Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 07:58 pm GMT

PDB ID	:	5IV7
EMDB ID	:	EMD-3396
Title	:	Cryo-electron microscopy structure of the star-shaped, hubless post-attachment T4 baseplate
Authors	:	Taylor, N.M.I.; Guerrero-Ferreira, R.C.; Goldie, K.N.; Stahlberg, H.; Leiman, P.G.
Deposited on	:	2016-03-19
Resolution	:	6.77 Å(reported)
Based on initial model	:	5IV5

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:

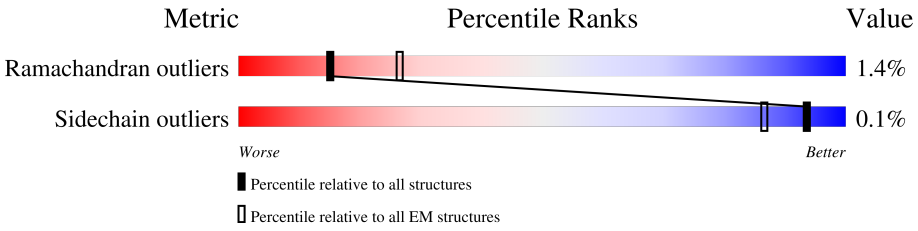
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 6.77 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	660	9% 98%
1	B	660	8% 97%
1	BF	660	9% 98%
1	BG	660	7% 97%
1	EA	660	9% 98%
1	EB	660	8% 97%
1	Q	660	9% 98%
1	R	660	7% 97%
1	g	660	9% 98%

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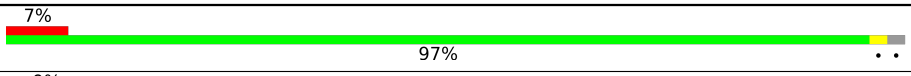
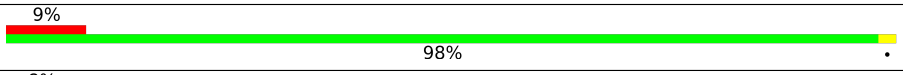
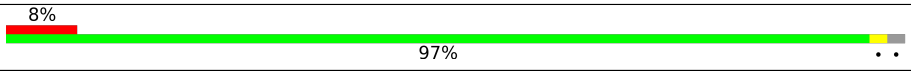
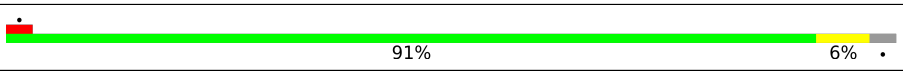
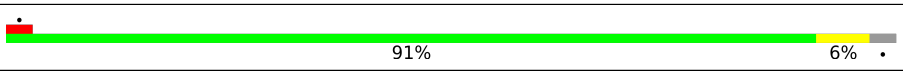
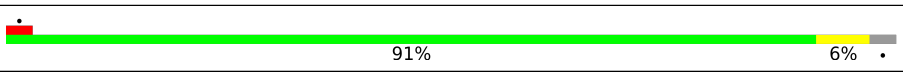
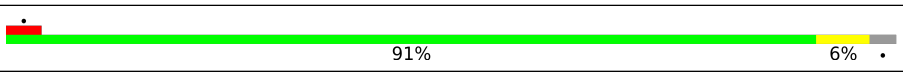
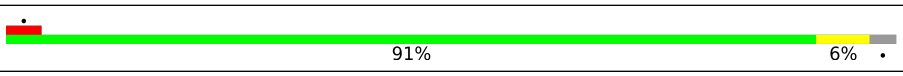
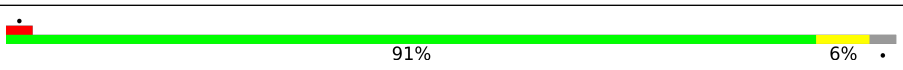
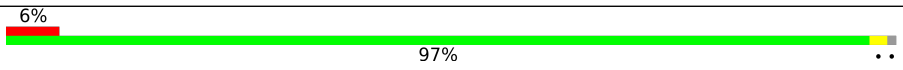
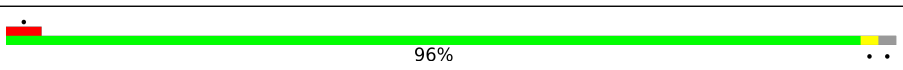
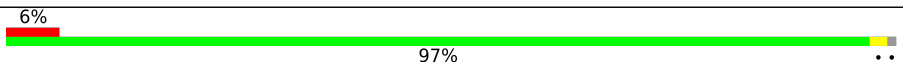
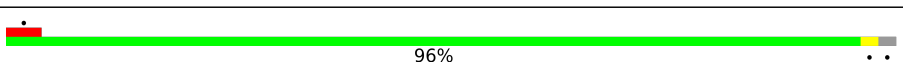
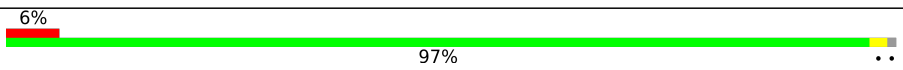
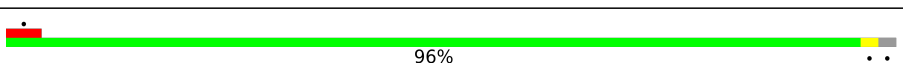
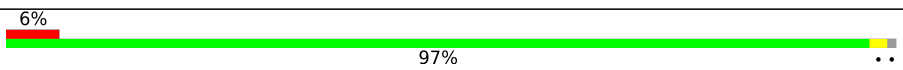
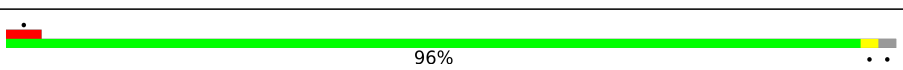
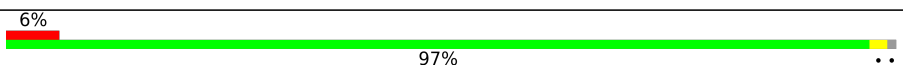
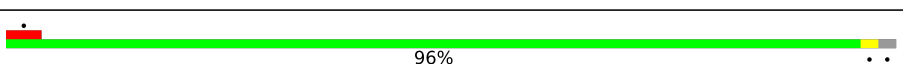
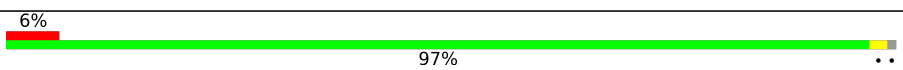
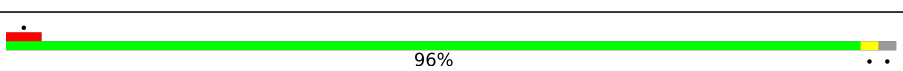
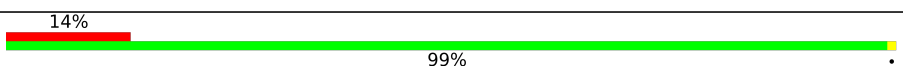
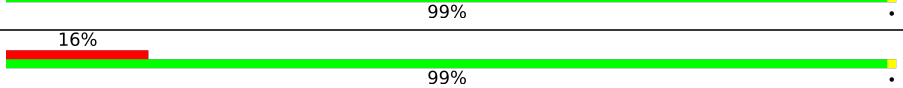
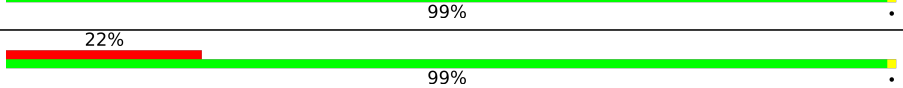
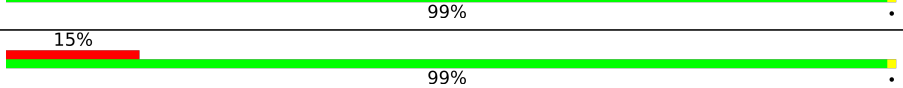
Mol	Chain	Length	Quality of chain
1	h	660	
1	w	660	
1	x	660	
2	C	1032	
2	CA	1032	
2	EC	1032	
2	S	1032	
2	i	1032	
2	y	1032	
3	AA	334	
3	CB	334	
3	CC	334	
3	D	334	
3	E	334	
3	ED	334	
3	EE	334	
3	T	334	
3	U	334	
3	j	334	
3	k	334	
3	z	334	
4	AB	288	
4	AC	288	
4	AD	288	
4	CD	288	

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Mol	Chain	Length	Quality of chain
4	CE	288	12% 99%
4	CF	288	24% 99%
4	EF	288	15% 99%
4	EG	288	12% 99%
4	F	288	15% 99%
4	FA	288	25% 99%
4	G	288	14% 99%
4	H	288	22% 99%
4	V	288	14% 99%
4	W	288	12% 99%
4	X	288	24% 99%
4	l	288	15% 99%
4	m	288	13% 99%
4	n	288	25% 99%
5	AE	602	15% 95% 5%
5	AF	602	20% 94% 6%
5	AG	602	16% 95% 5%
5	CG	602	14% 95% 5%
5	DA	602	20% 94% 6%
5	DB	602	16% 95% 5%
5	FB	602	14% 95% 5%
5	FC	602	19% 94% 6%
5	FD	602	17% 95% 5%
5	I	602	15% 95% 5%
5	J	602	19% 94% 6%

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Mol	Chain	Length	Quality of chain
5	K	602	15% 95% 5%
5	Y	602	14% 95% 5%
5	Z	602	20% 94% 6%
5	a	602	16% 95% 5%
5	o	602	14% 95% 5%
5	p	602	20% 94% 6%
5	q	602	17% 95% 5%
6	BA	219	18% 98%
6	BB	219	20% 98%
6	BC	219	10% 98%
6	DC	219	16% 98%
6	DD	219	25% 98%
6	DE	219	12% 98%
6	FE	219	20% 98%
6	FF	219	19% 98%
6	FG	219	9% 98%
6	L	219	18% 98%
6	M	219	20% 98%
6	N	219	10% 98%
6	b	219	17% 98%
6	c	219	25% 98%
6	d	219	11% 98%
6	r	219	20% 98%
6	s	219	19% 98%
6	t	219	9% 98%

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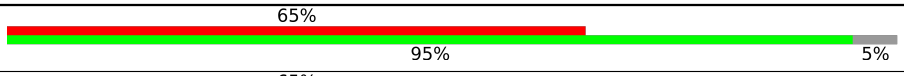
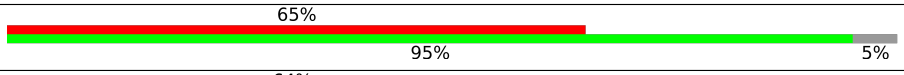
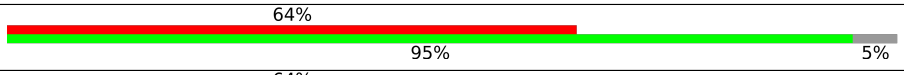
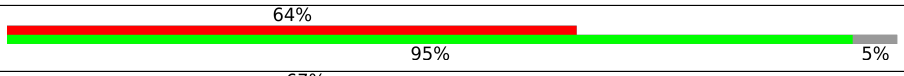
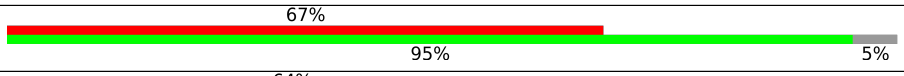
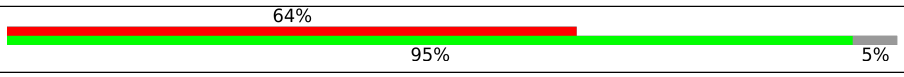
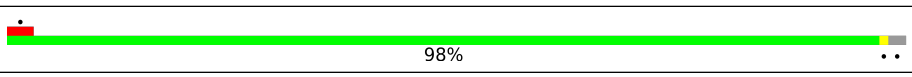
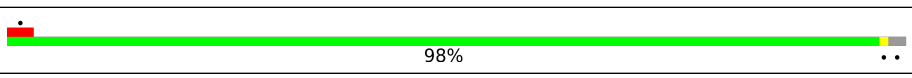
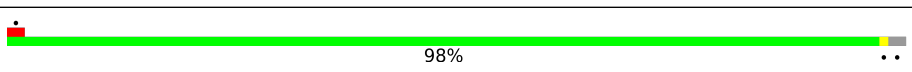
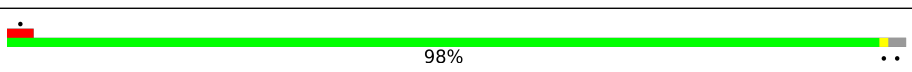
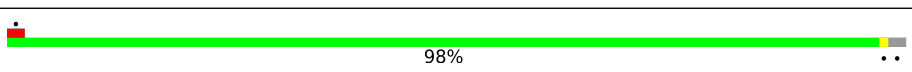
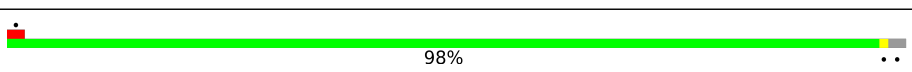
Mol	Chain	Length	Quality of chain
7	BD	132	
7	DF	132	
7	GA	132	
7	O	132	
7	e	132	
7	u	132	
8	BE	196	
8	DG	196	
8	GB	196	
8	P	196	
8	f	196	
8	v	196	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 312210 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	A	658	Total 5235	C 3308	N 867	O 1050	S 10	0	0
1	B	648	Total 5157	C 3259	N 854	O 1034	S 10	0	0
1	Q	658	Total 5235	C 3308	N 867	O 1050	S 10	0	0
1	R	648	Total 5157	C 3259	N 854	O 1034	S 10	0	0
1	g	658	Total 5235	C 3308	N 867	O 1050	S 10	0	0
1	h	648	Total 5157	C 3259	N 854	O 1034	S 10	0	0
1	w	658	Total 5235	C 3308	N 867	O 1050	S 10	0	0
1	x	648	Total 5157	C 3259	N 854	O 1034	S 10	0	0
1	BF	658	Total 5235	C 3308	N 867	O 1050	S 10	0	0
1	BG	648	Total 5157	C 3259	N 854	O 1034	S 10	0	0
1	EA	658	Total 5235	C 3308	N 867	O 1050	S 10	0	0
1	EB	648	Total 5157	C 3259	N 854	O 1034	S 10	0	0

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	E	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	T	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	U	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	j	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	k	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	z	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	AA	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	CB	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	CC	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		
3	ED	328	Total	C	N	O	S	0	0
			2631	1677	430	507	17		
3	EE	332	Total	C	N	O	S	0	0
			2658	1692	434	515	17		

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	V	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	W	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	X	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	l	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	m	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	n	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	AB	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	AC	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	AD	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	CD	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	CE	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	CF	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	EF	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	EG	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
4	FA	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	Z	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	a	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	o	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	p	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	q	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	AE	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	AF	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	AG	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	CG	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	DA	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	DB	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	FB	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	FC	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		
5	FD	602	Total	C	N	O	S	0	0
			4675	2933	779	953	10		

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	c	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	d	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	r	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	s	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	t	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	BA	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	BB	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	BC	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	DC	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	DD	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	DE	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FE	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FF	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		
6	FG	218	Total	C	N	O	S	0	0
			1665	1056	273	334	2		

- Molecule 7 is a protein called Baseplate wedge protein gp25.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
7	e	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
7	u	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
7	BD	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		
7	DF	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	GA	126	Total	C	N	O	S	0	0
			1011	636	169	202	4		

- Molecule 8 is a protein called Baseplate wedge protein gp53.

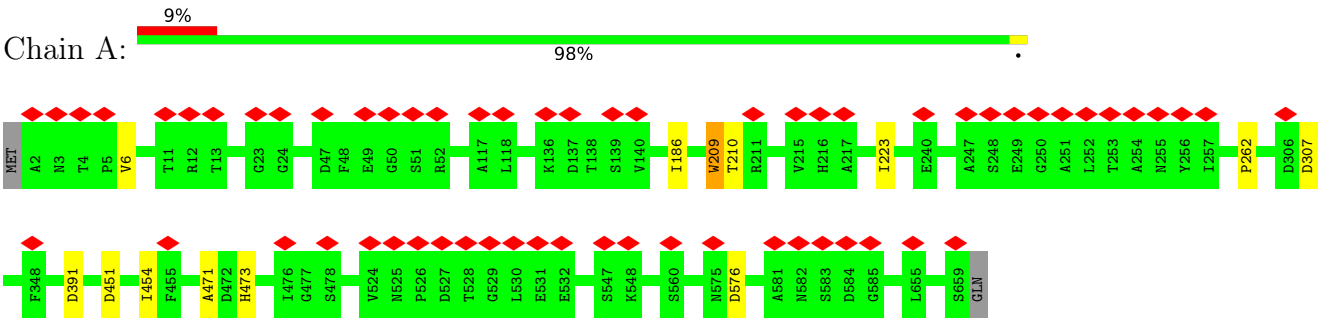
Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	f	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	v	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	BE	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	DG	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		
8	GB	193	Total	C	N	O	S	0	0
			1599	1035	259	299	6		

3 Residue-property plots (i)

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

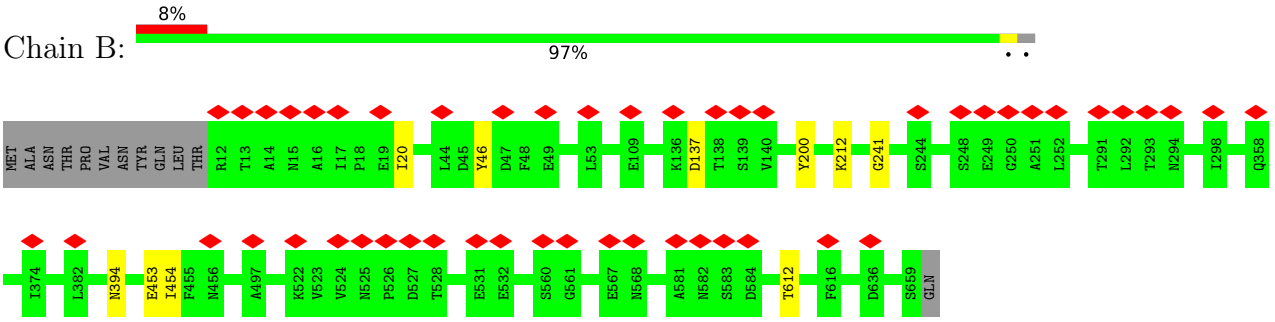
• Molecule 1: Baseplate wedge protein gp6

Chain A:



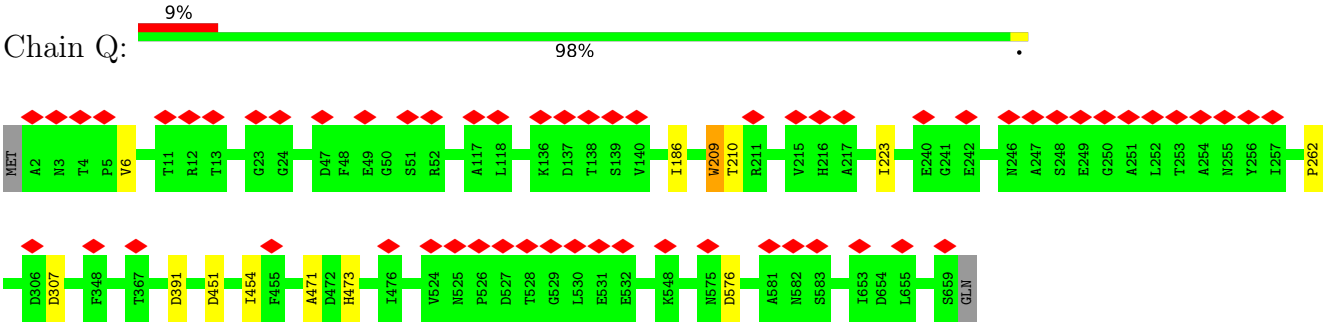
• Molecule 1: Baseplate wedge protein gp6

Chain B:



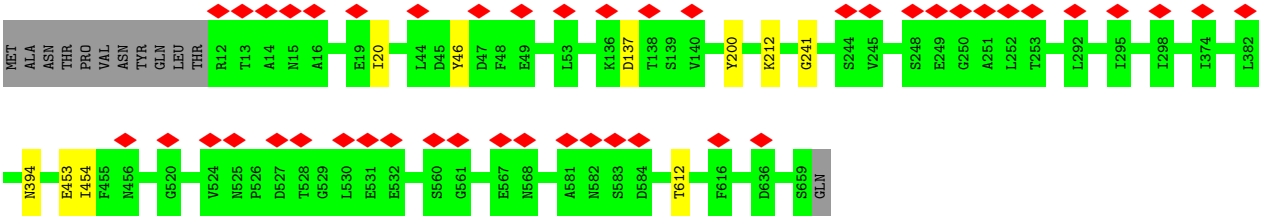
• Molecule 1: Baseplate wedge protein gp6

Chain Q:

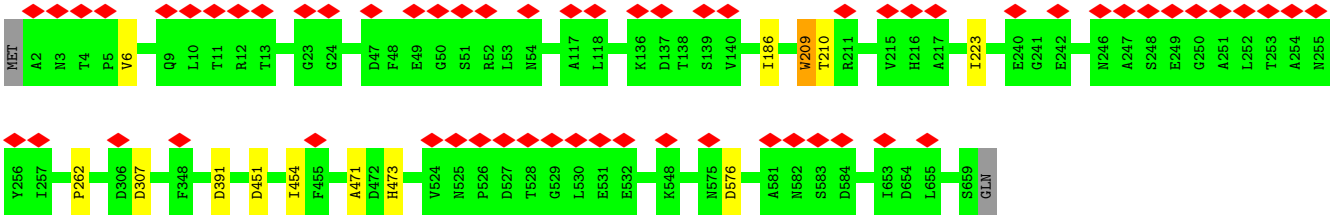


• Molecule 1: Baseplate wedge protein gp6

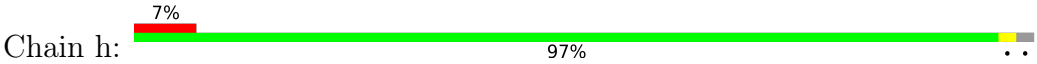
Chain R:

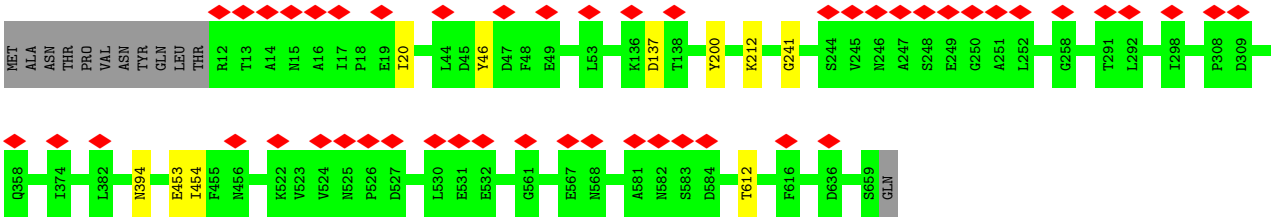


• Molecule 1: Baseplate wedge protein gp6

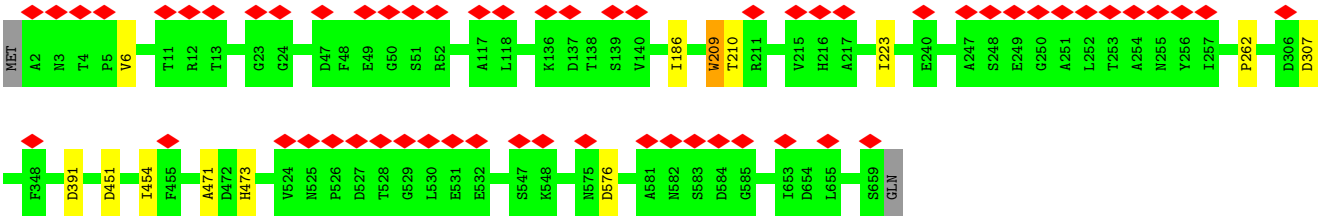


• Molecule 1: Baseplate wedge protein gp6

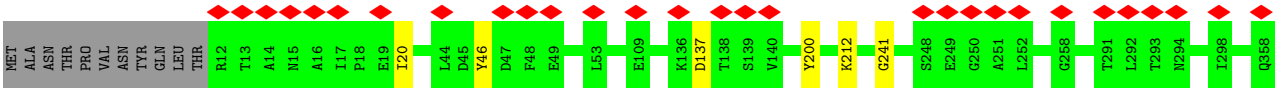


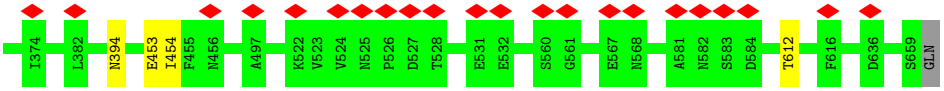


• Molecule 1: Baseplate wedge protein gp6



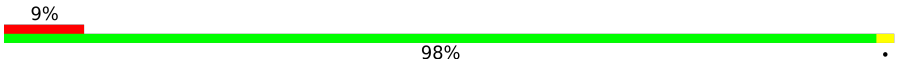
• Molecule 1: Baseplate wedge protein gp6

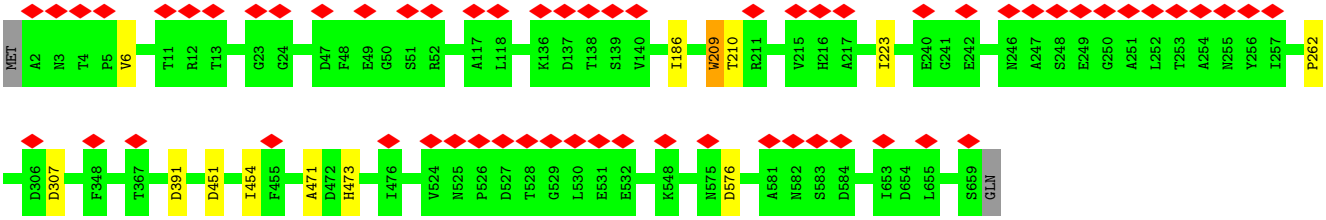




• Molecule 1: Baseplate wedge protein gp6

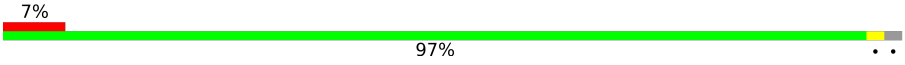
Chain BF:

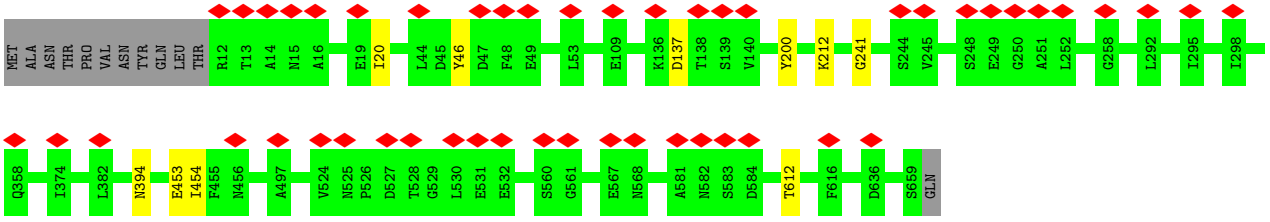




• Molecule 1: Baseplate wedge protein gp6

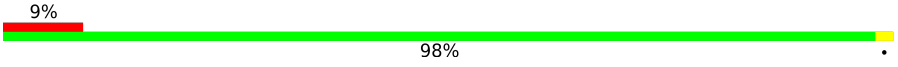
Chain BG:

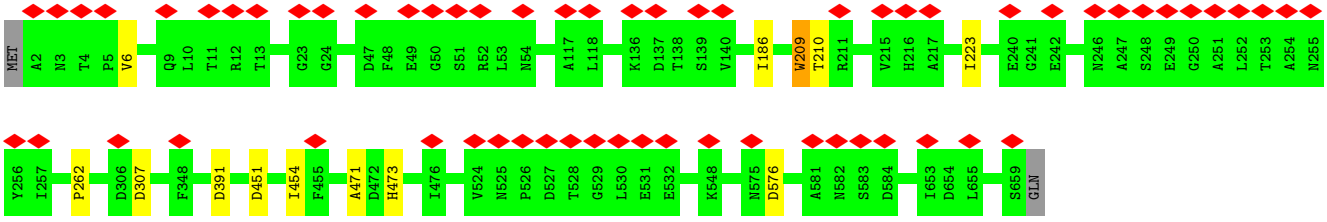




• Molecule 1: Baseplate wedge protein gp6

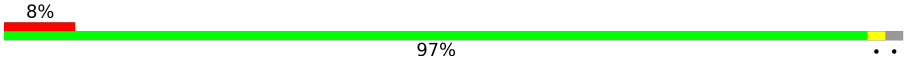
Chain EA:

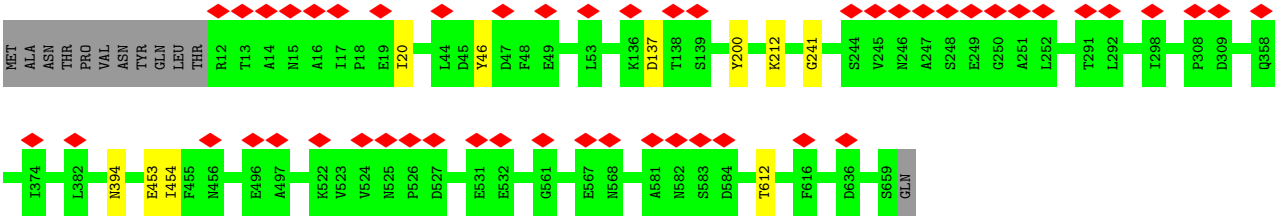




• Molecule 1: Baseplate wedge protein gp6

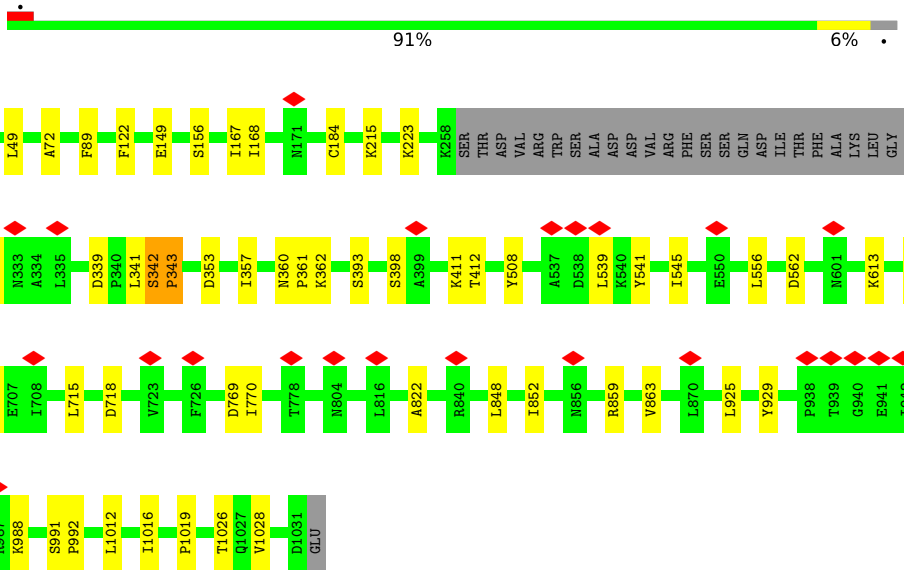
Chain EB:





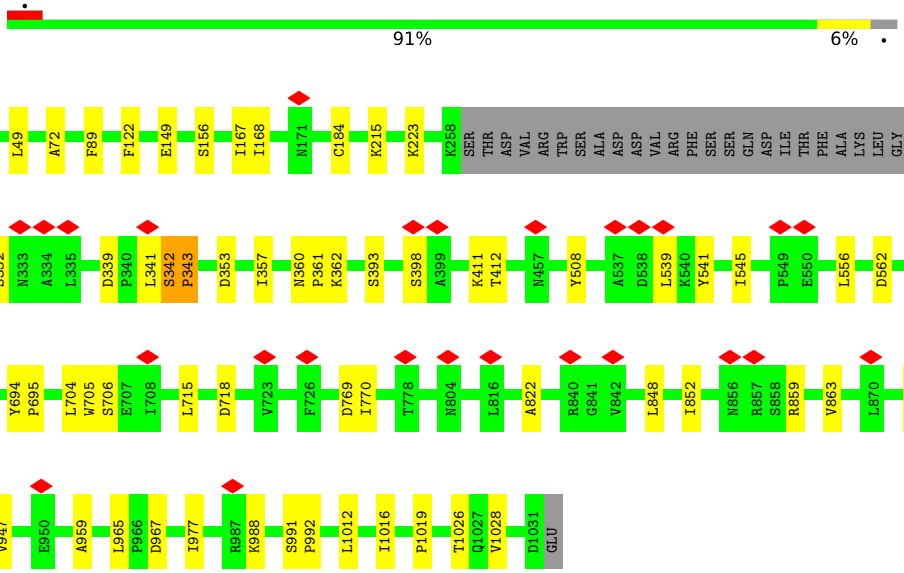
• Molecule 2: Baseplate wedge protein gp7

Chain C:



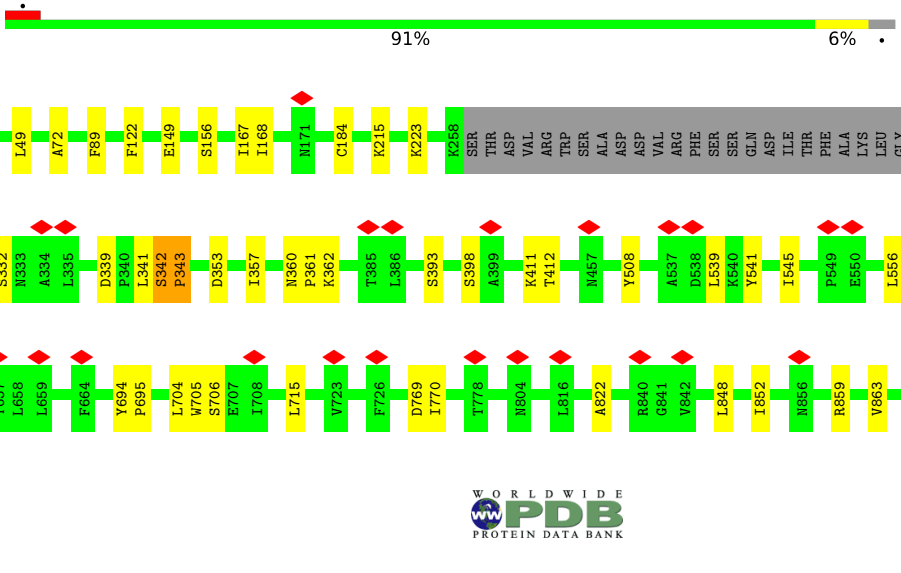
• Molecule 2: Baseplate wedge protein gp7

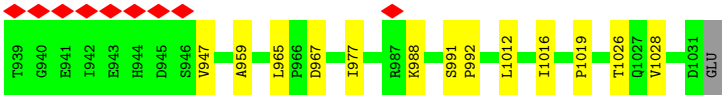
Chain S:



• Molecule 2: Baseplate wedge protein gp7

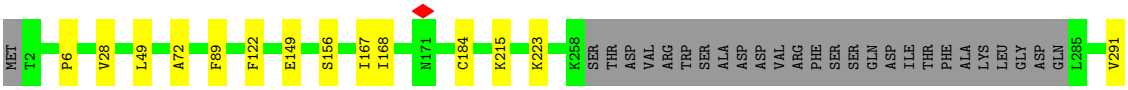
Chain i:

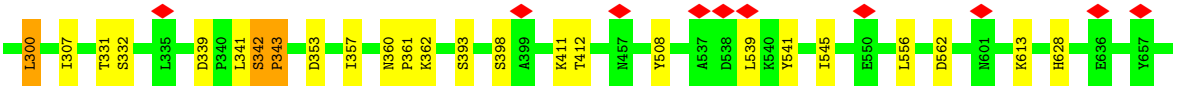


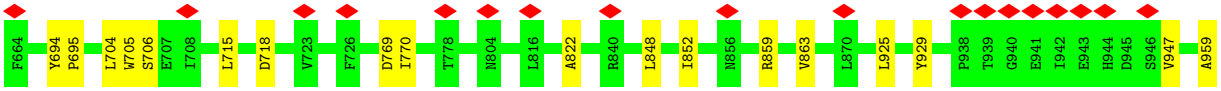


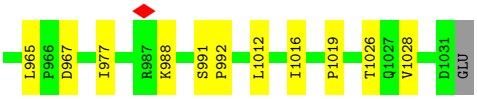
• Molecule 2: Baseplate wedge protein gp7

Chain y:



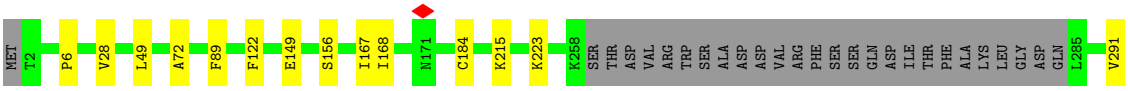


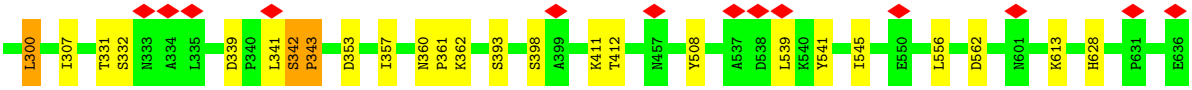


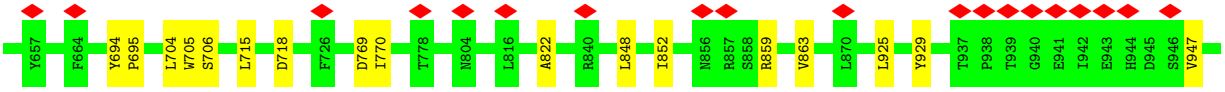


• Molecule 2: Baseplate wedge protein gp7

Chain CA:

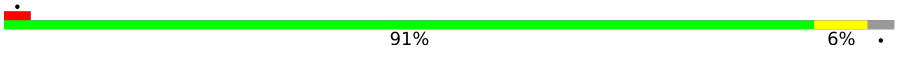


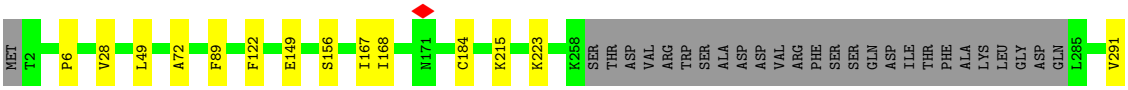


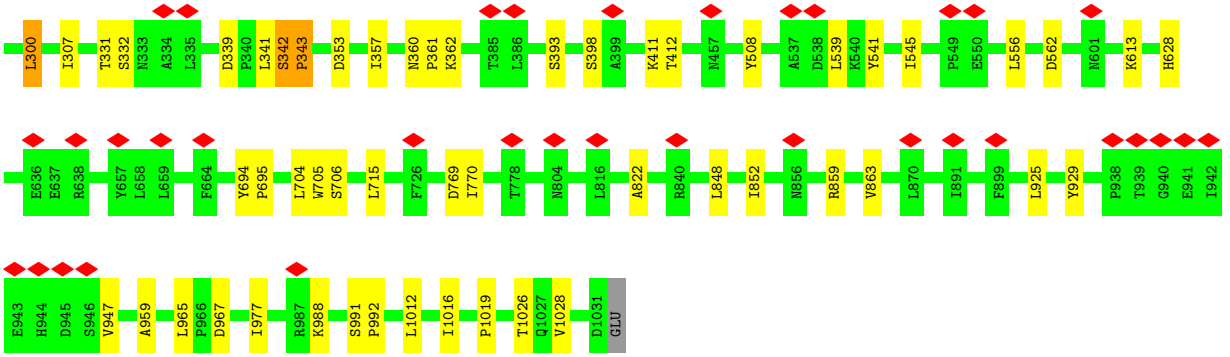


• Molecule 2: Baseplate wedge protein gp7

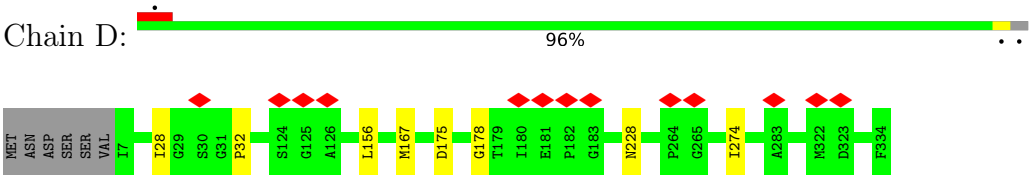
Chain EC:



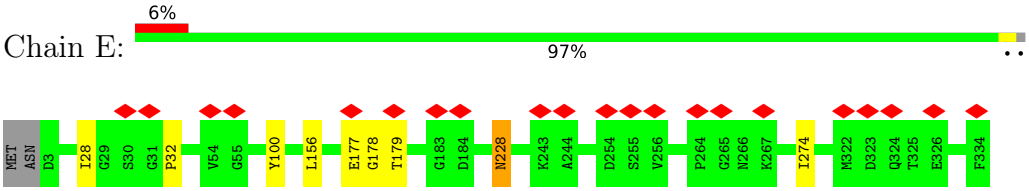




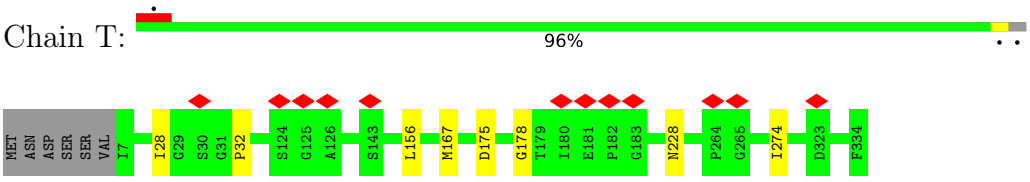
• Molecule 3: Baseplate wedge protein gp8



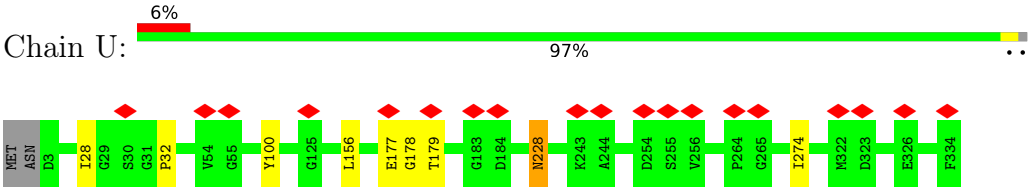
• Molecule 3: Baseplate wedge protein gp8



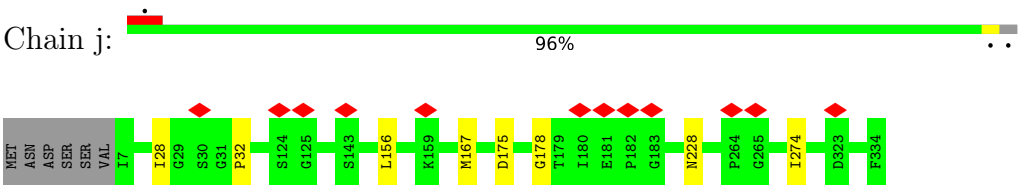
• Molecule 3: Baseplate wedge protein gp8



• Molecule 3: Baseplate wedge protein gp8

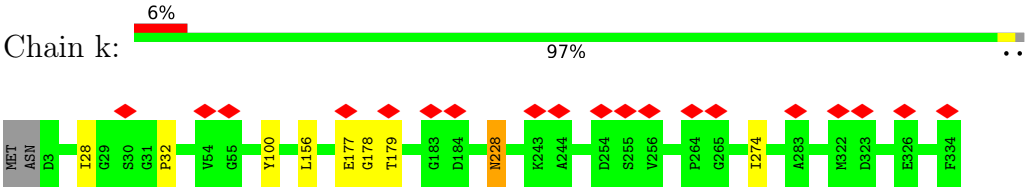


• Molecule 3: Baseplate wedge protein gp8



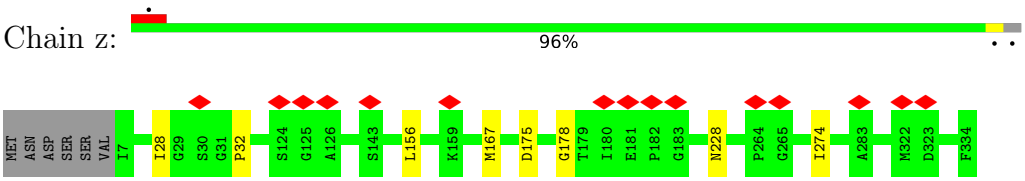
• Molecule 3: Baseplate wedge protein gp8

Chain k:



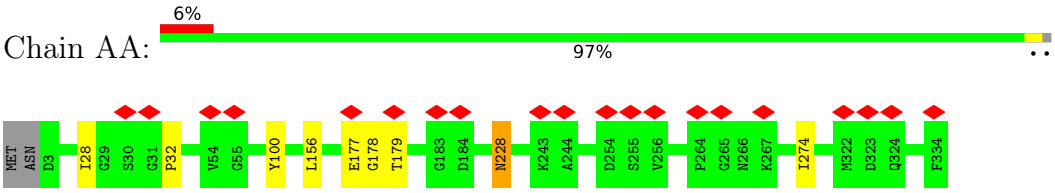
• Molecule 3: Baseplate wedge protein gp8

Chain z:



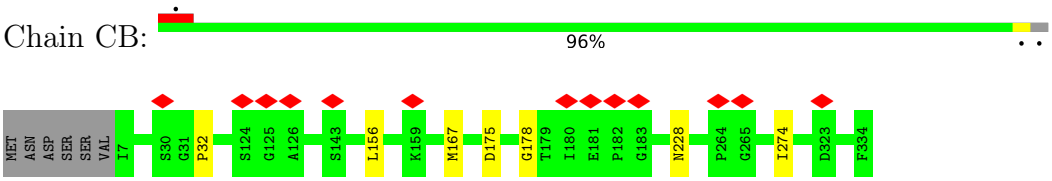
• Molecule 3: Baseplate wedge protein gp8

Chain AA:



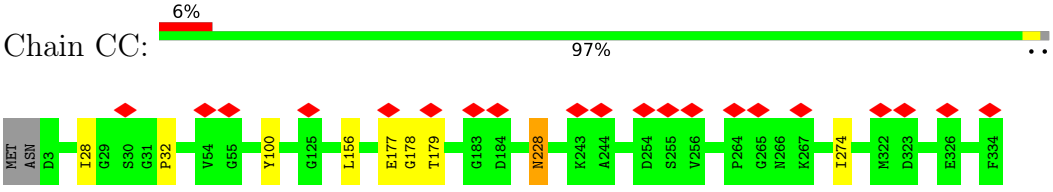
• Molecule 3: Baseplate wedge protein gp8

Chain CB:



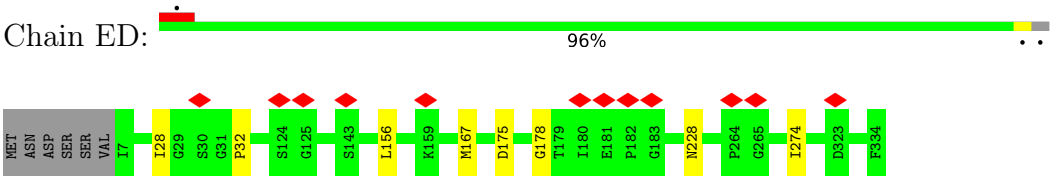
• Molecule 3: Baseplate wedge protein gp8

Chain CC:



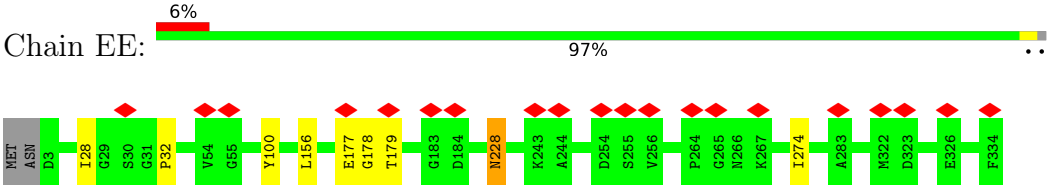
• Molecule 3: Baseplate wedge protein gp8

Chain ED:



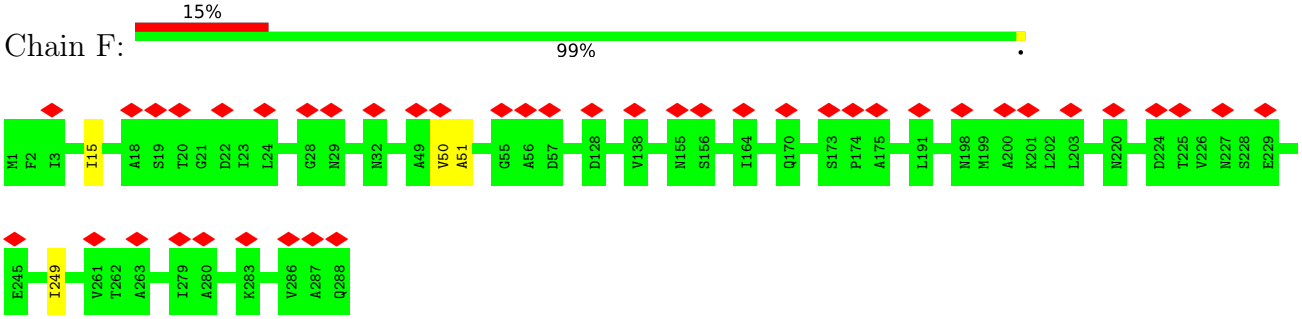
• Molecule 3: Baseplate wedge protein gp8

Chain EE:



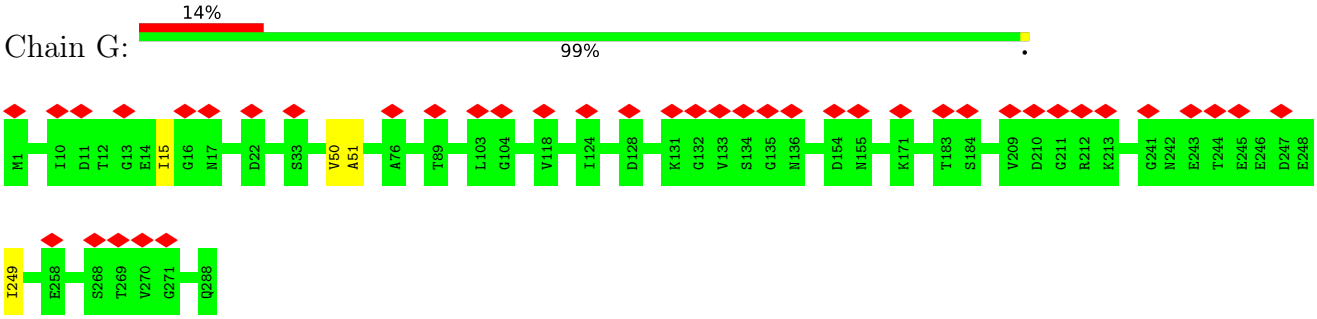
• Molecule 4: Baseplate wedge protein gp9

Chain F:



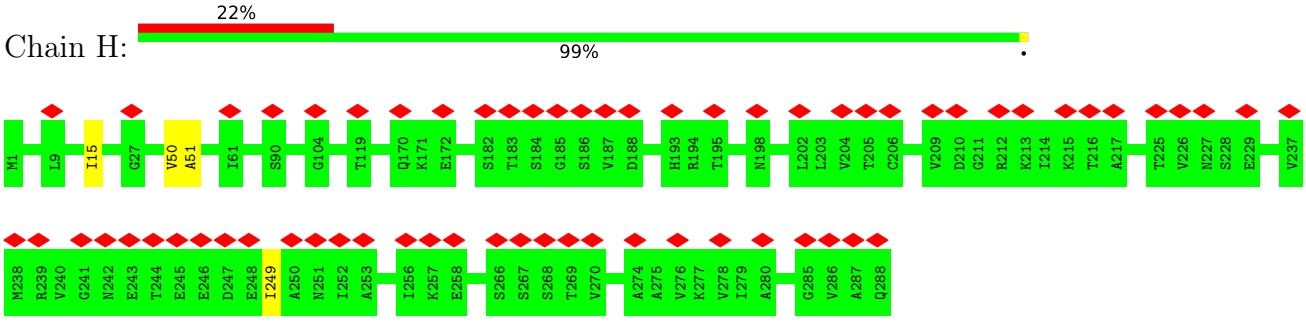
• Molecule 4: Baseplate wedge protein gp9

Chain G:



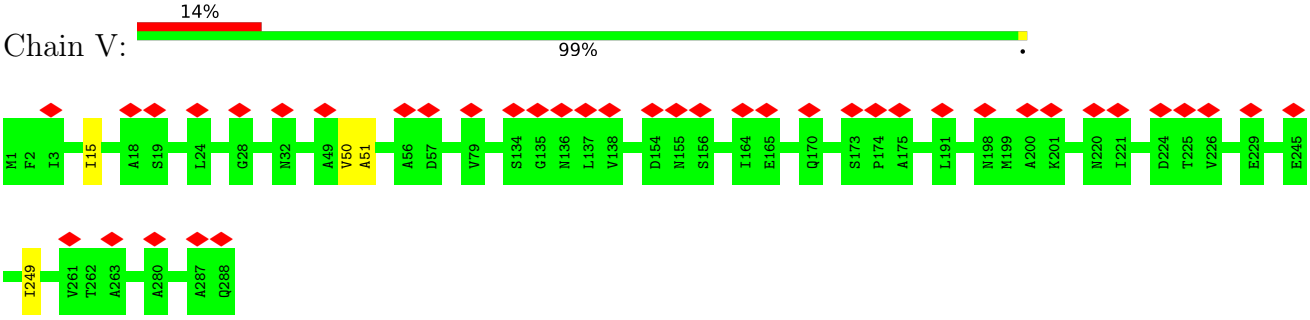
• Molecule 4: Baseplate wedge protein gp9

Chain H:



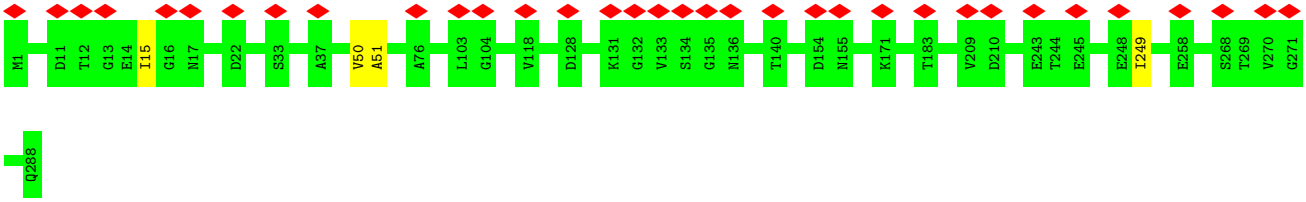
• Molecule 4: Baseplate wedge protein gp9

Chain V:

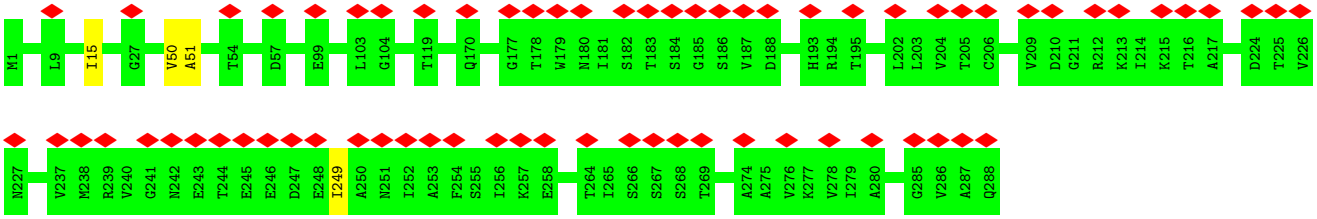


• Molecule 4: Baseplate wedge protein gp9

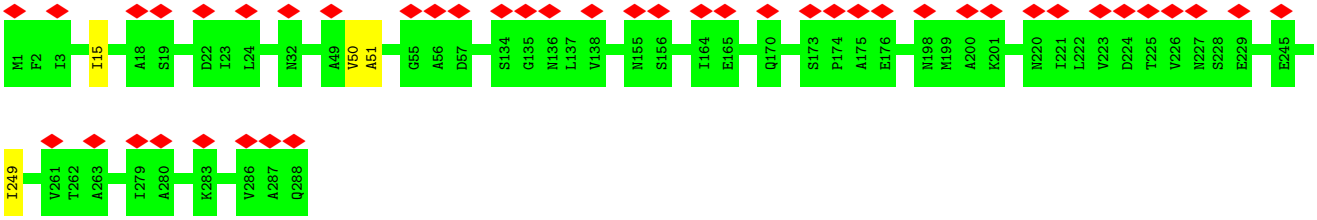
Chain W:



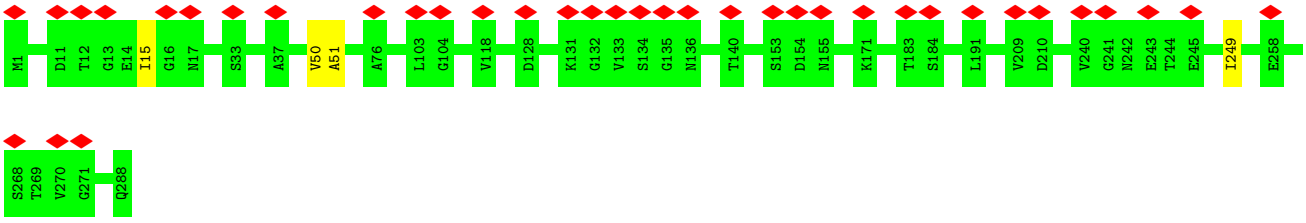
• Molecule 4: Baseplate wedge protein gp9



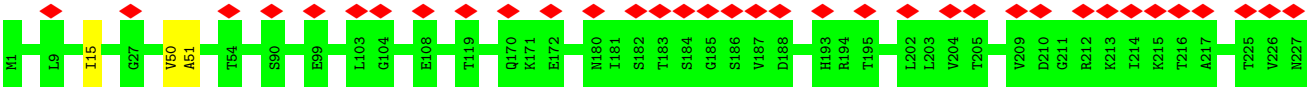
• Molecule 4: Baseplate wedge protein gp9

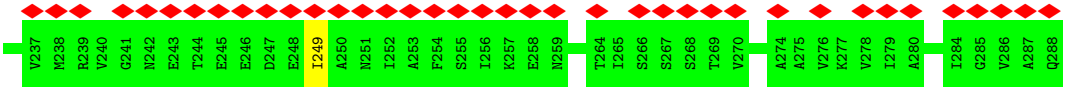


• Molecule 4: Baseplate wedge protein gp9



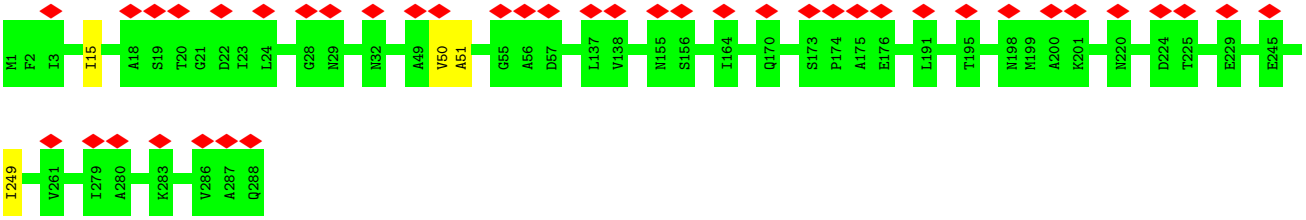
• Molecule 4: Baseplate wedge protein gp9





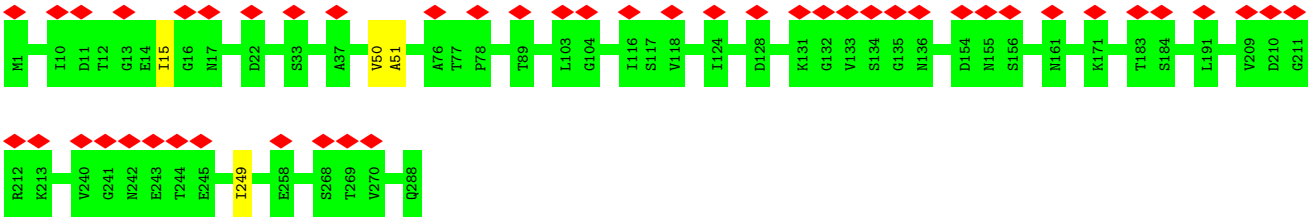
• Molecule 4: Baseplate wedge protein gp9

Chain AB:



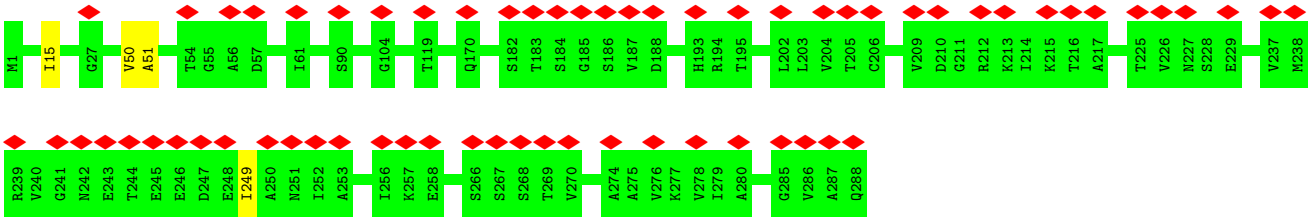
• Molecule 4: Baseplate wedge protein gp9

Chain AC:



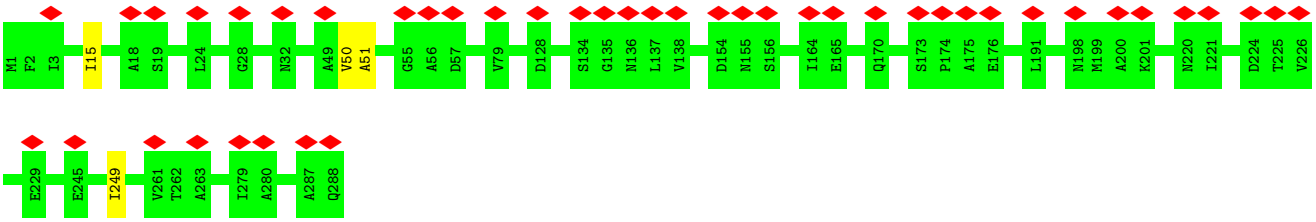
• Molecule 4: Baseplate wedge protein gp9

Chain AD:



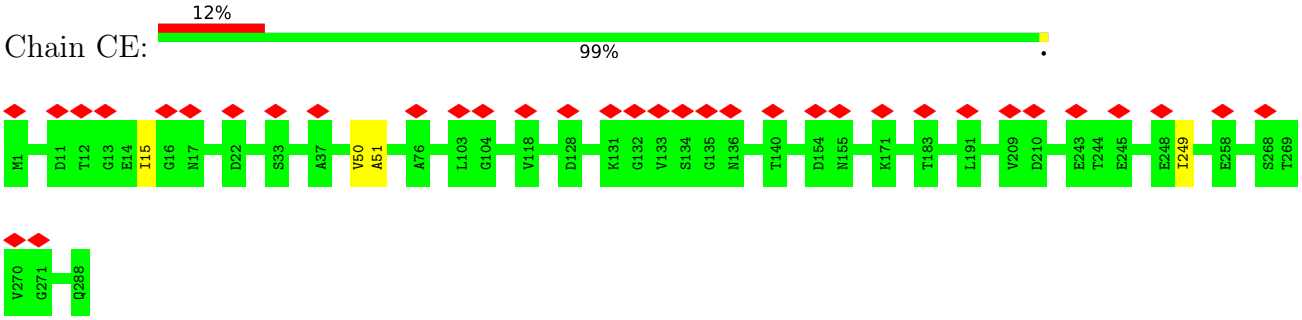
• Molecule 4: Baseplate wedge protein gp9

Chain CD:



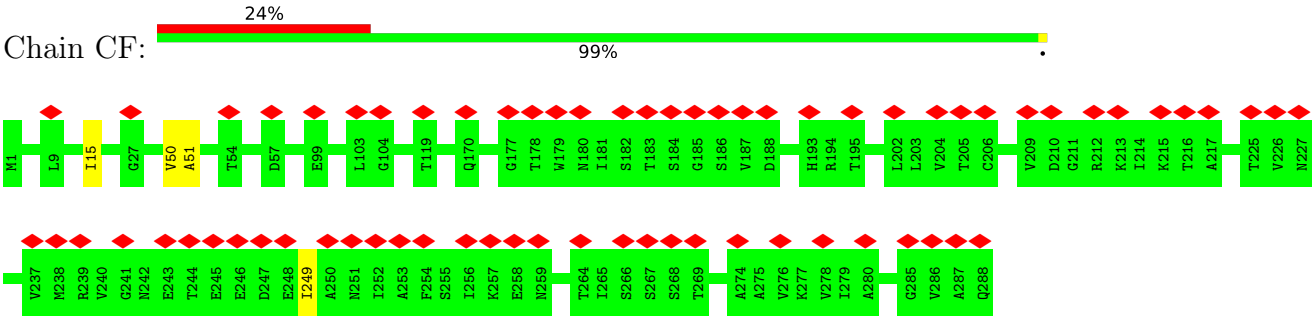
• Molecule 4: Baseplate wedge protein gp9

Chain CE:



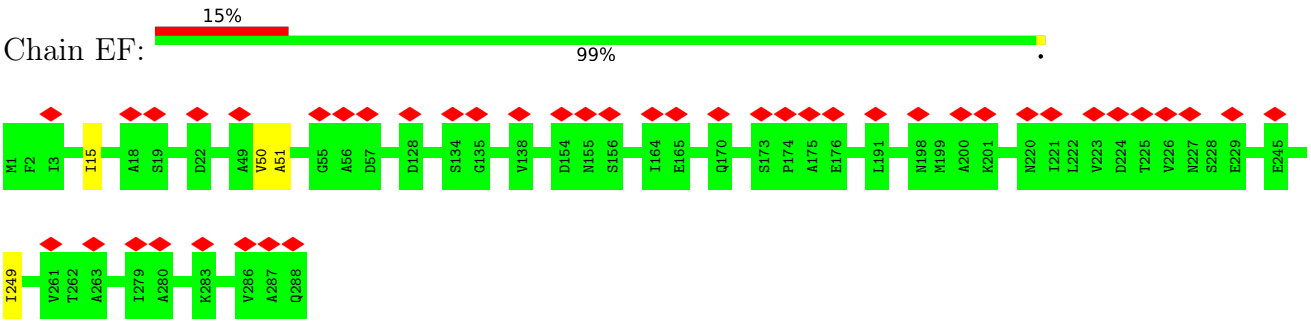
• Molecule 4: Baseplate wedge protein gp9

Chain CF:



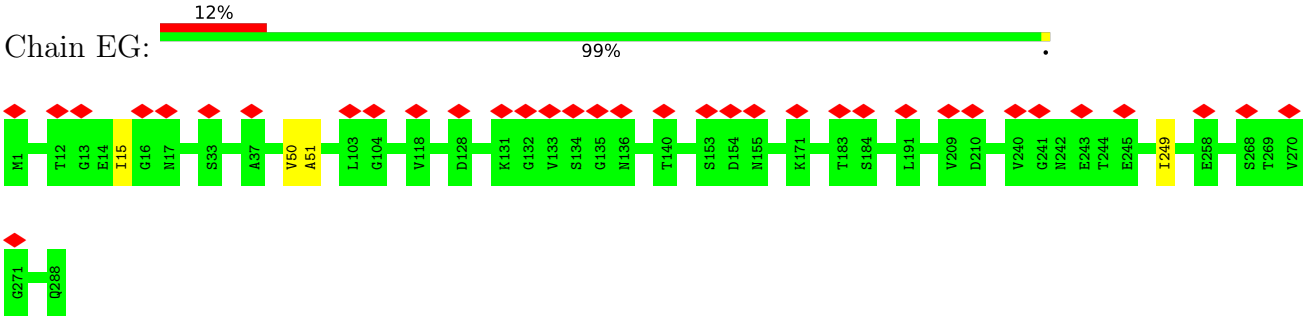
• Molecule 4: Baseplate wedge protein gp9

Chain EF:



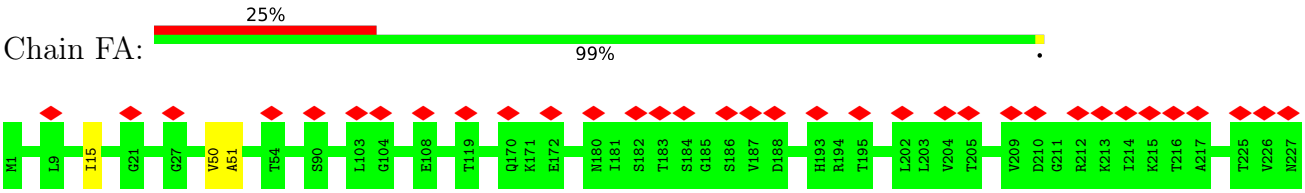
• Molecule 4: Baseplate wedge protein gp9

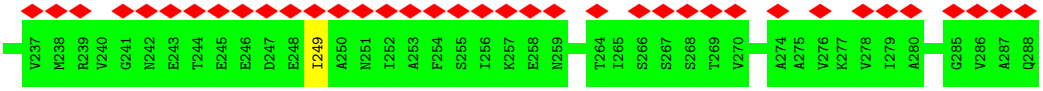
Chain EG:



• Molecule 4: Baseplate wedge protein gp9

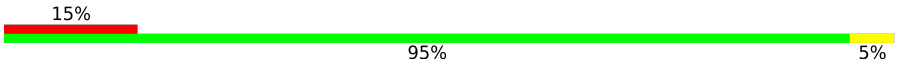
Chain FA:

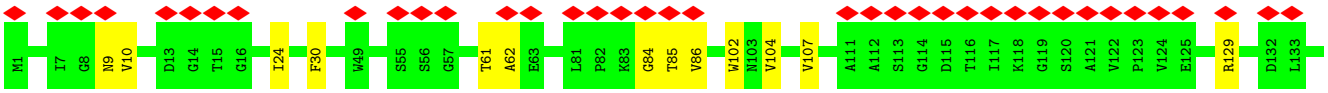


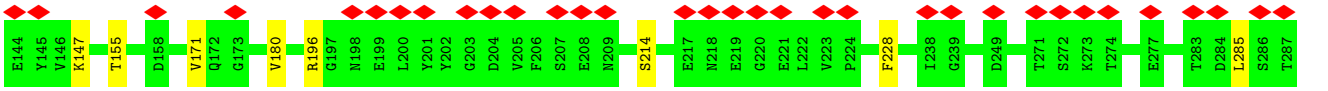


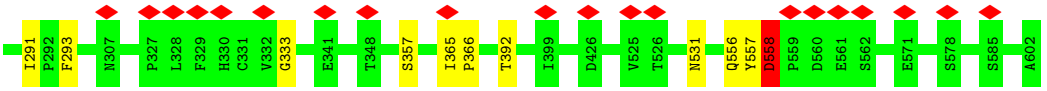
• Molecule 5: Baseplate wedge protein gp10

Chain I:









• Molecule 5: Baseplate wedge protein gp10

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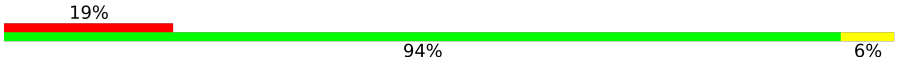
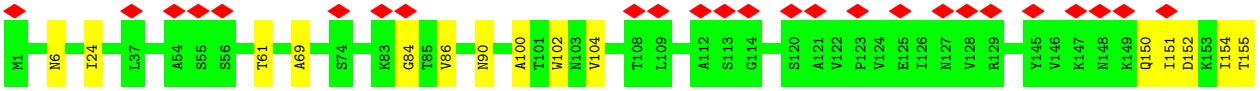
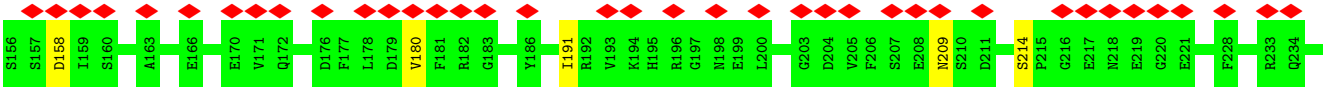
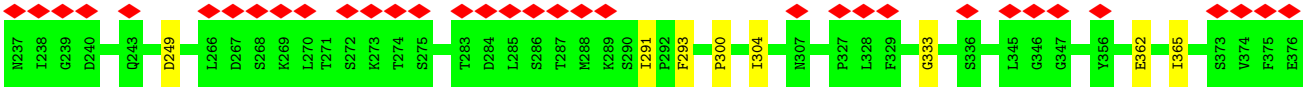
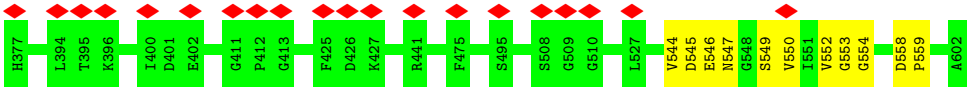




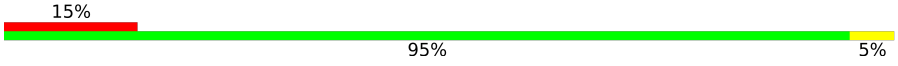


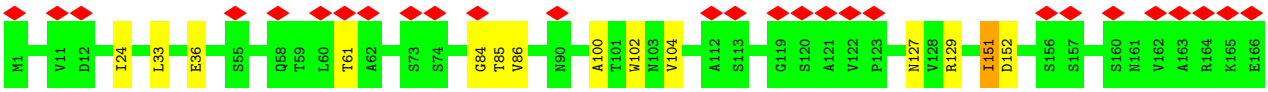


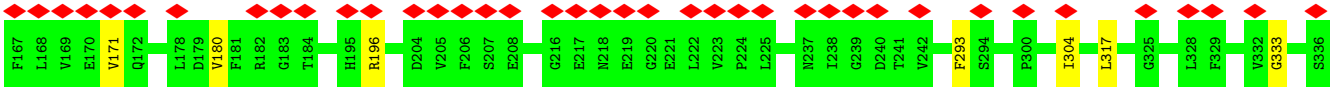


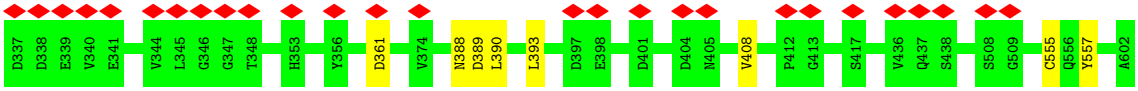
• Molecule 5: Baseplate wedge protein gp10

Chain K:









• Molecule 5: Baseplate wedge protein gp10

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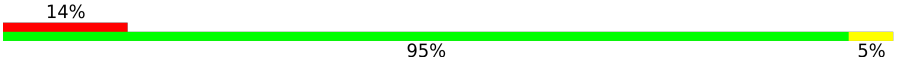
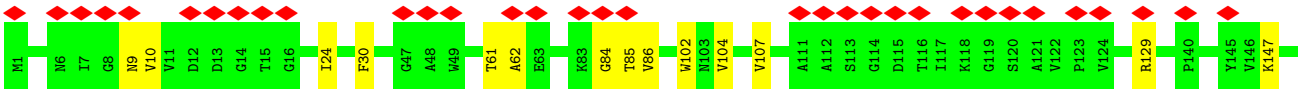
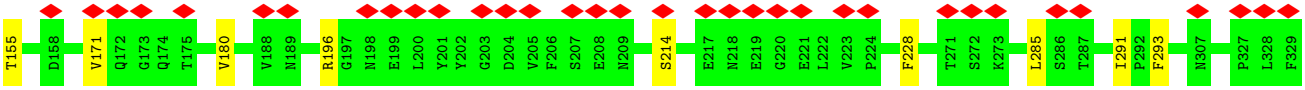
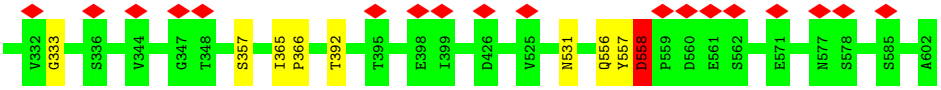


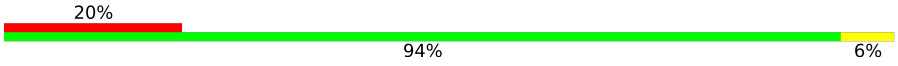


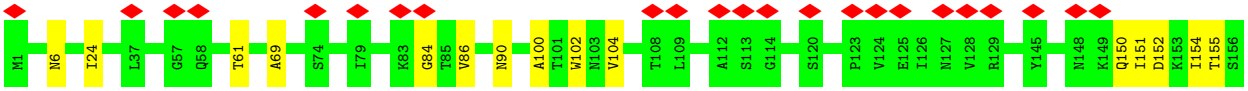


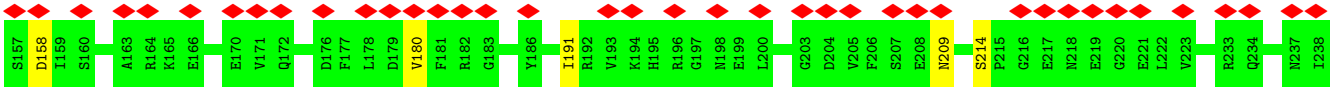


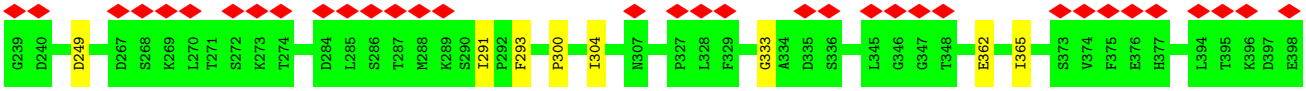
• Molecule 5: Baseplate wedge protein gp10

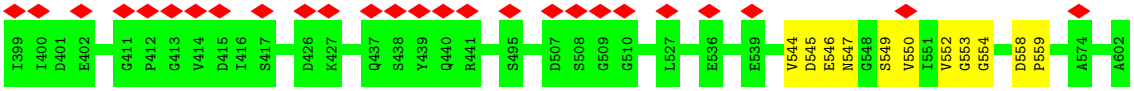
Chain Z:





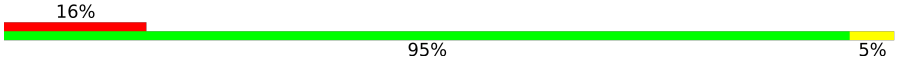


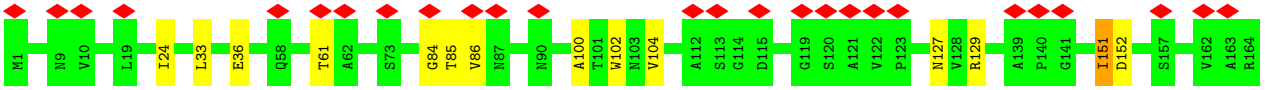


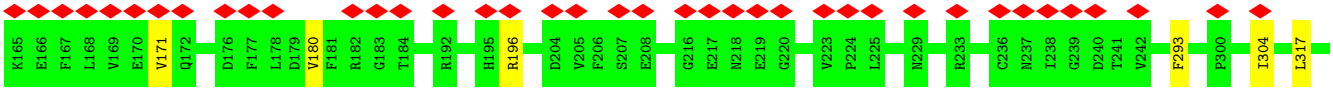


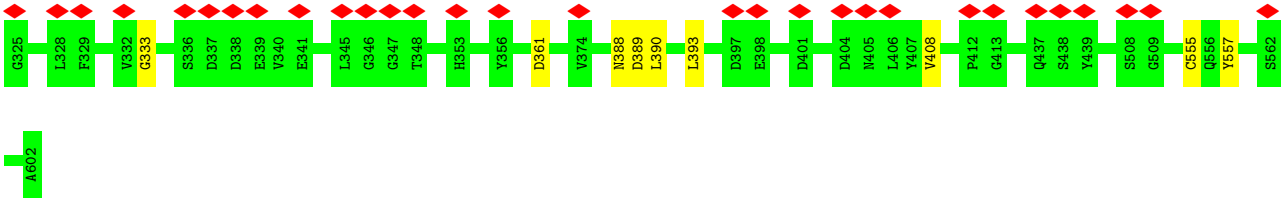
• Molecule 5: Baseplate wedge protein gp10

Chain a:

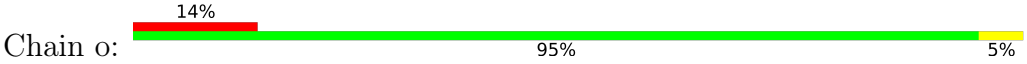


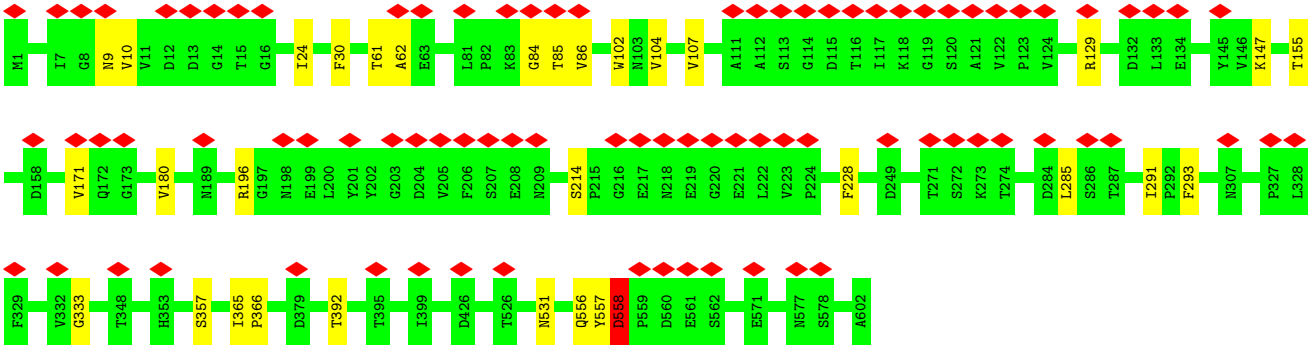




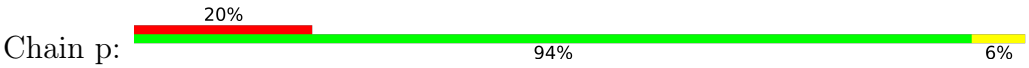


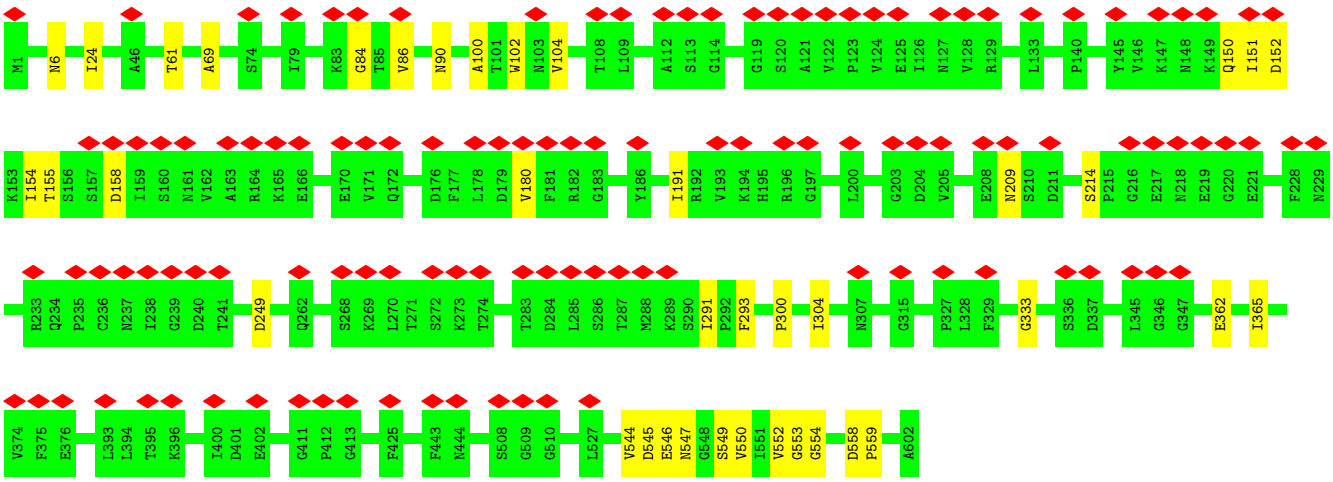
• Molecule 5: Baseplate wedge protein gp10



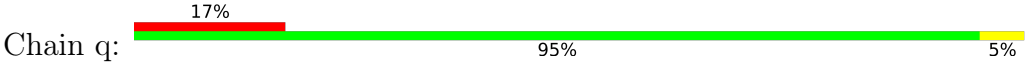


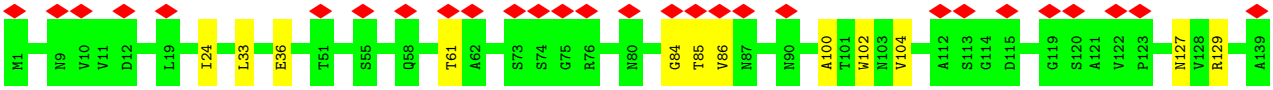
• Molecule 5: Baseplate wedge protein gp10

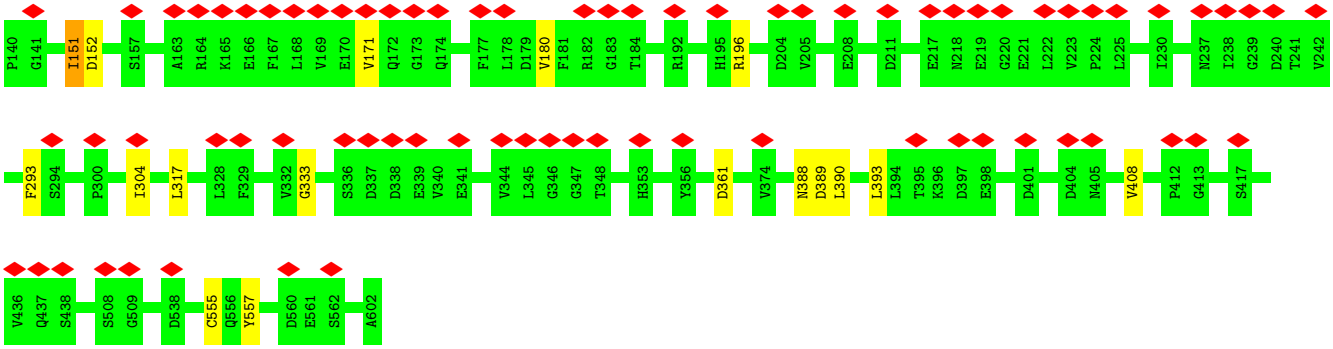




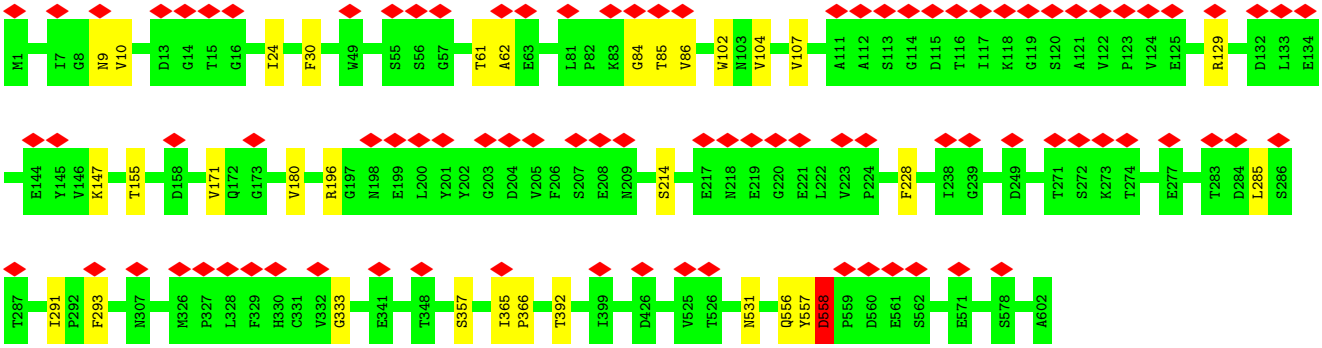
• Molecule 5: Baseplate wedge protein gp10



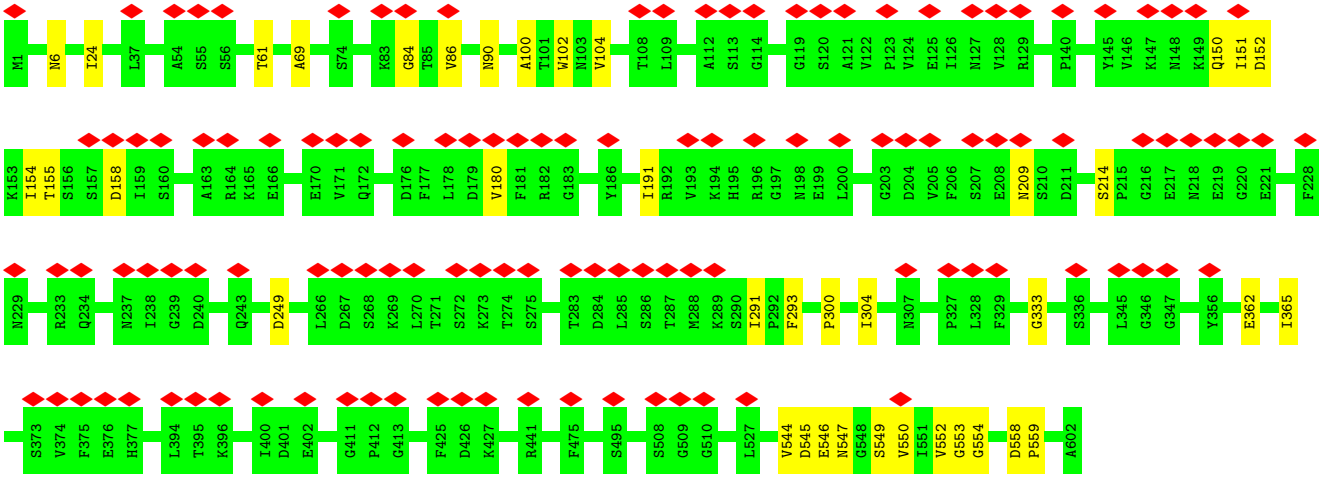




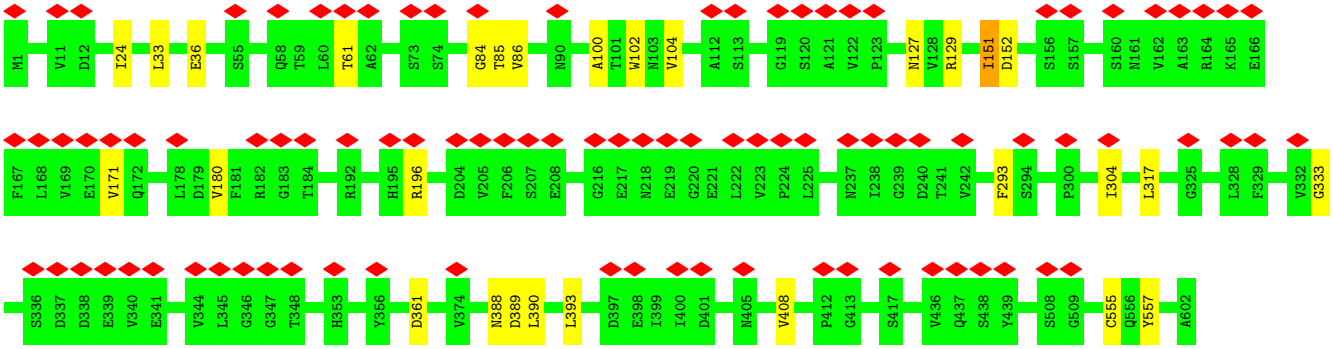
• Molecule 5: Baseplate wedge protein gp10



• Molecule 5: Baseplate wedge protein gp10



• Molecule 5: Baseplate wedge protein gp10



• Molecule 5: Baseplate wedge protein gp10

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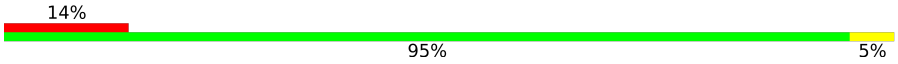
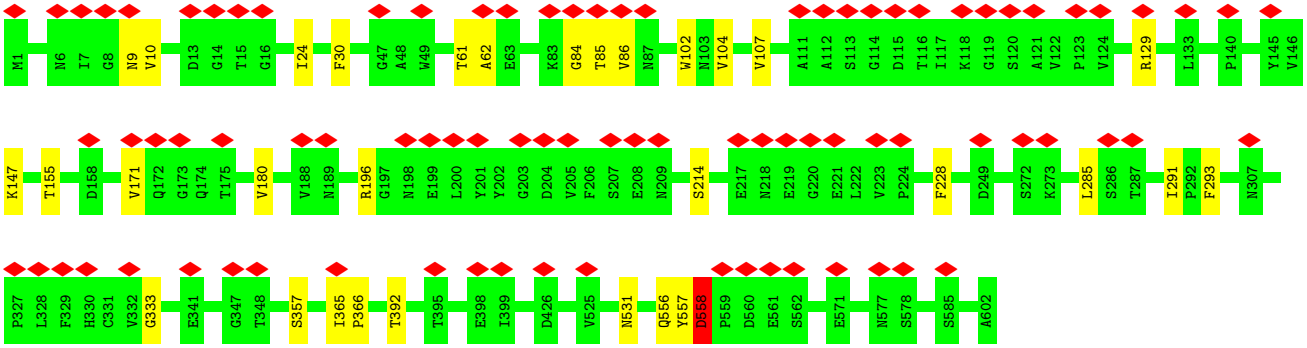
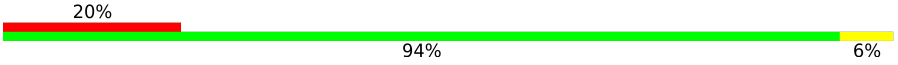
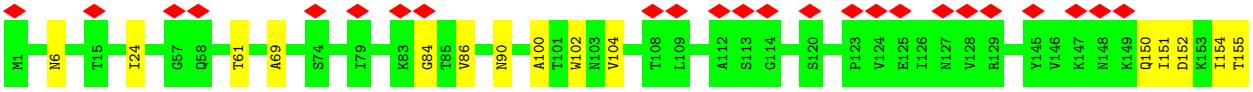


