



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:54 AM UTC

PDB ID : 8H2I / pdb_00008h2i
EMDB ID : EMD-34438
Title : Near-atomic structure of five-fold averaged PBCV-1 capsid
Authors : Shao, Q.; Agarkova, I.V.; Noel, E.A.; Dunigan, D.D.; Liu, Y.; Wang, A.; Guo, M.; Xie, L.; Zhao, X.; Rossmann, M.G.; Van Etten, J.L.; Klose, T.; Fang, Q.
Deposited on : 2022-10-06
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

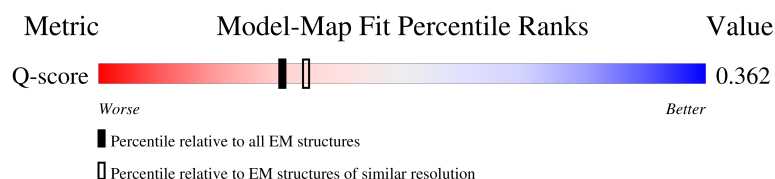
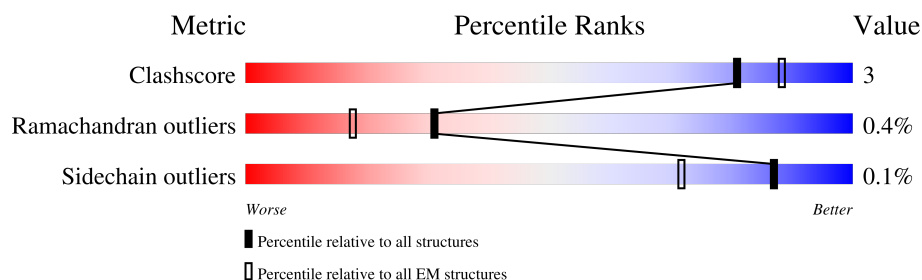
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	aA	437	85% 94% 5%
1	aB	437	81% 95% 5%
1	aC	437	78% 95% .
1	aD	437	78% 91% 8% .

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Mol	Chain	Length	Quality of chain
1	aE	437	52% 95% 5%
1	aF	437	44% 95% ..
1	aG	437	59% 96% .
1	aH	437	38% 95% ..
1	aI	437	40% 93% 6%
1	aJ	437	46% 94% 5%
1	aK	437	54% 94% 5%
1	aL	437	60% 95% .
1	aM	437	62% 95% 5%
1	aN	437	58% 96% .
1	aO	437	63% 97% .
1	aP	437	57% 97% .
1	aQ	437	68% 94% 5% .
1	aR	437	71% 95% 5%
1	aS	437	65% 96% .
1	aT	437	62% 96% .
1	aU	437	56% 96% .
1	aV	437	57% 97% .
1	aW	437	70% 95% 5%
1	aX	437	70% 97% .
1	aY	437	72% 96% .
1	aZ	437	66% 97% .
1	aa	437	45% 86% 12% .
1	ab	437	45% 89% 9% .
1	ac	437	42% 87% 12%

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Mol	Chain	Length	Quality of chain
1	ad	437	43% 95% .
1	ae	437	42% 97% .
1	af	437	47% 95% 5%
1	ag	437	45% 96% .
1	ah	437	37% 96% .
1	ai	437	44% 96% .
1	aj	437	75% 95% 5%
1	ak	437	62% 94% 5%
1	al	437	78% 94% 5%
1	am	437	41% 93% 6%
1	an	437	41% 96% .
1	ao	437	41% 96% .
1	ap	437	38% 95% .
1	aq	437	33% 95% 5%
1	ar	437	31% 95% ..
1	as	437	44% 95% .
1	at	437	58% 97% .
1	au	437	51% 94% 5%.
1	av	437	69% 98% .
1	aw	437	75% 96% .
1	ax	437	65% 96% ..
1	ay	437	88% 96% .
1	az	437	89% 97% ..
1	ba	437	57% 98% .
1	bb	437	67% 95% .

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Mol	Chain	Length	Quality of chain
1	bc	437	58% 96% .
1	bd	437	62% 95% 5%
1	be	437	61% 96% .
1	bf	437	55% 95% 5%
1	bg	437	58% 96% .
1	bh	437	55% 95% 5%
1	bi	437	62% 96% .
1	bj	437	68% 96% .
1	bk	437	61% 97% .
1	bl	437	67% 95% 5%
1	bm	437	66% 94% 6%
1	bn	437	70% 95% ..
1	bo	437	68% 94% 5%
1	bp	437	60% 94% 5%
1	bq	437	68% 97% .
1	br	437	48% 96% .
1	bs	437	58% 96% .
1	bt	437	56% 96% .
2	bA	520	58% 91% 8% .
2	bB	520	79% 94% 5% .
2	bu	520	31% 89% 10% ..
2	bv	520	36% 88% 11% ..
2	bw	520	34% 89% 10% ..
2	bx	520	42% 86% 12% ..
2	by	520	49% 88% 11% ..

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Mol	Chain	Length	Quality of chain
2	bz	520	
3	bC	486	
4	bD	403	
4	bF	403	
4	cX	403	
4	cZ	403	
4	dd	403	
4	df	403	
4	dj	403	
4	dk	403	
4	dl	403	
4	dp	403	
4	dr	403	
5	bE	401	
5	cY	401	
5	de	401	
5	dq	401	
6	bG	530	
7	bH	576	
8	bI	171	
8	bJ	171	
8	bK	171	
9	bL	181	
9	bM	181	
9	bN	181	

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Mol	Chain	Length	Quality of chain
9	bO	181	
10	bP	146	
11	bQ	216	
12	bR	173	
13	bS	210	
14	bT	207	
14	bU	207	
14	bV	207	
14	bW	207	
14	bX	207	
14	bY	207	
14	bZ	207	
14	ca	207	
14	cb	207	
14	cc	207	
14	cd	207	
14	ce	207	
15	cf	151	
16	cg	98	
17	ch	155	
18	ci	93	
19	cj	80	
19	ck	80	
19	cl	80	
19	cm	80	

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Mol	Chain	Length	Quality of chain
20	cn	148	
20	co	148	
21	cA	378	
21	cB	378	
21	cC	378	
21	cD	378	
21	cE	378	
21	cF	378	
21	cG	378	
21	cH	378	
21	cI	378	
21	cJ	378	
21	cK	378	
21	cL	378	
21	cM	378	
21	cN	378	
21	cp	378	
21	cq	378	
21	cr	378	
21	cs	378	
21	ct	378	
21	cu	378	
21	cv	378	
21	cw	378	
21	cx	378	

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Mol	Chain	Length	Quality of chain
21	cy	378	
21	cz	378	
22	cO	1335	
22	cQ	1335	
22	da	1335	
22	dc	1335	
22	dg	1335	
22	di	1335	
22	ds	1335	
22	du	1335	
23	cP	1369	
23	db	1369	
23	dh	1369	
23	dt	1369	
24	cR	400	
24	cS	400	
24	cT	400	
25	cU	1343	
25	cV	1343	
25	cW	1343	
26	dm	1359	
26	dn	1359	
26	do	1359	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 427569 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 Major capsid protein (MCP).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aa	432	Total	C	N	O	S	0	0
			3374	2145	571	650	8		
1	ab	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ac	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ad	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ae	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	af	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ag	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ah	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ai	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aj	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ak	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	al	435	Total	C	N	O	S	0	0
			3387	2152	574	653	8		
1	am	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	an	435	Total	C	N	O	S	0	0
			3387	2152	574	653	8		
1	ao	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	ap	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aq	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ar	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	as	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	at	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	au	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	av	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aw	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ax	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	ay	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	az	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aA	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aB	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aC	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aD	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aE	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aF	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aG	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aH	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aI	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aJ	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aK	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aL	435	Total	C	N	O	S	0	0
			3387	2152	574	653	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	aM	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aN	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aO	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aP	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aQ	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	aR	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aS	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aT	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aU	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aV	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aW	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aX	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		
1	aY	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	aZ	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	ba	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bb	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bc	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bd	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	be	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bf	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bg	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	bh	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bi	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bj	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bk	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bl	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bm	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bn	434	Total	C	N	O	S	0	0
			3382	2149	573	652	8		
1	bo	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bp	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bq	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	br	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bs	436	Total	C	N	O	S	0	0
			3395	2156	576	655	8		
1	bt	435	Total	C	N	O	S	0	0
			3390	2153	575	654	8		

- Molecule 2 is a protein called MCPv1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	bu	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		
2	bv	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		
2	bw	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		
2	bx	514	Total	C	N	O	S	0	0
			4074	2611	677	775	11		
2	by	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		
2	bz	508	Total	C	N	O	S	0	0
			4030	2583	670	766	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	bA	516	Total	C	N	O	S	0	0
			4079	2612	679	777	11		
2	bB	517	Total	C	N	O	S	0	0
			4090	2621	680	778	11		

- Molecule 3 is a protein called MCPv2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	bC	485	Total	C	N	O	S	0	0
			3921	2518	645	742	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
bC	343	SER	GLY	variant	UNP M1I493

- Molecule 4 is a protein called MCPv3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	bF	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	cX	401	Total	C	N	O	S	0	0
			3165	2029	521	605	10		
4	cZ	401	Total	C	N	O	S	0	0
			3165	2029	521	605	10		
4	dd	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	df	401	Total	C	N	O	S	0	0
			3165	2029	521	605	10		
4	dj	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	dk	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	dl	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	dp	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		
4	dr	401	Total	C	N	O	S	0	0
			3169	2031	521	607	10		

- Molecule 5 is a protein called MCPv4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	bE	397	Total	C	N	O	S	0	0
			3146	2021	513	601	11		
5	cY	397	Total	C	N	O	S	0	0
			3146	2021	513	601	11		
5	de	397	Total	C	N	O	S	0	0
			3146	2021	513	601	11		
5	dq	397	Total	C	N	O	S	0	0
			3146	2021	513	601	11		

- Molecule 6 is a protein called P1v1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	bG	504	Total	C	N	O	S	0	0
			3864	2454	633	771	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
bG	113	ASN	SER	variant	UNP M1I677
bG	348	ILE	VAL	variant	UNP M1I677
bG	364	SER	THR	variant	UNP M1I677

- Molecule 7 is a protein called P2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	bH	424	Total	C	N	O	S	0	0
			3258	2015	591	642	10		

- Molecule 8 is a protein called P3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	bI	141	Total	C	N	O	S	0	0
			1096	691	191	209	5		
8	bJ	147	Total	C	N	O	S	0	0
			1146	724	198	219	5		
8	bK	116	Total	C	N	O	S	0	0
			892	560	157	170	5		

- Molecule 9 is a protein called P4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	bL	63	Total	C	N	O	S	0	0
			526	340	88	97	1		
9	bM	63	Total	C	N	O	S	0	0
			526	340	88	97	1		
9	bN	62	Total	C	N	O	S	0	0
			519	336	87	95	1		
9	bO	62	Total	C	N	O	S	0	0
			519	336	87	95	1		

- Molecule 10 is a protein called P5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	bP	142	Total	C	N	O	S	0	0
			1126	724	192	208	2		

- Molecule 11 is a protein called P6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	bQ	162	Total	C	N	O	S	0	0
			1275	830	202	242	1		

- Molecule 12 is a protein called P8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	bR	159	Total	C	N	O	S	0	0
			1244	798	207	235	4		

- Molecule 13 is a protein called P9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	bS	191	Total	C	N	O	S	0	0
			1504	953	258	285	8		

- Molecule 14 is a protein called P11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	bT	48	Total	C	N	O	S	0	0
			373	237	65	69	2		
14	bU	54	Total	C	N	O	S	0	0
			424	273	70	79	2		
14	bV	53	Total	C	N	O	S	0	0
			416	269	68	77	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	bW	52	Total	C	N	O	S	0	0
			405	260	67	76	2		
14	bX	41	Total	C	N	O	S	0	0
			312	195	53	62	2		
14	bY	74	Total	C	N	O	S	0	0
			576	370	96	108	2		
14	bZ	52	Total	C	N	O	S	0	0
			405	260	67	76	2		
14	ca	52	Total	C	N	O	S	0	0
			405	260	67	76	2		
14	cb	52	Total	C	N	O	S	0	0
			405	260	67	76	2		
14	cc	84	Total	C	N	O	S	0	0
			646	415	107	122	2		
14	cd	75	Total	C	N	O	S	0	0
			583	375	97	109	2		
14	ce	72	Total	C	N	O	S	0	0
			560	359	93	106	2		

- Molecule 15 is a protein called P12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	cf	78	Total	C	N	O	S	0	0
			631	408	103	116	4		

- Molecule 16 is a protein called P13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	cg	66	Total	C	N	O	S	0	0
			521	333	89	96	3		

- Molecule 17 is a protein called P15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	ch	152	Total	C	N	O	S	0	0
			1288	838	212	233	5		

- Molecule 18 is a protein called P16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	ci	80	Total	C	N	O	S	0	0
			553	358	95	94	6		

- Molecule 19 is a protein called P17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	cj	59	Total	C	N	O	S	0	0
			463	295	76	90	2		
19	ck	57	Total	C	N	O	S	0	0
			455	293	76	84	2		
19	cl	55	Total	C	N	O	S	0	0
			431	275	71	82	3		
19	cm	63	Total	C	N	O	S	0	0
			503	320	86	95	2		

- Molecule 20 is a protein called P18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	cn	98	Total	C	N	O	S	0	0
			769	488	134	146	1		
20	co	95	Total	C	N	O	S	0	0
			733	470	123	139	1		

- Molecule 21 is a protein called P19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	cp	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cq	282	Total	C	N	O	S	0	0
			2212	1420	371	413	8		
21	cr	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cs	275	Total	C	N	O	S	0	0
			2159	1387	363	402	7		
21	ct	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cu	280	Total	C	N	O	S	0	0
			2199	1413	369	410	7		
21	cv	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cw	280	Total	C	N	O	S	0	0
			2199	1413	369	410	7		
21	cx	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cy	280	Total	C	N	O	S	0	0
			2199	1413	369	410	7		
21	cz	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	cA	279	Total	C	N	O	S	0	0
			2191	1409	367	408	7		
21	cB	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cC	279	Total	C	N	O	S	0	0
			2191	1409	367	408	7		
21	cD	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cE	280	Total	C	N	O	S	0	0
			2199	1413	369	410	7		
21	cF	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cG	282	Total	C	N	O	S	0	0
			2212	1420	371	413	8		
21	cH	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cI	279	Total	C	N	O	S	0	0
			2191	1409	367	408	7		
21	cJ	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cK	279	Total	C	N	O	S	0	0
			2191	1409	367	408	7		
21	cL	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		
21	cM	277	Total	C	N	O	S	0	0
			2173	1396	365	405	7		
21	cN	292	Total	C	N	O	S	0	0
			2299	1479	385	426	9		

- Molecule 22 is a protein called P20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	cO	30	Total	C	N	O	S	0	0
			218	142	35	39	2		
22	cQ	31	Total	C	N	O	S	0	0
			233	149	38	44	2		
22	da	32	Total	C	N	O	S	0	0
			228	144	37	45	2		
22	dc	28	Total	C	N	O	S	0	0
			209	134	34	39	2		
22	dg	32	Total	C	N	O	S	0	0
			241	153	40	46	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
22	di	29	Total	C	N	O	S	0	0
			211	137	32	40	2		
22	ds	32	Total	C	N	O	S	0	0
			238	152	40	44	2		
22	du	30	Total	C	N	O	S	0	0
			224	144	36	42	2		

- Molecule 23 is a protein called P21.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	cP	35	Total	C	N	O	0	0
			239	152	42	45		
23	db	30	Total	C	N	O	0	0
			200	127	36	37		
23	dh	35	Total	C	N	O	0	0
			249	157	45	47		
23	dt	35	Total	C	N	O	0	0
			236	147	44	45		

- Molecule 24 is a protein called MCPv5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	cR	399	Total	C	N	O	S	0	0
			3203	2060	518	611	14		
24	cS	399	Total	C	N	O	S	0	0
			3203	2060	518	611	14		
24	cT	399	Total	C	N	O	S	0	0
			3203	2060	518	611	14		

- Molecule 25 is a protein called P22.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	cU	43	Total	C	N	O	0	0
			311	203	51	57		
25	cV	43	Total	C	N	O	0	0
			305	201	50	54		
25	cW	43	Total	C	N	O	0	0
			308	202	51	55		

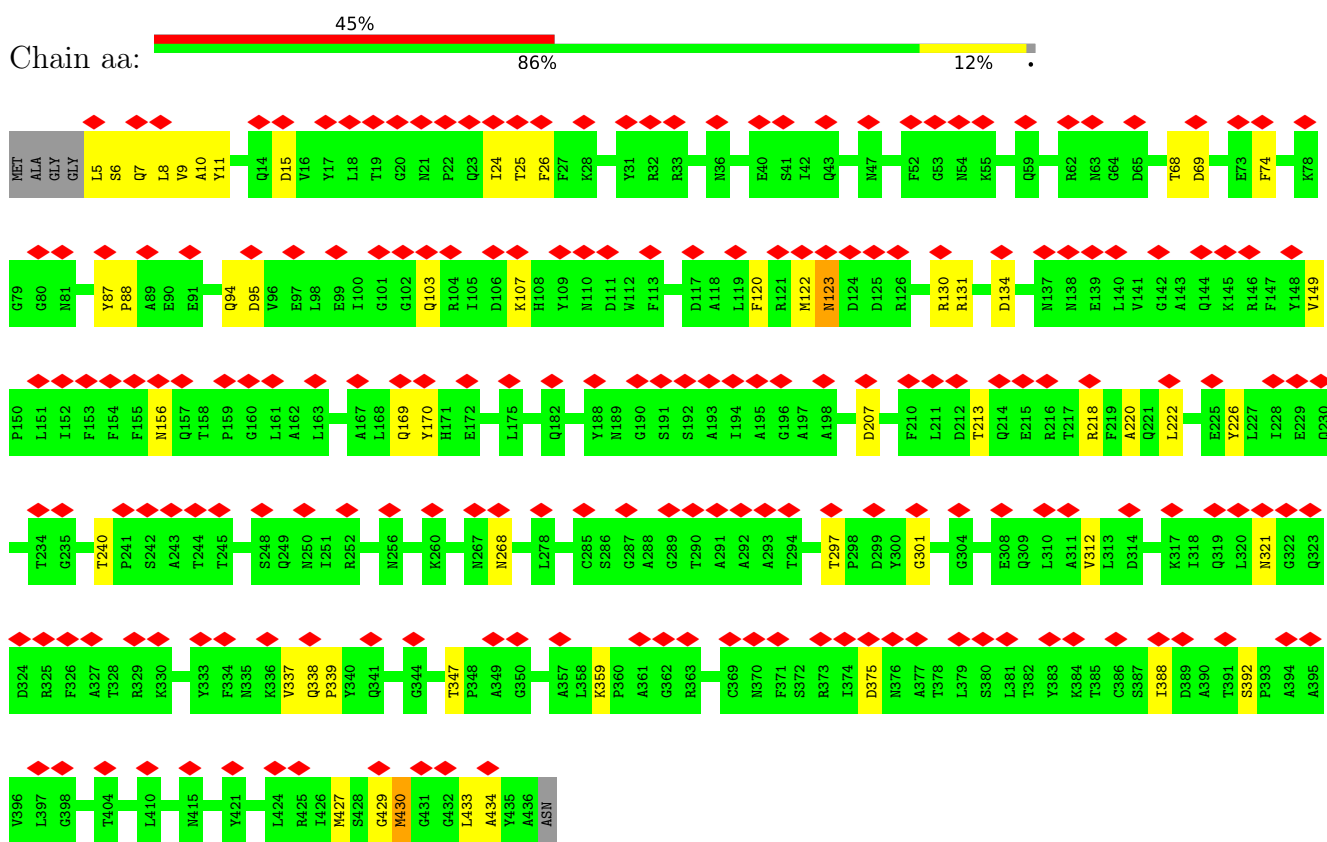
- Molecule 26 is a protein called P23.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	dm	25	Total 174	C 111	N 28	O 35	0	0
26	dn	25	Total 181	C 116	N 29	O 36	0	0
26	do	25	Total 182	C 121	N 28	O 33	0	0

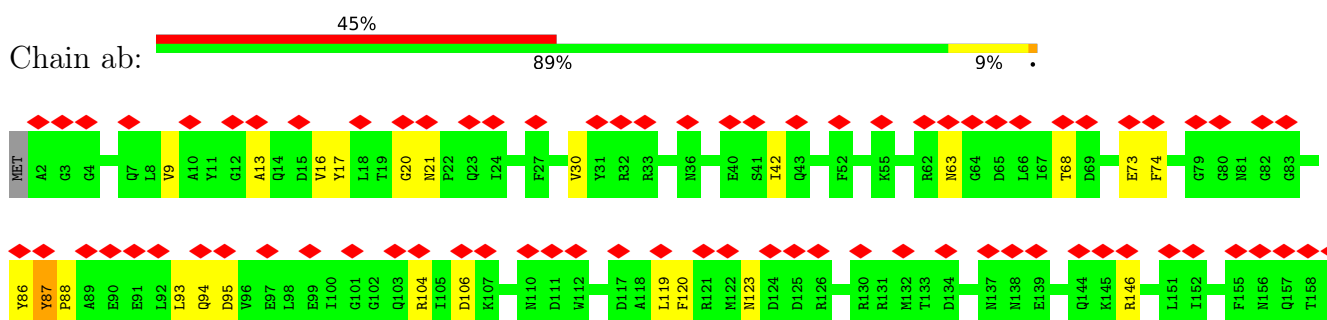
3 Residue-property plots

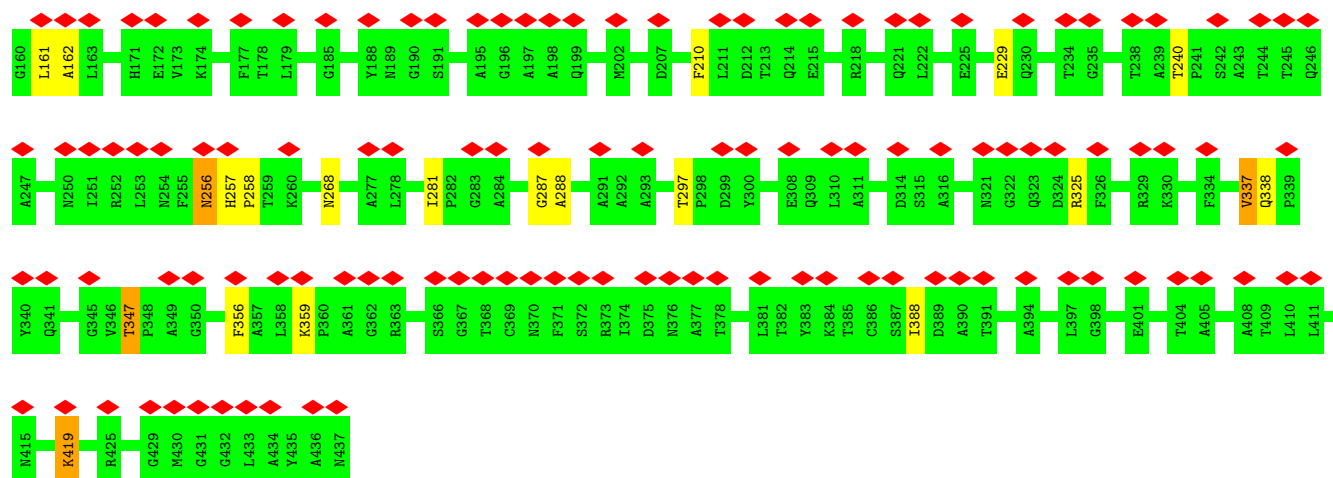
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Major capsid protein (MCP)

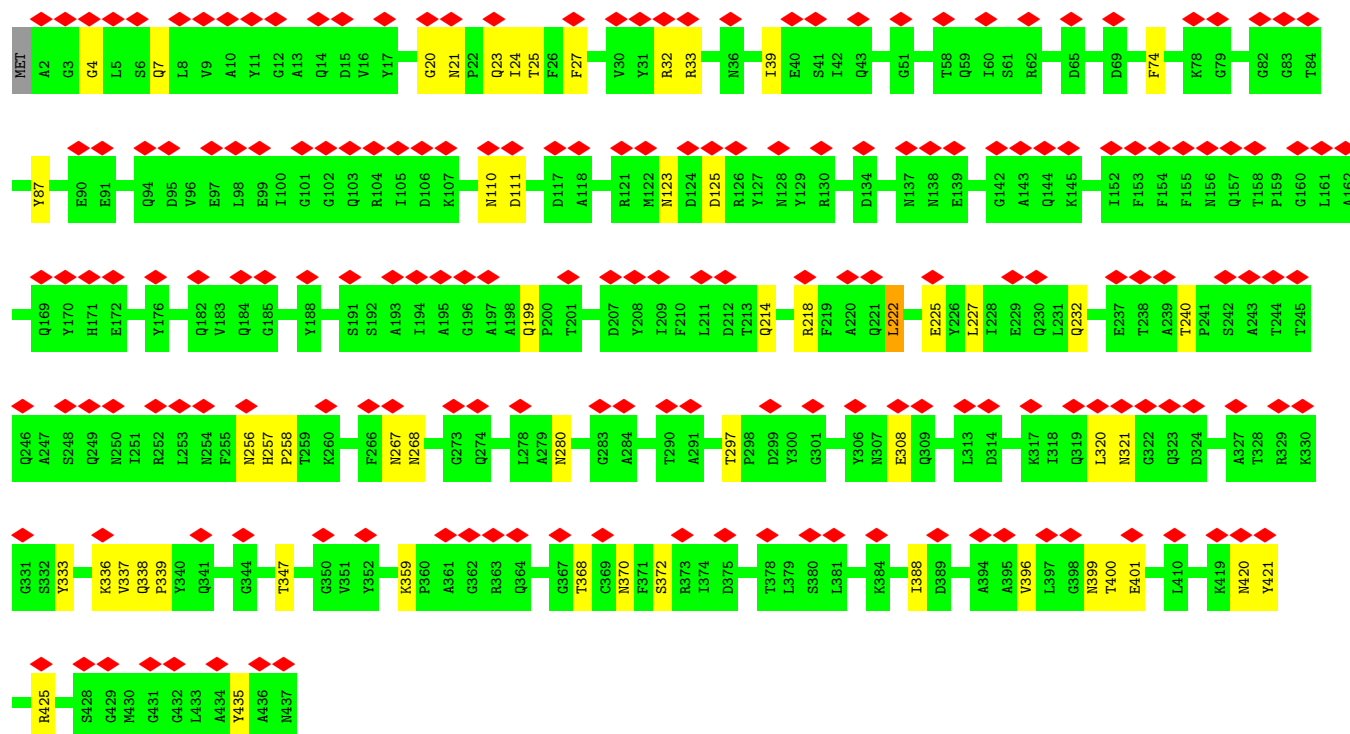
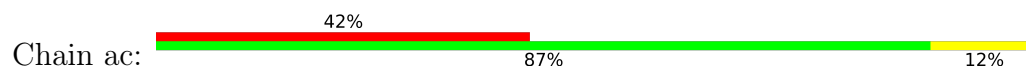


• Molecule 1: Major capsid protein (MCP)

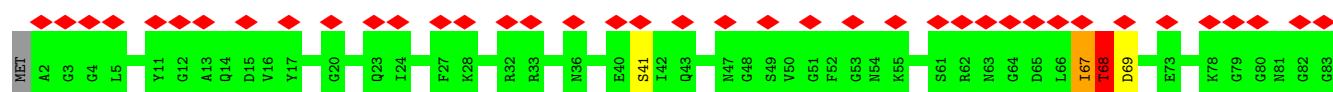
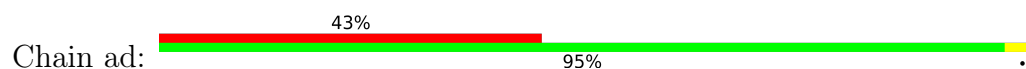


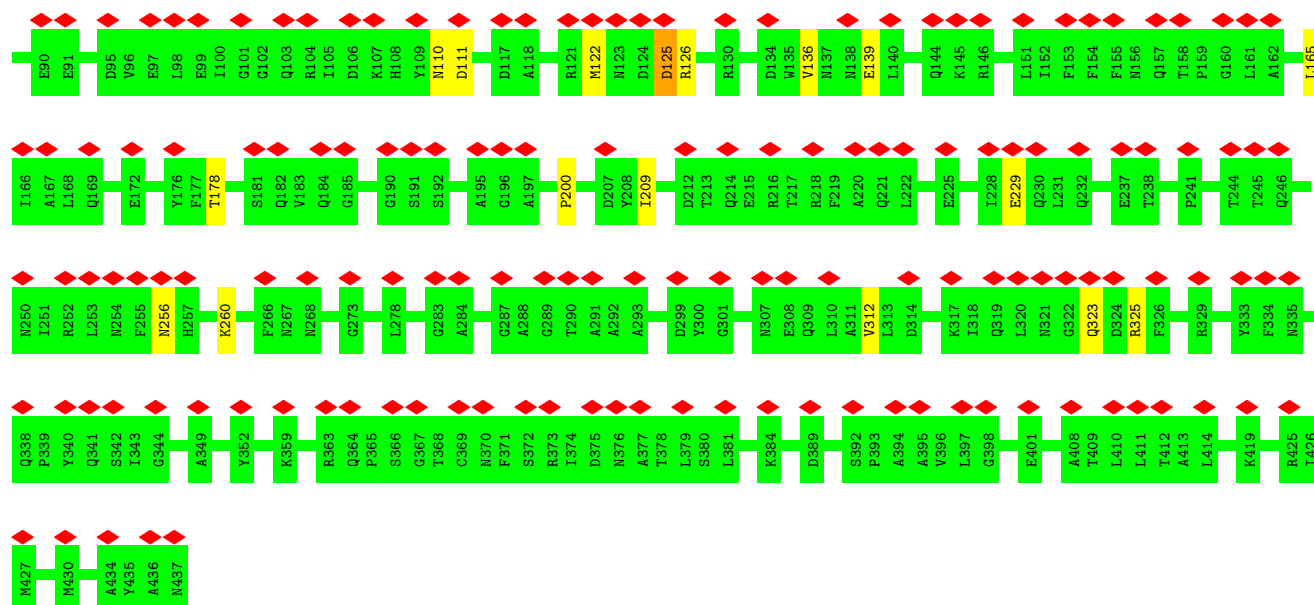


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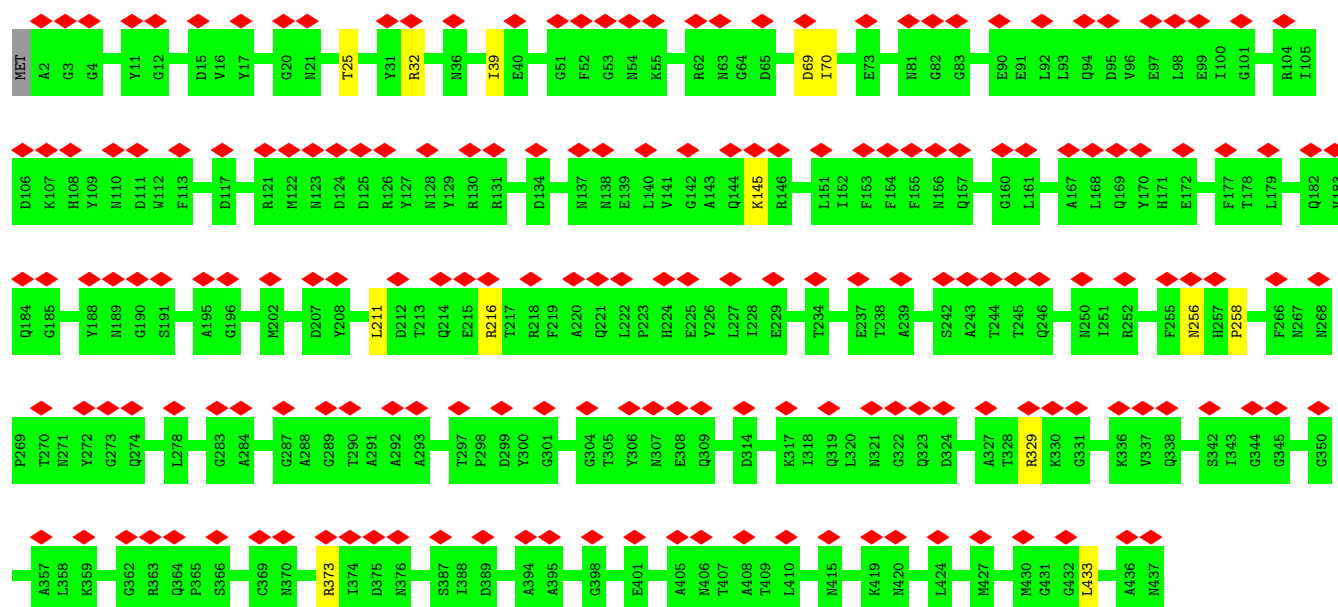
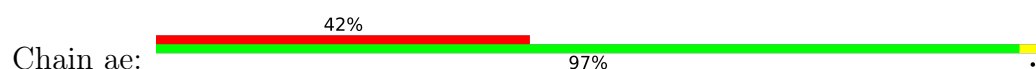


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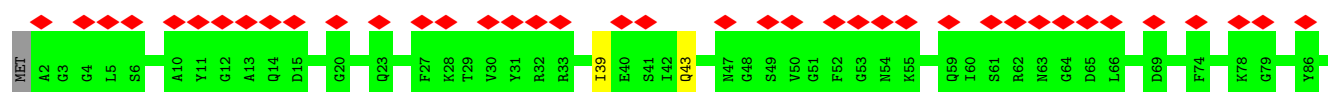


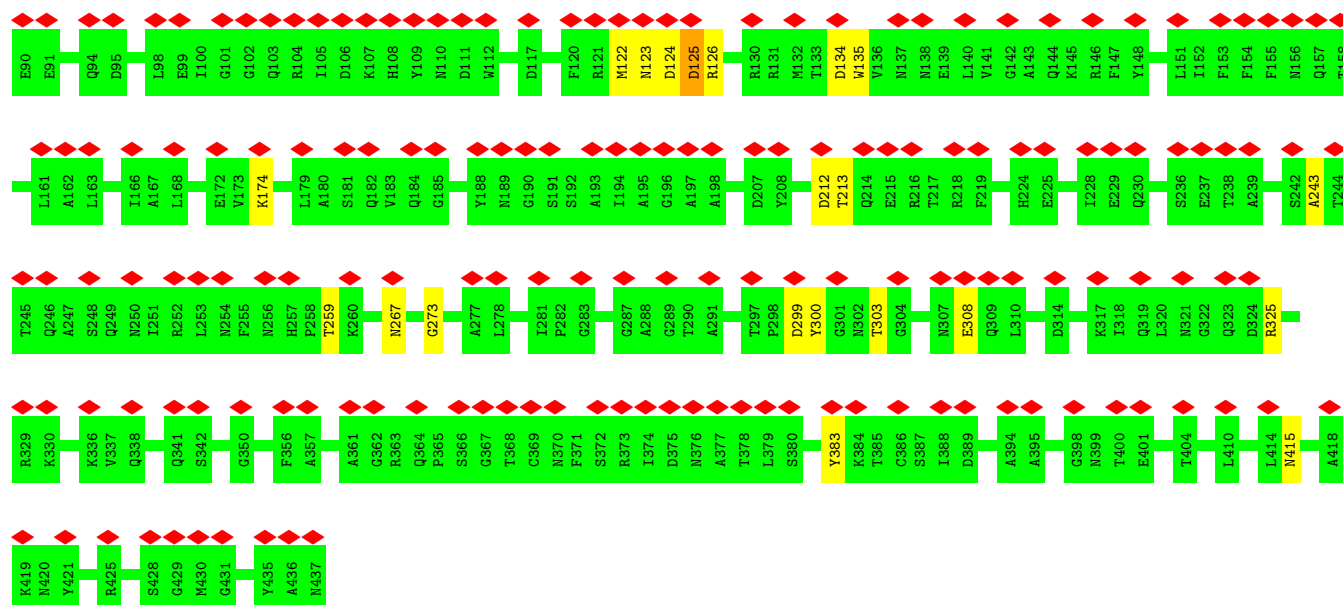


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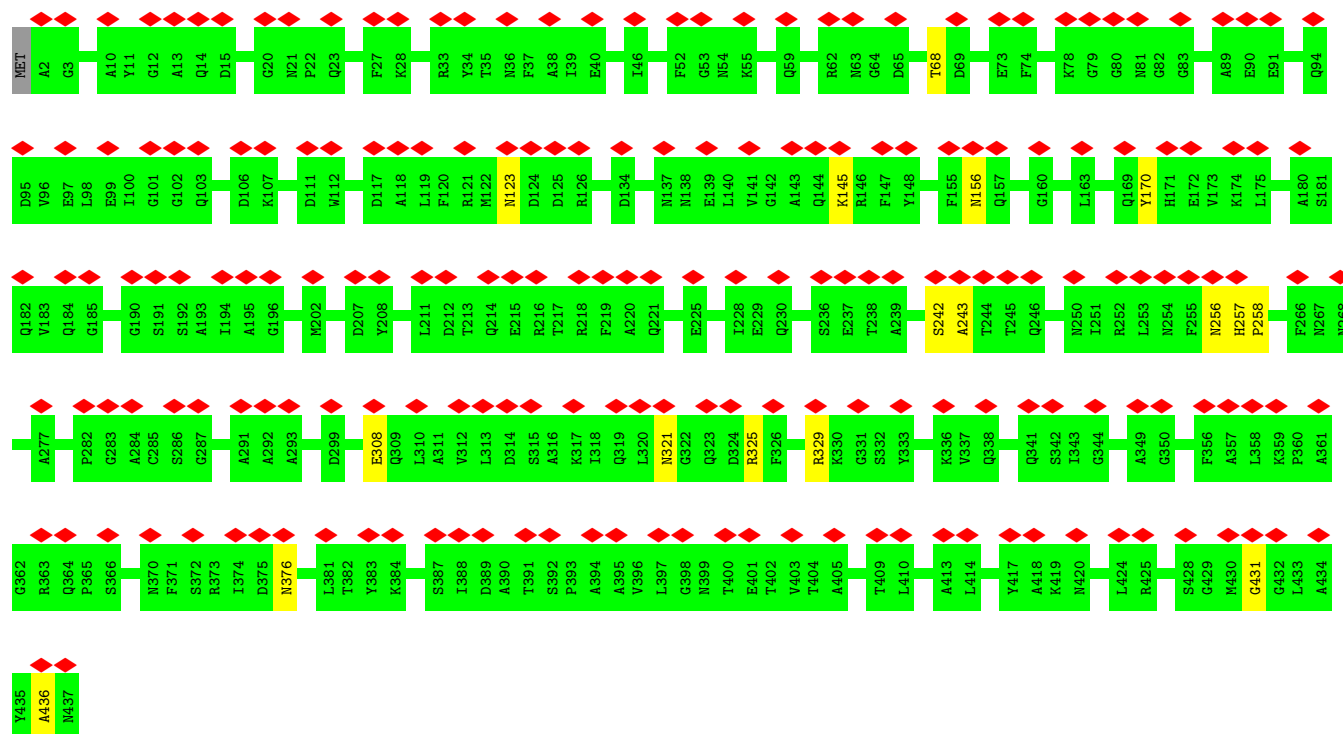


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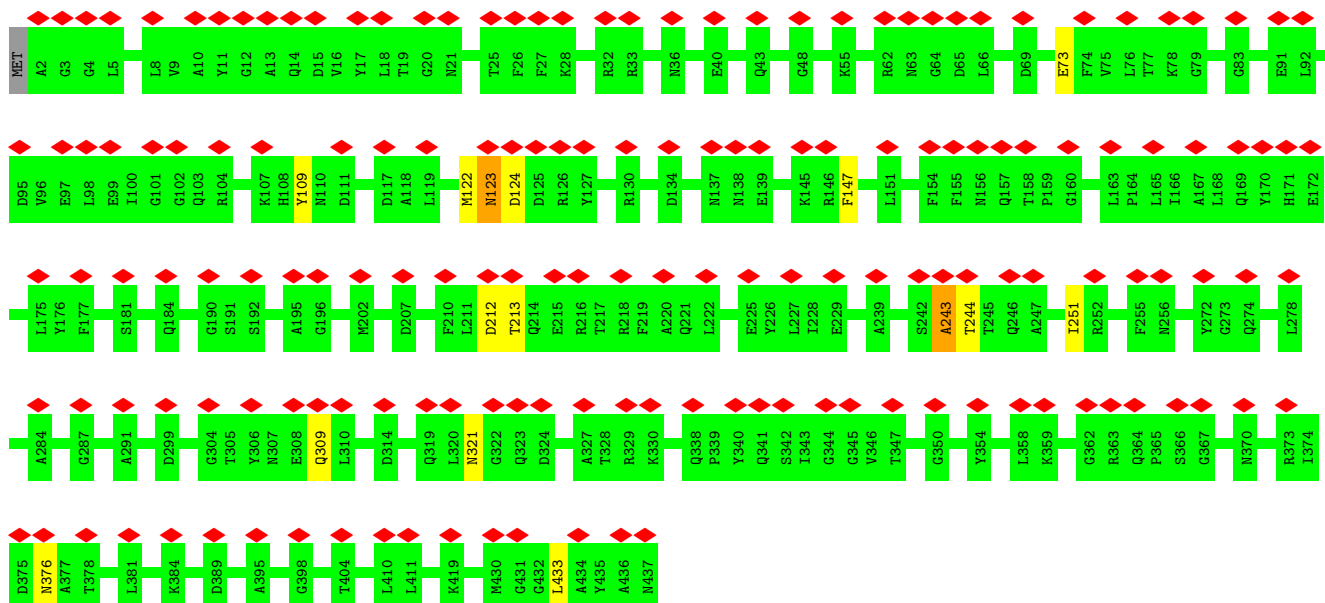


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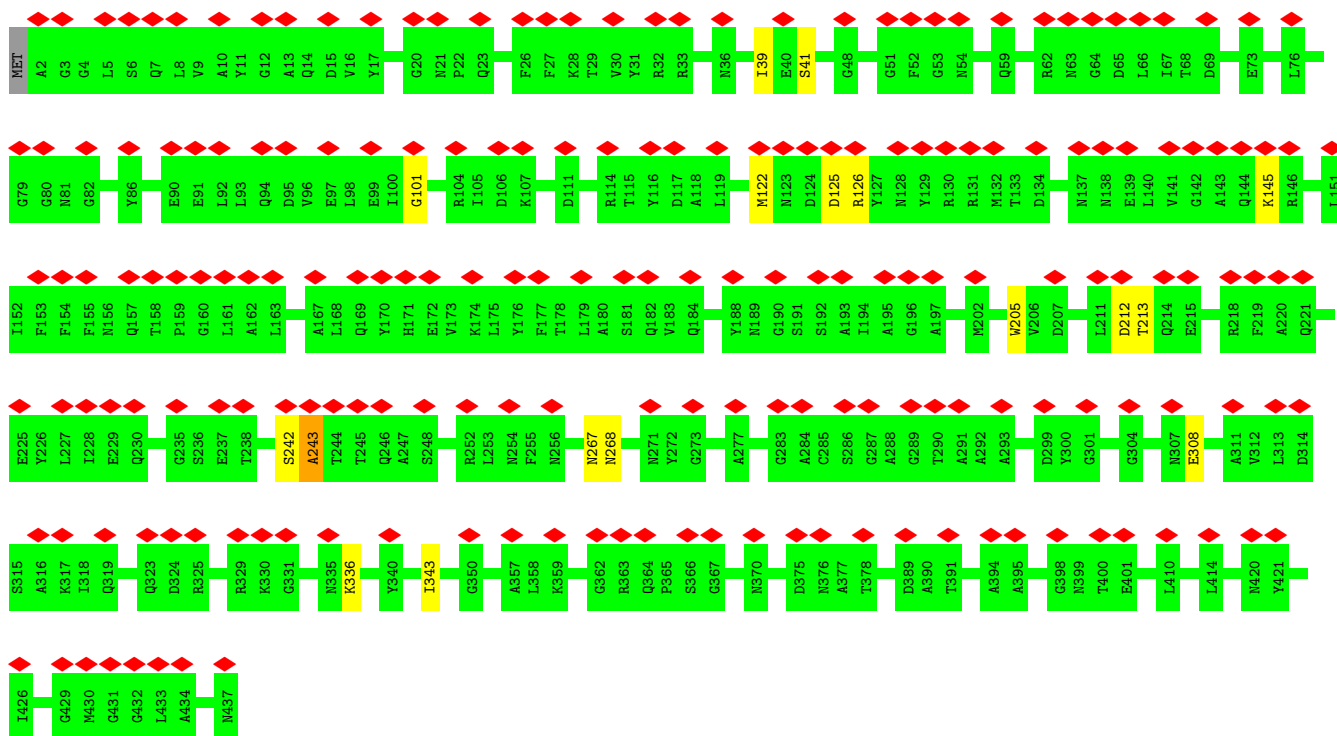


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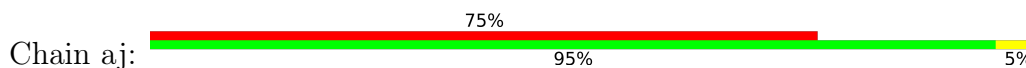


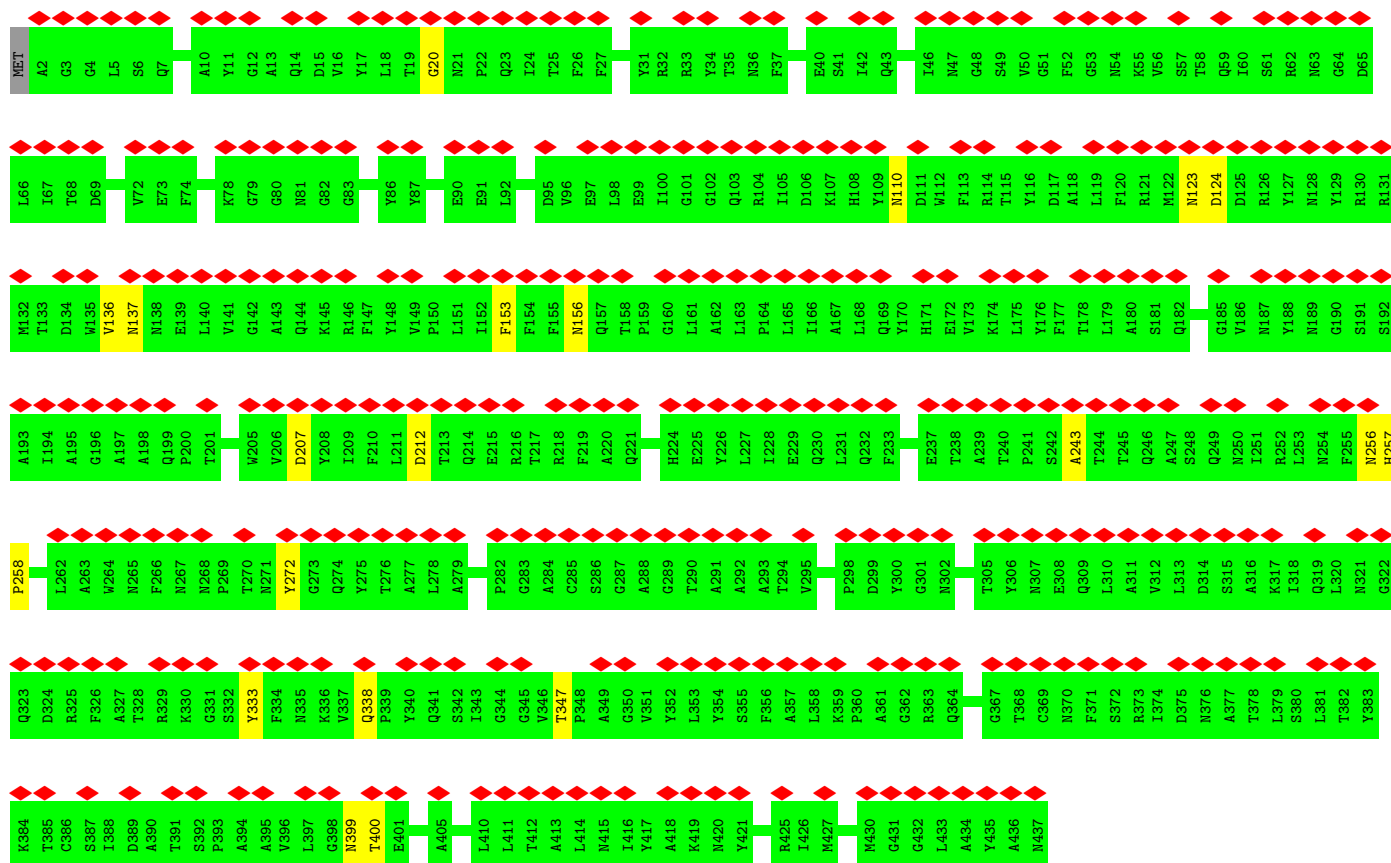


- Molecule 1: Major capsid protein (MCP)

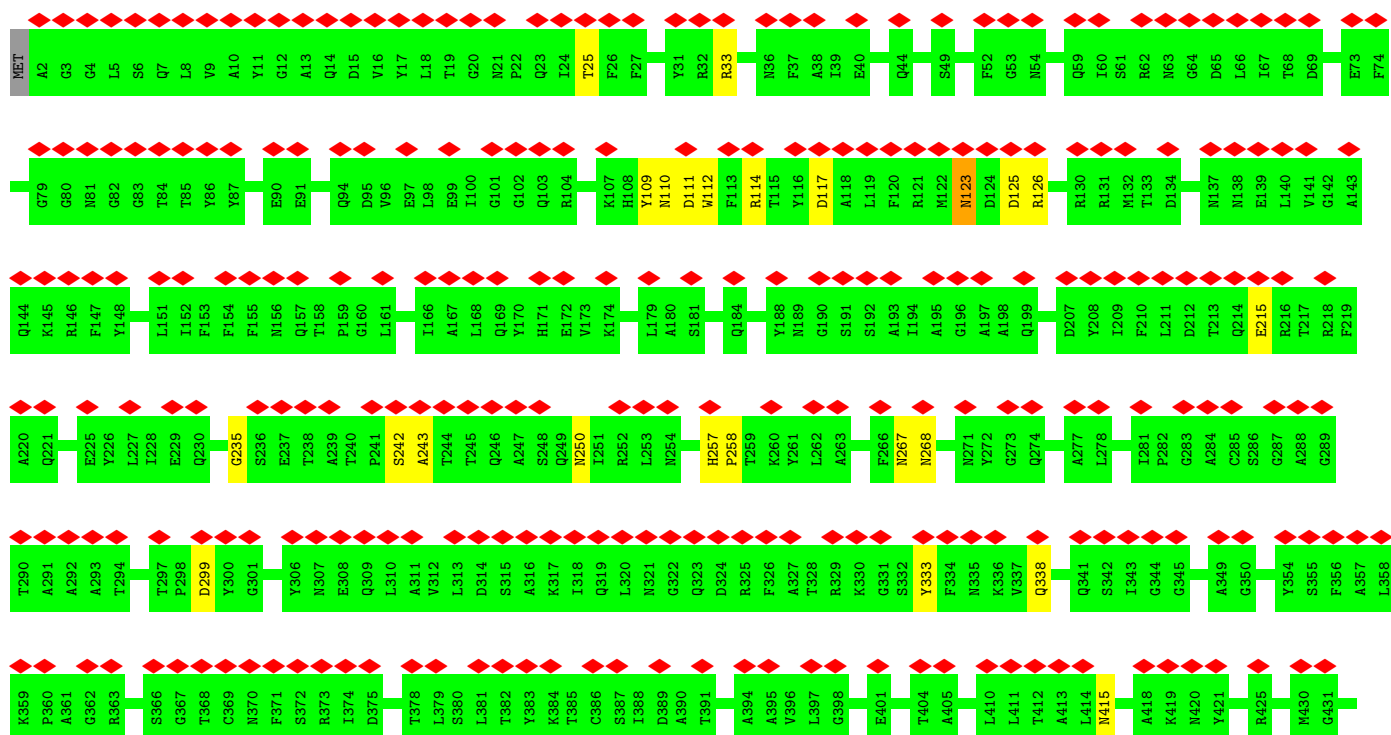


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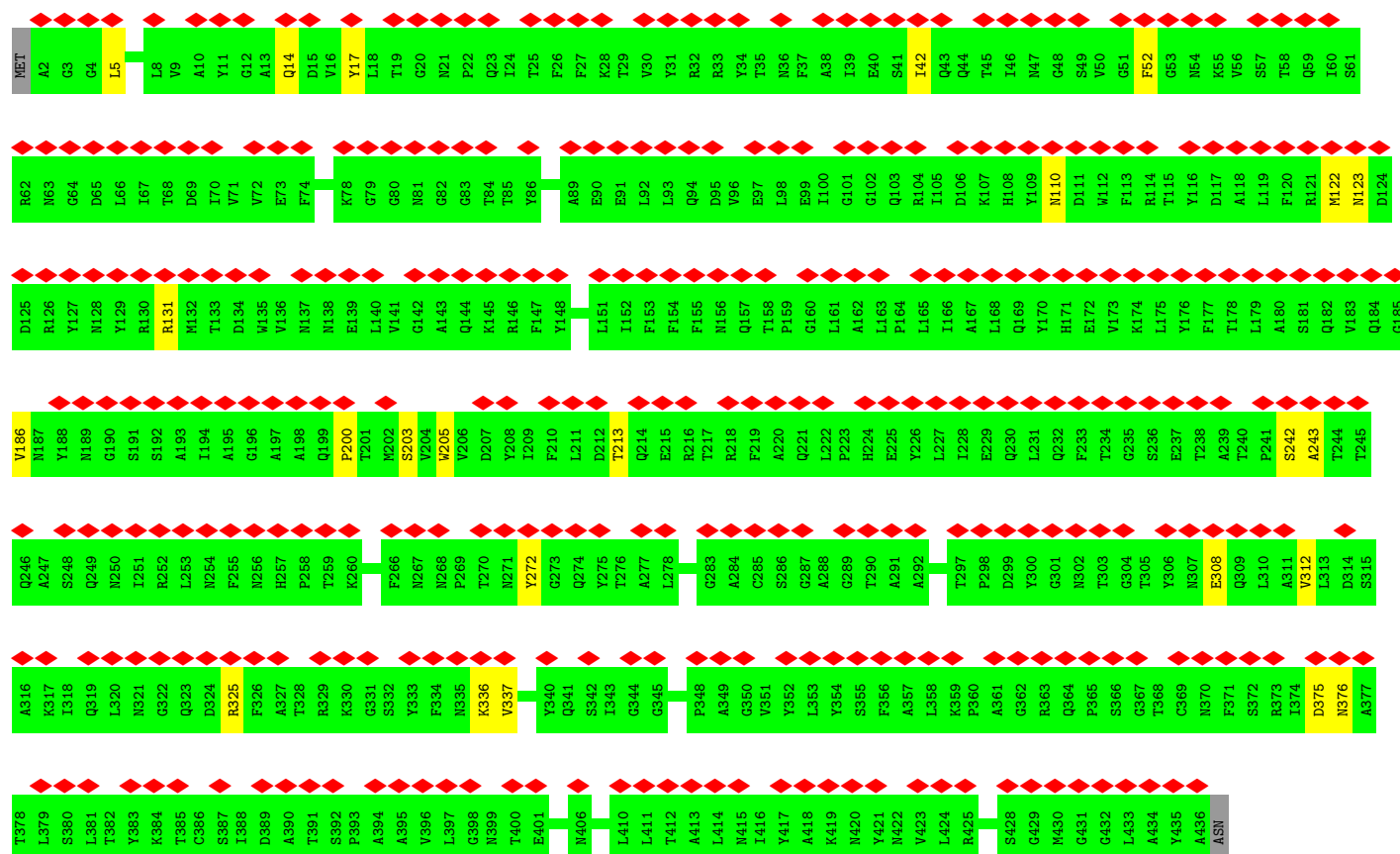
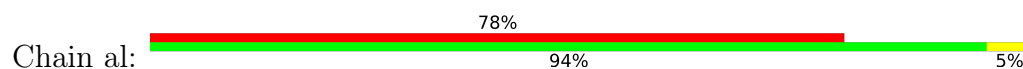


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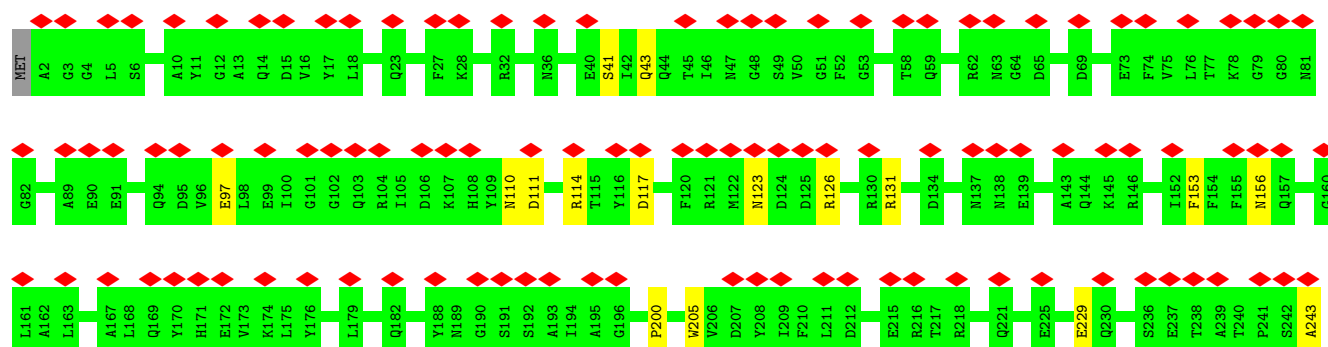
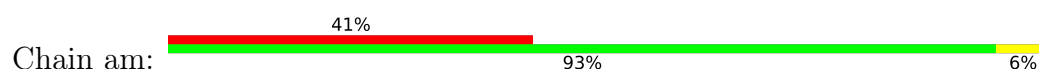


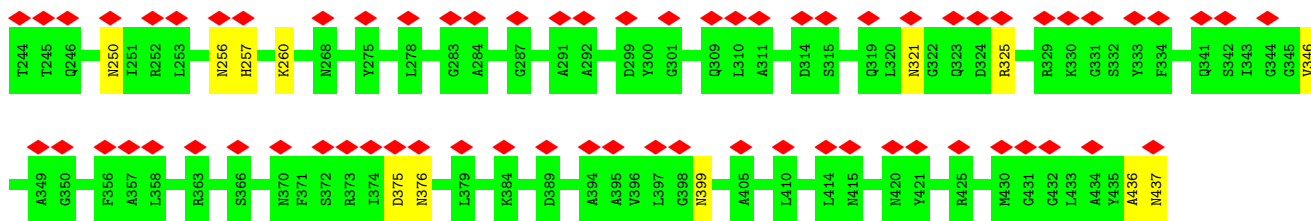


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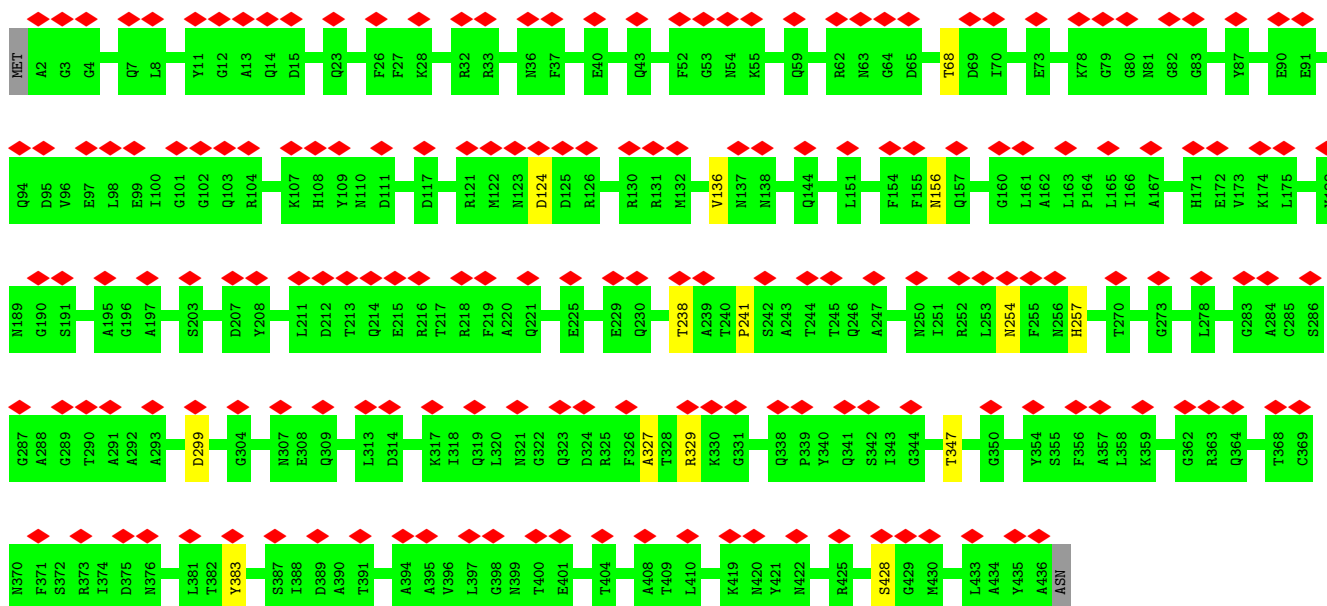
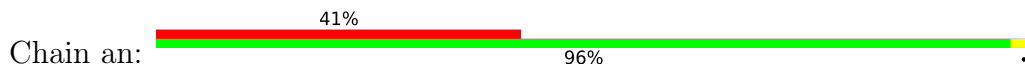


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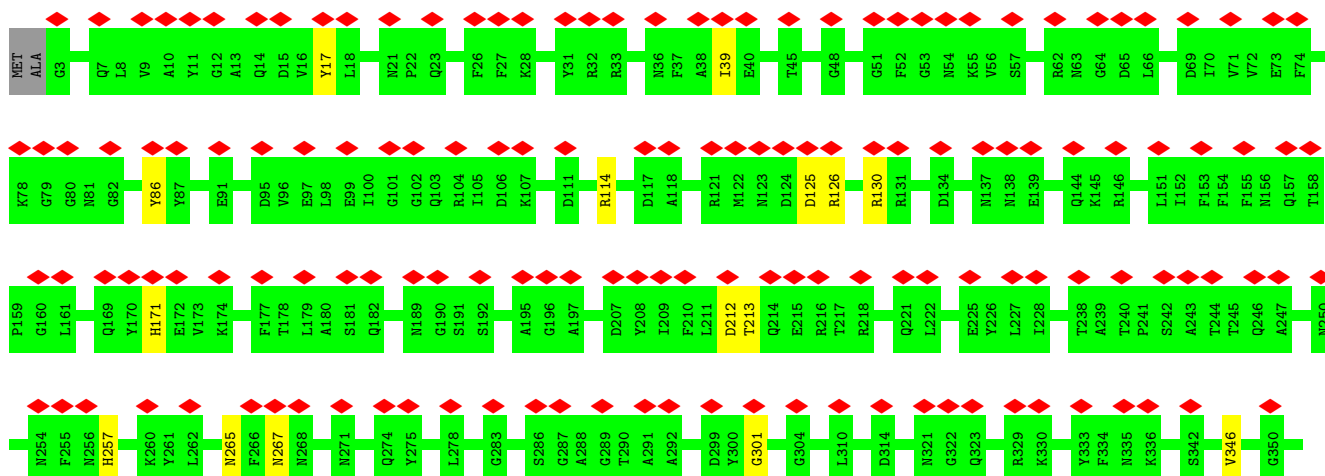
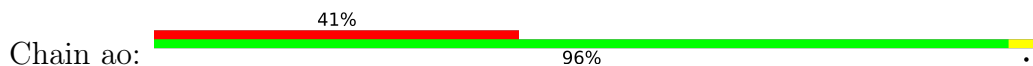


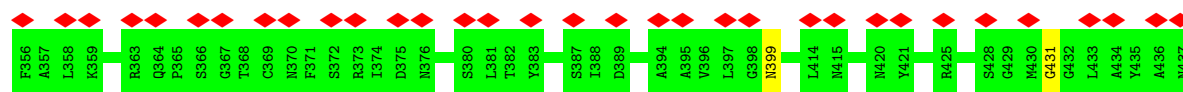


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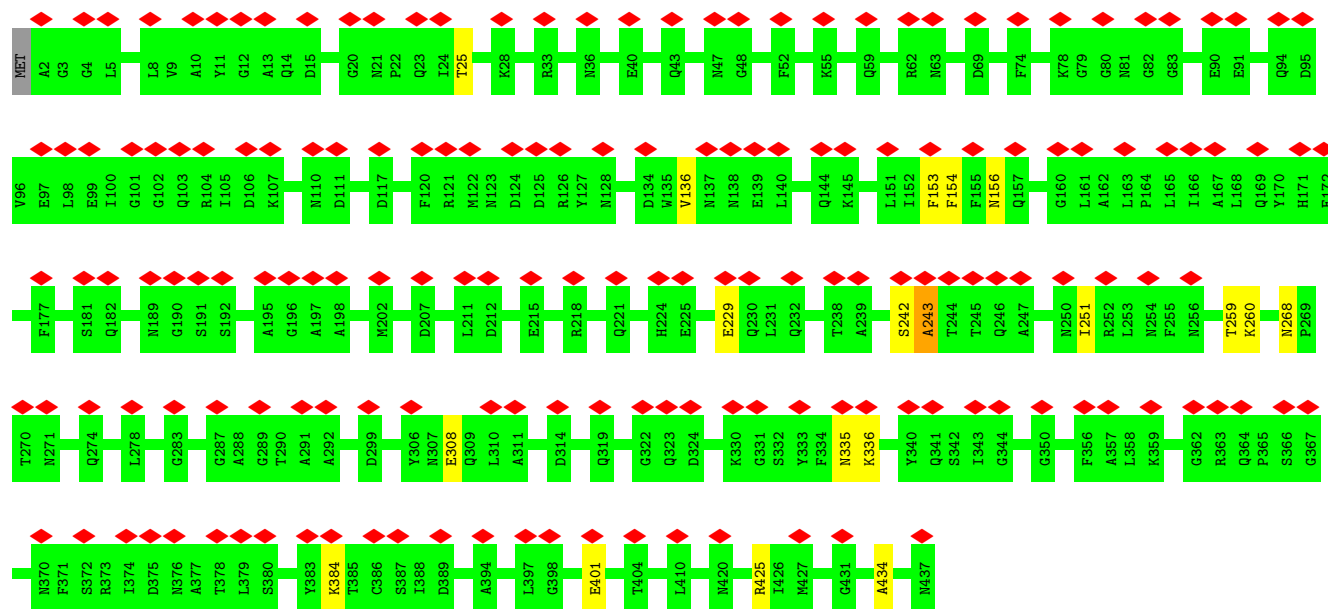
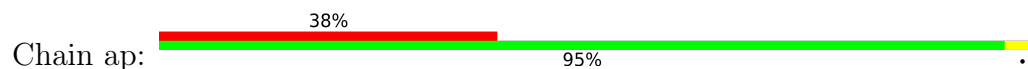


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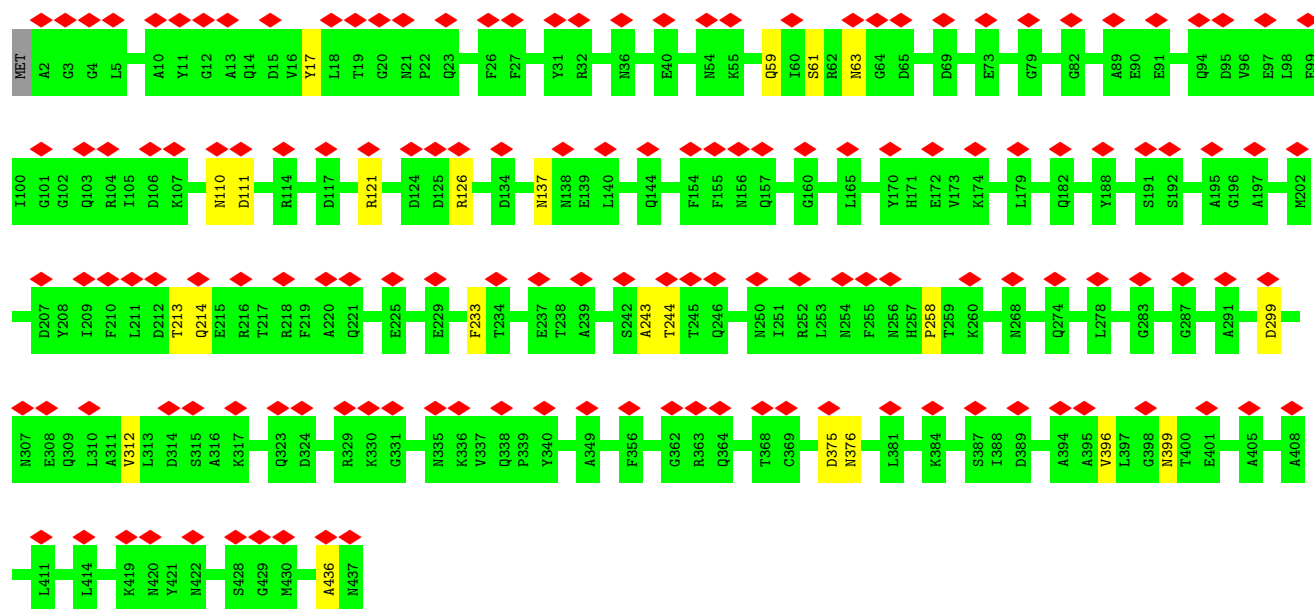




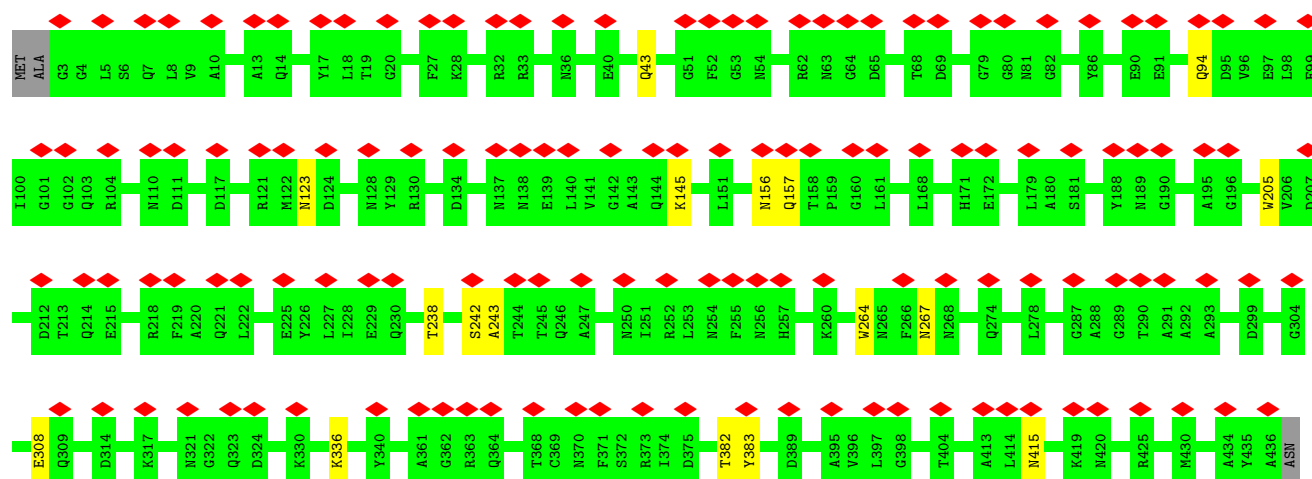
• Molecule 1: Major capsid protein (MCP)



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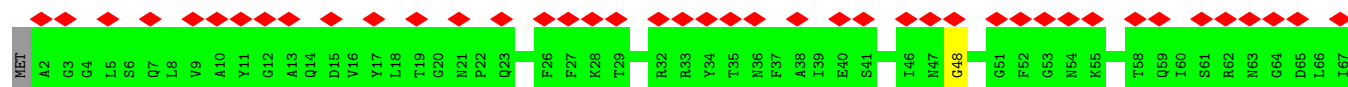
• Molecule 1: Major capsid protein (MCP)

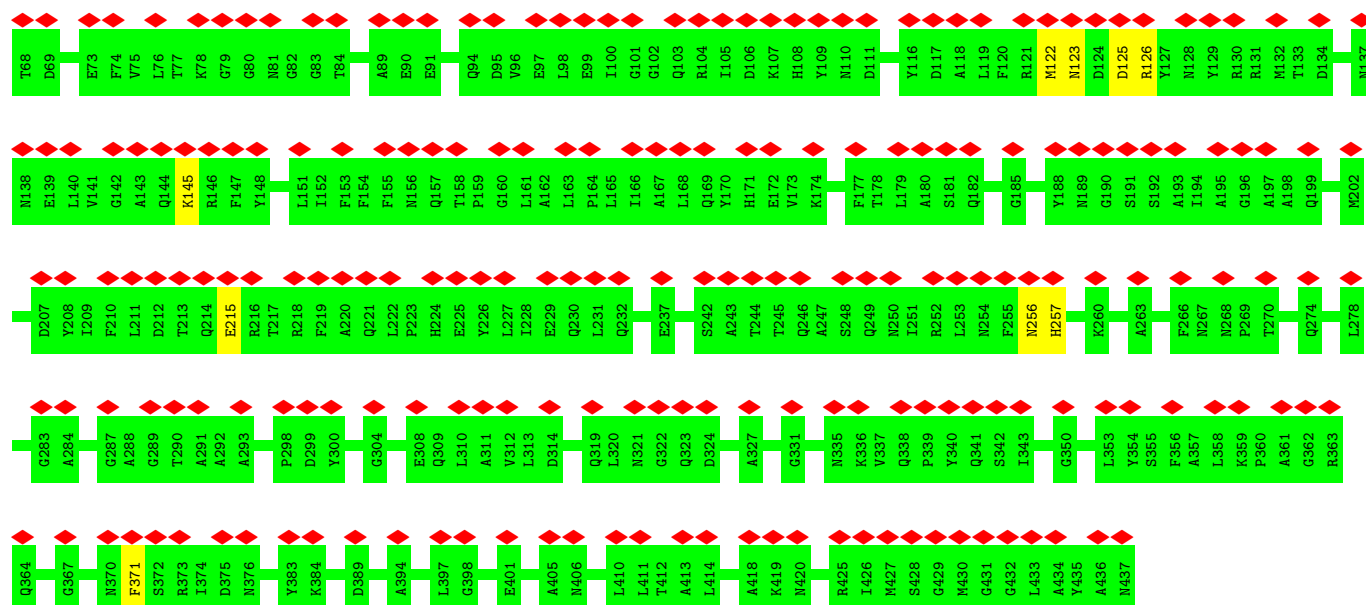


• Molecule 1: Major capsid protein (MCP)

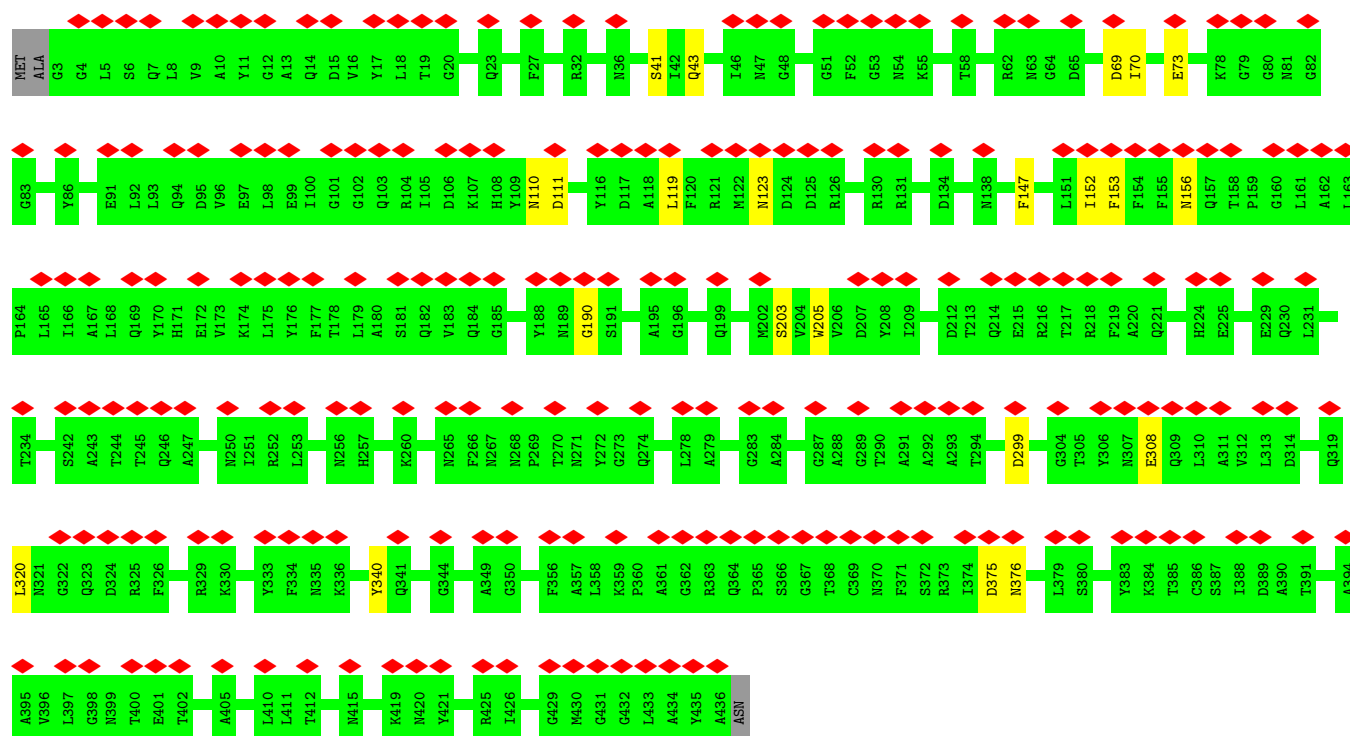


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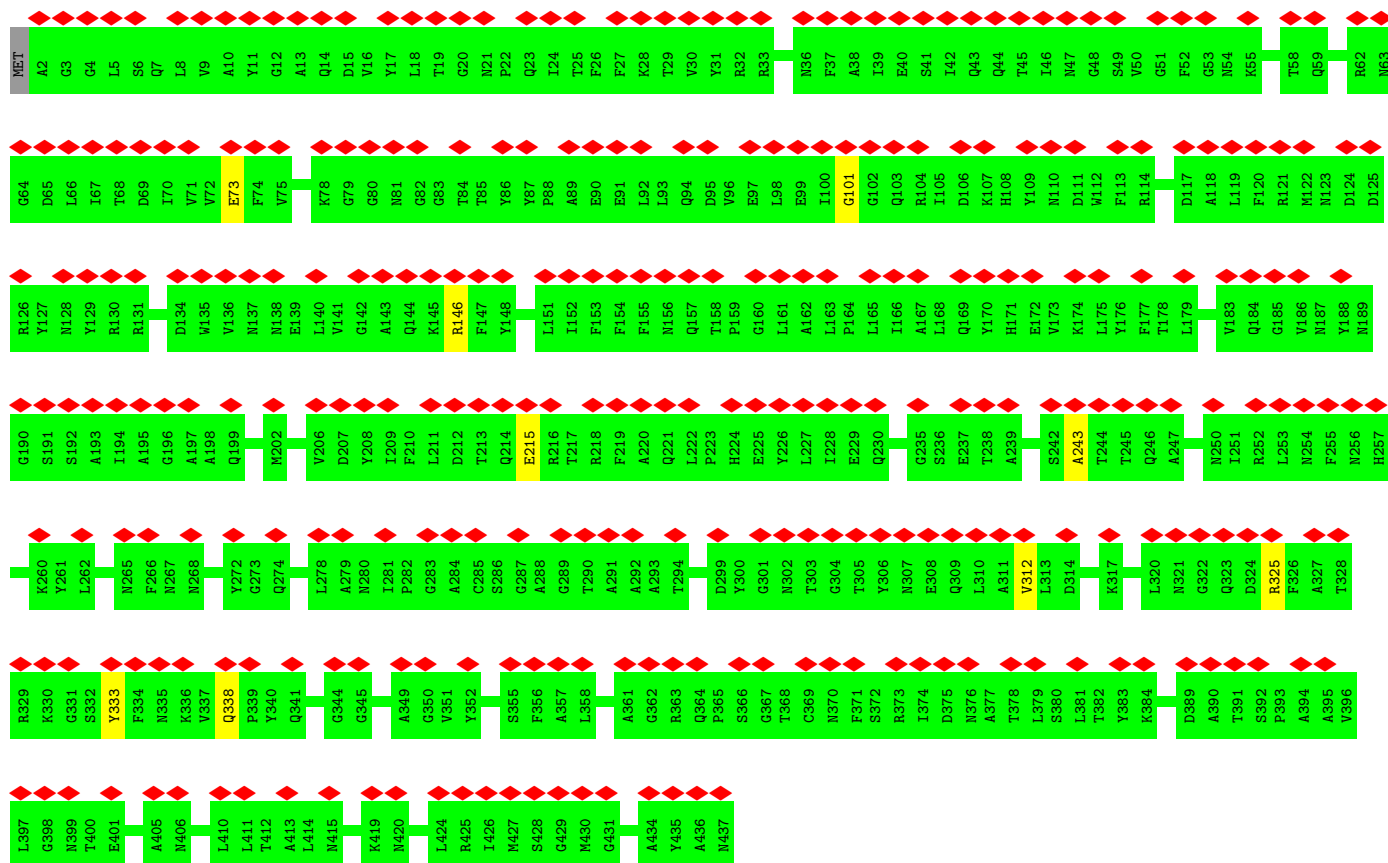


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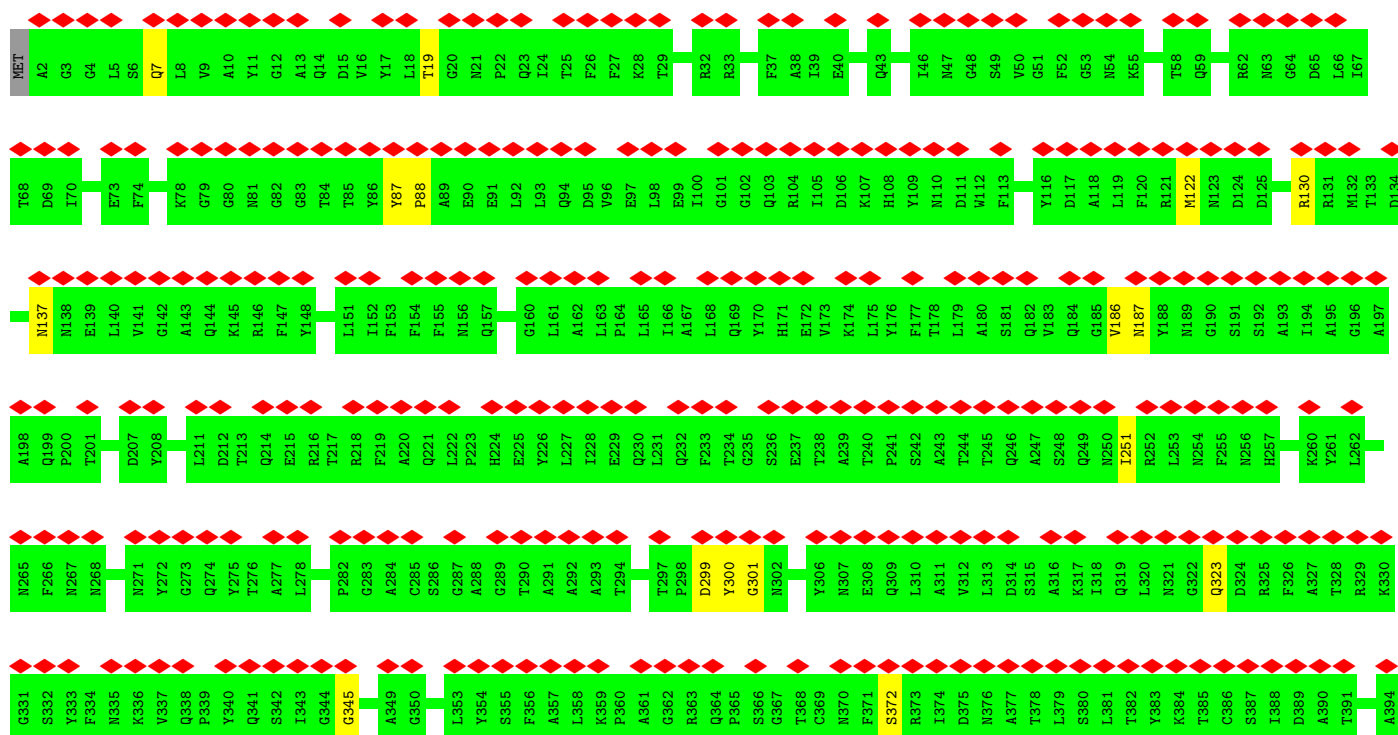
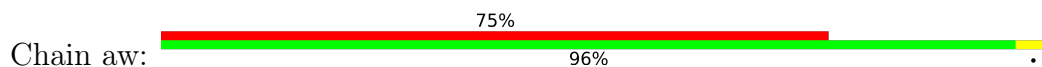


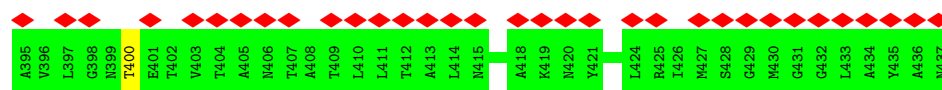
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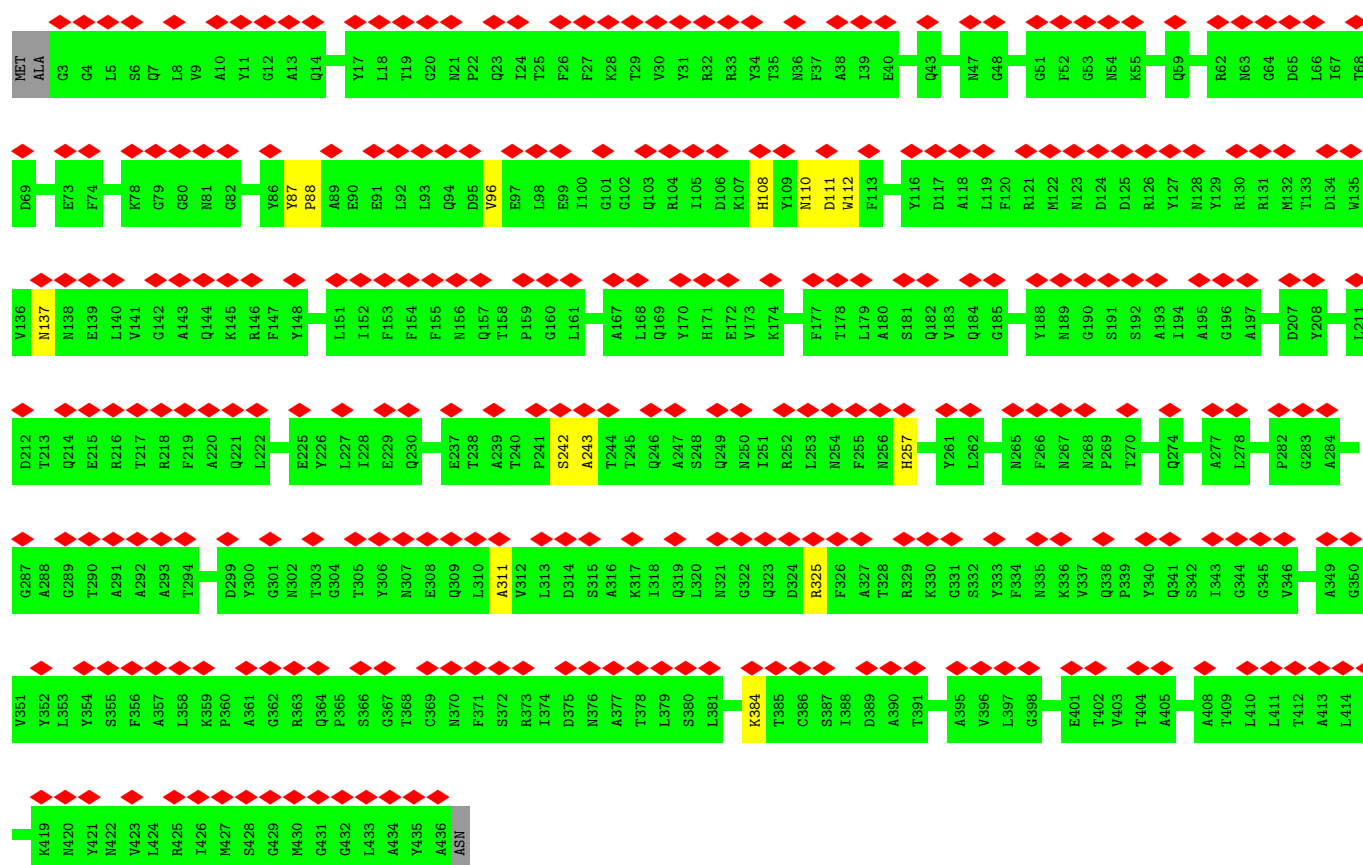


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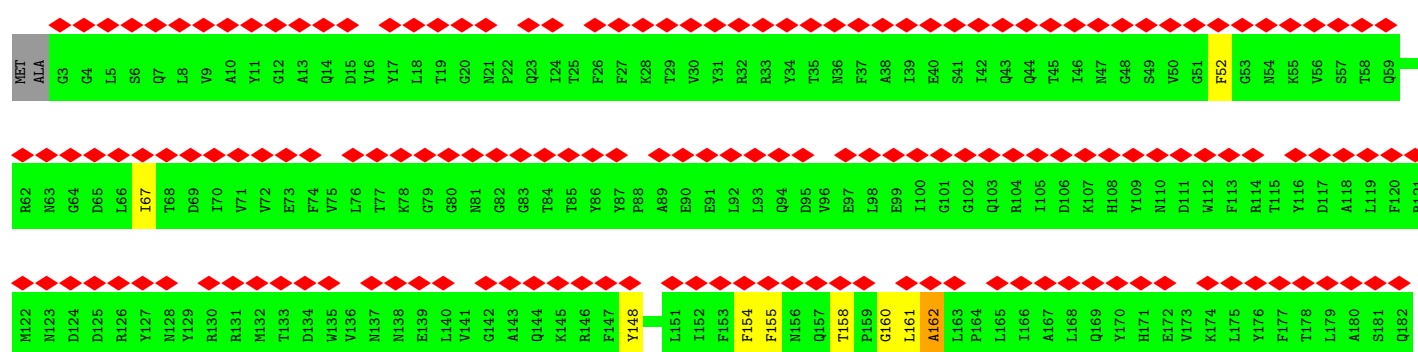


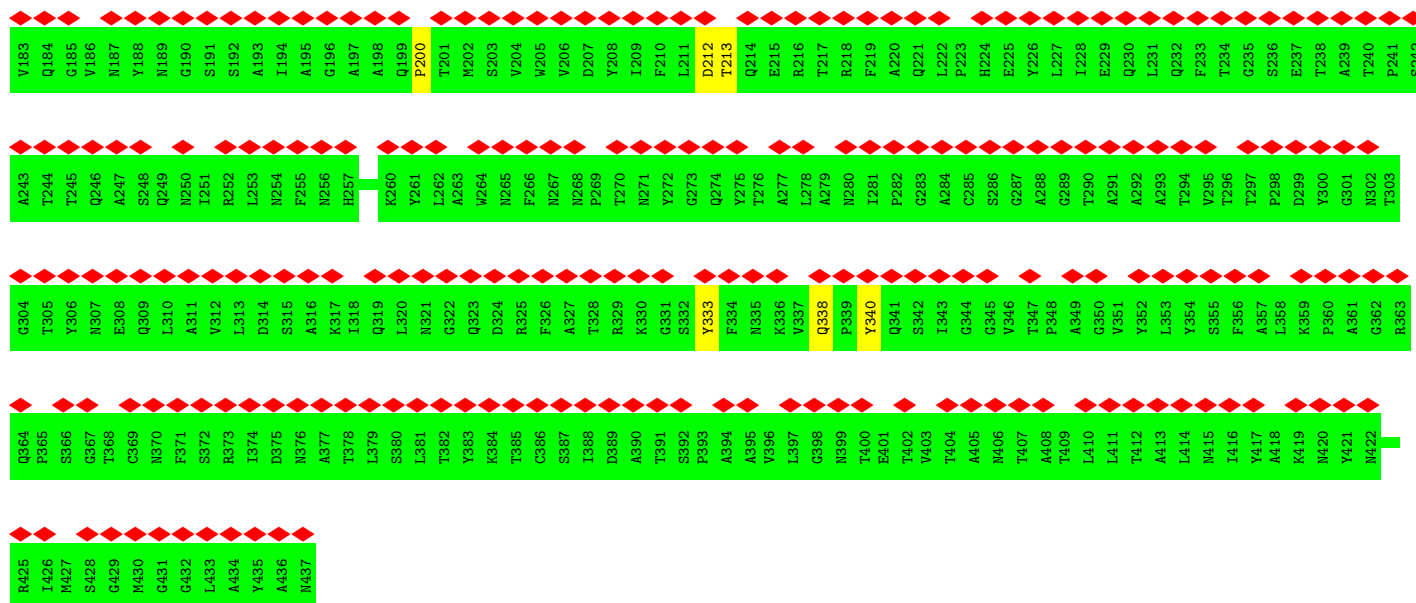


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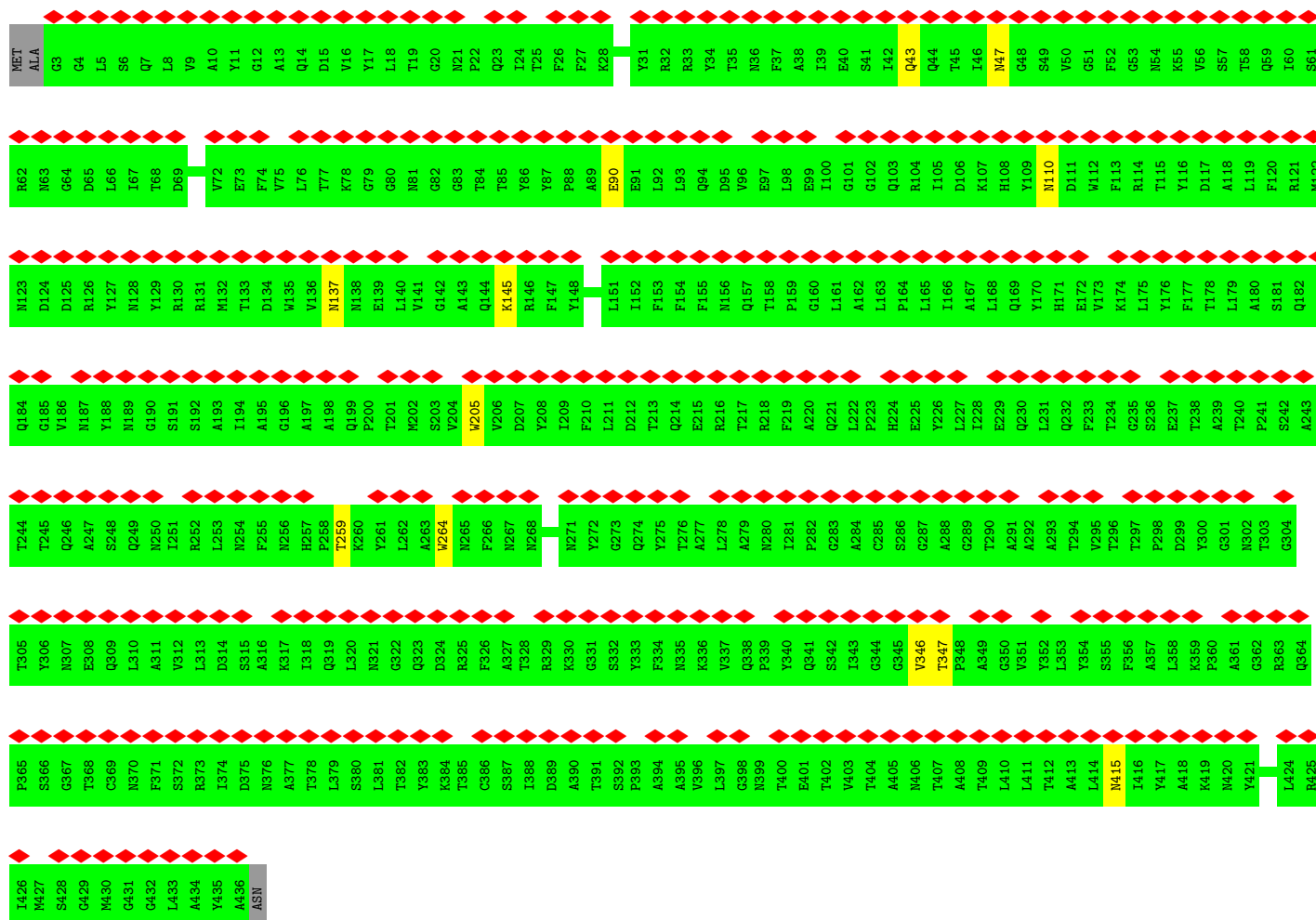


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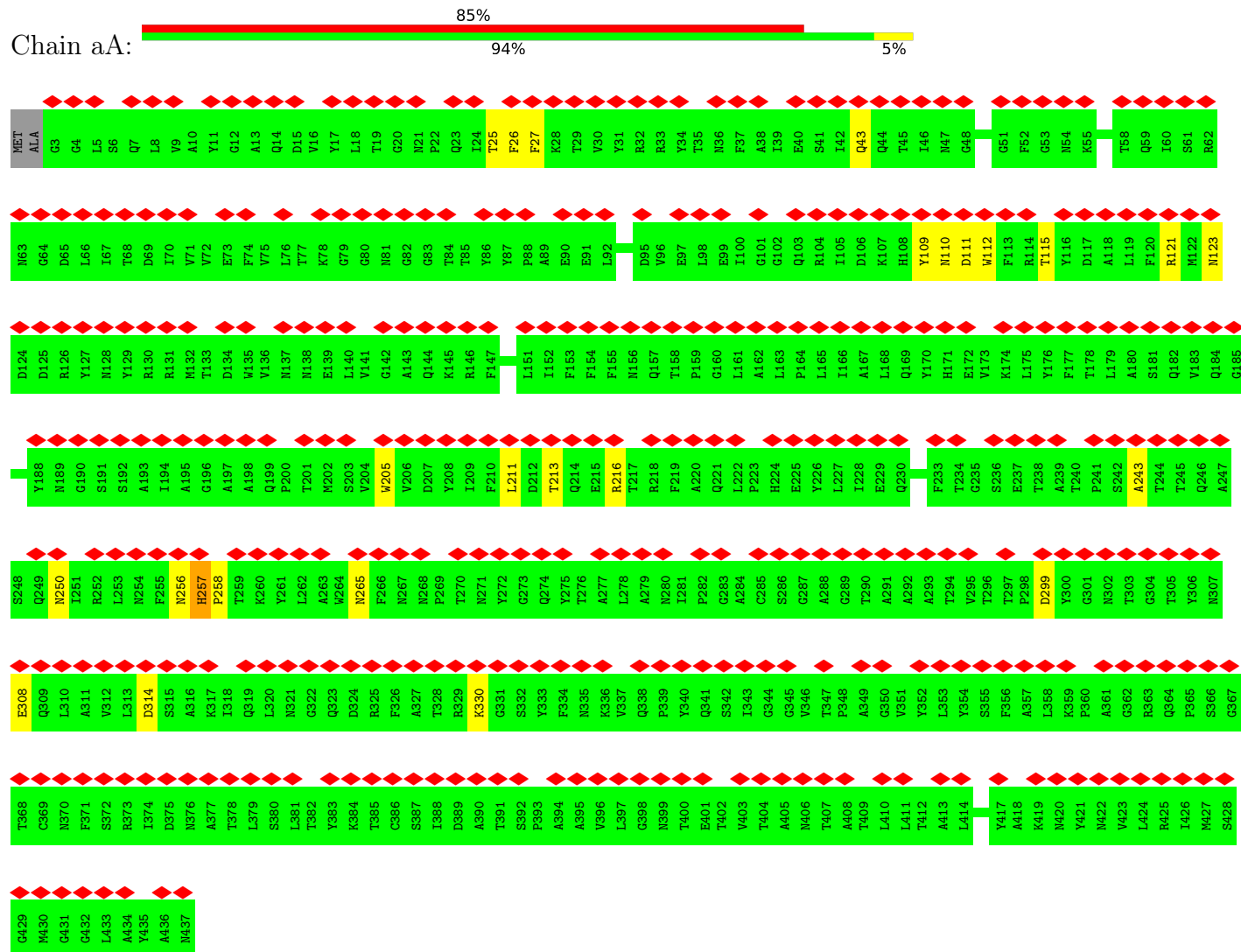




