8	A9	245	LEU
8	A9	327	ARG
9	LA	234	THR
9	LC	278	CYS

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Mol	Chain	Res	Type
9	LD	234	THR
9	LF	278	CYS
9	LG	234	THR
9	LI	278	CYS
9	LJ	234	THR
9	LL	278	CYS
9	LM	234	THR
9	LO	278	CYS
9	LP	234	THR
9	LR	278	CYS
10	FA	176	ASP
10	FA	198	ASN
10	FA	212	ASN
10	FA	380	GLU
10	FA	558	ILE
10	FA	564	ASP
10	FB	91	ASN
10	FB	161	SER
10	FB	369	ASN
10	FB	394	ILE
10	FC	2	LYS
10	FC	214	ASP
10	FJ	176	ASP
10	FJ	198	ASN
10	FJ	212	ASN
10	FJ	380	GLU
10	FJ	558	ILE
10	FJ	564	ASP
10	FK	91	ASN
10	FK	161	SER
10	FK	369	ASN
10	FK	394	ILE
10	FK	531	THR
10	FL	2	LYS
10	FL	198	ASN
10	FL	214	ASP
10	FS	176	ASP
10	FS	198	ASN
10	FS	212	ASN
10	FS	380	GLU
10	FS	558	ILE
10	FS	564	ASP

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Mol	Chain	Res	Type
10	FT	91	ASN
10	FT	161	SER
10	FT	369	ASN
10	FT	394	ILE
10	FT	531	THR
10	FU	2	LYS
10	FU	214	ASP
10	Fb	176	ASP
10	Fb	198	ASN
10	Fb	212	ASN
10	Fb	380	GLU
10	Fb	558	ILE
10	Fb	564	ASP
10	Fc	91	ASN
10	Fc	161	SER
10	Fc	369	ASN
10	Fc	394	ILE
10	Fc	531	THR
10	Fd	2	LYS
10	Fd	198	ASN
10	Fd	214	ASP
10	Fk	176	ASP
10	Fk	198	ASN
10	Fk	212	ASN
10	Fk	380	GLU
10	Fk	558	ILE
10	Fk	564	ASP
10	Fl	91	ASN
10	Fl	161	SER
10	Fl	369	ASN
10	Fl	394	ILE
10	Fl	531	THR
10	Fm	2	LYS
10	Fm	214	ASP
10	Ft	176	ASP
10	Ft	198	ASN
10	Ft	212	ASN
10	Ft	380	GLU
10	Ft	558	ILE
10	Ft	564	ASP
10	Fu	91	ASN
10	Fu	161	SER

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Mol	Chain	Res	Type
10	Fu	369	ASN
10	Fu	394	ILE
10	Fv	2	LYS
10	Fv	198	ASN
10	Fv	214	ASP
11	FD	4	GLU
11	FD	16	ARG
11	FE	168	ASP
11	FF	42	THR
11	FF	59	ILE
11	FF	86	GLN
11	FM	4	GLU
11	FM	16	ARG
11	FN	168	ASP
11	FO	42	THR
11	FO	59	ILE
11	FO	86	GLN
11	FV	4	GLU
11	FV	16	ARG
11	FW	168	ASP
11	FX	42	THR
11	FX	59	ILE
11	FX	86	GLN
11	Fe	4	GLU
11	Fe	16	ARG
11	Ff	168	ASP
11	Fg	42	THR
11	Fg	59	ILE
11	Fg	86	GLN
11	Fn	4	GLU
11	Fn	16	ARG
11	Fo	168	ASP
11	Fp	42	THR
11	Fp	59	ILE
11	Fp	86	GLN
11	Fw	4	GLU
11	Fw	16	ARG
11	Fx	168	ASP
11	Fy	42	THR
11	Fy	59	ILE
11	Fy	86	GLN
12	FG	49	LEU

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Mol	Chain	Res	Type
12	FG	116	ARG
12	FG	447	ARG
12	FI	3	GLN
12	FI	235	SER
12	FI	260	LEU
12	FI	293	ASP
12	FI	373	ARG
12	FI	411	SER
12	FH	208	THR
12	FH	285	ARG
12	FH	288	ASN
12	FH	369	ASN
12	FH	430	GLU
12	FP	49	LEU
12	FP	116	ARG
12	FP	447	ARG
12	FR	3	GLN
12	FR	235	SER
12	FR	260	LEU
12	FR	293	ASP
12	FR	373	ARG
12	FR	411	SER
12	FQ	208	THR
12	FQ	285	ARG
12	FQ	288	ASN
12	FQ	369	ASN
12	FQ	430	GLU
12	FY	49	LEU
12	FY	116	ARG
12	FY	447	ARG
12	Fa	3	GLN
12	Fa	235	SER
12	Fa	260	LEU
12	Fa	293	ASP
12	Fa	373	ARG
12	Fa	411	SER
12	FZ	208	THR
12	FZ	285	ARG
12	FZ	288	ASN
12	FZ	369	ASN
12	FZ	430	GLU
12	Fh	49	LEU

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Mol	Chain	Res	Type
12	Fh	116	ARG
12	Fh	447	ARG
12	Fj	3	GLN
12	Fj	235	SER
12	Fj	260	LEU
12	Fj	293	ASP
12	Fj	373	ARG
12	Fj	411	SER
12	Fi	208	THR
12	Fi	285	ARG
12	Fi	288	ASN
12	Fi	369	ASN
12	Fi	430	GLU
12	Fq	49	LEU
12	Fq	116	ARG
12	Fq	447	ARG
12	Fs	3	GLN
12	Fs	235	SER
12	Fs	260	LEU
12	Fs	293	ASP
12	Fs	373	ARG
12	Fs	411	SER
12	Fr	208	THR
12	Fr	285	ARG
12	Fr	288	ASN
12	Fr	369	ASN
12	Fr	430	GLU
12	Fz	49	LEU
12	Fz	116	ARG
12	Fz	447	ARG
12	F2	3	GLN
12	F2	235	SER
12	F2	260	LEU
12	F2	293	ASP
12	F2	373	ARG
12	F2	411	SER
12	F1	208	THR
12	F1	285	ARG
12	F1	288	ASN
12	F1	369	ASN
12	F1	430	GLU
14	AA	66	THR

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Mol	Chain	Res	Type
14	AB	66	THR
14	AB	113	VAL
14	AC	113	VAL
14	AD	113	VAL
14	AE	66	THR
14	AF	113	VAL
15	BE	47	ASN
15	BE	215	GLN
15	BE	231	ASP
15	BE	370	VAL
15	BE	379	SER
15	BF	47	ASN
15	BF	64	ASN
15	BF	215	GLN
15	BF	326	ASP
15	BF	375	LYS
15	BG	47	ASN
15	BG	64	ASN
15	BG	215	GLN
15	BG	370	VAL
16	BH	558	ARG
16	BI	554	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (645) such sidechains are listed below:

Mol	Chain	Res	Type
1	AT	16	ASN
1	AT	33	GLN
1	AT	45	GLN
1	AT	96	GLN
1	AT	172	ASN
1	AT	239	ASN
1	AT	304	ASN
1	AT	509	ASN
1	AT	624	GLN
1	AT	639	ASN
1	AV	16	ASN
1	AV	96	GLN
1	AV	172	ASN
1	AV	239	ASN
1	AV	304	ASN
1	AV	509	ASN

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Mol	Chain	Res	Type
1	AV	624	GLN
1	AX	16	ASN
1	AX	33	GLN
1	AX	96	GLN
1	AX	172	ASN
1	AX	239	ASN
1	AX	304	ASN
1	AX	367	GLN
1	AX	451	ASN
1	AX	462	ASN
1	AX	509	ASN
1	AX	624	GLN
1	AS	33	GLN
1	AS	55	ASN
1	AS	64	ASN
1	AS	70	GLN
1	AS	145	ASN
1	AS	222	HIS
1	AS	239	ASN
1	AS	304	ASN
1	AS	451	ASN
1	AS	462	ASN
1	AS	464	ASN
1	AS	509	ASN
1	AU	10	GLN
1	AU	55	ASN
1	AU	64	ASN
1	AU	145	ASN
1	AU	222	HIS
1	AU	367	GLN
1	AU	451	ASN
1	AU	464	ASN
1	AU	509	ASN
1	AW	64	ASN
1	AW	70	GLN
1	AW	145	ASN
1	AW	222	HIS
1	AW	451	ASN
1	AW	464	ASN
1	AN	92	GLN
1	AN	273	GLN
1	AN	336	GLN