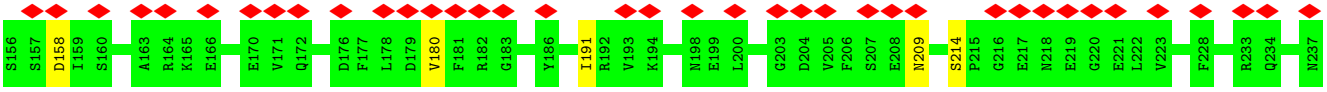


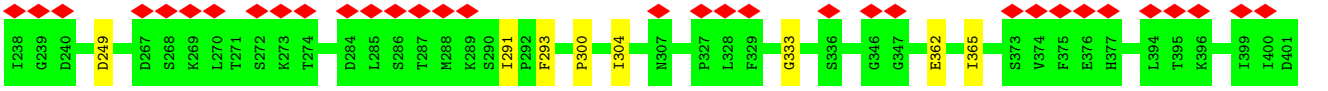
• Molecule 5: Baseplate wedge protein gp10

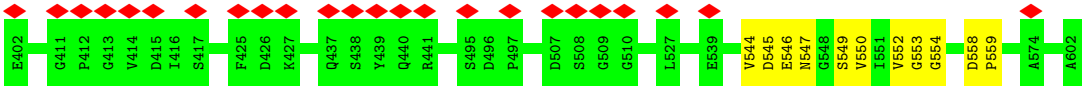
Chain DA:





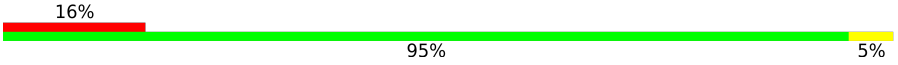


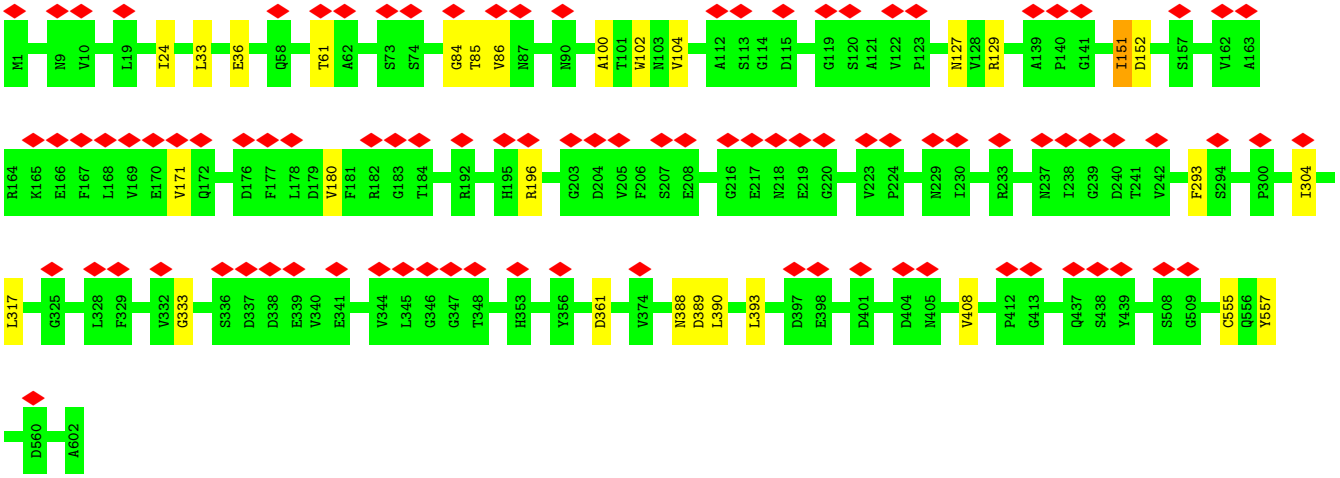




• Molecule 5: Baseplate wedge protein gp10

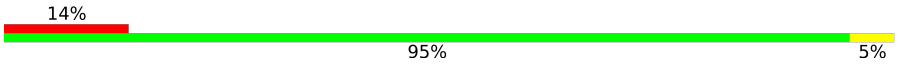
Chain DB:

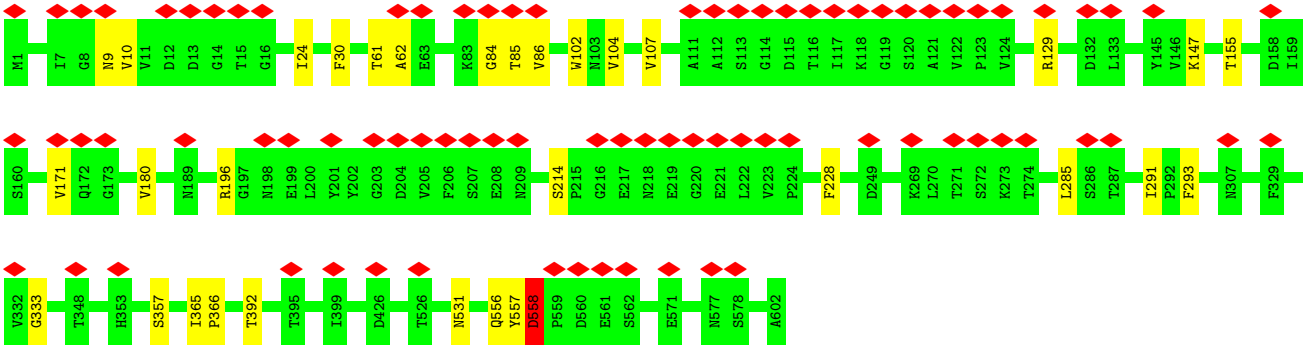




• Molecule 5: Baseplate wedge protein gp10

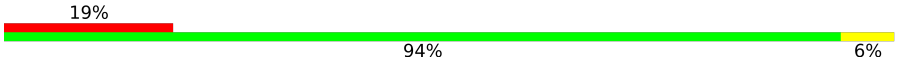
Chain FB:

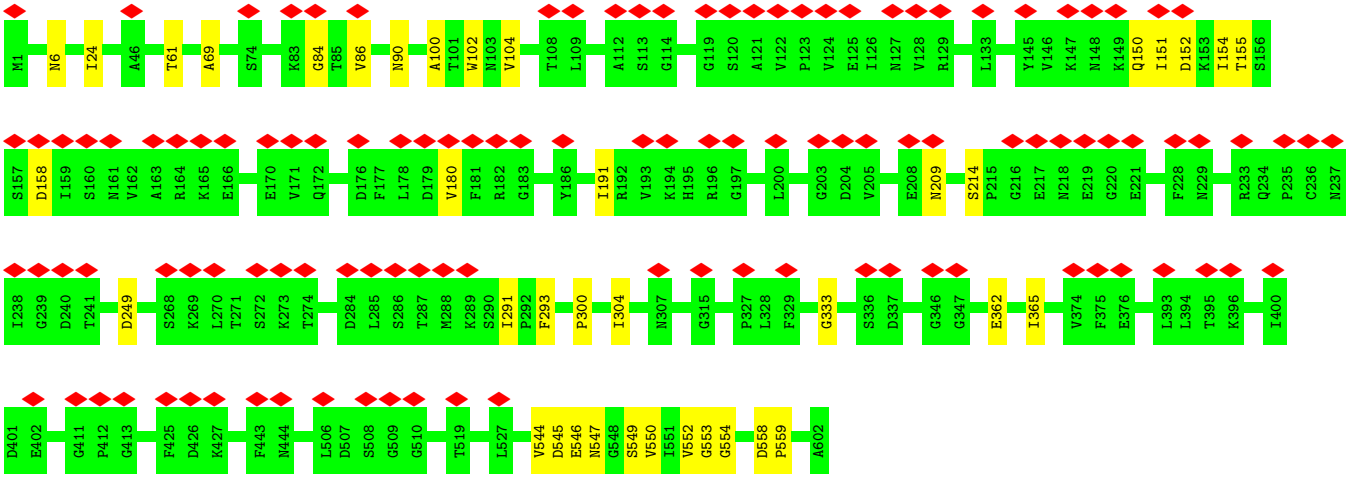




• Molecule 5: Baseplate wedge protein gp10

Chain FC:





• Molecule 5: Baseplate wedge protein gp10

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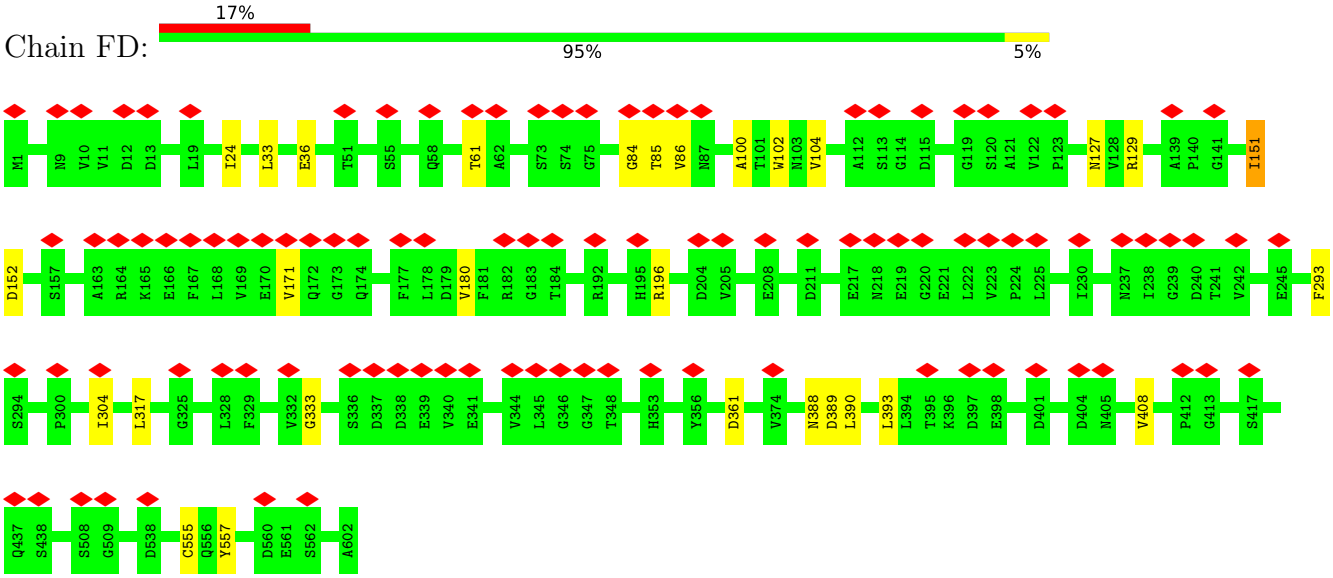
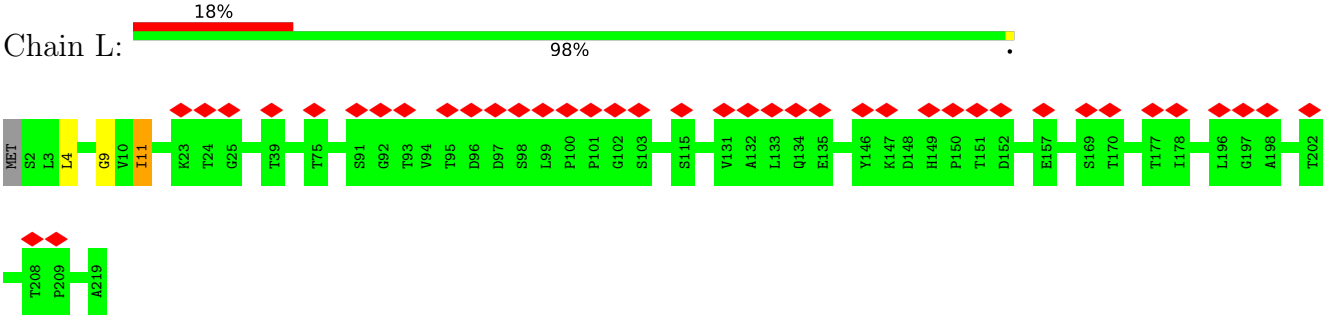


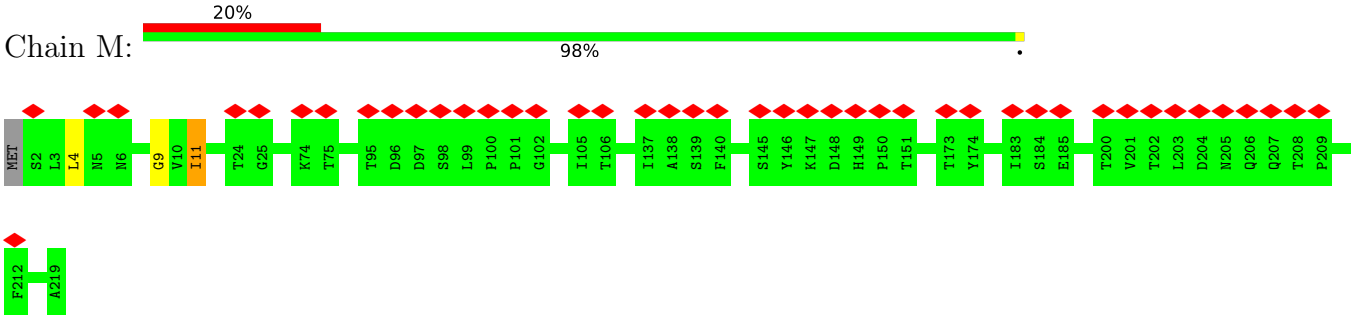
• Molecule 6: Baseplate wedge protein gp11

Chain L:



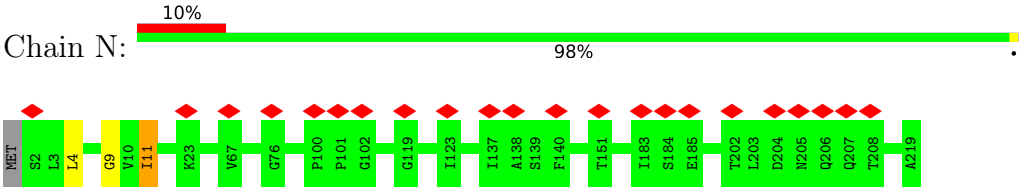
• Molecule 6: Baseplate wedge protein gp11

Chain M:



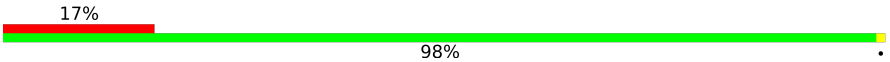
• Molecule 6: Baseplate wedge protein gp11

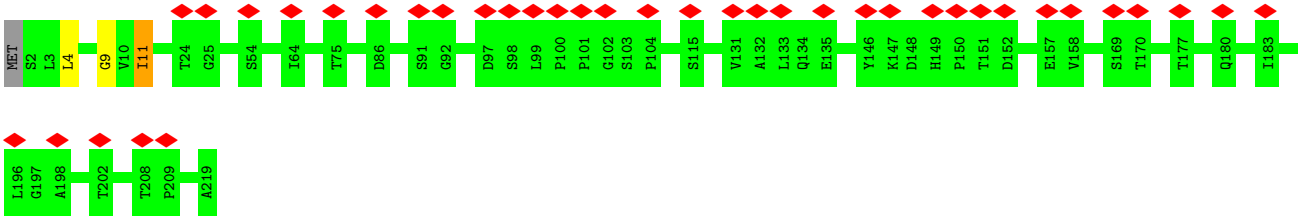
Chain N:



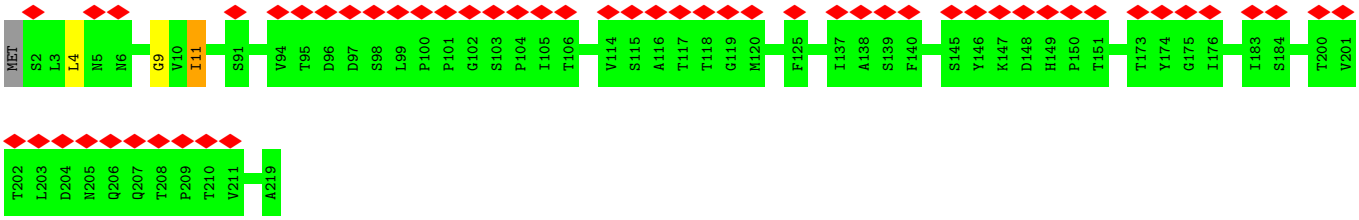
• Molecule 6: Baseplate wedge protein gp11

Chain b:

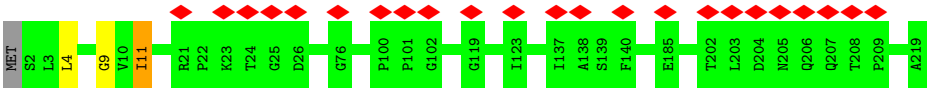




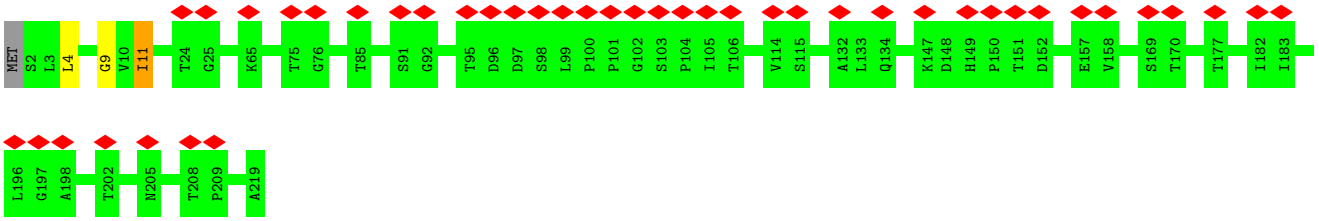
• Molecule 6: Baseplate wedge protein gp11



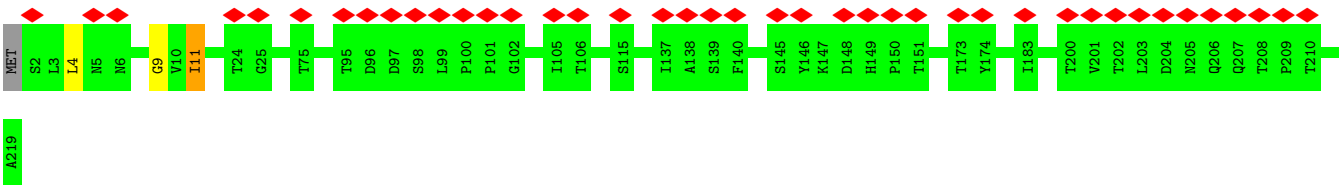
• Molecule 6: Baseplate wedge protein gp11



• Molecule 6: Baseplate wedge protein gp11

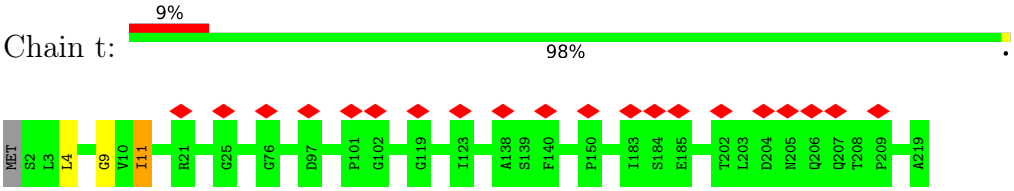


• Molecule 6: Baseplate wedge protein gp11



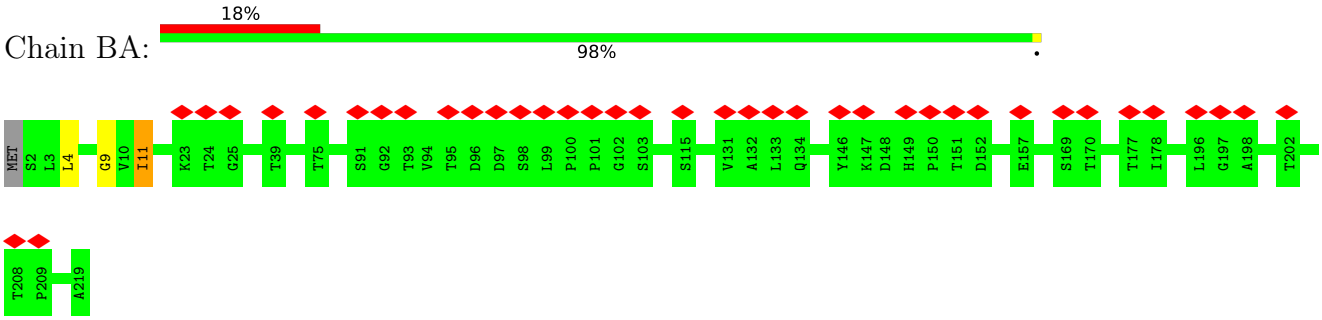
• Molecule 6: Baseplate wedge protein gp11

Chain t:



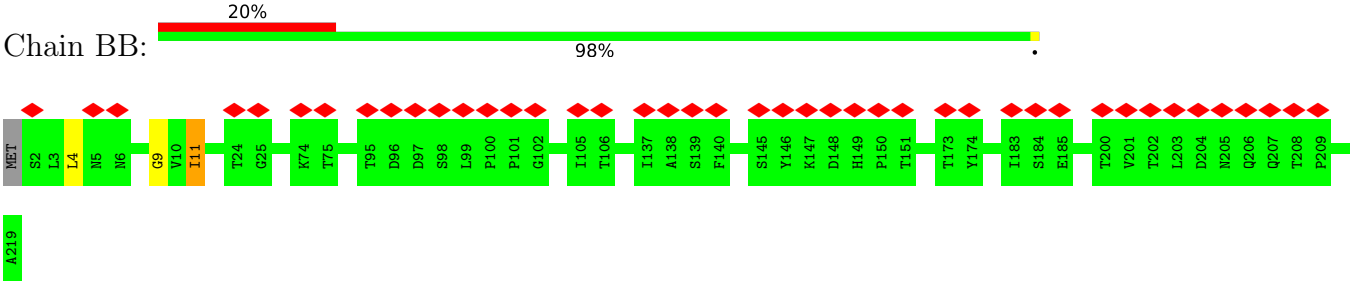
• Molecule 6: Baseplate wedge protein gp11

Chain BA:



• Molecule 6: Baseplate wedge protein gp11

Chain BB:



• Molecule 6: Baseplate wedge protein gp11

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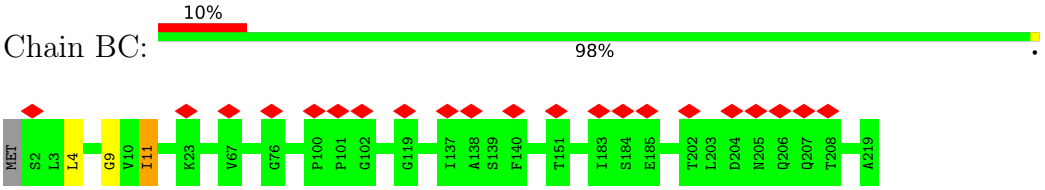

• Molecule 6: Baseplate wedge protein gp11

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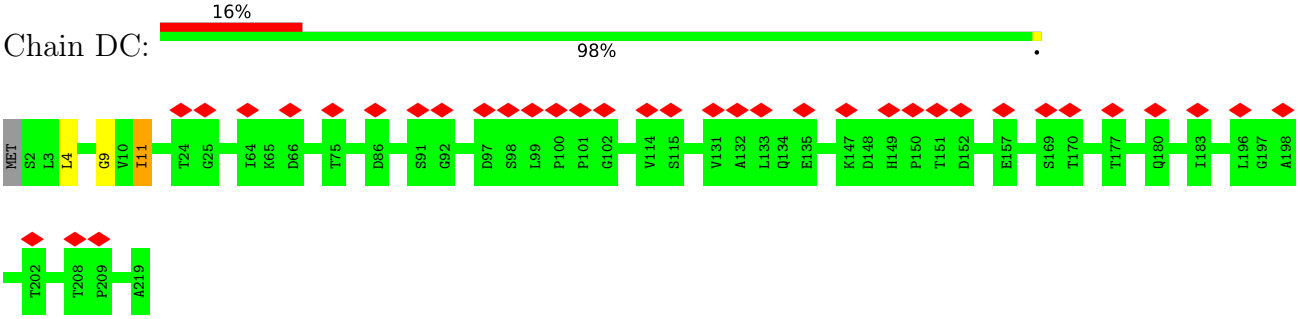

• Molecule 6: Baseplate wedge protein gp11

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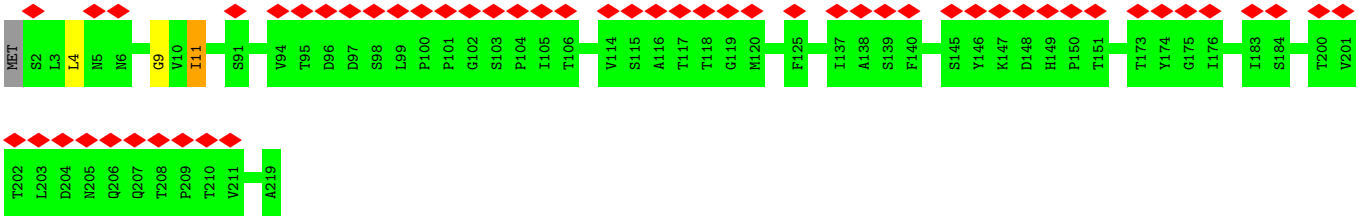

• Molecule 6: Baseplate wedge protein gp11

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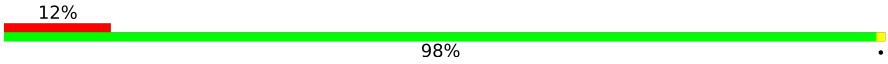
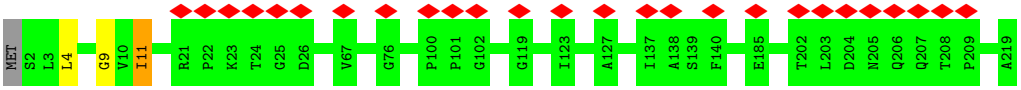
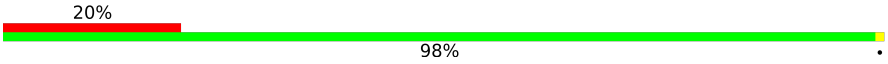
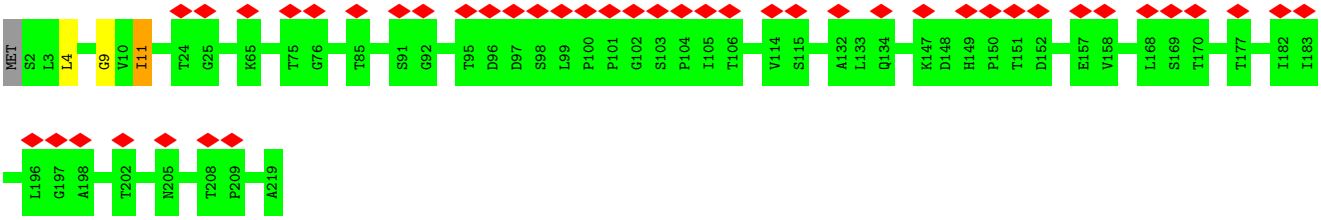




• Molecule 6: Baseplate wedge protein gp11

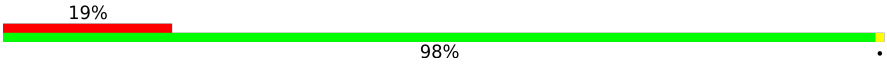
Chain FE:

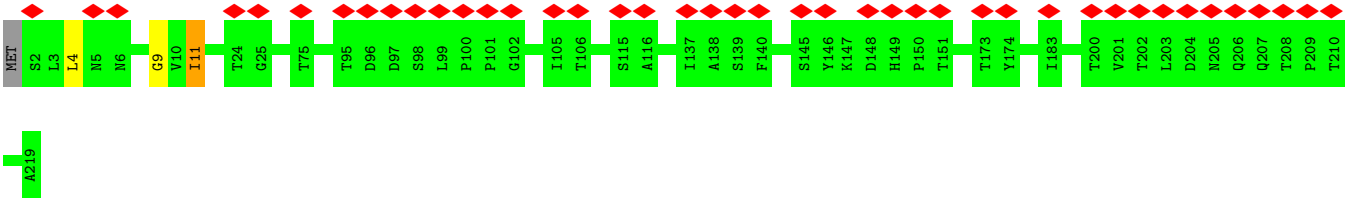




• Molecule 6: Baseplate wedge protein gp11

Chain FF:





• Molecule 6: Baseplate wedge protein gp11

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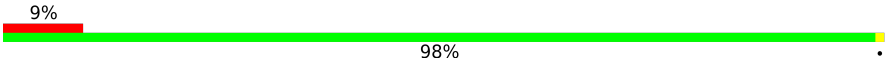
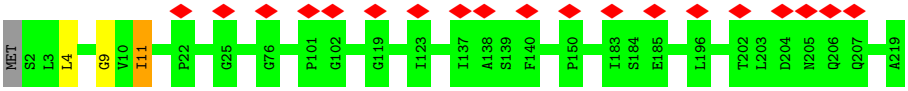
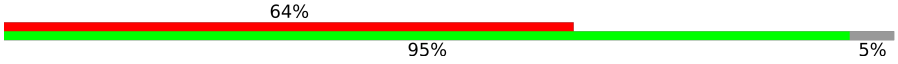
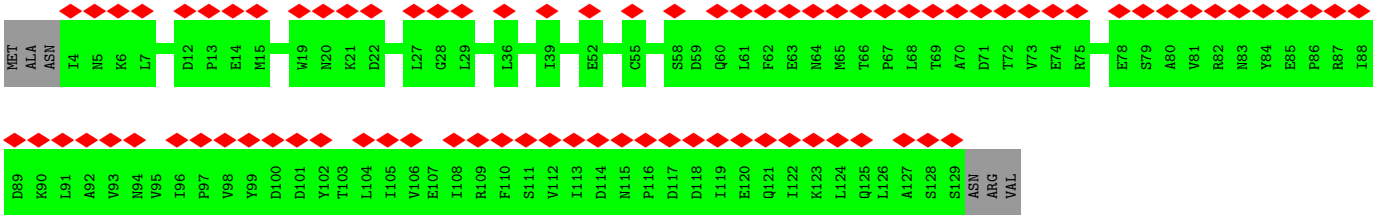




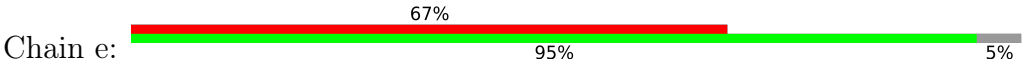
• Molecule 7: Baseplate wedge protein gp25