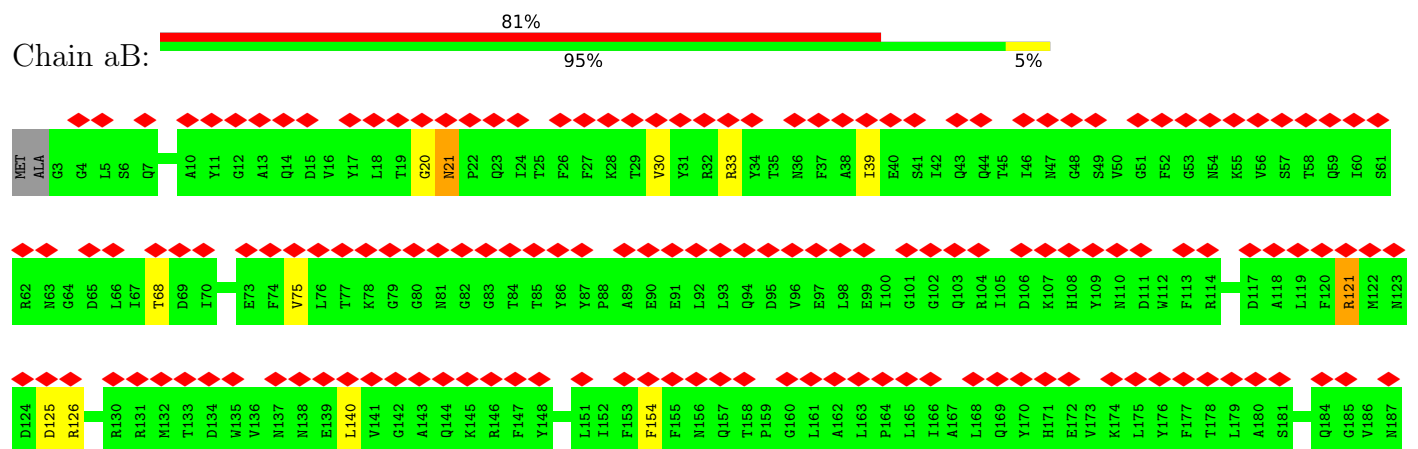
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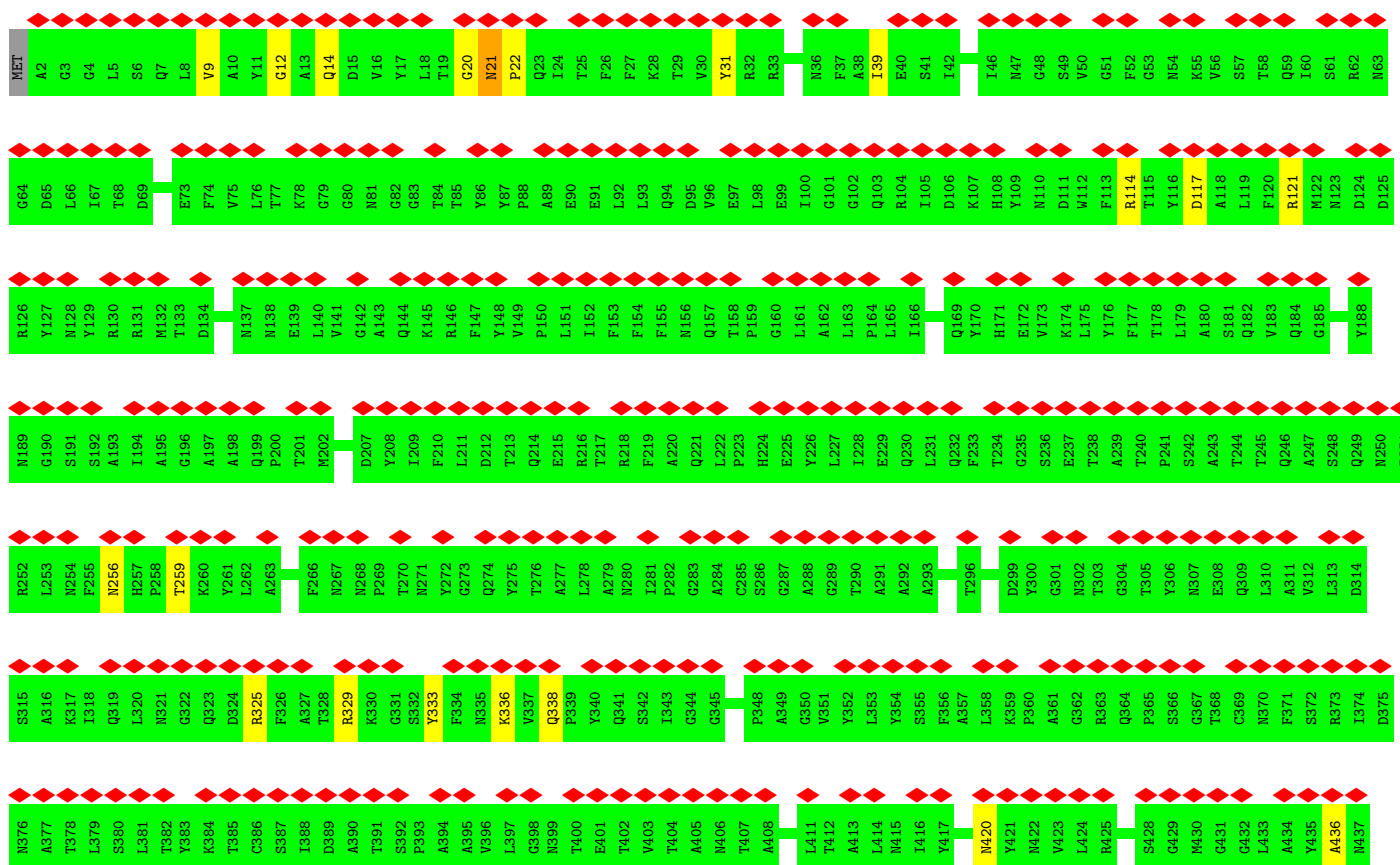
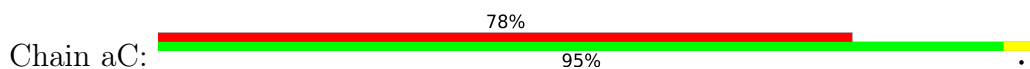


• Molecule 1: Major capsid protein (MCP)

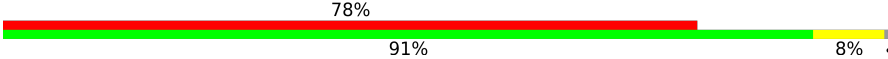


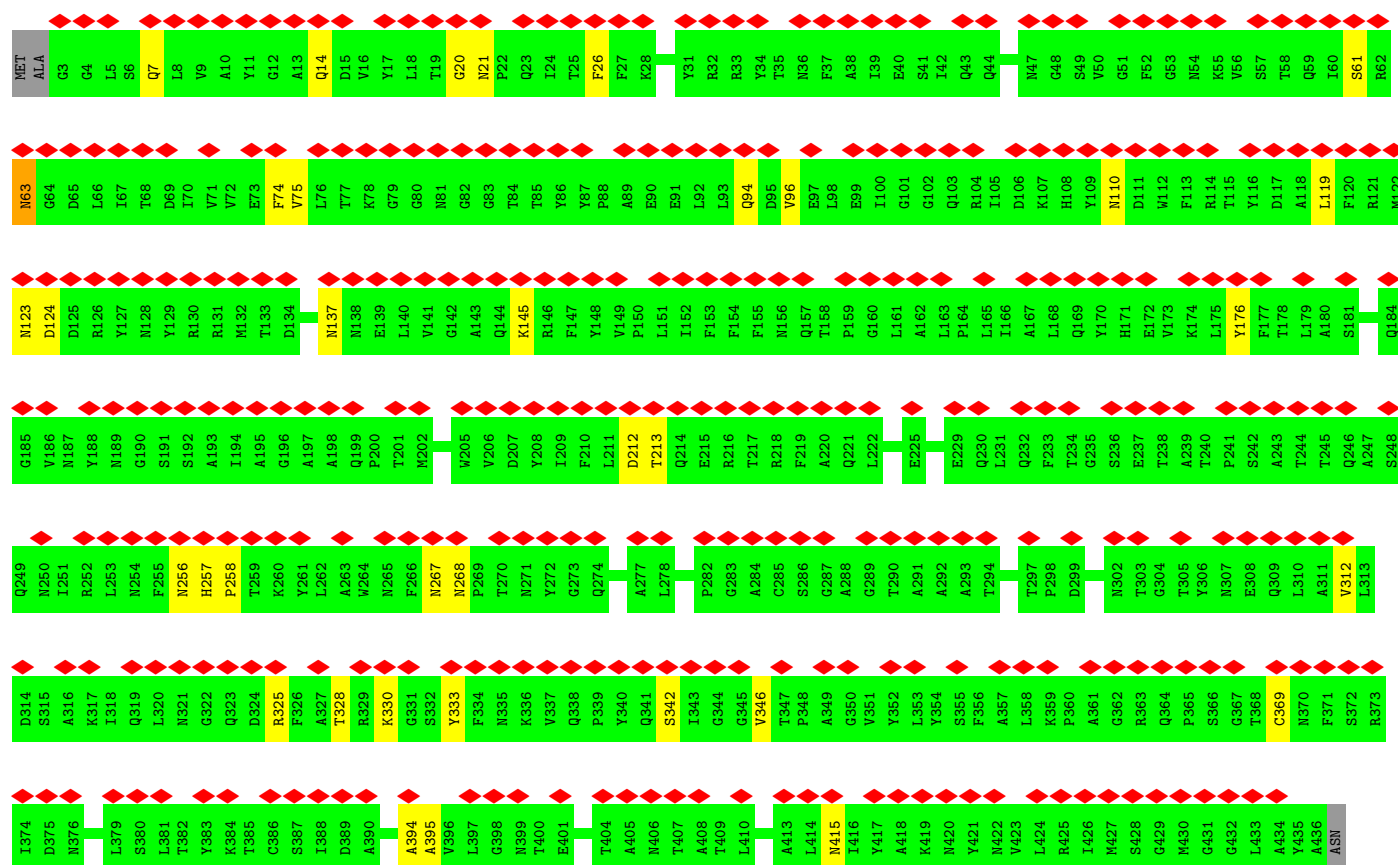


• Molecule 1: Major capsid protein (MCP)

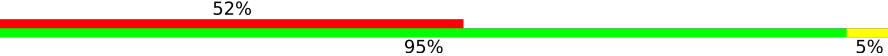


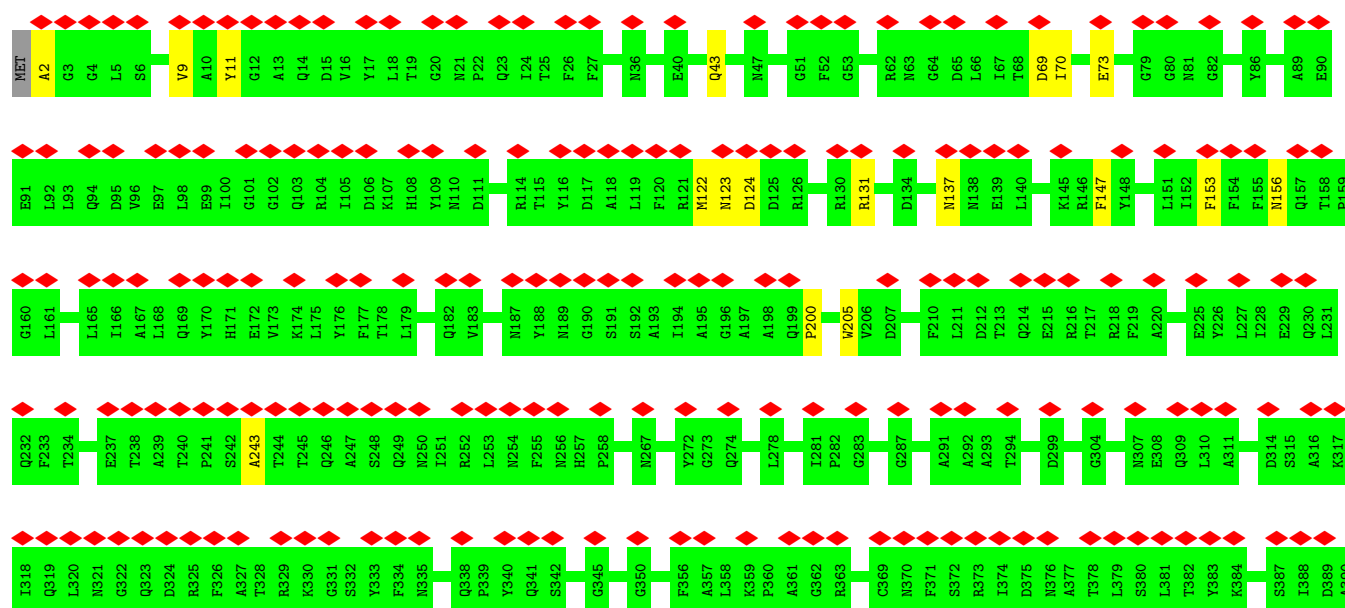
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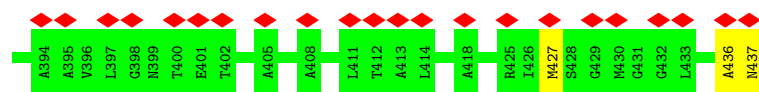
Chain aD: 



• Molecule 1: Major capsid protein (MCP)

Chain aE: 





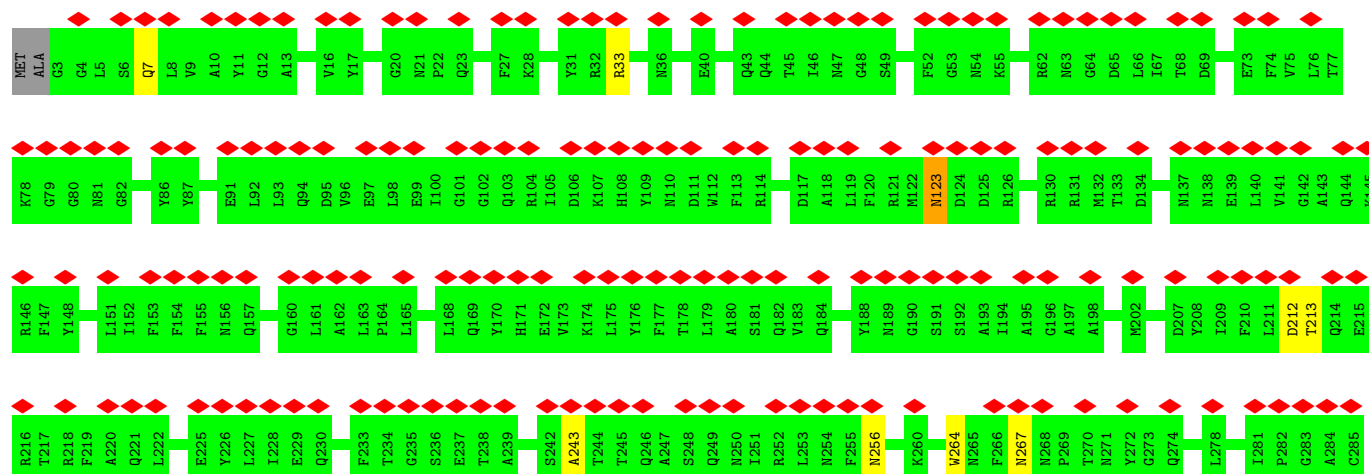
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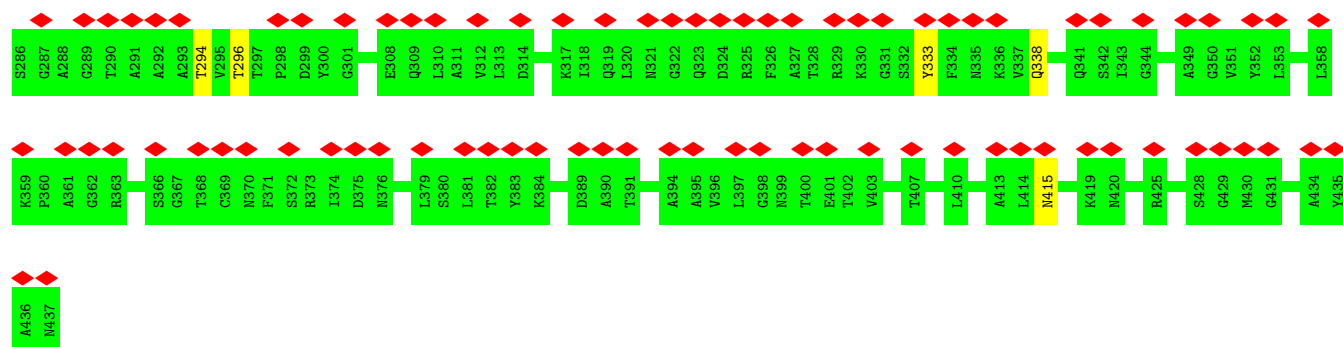
Chain aF: 44% 95%



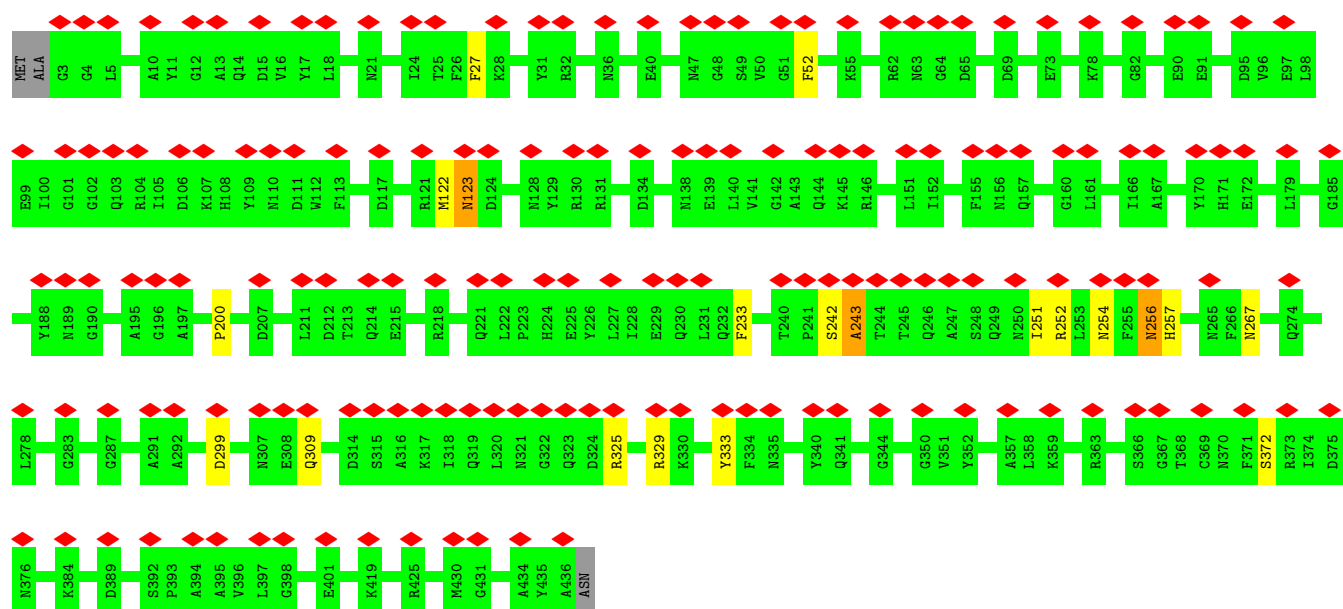
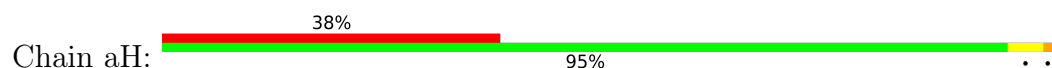
• Molecule 1: Major capsid protein (MCP)

Chain aG: 59% 96%

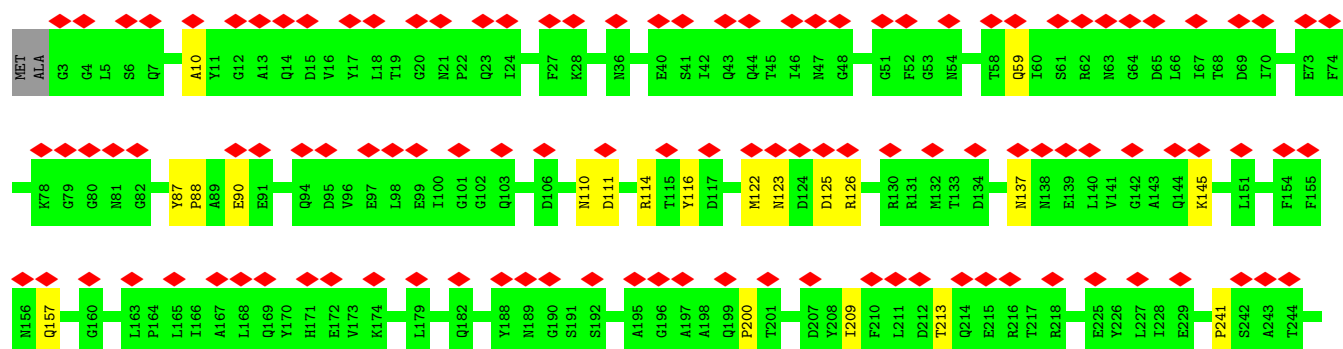
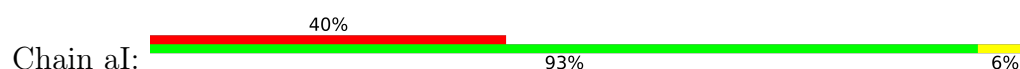


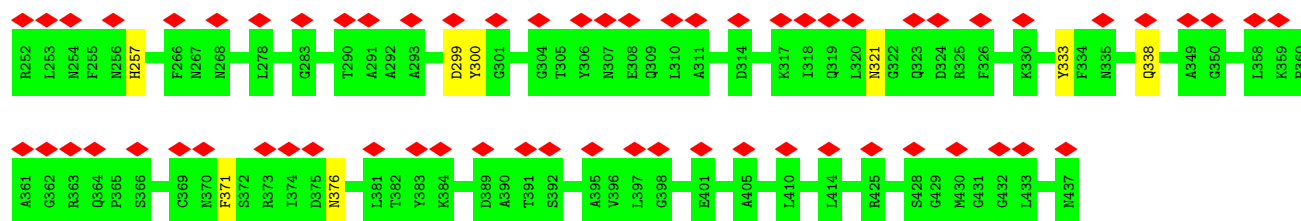


• Molecule 1: Major capsid protein (MCP)

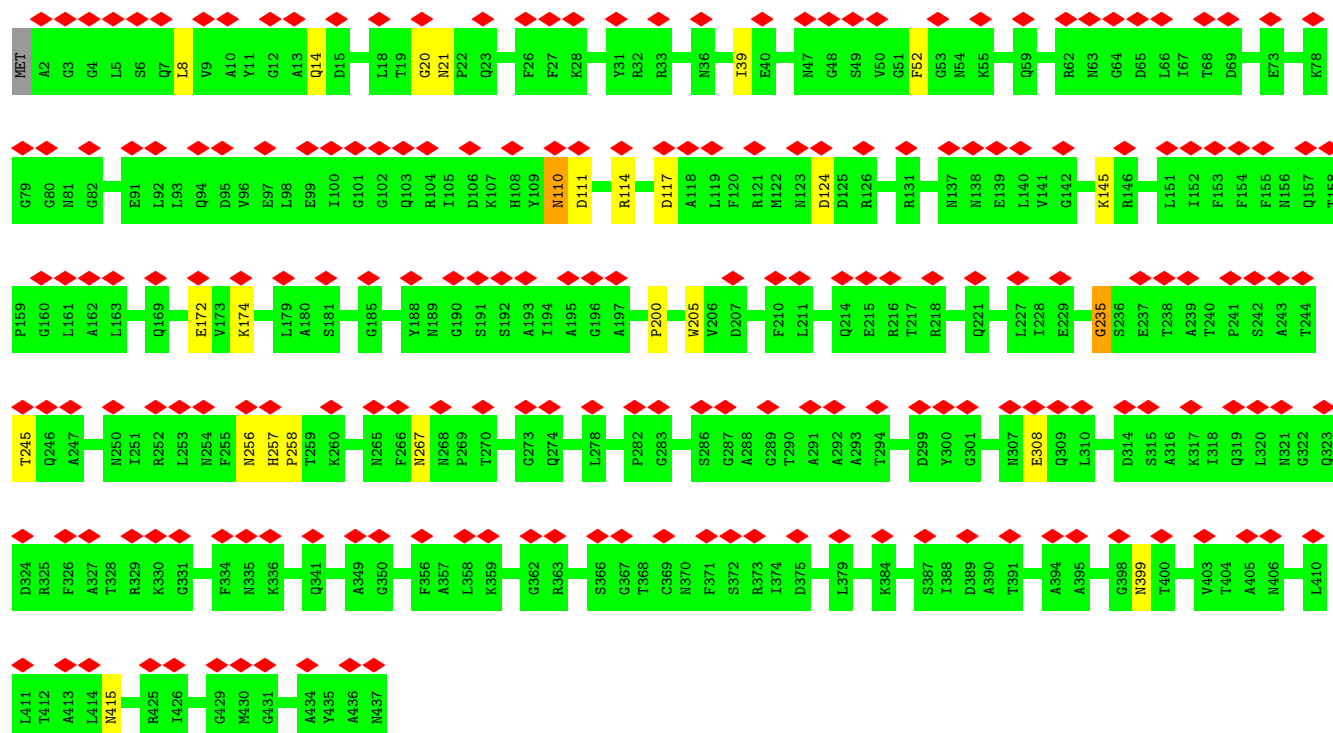


• Molecule 1: Major capsid protein (MCP)

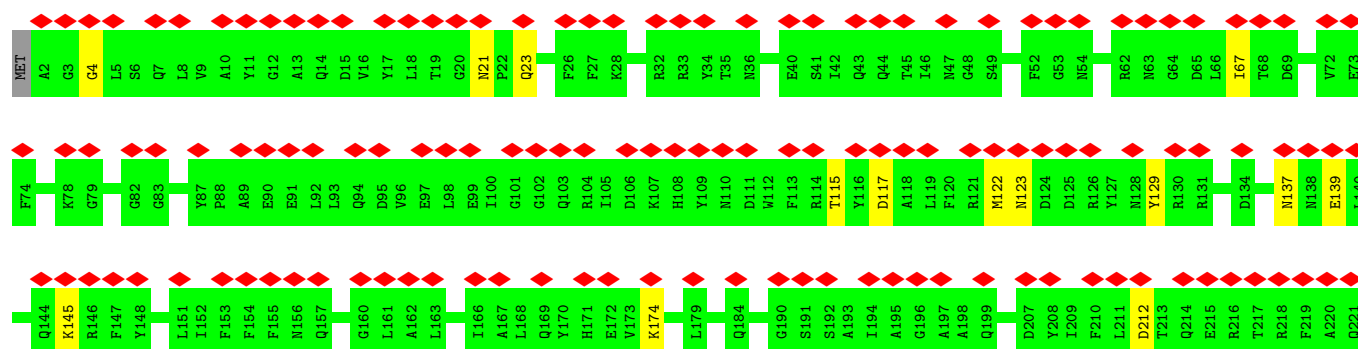


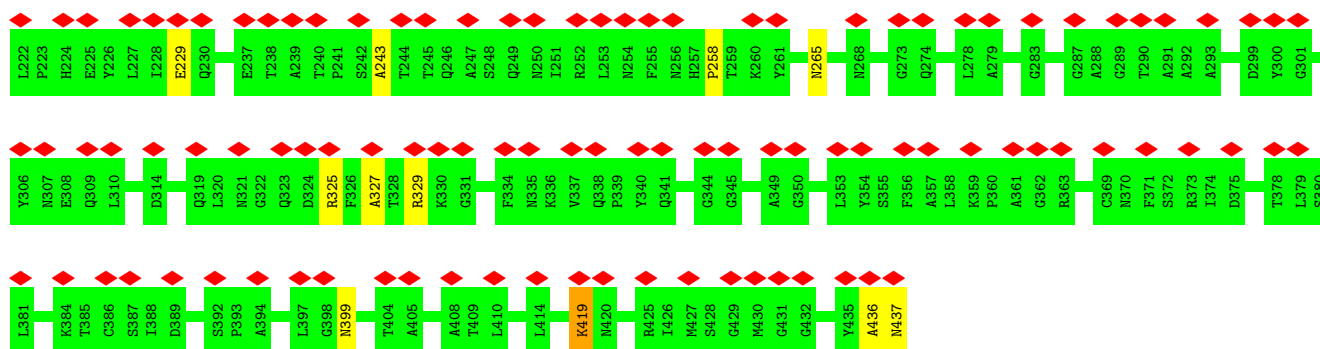


• Molecule 1: Major capsid protein (MCP)

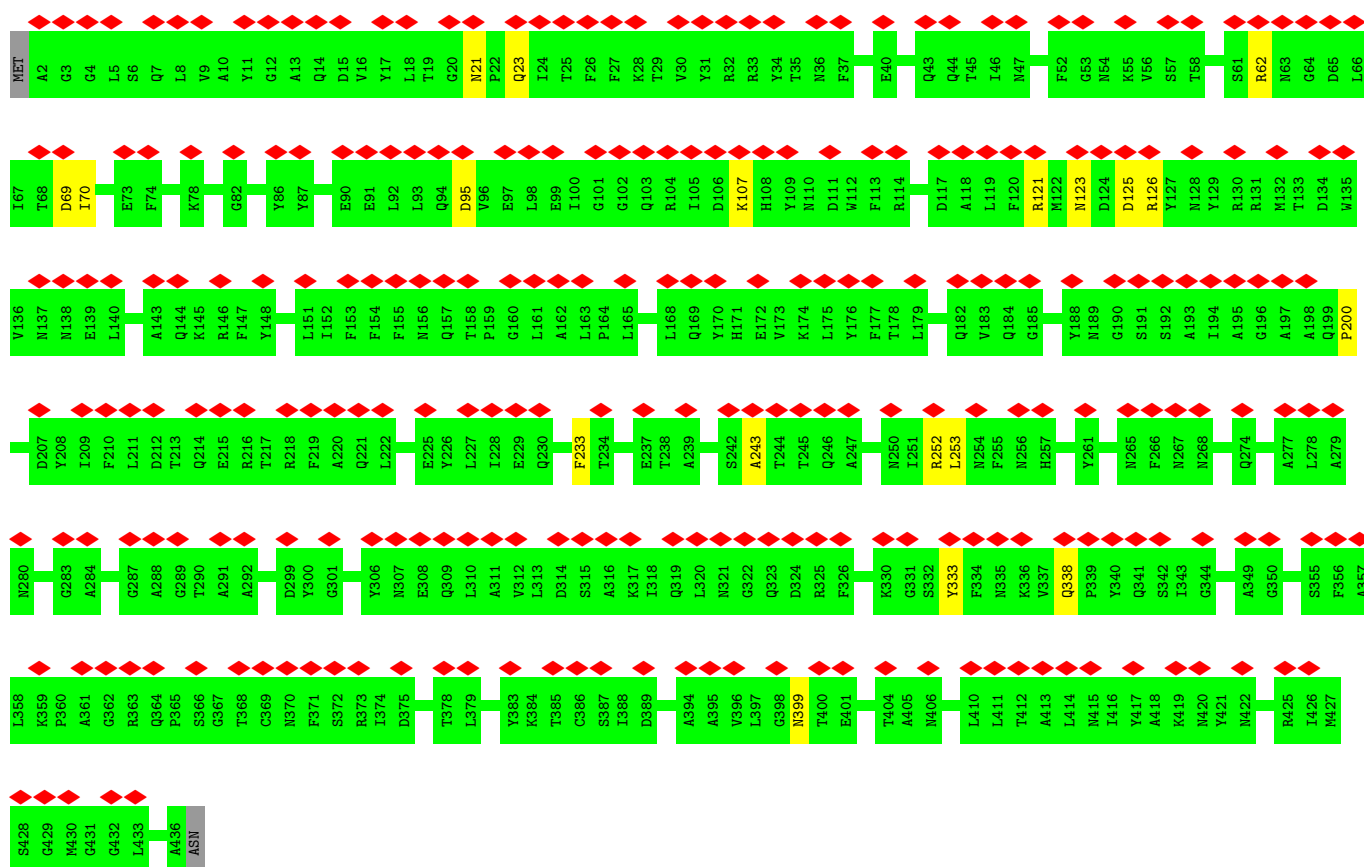


• Molecule 1: Major capsid protein (MCP)

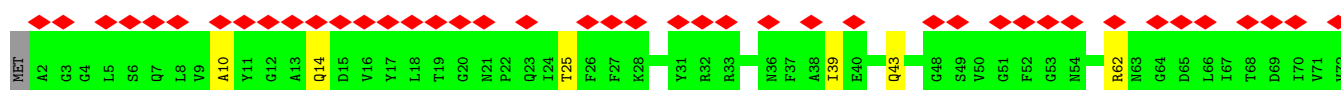


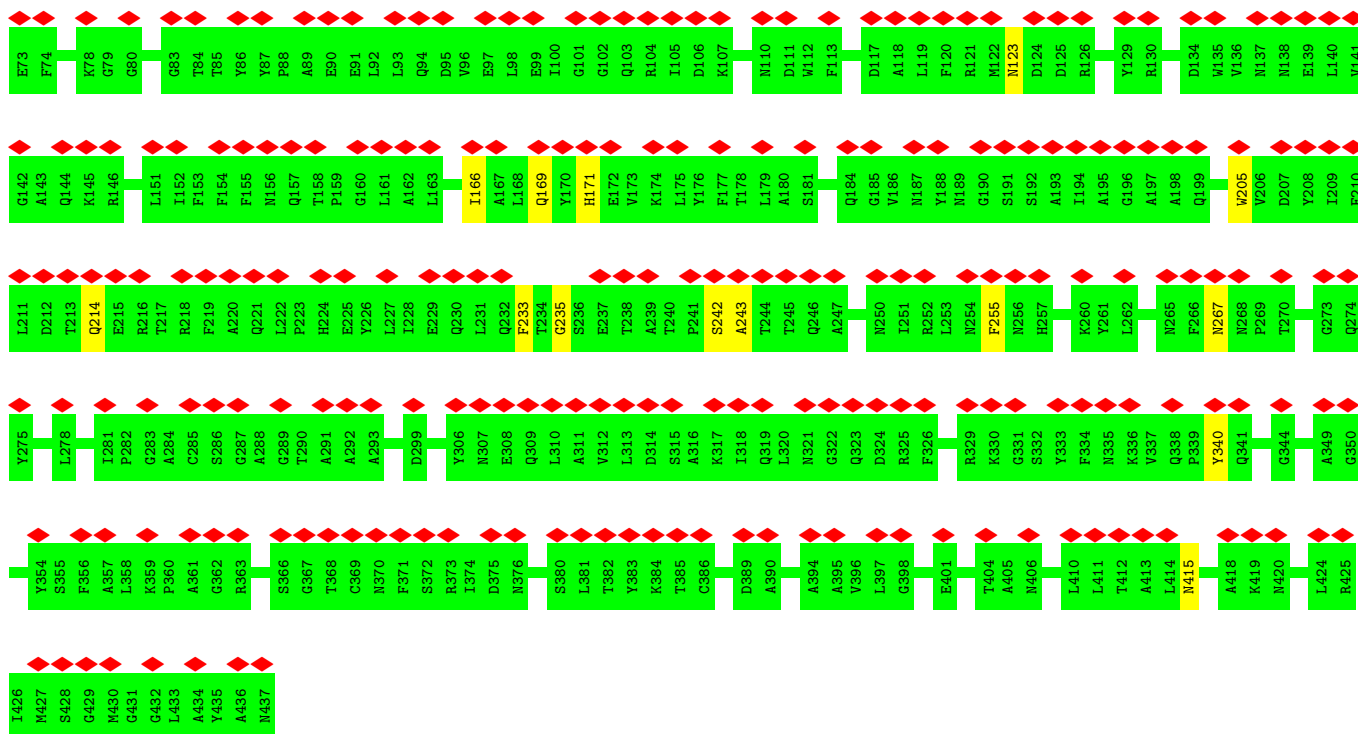


• Molecule 1: Major capsid protein (MCP)

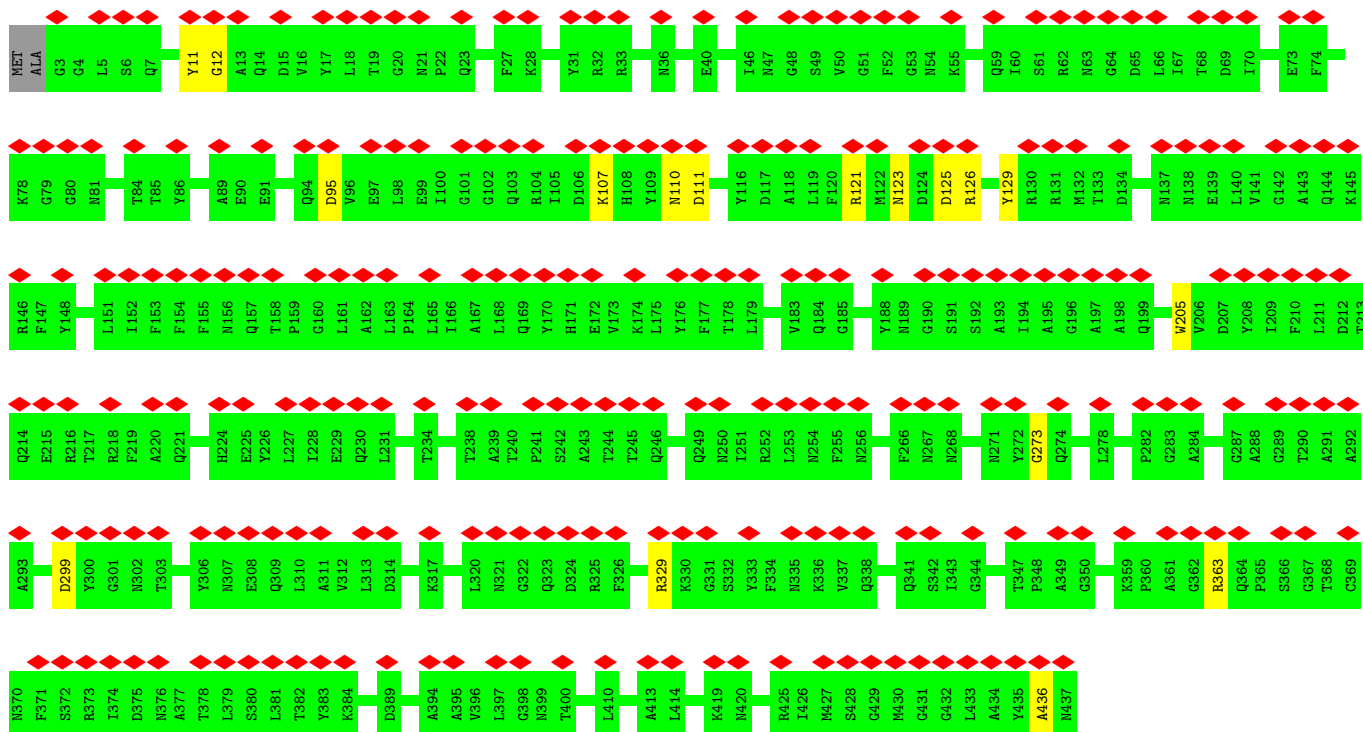


• Molecule 1: Major capsid protein (MCP)

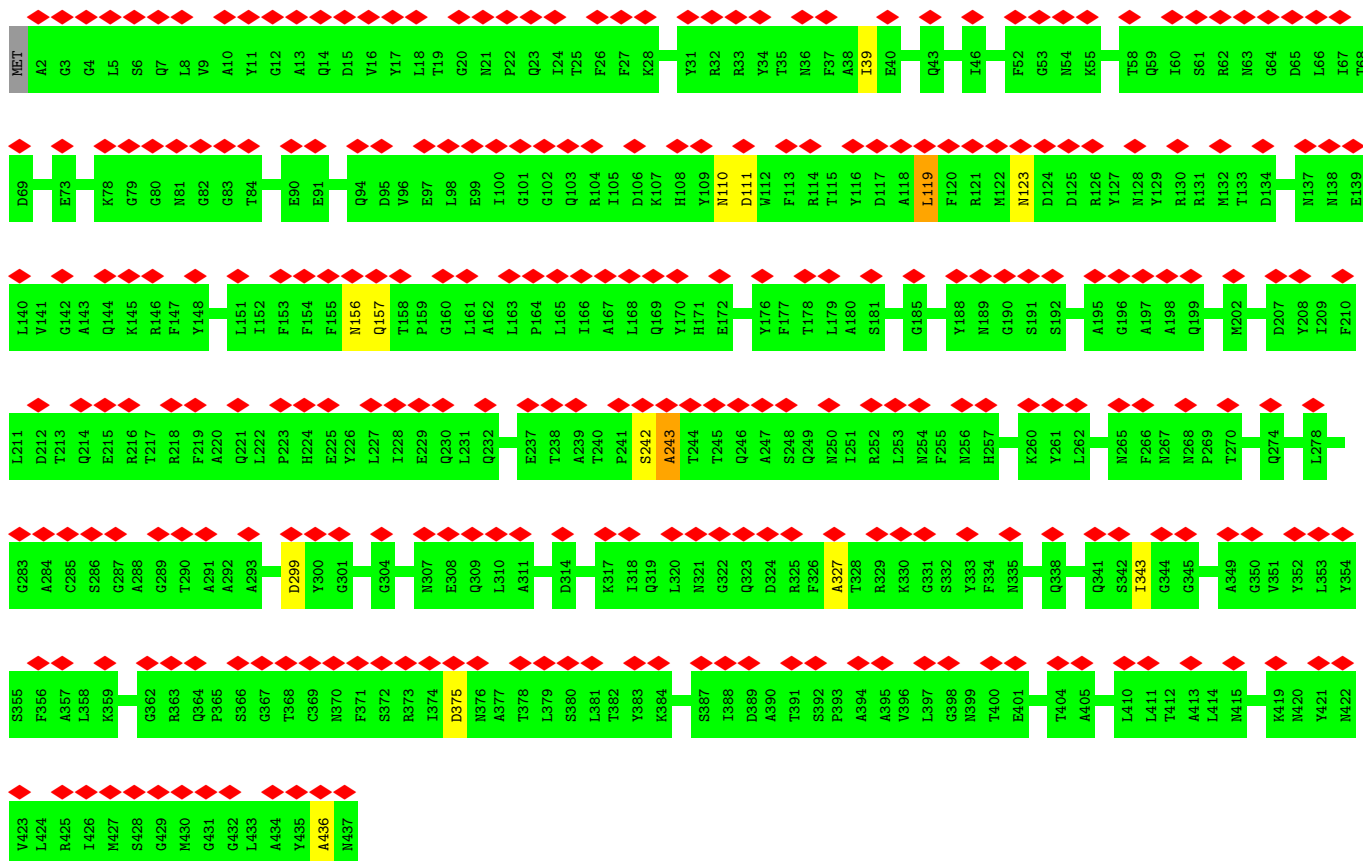




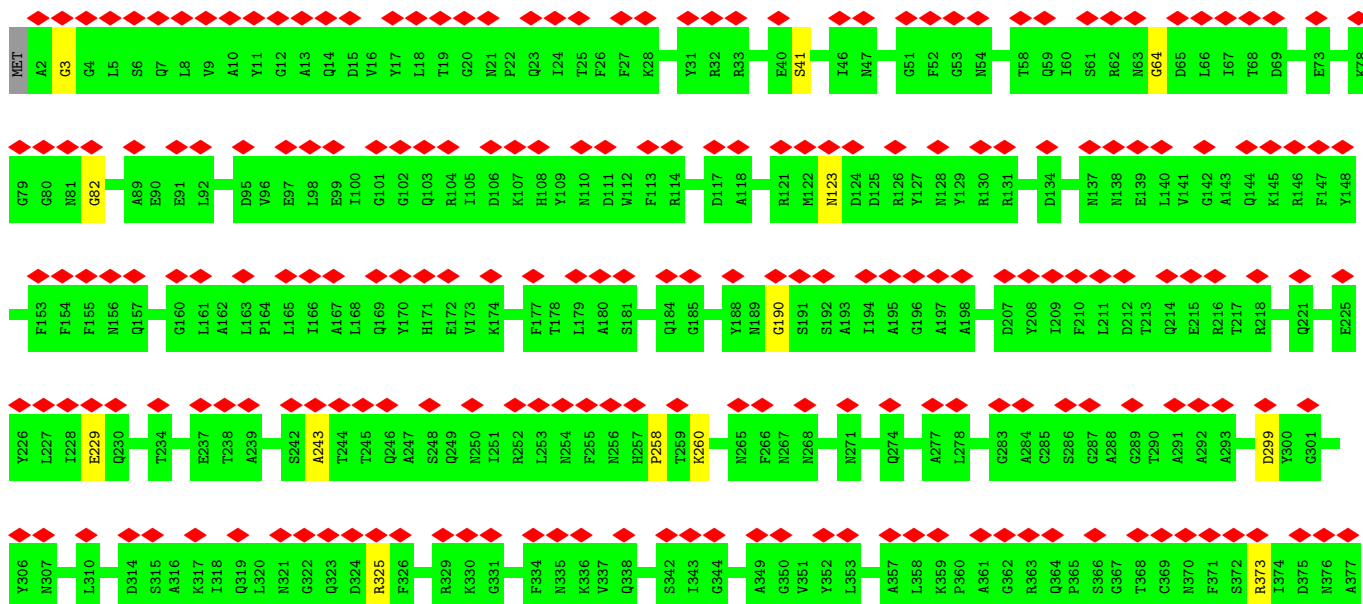
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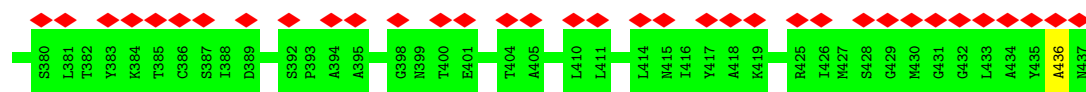


• Molecule 1: Major capsid protein (MCP)

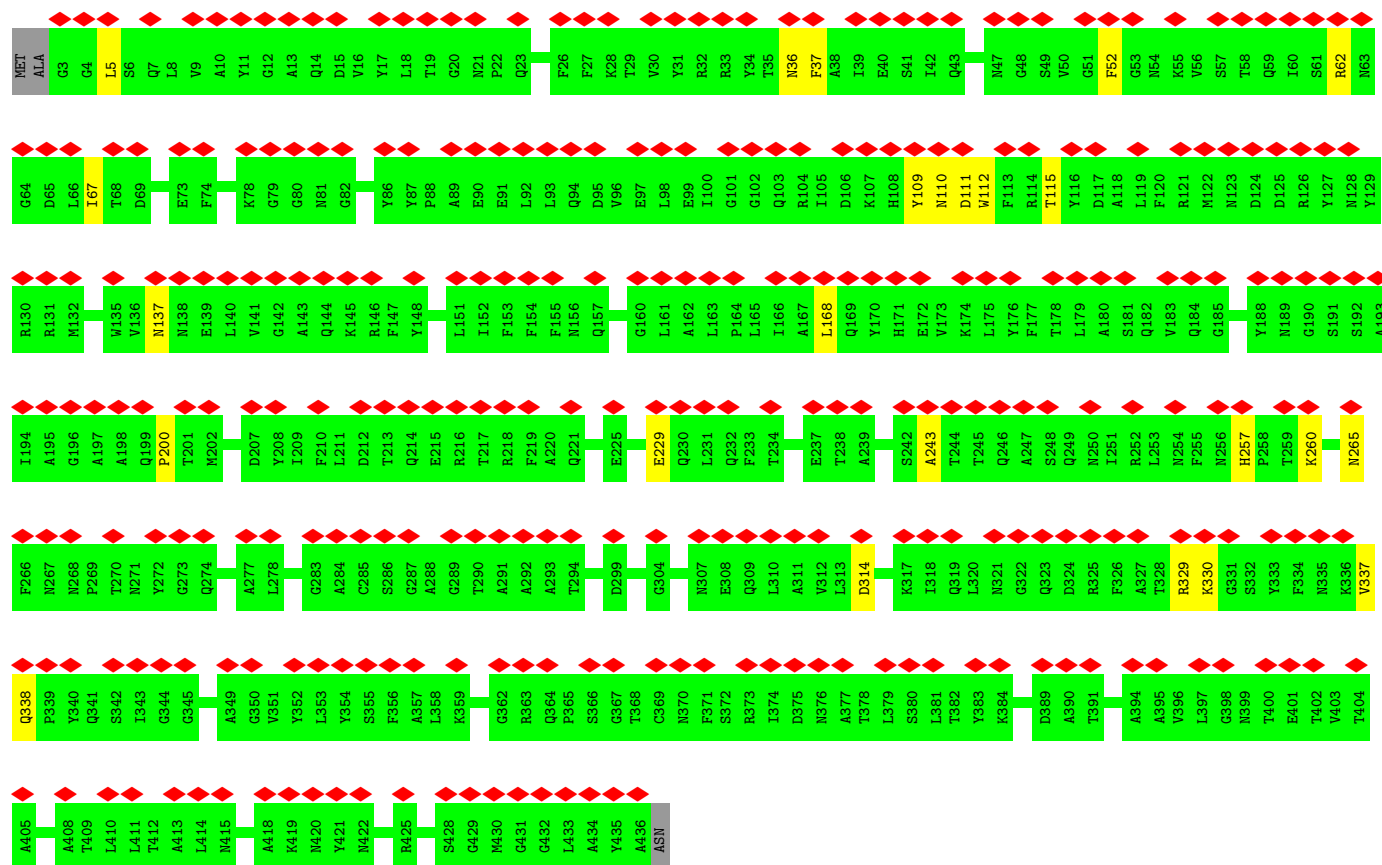


• Molecule 1: Major capsid protein (MCP)

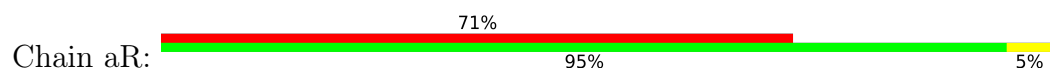


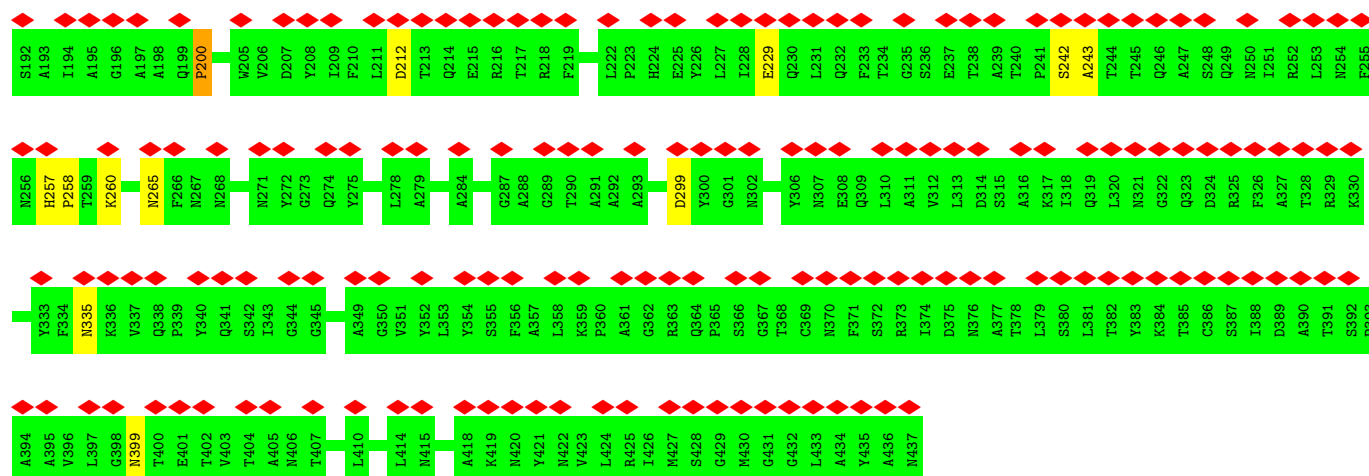


• Molecule 1: Major capsid protein (MCP)

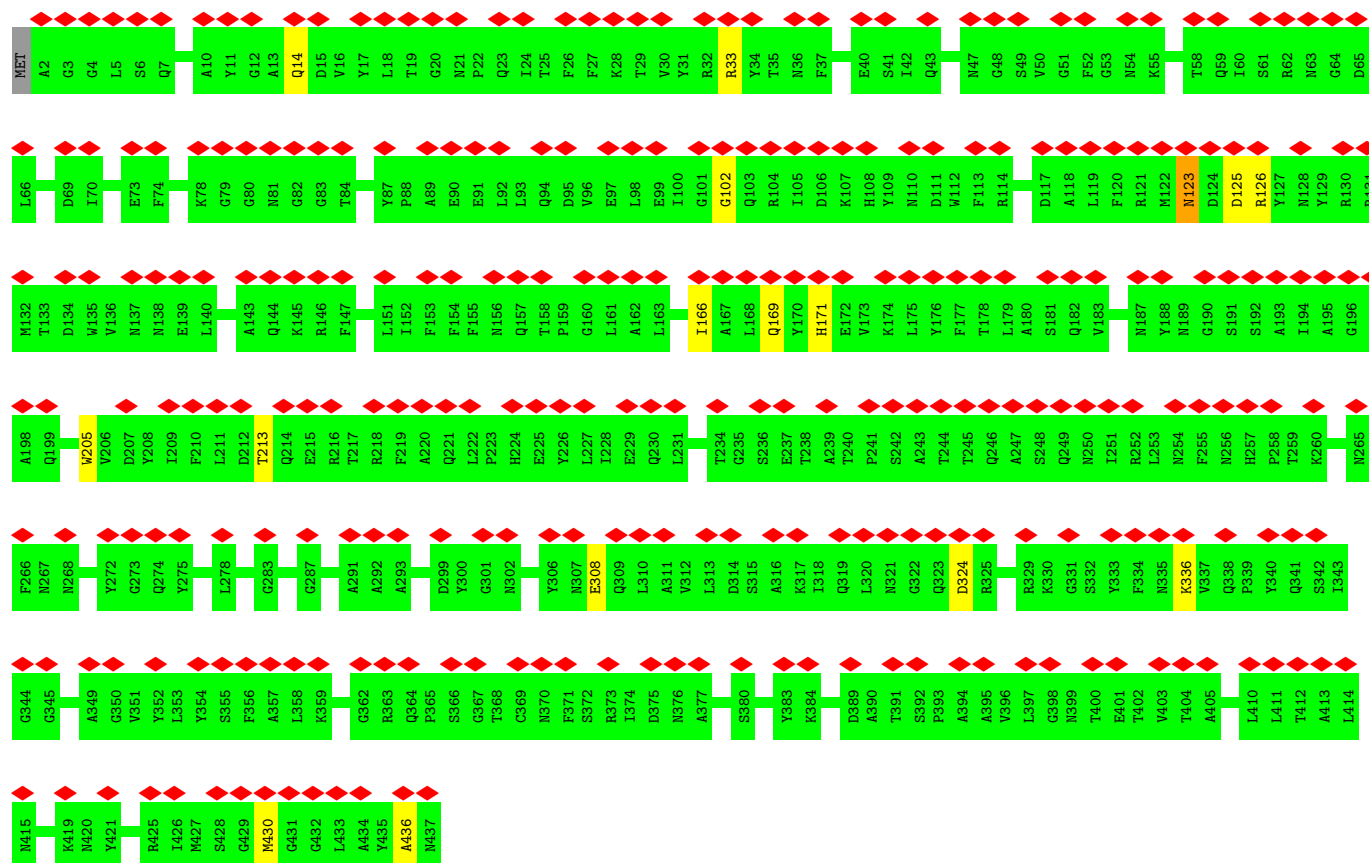


• Molecule 1: Major capsid protein (MCP)



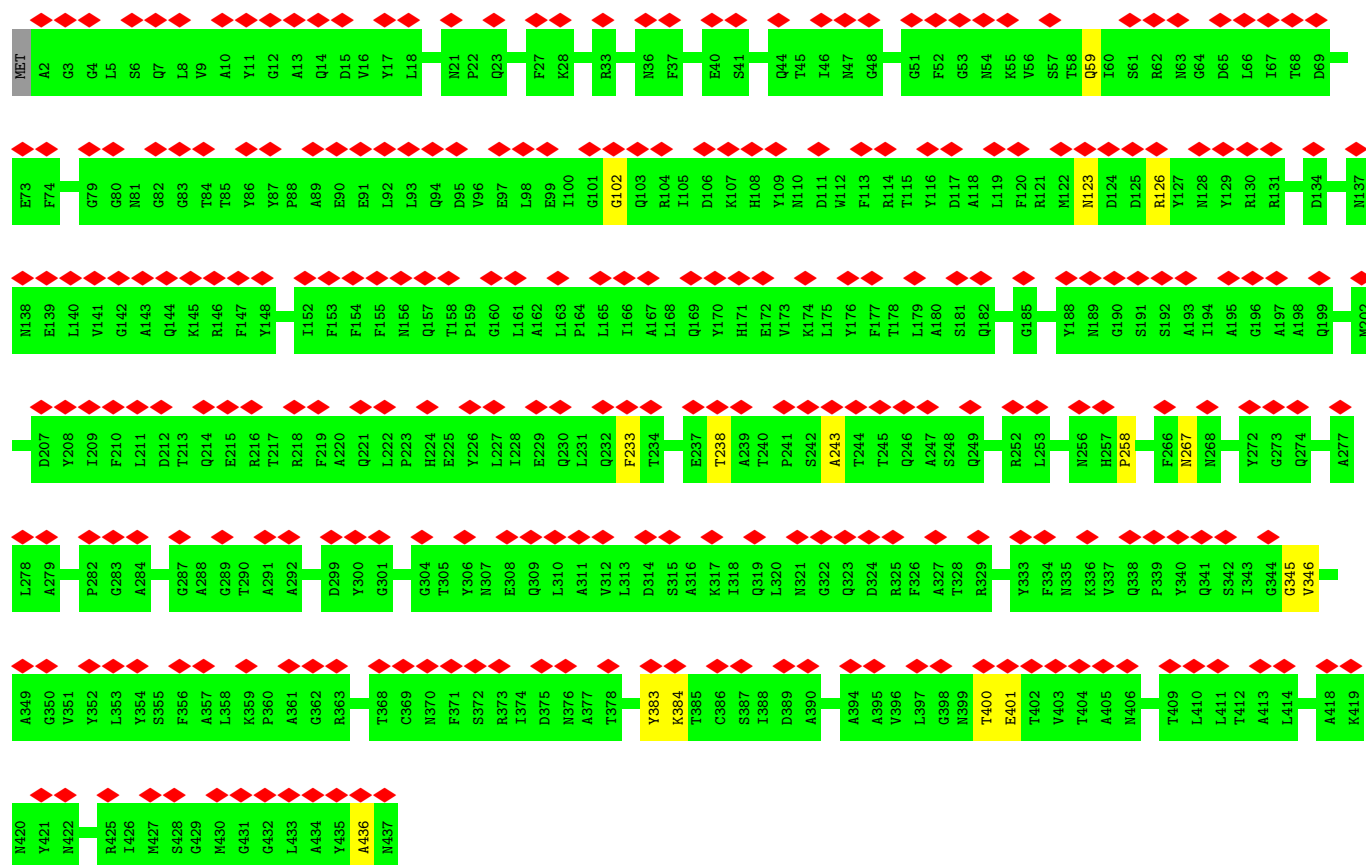


• Molecule 1: Major capsid protein (MCP)

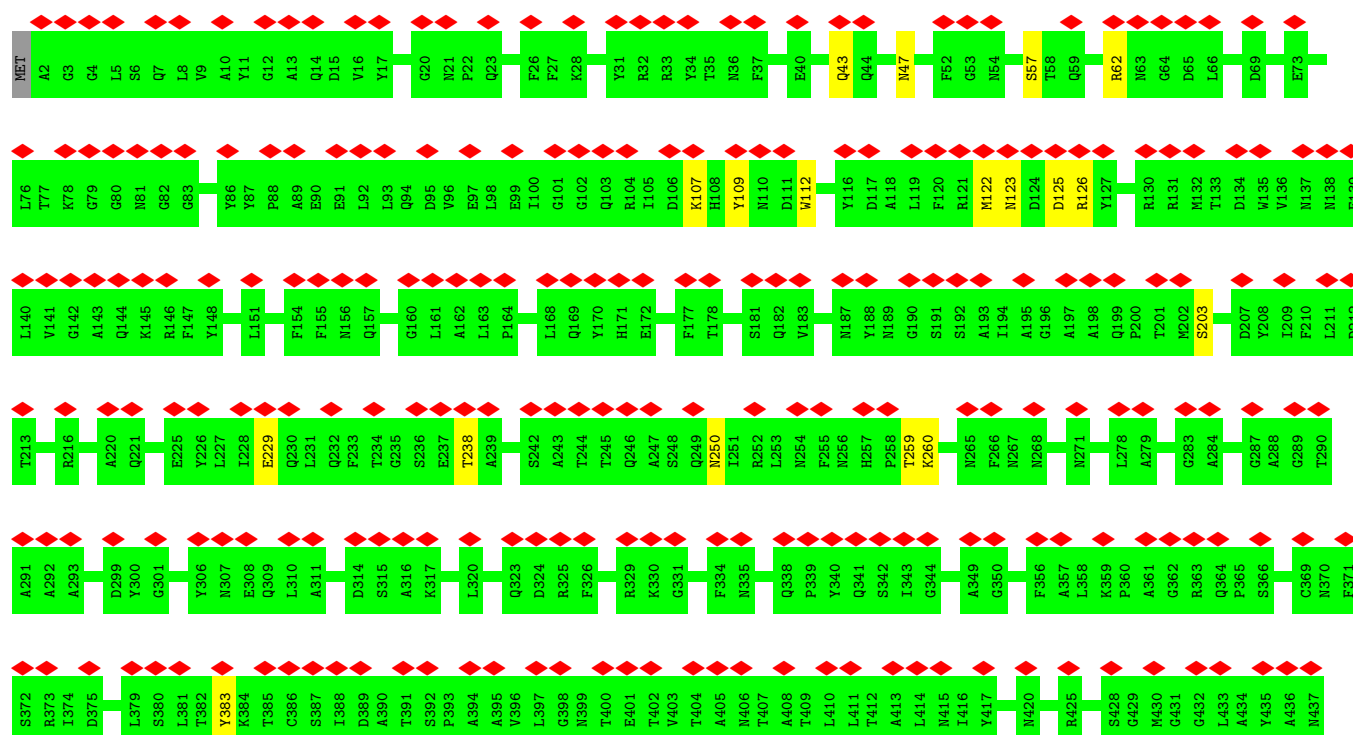


• Molecule 1: Major capsid protein (MCP)

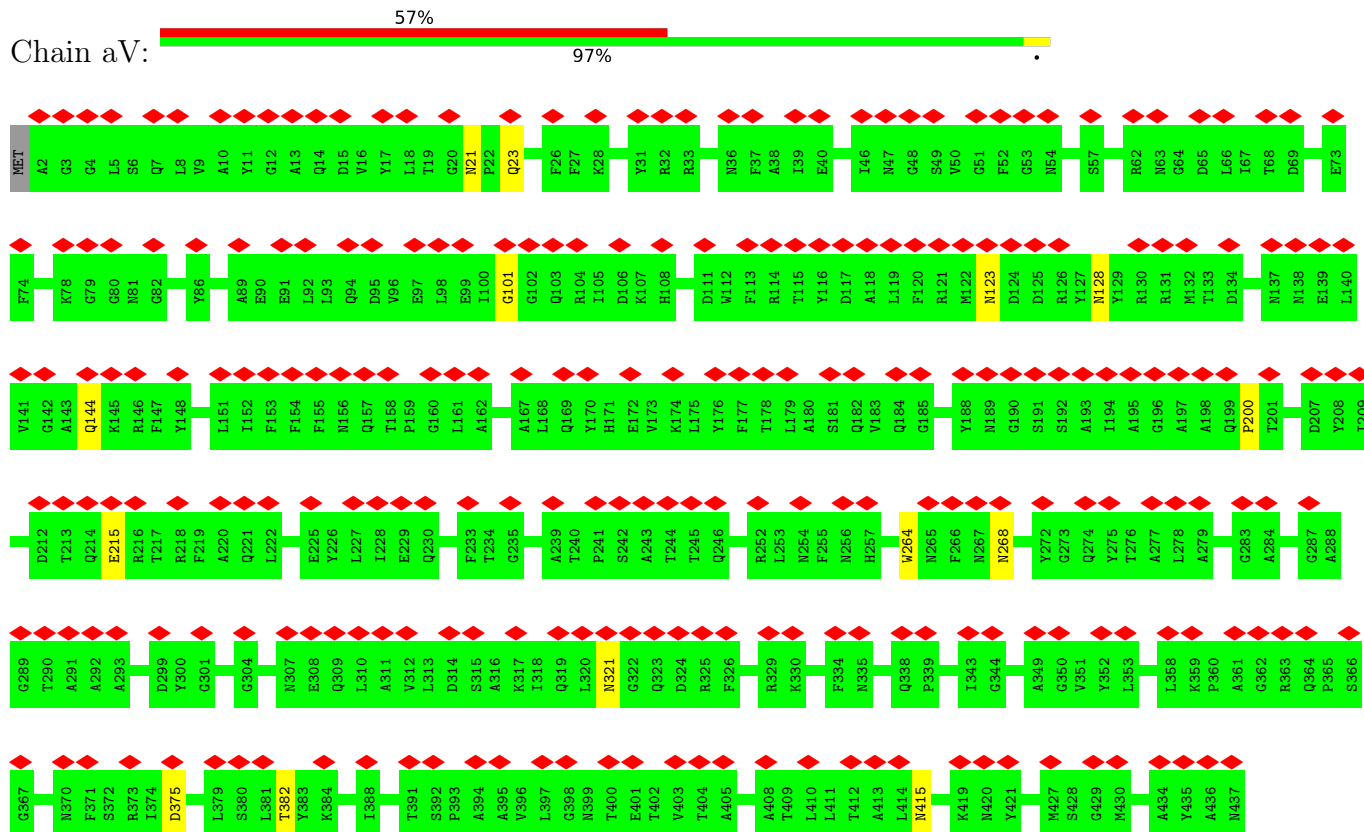




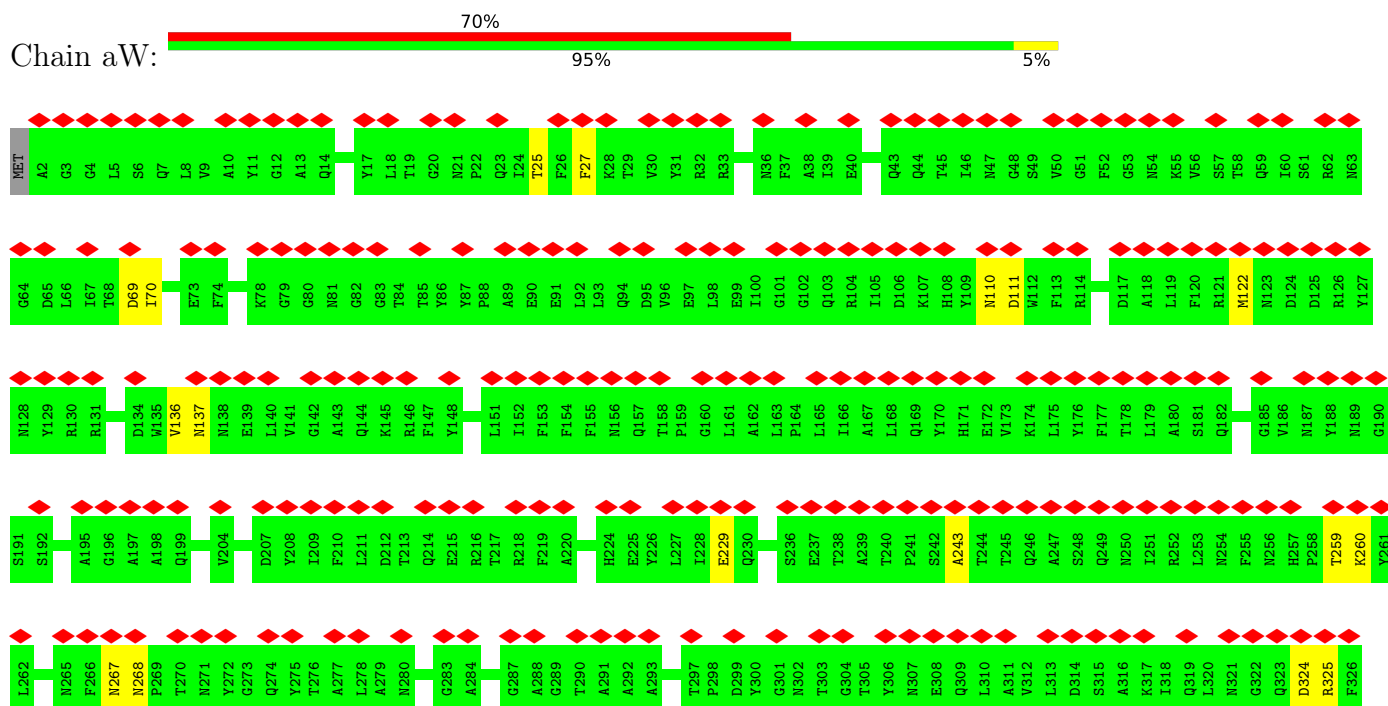
• Molecule 1: Major capsid protein (MCP)

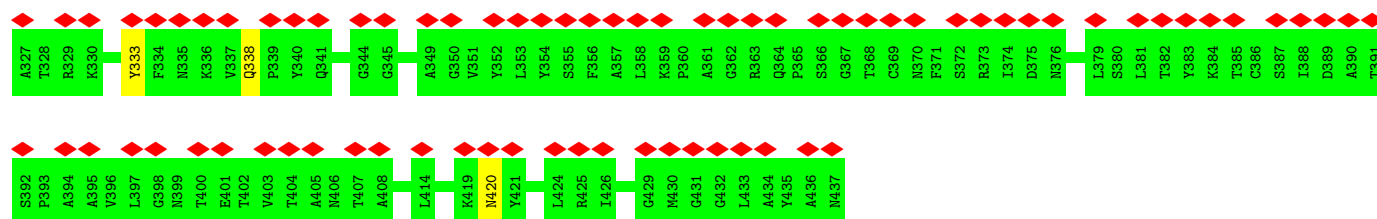


- Molecule 1: Major capsid protein (MCP)

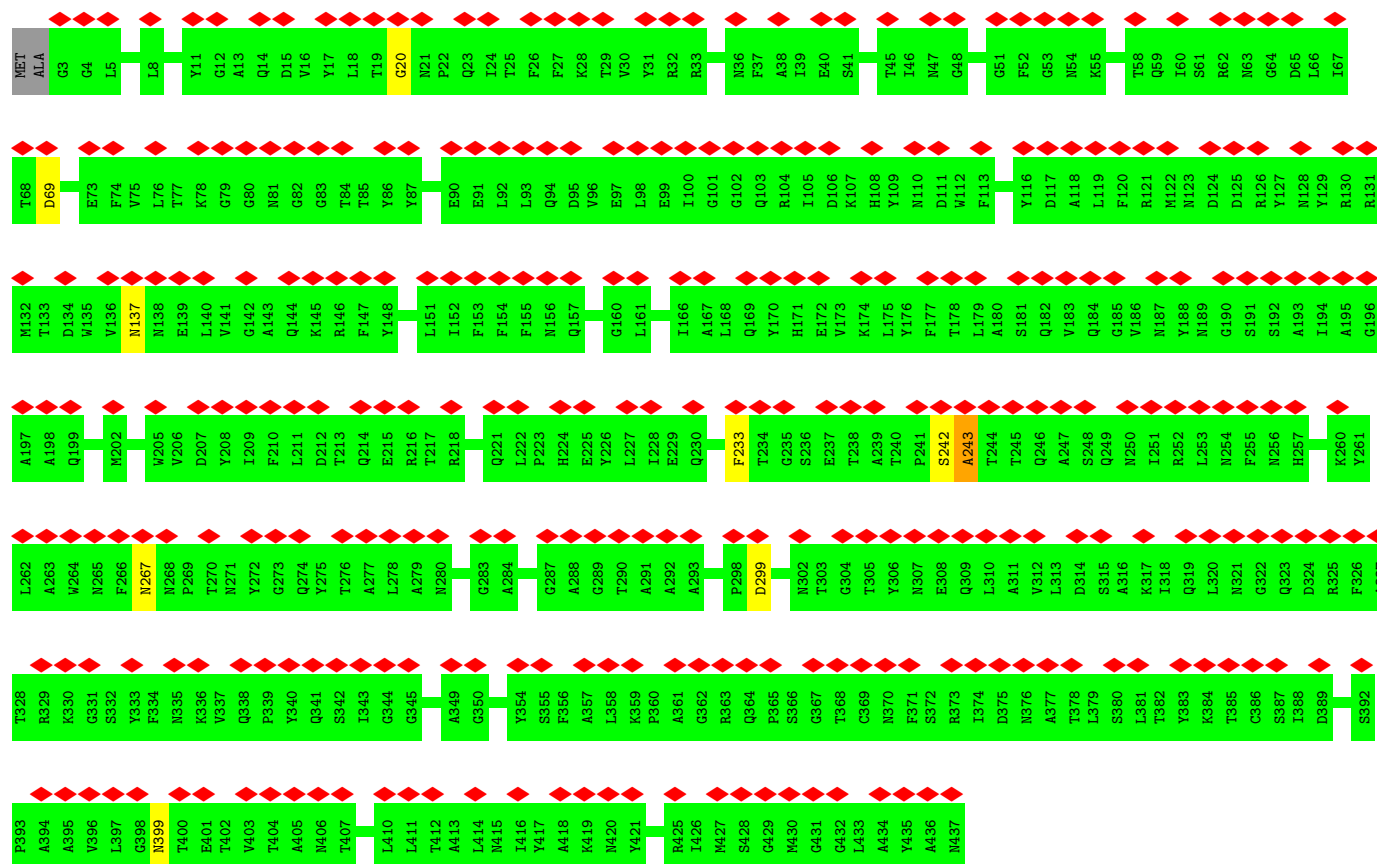
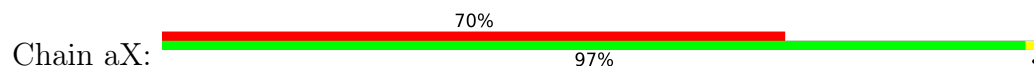


- Molecule 1: Major capsid protein (MCP)

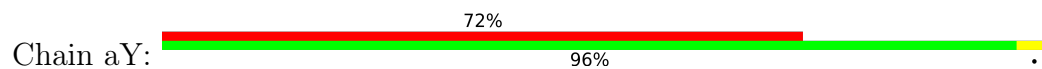


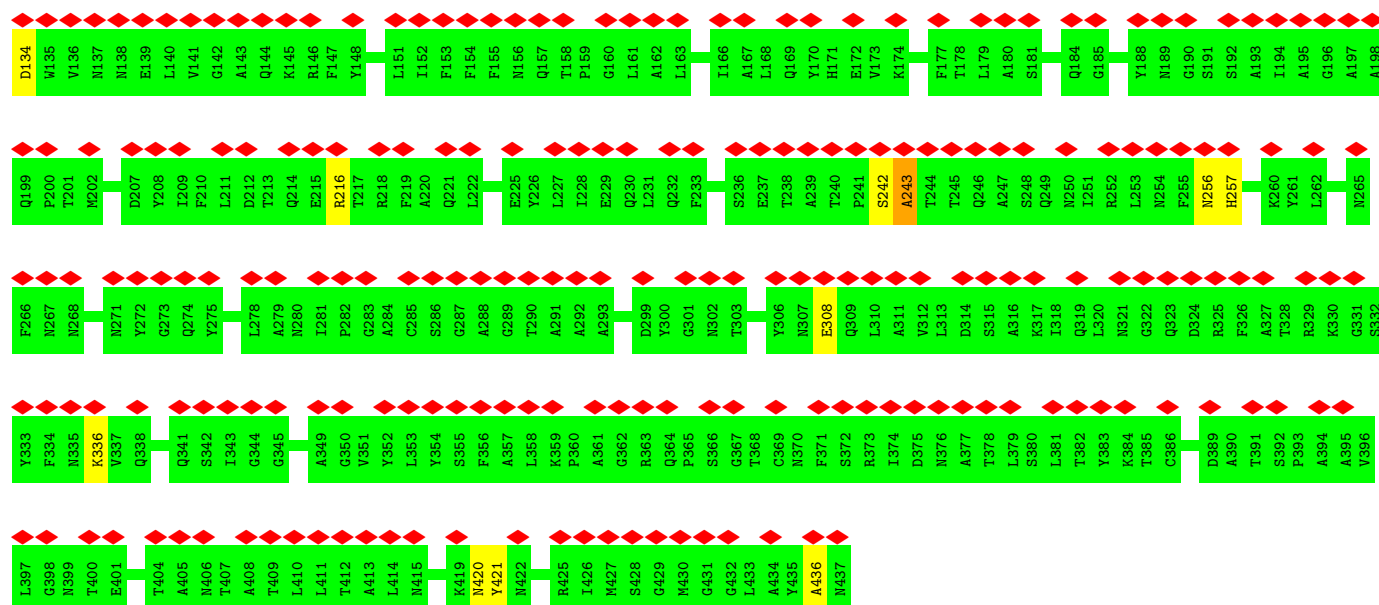


• Molecule 1: Major capsid protein (MCP)

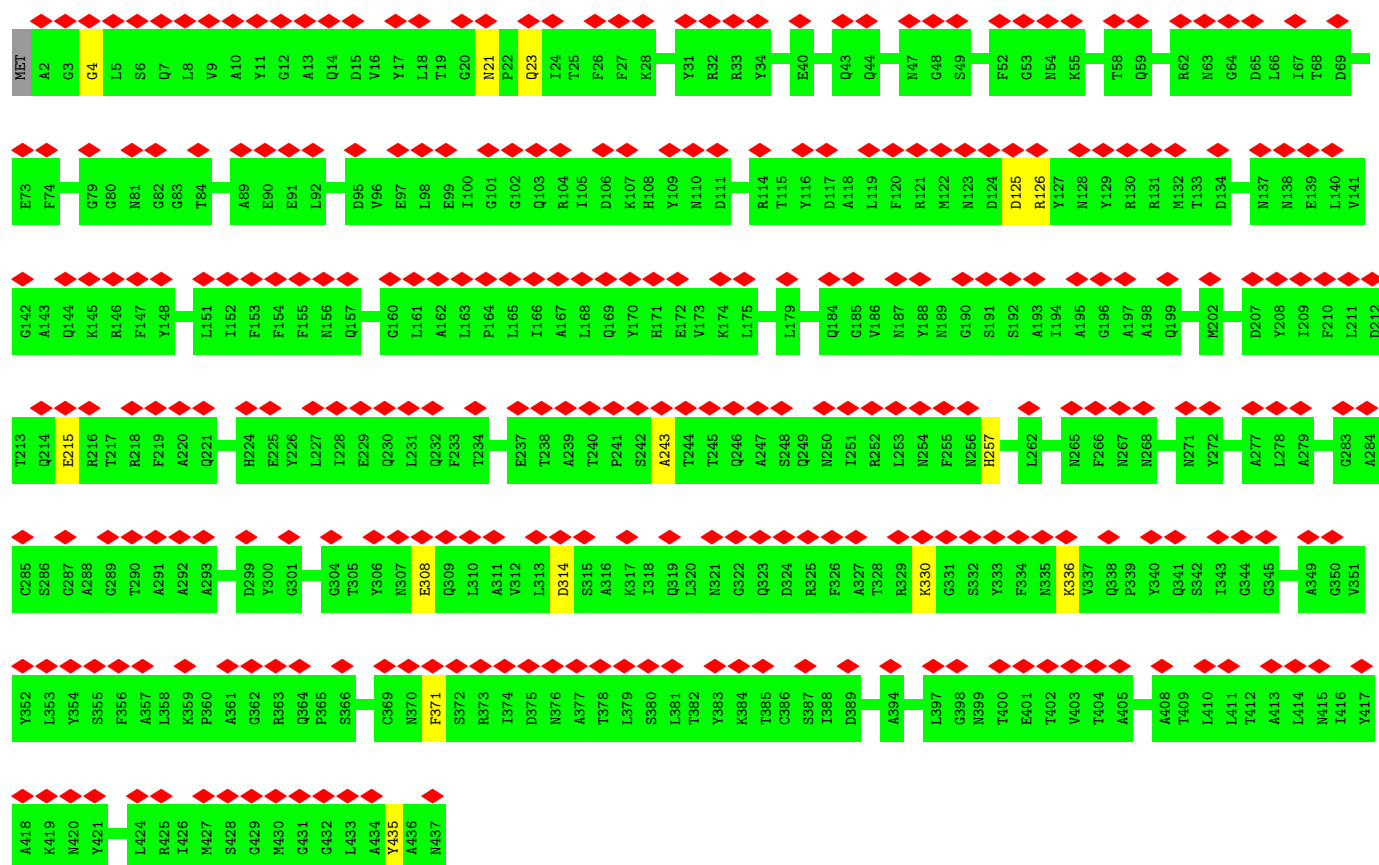


• Molecule 1: Major capsid protein (MCP)

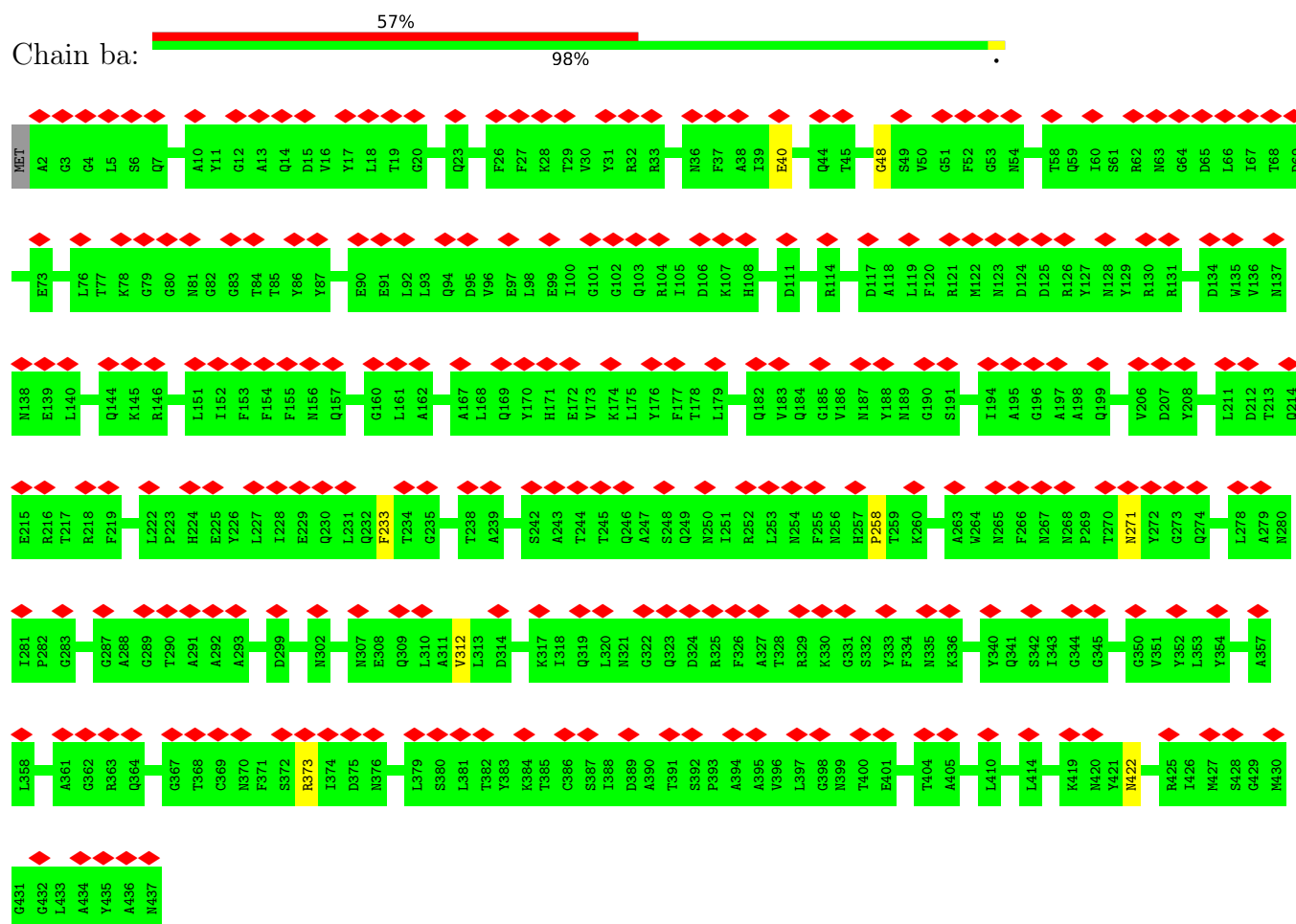




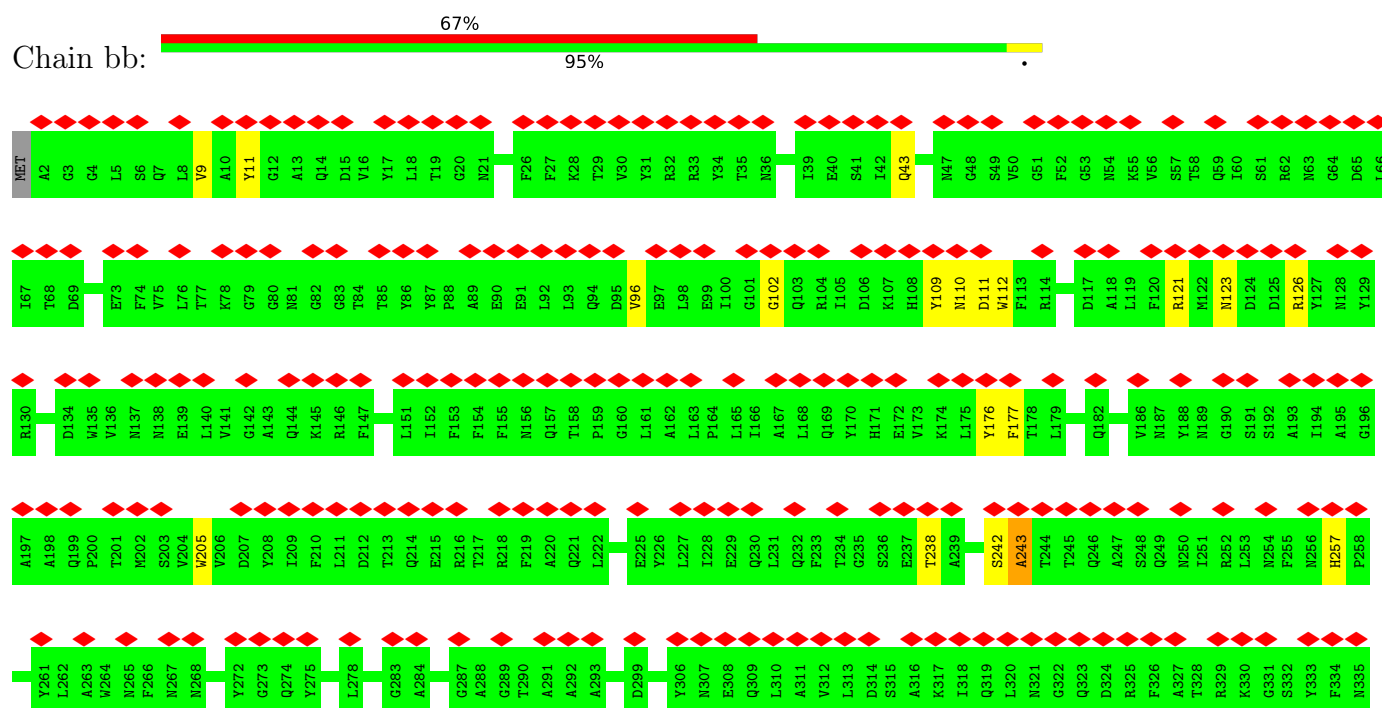
- Molecule 1: Major capsid protein (MCP)

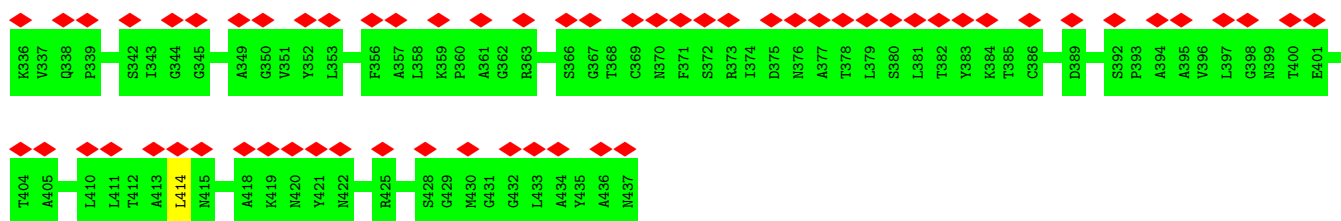


- Molecule 1: Major capsid protein (MCP)

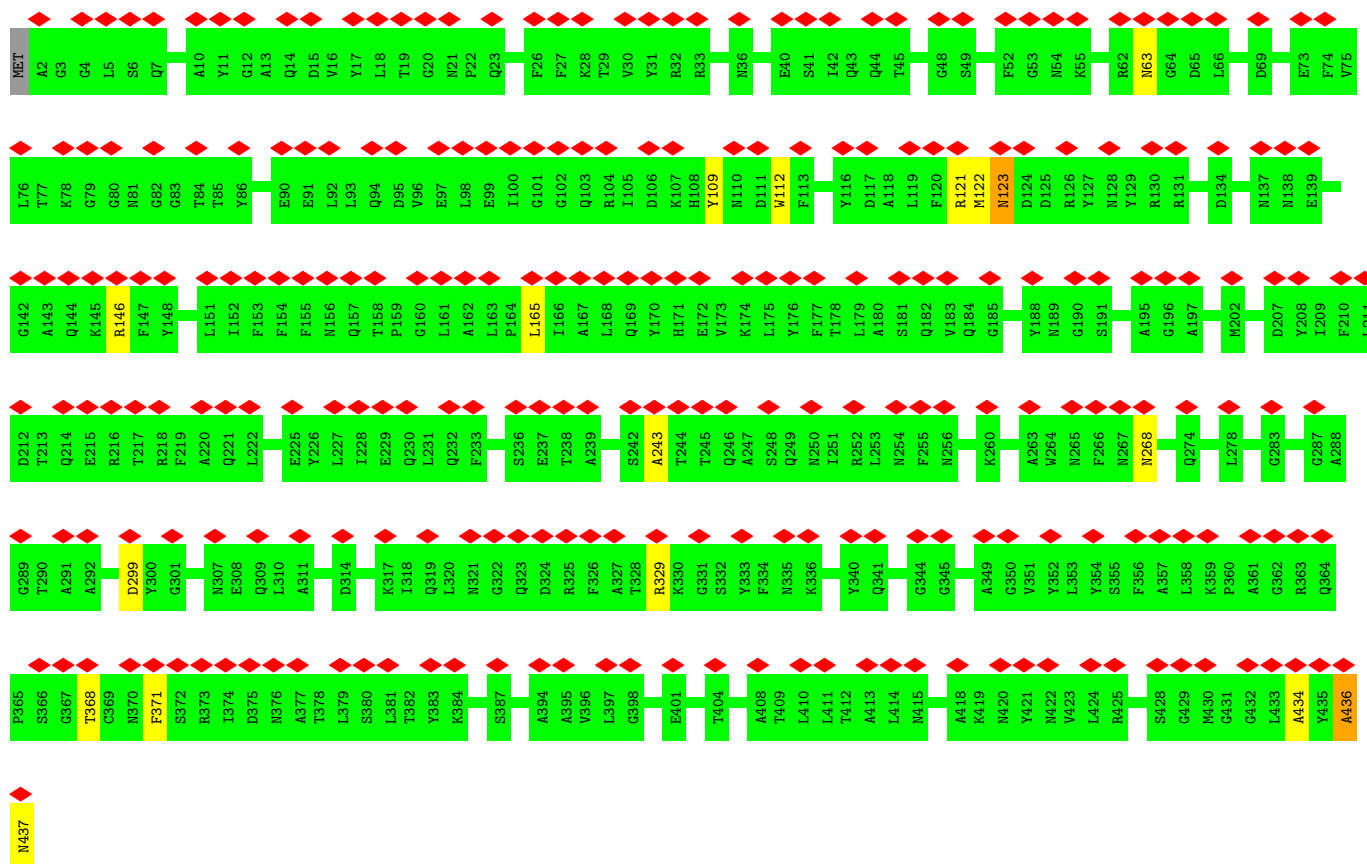


- Molecule 1: Major capsid protein (MCP)

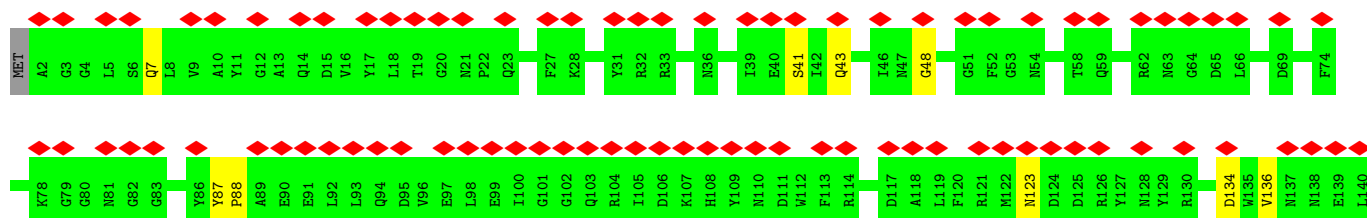


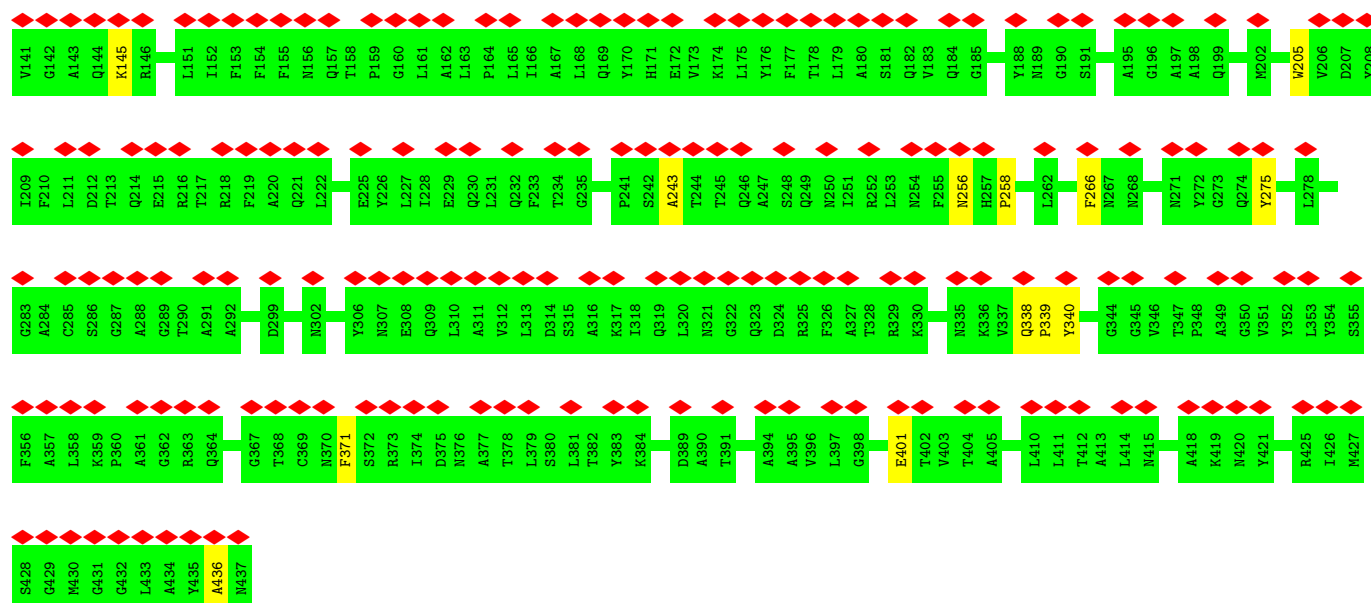


• Molecule 1: Major capsid protein (MCP)

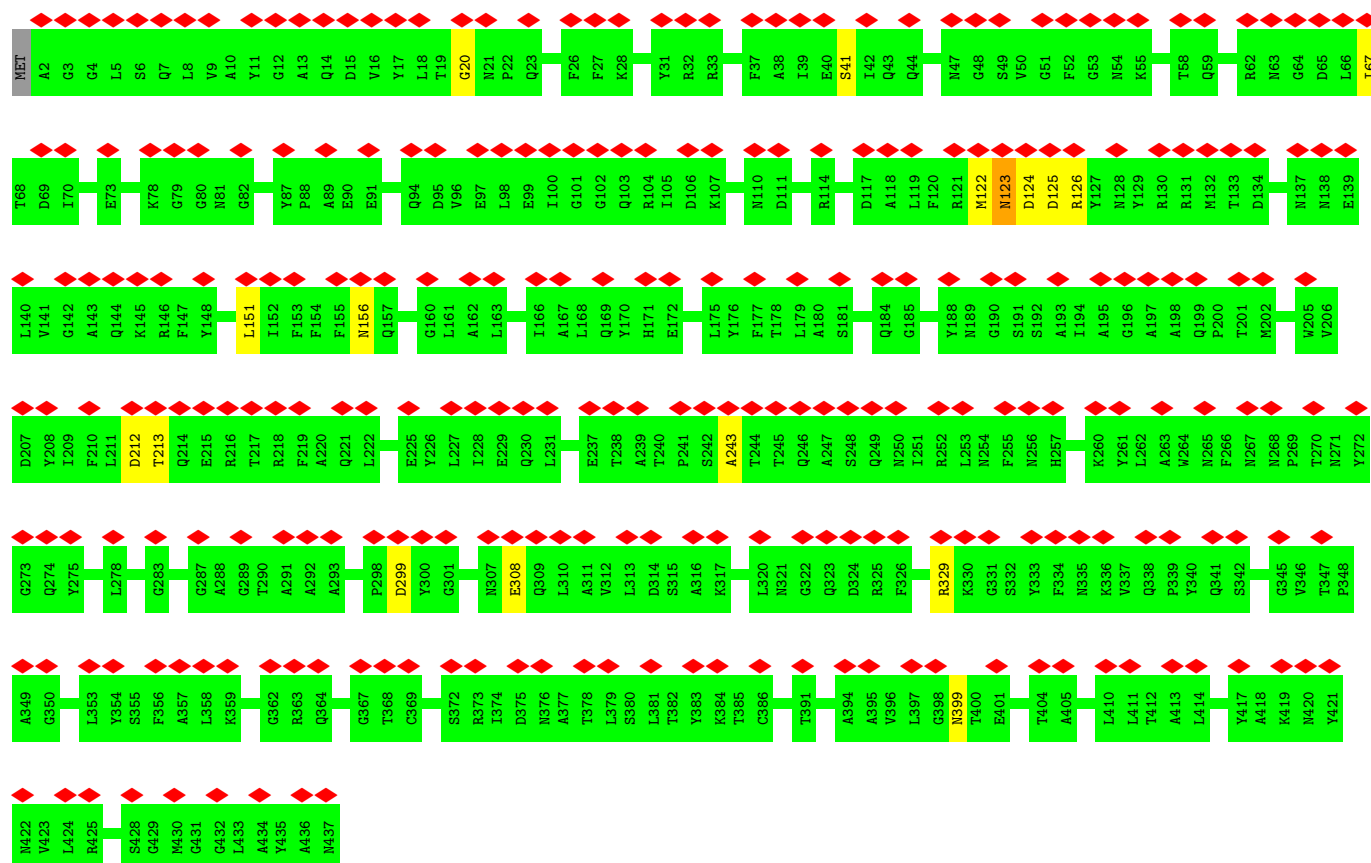


• Molecule 1: Major capsid protein (MCP)