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Mol	Chain	Res	Type
1	AN	372	GLN
1	AN	425	ASN
1	AN	436	GLN
1	AN	479	HIS
1	AN	548	ASN
1	AN	566	GLN
1	AP	182	GLN
1	AP	273	GLN
1	AP	309	ASN
1	AP	367	GLN
1	AP	425	ASN
1	AP	464	ASN
1	AP	548	ASN
1	AP	566	GLN
1	AR	145	ASN
1	AR	182	GLN
1	AR	273	GLN
1	AR	309	ASN
1	AR	336	GLN
1	AR	367	GLN
1	AR	372	GLN
1	AR	425	ASN
1	AR	464	ASN
1	AR	479	HIS
1	AR	548	ASN
1	AR	566	GLN
1	AR	596	ASN
1	AR	610	GLN
1	AM	8	ASN
1	AM	97	ASN
1	AM	182	GLN
1	AM	336	GLN
1	AM	451	ASN
1	AO	8	ASN
1	AO	64	ASN
1	AO	92	GLN
1	AO	97	ASN
1	AO	165	ASN
1	AO	336	GLN
1	AO	451	ASN
1	AO	548	ASN
1	AO	596	ASN

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Mol	Chain	Res	Type
1	AQ	64	ASN
1	AQ	97	ASN
1	AQ	165	ASN
1	AQ	182	GLN
1	AQ	304	ASN
1	AQ	336	GLN
1	AQ	425	ASN
1	AQ	451	ASN
1	AQ	596	ASN
2	BL	46	ASN
2	BL	188	ASN
2	BL	302	GLN
2	BL	313	HIS
2	BN	46	ASN
2	BN	313	HIS
2	BP	188	ASN
2	BP	313	HIS
2	BK	207	GLN
2	BK	225	ASN
2	BK	302	GLN
2	BK	313	HIS
2	BK	343	ASN
2	BM	300	GLN
2	BM	302	GLN
2	BO	127	HIS
2	BO	225	ASN
2	BO	302	GLN
2	BO	313	HIS
2	BO	343	ASN
3	BR	35	GLN
3	BT	35	GLN
3	BU	235	ASN
3	BU	250	GLN
3	BV	35	GLN
3	BV	193	GLN
4	AH	100	GLN
4	AH	146	GLN
4	AJ	142	HIS
4	AL	141	ASN
4	AL	143	GLN
4	AI	141	ASN
4	AI	142	HIS

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Mol	Chain	Res	Type
5	BB	145	ASN
5	BB	283	GLN
5	BB	318	ASN
5	BB	400	HIS
5	BC	145	ASN
5	BC	318	ASN
5	BC	385	ASN
5	BC	400	HIS
5	BC	479	ASN
5	BD	145	ASN
5	BD	318	ASN
7	AY	207	HIS
7	AY	408	GLN
7	AY	420	ASN
7	AY	532	HIS
7	AY	664	ASN
7	AY	680	ASN
7	AY	918	ASN
7	AY	1027	GLN
7	A2	136	ASN
7	A2	207	HIS
7	A2	267	ASN
7	A2	408	GLN
7	A2	420	ASN
7	A2	485	HIS
7	A2	532	HIS
7	A2	581	GLN
7	A2	667	HIS
7	A2	683	HIS
7	A2	850	ASN
7	A2	908	HIS
7	A2	918	ASN
7	A2	1027	GLN
7	AZ	207	HIS
7	AZ	267	ASN
7	AZ	360	ASN
7	AZ	408	GLN
7	AZ	420	ASN
7	AZ	532	HIS
7	AZ	683	HIS
7	AZ	850	ASN
7	AZ	908	HIS

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Mol	Chain	Res	Type
7	AZ	918	ASN
7	AZ	1027	GLN
7	A0	207	HIS
7	A0	267	ASN
7	A0	360	ASN
7	A0	408	GLN
7	A0	532	HIS
7	A0	683	HIS
7	A0	908	HIS
7	A0	918	ASN
7	A0	1027	GLN
7	A1	207	HIS
7	A1	267	ASN
7	A1	408	GLN
7	A1	420	ASN
7	A1	532	HIS
7	A1	664	ASN
7	A1	667	HIS
7	A1	683	HIS
7	A1	908	HIS
7	A1	918	ASN
7	A1	1027	GLN
7	A3	207	HIS
7	A3	223	GLN
7	A3	267	ASN
7	A3	408	GLN
7	A3	420	ASN
7	A3	532	HIS
7	A3	908	HIS
7	A3	918	ASN
7	A3	1027	GLN
8	Ad	208	ASN
8	Ad	239	GLN
8	Ad	278	GLN
8	Ac	208	ASN
8	Ac	239	GLN
8	Ac	278	GLN
8	Ab	208	ASN
8	Ab	239	GLN
8	Ab	278	GLN
8	Aa	208	ASN
8	Aa	239	GLN

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Mol	Chain	Res	Type
8	Aa	278	GLN
8	Ae	208	ASN
8	Ae	239	GLN
8	Ae	278	GLN
8	Af	208	ASN
8	Af	239	GLN
8	Af	278	GLN
8	A4	81	ASN
8	A4	244	ASN
8	A4	312	GLN
8	A4	336	ASN
8	A5	41	GLN
8	A5	71	ASN
8	A5	81	ASN
8	A5	278	GLN
8	A5	336	ASN
8	A6	234	ASN
8	A6	336	ASN
8	A7	71	ASN
8	A7	153	ASN
8	A7	244	ASN
8	A7	336	ASN
8	A8	239	GLN
8	A8	312	GLN
8	A8	336	ASN
8	A9	41	GLN
8	A9	71	ASN
8	A9	244	ASN
8	A9	278	GLN
8	A9	323	GLN
8	A9	336	ASN
9	LA	32	ASN
9	LB	145	ASN
9	LB	218	GLN
9	LC	17	ASN
9	LC	145	ASN
9	LD	32	ASN
9	LE	145	ASN
9	LE	218	GLN
9	LF	17	ASN
9	LF	145	ASN
9	LH	145	ASN

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Mol	Chain	Res	Type
9	LH	218	GLN
9	LI	17	ASN
9	LI	145	ASN
9	LJ	32	ASN
9	LK	145	ASN
9	LK	218	GLN
9	LL	17	ASN
9	LL	145	ASN
9	LN	145	ASN
9	LN	218	GLN
9	LO	145	ASN
9	LQ	145	ASN
9	LQ	218	GLN
9	LR	17	ASN
9	LR	145	ASN
10	FA	3	GLN
10	FA	179	ASN
10	FA	212	ASN
10	FA	409	GLN
10	FA	512	ASN
10	FA	553	HIS
10	FA	589	ASN
10	FB	62	ASN
10	FB	192	ASN
10	FB	354	ASN
10	FB	357	GLN
10	FB	369	ASN
10	FB	471	HIS
10	FB	509	ASN
10	FC	212	ASN
10	FC	262	ASN
10	FC	369	ASN
10	FC	393	ASN
10	FC	514	ASN
10	FC	562	GLN
10	FJ	3	GLN
10	FJ	79	ASN
10	FJ	179	ASN
10	FJ	409	GLN
10	FJ	512	ASN
10	FJ	553	HIS
10	FJ	562	GLN

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Mol	Chain	Res	Type
10	FJ	589	ASN
10	FK	62	ASN
10	FK	192	ASN
10	FK	198	ASN
10	FK	354	ASN
10	FK	357	GLN
10	FK	369	ASN
10	FK	471	HIS
10	FK	509	ASN
10	FL	262	ASN
10	FL	369	ASN
10	FL	393	ASN
10	FL	514	ASN
10	FL	562	GLN
10	FS	3	GLN
10	FS	79	ASN
10	FS	179	ASN
10	FS	212	ASN
10	FS	409	GLN
10	FS	512	ASN
10	FS	553	HIS
10	FS	562	GLN
10	FS	589	ASN
10	FT	62	ASN
10	FT	310	ASN
10	FT	354	ASN
10	FT	357	GLN
10	FT	369	ASN
10	FT	471	HIS
10	FT	509	ASN
10	FU	3	GLN
10	FU	212	ASN
10	FU	262	ASN
10	FU	369	ASN
10	FU	393	ASN
10	FU	514	ASN
10	FU	562	GLN
10	Fb	3	GLN
10	Fb	79	ASN
10	Fb	179	ASN
10	Fb	198	ASN
10	Fb	212	ASN

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Mol	Chain	Res	Type
10	Fb	409	GLN
10	Fb	512	ASN
10	Fb	562	GLN
10	Fb	589	ASN
10	Fc	62	ASN
10	Fc	198	ASN
10	Fc	354	ASN
10	Fc	357	GLN
10	Fc	369	ASN
10	Fc	471	HIS
10	Fc	509	ASN
10	Fd	262	ASN
10	Fd	369	ASN
10	Fd	393	ASN
10	Fd	514	ASN
10	Fd	562	GLN
10	Fk	3	GLN
10	Fk	179	ASN
10	Fk	198	ASN
10	Fk	212	ASN
10	Fk	409	GLN
10	Fk	512	ASN
10	Fk	553	HIS
10	Fk	589	ASN
10	Fl	62	ASN
10	Fl	354	ASN
10	Fl	357	GLN
10	Fl	369	ASN
10	Fl	471	HIS
10	Fl	553	HIS
10	Fm	79	ASN
10	Fm	212	ASN
10	Fm	262	ASN
10	Fm	369	ASN
10	Fm	393	ASN
10	Fm	514	ASN
10	Ft	3	GLN
10	Ft	79	ASN
10	Ft	179	ASN
10	Ft	409	GLN
10	Ft	512	ASN
10	Ft	553	HIS