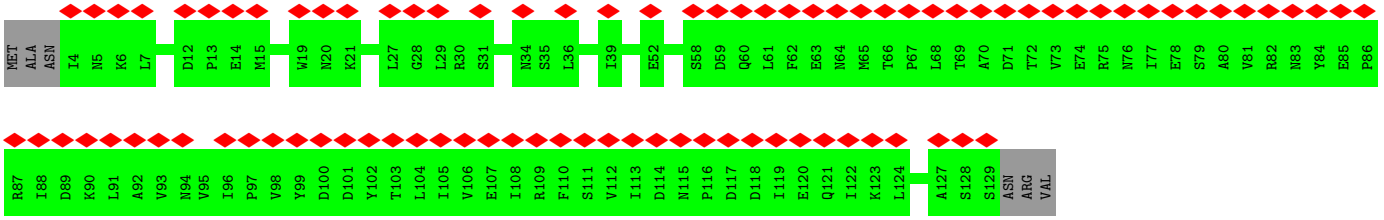
Chain O:



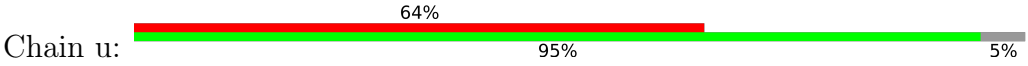


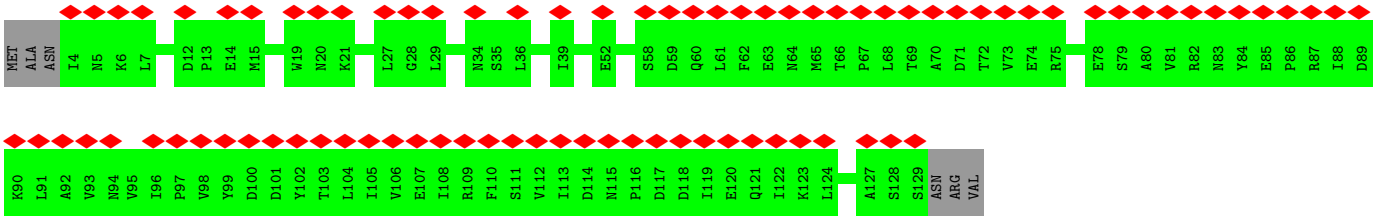
• Molecule 7: Baseplate wedge protein gp25



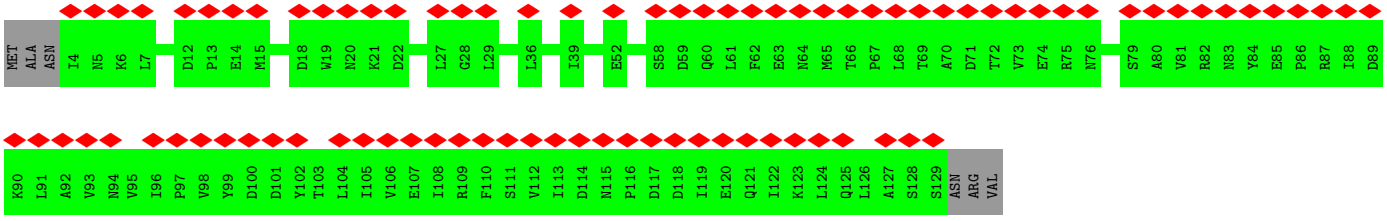


• Molecule 7: Baseplate wedge protein gp25

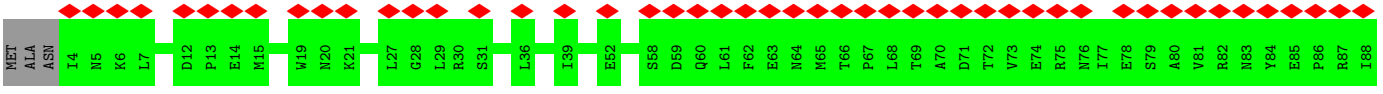




• Molecule 7: Baseplate wedge protein gp25

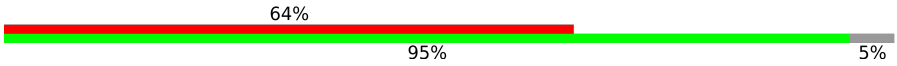


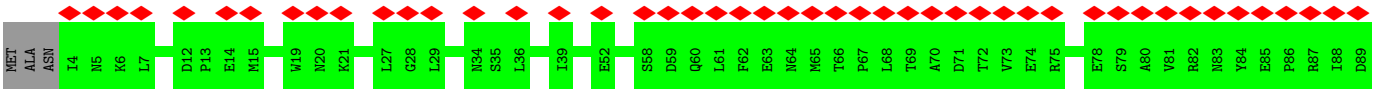
• Molecule 7: Baseplate wedge protein gp25

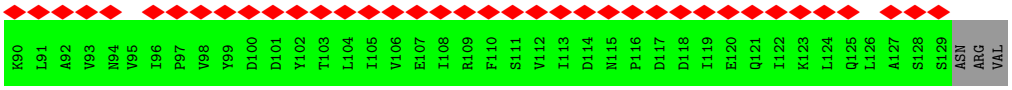


• Molecule 7: Baseplate wedge protein gp25

Chain GA:

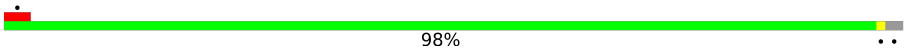


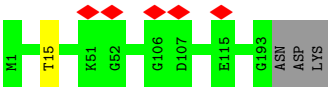




• Molecule 8: Baseplate wedge protein gp53

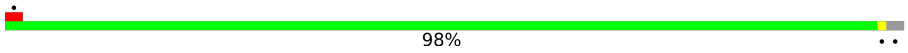
Chain P:

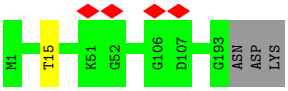




• Molecule 8: Baseplate wedge protein gp53

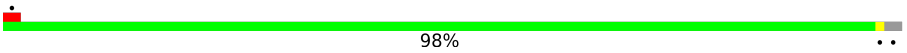
Chain f:

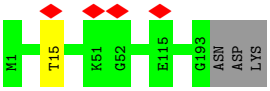




• Molecule 8: Baseplate wedge protein gp53

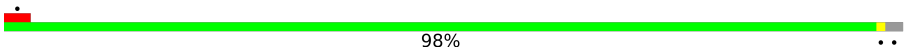
Chain v:

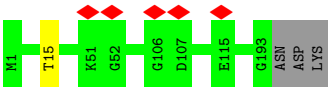




• Molecule 8: Baseplate wedge protein gp53

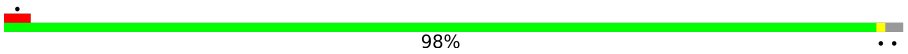
Chain BE:

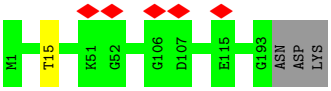




• Molecule 8: Baseplate wedge protein gp53

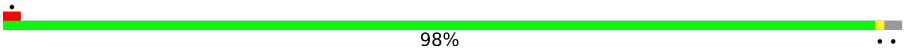
Chain DG:

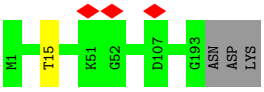




• Molecule 8: Baseplate wedge protein gp53

Chain GB:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	5176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37700	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0095	Depositor
Map size (Å)	636.48, 636.48, 636.48	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.326, 1.326, 1.326	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.45	0/5337	0.63	1/7256 (0.0%)
1	B	0.47	0/5257	0.65	0/7144
1	BF	0.45	0/5337	0.63	1/7256 (0.0%)
1	BG	0.47	0/5257	0.65	0/7144
1	EA	0.45	0/5337	0.63	1/7256 (0.0%)
1	EB	0.47	0/5257	0.65	0/7144
1	Q	0.45	0/5337	0.63	1/7256 (0.0%)
1	R	0.47	0/5257	0.65	0/7144
1	g	0.45	0/5337	0.63	1/7256 (0.0%)
1	h	0.47	0/5257	0.65	0/7144
1	w	0.45	0/5337	0.63	1/7256 (0.0%)
1	x	0.47	0/5257	0.65	0/7144
2	C	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	CA	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	EC	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	S	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	i	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
2	y	0.51	3/8405 (0.0%)	0.75	7/11412 (0.1%)
3	AA	0.56	0/2736	0.79	3/3731 (0.1%)
3	CB	0.56	0/2709	0.79	3/3694 (0.1%)
3	CC	0.56	0/2736	0.79	3/3731 (0.1%)
3	D	0.56	0/2709	0.79	3/3694 (0.1%)
3	E	0.56	0/2736	0.79	3/3731 (0.1%)
3	ED	0.56	0/2709	0.79	3/3694 (0.1%)
3	EE	0.56	0/2736	0.79	3/3731 (0.1%)
3	T	0.56	0/2709	0.79	3/3694 (0.1%)
3	U	0.56	0/2736	0.79	3/3731 (0.1%)
3	j	0.56	0/2709	0.79	3/3694 (0.1%)
3	k	0.56	0/2736	0.79	3/3731 (0.1%)
3	z	0.56	0/2709	0.80	3/3694 (0.1%)
4	AB	0.40	0/2205	0.58	0/2988
4	AC	0.40	0/2205	0.58	0/2988
4	AD	0.40	0/2205	0.58	0/2988
4	CD	0.40	0/2205	0.58	0/2988

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	CE	0.40	0/2205	0.58	0/2988
4	CF	0.40	0/2205	0.58	0/2988
4	EF	0.40	0/2205	0.58	0/2988
4	EG	0.40	0/2205	0.58	0/2988
4	F	0.40	0/2205	0.58	0/2988
4	FA	0.40	0/2205	0.58	0/2988
4	G	0.40	0/2205	0.58	0/2988
4	H	0.40	0/2205	0.58	0/2988
4	V	0.40	0/2205	0.58	0/2988
4	W	0.40	0/2205	0.58	0/2988
4	X	0.40	0/2205	0.58	0/2988
4	l	0.40	0/2205	0.58	0/2988
4	m	0.40	0/2205	0.58	0/2988
4	n	0.40	0/2205	0.58	0/2988
5	AE	0.42	0/4777	0.68	4/6510 (0.1%)
5	AF	0.43	0/4778	0.71	3/6513 (0.0%)
5	AG	0.44	0/4778	0.69	3/6513 (0.0%)
5	CG	0.42	0/4777	0.68	4/6510 (0.1%)
5	DA	0.43	0/4778	0.71	3/6513 (0.0%)
5	DB	0.44	0/4778	0.69	3/6513 (0.0%)
5	FB	0.42	0/4777	0.68	4/6510 (0.1%)
5	FC	0.43	0/4778	0.71	3/6513 (0.0%)
5	FD	0.44	0/4778	0.69	3/6513 (0.0%)
5	I	0.42	0/4777	0.68	4/6510 (0.1%)
5	J	0.43	0/4778	0.71	3/6513 (0.0%)
5	K	0.44	0/4778	0.69	3/6513 (0.0%)
5	Y	0.42	0/4777	0.68	4/6510 (0.1%)
5	Z	0.43	0/4778	0.71	3/6513 (0.0%)
5	a	0.44	0/4778	0.69	3/6513 (0.0%)
5	o	0.42	0/4777	0.68	4/6510 (0.1%)
5	p	0.43	0/4778	0.71	3/6513 (0.0%)
5	q	0.44	0/4778	0.69	3/6513 (0.0%)
6	BA	0.42	0/1700	0.62	0/2318
6	BB	0.42	0/1700	0.62	0/2318
6	BC	0.42	0/1700	0.63	0/2318
6	DC	0.42	0/1700	0.62	0/2318
6	DD	0.42	0/1700	0.62	0/2318
6	DE	0.42	0/1700	0.62	0/2318
6	FE	0.42	0/1700	0.62	0/2318
6	FF	0.42	0/1700	0.62	0/2318
6	FG	0.42	0/1700	0.62	0/2318
6	L	0.42	0/1700	0.62	0/2318
6	M	0.42	0/1700	0.62	0/2318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
6	N	0.42	0/1700	0.62	0/2318
6	b	0.42	0/1700	0.62	0/2318
6	c	0.42	0/1700	0.62	0/2318
6	d	0.42	0/1700	0.63	0/2318
6	r	0.42	0/1700	0.62	0/2318
6	s	0.42	0/1700	0.62	0/2318
6	t	0.42	0/1700	0.62	0/2318
7	BD	0.35	0/1027	0.58	0/1392
7	DF	0.35	0/1027	0.57	0/1392
7	GA	0.35	0/1027	0.58	0/1392
7	O	0.35	0/1027	0.58	0/1392
7	e	0.35	0/1027	0.57	0/1392
7	u	0.35	0/1027	0.58	0/1392
8	BE	0.48	0/1643	0.62	0/2228
8	DG	0.48	0/1643	0.62	0/2228
8	GB	0.48	0/1643	0.62	0/2228
8	P	0.48	0/1643	0.62	0/2228
8	f	0.48	0/1643	0.62	0/2228
8	v	0.48	0/1643	0.62	0/2228
All	All	0.46	18/318972 (0.0%)	0.68	144/433866 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	7
1	BF	0	6
1	BG	0	7
1	EA	0	6
1	EB	0	7
1	Q	0	6
1	R	0	7
1	g	0	6
1	h	0	7
1	w	0	6
1	x	0	7
2	C	0	31
2	CA	0	31
2	EC	0	31

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	S	0	31
2	i	0	31
2	y	0	31
3	AA	0	4
3	CB	0	3
3	CC	0	4
3	D	0	3
3	E	0	4
3	ED	0	3
3	EE	0	4
3	T	0	3
3	U	0	4
3	j	0	3
3	k	0	4
3	z	0	3
5	AE	0	16
5	AF	0	24
5	AG	0	15
5	CG	0	16
5	DA	0	24
5	DB	0	15
5	FB	0	16
5	FC	0	24
5	FD	0	15
5	I	0	16
5	J	0	24
5	K	0	15
5	Y	0	16
5	Z	0	24
5	a	0	15
5	o	0	16
5	p	0	24
5	q	0	15
6	BA	0	2
6	BB	0	2
6	BC	0	2
6	DC	0	2
6	DD	0	2
6	DE	0	2
6	FE	0	2
6	FF	0	2
6	FG	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	L	0	2
6	M	0	2
6	N	0	2
6	b	0	2
6	c	0	2
6	d	0	2
6	r	0	2
6	s	0	2
6	t	0	2
All	All	0	672

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	613	LYS	C-N	6.92	1.47	1.34
2	i	613	LYS	C-N	6.91	1.47	1.34
2	EC	613	LYS	C-N	6.91	1.47	1.34
2	y	613	LYS	C-N	6.90	1.47	1.34
2	CA	613	LYS	C-N	6.90	1.47	1.34
2	S	613	LYS	C-N	6.88	1.47	1.34
2	C	49	LEU	C-N	6.76	1.47	1.34
2	EC	49	LEU	C-N	6.76	1.47	1.34
2	CA	49	LEU	C-N	6.76	1.47	1.34
2	i	49	LEU	C-N	6.75	1.47	1.34
2	S	49	LEU	C-N	6.74	1.47	1.34
2	y	49	LEU	C-N	6.72	1.47	1.34
2	C	72	ALA	C-N	-6.58	1.19	1.34
2	S	72	ALA	C-N	-6.58	1.19	1.34
2	y	72	ALA	C-N	-6.58	1.19	1.34
2	CA	72	ALA	C-N	-6.56	1.19	1.34
2	i	72	ALA	C-N	-6.55	1.19	1.34
2	EC	72	ALA	C-N	-6.55	1.19	1.34

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AG	317	LEU	CA-CB-CG	7.88	133.42	115.30
5	DB	317	LEU	CA-CB-CG	7.87	133.41	115.30
5	q	317	LEU	CA-CB-CG	7.86	133.39	115.30
5	FD	317	LEU	CA-CB-CG	7.86	133.39	115.30
5	K	317	LEU	CA-CB-CG	7.85	133.35	115.30
5	a	317	LEU	CA-CB-CG	7.84	133.32	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	EC	715	LEU	CA-CB-CG	7.35	132.19	115.30
2	CA	715	LEU	CA-CB-CG	7.34	132.18	115.30
2	i	715	LEU	CA-CB-CG	7.33	132.17	115.30
2	y	715	LEU	CA-CB-CG	7.33	132.16	115.30
2	S	715	LEU	CA-CB-CG	7.33	132.16	115.30
2	C	715	LEU	CA-CB-CG	7.33	132.15	115.30
5	FB	558	ASP	C-N-CD	7.02	143.15	128.40
5	Y	558	ASP	C-N-CD	7.01	143.13	128.40
5	I	558	ASP	C-N-CD	7.01	143.12	128.40
5	CG	558	ASP	C-N-CD	7.01	143.12	128.40
5	AE	558	ASP	C-N-CD	7.00	143.10	128.40
5	o	558	ASP	C-N-CD	7.00	143.09	128.40
5	Z	553	GLY	N-CA-C	6.47	129.28	113.10
5	FC	553	GLY	N-CA-C	6.46	129.26	113.10
5	J	553	GLY	N-CA-C	6.46	129.26	113.10
5	p	553	GLY	N-CA-C	6.46	129.25	113.10
5	AF	553	GLY	N-CA-C	6.46	129.24	113.10
5	DA	553	GLY	N-CA-C	6.45	129.24	113.10
3	k	228	ASN	N-CA-C	6.31	128.03	111.00
3	CC	228	ASN	N-CA-C	6.31	128.03	111.00
3	U	228	ASN	N-CA-C	6.30	128.01	111.00
3	EE	228	ASN	N-CA-C	6.29	127.99	111.00
3	AA	228	ASN	N-CA-C	6.29	127.98	111.00
3	E	228	ASN	N-CA-C	6.28	127.95	111.00
2	C	694	TYR	C-N-CD	-6.14	107.09	120.60
2	S	694	TYR	C-N-CD	-6.14	107.09	120.60
2	CA	694	TYR	C-N-CD	-6.13	107.11	120.60
2	i	694	TYR	C-N-CD	-6.13	107.12	120.60
2	EC	694	TYR	C-N-CD	-6.13	107.12	120.60
2	y	694	TYR	C-N-CD	-6.13	107.12	120.60
3	CB	175	ASP	N-CA-C	-5.94	94.96	111.00
3	j	175	ASP	N-CA-C	-5.94	94.97	111.00
3	D	175	ASP	N-CA-C	-5.92	95.00	111.00
3	ED	175	ASP	N-CA-C	-5.92	95.00	111.00
3	z	175	ASP	N-CA-C	-5.92	95.03	111.00
3	T	175	ASP	N-CA-C	-5.91	95.04	111.00
5	CG	62	ALA	N-CA-C	5.78	126.62	111.00
5	I	62	ALA	N-CA-C	5.78	126.61	111.00
5	o	62	ALA	N-CA-C	5.78	126.61	111.00
5	FB	62	ALA	N-CA-C	5.78	126.60	111.00
5	FB	285	LEU	CB-CG-CD1	-5.78	101.18	111.00
5	AE	285	LEU	CB-CG-CD1	-5.77	101.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	62	ALA	N-CA-C	5.77	126.59	111.00
5	CG	285	LEU	CB-CG-CD1	-5.77	101.19	111.00
5	o	285	LEU	CB-CG-CD1	-5.76	101.20	111.00
5	AE	62	ALA	N-CA-C	5.76	126.56	111.00
5	I	285	LEU	CB-CG-CD1	-5.75	101.22	111.00
5	Y	285	LEU	CB-CG-CD1	-5.75	101.22	111.00
3	z	156	LEU	CA-CB-CG	5.72	128.45	115.30
3	j	156	LEU	CA-CB-CG	5.72	128.45	115.30
3	CB	156	LEU	CA-CB-CG	5.71	128.43	115.30
3	T	156	LEU	CA-CB-CG	5.71	128.42	115.30
3	D	156	LEU	CA-CB-CG	5.70	128.40	115.30
3	ED	156	LEU	CA-CB-CG	5.69	128.39	115.30
3	CB	167	MET	CA-CB-CG	5.62	122.85	113.30
3	z	167	MET	CA-CB-CG	5.61	122.84	113.30
3	ED	167	MET	CA-CB-CG	5.61	122.83	113.30
3	j	167	MET	CA-CB-CG	5.60	122.83	113.30
3	T	167	MET	CA-CB-CG	5.60	122.82	113.30
3	D	167	MET	CA-CB-CG	5.58	122.78	113.30
5	DB	33	LEU	CA-CB-CG	5.56	128.09	115.30
5	q	33	LEU	CA-CB-CG	5.56	128.08	115.30
5	K	33	LEU	CA-CB-CG	5.55	128.07	115.30
5	a	33	LEU	CA-CB-CG	5.55	128.06	115.30
5	FD	33	LEU	CA-CB-CG	5.55	128.06	115.30
5	AG	33	LEU	CA-CB-CG	5.54	128.05	115.30
3	AA	156	LEU	CA-CB-CG	5.40	127.72	115.30
3	U	156	LEU	CA-CB-CG	5.39	127.70	115.30
3	E	156	LEU	CA-CB-CG	5.39	127.69	115.30
3	k	156	LEU	CA-CB-CG	5.39	127.69	115.30
3	CC	156	LEU	CA-CB-CG	5.38	127.67	115.30
3	EE	156	LEU	CA-CB-CG	5.38	127.66	115.30
2	y	539	LEU	CA-CB-CG	5.31	127.51	115.30
2	C	539	LEU	CA-CB-CG	5.30	127.50	115.30
2	CA	539	LEU	CA-CB-CG	5.30	127.50	115.30
2	EC	539	LEU	CA-CB-CG	5.30	127.48	115.30
2	i	539	LEU	CA-CB-CG	5.29	127.47	115.30
2	S	539	LEU	CA-CB-CG	5.28	127.44	115.30
2	C	848	LEU	CA-CB-CG	5.28	127.43	115.30
2	S	1012	LEU	CB-CG-CD1	5.28	119.97	111.00
2	EC	848	LEU	CA-CB-CG	5.27	127.42	115.30
2	i	848	LEU	CA-CB-CG	5.26	127.41	115.30
2	y	848	LEU	CA-CB-CG	5.26	127.41	115.30
2	S	848	LEU	CA-CB-CG	5.26	127.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	531	ASN	C-N-CA	-5.25	108.58	121.70
5	o	531	ASN	C-N-CA	-5.25	108.58	121.70
5	AE	531	ASN	C-N-CA	-5.25	108.58	121.70
5	AF	158	ASP	CB-CG-OD1	5.25	123.02	118.30
2	CA	848	LEU	CA-CB-CG	5.24	127.36	115.30
5	CG	531	ASN	C-N-CA	-5.24	108.60	121.70
5	FB	531	ASN	C-N-CA	-5.24	108.61	121.70
2	i	1012	LEU	CB-CG-CD1	5.23	119.90	111.00
5	I	531	ASN	C-N-CA	-5.23	108.62	121.70
2	CA	1012	LEU	CB-CG-CD1	5.23	119.89	111.00
2	EC	1012	LEU	CB-CG-CD1	5.23	119.89	111.00
5	DA	158	ASP	CB-CG-OD1	5.23	123.00	118.30
2	C	1012	LEU	CB-CG-CD1	5.22	119.88	111.00
5	Z	158	ASP	CB-CG-OD1	5.22	123.00	118.30
3	E	100	TYR	CA-CB-CG	-5.22	103.48	113.40
1	w	307	ASP	C-N-CD	-5.22	109.12	120.60
3	AA	100	TYR	CA-CB-CG	-5.22	103.49	113.40
3	CC	100	TYR	CA-CB-CG	-5.22	103.49	113.40
3	EE	100	TYR	CA-CB-CG	-5.21	103.49	113.40
3	k	100	TYR	CA-CB-CG	-5.21	103.50	113.40
2	y	1012	LEU	CB-CG-CD1	5.21	119.85	111.00
1	BF	307	ASP	C-N-CD	-5.21	109.15	120.60
1	g	307	ASP	C-N-CD	-5.20	109.15	120.60
1	EA	307	ASP	C-N-CD	-5.20	109.16	120.60
1	A	307	ASP	C-N-CD	-5.20	109.16	120.60
5	J	158	ASP	CB-CG-OD1	5.20	122.98	118.30
5	p	158	ASP	CB-CG-OD1	5.20	122.98	118.30
3	U	100	TYR	CA-CB-CG	-5.20	103.53	113.40
5	FC	158	ASP	CB-CG-OD1	5.20	122.98	118.30
1	Q	307	ASP	C-N-CD	-5.19	109.18	120.60
2	S	556	LEU	CA-CB-CG	5.17	127.19	115.30
2	EC	556	LEU	CA-CB-CG	5.17	127.18	115.30
2	C	556	LEU	CA-CB-CG	5.16	127.17	115.30
2	y	556	LEU	CA-CB-CG	5.15	127.15	115.30
2	i	556	LEU	CA-CB-CG	5.15	127.15	115.30
2	CA	556	LEU	CA-CB-CG	5.15	127.14	115.30
5	DA	544	VAL	C-N-CA	5.12	134.49	121.70
5	Z	544	VAL	C-N-CA	5.11	134.48	121.70
5	p	544	VAL	C-N-CA	5.10	134.45	121.70
5	J	544	VAL	C-N-CA	5.09	134.43	121.70
5	AF	544	VAL	C-N-CA	5.09	134.44	121.70
5	FC	544	VAL	C-N-CA	5.09	134.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	LEU	CA-CB-CG	-5.09	103.60	115.30
2	y	300	LEU	CA-CB-CG	-5.08	103.62	115.30
2	CA	300	LEU	CA-CB-CG	-5.07	103.63	115.30
2	i	300	LEU	CA-CB-CG	-5.07	103.64	115.30
2	EC	300	LEU	CA-CB-CG	-5.06	103.66	115.30
5	DB	557	TYR	C-N-CA	5.06	134.35	121.70
2	S	300	LEU	CA-CB-CG	-5.06	103.66	115.30
5	K	557	TYR	C-N-CA	5.06	134.34	121.70
5	q	557	TYR	C-N-CA	5.06	134.34	121.70
5	a	557	TYR	C-N-CA	5.04	134.30	121.70
5	AG	557	TYR	C-N-CA	5.03	134.27	121.70
5	FD	557	TYR	C-N-CA	5.03	134.27	121.70

There are no chirality outliers.

All (672) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ILE	Peptide
1	A	209	TRP	Peptide
1	A	262	PRO	Peptide
1	A	451	ASP	Peptide
1	A	576	ASP	Peptide
1	A	6	VAL	Peptide
3	AA	177	GLU	Peptide
3	AA	178	GLY	Peptide
3	AA	228	ASN	Peptide
3	AA	32	PRO	Peptide
5	AE	102	TRP	Peptide
5	AE	107	VAL	Peptide
5	AE	155	THR	Peptide
5	AE	196	ARG	Peptide
5	AE	214	SER	Peptide
5	AE	291	ILE	Peptide
5	AE	293	PHE	Peptide
5	AE	333	GLY	Peptide
5	AE	357	SER	Peptide
5	AE	365	ILE	Peptide
5	AE	366	PRO	Peptide
5	AE	556	GLN	Peptide
5	AE	558	ASP	Peptide
5	AE	61	THR	Peptide
5	AE	84	GLY	Peptide

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Mol	Chain	Res	Type	Group
5	AE	9	ASN	Peptide
5	AF	100	ALA	Peptide
5	AF	102	TRP	Peptide
5	AF	150	GLN	Peptide
5	AF	152	ASP	Peptide
5	AF	155	THR	Peptide
5	AF	191	ILE	Peptide
5	AF	214	SER	Peptide
5	AF	291	ILE	Peptide
5	AF	293	PHE	Peptide
5	AF	300	PRO	Peptide
5	AF	304	ILE	Peptide
5	AF	333	GLY	Peptide
5	AF	362	GLU	Peptide
5	AF	545	ASP	Peptide
5	AF	547	ASN	Peptide
5	AF	549	SER	Peptide
5	AF	550	VAL	Peptide
5	AF	552	VAL	Peptide
5	AF	554	GLY	Peptide
5	AF	558	ASP	Peptide
5	AF	6	ASN	Peptide
5	AF	61	THR	Peptide
5	AF	69	ALA	Peptide
5	AF	84	GLY	Peptide
5	AG	100	ALA	Peptide
5	AG	102	TRP	Peptide
5	AG	127	ASN	Peptide
5	AG	151	ILE	Peptide
5	AG	196	ARG	Peptide
5	AG	293	PHE	Peptide
5	AG	333	GLY	Peptide
5	AG	361	ASP	Peptide
5	AG	388	ASN	Peptide
5	AG	389	ASP	Peptide
5	AG	390	LEU	Peptide
5	AG	393	LEU	Peptide
5	AG	555	CYS	Peptide
5	AG	61	THR	Peptide
5	AG	84	GLY	Peptide
1	B	137	ASP	Peptide
1	B	20	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	200	TYR	Peptide
1	B	212	LYS	Peptide
1	B	241	GLY	Peptide
1	B	453	GLU	Peptide
1	B	612	THR	Peptide
6	BA	11	ILE	Peptide
6	BA	9	GLY	Peptide
6	BB	11	ILE	Peptide
6	BB	9	GLY	Peptide
6	BC	11	ILE	Peptide
6	BC	9	GLY	Peptide
1	BF	186	ILE	Peptide
1	BF	209	TRP	Peptide
1	BF	262	PRO	Peptide
1	BF	451	ASP	Peptide
1	BF	576	ASP	Peptide
1	BF	6	VAL	Peptide
1	BG	137	ASP	Peptide
1	BG	20	ILE	Peptide
1	BG	200	TYR	Peptide
1	BG	212	LYS	Peptide
1	BG	241	GLY	Peptide
1	BG	453	GLU	Peptide
1	BG	612	THR	Peptide
2	C	1016	ILE	Peptide
2	C	156	SER	Peptide
2	C	167	ILE	Peptide
2	C	184	CYS	Peptide
2	C	215	LYS	Peptide
2	C	300	LEU	Peptide
2	C	331	THR	Peptide
2	C	332	SER	Peptide
2	C	339	ASP	Peptide
2	C	342	SER	Peptide
2	C	343	PRO	Peptide
2	C	353	ASP	Peptide
2	C	393	SER	Peptide
2	C	398	SER	Peptide
2	C	508	TYR	Peptide
2	C	545	ILE	Peptide
2	C	562	ASP	Peptide
2	C	628	HIS	Peptide

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Mol	Chain	Res	Type	Group
2	C	695	PRO	Peptide
2	C	705	TRP	Peptide
2	C	706	SER	Peptide
2	C	769	ASP	Peptide
2	C	859	ARG	Peptide
2	C	863	VAL	Peptide
2	C	89	PHE	Peptide
2	C	925	LEU	Peptide
2	C	929	TYR	Peptide
2	C	965	LEU	Peptide
2	C	967	ASP	Peptide
2	C	988	LYS	Peptide
2	C	991	SER	Peptide
2	CA	1016	ILE	Peptide
2	CA	156	SER	Peptide
2	CA	167	ILE	Peptide
2	CA	184	CYS	Peptide
2	CA	215	LYS	Peptide
2	CA	300	LEU	Peptide
2	CA	331	THR	Peptide
2	CA	332	SER	Peptide
2	CA	339	ASP	Peptide
2	CA	342	SER	Peptide
2	CA	343	PRO	Peptide
2	CA	353	ASP	Peptide
2	CA	393	SER	Peptide
2	CA	398	SER	Peptide
2	CA	508	TYR	Peptide
2	CA	545	ILE	Peptide
2	CA	562	ASP	Peptide
2	CA	628	HIS	Peptide
2	CA	695	PRO	Peptide
2	CA	705	TRP	Peptide
2	CA	706	SER	Peptide
2	CA	769	ASP	Peptide
2	CA	859	ARG	Peptide
2	CA	863	VAL	Peptide
2	CA	89	PHE	Peptide
2	CA	925	LEU	Peptide
2	CA	929	TYR	Peptide
2	CA	965	LEU	Peptide
2	CA	967	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	CA	988	LYS	Peptide
2	CA	991	SER	Peptide
3	CB	178	GLY	Peptide
3	CB	228	ASN	Peptide
3	CB	32	PRO	Peptide
3	CC	177	GLU	Peptide
3	CC	178	GLY	Peptide
3	CC	228	ASN	Peptide
3	CC	32	PRO	Peptide
5	CG	102	TRP	Peptide
5	CG	107	VAL	Peptide
5	CG	155	THR	Peptide
5	CG	196	ARG	Peptide
5	CG	214	SER	Peptide
5	CG	291	ILE	Peptide
5	CG	293	PHE	Peptide
5	CG	333	GLY	Peptide
5	CG	357	SER	Peptide
5	CG	365	ILE	Peptide
5	CG	366	PRO	Peptide
5	CG	556	GLN	Peptide
5	CG	558	ASP	Peptide
5	CG	61	THR	Peptide
5	CG	84	GLY	Peptide
5	CG	9	ASN	Peptide
3	D	178	GLY	Peptide
3	D	228	ASN	Peptide
3	D	32	PRO	Peptide
5	DA	100	ALA	Peptide
5	DA	102	TRP	Peptide
5	DA	150	GLN	Peptide
5	DA	152	ASP	Peptide
5	DA	155	THR	Peptide
5	DA	191	ILE	Peptide
5	DA	214	SER	Peptide
5	DA	291	ILE	Peptide
5	DA	293	PHE	Peptide
5	DA	300	PRO	Peptide
5	DA	304	ILE	Peptide
5	DA	333	GLY	Peptide
5	DA	362	GLU	Peptide
5	DA	545	ASP	Peptide