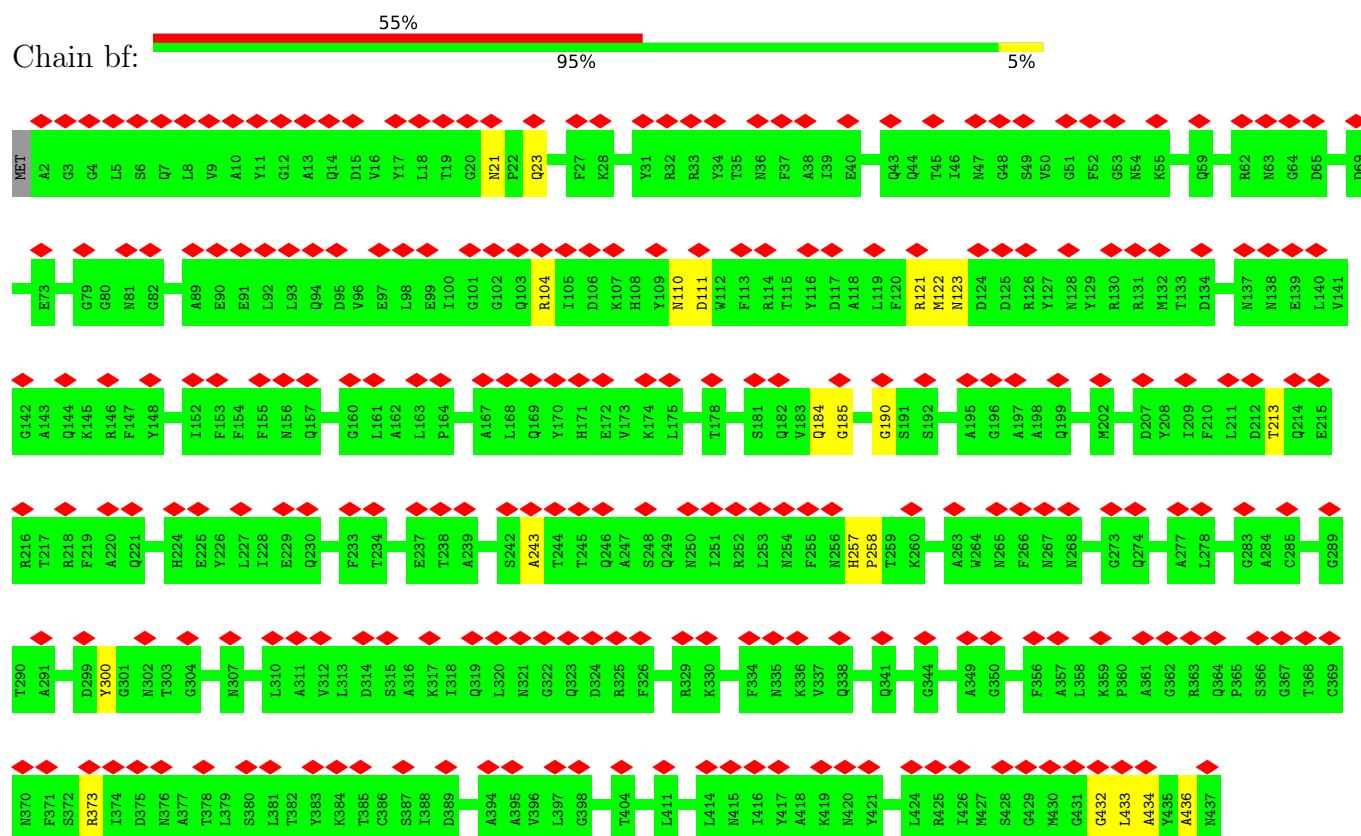




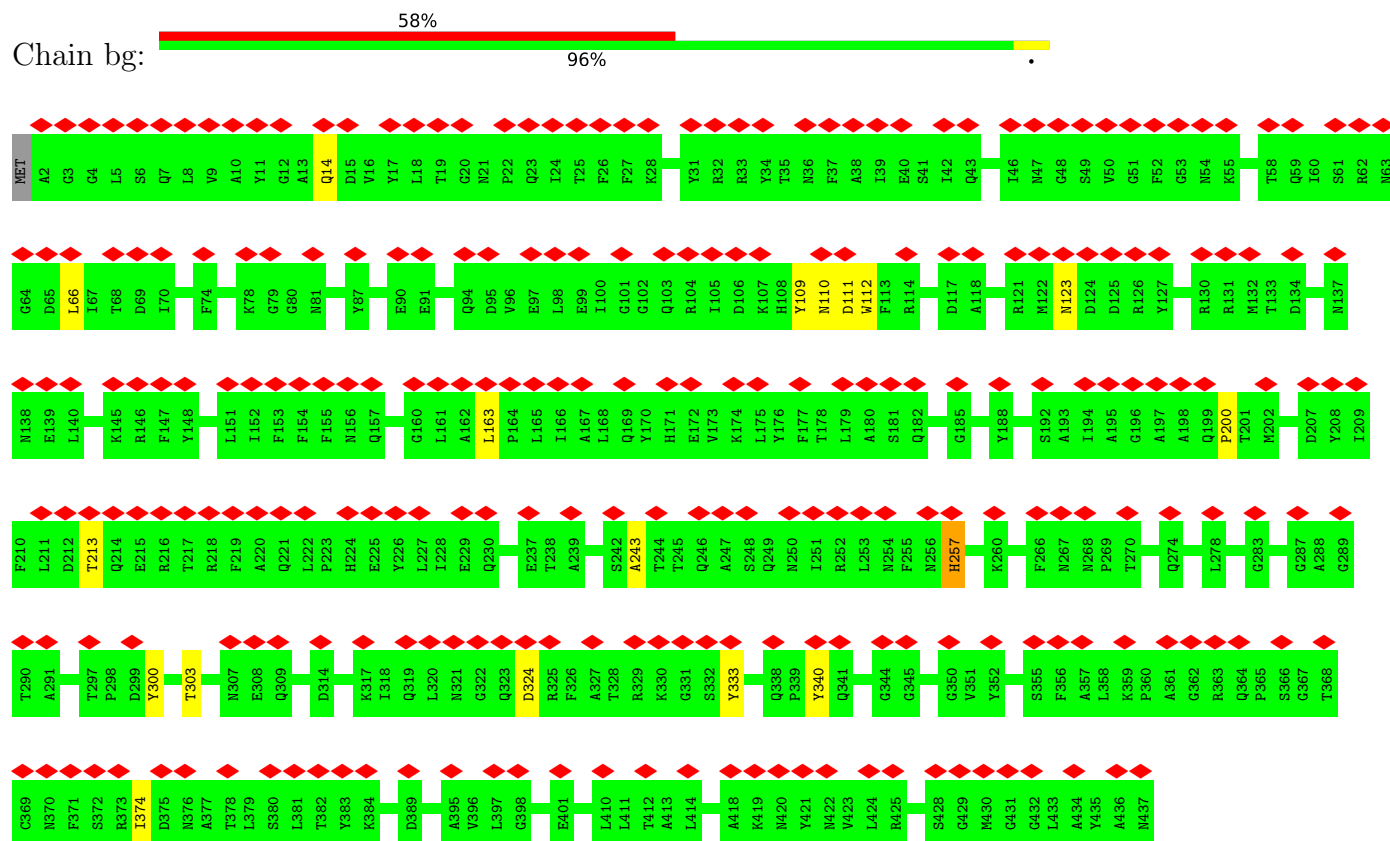
• Molecule 1: Major capsid protein (MCP)



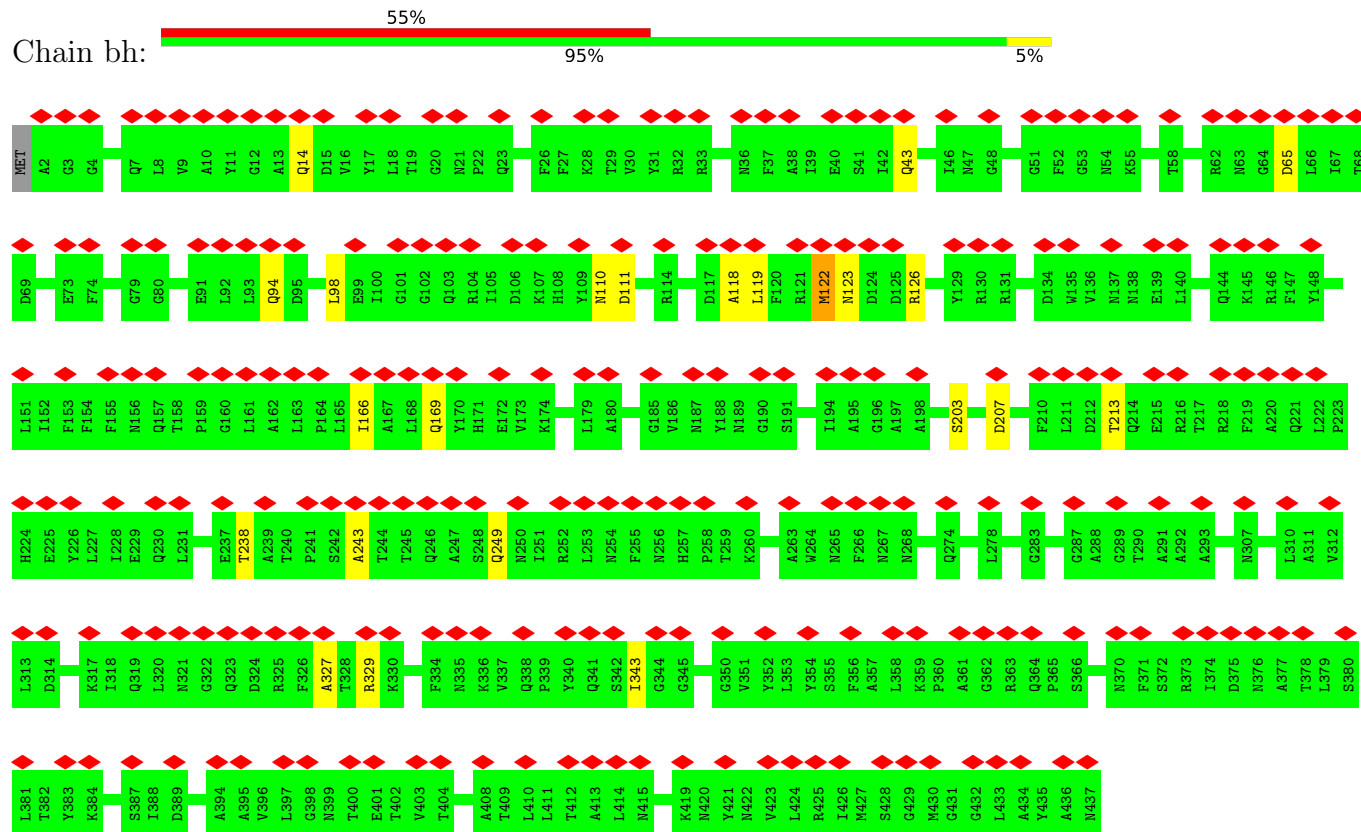
• Molecule 1: Major capsid protein (MCP)



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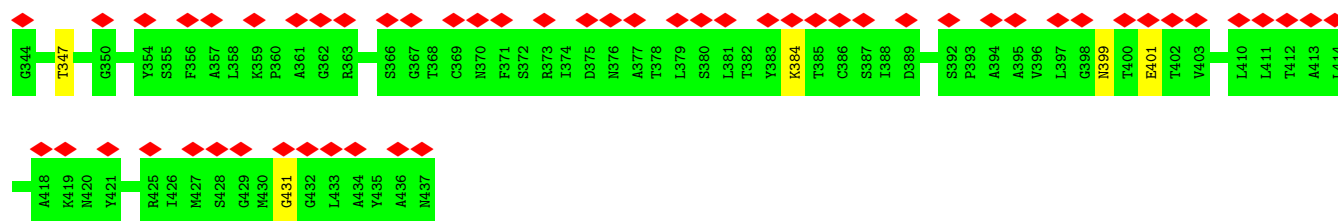


- Molecule 1: Major capsid protein (MCP)

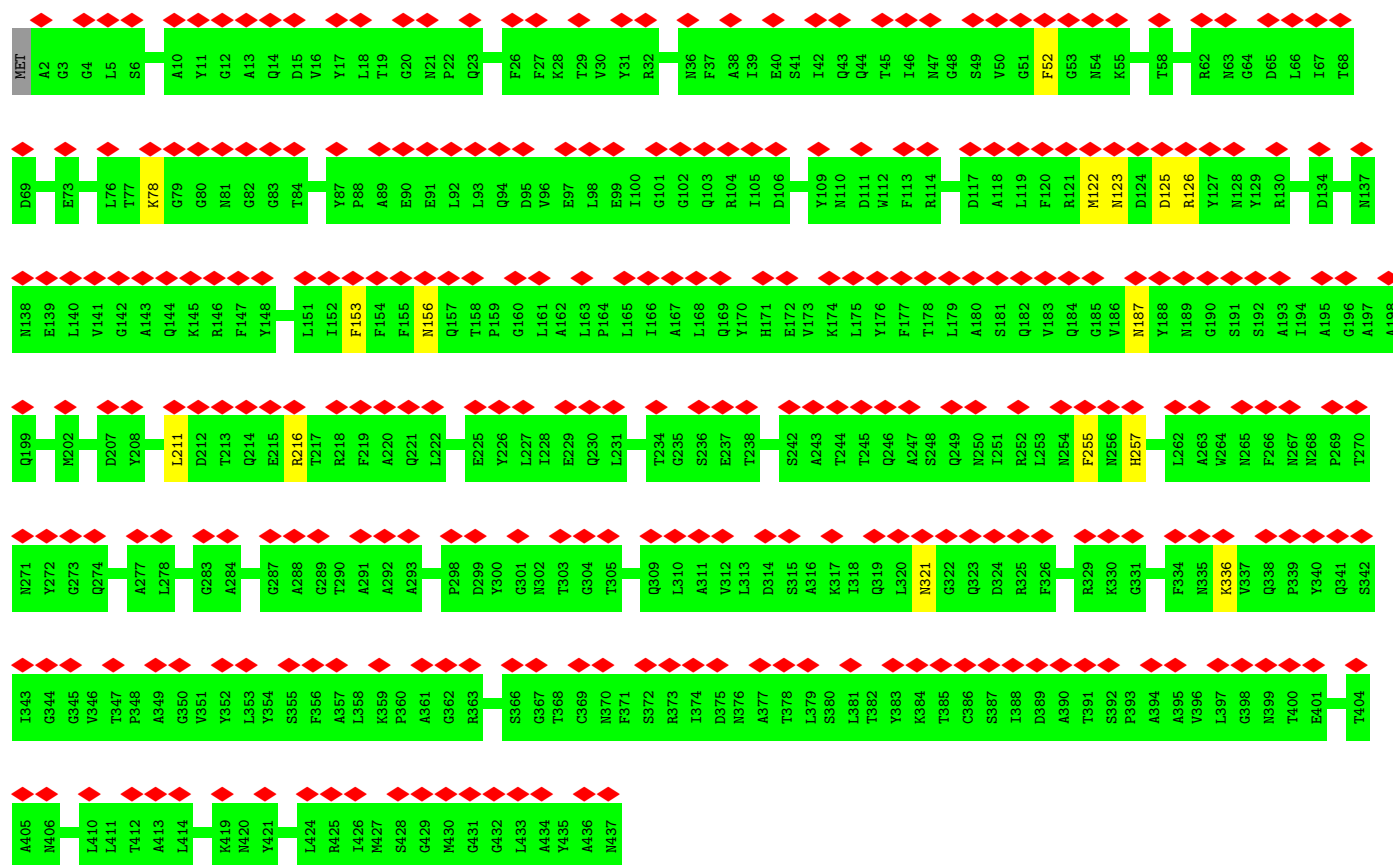


- Molecule 1: Major capsid protein (MCP)

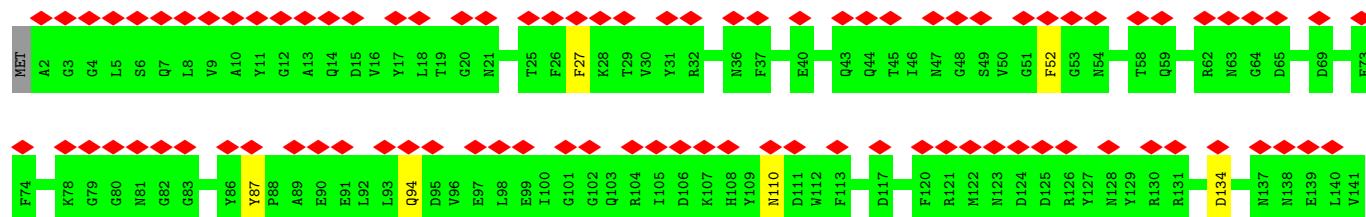


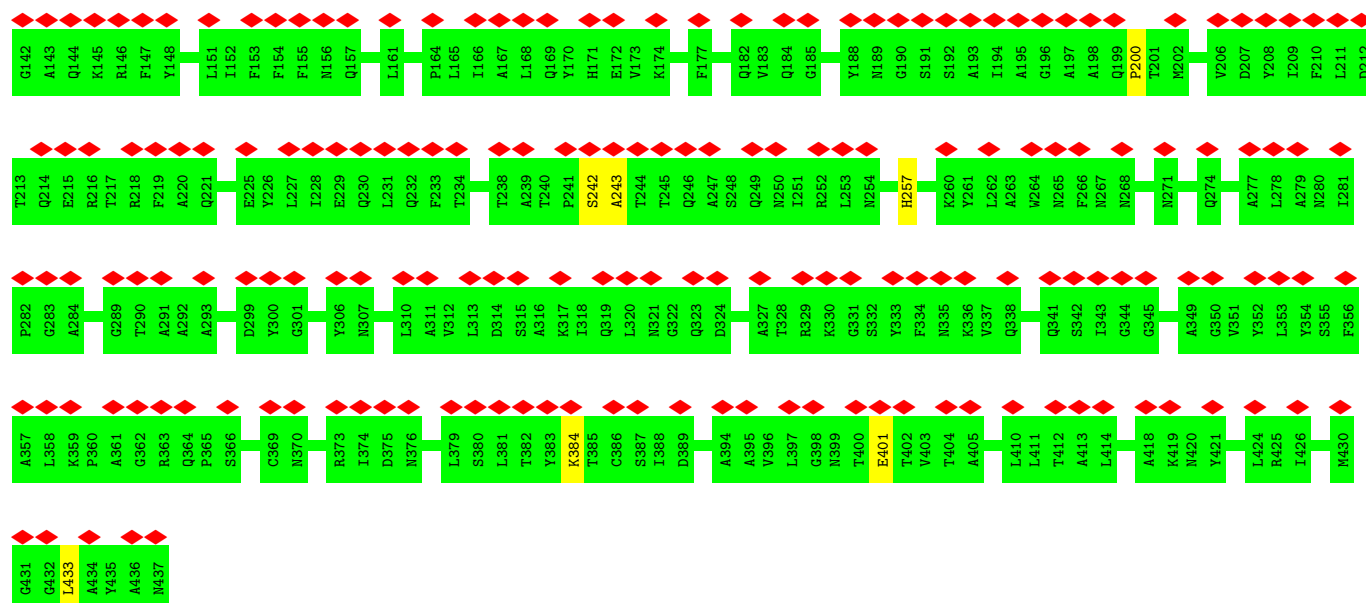


• Molecule 1: Major capsid protein (MCP)

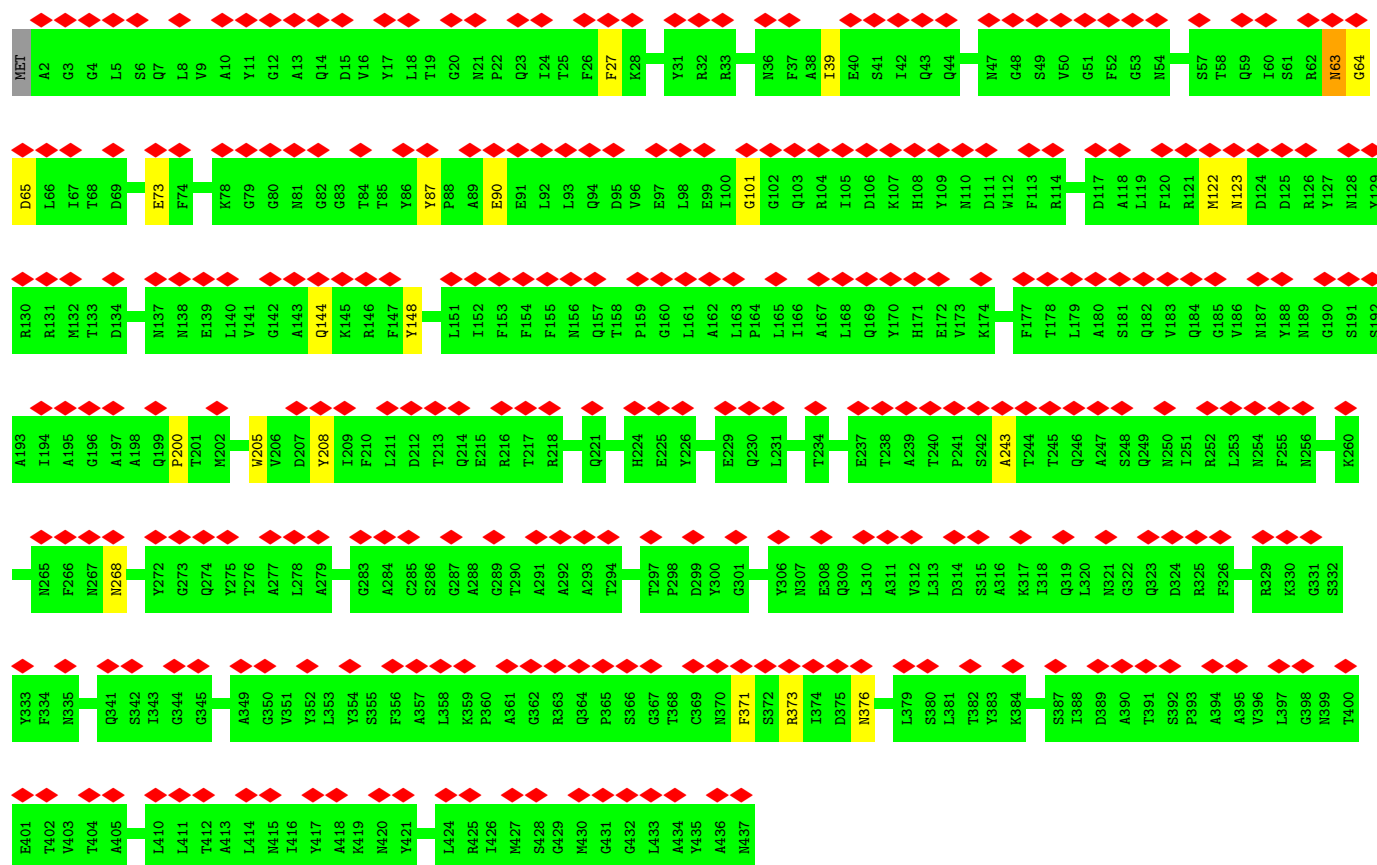


• Molecule 1: Major capsid protein (MCP)

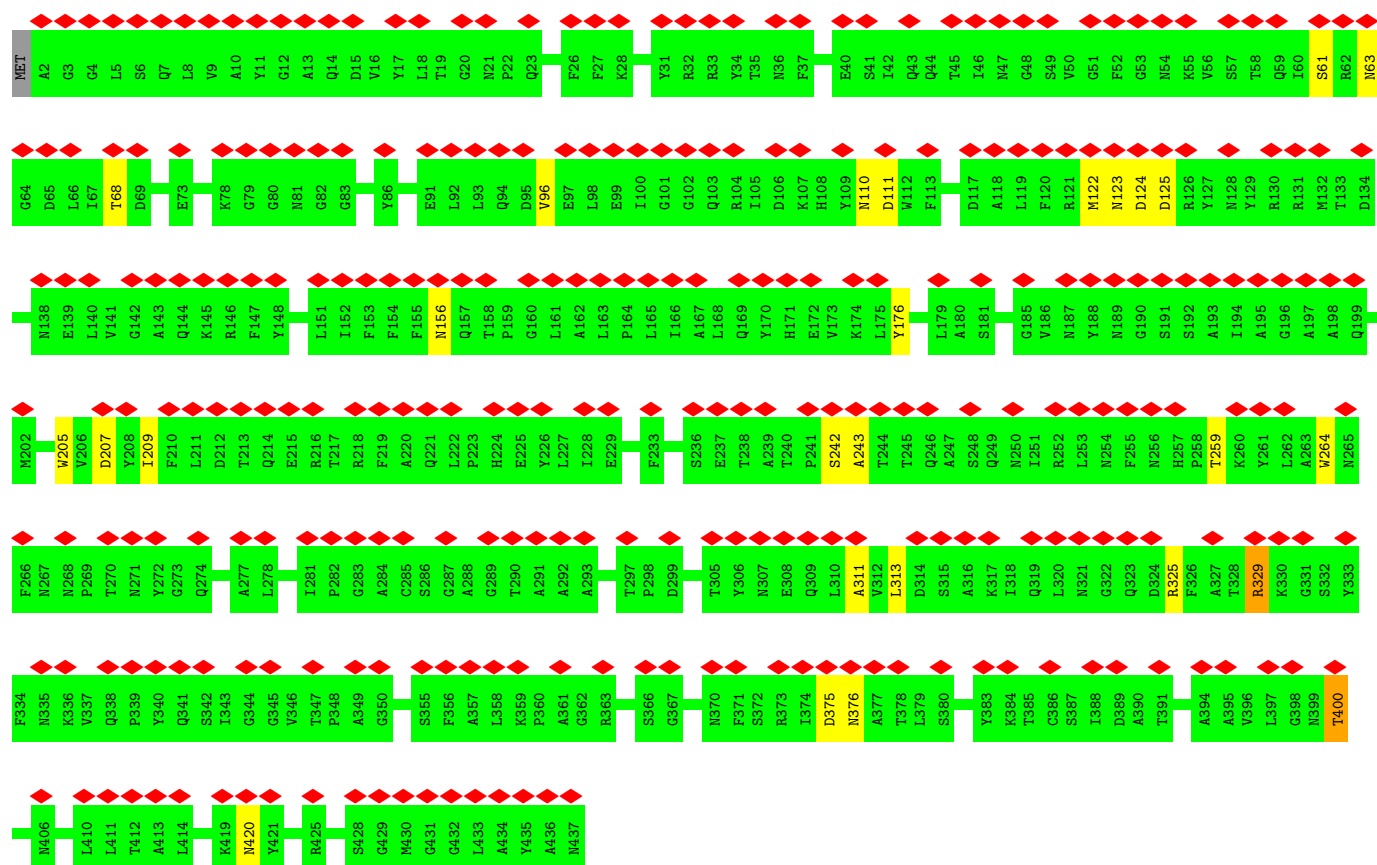




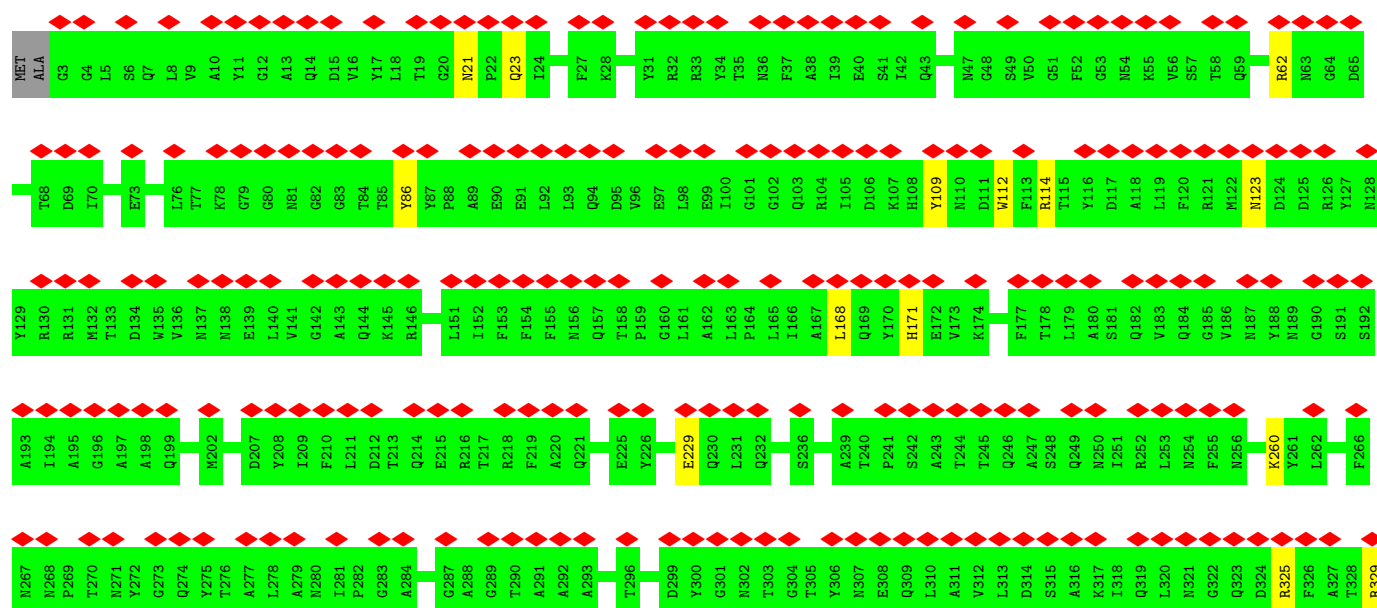
• Molecule 1: Major capsid protein (MCP)

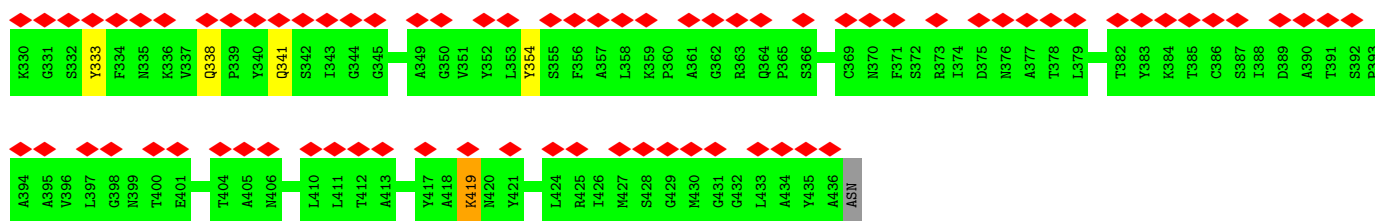


• Molecule 1: Major capsid protein (MCP)

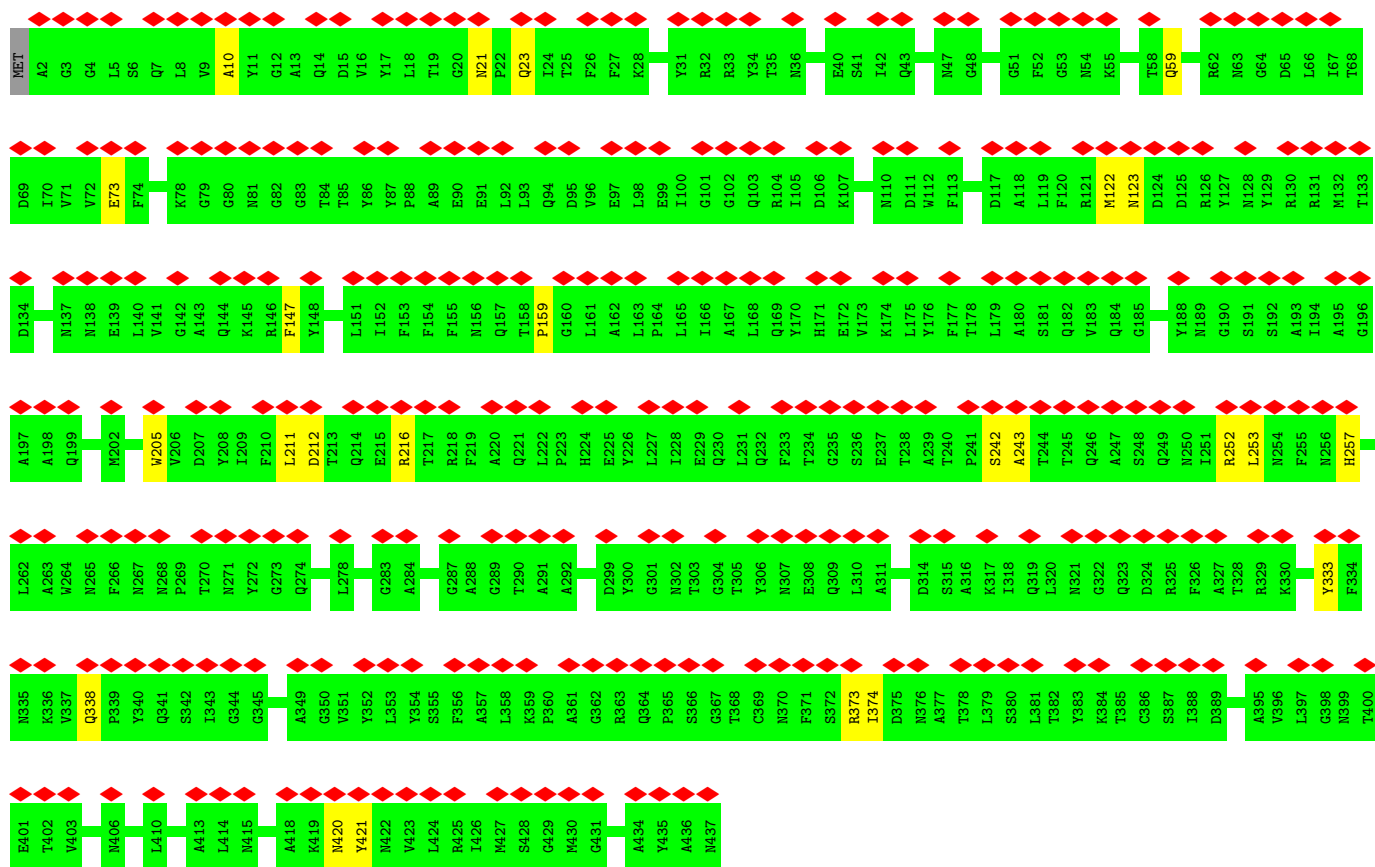


• Molecule 1: Major capsid protein (MCP)

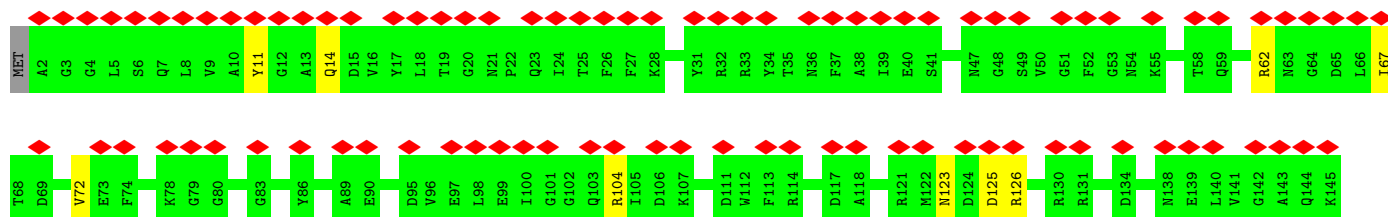


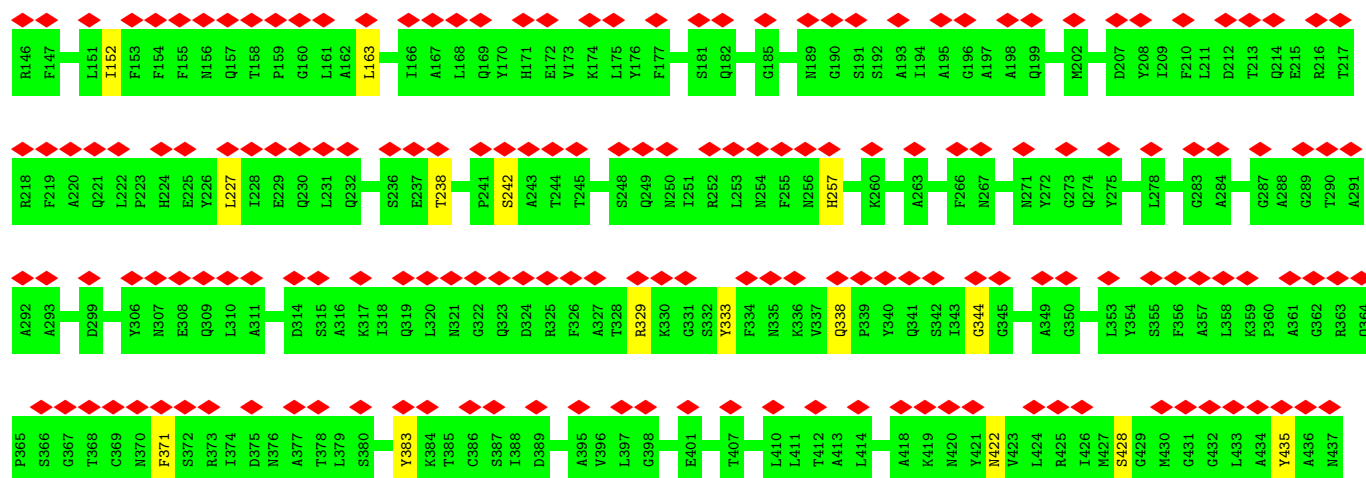


• Molecule 1: Major capsid protein (MCP)

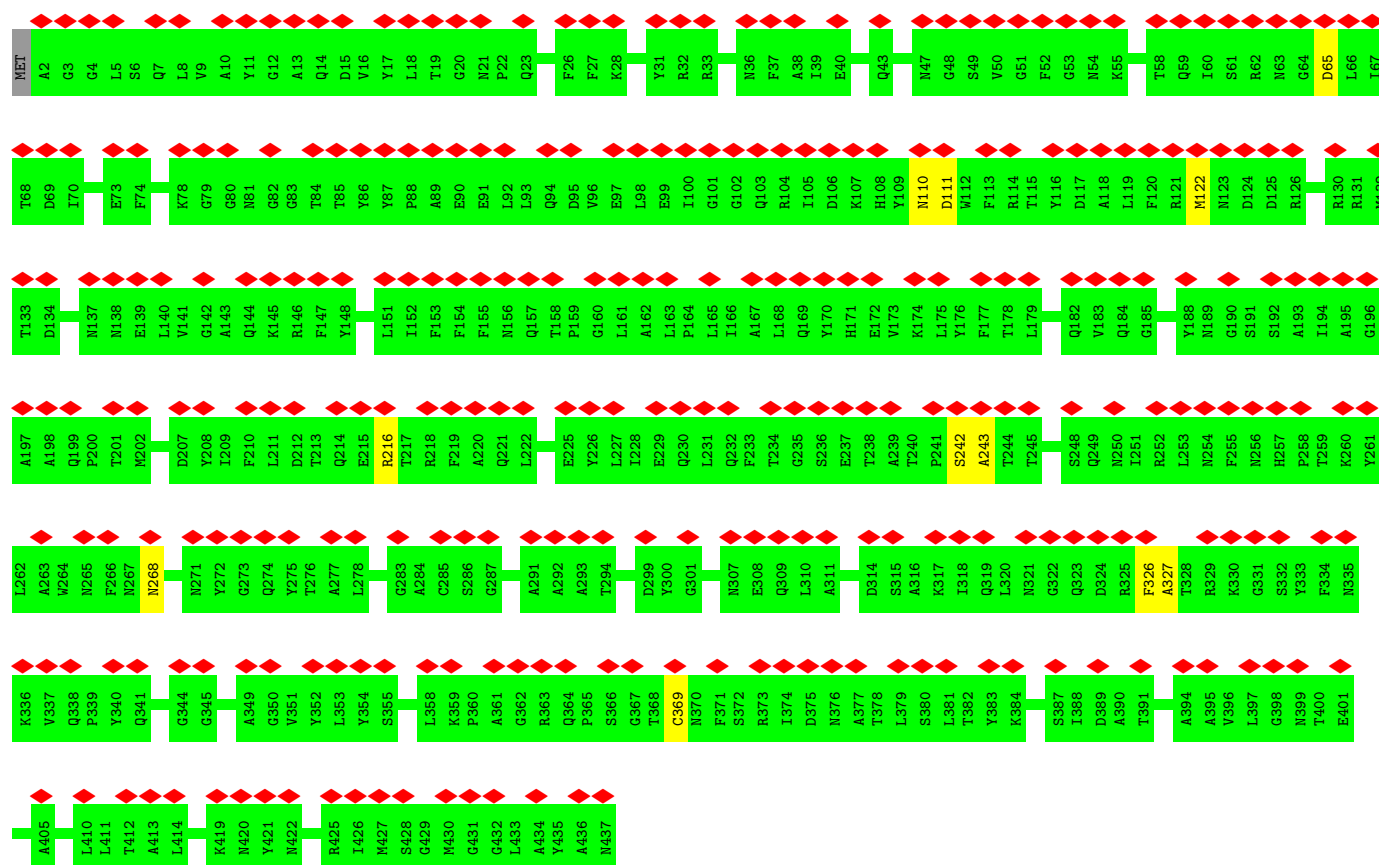


• Molecule 1: Major capsid protein (MCP)





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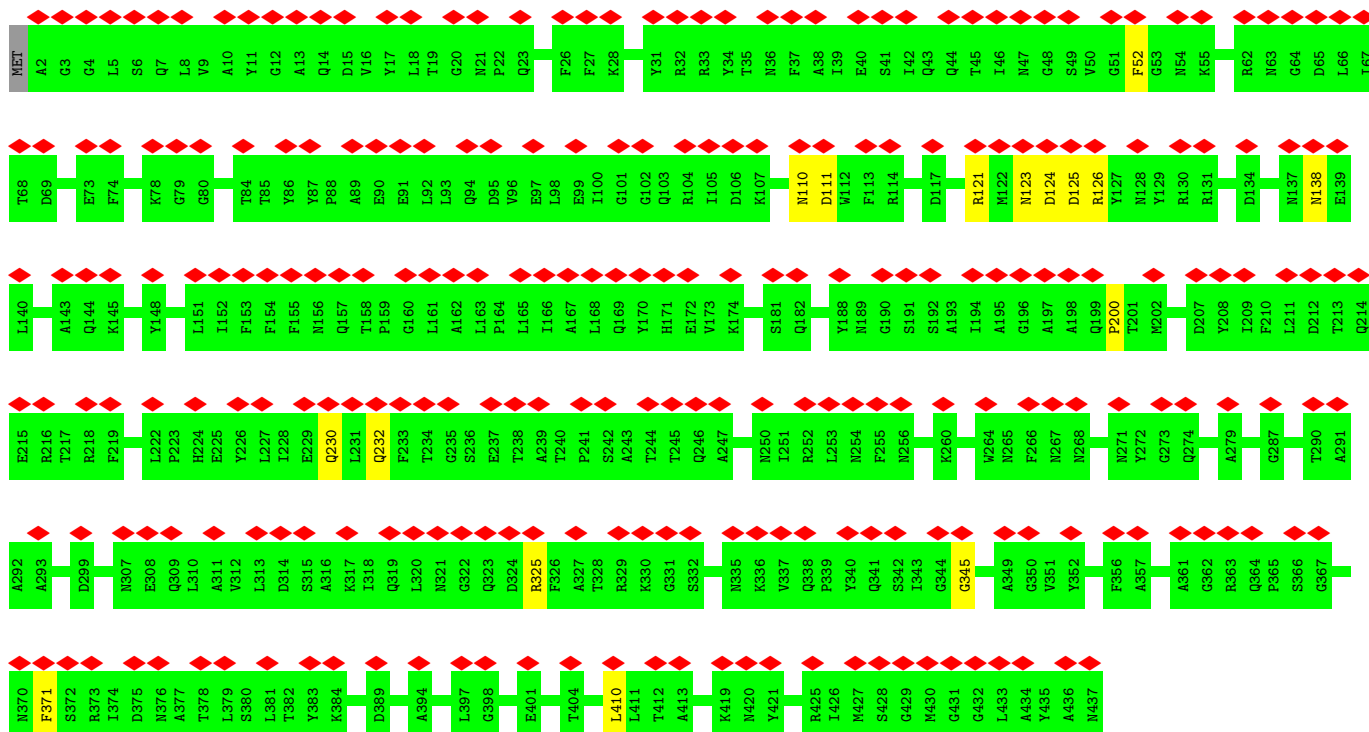


• Molecule 1: Major capsid protein (MCP)





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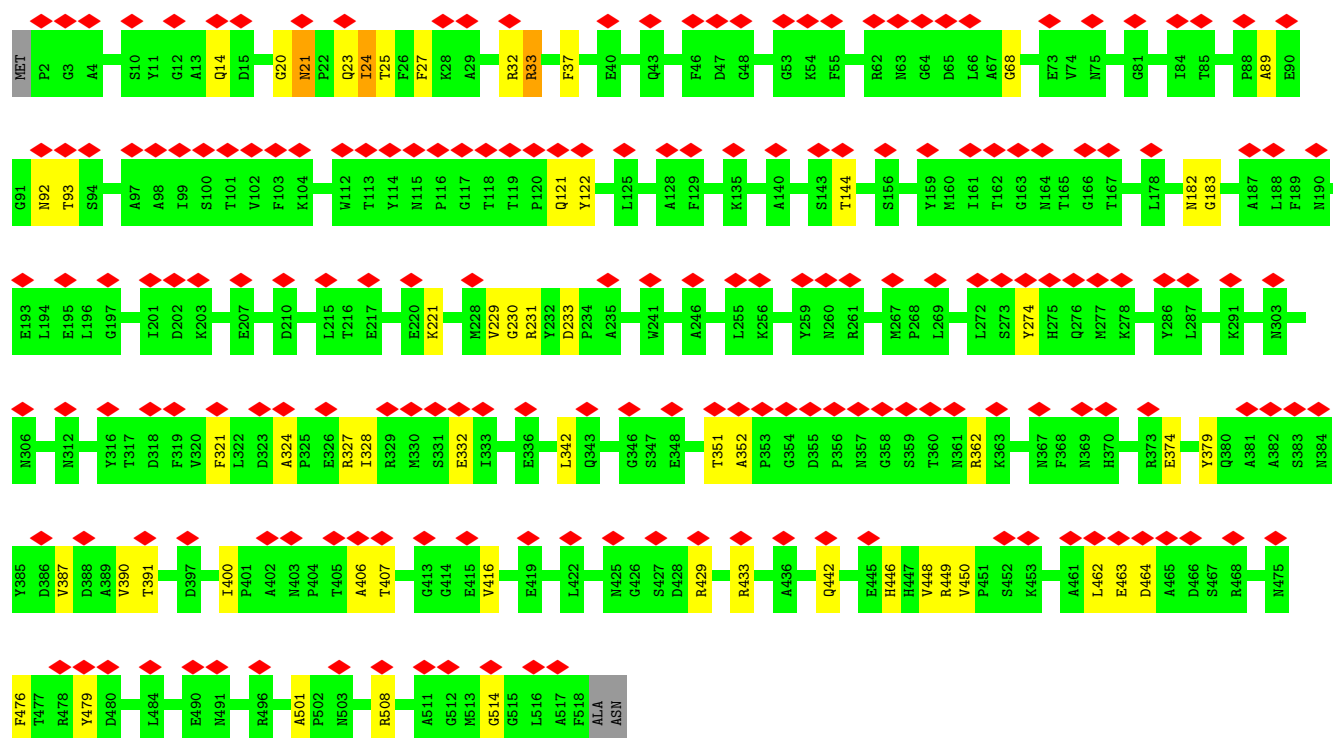


• Molecule 2: MCPv1



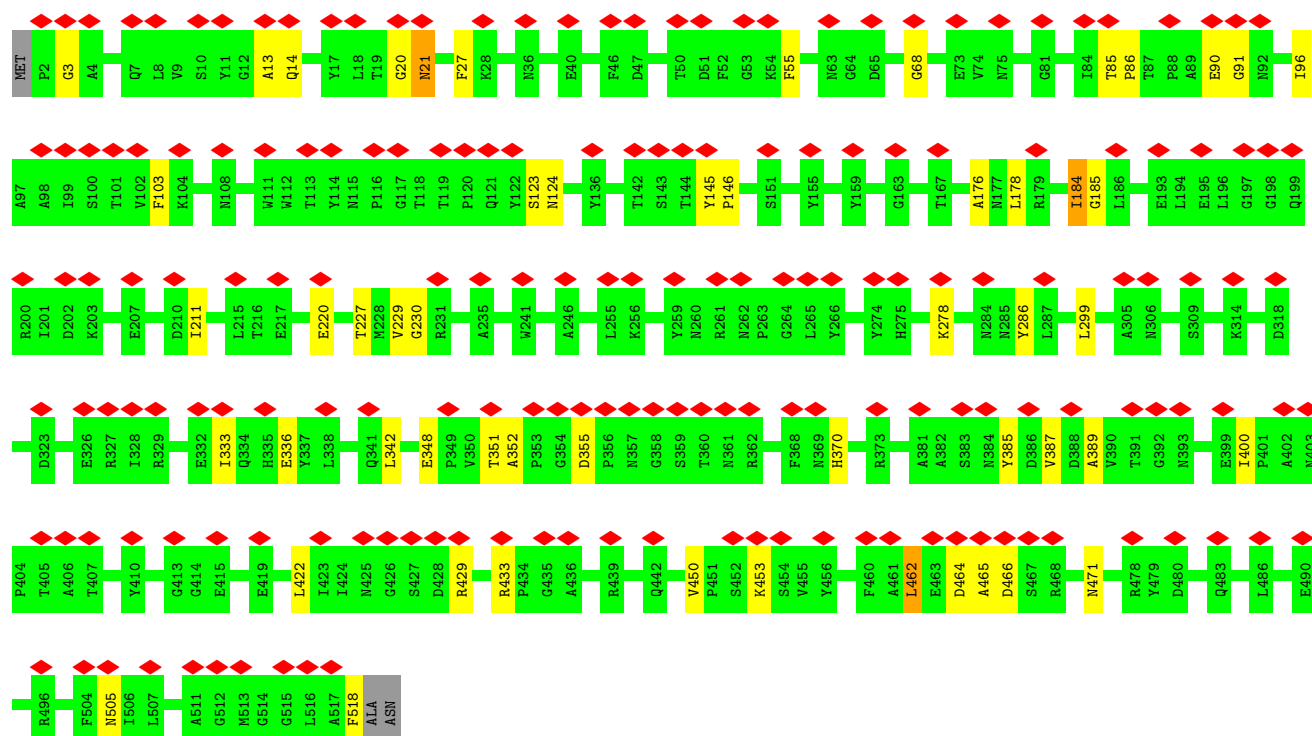
• Molecule 2: MCPv1

Chain bv: 



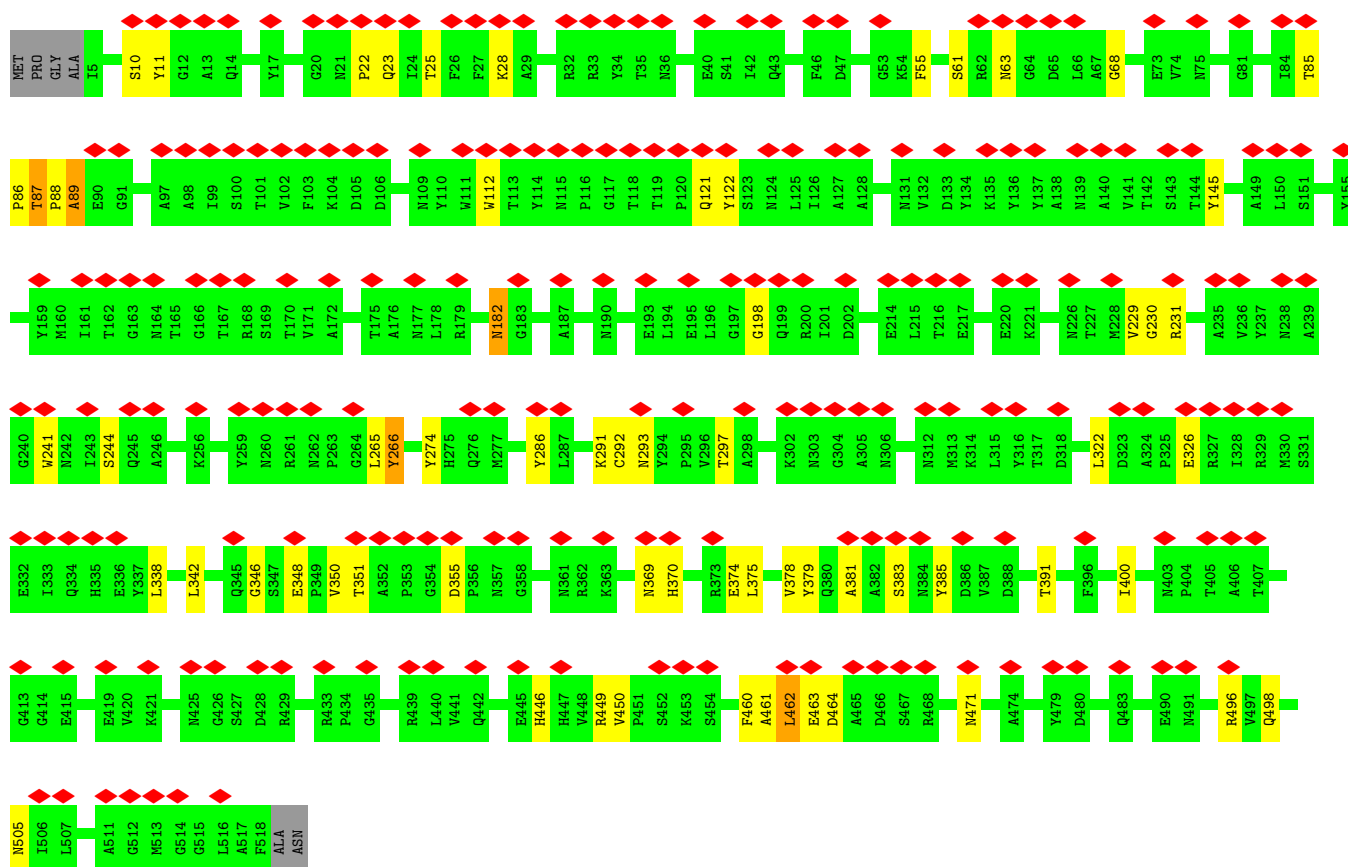
• Molecule 2: MCPv1

Chain bw: 



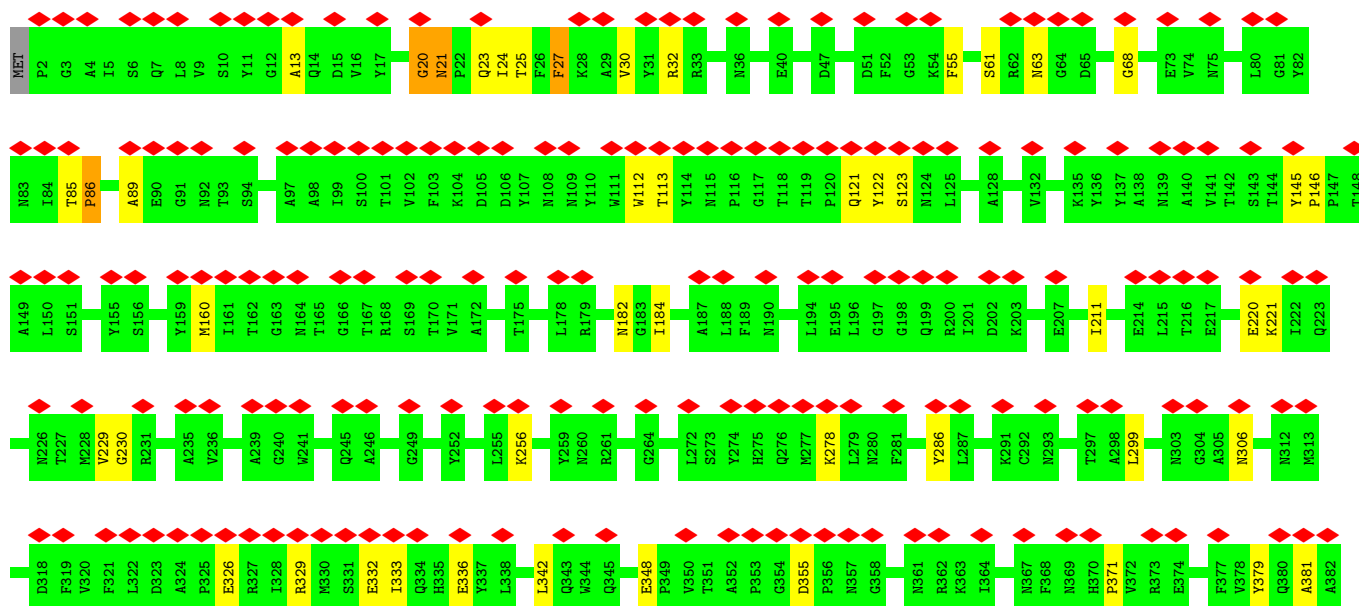
• Molecule 2: MCPv1

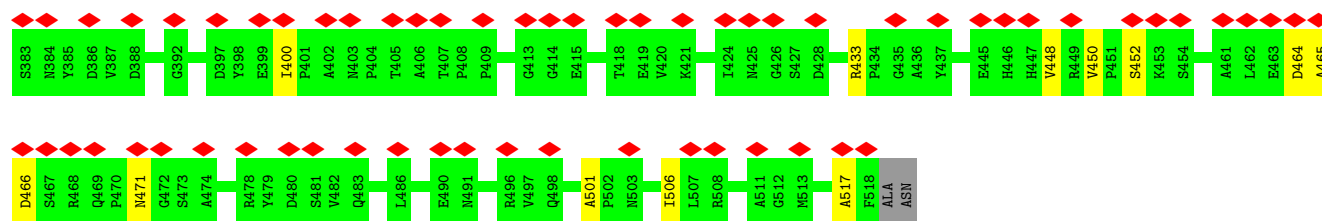
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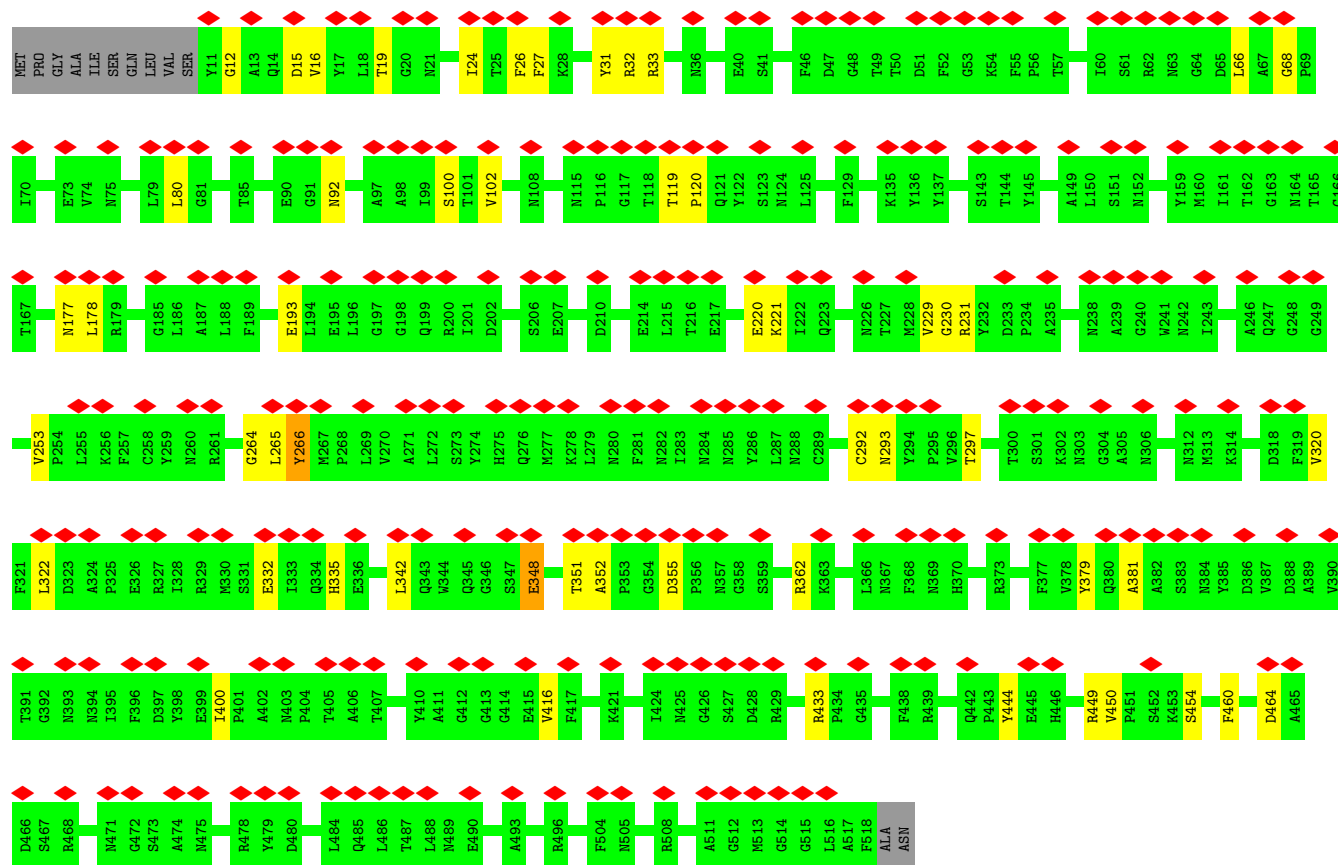
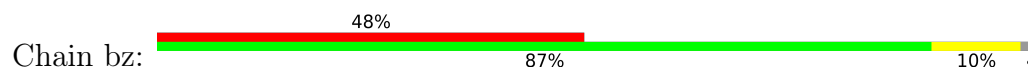
• Molecule 2: MCPv1

Chain by: 

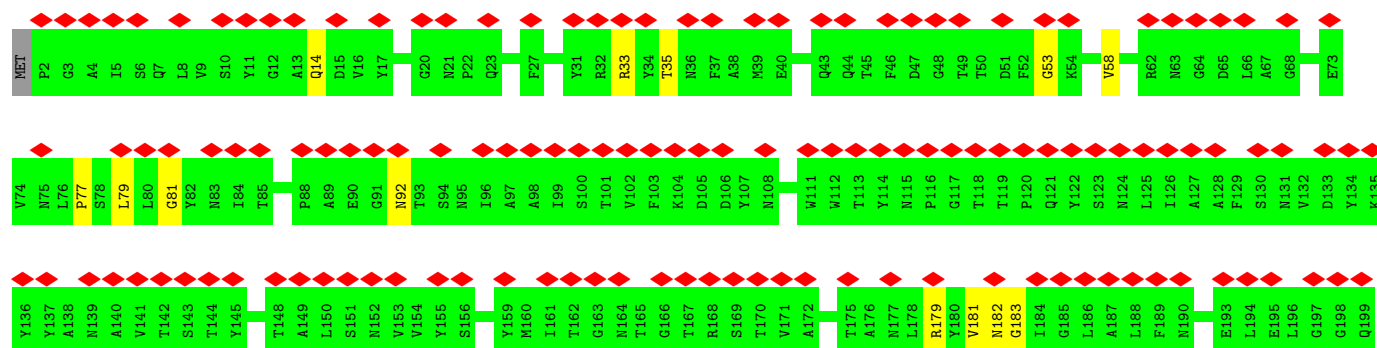


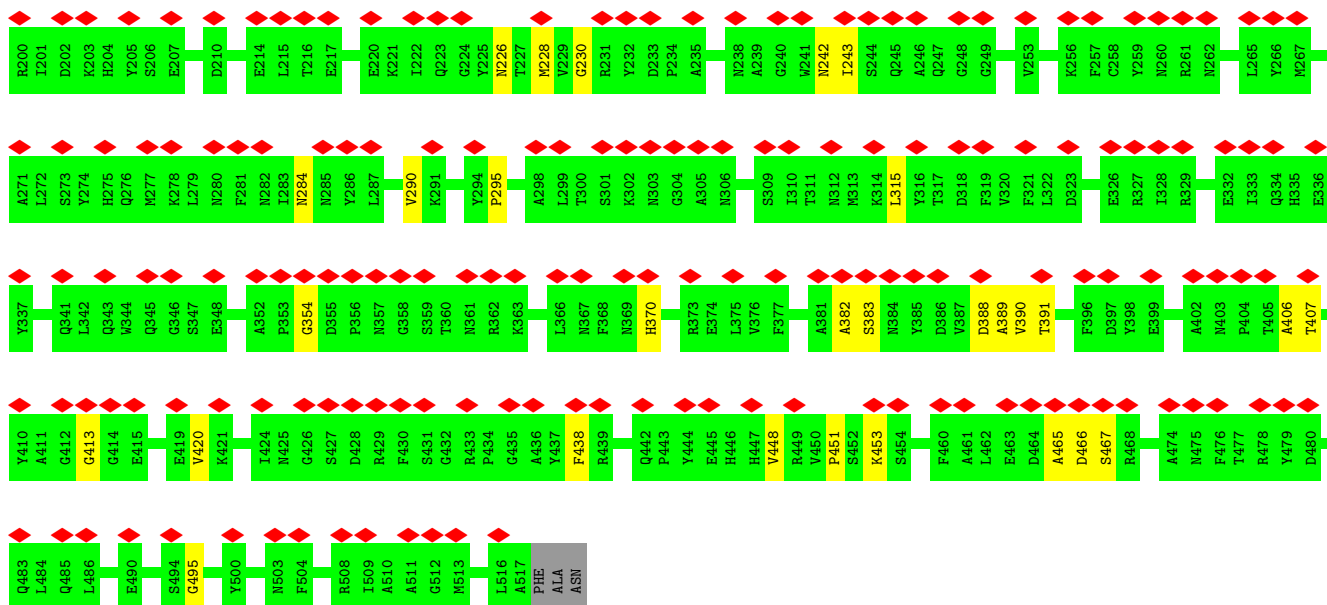


• Molecule 2: MCPv1

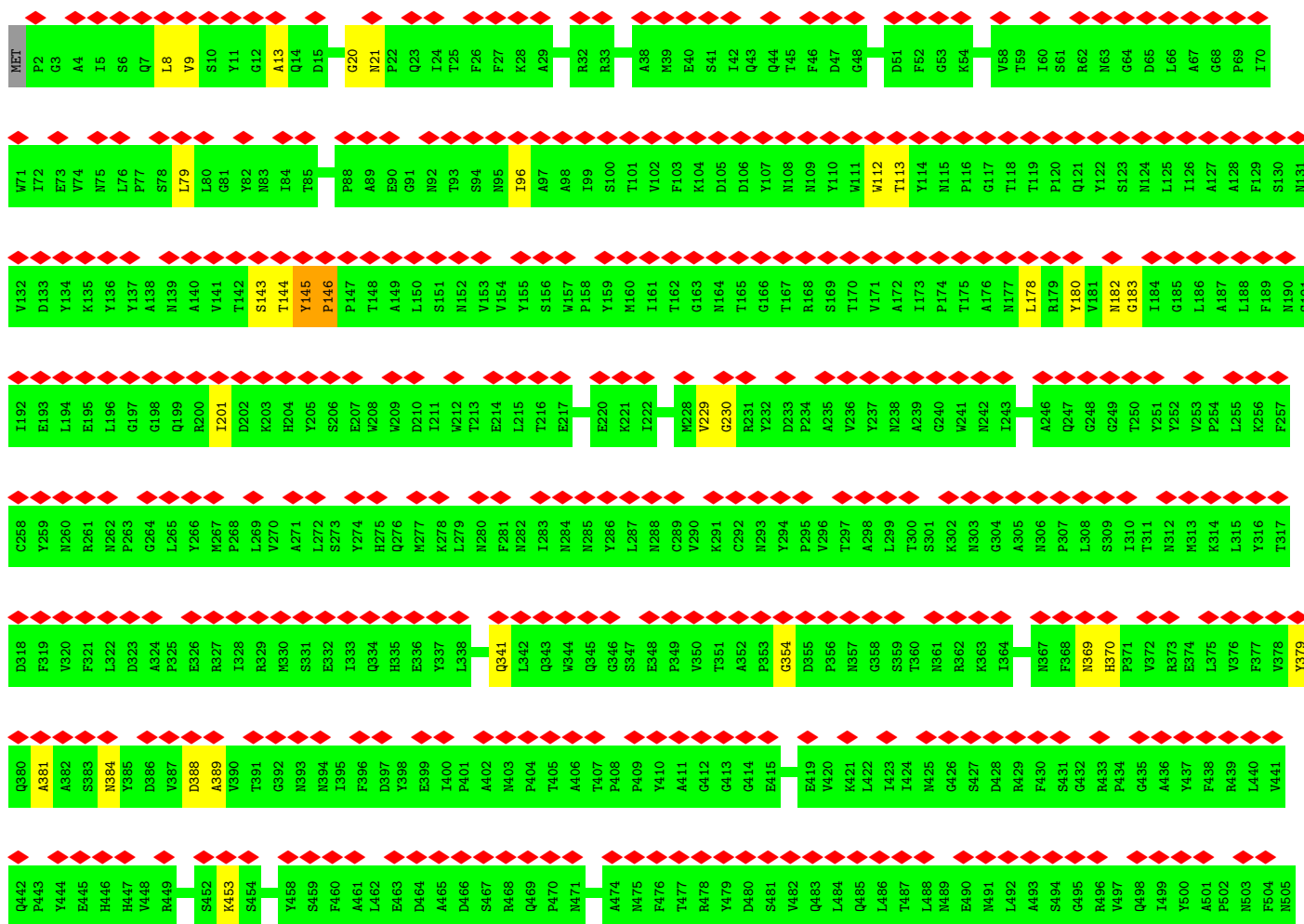
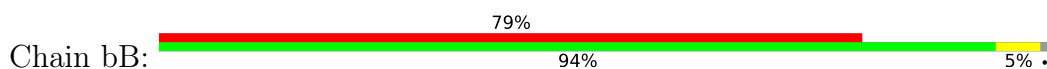


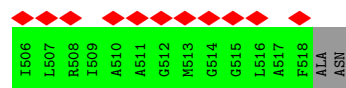
• Molecule 2: MCPv1



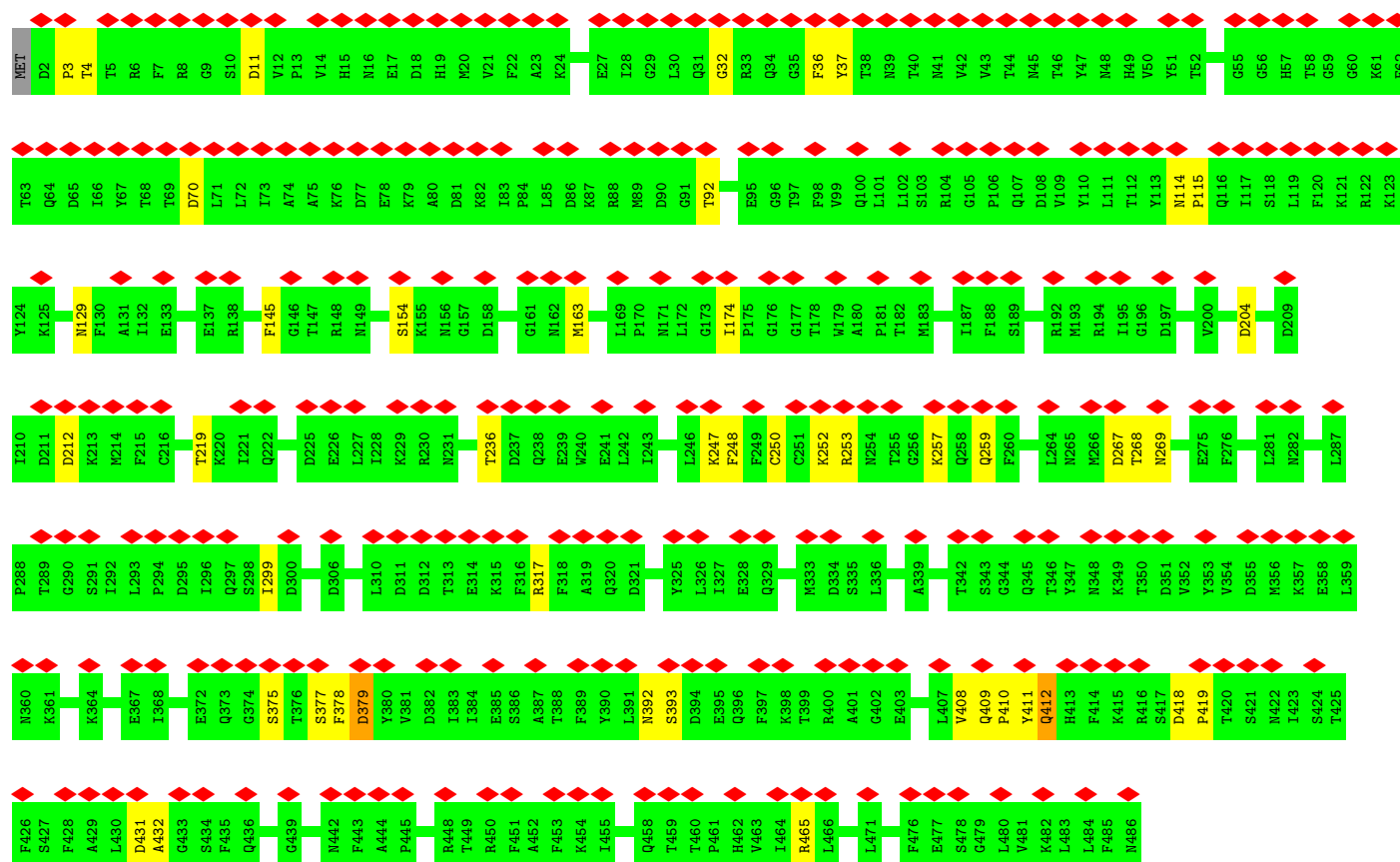
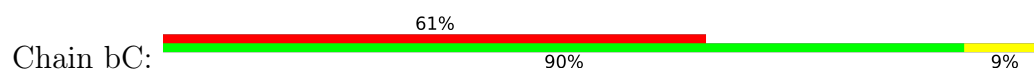


• Molecule 2: MCPv1

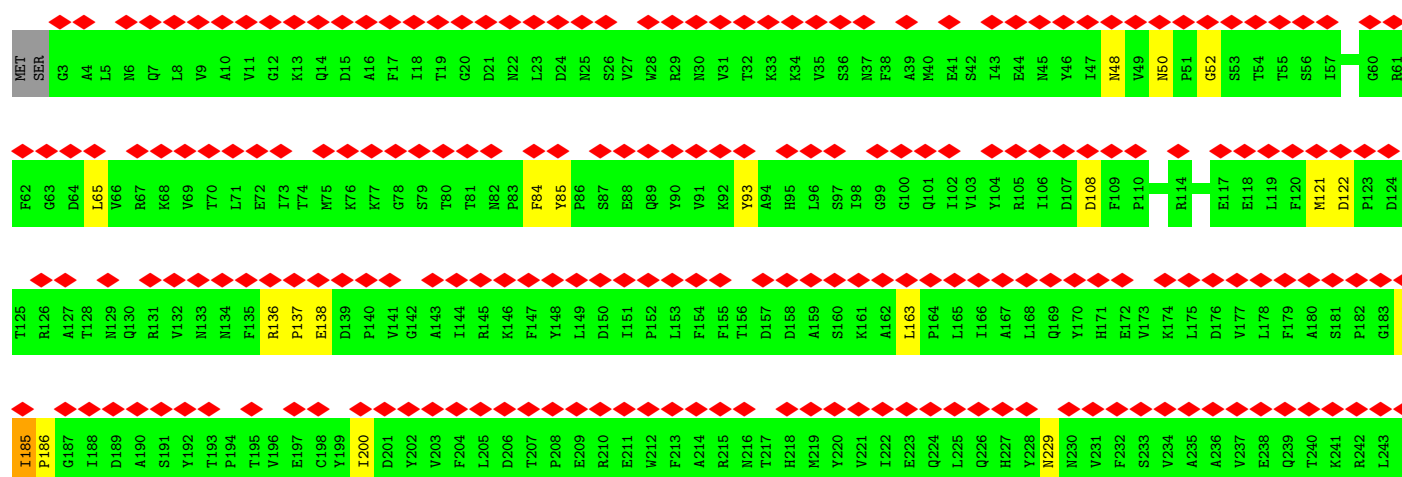
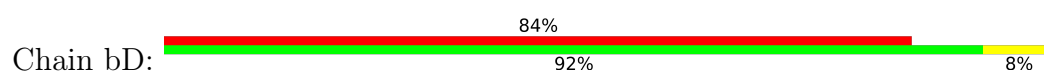


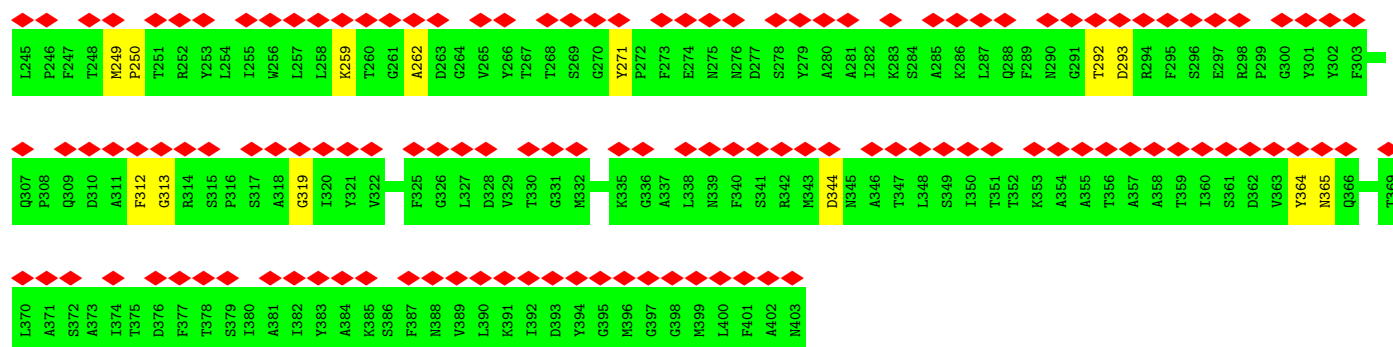


• Molecule 3: MCPv2

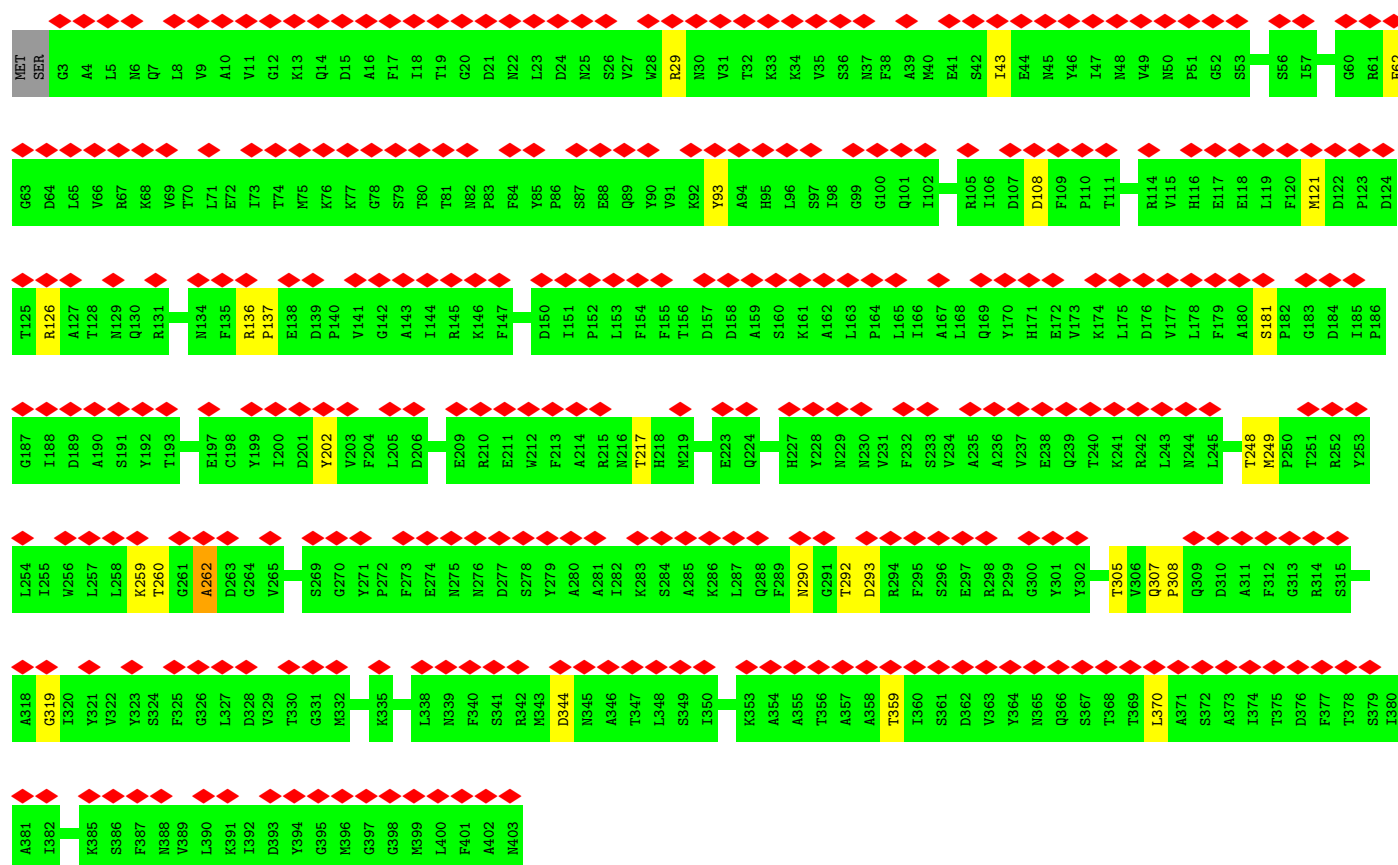
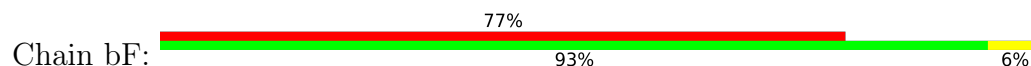


• Molecule 4: MCPv3

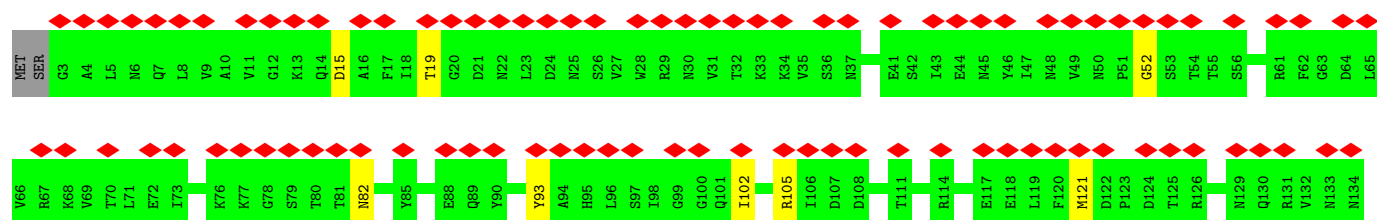


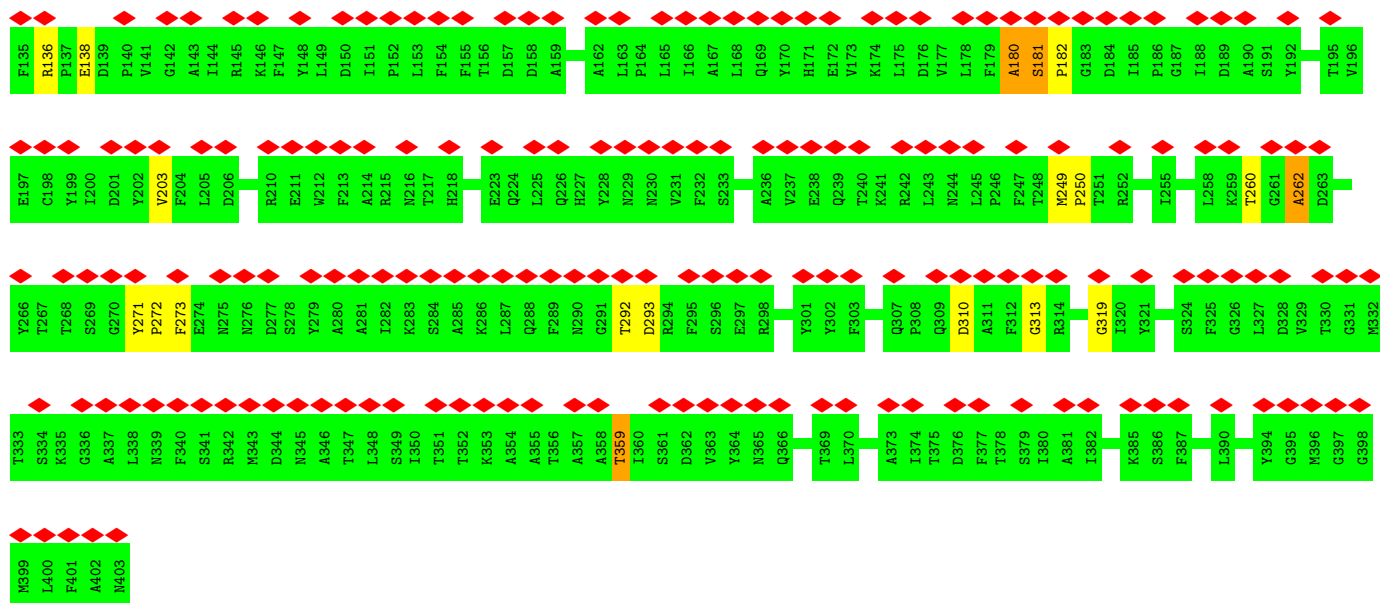


• Molecule 4: MCPv3

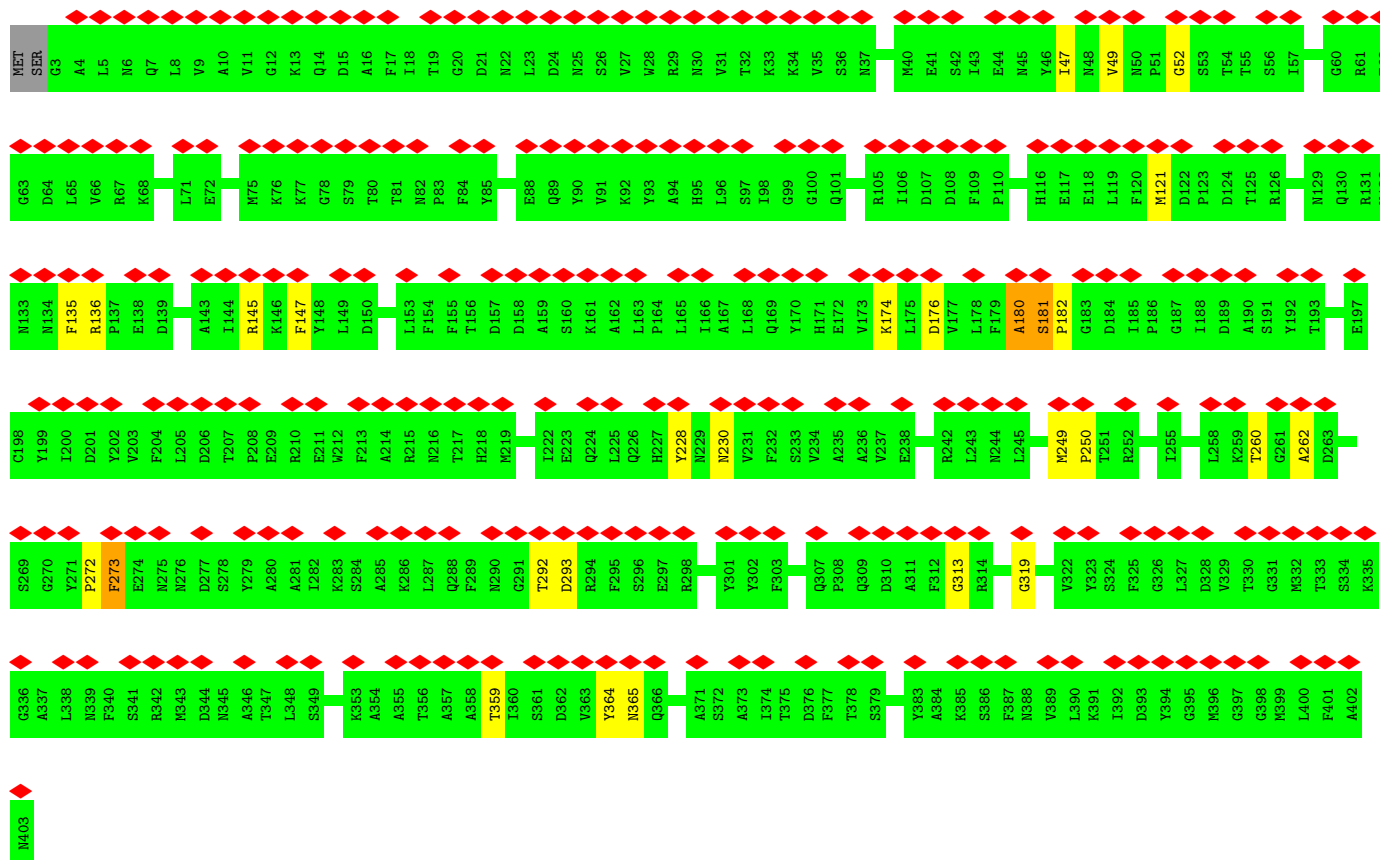


• Molecule 4: MCPv3

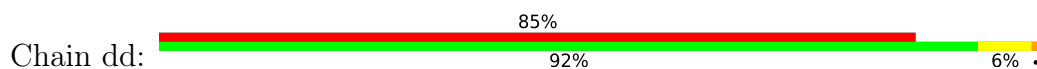


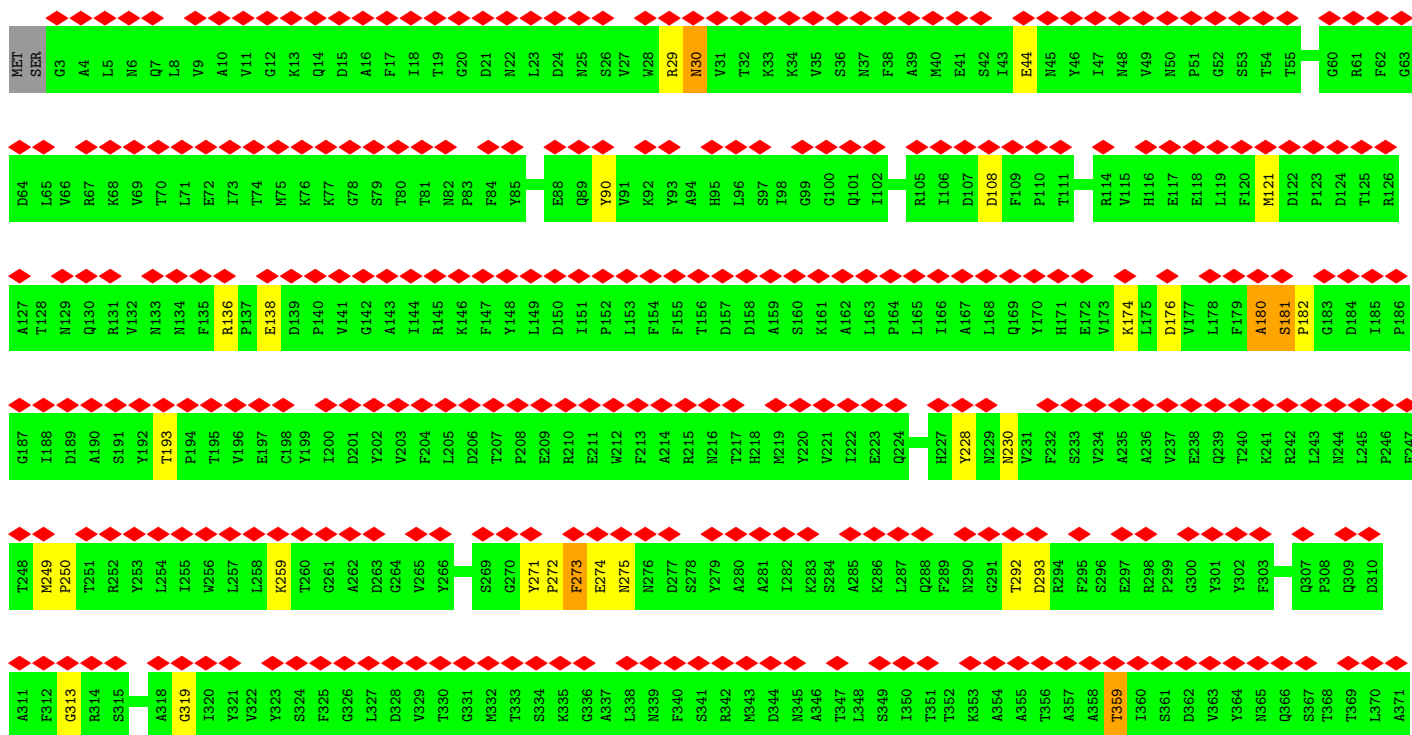


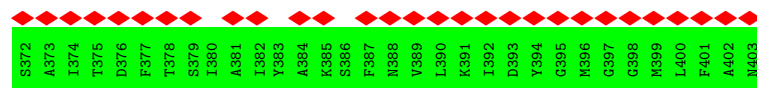
• Molecule 4: MCPv3



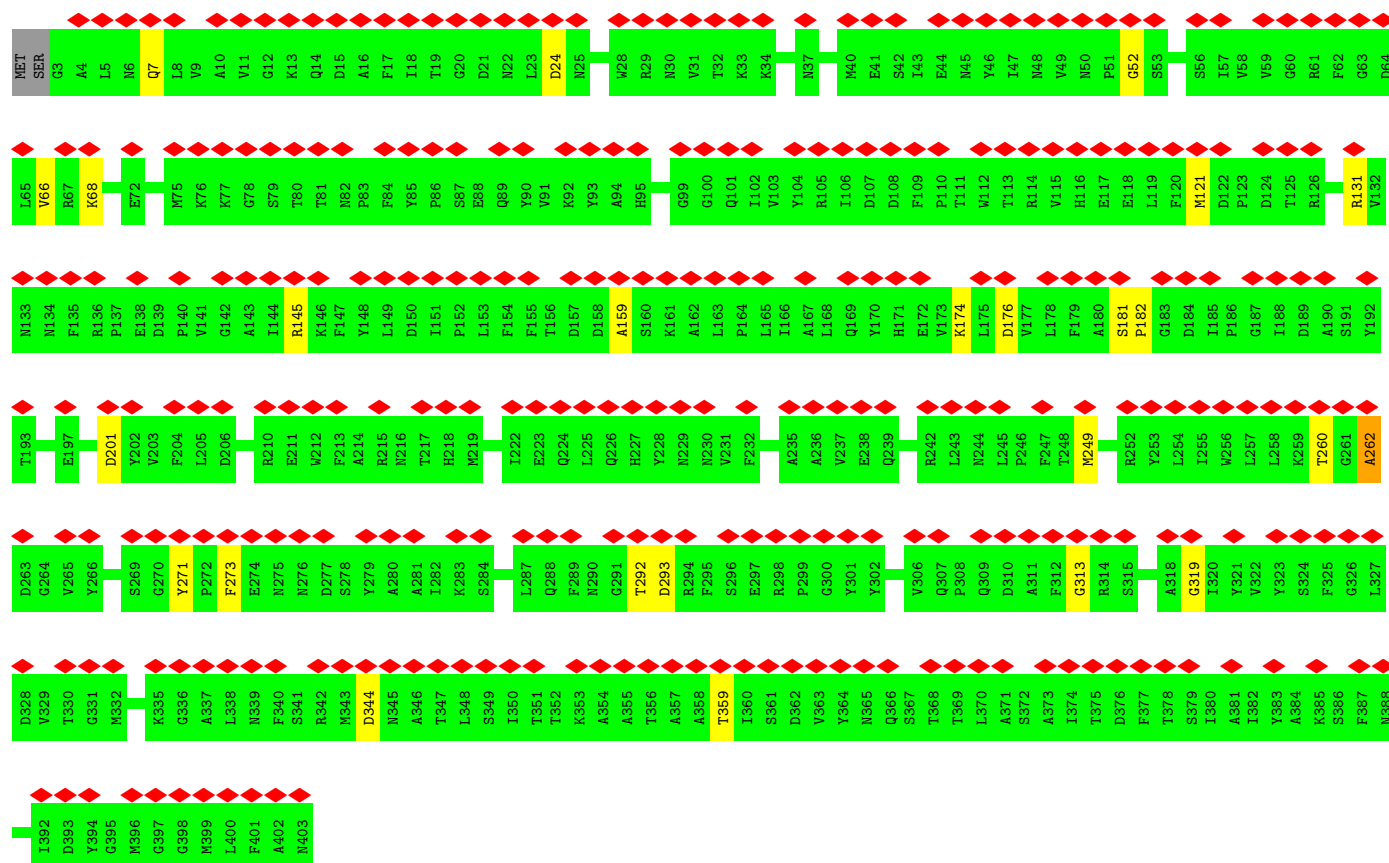
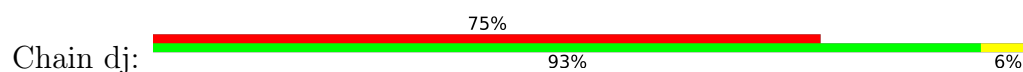
• Molecule 4: MCPv3



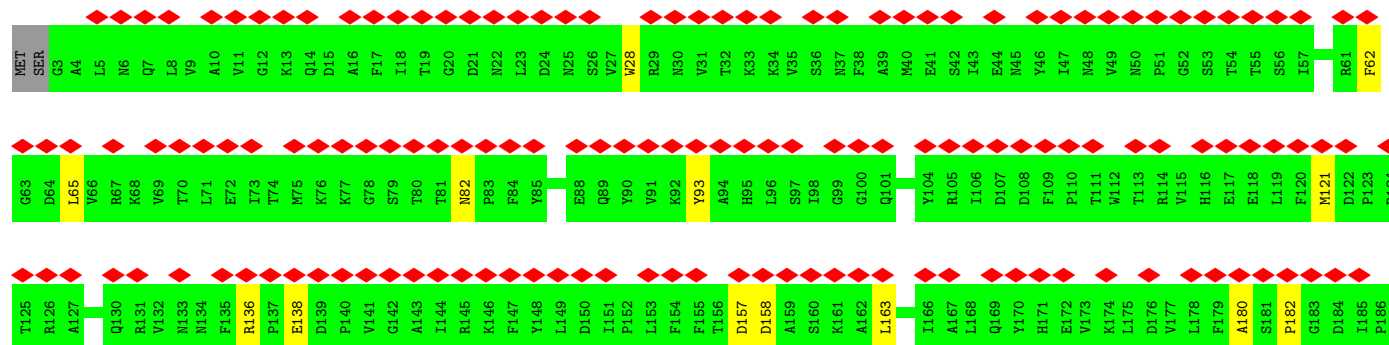
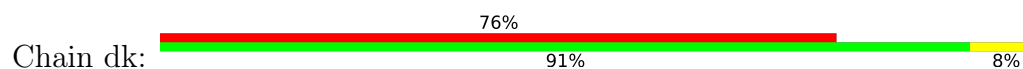


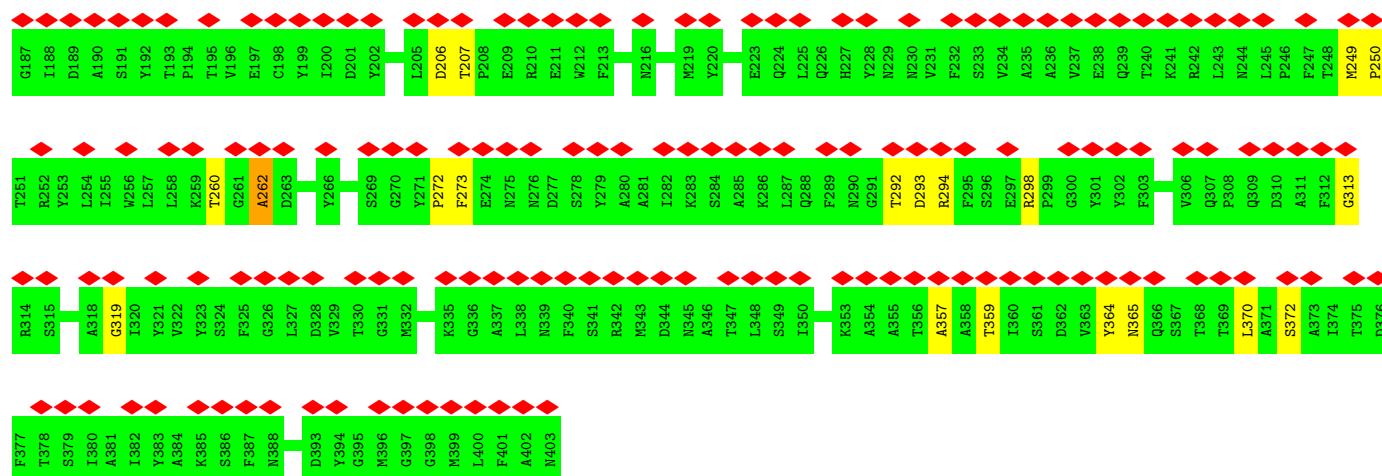


• Molecule 4: MCPv3

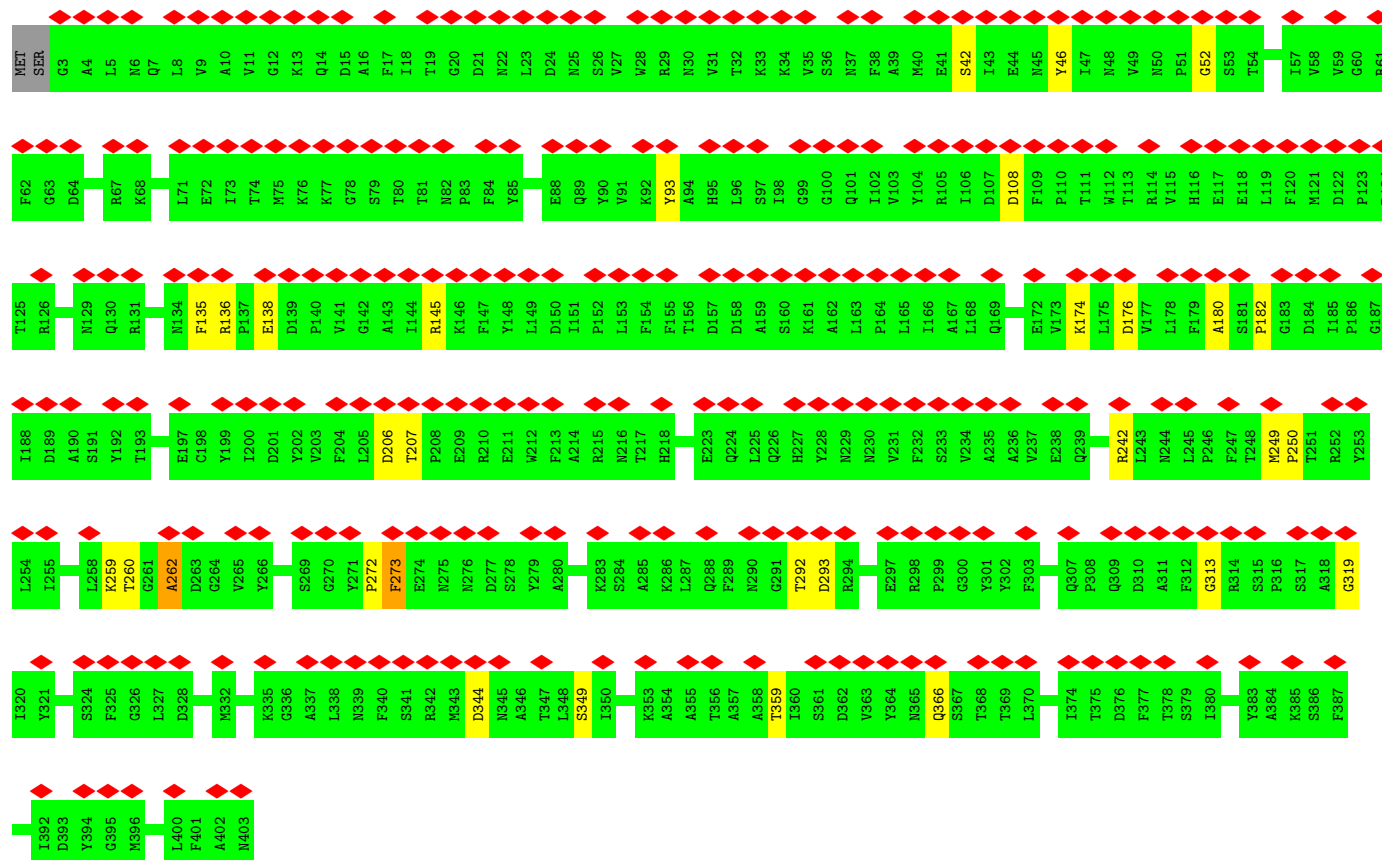
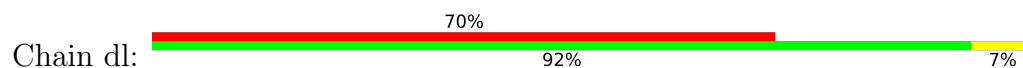