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Mol	Chain	Res	Type
10	Ft	562	GLN
10	Ft	589	ASN
10	Fu	62	ASN
10	Fu	192	ASN
10	Fu	198	ASN
10	Fu	354	ASN
10	Fu	357	GLN
10	Fu	369	ASN
10	Fu	471	HIS
10	Fv	262	ASN
10	Fv	369	ASN
10	Fv	393	ASN
10	Fv	514	ASN
10	Fv	562	GLN
11	FD	45	GLN
11	FD	54	ASN
11	FD	150	GLN
11	FD	170	GLN
11	FD	198	GLN
11	FE	14	ASN
11	FE	34	ASN
11	FE	173	ASN
11	FF	14	ASN
11	FF	66	GLN
11	FF	86	GLN
11	FF	198	GLN
11	FF	212	ASN
11	FM	150	GLN
11	FM	170	GLN
11	FM	198	GLN
11	FN	14	ASN
11	FN	34	ASN
11	FN	173	ASN
11	FO	14	ASN
11	FO	66	GLN
11	FO	86	GLN
11	FO	198	GLN
11	FO	212	ASN
11	FV	150	GLN
11	FV	170	GLN
11	FV	198	GLN
11	FW	14	ASN

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Mol	Chain	Res	Type
11	FW	173	ASN
11	FX	14	ASN
11	FX	66	GLN
11	FX	86	GLN
11	FX	212	ASN
11	Fe	150	GLN
11	Fe	170	GLN
11	Fe	198	GLN
11	Ff	14	ASN
11	Ff	173	ASN
11	Fg	14	ASN
11	Fg	66	GLN
11	Fg	86	GLN
11	Fg	212	ASN
11	Fn	150	GLN
11	Fn	170	GLN
11	Fn	198	GLN
11	Fo	14	ASN
11	Fo	173	ASN
11	Fp	14	ASN
11	Fp	66	GLN
11	Fp	86	GLN
11	Fp	212	ASN
11	Fw	150	GLN
11	Fw	170	GLN
11	Fw	198	GLN
11	Fx	14	ASN
11	Fx	34	ASN
11	Fx	173	ASN
11	Fy	14	ASN
11	Fy	66	GLN
11	Fy	86	GLN
11	Fy	198	GLN
11	Fy	212	ASN
12	FG	4	ASN
12	FG	65	GLN
12	FG	125	HIS
12	FG	149	GLN
12	FG	324	ASN
12	FG	355	ASN
12	FG	357	ASN
12	FG	369	ASN

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Mol	Chain	Res	Type
12	FG	390	ASN
12	FG	393	ASN
12	FG	401	HIS
12	FI	8	HIS
12	FI	65	GLN
12	FI	149	GLN
12	FI	193	GLN
12	FI	294	ASN
12	FI	399	ASN
12	FI	412	ASN
12	FI	446	ASN
12	FH	65	GLN
12	FH	133	GLN
12	FH	193	GLN
12	FH	331	GLN
12	FH	343	ASN
12	FH	369	ASN
12	FH	417	ASN
12	FP	3	GLN
12	FP	65	GLN
12	FP	184	ASN
12	FP	324	ASN
12	FP	355	ASN
12	FP	357	ASN
12	FP	369	ASN
12	FP	390	ASN
12	FP	401	HIS
12	FR	4	ASN
12	FR	65	GLN
12	FR	149	GLN
12	FR	193	GLN
12	FR	294	ASN
12	FR	399	ASN
12	FR	412	ASN
12	FR	446	ASN
12	FQ	65	GLN
12	FQ	133	GLN
12	FQ	193	GLN
12	FQ	331	GLN
12	FQ	417	ASN
12	FY	4	ASN
12	FY	65	GLN

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Mol	Chain	Res	Type
12	FY	125	HIS
12	FY	324	ASN
12	FY	355	ASN
12	FY	357	ASN
12	FY	369	ASN
12	FY	390	ASN
12	Fa	8	HIS
12	Fa	149	GLN
12	Fa	193	GLN
12	Fa	294	ASN
12	Fa	399	ASN
12	Fa	412	ASN
12	Fa	446	ASN
12	FZ	65	GLN
12	FZ	193	GLN
12	FZ	331	GLN
12	FZ	369	ASN
12	FZ	417	ASN
12	Fh	3	GLN
12	Fh	65	GLN
12	Fh	125	HIS
12	Fh	324	ASN
12	Fh	355	ASN
12	Fh	357	ASN
12	Fh	369	ASN
12	Fh	390	ASN
12	Fh	401	HIS
12	Fj	4	ASN
12	Fj	193	GLN
12	Fj	294	ASN
12	Fj	399	ASN
12	Fj	412	ASN
12	Fj	446	ASN
12	Fi	65	GLN
12	Fi	193	GLN
12	Fi	331	GLN
12	Fi	343	ASN
12	Fi	417	ASN
12	Fq	4	ASN
12	Fq	65	GLN
12	Fq	125	HIS
12	Fq	324	ASN

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Mol	Chain	Res	Type
12	Fq	355	ASN
12	Fq	357	ASN
12	Fq	369	ASN
12	Fq	390	ASN
12	Fq	401	HIS
12	Fs	65	GLN
12	Fs	149	GLN
12	Fs	193	GLN
12	Fs	294	ASN
12	Fs	399	ASN
12	Fs	412	ASN
12	Fs	446	ASN
12	Fr	65	GLN
12	Fr	193	GLN
12	Fr	331	GLN
12	Fr	369	ASN
12	Fr	417	ASN
12	Fz	3	GLN
12	Fz	65	GLN
12	Fz	125	HIS
12	Fz	324	ASN
12	Fz	355	ASN
12	Fz	357	ASN
12	Fz	369	ASN
12	Fz	390	ASN
12	Fz	401	HIS
12	F2	4	ASN
12	F2	149	GLN
12	F2	193	GLN
12	F2	294	ASN
12	F2	399	ASN
12	F2	412	ASN
12	F2	446	ASN
12	F1	65	GLN
12	F1	133	GLN
12	F1	193	GLN
12	F1	331	GLN
12	F1	343	ASN
12	F1	369	ASN
12	F1	417	ASN
13	BW	95	GLN
13	BW	97	ASN

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Mol	Chain	Res	Type
13	BX	97	ASN
13	BY	59	ASN
13	BY	97	ASN
13	BZ	95	GLN
13	B1	59	ASN
13	B1	97	ASN
13	B2	59	ASN
13	B2	95	GLN
13	B2	97	ASN
13	B3	59	ASN
13	B4	59	ASN
13	B5	97	ASN
13	B6	59	ASN
13	B7	97	ASN
13	B8	89	GLN
13	B8	91	GLN
14	AA	3	ASN
14	AA	64	ASN
14	AB	3	ASN
14	AB	64	ASN
14	AC	64	ASN
14	AE	64	ASN
14	AF	64	ASN
15	BE	70	GLN
15	BE	180	ASN
15	BE	207	ASN
15	BE	242	ASN
15	BE	248	ASN
15	BE	323	ASN
15	BF	180	ASN
15	BF	242	ASN
15	BF	248	ASN
15	BF	323	ASN
15	BG	82	GLN
15	BG	173	ASN
15	BG	180	ASN
15	BG	207	ASN
15	BG	242	ASN
15	BG	270	GLN
15	BG	323	ASN
16	BJ	562	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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](#)

There are no chain breaks in this entry.

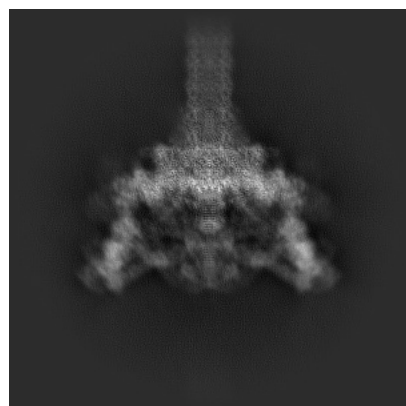
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50187. These allow visual inspection of the internal detail of the map and identification of artifacts.