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Mol	Chain	Res	Type	Group
5	DA	547	ASN	Peptide
5	DA	549	SER	Peptide
5	DA	550	VAL	Peptide
5	DA	552	VAL	Peptide
5	DA	554	GLY	Peptide
5	DA	558	ASP	Peptide
5	DA	6	ASN	Peptide
5	DA	61	THR	Peptide
5	DA	69	ALA	Peptide
5	DA	84	GLY	Peptide
5	DB	100	ALA	Peptide
5	DB	102	TRP	Peptide
5	DB	127	ASN	Peptide
5	DB	151	ILE	Peptide
5	DB	196	ARG	Peptide
5	DB	293	PHE	Peptide
5	DB	333	GLY	Peptide
5	DB	361	ASP	Peptide
5	DB	388	ASN	Peptide
5	DB	389	ASP	Peptide
5	DB	390	LEU	Peptide
5	DB	393	LEU	Peptide
5	DB	555	CYS	Peptide
5	DB	61	THR	Peptide
5	DB	84	GLY	Peptide
6	DC	11	ILE	Peptide
6	DC	9	GLY	Peptide
6	DD	11	ILE	Peptide
6	DD	9	GLY	Peptide
6	DE	11	ILE	Peptide
6	DE	9	GLY	Peptide
3	E	177	GLU	Peptide
3	E	178	GLY	Peptide
3	E	228	ASN	Peptide
3	E	32	PRO	Peptide
1	EA	186	ILE	Peptide
1	EA	209	TRP	Peptide
1	EA	262	PRO	Peptide
1	EA	451	ASP	Peptide
1	EA	576	ASP	Peptide
1	EA	6	VAL	Peptide
1	EB	137	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	EB	20	ILE	Peptide
1	EB	200	TYR	Peptide
1	EB	212	LYS	Peptide
1	EB	241	GLY	Peptide
1	EB	453	GLU	Peptide
1	EB	612	THR	Peptide
2	EC	1016	ILE	Peptide
2	EC	156	SER	Peptide
2	EC	167	ILE	Peptide
2	EC	184	CYS	Peptide
2	EC	215	LYS	Peptide
2	EC	300	LEU	Peptide
2	EC	331	THR	Peptide
2	EC	332	SER	Peptide
2	EC	339	ASP	Peptide
2	EC	342	SER	Peptide
2	EC	343	PRO	Peptide
2	EC	353	ASP	Peptide
2	EC	393	SER	Peptide
2	EC	398	SER	Peptide
2	EC	508	TYR	Peptide
2	EC	545	ILE	Peptide
2	EC	562	ASP	Peptide
2	EC	628	HIS	Peptide
2	EC	695	PRO	Peptide
2	EC	705	TRP	Peptide
2	EC	706	SER	Peptide
2	EC	769	ASP	Peptide
2	EC	859	ARG	Peptide
2	EC	863	VAL	Peptide
2	EC	89	PHE	Peptide
2	EC	925	LEU	Peptide
2	EC	929	TYR	Peptide
2	EC	965	LEU	Peptide
2	EC	967	ASP	Peptide
2	EC	988	LYS	Peptide
2	EC	991	SER	Peptide
3	ED	178	GLY	Peptide
3	ED	228	ASN	Peptide
3	ED	32	PRO	Peptide
3	EE	177	GLU	Peptide
3	EE	178	GLY	Peptide

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Mol	Chain	Res	Type	Group
3	EE	228	ASN	Peptide
3	EE	32	PRO	Peptide
5	FB	102	TRP	Peptide
5	FB	107	VAL	Peptide
5	FB	155	THR	Peptide
5	FB	196	ARG	Peptide
5	FB	214	SER	Peptide
5	FB	291	ILE	Peptide
5	FB	293	PHE	Peptide
5	FB	333	GLY	Peptide
5	FB	357	SER	Peptide
5	FB	365	ILE	Peptide
5	FB	366	PRO	Peptide
5	FB	556	GLN	Peptide
5	FB	558	ASP	Peptide
5	FB	61	THR	Peptide
5	FB	84	GLY	Peptide
5	FB	9	ASN	Peptide
5	FC	100	ALA	Peptide
5	FC	102	TRP	Peptide
5	FC	150	GLN	Peptide
5	FC	152	ASP	Peptide
5	FC	155	THR	Peptide
5	FC	191	ILE	Peptide
5	FC	214	SER	Peptide
5	FC	291	ILE	Peptide
5	FC	293	PHE	Peptide
5	FC	300	PRO	Peptide
5	FC	304	ILE	Peptide
5	FC	333	GLY	Peptide
5	FC	362	GLU	Peptide
5	FC	545	ASP	Peptide
5	FC	547	ASN	Peptide
5	FC	549	SER	Peptide
5	FC	550	VAL	Peptide
5	FC	552	VAL	Peptide
5	FC	554	GLY	Peptide
5	FC	558	ASP	Peptide
5	FC	6	ASN	Peptide
5	FC	61	THR	Peptide
5	FC	69	ALA	Peptide
5	FC	84	GLY	Peptide

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Mol	Chain	Res	Type	Group
5	FD	100	ALA	Peptide
5	FD	102	TRP	Peptide
5	FD	127	ASN	Peptide
5	FD	151	ILE	Peptide
5	FD	196	ARG	Peptide
5	FD	293	PHE	Peptide
5	FD	333	GLY	Peptide
5	FD	361	ASP	Peptide
5	FD	388	ASN	Peptide
5	FD	389	ASP	Peptide
5	FD	390	LEU	Peptide
5	FD	393	LEU	Peptide
5	FD	555	CYS	Peptide
5	FD	61	THR	Peptide
5	FD	84	GLY	Peptide
6	FE	11	ILE	Peptide
6	FE	9	GLY	Peptide
6	FF	11	ILE	Peptide
6	FF	9	GLY	Peptide
6	FG	11	ILE	Peptide
6	FG	9	GLY	Peptide
5	I	102	TRP	Peptide
5	I	107	VAL	Peptide
5	I	155	THR	Peptide
5	I	196	ARG	Peptide
5	I	214	SER	Peptide
5	I	291	ILE	Peptide
5	I	293	PHE	Peptide
5	I	333	GLY	Peptide
5	I	357	SER	Peptide
5	I	365	ILE	Peptide
5	I	366	PRO	Peptide
5	I	556	GLN	Peptide
5	I	558	ASP	Peptide
5	I	61	THR	Peptide
5	I	84	GLY	Peptide
5	I	9	ASN	Peptide
5	J	100	ALA	Peptide
5	J	102	TRP	Peptide
5	J	150	GLN	Peptide
5	J	152	ASP	Peptide
5	J	155	THR	Peptide

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Mol	Chain	Res	Type	Group
5	J	191	ILE	Peptide
5	J	214	SER	Peptide
5	J	291	ILE	Peptide
5	J	293	PHE	Peptide
5	J	300	PRO	Peptide
5	J	304	ILE	Peptide
5	J	333	GLY	Peptide
5	J	362	GLU	Peptide
5	J	545	ASP	Peptide
5	J	547	ASN	Peptide
5	J	549	SER	Peptide
5	J	550	VAL	Peptide
5	J	552	VAL	Peptide
5	J	554	GLY	Peptide
5	J	558	ASP	Peptide
5	J	6	ASN	Peptide
5	J	61	THR	Peptide
5	J	69	ALA	Peptide
5	J	84	GLY	Peptide
5	K	100	ALA	Peptide
5	K	102	TRP	Peptide
5	K	127	ASN	Peptide
5	K	151	ILE	Peptide
5	K	196	ARG	Peptide
5	K	293	PHE	Peptide
5	K	333	GLY	Peptide
5	K	361	ASP	Peptide
5	K	388	ASN	Peptide
5	K	389	ASP	Peptide
5	K	390	LEU	Peptide
5	K	393	LEU	Peptide
5	K	555	CYS	Peptide
5	K	61	THR	Peptide
5	K	84	GLY	Peptide
6	L	11	ILE	Peptide
6	L	9	GLY	Peptide
6	M	11	ILE	Peptide
6	M	9	GLY	Peptide
6	N	11	ILE	Peptide
6	N	9	GLY	Peptide
1	Q	186	ILE	Peptide
1	Q	209	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	Q	262	PRO	Peptide
1	Q	451	ASP	Peptide
1	Q	576	ASP	Peptide
1	Q	6	VAL	Peptide
1	R	137	ASP	Peptide
1	R	20	ILE	Peptide
1	R	200	TYR	Peptide
1	R	212	LYS	Peptide
1	R	241	GLY	Peptide
1	R	453	GLU	Peptide
1	R	612	THR	Peptide
2	S	1016	ILE	Peptide
2	S	156	SER	Peptide
2	S	167	ILE	Peptide
2	S	184	CYS	Peptide
2	S	215	LYS	Peptide
2	S	300	LEU	Peptide
2	S	331	THR	Peptide
2	S	332	SER	Peptide
2	S	339	ASP	Peptide
2	S	342	SER	Peptide
2	S	343	PRO	Peptide
2	S	353	ASP	Peptide
2	S	393	SER	Peptide
2	S	398	SER	Peptide
2	S	508	TYR	Peptide
2	S	545	ILE	Peptide
2	S	562	ASP	Peptide
2	S	628	HIS	Peptide
2	S	695	PRO	Peptide
2	S	705	TRP	Peptide
2	S	706	SER	Peptide
2	S	769	ASP	Peptide
2	S	859	ARG	Peptide
2	S	863	VAL	Peptide
2	S	89	PHE	Peptide
2	S	925	LEU	Peptide
2	S	929	TYR	Peptide
2	S	965	LEU	Peptide
2	S	967	ASP	Peptide
2	S	988	LYS	Peptide
2	S	991	SER	Peptide

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Mol	Chain	Res	Type	Group
3	T	178	GLY	Peptide
3	T	228	ASN	Peptide
3	T	32	PRO	Peptide
3	U	177	GLU	Peptide
3	U	178	GLY	Peptide
3	U	228	ASN	Peptide
3	U	32	PRO	Peptide
5	Y	102	TRP	Peptide
5	Y	107	VAL	Peptide
5	Y	155	THR	Peptide
5	Y	196	ARG	Peptide
5	Y	214	SER	Peptide
5	Y	291	ILE	Peptide
5	Y	293	PHE	Peptide
5	Y	333	GLY	Peptide
5	Y	357	SER	Peptide
5	Y	365	ILE	Peptide
5	Y	366	PRO	Peptide
5	Y	556	GLN	Peptide
5	Y	558	ASP	Peptide
5	Y	61	THR	Peptide
5	Y	84	GLY	Peptide
5	Y	9	ASN	Peptide
5	Z	100	ALA	Peptide
5	Z	102	TRP	Peptide
5	Z	150	GLN	Peptide
5	Z	152	ASP	Peptide
5	Z	155	THR	Peptide
5	Z	191	ILE	Peptide
5	Z	214	SER	Peptide
5	Z	291	ILE	Peptide
5	Z	293	PHE	Peptide
5	Z	300	PRO	Peptide
5	Z	304	ILE	Peptide
5	Z	333	GLY	Peptide
5	Z	362	GLU	Peptide
5	Z	545	ASP	Peptide
5	Z	547	ASN	Peptide
5	Z	549	SER	Peptide
5	Z	550	VAL	Peptide
5	Z	552	VAL	Peptide
5	Z	554	GLY	Peptide

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Mol	Chain	Res	Type	Group
5	Z	558	ASP	Peptide
5	Z	6	ASN	Peptide
5	Z	61	THR	Peptide
5	Z	69	ALA	Peptide
5	Z	84	GLY	Peptide
5	a	100	ALA	Peptide
5	a	102	TRP	Peptide
5	a	127	ASN	Peptide
5	a	151	ILE	Peptide
5	a	196	ARG	Peptide
5	a	293	PHE	Peptide
5	a	333	GLY	Peptide
5	a	361	ASP	Peptide
5	a	388	ASN	Peptide
5	a	389	ASP	Peptide
5	a	390	LEU	Peptide
5	a	393	LEU	Peptide
5	a	555	CYS	Peptide
5	a	61	THR	Peptide
5	a	84	GLY	Peptide
6	b	11	ILE	Peptide
6	b	9	GLY	Peptide
6	c	11	ILE	Peptide
6	c	9	GLY	Peptide
6	d	11	ILE	Peptide
6	d	9	GLY	Peptide
1	g	186	ILE	Peptide
1	g	209	TRP	Peptide
1	g	262	PRO	Peptide
1	g	451	ASP	Peptide
1	g	576	ASP	Peptide
1	g	6	VAL	Peptide
1	h	137	ASP	Peptide
1	h	20	ILE	Peptide
1	h	200	TYR	Peptide
1	h	212	LYS	Peptide
1	h	241	GLY	Peptide
1	h	453	GLU	Peptide
1	h	612	THR	Peptide
2	i	1016	ILE	Peptide
2	i	156	SER	Peptide
2	i	167	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	i	184	CYS	Peptide
2	i	215	LYS	Peptide
2	i	300	LEU	Peptide
2	i	331	THR	Peptide
2	i	332	SER	Peptide
2	i	339	ASP	Peptide
2	i	342	SER	Peptide
2	i	343	PRO	Peptide
2	i	353	ASP	Peptide
2	i	393	SER	Peptide
2	i	398	SER	Peptide
2	i	508	TYR	Peptide
2	i	545	ILE	Peptide
2	i	562	ASP	Peptide
2	i	628	HIS	Peptide
2	i	695	PRO	Peptide
2	i	705	TRP	Peptide
2	i	706	SER	Peptide
2	i	769	ASP	Peptide
2	i	859	ARG	Peptide
2	i	863	VAL	Peptide
2	i	89	PHE	Peptide
2	i	925	LEU	Peptide
2	i	929	TYR	Peptide
2	i	965	LEU	Peptide
2	i	967	ASP	Peptide
2	i	988	LYS	Peptide
2	i	991	SER	Peptide
3	j	178	GLY	Peptide
3	j	228	ASN	Peptide
3	j	32	PRO	Peptide
3	k	177	GLU	Peptide
3	k	178	GLY	Peptide
3	k	228	ASN	Peptide
3	k	32	PRO	Peptide
5	o	102	TRP	Peptide
5	o	107	VAL	Peptide
5	o	155	THR	Peptide
5	o	196	ARG	Peptide
5	o	214	SER	Peptide
5	o	291	ILE	Peptide
5	o	293	PHE	Peptide

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Mol	Chain	Res	Type	Group
5	o	333	GLY	Peptide
5	o	357	SER	Peptide
5	o	365	ILE	Peptide
5	o	366	PRO	Peptide
5	o	556	GLN	Peptide
5	o	558	ASP	Peptide
5	o	61	THR	Peptide
5	o	84	GLY	Peptide
5	o	9	ASN	Peptide
5	p	100	ALA	Peptide
5	p	102	TRP	Peptide
5	p	150	GLN	Peptide
5	p	152	ASP	Peptide
5	p	155	THR	Peptide
5	p	191	ILE	Peptide
5	p	214	SER	Peptide
5	p	291	ILE	Peptide
5	p	293	PHE	Peptide
5	p	300	PRO	Peptide
5	p	304	ILE	Peptide
5	p	333	GLY	Peptide
5	p	362	GLU	Peptide
5	p	545	ASP	Peptide
5	p	547	ASN	Peptide
5	p	549	SER	Peptide
5	p	550	VAL	Peptide
5	p	552	VAL	Peptide
5	p	554	GLY	Peptide
5	p	558	ASP	Peptide
5	p	6	ASN	Peptide
5	p	61	THR	Peptide
5	p	69	ALA	Peptide
5	p	84	GLY	Peptide
5	q	100	ALA	Peptide
5	q	102	TRP	Peptide
5	q	127	ASN	Peptide
5	q	151	ILE	Peptide
5	q	196	ARG	Peptide
5	q	293	PHE	Peptide
5	q	333	GLY	Peptide
5	q	361	ASP	Peptide
5	q	388	ASN	Peptide

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Mol	Chain	Res	Type	Group
5	q	389	ASP	Peptide
5	q	390	LEU	Peptide
5	q	393	LEU	Peptide
5	q	555	CYS	Peptide
5	q	61	THR	Peptide
5	q	84	GLY	Peptide
6	r	11	ILE	Peptide
6	r	9	GLY	Peptide
6	s	11	ILE	Peptide
6	s	9	GLY	Peptide
6	t	11	ILE	Peptide
6	t	9	GLY	Peptide
1	w	186	ILE	Peptide
1	w	209	TRP	Peptide
1	w	262	PRO	Peptide
1	w	451	ASP	Peptide
1	w	576	ASP	Peptide
1	w	6	VAL	Peptide
1	x	137	ASP	Peptide
1	x	20	ILE	Peptide
1	x	200	TYR	Peptide
1	x	212	LYS	Peptide
1	x	241	GLY	Peptide
1	x	453	GLU	Peptide
1	x	612	THR	Peptide
2	y	1016	ILE	Peptide
2	y	156	SER	Peptide
2	y	167	ILE	Peptide
2	y	184	CYS	Peptide
2	y	215	LYS	Peptide
2	y	300	LEU	Peptide
2	y	331	THR	Peptide
2	y	332	SER	Peptide
2	y	339	ASP	Peptide
2	y	342	SER	Peptide
2	y	343	PRO	Peptide
2	y	353	ASP	Peptide
2	y	393	SER	Peptide
2	y	398	SER	Peptide
2	y	508	TYR	Peptide
2	y	545	ILE	Peptide
2	y	562	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	y	628	HIS	Peptide
2	y	695	PRO	Peptide
2	y	705	TRP	Peptide
2	y	706	SER	Peptide
2	y	769	ASP	Peptide
2	y	859	ARG	Peptide
2	y	863	VAL	Peptide
2	y	89	PHE	Peptide
2	y	925	LEU	Peptide
2	y	929	TYR	Peptide
2	y	965	LEU	Peptide
2	y	967	ASP	Peptide
2	y	988	LYS	Peptide
2	y	991	SER	Peptide
3	z	178	GLY	Peptide
3	z	228	ASN	Peptide
3	z	32	PRO	Peptide

5.2 Too-close contacts

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

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	A	656/660 (99%)	590 (90%)	59 (9%)	7 (1%)	14 52
1	B	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	29 69
1	BF	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	14 52
1	BG	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	29 69
1	EA	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	14 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EB	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	29	69
1	Q	656/660 (99%)	590 (90%)	59 (9%)	7 (1%)	14	52
1	R	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	29	69
1	g	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	14	52
1	h	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	29	69
1	w	656/660 (99%)	589 (90%)	60 (9%)	7 (1%)	14	52
1	x	646/660 (98%)	587 (91%)	56 (9%)	3 (0%)	29	69
2	C	1000/1032 (97%)	817 (82%)	155 (16%)	28 (3%)	5	30
2	CA	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	5	30
2	EC	1000/1032 (97%)	818 (82%)	155 (16%)	27 (3%)	5	31
2	S	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	5	30
2	i	1000/1032 (97%)	818 (82%)	155 (16%)	27 (3%)	5	31
2	y	1000/1032 (97%)	818 (82%)	154 (15%)	28 (3%)	5	30
3	AA	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	41	76
3	CB	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	CC	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	41	76
3	D	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	E	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	41	76
3	ED	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	EE	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	41	76
3	T	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	U	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	41	76
3	j	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
3	k	330/334 (99%)	308 (93%)	21 (6%)	1 (0%)	41	76
3	z	326/334 (98%)	307 (94%)	19 (6%)	0	100	100
4	AB	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	AC	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	AD	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	CD	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	CE	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	CF	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	EF	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	EG	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	F	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	FA	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	G	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	H	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	V	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	W	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	X	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	l	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	m	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
4	n	286/288 (99%)	262 (92%)	20 (7%)	4 (1%)	11	46
5	AE	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	6	34
5	AF	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	8	40
5	AG	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	7	38
5	CG	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	6	34
5	DA	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	8	40
5	DB	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	7	38
5	FB	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	6	34
5	FC	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	8	40
5	FD	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	7	38
5	I	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	6	34
5	J	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	8	40
5	K	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	7	38
5	Y	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	6	34
5	Z	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	8	40
5	a	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	7	38
5	o	598/602 (99%)	531 (89%)	53 (9%)	14 (2%)	6	34
5	p	600/602 (100%)	518 (86%)	71 (12%)	11 (2%)	8	40
5	q	600/602 (100%)	519 (86%)	69 (12%)	12 (2%)	7	38
6	BA	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	BB	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	BC	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	DC	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	DD	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	DE	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	FE	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	FF	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	FG	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	L	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	M	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	N	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	b	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	c	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	d	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	r	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	s	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
6	t	216/219 (99%)	205 (95%)	9 (4%)	2 (1%)	17	57
7	BD	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	DF	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	GA	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	O	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	e	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
7	u	124/132 (94%)	116 (94%)	8 (6%)	0	100	100
8	BE	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	DG	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	GB	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	P	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	f	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
8	v	191/196 (97%)	172 (90%)	19 (10%)	0	100	100
All	All	39462/40050 (98%)	35197 (89%)	3703 (9%)	562 (1%)	15	46

All (562) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	249	ILE
4	G	249	ILE
4	H	249	ILE
5	I	10	VAL
5	I	24	ILE
5	J	24	ILE
5	K	24	ILE
4	V	249	ILE
4	W	249	ILE
4	X	249	ILE
5	Y	10	VAL
5	Y	24	ILE
5	Z	24	ILE
5	a	24	ILE
4	l	249	ILE
4	m	249	ILE
4	n	249	ILE
5	o	10	VAL
5	o	24	ILE
5	p	24	ILE
5	q	24	ILE
4	AB	249	ILE
4	AC	249	ILE
4	AD	249	ILE
5	AE	10	VAL
5	AE	24	ILE
5	AF	24	ILE
5	AG	24	ILE
4	CD	249	ILE
4	CE	249	ILE
4	CF	249	ILE
5	CG	10	VAL
5	CG	24	ILE
5	DA	24	ILE
5	DB	24	ILE
4	EF	249	ILE
4	EG	249	ILE
4	FA	249	ILE
5	FB	10	VAL
5	FB	24	ILE
5	FC	24	ILE
5	FD	24	ILE
1	B	46	TYR

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Mol	Chain	Res	Type
1	B	454	ILE
2	C	168	ILE
2	C	343	PRO
2	C	852	ILE
2	C	947	VAL
5	I	104	VAL
5	I	171	VAL
5	I	392	THR
5	J	86	VAL
5	J	151	ILE
5	J	154	ILE
5	K	85	THR
5	K	86	VAL
5	K	152	ASP
5	K	171	VAL
5	K	408	VAL
1	R	46	TYR
1	R	454	ILE
2	S	168	ILE
2	S	343	PRO
2	S	852	ILE
2	S	947	VAL
5	Y	104	VAL
5	Y	171	VAL
5	Y	392	THR
5	Z	86	VAL
5	Z	151	ILE
5	Z	154	ILE
5	a	85	THR
5	a	86	VAL
5	a	152	ASP
5	a	171	VAL
5	a	408	VAL
1	h	46	TYR
1	h	454	ILE
2	i	168	ILE
2	i	343	PRO
2	i	852	ILE
2	i	947	VAL
5	o	104	VAL
5	o	171	VAL
5	o	392	THR

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Mol	Chain	Res	Type
5	p	86	VAL
5	p	151	ILE
5	p	154	ILE
5	q	85	THR
5	q	86	VAL
5	q	152	ASP
5	q	171	VAL
5	q	408	VAL
1	x	46	TYR
1	x	454	ILE
2	y	168	ILE
2	y	343	PRO
2	y	411	LYS
2	y	852	ILE
2	y	947	VAL
5	AE	104	VAL
5	AE	171	VAL
5	AE	392	THR
5	AF	86	VAL
5	AF	151	ILE
5	AF	154	ILE
5	AG	85	THR
5	AG	86	VAL
5	AG	152	ASP
5	AG	171	VAL
5	AG	408	VAL
1	BG	46	TYR
1	BG	454	ILE
2	CA	168	ILE
2	CA	343	PRO
2	CA	411	LYS
2	CA	852	ILE
2	CA	947	VAL
5	CG	104	VAL
5	CG	171	VAL
5	CG	392	THR
5	DA	86	VAL
5	DA	151	ILE
5	DA	154	ILE
5	DB	85	THR
5	DB	86	VAL
5	DB	152	ASP

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Mol	Chain	Res	Type
5	DB	171	VAL
5	DB	408	VAL
1	EB	46	TYR
1	EB	454	ILE
2	EC	168	ILE
2	EC	343	PRO
2	EC	852	ILE
2	EC	947	VAL
5	FB	104	VAL
5	FB	171	VAL
5	FB	392	THR
5	FC	86	VAL
5	FC	151	ILE
5	FC	154	ILE
5	FD	85	THR
5	FD	86	VAL
5	FD	152	ASP
5	FD	171	VAL
5	FD	408	VAL
1	A	210	THR
1	A	223	ILE
1	A	473	HIS
2	C	341	LEU
2	C	411	LYS
2	C	992	PRO
3	E	179	THR
4	F	15	ILE
4	F	50	VAL
4	G	15	ILE
4	G	50	VAL
4	H	15	ILE
4	H	50	VAL
5	I	85	THR
5	I	86	VAL
5	I	557	TYR
5	J	104	VAL
5	J	559	PRO
5	K	104	VAL
5	K	151	ILE
5	K	304	ILE
6	L	11	ILE
6	M	11	ILE

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Mol	Chain	Res	Type
6	N	11	ILE
1	Q	210	THR
1	Q	223	ILE
1	Q	473	HIS
2	S	341	LEU
2	S	411	LYS
2	S	992	PRO
3	U	179	THR
4	V	15	ILE
4	V	50	VAL
4	W	15	ILE
4	W	50	VAL
4	X	15	ILE
4	X	50	VAL
5	Y	85	THR
5	Y	86	VAL
5	Y	557	TYR
5	Z	104	VAL
5	Z	559	PRO
5	a	104	VAL
5	a	151	ILE
5	a	304	ILE
6	b	11	ILE
6	c	11	ILE
6	d	11	ILE
1	g	210	THR
1	g	223	ILE
1	g	473	HIS
2	i	341	LEU
2	i	411	LYS
2	i	992	PRO
3	k	179	THR
4	l	15	ILE
4	l	50	VAL
4	m	15	ILE
4	m	50	VAL
4	n	15	ILE
4	n	50	VAL
5	o	85	THR
5	o	86	VAL
5	o	557	TYR
5	p	104	VAL

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Mol	Chain	Res	Type
5	p	559	PRO
5	q	104	VAL
5	q	151	ILE
5	q	304	ILE
6	r	11	ILE
6	s	11	ILE
6	t	11	ILE
1	w	210	THR
1	w	223	ILE
1	w	473	HIS
2	y	341	LEU
2	y	992	PRO
3	AA	179	THR
4	AB	15	ILE
4	AB	50	VAL
4	AC	15	ILE
4	AC	50	VAL
4	AD	15	ILE
4	AD	50	VAL
5	AE	85	THR
5	AE	86	VAL
5	AE	557	TYR
5	AF	104	VAL
5	AF	559	PRO
5	AG	104	VAL
5	AG	151	ILE
5	AG	304	ILE
6	BA	11	ILE
6	BB	11	ILE
6	BC	11	ILE
1	BF	210	THR
1	BF	223	ILE
1	BF	473	HIS
2	CA	341	LEU
2	CA	992	PRO
3	CC	179	THR
4	CD	15	ILE
4	CD	50	VAL
4	CE	15	ILE
4	CE	50	VAL
4	CF	15	ILE
4	CF	50	VAL

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Mol	Chain	Res	Type
5	CG	85	THR
5	CG	86	VAL
5	CG	557	TYR
5	DA	104	VAL
5	DA	559	PRO
5	DB	104	VAL
5	DB	151	ILE
5	DB	304	ILE
6	DC	11	ILE
6	DD	11	ILE
6	DE	11	ILE
1	EA	210	THR
1	EA	223	ILE
1	EA	473	HIS
2	EC	341	LEU
2	EC	411	LYS
2	EC	992	PRO
3	EE	179	THR
4	EF	15	ILE
4	EF	50	VAL
4	EG	15	ILE
4	EG	50	VAL
4	FA	15	ILE
4	FA	50	VAL
5	FB	85	THR
5	FB	86	VAL
5	FB	557	TYR
5	FC	104	VAL
5	FC	559	PRO
5	FD	104	VAL
5	FD	151	ILE
5	FD	304	ILE
6	FE	11	ILE
6	FF	11	ILE
6	FG	11	ILE
2	C	28	VAL
2	C	122	PHE
2	C	223	LYS
2	C	307	ILE
2	C	361	PRO
2	C	541	TYR
2	C	1026	THR

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Mol	Chain	Res	Type
5	I	129	ARG
5	I	147	LYS
5	I	180	VAL
5	I	228	PHE
5	I	558	ASP
5	J	180	VAL
5	K	36	GLU
5	K	129	ARG
5	K	180	VAL
6	L	4	LEU
6	M	4	LEU
6	N	4	LEU
2	S	28	VAL
2	S	122	PHE
2	S	223	LYS
2	S	307	ILE
2	S	361	PRO
2	S	541	TYR
2	S	1026	THR
5	Y	129	ARG
5	Y	147	LYS
5	Y	180	VAL
5	Y	228	PHE
5	Y	558	ASP
5	Z	180	VAL
5	a	36	GLU
5	a	129	ARG
5	a	180	VAL
6	b	4	LEU
6	c	4	LEU
6	d	4	LEU
2	i	28	VAL
2	i	122	PHE
2	i	223	LYS
2	i	307	ILE
2	i	361	PRO
2	i	541	TYR
2	i	1026	THR
5	o	129	ARG
5	o	147	LYS
5	o	180	VAL
5	o	228	PHE

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Mol	Chain	Res	Type
5	o	558	ASP
5	p	180	VAL
5	q	36	GLU
5	q	129	ARG
5	q	180	VAL
6	r	4	LEU
6	s	4	LEU
6	t	4	LEU
2	y	28	VAL
2	y	122	PHE
2	y	223	LYS
2	y	307	ILE
2	y	361	PRO
2	y	541	TYR
2	y	1026	THR
5	AE	129	ARG
5	AE	147	LYS
5	AE	180	VAL
5	AE	228	PHE
5	AE	558	ASP
5	AF	180	VAL
5	AG	36	GLU
5	AG	129	ARG
5	AG	180	VAL
6	BA	4	LEU
6	BB	4	LEU
6	BC	4	LEU
2	CA	28	VAL
2	CA	122	PHE
2	CA	223	LYS
2	CA	307	ILE
2	CA	361	PRO
2	CA	541	TYR
2	CA	1026	THR
5	CG	129	ARG
5	CG	147	LYS
5	CG	180	VAL
5	CG	228	PHE
5	CG	558	ASP
5	DA	180	VAL
5	DB	36	GLU
5	DB	129	ARG