• Molecule 4: MCPv3

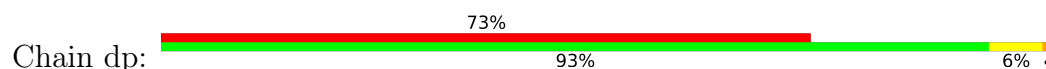


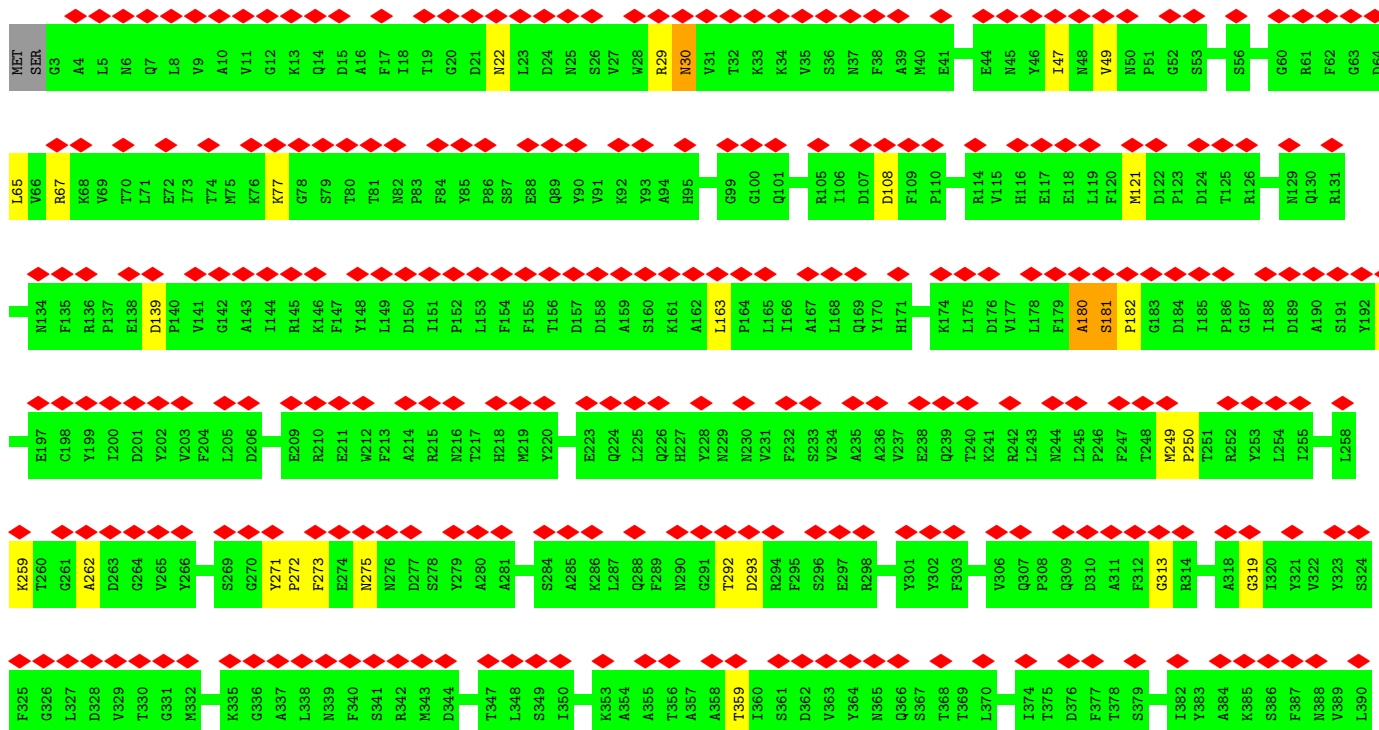


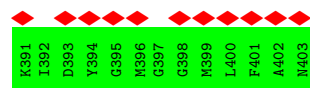
• Molecule 4: MCPv3



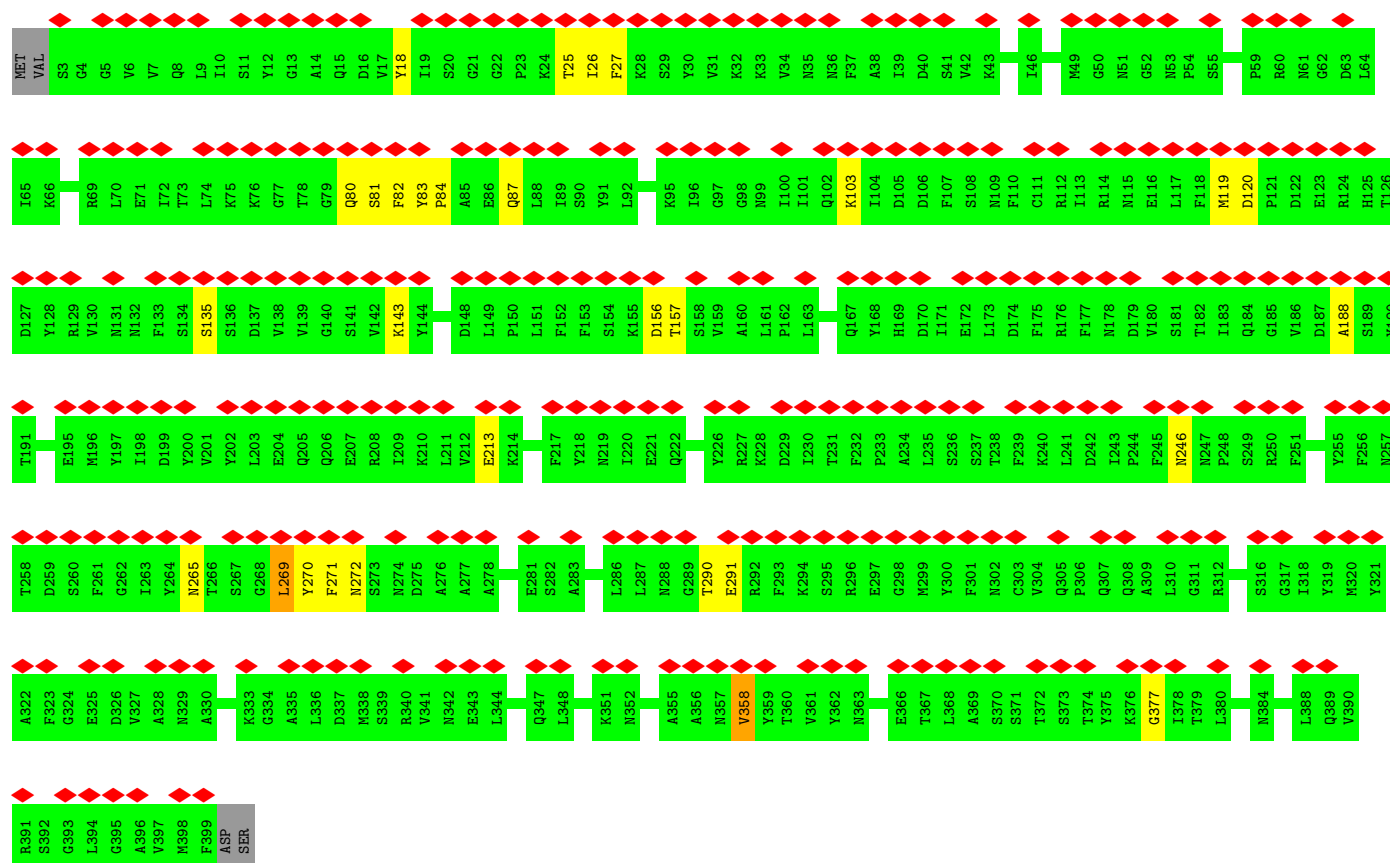
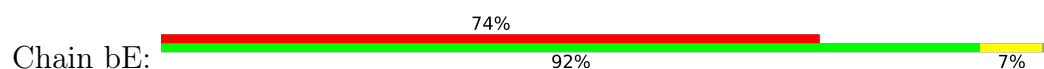
• Molecule 4: MCPv3



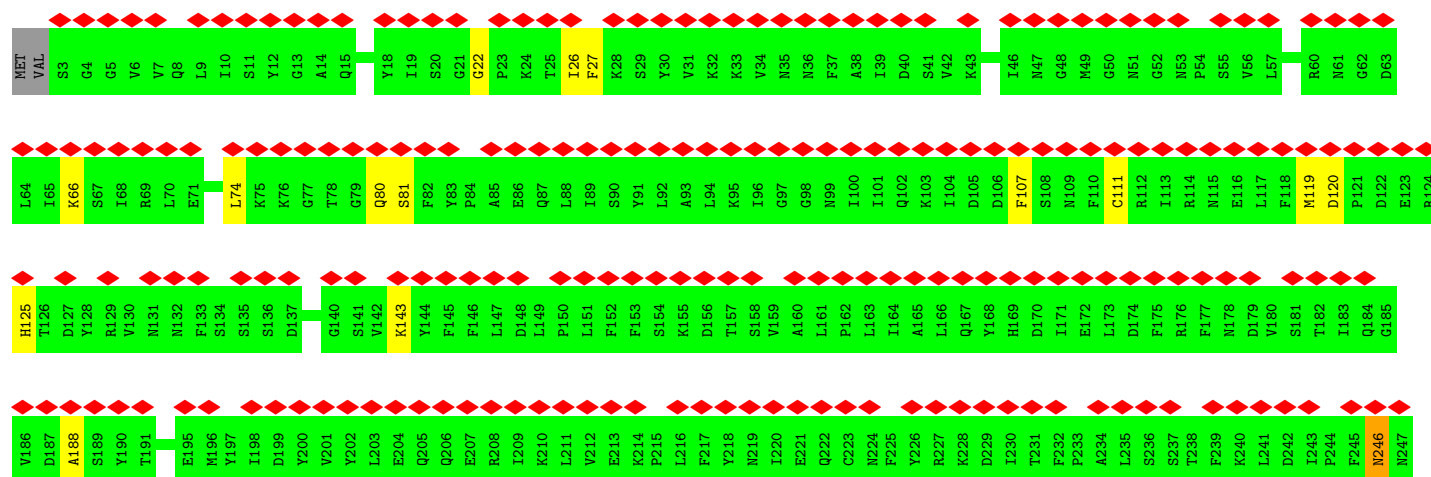
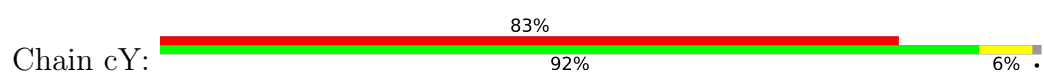


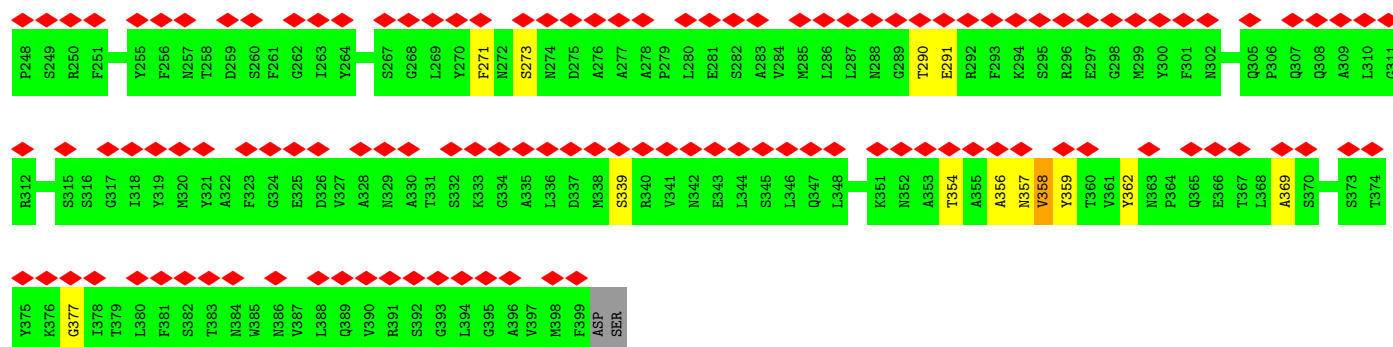


● Molecule 5: MCPv4

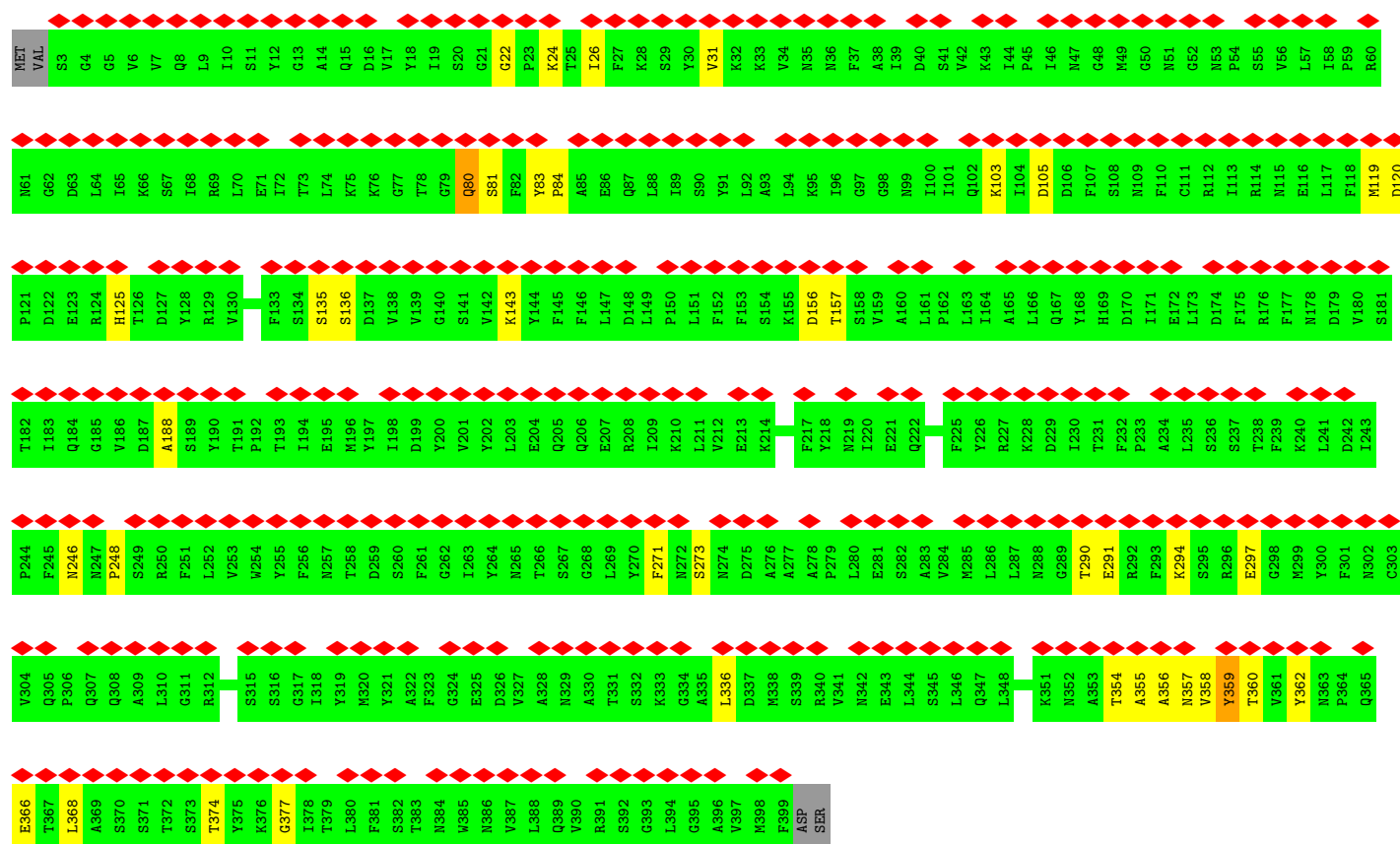
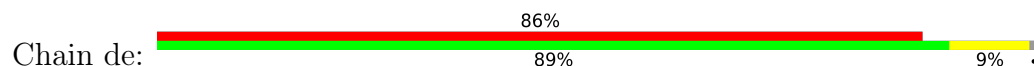


● Molecule 5: MCPv4

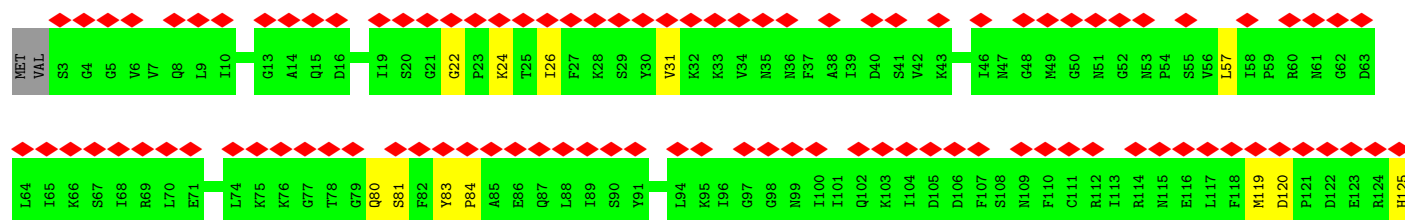
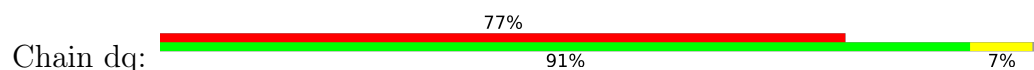


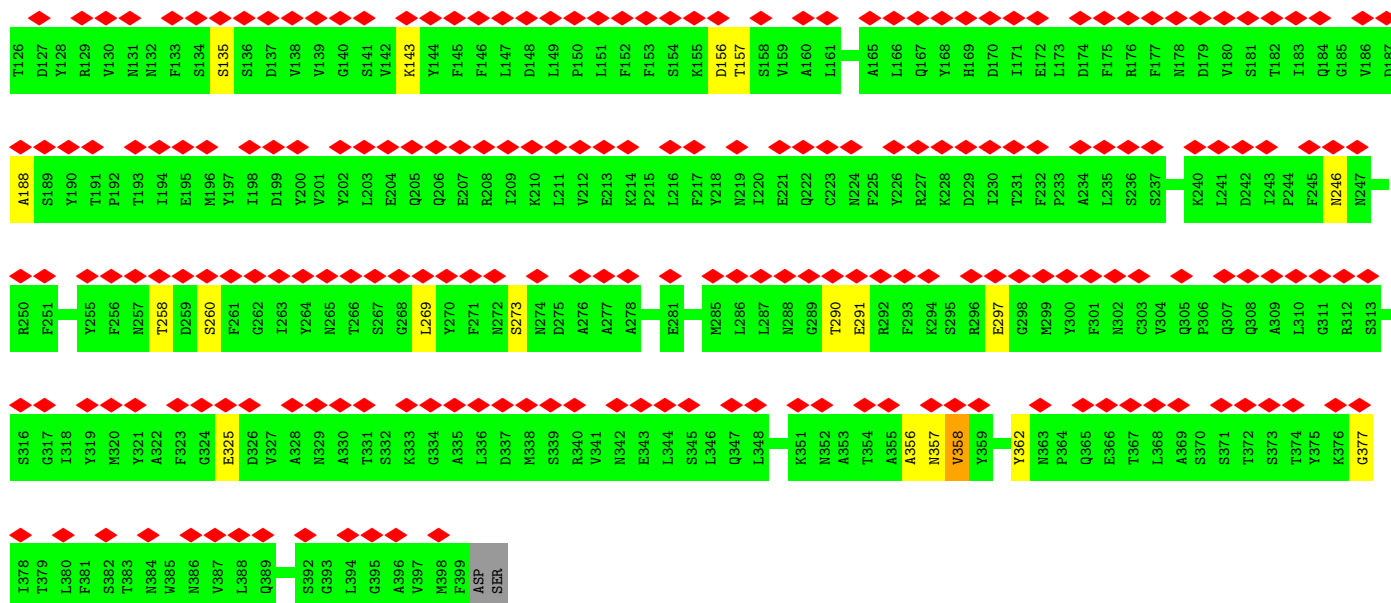


• Molecule 5: MCPv4

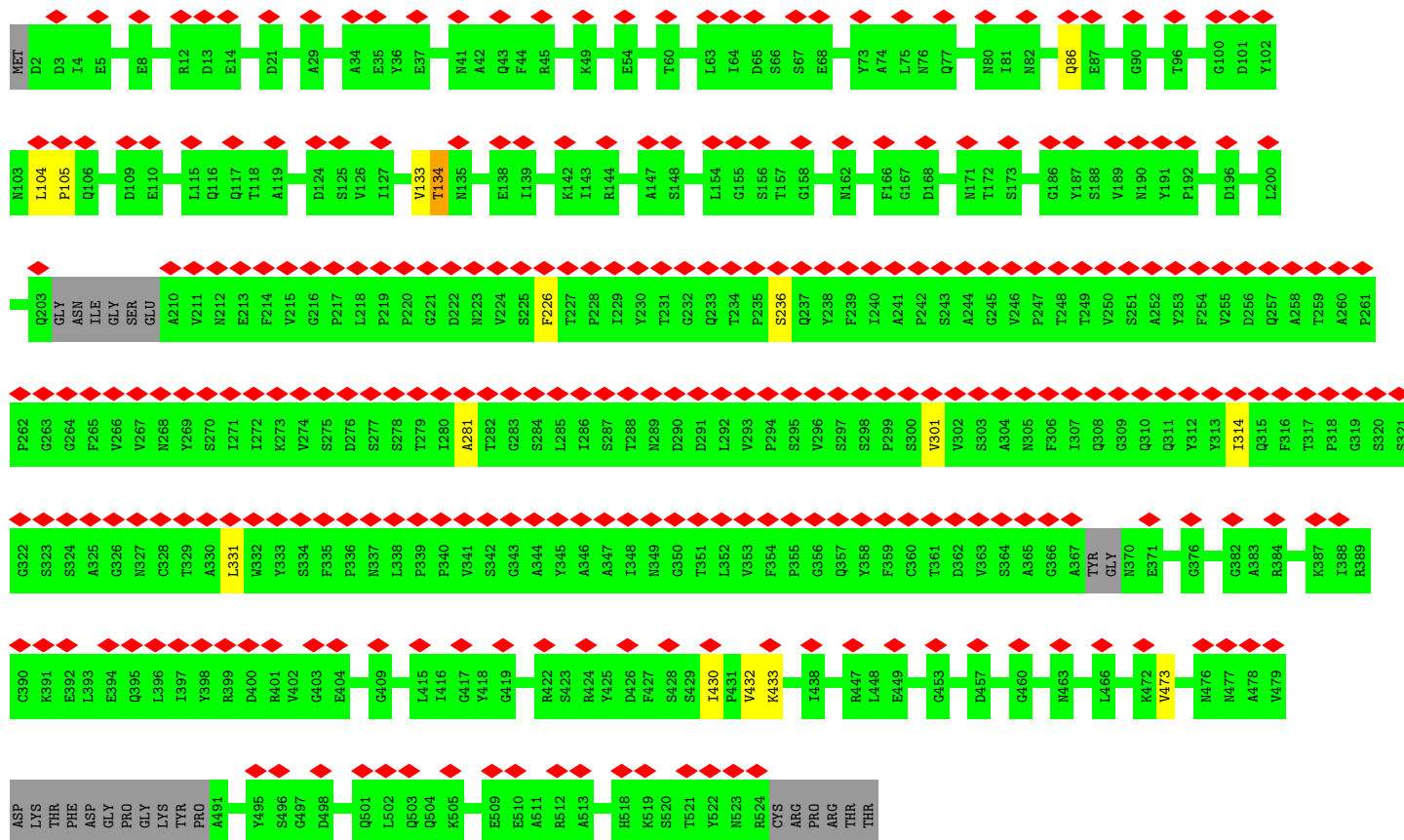


• Molecule 5: MCPv4



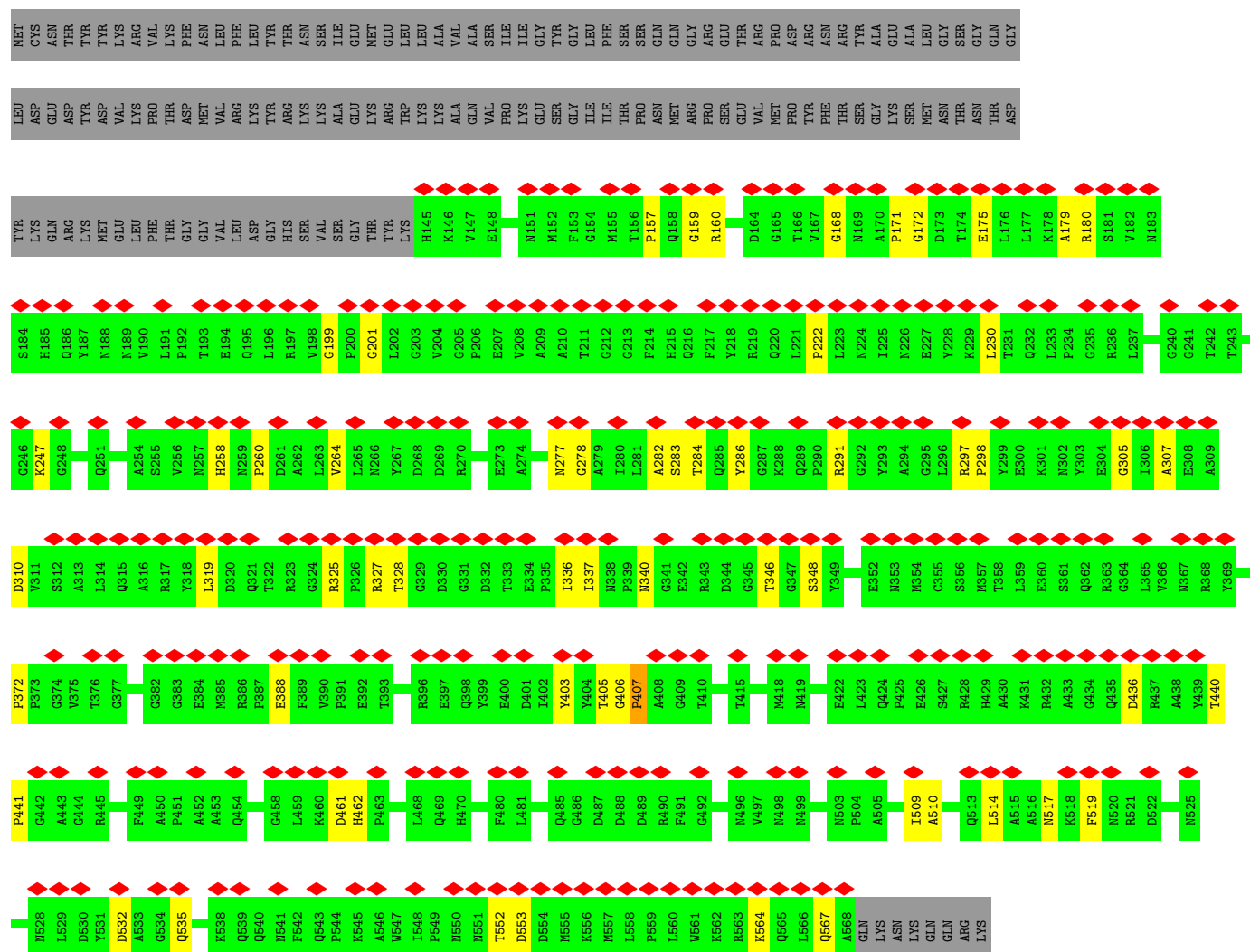


• Molecule 6: P1v1

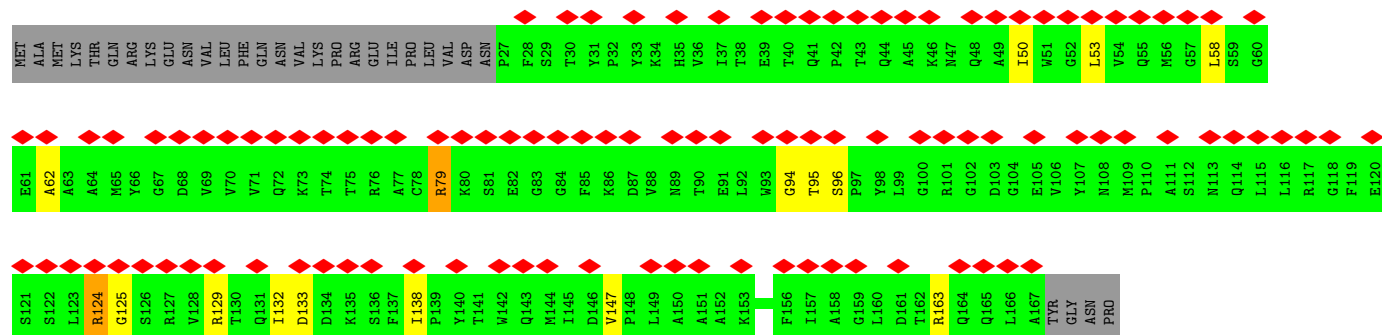
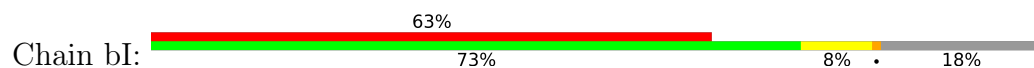


• Molecule 7: P2

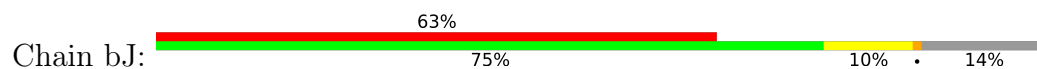


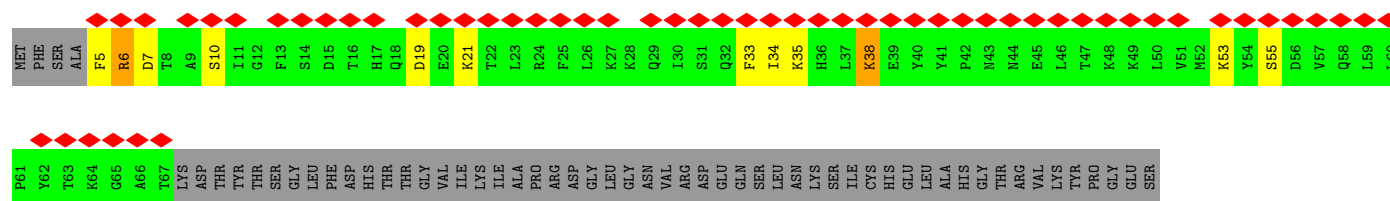


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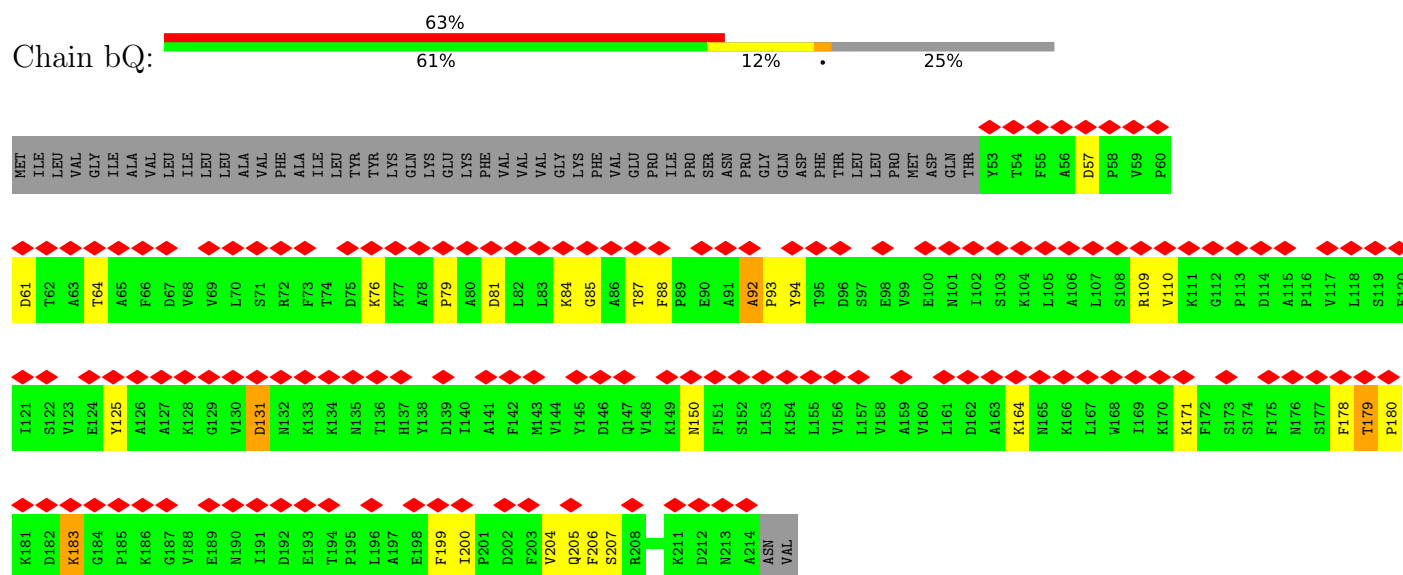


• Molecule 8: P3

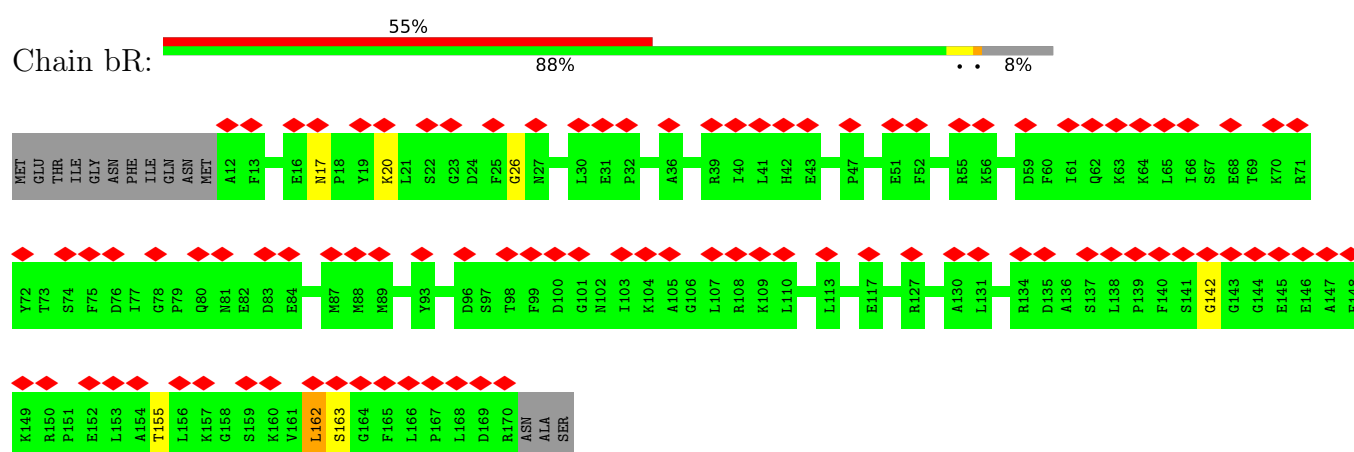




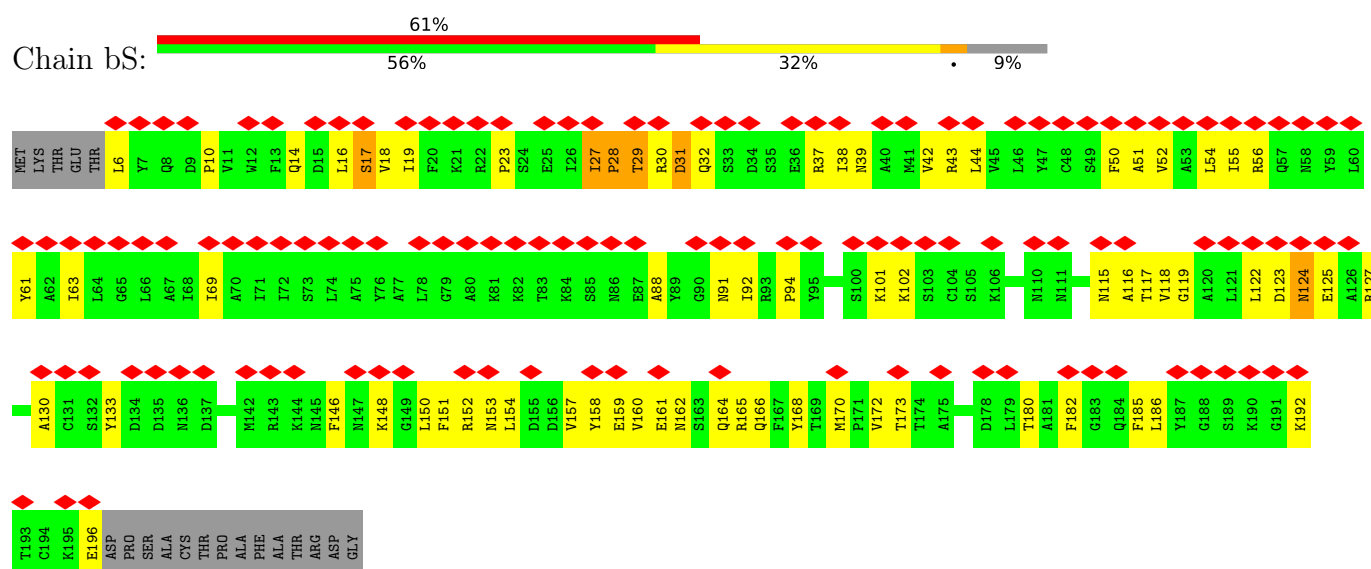
- Molecule 11: P6



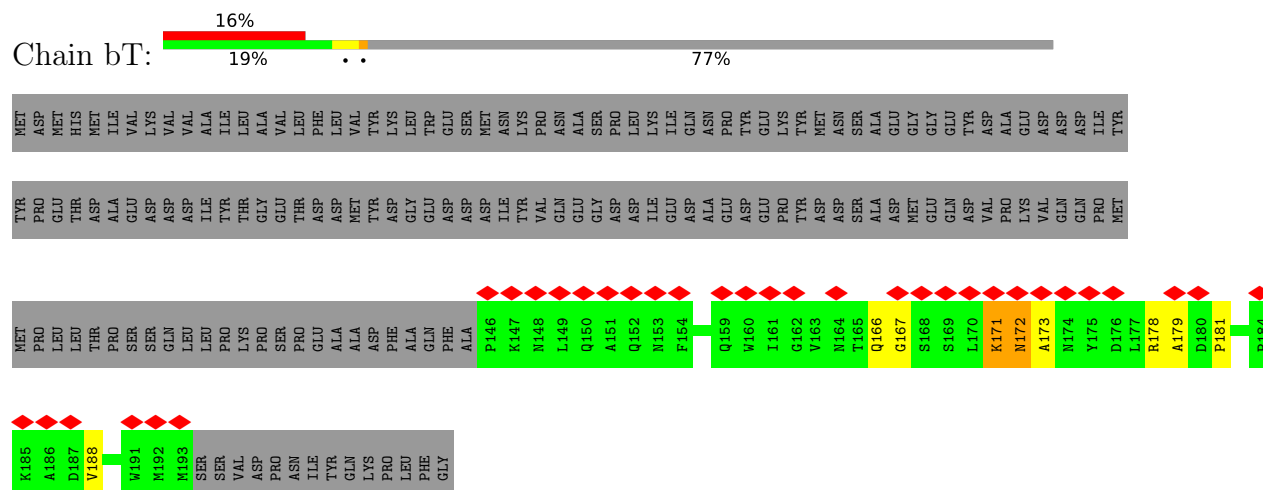
- Molecule 12: P8



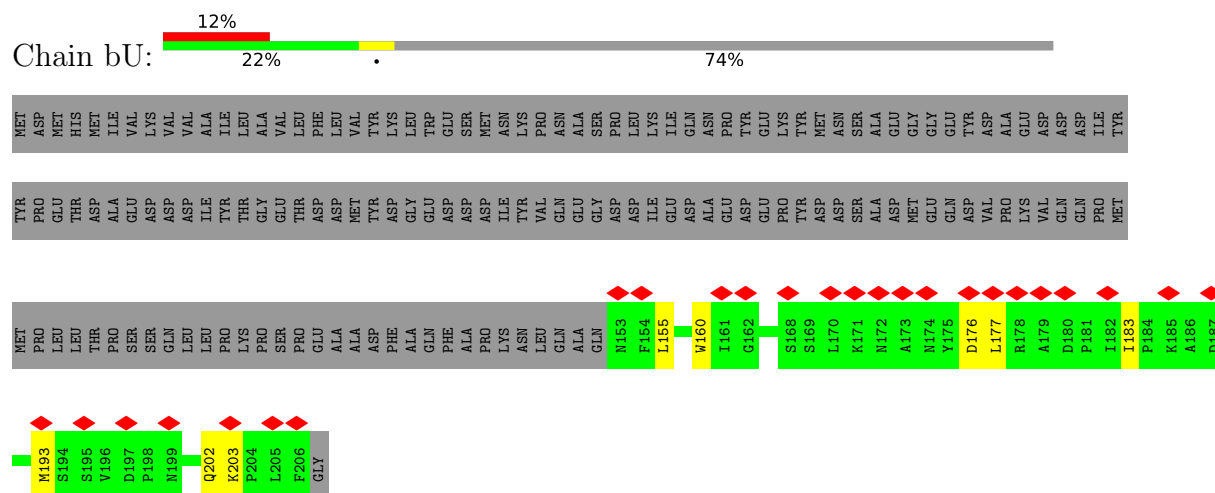
- Molecule 13: P9



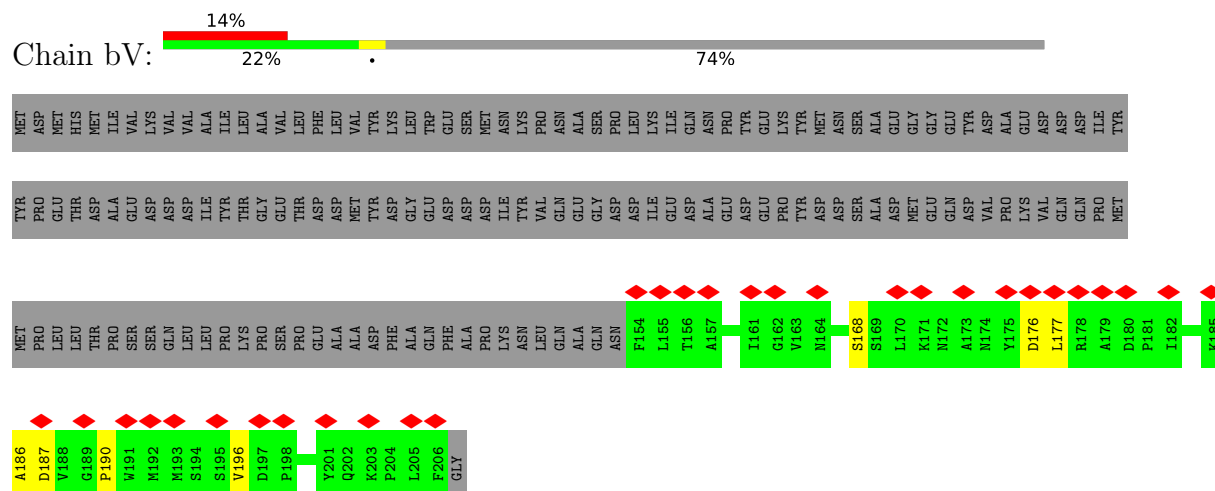
• Molecule 14: P11



• Molecule 14: P11



• Molecule 14: P11



• Molecule 14: P11

- Molecule 14: P11

- Molecule 14: P11

- Molecule 14: P11



P181	P182	P183	P184	P185	P186	P187	P188	P189	P190	P191	P192	P193	P194	P195	P196	P197	P198	P199	T200	Z201	Z202	Z203	P204	L205	PHE	GLY
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Chain ca:

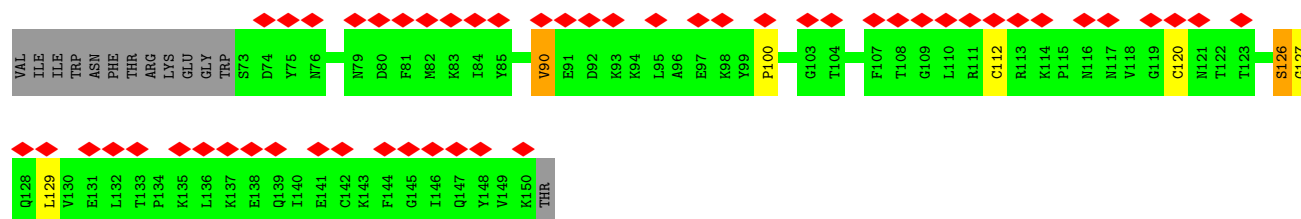
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Chain cb:

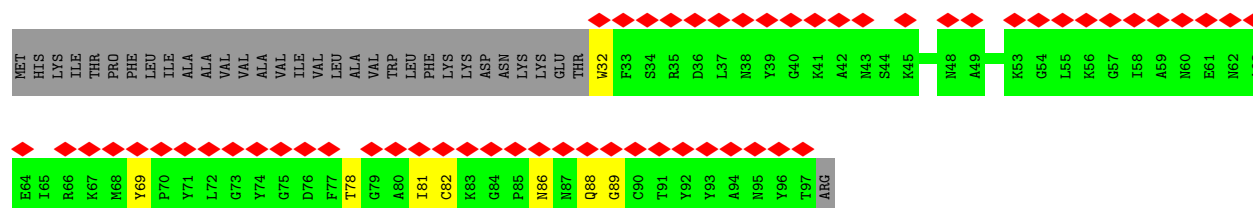
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Chain cc:

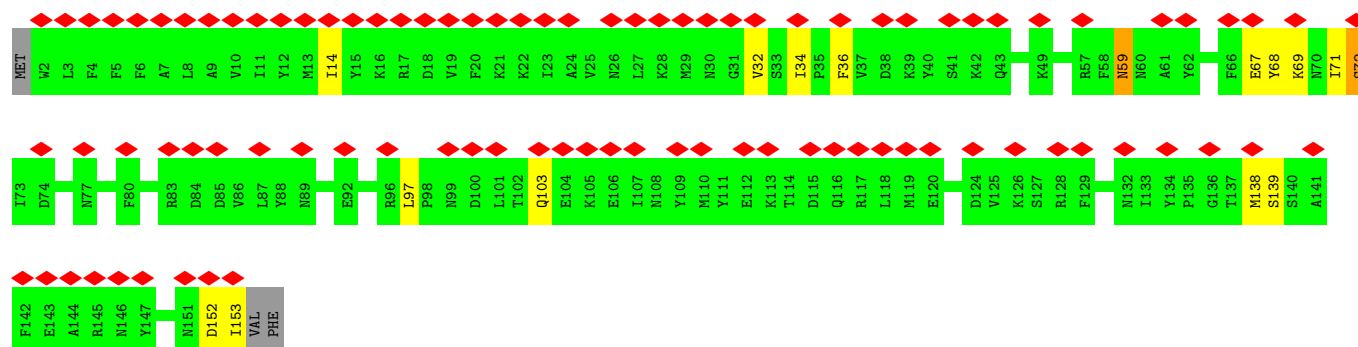
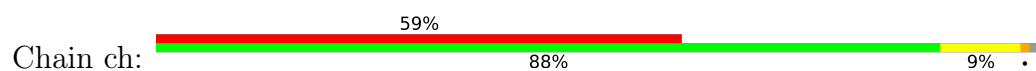
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-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



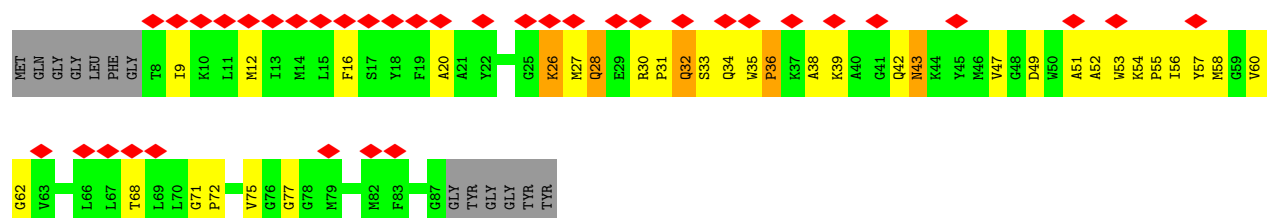
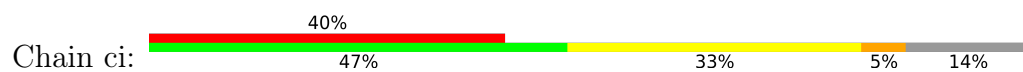
• Molecule 16: P13



• Molecule 17: P15



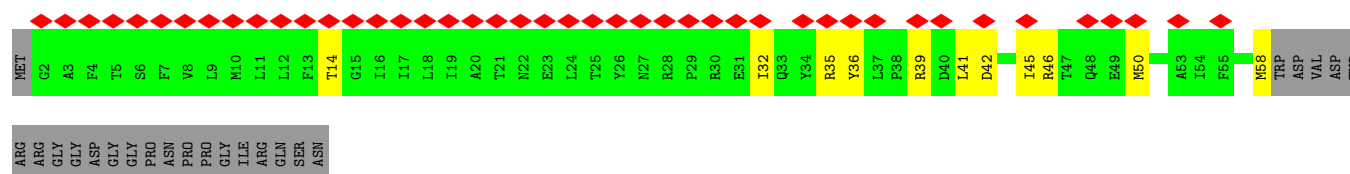
• Molecule 18: P16



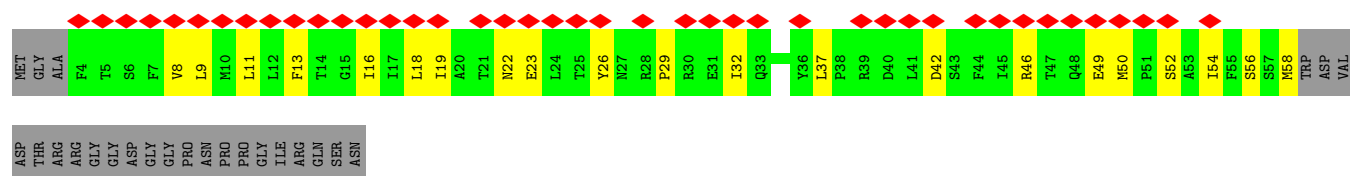
• Molecule 19: P17



- Molecule 19: P17



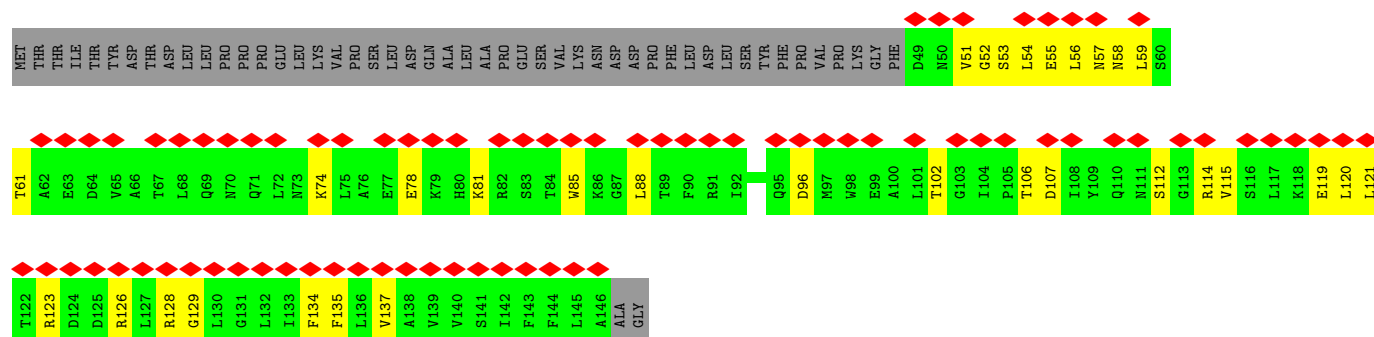
- Molecule 19: P17



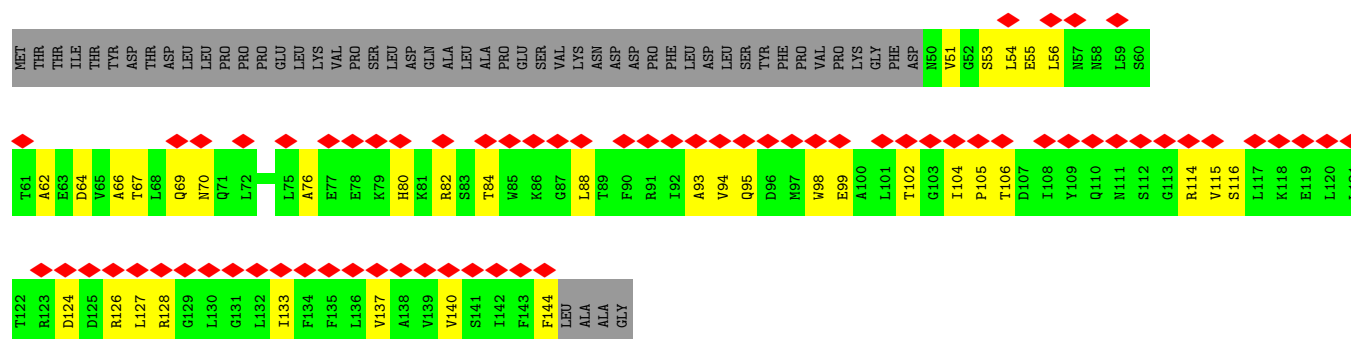
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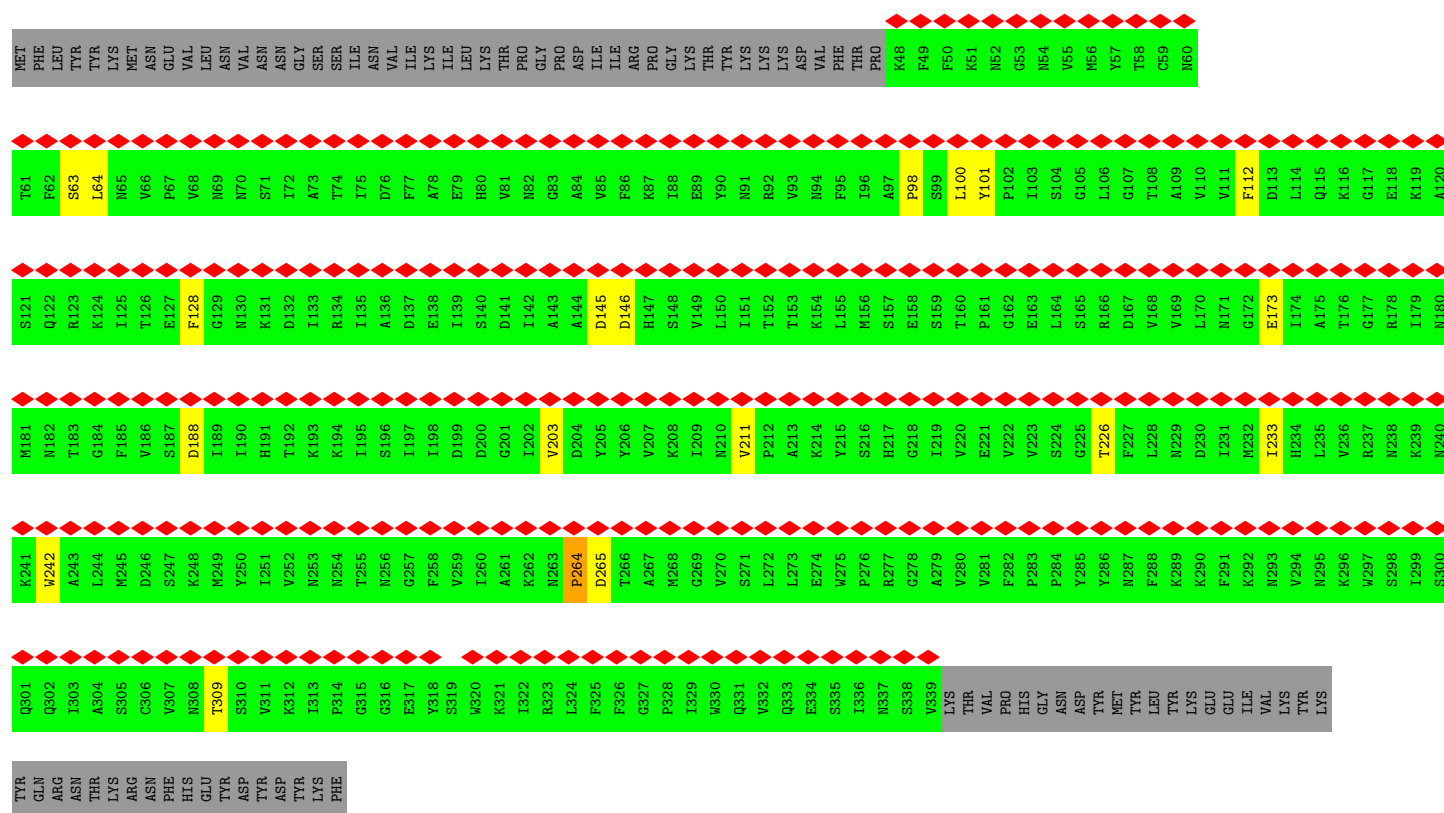
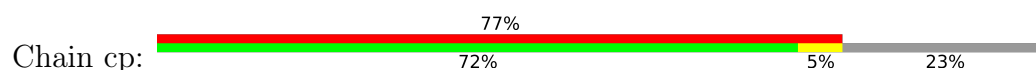
- Molecule 20: P18



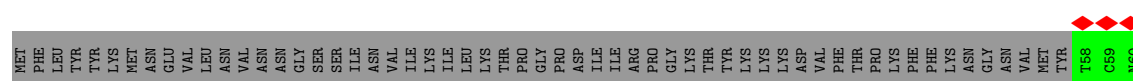
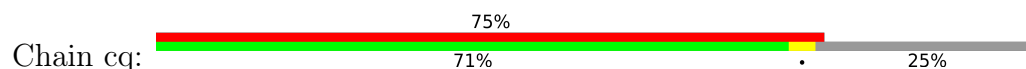
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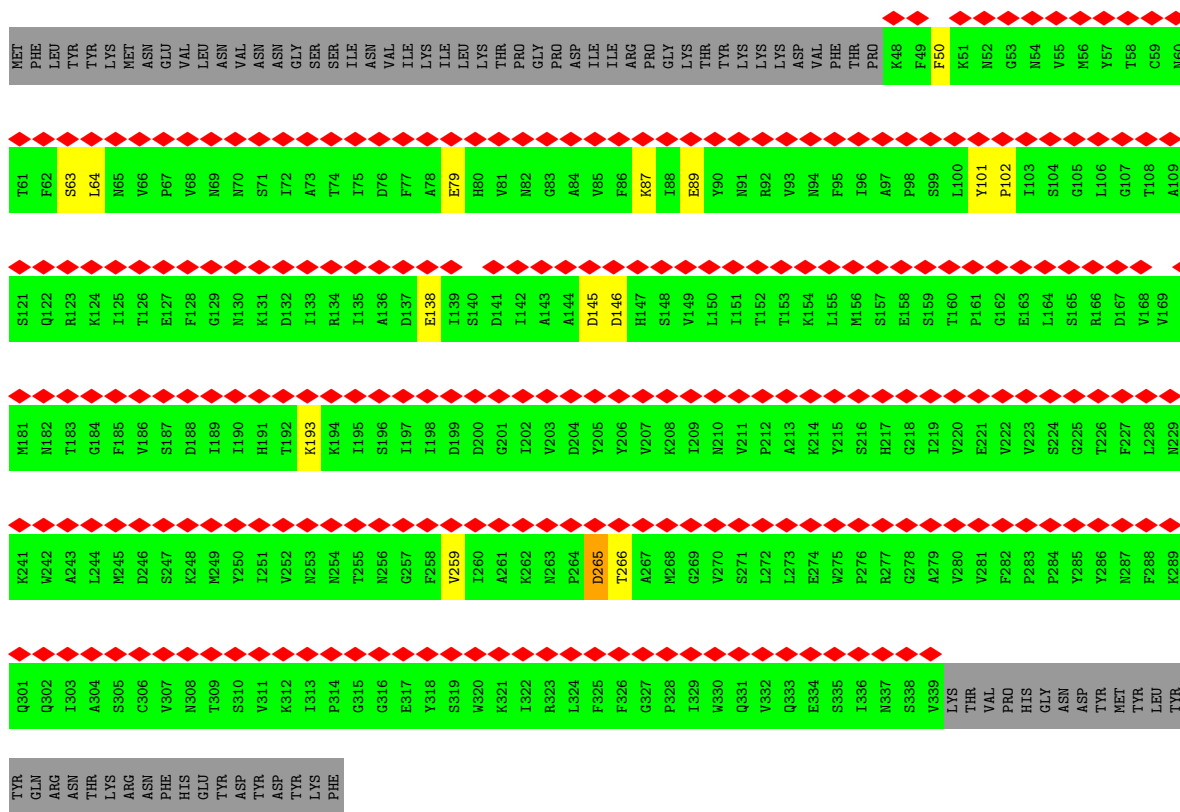
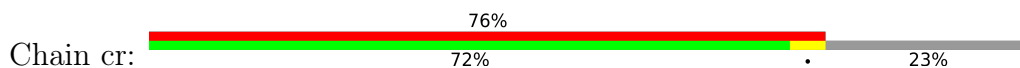
• Molecule 21: P19



• Molecule 21: P19



- Molecule 21: P19



- Molecule 21: P19

Chain cs:

- Molecule 21: P19

Chain ct:

1 2 3 4 5

TYR
GLN
ARG
ASN
THR
LYS
LYS
ARG
ASN
PHE
HIS
GLU
TYR
ASP
TYR
PHE

● Molecule 21: P19

Chain cu: 

MET PHE LEU TYR TYR LYS MET ASN GLU VAL ASN VAL ASN GLY SER ILE ASN VAL ILE LYS LYS LYS THR LYS THR PRO PRO ASP ASP ILE ILE ARG PRO GLY LYS THR TYR LYS LYS ASP VAL PHE THR PRO LYS PHE PHE LYS ASN ASN VAL MET THR CYS N60

T61 F62 S63 L64 N65 V66 P67 V68 N69 N70 S71 I72 A73 T74 I75 D76 F77 A78 E79 H80 H82 N82 G83 A84 V85 V86 F86 K87 I88 E89 Y90 N91 N92 N93 N94 N95 I96 I97 P98 S99 L100 Y101 P102 I103 S104 G105 L106 G107 T108 A109 V110 V111 F112 D113 L114 Q115 K116 G117 E118 K119 A120

S121 Q122 K124 T125 T126 E127 F128 G129 N130 K131 I132 D132 I133 R134 I135 A136 D137 E138 I139 S140 D141 I142 A143 A144 D145 D146 H147 S148 V149 L150 L151 I152 T153 T154 K154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 S165 R166 D167 V168 L169 N170 N171 G172 E173 I174 A175 T176 G177 I179 N180

M181 N182 T183 G184 F185 V186 S187 D188 M189 I190 H191 T192 K193 K194 I195 S196 I197 N198 D199 D200 G201 T202 V203 D204 Y205 Y206 V207 K208 I209 N210 V211 P212 A213 K214 Y215 S216 H217 G218 I219 V220 E221 V222 V223 S224 G225 T226 F227 L228 N229 D230 I231 M232 K233 H234 L235 V236 K237 N238 K239 N240

K241 W242 A243 L244 M245 S247 K248 M249 Y250 I251 V252 M253 T254 T255 N256 G257 F258 V259 T260 A261 K262 M263 P264 D265 T266 A267 M268 G269 V270 S271 L272 L273 E274 W275 P276 R277 G278 A279 V280 V281 F282 P283 P284 V285 Y286 M287 F288 K289 K290 F291 K292 M293 V294 N295 K296 W297 I299 S300

Q301 Q302 T303 A304 S305 C306 V307 N308 T309 S310 V311 K312 L313 P314 G315 G316 E317 Y318 S319 W320 K321 R322 R323 L324 F325 F326 G327 P328 I329 W330 Q331 V332 Q333 E334 S335 I336 N337 S338 V339 LYS THR VAL PRO HIS GLY ASN ASP TYR MET LEU TYR LYS GLU ILE VAL LYS LYS

TYR
GLN
ARG
ASN
THR
LYS
LYS
ARG
ASN
PHE
HIS
GLU
TYR
ASP
TYR
PHE

● Molecule 21: P19

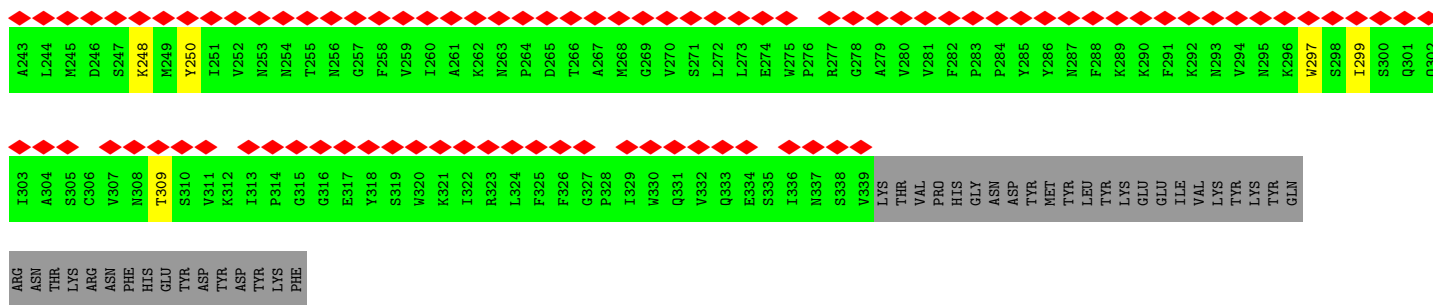
Chain cv: 

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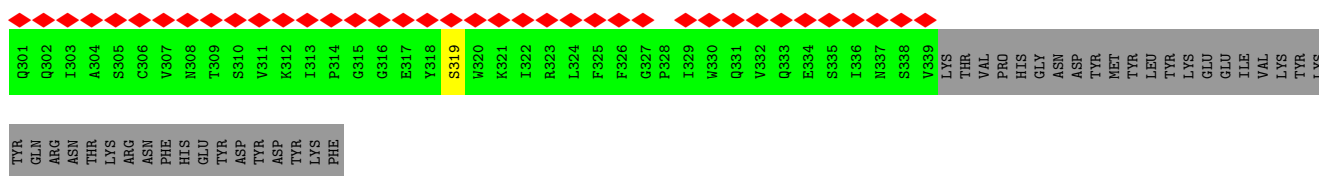
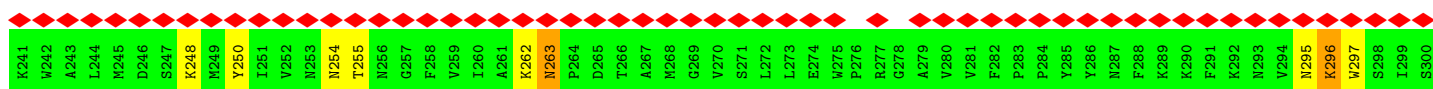
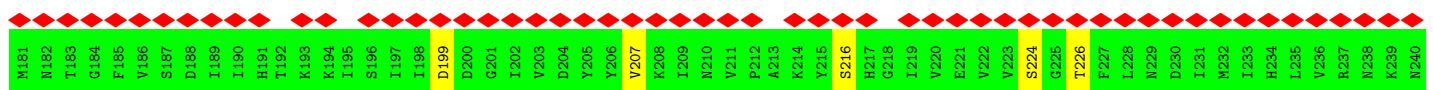
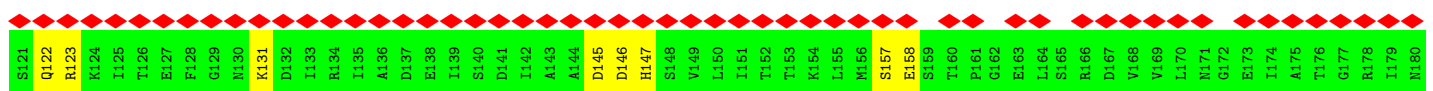
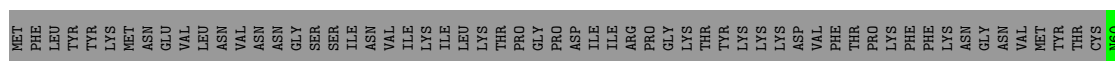
T61 F62 S63 L64 N65 V66 P67 V68 N69 N70 S71 I72 A73 D76 F77 A78 E79 H80 H82 N82 G83 A84 V85 V86 F86 K87 I88 E89 Y90 N91 N92 N93 N94 N95 I96 I97 P98 S99 L100 Y101 P102 I103 S104 G105 L106 G107 T108 A109 V110 V111 F112 D113 L114 Q115 K116 G117 E118 S121 Q122

R123 K124 I125 T126 T127 F128 G129 N130 K131 D132 I133 R134 I135 A136 D137 I138 I139 S140 D141 I142 A143 A144 D145 D146 H147 S148 V149 L150 I151 T152 T153 K154 L155 M156 S157 E158 S159 T160 P161 G162 E163 L164 R166 D167 V168 L169 N170 N171 G172 E173 I174 A175 T176 G177 R178 I179 N180 M181 N182

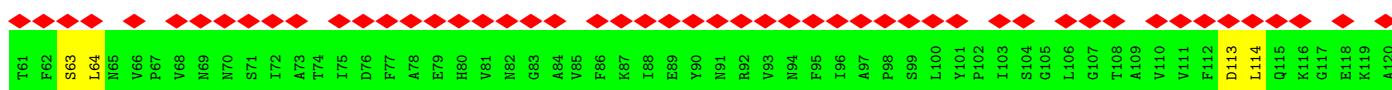
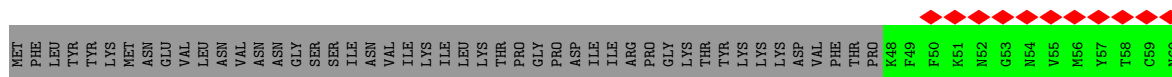
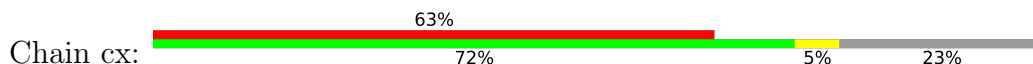
T183 G184 F185 V186 S187 D188 I189 I190 H191 T192 K193 K194 I195 S196 I197 I198 D199 D200 G201 I202 V203 D204 Y205 Y206 V207 K208 I209 N210 V211 P212 A213 K214 L215 M216 S217 E218 S219 H217 G218 I219 V220 E221 V222 S224 G225 T226 F227 L228 N229 D230 I231 M232 K233 L234 L235 V236 R237 N238 K239 K241 W242

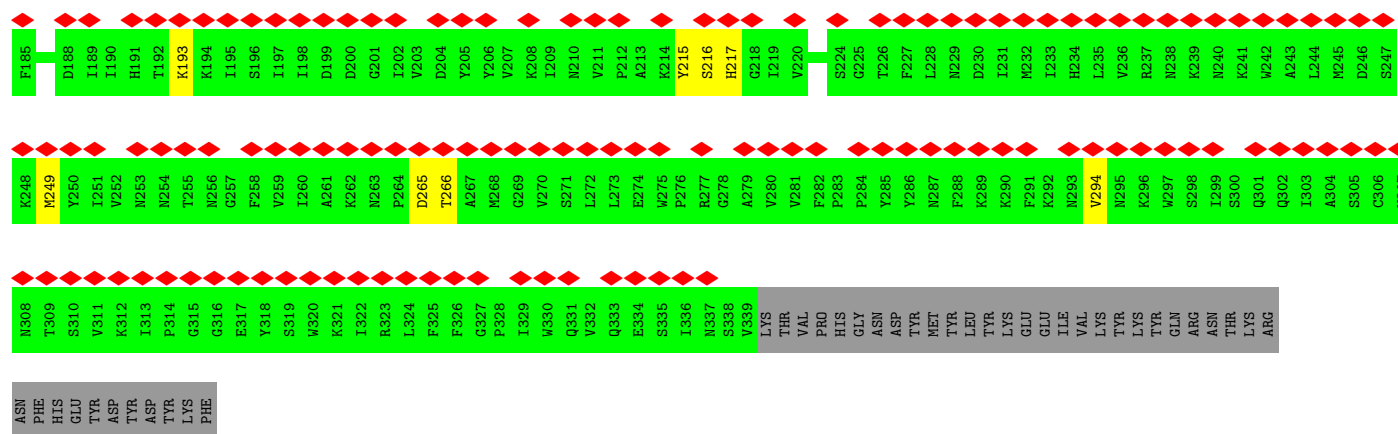


• Molecule 21: P19

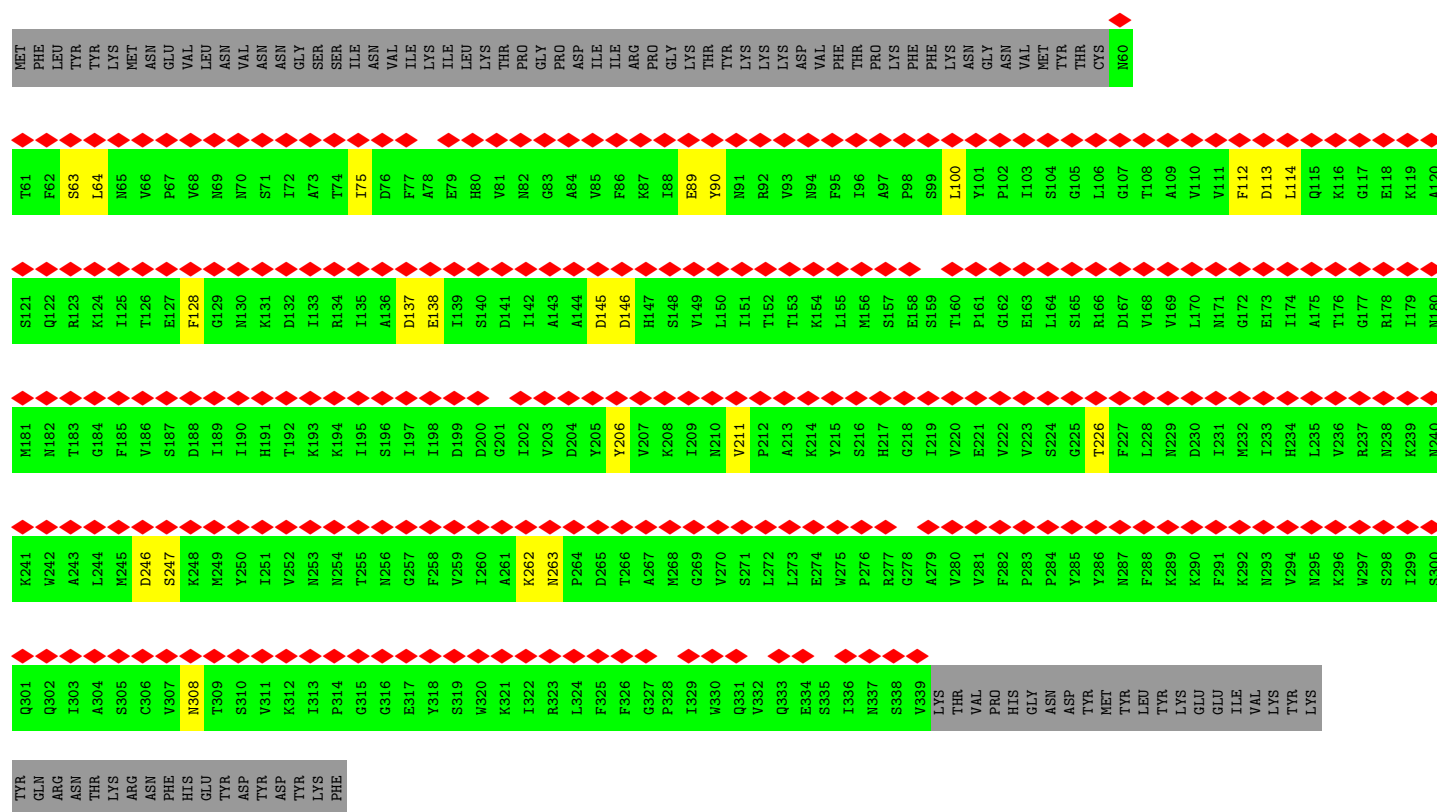
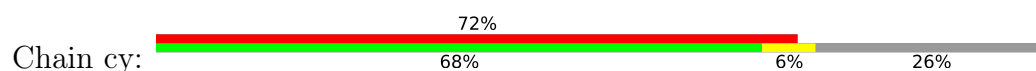


• Molecule 21: P19

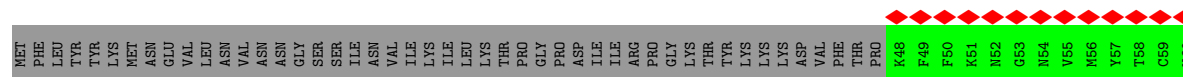
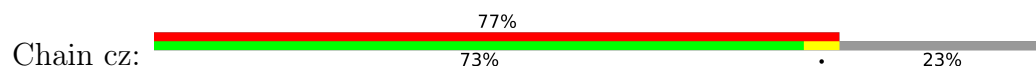




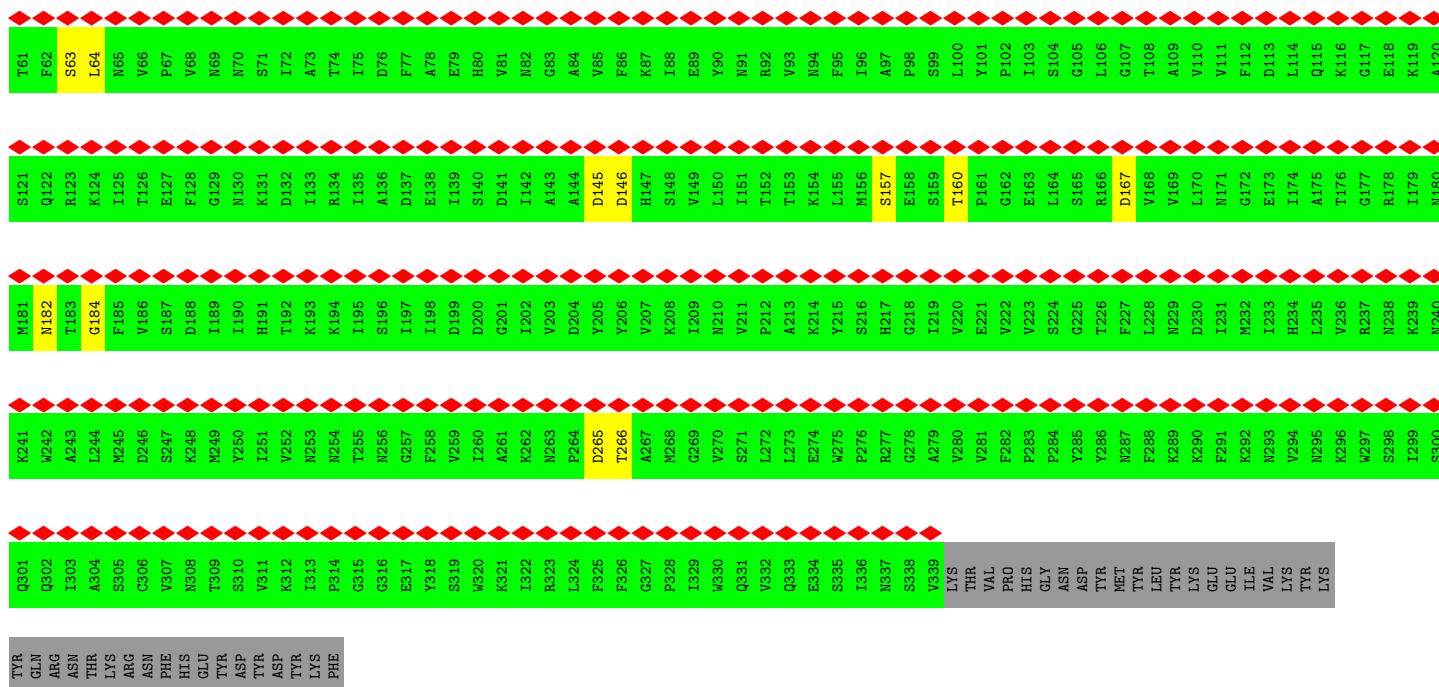
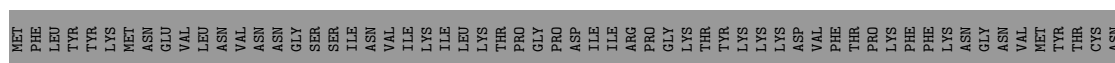
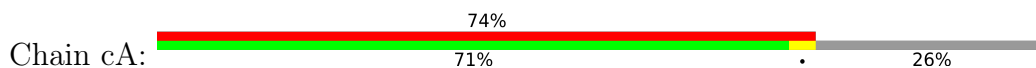
• Molecule 21: P19



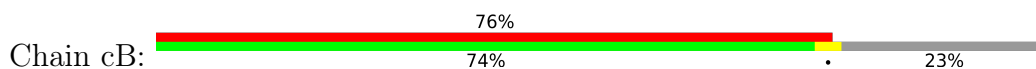
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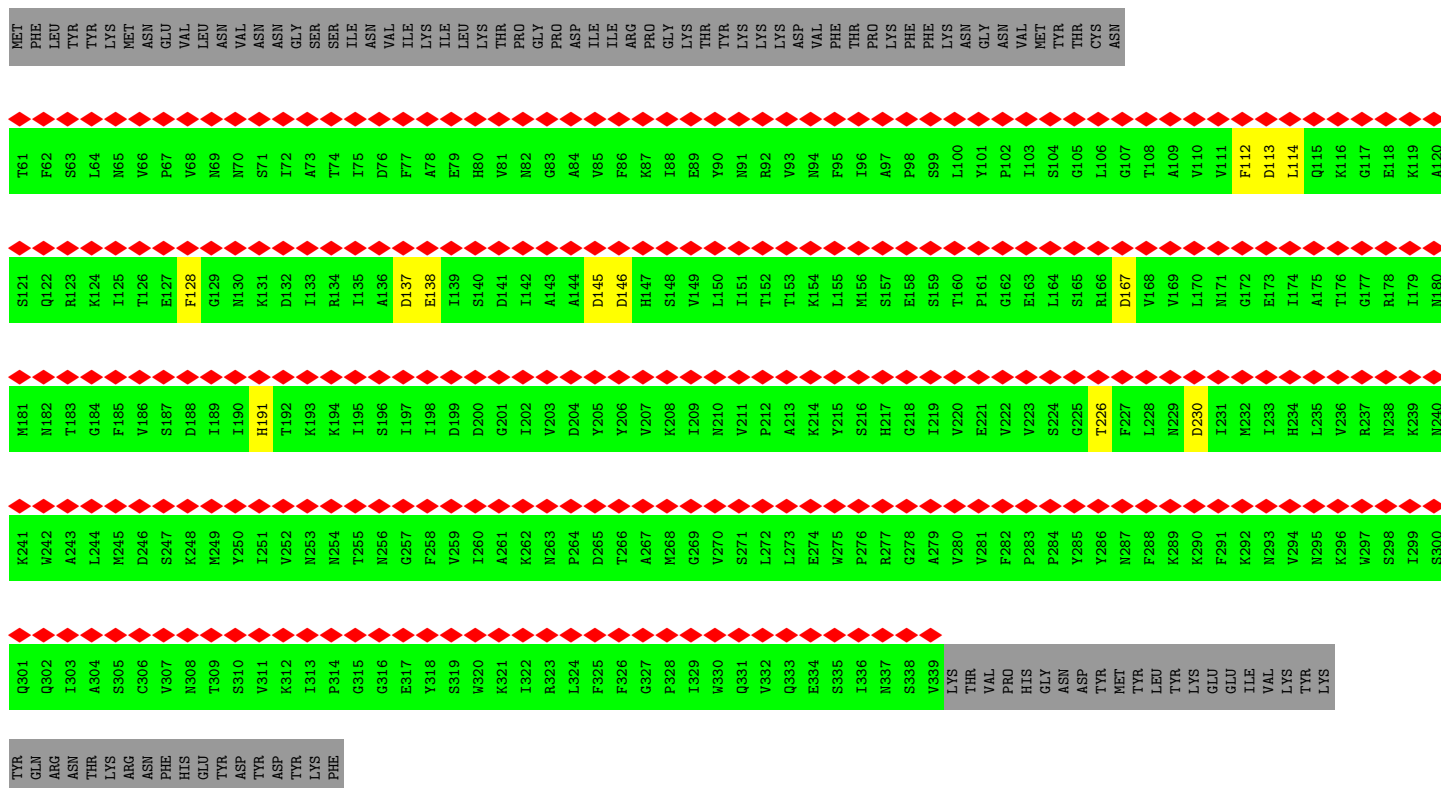
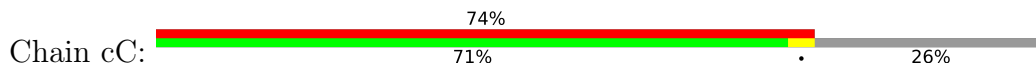
- Molecule 21: P19



- Molecule 21: P19

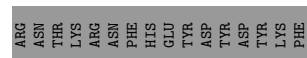
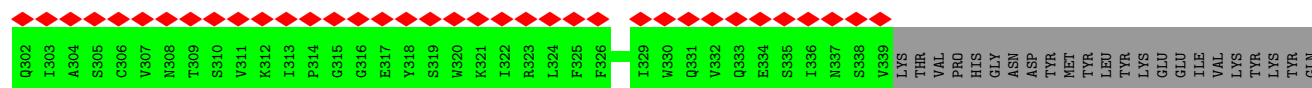
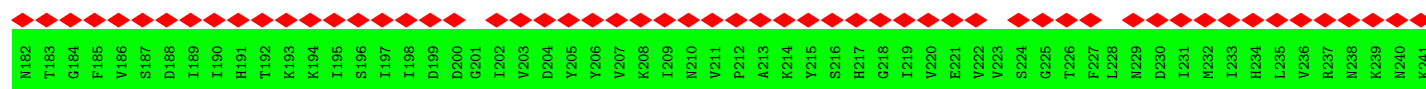
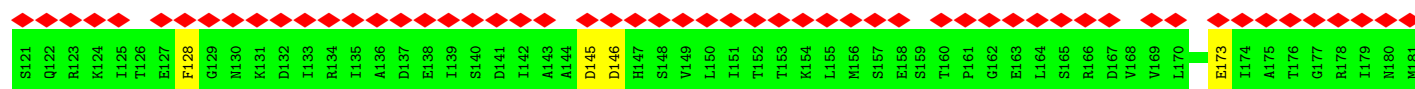
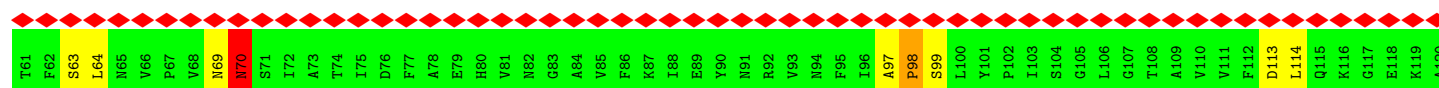
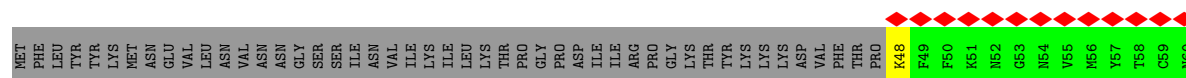
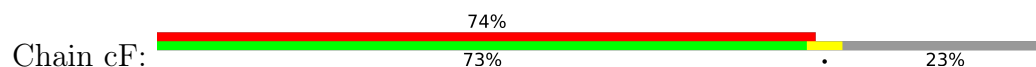


- Molecule 21: P19

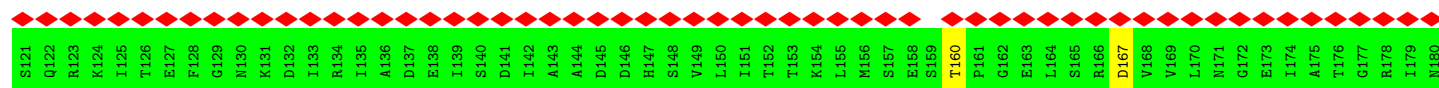
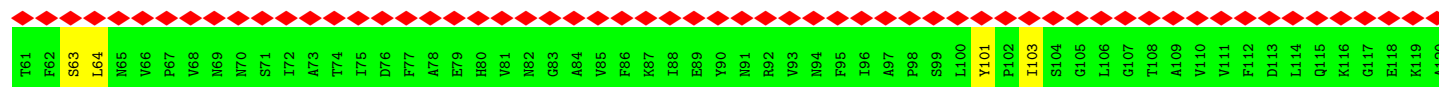
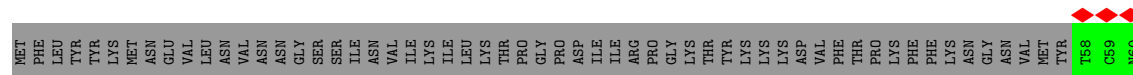
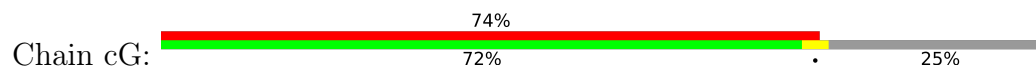


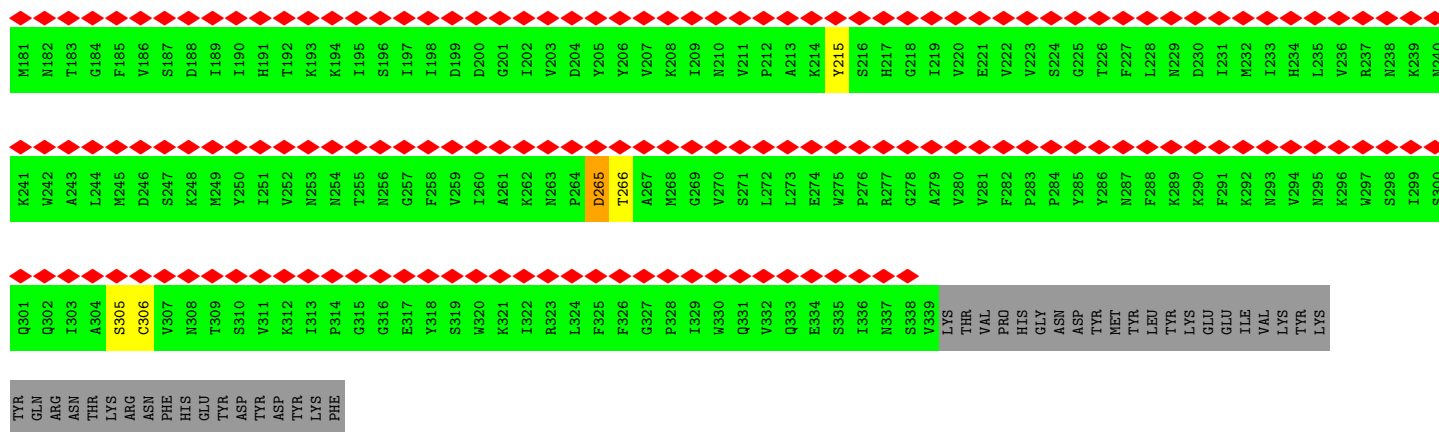


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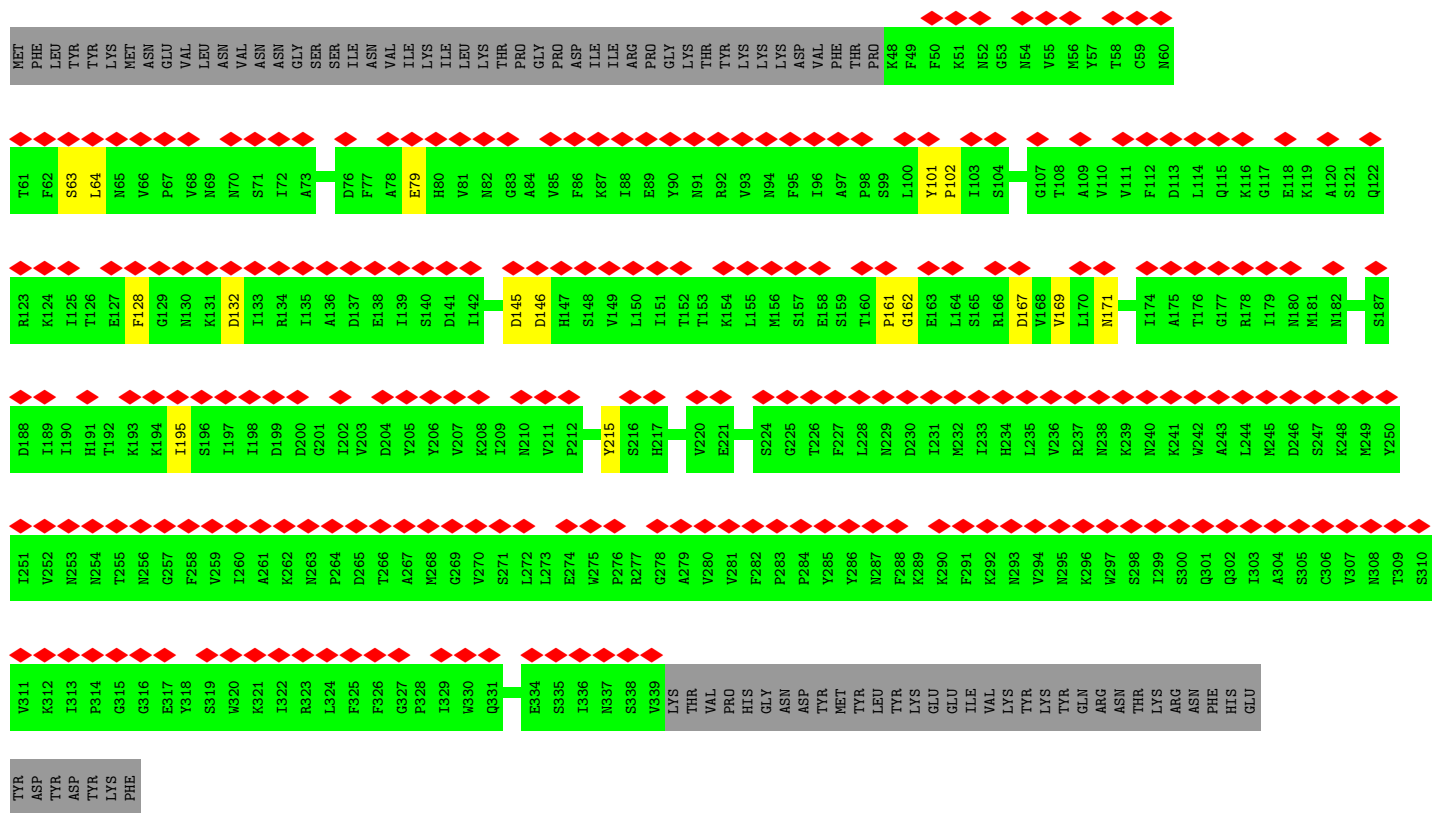
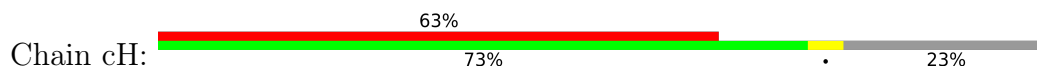


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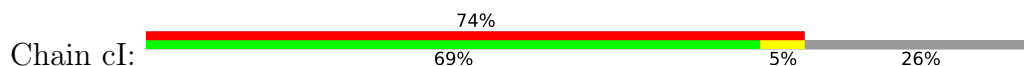




• Molecule 21: P19



• Molecule 21: P19



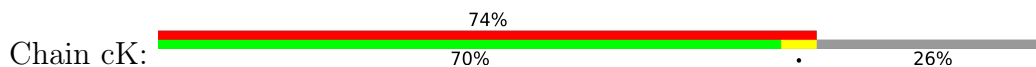
S121	M181	K241	Q301	TYR
Q122	N182	W242	Q302	GLN
R123	T183	A243	I303	ARG
K124	G184	L244	A304	THR
I125	F185	M245	S305	LYS
T126	V186	D246	C306	ARG
E127	S187	S247	V307	ASN
F128	D188	K248	N308	PHE
G129	I189	M249	T309	HIS
M130	I190	Y250	LEU	GLU
K131	H191	I251	ASN	TYR
D132	T192	V252	S310	ASP
R133	K193	N253	V311	TYR
K134	K194	N254	K312	ASP
I135	I195	T255	I313	LYS
A136	S196	N256	P314	PHE
D137	I197	E257	G315	
E138	I198	F258	G316	
I139	D199	V259	Y318	
S140	D200	I260	S319	
D141	G201	A261	W320	
I142	I202	K262	K321	
A143	V203	N263	I322	
A144	D204	P264	R523	
D145	Y205	D265	L324	
D146	Y206	T266	F325	
H147	V207	A267	F326	
S148	K208	M268	G327	
V149	I209	G269	P328	
L150	N210	V270	I329	
I151	V211	S271	W330	
T152	P212	L272	Q331	
T153	A213	L273	V332	
K154	K214	E274	Q333	
L155	Y215	W275	E334	
M156	S216	P276	S335	
S157	H217	R277	I336	
E158	G218	G278	N337	
S159	I219	A279	S338	
T160	V220	V280	V339	
P161	E221	V281	LYS	
G162	V222	F282	THR	
E163	V223	P283	VAL	
L164	S224	G284	PRO	
S165	G225	Y285	HIS	
R166	T226	Y286	GLY	
D167	F227	N287	ASN	
V168	L228	F288	ASP	
V169	N229	K289	TYR	
L170	D230	K290	LEU	
N171	I231	F291	LYS	
G172	M232	K292	GLU	
E173	I233	N293	ILE	
I174	H234	V294	VAL	
A175	L235	N295	LYS	
T176	V236	K296	THR	
G177	R237	W297	LYS	
R178	N238	S298		
I179	K239	I299		
N180	N240	S300		

• Molecule 21: P19



MET	T61	S121	M182	A243	I303	ARG
PHE	F62	Q122	T183	L244	A304	ASN
LEU	S63	R123	G184	M245	S305	THR
TYR	L64	K124	F185	D246	C306	LYS
LYS	N65	I125	V186	S247	V307	ARG
THR	P67	T126	D188	K248	N308	PHE
ASN	V68	E127	I189	M249	T309	HIS
VAL	N69	F128	T192	Y250	S310	GLU
ASN	N70	G129	K193	I251	V311	TYR
ASN	S71	M130	K194	V252	K312	ASP
GLY	I72	D132	I195	N253	I313	TYR
SER	A73	P314	S196	N254	P314	LYS
THR	T74	I133	S197	T255	G315	PHE
ILE	I75	I135	I197	N256	G316	
ASN	D76	A136	I198	G257	E317	
VAL	F77	D137	V258	F258	Y318	
ILE	A78	E138	V259	I260	S319	
LYS	E79	I139	I261	A261	W320	
LEU	H80	S140	K262	N263	I322	
LYS	N82	D141	Y205	P264	R523	
THR	C83	I142	Y206	T266	L324	
PRO	A84	D145	V207	A267	F325	
GLY	R85	D146	K208	M268	F326	
THR	F86	H147	I209	G269	G327	
ARG	K87	S148	N210	V270	P328	
PRO	T88	V149	V211	S271	I329	
GLY	E89	L150	P212	L272	W330	
LYS	Y90	I151	A213	L273	Q331	
THR	N91	T152	K214	E274	Q333	
LYS	A92	T153	Y215	W275	E334	
LYS	V93	K154	S216	P276	S335	
ASP	N94	L155	H217	R277	I336	
VAL	F95	M156	G218	G278	N337	
PHE	I96	S157	I219	A279	S338	
THR	A97	E158	V220	V280	V339	
PRO	P98	S159	E221	V281	LYS	
K48	S99	T160	V222	F282	THR	
F49	L100	P161	V223	P283	VAL	
F50	X51	G162	S224	P284	PRO	
X51	Y101	E163	G225	Y285	GLY	
N52	P102	L164	T226	Y286	ASN	
G53	I103	S165	F227	N287	TYR	
N54	S104	R166	L228	F288	MET	
G105	G105	D167	N229	K289	THR	
V55	L106	V168	D230	F291	LEU	
M56	G107	V169	I231	K292	LYS	
V57	T108	L170	M232	G293	GLU	
T58	A109	N171	G172	I174	ILE	
C59	V110	E173	I174	A175	VAL	
N60	F112	D113	T176	K296	LYS	
	D114	Q115	G177	W297	THR	
	K116	E117	R178	I298	GLN	
	E118	K119	N180	S300		
	A120		M181	Q301		
				Q302		