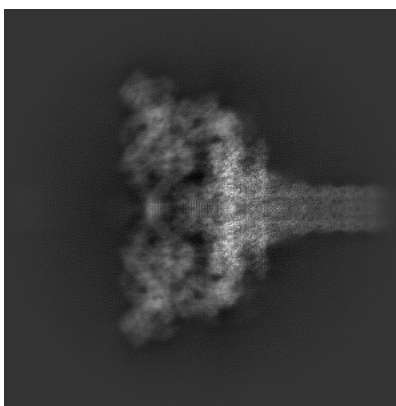
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

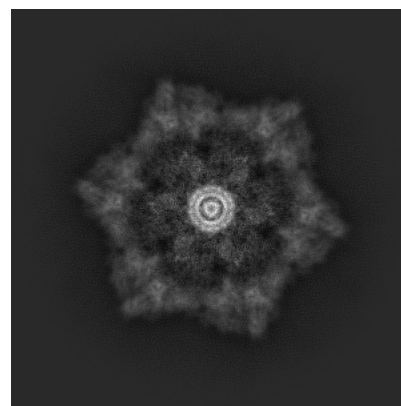
6.1.1 Primary map



X

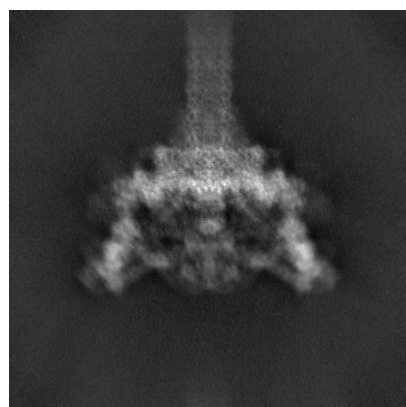


Y

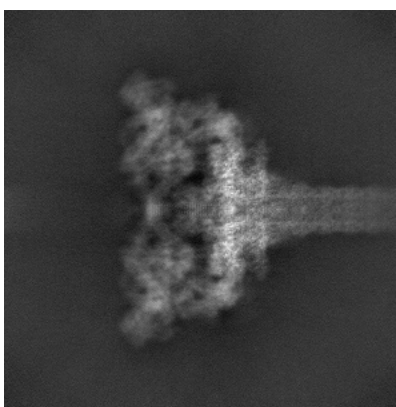


Z

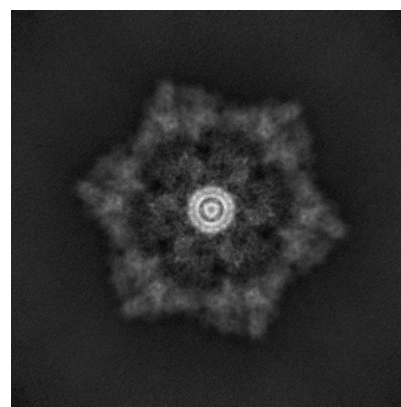
6.1.2 Raw map



X



Y

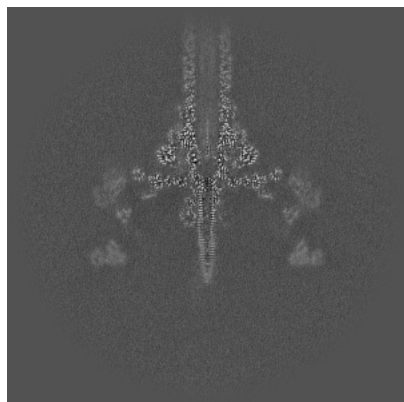


Z

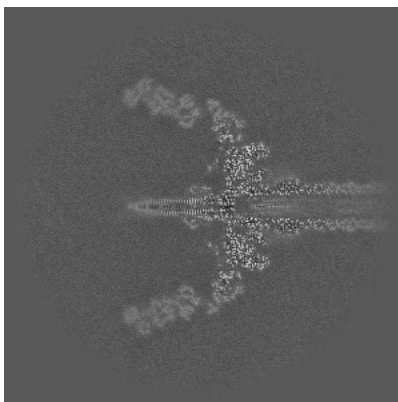
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

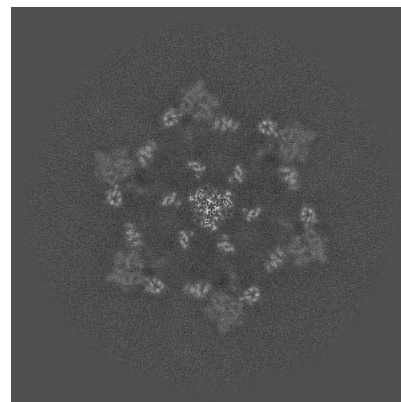
6.2.1 Primary map



X Index: 324

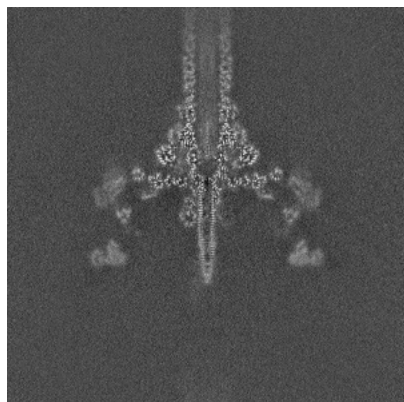


Y Index: 324

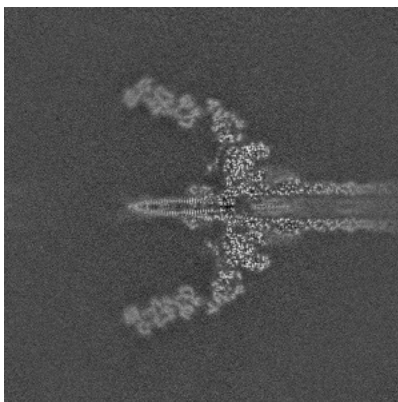


Z Index: 324

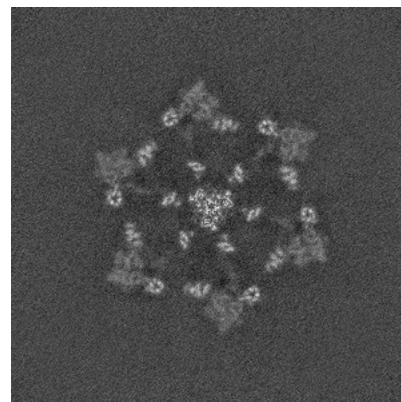
6.2.2 Raw map



X Index: 324



Y Index: 324

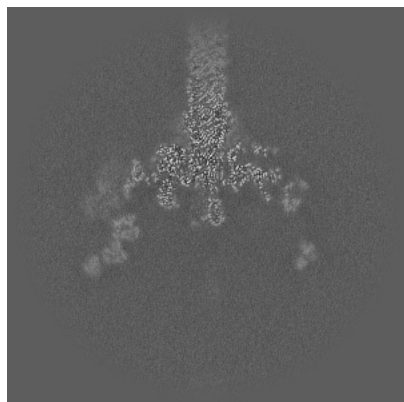


Z Index: 324

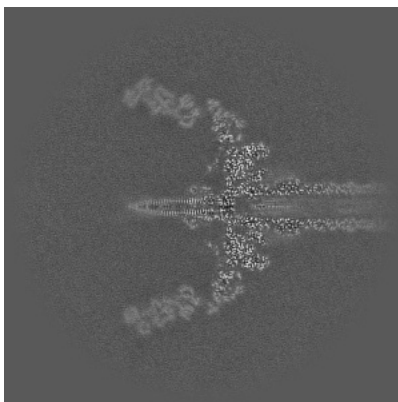
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

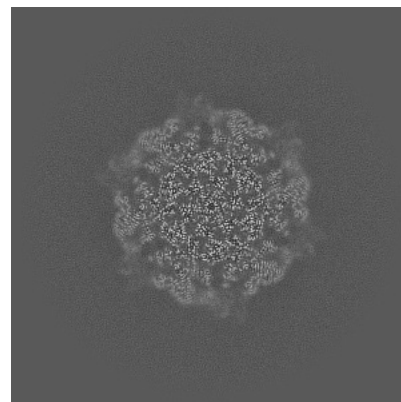
6.3.1 Primary map



X Index: 346

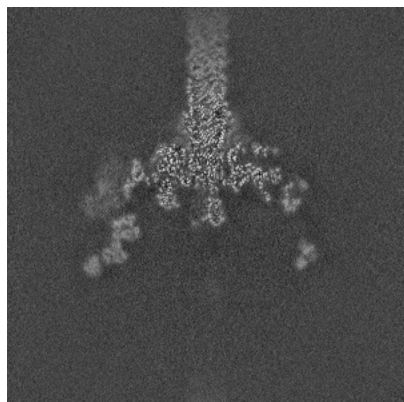


Y Index: 324

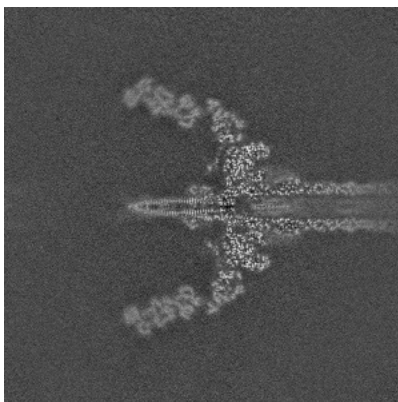


Z Index: 366

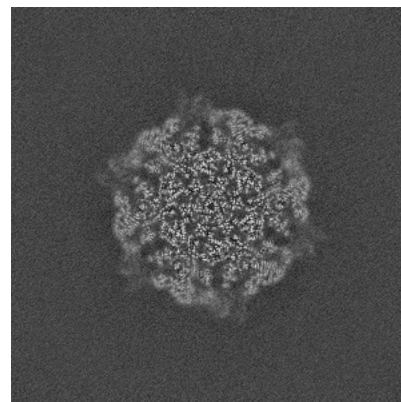
6.3.2 Raw map



X Index: 346



Y Index: 324

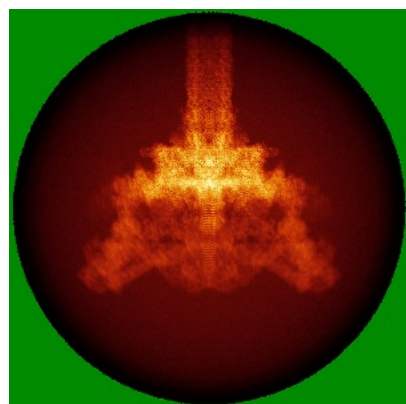


Z Index: 366

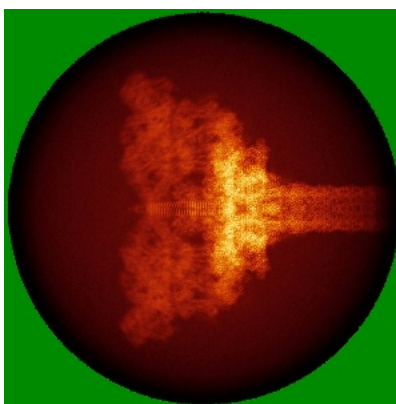
The images above show the largest variance slices of the map in three orthogonal directions.