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Mol	Chain	Res	Type
5	DB	180	VAL
6	DC	4	LEU
6	DD	4	LEU
6	DE	4	LEU
2	EC	28	VAL
2	EC	122	PHE
2	EC	223	LYS
2	EC	307	ILE
2	EC	361	PRO
2	EC	541	TYR
2	EC	1026	THR
5	FB	129	ARG
5	FB	147	LYS
5	FB	180	VAL
5	FB	228	PHE
5	FB	558	ASP
5	FC	180	VAL
5	FD	36	GLU
5	FD	129	ARG
5	FD	180	VAL
6	FE	4	LEU
6	FF	4	LEU
6	FG	4	LEU
1	A	209	TRP
1	A	391	ASP
1	A	471	ALA
1	B	394	ASN
2	C	149	GLU
2	C	342	SER
2	C	360	ASN
2	C	362	LYS
2	C	822	ALA
2	C	959	ALA
4	F	51	ALA
4	G	51	ALA
4	H	51	ALA
5	J	90	ASN
5	J	546	GLU
1	Q	209	TRP
1	Q	391	ASP
1	Q	471	ALA
1	R	394	ASN

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Mol	Chain	Res	Type
2	S	149	GLU
2	S	342	SER
2	S	360	ASN
2	S	362	LYS
2	S	822	ALA
2	S	959	ALA
4	V	51	ALA
4	W	51	ALA
4	X	51	ALA
5	Z	90	ASN
5	Z	546	GLU
1	g	209	TRP
1	g	391	ASP
1	g	471	ALA
1	h	394	ASN
2	i	149	GLU
2	i	342	SER
2	i	360	ASN
2	i	362	LYS
2	i	822	ALA
2	i	959	ALA
4	l	51	ALA
4	m	51	ALA
4	n	51	ALA
5	p	90	ASN
5	p	546	GLU
1	w	209	TRP
1	w	391	ASP
1	w	471	ALA
1	x	394	ASN
2	y	149	GLU
2	y	342	SER
2	y	360	ASN
2	y	362	LYS
2	y	822	ALA
2	y	959	ALA
4	AB	51	ALA
4	AC	51	ALA
4	AD	51	ALA
5	AF	90	ASN
5	AF	546	GLU
1	BF	209	TRP

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Mol	Chain	Res	Type
1	BF	391	ASP
1	BF	471	ALA
1	BG	394	ASN
2	CA	149	GLU
2	CA	342	SER
2	CA	360	ASN
2	CA	362	LYS
2	CA	822	ALA
2	CA	959	ALA
4	CD	51	ALA
4	CE	51	ALA
4	CF	51	ALA
5	DA	90	ASN
5	DA	546	GLU
1	EA	209	TRP
1	EA	391	ASP
1	EA	471	ALA
1	EB	394	ASN
2	EC	149	GLU
2	EC	342	SER
2	EC	360	ASN
2	EC	362	LYS
2	EC	412	THR
2	EC	822	ALA
2	EC	959	ALA
4	EF	51	ALA
4	EG	51	ALA
4	FA	51	ALA
5	FC	90	ASN
5	FC	546	GLU
2	C	6	PRO
2	C	412	THR
2	C	718	ASP
5	I	30	PHE
5	J	209	ASN
2	S	6	PRO
2	S	412	THR
2	S	718	ASP
5	Y	30	PHE
5	Z	209	ASN
2	i	6	PRO
2	i	412	THR

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Mol	Chain	Res	Type
5	o	30	PHE
5	p	209	ASN
2	y	6	PRO
2	y	412	THR
2	y	718	ASP
5	AE	30	PHE
5	AF	209	ASN
2	CA	6	PRO
2	CA	412	THR
2	CA	718	ASP
5	CG	30	PHE
5	DA	209	ASN
2	EC	6	PRO
5	FB	30	PHE
5	FC	209	ASN
1	A	454	ILE
2	C	357	ILE
1	Q	454	ILE
2	S	357	ILE
1	g	454	ILE
2	i	357	ILE
1	w	454	ILE
2	y	357	ILE
1	BF	454	ILE
2	CA	357	ILE
1	EA	454	ILE
2	EC	357	ILE
2	C	1019	PRO
2	S	1019	PRO
2	i	1019	PRO
2	y	1019	PRO
2	CA	1019	PRO
2	EC	1019	PRO
2	C	291	VAL
2	S	291	VAL
2	i	291	VAL
2	y	291	VAL
2	CA	291	VAL
2	EC	291	VAL
2	C	770	ILE
5	J	365	ILE
2	S	770	ILE

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Mol	Chain	Res	Type
2	S	977	ILE
5	Z	365	ILE
2	i	770	ILE
2	i	977	ILE
5	p	365	ILE
2	y	770	ILE
2	y	977	ILE
5	AF	365	ILE
2	CA	770	ILE
2	CA	977	ILE
5	DA	365	ILE
2	EC	770	ILE
2	EC	977	ILE
5	FC	365	ILE
2	C	977	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/578 (100%)	576 (100%)	0	100	100
1	B	567/578 (98%)	567 (100%)	0	100	100
1	BF	576/578 (100%)	576 (100%)	0	100	100
1	BG	567/578 (98%)	567 (100%)	0	100	100
1	EA	576/578 (100%)	576 (100%)	0	100	100
1	EB	567/578 (98%)	567 (100%)	0	100	100
1	Q	576/578 (100%)	576 (100%)	0	100	100
1	R	567/578 (98%)	567 (100%)	0	100	100
1	g	576/578 (100%)	576 (100%)	0	100	100
1	h	567/578 (98%)	567 (100%)	0	100	100
1	w	576/578 (100%)	576 (100%)	0	100	100
1	x	567/578 (98%)	567 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	896/921 (97%)	894 (100%)	2 (0%)	93	96
2	CA	896/921 (97%)	894 (100%)	2 (0%)	93	96
2	EC	896/921 (97%)	894 (100%)	2 (0%)	93	96
2	S	896/921 (97%)	894 (100%)	2 (0%)	93	96
2	i	896/921 (97%)	894 (100%)	2 (0%)	93	96
2	y	896/921 (97%)	894 (100%)	2 (0%)	93	96
3	AA	293/295 (99%)	291 (99%)	2 (1%)	84	90
3	CB	289/295 (98%)	288 (100%)	1 (0%)	92	95
3	CC	293/295 (99%)	291 (99%)	2 (1%)	84	90
3	D	289/295 (98%)	287 (99%)	2 (1%)	84	90
3	E	293/295 (99%)	291 (99%)	2 (1%)	84	90
3	ED	289/295 (98%)	287 (99%)	2 (1%)	84	90
3	EE	293/295 (99%)	291 (99%)	2 (1%)	84	90
3	T	289/295 (98%)	287 (99%)	2 (1%)	84	90
3	U	293/295 (99%)	291 (99%)	2 (1%)	84	90
3	j	289/295 (98%)	287 (99%)	2 (1%)	84	90
3	k	293/295 (99%)	291 (99%)	2 (1%)	84	90
3	z	289/295 (98%)	287 (99%)	2 (1%)	84	90
4	AB	244/244 (100%)	244 (100%)	0	100	100
4	AC	244/244 (100%)	244 (100%)	0	100	100
4	AD	244/244 (100%)	244 (100%)	0	100	100
4	CD	244/244 (100%)	244 (100%)	0	100	100
4	CE	244/244 (100%)	244 (100%)	0	100	100
4	CF	244/244 (100%)	244 (100%)	0	100	100
4	EF	244/244 (100%)	244 (100%)	0	100	100
4	EG	244/244 (100%)	244 (100%)	0	100	100
4	F	244/244 (100%)	244 (100%)	0	100	100
4	FA	244/244 (100%)	244 (100%)	0	100	100
4	G	244/244 (100%)	244 (100%)	0	100	100
4	H	244/244 (100%)	244 (100%)	0	100	100
4	V	244/244 (100%)	244 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	W	244/244 (100%)	244 (100%)	0	100	100
4	X	244/244 (100%)	244 (100%)	0	100	100
4	l	244/244 (100%)	244 (100%)	0	100	100
4	m	244/244 (100%)	244 (100%)	0	100	100
4	n	244/244 (100%)	244 (100%)	0	100	100
5	AE	519/519 (100%)	519 (100%)	0	100	100
5	AF	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	AG	519/519 (100%)	519 (100%)	0	100	100
5	CG	519/519 (100%)	519 (100%)	0	100	100
5	DA	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	DB	519/519 (100%)	519 (100%)	0	100	100
5	FB	519/519 (100%)	519 (100%)	0	100	100
5	FC	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	FD	519/519 (100%)	519 (100%)	0	100	100
5	I	519/519 (100%)	519 (100%)	0	100	100
5	J	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	K	519/519 (100%)	519 (100%)	0	100	100
5	Y	519/519 (100%)	519 (100%)	0	100	100
5	Z	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	a	519/519 (100%)	519 (100%)	0	100	100
5	o	519/519 (100%)	519 (100%)	0	100	100
5	p	519/519 (100%)	518 (100%)	1 (0%)	93	96
5	q	519/519 (100%)	519 (100%)	0	100	100
6	BA	187/188 (100%)	187 (100%)	0	100	100
6	BB	187/188 (100%)	187 (100%)	0	100	100
6	BC	187/188 (100%)	187 (100%)	0	100	100
6	DC	187/188 (100%)	187 (100%)	0	100	100
6	DD	187/188 (100%)	187 (100%)	0	100	100
6	DE	187/188 (100%)	187 (100%)	0	100	100
6	FE	187/188 (100%)	187 (100%)	0	100	100
6	FF	187/188 (100%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	FG	187/188 (100%)	187 (100%)	0	100	100
6	L	187/188 (100%)	187 (100%)	0	100	100
6	M	187/188 (100%)	187 (100%)	0	100	100
6	N	187/188 (100%)	187 (100%)	0	100	100
6	b	187/188 (100%)	187 (100%)	0	100	100
6	c	187/188 (100%)	187 (100%)	0	100	100
6	d	187/188 (100%)	187 (100%)	0	100	100
6	r	187/188 (100%)	187 (100%)	0	100	100
6	s	187/188 (100%)	187 (100%)	0	100	100
6	t	187/188 (100%)	187 (100%)	0	100	100
7	BD	118/123 (96%)	118 (100%)	0	100	100
7	DF	118/123 (96%)	118 (100%)	0	100	100
7	GA	118/123 (96%)	118 (100%)	0	100	100
7	O	118/123 (96%)	118 (100%)	0	100	100
7	e	118/123 (96%)	118 (100%)	0	100	100
7	u	118/123 (96%)	118 (100%)	0	100	100
8	BE	166/169 (98%)	165 (99%)	1 (1%)	86	92
8	DG	166/169 (98%)	165 (99%)	1 (1%)	86	92
8	GB	166/169 (98%)	165 (99%)	1 (1%)	86	92
8	P	166/169 (98%)	165 (99%)	1 (1%)	86	92
8	f	166/169 (98%)	165 (99%)	1 (1%)	86	92
8	v	166/169 (98%)	165 (99%)	1 (1%)	86	92
All	All	34530/34872 (99%)	34483 (100%)	47 (0%)	93	97

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	704	LEU
2	C	1028	VAL
3	D	28	ILE
3	D	274	ILE
3	E	28	ILE
3	E	274	ILE
5	J	249	ASP

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Mol	Chain	Res	Type
8	P	15	THR
2	S	704	LEU
2	S	1028	VAL
3	T	28	ILE
3	T	274	ILE
3	U	28	ILE
3	U	274	ILE
5	Z	249	ASP
8	f	15	THR
2	i	704	LEU
2	i	1028	VAL
3	j	28	ILE
3	j	274	ILE
3	k	28	ILE
3	k	274	ILE
5	p	249	ASP
8	v	15	THR
2	y	704	LEU
2	y	1028	VAL
3	z	28	ILE
3	z	274	ILE
3	AA	28	ILE
3	AA	274	ILE
5	AF	249	ASP
8	BE	15	THR
2	CA	704	LEU
2	CA	1028	VAL
3	CB	274	ILE
3	CC	28	ILE
3	CC	274	ILE
5	DA	249	ASP
8	DG	15	THR
2	EC	704	LEU
2	EC	1028	VAL
3	ED	28	ILE
3	ED	274	ILE
3	EE	28	ILE
3	EE	274	ILE
5	FC	249	ASP
8	GB	15	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (671) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	40	GLN
1	A	69	GLN
1	A	159	ASN
1	A	216	HIS
1	A	294	ASN
1	A	303	ASN
1	A	394	ASN
1	A	456	ASN
1	A	490	ASN
1	B	84	ASN
1	B	91	GLN
1	B	169	GLN
1	B	195	ASN
1	B	281	ASN
1	B	305	ASN
1	B	337	GLN
1	B	361	GLN
1	B	388	GLN
1	B	400	ASN
1	B	434	GLN
1	B	503	ASN
1	B	582	ASN
2	C	22	GLN
2	C	91	GLN
2	C	130	ASN
2	C	333	ASN
2	C	486	HIS
2	C	528	ASN
2	C	601	ASN
2	C	626	GLN
2	C	673	GLN
2	C	684	ASN
2	C	716	ASN
2	C	914	ASN
2	C	1018	ASN
3	D	23	ASN
3	D	26	ASN
3	D	50	ASN
3	D	74	HIS
3	D	232	GLN
3	D	233	GLN
3	D	314	ASN

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Mol	Chain	Res	Type
3	E	26	ASN
3	E	115	ASN
3	E	271	GLN
3	E	314	ASN
4	F	45	GLN
4	F	52	ASN
4	F	70	HIS
4	F	170	GLN
4	F	193	HIS
4	F	282	GLN
4	G	45	GLN
4	G	52	ASN
4	G	70	HIS
4	G	170	GLN
4	G	193	HIS
4	H	45	GLN
4	H	52	ASN
4	H	70	HIS
4	H	170	GLN
4	H	193	HIS
4	H	282	GLN
5	I	3	GLN
5	I	161	ASN
5	I	198	ASN
5	I	262	GLN
5	I	318	GLN
5	I	377	HIS
5	I	387	ASN
5	I	410	GLN
5	I	437	GLN
5	I	444	ASN
5	I	467	ASN
5	I	504	ASN
5	I	580	HIS
5	J	187	ASN
5	J	198	ASN
5	J	318	GLN
5	J	377	HIS
5	J	410	GLN
5	J	421	ASN
5	J	444	ASN
5	J	504	ASN

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Mol	Chain	Res	Type
5	J	514	HIS
5	J	588	ASN
5	K	87	ASN
5	K	195	HIS
5	K	243	GLN
5	K	262	GLN
5	K	307	ASN
5	K	377	HIS
5	K	388	ASN
5	K	421	ASN
5	K	467	ASN
5	K	504	ASN
6	L	31	ASN
6	L	61	ASN
6	L	164	GLN
6	L	180	GLN
6	M	31	ASN
6	M	61	ASN
6	M	164	GLN
6	M	180	GLN
6	N	31	ASN
6	N	61	ASN
6	N	164	GLN
6	N	180	GLN
8	P	79	ASN
8	P	103	ASN
1	Q	3	ASN
1	Q	40	GLN
1	Q	69	GLN
1	Q	159	ASN
1	Q	216	HIS
1	Q	294	ASN
1	Q	303	ASN
1	Q	456	ASN
1	Q	490	ASN
1	R	40	GLN
1	R	84	ASN
1	R	91	GLN
1	R	169	GLN
1	R	195	ASN
1	R	281	ASN
1	R	337	GLN

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Mol	Chain	Res	Type
1	R	361	GLN
1	R	388	GLN
1	R	400	ASN
1	R	434	GLN
1	R	503	ASN
1	R	518	ASN
1	R	570	GLN
1	R	582	ASN
2	S	22	GLN
2	S	91	GLN
2	S	130	ASN
2	S	243	ASN
2	S	333	ASN
2	S	486	HIS
2	S	528	ASN
2	S	601	ASN
2	S	626	GLN
2	S	673	GLN
2	S	684	ASN
2	S	716	ASN
2	S	914	ASN
3	T	23	ASN
3	T	26	ASN
3	T	232	GLN
3	T	233	GLN
3	T	271	GLN
3	T	314	ASN
3	U	26	ASN
3	U	115	ASN
3	U	232	GLN
3	U	271	GLN
3	U	314	ASN
4	V	45	GLN
4	V	70	HIS
4	V	170	GLN
4	V	193	HIS
4	W	45	GLN
4	W	52	ASN
4	W	70	HIS
4	W	170	GLN
4	W	193	HIS
4	X	45	GLN

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Mol	Chain	Res	Type
4	X	52	ASN
4	X	70	HIS
4	X	170	GLN
4	X	193	HIS
5	Y	3	GLN
5	Y	127	ASN
5	Y	161	ASN
5	Y	262	GLN
5	Y	377	HIS
5	Y	387	ASN
5	Y	410	GLN
5	Y	444	ASN
5	Y	467	ASN
5	Y	504	ASN
5	Y	580	HIS
5	Z	27	ASN
5	Z	187	ASN
5	Z	198	ASN
5	Z	318	GLN
5	Z	377	HIS
5	Z	410	GLN
5	Z	421	ASN
5	Z	444	ASN
5	Z	504	ASN
5	Z	514	HIS
5	Z	588	ASN
5	a	27	ASN
5	a	87	ASN
5	a	161	ASN
5	a	195	HIS
5	a	198	ASN
5	a	243	GLN
5	a	262	GLN
5	a	307	ASN
5	a	377	HIS
5	a	421	ASN
5	a	467	ASN
5	a	498	ASN
5	a	504	ASN
6	b	31	ASN
6	b	61	ASN
6	b	164	GLN

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Mol	Chain	Res	Type
6	b	180	GLN
6	c	31	ASN
6	c	61	ASN
6	c	164	GLN
6	c	180	GLN
6	d	31	ASN
6	d	61	ASN
6	d	164	GLN
6	d	180	GLN
8	f	79	ASN
8	f	103	ASN
1	g	40	GLN
1	g	69	GLN
1	g	159	ASN
1	g	216	HIS
1	g	294	ASN
1	g	303	ASN
1	g	394	ASN
1	g	456	ASN
1	g	490	ASN
1	h	40	GLN
1	h	84	ASN
1	h	91	GLN
1	h	169	GLN
1	h	195	ASN
1	h	281	ASN
1	h	305	ASN
1	h	337	GLN
1	h	361	GLN
1	h	388	GLN
1	h	400	ASN
1	h	434	GLN
1	h	503	ASN
1	h	518	ASN
1	h	570	GLN
1	h	582	ASN
2	i	22	GLN
2	i	91	GLN
2	i	130	ASN
2	i	243	ASN
2	i	333	ASN
2	i	486	HIS

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Mol	Chain	Res	Type
2	i	528	ASN
2	i	601	ASN
2	i	626	GLN
2	i	663	ASN
2	i	673	GLN
2	i	684	ASN
2	i	716	ASN
2	i	914	ASN
3	j	23	ASN
3	j	26	ASN
3	j	232	GLN
3	j	233	GLN
3	j	314	ASN
3	k	26	ASN
3	k	115	ASN
3	k	232	GLN
3	k	271	GLN
3	k	314	ASN
4	l	45	GLN
4	l	52	ASN
4	l	70	HIS
4	l	170	GLN
4	l	193	HIS
4	m	45	GLN
4	m	52	ASN
4	m	70	HIS
4	m	170	GLN
4	m	193	HIS
4	n	45	GLN
4	n	52	ASN
4	n	70	HIS
4	n	170	GLN
4	n	193	HIS
5	o	3	GLN
5	o	161	ASN
5	o	198	ASN
5	o	262	GLN
5	o	318	GLN
5	o	377	HIS
5	o	387	ASN
5	o	410	GLN
5	o	437	GLN

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Mol	Chain	Res	Type
5	o	444	ASN
5	o	467	ASN
5	o	504	ASN
5	o	580	HIS
5	p	27	ASN
5	p	187	ASN
5	p	198	ASN
5	p	318	GLN
5	p	377	HIS
5	p	410	GLN
5	p	421	ASN
5	p	444	ASN
5	p	504	ASN
5	p	514	HIS
5	p	588	ASN
5	q	87	ASN
5	q	161	ASN
5	q	195	HIS
5	q	198	ASN
5	q	243	GLN
5	q	262	GLN
5	q	307	ASN
5	q	377	HIS
5	q	421	ASN
5	q	467	ASN
5	q	498	ASN
5	q	504	ASN
6	r	31	ASN
6	r	61	ASN
6	r	164	GLN
6	r	180	GLN
6	s	31	ASN
6	s	33	GLN
6	s	61	ASN
6	s	164	GLN
6	s	180	GLN
6	t	31	ASN
6	t	61	ASN
6	t	164	GLN
6	t	180	GLN
8	v	79	ASN
1	w	3	ASN

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Mol	Chain	Res	Type
1	w	40	GLN
1	w	69	GLN
1	w	159	ASN
1	w	216	HIS
1	w	294	ASN
1	w	303	ASN
1	w	456	ASN
1	w	490	ASN
1	x	84	ASN
1	x	91	GLN
1	x	169	GLN
1	x	195	ASN
1	x	281	ASN
1	x	305	ASN
1	x	337	GLN
1	x	361	GLN
1	x	400	ASN
1	x	434	GLN
1	x	503	ASN
1	x	518	ASN
1	x	582	ASN
2	y	22	GLN
2	y	91	GLN
2	y	130	ASN
2	y	243	ASN
2	y	333	ASN
2	y	528	ASN
2	y	601	ASN
2	y	626	GLN
2	y	673	GLN
2	y	684	ASN
2	y	716	ASN
2	y	914	ASN
2	y	1018	ASN
3	z	23	ASN
3	z	26	ASN
3	z	232	GLN
3	z	233	GLN
3	z	314	ASN
3	AA	26	ASN
3	AA	115	ASN
3	AA	232	GLN

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Mol	Chain	Res	Type
3	AA	271	GLN
3	AA	314	ASN
4	AB	45	GLN
4	AB	52	ASN
4	AB	70	HIS
4	AB	170	GLN
4	AB	193	HIS
4	AC	4	GLN
4	AC	45	GLN
4	AC	52	ASN
4	AC	70	HIS
4	AC	120	ASN
4	AC	170	GLN
4	AC	193	HIS
4	AD	45	GLN
4	AD	52	ASN
4	AD	70	HIS
4	AD	170	GLN
4	AD	193	HIS
5	AE	3	GLN
5	AE	161	ASN
5	AE	190	ASN
5	AE	198	ASN
5	AE	262	GLN
5	AE	377	HIS
5	AE	387	ASN
5	AE	410	GLN
5	AE	437	GLN
5	AE	444	ASN
5	AE	467	ASN
5	AE	504	ASN
5	AE	580	HIS
5	AF	27	ASN
5	AF	187	ASN
5	AF	198	ASN
5	AF	318	GLN
5	AF	377	HIS
5	AF	410	GLN
5	AF	421	ASN
5	AF	444	ASN
5	AF	504	ASN
5	AF	514	HIS

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Mol	Chain	Res	Type
5	AF	588	ASN
5	AG	87	ASN
5	AG	161	ASN
5	AG	195	HIS
5	AG	198	ASN
5	AG	243	GLN
5	AG	262	GLN
5	AG	307	ASN
5	AG	377	HIS
5	AG	421	ASN
5	AG	467	ASN
5	AG	498	ASN
5	AG	504	ASN
6	BA	31	ASN
6	BA	61	ASN
6	BA	164	GLN
6	BA	180	GLN
6	BB	31	ASN
6	BB	33	GLN
6	BB	61	ASN
6	BB	164	GLN
6	BB	180	GLN
6	BC	31	ASN
6	BC	33	GLN
6	BC	61	ASN
6	BC	164	GLN
6	BC	180	GLN
8	BE	79	ASN
1	BF	3	ASN
1	BF	40	GLN
1	BF	69	GLN
1	BF	159	ASN
1	BF	216	HIS
1	BF	294	ASN
1	BF	303	ASN
1	BF	456	ASN
1	BF	490	ASN
1	BG	40	GLN
1	BG	84	ASN
1	BG	91	GLN
1	BG	169	GLN
1	BG	195	ASN

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Mol	Chain	Res	Type
1	BG	281	ASN
1	BG	305	ASN
1	BG	337	GLN
1	BG	361	GLN
1	BG	388	GLN
1	BG	400	ASN
1	BG	434	GLN
1	BG	503	ASN
1	BG	582	ASN
2	CA	22	GLN
2	CA	91	GLN
2	CA	130	ASN
2	CA	243	ASN
2	CA	333	ASN
2	CA	528	ASN
2	CA	601	ASN
2	CA	626	GLN
2	CA	663	ASN
2	CA	673	GLN
2	CA	684	ASN
2	CA	716	ASN
2	CA	914	ASN
2	CA	1018	ASN
3	CB	23	ASN
3	CB	26	ASN
3	CB	50	ASN
3	CB	74	HIS
3	CB	232	GLN
3	CB	233	GLN
3	CB	314	ASN
3	CC	26	ASN
3	CC	271	GLN
3	CC	314	ASN
4	CD	45	GLN
4	CD	52	ASN
4	CD	70	HIS
4	CD	170	GLN
4	CD	193	HIS
4	CE	45	GLN
4	CE	52	ASN
4	CE	70	HIS
4	CE	170	GLN

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Mol	Chain	Res	Type
4	CE	193	HIS
4	CE	288	GLN
4	CF	45	GLN
4	CF	52	ASN
4	CF	70	HIS
4	CF	170	GLN
4	CF	193	HIS
4	CF	282	GLN
5	CG	3	GLN
5	CG	161	ASN
5	CG	190	ASN
5	CG	198	ASN
5	CG	262	GLN
5	CG	318	GLN
5	CG	377	HIS
5	CG	387	ASN
5	CG	410	GLN
5	CG	437	GLN
5	CG	444	ASN
5	CG	467	ASN
5	CG	504	ASN
5	CG	580	HIS
5	DA	27	ASN
5	DA	187	ASN
5	DA	198	ASN
5	DA	318	GLN
5	DA	377	HIS
5	DA	410	GLN
5	DA	421	ASN
5	DA	444	ASN
5	DA	467	ASN
5	DA	504	ASN
5	DA	514	HIS
5	DA	588	ASN
5	DB	87	ASN
5	DB	195	HIS
5	DB	198	ASN
5	DB	243	GLN
5	DB	262	GLN
5	DB	307	ASN
5	DB	377	HIS
5	DB	388	ASN

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Mol	Chain	Res	Type
5	DB	421	ASN
5	DB	467	ASN
5	DB	498	ASN
5	DB	504	ASN
6	DC	31	ASN
6	DC	61	ASN
6	DC	164	GLN
6	DC	180	GLN
6	DD	31	ASN
6	DD	33	GLN
6	DD	61	ASN
6	DD	164	GLN
6	DD	180	GLN
6	DE	31	ASN
6	DE	61	ASN
6	DE	164	GLN
6	DE	180	GLN
8	DG	79	ASN
1	EA	40	GLN
1	EA	69	GLN
1	EA	159	ASN
1	EA	216	HIS
1	EA	294	ASN
1	EA	303	ASN
1	EA	456	ASN
1	EA	490	ASN
1	EB	84	ASN
1	EB	91	GLN
1	EB	169	GLN
1	EB	195	ASN
1	EB	281	ASN
1	EB	337	GLN
1	EB	361	GLN
1	EB	400	ASN
1	EB	434	GLN
1	EB	503	ASN
1	EB	582	ASN
2	EC	22	GLN
2	EC	91	GLN
2	EC	130	ASN
2	EC	243	ASN
2	EC	333	ASN

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Mol	Chain	Res	Type
2	EC	528	ASN
2	EC	626	GLN
2	EC	663	ASN
2	EC	673	GLN
2	EC	684	ASN
2	EC	716	ASN
2	EC	914	ASN
2	EC	1018	ASN
3	ED	23	ASN
3	ED	26	ASN
3	ED	232	GLN
3	ED	233	GLN
3	ED	314	ASN
3	EE	26	ASN
3	EE	115	ASN
3	EE	232	GLN
3	EE	271	GLN
3	EE	314	ASN
4	EF	45	GLN
4	EF	52	ASN
4	EF	70	HIS
4	EF	170	GLN
4	EF	193	HIS
4	EG	4	GLN
4	EG	45	GLN
4	EG	70	HIS
4	EG	170	GLN
4	EG	193	HIS
4	FA	45	GLN
4	FA	70	HIS
4	FA	170	GLN
4	FA	193	HIS
4	FA	282	GLN
5	FB	3	GLN
5	FB	161	ASN
5	FB	198	ASN
5	FB	262	GLN
5	FB	318	GLN
5	FB	377	HIS
5	FB	387	ASN
5	FB	410	GLN
5	FB	437	GLN

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Mol	Chain	Res	Type
5	FB	444	ASN
5	FB	467	ASN
5	FB	504	ASN
5	FB	580	HIS
5	FC	187	ASN
5	FC	198	ASN
5	FC	318	GLN
5	FC	377	HIS
5	FC	410	GLN
5	FC	421	ASN
5	FC	444	ASN
5	FC	467	ASN
5	FC	504	ASN
5	FC	514	HIS
5	FC	588	ASN
5	FD	87	ASN
5	FD	195	HIS
5	FD	198	ASN
5	FD	243	GLN
5	FD	262	GLN
5	FD	307	ASN
5	FD	377	HIS
5	FD	388	ASN
5	FD	421	ASN
5	FD	467	ASN
5	FD	498	ASN
5	FD	504	ASN
6	FE	31	ASN
6	FE	61	ASN
6	FE	164	GLN
6	FE	180	GLN
6	FF	31	ASN
6	FF	33	GLN
6	FF	61	ASN
6	FF	164	GLN
6	FF	180	GLN
6	FG	31	ASN
6	FG	61	ASN
6	FG	164	GLN
6	FG	180	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	I	1
5	Y	1
5	o	1
5	CG	1
5	FB	1
5	AE	1
2	i	1
2	CA	1
2	EC	1
2	C	1
2	S	1
2	y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	570:ARG	C	571:GLU	N	3.75
1	Y	570:ARG	C	571:GLU	N	3.75
1	o	570:ARG	C	571:GLU	N	3.75
1	CG	570:ARG	C	571:GLU	N	3.75
1	FB	570:ARG	C	571:GLU	N	3.75
1	AE	570:ARG	C	571:GLU	N	3.74
1	i	72:ALA	C	73:ASP	N	1.19
1	CA	72:ALA	C	73:ASP	N	1.19
1	EC	72:ALA	C	73:ASP	N	1.19
1	C	72:ALA	C	73:ASP	N	1.18
1	S	72:ALA	C	73:ASP	N	1.18
1	y	72:ALA	C	73:ASP	N	1.18

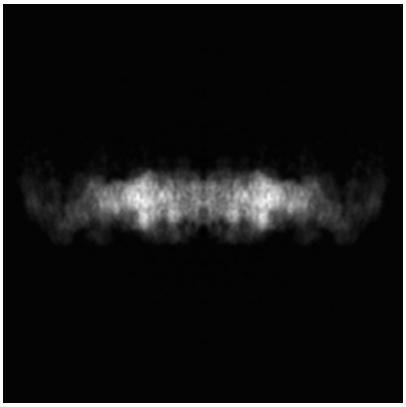
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3396. These allow visual inspection of the internal detail of the map and identification of artifacts.