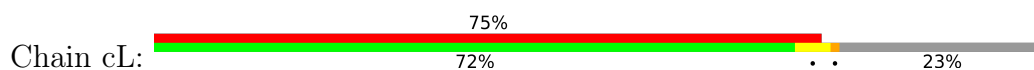
• Molecule 21: P19



MET	ARG
PHE	ASN
LEU	THR
TYR	LYS
LYS	ARG
LYS	ASN
MET	PHE
ASN	HIS
GLU	GLU
VAL	TYR
LEU	ASP
ASN	TYR
ASN	ASP
VAL	TYR
ASN	LYS
ASN	PHE

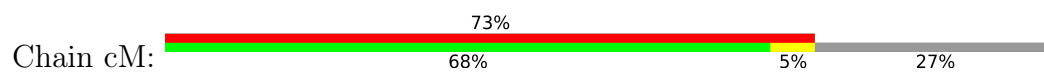
T61	S121	M181	K241	Q301	TYR
F62	Q122	N182	W242	Q302	GLN
S63	R123	T183	A243	I303	ARG
L64	K124	G184	L244	A304	ASN
N65	I125	F185	M245	S305	THR
V66	T126	V186	D246	C306	LYS
P67	E127	S187	S247	V307	ARG
V68	F128	D188	K248	N308	ASN
N69	G129	I189	M249	T309	PHE
N70	M130	I190	Y250	S310	HIS
S71	K131	H191	I251	V311	GLU
I72	D132	T192	V252	K312	TYR
A73	I133	K193	N253	I313	ASP
T74	R134	K194	N254	P314	LYS
I75	I135	I195	T255	G315	PHE
D76	A136	S196	N256	G316	
F77	D137	I197	G257	E317	
A78	E138	I198	F258	Y318	
E79	I139	D199	V259	S319	
H80	S140	D200	I260	W320	
V81	D141	G201	A261	K321	
N82	I142	I202	K262	I322	
G83	A143	V203	N263	R323	
A84	A144	D204	P264	L324	
V85	D145	Y205	D265	F325	
F86	D146	Y206	T266	F326	
K87	H147	V207	A267	G327	
I88	S148	K208	M268	P328	
E89	V149	I209	G269	I329	
Y90	L150	N210	V270	W330	
N91	I151	V211	S271	Q331	
R92	T152	P212	L272	V332	
V93	T153	A213	L273	Q333	
N94	K154	K214	E274	E334	
F95	L155	Y215	W275	S335	
I96	M156	S216	P276	I336	
A97	S157	H217	R277	N337	
P98	E158	G218	G278	S338	
S99	S159	I219	A279	V339	
L100	T160	V220	V280	LYS	LYS
Y101	P161	E221	V281	THR	THR
P102	G162	V222	F282	VAL	VAL
I103	E163	V223	P283	HIS	PRO
S104	L164	S224	P284	GLY	HIS
G105	S165	G225	Y285	ASN	GLY
L106	R166	T226	Y286	ASP	ASP
G107	D167	F227	N287	TYR	TYR
T108	V168	L228	F288	LEU	MET
A109	V169	N229	K289	TYR	TYR
V110	L170	D230	K290	LYS	LEU
V111	M171	I231	F291	GLU	LYS
F112	G172	M232	K292	ILE	GLU
D113	E173	I233	M293	VAL	ILE
L114	I174	H234	V294	LYS	VAL
Q115	A175	L235	N295	TYR	LYS
K116	T176	V236	K296		
G117	G177	R237	W297		
E118	R178	N238	S298		
K119	I179	K239	I299		
A120	N180	N240	S300		

• Molecule 21: P19



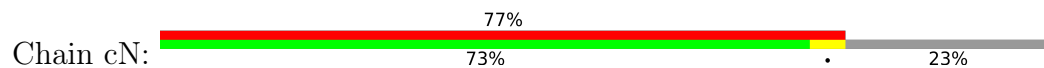
MET	T61	S121	M181	K241	Q301	TYR
PHE	F62	Q122	N182	W242	Q302	GLN
LEU	S63	R123	T183	A243	I303	ARG
TYR	L64	K124	G184	L244	A304	ASN
LYS	N65	I125	F185	M245	S305	THR
MET	V66	T126	V186	D246	C306	LYS
ASN	P67	E127	S187	S247	V307	ARG
GLU	F128	F128	D188	K248	N308	ASN
VAL	G129	F129	I189	M249	T309	PHE
ASN	M130	M130	I190	Y250	S310	HIS
VAL	K131	K131	H191	I251	V311	GLU
ASN	D132	D132	T192	V252	K312	TYR
GLY	I133	I133	K193	N253	I313	ASP
SER	R134	R134	K194	N254	P314	LYS
ILE	I75	I135	I195	T255	G315	PHE
ASN	D76	A136	S196	N256	G316	
VAL	F77	D137	I197	G257	E317	
LYS	A78	E138	I198	F258	Y318	
ILE	E79	I139	D199	V259	S319	
LYS	H80	S140	D200	I260	W320	
THR	V81	D141	G201	A261	K321	
PRO	N82	I142	I202	K262	I322	
GLY	G83	A143	V203	N263	R323	
PRO	A84	A144	D204	P264	L324	
ASP	V85	D145	Y205	D265	F325	
ILE	F86	D146	Y206	T266	F326	
ILE	K87	H147	V207	A267	G327	
ARG	I88	S148	K208	M268	P328	
GLY	E89	V149	G269	I329	I329	
LYS	Y90	L150	V270	W330	W330	
THR	N91	I151	S271	Q331	Q331	
LYS	R92	T152	P212	V332	V332	
LYS	V93	T153	L273	Q333	Q333	
ASP	N94	K154	E274	E334	E334	
VAL	F95	L155	W275	S335	S335	
PHE	I96	M156	P276	I336	I336	
THR	A97	S157	R277	N337	N337	
PRO	P98	E158	G278	S338	S338	
K48	S99	S159	A279	V339	V339	
F49	L100	T160	V280	LYS	LYS	LYS
F50	Y101	P161	V281	THR	THR	THR
K51	P102	G162	F282	VAL	VAL	VAL
N52	I103	E163	P283	HIS	HIS	PRO
G53	S104	L164	P284	GLY	GLY	HIS
N54	G105	S165	Y285	ASN	ASN	GLY
V55	L106	R166	Y286	ASP	ASP	ASP
N56	G107	D167	N287	TYR	TYR	TYR
Y57	T108	V168	L228	MET	MET	MET
F58	A109	V169	N229	TYR	TYR	TYR
C59	V110	L170	K290	LEU	LEU	LEU
N60	V111	M171	F291	LYS	LYS	LYS
	F112	G172	K292	GLU	GLU	GLU
	D113	E173	M293	ILE	ILE	ILE
	L114	I174	H294	VAL	VAL	VAL
	Q115	A175	L295	LYS	LYS	LYS
	K116	T176	V296	TYR	TYR	TYR
	G117	G177	R297			
	E118	R178	S298			
	K119	I179	I299			
	A120	N180	S300			

• Molecule 21: P19



TYR	GLN	ARG	ASN	THR	LYS	ARG	ASN	PHE	HIS	GLU	TYR	ASP	TYR	ASP	LYS	LYS	PHE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
Q301	Q302	I303	A304	S305	C306	V307	N308	T309	S310	V311	K312	I313	P314	G315	G316	E317	Y318	S319	W320	K321	I322	K323	L324	F325	F326	G327	P328	I329	W330	Q331	V332	Q333	E334	S335	I336	N337	S338	V339																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
LYS	THR	VAL	PRO	HIS	GLY	ASN	ASP	TYR	MET	THR	LEU	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	GLU	ILE	VAL	LYS	TY

• Molecule 21: P19



Q301	Q302	I303	A304	S305	C306	V307	N308	T309	S310	V311	K312	I313	P314	G315	G316	E317	Y318	S319	W320	K321	I322	K323	L324	F325	F326	G327	P328	I329	W330	Q331	V332	Q333	E334	S335	I336	N337	S338	V339	LYS	THR	VAL	PRO	HIS	GLY	ASN	ASP	TYR	MET	THR	LEU	TYR	LYS	GLU	ILE	VAL	LYS	TYR	LYS	
K241	W242	A243	L244	M245	D246	S247	K248	M249	Y250	I251	V252	N253	N254	T255	N256	G257	F258	V259	L260	A261	K262	N263	P264	D265	T266	A267	M268	G269	V270	S271	L272	L273	E274	W275	P276	R277	G278	A279	V280	V281	F282	P283	P284	Y285	Y286	N287	F288	K289	L290	F291	K292	N293	V294	N295	K296	W297	S298	I299	C300
M181	N182	T183	G184	F185	V186	S187	D188	I189	I190	H191	T192	K193	K194	I195	S196	I197	I198	D199	D200	G201	T202	V203	D204	Y205	Y206	V207	K208	I209	N210	V211	P212	A213	K214	Y215	S216	H217	G218	I219	V220	E221	V222	V223	S224	G225	T226	F227	L228	N229	D230	I231	M232	I233	H234	L235	V236	R237	N238	K239	N240
S121	Q122	R123	K124	I125	T126	E127	F128	G129	N130	K131	D132	I133	R134	I135	A136	D137	E138	I139	D140	D141	I142	A143	A144	D145	D146	H147	S148	V149	L150	I151	T152	T153	K154	L155	M156	S157	E158	S159	T160	P161	G162	E163	L164	S165	R166	D167	V168	V169	L170	N171	G172	D173	I174	A175	T176	G177	R178	I179	N180
T61	F62	S63	L64	N65	V66	P67	V68	N69	N70	S71	I72	A73	T74	I75	D76	F77	A78	E79	H80	V81	N82	G83	A84	V85	F86	K87	I88	E89	Y90	N91	R92	V93	N94	F95	I96	A97	P98	S99	L100	Y101	P102	I103	S104	G105	L106	G107	T108	A109	V110	V111	F112	D113	L114	Q115	K116	G117	E118	K119	A120
MET	PHE	LEU	TYR	LYS	MET	ASN	GLU	LEU	ASN	VAL	ASN	GLY	SER	SER	ILE	ASN	VAL	LEU	LYS	LEU	PRO	GLY	PRO	ASP	ILE	ILE	ARG	PRO	GLY	LYS	THR	LYS	LYS	ASP	VAL	PHE	THR	PRO	K48	F49	F50	K51	N52	G53	N54	V55	M56	Y57	T58	C59	N60								









SER
THR
SER
PHE
PHE
GLY
LEU
MET
VAL
THR
ALA
VAL
GLN
THR
VAL

- Molecule 22: P20

[illegible]









ASN	PHE	SER	ILE	ASN	CYS	LEU	ILE	ILE	ASN	ALA	THR	THR	THR	GLY	LEU	GLU	VAL	ILE	ILE	TYR	ASN	PRO	PHE	GLY	ILE	ALA	ALA	SER	SER	LEU	SER	SER	SER	THR	THR	PRO	GLU	LEU	LEU	TYR	PHE	THR	ILE	THR	THR	SER	ILE	ALA	THR	SER	THR	GLN
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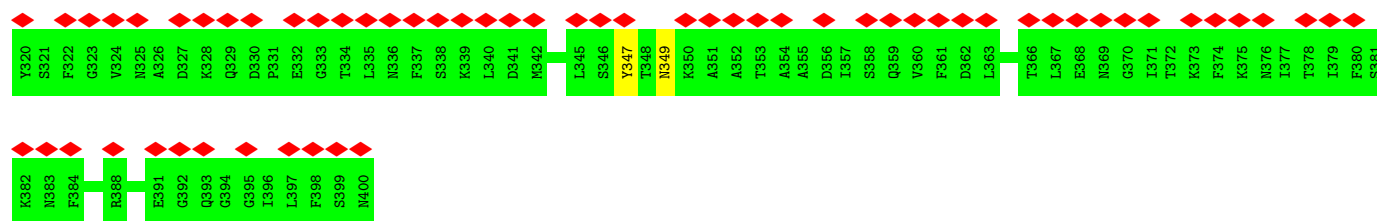
- Molecule 23: P21

Chain dh: 97%

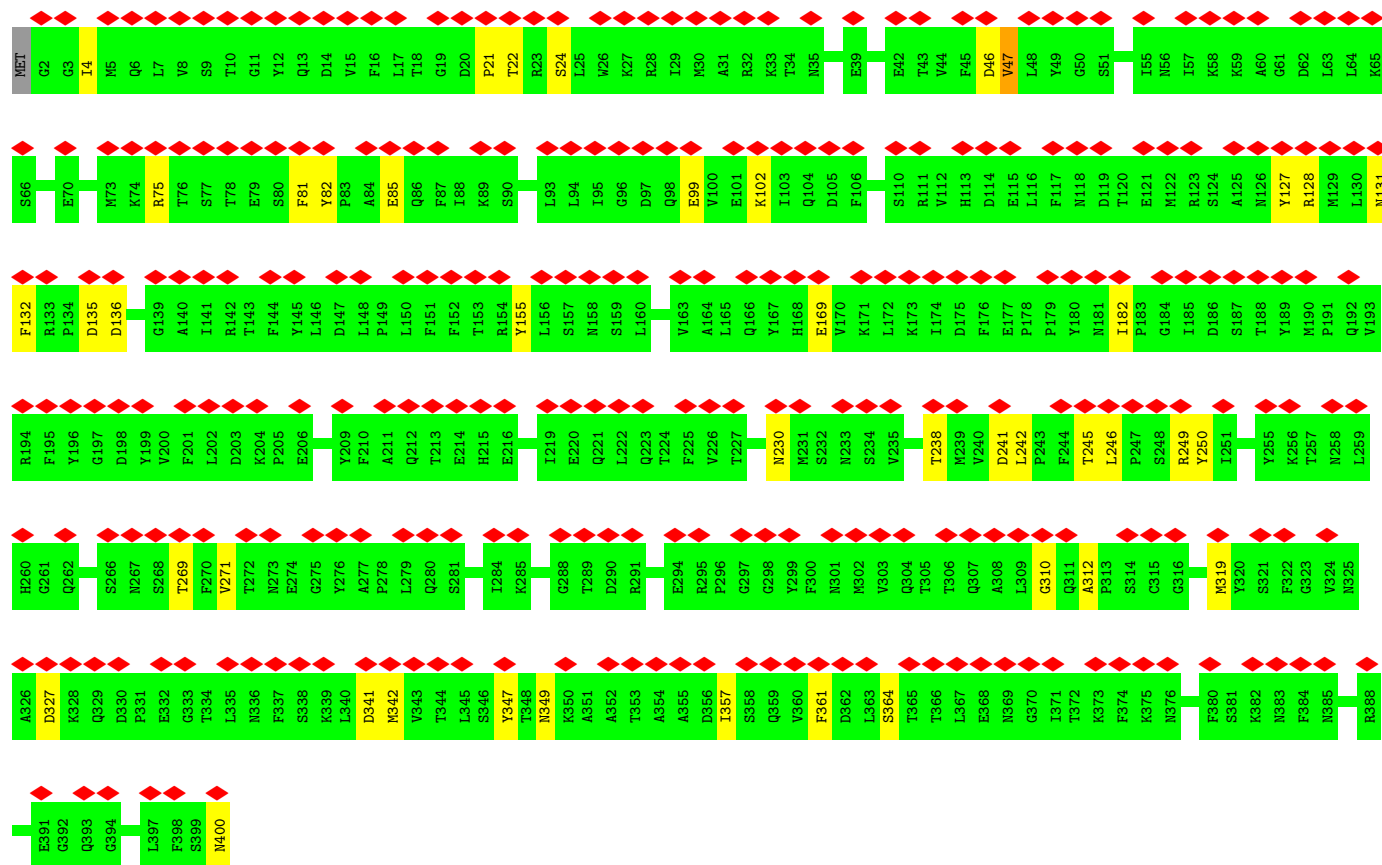
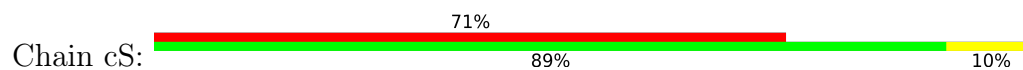
[illegible]



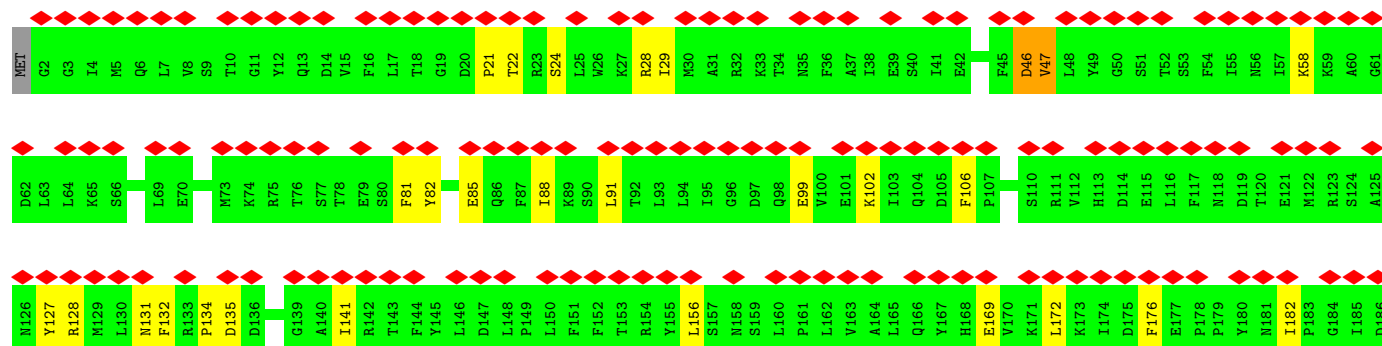
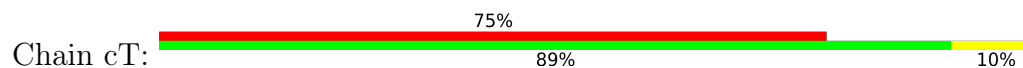


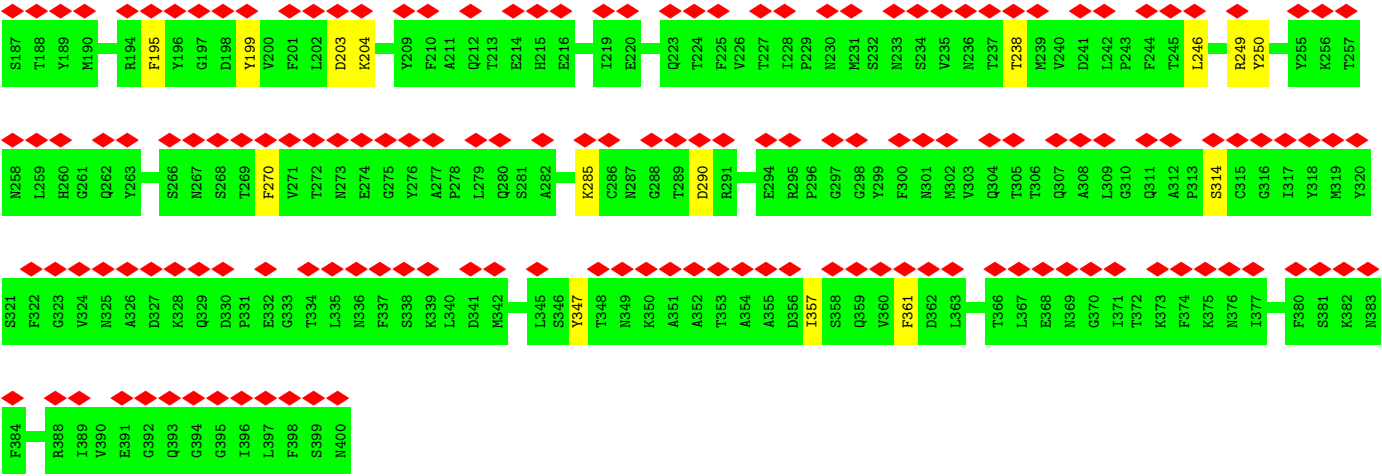


• Molecule 24: MCPv5

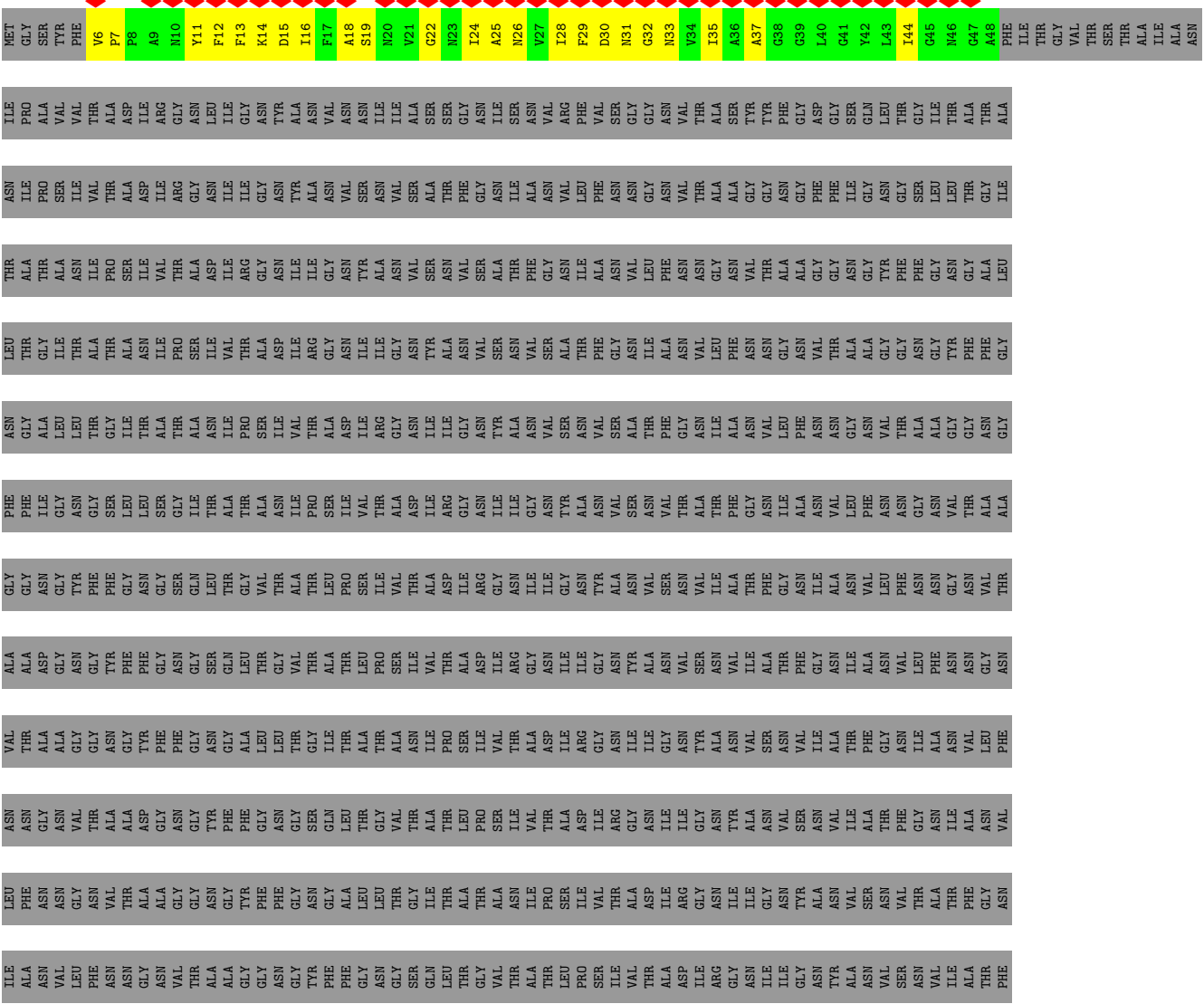


• Molecule 24: MCPv5





• Molecule 25: P22





- Molecule 26: P23

98%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56500	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 ($e^-/\text{\AA}^2$)	24.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.269	Depositor
Minimum map value	-1.541	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.098	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	1944.0, 1944.0, 1944.0	wwPDB
Map dimensions	1200, 1200, 1200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.62, 1.62, 1.62	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	aA	0.51	0/3468	0.88	8/4728 (0.2%)
1	aB	0.56	3/3468 (0.1%)	0.97	15/4728 (0.3%)
1	aC	0.58	0/3473	0.95	13/4735 (0.3%)
1	aD	0.60	1/3460 (0.0%)	1.06	21/4717 (0.4%)
1	aE	0.53	0/3473	0.90	10/4735 (0.2%)
1	aF	0.54	1/3460 (0.0%)	0.88	7/4717 (0.1%)
1	aG	0.52	0/3468	0.86	3/4728 (0.1%)
1	aH	0.51	0/3460	0.91	13/4717 (0.3%)
1	aI	0.53	1/3468 (0.0%)	0.91	16/4728 (0.3%)
1	aJ	0.56	0/3473	0.92	8/4735 (0.2%)
1	aK	0.51	0/3473	0.96	13/4735 (0.3%)
1	aL	0.53	0/3465	0.91	7/4724 (0.1%)
1	aM	0.52	0/3473	0.91	7/4735 (0.1%)
1	aN	0.54	0/3468	0.91	7/4728 (0.1%)
1	aO	0.53	0/3473	0.89	12/4735 (0.3%)
1	aP	0.51	0/3473	0.89	10/4735 (0.2%)
1	aQ	0.55	0/3460	0.91	5/4717 (0.1%)
1	aR	0.54	0/3473	0.94	13/4735 (0.3%)
1	aS	0.53	0/3473	0.89	5/4735 (0.1%)
1	aT	0.53	0/3473	0.87	10/4735 (0.2%)
1	aU	0.53	0/3473	0.89	3/4735 (0.1%)
1	aV	0.52	0/3473	0.85	5/4735 (0.1%)
1	aW	0.51	0/3473	0.94	10/4735 (0.2%)
1	aX	0.53	0/3468	0.92	11/4728 (0.2%)
1	aY	0.53	0/3473	0.90	9/4735 (0.2%)
1	aZ	0.54	0/3473	0.90	2/4735 (0.0%)
1	aa	0.91	0/3452	1.24	31/4707 (0.7%)
1	ab	0.91	0/3473	1.26	27/4735 (0.6%)
1	ac	0.90	0/3473	1.24	29/4735 (0.6%)
1	ad	0.54	0/3473	0.91	9/4735 (0.2%)
1	ae	0.51	0/3473	0.86	5/4735 (0.1%)
1	af	0.52	0/3473	0.91	12/4735 (0.3%)
1	ag	0.53	2/3473 (0.1%)	0.87	6/4735 (0.1%)
1	ah	0.51	0/3473	0.89	5/4735 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ai	0.52	0/3473	0.89	12/4735 (0.3%)
1	aj	0.53	0/3473	0.90	13/4735 (0.3%)
1	ak	0.51	0/3473	0.85	7/4735 (0.1%)
1	al	0.51	0/3465	0.91	11/4724 (0.2%)
1	am	0.53	1/3473 (0.0%)	0.93	10/4735 (0.2%)
1	an	0.53	0/3465	0.86	8/4724 (0.2%)
1	ao	0.52	0/3468	0.89	4/4728 (0.1%)
1	ap	0.52	0/3473	0.93	11/4735 (0.2%)
1	aq	0.52	0/3473	0.90	10/4735 (0.2%)
1	ar	0.53	0/3460	0.91	6/4717 (0.1%)
1	as	0.52	0/3473	0.90	11/4735 (0.2%)
1	at	0.52	1/3473 (0.0%)	0.83	5/4735 (0.1%)
1	au	0.51	0/3460	0.89	10/4717 (0.2%)
1	av	0.52	0/3473	0.89	3/4735 (0.1%)
1	aw	0.52	0/3473	0.94	11/4735 (0.2%)
1	ax	0.53	0/3460	0.84	6/4717 (0.1%)
1	ay	0.53	1/3468 (0.0%)	0.83	5/4728 (0.1%)
1	az	0.53	0/3460	0.85	4/4717 (0.1%)
1	ba	0.55	0/3473	0.92	6/4735 (0.1%)
1	bb	0.52	0/3473	0.85	4/4735 (0.1%)
1	bc	0.53	0/3473	0.93	10/4735 (0.2%)
1	bd	0.52	0/3473	0.91	5/4735 (0.1%)
1	be	0.52	0/3473	0.91	14/4735 (0.3%)
1	bf	0.51	0/3473	0.95	17/4735 (0.4%)
1	bg	0.53	1/3473 (0.0%)	0.89	6/4735 (0.1%)
1	bh	0.53	0/3473	0.85	7/4735 (0.1%)
1	bi	0.51	0/3473	0.89	14/4735 (0.3%)
1	bj	0.53	1/3473 (0.0%)	0.86	3/4735 (0.1%)
1	bk	0.51	0/3473	0.84	2/4735 (0.0%)
1	bl	0.51	0/3473	0.87	11/4735 (0.2%)
1	bm	0.53	0/3473	0.93	8/4735 (0.2%)
1	bn	0.50	0/3460	0.86	0/4717
1	bo	0.52	0/3473	0.87	6/4735 (0.1%)
1	bp	0.55	0/3473	0.97	12/4735 (0.3%)
1	bq	0.54	0/3473	0.91	5/4735 (0.1%)
1	br	0.53	0/3473	0.90	4/4735 (0.1%)
1	bs	0.53	0/3473	0.89	3/4735 (0.1%)
1	bt	0.52	0/3468	0.90	15/4728 (0.3%)
2	bA	0.56	1/4196 (0.0%)	0.94	20/5743 (0.3%)
2	bB	0.55	1/4208 (0.0%)	0.72	11/5759 (0.2%)
2	bu	0.87	0/4208	1.18	31/5759 (0.5%)
2	bv	0.86	0/4208	1.16	28/5759 (0.5%)
2	bw	0.85	1/4208 (0.0%)	1.16	28/5759 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	bx	0.86	1/4191 (0.0%)	1.19	32/5736 (0.6%)
2	by	0.85	0/4208	1.16	32/5759 (0.6%)
2	bz	0.86	1/4147 (0.0%)	1.19	26/5676 (0.5%)
3	bC	0.52	0/4020	0.66	2/5461 (0.0%)
4	bD	0.57	1/3248 (0.0%)	0.92	16/4423 (0.4%)
4	bF	0.56	1/3248 (0.0%)	0.92	15/4423 (0.3%)
4	cX	0.55	0/3244	0.96	15/4418 (0.3%)
4	cZ	0.55	0/3244	0.95	14/4418 (0.3%)
4	dd	0.55	0/3248	0.96	18/4423 (0.4%)
4	df	0.56	0/3244	0.95	13/4418 (0.3%)
4	dj	0.55	0/3248	0.94	14/4423 (0.3%)
4	dk	0.55	0/3248	0.94	14/4423 (0.3%)
4	dl	0.55	0/3248	0.94	14/4423 (0.3%)
4	dp	0.55	0/3248	0.96	16/4423 (0.4%)
4	dr	0.55	0/3248	0.95	14/4423 (0.3%)
5	bE	0.56	0/3218	0.96	14/4365 (0.3%)
5	cY	0.56	0/3218	0.98	17/4365 (0.4%)
5	de	0.56	0/3218	0.97	17/4365 (0.4%)
5	dq	0.56	0/3218	1.00	19/4365 (0.4%)
6	bG	0.54	0/3957	0.62	3/5413 (0.1%)
7	bH	0.63	2/3333 (0.1%)	1.13	35/4542 (0.8%)
8	bI	0.70	1/1120 (0.1%)	1.29	10/1517 (0.7%)
8	bJ	0.70	0/1172	1.32	20/1590 (1.3%)
8	bK	0.68	0/909	1.32	18/1228 (1.5%)
9	bL	0.62	0/537	1.24	8/720 (1.1%)
9	bM	0.67	0/537	1.13	7/720 (1.0%)
9	bN	0.67	0/530	1.27	6/710 (0.8%)
9	bO	0.60	0/530	1.08	1/710 (0.1%)
10	bP	0.77	0/1155	1.11	6/1573 (0.4%)
11	bQ	0.79	0/1307	1.41	26/1775 (1.5%)
12	bR	0.62	0/1270	1.05	8/1716 (0.5%)
13	bS	0.18	0/1534	0.53	4/2075 (0.2%)
14	bT	0.64	0/382	1.50	9/520 (1.7%)
14	bU	0.77	0/436	1.25	5/596 (0.8%)
14	bV	0.57	0/428	1.06	2/585 (0.3%)
14	bW	0.59	0/416	1.16	5/569 (0.9%)
14	bX	0.65	0/319	1.17	2/435 (0.5%)
14	bY	0.71	0/593	1.41	9/810 (1.1%)
14	bZ	0.65	0/416	1.12	2/569 (0.4%)
14	ca	0.60	0/416	1.07	0/569
14	cb	0.75	1/416 (0.2%)	1.39	6/569 (1.1%)
14	cc	0.67	1/665 (0.2%)	1.16	8/911 (0.9%)
14	cd	0.75	0/601	1.41	14/821 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
14	ce	0.66	0/576	1.13	2/787 (0.3%)
15	cf	0.68	0/647	1.08	6/873 (0.7%)
16	cg	0.72	0/535	1.06	2/723 (0.3%)
17	ch	0.83	0/1319	1.10	7/1781 (0.4%)
18	ci	0.63	0/565	1.19	8/760 (1.1%)
19	cj	0.19	0/471	0.38	0/643
19	ck	0.12	0/464	0.27	0/629
19	cl	0.16	0/438	0.38	0/595
19	cm	0.14	0/513	0.37	0/697
20	cn	0.16	0/778	0.49	0/1051
20	co	0.18	0/744	0.46	0/1010
21	cA	0.48	0/2239	0.56	0/3040
21	cB	0.54	0/2350	0.70	0/3188
21	cC	0.50	0/2239	0.58	0/3040
21	cD	0.51	0/2350	0.64	0/3188
21	cE	0.51	0/2247	0.66	1/3051 (0.0%)
21	cF	0.55	0/2350	0.70	1/3188 (0.0%)
21	cG	0.51	0/2260	0.64	0/3069
21	cH	0.58	0/2350	0.73	2/3188 (0.1%)
21	cI	0.50	0/2239	0.63	0/3040
21	cJ	0.56	1/2350 (0.0%)	0.70	0/3188
21	cK	0.50	0/2239	0.60	0/3040
21	cL	0.53	0/2350	0.72	3/3188 (0.1%)
21	cM	0.48	0/2220	0.60	0/3014
21	cN	0.50	0/2350	0.62	0/3188
21	cp	0.52	0/2350	0.63	0/3188
21	cq	0.50	0/2260	0.61	0/3069
21	cr	0.53	0/2350	0.67	2/3188 (0.1%)
21	cs	0.50	0/2206	0.59	0/2995
21	ct	0.53	0/2350	0.69	0/3188
21	cu	0.49	0/2247	0.62	0/3051
21	cv	0.56	0/2350	0.70	0/3188
21	cw	0.57	1/2247 (0.0%)	0.73	0/3051
21	cx	0.58	0/2350	0.72	3/3188 (0.1%)
21	cy	0.52	0/2247	0.65	2/3051 (0.1%)
21	cz	0.51	0/2350	0.63	0/3188
22	cO	0.39	0/222	0.72	0/302
22	cQ	0.39	0/237	0.59	0/322
22	da	0.38	0/231	0.58	0/316
22	dc	0.39	0/213	0.62	0/289
22	dg	0.32	0/245	0.55	0/334
22	di	0.31	0/215	0.59	0/293
22	ds	0.29	0/242	0.50	0/330

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	du	0.27	0/228	0.60	0/310
23	cP	0.36	0/244	0.66	0/333
23	db	0.38	0/203	0.68	0/277
23	dh	0.32	0/254	0.69	0/345
23	dt	0.23	0/239	0.65	0/324
24	cR	0.56	0/3281	0.98	4/4457 (0.1%)
24	cS	0.56	0/3281	0.97	4/4457 (0.1%)
24	cT	0.56	0/3281	0.98	4/4457 (0.1%)
25	cU	0.30	0/318	0.62	0/433
25	cV	0.30	0/312	0.66	0/425
25	cW	0.31	0/315	0.59	0/429
26	dm	0.37	0/176	0.82	0/243
26	dn	0.36	0/183	0.76	0/252
26	do	0.47	0/185	1.19	1/255 (0.4%)
All	All	0.57	27/437605 (0.0%)	0.91	1372/596073 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	bH	372	PRO	C-O	-9.01	1.17	1.25
4	bD	50	ASN	C-N	7.35	1.40	1.33
1	at	257	HIS	C-N	7.02	1.41	1.33
4	bF	181	SER	C-N	6.96	1.40	1.34
1	aB	257	HIS	C-N	6.63	1.41	1.33
1	am	257	HIS	C-N	6.49	1.41	1.33
1	aI	257	HIS	C-N	6.33	1.41	1.33
1	bj	257	HIS	C-N	6.13	1.40	1.33
1	bg	257	HIS	C-N	5.93	1.40	1.33
1	ay	158	THR	C-N	5.88	1.41	1.33
14	cc	125	THR	C-N	5.85	1.41	1.33
1	aB	281	ILE	C-N	5.75	1.41	1.33
1	aB	21	ASN	C-N	5.74	1.41	1.33
1	ag	256	ASN	CA-C	5.73	1.57	1.52
1	aF	158	THR	C-N	5.67	1.41	1.33
21	cJ	147	HIS	CA-CB	-5.66	1.46	1.52
7	bH	260	PRO	C-O	-5.63	1.16	1.24
1	ag	256	ASN	N-CA	5.63	1.52	1.47
2	bx	446	HIS	CB-CG	-5.60	1.42	1.50
2	bB	146	PRO	C-N	5.59	1.41	1.33
1	aD	21	ASN	C-N	5.44	1.40	1.33
8	bI	62	ALA	C-O	-5.38	1.17	1.24
2	bw	184	ILE	CA-C	-5.33	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	cw	131	LYS	CA-C	-5.12	1.48	1.52
2	bA	77	PRO	C-N	5.08	1.40	1.33
14	cb	183	ILE	C-N	5.07	1.40	1.33
2	bz	335	HIS	CB-CG	-5.05	1.43	1.50