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

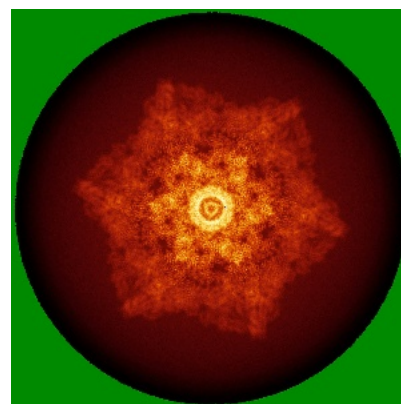
6.4.1 Primary map



X

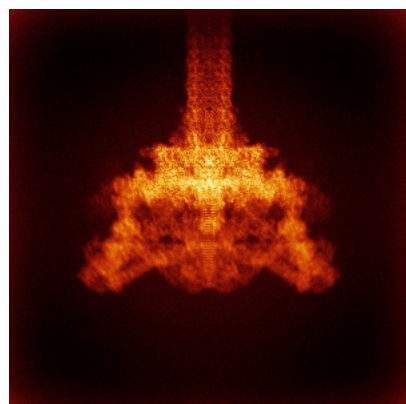


Y

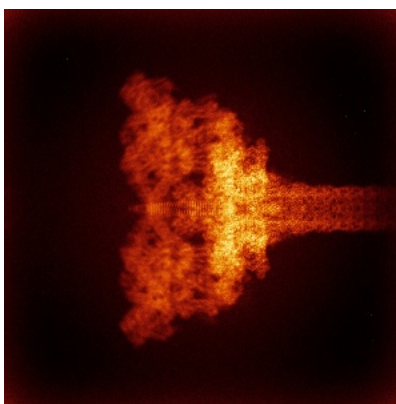


Z

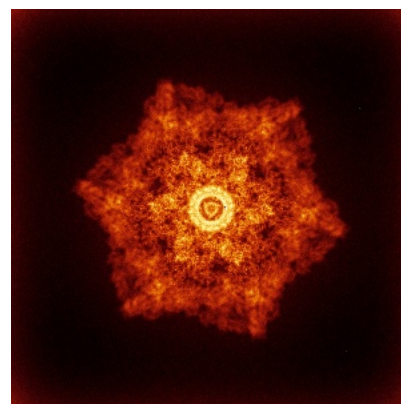
6.4.2 Raw map



X



Y

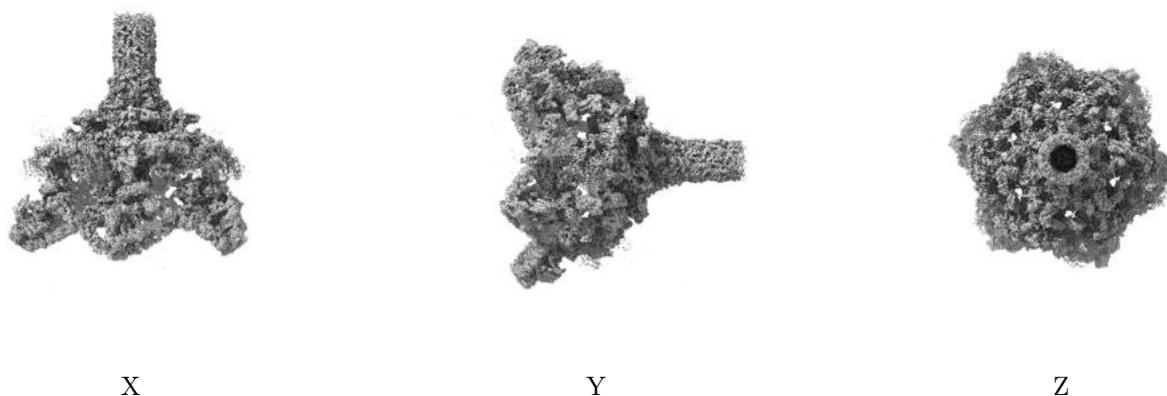


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

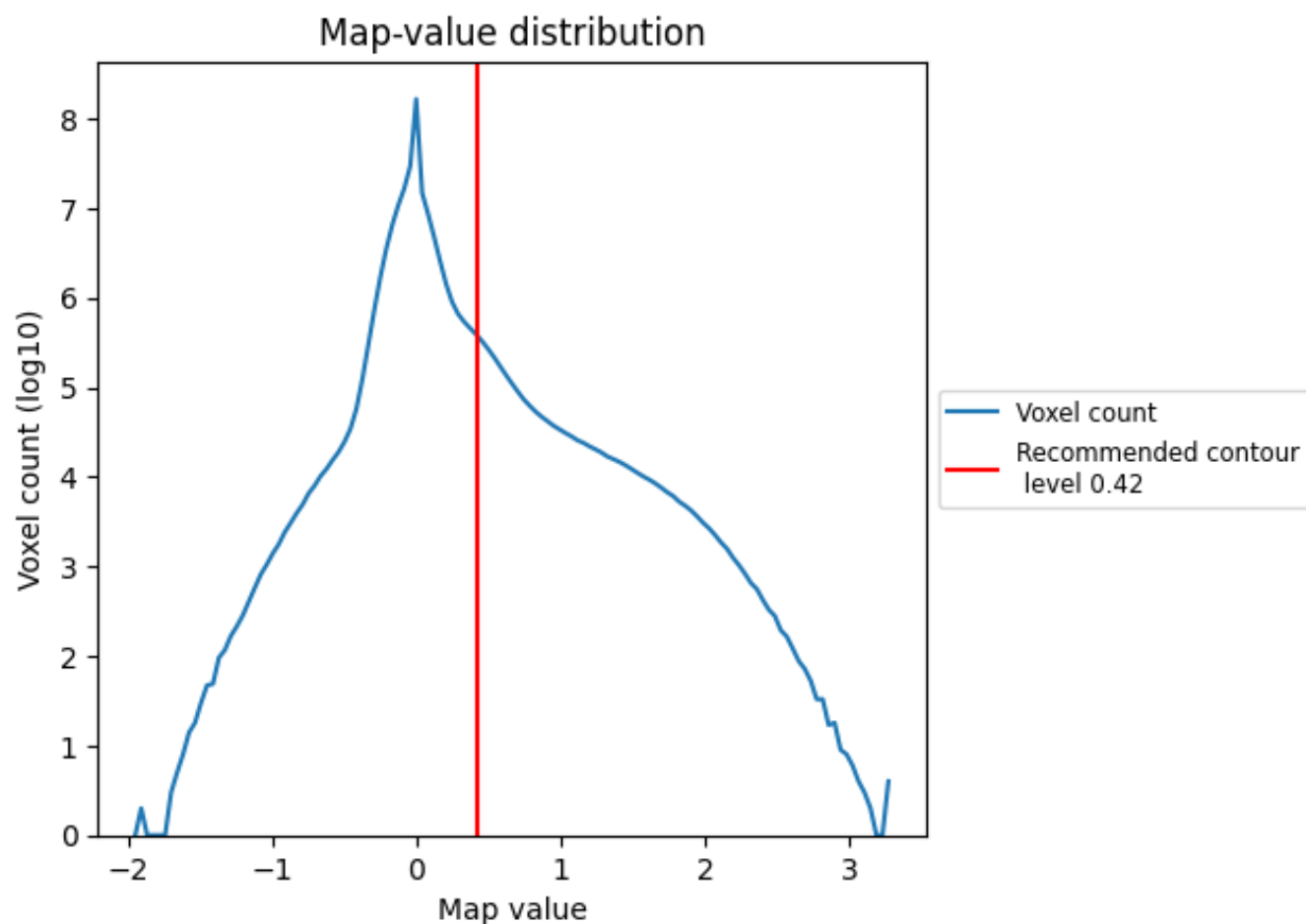
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