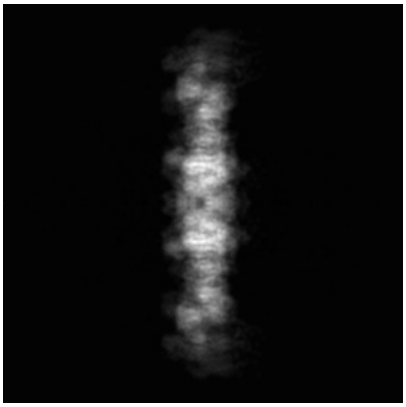
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

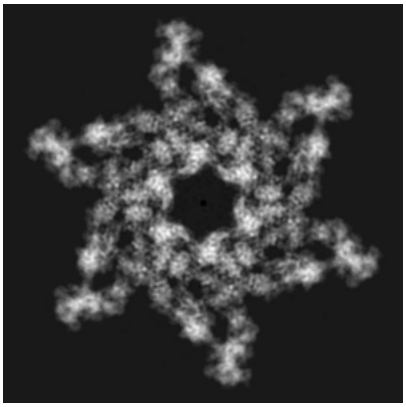
6.1.1 Primary map



X



Y

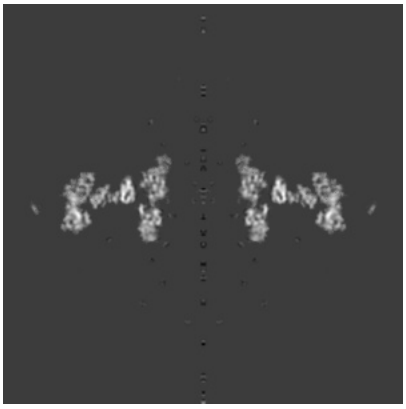


Z

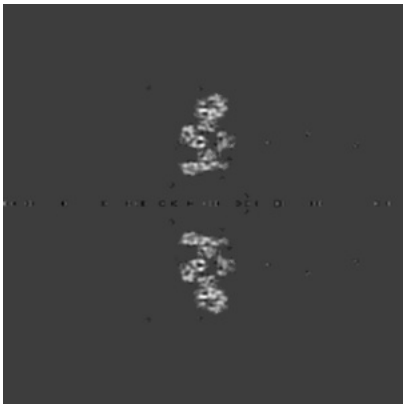
The images above show the map projected in three orthogonal directions.

6.2 Central slices

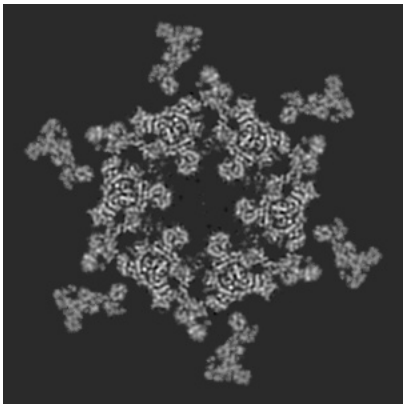
6.2.1 Primary map



X Index: 240



Y Index: 240

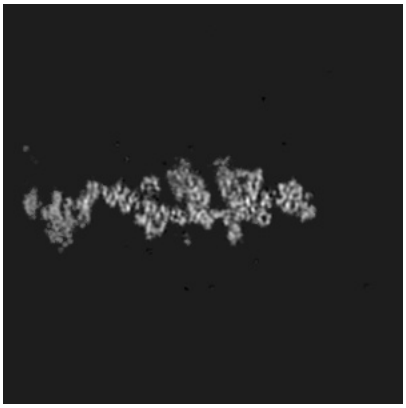


Z Index: 240

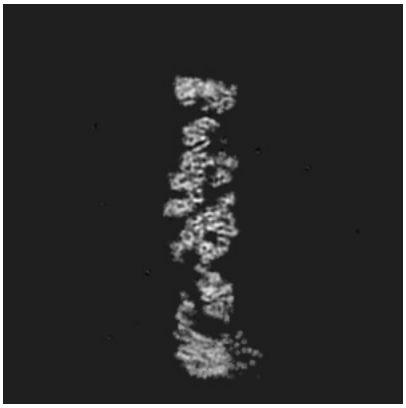
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

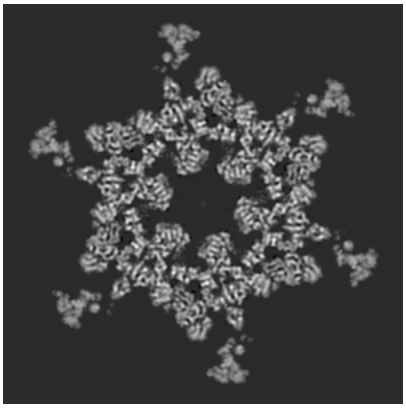
6.3.1 Primary map



X Index: 286



Y Index: 310



Z Index: 247

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0095. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

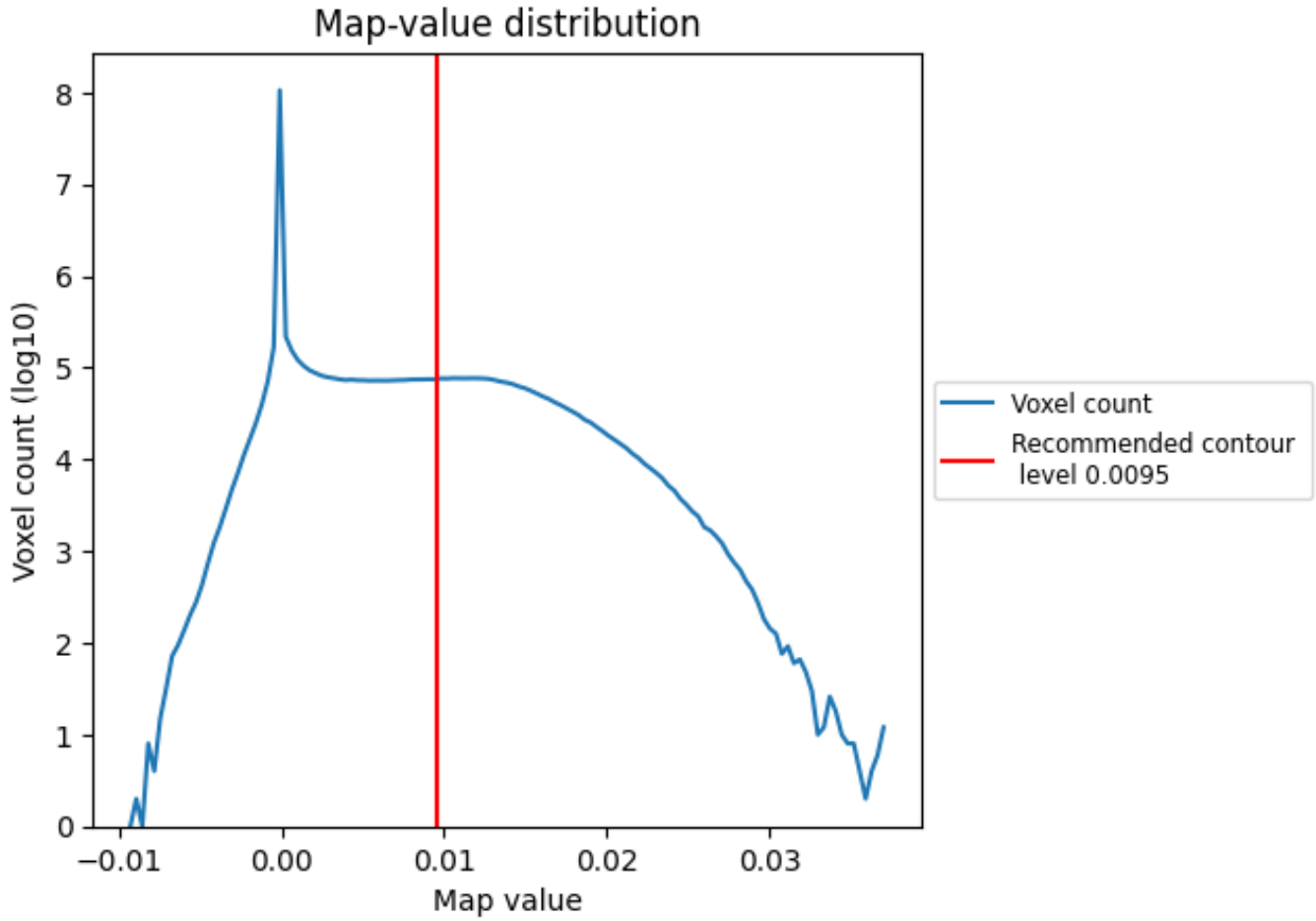
6.5 Mask visualisation (i)

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

7 Map analysis

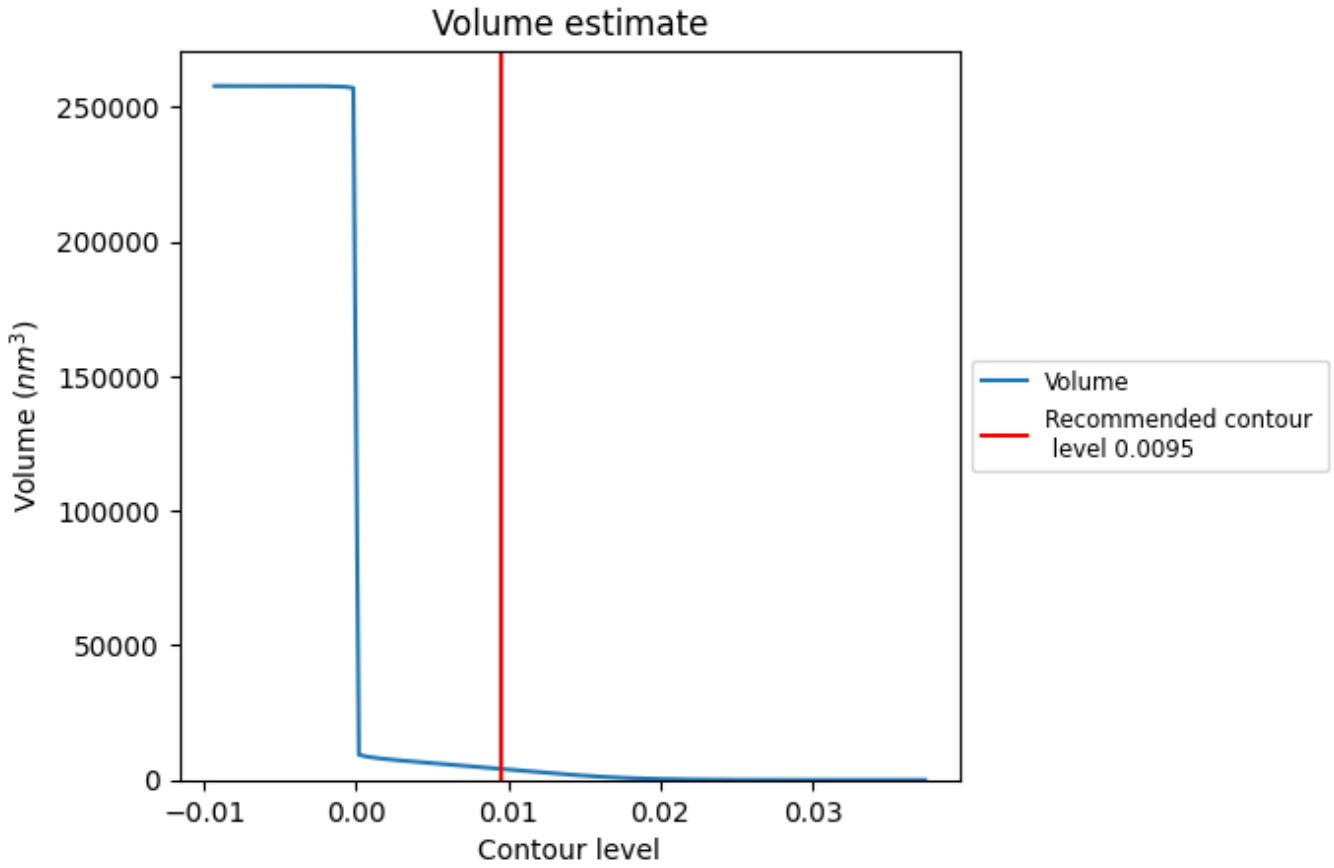
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

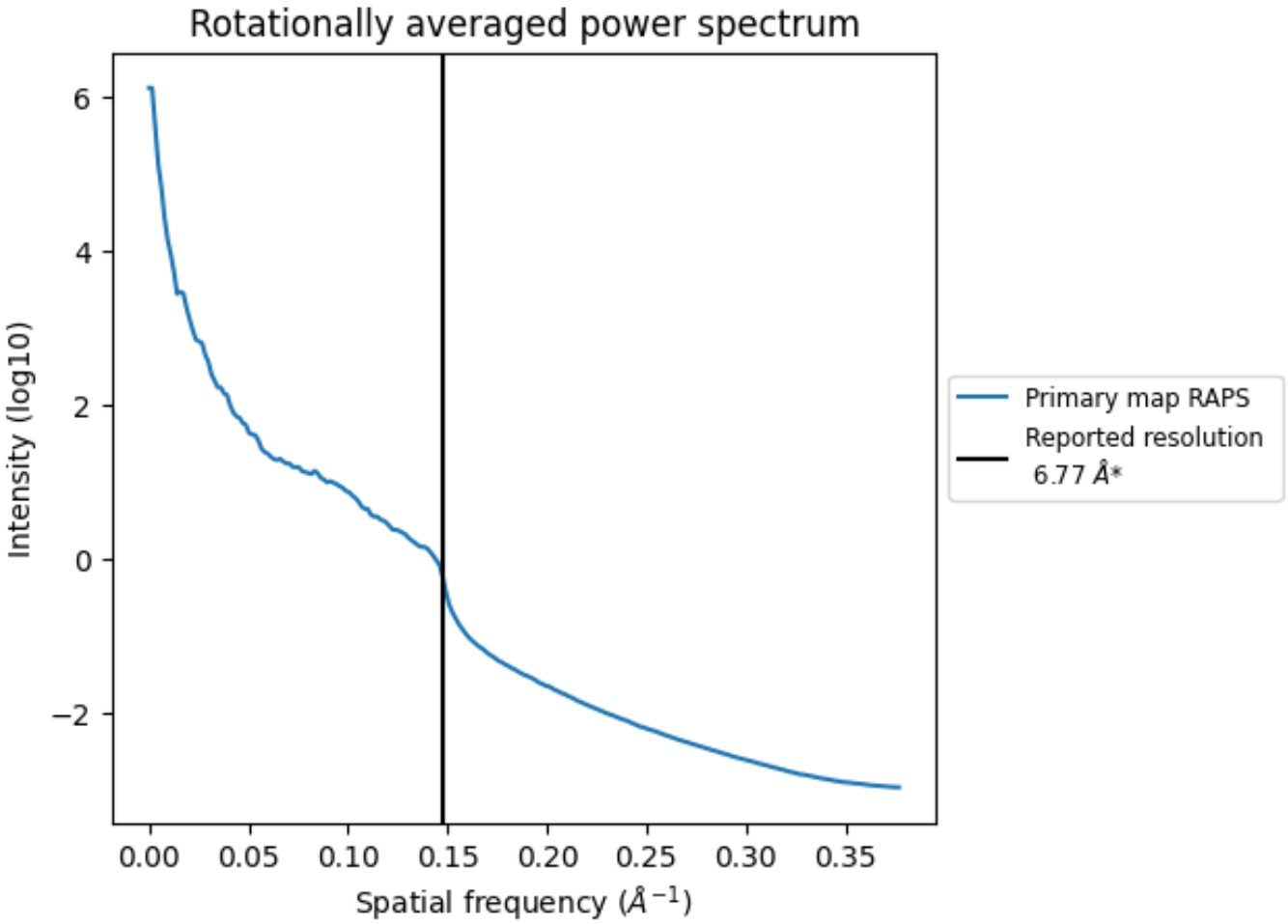
7.2 Volume estimate



The volume at the recommended contour level is 4148 nm^3; this corresponds to an approximate mass of 3747 kDa.

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

7.3 Rotationally averaged power spectrum (i)

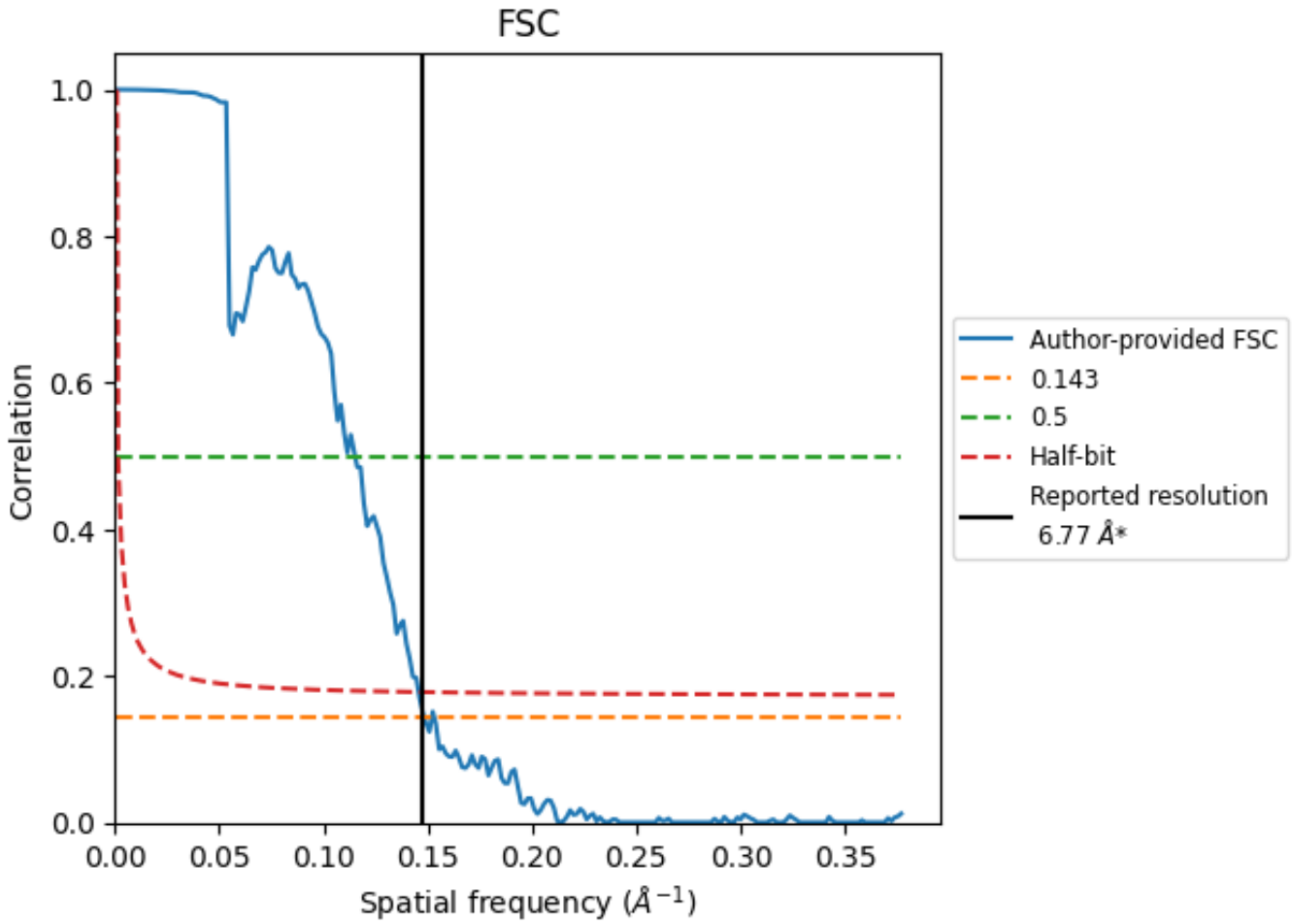


*Reported resolution corresponds to spatial frequency of 0.148 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.148 Å^{-1}

8.2 Resolution estimates (i)

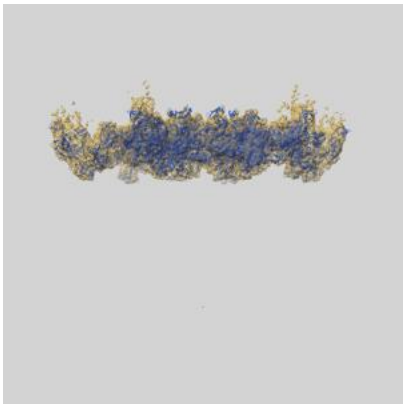
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.77	-	-
Author-provided FSC curve	6.74	8.69	6.87
Unmasked-calculated*	-	-	-

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

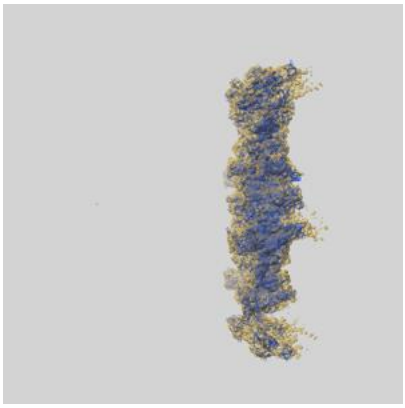
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3396 and PDB model 5IV7. Per-residue inclusion information can be found in section 3 on page 13.

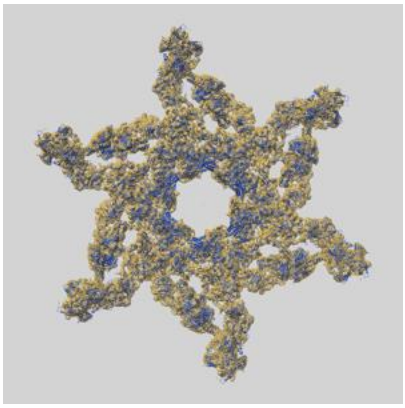
9.1 Map-model overlay



X



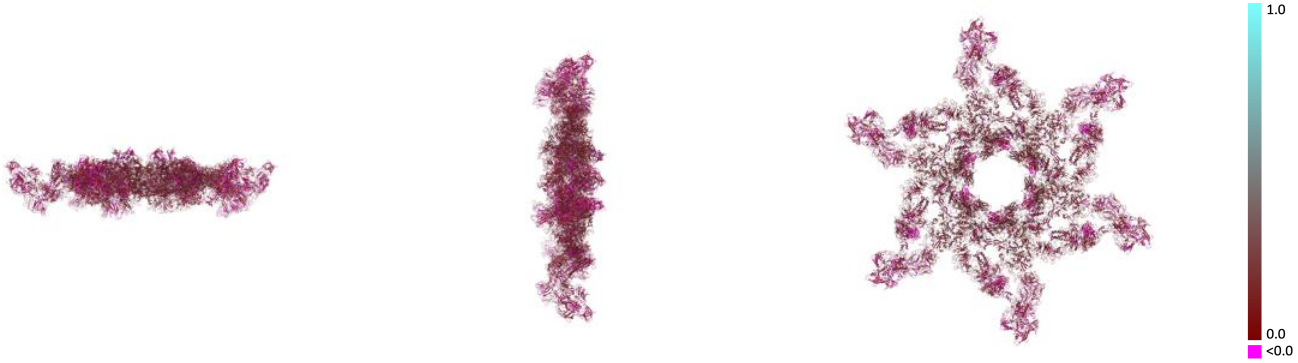
Y



Z

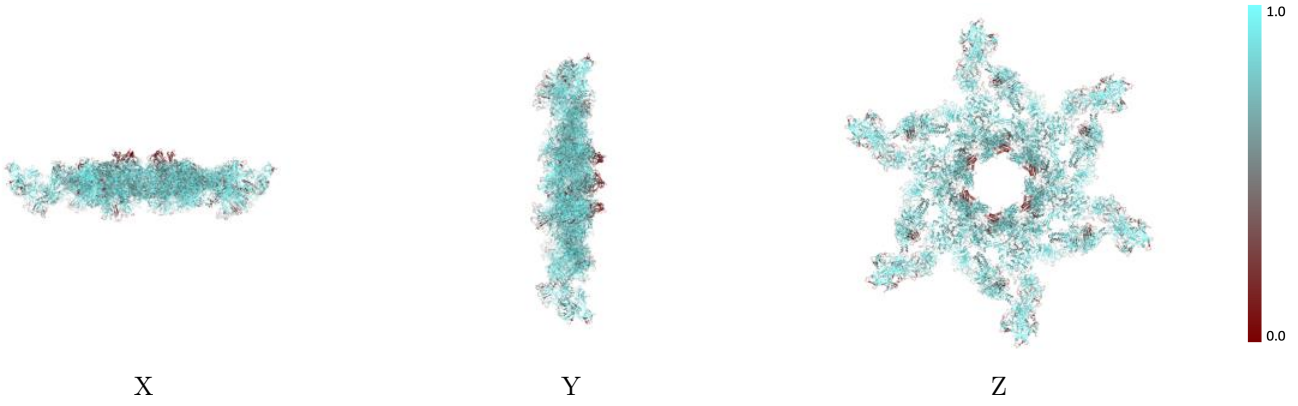
The images above show the 3D surface view of the map at the recommended contour level 0.0095 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



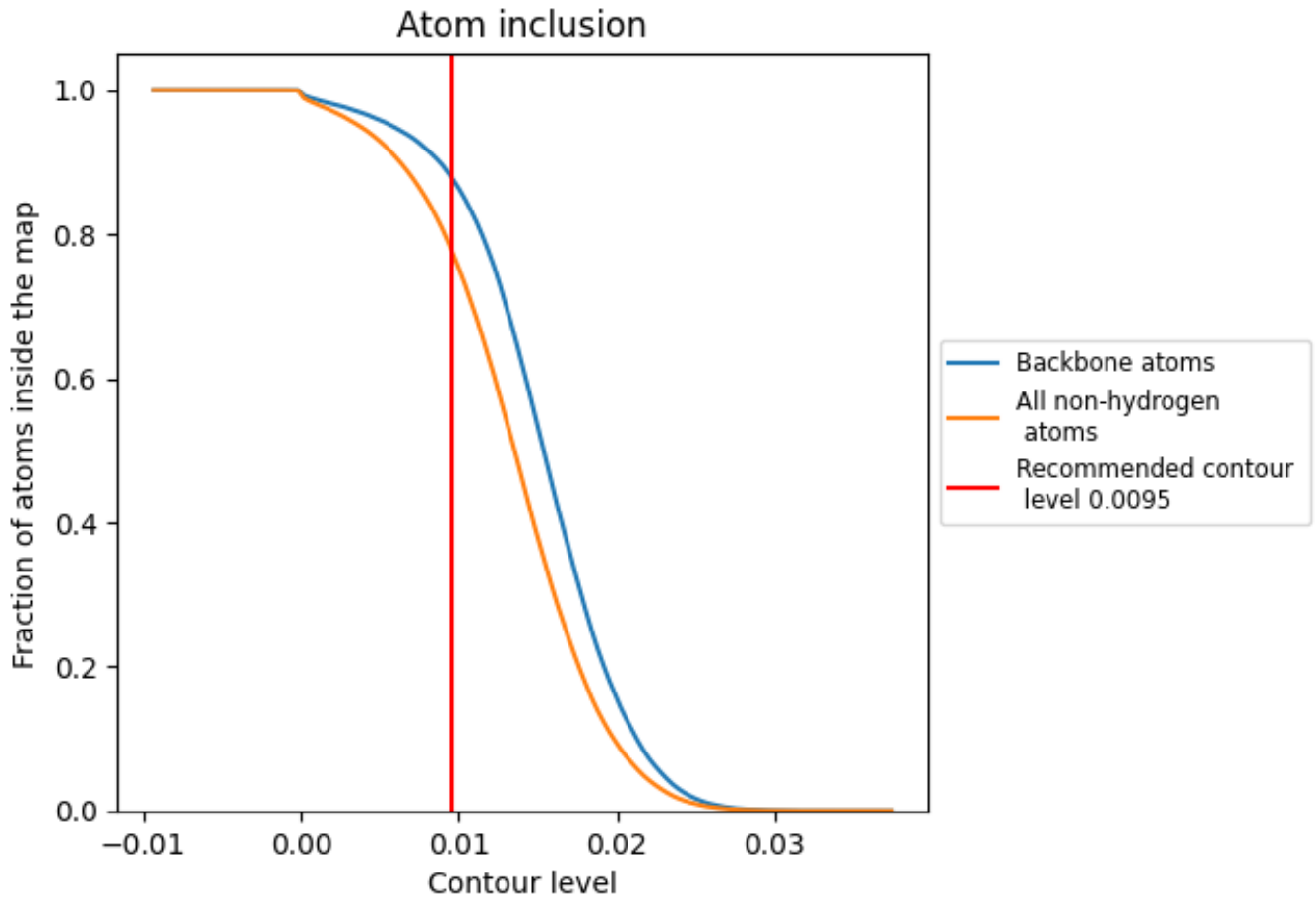
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0095).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.0095) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7794	0.1500
A	0.8073	0.1770
AA	0.8179	0.1670
AB	0.7570	0.1360
AC	0.7365	0.1300
AD	0.6909	0.1170
AE	0.7801	0.1310
AF	0.7292	0.1260
AG	0.7620	0.1440
B	0.7964	0.1830
BA	0.7204	0.0920
BB	0.7374	0.0890
BC	0.8316	0.0980
BD	0.2747	0.0820
BE	0.8293	0.1800
BF	0.8111	0.1750
BG	0.8011	0.1820
C	0.8602	0.1800
CA	0.8582	0.1810
CB	0.8495	0.1760
CC	0.8183	0.1700
CD	0.7505	0.1350
CE	0.7630	0.1420
CF	0.6741	0.1060
CG	0.7840	0.1310
D	0.8471	0.1750
DA	0.7329	0.1290
DB	0.7605	0.1420
DC	0.7362	0.1050
DD	0.6967	0.0750
DE	0.8091	0.0940
DF	0.2556	0.0670
DG	0.8318	0.1800
E	0.8183	0.1700
EA	0.8078	0.1770

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Chain	Atom inclusion	Q-score
EB	0.7968	0.1820
EC	0.8564	0.1810
ED	0.8475	0.1760
EE	0.8168	0.1700
EF	0.7588	0.1340
EG	0.7602	0.1410
F	0.7486	0.1260
FA	0.6788	0.1150
FB	0.7853	0.1350
FC	0.7266	0.1250
FD	0.7627	0.1400
FE	0.7210	0.1000
FF	0.7429	0.0870
FG	0.8298	0.1000
G	0.7565	0.1410
GA	0.2606	0.0790
GB	0.8363	0.1820
H	0.6848	0.1130
I	0.7809	0.1310
J	0.7298	0.1280
K	0.7622	0.1450
L	0.7155	0.0900
M	0.7380	0.0870
N	0.8274	0.0970
O	0.2758	0.0740
P	0.8293	0.1810
Q	0.8115	0.1740
R	0.8027	0.1840
S	0.8560	0.1800
T	0.8510	0.1730
U	0.8195	0.1710
V	0.7514	0.1370
W	0.7649	0.1460
X	0.6736	0.1090
Y	0.7766	0.1290
Z	0.7329	0.1290
a	0.7596	0.1410
b	0.7356	0.1020
c	0.6942	0.0710
d	0.8140	0.0920
e	0.2626	0.0700
f	0.8267	0.1770

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Chain	Atom inclusion	Q-score
g	0.8078	0.1760
h	0.7958	0.1830
i	0.8572	0.1810
j	0.8491	0.1750
k	0.8172	0.1690
l	0.7500	0.1340
m	0.7598	0.1430
n	0.6750	0.1110
o	0.7866	0.1340
p	0.7246	0.1240
q	0.7603	0.1410
r	0.7228	0.0990
s	0.7429	0.0820
t	0.8255	0.0990
u	0.2626	0.0850
v	0.8344	0.1800
w	0.8082	0.1790
x	0.7958	0.1820
y	0.8601	0.1810
z	0.8440	0.1770