All (1372) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	do	17	GLN	N-CA-C	12.75	125.18	111.03
8	bI	125	GLY	N-CA-C	-11.33	101.46	113.58
8	bJ	69	VAL	N-CA-C	10.96	120.78	111.90
14	bT	179	ALA	N-CA-C	10.88	124.22	111.71
9	bL	55	SER	N-CA-C	10.10	122.83	110.41
1	al	312	VAL	N-CA-C	10.04	122.53	112.90
1	aD	26	PHE	N-CA-C	9.98	123.40	111.82
1	be	213	THR	N-CA-C	9.88	123.28	111.82
1	ab	106	ASP	CA-CB-CG	9.81	122.41	112.60
7	bH	337	ILE	N-CA-C	9.58	120.49	111.48
1	ba	48	GLY	N-CA-C	9.54	121.71	112.08
14	cb	157	ALA	N-CA-C	9.53	121.67	111.28
5	dq	362	TYR	N-CA-C	9.36	124.83	113.23
12	bR	142	GLY	N-CA-C	-9.34	102.78	114.92
5	de	362	TYR	N-CA-C	9.27	124.78	113.38
5	cY	362	TYR	N-CA-C	9.27	124.83	112.88
8	bK	106	VAL	N-CA-C	-9.25	102.85	111.45
2	bB	354	GLY	N-CA-C	-9.24	101.64	112.73
8	bI	147	VAL	N-CA-C	9.12	119.39	108.45
9	bN	55	SER	N-CA-C	8.92	122.31	110.53
1	aC	256	ASN	N-CA-C	8.90	124.45	113.50
2	bz	297	THR	N-CA-C	-8.87	103.04	114.04
8	bJ	137	PHE	CA-C-N	8.83	128.91	120.43
8	bJ	137	PHE	C-N-CA	8.83	128.91	120.43
11	bQ	150	ASN	N-CA-C	8.78	123.81	111.52
1	ae	256	ASN	N-CA-C	8.73	123.76	112.41
5	cY	273	SER	N-CA-C	-8.71	102.43	113.23
5	de	273	SER	N-CA-C	-8.70	102.41	113.72
1	bf	213	THR	N-CA-C	8.68	121.52	111.11
5	dq	273	SER	N-CA-C	-8.65	102.47	113.72
2	bv	463	GLU	N-CA-C	8.54	121.70	111.02
1	bt	213	THR	N-CA-C	8.53	121.43	111.02
13	bS	27	ILE	C-N-CD	-8.52	90.05	125.00
4	dd	319	GLY	N-CA-C	-8.38	104.51	114.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	bP	122	PRO	N-CA-C	8.35	124.38	111.11
2	bu	463	GLU	N-CA-C	8.30	120.62	110.91
2	by	27	PHE	N-CA-C	8.27	120.30	111.28
16	cg	86	ASN	N-CA-C	-8.25	98.07	109.95
14	bY	153	ASN	N-CA-C	8.23	124.42	113.72
4	dk	262	ALA	N-CA-C	-8.23	105.24	114.62
4	cX	262	ALA	N-CA-C	-8.14	105.34	114.62
14	cd	172	ASN	CA-C-N	-8.13	107.69	121.75
14	cd	172	ASN	C-N-CA	-8.13	107.69	121.75
2	bA	354	GLY	CA-C-N	8.11	133.01	120.60
2	bA	354	GLY	C-N-CA	8.11	133.01	120.60
9	bL	16	THR	N-CA-C	8.11	120.84	111.11
8	bK	162	THR	N-CA-C	-8.05	103.03	113.17
5	cY	80	GLN	N-CA-C	8.05	122.50	111.39
2	bv	21	ASN	CA-C-N	7.99	127.92	119.85
2	bv	21	ASN	C-N-CA	7.99	127.92	119.85
1	bi	267	ASN	CA-C-N	7.98	132.28	121.74
1	bi	267	ASN	C-N-CA	7.98	132.28	121.74
5	de	80	GLN	N-CA-C	7.97	122.44	112.24
5	bE	80	GLN	N-CA-C	7.95	122.47	111.74
1	am	123	ASN	N-CA-C	7.94	120.94	111.33
5	dq	80	GLN	N-CA-C	7.94	122.40	112.24
14	cb	183	ILE	CA-C-N	7.93	127.95	119.78
14	cb	183	ILE	C-N-CA	7.93	127.95	119.78
5	cY	81	SER	N-CA-C	7.93	120.76	110.53
4	dk	319	GLY	N-CA-C	-7.90	104.65	114.92
5	de	26	ILE	N-CA-C	-7.89	105.45	113.10
1	ai	267	ASN	CA-C-N	7.89	132.15	121.74
1	ai	267	ASN	C-N-CA	7.89	132.15	121.74
8	bJ	164	GLN	N-CA-C	7.88	121.92	111.28
7	bH	519	PHE	N-CA-C	7.88	119.86	111.28
11	bQ	85	GLY	N-CA-C	7.84	123.52	113.24
7	bH	199	GLY	CA-C-N	7.84	127.84	119.76
7	bH	199	GLY	C-N-CA	7.84	127.84	119.76
2	bx	463	GLU	N-CA-C	7.83	120.08	110.91
1	ag	256	ASN	N-CA-C	7.83	124.16	113.21
1	br	400	THR	N-CA-C	7.82	121.11	110.55
4	dp	319	GLY	N-CA-C	-7.80	104.54	114.37
4	cX	319	GLY	N-CA-C	-7.80	104.55	114.37
4	cZ	319	GLY	N-CA-C	-7.75	104.60	114.37
10	bP	32	GLU	N-CA-C	7.75	123.41	113.88
4	df	319	GLY	N-CA-C	-7.75	104.61	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	bD	319	GLY	N-CA-C	-7.75	104.61	114.37
1	ac	359	LYS	CA-C-N	7.74	127.38	119.56
1	ac	359	LYS	C-N-CA	7.74	127.38	119.56
4	dr	319	GLY	N-CA-C	-7.71	104.66	114.37
2	bx	348	GLU	CA-C-N	7.69	127.70	119.78
2	bx	348	GLU	C-N-CA	7.69	127.70	119.78
1	ab	68	THR	N-CA-C	7.67	120.76	111.40
4	bF	319	GLY	N-CA-C	-7.67	104.70	114.37
1	aC	22	PRO	CA-C-N	7.66	131.16	120.29
1	aC	22	PRO	C-N-CA	7.66	131.16	120.29
2	bz	355	ASP	CA-C-N	7.64	127.36	119.56
2	bz	355	ASP	C-N-CA	7.64	127.36	119.56
5	bE	81	SER	N-CA-C	7.64	120.62	110.53
14	cb	184	PRO	N-CA-C	7.64	123.36	111.21
2	bA	495	GLY	N-CA-C	7.62	124.42	112.31
1	ac	388	ILE	N-CA-C	7.61	118.94	108.89
8	bJ	163	ARG	N-CA-C	7.58	120.09	110.61
2	bw	355	ASP	CA-C-N	7.58	127.29	119.56
2	bw	355	ASP	C-N-CA	7.58	127.29	119.56
14	ce	198	PRO	N-CA-C	7.57	123.68	113.84
5	dq	57	LEU	CA-C-N	-7.56	117.46	122.60
5	dq	57	LEU	C-N-CA	-7.56	117.46	122.60
2	bw	348	GLU	CA-C-N	7.53	127.49	120.03
2	bw	348	GLU	C-N-CA	7.53	127.49	120.03
4	bF	262	ALA	N-CA-C	-7.51	105.28	114.75
4	dl	262	ALA	N-CA-C	-7.51	105.29	114.75
1	be	123	ASN	CA-C-N	7.48	130.31	120.28
1	be	123	ASN	C-N-CA	7.48	130.31	120.28
11	bQ	61	ASP	CA-C-N	-7.44	112.87	122.77
11	bQ	61	ASP	C-N-CA	-7.44	112.87	122.77
15	cf	127	GLY	N-CA-C	7.44	116.98	110.21
1	aA	256	ASN	N-CA-C	7.43	120.68	110.06
2	by	86	PRO	N-CA-C	-7.43	99.53	111.19
7	bH	278	GLY	N-CA-C	7.43	121.64	112.73
2	bw	385	TYR	N-CA-C	-7.41	103.86	113.12
2	bA	35	THR	N-CA-C	-7.39	99.34	110.28
2	bv	221	LYS	N-CA-C	-7.38	104.80	113.88
1	ab	347	THR	CA-C-N	7.34	127.38	119.89
1	ab	347	THR	C-N-CA	7.34	127.38	119.89
1	aK	399	ASN	CA-C-N	7.34	132.46	120.94
1	aK	399	ASN	C-N-CA	7.34	132.46	120.94
1	bi	105	ILE	N-CA-C	-7.33	105.51	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	bw	464	ASP	N-CA-C	7.30	119.26	108.60
7	bH	258	HIS	CA-C-N	-7.28	114.54	123.21
7	bH	258	HIS	C-N-CA	-7.28	114.54	123.21
11	bQ	109	ARG	CA-C-N	-7.28	113.21	123.11
11	bQ	109	ARG	C-N-CA	-7.28	113.21	123.11
2	bz	24	ILE	N-CA-C	-7.27	100.20	109.58
1	bd	48	GLY	N-CA-C	7.25	119.41	112.08
4	dd	262	ALA	N-CA-C	-7.25	105.35	114.56
1	aJ	110	ASN	N-CA-C	-7.24	100.51	110.35
1	ac	256	ASN	N-CA-C	7.23	122.14	112.30
2	bB	180	TYR	N-CA-C	-7.23	100.98	110.53
1	bc	434	ALA	N-CA-C	7.23	120.02	111.71
4	dp	262	ALA	N-CA-C	-7.22	105.39	114.56
21	cL	263	ASN	N-CA-C	7.22	114.72	108.22
4	bD	262	ALA	N-CA-C	-7.22	105.39	114.56
1	ac	240	THR	CA-C-N	7.21	127.13	119.85
1	ac	240	THR	C-N-CA	7.21	127.13	119.85
1	ar	157	GLN	N-CA-C	7.21	122.34	112.90
9	bM	33	PHE	CA-C-N	7.19	131.50	120.13
9	bM	33	PHE	C-N-CA	7.19	131.50	120.13
4	dj	319	GLY	N-CA-C	-7.19	104.58	114.64
1	az	347	THR	N-CA-C	-7.18	98.44	109.64
7	bH	348	SER	N-CA-C	-7.17	104.00	112.89
4	dj	262	ALA	N-CA-C	-7.17	105.45	114.56
4	bF	305	THR	CA-C-N	-7.16	115.85	123.08
4	bF	305	THR	C-N-CA	-7.16	115.85	123.08
14	cd	161	ILE	N-CA-C	-7.16	103.80	110.53
5	de	81	SER	N-CA-C	7.15	120.60	110.23
2	by	348	GLU	CA-C-N	7.15	127.07	119.85
2	by	348	GLU	C-N-CA	7.15	127.07	119.85
1	aM	214	GLN	N-CA-C	7.14	118.71	111.07
4	dl	319	GLY	N-CA-C	-7.14	104.65	114.64
1	aO	156	ASN	N-CA-C	7.13	120.10	111.82
11	bQ	64	THR	CA-C-N	7.13	130.55	120.28
11	bQ	64	THR	C-N-CA	7.13	130.55	120.28
14	bU	183	ILE	N-CA-C	-7.13	99.78	107.77
1	bf	433	LEU	CA-C-N	7.13	129.70	120.44
1	bf	433	LEU	C-N-CA	7.13	129.70	120.44
14	bT	166	GLN	N-CA-C	-7.12	98.77	108.38
1	aD	394	ALA	N-CA-C	-7.12	103.52	111.28
5	dq	81	SER	N-CA-C	7.12	120.55	110.23
1	aa	392	SER	CA-C-N	7.09	127.69	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aa	392	SER	C-N-CA	7.09	127.69	119.47
2	bA	181	VAL	N-CA-C	-7.08	99.43	109.63
2	bv	400	ILE	CA-C-N	7.08	127.01	120.21
2	bv	400	ILE	C-N-CA	7.08	127.01	120.21
9	bN	18	GLN	N-CA-C	7.07	121.66	112.89
8	bJ	88	VAL	N-CA-C	7.07	113.77	106.21
2	by	464	ASP	N-CA-C	7.06	117.91	108.38
1	as	273	GLY	N-CA-C	7.05	125.10	115.30
1	aD	21	ASN	CA-C-N	-7.05	112.70	119.89
1	aD	21	ASN	C-N-CA	-7.05	112.70	119.89
1	am	257	HIS	CA-C-N	-7.04	112.22	119.83
1	am	257	HIS	C-N-CA	-7.04	112.22	119.83
17	ch	36	PHE	N-CA-C	7.04	119.04	111.36
9	bM	55	SER	N-CA-C	7.03	120.04	110.55
12	bR	155	THR	CA-C-N	-7.02	111.39	123.25
12	bR	155	THR	C-N-CA	-7.02	111.39	123.25
1	ab	388	ILE	N-CA-C	7.01	118.15	108.89
1	aK	137	ASN	N-CA-C	7.01	121.75	111.87
1	ay	162	ALA	N-CA-C	7.00	120.00	110.55
4	bF	359	THR	CA-C-N	7.00	130.05	120.46
4	bF	359	THR	C-N-CA	7.00	130.05	120.46
4	df	359	THR	CA-C-N	7.00	130.04	120.46
4	df	359	THR	C-N-CA	7.00	130.04	120.46
7	bH	286	TYR	N-CA-C	-6.99	98.22	109.96
1	bf	434	ALA	N-CA-C	6.97	118.53	111.07
2	bA	14	GLN	N-CA-C	-6.96	104.05	112.54
14	bT	178	ARG	CA-C-N	6.96	130.30	120.28
14	bT	178	ARG	C-N-CA	6.96	130.30	120.28
1	ac	347	THR	CA-C-N	6.94	126.97	119.89
1	ac	347	THR	C-N-CA	6.94	126.97	119.89
1	ab	94	GLN	N-CA-C	6.94	118.84	111.28
11	bQ	94	TYR	N-CA-C	-6.93	103.40	112.41
2	bw	68	GLY	CA-C-N	6.92	126.88	119.76
2	bw	68	GLY	C-N-CA	6.92	126.88	119.76
1	bq	369	CYS	CA-C-N	-6.91	113.86	122.84
1	bq	369	CYS	C-N-CA	-6.91	113.86	122.84
1	at	257	HIS	CA-C-N	-6.90	111.97	119.98
1	at	257	HIS	C-N-CA	-6.90	111.97	119.98
4	dd	359	THR	CA-C-N	6.90	129.91	120.46
4	dd	359	THR	C-N-CA	6.90	129.91	120.46
2	bw	400	ILE	CA-C-N	6.90	126.83	120.21
2	bw	400	ILE	C-N-CA	6.90	126.83	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	bI	50	ILE	N-CA-C	6.89	117.91	109.30
4	dr	262	ALA	N-CA-C	-6.88	105.43	114.31
1	aK	212	ASP	CA-C-N	6.87	129.81	120.54
1	aK	212	ASP	C-N-CA	6.87	129.81	120.54
1	bl	101	GLY	N-CA-C	6.87	125.48	114.90
1	ad	68	THR	N-CA-C	6.87	125.42	110.80
4	cX	359	THR	CA-C-N	6.86	129.86	120.46
4	cX	359	THR	C-N-CA	6.86	129.86	120.46
2	bu	92	ASN	N-CA-C	6.86	118.41	111.07
21	cy	100	LEU	CA-C-N	-6.86	110.34	122.48
21	cy	100	LEU	C-N-CA	-6.86	110.34	122.48
5	cY	246	ASN	N-CA-C	6.85	121.30	112.12
1	aD	369	CYS	N-CA-C	-6.82	98.12	109.24
2	bB	453	LYS	N-CA-C	-6.81	98.74	109.50
1	as	257	HIS	N-CA-C	6.80	116.14	108.25
18	ci	71	GLY	CA-C-N	6.80	126.50	119.56
18	ci	71	GLY	C-N-CA	6.80	126.50	119.56
1	aM	25	THR	N-CA-C	-6.80	98.97	109.24
2	bx	182	ASN	N-CA-C	6.79	119.31	111.02
2	bu	68	GLY	CA-C-N	6.79	126.75	119.76
2	bu	68	GLY	C-N-CA	6.79	126.75	119.76
2	bu	27	PHE	CA-CB-CG	-6.78	107.02	113.80
4	dr	359	THR	CA-C-N	6.78	130.08	120.53
4	dr	359	THR	C-N-CA	6.78	130.08	120.53
1	aj	136	VAL	N-CA-C	6.77	117.38	111.90
2	bx	355	ASP	CA-C-N	6.77	128.22	120.98
2	bx	355	ASP	C-N-CA	6.77	128.22	120.98
4	dk	359	THR	CA-C-N	6.76	130.07	120.53
4	dk	359	THR	C-N-CA	6.76	130.07	120.53
8	bI	53	LEU	N-CA-C	-6.76	97.88	108.90
1	aq	312	VAL	N-CA-C	6.76	119.50	111.05
1	aC	436	ALA	CA-C-N	6.74	133.84	121.70
1	aC	436	ALA	C-N-CA	6.74	133.84	121.70
4	cZ	359	THR	CA-C-N	6.74	130.04	120.53
4	cZ	359	THR	C-N-CA	6.74	130.04	120.53
7	bH	168	GLY	CA-C-N	-6.74	113.48	122.85
7	bH	168	GLY	C-N-CA	-6.74	113.48	122.85
1	au	123	ASN	N-CA-C	6.74	119.19	111.11
1	aC	336	LYS	N-CA-C	6.73	122.03	113.55
2	bz	68	GLY	CA-C-N	6.73	126.69	119.76
2	bz	68	GLY	C-N-CA	6.73	126.69	119.76
1	bp	344	GLY	N-CA-C	-6.73	104.05	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aB	281	ILE	CA-C-N	-6.73	112.83	119.76
1	aB	281	ILE	C-N-CA	-6.73	112.83	119.76
1	aW	137	ASN	CA-C-N	6.71	131.67	122.07
1	aW	137	ASN	C-N-CA	6.71	131.67	122.07
1	aj	400	THR	CA-C-N	6.71	129.57	120.38
1	aj	400	THR	C-N-CA	6.71	129.57	120.38
1	al	213	THR	N-CA-C	6.71	118.25	111.07
5	bE	246	ASN	N-CA-C	6.70	121.30	112.72
4	dl	359	THR	CA-C-N	6.70	129.98	120.53
4	dl	359	THR	C-N-CA	6.70	129.98	120.53
9	bO	23	LEU	N-CA-C	-6.70	104.97	113.01
1	ad	136	VAL	CA-C-N	-6.69	113.20	123.17
1	ad	136	VAL	C-N-CA	-6.69	113.20	123.17
1	ak	268	ASN	N-CA-C	-6.69	99.53	109.42
5	de	246	ASN	N-CA-C	6.68	121.28	112.13
1	af	125	ASP	N-CA-C	-6.67	103.82	112.23
14	cd	199	ASN	CA-C-N	-6.67	113.37	122.91
14	cd	199	ASN	C-N-CA	-6.67	113.37	122.91
1	aa	94	GLN	N-CA-C	6.66	118.54	111.28
4	dj	359	THR	CA-C-N	6.66	129.92	120.53
4	dj	359	THR	C-N-CA	6.66	129.92	120.53
14	cc	125	THR	CA-C-N	-6.66	113.12	119.85
14	cc	125	THR	C-N-CA	-6.66	113.12	119.85
14	cd	177	LEU	N-CA-C	6.66	119.54	111.82
2	bu	450	VAL	CA-C-N	6.66	126.60	119.28
2	bu	450	VAL	C-N-CA	6.66	126.60	119.28
5	dq	246	ASN	N-CA-C	6.66	121.24	112.72
4	dp	359	THR	CA-C-N	6.65	129.91	120.53
4	dp	359	THR	C-N-CA	6.65	129.91	120.53
2	by	221	LYS	N-CA-C	-6.65	105.79	114.04
14	bT	171	LYS	N-CA-C	-6.65	102.21	111.39
8	bJ	154	THR	N-CA-C	6.65	118.53	111.28
14	bU	203	LYS	N-CA-C	6.64	117.74	109.57
1	aB	257	HIS	CA-C-N	-6.63	112.29	119.98
1	aB	257	HIS	C-N-CA	-6.63	112.29	119.98
1	bc	436	ALA	CA-C-N	6.63	133.63	121.70
1	bc	436	ALA	C-N-CA	6.63	133.63	121.70
1	ab	297	THR	CA-C-N	6.63	127.08	120.52
1	ab	297	THR	C-N-CA	6.63	127.08	120.52
24	cT	24	SER	N-CA-C	-6.62	100.03	109.96
24	cR	24	SER	N-CA-C	-6.60	100.06	109.96
1	bo	122	MET	CA-C-N	6.59	134.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bo	122	MET	C-N-CA	6.59	134.13	121.54
12	bR	26	GLY	N-CA-C	-6.59	103.05	112.81
9	bL	7	ASP	CA-C-N	-6.59	113.08	123.23
9	bL	7	ASP	C-N-CA	-6.59	113.08	123.23
1	ah	243	ALA	N-CA-C	6.58	120.48	111.39
1	aP	64	GLY	N-CA-C	6.58	120.74	111.19
1	ac	21	ASN	CA-C-N	6.57	126.53	119.76
1	ac	21	ASN	C-N-CA	6.57	126.53	119.76
1	bp	62	ARG	CA-C-N	6.57	131.69	120.72
1	bp	62	ARG	C-N-CA	6.57	131.69	120.72
2	bA	383	SER	CA-C-N	6.57	133.86	122.56
2	bA	383	SER	C-N-CA	6.57	133.86	122.56
8	bK	95	THR	N-CA-C	-6.57	104.05	111.14
1	aR	105	ILE	N-CA-C	-6.56	105.44	111.67
1	bm	122	MET	CA-C-N	6.55	134.06	121.54
1	bm	122	MET	C-N-CA	6.55	134.06	121.54
2	bz	221	LYS	N-CA-C	-6.55	105.82	113.88
1	ab	240	THR	CA-C-N	6.53	127.06	120.14
1	ab	240	THR	C-N-CA	6.53	127.06	120.14
2	bz	348	GLU	N-CA-C	6.53	119.86	108.82
2	bw	333	ILE	N-CA-C	6.53	118.09	109.21
1	af	213	THR	N-CA-C	6.52	118.97	111.02
1	ay	158	THR	CA-C-N	-6.52	112.91	119.56
1	ay	158	THR	C-N-CA	-6.52	112.91	119.56
4	cX	121	MET	CA-C-N	6.51	131.27	120.86
4	cX	121	MET	C-N-CA	6.51	131.27	120.86
8	bK	62	ALA	CA-C-N	-6.50	111.06	120.29
8	bK	62	ALA	C-N-CA	-6.50	111.06	120.29
4	cZ	121	MET	CA-C-N	6.50	131.27	120.86
4	cZ	121	MET	C-N-CA	6.50	131.27	120.86
7	bH	247	LYS	CA-C-N	6.50	126.27	120.10
7	bH	247	LYS	C-N-CA	6.50	126.27	120.10
1	aw	137	ASN	CA-C-N	6.49	131.33	122.19
1	aw	137	ASN	C-N-CA	6.49	131.33	122.19
12	bR	17	ASN	N-CA-C	6.49	119.02	109.42
2	bx	68	GLY	CA-C-N	6.48	126.44	119.76
2	bx	68	GLY	C-N-CA	6.48	126.44	119.76
21	cE	100	LEU	N-CA-C	-6.48	105.34	113.18
4	dd	121	MET	CA-C-N	6.48	131.39	121.03
4	dd	121	MET	C-N-CA	6.48	131.39	121.03
1	bs	121	ARG	N-CA-C	-6.47	99.47	109.76
2	by	68	GLY	CA-C-N	6.47	126.42	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	by	68	GLY	C-N-CA	6.47	126.42	119.76
1	aU	122	MET	CA-C-N	6.47	133.89	121.54
1	aU	122	MET	C-N-CA	6.47	133.89	121.54
2	bB	13	ALA	N-CA-C	6.46	118.41	111.36
17	ch	34	ILE	CA-C-N	6.46	126.49	119.90
17	ch	34	ILE	C-N-CA	6.46	126.49	119.90
4	dp	121	MET	CA-C-N	6.46	131.37	121.03
4	dp	121	MET	C-N-CA	6.46	131.37	121.03
4	dp	180	ALA	CA-C-O	-6.46	114.59	122.41
2	bx	23	GLN	N-CA-C	6.45	118.31	111.28
8	bK	63	ALA	N-CA-C	-6.45	104.33	111.36
1	aq	137	ASN	CA-C-N	6.45	131.28	122.19
1	aq	137	ASN	C-N-CA	6.45	131.28	122.19
1	ab	359	LYS	CA-C-N	6.44	126.07	119.56
1	ab	359	LYS	C-N-CA	6.44	126.07	119.56
4	dk	121	MET	CA-C-N	6.44	131.34	121.03
4	dk	121	MET	C-N-CA	6.44	131.34	121.03
1	aY	436	ALA	CA-C-N	6.43	133.27	121.70
1	aY	436	ALA	C-N-CA	6.43	133.27	121.70
8	bJ	158	ALA	N-CA-C	6.43	118.28	111.28
4	dj	121	MET	CA-C-N	6.43	131.31	121.03
4	dj	121	MET	C-N-CA	6.43	131.31	121.03
1	av	312	VAL	N-CA-C	6.42	121.42	112.50
4	cZ	180	ALA	CA-C-O	-6.40	114.64	122.64
1	aa	268	ASN	CA-C-N	6.39	126.08	119.56
1	aa	268	ASN	C-N-CA	6.39	126.08	119.56
4	dr	121	MET	CA-C-N	6.39	131.26	121.03
4	dr	121	MET	C-N-CA	6.39	131.26	121.03
4	df	180	ALA	CA-C-O	-6.39	114.65	122.64
4	dr	180	ALA	CA-C-O	-6.38	114.69	122.41
1	bh	213	THR	N-CA-C	6.38	118.81	111.02
4	cX	180	ALA	CA-C-O	-6.38	114.67	122.64
4	dl	180	ALA	CA-C-O	-6.38	114.67	122.64
4	df	121	MET	CA-C-N	6.38	131.23	121.03
4	df	121	MET	C-N-CA	6.38	131.23	121.03
7	bH	172	GLY	N-CA-C	6.37	120.41	110.91
1	aj	123	ASN	CB-CA-C	-6.37	109.24	116.63
11	bQ	131	ASP	CA-C-N	-6.37	112.46	122.65
11	bQ	131	ASP	C-N-CA	-6.37	112.46	122.65
1	ba	312	VAL	N-CA-C	6.37	117.94	111.00
1	bf	123	ASN	CA-C-N	6.37	128.82	120.28
1	bf	123	ASN	C-N-CA	6.37	128.82	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	cd	177	LEU	CA-C-N	-6.37	110.94	120.94
14	cd	177	LEU	C-N-CA	-6.37	110.94	120.94
11	bQ	76	LYS	N-CA-C	-6.37	105.51	113.28
2	bv	416	VAL	N-CA-C	6.36	116.51	110.53
1	aI	257	HIS	CA-C-N	-6.36	112.96	119.83
1	aI	257	HIS	C-N-CA	-6.36	112.96	119.83
1	be	399	ASN	N-CA-C	6.35	117.82	108.86
10	bP	20	PRO	N-CA-C	6.35	121.19	111.15
14	cc	145	ALA	N-CA-C	-6.34	101.03	109.84
4	bD	293	ASP	N-CA-C	6.33	118.61	108.41
1	aT	233	PHE	CA-C-N	6.32	133.77	121.63
1	aT	233	PHE	C-N-CA	6.32	133.77	121.63
1	am	200	PRO	CA-C-N	-6.32	114.00	122.72
1	am	200	PRO	C-N-CA	-6.32	114.00	122.72
2	bz	348	GLU	CA-C-N	6.32	127.54	120.66
2	bz	348	GLU	C-N-CA	6.32	127.54	120.66
1	ab	356	PHE	N-CA-C	-6.30	105.72	113.41
21	cL	102	PRO	N-CA-C	6.30	121.73	113.86
4	dk	180	ALA	CA-C-O	-6.30	114.77	122.64
1	bf	122	MET	CA-C-N	6.29	133.55	122.66
1	bf	122	MET	C-N-CA	6.29	133.55	122.66
4	dd	180	ALA	CA-C-O	-6.29	114.78	122.64
1	ap	251	ILE	CA-C-N	6.27	129.73	120.95
1	ap	251	ILE	C-N-CA	6.27	129.73	120.95
2	bx	112	TRP	N-CA-C	-6.26	101.83	110.35
1	aL	200	PRO	CA-C-N	-6.26	114.16	122.99
1	aL	200	PRO	C-N-CA	-6.26	114.16	122.99
2	bw	13	ALA	N-CA-C	-6.26	106.27	114.04
1	aj	256	ASN	N-CA-C	6.26	120.23	112.03
11	bQ	64	THR	CA-C-O	-6.25	114.43	121.81
12	bR	162	LEU	CA-C-N	-6.25	112.08	120.90
12	bR	162	LEU	C-N-CA	-6.25	112.08	120.90
1	aI	10	ALA	N-CA-C	-6.25	99.45	109.39
1	aX	137	ASN	CA-C-N	6.24	130.99	122.19
1	aX	137	ASN	C-N-CA	6.24	130.99	122.19
1	aD	123	ASN	CB-CA-C	-6.24	109.39	116.63
2	bA	228	MET	N-CA-C	6.24	119.06	111.82
8	bK	119	PHE	N-CA-C	-6.24	101.70	110.50
4	bF	181	SER	CA-C-N	-6.24	113.80	120.47
4	bF	181	SER	C-N-CA	-6.24	113.80	120.47
4	dr	313	GLY	CA-C-N	6.23	129.68	120.95
4	dr	313	GLY	C-N-CA	6.23	129.68	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aa	359	LYS	CA-C-N	6.23	125.92	119.56
1	aa	359	LYS	C-N-CA	6.23	125.92	119.56
4	dp	313	GLY	CA-C-N	6.23	129.56	120.71
4	dp	313	GLY	C-N-CA	6.23	129.56	120.71
2	bx	464	ASP	N-CA-C	6.23	117.69	108.60
2	bx	400	ILE	CA-C-N	6.23	126.19	120.21
2	bx	400	ILE	C-N-CA	6.23	126.19	120.21
2	bz	400	ILE	CA-C-N	6.22	126.19	120.21
2	bz	400	ILE	C-N-CA	6.22	126.19	120.21
8	bI	138	ILE	CB-CA-C	-6.22	107.79	113.70
1	be	67	ILE	CA-C-N	-6.21	113.60	121.98
1	be	67	ILE	C-N-CA	-6.21	113.60	121.98
8	bI	58	LEU	O-C-N	6.21	130.24	123.10
4	dd	313	GLY	CA-C-N	6.21	129.53	120.71
4	dd	313	GLY	C-N-CA	6.21	129.53	120.71
2	by	400	ILE	CA-C-N	6.21	126.17	120.21
2	by	400	ILE	C-N-CA	6.21	126.17	120.21
4	df	313	GLY	CA-C-N	6.21	129.64	120.95
4	df	313	GLY	C-N-CA	6.21	129.64	120.95
1	aN	12	GLY	N-CA-C	6.20	122.36	112.06
4	cZ	313	GLY	CA-C-N	6.20	129.63	120.95
4	cZ	313	GLY	C-N-CA	6.20	129.63	120.95
4	dd	293	ASP	N-CA-C	6.20	118.71	109.59
1	aa	9	VAL	N-CA-C	6.20	117.41	108.48
1	bt	436	ALA	CA-C-N	6.20	132.85	121.70
1	bt	436	ALA	C-N-CA	6.20	132.85	121.70
4	dj	313	GLY	CA-C-N	6.20	129.56	120.82
4	dj	313	GLY	C-N-CA	6.20	129.56	120.82
1	aD	137	ASN	CA-C-N	6.19	130.91	122.19
1	aD	137	ASN	C-N-CA	6.19	130.91	122.19
4	bD	50	ASN	CA-C-N	-6.18	113.58	120.45
4	bD	50	ASN	C-N-CA	-6.18	113.58	120.45
4	cZ	293	ASP	N-CA-C	6.18	118.68	109.59
1	aJ	399	ASN	N-CA-C	6.18	117.96	109.18
4	df	293	ASP	N-CA-C	6.18	118.68	109.59
2	bz	460	PHE	N-CA-C	-6.18	104.91	112.88
14	bY	154	PHE	N-CA-C	6.17	117.67	111.07
4	dj	344	ASP	N-CA-C	6.16	117.80	111.14
1	aD	14	GLN	N-CA-C	-6.16	106.30	113.88
1	aR	212	ASP	CA-C-N	6.16	130.06	120.82
1	aR	212	ASP	C-N-CA	6.16	130.06	120.82
4	cX	313	GLY	CA-C-N	6.16	129.57	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	cX	313	GLY	C-N-CA	6.16	129.57	120.95
12	bR	20	LYS	N-CA-C	-6.15	104.49	111.07
6	bG	473	VAL	CA-C-N	-6.14	118.17	122.59
6	bG	473	VAL	C-N-CA	-6.14	118.17	122.59
14	bT	188	VAL	CA-C-N	6.14	131.52	121.87
14	bT	188	VAL	C-N-CA	6.14	131.52	121.87
4	dr	293	ASP	N-CA-C	6.14	118.62	109.59
4	dp	293	ASP	N-CA-C	6.14	118.61	109.59
1	bj	336	LYS	N-CA-C	6.14	121.43	113.88
24	cS	24	SER	N-CA-C	-6.13	100.01	109.76
4	dk	313	GLY	CA-C-N	6.13	129.53	120.95
4	dk	313	GLY	C-N-CA	6.13	129.53	120.95
2	bv	464	ASP	N-CA-C	6.12	117.49	108.86
4	bF	293	ASP	N-CA-C	6.12	118.59	109.59
2	bB	146	PRO	CA-C-N	-6.12	113.64	119.76
2	bB	146	PRO	C-N-CA	-6.12	113.64	119.76
1	aa	297	THR	CA-C-N	6.11	126.57	120.52
1	aa	297	THR	C-N-CA	6.11	126.57	120.52
1	aK	4	GLY	CA-C-N	-6.11	109.08	121.18
1	aK	4	GLY	C-N-CA	-6.11	109.08	121.18
2	bv	68	GLY	CA-C-N	6.11	126.05	119.76
2	bv	68	GLY	C-N-CA	6.11	126.05	119.76
1	aD	124	ASP	N-CA-C	-6.11	104.73	111.82
1	aI	213	THR	N-CA-C	6.11	118.47	111.02
1	aJ	235	GLY	N-CA-C	6.11	121.22	111.64
1	as	137	ASN	N-CA-C	6.10	119.98	111.56
2	bu	400	ILE	CA-C-N	6.09	126.06	120.21
2	bu	400	ILE	C-N-CA	6.09	126.06	120.21
1	bq	122	MET	CA-C-N	6.09	133.17	121.54
1	bq	122	MET	C-N-CA	6.09	133.17	121.54
1	aV	101	GLY	N-CA-C	6.09	123.68	114.61
4	dl	292	THR	CA-C-N	6.08	129.39	120.82
4	dl	292	THR	C-N-CA	6.08	129.39	120.82
7	bH	179	ALA	N-CA-C	-6.06	104.68	111.28
2	bA	33	ARG	N-CA-C	6.05	119.33	109.59
14	bY	205	LEU	CA-C-N	6.05	132.59	121.70
14	bY	205	LEU	C-N-CA	6.05	132.59	121.70
1	bg	213	THR	N-CA-C	6.05	118.37	111.11
1	au	156	ASN	CA-C-N	-6.04	112.57	122.54
1	au	156	ASN	C-N-CA	-6.04	112.57	122.54
1	an	257	HIS	CA-C-N	-6.03	112.30	119.84
1	an	257	HIS	C-N-CA	-6.03	112.30	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ao	399	ASN	CA-C-N	6.03	131.94	120.97
1	ao	399	ASN	C-N-CA	6.03	131.94	120.97
1	aS	213	THR	N-CA-C	6.03	117.52	111.07
1	ao	257	HIS	CA-C-N	-6.02	112.32	119.84
1	ao	257	HIS	C-N-CA	-6.02	112.32	119.84
1	aB	21	ASN	CA-C-N	-6.02	113.56	119.76
1	aB	21	ASN	C-N-CA	-6.02	113.56	119.76
2	bx	385	TYR	N-CA-C	-6.02	105.02	112.90
1	ab	74	PHE	CA-CB-CG	6.01	119.81	113.80
4	bF	121	MET	CA-C-N	6.01	131.31	121.57
4	bF	121	MET	C-N-CA	6.01	131.31	121.57
1	aa	347	THR	CA-C-N	6.01	125.98	120.03
1	aa	347	THR	C-N-CA	6.01	125.98	120.03
9	bL	15	ASP	CA-C-N	6.01	128.65	120.54
9	bL	15	ASP	C-N-CA	6.01	128.65	120.54
8	bK	83	GLY	N-CA-C	6.01	124.33	115.08
1	aN	436	ALA	CA-C-N	6.00	132.51	121.70
1	aN	436	ALA	C-N-CA	6.00	132.51	121.70
1	bh	122	MET	CA-C-N	6.00	133.01	121.54
1	bh	122	MET	C-N-CA	6.00	133.01	121.54
2	bv	462	LEU	N-CA-C	6.00	118.52	108.73
8	bK	84	GLY	N-CA-C	6.00	119.93	112.73
1	aa	120	PHE	N-CA-C	5.99	121.51	113.72
1	ab	268	ASN	CA-C-N	5.99	125.67	119.56
1	ab	268	ASN	C-N-CA	5.99	125.67	119.56
1	aQ	137	ASN	N-CA-C	5.99	119.87	111.30
14	bY	148	ASN	CA-C-N	-5.99	114.81	122.77
14	bY	148	ASN	C-N-CA	-5.99	114.81	122.77
2	bB	178	LEU	N-CA-C	5.98	119.02	110.10
4	dd	344	ASP	N-CA-C	5.98	117.80	111.28
4	dp	344	ASP	N-CA-C	5.98	117.80	111.28
2	bz	450	VAL	CA-C-N	5.98	126.41	119.47
2	bz	450	VAL	C-N-CA	5.98	126.41	119.47
14	cd	150	GLN	N-CA-C	5.97	119.81	110.32
1	bf	436	ALA	CA-C-N	5.97	132.44	121.70
1	bf	436	ALA	C-N-CA	5.97	132.44	121.70
1	aF	257	HIS	CA-C-N	-5.96	113.06	119.98
1	aF	257	HIS	C-N-CA	-5.96	113.06	119.98
1	aa	312	VAL	N-CA-C	5.96	118.73	112.83
1	bp	428	SER	N-CA-C	5.96	119.64	111.54
4	cX	292	THR	CA-C-N	5.96	129.57	121.05
4	cX	292	THR	C-N-CA	5.96	129.57	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	bD	344	ASP	N-CA-C	5.95	117.77	111.28
1	ap	25	THR	N-CA-C	-5.95	99.31	109.24
1	aH	256	ASN	N-CA-C	5.95	123.47	110.80
1	aq	59	GLN	N-CA-C	-5.94	99.04	108.73
1	aS	123	ASN	CA-C-N	5.94	129.34	120.31
1	aS	123	ASN	C-N-CA	5.94	129.34	120.31
1	aH	233	PHE	CA-C-N	5.94	132.40	121.94
1	aH	233	PHE	C-N-CA	5.94	132.40	121.94
1	bi	431	GLY	N-CA-C	5.94	119.85	111.42
8	bJ	150	ALA	N-CA-C	5.94	119.28	112.57
2	bz	332	GLU	N-CA-C	5.93	118.70	111.82
1	ad	256	ASN	N-CA-C	5.93	120.18	111.34
1	ad	312	VAL	N-CA-C	5.93	118.70	112.83
1	aM	123	ASN	CB-CA-C	-5.93	109.75	116.63
7	bH	201	GLY	N-CA-C	-5.93	102.03	110.63
11	bQ	64	THR	O-C-N	5.93	129.61	122.85
1	aj	137	ASN	CA-C-N	5.93	130.54	122.07
1	aj	137	ASN	C-N-CA	5.93	130.54	122.07
2	by	20	GLY	N-CA-C	-5.92	104.08	112.37
9	bN	34	ILE	N-CA-C	5.92	121.66	109.34
1	bp	104	ARG	CA-C-N	-5.92	117.10	123.08
1	bp	104	ARG	C-N-CA	-5.92	117.10	123.08
17	ch	97	LEU	CA-C-N	5.91	125.88	120.21
17	ch	97	LEU	C-N-CA	5.91	125.88	120.21
2	bw	21	ASN	CA-C-N	5.91	125.82	119.85
2	bw	21	ASN	C-N-CA	5.91	125.82	119.85
10	bP	129	ILE	N-CA-C	-5.91	106.99	112.43
2	bv	379	TYR	N-CA-C	5.91	118.15	108.52
24	cT	127	TYR	CA-CB-CG	5.90	124.52	113.90
8	bK	157	ILE	N-CA-C	-5.90	105.94	111.48
1	ar	123	ASN	CB-CA-C	-5.89	109.22	117.23
2	bw	387	VAL	N-CA-C	5.89	118.13	111.88
1	as	233	PHE	CA-C-N	5.89	132.01	122.29
1	as	233	PHE	C-N-CA	5.89	132.01	122.29
24	cS	127	TYR	CA-CB-CG	5.89	124.50	113.90
4	dj	292	THR	CA-C-N	5.89	129.47	121.05
4	dj	292	THR	C-N-CA	5.89	129.47	121.05
1	aK	67	ILE	CA-C-N	-5.88	113.85	121.79
1	aK	67	ILE	C-N-CA	-5.88	113.85	121.79
1	aW	122	MET	CA-C-N	5.88	132.78	121.54
1	aW	122	MET	C-N-CA	5.88	132.78	121.54
1	bi	399	ASN	CA-C-N	5.88	131.68	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bi	399	ASN	C-N-CA	5.88	131.68	120.97
24	cR	127	TYR	CA-CB-CG	5.88	124.48	113.90
14	bW	198	PRO	N-CA-C	5.88	121.58	113.65
2	bz	464	ASP	N-CA-C	5.88	119.29	109.95
4	bD	121	MET	CA-C-N	5.87	131.31	121.92
4	bD	121	MET	C-N-CA	5.87	131.31	121.92
10	bP	33	GLY	N-CA-C	5.87	122.24	110.97
2	bv	387	VAL	N-CA-C	5.87	117.74	112.17
1	ap	434	ALA	N-CA-C	5.86	117.75	111.36
14	bU	202	GLN	CA-C-N	5.85	129.20	120.83
14	bU	202	GLN	C-N-CA	5.85	129.20	120.83
1	aO	436	ALA	CA-C-N	5.84	132.22	121.70
1	aO	436	ALA	C-N-CA	5.84	132.22	121.70
24	cS	22	THR	N-CA-C	-5.84	99.90	107.73
2	by	13	ALA	N-CA-C	-5.84	107.14	114.56
4	bD	184	ASP	N-CA-C	5.84	118.53	111.40
4	dp	292	THR	CA-C-N	5.84	129.65	121.24
4	dp	292	THR	C-N-CA	5.84	129.65	121.24
5	cY	377	GLY	N-CA-C	5.84	119.29	110.18
24	cR	22	THR	N-CA-C	-5.84	99.91	107.73
5	dq	119	MET	CA-C-N	5.84	130.93	122.29
5	dq	119	MET	C-N-CA	5.84	130.93	122.29
2	bA	451	PRO	N-CA-C	5.83	120.35	111.19
21	cH	162	GLY	CA-C-N	-5.83	112.67	122.29
21	cH	162	GLY	C-N-CA	-5.83	112.67	122.29
1	aa	388	ILE	N-CA-C	5.83	116.59	108.89
1	aR	148	TYR	CA-C-N	-5.83	116.84	123.25
1	aR	148	TYR	C-N-CA	-5.83	116.84	123.25
1	aY	10	ALA	N-CA-C	-5.83	100.88	109.62
2	by	184	ILE	CB-CA-C	-5.83	104.27	112.14
5	cY	290	THR	CA-C-N	5.83	129.04	120.82
5	cY	290	THR	C-N-CA	5.83	129.04	120.82
1	bp	152	ILE	N-CA-C	5.83	121.46	109.34
1	aa	213	THR	N-CA-C	5.82	117.30	111.07
1	aP	123	ASN	CB-CA-C	-5.81	109.89	116.63
5	bE	290	THR	CA-C-N	5.81	129.01	120.82
5	bE	290	THR	C-N-CA	5.81	129.01	120.82
5	dq	290	THR	CA-C-N	5.81	128.96	120.71
5	dq	290	THR	C-N-CA	5.81	128.96	120.71
1	bc	243	ALA	CA-C-N	5.80	132.63	121.54
1	bc	243	ALA	C-N-CA	5.80	132.63	121.54
5	bE	119	MET	CA-C-N	5.80	130.88	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	bE	119	MET	C-N-CA	5.80	130.88	122.29
1	ab	119	LEU	N-CA-C	5.80	120.37	113.12
2	bA	370	HIS	CA-C-N	-5.80	113.57	119.83
2	bA	370	HIS	C-N-CA	-5.80	113.57	119.83
5	cY	119	MET	CA-C-N	5.80	130.87	122.29
5	cY	119	MET	C-N-CA	5.80	130.87	122.29
1	aQ	243	ALA	CA-C-N	5.79	132.61	121.54
1	aQ	243	ALA	C-N-CA	5.79	132.61	121.54
5	de	290	THR	CA-C-N	5.79	128.98	120.82
5	de	290	THR	C-N-CA	5.79	128.98	120.82
21	cx	294	VAL	N-CA-C	-5.79	101.76	108.82
7	bH	264	VAL	CA-C-N	5.79	130.36	122.84
7	bH	264	VAL	C-N-CA	5.79	130.36	122.84
1	ad	125	ASP	N-CA-C	-5.78	105.11	111.82
2	bx	446	HIS	N-CA-C	5.78	121.24	113.72
11	bQ	87	THR	N-CA-C	5.78	118.38	109.07
1	aX	267	ASN	CA-C-N	5.78	129.37	121.74
1	aX	267	ASN	C-N-CA	5.78	129.37	121.74
1	ab	93	LEU	CA-C-N	5.78	128.02	120.28
1	ab	93	LEU	C-N-CA	5.78	128.02	120.28
2	bx	462	LEU	N-CA-C	5.77	118.14	108.73
14	bX	191	TRP	CA-C-N	-5.77	114.34	123.12
14	bX	191	TRP	C-N-CA	-5.77	114.34	123.12
2	bu	449	ARG	CA-C-N	-5.77	118.44	122.59
2	bu	449	ARG	C-N-CA	-5.77	118.44	122.59
1	aj	212	ASP	CA-C-N	5.77	129.47	120.82
1	aj	212	ASP	C-N-CA	5.77	129.47	120.82
4	bD	313	GLY	CA-C-N	5.77	129.46	120.75
4	bD	313	GLY	C-N-CA	5.77	129.46	120.75
18	ci	26	LYS	O-C-N	-5.77	116.59	123.28
1	ah	109	TYR	CA-C-N	5.77	128.28	120.38
1	ah	109	TYR	C-N-CA	5.77	128.28	120.38
14	cc	134	PRO	CA-N-CD	-5.77	103.92	112.00
4	dr	292	THR	CA-C-N	5.77	129.55	121.24
4	dr	292	THR	C-N-CA	5.77	129.55	121.24
1	aT	243	ALA	CA-C-N	5.76	132.55	121.54
1	aT	243	ALA	C-N-CA	5.76	132.55	121.54
1	ag	431	GLY	N-CA-C	5.76	119.01	110.42
1	bi	347	THR	N-CA-C	-5.76	100.18	109.40
1	ar	156	ASN	N-CA-C	5.76	118.50	111.82
9	bN	54	TYR	CA-C-N	5.76	131.46	120.97
9	bN	54	TYR	C-N-CA	5.76	131.46	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bc	122	MET	CA-C-N	5.76	132.53	121.54
1	bc	122	MET	C-N-CA	5.76	132.53	121.54
1	bi	123	ASN	N-CA-C	-5.76	98.54	110.80
4	dd	292	THR	CA-C-N	5.76	129.53	121.24
4	dd	292	THR	C-N-CA	5.76	129.53	121.24
1	aA	123	ASN	CB-CA-C	-5.75	109.95	116.63
5	cY	359	TYR	N-CA-C	-5.75	106.11	113.01
2	by	501	ALA	CA-C-N	5.75	125.69	119.76
2	by	501	ALA	C-N-CA	5.75	125.69	119.76
4	df	292	THR	CA-C-N	5.75	129.52	121.24
4	df	292	THR	C-N-CA	5.75	129.52	121.24
14	bY	156	THR	CA-C-N	5.75	127.91	120.44
14	bY	156	THR	C-N-CA	5.75	127.91	120.44
1	bo	10	ALA	N-CA-C	-5.74	101.00	109.62
2	bw	342	LEU	N-CA-C	5.74	118.57	109.50
1	af	259	THR	N-CA-C	5.74	118.91	109.85
1	aH	122	MET	CA-C-N	5.74	132.50	121.54
1	aH	122	MET	C-N-CA	5.74	132.50	121.54
1	bt	140	LEU	CA-C-N	5.74	129.06	120.69
1	bt	140	LEU	C-N-CA	5.74	129.06	120.69
16	cg	78	THR	N-CA-C	5.74	118.31	111.71
8	bJ	124	ARG	CA-C-N	5.73	129.50	123.08
8	bJ	124	ARG	C-N-CA	5.73	129.50	123.08
1	aw	400	THR	CA-C-N	5.73	128.42	120.29
1	aw	400	THR	C-N-CA	5.73	128.42	120.29
14	cb	189	GLY	N-CA-C	-5.73	100.66	112.34
8	bJ	125	GLY	N-CA-C	-5.73	107.67	114.48
1	aO	157	GLN	CA-C-N	-5.72	111.38	122.70
1	aO	157	GLN	C-N-CA	-5.72	111.38	122.70
1	bl	122	MET	N-CA-C	5.72	117.16	110.41
2	by	332	GLU	N-CA-C	5.72	118.72	111.69
1	aI	137	ASN	CA-C-N	5.72	130.25	122.19
1	aI	137	ASN	C-N-CA	5.72	130.25	122.19
4	bF	292	THR	CA-C-N	5.72	129.47	121.24
4	bF	292	THR	C-N-CA	5.72	129.47	121.24
4	cX	293	ASP	N-CA-C	5.72	118.65	110.24
1	al	325	ARG	CA-C-N	5.71	132.07	121.62
1	al	325	ARG	C-N-CA	5.71	132.07	121.62
1	bo	159	PRO	CA-C-N	5.71	127.28	120.14
1	bo	159	PRO	C-N-CA	5.71	127.28	120.14
2	bz	80	LEU	N-CA-C	-5.71	101.39	109.96
1	ac	297	THR	CA-C-N	5.71	125.90	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	ac	297	THR	C-N-CA	5.71	125.90	120.31
4	dl	293	ASP	N-CA-C	5.71	118.61	110.10
1	be	299	ASP	CA-C-N	5.71	129.38	120.82
1	be	299	ASP	C-N-CA	5.71	129.38	120.82
14	bW	203	LYS	N-CA-C	-5.70	101.35	109.62
4	dj	293	ASP	N-CA-C	5.70	118.62	110.24
1	av	243	ALA	N-CA-C	5.69	117.50	108.79
1	bf	185	GLY	CA-C-N	-5.69	117.33	123.08
1	bf	185	GLY	C-N-CA	-5.69	117.33	123.08
1	aI	241	PRO	N-CA-C	5.68	119.60	111.13
4	dp	52	GLY	N-CA-C	-5.68	107.42	115.43
7	bH	372	PRO	N-CA-C	5.68	115.92	110.47
4	cZ	292	THR	CA-C-N	5.68	129.42	121.24
4	cZ	292	THR	C-N-CA	5.68	129.42	121.24
2	by	342	LEU	N-CA-C	5.68	118.47	109.50
2	bA	295	PRO	N-CA-C	-5.68	102.28	111.14
9	bM	6	ARG	N-CA-C	5.67	122.89	110.80
2	bu	464	ASP	N-CA-C	5.67	116.88	108.60
2	bz	92	ASN	CB-CA-C	-5.66	110.06	116.63
4	dd	52	GLY	N-CA-C	-5.66	107.45	115.43
17	ch	59	ASN	CA-CB-CG	-5.65	106.95	112.60
1	aL	399	ASN	N-CA-C	5.65	116.83	108.86
13	bS	17	SER	CB-CA-C	-5.65	110.08	116.63
1	ac	267	ASN	N-CA-C	5.65	117.38	108.96
1	aq	436	ALA	CA-C-N	5.64	131.86	121.70
1	aq	436	ALA	C-N-CA	5.64	131.86	121.70
1	aH	267	ASN	CA-C-N	5.64	129.19	121.74
1	aH	267	ASN	C-N-CA	5.64	129.19	121.74
1	ac	280	ASN	CA-C-N	5.64	128.24	123.33
1	ac	280	ASN	C-N-CA	5.64	128.24	123.33
5	cY	26	ILE	N-CA-C	-5.64	105.40	113.07
1	ae	433	LEU	CA-C-N	5.64	127.83	120.28
1	ae	433	LEU	C-N-CA	5.64	127.83	120.28
18	ci	32	GLN	CB-CA-C	-5.64	110.09	116.63
1	bs	138	ASN	N-CA-C	5.64	119.45	112.24
15	cf	100	PRO	N-CA-C	5.64	120.96	114.03
18	ci	43	ASN	N-CA-C	5.64	122.81	110.80
1	aR	123	ASN	CA-C-N	5.63	128.60	120.38
1	aR	123	ASN	C-N-CA	5.63	128.60	120.38
2	bu	221	LYS	N-CA-C	-5.63	106.76	113.97
1	aH	243	ALA	CA-C-N	5.63	132.29	121.54
1	aH	243	ALA	C-N-CA	5.63	132.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aD	63	ASN	CA-C-N	5.63	129.68	120.51
1	aD	63	ASN	C-N-CA	5.63	129.68	120.51
2	bA	14	GLN	CA-C-N	-5.62	111.33	120.72
2	bA	14	GLN	C-N-CA	-5.62	111.33	120.72
1	aa	123	ASN	CB-CA-C	-5.62	110.07	116.54
1	aI	122	MET	CA-C-N	5.62	132.28	121.54
1	aI	122	MET	C-N-CA	5.62	132.28	121.54
9	bM	7	ASP	N-CA-C	5.62	119.15	111.39
5	de	359	TYR	N-CA-C	-5.62	106.12	112.87
5	dq	26	ILE	N-CA-C	-5.62	105.43	113.07
1	aG	123	ASN	CB-CA-C	-5.62	110.08	116.54
1	aY	64	GLY	CA-C-N	5.61	130.08	120.71
1	aY	64	GLY	C-N-CA	5.61	130.08	120.71
5	dq	188	ALA	N-CA-C	5.61	117.38	108.79
7	bH	157	PRO	N-CA-C	-5.61	102.33	110.80
24	cT	22	THR	N-CA-C	-5.61	99.97	107.88
14	cc	199	ASN	CA-C-N	5.61	128.61	120.98
14	cc	199	ASN	C-N-CA	5.61	128.61	120.98
7	bH	160	ARG	N-CA-C	-5.61	100.05	108.96
1	bt	141	VAL	N-CA-C	5.60	116.64	109.30
14	cb	198	PRO	N-CA-C	5.60	124.01	112.47
14	cd	175	TYR	N-CA-C	-5.60	105.32	111.82
7	bH	159	GLY	N-CA-C	-5.60	102.60	110.88
14	cd	152	GLN	N-CA-C	5.60	116.77	108.60
1	aa	226	TYR	CA-C-N	-5.59	113.42	121.42
1	aa	226	TYR	C-N-CA	-5.59	113.42	121.42
2	bB	146	PRO	O-C-N	5.59	123.78	121.15
8	bJ	88	VAL	N-CA-CB	-5.59	106.69	112.28
1	aJ	256	ASN	N-CA-C	5.59	119.91	112.30
5	de	119	MET	CA-C-N	5.59	130.86	121.92
5	de	119	MET	C-N-CA	5.59	130.86	121.92
4	dk	293	ASP	N-CA-C	5.58	118.67	110.30
11	bQ	199	PHE	N-CA-C	-5.58	100.89	109.76
3	bC	70	ASP	CB-CA-C	-5.58	110.16	116.63
8	bJ	60	GLY	N-CA-C	-5.58	106.04	112.73
14	bY	164	ASN	N-CA-C	5.58	122.68	110.80
4	cZ	52	GLY	N-CA-C	-5.58	107.55	115.30
5	dq	291	GLU	N-CA-C	5.58	118.32	110.23
14	bV	190	PRO	CA-C-N	-5.58	113.80	122.67
14	bV	190	PRO	C-N-CA	-5.58	113.80	122.67
2	bu	13	ALA	N-CA-C	-5.58	107.12	114.31
1	bq	268	ASN	N-CA-C	-5.57	98.49	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	cr	50	PHE	CA-C-N	-5.57	113.85	122.49
21	cr	50	PHE	C-N-CA	-5.57	113.85	122.49
1	aP	190	GLY	N-CA-C	-5.57	100.61	110.86
1	bk	433	LEU	CA-C-N	5.57	127.74	120.28
1	bk	433	LEU	C-N-CA	5.57	127.74	120.28
14	cd	154	PHE	N-CA-C	5.57	119.65	112.86
1	am	243	ALA	N-CA-C	5.57	117.57	108.55
1	aL	233	PHE	CA-C-N	5.56	132.31	121.63
1	aL	233	PHE	C-N-CA	5.56	132.31	121.63
1	ai	243	ALA	CA-C-N	5.56	132.16	121.54
1	ai	243	ALA	C-N-CA	5.56	132.16	121.54
5	de	188	ALA	N-CA-C	5.56	117.30	108.79
1	aX	299	ASP	CA-C-N	5.56	129.16	120.82
1	aX	299	ASP	C-N-CA	5.56	129.16	120.82
1	ap	335	ASN	CA-C-N	-5.55	111.08	122.58
1	ap	335	ASN	C-N-CA	-5.55	111.08	122.58
8	bK	161	ASP	N-CA-C	-5.55	100.75	109.25
5	cY	188	ALA	N-CA-C	5.55	117.29	108.79
2	bv	450	VAL	CA-C-N	5.55	125.91	119.47
2	bv	450	VAL	C-N-CA	5.55	125.91	119.47
1	ai	268	ASN	N-CA-C	-5.55	98.54	108.47
1	aN	273	GLY	N-CA-C	5.55	122.74	115.36
8	bJ	90	THR	CA-C-N	5.54	128.72	120.90
8	bJ	90	THR	C-N-CA	5.54	128.72	120.90
1	aB	154	PHE	N-CA-C	5.54	119.14	112.38
1	az	137	ASN	CA-C-N	5.54	130.00	122.19
1	az	137	ASN	C-N-CA	5.54	130.00	122.19
1	aK	122	MET	CA-C-N	5.54	132.11	121.54
1	aK	122	MET	C-N-CA	5.54	132.11	121.54
1	aO	299	ASP	N-CA-C	-5.53	98.93	108.56
2	bx	378	VAL	N-CA-C	5.53	115.83	107.75
1	bm	400	THR	CA-C-N	5.53	127.69	120.28
1	bm	400	THR	C-N-CA	5.53	127.69	120.28
2	by	448	VAL	N-CA-C	5.53	116.19	110.82
8	bK	81	SER	CA-C-N	5.53	130.02	122.34
8	bK	81	SER	C-N-CA	5.53	130.02	122.34
5	de	291	GLU	N-CA-C	5.53	118.33	110.10
1	aw	251	ILE	CA-C-N	5.53	128.69	120.95
1	aw	251	ILE	C-N-CA	5.53	128.69	120.95
1	aj	399	ASN	CA-C-N	5.52	128.55	120.71
1	aj	399	ASN	C-N-CA	5.52	128.55	120.71
1	aa	240	THR	CA-C-N	5.52	125.42	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aa	240	THR	C-N-CA	5.52	125.42	119.85
8	bK	68	ASP	N-CA-C	5.52	118.48	111.69
4	dl	52	GLY	N-CA-C	-5.52	107.38	115.72
1	aU	259	THR	N-CA-C	5.52	117.73	108.96
1	aV	268	ASN	N-CA-C	-5.51	97.62	109.81
2	bw	211	ILE	CB-CA-C	-5.51	104.91	111.97
1	ap	243	ALA	CA-C-N	5.51	132.07	121.54
1	ap	243	ALA	C-N-CA	5.51	132.07	121.54
1	br	268	ASN	N-CA-C	-5.51	97.78	108.59
2	bv	144	THR	N-CA-C	-5.51	100.05	108.76
24	cS	182	ILE	N-CA-C	5.51	120.78	108.88
1	aY	122	MET	CA-C-N	5.51	132.06	121.54
1	aY	122	MET	C-N-CA	5.51	132.06	121.54
1	aC	14	GLN	N-CA-C	-5.51	105.36	111.36
5	bE	291	GLU	N-CA-C	5.50	118.30	110.10
2	bz	266	TYR	N-CA-C	-5.50	102.25	110.23
7	bH	159	GLY	CA-C-N	-5.50	114.87	122.30
7	bH	159	GLY	C-N-CA	-5.50	114.87	122.30
2	bu	89	ALA	CB-CA-C	-5.50	110.25	116.63
1	aw	299	ASP	CA-C-N	5.50	127.64	120.28
1	aw	299	ASP	C-N-CA	5.50	127.64	120.28
1	aE	2	ALA	CA-C-N	5.49	130.78	120.07
1	aE	2	ALA	C-N-CA	5.49	130.78	120.07
5	cY	291	GLU	N-CA-C	5.49	118.28	110.10
1	aV	200	PRO	CA-C-N	-5.49	115.42	123.00
1	aV	200	PRO	C-N-CA	-5.49	115.42	123.00
2	bv	24	ILE	N-CA-C	5.49	117.81	108.86
1	aB	75	VAL	N-CA-C	-5.49	99.84	107.80
1	aD	312	VAL	N-CA-C	5.49	119.41	113.43
24	cT	182	ILE	N-CA-C	5.49	120.74	108.88
2	bv	448	VAL	N-CA-C	5.49	116.26	110.72
1	aO	243	ALA	CA-C-N	5.49	132.01	121.54
1	aO	243	ALA	C-N-CA	5.49	132.01	121.54
1	bm	329	ARG	CA-C-N	-5.49	111.00	122.03
1	bm	329	ARG	C-N-CA	-5.49	111.00	122.03
1	aJ	14	GLN	CA-C-N	5.48	128.17	120.28
1	aJ	14	GLN	C-N-CA	5.48	128.17	120.28
1	bd	436	ALA	CA-C-N	5.48	131.57	121.70
1	bd	436	ALA	C-N-CA	5.48	131.57	121.70
1	aF	158	THR	CA-C-N	-5.48	113.25	119.28
1	aF	158	THR	C-N-CA	-5.48	113.25	119.28
24	cR	182	ILE	N-CA-C	5.47	120.69	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aR	299	ASP	N-CA-C	-5.47	99.05	108.56
14	ce	145	ALA	N-CA-C	5.47	121.89	109.81
1	ac	87	TYR	CA-C-N	5.46	124.98	119.19
1	ac	87	TYR	C-N-CA	5.46	124.98	119.19
2	bu	433	ARG	CA-C-N	5.46	125.41	119.78
2	bu	433	ARG	C-N-CA	5.46	125.41	119.78
3	bC	412	GLN	O-C-N	5.46	128.99	122.27
1	bf	243	ALA	CA-C-N	5.46	131.97	121.54
1	bf	243	ALA	C-N-CA	5.46	131.97	121.54
14	bZ	198	PRO	CA-C-N	5.46	129.93	122.34
14	bZ	198	PRO	C-N-CA	5.46	129.93	122.34
1	aa	222	LEU	CA-C-N	5.46	125.36	119.85
1	aa	222	LEU	C-N-CA	5.46	125.36	119.85
1	aD	268	ASN	N-CA-C	-5.46	101.48	109.50
1	aW	136	VAL	N-CA-C	5.46	116.32	111.90
1	aA	213	THR	N-CA-C	5.46	116.91	111.07
8	bK	66	TYR	CA-C-O	-5.45	115.06	120.90
2	bu	448	VAL	N-CA-C	5.45	116.23	110.72
4	cX	250	PRO	N-CA-C	5.45	120.14	111.26
1	aO	327	ALA	CA-C-N	5.44	128.84	121.05
1	aO	327	ALA	C-N-CA	5.44	128.84	121.05
1	al	186	VAL	N-CA-C	-5.44	107.32	111.62
1	aI	200	PRO	CA-C-N	-5.44	115.49	123.00
1	aI	200	PRO	C-N-CA	-5.44	115.49	123.00
2	bu	462	LEU	N-CA-C	5.44	117.50	108.20
5	dq	31	VAL	N-CA-C	5.44	115.69	107.75
1	au	340	TYR	CA-C-N	5.43	128.00	120.29
1	au	340	TYR	C-N-CA	5.43	128.00	120.29
1	al	122	MET	CA-C-N	5.43	131.91	121.54
1	al	122	MET	C-N-CA	5.43	131.91	121.54
1	bg	374	ILE	N-CA-C	-5.43	100.60	108.36
2	bx	286	TYR	N-CA-C	5.43	117.00	111.14
1	at	122	MET	CA-C-N	5.42	131.89	121.54
1	at	122	MET	C-N-CA	5.42	131.89	121.54
14	cd	176	ASP	N-CA-C	-5.42	102.26	110.28
1	bt	212	ASP	CA-C-N	5.41	128.31	120.79
1	bt	212	ASP	C-N-CA	5.41	128.31	120.79
7	bH	307	ALA	CA-C-N	-5.41	115.14	122.77
7	bH	307	ALA	C-N-CA	-5.41	115.14	122.77
5	de	31	VAL	N-CA-C	5.41	115.65	107.75
4	dl	313	GLY	CA-C-N	5.41	129.43	120.94
4	dl	313	GLY	C-N-CA	5.41	129.43	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bp	257	HIS	N-CA-C	5.41	121.77	109.81
2	bw	55	PHE	CA-C-N	5.41	125.38	120.03
2	bw	55	PHE	C-N-CA	5.41	125.38	120.03
5	bE	188	ALA	N-CA-C	5.41	117.31	108.76
4	dk	250	PRO	N-CA-C	5.41	120.08	111.26
2	bA	92	ASN	CB-CA-C	-5.40	109.88	117.23
21	cL	264	PRO	N-CA-C	-5.40	101.34	112.47
4	cZ	250	PRO	N-CA-C	5.40	120.06	111.26
1	ab	281	ILE	N-CA-C	-5.40	101.97	108.45
18	ci	28	GLN	N-CA-C	5.39	117.27	109.07
1	aX	243	ALA	CA-C-N	5.39	131.84	121.54
1	aX	243	ALA	C-N-CA	5.39	131.84	121.54
1	be	243	ALA	CA-C-N	5.39	131.84	121.54
1	be	243	ALA	C-N-CA	5.39	131.84	121.54
1	ae	25	THR	N-CA-C	-5.39	100.24	109.24
15	cf	126	SER	CA-C-N	-5.39	115.86	123.95
15	cf	126	SER	C-N-CA	-5.39	115.86	123.95
1	bj	122	MET	CA-C-N	5.39	131.83	121.54
1	bj	122	MET	C-N-CA	5.39	131.83	121.54
2	bx	55	PHE	CA-C-N	5.39	125.36	120.03
2	bx	55	PHE	C-N-CA	5.39	125.36	120.03
4	dd	250	PRO	N-CA-C	5.38	120.04	111.26
4	dp	250	PRO	N-CA-C	5.38	120.03	111.26
1	ah	251	ILE	CA-C-N	5.38	128.48	120.95
1	ah	251	ILE	C-N-CA	5.38	128.48	120.95
2	by	55	PHE	CA-C-N	5.38	125.58	120.31
2	by	55	PHE	C-N-CA	5.38	125.58	120.31
1	aF	268	ASN	N-CA-C	-5.38	99.01	108.69
4	bD	250	PRO	N-CA-C	5.38	120.02	111.26
4	bD	292	THR	CA-C-N	5.38	129.57	122.42
4	bD	292	THR	C-N-CA	5.38	129.57	122.42
6	bG	430	ILE	CB-CA-C	-5.38	108.65	114.35
1	ab	87	TYR	CA-C-N	5.37	125.19	119.28
1	ab	87	TYR	C-N-CA	5.37	125.19	119.28
4	df	250	PRO	N-CA-C	5.37	120.02	111.26
1	aT	59	GLN	N-CA-C	-5.37	101.78	110.32
1	bl	122	MET	CA-C-N	5.37	131.80	121.54
1	bl	122	MET	C-N-CA	5.37	131.80	121.54
8	bI	124	ARG	CA-C-N	-5.37	117.61	123.30
8	bI	124	ARG	C-N-CA	-5.37	117.61	123.30
1	af	383	TYR	CA-CB-CG	-5.37	104.23	113.90
13	bS	29	THR	N-CA-C	5.37	118.23	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aq	233	PHE	CA-C-N	5.37	131.38	121.94
1	aq	233	PHE	C-N-CA	5.37	131.38	121.94
2	bA	453	LYS	N-CA-C	-5.37	102.54	110.48
15	cf	90	VAL	N-CA-C	5.37	120.50	109.34
1	ag	123	ASN	CB-CA-C	-5.37	110.37	116.54
1	aq	299	ASP	N-CA-C	-5.37	99.22	108.56
1	ar	94	GLN	CA-C-N	-5.37	113.07	121.87
1	ar	94	GLN	C-N-CA	-5.37	113.07	121.87
5	bE	269	LEU	CA-C-N	-5.36	110.21	121.80
5	bE	269	LEU	C-N-CA	-5.36	110.21	121.80
1	aQ	67	ILE	CA-C-N	-5.36	111.30	121.54
1	aQ	67	ILE	C-N-CA	-5.36	111.30	121.54
7	bH	175	GLU	N-CA-C	5.36	117.12	111.28
14	bW	204	PRO	CA-C-N	5.36	131.35	121.70
14	bW	204	PRO	C-N-CA	5.36	131.35	121.70
1	ap	268	ASN	N-CA-C	-5.36	98.88	108.47
2	bv	449	ARG	CA-C-N	-5.35	118.73	122.59
2	bv	449	ARG	C-N-CA	-5.35	118.73	122.59
1	bf	122	MET	N-CA-C	5.35	117.32	109.24
1	bo	59	GLN	N-CA-C	-5.35	100.98	109.59
1	aW	267	ASN	CA-C-N	5.35	128.80	121.74
1	aW	267	ASN	C-N-CA	5.35	128.80	121.74
1	aB	400	THR	N-CA-C	5.35	118.65	110.36
8	bJ	162	THR	CA-C-N	-5.35	112.81	122.54
8	bJ	162	THR	C-N-CA	-5.35	112.81	122.54
1	ag	436	ALA	CA-C-N	5.34	131.32	121.70
1	ag	436	ALA	C-N-CA	5.34	131.32	121.70
1	bt	200	PRO	CA-C-N	-5.34	115.18	122.93
1	bt	200	PRO	C-N-CA	-5.34	115.18	122.93
1	as	122	MET	CA-C-N	5.34	131.74	121.54
1	as	122	MET	C-N-CA	5.34	131.74	121.54
1	aR	335	ASN	CA-C-N	-5.34	111.52	122.58
1	aR	335	ASN	C-N-CA	-5.34	111.52	122.58
2	bv	446	HIS	N-CA-C	5.34	120.46	113.30
2	bB	9	VAL	N-CA-C	5.34	115.55	110.53
1	aE	427	MET	CA-C-N	5.34	129.70	122.07
1	aE	427	MET	C-N-CA	5.34	129.70	122.07
1	bh	243	ALA	CA-C-N	5.34	131.73	121.54
1	bh	243	ALA	C-N-CA	5.34	131.73	121.54
4	dl	182	PRO	N-CA-C	5.34	121.55	113.81
1	ab	256	ASN	N-CA-C	5.33	118.86	111.71
1	ai	213	THR	N-CA-C	5.33	117.51	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	bE	377	GLY	N-CA-C	5.33	119.28	110.55
1	aT	258	PRO	CA-C-N	5.32	129.70	122.19
1	aT	258	PRO	C-N-CA	5.32	129.70	122.19
9	bM	5	PHE	CA-C-N	5.32	131.71	121.54
9	bM	5	PHE	C-N-CA	5.32	131.71	121.54
2	by	433	ARG	CA-C-N	5.32	125.26	119.78
2	by	433	ARG	C-N-CA	5.32	125.26	119.78
4	dk	182	PRO	N-CA-C	5.32	121.53	113.81
1	aD	395	ALA	N-CA-C	5.32	118.23	111.69
1	aA	299	ASP	CA-C-N	5.32	127.41	120.28
1	aA	299	ASP	C-N-CA	5.32	127.41	120.28
1	bt	427	MET	CA-C-N	5.32	129.67	122.07
1	bt	427	MET	C-N-CA	5.32	129.67	122.07
4	cZ	182	PRO	N-CA-C	5.32	121.52	113.81
1	bf	190	GLY	N-CA-C	-5.32	101.08	110.86
2	bw	453	LYS	N-CA-C	-5.31	100.99	109.23
1	aN	205	TRP	CA-C-N	5.31	129.78	123.19
1	aN	205	TRP	C-N-CA	5.31	129.78	123.19
13	bS	124	ASN	N-CA-C	5.31	117.07	111.28
1	ai	122	MET	CA-C-N	5.31	131.68	121.54
1	ai	122	MET	C-N-CA	5.31	131.68	121.54
21	cF	70	ASN	N-CA-CB	5.31	119.46	110.49
9	bL	6	ARG	CA-C-N	-5.31	114.61	122.41
9	bL	6	ARG	C-N-CA	-5.31	114.61	122.41
7	bH	291	ARG	N-CA-C	5.30	117.25	109.24
4	dr	250	PRO	N-CA-C	5.30	119.91	111.26
1	af	135	TRP	N-CA-C	-5.30	99.13	108.20
1	aY	243	ALA	CA-C-N	5.30	131.67	121.54
1	aY	243	ALA	C-N-CA	5.30	131.67	121.54
4	dl	250	PRO	N-CA-C	5.30	119.90	111.26
4	bD	52	GLY	N-CA-C	-5.30	104.87	114.46
1	bg	243	ALA	CA-C-N	5.29	131.65	121.54
1	bg	243	ALA	C-N-CA	5.29	131.65	121.54
4	cX	52	GLY	N-CA-C	-5.29	107.48	115.32
1	bc	165	LEU	N-CA-C	-5.29	105.62	111.71
4	dp	182	PRO	N-CA-C	5.29	121.49	113.81
4	dr	182	PRO	N-CA-C	5.29	121.48	113.81
2	bz	253	VAL	CA-C-N	5.29	125.49	120.31
2	bz	253	VAL	C-N-CA	5.29	125.49	120.31
1	aC	31	TYR	N-CA-C	-5.29	101.54	109.95
21	cx	215	TYR	CA-C-N	-5.29	111.44	121.54
21	cx	215	TYR	C-N-CA	-5.29	111.44	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aM	235	GLY	N-CA-C	5.28	119.94	111.64
1	bm	311	ALA	CA-C-N	-5.28	115.50	122.16
1	bm	311	ALA	C-N-CA	-5.28	115.50	122.16
1	aH	251	ILE	CA-C-N	5.28	128.34	120.95
1	aH	251	ILE	C-N-CA	5.28	128.34	120.95
2	bu	253	VAL	CA-C-N	5.28	125.48	120.31
2	bu	253	VAL	C-N-CA	5.28	125.48	120.31
4	df	182	PRO	N-CA-C	5.28	121.46	113.81
1	aB	30	VAL	N-CA-C	5.27	115.49	108.11
1	bl	243	ALA	CA-C-N	5.27	131.61	121.54
1	bl	243	ALA	C-N-CA	5.27	131.61	121.54
1	bf	432	GLY	N-CA-C	5.27	118.18	110.38
1	al	42	ILE	CA-C-N	5.26	128.95	121.42
1	al	42	ILE	C-N-CA	5.26	128.95	121.42
1	bp	72	VAL	CA-C-N	5.26	129.77	122.77
1	bp	72	VAL	C-N-CA	5.26	129.77	122.77
1	aC	9	VAL	N-CA-C	5.26	120.23	113.07
2	bw	450	VAL	CA-C-N	5.26	125.57	119.47
2	bw	450	VAL	C-N-CA	5.26	125.57	119.47
4	bF	29	ARG	N-CA-C	-5.26	104.16	111.52
1	aB	336	LYS	N-CA-C	5.26	119.92	112.93
1	br	436	ALA	CA-C-N	5.26	131.16	121.70
1	br	436	ALA	C-N-CA	5.26	131.16	121.70
1	aW	243	ALA	CA-C-N	5.25	131.57	121.54
1	aW	243	ALA	C-N-CA	5.25	131.57	121.54
8	bJ	162	THR	O-C-N	-5.25	115.43	122.68
4	dl	344	ASP	N-CA-C	5.25	117.80	111.40
1	aX	233	PHE	CA-C-N	5.25	131.39	122.37
1	aX	233	PHE	C-N-CA	5.25	131.39	122.37
1	aD	74	PHE	CA-C-N	-5.24	116.30	123.12
1	aD	74	PHE	C-N-CA	-5.24	116.30	123.12
1	aW	268	ASN	N-CA-C	-5.24	99.08	108.47
1	af	134	ASP	N-CA-C	5.24	116.25	108.86
1	an	136	VAL	CA-C-N	-5.24	114.25	122.79
1	an	136	VAL	C-N-CA	-5.24	114.25	122.79
1	aG	243	ALA	CA-C-N	5.24	131.54	121.54
1	aG	243	ALA	C-N-CA	5.24	131.54	121.54
1	an	241	PRO	N-CA-C	5.23	119.53	111.57
2	bu	342	LEU	N-CA-C	5.23	117.77	109.50
1	ak	258	PRO	CA-C-N	5.23	129.57	122.19
1	ak	258	PRO	C-N-CA	5.23	129.57	122.19
1	aE	137	ASN	CA-C-N	5.23	129.57	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	aE	137	ASN	C-N-CA	5.23	129.57	122.19
2	bw	227	THR	N-CA-C	-5.23	106.58	113.12
5	de	377	GLY	N-CA-C	5.23	119.24	110.56
1	an	428	SER	N-CA-C	5.23	118.80	111.90
1	be	299	ASP	N-CA-C	-5.23	99.46	108.56
1	bi	213	THR	N-CA-C	5.23	117.38	111.11
1	al	337	VAL	N-CA-C	5.23	115.89	110.82
4	cX	182	PRO	N-CA-C	5.22	121.39	113.81
4	dd	182	PRO	N-CA-C	5.22	121.38	113.81
1	as	243	ALA	CA-C-N	5.22	131.51	121.54
1	as	243	ALA	C-N-CA	5.22	131.51	121.54
2	bv	433	ARG	CA-C-N	5.22	125.22	119.89
2	bv	433	ARG	C-N-CA	5.22	125.22	119.89
2	by	21	ASN	CA-C-N	5.22	125.14	119.76
2	by	21	ASN	C-N-CA	5.22	125.14	119.76
2	bx	297	THR	N-CA-C	-5.22	107.58	114.31
2	bz	342	LEU	N-CA-C	5.22	117.75	109.50
4	dj	52	GLY	N-CA-C	-5.22	107.37	115.67
1	bi	212	ASP	CA-C-N	5.22	127.58	120.54
1	bi	212	ASP	C-N-CA	5.22	127.58	120.54
1	af	299	ASP	N-CA-C	-5.21	99.48	108.56
1	au	320	LEU	CA-C-N	5.21	129.53	122.07
1	au	320	LEU	C-N-CA	5.21	129.53	122.07
11	bQ	110	VAL	CA-C-N	5.21	131.12	122.62
11	bQ	110	VAL	C-N-CA	5.21	131.12	122.62
1	aP	243	ALA	CA-C-N	5.21	131.49	121.54
1	aP	243	ALA	C-N-CA	5.21	131.49	121.54
1	ba	233	PHE	CA-C-N	5.21	130.50	121.64
1	ba	233	PHE	C-N-CA	5.21	130.50	121.64
1	ab	9	VAL	N-CA-C	5.21	116.68	111.00
1	aZ	243	ALA	CA-C-N	5.21	131.48	121.54
1	aZ	243	ALA	C-N-CA	5.21	131.48	121.54
1	ac	268	ASN	CA-C-N	5.20	124.86	119.56
1	ac	268	ASN	C-N-CA	5.20	124.86	119.56
2	bz	433	ARG	CA-C-N	5.20	125.14	119.78
2	bz	433	ARG	C-N-CA	5.20	125.14	119.78
1	ac	39	ILE	N-CA-C	5.20	115.61	108.12
1	av	101	GLY	N-CA-C	5.20	122.36	114.61
1	an	299	ASP	N-CA-C	-5.20	99.52	108.56
1	aq	63	ASN	N-CA-C	-5.19	106.25	112.59
1	bt	105	ILE	N-CA-C	-5.19	106.74	111.67
1	ap	259	THR	N-CA-C	5.19	117.42	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	by	450	VAL	CA-C-N	5.19	125.49	119.47
2	by	450	VAL	C-N-CA	5.19	125.49	119.47
1	aa	149	VAL	CA-C-N	5.18	125.09	119.85
1	aa	149	VAL	C-N-CA	5.18	125.09	119.85
1	af	273	GLY	N-CA-C	5.18	122.51	115.30
1	aN	299	ASP	N-CA-C	-5.18	99.54	108.56
1	ac	199	GLN	CA-C-N	5.18	125.08	119.85
1	ac	199	GLN	C-N-CA	5.18	125.08	119.85
1	aA	257	HIS	CA-C-N	-5.18	114.23	119.83
1	aA	257	HIS	C-N-CA	-5.18	114.23	119.83
1	aO	299	ASP	CA-C-N	5.18	128.59	120.82
1	aO	299	ASP	C-N-CA	5.18	128.59	120.82
1	be	20	GLY	N-CA-C	-5.18	105.46	112.14
2	bx	266	TYR	N-CA-C	-5.18	102.38	110.10
2	bx	450	VAL	CA-C-N	5.18	125.48	119.47
2	bx	450	VAL	C-N-CA	5.18	125.48	119.47
9	bN	62	TYR	N-CA-C	5.18	118.39	110.20
1	au	119	LEU	N-CA-C	5.18	119.50	112.04
2	bu	252	TYR	CA-C-N	-5.18	118.83	123.33
2	bu	252	TYR	C-N-CA	-5.18	118.83	123.33
1	ax	137	ASN	CA-C-N	5.18	129.47	122.07
1	ax	137	ASN	C-N-CA	5.18	129.47	122.07
1	aI	300	TYR	N-CA-C	5.18	117.59	111.33
1	bi	243	ALA	CA-C-N	5.18	131.43	121.54
1	bi	243	ALA	C-N-CA	5.18	131.43	121.54
4	dj	182	PRO	N-CA-C	5.17	121.46	113.75
1	aa	74	PHE	CA-CB-CG	5.17	118.97	113.80
1	at	48	GLY	N-CA-C	5.17	117.31	112.04
1	au	299	ASP	N-CA-C	-5.17	99.57	108.56
7	bH	180	ARG	CA-C-N	-5.17	114.27	122.23
7	bH	180	ARG	C-N-CA	-5.17	114.27	122.23
1	ay	148	TYR	CA-C-N	-5.16	117.57	123.25
1	ay	148	TYR	C-N-CA	-5.16	117.57	123.25
1	aD	328	THR	N-CA-C	5.16	118.28	110.64
1	aI	299	ASP	CA-C-N	5.16	127.45	120.38
1	aI	299	ASP	C-N-CA	5.16	127.45	120.38
1	am	399	ASN	CA-C-N	5.16	130.36	120.97
1	am	399	ASN	C-N-CA	5.16	130.36	120.97
4	dk	292	THR	CA-C-N	5.16	129.46	121.26
4	dk	292	THR	C-N-CA	5.16	129.46	121.26
1	ai	343	ILE	N-CA-C	-5.16	107.12	111.56
1	bd	243	ALA	CA-C-N	5.16	131.39	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bd	243	ALA	C-N-CA	5.16	131.39	121.54
4	bF	344	ASP	N-CA-C	5.16	117.80	111.82
1	af	243	ALA	CA-C-N	5.16	131.39	121.54
1	af	243	ALA	C-N-CA	5.16	131.39	121.54
1	aD	342	SER	CA-C-N	-5.15	117.88	123.08
1	aD	342	SER	C-N-CA	-5.15	117.88	123.08
5	dq	377	GLY	N-CA-C	5.15	119.11	110.56
1	am	97	GLU	CA-C-N	-5.15	114.81	122.74
1	am	97	GLU	C-N-CA	-5.15	114.81	122.74
1	aP	82	GLY	N-CA-C	5.15	117.39	111.36
2	bu	233	ASP	CA-C-N	5.15	125.44	119.47
2	bu	233	ASP	C-N-CA	5.15	125.44	119.47
8	bI	79	ARG	CA-C-N	5.15	127.18	120.28
8	bI	79	ARG	C-N-CA	5.15	127.18	120.28
2	by	452	SER	CA-C-N	5.15	130.55	122.21
2	by	452	SER	C-N-CA	5.15	130.55	122.21
1	aP	299	ASP	N-CA-C	-5.15	99.60	108.56
2	bz	33	ARG	N-CA-C	5.15	118.33	110.20
1	aD	75	VAL	N-CA-C	-5.15	100.34	107.80
2	bx	496	ARG	N-CA-C	5.15	118.61	109.96
1	ac	27	PHE	CA-CB-CG	-5.14	108.66	113.80
1	ac	420	ASN	N-CA-C	5.14	116.11	108.86
1	ab	120	PHE	CA-CB-CG	-5.14	108.66	113.80
1	aK	243	ALA	CA-C-N	5.14	131.36	121.54
1	aK	243	ALA	C-N-CA	5.14	131.36	121.54
1	bb	243	ALA	CA-C-N	5.14	131.36	121.54
1	bb	243	ALA	C-N-CA	5.14	131.36	121.54
2	by	182	ASN	N-CA-C	5.14	119.80	111.37
1	ak	250	ASN	CA-C-N	-5.14	116.81	123.19
1	ak	250	ASN	C-N-CA	-5.14	116.81	123.19
1	ad	200	PRO	CA-C-N	-5.14	115.91	123.00
1	ad	200	PRO	C-N-CA	-5.14	115.91	123.00
1	aI	59	GLN	N-CA-C	-5.14	100.93	109.46
1	aT	267	ASN	N-CA-C	5.14	117.78	109.40
1	bc	268	ASN	N-CA-C	-5.14	98.45	109.81
2	by	211	ILE	CB-CA-C	-5.14	105.39	111.97
2	bA	413	GLY	N-CA-C	5.14	121.20	115.08
1	bl	268	ASN	N-CA-C	-5.14	98.52	108.59
1	ak	299	ASP	CA-C-N	5.14	127.48	120.54
1	ak	299	ASP	C-N-CA	5.14	127.48	120.54
2	bw	389	ALA	CA-C-N	-5.13	114.06	122.33
2	bw	389	ALA	C-N-CA	-5.13	114.06	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	bw	433	ARG	CA-C-N	5.13	125.07	119.78
2	bw	433	ARG	C-N-CA	5.13	125.07	119.78
7	bH	388	GLU	N-CA-C	5.13	116.87	111.28
1	aB	121	ARG	N-CA-C	-5.13	101.39	109.50
4	bD	312	PHE	N-CA-C	5.13	118.75	112.03
1	as	256	ASN	N-CA-C	5.12	118.74	112.03
2	bx	461	ALA	CA-C-N	-5.12	115.96	122.77
2	bx	461	ALA	C-N-CA	-5.12	115.96	122.77
1	aw	19	THR	CA-C-N	5.12	124.83	119.92
1	aw	19	THR	C-N-CA	5.12	124.83	119.92
1	bh	118	ALA	CA-C-N	-5.12	113.55	122.36
1	bh	118	ALA	C-N-CA	-5.12	113.55	122.36
2	bw	462	LEU	N-CA-C	5.12	117.08	108.73
1	bb	177	PHE	CA-C-N	-5.12	115.66	122.72
1	bb	177	PHE	C-N-CA	-5.12	115.66	122.72
1	ac	222	LEU	CA-C-N	5.12	125.02	119.85
1	ac	222	LEU	C-N-CA	5.12	125.02	119.85
1	be	122	MET	CA-C-N	5.12	131.31	121.54
1	be	122	MET	C-N-CA	5.12	131.31	121.54
1	ac	20	GLY	N-CA-C	-5.11	105.54	112.14
1	ag	170	TYR	CA-C-O	-5.11	113.58	119.56
1	aa	134	ASP	CA-CB-CG	5.11	117.71	112.60
10	bP	108	LYS	N-CA-C	-5.11	101.63	109.76
2	bB	145	TYR	CA-C-N	5.11	123.34	119.66
2	bB	145	TYR	C-N-CA	5.11	123.34	119.66
11	bQ	183	LYS	CA-C-N	-5.11	113.84	121.87
11	bQ	183	LYS	C-N-CA	-5.11	113.84	121.87
1	bp	242	SER	N-CA-C	5.11	118.95	111.04
1	ab	337	VAL	CA-C-N	-5.11	113.42	120.26
1	ab	337	VAL	C-N-CA	-5.11	113.42	120.26
1	aC	12	GLY	N-CA-C	-5.11	107.10	111.95
1	aX	399	ASN	N-CA-C	5.11	116.43	109.18
1	aE	200	PRO	CA-C-N	-5.10	115.53	122.93
1	aE	200	PRO	C-N-CA	-5.10	115.53	122.93
1	aB	68	THR	N-CA-C	5.10	121.95	113.89
1	aE	243	ALA	CA-C-N	5.10	131.29	121.54
1	aE	243	ALA	C-N-CA	5.10	131.29	121.54
2	bv	501	ALA	CA-C-N	5.10	125.04	119.78
2	bv	501	ALA	C-N-CA	5.10	125.04	119.78
11	bQ	179	THR	CA-C-N	5.10	124.76	119.56
11	bQ	179	THR	C-N-CA	5.10	124.76	119.56
5	dq	22	GLY	CA-C-N	5.10	124.76	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	dq	22	GLY	C-N-CA	5.10	124.76	119.56
2	bx	342	LEU	N-CA-C	5.10	117.55	109.50
8	bJ	138	ILE	CB-CA-C	-5.10	108.86	113.70
14	cc	161	ILE	CA-C-N	5.10	131.40	121.41
14	cc	161	ILE	C-N-CA	5.10	131.40	121.41
1	aa	122	MET	N-CA-C	5.09	116.93	109.24
8	bK	120	GLU	CA-C-N	-5.09	115.30	122.94
8	bK	120	GLU	C-N-CA	-5.09	115.30	122.94
1	ax	96	VAL	CA-C-N	5.09	130.03	123.00
1	ax	96	VAL	C-N-CA	5.09	130.03	123.00
1	aC	21	ASN	CA-C-N	5.09	126.20	119.84
1	aC	21	ASN	C-N-CA	5.09	126.20	119.84
5	bE	26	ILE	N-CA-C	-5.09	105.42	112.50
1	aj	123	ASN	N-CA-C	5.09	116.68	108.08
1	aj	243	ALA	N-CA-C	5.09	116.25	108.42
5	de	22	GLY	CA-C-N	5.09	124.75	119.56
5	de	22	GLY	C-N-CA	5.09	124.75	119.56
11	bQ	84	LYS	N-CA-C	-5.08	107.05	114.12
1	aA	243	ALA	N-CA-C	5.08	116.57	108.79
1	aP	3	GLY	N-CA-C	5.08	121.48	112.02
1	aa	430	MET	CA-C-N	-5.08	117.08	122.67
1	aa	430	MET	C-N-CA	-5.08	117.08	122.67
14	bT	181	PRO	CA-C-N	5.08	127.89	120.98
14	bT	181	PRO	C-N-CA	5.08	127.89	120.98
17	ch	103	GLN	N-CA-C	-5.08	106.24	112.90
1	al	5	LEU	N-CA-C	-5.08	106.59	112.89
1	aH	299	ASP	CA-C-N	5.08	128.44	120.82
1	aH	299	ASP	C-N-CA	5.08	128.44	120.82
2	bu	332	GLU	N-CA-C	5.08	116.90	111.36
14	bU	193	MET	N-CA-C	-5.08	102.24	110.32
5	cY	22	GLY	CA-C-N	5.08	124.69	119.56
5	cY	22	GLY	C-N-CA	5.08	124.69	119.56
1	ar	382	THR	N-CA-C	-5.08	100.90	109.07
1	aC	121	ARG	N-CA-C	-5.08	101.69	109.76
1	bs	410	LEU	N-CA-C	-5.07	107.04	113.18
1	ae	258	PRO	N-CA-C	-5.07	102.73	110.95
1	ap	136	VAL	N-CA-C	5.07	116.38	112.12
1	az	259	THR	N-CA-C	5.07	117.86	109.85
2	bv	342	LEU	N-CA-C	5.07	117.51	109.50
18	ci	30	ARG	CA-C-N	5.07	125.54	120.52
18	ci	30	ARG	C-N-CA	5.07	125.54	120.52
1	bt	299	ASP	CA-C-N	5.07	128.42	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bt	299	ASP	C-N-CA	5.07	128.42	120.82
1	aP	436	ALA	CA-C-N	5.07	130.82	121.70
1	aP	436	ALA	C-N-CA	5.07	130.82	121.70
1	ac	125	ASP	CA-CB-CG	5.06	117.66	112.60
2	bA	467	SER	N-CA-C	5.06	119.30	113.38
14	cd	182	ILE	N-CA-C	5.06	115.60	108.36
1	aL	243	ALA	CA-C-N	5.06	131.21	121.54
1	aL	243	ALA	C-N-CA	5.06	131.21	121.54
7	bH	230	LEU	N-CA-C	-5.06	101.46	109.76
8	bK	104	GLY	N-CA-C	5.06	120.28	114.16
1	aa	24	ILE	N-CA-C	5.05	115.13	107.80
1	bi	336	LYS	N-CA-C	5.05	119.92	113.55
11	bQ	81	ASP	N-CA-C	-5.05	104.92	111.74
1	aw	300	TYR	N-CA-C	5.05	116.79	111.28
1	aM	233	PHE	CA-C-N	5.05	131.06	122.37
1	aM	233	PHE	C-N-CA	5.05	131.06	122.37
1	aJ	8	LEU	N-CA-C	-5.05	106.28	112.90
5	cY	358	VAL	N-CA-C	5.05	119.84	109.34
2	bv	233	ASP	CA-C-N	5.05	125.32	119.47
2	bv	233	ASP	C-N-CA	5.05	125.32	119.47
1	ac	74	PHE	CA-CB-CG	5.04	118.84	113.80
1	aT	436	ALA	CA-C-N	5.04	130.78	121.70
1	aT	436	ALA	C-N-CA	5.04	130.78	121.70
1	bl	148	TYR	CA-C-N	-5.04	117.70	123.25
1	bl	148	TYR	C-N-CA	-5.04	117.70	123.25
2	bu	501	ALA	CA-C-N	5.04	124.95	119.76
2	bu	501	ALA	C-N-CA	5.04	124.95	119.76
11	bQ	164	LYS	CA-C-N	5.04	129.71	122.40
11	bQ	164	LYS	C-N-CA	5.04	129.71	122.40
1	aF	97	GLU	CA-C-N	-5.04	116.05	123.00
1	aF	97	GLU	C-N-CA	-5.04	116.05	123.00
1	bc	299	ASP	N-CA-C	-5.04	99.80	108.56
2	bu	442	GLN	CA-C-N	5.04	124.48	119.24
2	bu	442	GLN	C-N-CA	5.04	124.48	119.24
2	bx	286	TYR	CA-C-N	-5.04	114.59	122.05
2	bx	286	TYR	C-N-CA	-5.04	114.59	122.05
1	ad	178	THR	N-CA-C	-5.04	100.69	108.90
1	bl	200	PRO	CA-C-N	-5.04	116.05	123.00
1	bl	200	PRO	C-N-CA	-5.04	116.05	123.00
1	aM	10	ALA	N-CA-C	-5.03	102.08	109.62
1	aR	399	ASN	N-CA-C	5.03	116.32	109.18
2	by	355	ASP	CA-C-N	5.03	126.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	by	355	ASP	C-N-CA	5.03	126.12	119.84
5	dq	358	VAL	N-CA-C	5.03	119.80	109.34
1	af	212	ASP	CA-C-N	5.02	127.77	120.79
1	af	212	ASP	C-N-CA	5.02	127.77	120.79
1	bp	227	LEU	N-CA-C	-5.02	100.97	108.96
14	bW	183	ILE	N-CA-C	-5.02	102.58	107.55
7	bH	336	ILE	CA-C-N	-5.02	118.05	122.97
7	bH	336	ILE	C-N-CA	-5.02	118.05	122.97
1	au	190	GLY	N-CA-C	-5.02	101.08	110.77
1	ax	325	ARG	CA-C-N	5.02	130.81	121.62
1	ax	325	ARG	C-N-CA	5.02	130.81	121.62
4	dd	84	PHE	CA-C-N	5.02	128.25	122.83
4	dd	84	PHE	C-N-CA	5.02	128.25	122.83
1	aI	122	MET	N-CA-C	5.02	116.87	108.99
5	bE	358	VAL	N-CA-C	5.02	119.78	109.34
1	an	254	ASN	N-CA-C	-5.02	104.13	111.30
1	aB	140	LEU	CA-C-N	5.02	128.01	120.69
1	aB	140	LEU	C-N-CA	5.02	128.01	120.69
1	aJ	245	THR	N-CA-C	5.01	116.81	109.24
1	ai	101	GLY	N-CA-C	5.01	121.67	114.10
1	bg	200	PRO	CA-C-N	-5.01	116.09	123.00
1	bg	200	PRO	C-N-CA	-5.01	116.09	123.00
2	bx	498	GLN	CA-C-N	-5.01	116.98	123.19
2	bx	498	GLN	C-N-CA	-5.01	116.98	123.19
7	bH	171	PRO	N-CA-C	-5.01	103.41	111.38
1	aS	436	ALA	CA-C-N	5.01	130.72	121.70
1	aS	436	ALA	C-N-CA	5.01	130.72	121.70
1	ai	212	ASP	CA-C-N	5.00	127.30	120.54
1	ai	212	ASP	C-N-CA	5.00	127.30	120.54
1	as	256	ASN	CA-C-O	-5.00	115.27	119.97
15	cf	129	LEU	N-CA-C	-5.00	102.88	110.28
1	aR	200	PRO	CA-C-N	-5.00	115.68	122.93
1	aR	200	PRO	C-N-CA	-5.00	115.68	122.93
1	aV	382	THR	N-CA-C	-5.00	100.75	108.90
1	ba	271	ASN	CA-C-N	5.00	127.87	120.82
1	ba	271	ASN	C-N-CA	5.00	127.87	120.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	3390	0	3284	13	0
1	aB	3390	0	3284	9	0
1	aC	3395	0	3289	8	0
1	aD	3382	0	3278	13	0
1	aE	3395	0	3289	9	0
1	aF	3382	0	3278	11	0
1	aG	3390	0	3284	8	0
1	aH	3382	0	3278	11	0
1	aI	3390	0	3284	10	0
1	aJ	3395	0	3289	13	0
1	aK	3395	0	3289	9	0
1	aL	3387	0	3283	8	0
1	aM	3395	0	3289	9	0
1	aN	3390	0	3284	7	0
1	aO	3395	0	3289	5	0
1	aP	3395	0	3289	4	0
1	aQ	3382	0	3278	12	0
1	aR	3395	0	3289	8	0
1	aS	3395	0	3289	9	0
1	aT	3395	0	3289	5	0
1	aU	3395	0	3289	9	0
1	aV	3395	0	3289	6	0
1	aW	3395	0	3289	8	0
1	aX	3390	0	3284	3	0
1	aY	3395	0	3289	8	0
1	aZ	3395	0	3289	8	0
1	aa	3374	0	3272	99	0
1	ab	3395	0	3289	32	0
1	ac	3395	0	3289	58	0
1	ad	3395	0	3289	10	0
1	ae	3395	0	3289	6	0
1	af	3395	0	3289	10	0
1	ag	3395	0	3289	9	0
1	ah	3395	0	3289	9	0
1	ai	3395	0	3289	7	0
1	aj	3395	0	3289	8	0
1	ak	3395	0	3289	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	al	3387	0	3283	8	0
1	am	3395	0	3289	16	0
1	an	3387	0	3283	7	0
1	ao	3390	0	3284	9	0
1	ap	3395	0	3289	8	0
1	aq	3395	0	3289	9	0
1	ar	3382	0	3278	7	0
1	as	3395	0	3289	9	0
1	at	3395	0	3289	4	0
1	au	3382	0	3278	11	0
1	av	3395	0	3289	4	0
1	aw	3395	0	3289	6	0
1	ax	3382	0	3278	6	0
1	ay	3390	0	3284	9	0
1	az	3382	0	3278	6	0
1	ba	3395	0	3289	3	0
1	bb	3395	0	3289	22	0
1	bc	3395	0	3289	9	0
1	bd	3395	0	3289	13	0
1	be	3395	0	3289	7	0
1	bf	3395	0	3289	7	0
1	bg	3395	0	3289	10	0
1	bh	3395	0	3289	13	0
1	bi	3395	0	3289	3	0
1	bj	3395	0	3289	6	0
1	bk	3395	0	3289	6	0
1	bl	3395	0	3289	22	0
1	bm	3395	0	3289	16	0
1	bn	3382	0	3278	11	0
1	bo	3395	0	3289	11	0
1	bp	3395	0	3289	9	0
1	bq	3395	0	3289	4	0
1	br	3395	0	3289	8	0
1	bs	3395	0	3289	8	0
1	bt	3390	0	3284	3	0
2	bA	4079	0	3911	13	0
2	bB	4090	0	3920	18	0
2	bu	4090	0	3920	47	0
2	bv	4090	0	3920	38	0
2	bw	4090	0	3920	22	0
2	bx	4074	0	3904	37	0
2	by	4090	0	3920	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	bz	4030	0	3855	48	0
3	bC	3921	0	3830	30	0
4	bD	3169	0	3084	19	0
4	bF	3169	0	3084	19	0
4	cX	3165	0	3080	18	0
4	cZ	3165	0	3080	10	0
4	dd	3169	0	3084	24	0
4	df	3165	0	3080	32	0
4	dj	3169	0	3084	9	0
4	dk	3169	0	3084	14	0
4	dl	3169	0	3084	13	0
4	dp	3169	0	3084	54	0
4	dr	3169	0	3084	13	0
5	bE	3146	0	3091	28	0
5	cY	3146	0	3091	12	0
5	de	3146	0	3091	50	0
5	dq	3146	0	3091	34	0
6	bG	3864	0	3724	7	0
7	bH	3258	0	3136	31	0
8	bI	1096	0	1079	15	0
8	bJ	1146	0	1125	5	0
8	bK	892	0	879	8	0
9	bL	526	0	535	7	0
9	bM	526	0	535	5	0
9	bN	519	0	528	4	0
9	bO	519	0	528	1	0
10	bP	1126	0	1142	7	0
11	bQ	1275	0	1274	13	0
12	bR	1244	0	1254	1	0
13	bS	1504	0	1497	163	0
14	bT	373	0	370	1	0
14	bU	424	0	415	2	0
14	bV	416	0	409	3	0
14	bW	405	0	400	3	0
14	bX	312	0	301	4	0
14	bY	576	0	561	6	0
14	bZ	405	0	400	5	0
14	ca	405	0	400	2	0
14	cb	405	0	400	1	0
14	cc	646	0	643	4	0
14	cd	583	0	569	2	0
14	ce	560	0	541	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	cf	631	0	625	1	0
16	cg	521	0	494	2	0
17	ch	1288	0	1280	11	0
18	ci	553	0	539	83	0
19	cj	463	0	449	49	0
19	ck	455	0	448	32	0
19	cl	431	0	422	33	0
19	cm	503	0	486	51	0
20	cn	769	0	785	40	0
20	co	733	0	728	91	0
21	cA	2191	0	2203	6	0
21	cB	2299	0	2307	8	0
21	cC	2191	0	2203	6	0
21	cD	2299	0	2307	8	0
21	cE	2199	0	2209	11	0
21	cF	2299	0	2307	10	0
21	cG	2212	0	2221	7	0
21	cH	2299	0	2307	9	0
21	cI	2191	0	2203	9	0
21	cJ	2299	0	2307	13	0
21	cK	2191	0	2203	8	0
21	cL	2299	0	2307	10	0
21	cM	2173	0	2187	11	0
21	cN	2299	0	2307	7	0
21	cp	2299	0	2307	11	0
21	cq	2212	0	2221	5	0
21	cr	2299	0	2307	9	0
21	cs	2159	0	2171	13	0
21	ct	2299	0	2307	14	0
21	cu	2199	0	2209	4	0
21	cv	2299	0	2307	13	0
21	cw	2199	0	2209	16	0
21	cx	2299	0	2307	10	0
21	cy	2199	0	2209	11	0
21	cz	2299	0	2307	8	0
22	cO	218	0	220	28	0
22	cQ	233	0	234	35	0
22	da	228	0	221	22	0
22	dc	209	0	208	36	0
22	dg	241	0	239	39	0
22	di	211	0	208	36	0
22	ds	238	0	237	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	du	224	0	226	41	0
23	cP	239	0	226	32	0
23	db	200	0	188	45	0
23	dh	249	0	241	32	0
23	dt	236	0	229	27	0
24	cR	3203	0	3142	27	0
24	cS	3203	0	3142	24	0
24	cT	3203	0	3142	34	0
25	cU	311	0	299	37	0
25	cV	305	0	293	32	0
25	cW	308	0	297	28	0
26	dm	174	0	154	37	0
26	dn	181	0	169	36	0
26	do	182	0	175	37	0
All	All	427569	0	416835	2222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (2222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:dp:138:GLU:CD	23:dt:17:ILE:HD11	1.38	1.46
5:dq:269:LEU:HD22	22:du:15:ARG:CD	1.46	1.44
4:dd:272:PRO:CD	22:dg:14:ILE:HD13	1.47	1.42
5:dq:269:LEU:HD22	22:du:15:ARG:CG	1.48	1.39
4:dp:84:PHE:HZ	4:dp:273:PHE:CZ	1.43	1.34
2:by:27:PHE:CZ	2:bz:320:VAL:HG11	1.66	1.28
4:dd:272:PRO:HD2	22:dg:14:ILE:CD1	1.65	1.27
1:aa:7:GLN:CB	20:co:54:LEU:HD11	1.63	1.26
1:aa:427:MET:HE1	13:bS:146:PHE:CE1	1.68	1.25
13:bS:27:ILE:CB	13:bS:28:PRO:HD3	1.41	1.25
1:ab:210:PHE:O	19:cm:63:THR:HG21	1.31	1.23
4:df:271:TYR:HB2	23:dh:14:ARG:NH2	1.56	1.21
24:cR:134:PRO:HA	25:cV:12:PHE:CE1	1.75	1.20
5:dq:269:LEU:CD2	22:du:15:ARG:HG2	1.73	1.19
4:dp:84:PHE:CZ	4:dp:273:PHE:CZ	2.31	1.18
13:bS:27:ILE:HB	13:bS:28:PRO:CD	1.74	1.18
5:de:135:SER:CB	22:di:12:ILE:HD13	1.77	1.15
2:by:27:PHE:O	2:bz:264:GLY:HA2	1.46	1.14
26:dm:32:GLY:HA3	26:dn:27:VAL:HG22	1.22	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:de:355:ALA:HB3	5:de:360:THR:HG21	1.18	1.12
5:dq:135:SER:HB2	22:du:12:ILE:HG21	1.23	1.12
5:de:135:SER:HB2	22:di:12:ILE:HG21	1.25	1.12
1:ac:320:LEU:HD12	19:cm:64:ARG:NH2	1.64	1.11
4:df:275:ASN:HB2	22:dg:10:ASP:OD2	1.49	1.11
26:do:27:VAL:CG2	26:do:30:LEU:HD23	1.78	1.11
7:bH:514:LEU:HD22	7:bH:517:ASN:HD22	1.11	1.11
15:cf:112:CYS:SG	15:cf:120:CYS:SG	2.36	1.11
5:dq:269:LEU:HD22	22:du:15:ARG:HG2	1.17	1.10
1:ac:370:ASN:ND2	19:cm:59:TRP:HB2	1.65	1.09
4:dd:272:PRO:CG	22:dg:14:ILE:HD13	1.82	1.09
2:by:329:ARG:HD3	19:ck:42:ASP:OD1	1.53	1.09
13:bS:27:ILE:CB	13:bS:28:PRO:CD	2.30	1.09
1:aa:429:GLY:CA	13:bS:117:THR:HG21	1.82	1.09
18:ci:49:ASP:HB2	18:ci:52:ALA:HB2	1.29	1.09
26:dm:32:GLY:CA	26:dn:27:VAL:HG22	1.81	1.09
26:do:27:VAL:HG21	26:do:30:LEU:HB3	1.24	1.09
2:bz:16:VAL:HG22	20:cn:56:LEU:CD2	1.83	1.08
5:de:135:SER:HB3	22:di:12:ILE:HD13	1.30	1.08
13:bS:27:ILE:HB	13:bS:28:PRO:HD3	1.08	1.07
4:df:271:TYR:HB2	23:dh:14:ARG:HH21	1.02	1.07
1:aa:7:GLN:HB2	20:co:54:LEU:CD1	1.82	1.07
4:bF:126:ARG:HH21	22:cQ:8:LEU:HD23	1.11	1.07
1:aa:427:MET:HE1	13:bS:146:PHE:CD1	1.88	1.07
13:bS:56:ARG:NE	18:ci:9:ILE:HD11	1.71	1.06
24:cT:134:PRO:HA	25:cU:12:PHE:CE1	1.90	1.06
4:dk:138:GLU:OE1	26:dm:22:PHE:HZ	1.38	1.05
13:bS:29:THR:CG2	13:bS:37:ARG:HG2	1.87	1.05
4:dp:138:GLU:CD	23:dt:17:ILE:CD1	2.29	1.05
2:by:333:ILE:CD1	19:ck:46:ARG:HD3	1.86	1.05
5:dq:269:LEU:HD22	22:du:15:ARG:HD3	1.34	1.05
18:ci:49:ASP:HB2	18:ci:52:ALA:CB	1.87	1.04
5:de:135:SER:HB2	22:di:12:ILE:CG2	1.87	1.03
1:aa:7:GLN:CB	20:co:54:LEU:HD21	1.87	1.03
5:dq:269:LEU:CD2	22:du:15:ARG:CD	2.35	1.03
2:by:27:PHE:HZ	2:bz:320:VAL:HG11	0.86	1.02
5:de:271:PHE:HB2	23:dh:9:ASN:HD22	1.18	1.01
4:df:275:ASN:HD21	22:dg:6:ASN:HB3	1.21	1.01
5:dq:269:LEU:HB3	22:du:15:ARG:HD3	1.40	1.01
13:bS:28:PRO:CG	18:ci:20:ALA:HB1	1.90	1.01
1:aa:7:GLN:CB	20:co:54:LEU:CD1	2.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aa:7:GLN:C	20:co:54:LEU:HD11	1.85	1.00
5:bE:269:LEU:HD21	22:cO:16:THR:HB	1.42	1.00
26:do:15:VAL:HG11	26:do:19:VAL:HG13	1.43	1.00
1:aa:8:LEU:CD2	20:co:70:ASN:HD21	1.74	1.00
13:bS:27:ILE:CG2	13:bS:28:PRO:HD3	1.92	1.00
2:by:23:GLN:HG2	19:cj:57:SER:CB	1.92	1.00
24:cR:134:PRO:CA	25:cV:12:PHE:CE1	2.44	0.99
1:ac:258:PRO:HG2	19:cm:59:TRP:HE3	1.24	0.99
13:bS:30:ARG:O	13:bS:32:GLN:HG3	1.60	0.99
4:df:275:ASN:HD21	22:dg:6:ASN:CB	1.75	0.99
26:dn:15:VAL:HG11	26:dn:19:VAL:HG23	1.42	0.99
4:dp:138:GLU:OE2	23:dt:17:ILE:HD11	1.63	0.98
13:bS:56:ARG:NE	18:ci:9:ILE:CD1	2.26	0.98
1:aa:7:GLN:HB2	20:co:54:LEU:HD11	1.42	0.96
23:db:10:PRO:HB2	22:dc:17:MET:HG3	1.45	0.96
1:ac:258:PRO:HG3	19:cm:59:TRP:HB3	1.45	0.96
1:bb:238:THR:CG2	1:bb:414:LEU:HB2	1.96	0.95
2:bz:16:VAL:CG2	20:cn:56:LEU:HD21	1.96	0.95
26:dn:15:VAL:HG11	26:dn:19:VAL:CG2	1.96	0.95
7:bH:514:LEU:HD22	7:bH:517:ASN:ND2	1.82	0.95
5:bE:135:SER:HB2	22:cO:12:ILE:HD12	1.49	0.95
13:bS:157:VAL:HG21	18:ci:61:LEU:CD1	1.97	0.95
1:ac:23:GLN:O	19:cl:52:SER:HB2	1.65	0.94
1:ac:321:ASN:HD22	19:cm:65:ARG:NH1	1.65	0.94
1:bb:238:THR:HG23	1:bb:414:LEU:HB2	1.47	0.94
5:de:135:SER:HB3	22:di:12:ILE:CD1	1.97	0.94
1:ac:370:ASN:HD22	19:cm:59:TRP:HB2	1.25	0.94
4:dp:272:PRO:HG2	22:ds:14:ILE:HD12	1.50	0.94
23:db:10:PRO:HB2	22:dc:17:MET:CG	1.96	0.94
2:by:23:GLN:HG2	19:cj:57:SER:OG	1.66	0.94
24:cR:134:PRO:CB	25:cV:12:PHE:CZ	2.49	0.94
1:aa:429:GLY:HA3	13:bS:117:THR:CG2	1.96	0.94
2:by:25:THR:N	19:cj:54:ILE:HD11	1.83	0.94
24:cT:135:ASP:N	25:cU:12:PHE:HE1	1.64	0.94
24:cT:135:ASP:H	25:cU:12:PHE:HE1	1.16	0.94
4:dp:84:PHE:CZ	4:dp:273:PHE:CE2	2.57	0.93
24:cR:134:PRO:HA	25:cV:12:PHE:CD1	2.01	0.93
4:dp:84:PHE:HZ	4:dp:273:PHE:HZ	1.09	0.93
5:de:271:PHE:CB	23:dh:9:ASN:HD22	1.82	0.92
1:bl:65:ASP:OD1	8:bl:95:THR:HG22	1.69	0.92
5:dq:269:LEU:CD2	22:du:15:ARG:CG	2.37	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bu:11:TYR:HE2	13:bS:158:TYR:HD2	1.05	0.91
1:aa:427:MET:HE1	13:bS:146:PHE:HE1	1.36	0.91
26:dm:21:VAL:HG12	26:dn:15:VAL:HB	1.53	0.91
2:bv:327:ARG:NH2	13:bS:168:TYR:CE2	2.39	0.91
4:dk:138:GLU:OE1	26:dm:22:PHE:CZ	2.24	0.91
4:bD:136:ARG:O	22:cQ:12:ILE:HD13	1.71	0.91
4:dp:272:PRO:HD2	22:ds:14:ILE:CD1	2.00	0.91
2:bu:21:ASN:ND2	18:ci:53:TRP:HH2	1.69	0.90
2:bv:274:TYR:OH	13:bS:172:VAL:HG21	1.71	0.90
1:aa:10:ALA:HB2	19:cm:37:LEU:HD23	1.53	0.90
1:ac:320:LEU:HD12	19:cm:64:ARG:HH22	1.33	0.90
26:do:15:VAL:HG11	26:do:19:VAL:CG1	2.00	0.90
1:aa:429:GLY:HA3	13:bS:117:THR:HG21	1.50	0.90
13:bS:32:GLN:HG2	18:ci:26:LYS:HD3	1.54	0.90
4:dp:136:ARG:C	22:ds:12:ILE:HD13	1.96	0.89
4:dp:272:PRO:HD2	22:ds:14:ILE:HD12	1.54	0.89
26:do:27:VAL:CG2	26:do:30:LEU:HB3	2.03	0.89
4:dd:272:PRO:HD2	22:dg:14:ILE:HD13	0.89	0.89
5:dq:269:LEU:CD2	22:du:15:ARG:HD3	1.97	0.89
4:dp:272:PRO:CD	22:ds:14:ILE:HD12	2.03	0.89
13:bS:148:LYS:HE2	20:co:56:LEU:HD13	1.55	0.89
2:bu:11:TYR:HE2	13:bS:158:TYR:CD2	1.89	0.89
5:dq:269:LEU:CB	22:du:15:ARG:HD3	2.02	0.88
19:cl:23:GLU:HG2	20:co:128:ARG:HB2	1.55	0.88
22:cO:14:ILE:HG22	22:cO:15:ARG:HG2	1.53	0.88
1:ab:30:VAL:HG22	19:cm:48:GLN:HE22	1.38	0.88
1:aa:7:GLN:CA	20:co:54:LEU:HD11	2.03	0.88
1:aa:123:ASN:OD1	1:ac:123:ASN:HB3	1.74	0.88
26:dm:27:VAL:HG21	26:dm:30:LEU:HD23	1.56	0.88
4:dp:272:PRO:CG	22:ds:14:ILE:HD12	2.04	0.88
18:ci:26:LYS:NZ	18:ci:28:GLN:HG3	1.88	0.87
4:dp:136:ARG:HH11	22:ds:14:ILE:CG2	1.86	0.87
26:dm:29:TYR:HB3	26:dn:24:ASN:HB3	1.53	0.87
17:ch:68:TYR:O	17:ch:71:ILE:HG13	1.73	0.87
13:bS:56:ARG:CD	18:ci:9:ILE:HD11	2.04	0.87
5:dq:269:LEU:HD13	22:du:15:ARG:HD2	1.57	0.87
1:ac:258:PRO:HG2	19:cm:59:TRP:CE3	2.10	0.87
24:cT:134:PRO:CA	25:cU:12:PHE:CE1	2.58	0.86
1:ab:30:VAL:HG22	19:cm:48:GLN:NE2	1.90	0.86
13:bS:157:VAL:HG21	18:ci:61:LEU:HD11	1.55	0.86
23:db:10:PRO:CB	22:dc:17:MET:HG3	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:dp:138:GLU:CG	23:dt:17:ILE:HD11	2.05	0.86
13:bS:29:THR:HG22	13:bS:37:ARG:HA	1.57	0.86
5:de:135:SER:CB	22:di:12:ILE:CG2	2.54	0.86
1:aa:6:SER:O	20:co:64:ASP:CB	2.24	0.86
2:by:23:GLN:HG2	19:cj:57:SER:HB2	1.54	0.86
4:bD:138:GLU:HB2	23:cP:17:ILE:HD13	1.57	0.86
1:aa:427:MET:CE	13:bS:146:PHE:CE1	2.56	0.86
1:aa:103:GLN:HB2	13:bS:166:GLN:CD	2.01	0.85
18:ci:57:TYR:O	18:ci:61:LEU:HD13	1.75	0.85
4:df:275:ASN:HD21	22:dg:6:ASN:CG	1.84	0.85
2:bz:15:ASP:HB2	20:cn:54:LEU:O	1.76	0.85
1:bb:238:THR:CG2	1:bb:414:LEU:HD22	2.06	0.85
13:bS:28:PRO:HG2	18:ci:20:ALA:HB1	1.59	0.85
5:de:135:SER:H	22:di:12:ILE:HD13	1.42	0.85
13:bS:28:PRO:CD	18:ci:20:ALA:HB1	2.07	0.85
2:by:333:ILE:HD11	19:ck:46:ARG:HD3	1.56	0.84
23:dt:18:VAL:HG22	23:dt:20:GLY:H	1.41	0.84
1:aa:7:GLN:HB3	20:co:54:LEU:HD21	1.58	0.84
5:dq:135:SER:CB	22:du:12:ILE:HG21	2.06	0.84
1:aa:8:LEU:CD2	20:co:70:ASN:ND2	2.40	0.84
2:by:27:PHE:HZ	2:bz:320:VAL:CG1	1.82	0.84
2:bz:16:VAL:HG22	20:cn:56:LEU:HD21	1.52	0.84
23:db:11:PHE:O	23:db:12:PHE:CD2	2.31	0.84
1:bb:238:THR:HG23	1:bb:414:LEU:CB	2.07	0.84
1:ab:210:PHE:O	19:cm:63:THR:CG2	2.21	0.84
26:do:27:VAL:HG21	26:do:30:LEU:CB	2.08	0.84
26:dm:32:GLY:HA3	26:dn:27:VAL:CG2	2.06	0.83
1:aa:7:GLN:HB3	20:co:54:LEU:HD11	1.58	0.83
1:aa:7:GLN:CB	20:co:54:LEU:CD2	2.55	0.83
1:aa:8:LEU:HD22	20:co:70:ASN:ND2	1.93	0.83
26:do:27:VAL:HG22	26:do:30:LEU:HD23	1.59	0.83
4:dp:136:ARG:NH1	22:ds:14:ILE:CG2	2.42	0.83
4:bF:126:ARG:HH21	22:cQ:8:LEU:CD2	1.90	0.83
23:db:8:TRP:O	23:db:9:ASN:HB3	1.78	0.83
24:cT:135:ASP:N	25:cU:12:PHE:CE1	2.47	0.83
23:db:10:PRO:HB2	22:dc:17:MET:CB	2.08	0.83
7:bH:403:TYR:CE2	7:bH:405:THR:HG23	2.13	0.82
4:df:275:ASN:ND2	22:dg:6:ASN:HB3	1.94	0.82
2:by:27:PHE:CE1	2:bz:66:LEU:HD12	2.15	0.82
5:bE:271:PHE:HD2	23:cP:9:ASN:ND2	1.77	0.81
13:bS:29:THR:HG21	13:bS:37:ARG:CG	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:ch:68:TYR:CD1	17:ch:71:ILE:HD12	2.14	0.81
25:cU:14:LYS:HA	25:cW:19:SER:HB3	1.62	0.81
22:dg:28:PHE:HB3	22:di:23:LEU:HB3	1.62	0.81
4:dj:271:TYR:CE2	26:dm:17:GLN:CB	2.62	0.81
2:by:24:ILE:HD13	19:cj:51:PRO:HG3	1.63	0.81
2:bv:327:ARG:NH2	13:bS:168:TYR:HE2	1.77	0.81
1:aa:8:LEU:HD21	20:co:70:ASN:HD21	1.45	0.81
1:ay:67:ILE:O	1:ay:162:ALA:HB1	1.81	0.81
13:bS:29:THR:CG2	13:bS:37:ARG:CG	2.58	0.81
1:ac:421:TYR:CD2	19:cm:58:MET:HE1	2.15	0.80
5:de:135:SER:H	22:di:12:ILE:CD1	1.94	0.80
18:ci:32:GLN:HG2	18:ci:33:SER:H	1.46	0.80
1:ac:218:ARG:HD3	19:cm:42:ASP:OD1	1.82	0.80
18:ci:26:LYS:HZ2	18:ci:28:GLN:HG3	1.44	0.80
1:ab:210:PHE:C	19:cm:63:THR:HG21	2.05	0.80
7:bH:514:LEU:CD2	7:bH:517:ASN:ND2	2.45	0.80
2:bu:11:TYR:CE2	13:bS:158:TYR:CD2	2.70	0.79
13:bS:56:ARG:CZ	18:ci:9:ILE:HD12	2.12	0.79
24:cR:135:ASP:H	25:cV:12:PHE:HE1	1.27	0.79
2:by:32:ARG:HH21	19:cj:50:MET:HG2	1.47	0.79
4:dp:136:ARG:O	22:ds:12:ILE:HD13	1.82	0.79
1:aa:169:GLN:HG3	13:bS:117:THR:HB	1.64	0.79
5:dq:135:SER:OG	22:du:12:ILE:HD12	1.82	0.79
1:aa:7:GLN:C	20:co:54:LEU:CD1	2.56	0.78
1:aa:7:GLN:C	20:co:64:ASP:HB2	2.08	0.78
1:bl:63:ASN:O	1:bl:208:TYR:CD2	2.37	0.78
2:bu:21:ASN:ND2	18:ci:53:TRP:CH2	2.52	0.78
4:df:275:ASN:CB	22:dg:10:ASP:OD2	2.31	0.78
22:ds:28:PHE:HB3	22:du:23:LEU:HB3	1.63	0.78
13:bS:29:THR:HG21	13:bS:37:ARG:CB	2.14	0.78
1:aa:5:LEU:HD11	1:ab:17:TYR:CD1	2.19	0.78
18:ci:52:ALA:C	18:ci:55:PRO:HD2	2.09	0.77
26:dn:30:LEU:HD13	26:do:25:VAL:HB	1.64	0.77
1:ab:210:PHE:HB3	19:cm:63:THR:HG22	1.64	0.77
2:by:329:ARG:CD	19:ck:42:ASP:OD1	2.33	0.77
1:aa:429:GLY:N	13:bS:117:THR:HG21	2.00	0.77
1:ac:321:ASN:HD22	19:cm:65:ARG:HH12	1.29	0.77
5:bE:271:PHE:CD2	23:cP:9:ASN:ND2	2.53	0.77
13:bS:56:ARG:CZ	18:ci:9:ILE:CD1	2.63	0.77
4:bD:138:GLU:CB	23:cP:17:ILE:HD13	2.13	0.77
1:aa:7:GLN:HB2	20:co:54:LEU:CD2	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aa:169:GLN:CG	13:bS:117:THR:HB	2.14	0.77
2:bu:16:VAL:HG21	18:ci:57:TYR:HB2	1.66	0.77
4:dp:136:ARG:NH1	22:ds:14:ILE:HG23	2.00	0.77
2:bu:11:TYR:CE2	13:bS:158:TYR:HD2	1.95	0.76
24:cR:134:PRO:HB3	25:cV:12:PHE:CZ	2.18	0.76
18:ci:52:ALA:O	18:ci:55:PRO:HD2	1.86	0.76
4:dd:272:PRO:HG2	22:dg:14:ILE:HD13	1.67	0.76
26:dm:29:TYR:O	26:dn:24:ASN:HA	1.85	0.76
2:bz:15:ASP:O	19:cj:55:PHE:HA	1.86	0.76
2:by:27:PHE:CZ	2:bz:320:VAL:CG1	2.60	0.76
2:bz:16:VAL:CG2	20:cn:56:LEU:CD2	2.58	0.76
17:ch:68:TYR:CE1	17:ch:71:ILE:HD12	2.21	0.76
1:ab:17:TYR:OH	13:bS:150:LEU:HA	1.85	0.76
2:bv:508:ARG:HB2	13:bS:186:LEU:HG	1.68	0.76
1:ac:24:ILE:HB	19:cl:50:MET:HB2	1.67	0.75
1:aa:11:TYR:CE2	20:co:51:VAL:O	2.39	0.75
5:cY:271:PHE:CD1	22:da:6:ASN:HA	2.19	0.75
1:ac:24:ILE:HB	19:cl:50:MET:CB	2.17	0.75
2:bu:5:ILE:HG12	13:bS:165:ARG:HH21	1.51	0.75
23:db:10:PRO:CB	22:dc:17:MET:CB	2.64	0.75
2:bx:22:PRO:HB2	19:ck:41:LEU:HD23	1.69	0.75
7:bH:403:TYR:OH	7:bH:405:THR:CG2	2.35	0.75
22:dc:14:ILE:O	22:dc:15:ARG:HG2	1.87	0.75
25:cU:26:ASN:HA	25:cW:32:GLY:HA3	1.69	0.74
9:bL:21:LYS:NZ	14:cc:135:SER:OG	2.20	0.74
2:bu:9:VAL:HA	13:bS:160:VAL:CG1	2.17	0.74
2:bu:5:ILE:HD11	13:bS:166:GLN:NE2	2.03	0.74
2:bv:327:ARG:HH22	13:bS:168:TYR:HE2	1.35	0.74
2:by:329:ARG:HG2	19:ck:46:ARG:NH1	2.02	0.74
2:bz:16:VAL:HG21	20:cn:56:LEU:HD21	1.70	0.74
2:bz:15:ASP:HB3	20:cn:55:GLU:HG2	1.69	0.74
4:dd:272:PRO:HG2	22:dg:14:ILE:CB	2.18	0.74
22:dg:13:MET:HE1	22:dg:17:MET:HE3	1.69	0.74
2:by:333:ILE:HD11	19:ck:46:ARG:HH11	1.51	0.74
4:dd:272:PRO:CG	22:dg:14:ILE:CD1	2.66	0.74
26:dn:30:LEU:CD1	26:do:25:VAL:HB	2.18	0.74
1:aa:6:SER:O	20:co:64:ASP:HB3	1.87	0.74
2:by:24:ILE:C	19:cj:54:ILE:HD11	2.13	0.74
1:aa:170:TYR:CE1	13:bS:115:ASN:O	2.40	0.74
1:aa:218:ARG:HE	19:cl:54:ILE:HG12	1.52	0.74
2:bu:5:ILE:HD11	13:bS:166:GLN:HE22	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:bS:148:LYS:CE	20:co:56:LEU:HD13	2.17	0.73
1:aa:6:SER:C	20:co:64:ASP:HB3	2.13	0.73
2:by:24:ILE:HD13	19:cj:51:PRO:CG	2.18	0.73
5:de:271:PHE:HB2	23:dh:9:ASN:ND2	1.99	0.73
1:aa:8:LEU:CD1	20:co:70:ASN:ND2	2.51	0.73
1:bb:238:THR:HG22	1:bb:414:LEU:HD22	1.70	0.73
1:af:174:LYS:NZ	3:bC:154:SER:OG	2.22	0.73
13:bS:29:THR:HG22	13:bS:37:ARG:HG2	1.70	0.73
26:do:30:LEU:HD12	26:do:30:LEU:O	1.89	0.73
2:bx:22:PRO:O	19:ck:41:LEU:HD22	1.89	0.73
4:dr:271:TYR:CD2	23:dt:14:ARG:HD2	2.23	0.73
22:du:15:ARG:HH11	22:du:15:ARG:HG3	1.54	0.73
7:bH:403:TYR:CZ	7:bH:405:THR:CG2	2.71	0.73
4:dd:272:PRO:HG2	22:dg:14:ILE:CG1	2.18	0.73
26:dm:15:VAL:HB	26:do:21:VAL:HG12	1.71	0.73
26:dm:30:LEU:O	26:dm:30:LEU:HD12	1.89	0.73
1:bc:329:ARG:NH2	1:be:41:SER:OG	2.22	0.73
5:bE:135:SER:HB2	22:cO:12:ILE:CD1	2.17	0.72
7:bH:406:GLY:O	7:bH:407:PRO:O	2.06	0.72
1:aa:103:GLN:HB2	13:bS:166:GLN:OE1	1.89	0.72
26:do:27:VAL:CG2	26:do:30:LEU:CD2	2.62	0.72
4:dk:82:ASN:ND2	26:dm:22:PHE:CE2	2.57	0.72
1:ab:210:PHE:C	19:cm:63:THR:CG2	2.62	0.72
7:bH:514:LEU:CD2	7:bH:517:ASN:HD22	1.94	0.72
13:bS:157:VAL:HG21	18:ci:61:LEU:HD12	1.69	0.72
5:dq:135:SER:HB2	22:du:12:ILE:CG2	2.12	0.72
13:bS:27:ILE:CG2	13:bS:44:LEU:HD13	2.20	0.72
24:cT:134:PRO:HA	25:cU:12:PHE:CD1	2.24	0.72
1:ac:320:LEU:CD1	19:cm:64:ARG:NH2	2.50	0.72
2:bz:12:GLY:HA2	20:cn:55:GLU:OE2	1.90	0.71
17:ch:71:ILE:O	17:ch:72:SER:HB2	1.90	0.71
5:de:135:SER:N	22:di:12:ILE:HD13	2.04	0.71
5:dq:125:HIS:CE1	22:du:7:PRO:HD2	2.25	0.71
23:cP:18:VAL:HA	22:cQ:13:MET:HB2	1.71	0.71
18:ci:33:SER:O	18:ci:35:TRP:NE1	2.24	0.71
4:dp:136:ARG:O	22:ds:12:ILE:HG21	1.91	0.71
5:dq:269:LEU:CG	22:du:15:ARG:HD3	2.19	0.71
2:bv:332:GLU:HB3	13:bS:6:LEU:HD11	1.71	0.71
23:cP:16:ILE:HA	22:cQ:11:PRO:HG2	1.72	0.71
5:de:357:ASN:O	5:de:360:THR:HB	1.90	0.71
4:dp:272:PRO:HG2	22:ds:14:ILE:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aa:8:LEU:HD13	20:co:70:ASN:ND2	2.06	0.71
13:bS:29:THR:CB	13:bS:37:ARG:HG2	2.20	0.71
23:db:10:PRO:CB	22:dc:17:MET:HB2	2.20	0.70
2:by:326:GLU:HG3	2:by:329:ARG:NH2	2.05	0.70
4:bF:126:ARG:NH2	22:cQ:8:LEU:HD23	1.96	0.70
7:bH:403:TYR:CZ	7:bH:405:THR:HG23	2.26	0.70
1:aa:7:GLN:CG	20:co:54:LEU:HD21	2.20	0.70
1:aa:220:ALA:HB1	13:bS:118:VAL:HG21	1.73	0.70
26:dm:31:ILE:O	26:dn:26:PHE:HA	1.90	0.70
5:bE:135:SER:CB	22:cO:12:ILE:HD12	2.21	0.70
4:bF:136:ARG:NH2	23:cP:13:ASN:OD1	2.21	0.70
21:cu:122:GLN:NE2	21:cu:216:SER:OG	2.25	0.70
21:cL:263:ASN:HB3	21:cL:267:ALA:HA	1.72	0.70
5:de:135:SER:CB	22:di:12:ILE:HG23	2.19	0.70
26:do:27:VAL:HG21	26:do:30:LEU:CD2	2.21	0.70
23:db:8:TRP:CG	23:db:9:ASN:H	2.10	0.70
1:aa:123:ASN:HB3	1:ab:123:ASN:OD1	1.92	0.70
2:by:27:PHE:CE1	2:bz:66:LEU:CD1	2.75	0.70
4:dr:271:TYR:CD2	23:dt:14:ARG:CD	2.75	0.69
1:ac:258:PRO:HB2	19:cm:58:MET:HE2	1.74	0.69
2:by:24:ILE:HG22	19:cj:59:TRP:HZ2	1.57	0.69
1:ap:425:ARG:NH2	1:aq:17:TYR:OH	2.25	0.69
20:co:66:ALA:HB1	20:co:69:GLN:HB2	1.74	0.69
20:co:76:ALA:O	20:co:80:HIS:ND1	2.21	0.69
1:aa:8:LEU:O	20:co:54:LEU:HD12	1.93	0.69
2:by:112:TRP:CD1	2:by:113:THR:HG1	2.09	0.69
23:db:10:PRO:HG2	22:dc:17:MET:HA	1.74	0.69
26:dn:25:VAL:HG23	26:do:19:VAL:HG23	1.74	0.69
26:dn:32:GLY:HA3	26:do:30:LEU:CD2	2.21	0.69
22:cO:11:PRO:HB2	22:cQ:17:MET:HG3	1.73	0.69
5:de:271:PHE:CB	23:dh:9:ASN:ND2	2.54	0.69
1:aa:5:LEU:HD11	1:ab:17:TYR:HD1	1.58	0.69
1:aa:6:SER:C	20:co:64:ASP:CB	2.66	0.69
2:by:23:GLN:O	19:cj:54:ILE:HG12	1.92	0.69
17:ch:68:TYR:CD1	17:ch:71:ILE:CD1	2.75	0.69
18:ci:54:LYS:HE2	18:ci:58:MET:CE	2.23	0.69
1:aa:429:GLY:HA3	13:bS:117:THR:HG22	1.75	0.69
1:aA:115:THR:OG1	1:aA:265:ASN:ND2	2.26	0.69
4:dp:118:GLU:OE2	4:dp:273:PHE:CD1	2.46	0.69
13:bS:27:ILE:HG22	13:bS:28:PRO:HD3	1.73	0.68
13:bS:27:ILE:HB	13:bS:28:PRO:HD2	1.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:df:274:GLU:OE2	23:dh:14:ARG:NH2	2.25	0.68
4:dp:84:PHE:CE1	4:dp:273:PHE:CE2	2.81	0.68
18:ci:32:GLN:HG2	18:ci:33:SER:N	2.08	0.68
4:dd:273:PHE:HB2	4:dd:317:SER:HB3	1.75	0.68
3:bC:268:THR:OG1	3:bC:269:ASN:N	2.27	0.68
13:bS:56:ARG:NE	18:ci:9:ILE:HD12	2.09	0.68
4:df:271:TYR:CG	23:dh:14:ARG:NE	2.58	0.68
24:cR:135:ASP:N	25:cV:12:PHE:HE1	1.89	0.68
2:bu:5:ILE:CD1	13:bS:166:GLN:NE2	2.56	0.68
19:ck:35:ARG:HG2	20:cn:53:SER:OG	1.94	0.68
2:bv:274:TYR:OH	13:bS:172:VAL:CG2	2.42	0.68
13:bS:92:ILE:HG12	13:bS:94:PRO:HD3	1.76	0.68
2:bu:9:VAL:HA	13:bS:160:VAL:HG13	1.76	0.67
18:ci:49:ASP:O	18:ci:52:ALA:HB3	1.94	0.67
4:df:138:GLU:CB	23:dh:11:PHE:CZ	2.77	0.67
13:bS:148:LYS:HE2	20:co:56:LEU:CD1	2.23	0.67
23:db:8:TRP:HZ2	22:dc:13:MET:HE2	1.58	0.67
5:de:80:GLN:OE1	22:di:14:ILE:HD13	1.94	0.67
9:bL:19:ASP:OD2	9:bL:53:LYS:NZ	2.28	0.67
23:db:10:PRO:CG	22:dc:17:MET:HA	2.25	0.67
26:dm:26:PHE:O	26:dn:20:VAL:HA	1.95	0.67
1:ac:25:THR:O	19:cl:50:MET:SD	2.52	0.67
1:bb:238:THR:HG21	1:bb:414:LEU:HB2	1.76	0.67
2:by:23:GLN:CG	19:cj:57:SER:HB2	2.22	0.67
22:cO:15:ARG:NH2	22:cQ:20:TYR:O	2.28	0.67
25:cU:25:ALA:O	25:cW:32:GLY:N	2.27	0.67
2:by:333:ILE:CG1	19:ck:46:ARG:HD3	2.24	0.67
4:df:271:TYR:HB2	23:dh:14:ARG:CZ	2.23	0.67
26:dm:32:GLY:HA2	26:dn:27:VAL:HG22	1.77	0.66
4:bF:217:THR:OG1	10:bP:47:LYS:NZ	2.26	0.66
5:de:80:GLN:OE1	22:di:14:ILE:CD1	2.43	0.66
5:de:358:VAL:HG22	5:de:368:LEU:HD11	1.75	0.66
1:ac:421:TYR:HD2	19:cm:58:MET:HE1	1.59	0.66
26:do:27:VAL:HG21	26:do:30:LEU:HD23	1.69	0.66
11:bQ:92:ALA:N	11:bQ:93:PRO:CD	2.58	0.66
14:bY:135:SER:N	14:bY:136:PRO:CD	2.59	0.66
25:cV:32:GLY:HA3	25:cW:26:ASN:HA	1.75	0.66
4:df:275:ASN:ND2	22:dg:6:ASN:CG	2.52	0.66
4:dp:137:PRO:CA	22:ds:12:ILE:HD13	2.24	0.66
1:aa:7:GLN:HB2	20:co:54:LEU:HD13	1.78	0.66
25:cV:33:ASN:N	25:cW:26:ASN:O	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:db:11:PHE:O	23:db:12:PHE:CG	2.49	0.66
1:ac:225:GLU:OE1	19:cm:50:MET:HB3	1.96	0.66
18:ci:56:ILE:O	18:ci:60:VAL:HG23	1.96	0.66
5:de:135:SER:CB	22:di:12:ILE:HG21	2.11	0.66
26:do:11:ASP:H	26:do:12:PRO:HD2	1.61	0.66
1:bn:325:ARG:NH1	1:bn:354:TYR:OH	2.28	0.66
2:by:333:ILE:HD11	19:ck:46:ARG:NH1	2.11	0.66
13:bS:29:THR:CG2	13:bS:37:ARG:HA	2.26	0.66
5:de:355:ALA:HB3	5:de:360:THR:CG2	2.12	0.66
5:dq:135:SER:OG	22:du:12:ILE:CD1	2.44	0.66
25:cU:26:ASN:O	25:cW:33:ASN:N	2.26	0.65
24:cR:134:PRO:HB2	25:cV:12:PHE:CZ	2.31	0.65
4:bD:108:ASP:OD2	4:bD:259:LYS:NZ	2.30	0.65
1:aZ:435:TYR:OH	9:bM:53:LYS:NZ	2.25	0.65
1:aW:259:THR:OG1	1:aW:420:ASN:ND2	2.29	0.65
1:bm:259:THR:OG1	1:bm:420:ASN:ND2	2.30	0.65
2:by:24:ILE:HA	19:cj:54:ILE:HG12	1.77	0.65
5:de:359:TYR:CE1	4:df:138:GLU:CB	2.80	0.65
1:aa:7:GLN:OE1	20:co:56:LEU:HD12	1.96	0.65
2:by:27:PHE:CD1	2:bz:66:LEU:CD1	2.79	0.65
4:dp:272:PRO:HD2	22:ds:14:ILE:HD11	1.78	0.65
23:db:8:TRP:O	23:db:9:ASN:CB	2.45	0.64
5:bE:82:PHE:HB2	5:bE:270:TYR:CZ	2.31	0.64
4:dp:136:ARG:HH11	22:ds:14:ILE:HG22	1.61	0.64
2:by:27:PHE:CZ	2:bz:66:LEU:HD12	2.33	0.64
17:ch:67:GLU:OE1	17:ch:69:LYS:HE2	1.97	0.64
20:co:55:GLU:O	20:co:55:GLU:HG2	1.97	0.64
18:ci:54:LYS:HE2	18:ci:58:MET:HE3	1.79	0.64
4:dd:272:PRO:HG2	22:dg:14:ILE:CD1	2.26	0.64
5:de:356:ALA:O	5:de:368:LEU:HD22	1.98	0.64
4:dp:84:PHE:CZ	4:dp:273:PHE:HZ	1.95	0.64
4:dr:271:TYR:CE2	23:dt:14:ARG:HD3	2.33	0.64
19:cl:16:ILE:HD13	19:cl:19:ILE:HD12	1.79	0.64
26:dm:32:GLY:CA	26:dn:27:VAL:CG2	2.68	0.64
5:de:358:VAL:CG2	5:de:368:LEU:HD11	2.27	0.64
1:bb:102:GLY:C	1:bl:63:ASN:HD21	2.06	0.64
18:ci:54:LYS:O	18:ci:57:TYR:HB3	1.97	0.64
13:bS:17:SER:HB2	20:co:115:VAL:HB	1.80	0.63
13:bS:42:VAL:HG13	13:bS:69:ILE:HD12	1.80	0.63
4:dd:275:ASN:HD21	22:di:7:PRO:HD2	1.63	0.63
4:dp:272:PRO:CD	22:ds:14:ILE:CD1	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aa:6:SER:O	20:co:64:ASP:HB2	1.98	0.63
26:dn:21:VAL:HG12	26:do:15:VAL:HB	1.81	0.63
23:dt:13:ASN:O	23:dt:14:ARG:HG3	1.99	0.63
13:bS:29:THR:HB	13:bS:37:ARG:HG2	1.78	0.63
4:dp:272:PRO:CG	22:ds:14:ILE:CD1	2.77	0.63
1:bb:102:GLY:HA3	1:bl:63:ASN:HD21	1.63	0.63
4:dp:137:PRO:N	22:ds:12:ILE:HD13	2.14	0.63
17:ch:68:TYR:CG	20:cn:112:SER:O	2.52	0.63
21:cw:122:GLN:NE2	21:cw:216:SER:OG	2.31	0.63
2:bx:88:PRO:O	2:bx:89:ALA:CB	2.46	0.63
4:dp:137:PRO:HA	22:ds:12:ILE:HD13	1.79	0.63
4:bF:307:GLN:N	4:bF:308:PRO:CD	2.62	0.63
23:cP:32:ASN:HB2	22:cQ:27:TYR:CD1	2.33	0.63
26:dm:27:VAL:CG2	26:dm:30:LEU:HD23	2.28	0.63
1:aR:115:THR:OG1	1:aR:265:ASN:ND2	2.32	0.62
5:de:135:SER:CA	22:di:12:ILE:HD13	2.30	0.62
4:df:271:TYR:CB	23:dh:14:ARG:HH21	1.95	0.62
25:cV:37:ALA:N	25:cW:30:ASP:O	2.32	0.62
1:aZ:125:ASP:OD1	1:aZ:126:ARG:N	2.32	0.62
1:ae:145:LYS:NZ	1:af:308:GLU:OE2	2.32	0.62
2:by:329:ARG:HD3	19:ck:42:ASP:CG	2.25	0.62
4:cX:138:GLU:CB	22:da:18:ILE:HD13	2.29	0.62
1:aI:125:ASP:OD1	1:aI:126:ARG:N	2.33	0.62
2:by:23:GLN:CG	19:cj:57:SER:CB	2.73	0.62
22:cO:17:MET:SD	22:cO:18:ILE:N	2.73	0.62
24:cR:134:PRO:CA	25:cV:12:PHE:CZ	2.82	0.62
2:by:27:PHE:CE2	2:bz:322:LEU:HD21	2.35	0.62
5:de:359:TYR:HE1	4:df:138:GLU:CB	2.13	0.62
1:ak:25:THR:OG1	21:cF:48:LYS:NZ	2.30	0.62
1:bb:238:THR:CG2	1:bb:414:LEU:CB	2.70	0.62
1:aM:14:GLN:NE2	8:bJ:162:THR:OG1	2.32	0.61
4:bF:43:ILE:HD13	4:bF:62:PHE:HB3	1.81	0.61
23:cP:29:ILE:N	22:cQ:23:LEU:O	2.31	0.61
1:af:125:ASP:OD1	1:af:126:ARG:N	2.33	0.61
26:dm:29:TYR:HE1	26:dm:31:ILE:HG23	1.65	0.61
22:du:15:ARG:HG3	22:du:15:ARG:NH1	2.15	0.61
1:ab:210:PHE:CB	19:cm:63:THR:HG22	2.30	0.61
1:ac:258:PRO:CB	19:cm:58:MET:HE2	2.30	0.61
4:bF:137:PRO:HA	23:cP:11:PHE:HZ	1.66	0.61
13:bS:148:LYS:CE	20:co:56:LEU:CD1	2.78	0.61
23:cP:21:ASN:HB2	22:cQ:16:THR:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:db:10:PRO:HB2	22:dc:17:MET:CA	2.31	0.61
13:bS:152:ARG:CZ	18:ci:75:VAL:HG11	2.31	0.61
25:cU:19:SER:HA	25:cW:25:ALA:HB2	1.82	0.61
22:ds:16:THR:HG22	23:dt:21:ASN:H	1.63	0.61
1:ag:308:GLU:OE2	1:ai:145:LYS:NZ	2.33	0.61
2:by:24:ILE:HG21	19:cj:51:PRO:HG2	1.82	0.61
22:cO:11:PRO:HA	23:cP:8:TRP:HZ2	1.64	0.61
1:aC:259:THR:OG1	1:aC:420:ASN:ND2	2.33	0.61
1:aL:125:ASP:OD1	1:aL:126:ARG:N	2.33	0.61
13:bS:30:ARG:O	13:bS:31:ASP:C	2.43	0.61
19:cl:56:SER:HB3	20:co:53:SER:HA	1.83	0.61
25:cU:30:ASP:HA	25:cV:24:ILE:O	2.01	0.61
25:cW:19:SER:OG	25:cW:20:ASN:N	2.34	0.61
23:dt:21:ASN:OD1	22:du:27:TYR:HB2	2.00	0.61
2:by:24:ILE:HD13	19:cj:51:PRO:CB	2.30	0.61
20:cn:54:LEU:HG	20:cn:56:LEU:HD22	1.83	0.61
1:ac:232:GLN:NE2	1:ac:257:HIS:ND1	2.49	0.61
7:bH:532:ASP:HB3	7:bH:535:GLN:HG3	1.83	0.61
20:cn:107:ASP:OD2	20:cn:126:ARG:NH1	2.32	0.61
4:dj:174:LYS:NZ	4:dj:176:ASP:OD2	2.33	0.61
12:bR:162:LEU:O	12:bR:163:SER:C	2.43	0.60
23:db:10:PRO:HB2	22:dc:17:MET:HA	1.83	0.60
1:aa:7:GLN:HG3	20:co:54:LEU:HD21	1.81	0.60
1:aa:434:ALA:HB1	13:bS:150:LEU:HD11	1.81	0.60
2:bv:327:ARG:NH1	13:bS:165:ARG:O	2.29	0.60
2:bx:28:LYS:HG2	19:ck:45:ILE:HD12	1.83	0.60
1:aa:427:MET:CE	13:bS:146:PHE:HE1	2.07	0.60
2:bu:5:ILE:CG1	13:bS:165:ARG:HH21	2.13	0.60
17:ch:152:ASP:O	17:ch:153:ILE:C	2.45	0.60
26:do:29:TYR:HE1	26:do:31:ILE:HG22	1.67	0.60
13:bS:16:LEU:O	13:bS:17:SER:OG	2.17	0.60
4:dd:272:PRO:HG2	22:dg:14:ILE:HB	1.83	0.60
5:bE:82:PHE:CB	5:bE:270:TYR:CZ	2.85	0.60
24:cT:134:PRO:CB	25:cU:12:PHE:CZ	2.84	0.60
18:ci:27:MET:C	18:ci:28:GLN:HG2	2.27	0.60
19:cj:16:ILE:HD12	20:cn:135:PHE:HA	1.84	0.60
22:da:17:MET:HG3	22:dc:11:PRO:HB2	1.83	0.60
4:dd:272:PRO:CD	22:dg:14:ILE:CD1	2.41	0.60
4:dp:136:ARG:NH1	22:ds:12:ILE:O	2.35	0.60
1:bj:125:ASP:OD1	1:bj:126:ARG:N	2.35	0.60
5:bE:82:PHE:CD1	5:bE:270:TYR:CD1	2.90	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:cS:75:ARG:NH2	24:cS:136:ASP:O	2.34	0.60
10:bP:61:ASP:OD2	10:bP:65:LYS:NZ	2.35	0.60
24:cT:99:GLU:OE1	24:cT:102:LYS:NZ	2.35	0.60
22:da:9:ASN:HA	23:db:12:PHE:HE1	1.65	0.60
1:bd:371:PHE:O	8:bK:127:ARG:NH1	2.34	0.59
18:ci:49:ASP:HB2	18:ci:52:ALA:HB3	1.78	0.59
22:cO:17:MET:HE1	23:cP:11:PHE:HA	1.84	0.59
1:aa:169:GLN:HG3	13:bS:117:THR:CB	2.30	0.59
14:bU:176:ASP:OD1	14:bU:177:LEU:N	2.35	0.59
24:cR:135:ASP:N	25:cV:12:PHE:CE1	2.69	0.59
1:ac:227:LEU:HD22	19:cm:55:PHE:CZ	2.38	0.59
2:bB:388:ASP:OD1	2:bB:389:ALA:N	2.35	0.59
26:do:11:ASP:N	26:do:12:PRO:HD2	2.16	0.59
4:dp:138:GLU:CG	23:dt:17:ILE:CD1	2.76	0.59