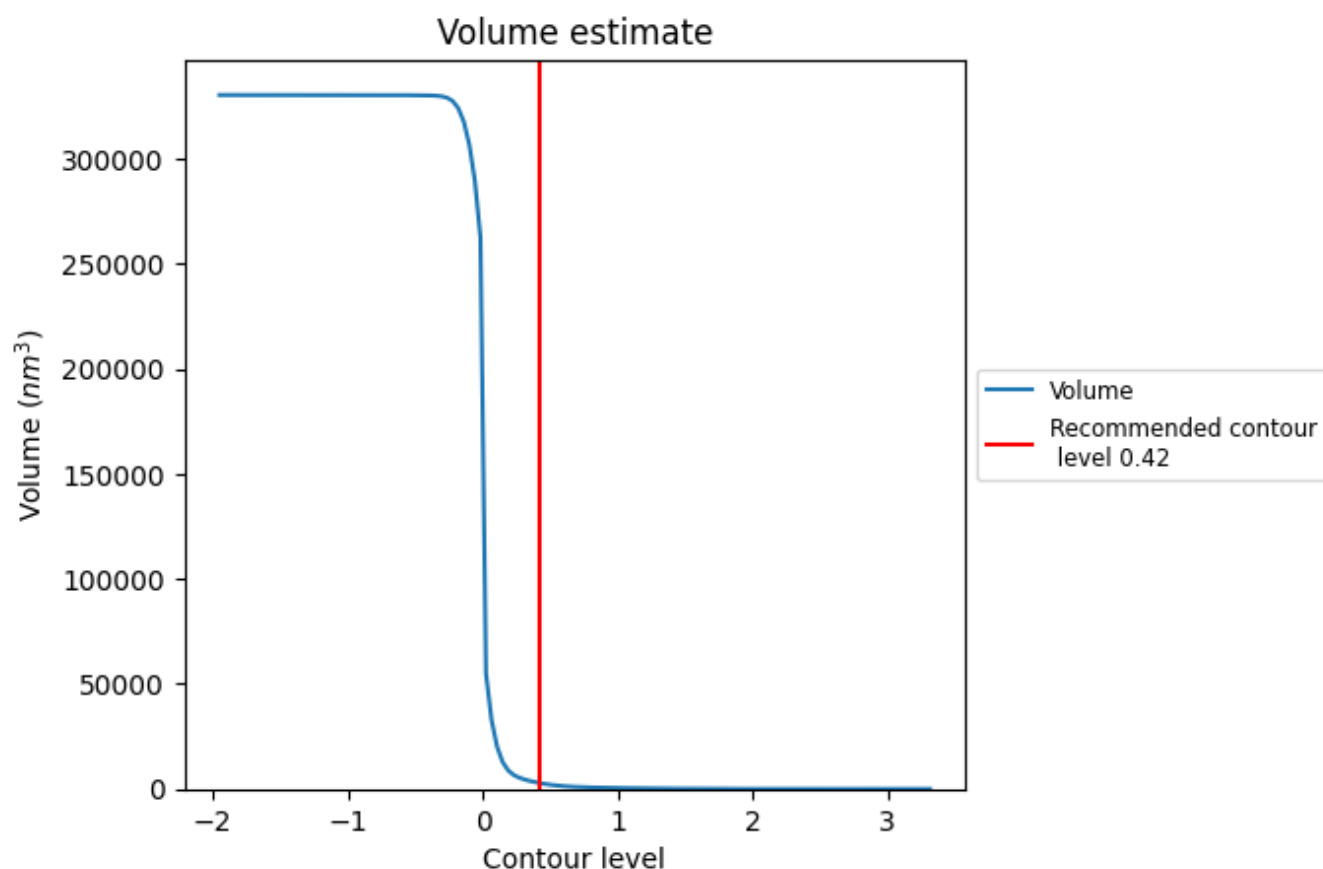
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

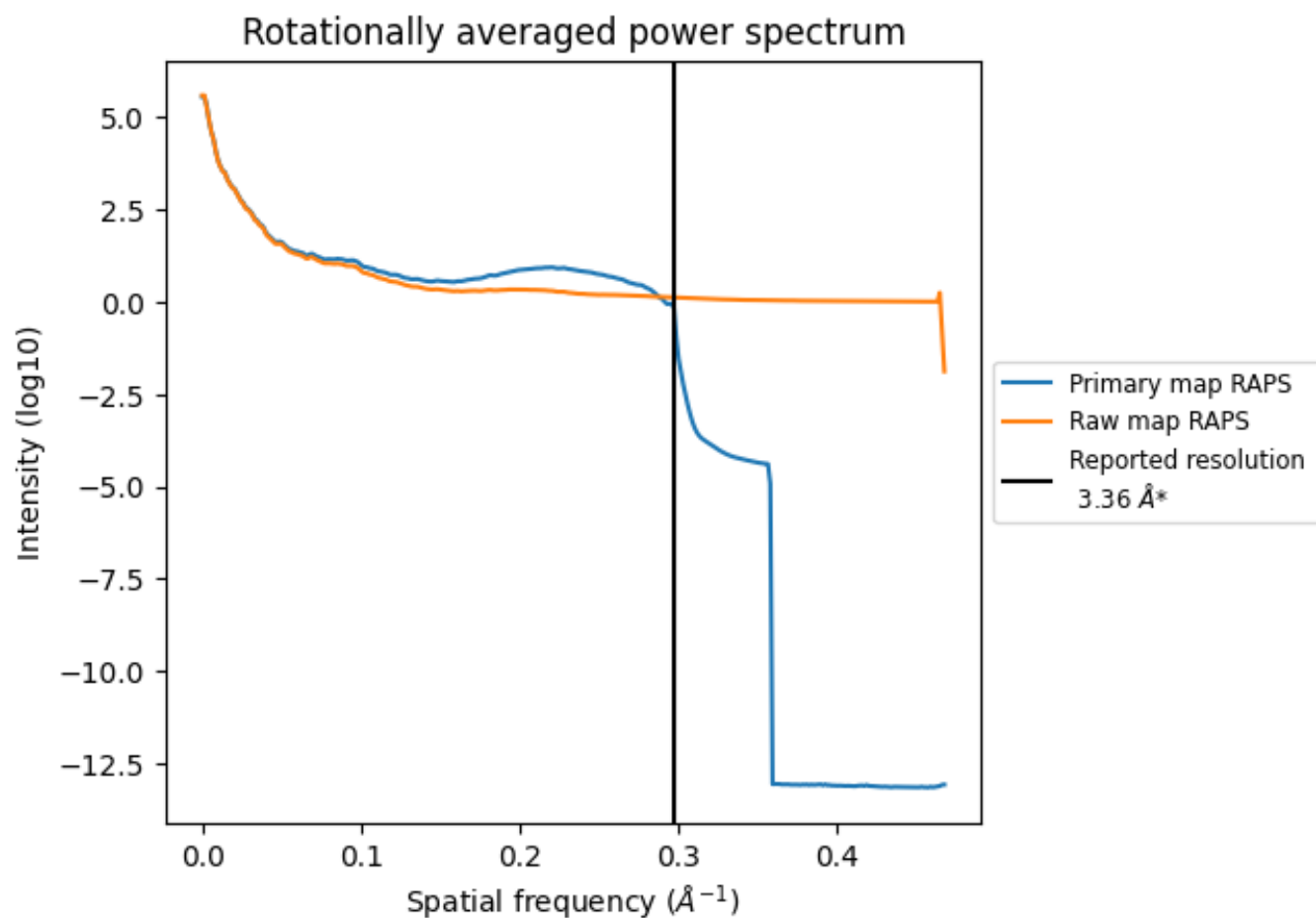
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2851 nm^3 ; this corresponds to an approximate mass of 2576 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