5:dq:269:LEU:HD13	22:du:15:ARG:CD	2.31	0.59
4:bF:108:ASP:OD2	4:bF:259:LYS:NZ	2.36	0.59
7:bH:403:TYR:OH	7:bH:405:THR:HG21	2.03	0.59
7:bH:403:TYR:CE2	7:bH:405:THR:CG2	2.86	0.59
5:dq:269:LEU:CD1	22:du:15:ARG:HD2	2.31	0.59
4:cX:271:TYR:CG	22:dc:15:ARG:HD2	2.38	0.59
26:dn:29:TYR:HB3	26:do:24:ASN:HB3	1.83	0.59
20:co:93:ALA:HB3	20:co:95:GLN:HE22	1.68	0.59
25:cU:16:ILE:O	25:cW:23:ASN:N	2.35	0.59
5:cY:271:PHE:HD1	22:da:6:ASN:HA	1.66	0.59
23:db:8:TRP:HA	23:db:8:TRP:CE3	2.37	0.59
26:dm:33:ASN:O	26:dm:34:ALA:C	2.45	0.59
1:aa:68:THR:O	1:aa:156:ASN:HA	2.03	0.59
1:ao:86:TYR:OH	1:ao:114:ARG:NH2	2.35	0.59
2:bw:90:GLU:O	2:bw:91:GLY:C	2.46	0.59
2:bx:88:PRO:O	2:bx:89:ALA:HB3	2.02	0.59
1:aa:169:GLN:HG3	13:bS:117:THR:CA	2.33	0.58
2:bv:321:PHE:HD2	13:bS:165:ARG:CZ	2.16	0.58
14:bW:176:ASP:OD1	14:bW:177:LEU:N	2.36	0.58
25:cU:33:ASN:N	25:cV:26:ASN:O	2.25	0.58
1:ap:384:LYS:NZ	1:ap:401:GLU:O	2.37	0.58
19:cj:54:ILE:O	19:cj:54:ILE:HG22	2.02	0.58
4:dp:137:PRO:CA	22:ds:12:ILE:CD1	2.80	0.58
1:aH:123:ASN:N	1:aJ:124:ASP:OD2	2.37	0.58
2:by:333:ILE:HG12	19:ck:46:ARG:HD3	1.85	0.58
4:dp:136:ARG:C	22:ds:12:ILE:CD1	2.75	0.58
4:dp:137:PRO:HA	22:ds:12:ILE:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aa:123:ASN:CG	1:ac:123:ASN:HB3	2.28	0.58
1:aV:215:GLU:OE2	21:cJ:48:LYS:NZ	2.36	0.58
13:bS:157:VAL:CG2	18:ci:61:LEU:HD11	2.32	0.58
5:de:271:PHE:CD2	23:dh:9:ASN:ND2	2.72	0.58
26:dm:33:ASN:CB	26:dn:28:ASP:O	2.51	0.58
5:cY:271:PHE:HD2	22:da:9:ASN:HD22	1.47	0.58
1:am:153:PHE:H	1:am:156:ASN:HD21	1.50	0.58
1:bb:238:THR:CG2	1:bb:414:LEU:CD2	2.79	0.58
21:cw:262:LYS:O	21:cw:263:ASN:CB	2.51	0.58
1:aT:238:THR:HG1	1:aT:383:TYR:HH	1.51	0.58
5:de:135:SER:HB2	22:di:12:ILE:HD13	1.81	0.58
4:df:271:TYR:CD1	23:dh:14:ARG:NE	2.68	0.58
4:df:275:ASN:OD1	22:dg:6:ASN:CG	2.46	0.58
1:ad:67:ILE:HD11	1:ad:165:LEU:HD21	1.85	0.58
2:bz:19:THR:O	19:cj:61:VAL:HG12	2.04	0.58
2:bA:388:ASP:OD1	2:bA:389:ALA:N	2.37	0.58
18:ci:27:MET:O	18:ci:28:GLN:HG2	2.03	0.58
19:cl:9:LEU:HD22	20:co:140:VAL:HG21	1.86	0.58
4:cX:310:ASP:OD2	5:cY:66:LYS:NZ	2.37	0.58
26:dm:29:TYR:HE1	26:dm:31:ILE:CG2	2.17	0.58
26:dm:31:ILE:O	26:dm:31:ILE:HG13	2.03	0.58
4:dp:272:PRO:HB2	4:dp:273:PHE:CD2	2.38	0.58
2:bz:32:ARG:NH1	19:cj:59:TRP:CE3	2.72	0.58
24:cT:134:PRO:C	25:cU:12:PHE:CE1	2.81	0.58
24:cT:249:ARG:HG3	24:cT:250:TYR:CD2	2.39	0.58
2:by:333:ILE:HD13	19:ck:46:ARG:HD3	1.84	0.58
5:bE:18:TYR:OH	10:bP:27:VAL:N	2.34	0.58
14:bV:176:ASP:OD1	14:bV:177:LEU:N	2.37	0.58
18:ci:54:LYS:HG2	18:ci:58:MET:HE3	1.86	0.58
1:ap:308:GLU:OE2	1:ar:145:LYS:NZ	2.36	0.57
13:bS:56:ARG:NH2	18:ci:9:ILE:HD12	2.18	0.57
13:bS:152:ARG:NE	18:ci:75:VAL:HG11	2.19	0.57
22:da:17:MET:HA	22:dc:11:PRO:HG2	1.86	0.57
23:db:10:PRO:HB3	22:dc:13:MET:SD	2.43	0.57
5:de:125:HIS:NE2	22:di:7:PRO:N	2.52	0.57
1:at:145:LYS:NZ	1:au:308:GLU:OE2	2.37	0.57
1:bl:63:ASN:HA	8:bI:94:GLY:O	2.04	0.57
4:dp:118:GLU:OE2	4:dp:273:PHE:CE1	2.57	0.57
1:aE:122:MET:O	1:aE:123:ASN:C	2.48	0.57
1:aY:308:GLU:OE1	1:aY:336:LYS:NZ	2.37	0.57
20:cn:134:PHE:HA	20:cn:137:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:co:114:ARG:HD2	20:co:115:VAL:HG13	1.86	0.57
24:cR:134:PRO:CB	25:cV:12:PHE:CE1	2.85	0.57
21:cJ:238:ASN:O	21:cJ:239:LYS:C	2.48	0.57
4:df:275:ASN:OD1	22:dg:6:ASN:ND2	2.37	0.57
2:by:27:PHE:O	2:bz:264:GLY:CA	2.38	0.57
21:cw:262:LYS:O	21:cw:263:ASN:HB3	2.04	0.57
4:df:108:ASP:OD2	4:df:259:LYS:NZ	2.37	0.57
22:dg:14:ILE:HD12	22:dg:15:ARG:HB3	1.86	0.57
1:aS:308:GLU:OE1	1:aS:336:LYS:NZ	2.38	0.57
13:bS:10:PRO:HA	18:ci:31:PRO:HB3	1.86	0.57
23:cP:35:GLY:N	22:cQ:30:GLY:O	2.38	0.57
1:az:145:LYS:NZ	1:aA:308:GLU:OE2	2.38	0.57
1:aK:139:GLU:CD	1:aK:139:GLU:H	2.13	0.57
1:bb:102:GLY:CA	1:bl:63:ASN:HD21	2.18	0.57
1:bn:86:TYR:OH	1:bn:114:ARG:NH2	2.37	0.57
2:bv:321:PHE:HD2	13:bS:165:ARG:NH1	2.02	0.57
9:bL:30:ILE:O	9:bL:34:ILE:N	2.37	0.57
22:cO:11:PRO:HG2	22:cQ:17:MET:HA	1.87	0.57
25:cU:30:ASP:O	25:cW:37:ALA:N	2.37	0.57
5:de:135:SER:HB3	22:di:12:ILE:CG1	2.35	0.57
4:dl:136:ARG:O	26:do:14:ILE:HD11	2.04	0.57
4:dr:271:TYR:CE2	23:dt:14:ARG:CD	2.88	0.57
1:ad:125:ASP:OD1	1:ad:126:ARG:N	2.37	0.57
1:ak:125:ASP:OD1	1:ak:126:ARG:N	2.38	0.57
13:bS:28:PRO:HG2	18:ci:20:ALA:CB	2.32	0.57
19:cl:13:PHE:HA	20:co:137:VAL:HG21	1.85	0.57
22:dg:11:PRO:HG2	23:dh:16:ILE:HA	1.86	0.57
19:cl:37:LEU:HD23	19:cm:36:TYR:HB3	1.87	0.57
26:dm:28:ASP:OD2	26:dn:22:PHE:HA	2.04	0.57
1:bf:257:HIS:ND1	1:bg:14:GLN:NE2	2.53	0.57
5:bE:82:PHE:CD1	5:bE:270:TYR:CE1	2.93	0.57
1:bp:333:TYR:OH	1:bp:338:GLN:NE2	2.37	0.56
7:bH:406:GLY:O	7:bH:407:PRO:C	2.47	0.56
1:aa:11:TYR:N	19:cm:36:TYR:O	2.35	0.56
21:cz:173:GLU:OE1	21:cz:173:GLU:N	2.38	0.56
22:cQ:13:MET:HG3	22:cQ:17:MET:HE3	1.86	0.56
22:ds:26:THR:OG1	22:du:20:TYR:O	2.23	0.56
1:aB:125:ASP:OD1	1:aB:126:ARG:N	2.39	0.56
1:bb:238:THR:HG21	1:bb:414:LEU:HD22	1.86	0.56
2:bu:13:ALA:HB2	18:ci:57:TYR:CE2	2.40	0.56
18:ci:57:TYR:O	18:ci:61:LEU:CD1	2.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:cj:54:ILE:O	19:cj:55:PHE:HB2	2.04	0.56
22:da:11:PRO:HB2	23:db:16:ILE:HG12	1.86	0.56
22:di:25:ALA:HB3	22:di:28:PHE:HE1	1.70	0.56
1:aW:333:TYR:OH	1:aW:338:GLN:NE2	2.38	0.56
26:dm:25:VAL:HG11	26:do:27:VAL:HG11	1.87	0.56
1:aS:166:ILE:O	1:aS:169:GLN:NE2	2.39	0.56
2:bu:21:ASN:HB2	18:ci:53:TRP:CZ2	2.40	0.56
2:by:329:ARG:HG2	19:ck:46:ARG:HH12	1.71	0.56
24:cS:249:ARG:HG3	24:cS:250:TYR:CD2	2.41	0.56
3:bC:163:MET:O	3:bC:253:ARG:NH1	2.39	0.56
9:bM:34:ILE:O	9:bM:38:LYS:NZ	2.38	0.56
20:cn:119:GLU:O	20:cn:123:ARG:N	2.38	0.56
21:ct:254:ASN:C	21:ct:256:ASN:H	2.12	0.56
21:cv:173:GLU:OE1	21:cv:173:GLU:N	2.39	0.56
1:ap:153:PHE:H	1:ap:156:ASN:HD21	1.52	0.56
14:bY:139:ALA:O	14:bY:140:ASP:C	2.44	0.56
2:by:371:PRO:HG2	19:ck:58:MET:HG2	1.88	0.56
19:cl:29:PRO:HG2	20:co:82:ARG:HH21	1.71	0.56
23:db:18:VAL:HG12	23:db:20:GLY:H	1.71	0.56
4:dl:108:ASP:OD2	4:dl:259:LYS:NZ	2.39	0.56
1:aS:125:ASP:OD1	1:aS:126:ARG:N	2.38	0.56
1:bp:125:ASP:OD1	1:bp:126:ARG:N	2.39	0.56
2:bx:61:SER:OG	2:bx:63:ASN:ND2	2.39	0.56
2:bx:370:HIS:ND1	2:bx:505:ASN:OD1	2.39	0.56
2:bB:229:VAL:O	2:bB:230:GLY:C	2.49	0.56
13:bS:29:THR:HG21	13:bS:37:ARG:HB3	1.85	0.56
21:cw:100:LEU:O	21:cw:147:HIS:ND1	2.37	0.56
5:de:271:PHE:CG	23:dh:9:ASN:ND2	2.74	0.56
1:aN:121:ARG:O	1:aN:126:ARG:NE	2.39	0.56
20:cn:120:LEU:HD12	20:cn:121:LEU:HD22	1.87	0.56
24:cS:245:THR:OG1	24:cS:400:ASN:ND2	2.38	0.56
1:bm:61:SER:OG	1:bm:63:ASN:ND2	2.39	0.55
1:bs:125:ASP:OD1	1:bs:126:ARG:N	2.39	0.55
13:bS:29:THR:CG2	13:bS:37:ARG:CB	2.83	0.55
18:ci:54:LYS:N	18:ci:55:PRO:CD	2.69	0.55
4:dp:84:PHE:CE1	4:dp:273:PHE:HE2	2.21	0.55
1:aa:169:GLN:HG3	13:bS:117:THR:C	2.31	0.55
5:bE:213:GLU:OE1	9:bO:64:LYS:NZ	2.40	0.55
21:cq:137:ASP:OD1	21:cq:138:GLU:N	2.39	0.55
25:cU:44:ILE:HG22	25:cV:39:GLY:HA2	1.88	0.55
5:cY:125:HIS:CE1	23:db:7:ASN:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:bF:43:ILE:HD13	4:bF:62:PHE:CB	2.35	0.55
11:bQ:57:ASP:OD2	11:bQ:171:LYS:NZ	2.39	0.55
18:ci:49:ASP:CB	18:ci:52:ALA:CB	2.75	0.55
21:cK:137:ASP:OD1	21:cK:138:GLU:N	2.40	0.55
24:cT:131:ASN:OD1	24:cT:132:PHE:N	2.40	0.55
25:cV:24:ILE:HA	25:cW:18:ALA:HB3	1.88	0.55
5:de:358:VAL:C	5:de:360:THR:N	2.61	0.55
4:dr:29:ARG:O	4:dr:30:ASN:C	2.49	0.55
1:bn:229:GLU:OE1	1:bn:419:LYS:NZ	2.40	0.55
22:cO:13:MET:HB2	22:cQ:19:VAL:HG22	1.88	0.55
25:cU:18:ALA:HB3	25:cW:24:ILE:HA	1.88	0.55
4:dp:136:ARG:HG3	22:ds:12:ILE:HD12	1.89	0.55
3:bC:36:PHE:CG	3:bC:37:TYR:N	2.74	0.55
1:bl:65:ASP:CG	8:bl:95:THR:HG22	2.31	0.55
1:br:62:ARG:NH2	8:bK:96:SER:OG	2.40	0.55
2:bu:471:ASN:OD1	2:bu:471:ASN:N	2.37	0.55
21:cs:122:GLN:NE2	21:cs:216:SER:OG	2.39	0.55
21:cN:137:ASP:OD1	21:cN:138:GLU:N	2.40	0.55
2:bu:9:VAL:HA	13:bS:160:VAL:HG11	1.89	0.55
14:bY:185:LYS:H	16:cg:32:TRP:HE1	1.54	0.55
19:cj:31:GLU:HB3	19:ck:32:ILE:HG22	1.87	0.55
4:df:29:ARG:O	4:df:30:ASN:C	2.49	0.55
2:bw:351:THR:O	2:bw:352:ALA:C	2.50	0.55
2:by:24:ILE:CG2	19:cj:59:TRP:CZ2	2.90	0.55
2:bz:15:ASP:CB	20:cn:55:GLU:HA	2.37	0.55
9:bL:25:PHE:C	9:bL:25:PHE:CD1	2.85	0.55
24:cR:131:ASN:OD1	24:cR:132:PHE:N	2.40	0.55
4:cX:15:ASP:O	4:cX:19:THR:N	2.39	0.55
5:de:358:VAL:C	5:de:360:THR:H	2.15	0.55
22:di:10:ASP:OD1	22:di:10:ASP:N	2.37	0.55
1:bm:375:ASP:OD1	1:bm:376:ASN:N	2.39	0.55
2:by:24:ILE:HG22	19:cj:59:TRP:CZ2	2.40	0.55
2:bB:112:TRP:O	2:bB:113:THR:C	2.50	0.55
1:aa:6:SER:C	20:co:64:ASP:HB2	2.32	0.55
1:aB:308:GLU:OE2	1:aD:145:LYS:NZ	2.40	0.55
1:aI:145:LYS:NZ	1:aJ:308:GLU:OE2	2.40	0.55
1:bp:371:PHE:O	8:bJ:76:ARG:NH2	2.40	0.55
2:by:220:GLU:HB3	2:bz:449:ARG:HG3	1.89	0.55
18:ci:49:ASP:CA	18:ci:52:ALA:HB3	2.37	0.55
21:cM:119:LYS:NZ	21:cM:141:ASP:OD2	2.40	0.55
1:bg:324:ASP:OD2	5:bE:103:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:by:471:ASN:N	2:by:471:ASN:OD1	2.37	0.54
23:db:8:TRP:CZ2	22:dc:13:MET:HE2	2.42	0.54
1:aF:257:HIS:O	1:aF:258:PRO:C	2.46	0.54
1:aQ:115:THR:OG1	1:aQ:265:ASN:ND2	2.35	0.54
2:bu:9:VAL:O	13:bS:160:VAL:CG1	2.56	0.54
3:bC:378:PHE:O	3:bC:379:ASP:CB	2.54	0.54
13:bS:154:LEU:HD23	18:ci:77:GLY:HA2	1.88	0.54
19:cl:23:GLU:HA	20:co:127:LEU:HD23	1.88	0.54
23:cP:32:ASN:HB3	22:cQ:28:PHE:H	1.72	0.54
5:de:356:ALA:O	5:de:368:LEU:HD13	2.06	0.54
22:ds:19:VAL:HG12	22:du:13:MET:HE3	1.89	0.54
20:co:106:THR:HB	20:co:126:ARG:HH22	1.72	0.54
5:dq:269:LEU:HB3	22:du:15:ARG:CD	2.27	0.54
1:ac:24:ILE:CB	19:cl:50:MET:HB2	2.35	0.54
1:as:327:ALA:O	1:as:329:ARG:NH1	2.41	0.54
1:ay:160:GLY:HA2	1:aA:26:PHE:O	2.07	0.54
1:bh:238:THR:HG22	1:bh:249:GLN:OE1	2.08	0.54
2:bu:9:VAL:HG13	13:bS:161:GLU:HA	1.90	0.54
18:ci:72:PRO:O	20:co:62:ALA:HA	2.07	0.54
21:cs:242:TRP:HE1	21:cs:337:ASN:HD21	1.55	0.54
4:cX:102:ILE:HG21	4:cX:105:ARG:HD3	1.89	0.54
2:bx:22:PRO:HB2	19:ck:41:LEU:CD2	2.36	0.54
24:cR:134:PRO:HA	25:cV:12:PHE:CZ	2.34	0.54
22:dg:37:GLN:NE2	23:dh:37:THR:OG1	2.35	0.54
1:ac:258:PRO:CG	19:cm:59:TRP:HB3	2.30	0.54
13:bS:27:ILE:HB	18:ci:20:ALA:CB	2.38	0.54
20:co:94:VAL:HG13	20:co:98:TRP:HZ3	1.72	0.54
5:cY:354:THR:O	5:cY:369:ALA:N	2.41	0.54
26:dn:32:GLY:HA3	26:do:30:LEU:HD21	1.89	0.54
26:do:25:VAL:HG12	26:do:27:VAL:HG13	1.90	0.54
1:bj:211:LEU:O	1:bj:216:ARG:NH1	2.41	0.54
19:cj:37:LEU:HD22	19:ck:36:TYR:HB3	1.90	0.54
21:cr:145:ASP:OD1	21:cr:146:ASP:N	2.41	0.54
21:cw:113:ASP:OD1	21:cw:114:LEU:N	2.39	0.54
23:db:10:PRO:CB	22:dc:17:MET:HA	2.38	0.54
1:aJ:235:GLY:O	1:aU:250:ASN:ND2	2.40	0.54
1:bh:94:GLN:O	1:bh:110:ASN:N	2.41	0.54
1:ah:123:ASN:CG	1:ah:124:ASP:H	2.16	0.54
1:ay:333:TYR:OH	1:ay:338:GLN:NE2	2.41	0.54
5:dq:269:LEU:CG	22:du:15:ARG:CD	2.82	0.54
1:aA:250:ASN:ND2	4:bD:229:ASN:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:dg:6:ASN:O	22:dg:8:LEU:N	2.41	0.54
26:dm:27:VAL:HA	26:dn:21:VAL:HG22	1.90	0.54
1:aa:6:SER:O	20:co:64:ASP:N	2.41	0.53
1:ar:238:THR:OG1	1:ar:383:TYR:OH	2.25	0.53
10:bP:34:GLY:O	10:bP:35:GLU:C	2.49	0.53
13:bS:148:LYS:HD2	20:co:56:LEU:HD11	1.91	0.53
23:cP:35:GLY:HA3	22:cQ:32:GLY:N	2.23	0.53
4:df:174:LYS:NZ	4:df:176:ASP:OD2	2.41	0.53
22:di:9:ASN:OD1	22:di:10:ASP:N	2.41	0.53
1:ak:333:TYR:OH	1:ak:338:GLN:NE2	2.41	0.53
1:at:125:ASP:OD1	1:at:126:ARG:N	2.39	0.53
1:bc:371:PHE:O	8:bJ:124:ARG:NH2	2.41	0.53
2:bx:25:THR:HG21	19:ck:45:ILE:HD11	1.91	0.53
2:bz:16:VAL:N	20:cn:54:LEU:O	2.36	0.53
21:cE:113:ASP:OD1	21:cE:114:LEU:N	2.42	0.53
1:ar:308:GLU:OE1	1:ar:336:LYS:NZ	2.41	0.53
2:by:27:PHE:CE2	2:bz:322:LEU:CD2	2.91	0.53
13:bS:30:ARG:O	13:bS:32:GLN:N	2.42	0.53
18:ci:68:THR:HG22	18:ci:75:VAL:O	2.09	0.53
22:dg:24:SER:HA	23:dh:29:ILE:HB	1.90	0.53
1:aj:207:ASP:C	1:aj:207:ASP:OD1	2.51	0.53
1:bk:384:LYS:NZ	1:bk:401:GLU:O	2.42	0.53
2:by:25:THR:OG1	19:cj:54:ILE:CD1	2.57	0.53
2:by:336:GLU:OE2	19:ck:50:MET:SD	2.67	0.53
8:bl:95:THR:HG22	8:bl:95:THR:O	2.08	0.53
21:cE:71:SER:OG	21:cE:319:SER:N	2.41	0.53
1:aa:8:LEU:CD1	20:co:70:ASN:HD21	2.21	0.53
1:ai:308:GLU:OE1	1:ai:336:LYS:NZ	2.41	0.53
1:av:333:TYR:OH	1:av:338:GLN:NE2	2.41	0.53
21:cr:113:ASP:OD1	21:cr:114:LEU:N	2.41	0.53
25:cV:30:ASP:HA	25:cW:24:ILE:O	2.08	0.53
4:cX:102:ILE:HG21	4:cX:105:ARG:CG	2.38	0.53
1:aS:324:ASP:OD2	1:bf:104:ARG:NH1	2.41	0.53
1:aT:400:THR:OG1	1:aV:144:GLN:OE1	2.25	0.53
25:cU:44:ILE:HD13	25:cV:35:ILE:HG12	1.91	0.53
1:aa:429:GLY:CA	13:bS:117:THR:CG2	2.59	0.53
1:aB:20:GLY:O	1:aB:21:ASN:C	2.51	0.53
1:aC:333:TYR:OH	1:aC:338:GLN:NE2	2.39	0.53
1:aJ:172:GLU:OE1	1:aJ:174:LYS:NZ	2.42	0.53
1:aK:327:ALA:O	1:aK:329:ARG:NH1	2.42	0.53
1:bo:252:ARG:NH1	1:bo:253:LEU:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bv:332:GLU:HB3	13:bS:6:LEU:CD1	2.38	0.53
5:bE:82:PHE:O	5:bE:87:GLN:NE2	2.42	0.53
13:bS:116:ALA:HB2	13:bS:127:ARG:HE	1.74	0.53
13:bS:192:LYS:NZ	13:bS:196:GLU:O	2.28	0.53
14:ca:156:THR:HG1	14:ca:160:TRP:CD1	2.26	0.53
20:co:94:VAL:H	20:co:95:GLN:NE2	2.07	0.53
4:dp:136:ARG:O	22:ds:12:ILE:CG2	2.56	0.53
1:ad:229:GLU:OE2	1:ad:260:LYS:NZ	2.40	0.53
2:bw:229:VAL:O	2:bw:230:GLY:C	2.50	0.53
25:cV:24:ILE:HG13	25:cV:28:ILE:HD12	1.91	0.53
23:db:8:TRP:CG	23:db:9:ASN:N	2.76	0.53
1:ac:33:ARG:NH2	20:co:64:ASP:O	2.34	0.53
1:aZ:371:PHE:O	8:bI:124:ARG:NH2	2.42	0.53
2:bv:508:ARG:NE	13:bS:185:PHE:CE2	2.74	0.53
19:cl:18:LEU:HD11	19:cm:18:LEU:HD12	1.91	0.53
21:cx:265:ASP:OD1	21:cx:266:THR:N	2.40	0.53
24:cT:85:GLU:OE1	24:cT:85:GLU:N	2.41	0.53
5:dq:120:ASP:C	5:dq:120:ASP:OD1	2.52	0.53
1:aa:170:TYR:CZ	13:bS:115:ASN:O	2.62	0.53
1:aa:170:TYR:HE1	13:bS:115:ASN:O	1.89	0.53
1:ah:122:MET:O	1:ah:123:ASN:C	2.52	0.53
1:aM:255:PHE:O	8:bI:129:ARG:NH1	2.42	0.53
1:bl:65:ASP:OD1	8:bI:95:THR:CG2	2.52	0.53
13:bS:124:ASN:O	13:bS:125:GLU:HB2	2.08	0.53
26:dm:29:TYR:CE1	26:dm:31:ILE:HG23	2.45	0.53
1:aa:103:GLN:HB2	13:bS:166:GLN:NE2	2.24	0.52
1:bn:21:ASN:O	1:bn:23:GLN:NE2	2.42	0.52
2:by:23:GLN:CG	19:cj:57:SER:OG	2.49	0.52
21:cw:295:ASN:O	21:cw:296:LYS:C	2.52	0.52
21:cx:113:ASP:OD1	21:cx:114:LEU:N	2.40	0.52
22:cO:20:TYR:O	22:cQ:26:THR:OG1	2.27	0.52
23:dh:18:VAL:HG22	23:dh:20:GLY:H	1.73	0.52
4:dr:108:ASP:OD2	4:dr:259:LYS:NZ	2.42	0.52
1:aa:7:GLN:HB2	20:co:54:LEU:CG	2.40	0.52
1:bh:166:ILE:O	1:bh:169:GLN:NE2	2.42	0.52
25:cV:43:LEU:HG	25:cW:34:VAL:HB	1.90	0.52
26:dm:33:ASN:HB3	26:dn:28:ASP:O	2.09	0.52
4:dp:137:PRO:N	22:ds:12:ILE:CD1	2.72	0.52
1:aF:325:ARG:HE	1:aG:7:GLN:CD	2.17	0.52
1:aU:107:LYS:NZ	1:aW:324:ASP:OD2	2.43	0.52
25:cU:24:ILE:HG21	25:cU:28:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:cX:82:ASN:HD22	4:cX:136:ARG:HB2	1.74	0.52
4:dp:138:GLU:HG3	23:dt:17:ILE:CD1	2.40	0.52
1:aH:256:ASN:O	1:aH:372:SER:N	2.42	0.52
1:bi:384:LYS:NZ	1:bi:401:GLU:O	2.42	0.52
2:bx:383:SER:OG	2:bx:391:THR:O	2.26	0.52
4:bD:185:ILE:H	4:bD:186:PRO:CD	2.22	0.52
24:cS:364:SER:OG	24:cT:141:ILE:O	2.26	0.52
22:ds:14:ILE:HG12	22:du:9:ASN:OD1	2.09	0.52
26:dm:24:ASN:HB3	26:do:29:TYR:HB3	1.91	0.52
4:dp:138:GLU:HG3	23:dt:17:ILE:HD11	1.90	0.52
1:aF:327:ALA:O	1:aF:329:ARG:NH1	2.43	0.52
11:bQ:125:TYR:CG	11:bQ:125:TYR:O	2.62	0.52
21:cB:145:ASP:OD1	21:cB:146:ASP:N	2.43	0.52
21:cN:113:ASP:OD1	21:cN:114:LEU:N	2.43	0.52
25:cU:28:ILE:HD11	25:cV:24:ILE:HG12	1.91	0.52
5:de:360:THR:O	5:de:360:THR:HG22	2.09	0.52
4:dl:242:ARG:NH1	4:dl:349:SER:OG	2.43	0.52
4:dr:271:TYR:HD2	23:dt:14:ARG:HD2	1.73	0.52
1:aQ:314:ASP:OD1	1:aQ:330:LYS:NZ	2.42	0.52
18:ci:49:ASP:N	18:ci:52:ALA:HB3	2.25	0.52
20:cn:115:VAL:HG13	20:cn:119:GLU:OE1	2.09	0.52
23:dh:11:PHE:HE1	22:di:18:ILE:HD12	1.74	0.52
1:bj:153:PHE:H	1:bj:156:ASN:HD21	1.58	0.52
1:bo:373:ARG:NH1	1:bp:11:TYR:O	2.42	0.52
5:bE:120:ASP:C	5:bE:120:ASP:OD1	2.53	0.52
21:cw:254:ASN:CG	21:cw:255:THR:H	2.17	0.52
1:bs:371:PHE:O	8:bK:76:ARG:NH2	2.43	0.52
21:cM:145:ASP:OD1	21:cM:146:ASP:N	2.43	0.52
24:cT:134:PRO:HA	25:cU:12:PHE:CZ	2.40	0.52
1:af:43:GLN:O	2:by:278:LYS:NZ	2.43	0.51
4:cX:82:ASN:OD1	22:dc:14:ILE:HD12	2.09	0.51
23:dt:24:VAL:HG22	22:du:29:THR:O	2.10	0.51
13:bS:63:ILE:HD11	19:cl:8:VAL:HG23	1.92	0.51
21:cC:137:ASP:OD1	21:cC:138:GLU:N	2.43	0.51
23:dh:9:ASN:HA	22:di:13:MET:HE1	1.93	0.51
4:dk:136:ARG:O	26:dn:14:ILE:HD11	2.10	0.51
26:dn:29:TYR:O	26:do:24:ASN:HA	2.09	0.51
1:bd:145:LYS:NZ	1:be:308:GLU:OE2	2.40	0.51
2:bz:292:CYS:SG	2:bz:293:ASN:N	2.82	0.51
2:bB:145:TYR:N	2:bB:146:PRO:HD2	2.25	0.51
21:cv:248:LYS:C	21:cv:250:TYR:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:cJ:265:ASP:OD1	21:cJ:266:THR:N	2.44	0.51
21:cK:145:ASP:OD1	21:cK:146:ASP:N	2.43	0.51
22:cQ:13:MET:SD	22:cQ:13:MET:N	2.84	0.51
5:de:103:LYS:NZ	5:de:105:ASP:OD2	2.44	0.51
22:dg:28:PHE:CG	22:di:23:LEU:HD23	2.46	0.51
1:aa:10:ALA:HB2	19:cm:37:LEU:CD2	2.32	0.51
1:ac:24:ILE:CG2	19:cl:50:MET:HB2	2.40	0.51
8:bJ:81:SER:O	8:bJ:82:GLU:C	2.53	0.51
20:cn:114:ARG:C	20:cn:115:VAL:HG23	2.36	0.51
22:cO:29:THR:HG22	23:cP:23:VAL:HA	1.93	0.51
1:as:125:ASP:OD1	1:as:126:ARG:N	2.43	0.51
21:cs:113:ASP:OD1	21:cs:114:LEU:N	2.43	0.51
21:cJ:248:LYS:C	21:cJ:250:TYR:H	2.19	0.51
25:cU:32:GLY:HA3	25:cV:26:ASN:HA	1.92	0.51
13:bS:19:ILE:O	13:bS:23:PRO:HD2	2.10	0.51
17:ch:71:ILE:O	17:ch:72:SER:CB	2.59	0.51
19:cl:16:ILE:HG13	20:co:133:ILE:HB	1.93	0.51
5:cY:120:ASP:C	5:cY:120:ASP:OD1	2.53	0.51
1:aa:7:GLN:CB	20:co:54:LEU:CG	2.88	0.51
1:aT:384:LYS:NZ	1:aT:401:GLU:O	2.43	0.51
2:bx:25:THR:HB	19:ck:41:LEU:HD11	1.92	0.51
21:cq:145:ASP:OD1	21:cq:146:ASP:N	2.43	0.51
24:cS:155:TYR:OH	24:cS:327:ASP:O	2.29	0.51
4:cZ:273:PHE:CD2	22:dc:9:ASN:ND2	2.79	0.51
1:as:329:ARG:HH21	1:au:41:SER:HB3	1.75	0.51
2:bx:322:LEU:HB3	2:bx:326:GLU:HB2	1.93	0.51
4:bF:43:ILE:HD12	4:bF:202:TYR:CD1	2.45	0.51
21:cI:145:ASP:OD1	21:cI:146:ASP:N	2.43	0.51
5:cY:246:ASN:O	5:cY:339:SER:N	2.44	0.51
22:da:19:VAL:HG12	22:dc:13:MET:HB2	1.92	0.51
1:ab:229:GLU:OE1	1:ab:419:LYS:NZ	2.44	0.51
1:bt:211:LEU:O	1:bt:216:ARG:NH2	2.44	0.51
21:cv:145:ASP:OD1	21:cv:146:ASP:N	2.42	0.51
23:dt:13:ASN:O	23:dt:14:ARG:CG	2.58	0.51
1:aa:8:LEU:HD13	20:co:70:ASN:CG	2.35	0.51
1:aa:430:MET:HE2	13:bS:170:MET:SD	2.51	0.51
1:ac:320:LEU:HD12	19:cm:64:ARG:HH21	1.65	0.51
1:ah:243:ALA:O	1:ah:244:THR:OG1	2.20	0.51
1:aC:20:GLY:O	1:aC:21:ASN:C	2.53	0.51
1:aI:116:TYR:OH	1:aI:157:GLN:NE2	2.42	0.51
2:bw:20:GLY:O	2:bw:21:ASN:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:bC:431:ASP:OD1	3:bC:432:ALA:N	2.43	0.51
5:bE:271:PHE:HB2	23:cP:9:ASN:HD22	1.75	0.51
11:bQ:179:THR:N	11:bQ:180:PRO:CD	2.74	0.51
4:cX:102:ILE:CG2	4:cX:105:ARG:CG	2.89	0.51
5:cY:271:PHE:HB2	22:da:9:ASN:HB2	1.93	0.51
4:cZ:135:PHE:CE1	4:cZ:147:PHE:CE1	2.99	0.51
5:de:356:ALA:C	5:de:368:LEU:HD22	2.35	0.51
1:aa:337:VAL:O	1:aa:338:GLN:C	2.53	0.50
1:am:43:GLN:HB2	1:am:205:TRP:CZ3	2.46	0.50
22:dg:6:ASN:O	22:dg:9:ASN:N	2.41	0.50
1:aC:114:ARG:NH2	1:aC:117:ASP:OD2	2.42	0.50
1:aH:252:ARG:NH1	1:aH:254:ASN:OD1	2.43	0.50
2:bu:465:ALA:O	2:bu:466:ASP:HB2	2.11	0.50
2:bA:448:VAL:O	3:bC:219:THR:OG1	2.29	0.50
18:ci:49:ASP:CB	18:ci:52:ALA:HB3	2.41	0.50
21:cz:113:ASP:OD1	21:cz:114:LEU:N	2.41	0.50
1:aL:21:ASN:O	1:aL:23:GLN:NE2	2.44	0.50
1:aM:62:ARG:NH2	1:aM:171:HIS:O	2.44	0.50
19:cj:12:LEU:O	19:cj:16:ILE:HG23	2.11	0.50
20:cn:88:LEU:HD23	20:cn:88:LEU:H	1.77	0.50
21:cx:173:GLU:OE1	21:cx:173:GLU:N	2.45	0.50
1:ac:321:ASN:ND2	19:cm:65:ARG:HH12	2.02	0.50
1:as:212:ASP:OD2	14:bY:203:LYS:NZ	2.39	0.50
1:aM:267:ASN:OD1	1:aM:415:ASN:ND2	2.43	0.50
1:aY:256:ASN:ND2	1:bj:321:ASN:O	2.44	0.50
1:bl:63:ASN:O	1:bl:208:TYR:HD2	1.91	0.50
2:bx:182:ASN:C	2:bx:182:ASN:OD1	2.55	0.50
20:co:104:ILE:HB	20:co:105:PRO:HD3	1.93	0.50
21:ct:305:SER:O	21:ct:307:VAL:N	2.44	0.50
1:be:151:LEU:O	1:be:156:ASN:ND2	2.45	0.50
1:bo:420:ASN:OD1	1:bo:421:TYR:N	2.42	0.50
20:co:95:GLN:HA	20:co:98:TRP:HE3	1.75	0.50
21:cp:145:ASP:OD1	21:cp:146:ASP:N	2.44	0.50
21:cx:167:ASP:C	21:cx:167:ASP:OD1	2.55	0.50
4:dk:206:ASP:OD1	4:dk:207:THR:N	2.45	0.50
4:dl:273:PHE:HD2	26:dm:12:PRO:HG3	1.77	0.50
1:aa:170:TYR:CE1	13:bS:115:ASN:HB3	2.46	0.50
2:bw:278:LYS:NZ	2:bx:346:GLY:O	2.44	0.50
2:by:24:ILE:HA	19:cj:54:ILE:CG1	2.41	0.50
3:bC:375:SER:O	3:bC:377:SER:N	2.44	0.50
5:bE:269:LEU:HD21	22:cO:16:THR:CB	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:bM:19:ASP:OD1	9:bM:21:LYS:NZ	2.41	0.50
21:ct:138:GLU:OE2	21:ct:193:LYS:NZ	2.42	0.50
21:cM:182:ASN:OD1	21:cM:183:THR:N	2.44	0.50
25:cU:31:ASN:O	25:cW:37:ALA:HB2	2.12	0.50
4:dr:180:ALA:O	4:dr:181:SER:C	2.55	0.50
1:aP:229:GLU:OE2	1:aP:260:LYS:NZ	2.44	0.50
1:aS:14:GLN:NE2	10:bP:133:SER:OG	2.44	0.50
3:bC:267:ASP:O	3:bC:268:THR:C	2.55	0.50
13:bS:27:ILE:HG21	18:ci:20:ALA:HB2	1.94	0.50
13:bS:29:THR:CG2	13:bS:37:ARG:CA	2.89	0.50
24:cR:85:GLU:OE1	24:cR:85:GLU:N	2.44	0.50
24:cT:270:PHE:CE2	24:cT:314:SER:HB3	2.47	0.50
4:cZ:180:ALA:O	4:cZ:181:SER:C	2.54	0.50
1:aa:7:GLN:O	20:co:54:LEU:CD1	2.60	0.50
1:aa:170:TYR:CG	13:bS:170:MET:HG3	2.47	0.50
1:bo:333:TYR:OH	1:bo:338:GLN:NE2	2.45	0.50
2:bx:274:TYR:OH	13:bS:154:LEU:CD1	2.60	0.50
2:by:23:GLN:C	19:cj:54:ILE:HG12	2.37	0.50
2:by:23:GLN:C	19:cj:54:ILE:CG1	2.85	0.50
20:co:88:LEU:HA	20:co:128:ARG:HH22	1.75	0.50
20:co:140:VAL:O	20:co:144:PHE:N	2.28	0.50
21:ct:305:SER:O	21:ct:306:CYS:C	2.54	0.50
21:cN:119:LYS:NZ	21:cN:141:ASP:OD2	2.44	0.50
22:da:13:MET:SD	22:da:17:MET:HE2	2.52	0.50
1:aa:8:LEU:CD1	20:co:70:ASN:CG	2.85	0.50
8:bI:94:GLY:O	8:bI:95:THR:HB	2.12	0.50
21:cr:87:LYS:NZ	21:cr:89:GLU:OE1	2.45	0.50
22:cO:27:TYR:OH	22:cQ:31:ASN:ND2	2.45	0.50
23:db:10:PRO:CB	22:dc:17:MET:CG	2.71	0.50
1:au:152:ILE:O	1:au:152:ILE:HG22	2.11	0.49
1:bn:229:GLU:OE2	1:bn:260:LYS:NZ	2.44	0.49
2:bv:24:ILE:HG21	18:ci:42:GLN:OE1	2.12	0.49
2:by:24:ILE:CG2	19:cj:59:TRP:HZ2	2.21	0.49
9:bM:34:ILE:O	9:bM:35:LYS:HB2	2.12	0.49
11:bQ:131:ASP:C	11:bQ:131:ASP:OD1	2.53	0.49
21:cs:305:SER:O	21:cs:306:CYS:C	2.55	0.49
21:cB:300:SER:OG	21:cB:302:GLN:NE2	2.45	0.49
21:cF:98:PRO:O	21:cF:99:SER:CB	2.59	0.49
24:cT:28:ARG:NH1	24:cT:29:ILE:O	2.46	0.49
4:dp:136:ARG:HG3	22:ds:12:ILE:HG21	1.94	0.49
1:bl:64:GLY:H	8:bI:95:THR:HB	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bv:32:ARG:NH1	18:ci:39:LYS:O	2.45	0.49
2:bv:514:GLY:O	13:bS:182:PHE:HZ	1.95	0.49
24:cS:230:ASN:O	24:cS:349:ASN:ND2	2.45	0.49
22:da:24:SER:HA	23:db:29:ILE:O	2.12	0.49
22:dg:17:MET:HA	22:di:11:PRO:HG2	1.94	0.49
1:aZ:215:GLU:OE1	21:cD:48:LYS:NZ	2.45	0.49
1:bk:94:GLN:O	1:bk:110:ASN:N	2.45	0.49
2:bv:92:ASN:O	2:bv:93:THR:HB	2.12	0.49
4:bF:43:ILE:CD1	4:bF:62:PHE:HB3	2.42	0.49
21:cB:173:GLU:OE1	21:cB:173:GLU:N	2.45	0.49
24:cS:85:GLU:OE1	24:cS:85:GLU:N	2.43	0.49
5:de:120:ASP:C	5:de:120:ASP:OD1	2.54	0.49
1:aa:430:MET:CE	13:bS:170:MET:SD	3.00	0.49
1:ab:16:VAL:CG1	13:bS:151:PHE:CE2	2.95	0.49
1:ac:333:TYR:OH	1:ac:338:GLN:NE2	2.45	0.49
1:ac:368:THR:HG21	19:cm:58:MET:CE	2.42	0.49
1:aU:125:ASP:OD1	1:aU:126:ARG:N	2.45	0.49
22:da:23:LEU:O	23:db:29:ILE:N	2.29	0.49
4:dp:90:TYR:CG	4:dp:90:TYR:O	2.64	0.49
1:aK:115:THR:OG1	1:aK:265:ASN:ND2	2.46	0.49
2:bA:390:VAL:O	2:bA:391:THR:OG1	2.21	0.49
2:bB:201:ILE:O	2:bB:341:GLN:NE2	2.44	0.49
18:ci:32:GLN:CG	18:ci:33:SER:N	2.73	0.49
21:cz:167:ASP:C	21:cz:167:ASP:OD1	2.54	0.49
21:cA:145:ASP:OD1	21:cA:146:ASP:N	2.46	0.49
21:cF:113:ASP:OD1	21:cF:114:LEU:N	2.43	0.49
21:cJ:173:GLU:OE1	21:cJ:173:GLU:N	2.45	0.49
23:db:10:PRO:HB3	22:dc:17:MET:HG3	1.93	0.49
22:dc:14:ILE:O	22:dc:14:ILE:HG12	2.11	0.49
1:ab:16:VAL:HG11	13:bS:151:PHE:CE2	2.48	0.49
1:ac:396:VAL:O	1:ac:399:ASN:ND2	2.45	0.49
1:az:43:GLN:HB2	1:az:205:TRP:CZ3	2.48	0.49
2:bw:370:HIS:ND1	2:bw:505:ASN:OD1	2.44	0.49
19:cj:13:PHE:O	19:cj:16:ILE:HG12	2.12	0.49
21:cz:123:ARG:O	21:cz:216:SER:OG	2.31	0.49
26:dm:20:VAL:HG13	26:dn:14:ILE:HG22	1.95	0.49
5:dq:325:GLU:OE1	4:dr:67:ARG:NH1	2.45	0.49
1:ac:227:LEU:HD22	19:cm:55:PHE:HZ	1.76	0.49
1:aj:124:ASP:OD2	1:ak:123:ASN:N	2.46	0.49
1:ay:340:TYR:OH	1:aA:121:ARG:NE	2.45	0.49
2:bB:112:TRP:CD1	2:bB:113:THR:HG1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:bS:148:LYS:CD	20:co:56:LEU:HD11	2.42	0.49
24:cS:131:ASN:OD1	24:cS:132:PHE:N	2.46	0.49
26:dn:17:GLN:NE2	26:dn:18:ASP:OD1	2.45	0.49
4:dp:118:GLU:OE2	4:dp:273:PHE:HD1	1.90	0.49
1:aM:166:ILE:O	1:aM:169:GLN:NE2	2.46	0.49
1:bo:374:ILE:O	8:bI:79:ARG:NH1	2.45	0.49
18:ci:33:SER:O	18:ci:35:TRP:CD1	2.66	0.49
21:cJ:145:ASP:OD1	21:cJ:146:ASP:N	2.44	0.49
1:an:327:ALA:O	1:an:329:ARG:NH1	2.45	0.49
2:bv:508:ARG:CB	13:bS:186:LEU:HG	2.42	0.49
2:bz:26:PHE:CG	2:bz:27:PHE:N	2.81	0.49
2:bB:20:GLY:O	2:bB:21:ASN:C	2.55	0.49
4:bD:137:PRO:HA	22:cQ:12:ILE:HD11	1.95	0.49
13:bS:101:LYS:HD3	13:bS:102:LYS:N	2.27	0.49
21:cs:145:ASP:OD1	21:cs:146:ASP:N	2.42	0.49
4:dp:136:ARG:CG	22:ds:12:ILE:HG21	2.43	0.49
5:dq:269:LEU:HD22	22:du:15:ARG:HD2	1.73	0.49
1:av:73:GLU:OE2	1:av:146:ARG:NH1	2.46	0.49
1:bq:65:ASP:OD1	1:bq:216:ARG:NH2	2.45	0.49
4:dl:138:GLU:HB2	26:do:14:ILE:HD13	1.94	0.49
1:ac:32:ARG:CZ	19:cl:46:ARG:O	2.61	0.48
1:aK:229:GLU:OE1	1:aK:419:LYS:NZ	2.46	0.48
1:aY:420:ASN:ND2	1:aY:421:TYR:O	2.46	0.48
1:be:212:ASP:C	1:be:212:ASP:OD1	2.56	0.48
1:br:123:ASN:CG	1:br:124:ASP:H	2.20	0.48
2:bu:9:VAL:CA	13:bS:160:VAL:HG13	2.43	0.48
2:bv:32:ARG:HD2	18:ci:38:ALA:HB1	1.93	0.48
2:by:256:LYS:NZ	2:bz:444:TYR:OH	2.46	0.48
26:dm:33:ASN:HB3	26:dn:29:TYR:HA	1.95	0.48
1:ab:17:TYR:HH	13:bS:150:LEU:HA	1.78	0.48
1:ag:257:HIS:HB3	1:ag:258:PRO:CD	2.43	0.48
1:am:436:ALA:O	1:am:437:ASN:HB2	2.13	0.48
2:bv:182:ASN:OD1	2:bv:183:GLY:N	2.46	0.48
5:bE:83:TYR:N	5:bE:84:PRO:HD3	2.28	0.48
9:bL:18:GLN:OE1	9:bL:18:GLN:N	2.46	0.48
19:cl:22:ASN:OD1	19:cm:22:ASN:ND2	2.43	0.48
21:cx:145:ASP:OD1	21:cx:146:ASP:N	2.42	0.48
4:dd:90:TYR:CG	4:dd:90:TYR:O	2.65	0.48
4:dj:7:GLN:OE1	4:dk:294:ARG:NH1	2.46	0.48
1:aa:131:ARG:NH2	1:ab:347:THR:O	2.44	0.48
5:bE:271:PHE:HD2	23:cP:9:ASN:HD22	1.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:bS:52:VAL:HG12	13:bS:61:TYR:CD2	2.48	0.48
13:bS:154:LEU:CD2	18:ci:77:GLY:HA2	2.43	0.48
24:cT:46:ASP:CG	24:cT:47:VAL:H	2.19	0.48
1:aV:321:ASN:ND2	1:aV:375:ASP:OD1	2.46	0.48
1:bl:73:GLU:OE2	1:bm:329:ARG:NH1	2.46	0.48
6:bG:133:VAL:O	6:bG:134:THR:HB	2.14	0.48
21:cN:265:ASP:OD1	21:cN:266:THR:N	2.42	0.48
23:db:10:PRO:CG	22:dc:17:MET:HB2	2.43	0.48
23:db:10:PRO:CG	22:dc:17:MET:CA	2.91	0.48
5:de:125:HIS:NE2	22:di:7:PRO:CD	2.76	0.48
22:du:23:LEU:HD23	22:du:24:SER:N	2.28	0.48
1:ay:67:ILE:O	1:ay:162:ALA:CB	2.58	0.48
1:bj:255:PHE:O	7:bH:325:ARG:NH2	2.46	0.48
1:bl:64:GLY:N	8:bl:95:THR:HB	2.28	0.48
7:bH:282:ALA:O	7:bH:284:THR:N	2.47	0.48
4:dr:275:ASN:ND2	22:ds:10:ASP:CB	2.77	0.48
1:at:256:ASN:HA	1:at:371:PHE:HB2	1.96	0.48
2:by:30:VAL:HG21	19:cj:52:SER:N	2.29	0.48
2:bA:465:ALA:O	2:bA:466:ASP:HB3	2.13	0.48
3:bC:92:THR:H	7:bH:222:PRO:CB	2.27	0.48
5:bE:82:PHE:CG	5:bE:270:TYR:CE2	3.01	0.48
20:co:102:THR:O	20:co:106:THR:OG1	2.21	0.48
21:cy:145:ASP:OD1	21:cy:146:ASP:N	2.42	0.48
24:cS:357:ILE:HA	24:cS:361:PHE:CD2	2.48	0.48
24:cT:134:PRO:CA	25:cU:12:PHE:CZ	2.95	0.48
4:cZ:364:TYR:CD2	4:cZ:365:ASN:O	2.67	0.48
4:dd:276:ASN:HD22	5:de:136:SER:HG	1.60	0.48
4:df:273:PHE:HD2	22:dg:9:ASN:ND2	2.11	0.48
1:aa:5:LEU:C	1:aa:5:LEU:HD12	2.38	0.48
1:aL:121:ARG:NE	1:aM:340:TYR:OH	2.47	0.48
1:bp:238:THR:OG1	1:bp:383:TYR:OH	2.31	0.48
13:bS:39:ASN:O	13:bS:43:ARG:HG2	2.13	0.48
23:cP:35:GLY:HA3	22:cQ:32:GLY:H	1.78	0.48
23:dt:9:ASN:OD1	22:du:15:ARG:NH2	2.43	0.48
1:ap:229:GLU:OE2	1:ap:260:LYS:NZ	2.45	0.48
1:bh:43:GLN:NE2	1:bh:203:SER:OG	2.46	0.48
2:bv:20:GLY:O	2:bv:21:ASN:C	2.57	0.48
2:bw:336:GLU:OE1	18:ci:51:ALA:HB2	2.13	0.48
13:bS:27:ILE:HG21	13:bS:44:LEU:HD13	1.94	0.48
22:dg:27:TYR:HB3	22:di:22:ASN:OD1	2.14	0.48
1:aa:207:ASP:C	1:aa:207:ASP:OD1	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ai:125:ASP:OD1	1:ai:126:ARG:N	2.46	0.48
2:by:24:ILE:CD1	19:cj:51:PRO:CB	2.91	0.48
13:bS:159:GLU:HB3	13:bS:164:GLN:HE22	1.79	0.48
19:cj:14:THR:HG23	19:ck:14:THR:OG1	2.14	0.48
21:cG:265:ASP:OD1	21:cG:266:THR:N	2.45	0.48
23:db:9:ASN:OD1	23:db:10:PRO:HD2	2.14	0.48
4:dk:65:LEU:HA	4:dk:163:LEU:O	2.14	0.48
1:aq:375:ASP:OD1	1:aq:376:ASN:N	2.47	0.48
3:bC:267:ASP:OD1	3:bC:268:THR:N	2.47	0.48
20:cn:114:ARG:O	20:cn:115:VAL:CG2	2.61	0.48
21:cp:101:TYR:OH	21:cp:145:ASP:N	2.46	0.48
22:cO:23:LEU:HB3	22:cQ:28:PHE:HD1	1.79	0.48
23:dh:12:PHE:CG	23:dh:16:ILE:HD11	2.49	0.48
1:aj:110:ASN:O	1:aj:272:TYR:OH	2.24	0.47
1:az:90:GLU:O	1:az:110:ASN:ND2	2.47	0.47
1:bh:65:ASP:OD2	8:bK:117:ARG:NH2	2.47	0.47
2:bw:176:ALA:O	2:bw:178:LEU:N	2.47	0.47
2:bx:121:GLN:O	2:bx:122:TYR:C	2.56	0.47
21:cy:137:ASP:OD1	21:cy:138:GLU:N	2.47	0.47
1:ab:325:ARG:CZ	1:ac:4:GLY:HA2	2.44	0.47
1:bb:102:GLY:C	1:bl:63:ASN:ND2	2.71	0.47
2:bz:265:LEU:O	2:bz:266:TYR:C	2.52	0.47
4:bF:43:ILE:CD1	4:bF:62:PHE:CB	2.92	0.47
20:cn:114:ARG:C	20:cn:115:VAL:CG2	2.87	0.47
20:co:99:GLU:HG3	20:co:128:ARG:HH11	1.79	0.47
21:ct:248:LYS:C	21:ct:250:TYR:H	2.22	0.47
21:cE:75:ILE:HB	21:cE:206:TYR:CE2	2.48	0.47
21:cF:69:ASN:O	21:cF:70:ASN:HB3	2.14	0.47
21:cK:265:ASP:OD1	21:cK:266:THR:N	2.44	0.47
24:cR:134:PRO:C	25:cV:12:PHE:CE1	2.92	0.47
1:am:110:ASN:OD1	1:am:111:ASP:N	2.47	0.47
21:cy:262:LYS:O	21:cy:263:ASN:HB2	2.14	0.47
24:cS:99:GLU:OE1	24:cS:102:LYS:NZ	2.36	0.47
24:cT:357:ILE:HA	24:cT:361:PHE:CD2	2.49	0.47
4:dd:272:PRO:O	4:dd:273:PHE:C	2.57	0.47
5:de:354:THR:HG21	5:de:366:GLU:CD	2.39	0.47
22:dg:10:ASP:O	22:dg:12:ILE:N	2.47	0.47
1:aa:7:GLN:CA	20:co:64:ASP:HB2	2.44	0.47
1:aI:90:GLU:OE1	1:aI:114:ARG:HD2	2.14	0.47
1:bd:87:TYR:H	1:bd:134:ASP:CG	2.22	0.47
1:bf:121:ARG:NE	1:bg:340:TYR:OH	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:by:329:ARG:CG	19:ck:42:ASP:OD1	2.62	0.47
14:cd:145:ALA:N	14:cd:146:PRO:CD	2.76	0.47
20:co:95:GLN:HA	20:co:98:TRP:CE3	2.49	0.47
21:cN:145:ASP:OD1	21:cN:146:ASP:N	2.47	0.47
1:ac:214:GLN:NE2	19:cm:42:ASP:OD2	2.38	0.47
1:ao:125:ASP:OD1	1:ao:126:ARG:N	2.48	0.47
1:aH:325:ARG:NH1	1:aJ:39:ILE:O	2.46	0.47
1:aU:238:THR:OG1	1:aU:383:TYR:OH	2.27	0.47
5:bE:82:PHE:HB2	5:bE:270:TYR:OH	2.15	0.47
21:cx:216:SER:OG	21:cx:217:HIS:N	2.44	0.47
26:dn:33:ASN:O	26:do:29:TYR:CD2	2.68	0.47
2:bv:33:ARG:HD2	18:ci:53:TRP:NE1	2.29	0.47
2:by:506:ILE:HD11	19:ck:58:MET:HE1	1.96	0.47
2:bz:26:PHE:O	2:bz:27:PHE:HB2	2.14	0.47
21:cF:145:ASP:OD1	21:cF:146:ASP:N	2.45	0.47
1:ac:222:LEU:HD21	19:cm:46:ARG:NE	2.30	0.47
1:al:203:SER:OG	1:al:205:TRP:NE1	2.47	0.47
1:ap:153:PHE:O	1:ap:154:PHE:C	2.57	0.47
1:ay:212:ASP:OD1	1:ay:213:THR:N	2.47	0.47
1:aF:47:ASN:N	1:aF:57:SER:O	2.47	0.47
1:aH:309:GLN:OE1	1:aJ:145:LYS:NZ	2.43	0.47
1:aV:21:ASN:O	1:aV:23:GLN:NE2	2.47	0.47
1:bg:257:HIS:CD2	1:bh:14:GLN:HE22	2.33	0.47
2:by:333:ILE:HD11	19:ck:46:ARG:CD	2.35	0.47
4:bD:138:GLU:HB2	23:cP:17:ILE:HG21	1.96	0.47
7:bH:552:THR:HG22	7:bH:553:ASP:H	1.80	0.47
10:bP:99:ARG:NH1	10:bP:100:VAL:O	2.48	0.47
11:bQ:92:ALA:H	11:bQ:93:PRO:HD3	1.79	0.47
13:bS:28:PRO:HD3	18:ci:20:ALA:HB1	1.93	0.47
13:bS:56:ARG:HD2	18:ci:9:ILE:HD11	1.94	0.47
20:co:84:THR:O	20:co:88:LEU:CB	2.63	0.47
20:co:99:GLU:HG3	20:co:128:ARG:NH1	2.30	0.47
20:co:137:VAL:HA	20:co:140:VAL:HG22	1.97	0.47
21:ct:50:PHE:CG	21:ct:51:LYS:N	2.82	0.47
21:cC:112:PHE:O	21:cC:226:THR:N	2.48	0.47
21:cE:285:TYR:O	21:cE:287:ASN:ND2	2.48	0.47
24:cR:312:ALA:O	24:cS:128:ARG:NH1	2.48	0.47
5:cY:356:ALA:O	5:cY:357:ASN:HB3	2.15	0.47
23:db:10:PRO:HG2	22:dc:16:THR:O	2.14	0.47
4:dj:68:LYS:NZ	4:dj:201:ASP:OD2	2.34	0.47
4:dj:131:ARG:O	4:dj:145:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aU:43:GLN:NE2	1:aU:203:SER:OG	2.48	0.47
1:bp:422:ASN:ND2	1:bp:435:TYR:O	2.47	0.47
2:bu:20:GLY:O	2:bu:21:ASN:C	2.55	0.47
2:bu:441:VAL:O	2:bu:442:GLN:C	2.56	0.47
3:bC:145:PHE:CD1	3:bC:299:ILE:HD11	2.50	0.47
5:bE:82:PHE:CG	5:bE:270:TYR:CZ	3.03	0.47
21:cz:63:SER:OG	21:cz:64:LEU:N	2.47	0.47
21:cA:157:SER:OG	21:cA:160:THR:OG1	2.33	0.47
21:cE:265:ASP:OD1	21:cE:266:THR:N	2.46	0.47
4:cX:102:ILE:CG2	4:cX:105:ARG:HG2	2.45	0.47
23:db:8:TRP:CD1	23:db:9:ASN:H	2.32	0.47
5:de:83:TYR:N	5:de:84:PRO:HD3	2.30	0.47
1:ab:73:GLU:CD	1:ab:146:ARG:HH11	2.23	0.47
1:aH:256:ASN:OD1	1:aH:257:HIS:N	2.48	0.47
1:aT:345:GLY:O	1:aV:128:ASN:ND2	2.46	0.47
2:bw:465:ALA:O	2:bw:466:ASP:HB2	2.15	0.47
2:bx:229:VAL:O	2:bx:230:GLY:C	2.57	0.47
18:ci:54:LYS:HB3	18:ci:55:PRO:HD3	1.97	0.47
21:cD:235:LEU:H	21:cD:259:VAL:CG2	2.28	0.47
21:cD:265:ASP:OD1	21:cD:266:THR:N	2.48	0.47
1:ab:42:ILE:CD1	1:ab:63:ASN:HD22	2.28	0.47
1:ac:227:LEU:HD13	19:cm:55:PHE:CZ	2.50	0.47
18:ci:49:ASP:O	18:ci:53:TRP:N	2.48	0.47
20:cn:96:ASP:OD2	20:cn:129:GLY:N	2.48	0.47
24:cT:91:LEU:HD13	24:cT:106:PHE:CD1	2.49	0.47
1:ar:267:ASN:OD1	1:ar:415:ASN:ND2	2.48	0.46
1:aU:47:ASN:N	1:aU:57:SER:O	2.38	0.46
2:bu:5:ILE:CD1	13:bS:166:GLN:HE21	2.26	0.46
2:bu:182:ASN:OD1	2:bu:183:GLY:N	2.48	0.46
24:cS:46:ASP:CG	24:cS:47:VAL:H	2.22	0.46
25:cV:24:ILE:HG21	25:cV:28:ILE:HB	1.96	0.46
1:aI:87:TYR:N	1:aI:88:PRO:HD3	2.29	0.46
2:bx:22:PRO:O	19:ck:41:LEU:CD2	2.60	0.46
18:ci:32:GLN:CG	18:ci:33:SER:H	2.16	0.46
21:cp:63:SER:OG	21:cp:64:LEU:N	2.49	0.46
4:dp:36:SER:N	5:dq:24:LYS:O	2.49	0.46
5:dq:125:HIS:NE2	22:du:7:PRO:HD2	2.29	0.46
1:ae:373:ARG:NH1	14:bV:168:SER:OG	2.49	0.46
1:am:375:ASP:OD1	1:am:376:ASN:N	2.49	0.46
1:bl:144:GLN:OE1	1:bm:400:THR:OG1	2.31	0.46
2:bu:292:CYS:SG	2:bu:293:ASN:N	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bv:406:ALA:O	2:bv:407:THR:C	2.57	0.46
2:bw:123:SER:OG	2:bw:124:ASN:N	2.48	0.46
3:bC:248:PHE:C	3:bC:250:CYS:H	2.22	0.46
4:bD:93:TYR:C	4:bD:93:TYR:CD1	2.93	0.46
5:bE:25:THR:HG22	5:bE:27:PHE:H	1.80	0.46
19:cl:58:MET:C	20:co:53:SER:OG	2.58	0.46
21:cF:97:ALA:HB1	21:cF:98:PRO:HD2	1.97	0.46
21:cM:63:SER:OG	21:cM:64:LEU:N	2.48	0.46
22:cO:13:MET:HE3	22:cO:14:ILE:N	2.30	0.46
4:dd:275:ASN:ND2	22:di:7:PRO:HD2	2.30	0.46
4:dk:364:TYR:CD2	4:dk:365:ASN:O	2.69	0.46
1:as:172:GLU:OE1	1:as:172:GLU:N	2.47	0.46
1:ay:154:PHE:CZ	1:ay:161:LEU:HD22	2.51	0.46
1:aD:61:SER:OG	1:aD:63:ASN:OD1	2.23	0.46
3:bC:411:TYR:CD1	3:bC:411:TYR:C	2.93	0.46
21:cC:113:ASP:OD1	21:cC:114:LEU:N	2.46	0.46
4:df:228:TYR:OH	4:df:230:ASN:ND2	2.48	0.46
22:ds:9:ASN:OD1	23:dt:13:ASN:ND2	2.41	0.46
1:ac:368:THR:HG21	19:cm:58:MET:HE3	1.98	0.46
1:al:308:GLU:OE2	1:al:336:LYS:NZ	2.49	0.46
1:aA:109:TYR:O	1:aA:112:TRP:N	2.49	0.46
1:bb:238:THR:HG23	1:bb:414:LEU:HB3	1.95	0.46
2:bB:8:LEU:O	3:bC:129:ASN:ND2	2.48	0.46
21:cG:63:SER:OG	21:cG:64:LEU:N	2.49	0.46
26:dn:20:VAL:HG13	26:do:14:ILE:HG22	1.98	0.46
1:be:125:ASP:OD1	1:be:126:ARG:N	2.49	0.46
2:bu:9:VAL:CG1	13:bS:161:GLU:HA	2.45	0.46
2:bx:471:ASN:OD1	2:bx:471:ASN:N	2.41	0.46
4:bF:137:PRO:HA	23:cP:11:PHE:CZ	2.47	0.46
25:cU:13:PHE:HB2	25:cW:17:PHE:O	2.16	0.46
4:cX:93:TYR:CD1	4:cX:93:TYR:C	2.94	0.46
5:de:294:LYS:NZ	4:df:44:GLU:OE2	2.43	0.46
1:aa:7:GLN:HB3	20:co:54:LEU:CD1	2.31	0.46
1:aa:7:GLN:HB3	20:co:54:LEU:CD2	2.31	0.46
1:ad:68:THR:OG1	1:ad:209:ILE:HG12	2.15	0.46
1:aA:314:ASP:OD2	1:aA:330:LYS:NZ	2.48	0.46
1:aE:43:GLN:HB2	1:aE:205:TRP:CZ3	2.51	0.46
2:by:229:VAL:O	2:by:230:GLY:C	2.57	0.46
2:bB:379:TYR:CZ	2:bB:381:ALA:HB3	2.51	0.46
8:bI:94:GLY:O	8:bI:95:THR:CB	2.63	0.46
21:cI:63:SER:OG	21:cI:64:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:do:27:VAL:HG23	26:do:27:VAL:O	2.15	0.46
1:ab:20:GLY:O	1:ab:21:ASN:C	2.57	0.46
1:ab:257:HIS:O	1:ab:258:PRO:C	2.56	0.46
1:aB:33:ARG:NE	1:aD:20:GLY:O	2.49	0.46
1:aF:20:GLY:O	1:aG:33:ARG:NE	2.47	0.46
1:aI:333:TYR:OH	1:aI:338:GLN:NE2	2.49	0.46
1:bb:109:TYR:O	1:bb:112:TRP:N	2.49	0.46
1:bm:68:THR:O	1:bm:156:ASN:ND2	2.46	0.46
2:bx:449:ARG:HG3	2:bz:220:GLU:HB3	1.98	0.46
13:bS:88:ALA:HB2	13:bS:102:LYS:HE3	1.98	0.46
18:ci:12:MET:O	18:ci:16:PHE:CD2	2.69	0.46
21:cq:118:GLU:OE2	21:cq:193:LYS:NZ	2.47	0.46
21:cr:63:SER:OG	21:cr:64:LEU:N	2.49	0.46
21:cs:173:GLU:N	21:cs:173:GLU:OE1	2.47	0.46
21:cu:220:VAL:N	21:cu:299:ILE:O	2.47	0.46
21:cL:263:ASN:HB3	21:cL:267:ALA:CA	2.43	0.46
25:cW:35:ILE:HD11	25:cW:38:GLY:HA2	1.98	0.46
22:da:27:TYR:O	22:dc:22:ASN:HA	2.16	0.46
4:dp:138:GLU:OE1	23:dt:17:ILE:CD1	2.63	0.46
1:aC:39:ILE:O	1:aD:325:ARG:NH2	2.48	0.46
1:aD:94:GLN:O	1:aD:110:ASN:N	2.49	0.46
1:aU:62:ARG:NH1	7:bH:310:ASP:OD2	2.49	0.46
2:bx:292:CYS:SG	2:bx:293:ASN:N	2.89	0.46
2:bA:58:VAL:HG11	2:bA:315:LEU:HD21	1.97	0.46
4:bD:122:ASP:C	4:bD:122:ASP:OD1	2.58	0.46
14:cc:133:LYS:O	14:cc:134:PRO:C	2.58	0.46
21:cG:215:TYR:O	21:cG:215:TYR:CD1	2.68	0.46
26:do:11:ASP:N	26:do:12:PRO:CD	2.79	0.46
1:ao:265:ASN:OD1	1:ao:267:ASN:ND2	2.49	0.46
1:aE:153:PHE:H	1:aE:156:ASN:HD21	1.62	0.46
1:aY:242:SER:OG	1:aY:243:ALA:N	2.49	0.46
1:aZ:314:ASP:OD2	1:aZ:330:LYS:NZ	2.43	0.46
1:bo:242:SER:OG	1:bo:243:ALA:N	2.49	0.46
2:bx:379:TYR:CZ	2:bx:381:ALA:HB3	2.51	0.46
6:bG:236:SER:HA	6:bG:314:ILE:O	2.16	0.46
17:ch:32:VAL:O	17:ch:59:ASN:ND2	2.48	0.46
21:cD:63:SER:OG	21:cD:64:LEU:N	2.49	0.46
25:cU:11:TYR:CD2	25:cW:15:ASP:HB2	2.51	0.46
25:cU:35:ILE:HA	25:cW:44:ILE:HB	1.98	0.46
1:aa:8:LEU:HB3	20:co:55:GLU:OE2	2.16	0.45
1:ac:370:ASN:ND2	1:ac:372:SER:OG	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aj:333:TYR:OH	1:aj:338:GLN:NE2	2.49	0.45
1:aA:257:HIS:O	1:aA:258:PRO:C	2.59	0.45
1:aZ:308:GLU:OE2	1:aZ:336:LYS:NZ	2.46	0.45
2:bv:514:GLY:O	13:bS:182:PHE:CZ	2.70	0.45
2:bA:226:ASN:O	2:bA:230:GLY:N	2.46	0.45
9:bL:33:PHE:O	9:bL:34:ILE:HB	2.17	0.45
13:bS:152:ARG:NE	13:bS:159:GLU:OE2	2.47	0.45
21:cy:246:ASP:OD1	21:cy:247:SER:N	2.48	0.45
21:cA:63:SER:OG	21:cA:64:LEU:N	2.49	0.45
21:cD:145:ASP:OD1	21:cD:146:ASP:N	2.45	0.45
22:cO:20:TYR:HB2	23:cP:13:ASN:O	2.16	0.45
24:cR:166:GLN:OE1	24:cR:166:GLN:N	2.44	0.45
1:ac:370:ASN:ND2	19:cm:59:TRP:CB	2.58	0.45
1:aQ:52:PHE:CE1	1:aQ:200:PRO:HD3	2.51	0.45
1:bf:21:ASN:O	1:bf:23:GLN:NE2	2.49	0.45
2:bv:327:ARG:CZ	13:bS:168:TYR:CD2	2.99	0.45
21:cL:112:PHE:O	21:cL:226:THR:N	2.50	0.45
22:cO:23:LEU:HD13	22:cQ:28:PHE:HE1	1.81	0.45
4:df:275:ASN:CG	22:dg:6:ASN:CG	2.83	0.45
5:dq:83:TYR:N	5:dq:84:PRO:HD3	2.31	0.45
1:al:375:ASP:OD2	1:al:376:ASN:ND2	2.50	0.45
1:aw:87:TYR:N	1:aw:88:PRO:HD3	2.31	0.45
2:bx:274:TYR:OH	13:bS:154:LEU:HD11	2.17	0.45
2:by:465:ALA:O	2:by:466:ASP:HB2	2.16	0.45
20:cn:51:VAL:HG13	20:cn:52:GLY:N	2.31	0.45
21:cw:63:SER:OG	21:cw:64:LEU:N	2.49	0.45
22:da:8:LEU:HD13	22:da:8:LEU:HA	1.78	0.45
22:di:23:LEU:HD21	22:di:28:PHE:HZ	1.81	0.45
26:do:29:TYR:HE1	26:do:31:ILE:CG2	2.28	0.45
23:dt:14:ARG:O	23:dt:15:SER:OG	2.34	0.45
1:ac:225:GLU:HG2	1:ac:425:ARG:HG2	1.98	0.45
1:ae:211:LEU:O	1:ae:216:ARG:NH2	2.50	0.45
1:ai:242:SER:OG	1:ai:243:ALA:N	2.49	0.45
1:aG:212:ASP:OD1	1:aG:213:THR:N	2.49	0.45
1:bl:65:ASP:OD1	8:bI:95:THR:O	2.34	0.45
2:bz:19:THR:OG1	19:cj:58:MET:HB3	2.15	0.45
18:ci:49:ASP:C	18:ci:52:ALA:HB3	2.41	0.45
19:cl:11:LEU:HA	19:cm:11:LEU:HD21	1.98	0.45
21:cq:113:ASP:OD1	21:cq:114:LEU:N	2.47	0.45
21:cJ:329:ILE:HG23	21:cJ:330:TRP:N	2.30	0.45
1:ab:87:TYR:N	1:ab:88:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ac:435:TYR:HE2	19:cm:59:TRP:CZ2	2.34	0.45
1:ao:130:ARG:NH2	1:ao:301:GLY:O	2.49	0.45
1:aL:333:TYR:OH	1:aL:338:GLN:NE2	2.49	0.45
1:aQ:337:VAL:O	1:aQ:338:GLN:C	2.58	0.45
2:bu:241:TRP:NE1	2:bu:244:SER:OG	2.49	0.45
2:bz:379:TYR:CZ	2:bz:381:ALA:HB3	2.52	0.45
3:bC:174:ILE:O	3:bC:236:THR:OG1	2.34	0.45
21:cv:63:SER:OG	21:cv:64:LEU:N	2.49	0.45
23:db:16:ILE:O	23:db:17:ILE:HD13	2.16	0.45
4:df:271:TYR:CB	23:dh:14:ARG:HE	2.28	0.45
1:ax:87:TYR:N	1:ax:88:PRO:HD3	2.32	0.45
1:ax:108:HIS:HD1	1:ax:112:TRP:CD1	2.34	0.45
1:aE:436:ALA:O	1:aE:437:ASN:HB2	2.17	0.45
1:aK:117:ASP:OD2	1:aK:129:TYR:CE2	2.69	0.45
3:bC:212:ASP:OD1	3:bC:247:LYS:NZ	2.34	0.45
21:cJ:63:SER:OG	21:cJ:64:LEU:N	2.49	0.45
1:aN:95:ASP:OD2	1:aN:107:LYS:NZ	2.50	0.45
2:bx:85:THR:N	2:bx:86:PRO:CD	2.80	0.45
3:bC:257:LYS:H	3:bC:259:GLN:HE22	1.65	0.45
4:dk:357:ALA:O	4:dk:372:SER:N	2.48	0.45
22:ds:36:THR:HG1	22:du:32:GLY:H	1.63	0.45
1:aa:8:LEU:C	20:co:54:LEU:HD12	2.42	0.45
1:an:124:ASP:OD1	1:ao:346:VAL:N	2.49	0.45
1:aF:169:GLN:O	7:bH:277:ASN:ND2	2.50	0.45
1:aL:95:ASP:OD2	1:aL:107:LYS:NZ	2.46	0.45
1:aQ:329:ARG:NH1	1:aS:205:TRP:CD2	2.84	0.45
1:br:110:ASN:OD1	1:br:111:ASP:N	2.50	0.45
2:bu:382:ALA:C	2:bu:384:ASN:H	2.25	0.45
2:bv:274:TYR:CZ	13:bS:172:VAL:HG21	2.50	0.45
3:bC:408:VAL:O	3:bC:409:GLN:C	2.59	0.45
14:cc:151:ALA:O	14:cc:152:GLN:HB2	2.17	0.45
17:ch:138:MET:O	17:ch:139:SER:C	2.56	0.45
19:cj:30:ARG:HG2	19:cj:30:ARG:HH11	1.81	0.45
20:co:95:GLN:H	20:co:95:GLN:CD	2.25	0.45
22:cO:35:LEU:O	22:cO:36:THR:OG1	2.29	0.45
25:cV:23:ASN:N	25:cW:16:ILE:O	2.50	0.45
4:df:271:TYR:CB	23:dh:14:ARG:NE	2.79	0.45
1:aW:325:ARG:NH2	1:aY:39:ILE:O	2.49	0.45
1:bd:136:VAL:O	1:bd:136:VAL:HG12	2.16	0.45
1:bs:123:ASN:OD1	1:bs:124:ASP:N	2.50	0.45
2:bz:15:ASP:CB	20:cn:54:LEU:O	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:bD:65:LEU:HA	4:bD:163:LEU:O	2.17	0.45
5:bE:82:PHE:CE1	5:bE:270:TYR:CD1	3.05	0.45
13:bS:51:ALA:O	13:bS:55:ILE:HG12	2.17	0.45
21:cv:161:PRO:HD2	21:cv:195:ILE:O	2.17	0.45
21:cy:75:ILE:HB	21:cy:206:TYR:CE2	2.52	0.45
4:dp:84:PHE:CZ	4:dp:272:PRO:HB3	2.51	0.45
1:aa:87:TYR:N	1:aa:88:PRO:HD3	2.32	0.45
1:aa:103:GLN:HE22	1:aa:433:LEU:H	1.64	0.45
1:aq:110:ASN:OD1	1:aq:111:ASP:N	2.50	0.45
1:ba:373:ARG:O	8:bJ:131:GLN:NE2	2.49	0.45
1:bm:207:ASP:OD2	1:bn:341:GLN:NE2	2.49	0.45
2:bu:16:VAL:HG21	18:ci:57:TYR:CB	2.41	0.45
2:bx:10:SER:O	2:bx:11:TYR:C	2.59	0.45
2:bz:12:GLY:CA	20:cn:55:GLU:OE2	2.61	0.45
8:bI:132:ILE:HG13	8:bI:133:ASP:N	2.32	0.45
13:bS:119:GLY:HA2	13:bS:122:LEU:HD12	1.98	0.45
14:cd:135:SER:N	14:cd:136:PRO:CD	2.80	0.45
21:cB:263:ASN:C	21:cB:263:ASN:OD1	2.59	0.45
22:da:17:MET:HB3	23:db:22:LEU:HD13	1.99	0.45
22:dg:28:PHE:HB3	22:di:23:LEU:CB	2.41	0.45
4:dk:298:ARG:NH2	4:dl:42:SER:O	2.50	0.45
1:aa:95:ASP:OD2	1:aa:107:LYS:NZ	2.47	0.44
1:aa:338:GLN:N	1:aa:339:PRO:HD2	2.33	0.44
1:aj:257:HIS:O	1:aj:258:PRO:C	2.60	0.44
1:aq:61:SER:OG	1:aK:174:LYS:NZ	2.50	0.44
1:aq:396:VAL:O	1:aq:399:ASN:ND2	2.49	0.44
1:aJ:20:GLY:O	1:aJ:21:ASN:C	2.60	0.44
1:bc:436:ALA:O	1:bc:437:ASN:ND2	2.50	0.44
1:bl:371:PHE:O	7:bH:327:ARG:NH1	2.49	0.44
19:cj:30:ARG:CZ	20:cn:81:LYS:HD2	2.48	0.44
21:cs:263:ASN:O	21:cs:263:ASN:ND2	2.50	0.44
21:cw:91:ASN:O	21:cw:92:ARG:HB3	2.17	0.44
21:cB:113:ASP:OD1	21:cB:114:LEU:N	2.49	0.44
21:cG:101:TYR:CE1	21:cG:103:ILE:O	2.70	0.44
21:cI:265:ASP:OD1	21:cI:266:THR:N	2.47	0.44
23:dh:13:ASN:O	22:di:20:TYR:HB2	2.17	0.44
4:dk:93:TYR:CD1	4:dk:93:TYR:C	2.95	0.44
1:au:375:ASP:OD2	1:au:376:ASN:ND2	2.50	0.44
1:aD:256:ASN:HD21	4:bF:290:ASN:HB3	1.81	0.44
1:bb:242:SER:OG	1:bb:243:ALA:N	2.50	0.44
1:bt:238:THR:OG1	1:bt:383:TYR:OH	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bz:16:VAL:HG22	20:cn:56:LEU:HD23	1.88	0.44
3:bC:378:PHE:O	3:bC:379:ASP:HB3	2.17	0.44
21:ct:91:ASN:O	21:ct:92:ARG:HB2	2.17	0.44
21:cv:223:VAL:HG22	21:cv:224:SER:N	2.33	0.44
5:cY:107:PHE:CZ	5:cY:111:CYS:SG	3.10	0.44
1:ac:400:THR:OG1	1:ac:401:GLU:N	2.50	0.44
1:aM:242:SER:OG	1:aM:243:ALA:N	2.50	0.44
1:aT:126:ARG:NH1	1:aT:346:VAL:O	2.49	0.44
2:bu:9:VAL:O	13:bS:160:VAL:HG13	2.18	0.44
2:bu:449:ARG:HG3	2:bw:220:GLU:HB3	2.00	0.44
2:by:24:ILE:CA	19:cj:54:ILE:CG1	2.95	0.44
6:bG:86:GLN:OE1	6:bG:86:GLN:N	2.47	0.44
21:cr:138:GLU:CD	21:cr:193:LYS:HZ1	2.26	0.44
21:cJ:237:ARG:NH1	21:cJ:255:THR:O	2.51	0.44
24:cS:245:THR:CB	24:cS:400:ASN:HD22	2.30	0.44
4:cZ:47:ILE:HG22	4:cZ:49:VAL:H	1.82	0.44
4:cZ:135:PHE:CZ	4:cZ:145:ARG:HB2	2.53	0.44
1:ac:25:THR:O	19:cl:50:MET:CG	2.65	0.44
1:ax:242:SER:OG	1:ax:243:ALA:N	2.50	0.44
1:aB:242:SER:OG	1:aB:243:ALA:N	2.50	0.44
1:aO:375:ASP:OD1	8:bK:163:ARG:NH2	2.51	0.44
1:bh:122:MET:O	1:bh:126:ARG:N	2.40	0.44
2:bB:145:TYR:HB2	2:bB:146:PRO:CD	2.48	0.44
20:co:124:ASP:O	20:co:126:ARG:HG3	2.17	0.44
21:ct:113:ASP:OD1	21:ct:114:LEU:N	2.51	0.44
21:cu:265:ASP:OD1	21:cu:266:THR:N	2.47	0.44
21:cw:157:SER:O	21:cw:158:GLU:C	2.58	0.44
4:dp:273:PHE:O	22:du:9:ASN:ND2	2.50	0.44
1:ag:325:ARG:NH1	1:ai:39:ILE:O	2.49	0.44
1:aH:242:SER:OG	1:aH:243:ALA:N	2.50	0.44
1:bg:300:TYR:O	1:bg:303:THR:OG1	2.32	0.44
20:cn:57:ASN:OD1	20:cn:58:ASN:N	2.51	0.44
21:cs:230:ASP:OD1	21:cs:230:ASP:N	2.51	0.44
4:cX:138:GLU:CB	22:da:18:ILE:CD1	2.95	0.44
22:dc:14:ILE:O	22:dc:14:ILE:HG23	2.17	0.44
1:aB:205:TRP:CE2	1:aC:329:ARG:NH1	2.86	0.44
1:aD:330:LYS:O	1:aD:333:TYR:HB2	2.18	0.44
1:aF:124:ASP:OD2	1:aG:123:ASN:N	2.46	0.44
1:aF:154:PHE:CB	1:aF:229:GLU:H	2.31	0.44
1:aR:229:GLU:OE2	1:aR:260:LYS:NZ	2.49	0.44
2:bu:433:ARG:HB2	2:bu:438:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bv:351:THR:O	2:bv:352:ALA:C	2.59	0.44
2:by:85:THR:HB	2:by:86:PRO:CD	2.47	0.44
2:bB:79:LEU:HD23	2:bB:79:LEU:H	1.82	0.44
7:bH:514:LEU:HD23	7:bH:517:ASN:ND2	2.31	0.44
9:bN:33:PHE:O	9:bN:34:ILE:HB	2.18	0.44
19:cj:30:ARG:HG2	19:cj:30:ARG:NH1	2.33	0.44
19:ck:39:ARG:HG2	19:ck:39:ARG:NH1	2.33	0.44
21:cw:295:ASN:O	21:cw:297:TRP:N	2.51	0.44
21:cH:63:SER:OG	21:cH:64:LEU:N	2.50	0.44
22:cO:8:LEU:HA	23:cP:8:TRP:CZ3	2.53	0.44
5:de:355:ALA:CB	5:de:360:THR:HG21	2.12	0.44
1:ad:110:ASN:OD1	1:ad:111:ASP:N	2.50	0.44
1:al:52:PHE:CE1	1:al:200:PRO:HD3	2.53	0.44
1:aQ:62:ARG:NH2	1:aQ:168:LEU:O	2.51	0.44
1:bd:256:ASN:OD1	8:bK:127:ARG:NH2	2.44	0.44
1:bh:110:ASN:OD1	1:bh:111:ASP:N	2.48	0.44
1:bn:62:ARG:NH2	1:bn:168:LEU:O	2.50	0.44
2:bu:406:ALA:O	2:bu:407:THR:C	2.61	0.44
13:bS:123:ASP:N	13:bS:123:ASP:OD1	2.50	0.44
21:cp:188:ASP:OD1	21:cp:188:ASP:N	2.48	0.44
21:ct:283:PRO:C	21:ct:285:TYR:H	2.25	0.44
22:cO:8:LEU:HD23	22:cQ:11:PRO:HA	1.99	0.44
23:cP:22:LEU:HD13	22:cQ:17:MET:HB3	1.99	0.44
1:ay:155:PHE:HA	1:ay:161:LEU:O	2.18	0.44
1:aJ:114:ARG:NH2	1:aJ:117:ASP:OD2	2.51	0.44
1:aR:14:GLN:O	1:aR:17:TYR:CE2	2.71	0.44
1:bo:211:LEU:O	1:bo:216:ARG:NH2	2.51	0.44
1:br:123:ASN:CG	1:br:124:ASP:N	2.75	0.44
2:bA:406:ALA:O	2:bA:407:THR:C	2.59	0.44
7:bH:461:ASP:OD1	7:bH:462:HIS:N	2.50	0.44
14:bY:135:SER:N	14:bY:136:PRO:HD2	2.32	0.44
18:ci:26:LYS:HZ3	18:ci:28:GLN:HG3	1.75	0.44
19:cj:62:ASP:OD1	19:cj:63:THR:N	2.48	0.44
20:cn:114:ARG:O	20:cn:115:VAL:HG22	2.17	0.44
21:ct:306:CYS:SG	21:ct:307:VAL:N	2.91	0.44
21:cJ:281:VAL:O	21:cJ:281:VAL:HG12	2.18	0.44
24:cS:250:TYR:C	24:cS:250:TYR:CD1	2.95	0.44
24:cT:169:GLU:OE1	24:cT:169:GLU:N	2.45	0.44
22:da:16:THR:HG23	23:db:21:ASN:O	2.18	0.44
1:aL:252:ARG:NH1	1:aL:253:LEU:O	2.51	0.44
1:bo:205:TRP:CE2	1:bp:329:ARG:NH1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bv:121:GLN:O	2:bv:122:TYR:C	2.60	0.44
2:by:20:GLY:O	2:by:21:ASN:C	2.60	0.44
2:bz:229:VAL:O	2:bz:230:GLY:C	2.60	0.44
2:bB:182:ASN:OD1	2:bB:183:GLY:N	2.51	0.44
2:bB:369:ASN:OD1	2:bB:370:HIS:N	2.49	0.44
3:bC:317:ARG:NH1	11:bQ:200:ILE:O	2.45	0.44
21:cD:215:TYR:O	21:cD:215:TYR:CD1	2.71	0.44
21:cH:79:GLU:OE1	21:cH:79:GLU:N	2.51	0.44
22:cO:13:MET:HE3	22:cO:14:ILE:H	1.83	0.44
23:cP:27:GLY:O	22:cQ:22:ASN:HA	2.18	0.44
23:db:8:TRP:HA	23:db:8:TRP:HE3	1.83	0.44
4:dj:271:TYR:CZ	26:dm:17:GLN:CB	3.01	0.44
22:ds:17:MET:HB2	23:dt:22:LEU:HD12	1.99	0.44
1:aA:216:ARG:NH1	14:bZ:156:THR:O	2.51	0.43
1:bc:146:ARG:NH2	1:bd:401:GLU:OE1	2.50	0.43
2:bv:37:PHE:CD2	2:bv:37:PHE:C	2.95	0.43
2:bx:274:TYR:CG	18:ci:61:LEU:HD23	2.53	0.43
11:bQ:204:VAL:O	11:bQ:204:VAL:HG12	2.17	0.43
18:ci:35:TRP:HA	18:ci:36:PRO:HD3	1.81	0.43
18:ci:61:LEU:O	18:ci:62:GLY:C	2.60	0.43
20:co:106:THR:OG1	20:co:126:ARG:NH1	2.49	0.43
21:cq:220:VAL:N	21:cq:299:ILE:O	2.51	0.43
21:cz:145:ASP:OD1	21:cz:146:ASP:N	2.44	0.43
21:cK:215:TYR:CG	21:cK:215:TYR:O	2.71	0.43
1:am:205:TRP:CE3	1:an:329:ARG:NH2	2.86	0.43
1:aD:212:ASP:OD1	1:aD:213:THR:N	2.50	0.43
1:aQ:229:GLU:OE2	1:aQ:260:LYS:NZ	2.41	0.43
1:bd:338:GLN:N	1:bd:339:PRO:HD2	2.33	0.43
1:bl:373:ARG:O	7:bH:328:THR:CG2	2.66	0.43
1:bs:52:PHE:CE1	1:bs:200:PRO:HD3	2.53	0.43
1:bt:21:ASN:O	1:bt:23:GLN:NE2	2.51	0.43
3:bC:409:GLN:N	3:bC:410:PRO:CD	2.82	0.43
7:bH:564:LYS:O	7:bH:567:GLN:HG2	2.17	0.43
9:bN:30:ILE:O	9:bN:34:ILE:N	2.51	0.43
10:bP:6:SER:O	10:bP:7:ALA:HB3	2.18	0.43
13:bS:152:ARG:CZ	18:ci:75:VAL:CG1	2.96	0.43
13:bS:162:ASN:OD1	13:bS:164:GLN:NE2	2.52	0.43
21:cx:138:GLU:OE2	21:cx:193:LYS:NZ	2.51	0.43
21:cD:173:GLU:CD	21:cD:173:GLU:N	2.76	0.43
21:cE:263:ASN:HB3	21:cE:267:ALA:HA	1.99	0.43
24:cS:341:ASP:CG	24:cS:342:MET:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:da:37:GLN:NE2	23:db:36:LEU:O	2.51	0.43
5:de:297:GLU:OE1	5:de:297:GLU:N	2.50	0.43
4:df:90:TYR:O	4:df:90:TYR:CG	2.70	0.43
4:dl:138:GLU:N	26:do:14:ILE:HD13	2.33	0.43
26:dm:21:VAL:CG1	26:dn:15:VAL:HB	2.37	0.43
1:aq:213:THR:O	1:aq:214:GLN:C	2.60	0.43
1:au:69:ASP:OD1	1:au:70:ILE:N	2.52	0.43
1:ax:110:ASN:OD1	1:ax:111:ASP:N	2.51	0.43
1:bd:266:PHE:O	1:bd:275:TYR:HA	2.19	0.43
1:bg:257:HIS:CG	1:bh:14:GLN:HE22	2.37	0.43
1:bo:73:GLU:HA	1:bo:147:PHE:O	2.19	0.43
1:br:314:ASP:O	1:br:331:GLY:N	2.47	0.43
2:bu:9:VAL:HG22	13:bS:160:VAL:HG22	2.01	0.43
13:bS:38:ILE:O	13:bS:42:VAL:HG23	2.18	0.43
14:ca:176:ASP:OD1	14:ca:177:LEU:N	2.48	0.43
14:cb:176:ASP:OD1	14:cb:177:LEU:N	2.50	0.43
14:cc:130:LEU:O	14:cc:131:LEU:HB2	2.19	0.43
19:cj:41:LEU:HB2	19:cj:61:VAL:HG23	2.00	0.43
21:cr:79:GLU:OE1	21:cr:79:GLU:N	2.51	0.43
21:cw:199:ASP:OD1	21:cw:199:ASP:N	2.51	0.43
21:cy:113:ASP:OD1	21:cy:114:LEU:N	2.47	0.43
21:cz:265:ASP:OD1	21:cz:266:THR:N	2.49	0.43
21:cF:173:GLU:OE1	21:cF:173:GLU:N	2.51	0.43
24:cS:269:THR:O	24:cS:271:VAL:HG13	2.18	0.43
24:cT:172:LEU:HD23	24:cT:172:LEU:C	2.43	0.43
4:df:180:ALA:O	4:df:181:SER:C	2.60	0.43
26:dm:33:ASN:HB2	26:dn:28:ASP:O	2.17	0.43
1:ac:320:LEU:CD1	19:cm:64:ARG:HH21	2.26	0.43
1:ag:242:SER:OG	1:ag:243:ALA:N	2.50	0.43
1:al:14:GLN:O	1:al:17:TYR:CE2	2.72	0.43
1:aK:436:ALA:O	1:aK:437:ASN:HB2	2.18	0.43
1:aY:130:ARG:O	1:aY:134:ASP:N	2.51	0.43
2:bv:25:THR:HG22	2:bv:27:PHE:H	1.83	0.43
2:bA:53:GLY:N	2:bA:284:ASN:O	2.52	0.43
3:bC:114:ASN:N	3:bC:115:PRO:HD3	2.34	0.43
5:bE:156:ASP:O	5:bE:157:THR:C	2.62	0.43
21:cC:230:ASP:OD1	21:cC:230:ASP:N	2.51	0.43
21:cD:167:ASP:C	21:cD:167:ASP:OD1	2.61	0.43
21:cE:248:LYS:C	21:cE:250:TYR:H	2.26	0.43
21:cH:145:ASP:OD1	21:cH:146:ASP:N	2.45	0.43
26:dm:20:VAL:HG22	26:dn:14:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aj:153:PHE:H	1:aj:156:ASN:HD21	1.67	0.43
1:am:41:SER:CB	1:an:329:ARG:HH21	2.31	0.43
1:am:436:ALA:O	1:am:437:ASN:ND2	2.52	0.43
1:ao:171:HIS:CD2	1:ao:431:GLY:H	2.37	0.43
1:aE:9:VAL:O	1:aE:11:TYR:N	2.51	0.43
1:aM:43:GLN:HB2	1:aM:205:TRP:CZ3	2.53	0.43
1:aW:229:GLU:OE2	1:aW:260:LYS:NZ	2.48	0.43
1:bm:110:ASN:OD1	1:bm:111:ASP:N	2.51	0.43
2:by:506:ILE:CD1	19:ck:58:MET:HE1	2.48	0.43
2:bA:79:LEU:H	2:bA:79:LEU:HG	1.69	0.43
13:bS:18:VAL:HG22	20:co:115:VAL:HA	1.99	0.43
14:bX:176:ASP:OD1	14:bX:177:LEU:N	2.52	0.43
14:bY:145:ALA:O	14:bY:147:LYS:N	2.52	0.43
18:ci:51:ALA:O	18:ci:55:PRO:HD3	2.19	0.43
19:ck:39:ARG:HG2	19:ck:39:ARG:HH11	1.82	0.43
21:cs:265:ASP:OD1	21:cs:266:THR:N	2.47	0.43
21:cE:145:ASP:OD1	21:cE:146:ASP:N	2.48	0.43
23:cP:8:TRP:O	23:cP:8:TRP:CD1	2.71	0.43
4:cX:203:VAL:HG11	5:cY:27:PHE:CZ	2.54	0.43
4:dd:36:SER:N	5:de:24:LYS:O	2.50	0.43
5:dq:269:LEU:CD1	22:du:15:ARG:CD	2.95	0.43
4:dr:77:LYS:NZ	4:dr:139:ASP:OD1	2.38	0.43
22:ds:27:TYR:CD1	23:dt:32:ASN:HB2	2.54	0.43
1:aa:7:GLN:HB3	20:co:54:LEU:CG	2.48	0.43
1:ab:16:VAL:HG11	13:bS:151:PHE:CZ	2.54	0.43
1:aE:122:MET:O	1:aE:124:ASP:N	2.50	0.43
1:aQ:110:ASN:CG	1:aQ:111:ASP:N	2.77	0.43
1:bh:207:ASP:C	1:bh:207:ASP:OD1	2.62	0.43
1:bs:110:ASN:OD1	1:bs:111:ASP:N	2.52	0.43
21:cH:161:PRO:HD2	21:cH:195:ILE:O	2.18	0.43
21:cN:305:SER:O	21:cN:306:CYS:C	2.61	0.43
24:cR:201:PHE:CD1	24:cS:4:ILE:HD11	2.53	0.43
4:cX:102:ILE:HG21	4:cX:105:ARG:HG2	1.98	0.43
23:db:22:LEU:HD23	22:dc:28:PHE:CE2	2.54	0.43
23:dh:23:VAL:HG22	22:di:29:THR:OG1	2.19	0.43
1:al:110:ASN:O	1:al:272:TYR:OH	2.33	0.43
1:am:229:GLU:OE2	1:am:260:LYS:NZ	2.50	0.43
1:aG:267:ASN:OD1	1:aG:415:ASN:ND2	2.52	0.43
1:aQ:110:ASN:CG	1:aQ:111:ASP:H	2.27	0.43
1:aS:102:GLY:O	1:bc:63:ASN:ND2	2.50	0.43
2:bu:385:TYR:C	2:bu:385:TYR:CD1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bw:85:THR:N	2:bw:86:PRO:HD2	2.34	0.43
2:bw:184:ILE:HG23	2:bw:185:GLY:N	2.34	0.43
11:bQ:179:THR:HB	11:bQ:180:PRO:HD3	2.00	0.43
13:bS:14:GLN:OE1	13:bS:16:LEU:HG	2.18	0.43
13:bS:27:ILE:HB	18:ci:20:ALA:HB1	2.00	0.43
20:co:94:VAL:HG13	20:co:98:TRP:CZ3	2.52	0.43
21:cw:145:ASP:OD1	21:cw:146:ASP:N	2.43	0.43
21:cC:167:ASP:OD1	21:cC:191:HIS:ND1	2.44	0.43
24:cS:169:GLU:OE1	24:cS:169:GLU:N	2.49	0.43
24:cT:238:THR:CG2	24:cT:347:TYR:CZ	3.02	0.43
4:dd:364:TYR:CE2	4:dd:365:ASN:O	2.72	0.43
1:aa:427:MET:CE	13:bS:146:PHE:CD1	2.80	0.43
1:ac:337:VAL:O	1:ac:338:GLN:C	2.61	0.43
1:au:43:GLN:HB2	1:au:205:TRP:CZ3	2.54	0.43
1:aU:229:GLU:OE2	1:aU:260:LYS:NZ	2.51	0.43
1:ba:422:ASN:OD1	1:ba:422:ASN:C	2.62	0.43
1:bo:212:ASP:C	1:bo:212:ASP:OD1	2.62	0.43
2:bB:145:TYR:HB2	2:bB:146:PRO:HD3	2.00	0.43
20:cn:54:LEU:HD12	20:cn:55:GLU:N	2.33	0.43
21:cs:167:ASP:C	21:cs:167:ASP:OD1	2.61	0.43
21:cL:216:SER:OG	21:cL:217:HIS:N	2.52	0.43
1:aa:429:GLY:HA2	13:bS:117:THR:HG21	1.88	0.43
1:ap:242:SER:OG	1:ap:243:ALA:N	2.51	0.43
1:as:338:GLN:NE2	1:as:355:SER:OG	2.52	0.43
1:aB:39:ILE:O	1:aC:325:ARG:NH2	2.49	0.43
1:aJ:110:ASN:O	1:aJ:111:ASP:HB2	2.19	0.43
1:aU:109:TYR:O	1:aU:112:TRP:N	2.51	0.43
1:bi:52:PHE:CE1	1:bi:200:PRO:HD3	2.53	0.43
2:bv:429:ARG:O	2:bw:3:GLY:HA2	2.19	0.43
2:bz:15:ASP:HB3	20:cn:55:GLU:HA	2.01	0.43
9:bN:40:TYR:CD1	9:bN:40:TYR:C	2.96	0.43
13:bS:92:ILE:HG12	13:bS:94:PRO:CD	2.48	0.43
21:cp:264:PRO:HG2	21:cp:265:ASP:H	1.84	0.43
21:cs:167:ASP:OD2	21:cs:191:HIS:NE2	2.50	0.43
23:cP:32:ASN:CG	23:cP:33:GLY:N	2.77	0.43
24:cT:88:ILE:HG12	24:cT:176:PHE:CE1	2.54	0.43
4:cX:102:ILE:HG21	4:cX:105:ARG:CD	2.49	0.43
5:dq:156:ASP:O	5:dq:157:THR:C	2.62	0.43
22:du:14:ILE:O	22:du:15:ARG:HG3	2.19	0.43
1:ad:41:SER:CB	1:ae:329:ARG:HH21	2.32	0.43
1:am:114:ARG:NH2	1:am:117:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ar:43:GLN:HB2	1:ar:205:TRP:CZ3	2.54	0.43
1:aw:122:MET:SD	1:aw:345:GLY:HA3	2.59	0.43
1:az:264:TRP:HA	1:az:415:ASN:O	2.19	0.43
1:aZ:4:GLY:N	1:ba:40:GLU:OE1	2.51	0.43
1:bb:9:VAL:O	1:bb:11:TYR:N	2.51	0.43
1:bc:109:TYR:O	1:bc:112:TRP:N	2.51	0.43
2:bA:420:VAL:HG22	2:bA:438:PHE:CE2	2.54	0.43
6:bG:104:LEU:HB3	6:bG:105:PRO:HD3	2.01	0.43
21:cK:220:VAL:N	21:cK:299:ILE:O	2.51	0.43
21:cL:126:THR:O	21:cL:127:GLU:C	2.60	0.43
24:cR:238:THR:CG2	24:cR:347:TYR:CZ	3.02	0.43
24:cT:91:LEU:CD1	24:cT:106:PHE:CD1	3.02	0.43
24:cT:250:TYR:CD1	24:cT:250:TYR:C	2.96	0.43
22:da:8:LEU:HD13	22:dc:8:LEU:HD12	2.00	0.43
26:dn:31:ILE:O	26:dn:31:ILE:HG23	2.18	0.43
1:ab:95:ASP:C	1:ab:95:ASP:OD1	2.62	0.42
1:bb:121:ARG:O	1:bb:126:ARG:NH2	2.52	0.42
3:bC:392:ASN:O	3:bC:393:SER:HB2	2.19	0.42
19:cj:42:ASP:OD1	19:cj:46:ARG:NH1	2.38	0.42
21:cw:248:LYS:C	21:cw:250:TYR:H	2.27	0.42
21:cG:160:THR:O	21:cG:160:THR:HG23	2.19	0.42
21:cL:75:ILE:HB	21:cL:206:TYR:CE2	2.53	0.42
21:cM:91:ASN:O	21:cM:92:ARG:HB2	2.19	0.42
24:cT:156:LEU:C	24:cT:156:LEU:HD12	2.44	0.42
4:dj:159:ALA:O	4:dk:28:TRP:NE1	2.52	0.42
26:dn:26:PHE:O	26:do:21:VAL:HG22	2.19	0.42
4:dp:180:ALA:O	4:dp:181:SER:C	2.61	0.42
5:dq:356:ALA:O	5:dq:357:ASN:HB2	2.19	0.42
1:aa:218:ARG:NE	19:cl:54:ILE:HG12	2.26	0.42
1:aL:69:ASP:OD1	1:aL:70:ILE:N	2.52	0.42
2:bu:145:TYR:CD1	2:bu:145:TYR:C	2.94	0.42
2:bz:100:SER:C	2:bz:102:VAL:H	2.26	0.42
3:bC:252:LYS:O	3:bC:253:ARG:HB2	2.19	0.42
7:bH:436:ASP:OD1	7:bH:436:ASP:N	2.52	0.42
14:bW:174:ASN:H	14:bW:199:ASN:ND2	2.18	0.42
21:cr:265:ASP:OD1	21:cr:266:THR:N	2.47	0.42
21:cy:112:PHE:O	21:cy:226:THR:N	2.52	0.42
21:cI:248:LYS:C	21:cI:250:TYR:H	2.27	0.42
24:cS:241:ASP:OD1	24:cS:242:LEU:N	2.52	0.42
4:cX:180:ALA:O	4:cX:181:SER:C	2.61	0.42
4:dk:157:ASP:OD1	4:dk:158:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ah:123:ASN:ND2	1:ah:124:ASP:H	2.17	0.42
1:au:43:GLN:NE2	1:au:203:SER:OG	2.51	0.42
1:aD:96:VAL:HA	1:aD:176:TYR:O	2.20	0.42
1:aN:110:ASN:OD1	1:aN:111:ASP:N	2.52	0.42
1:aO:110:ASN:OD1	1:aO:111:ASP:N	2.51	0.42
1:bd:41:SER:OG	1:be:329:ARG:NH2	2.48	0.42
1:br:327:ALA:O	1:br:329:ARG:NH1	2.53	0.42
13:bS:130:ALA:HB3	13:bS:173:THR:HG21	2.01	0.42
21:cv:123:ARG:HB3	21:cv:217:HIS:O	2.20	0.42
21:cv:297:TRP:HE1	21:cv:299:ILE:HG13	1.83	0.42
21:cy:75:ILE:HB	21:cy:206:TYR:CZ	2.54	0.42
21:cA:265:ASP:OD1	21:cA:266:THR:N	2.47	0.42
1:ab:161:LEU:O	1:ab:162:ALA:C	2.61	0.42
1:ah:321:ASN:N	1:ah:376:ASN:O	2.51	0.42
1:am:131:ARG:NH1	1:an:347:THR:O	2.53	0.42
1:as:329:ARG:NH2	1:au:41:SER:HB3	2.34	0.42
1:aw:130:ARG:NH2	1:aw:301:GLY:O	2.52	0.42
1:aA:25:THR:HG22	1:aA:27:PHE:H	1.84	0.42
1:aA:211:LEU:O	1:aA:216:ARG:NH2	2.49	0.42
1:aO:39:ILE:O	1:aP:325:ARG:NH2	2.49	0.42
1:aQ:36:ASN:OD1	1:aQ:37:PHE:N	2.53	0.42
1:aR:52:PHE:CE1	1:aR:200:PRO:HD3	2.54	0.42
1:bc:368:THR:O	1:bd:7:GLN:NE2	2.52	0.42
1:bd:87:TYR:N	1:bd:88:PRO:HD3	2.34	0.42
2:bx:338:LEU:HB3	2:bz:31:TYR:CD2	2.55	0.42
2:bz:379:TYR:CG	2:bz:416:VAL:HG11	2.55	0.42
8:bK:130:THR:O	8:bK:134:ASP:N	2.49	0.42
19:cl:49:GLU:O	19:cl:50:MET:HE2	2.19	0.42
19:cm:19:ILE:O	19:cm:23:GLU:HG3	2.19	0.42
21:cy:63:SER:OG	21:cy:64:LEU:N	2.52	0.42
21:cB:118:GLU:OE1	21:cB:118:GLU:N	2.52	0.42
21:cG:305:SER:O	21:cG:306:CYS:C	2.61	0.42
24:cR:169:GLU:OE1	24:cR:169:GLU:N	2.47	0.42
5:dq:297:GLU:OE1	5:dq:297:GLU:N	2.50	0.42
1:ac:258:PRO:CG	19:cm:59:TRP:CE3	2.94	0.42
1:af:300:TYR:O	1:af:303:THR:OG1	2.29	0.42
1:am:321:ASN:N	1:am:376:ASN:O	2.52	0.42
1:as:123:ASN:N	1:as:125:ASP:OD1	2.52	0.42
1:aH:329:ARG:NH1	1:aJ:205:TRP:CD2	2.87	0.42
1:aW:25:THR:HG22	1:aW:27:PHE:H	1.84	0.42
1:bc:123:ASN:N	1:be:124:ASP:OD2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bm:205:TRP:CE2	1:bn:329:ARG:NH1	2.87	0.42
2:bx:241:TRP:HE1	2:bx:244:SER:H	1.67	0.42
3:bC:3:PRO:O	3:bC:4:THR:C	2.63	0.42
13:bS:91:ASN:HB3	13:bS:180:THR:HG21	2.02	0.42
14:bV:186:ALA:O	14:bV:187:ASP:C	2.62	0.42
18:ci:12:MET:O	18:ci:16:PHE:HD2	2.03	0.42
20:cn:74:LYS:O	20:cn:78:GLU:HB2	2.19	0.42
21:cA:182:ASN:ND2	21:cA:184:GLY:O	2.53	0.42
25:cU:22:GLY:HA2	25:cV:16:ILE:HG23	2.01	0.42
4:df:274:GLU:CD	23:dh:14:ARG:HH22	2.27	0.42
1:aa:68:THR:HG1	1:aa:69:ASP:H	1.68	0.42
1:ab:86:TYR:O	1:ab:87:TYR:C	2.62	0.42
1:av:325:ARG:NH2	1:aw:7:GLN:OE1	2.48	0.42
1:bg:333:TYR:CD2	1:bg:333:TYR:C	2.98	0.42
1:bq:242:SER:OG	1:bq:243:ALA:N	2.52	0.42
2:bu:5:ILE:HD13	13:bS:166:GLN:NE2	2.31	0.42
2:bv:14:GLN:H	2:bv:14:GLN:CD	2.28	0.42
2:by:286:TYR:OH	2:by:299:LEU:O	2.37	0.42
2:by:326:GLU:HG3	2:by:329:ARG:HH21	1.81	0.42
5:bE:265:ASN:HD21	5:bE:272:ASN:HB3	1.85	0.42
4:bF:248:THR:O	4:bF:249:MET:HB2	2.19	0.42
4:bF:260:THR:O	4:bF:262:ALA:N	2.50	0.42
19:cl:26:TYR:CZ	20:co:127:LEU:HD22	2.55	0.42
21:cA:167:ASP:OD1	21:cA:167:ASP:C	2.62	0.42
21:cM:248:LYS:C	21:cM:250:TYR:H	2.28	0.42
24:cR:46:ASP:OD1	24:cR:46:ASP:N	2.52	0.42
24:cR:134:PRO:HB3	25:cV:12:PHE:CE2	2.54	0.42
4:cX:82:ASN:OD1	4:cX:82:ASN:O	2.38	0.42
4:dd:273:PHE:CB	4:dd:317:SER:HB3	2.47	0.42
5:de:354:THR:HG21	5:de:366:GLU:OE1	2.19	0.42
22:dg:13:MET:HE2	23:dh:8:TRP:CH2	2.55	0.42
1:ak:215:GLU:OE1	1:ak:215:GLU:N	2.50	0.42
1:aB:212:ASP:OD1	1:aB:213:THR:N	2.52	0.42
2:bu:382:ALA:O	2:bu:385:TYR:CD2	2.72	0.42
21:cr:235:LEU:H	21:cr:259:VAL:CG2	2.33	0.42
21:cM:297:TRP:CD1	21:cM:297:TRP:C	2.98	0.42
22:cO:23:LEU:HB3	22:cQ:28:PHE:CD1	2.54	0.42
24:cS:250:TYR:CG	24:cS:319:MET:HE3	2.54	0.42
4:cX:260:THR:O	4:cX:262:ALA:N	2.51	0.42
1:ag:68:THR:O	1:ag:156:ASN:ND2	2.52	0.42
1:ah:212:ASP:OD1	1:ah:213:THR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aq:375:ASP:OD2	14:bW:175:TYR:OH	2.30	0.42
1:ax:311:ALA:O	1:ax:384:LYS:CE	2.68	0.42
1:aA:43:GLN:HB2	1:aA:205:TRP:CZ3	2.55	0.42
1:aH:329:ARG:HH21	1:aH:333:TYR:HB2	1.84	0.42
1:aN:11:TYR:O	1:aP:373:ARG:NH1	2.52	0.42
1:aY:216:ARG:NH2	7:bH:305:GLY:O	2.52	0.42
2:bu:379:TYR:CG	2:bu:416:VAL:HG11	2.55	0.42
2:bB:144:THR:O	2:bB:145:TYR:C	2.63	0.42
3:bC:204:ASP:OD2	3:bC:465:ARG:NH2	2.51	0.42
4:bD:137:PRO:HA	22:cQ:12:ILE:CD1	2.48	0.42
11:bQ:92:ALA:N	11:bQ:93:PRO:HD3	2.33	0.42
19:cl:37:LEU:CD2	19:cm:36:TYR:HB3	2.50	0.42
20:cn:74:LYS:HE3	20:cn:74:LYS:HB3	1.82	0.42
21:ct:265:ASP:OD1	21:ct:266:THR:N	2.51	0.42
21:cC:145:ASP:OD1	21:cC:146:ASP:N	2.46	0.42
24:cR:62:ASP:O	24:cR:162:LEU:N	2.53	0.42
4:cZ:273:PHE:HD2	22:dc:9:ASN:ND2	2.15	0.42
5:de:156:ASP:O	5:de:157:THR:C	2.62	0.42
22:dg:25:ALA:HB3	22:dg:28:PHE:CE1	2.54	0.42
1:aa:25:THR:O	1:aa:26:PHE:C	2.63	0.42
1:ad:323:GLN:NE2	2:by:517:ALA:O	2.48	0.42
1:an:238:THR:OG1	1:an:383:TYR:CZ	2.72	0.42
1:aw:372:SER:OG	14:bZ:166:GLN:HG3	2.20	0.42
1:aN:125:ASP:O	1:aN:129:TYR:N	2.48	0.42
1:bn:333:TYR:OH	1:bn:338:GLN:NE2	2.52	0.42
2:by:32:ARG:NH2	19:cj:50:MET:HG2	2.25	0.42
4:bD:185:ILE:N	4:bD:186:PRO:CD	2.82	0.42
11:bQ:205:GLN:O	11:bQ:207:SER:N	2.51	0.42
21:cu:125:ILE:HG23	21:cu:125:ILE:O	2.19	0.42
21:cw:224:SER:OG	21:cw:226:THR:OG1	2.35	0.42
21:cN:63:SER:OG	21:cN:64:LEU:N	2.50	0.42
25:cU:29:PHE:HD1	25:cW:35:ILE:HG21	1.85	0.42
4:dd:180:ALA:O	4:dd:181:SER:C	2.62	0.42
4:dd:276:ASN:CG	4:dd:278:SER:HG	2.28	0.42
22:ds:20:TYR:HB2	22:du:14:ILE:HA	2.01	0.42
1:ac:32:ARG:NH2	19:cl:46:ARG:O	2.53	0.42
1:ac:308:GLU:OE2	1:ac:336:LYS:NZ	2.50	0.42
1:ag:321:ASN:N	1:ag:376:ASN:O	2.51	0.42
1:aB:121:ARG:O	1:aB:126:ARG:NH2	2.52	0.42
1:aG:264:TRP:HA	1:aG:415:ASN:O	2.20	0.42
1:aQ:109:TYR:O	1:aQ:112:TRP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:bh:110:ASN:CG	1:bh:111:ASP:N	2.78	0.42
1:bi:209:ILE:HD13	1:bk:27:PHE:CD1	2.55	0.42
2:bw:422:LEU:HD23	2:bw:429:ARG:HG2	2.02	0.42
2:by:145:TYR:CD1	2:by:145:TYR:C	2.96	0.42
2:bz:15:ASP:HA	20:cn:55:GLU:HA	2.01	0.42
11:bQ:178:PHE:C	11:bQ:180:PRO:HD2	2.45	0.42
21:cH:167:ASP:OD1	21:cH:167:ASP:C	2.62	0.42
21:cI:285:TYR:CG	21:cI:286:TYR:N	2.88	0.42
21:cK:161:PRO:HD2	21:cK:195:ILE:O	2.20	0.42
23:dt:13:ASN:C	23:dt:14:ARG:HG3	2.44	0.42
1:aa:8:LEU:HD22	20:co:70:ASN:HD22	1.78	0.41
1:aa:321:ASN:OD1	1:aa:375:ASP:N	2.49	0.41
1:af:122:MET:O	1:af:123:ASN:HB2	2.19	0.41
1:aJ:257:HIS:O	1:aJ:258:PRO:C	2.61	0.41
1:bp:67:ILE:CG2	1:bp:163:LEU:HB3	2.50	0.41
2:bv:390:VAL:O	2:bv:391:THR:OG1	2.26	0.41
2:bA:290:VAL:O	2:bA:290:VAL:HG23	2.18	0.41
4:bD:271:TYR:CD1	22:cQ:15:ARG:HG2	2.55	0.41
4:bF:126:ARG:NH2	22:cQ:8:LEU:CD2	2.70	0.41
21:cv:188:ASP:OD1	21:cv:188:ASP:N	2.49	0.41
21:cH:169:VAL:HG12	21:cH:171:ASN:H	1.85	0.41
21:cL:118:GLU:OE1	21:cL:118:GLU:N	2.53	0.41
5:dq:135:SER:CB	22:du:12:ILE:CG2	2.85	0.41
1:aa:130:ARG:NH2	1:aa:301:GLY:O	2.53	0.41
1:ad:122:MET:O	1:ad:125:ASP:CG	2.63	0.41
1:ak:109:TYR:O	1:ak:112:TRP:N	2.53	0.41
1:ar:242:SER:OG	1:ar:243:ALA:N	2.53	0.41
1:aC:325:ARG:NH2	1:aD:7:GLN:OE1	2.47	0.41
1:aF:67:ILE:CG2	1:aF:163:LEU:HB2	2.50	0.41
1:bl:376:ASN:OD1	1:bl:376:ASN:C	2.63	0.41
2:bv:23:GLN:O	18:ci:43:ASN:CG	2.63	0.41
2:bw:518:PHE:CG	2:bx:198:GLY:O	2.73	0.41
2:by:333:ILE:HG12	19:ck:46:ARG:CD	2.48	0.41
6:bG:226:PHE:HA	6:bG:331:LEU:O	2.20	0.41
14:bX:196:VAL:O	14:bX:197:ASP:HB3	2.20	0.41
14:bZ:176:ASP:OD1	14:bZ:177:LEU:N	2.51	0.41
21:cp:98:PRO:C	21:cp:100:LEU:H	2.28	0.41
21:cv:248:LYS:C	21:cv:250:TYR:N	2.79	0.41
21:cx:63:SER:OG	21:cx:64:LEU:N	2.52	0.41
22:cO:27:TYR:HB2	23:cP:21:ASN:OD1	2.20	0.41
4:cZ:174:LYS:NZ	4:cZ:176:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:di:34:ALA:C	22:di:35:LEU:HD12	2.44	0.41
4:dk:260:THR:O	4:dk:262:ALA:N	2.53	0.41
23:dt:10:PRO:C	22:du:17:MET:HE1	2.45	0.41
1:au:110:ASN:OD1	1:au:111:ASP:N	2.52	0.41
1:az:47:ASN:OD1	4:bD:48:ASN:ND2	2.53	0.41
1:aD:257:HIS:O	1:aD:258:PRO:C	2.61	0.41
1:aE:73:GLU:HA	1:aE:147:PHE:O	2.21	0.41
1:aI:371:PHE:O	8:bI:163:ARG:NH2	2.54	0.41
1:aK:325:ARG:NH2	1:aM:39:ILE:O	2.49	0.41
1:bg:66:LEU:HA	1:bg:163:LEU:O	2.20	0.41
2:bv:33:ARG:CD	18:ci:53:TRP:NE1	2.83	0.41
3:bC:11:ASP:OD1	3:bC:11:ASP:N	2.54	0.41
3:bC:418:ASP:N	3:bC:419:PRO:CD	2.84	0.41
7:bH:297:ARG:N	7:bH:298:PRO:CD	2.82	0.41
19:cl:18:LEU:HD12	19:cm:15:GLY:HA2	2.01	0.41
20:cn:96:ASP:OD2	20:cn:128:ARG:HB2	2.19	0.41
21:cF:63:SER:OG	21:cF:64:LEU:N	2.51	0.41
22:cO:28:PHE:HZ	23:cP:28:VAL:HG21	1.85	0.41
25:cW:19:SER:OG	25:cW:20:ASN:ND2	2.53	0.41
4:cZ:260:THR:O	4:cZ:262:ALA:N	2.53	0.41
26:dn:30:LEU:HD12	26:do:25:VAL:HB	2.00	0.41
1:ae:69:ASP:OD1	1:ae:70:ILE:N	2.53	0.41
1:aE:131:ARG:NH1	1:aF:347:THR:O	2.53	0.41
1:aJ:267:ASN:OD1	1:aJ:415:ASN:ND2	2.53	0.41
1:aN:95:ASP:OD1	1:aN:95:ASP:C	2.63	0.41
1:aR:242:SER:OG	1:aR:243:ALA:N	2.53	0.41
1:bk:52:PHE:CE1	1:bk:200:PRO:HD3	2.55	0.41
1:bl:87:TYR:CD2	1:bl:90:GLU:OE2	2.73	0.41
1:bs:230:GLN:HE21	1:bs:232:GLN:HE21	1.68	0.41
2:bA:242:ASN:O	2:bA:243:ILE:HB	2.21	0.41
7:bH:340:ASN:OD1	7:bH:340:ASN:C	2.63	0.41
13:bS:50:PHE:O	13:bS:54:LEU:HG	2.21	0.41
14:bZ:159:GLN:OE1	14:bZ:159:GLN:N	2.49	0.41
21:cx:123:ARG:O	21:cx:216:SER:HB3	2.19	0.41
21:cE:167:ASP:OD1	21:cE:167:ASP:C	2.62	0.41
24:cR:230:ASN:O	24:cR:349:ASN:ND2	2.51	0.41
24:cT:81:PHE:CG	24:cT:82:TYR:N	2.89	0.41
22:dg:16:THR:HG22	23:dh:21:ASN:H	1.84	0.41
4:dj:24:ASP:OD1	4:dj:24:ASP:N	2.54	0.41
4:dl:93:TYR:C	4:dl:93:TYR:CD1	2.99	0.41
4:dp:65:LEU:HA	4:dp:163:LEU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:af:123:ASN:O	1:af:124:ASP:HB2	2.19	0.41
1:ak:114:ARG:NH2	1:ak:117:ASP:OD2	2.52	0.41
1:az:346:VAL:O	1:az:346:VAL:HG13	2.19	0.41
1:aD:346:VAL:HG13	1:aD:346:VAL:O	2.20	0.41
1:aG:333:TYR:OH	1:aG:338:GLN:NE2	2.53	0.41
1:aI:321:ASN:N	1:aI:376:ASN:O	2.49	0.41
1:aX:242:SER:OG	1:aX:243:ALA:N	2.51	0.41
1:bc:121:ARG:NE	1:bd:340:TYR:OH	2.54	0.41
1:bp:14:GLN:H	1:bp:14:GLN:CD	2.28	0.41
1:bq:326:PHE:CD1	1:bq:327:ALA:O	2.74	0.41
2:bw:462:LEU:C	2:bw:471:ASN:HD22	2.27	0.41
2:bx:145:TYR:C	2:bx:145:TYR:CD1	2.96	0.41
2:bx:265:LEU:O	2:bx:266:TYR:C	2.61	0.41
2:bA:182:ASN:OD1	2:bA:183:GLY:N	2.54	0.41
13:bS:162:ASN:OD1	13:bS:164:GLN:CD	2.63	0.41
18:ci:54:LYS:N	18:ci:55:PRO:HD2	2.36	0.41
20:co:88:LEU:HA	20:co:128:ARG:NH2	2.35	0.41
21:cv:91:ASN:O	21:cv:92:ARG:HB2	2.20	0.41
21:cB:263:ASN:OD1	21:cB:266:THR:N	2.53	0.41
21:cG:167:ASP:OD1	21:cG:167:ASP:C	2.63	0.41
21:cI:87:LYS:NZ	21:cI:89:GLU:OE1	2.53	0.41
24:cR:91:LEU:HD13	24:cR:106:PHE:CD1	2.55	0.41
24:cR:203:ASP:OD1	24:cR:204:LYS:N	2.52	0.41
23:dh:37:THR:C	23:dh:39:SER:H	2.28	0.41
1:ab:21:ASN:OD1	20:co:67:THR:CG2	2.69	0.41
1:ab:325:ARG:HE	1:ac:7:GLN:HB2	1.85	0.41
1:ag:329:ARG:NH2	1:ai:41:SER:O	2.53	0.41
1:ap:308:GLU:OE2	1:ap:336:LYS:NZ	2.52	0.41
1:ay:52:PHE:CE2	1:ay:200:PRO:HD3	2.55	0.41
1:aE:69:ASP:OD1	1:aE:70:ILE:N	2.54	0.41
1:aO:242:SER:OG	1:aO:243:ALA:N	2.52	0.41
1:bb:110:ASN:OD1	1:bb:111:ASP:N	2.54	0.41
1:bo:21:ASN:O	1:bo:23:GLN:NE2	2.54	0.41
1:bq:110:ASN:OD1	1:bq:111:ASP:N	2.53	0.41
1:br:128:ASN:ND2	1:bs:345:GLY:O	2.54	0.41
2:bu:21:ASN:N	2:bu:22:PRO:HD3	2.36	0.41
2:by:160:MET:SD	2:by:160:MET:C	3.03	0.41
2:bB:182:ASN:CG	2:bB:183:GLY:N	2.79	0.41
4:bD:84:PHE:CE1	4:bD:85:TYR:CE1	3.09	0.41
14:bT:171:LYS:O	14:bT:172:ASN:C	2.64	0.41
20:cn:102:THR:O	20:cn:106:THR:OG1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:co:84:THR:O	20:co:88:LEU:HB3	2.21	0.41
21:cp:233:ILE:HG22	21:cp:242:TRP:CE3	2.56	0.41
21:cH:215:TYR:CD2	21:cH:215:TYR:O	2.73	0.41
21:cM:227:PHE:C	21:cM:229:ASN:H	2.28	0.41
23:cP:29:ILE:HB	22:cQ:24:SER:HB2	2.01	0.41
24:cR:91:LEU:CD1	24:cR:106:PHE:CD1	3.03	0.41
22:dc:27:TYR:HD1	22:dc:27:TYR:HA	1.75	0.41
5:de:248:PRO:HA	5:de:336:LEU:O	2.21	0.41
1:ac:110:ASN:OD1	1:ac:111:ASP:N	2.54	0.41
1:au:73:GLU:HA	1:au:147:PHE:O	2.21	0.41
1:aI:110:ASN:OD1	1:aI:111:ASP:N	2.52	0.41
1:aX:69:ASP:C	1:aX:69:ASP:OD1	2.63	0.41
1:bd:43:GLN:HB2	1:bd:205:TRP:CZ3	2.55	0.41
1:bh:119:LEU:O	1:bh:343:ILE:CD1	2.69	0.41
2:bu:119:THR:HB	2:bu:120:PRO:HD2	2.03	0.41
2:by:112:TRP:O	2:by:123:SER:OG	2.38	0.41
6:bG:432:VAL:O	6:bG:433:LYS:HB2	2.19	0.41
7:bH:440:THR:HA	7:bH:441:PRO:HD3	1.84	0.41
14:bX:196:VAL:O	14:bX:197:ASP:CB	2.69	0.41
21:cp:112:PHE:O	21:cp:226:THR:N	2.54	0.41
21:cJ:154:LYS:NZ	21:cJ:163:GLU:OE2	2.52	0.41
25:cU:15:ASP:HA	25:cW:21:VAL:O	2.20	0.41
4:dl:135:PHE:CZ	4:dl:145:ARG:HG3	2.55	0.41
1:ab:13:ALA:HB2	13:bS:153:ASN:HA	2.03	0.41
1:af:267:ASN:OD1	1:af:415:ASN:ND2	2.54	0.41
1:aj:20:GLY:O	1:ak:33:ARG:NE	2.53	0.41
1:an:68:THR:O	1:an:156:ASN:ND2	2.53	0.41
1:ao:17:TYR:CD1	14:bU:155:LEU:HB2	2.56	0.41
1:av:215:GLU:OE2	21:cv:48:LYS:NZ	2.42	0.41
1:aF:154:PHE:HB2	1:aF:229:GLU:H	1.85	0.41
1:aH:52:PHE:CE1	1:aH:200:PRO:HD3	2.56	0.41
1:aJ:52:PHE:CE1	1:aJ:200:PRO:HD3	2.56	0.41
1:aK:21:ASN:O	1:aK:23:GLN:NE2	2.54	0.41
1:aV:264:TRP:HA	1:aV:415:ASN:O	2.21	0.41
1:bg:110:ASN:OD1	1:bg:111:ASP:N	2.53	0.41
1:bn:171:HIS:CE1	7:bH:346:THR:O	2.74	0.41
2:bx:350:VAL:C	2:bx:351:THR:HG23	2.46	0.41
2:bx:462:LEU:C	2:bx:471:ASN:HD22	2.29	0.41
2:by:306:ASN:OD1	2:by:306:ASN:C	2.64	0.41
2:by:379:TYR:CZ	2:by:381:ALA:HB3	2.56	0.41
2:bz:348:GLU:O	2:bz:362:ARG:NE	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:cB:258:PHE:CD2	21:cB:259:VAL:HG23	2.56	0.41
21:cH:101:TYR:HB2	21:cH:102:PRO:HD2	2.02	0.41
21:cJ:210:ASN:OD1	21:cJ:211:VAL:N	2.53	0.41
21:cL:145:ASP:OD1	21:cL:146:ASP:N	2.47	0.41
21:cM:226:THR:HG22	21:cM:228:LEU:H	1.85	0.41
22:cO:23:LEU:HD23	22:cO:24:SER:N	2.36	0.41
25:cU:24:ILE:O	25:cW:30:ASP:HA	2.21	0.41
5:dq:258:THR:HG23	5:dq:260:SER:H	1.86	0.41
1:ab:337:VAL:O	1:ab:338:GLN:C	2.61	0.41
1:ac:338:GLN:N	1:ac:339:PRO:HD2	2.36	0.41
1:ae:39:ILE:O	1:af:325:ARG:NH2	2.50	0.41
1:ak:110:ASN:OD1	1:ak:111:ASP:N	2.53	0.41
1:al:242:SER:OG	1:al:243:ALA:N	2.53	0.41
1:aA:110:ASN:CG	1:aA:111:ASP:N	2.79	0.41
1:aD:267:ASN:OD1	1:aD:415:ASN:ND2	2.54	0.41
1:aR:169:GLN:OE1	1:aR:169:GLN:N	2.48	0.41
1:bf:110:ASN:CG	1:bf:111:ASP:N	2.79	0.41
1:bf:184:GLN:HG2	1:bf:300:TYR:CD2	2.56	0.41
1:bf:373:ARG:NH1	8:bK:124:ARG:O	2.53	0.41
1:bk:242:SER:OG	1:bk:243:ALA:N	2.51	0.41
1:bm:96:VAL:HA	1:bm:176:TYR:O	2.21	0.41
1:br:39:ILE:O	1:bs:325:ARG:NH1	2.52	0.41
2:bu:382:ALA:C	2:bu:384:ASN:N	2.77	0.41
2:bx:86:PRO:O	2:bx:87:THR:HB	2.21	0.41
2:by:145:TYR:HB3	2:by:146:PRO:CD	2.51	0.41
4:bD:271:TYR:CG	22:cQ:15:ARG:CG	3.04	0.41
4:bF:93:TYR:CD1	4:bF:93:TYR:C	2.98	0.41
6:bG:281:ALA:HA	6:bG:301:VAL:O	2.21	0.41
7:bH:509:ILE:HG13	7:bH:510:ALA:N	2.35	0.41
11:bQ:205:GLN:O	11:bQ:206:PHE:HB2	2.20	0.41
19:cj:24:LEU:HD21	20:cn:85:TRP:HA	2.02	0.41
19:cl:32:ILE:HA	19:cm:32:ILE:HG23	2.02	0.41
19:cl:42:ASP:OD2	19:cl:46:ARG:NH2	2.52	0.41
21:cs:137:ASP:OD1	21:cs:138:GLU:N	2.54	0.41
21:cv:112:PHE:O	21:cv:226:THR:N	2.54	0.41
21:cx:249:MET:O	21:cx:249:MET:HG3	2.20	0.41
21:cy:308:ASN:OD1	21:cy:308:ASN:C	2.64	0.41
21:cF:248:LYS:C	21:cF:250:TYR:H	2.29	0.41
21:cI:198:ILE:HG22	21:cI:199:ASP:N	2.35	0.41
21:cJ:82:ASN:CG	21:cJ:83:GLY:H	2.29	0.41
21:cM:248:LYS:O	21:cM:249:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:cS:238:THR:CG2	24:cS:347:TYR:CZ	3.04	0.41
25:cU:37:ALA:HA	25:cV:31:ASN:HA	2.02	0.41
25:cW:24:ILE:HD12	25:cW:28:ILE:HD12	2.02	0.41
25:cW:33:ASN:OD1	25:cW:34:VAL:N	2.54	0.41
23:db:10:PRO:HG3	22:dc:17:MET:HB2	2.02	0.41
4:dd:364:TYR:CD2	4:dd:365:ASN:O	2.74	0.41
23:dh:8:TRP:HZ2	22:di:11:PRO:HA	1.86	0.41
4:dl:206:ASP:OD1	4:dl:207:THR:N	2.54	0.41
26:do:25:VAL:CG1	26:do:27:VAL:HG13	2.50	0.41
4:dr:47:ILE:HG22	4:dr:49:VAL:H	1.86	0.41
1:ad:139:GLU:OE1	1:ad:139:GLU:N	2.46	0.41
1:ak:235:GLY:O	1:am:250:ASN:ND2	2.53	0.41
1:aq:121:ARG:O	1:aq:126:ARG:NH2	2.53	0.41
1:ax:311:ALA:O	1:ax:384:LYS:NZ	2.53	0.41
1:aX:20:GLY:O	1:aY:33:ARG:NE	2.52	0.41
1:aZ:21:ASN:O	1:aZ:23:GLN:NE2	2.54	0.41
1:bh:327:ALA:O	1:bh:329:ARG:NH1	2.55	0.41
1:bj:52:PHE:CZ	1:bj:187:ASN:OD1	2.74	0.41
1:bm:264:TRP:HE1	1:bm:313:LEU:CD1	2.33	0.41
2:bv:229:VAL:O	2:bv:230:GLY:C	2.62	0.41
2:by:23:GLN:HA	19:cj:57:SER:CB	2.51	0.41
2:by:27:PHE:CD1	2:bz:66:LEU:HD13	2.56	0.41
2:bz:119:THR:HB	2:bz:120:PRO:HD2	2.03	0.41
4:bD:136:ARG:C	22:cQ:12:ILE:HD13	2.40	0.41
5:bE:265:ASN:CG	5:bE:272:ASN:HD22	2.29	0.41
9:bL:29:GLN:OE1	9:bL:38:LYS:NZ	2.53	0.41
21:cp:173:GLU:OE1	21:cp:173:GLU:N	2.49	0.41
21:cr:101:TYR:HA	21:cr:102:PRO:HD3	1.96	0.41
21:ct:209:ILE:HD11	21:ct:320:TRP:CZ3	2.55	0.41
21:cK:113:ASP:OD1	21:cK:114:LEU:N	2.52	0.41
23:cP:8:TRP:HH2	22:cQ:13:MET:HE1	1.85	0.41
4:dj:260:THR:O	4:dj:262:ALA:N	2.53	0.41
1:ac:225:GLU:CD	19:cm:50:MET:SD	3.04	0.40
1:ag:145:LYS:NZ	1:ah:309:GLN:OE1	2.51	0.40
1:aS:171:HIS:CE1	1:aS:430:MET:HB2	2.57	0.40
1:aW:69:ASP:OD1	1:aW:70:ILE:N	2.54	0.40
1:bk:87:TYR:H	1:bk:134:ASP:CG	2.30	0.40
2:bx:375:LEU:HG	2:bx:460:PHE:HE2	1.86	0.40
2:bz:351:THR:O	2:bz:352:ALA:C	2.64	0.40
2:bB:96:ILE:HD12	2:bB:96:ILE:C	2.46	0.40
3:bC:410:PRO:C	3:bC:412:GLN:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:cj:41:LEU:O	19:cj:45:ILE:HG13	2.21	0.40
21:cp:203:VAL:O	21:cp:203:VAL:HG13	2.21	0.40
21:cs:325:PHE:N	21:cs:325:PHE:CD2	2.89	0.40
21:cE:328:PRO:O	21:cE:331:GLN:N	2.54	0.40
21:cF:64:LEU:H	21:cF:64:LEU:HD23	1.86	0.40
21:cH:132:ASP:OD1	21:cH:132:ASP:N	2.54	0.40
21:cL:296:LYS:O	21:cL:297:TRP:HB2	2.21	0.40
24:cT:134:PRO:HB2	25:cU:12:PHE:CZ	2.54	0.40
25:cU:6:VAL:N	25:cU:7:PRO:CD	2.84	0.40
22:da:9:ASN:HA	23:db:12:PHE:CE1	2.51	0.40
4:dd:65:LEU:HA	4:dd:163:LEU:O	2.22	0.40
4:dp:364:TYR:CE2	4:dp:365:ASN:O	2.74	0.40
1:ac:225:GLU:OE1	19:cm:52:SER:HB3	2.21	0.40
1:am:153:PHE:H	1:am:156:ASN:ND2	2.17	0.40
1:ao:212:ASP:OD1	1:ao:213:THR:N	2.53	0.40
1:ar:264:TRP:HA	1:ar:415:ASN:O	2.21	0.40
1:aw:186:VAL:HG23	1:aw:187:ASN:N	2.36	0.40
1:aG:294:THR:HG22	1:aG:296:THR:H	1.86	0.40
1:aH:27:PHE:CE1	1:aI:209:ILE:HD13	2.56	0.40
1:aL:62:ARG:NH2	9:bM:10:SER:O	2.52	0.40
1:bb:43:GLN:HB2	1:bb:205:TRP:CZ3	2.55	0.40
1:bb:96:VAL:HA	1:bb:176:TYR:O	2.21	0.40
1:bl:205:TRP:CD2	1:bm:329:ARG:NH1	2.89	0.40
1:bm:124:ASP:OD1	1:bm:125:ASP:N	2.54	0.40
2:bv:476:PHE:HA	2:bv:479:TYR:CD2	2.56	0.40
2:bw:96:ILE:O	2:bw:103:PHE:CE2	2.74	0.40
2:bx:369:ASN:OD1	2:bx:370:HIS:N	2.53	0.40
2:bz:177:ASN:O	2:bz:178:LEU:C	2.62	0.40
9:bN:17:HIS:N	9:bN:18:GLN:OE1	2.53	0.40
20:cn:59:LEU:HB3	20:cn:61:THR:HG23	2.03	0.40
21:cL:63:SER:OG	21:cL:64:LEU:N	2.54	0.40
21:cM:112:PHE:CD1	21:cM:112:PHE:C	3.00	0.40
22:da:17:MET:HB3	23:db:22:LEU:CD1	2.50	0.40
4:dl:174:LYS:NZ	4:dl:176:ASP:OD1	2.47	0.40
1:ab:287:GLY:O	1:ab:288:ALA:C	2.63	0.40
1:ac:25:THR:O	19:cl:50:MET:HG3	2.21	0.40
1:ag:329:ARG:CZ	1:ai:205:TRP:CZ3	3.05	0.40
1:ah:433:LEU:O	14:bX:191:TRP:O	2.38	0.40
1:aj:347:THR:O	1:al:131:ARG:NH1	2.54	0.40
1:ak:267:ASN:OD1	1:ak:415:ASN:ND2	2.54	0.40
1:au:152:ILE:O	1:au:153:PHE:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:aR:20:GLY:O	1:aS:33:ARG:NE	2.55	0.40
1:bl:27:PHE:CE1	1:bm:209:ILE:HD13	2.56	0.40
1:bn:109:TYR:O	1:bn:112:TRP:N	2.54	0.40
2:bu:21:ASN:HB2	18:ci:53:TRP:HZ2	1.85	0.40
2:bu:85:THR:OG1	2:bu:86:PRO:HD3	2.21	0.40
2:by:61:SER:OG	2:by:63:ASN:OD1	2.39	0.40
2:by:121:GLN:O	2:by:122:TYR:C	2.63	0.40
13:bS:17:SER:HA	20:co:116:SER:O	2.21	0.40
18:ci:34:GLN:C	18:ci:35:TRP:CD1	2.99	0.40
21:cp:211:VAL:O	21:cp:211:VAL:HG13	2.21	0.40
21:cE:210:ASN:OD1	21:cE:210:ASN:C	2.63	0.40
21:cI:112:PHE:O	21:cI:226:THR:N	2.55	0.40
21:cI:220:VAL:N	21:cI:299:ILE:O	2.51	0.40
24:cT:285:LYS:HE2	24:cT:290:ASP:OD1	2.21	0.40
25:cU:35:ILE:O	25:cV:29:PHE:HA	2.22	0.40
23:db:10:PRO:CB	22:dc:17:MET:CA	2.96	0.40
23:db:22:LEU:HD23	22:dc:28:PHE:CD2	2.57	0.40
4:dl:260:THR:O	4:dl:262:ALA:N	2.52	0.40
23:dt:24:VAL:HG21	23:dt:28:VAL:HG23	2.03	0.40
1:aa:15:ASP:OD2	20:co:51:VAL:HB	2.22	0.40
1:ak:242:SER:OG	1:ak:243:ALA:N	2.54	0.40
1:am:126:ARG:HH22	1:am:346:VAL:CG1	2.34	0.40
1:am:325:ARG:NH2	1:ao:39:ILE:O	2.53	0.40
1:aq:243:ALA:C	1:aq:244:THR:HG23	2.46	0.40
1:at:215:GLU:OE1	1:at:215:GLU:N	2.54	0.40
1:aQ:5:LEU:H	1:aQ:5:LEU:HD23	1.86	0.40
1:bl:39:ILE:O	1:bm:325:ARG:NH2	2.49	0.40
4:bD:364:TYR:CD2	4:bD:365:ASN:O	2.75	0.40
13:bS:165:ARG:NH2	13:bS:166:GLN:NE2	2.69	0.40
16:cg:69:TYR:CG	16:cg:81:ILE:HD12	2.56	0.40
21:ct:79:GLU:OE1	21:ct:79:GLU:N	2.55	0.40
21:ct:254:ASN:C	21:ct:256:ASN:N	2.79	0.40
21:cw:207:VAL:O	21:cw:319:SER:HA	2.20	0.40
21:cz:329:ILE:HG23	21:cz:330:TRP:N	2.35	0.40
21:cK:294:VAL:O	21:cK:295:ASN:C	2.63	0.40
24:cS:312:ALA:O	24:cT:128:ARG:NH1	2.54	0.40
24:cT:58:LYS:O	24:cT:199:TYR:OH	2.37	0.40
24:cT:203:ASP:OD1	24:cT:204:LYS:N	2.52	0.40
4:cZ:228:TYR:OH	4:cZ:230:ASN:ND2	2.54	0.40
4:df:271:TYR:CB	23:dh:14:ARG:CZ	2.94	0.40
23:dh:24:VAL:HG21	23:dh:28:VAL:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:dl:273:PHE:HD2	26:dm:12:PRO:CG	2.34	0.40
1:ac:23:GLN:C	19:cl:52:SER:HB2	2.41	0.40
1:ad:325:ARG:NH1	1:af:39:ILE:O	2.50	0.40
1:ah:73:GLU:HA	1:ah:147:PHE:O	2.22	0.40
1:as:110:ASN:OD1	1:as:111:ASP:N	2.53	0.40
1:aN:329:ARG:NH2	1:aP:41:SER:O	2.54	0.40
1:aO:119:LEU:O	1:aO:343:ILE:CD1	2.70	0.40
1:aR:166:ILE:O	1:aR:169:GLN:NE2	2.53	0.40
1:aW:110:ASN:OD1	1:aW:111:ASP:N	2.54	0.40
1:bb:238:THR:HG22	1:bb:414:LEU:CD2	2.46	0.40
1:bg:109:TYR:O	1:bg:112:TRP:N	2.55	0.40
1:bm:242:SER:OG	1:bm:243:ALA:N	2.55	0.40
2:bu:320:VAL:HG11	2:bw:27:PHE:CZ	2.57	0.40
2:bv:324:ALA:HB2	13:bS:165:ARG:HA	2.04	0.40
2:bv:328:ILE:HG21	13:bS:133:TYR:CG	2.56	0.40
2:bw:14:GLN:H	2:bw:14:GLN:CD	2.28	0.40
2:bw:145:TYR:HB3	2:bw:146:PRO:CD	2.51	0.40
2:bw:286:TYR:OH	2:bw:299:LEU:O	2.36	0.40
2:bx:241:TRP:NE1	2:bx:244:SER:H	2.20	0.40
2:by:24:ILE:CA	19:cj:54:ILE:HG12	2.49	0.40
2:bB:384:ASN:OD1	2:bB:384:ASN:C	2.65	0.40
5:bE:83:TYR:N	5:bE:84:PRO:CD	2.84	0.40
14:bZ:169:SER:O	14:bZ:199:ASN:ND2	2.55	0.40
21:cy:89:GLU:O	21:cy:90:TYR:HB2	2.22	0.40
24:cS:81:PHE:CG	24:cS:82:TYR:N	2.90	0.40
24:cS:135:ASP:N	25:cW:12:PHE:CE1	2.88	0.40
24:cT:195:PHE:CD1	24:cT:195:PHE:C	3.00	0.40
5:de:358:VAL:HA	5:de:368:LEU:HD21	2.03	0.40
22:dg:23:LEU:HA	22:di:17:MET:O	2.22	0.40
4:dr:65:LEU:HA	4:dr:163:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	433/437 (99%)	421 (97%)	12 (3%)	0	100	100
1	aB	433/437 (99%)	424 (98%)	9 (2%)	0	100	100
1	aC	434/437 (99%)	423 (98%)	11 (2%)	0	100	100
1	aD	432/437 (99%)	421 (98%)	11 (2%)	0	100	100
1	aE	434/437 (99%)	419 (96%)	15 (4%)	0	100	100
1	aF	432/437 (99%)	421 (98%)	11 (2%)	0	100	100
1	aG	433/437 (99%)	420 (97%)	13 (3%)	0	100	100
1	aH	432/437 (99%)	422 (98%)	9 (2%)	1 (0%)	43	73
1	aI	433/437 (99%)	422 (98%)	10 (2%)	1 (0%)	43	73
1	aJ	434/437 (99%)	421 (97%)	13 (3%)	0	100	100
1	aK	434/437 (99%)	420 (97%)	12 (3%)	2 (0%)	24	57
1	aL	433/437 (99%)	419 (97%)	13 (3%)	1 (0%)	43	73
1	aM	434/437 (99%)	418 (96%)	16 (4%)	0	100	100
1	aN	433/437 (99%)	419 (97%)	13 (3%)	1 (0%)	43	73
1	aO	434/437 (99%)	419 (96%)	14 (3%)	1 (0%)	43	73
1	aP	434/437 (99%)	422 (97%)	11 (2%)	1 (0%)	43	73
1	aQ	432/437 (99%)	420 (97%)	11 (2%)	1 (0%)	43	73
1	aR	434/437 (99%)	416 (96%)	14 (3%)	4 (1%)	14	45
1	aS	434/437 (99%)	418 (96%)	15 (4%)	1 (0%)	43	73
1	aT	434/437 (99%)	417 (96%)	15 (4%)	2 (0%)	24	57
1	aU	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	43	73
1	aV	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	43	73
1	aW	434/437 (99%)	420 (97%)	14 (3%)	0	100	100
1	aX	433/437 (99%)	420 (97%)	13 (3%)	0	100	100
1	aY	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	43	73
1	aZ	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	43	73
1	aa	430/437 (98%)	420 (98%)	10 (2%)	0	100	100
1	ab	434/437 (99%)	430 (99%)	4 (1%)	0	100	100
1	ac	434/437 (99%)	425 (98%)	9 (2%)	0	100	100
1	ad	434/437 (99%)	419 (96%)	13 (3%)	2 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	ae	434/437 (99%)	419 (96%)	15 (4%)	0	100	100
1	af	434/437 (99%)	422 (97%)	12 (3%)	0	100	100
1	ag	434/437 (99%)	415 (96%)	19 (4%)	0	100	100
1	ah	434/437 (99%)	417 (96%)	16 (4%)	1 (0%)	43	73
1	ai	434/437 (99%)	418 (96%)	16 (4%)	0	100	100
1	aj	434/437 (99%)	423 (98%)	11 (2%)	0	100	100
1	ak	434/437 (99%)	422 (97%)	10 (2%)	2 (0%)	24	57
1	al	433/437 (99%)	425 (98%)	7 (2%)	1 (0%)	43	73
1	am	434/437 (99%)	423 (98%)	11 (2%)	0	100	100
1	an	433/437 (99%)	423 (98%)	10 (2%)	0	100	100
1	ao	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	ap	434/437 (99%)	417 (96%)	17 (4%)	0	100	100
1	aq	434/437 (99%)	425 (98%)	8 (2%)	1 (0%)	43	73
1	ar	432/437 (99%)	420 (97%)	12 (3%)	0	100	100
1	as	434/437 (99%)	418 (96%)	14 (3%)	2 (0%)	24	57
1	at	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	43	73
1	au	432/437 (99%)	421 (98%)	11 (2%)	0	100	100
1	av	434/437 (99%)	425 (98%)	9 (2%)	0	100	100
1	aw	434/437 (99%)	418 (96%)	15 (4%)	1 (0%)	43	73
1	ax	432/437 (99%)	417 (96%)	14 (3%)	1 (0%)	43	73
1	ay	433/437 (99%)	419 (97%)	14 (3%)	0	100	100
1	az	432/437 (99%)	420 (97%)	12 (3%)	0	100	100
1	ba	434/437 (99%)	416 (96%)	17 (4%)	1 (0%)	43	73
1	bb	434/437 (99%)	420 (97%)	12 (3%)	2 (0%)	24	57
1	bc	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	43	73
1	bd	434/437 (99%)	423 (98%)	9 (2%)	2 (0%)	24	57
1	be	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	43	73
1	bf	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	43	73
1	bg	434/437 (99%)	421 (97%)	12 (3%)	1 (0%)	43	73
1	bh	434/437 (99%)	422 (97%)	11 (2%)	1 (0%)	43	73
1	bi	434/437 (99%)	419 (96%)	14 (3%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	bj	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	43	73
1	bk	434/437 (99%)	419 (96%)	14 (3%)	1 (0%)	43	73
1	bl	434/437 (99%)	418 (96%)	15 (4%)	1 (0%)	43	73
1	bm	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	43	73
1	bn	432/437 (99%)	416 (96%)	15 (4%)	1 (0%)	43	73
1	bo	434/437 (99%)	419 (96%)	13 (3%)	2 (0%)	24	57
1	bp	434/437 (99%)	422 (97%)	11 (2%)	1 (0%)	43	73
1	bq	434/437 (99%)	420 (97%)	14 (3%)	0	100	100
1	br	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	43	73
1	bs	434/437 (99%)	421 (97%)	13 (3%)	0	100	100
1	bt	433/437 (99%)	423 (98%)	9 (2%)	1 (0%)	43	73
2	bA	514/520 (99%)	486 (95%)	26 (5%)	2 (0%)	30	62
2	bB	515/520 (99%)	480 (93%)	34 (7%)	1 (0%)	43	73
2	bu	515/520 (99%)	489 (95%)	25 (5%)	1 (0%)	43	73
2	bv	515/520 (99%)	485 (94%)	29 (6%)	1 (0%)	43	73
2	bw	515/520 (99%)	490 (95%)	25 (5%)	0	100	100
2	bx	512/520 (98%)	483 (94%)	27 (5%)	2 (0%)	30	62
2	by	515/520 (99%)	482 (94%)	32 (6%)	1 (0%)	43	73
2	bz	506/520 (97%)	473 (94%)	32 (6%)	1 (0%)	43	73
3	bC	483/486 (99%)	459 (95%)	22 (5%)	2 (0%)	30	62
4	bD	399/403 (99%)	383 (96%)	14 (4%)	2 (0%)	24	57
4	bF	399/403 (99%)	385 (96%)	14 (4%)	0	100	100
4	cX	399/403 (99%)	380 (95%)	14 (4%)	5 (1%)	9	38
4	cZ	399/403 (99%)	380 (95%)	14 (4%)	5 (1%)	9	38
4	dd	399/403 (99%)	379 (95%)	15 (4%)	5 (1%)	9	38
4	df	399/403 (99%)	377 (94%)	14 (4%)	8 (2%)	6	32
4	dj	399/403 (99%)	376 (94%)	20 (5%)	3 (1%)	16	48
4	dk	399/403 (99%)	374 (94%)	22 (6%)	3 (1%)	16	48
4	dl	399/403 (99%)	374 (94%)	20 (5%)	5 (1%)	9	38
4	dp	399/403 (99%)	381 (96%)	14 (4%)	4 (1%)	12	43
4	dr	399/403 (99%)	378 (95%)	14 (4%)	7 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	bE	395/401 (98%)	382 (97%)	12 (3%)	1 (0%)	36	67
5	cY	395/401 (98%)	382 (97%)	12 (3%)	1 (0%)	36	67
5	de	395/401 (98%)	385 (98%)	10 (2%)	0	100	100
5	dq	395/401 (98%)	384 (97%)	10 (2%)	1 (0%)	36	67
6	bG	496/530 (94%)	478 (96%)	17 (3%)	1 (0%)	43	73
7	bH	422/576 (73%)	388 (92%)	32 (8%)	2 (0%)	24	57
8	bI	139/171 (81%)	131 (94%)	7 (5%)	1 (1%)	18	51
8	bJ	145/171 (85%)	135 (93%)	9 (6%)	1 (1%)	18	51
8	bK	114/171 (67%)	111 (97%)	3 (3%)	0	100	100
9	bL	61/181 (34%)	59 (97%)	1 (2%)	1 (2%)	7	35
9	bM	61/181 (34%)	55 (90%)	5 (8%)	1 (2%)	7	35
9	bN	60/181 (33%)	56 (93%)	3 (5%)	1 (2%)	7	34
9	bO	60/181 (33%)	54 (90%)	5 (8%)	1 (2%)	7	34
10	bP	140/146 (96%)	133 (95%)	7 (5%)	0	100	100
11	bQ	160/216 (74%)	149 (93%)	8 (5%)	3 (2%)	6	32
12	bR	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
13	bS	189/210 (90%)	172 (91%)	15 (8%)	2 (1%)	11	41
14	bT	46/207 (22%)	40 (87%)	3 (6%)	3 (6%)	1	14
14	bU	52/207 (25%)	48 (92%)	3 (6%)	1 (2%)	6	32
14	bV	51/207 (25%)	42 (82%)	8 (16%)	1 (2%)	6	32
14	bW	50/207 (24%)	45 (90%)	4 (8%)	1 (2%)	6	32
14	bX	39/207 (19%)	34 (87%)	4 (10%)	1 (3%)	4	27
14	bY	72/207 (35%)	58 (81%)	10 (14%)	4 (6%)	1	15
14	bZ	50/207 (24%)	46 (92%)	4 (8%)	0	100	100
14	ca	50/207 (24%)	47 (94%)	2 (4%)	1 (2%)	6	32
14	cb	50/207 (24%)	45 (90%)	4 (8%)	1 (2%)	6	32
14	cc	82/207 (40%)	73 (89%)	8 (10%)	1 (1%)	10	40
14	cd	73/207 (35%)	66 (90%)	7 (10%)	0	100	100
14	ce	70/207 (34%)	63 (90%)	6 (9%)	1 (1%)	9	37
15	cf	76/151 (50%)	67 (88%)	7 (9%)	2 (3%)	4	27
16	cg	64/98 (65%)	58 (91%)	3 (5%)	3 (5%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	ch	150/155 (97%)	143 (95%)	5 (3%)	2 (1%)	9	38
18	ci	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	9	38
19	cj	57/80 (71%)	51 (90%)	6 (10%)	0	100	100
19	ck	55/80 (69%)	52 (94%)	3 (6%)	0	100	100
19	cl	53/80 (66%)	51 (96%)	2 (4%)	0	100	100
19	cm	61/80 (76%)	58 (95%)	3 (5%)	0	100	100
20	cn	96/148 (65%)	93 (97%)	3 (3%)	0	100	100
20	co	93/148 (63%)	87 (94%)	6 (6%)	0	100	100
21	cA	277/378 (73%)	254 (92%)	23 (8%)	0	100	100
21	cB	290/378 (77%)	267 (92%)	23 (8%)	0	100	100
21	cC	277/378 (73%)	250 (90%)	26 (9%)	1 (0%)	30	62
21	cD	290/378 (77%)	267 (92%)	20 (7%)	3 (1%)	12	43
21	cE	278/378 (74%)	255 (92%)	21 (8%)	2 (1%)	18	51
21	cF	290/378 (77%)	257 (89%)	30 (10%)	3 (1%)	12	43
21	cG	280/378 (74%)	253 (90%)	26 (9%)	1 (0%)	30	62
21	cH	290/378 (77%)	261 (90%)	28 (10%)	1 (0%)	36	67
21	cI	277/378 (73%)	256 (92%)	21 (8%)	0	100	100
21	cJ	290/378 (77%)	263 (91%)	24 (8%)	3 (1%)	12	43
21	cK	277/378 (73%)	258 (93%)	18 (6%)	1 (0%)	30	62
21	cL	290/378 (77%)	265 (91%)	24 (8%)	1 (0%)	36	67
21	cM	275/378 (73%)	252 (92%)	22 (8%)	1 (0%)	30	62
21	cN	290/378 (77%)	267 (92%)	21 (7%)	2 (1%)	18	51
21	cp	290/378 (77%)	263 (91%)	24 (8%)	3 (1%)	12	43
21	cq	280/378 (74%)	257 (92%)	21 (8%)	2 (1%)	18	51
21	cr	290/378 (77%)	264 (91%)	25 (9%)	1 (0%)	36	67
21	cs	273/378 (72%)	248 (91%)	23 (8%)	2 (1%)	18	51
21	ct	290/378 (77%)	258 (89%)	30 (10%)	2 (1%)	18	51
21	cu	278/378 (74%)	260 (94%)	18 (6%)	0	100	100
21	cv	290/378 (77%)	254 (88%)	34 (12%)	2 (1%)	18	51
21	cw	278/378 (74%)	252 (91%)	22 (8%)	4 (1%)	9	37
21	cx	290/378 (77%)	260 (90%)	30 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	cy	278/378 (74%)	248 (89%)	29 (10%)	1 (0%)	30	62
21	cz	290/378 (77%)	267 (92%)	21 (7%)	2 (1%)	18	51
22	cO	28/1335 (2%)	21 (75%)	7 (25%)	0	100	100
22	cQ	29/1335 (2%)	22 (76%)	7 (24%)	0	100	100
22	da	30/1335 (2%)	24 (80%)	6 (20%)	0	100	100
22	dc	26/1335 (2%)	21 (81%)	5 (19%)	0	100	100
22	dg	30/1335 (2%)	27 (90%)	3 (10%)	0	100	100
22	di	27/1335 (2%)	21 (78%)	6 (22%)	0	100	100
22	ds	30/1335 (2%)	30 (100%)	0	0	100	100
22	du	28/1335 (2%)	24 (86%)	4 (14%)	0	100	100
23	cP	33/1369 (2%)	22 (67%)	11 (33%)	0	100	100
23	db	28/1369 (2%)	20 (71%)	6 (21%)	2 (7%)	1	12
23	dh	33/1369 (2%)	26 (79%)	7 (21%)	0	100	100
23	dt	33/1369 (2%)	25 (76%)	8 (24%)	0	100	100
24	cR	397/400 (99%)	358 (90%)	34 (9%)	5 (1%)	9	38
24	cS	397/400 (99%)	359 (90%)	34 (9%)	4 (1%)	12	43
24	cT	397/400 (99%)	358 (90%)	35 (9%)	4 (1%)	12	43
25	cU	41/1343 (3%)	36 (88%)	5 (12%)	0	100	100
25	cV	41/1343 (3%)	35 (85%)	5 (12%)	1 (2%)	4	29
25	cW	41/1343 (3%)	36 (88%)	5 (12%)	0	100	100
26	dm	23/1359 (2%)	19 (83%)	4 (17%)	0	100	100
26	dn	23/1359 (2%)	18 (78%)	5 (22%)	0	100	100
26	do	23/1359 (2%)	21 (91%)	2 (9%)	0	100	100
All	All	54281/83744 (65%)	51687 (95%)	2389 (4%)	205 (0%)	31	62

All (205) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	ah	123	ASN
1	aU	123	ASN
1	bm	123	ASN
1	bo	123	ASN
1	br	123	ASN
2	bA	382	ALA

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Mol	Chain	Res	Type
6	bG	134	THR
7	bH	407	PRO
9	bO	21	LYS
11	bQ	79	PRO
14	cb	197	ASP
14	cc	167	GLY
15	cf	90	VAL
15	cf	126	SER
16	cg	82	CYS
16	cg	88	GLN
21	ct	306	CYS
21	cF	70	ASN
1	al	123	ASN
1	as	123	ASN
1	at	123	ASN
1	aw	323	GLN
1	aI	123	ASN
1	aK	123	ASN
1	aO	123	ASN
1	aR	123	ASN
1	aT	123	ASN
1	aV	123	ASN
1	bg	123	ASN
1	bh	123	ASN
1	bj	123	ASN
1	bn	123	ASN
1	bp	123	ASN
2	bv	89	ALA
2	bx	89	ALA
2	by	89	ALA
2	bB	143	SER
13	bS	28	PRO
13	bS	31	ASP
14	bY	138	ALA
17	ch	72	SER
18	ci	36	PRO
21	cq	128	PHE
21	cF	98	PRO
21	cL	264	PRO
24	cR	310	GLY
24	cS	310	GLY
4	cX	273	PHE

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Mol	Chain	Res	Type
5	cY	358	VAL
4	df	272	PRO
4	dk	273	PHE
4	dr	272	PRO
1	aH	123	ASN
1	aK	258	PRO
1	aS	123	ASN
1	bd	123	ASN
2	bz	454	SER
3	bC	379	ASP
5	bE	358	VAL
7	bH	283	SER
9	bM	6	ARG
14	bT	172	ASN
14	bT	173	ALA
21	cp	264	PRO
21	cv	212	PRO
21	cv	309	THR
21	cw	263	ASN
21	cw	296	LYS
21	cE	128	PHE
21	cJ	239	LYS
21	cJ	265	ASP
24	cR	46	ASP
24	cR	47	VAL
24	cR	246	LEU
24	cS	246	LEU
24	cT	246	LEU
4	cZ	273	PHE
4	df	273	PHE
4	df	359	THR
4	dj	273	PHE
4	dl	272	PRO
4	dl	273	PHE
4	dr	30	ASN
4	dr	273	PHE
1	ad	68	THR
1	ad	69	ASP
1	ak	123	ASN
1	aq	258	PRO
1	aL	123	ASN
1	aN	123	ASN

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Mol	Chain	Res	Type
1	bc	123	ASN
1	be	123	ASN
17	ch	14	ILE
21	cs	128	PHE
21	cw	123	ARG
21	cy	128	PHE
21	cC	128	PHE
21	cD	128	PHE
21	cF	128	PHE
21	cM	264	PRO
21	cN	128	PHE
24	cS	21	PRO
24	cT	21	PRO
4	cX	272	PRO
4	cX	359	THR
23	db	9	ASN
4	dd	181	SER
4	dd	359	THR
4	df	30	ASN
4	dk	272	PRO
4	dr	22	ASN
1	aR	258	PRO
1	bb	123	ASN
4	bD	185	ILE
8	bJ	96	SER
9	bN	34	ILE
14	bX	197	ASP
21	cp	128	PHE
21	cq	255	THR
21	cr	265	ASP
21	cs	84	ALA
21	ct	267	ALA
21	cz	128	PHE
21	cD	265	ASP
21	cE	265	ASP
21	cG	265	ASP
21	cH	128	PHE
21	cK	265	ASP
21	cN	265	ASP
24	cT	46	ASP
25	cV	25	ALA
4	cX	181	SER

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Mol	Chain	Res	Type
4	cZ	249	MET
4	cZ	272	PRO
23	db	10	PRO
4	df	181	SER
4	df	249	MET
4	dj	181	SER
4	dp	181	SER
4	dr	249	MET
1	aR	15	ASP
1	aT	102	GLY
1	bd	258	PRO
1	bl	123	ASN
1	bo	257	HIS
1	bt	258	PRO
2	bx	87	THR
11	bQ	92	ALA
14	bU	160	TRP
14	bW	197	ASP
14	bY	164	ASN
16	cg	89	GLY
21	cp	309	THR
21	cD	309	THR
24	cR	21	PRO
24	cS	47	VAL
24	cT	47	VAL
4	cX	249	MET
4	dd	249	MET
4	df	193	THR
4	dk	249	MET
4	dl	46	TYR
4	dl	366	GLN
4	dp	136	ARG
4	dr	181	SER
1	as	258	PRO
1	ax	257	HIS
1	aR	257	HIS
1	bk	257	HIS
2	bA	81	GLY
4	bD	249	MET
8	bI	96	SER
9	bL	34	ILE
14	bV	196	VAL

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Mol	Chain	Res	Type
14	bY	146	PRO
14	bY	197	ASP
4	cZ	136	ARG
4	dj	249	MET
1	ba	258	PRO
14	bT	167	GLY
1	bf	258	PRO
1	bi	258	PRO
11	bQ	88	PHE
14	ce	197	ASP
4	dd	193	THR
4	dl	249	MET
5	dq	358	VAL
1	ak	257	HIS
1	aQ	257	HIS
1	bb	257	HIS
3	bC	32	GLY
14	ca	197	ASP
21	cz	294	VAL
21	cJ	294	VAL
4	cZ	181	SER
4	df	136	ARG
4	dp	193	THR
4	dp	249	MET
4	dr	193	THR
1	aP	258	PRO
1	aY	257	HIS
1	aZ	257	HIS
2	bu	120	PRO
21	cw	102	PRO
4	dd	136	ARG

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	357/358 (100%)	357 (100%)	0	100	100
1	aB	357/358 (100%)	357 (100%)	0	100	100
1	aC	357/358 (100%)	357 (100%)	0	100	100
1	aD	356/358 (99%)	355 (100%)	1 (0%)	86	84
1	aE	357/358 (100%)	357 (100%)	0	100	100
1	aF	356/358 (99%)	356 (100%)	0	100	100
1	aG	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	aH	356/358 (99%)	356 (100%)	0	100	100
1	aI	357/358 (100%)	357 (100%)	0	100	100
1	aJ	357/358 (100%)	357 (100%)	0	100	100
1	aK	357/358 (100%)	355 (99%)	2 (1%)	78	79
1	aL	356/358 (99%)	356 (100%)	0	100	100
1	aM	357/358 (100%)	357 (100%)	0	100	100
1	aN	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	aO	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	aP	357/358 (100%)	357 (100%)	0	100	100
1	aQ	356/358 (99%)	356 (100%)	0	100	100
1	aR	357/358 (100%)	357 (100%)	0	100	100
1	aS	357/358 (100%)	357 (100%)	0	100	100
1	aT	357/358 (100%)	357 (100%)	0	100	100
1	aU	357/358 (100%)	357 (100%)	0	100	100
1	aV	357/358 (100%)	357 (100%)	0	100	100
1	aW	357/358 (100%)	357 (100%)	0	100	100
1	aX	357/358 (100%)	357 (100%)	0	100	100
1	aY	357/358 (100%)	357 (100%)	0	100	100
1	aZ	357/358 (100%)	357 (100%)	0	100	100
1	aa	356/358 (99%)	356 (100%)	0	100	100
1	ab	357/358 (100%)	354 (99%)	3 (1%)	73	76
1	ac	357/358 (100%)	357 (100%)	0	100	100
1	ad	357/358 (100%)	356 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ae	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	af	357/358 (100%)	357 (100%)	0	100	100
1	ag	357/358 (100%)	357 (100%)	0	100	100
1	ah	357/358 (100%)	357 (100%)	0	100	100
1	ai	357/358 (100%)	357 (100%)	0	100	100
1	aj	357/358 (100%)	357 (100%)	0	100	100
1	ak	357/358 (100%)	357 (100%)	0	100	100
1	al	356/358 (99%)	356 (100%)	0	100	100
1	am	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	an	356/358 (99%)	356 (100%)	0	100	100
1	ao	357/358 (100%)	357 (100%)	0	100	100
1	ap	357/358 (100%)	357 (100%)	0	100	100
1	aq	357/358 (100%)	357 (100%)	0	100	100
1	ar	356/358 (99%)	356 (100%)	0	100	100
1	as	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	at	357/358 (100%)	357 (100%)	0	100	100
1	au	356/358 (99%)	356 (100%)	0	100	100
1	av	357/358 (100%)	357 (100%)	0	100	100
1	aw	357/358 (100%)	357 (100%)	0	100	100
1	ax	356/358 (99%)	356 (100%)	0	100	100
1	ay	357/358 (100%)	357 (100%)	0	100	100
1	az	356/358 (99%)	356 (100%)	0	100	100
1	ba	357/358 (100%)	357 (100%)	0	100	100
1	bb	357/358 (100%)	357 (100%)	0	100	100
1	bc	357/358 (100%)	357 (100%)	0	100	100
1	bd	357/358 (100%)	357 (100%)	0	100	100
1	be	357/358 (100%)	357 (100%)	0	100	100
1	bf	357/358 (100%)	357 (100%)	0	100	100
1	bg	357/358 (100%)	357 (100%)	0	100	100
1	bh	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	bi	357/358 (100%)	356 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	bj	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	bk	357/358 (100%)	357 (100%)	0	100	100
1	bl	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	bm	357/358 (100%)	357 (100%)	0	100	100
1	bn	356/358 (99%)	355 (100%)	1 (0%)	86	84
1	bo	357/358 (100%)	357 (100%)	0	100	100
1	bp	357/358 (100%)	357 (100%)	0	100	100
1	bq	357/358 (100%)	357 (100%)	0	100	100
1	br	357/358 (100%)	356 (100%)	1 (0%)	86	84
1	bs	357/358 (100%)	357 (100%)	0	100	100
1	bt	357/358 (100%)	357 (100%)	0	100	100
2	bA	438/441 (99%)	437 (100%)	1 (0%)	87	87
2	bB	439/441 (100%)	439 (100%)	0	100	100
2	bu	439/441 (100%)	434 (99%)	5 (1%)	65	73
2	bv	439/441 (100%)	434 (99%)	5 (1%)	65	73
2	bw	439/441 (100%)	439 (100%)	0	100	100
2	bx	438/441 (99%)	435 (99%)	3 (1%)	76	77
2	by	439/441 (100%)	439 (100%)	0	100	100
2	bz	432/441 (98%)	430 (100%)	2 (0%)	81	81
3	bC	439/440 (100%)	439 (100%)	0	100	100
4	bD	344/346 (99%)	343 (100%)	1 (0%)	86	84
4	bF	344/346 (99%)	343 (100%)	1 (0%)	86	84
4	cX	343/346 (99%)	343 (100%)	0	100	100
4	cZ	343/346 (99%)	343 (100%)	0	100	100
4	dd	344/346 (99%)	344 (100%)	0	100	100
4	df	343/346 (99%)	343 (100%)	0	100	100
4	dj	344/346 (99%)	343 (100%)	1 (0%)	86	84
4	dk	344/346 (99%)	342 (99%)	2 (1%)	78	79
4	dl	344/346 (99%)	344 (100%)	0	100	100
4	dp	344/346 (99%)	344 (100%)	0	100	100
4	dr	344/346 (99%)	344 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	bE	349/353 (99%)	348 (100%)	1 (0%)	86	84
5	cY	349/353 (99%)	347 (99%)	2 (1%)	78	79
5	de	349/353 (99%)	347 (99%)	2 (1%)	78	79
5	dq	349/353 (99%)	348 (100%)	1 (0%)	86	84
6	bG	424/446 (95%)	424 (100%)	0	100	100
7	bH	345/479 (72%)	344 (100%)	1 (0%)	86	84
8	bI	116/144 (81%)	116 (100%)	0	100	100
8	bJ	122/144 (85%)	122 (100%)	0	100	100
8	bK	93/144 (65%)	93 (100%)	0	100	100
9	bL	59/161 (37%)	59 (100%)	0	100	100
9	bM	59/161 (37%)	58 (98%)	1 (2%)	53	67
9	bN	58/161 (36%)	57 (98%)	1 (2%)	53	67
9	bO	58/161 (36%)	58 (100%)	0	100	100
10	bP	121/125 (97%)	121 (100%)	0	100	100
11	bQ	140/188 (74%)	139 (99%)	1 (1%)	76	77
12	bR	136/148 (92%)	136 (100%)	0	100	100
13	bS	164/179 (92%)	164 (100%)	0	100	100
14	bT	40/181 (22%)	40 (100%)	0	100	100
14	bU	47/181 (26%)	47 (100%)	0	100	100
14	bV	46/181 (25%)	46 (100%)	0	100	100
14	bW	45/181 (25%)	45 (100%)	0	100	100
14	bX	35/181 (19%)	35 (100%)	0	100	100
14	bY	62/181 (34%)	62 (100%)	0	100	100
14	bZ	45/181 (25%)	45 (100%)	0	100	100
14	ca	45/181 (25%)	45 (100%)	0	100	100
14	cb	45/181 (25%)	45 (100%)	0	100	100
14	cc	72/181 (40%)	71 (99%)	1 (1%)	59	70
14	cd	63/181 (35%)	62 (98%)	1 (2%)	55	68
14	ce	60/181 (33%)	60 (100%)	0	100	100
15	cf	70/139 (50%)	70 (100%)	0	100	100
16	cg	51/79 (65%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	ch	142/145 (98%)	142 (100%)	0	100	100
18	ci	47/63 (75%)	46 (98%)	1 (2%)	47	64
19	cj	51/70 (73%)	51 (100%)	0	100	100
19	ck	49/70 (70%)	49 (100%)	0	100	100
19	cl	47/70 (67%)	47 (100%)	0	100	100
19	cm	54/70 (77%)	54 (100%)	0	100	100
20	cn	84/130 (65%)	84 (100%)	0	100	100
20	co	78/130 (60%)	78 (100%)	0	100	100
21	cA	245/339 (72%)	245 (100%)	0	100	100
21	cB	257/339 (76%)	257 (100%)	0	100	100
21	cC	245/339 (72%)	245 (100%)	0	100	100
21	cD	257/339 (76%)	257 (100%)	0	100	100
21	cE	246/339 (73%)	246 (100%)	0	100	100
21	cF	257/339 (76%)	256 (100%)	1 (0%)	84	83
21	cG	248/339 (73%)	248 (100%)	0	100	100
21	cH	257/339 (76%)	257 (100%)	0	100	100
21	cI	245/339 (72%)	245 (100%)	0	100	100
21	cJ	257/339 (76%)	257 (100%)	0	100	100
21	cK	245/339 (72%)	245 (100%)	0	100	100
21	cL	257/339 (76%)	257 (100%)	0	100	100
21	cM	243/339 (72%)	243 (100%)	0	100	100
21	cN	257/339 (76%)	257 (100%)	0	100	100
21	cp	257/339 (76%)	257 (100%)	0	100	100
21	cq	248/339 (73%)	247 (100%)	1 (0%)	84	83
21	cr	257/339 (76%)	257 (100%)	0	100	100
21	cs	241/339 (71%)	241 (100%)	0	100	100
21	ct	257/339 (76%)	257 (100%)	0	100	100
21	cu	246/339 (73%)	246 (100%)	0	100	100
21	cv	257/339 (76%)	257 (100%)	0	100	100
21	cw	246/339 (73%)	246 (100%)	0	100	100
21	cx	257/339 (76%)	257 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	cy	246/339 (73%)	245 (100%)	1 (0%)	84	83
21	cz	257/339 (76%)	257 (100%)	0	100	100
22	cO	22/1123 (2%)	22 (100%)	0	100	100
22	cQ	25/1123 (2%)	24 (96%)	1 (4%)	28	52
22	da	24/1123 (2%)	24 (100%)	0	100	100
22	dc	22/1123 (2%)	22 (100%)	0	100	100
22	dg	26/1123 (2%)	26 (100%)	0	100	100
22	di	22/1123 (2%)	22 (100%)	0	100	100
22	ds	25/1123 (2%)	25 (100%)	0	100	100
22	du	24/1123 (2%)	24 (100%)	0	100	100
23	cP	24/1147 (2%)	24 (100%)	0	100	100
23	db	19/1147 (2%)	18 (95%)	1 (5%)	20	45
23	dh	26/1147 (2%)	25 (96%)	1 (4%)	29	53
23	dt	24/1147 (2%)	24 (100%)	0	100	100
24	cR	359/360 (100%)	359 (100%)	0	100	100
24	cS	359/360 (100%)	359 (100%)	0	100	100
24	cT	359/360 (100%)	359 (100%)	0	100	100
25	cU	30/1015 (3%)	30 (100%)	0	100	100
25	cV	28/1015 (3%)	28 (100%)	0	100	100
25	cW	29/1015 (3%)	29 (100%)	0	100	100
26	dm	17/1144 (2%)	16 (94%)	1 (6%)	18	43
26	dn	19/1144 (2%)	18 (95%)	1 (5%)	20	45
26	do	19/1144 (2%)	17 (90%)	2 (10%)	6	26
All	All	45770/70345 (65%)	45707 (100%)	63 (0%)	87	89

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ab	104	ARG
1	ab	256	ASN
1	ab	419	LYS
1	ad	67	ILE
1	ae	32	ARG
1	am	256	ASN

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Mol	Chain	Res	Type
1	as	256	ASN
1	aD	119	LEU
1	aG	256	ASN
1	aK	145	LYS
1	aK	419	LYS
1	aN	363	ARG
1	aO	119	LEU
1	bh	98	LEU
1	bi	78	LYS
1	bj	78	LYS
1	bl	63	ASN
1	bn	419	LYS
1	br	419	LYS
2	bu	33	ARG
2	bu	291	LYS
2	bu	344	TRP
2	bu	374	GLU
2	bu	442	GLN
2	bv	33	ARG
2	bv	231	ARG
2	bv	362	ARG
2	bv	374	GLU
2	bv	442	GLN
2	bx	231	ARG
2	bx	291	LYS
2	bx	374	GLU
2	bz	193	GLU
2	bz	231	ARG
2	bA	179	ARG
4	bD	200	ILE
5	bE	143	LYS
4	bF	370	LEU
7	bH	319	LEU
9	bM	38	LYS
9	bN	38	LYS
11	bQ	183	LYS
14	cc	134	PRO
14	cd	172	ASN
18	ci	47	VAL
21	cq	289	LYS
21	cy	211	VAL
21	cF	70	ASN

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Mol	Chain	Res	Type
22	cQ	27	TYR
5	cY	74	LEU
5	cY	143	LYS
23	db	28	VAL
5	de	143	LYS
5	de	374	THR
23	dh	14	ARG
4	dj	66	VAL
4	dk	62	PHE
4	dk	370	LEU
26	dm	20	VAL
26	dn	20	VAL
26	do	20	VAL
26	do	24	ASN
5	dq	143	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (359) such sidechains are listed below:

Mol	Chain	Res	Type
1	aa	265	ASN
1	aa	267	ASN
1	aa	415	ASN
1	ab	221	GLN
1	ab	309	GLN
1	ab	415	ASN
1	ac	94	GLN
1	ac	415	ASN
1	ad	21	ASN
1	ad	341	GLN
1	ae	309	GLN
1	ae	323	GLN
1	af	271	ASN
1	af	274	GLN
1	af	415	ASN
1	ag	257	HIS
1	ah	63	ASN
1	ah	256	ASN
1	ah	257	HIS
1	ah	323	GLN
1	ah	415	ASN
1	ai	103	GLN
1	aj	123	ASN

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Mol	Chain	Res	Type
1	aj	157	GLN
1	aj	256	ASN
1	aj	267	ASN
1	aj	341	GLN
1	ak	256	ASN
1	ak	415	ASN
1	ak	420	ASN
1	al	43	GLN
1	al	63	ASN
1	al	123	ASN
1	al	267	ASN
1	al	415	ASN
1	am	94	GLN
1	am	103	GLN
1	am	182	GLN
1	am	187	ASN
1	am	265	ASN
1	am	267	ASN
1	am	415	ASN
1	an	267	ASN
1	an	319	GLN
1	an	415	ASN
1	ao	250	ASN
1	ao	267	ASN
1	ao	323	GLN
1	ao	338	GLN
1	ap	265	ASN
1	ap	268	ASN
1	ap	341	GLN
1	ap	415	ASN
1	aq	47	ASN
1	aq	128	ASN
1	aq	187	ASN
1	ar	47	ASN
1	ar	265	ASN
1	ar	415	ASN
1	as	59	GLN
1	as	157	GLN
1	as	256	ASN
1	as	338	GLN
1	at	187	ASN
1	at	323	GLN

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Mol	Chain	Res	Type
1	au	63	ASN
1	au	137	ASN
1	au	156	ASN
1	av	323	GLN
1	av	335	ASN
1	av	415	ASN
1	aw	267	ASN
1	aw	271	ASN
1	aw	274	GLN
1	aw	415	ASN
1	ax	265	ASN
1	ax	267	ASN
1	ay	63	ASN
1	ay	187	ASN
1	ay	415	ASN
1	az	415	ASN
1	aA	137	ASN
1	aA	157	GLN
1	aA	187	ASN
1	aA	254	ASN
1	aB	123	ASN
1	aB	187	ASN
1	aB	256	ASN
1	aB	265	ASN
1	aB	267	ASN
1	aB	415	ASN
1	aC	128	ASN
1	aC	232	GLN
1	aC	249	GLN
1	aC	420	ASN
1	aD	187	ASN
1	aD	256	ASN
1	aE	254	ASN
1	aE	256	ASN
1	aF	47	ASN
1	aF	59	GLN
1	aF	128	ASN
1	aF	157	GLN
1	aF	338	GLN
1	aF	415	ASN
1	aG	63	ASN
1	aG	128	ASN

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Mol	Chain	Res	Type
1	aG	187	ASN
1	aG	250	ASN
1	aG	256	ASN
1	aG	321	ASN
1	aH	144	GLN
1	aH	187	ASN
1	aI	267	ASN
1	aI	309	GLN
1	aI	338	GLN
1	aI	415	ASN
1	aJ	47	ASN
1	aJ	59	GLN
1	aJ	108	HIS
1	aJ	128	ASN
1	aJ	157	GLN
1	aJ	187	ASN
1	aJ	323	GLN
1	aJ	415	ASN
1	aK	214	GLN
1	aL	187	ASN
1	aL	341	GLN
1	aL	415	ASN
1	aM	319	GLN
1	aM	415	ASN
1	aN	250	ASN
1	aN	415	ASN
1	aO	338	GLN
1	aP	144	GLN
1	aP	309	GLN
1	aQ	128	ASN
1	aQ	157	GLN
1	aQ	187	ASN
1	aQ	268	ASN
1	aR	187	ASN
1	aR	265	ASN
1	aR	267	ASN
1	aR	415	ASN
1	aS	108	HIS
1	aS	309	GLN
1	aS	338	GLN
1	aS	376	ASN
1	aS	415	ASN

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Mol	Chain	Res	Type
1	aT	137	ASN
1	aT	254	ASN
1	aT	267	ASN
1	aT	415	ASN
1	aU	267	ASN
1	aU	309	GLN
1	aU	415	ASN
1	aU	437	ASN
1	aV	256	ASN
1	aV	319	GLN
1	aV	321	ASN
1	aV	415	ASN
1	aW	94	GLN
1	aW	420	ASN
1	aY	265	ASN
1	aY	323	GLN
1	aY	415	ASN
1	ba	47	ASN
1	bb	123	ASN
1	bb	157	GLN
1	bb	415	ASN
1	bc	267	ASN
1	bc	309	GLN
1	bc	319	GLN
1	bd	415	ASN
1	be	47	ASN
1	be	59	GLN
1	be	256	ASN
1	be	415	ASN
1	bf	309	GLN
1	bg	256	ASN
1	bg	267	ASN
1	bh	43	GLN
1	bh	63	ASN
1	bh	137	ASN
1	bi	415	ASN
1	bj	14	GLN
1	bj	214	GLN
1	bj	250	ASN
1	bj	254	ASN
1	bj	341	GLN
1	bk	256	ASN

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Mol	Chain	Res	Type
1	bk	364	GLN
1	bl	63	ASN
1	bm	63	ASN
1	bm	144	GLN
1	bm	187	ASN
1	bm	224	HIS
1	bm	267	ASN
1	bm	415	ASN
1	bn	256	ASN
1	bn	309	GLN
1	bo	338	GLN
1	bo	341	GLN
1	bo	415	ASN
1	bp	267	ASN
1	bq	14	GLN
1	bq	364	GLN
1	br	415	ASN
1	br	437	ASN
1	bs	94	GLN
1	bs	230	GLN
1	bs	267	ASN
1	bs	338	GLN
1	bs	341	GLN
1	bs	364	GLN
1	bt	250	ASN
2	bu	361	ASN
2	bu	485	GLN
2	bv	36	ASN
2	bv	242	ASN
2	bw	403	ASN
2	bx	92	ASN
2	bx	483	GLN
2	by	276	GLN
2	by	403	ASN
2	by	447	HIS
2	bz	370	HIS
2	bA	485	GLN
2	bB	276	GLN
2	bB	341	GLN
2	bB	370	HIS
2	bB	483	GLN
4	bD	14	GLN

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Mol	Chain	Res	Type
4	bD	30	ASN
4	bD	116	HIS
4	bD	288	GLN
5	bE	131	ASN
6	bG	56	ASN
6	bG	77	GLN
6	bG	311	GLN
6	bG	357	GLN
6	bG	414	ASN
6	bG	518	HIS
7	bH	186	GLN
7	bH	462	HIS
7	bH	517	ASN
8	bJ	114	GLN
9	bL	17	HIS
13	bS	124	ASN
13	bS	166	GLN
14	bZ	202	GLN
14	cb	166	GLN
14	cb	202	GLN
14	cd	152	GLN
14	cd	166	GLN
17	ch	89	ASN
19	cl	33	GLN
19	cm	48	GLN
20	cn	111	ASN
20	co	70	ASN
21	cp	333	GLN
21	cq	234	HIS
21	cr	331	GLN
21	cs	65	ASN
21	cs	122	GLN
21	cs	253	ASN
21	cs	293	ASN
21	cs	302	GLN
21	cs	337	ASN
21	ct	295	ASN
21	ct	331	GLN
21	cu	69	ASN
21	cu	122	GLN
21	cu	234	HIS
21	cu	331	GLN

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Mol	Chain	Res	Type
21	cv	52	ASN
21	cv	234	HIS
21	cv	331	GLN
21	cv	333	GLN
21	cw	122	GLN
21	cw	308	ASN
21	cx	60	ASN
21	cx	234	HIS
21	cx	331	GLN
21	cz	287	ASN
21	cz	331	GLN
21	cA	229	ASN
21	cA	234	HIS
21	cA	331	GLN
21	cB	256	ASN
21	cB	302	GLN
21	cC	234	HIS
21	cC	331	GLN
21	cD	171	ASN
21	cD	331	GLN
21	cE	122	GLN
21	cE	229	ASN
21	cE	295	ASN
21	cE	302	GLN
21	cE	331	GLN
21	cF	171	ASN
21	cF	331	GLN
21	cH	331	GLN
21	cK	69	ASN
21	cK	331	GLN
21	cL	94	ASN
21	cL	263	ASN
21	cL	331	GLN
21	cM	234	HIS
21	cM	240	ASN
21	cM	331	GLN
21	cN	122	GLN
21	cN	331	GLN
23	cP	9	ASN
23	cP	32	ASN
22	cQ	31	ASN
24	cR	215	HIS

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Mol	Chain	Res	Type
24	cR	376	ASN
24	cR	393	GLN
24	cS	35	ASN
24	cS	280	GLN
24	cS	349	ASN
24	cS	400	ASN
24	cT	56	ASN
24	cT	349	ASN
24	cT	393	GLN
25	cU	20	ASN
25	cV	33	ASN
25	cW	20	ASN
4	cX	37	ASN
4	cX	239	GLN
4	cX	244	ASN
5	cY	307	GLN
4	cZ	244	ASN
23	db	32	ASN
4	dd	244	ASN
4	dd	288	GLN
4	df	50	ASN
4	df	116	HIS
4	df	133	ASN
23	dh	7	ASN
23	dh	9	ASN
4	dj	116	HIS
4	dj	129	ASN
4	dj	239	GLN
4	dj	275	ASN
4	dj	309	GLN
4	dk	239	GLN
4	dk	244	ASN
4	dl	30	ASN
4	dl	244	ASN
4	dl	309	GLN
26	dn	17	GLN
4	dp	48	ASN
4	dp	244	ASN
4	dr	22	ASN
4	dr	30	ASN
22	ds	37	GLN
23	dt	7	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

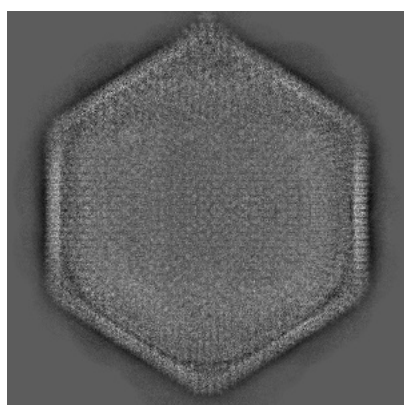
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34438. These allow visual inspection of the internal detail of the map and identification of artifacts.

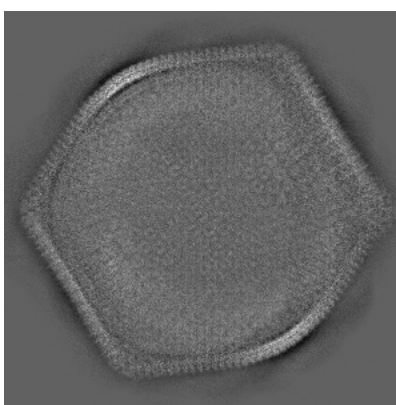
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

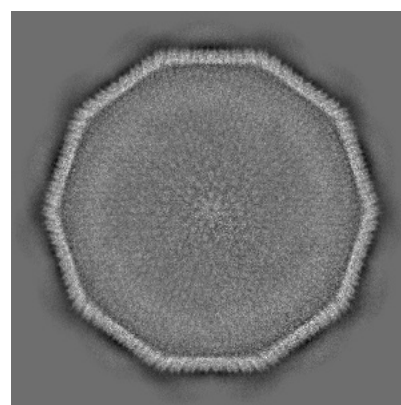
6.1.1 Primary map



X



Y

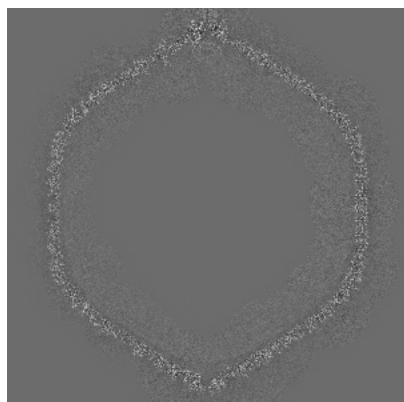


Z

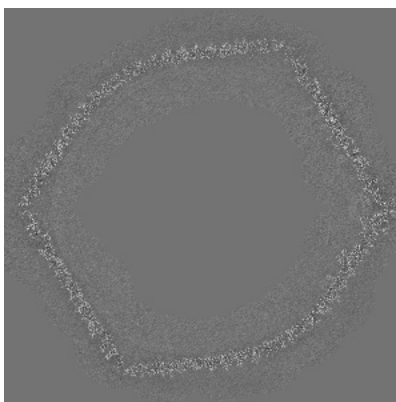
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

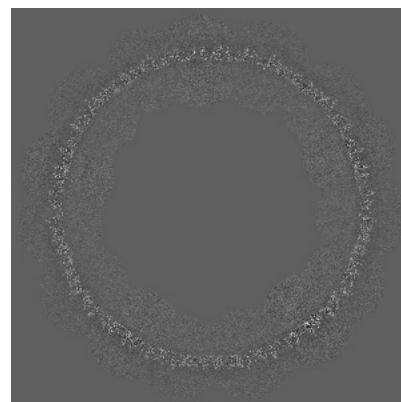
6.2.1 Primary map



X Index: 600



Y Index: 600

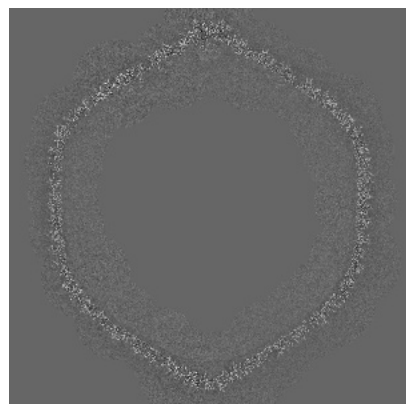


Z Index: 600

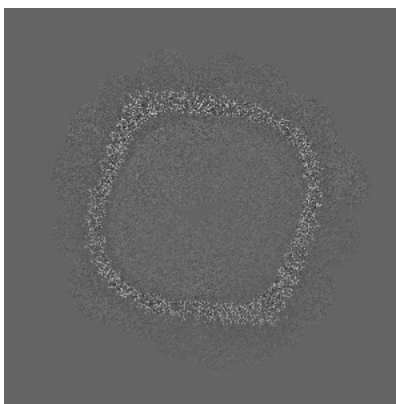
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

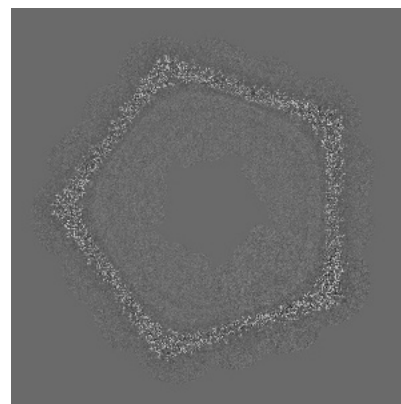
6.3.1 Primary map



X Index: 628



Y Index: 257

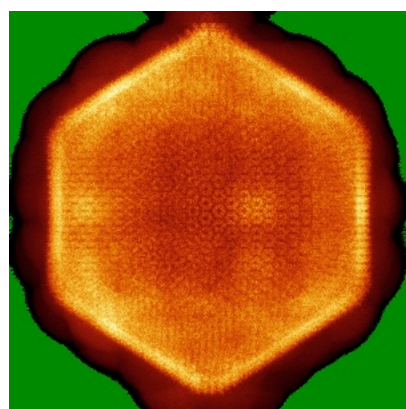


Z Index: 320

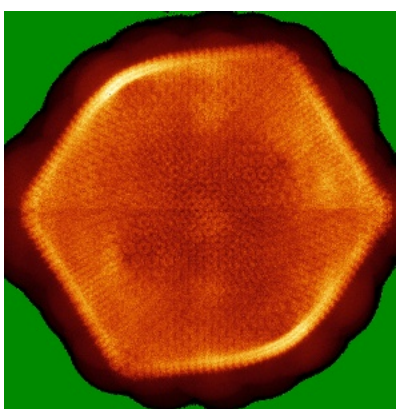
The images above show the largest variance slices of the map in three orthogonal directions.

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

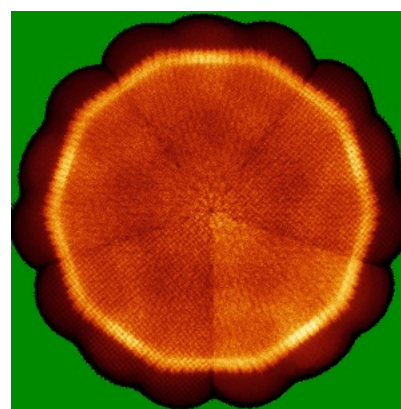
6.4.1 Primary map



X



Y

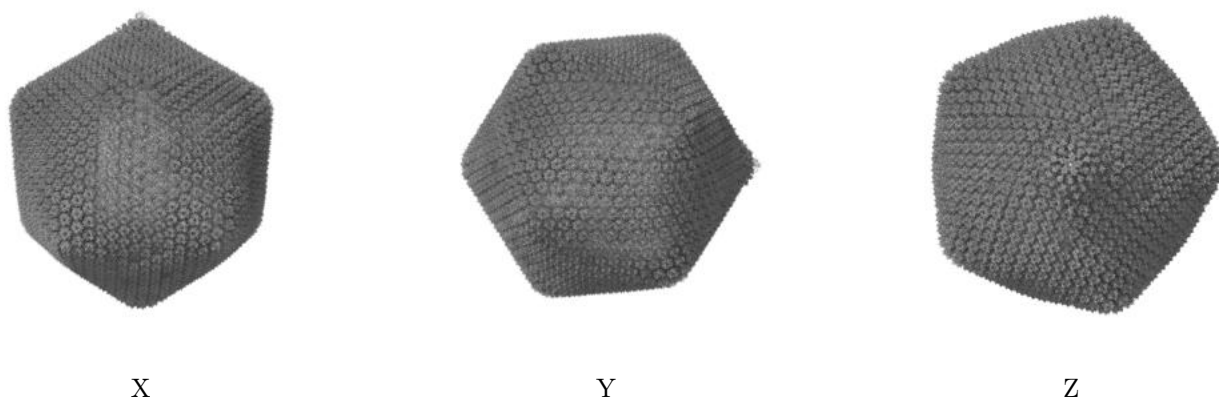


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

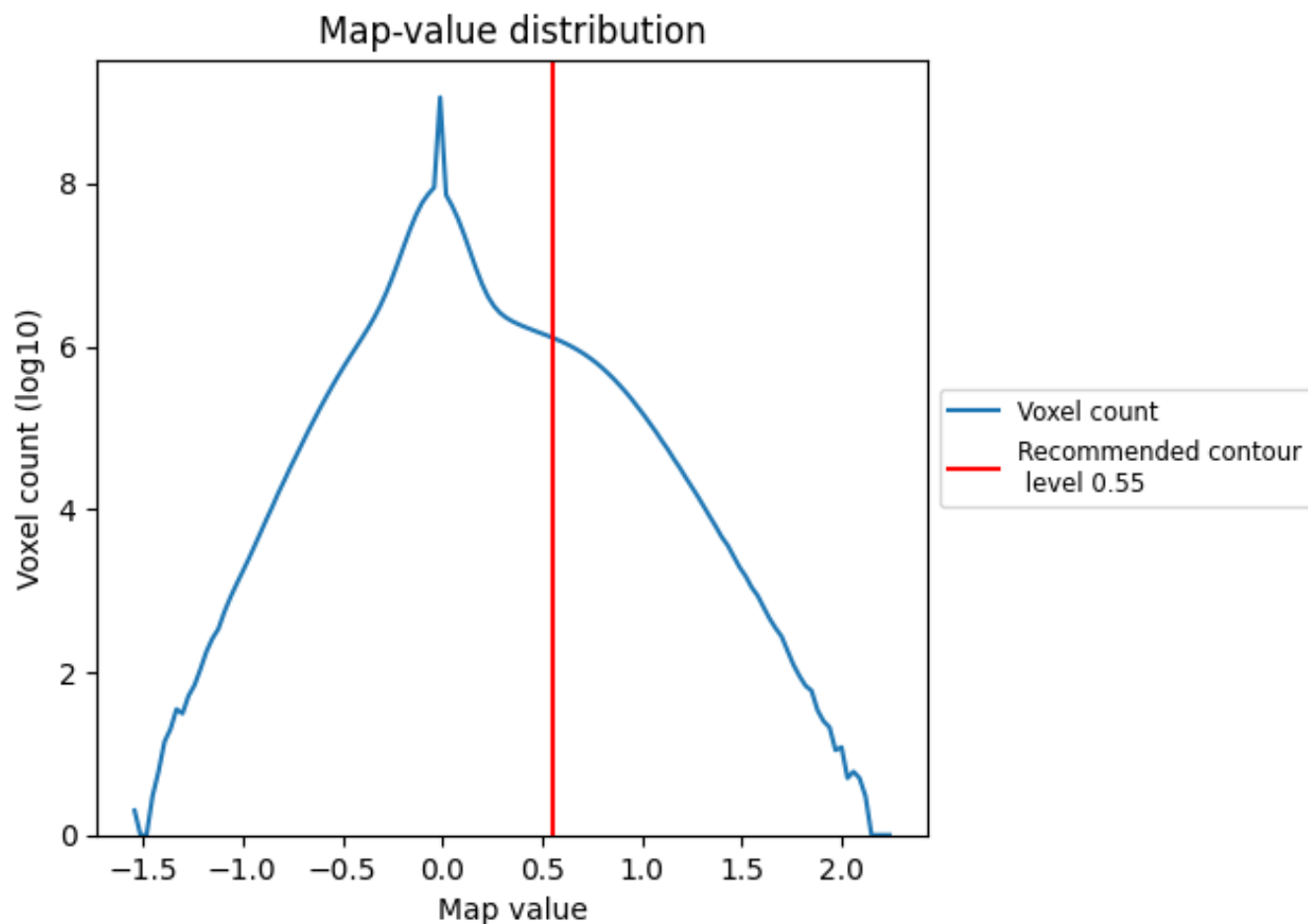
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

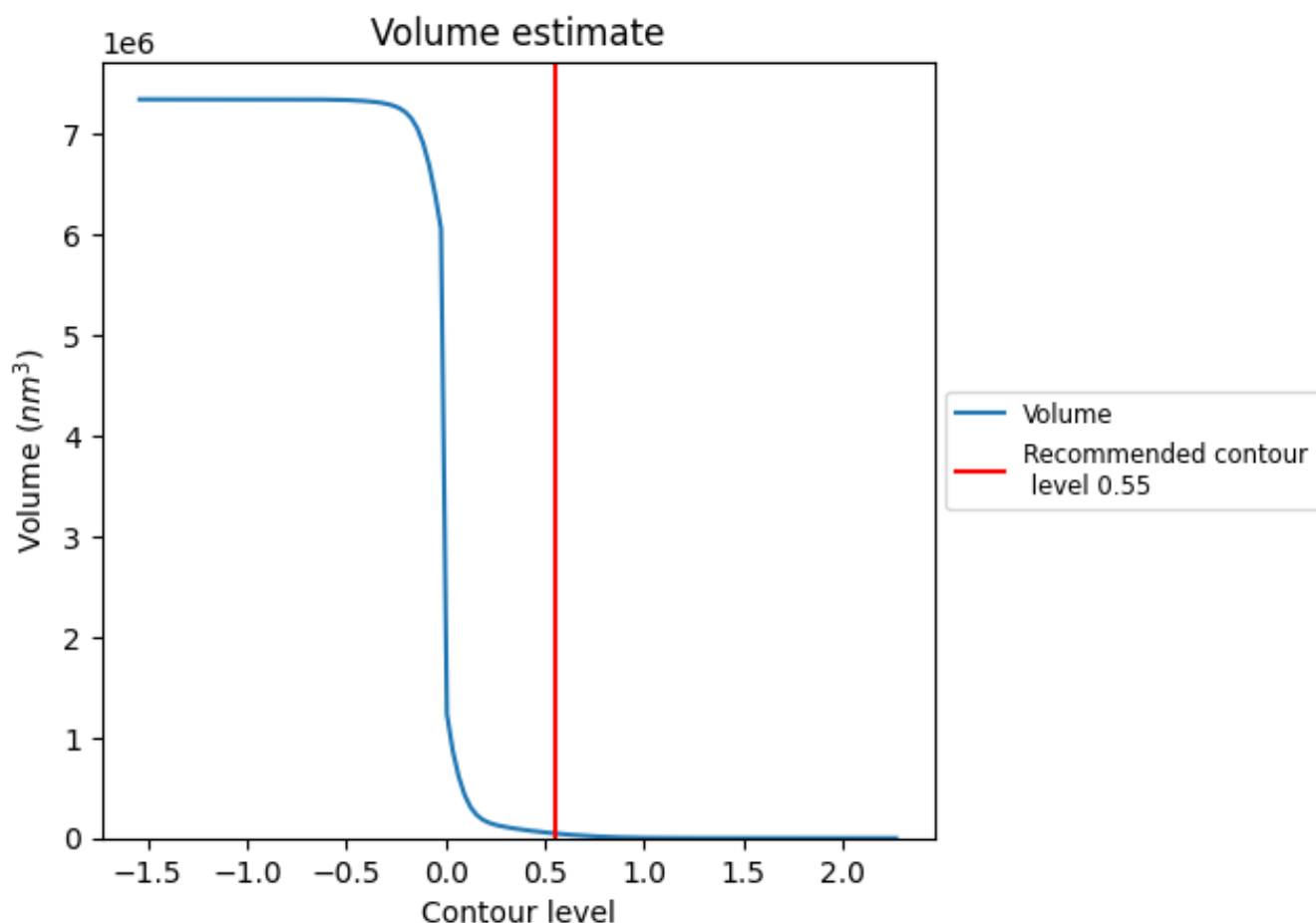
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

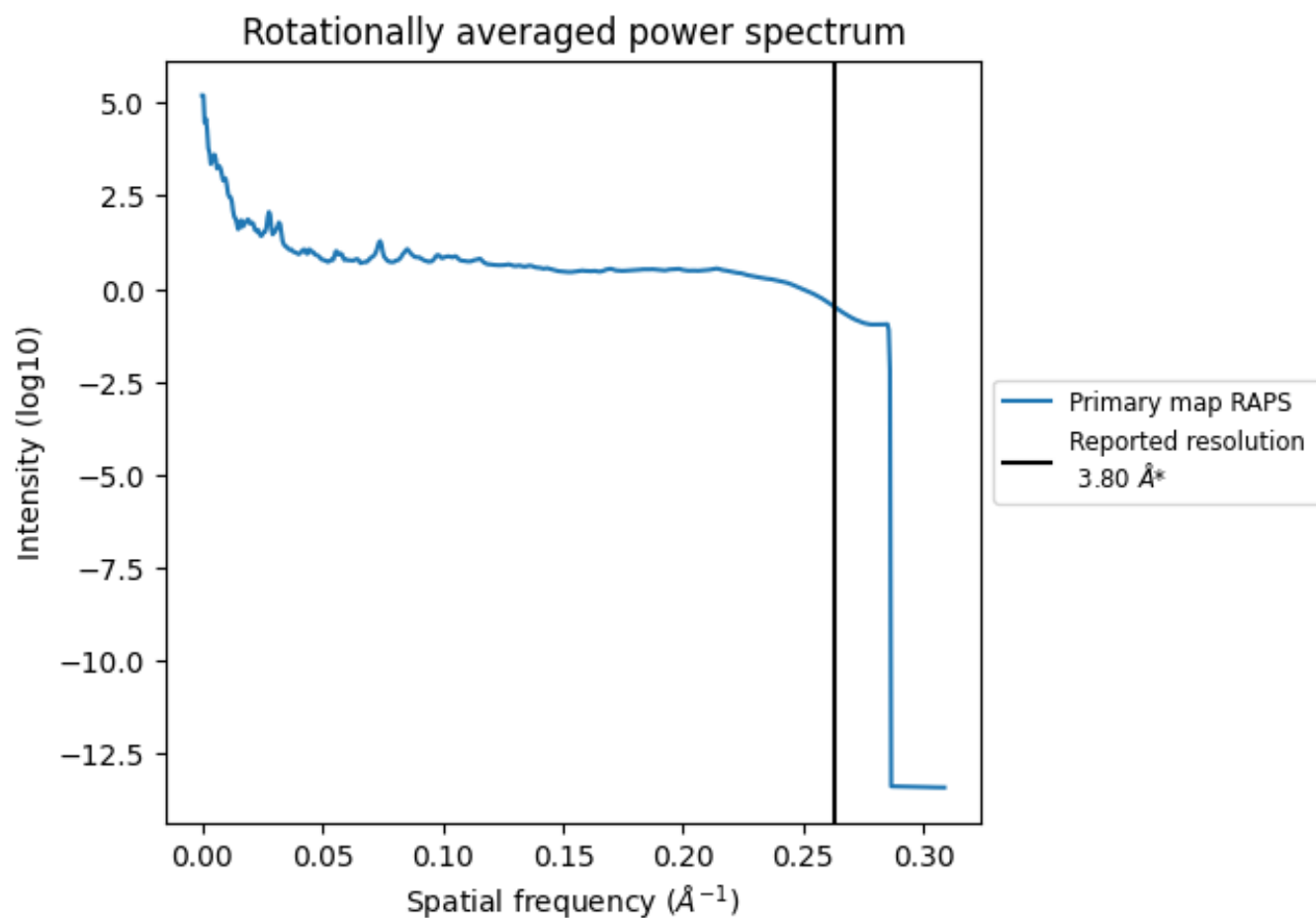
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46843 nm³; this corresponds to an approximate mass of 42315 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34438 and PDB model 8H2I. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)

This section was not generated.

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



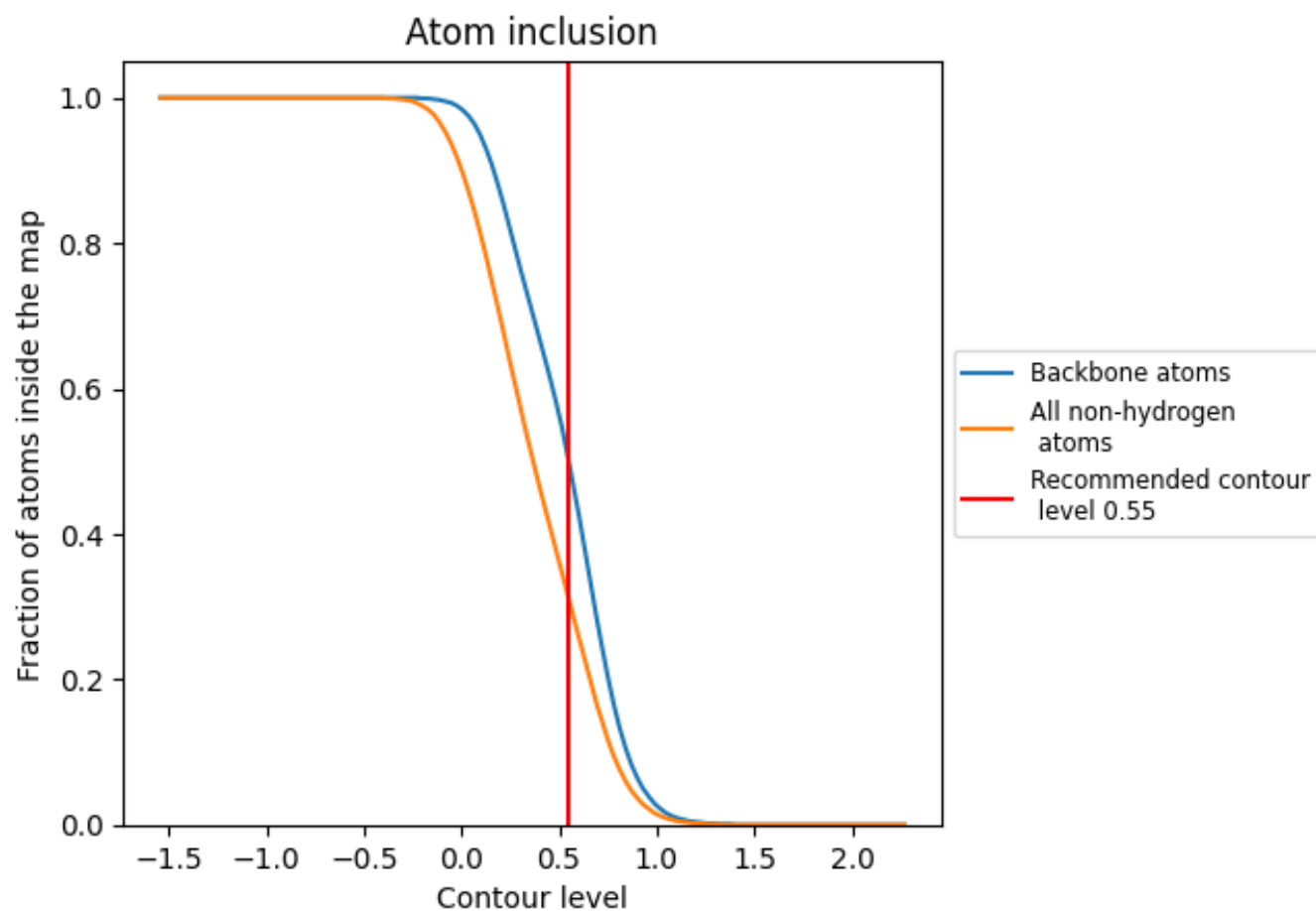
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 31% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3110	 0.3620
aA	 0.2580	 0.3860
aB	 0.2670	 0.3810
aC	 0.2860	 0.3790
aD	 0.2940	 0.3800
aE	 0.3830	 0.4000
aF	 0.4160	 0.3950
aG	 0.3710	 0.3900
aH	 0.4420	 0.4010
aI	 0.4390	 0.4000
aJ	 0.4140	 0.3930
aK	 0.3900	 0.3960
aL	 0.3660	 0.3930
aM	 0.3610	 0.3940
aN	 0.3690	 0.3970
aO	 0.3660	 0.3900
aP	 0.3750	 0.3960
aQ	 0.3370	 0.3910
aR	 0.3310	 0.3900
aS	 0.3510	 0.3970
aT	 0.3660	 0.3910
aU	 0.3800	 0.3960
aV	 0.3800	 0.3970
aW	 0.3310	 0.3900
aX	 0.3340	 0.3900
aY	 0.3320	 0.3900
aZ	 0.3520	 0.3910
aa	 0.4210	 0.3970
ab	 0.4250	 0.3940
ac	 0.4330	 0.4050
ad	 0.4340	 0.3980
ae	 0.4250	 0.4010
af	 0.4220	 0.4010
ag	 0.4150	 0.3910
ah	 0.4500	 0.4050



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Chain	Atom inclusion	Q-score
ai	0.4230	0.3990
aj	0.3020	0.3830
ak	0.3610	0.3940
al	0.2940	0.3800
am	0.4340	0.3980
an	0.4370	0.3950
ao	0.4260	0.3960
ap	0.4430	0.3980
aq	0.4620	0.3980
ar	0.4610	0.4010
as	0.4250	0.3900
at	0.3850	0.3990
au	0.3930	0.4020
av	0.3320	0.3890
aw	0.3030	0.3940
ax	0.3480	0.3980
ay	0.2330	0.3780
az	0.2220	0.3830
bA	0.3620	0.3680
bB	0.2710	0.3590
bC	0.3450	0.3730
bD	0.2300	0.3510
bE	0.2900	0.3580
bF	0.2640	0.3460
bG	0.3260	0.3190
bH	0.3210	0.3860
bI	0.3010	0.3470
bJ	0.3120	0.3430
bK	0.3060	0.3660
bL	0.2550	0.2560
bM	0.2370	0.2780
bN	0.2580	0.2770
bO	0.2130	0.2690
bP	0.2440	0.3230
bQ	0.2140	0.3340
bR	0.3370	0.3500
bS	0.3120	0.3890
bT	0.3150	0.3600
bU	0.4400	0.3720
bV	0.3780	0.3510
bW	0.3780	0.3380
bX	0.3420	0.3510

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Chain	Atom inclusion	Q-score
bY	 0.2230	 0.3100
bZ	 0.1960	 0.3360
ba	 0.3790	 0.3920
bb	 0.3440	 0.3980
bc	 0.3710	 0.3880
bd	 0.3590	 0.3920
be	 0.3650	 0.3910
bf	 0.3860	 0.3930
bg	 0.3700	 0.3880
bh	 0.3880	 0.3900
bi	 0.3690	 0.3950
bj	 0.3390	 0.3920
bk	 0.3720	 0.3900
bl	 0.3490	 0.3960
bm	 0.3400	 0.3930
bn	 0.3350	 0.4010
bo	 0.3390	 0.3910
bp	 0.3670	 0.3890
bq	 0.3350	 0.3870
br	 0.3990	 0.3920
bs	 0.3730	 0.3880
bt	 0.3840	 0.3930
bu	 0.4830	 0.3820
bv	 0.4510	 0.3760
bw	 0.4610	 0.3780
bx	 0.4270	 0.3790
by	 0.4070	 0.3760
bz	 0.4050	 0.3700
cA	 0.0000	 0.1280
cB	 0.0590	 0.2680
cC	 0.0010	 0.2080
cD	 0.0220	 0.2300
cE	 0.0380	 0.2070
cF	 0.1190	 0.2600
cG	 0.0270	 0.1770
cH	 0.2280	 0.2810
cI	 0.0090	 0.2100
cJ	 0.1480	 0.2890
cK	 0.0010	 0.1880
cL	 0.0800	 0.2810
cM	 0.0000	 0.1290
cN	 0.0110	 0.2370

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Chain	Atom inclusion	Q-score
cO	 0.0000	 0.4580
cP	 0.0080	 0.4540
cQ	 0.0130	 0.4490
cR	 0.2880	 0.3690
cS	 0.3090	 0.3610
cT	 0.2750	 0.3470
cU	 0.1420	 0.4210
cV	 0.1580	 0.4140
cW	 0.1700	 0.4200
cX	 0.3110	 0.3360
cY	 0.2550	 0.3320
cZ	 0.3020	 0.3400
ca	 0.2260	 0.3680
cb	 0.2460	 0.3550
cc	 0.2610	 0.3240
cd	 0.2650	 0.3370
ce	 0.3120	 0.3590
cf	 0.3640	 0.3430
cg	 0.1610	 0.3070
ch	 0.3600	 0.3560
ci	 0.4020	 0.3530
cj	 0.2720	 0.3750
ck	 0.2080	 0.3810
cl	 0.2500	 0.3610
cm	 0.2690	 0.3710
cn	 0.2410	 0.3910
co	 0.2670	 0.3680
cp	 0.0240	 0.2540
cq	 0.0000	 0.1670
cr	 0.0610	 0.2610
cs	 0.0020	 0.1780
ct	 0.0520	 0.2710
cu	 0.0010	 0.1850
cv	 0.1610	 0.2950
cw	 0.1090	 0.2620
cx	 0.2120	 0.2930
cy	 0.0350	 0.2420
cz	 0.0110	 0.2100
da	 0.0880	 0.4680
db	 0.1110	 0.4280
dc	 0.1120	 0.4710
dd	 0.2410	 0.3720

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Chain	Atom inclusion	Q-score
de	 0.2250	 0.3630
df	 0.2390	 0.3680
dg	 0.0080	 0.4510
dh	 0.0080	 0.4250
di	 0.0000	 0.4400
dj	 0.2870	 0.3620
dk	 0.2660	 0.3550
dl	 0.2990	 0.3340
dm	 0.0000	 0.3540
dn	 0.0110	 0.3860
do	 0.0000	 0.3280
dp	 0.3010	 0.3750
dq	 0.2960	 0.3750
dr	 0.3090	 0.3720
ds	 0.0300	 0.4410
dt	 0.0170	 0.4570
du	 0.0040	 0.4400