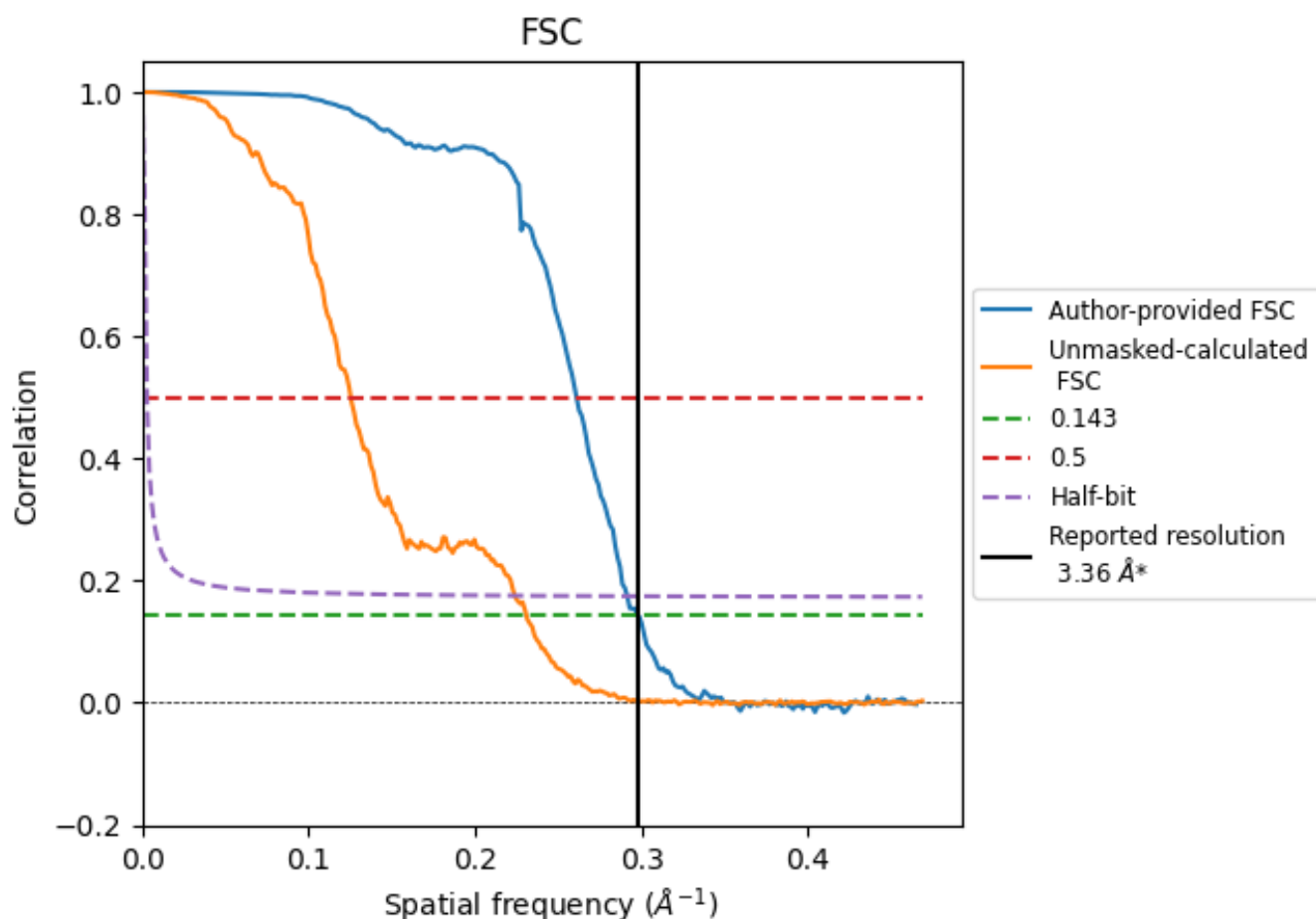


*Reported resolution corresponds to spatial frequency of 0.298 Å⁻¹

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 0.298 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

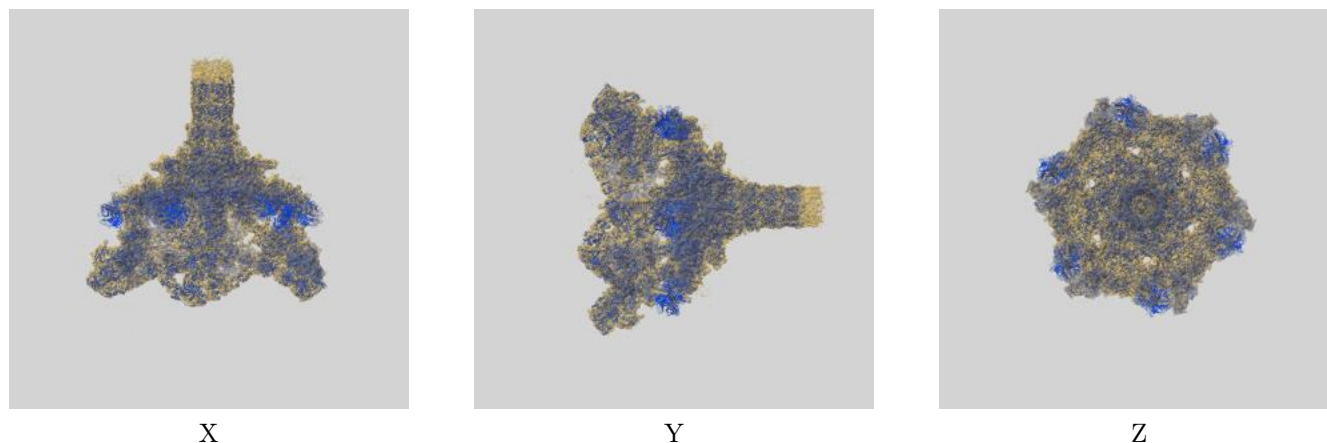
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.35	3.83	3.43
Unmasked-calculated*	4.33	7.98	4.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.33 differs from the reported value 3.36 by more than 10 %

9 Map-model fit [i](#)

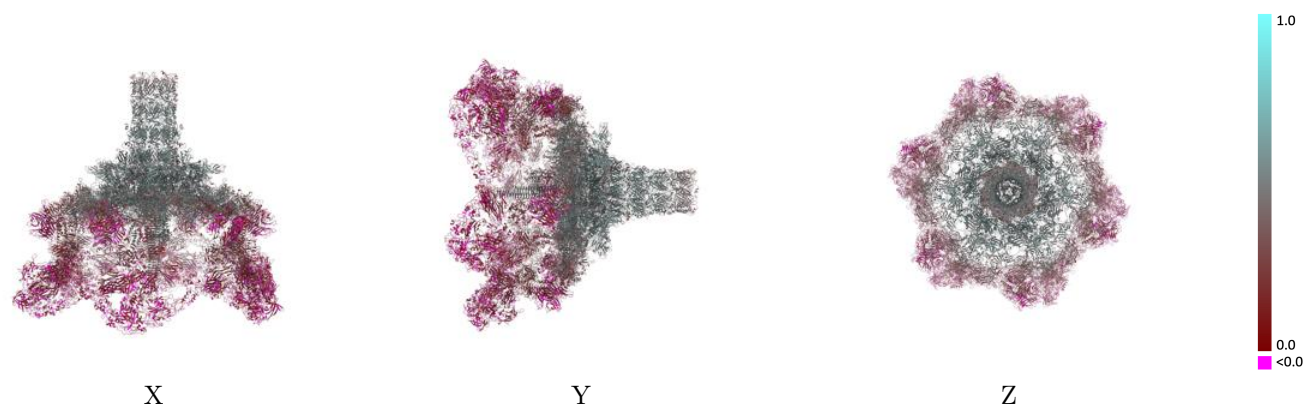
This section contains information regarding the fit between EMDB map EMD-50187 and PDB model 9F4B. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



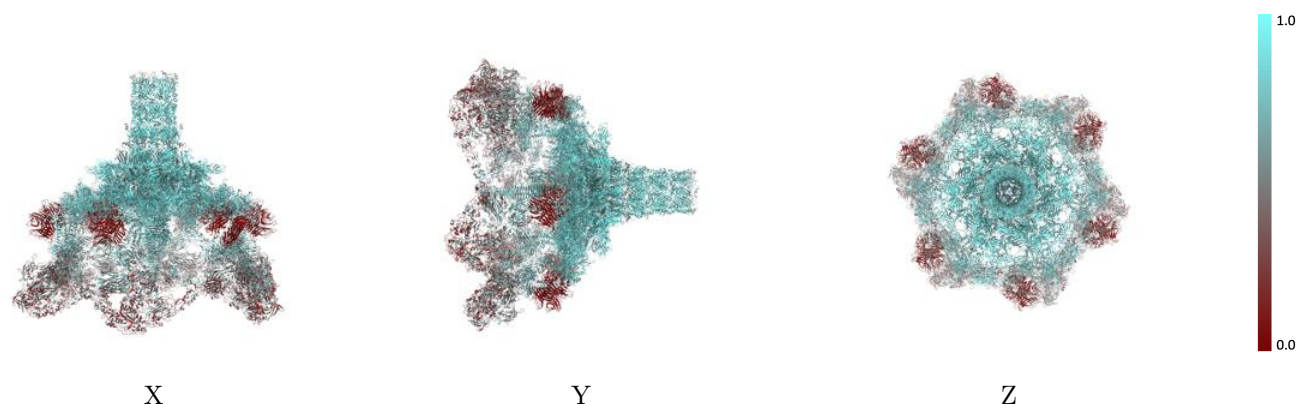
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



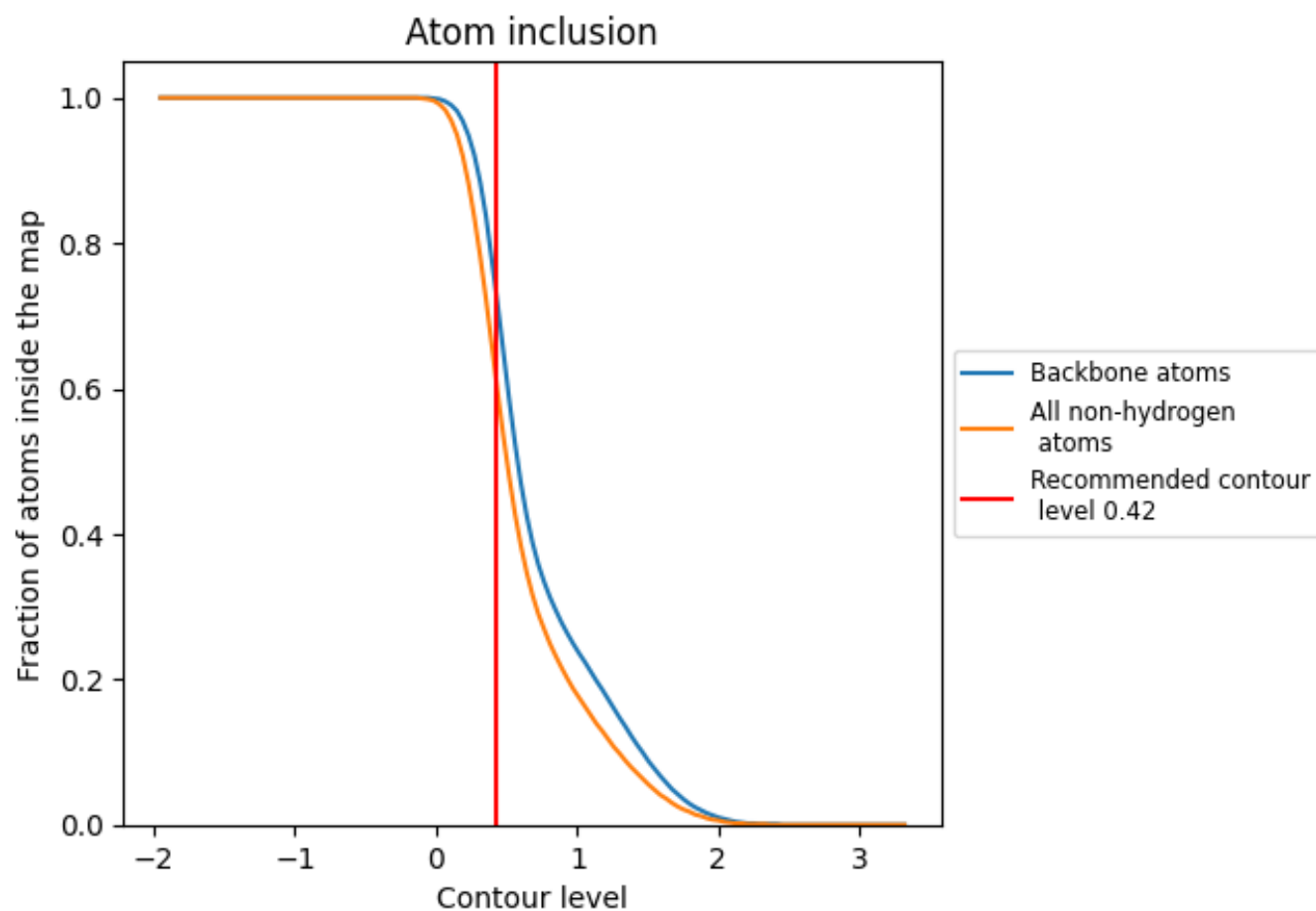
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.42).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6190	 0.3210
A0	 0.7760	 0.4120
A1	 0.7710	 0.4230
A2	 0.7690	 0.4220
A3	 0.7770	 0.4110
A4	 0.8480	 0.4860
A5	 0.8400	 0.4800
A6	 0.8500	 0.4850
A7	 0.8440	 0.4790
A8	 0.8450	 0.4870
A9	 0.8430	 0.4800
AA	 0.8640	 0.5080
AB	 0.8660	 0.5090
AC	 0.8660	 0.5090
AD	 0.8700	 0.5090
AE	 0.8650	 0.5080
AF	 0.8710	 0.5080
AG	 0.8810	 0.5230
AH	 0.8730	 0.5200
AI	 0.8800	 0.5200
AJ	 0.8750	 0.5210
AK	 0.8820	 0.5220
AL	 0.8730	 0.5210
AM	 0.8520	 0.5160
AN	 0.8670	 0.5150
AO	 0.8520	 0.5160
AP	 0.8680	 0.5150
AQ	 0.8540	 0.5170
AR	 0.8680	 0.5160
AS	 0.8690	 0.5100
AT	 0.8680	 0.5080
AU	 0.8670	 0.5090
AV	 0.8650	 0.5070
AW	 0.8640	 0.5090
AX	 0.8670	 0.5070



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Chain	Atom inclusion	Q-score
AY	 0.7790	 0.4080
AZ	 0.7720	 0.4240
Aa	 0.7850	 0.4080
Ab	 0.7800	 0.4070
Ac	 0.7870	 0.4060
Ad	 0.7790	 0.4070
Ae	 0.7870	 0.4060
Af	 0.7780	 0.4060
B1	 0.8300	 0.4960
B2	 0.8300	 0.4950
B3	 0.7230	 0.4190
B4	 0.7200	 0.4180
B5	 0.6980	 0.4150
B6	 0.7250	 0.4200
B7	 0.7030	 0.4150
B8	 0.6970	 0.4180
BA	 0.6770	 0.2750
BB	 0.8170	 0.5010
BC	 0.8160	 0.4990
BD	 0.8160	 0.5000
BE	 0.8650	 0.5310
BF	 0.8640	 0.5300
BG	 0.8640	 0.5290
BH	 0.6340	 0.4500
BI	 0.6010	 0.4360
BJ	 0.6220	 0.4420
BK	 0.7490	 0.4690
BL	 0.7880	 0.4940
BM	 0.7500	 0.4740
BN	 0.7850	 0.4920
BO	 0.7480	 0.4740
BP	 0.7840	 0.4930
BQ	 0.8530	 0.5110
BR	 0.8570	 0.5150
BS	 0.8630	 0.5120
BT	 0.8610	 0.5160
BU	 0.8620	 0.5120
BV	 0.8660	 0.5180
BW	 0.8350	 0.4930
BX	 0.8330	 0.4920
BY	 0.8260	 0.4950
BZ	 0.8350	 0.4940

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Chain	Atom inclusion	Q-score
F1	 0.3670	 0.1210
F2	 0.3850	 0.1210
FA	 0.5800	 0.2210
FB	 0.5780	 0.2040
FC	 0.5820	 0.2190
FD	 0.3610	 0.1250
FE	 0.3590	 0.1250
FF	 0.4000	 0.1190
FG	 0.4250	 0.1210
FH	 0.4180	 0.1270
FI	 0.4220	 0.1160
FJ	 0.5760	 0.2150
FK	 0.5500	 0.2090
FL	 0.5710	 0.2050
FM	 0.3780	 0.1230
FN	 0.3710	 0.1050
FO	 0.3500	 0.1040
FP	 0.4000	 0.1460
FQ	 0.3650	 0.1200
FR	 0.3780	 0.1190
FS	 0.5770	 0.2230
FT	 0.5770	 0.2060
FU	 0.5830	 0.2200
FV	 0.3620	 0.1250
FW	 0.3580	 0.1230
FX	 0.4100	 0.1220
FY	 0.4250	 0.1230
FZ	 0.4220	 0.1260
Fa	 0.4260	 0.1180
Fb	 0.5790	 0.2180
Fc	 0.5490	 0.2110
Fd	 0.5760	 0.2070
Fe	 0.3850	 0.1220
Ff	 0.3750	 0.1040
Fg	 0.3580	 0.1080
Fh	 0.3990	 0.1490
Fi	 0.3640	 0.1200
Fj	 0.3780	 0.1190
Fk	 0.5720	 0.2210
Fl	 0.5740	 0.2040
Fm	 0.5760	 0.2190
Fn	 0.3590	 0.1240

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Chain	Atom inclusion	Q-score
Fo	 0.3590	 0.1260
Fp	 0.4010	 0.1220
Fq	 0.4240	 0.1190
Fr	 0.4210	 0.1270
Fs	 0.4240	 0.1170
Ft	 0.5800	 0.2160
Fu	 0.5480	 0.2090
Fv	 0.5740	 0.2080
Fw	 0.3870	 0.1270
Fx	 0.3690	 0.1020
Fy	 0.3600	 0.1050
Fz	 0.4010	 0.1470
LA	 0.0950	 0.1360
LB	 0.1730	 0.1680
LC	 0.1160	 0.1400
LD	 0.1080	 0.1610
LE	 0.1810	 0.1650
LF	 0.1140	 0.1480
LG	 0.0940	 0.1370
LH	 0.1790	 0.1670
LI	 0.1170	 0.1410
LJ	 0.1070	 0.1610
LK	 0.1820	 0.1670
LL	 0.1150	 0.1510
LM	 0.0920	 0.1340
LN	 0.1710	 0.1650
LO	 0.1140	 0.1410
LP	 0.1070	 0.1610
LQ	 0.1840	 0.1680
LR	 0.1170	 0.1500