Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 01:43 PM JST

PDB ID	:	5ZAP
EMDB ID	:	EMD-6907
Title	:	Atomic structure of the herpes simplex virus type 2 B-capsid
Authors	:	Yuan, S.; Wang, J.L.; Zhu, D.J.; Wang, N.; Gao, Q.; Chen, W.Y.; Tang, H.; Wang, J.Z.; Zhang, X.Z.; Liu, H.R.; Rao, Z.H.; Wang, X.X.
Deposited on	:	2018-02-08
Resolution	:	3.10 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:

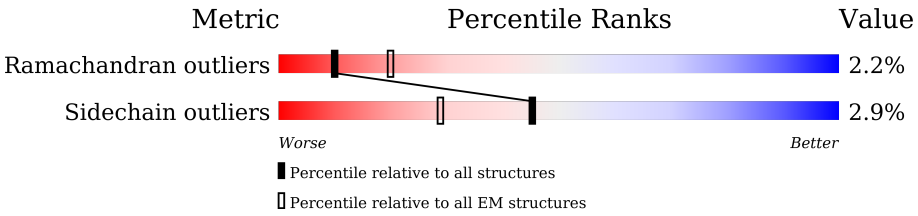
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1374	19% 95%
1	B	1374	16% 93%
1	C	1374	15% 95%
1	D	1374	18% 94% 5%
1	E	1374	18% 95%
1	F	1374	15% 95%
1	G	1374	48% 93% 5%
1	H	1374	21% 95%
1	I	1374	14% 94%

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Mol	Chain	Length	Quality of chain
1	J	1374	22% 93% 6%
1	K	1374	11% 92% 6%
1	L	1374	12% 93% 6%
1	M	1374	13% 91% 8%
1	N	1374	16% 93% 6%
1	O	1374	14% 92% 6%
1	P	1374	14% 93% 6%
2	Q	318	65% 91% 6%
2	R	318	72% 90% 6%
2	T	318	40% 91% 6%
2	U	318	37% 90% 6%
2	W	318	42% 92% 6%
2	X	318	39% 92% 5%
2	Z	318	41% 88% 6% 6%
2	a	318	44% 87% 8%
2	c	318	36% 92% 6%
2	d	318	30% 90% 6%
3	S	466	59% 63% 7% 29%
3	V	466	52% 65% 8% 26%
3	Y	466	51% 63% 10% 26%
3	b	466	51% 60% 12% 26%
3	e	466	50% 64% 8% 26%
4	f	112	80% 66% 25%
4	g	112	91% 70% 23%
4	h	112	92% 71% 21%

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Mol	Chain	Length	Quality of chain
4	i	112	88% 71% 21%
4	j	112	91% 71% 21%
4	k	112	89% 69% 24%
4	l	112	88% 71% 21%
4	m	112	94% 71% 22%
4	n	112	93% 71% 22%
4	o	112	92% 70% 21%
4	p	112	87% 71% 22%
4	q	112	88% 71% 22%
4	r	112	88% 66% 27%
4	s	112	90% 72% 21%
4	t	112	88% 70% 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 205925 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	1365	Total	C	N	O	S	0	0
			10104	6424	1819	1807	54		
1	A	1365	Total	C	N	O	S	0	0
			10160	6460	1837	1809	54		
1	B	1350	Total	C	N	O	S	0	0
			10105	6411	1825	1815	54		
1	C	1362	Total	C	N	O	S	0	0
			10220	6484	1852	1829	55		
1	D	1362	Total	C	N	O	S	0	0
			10229	6488	1849	1837	55		
1	E	1362	Total	C	N	O	S	0	0
			10233	6490	1853	1835	55		
1	F	1362	Total	C	N	O	S	0	0
			10239	6494	1857	1833	55		
1	H	1362	Total	C	N	O	S	0	0
			10245	6498	1851	1841	55		
1	I	1361	Total	C	N	O	S	0	0
			10239	6494	1850	1840	55		
1	J	1362	Total	C	N	O	S	0	0
			10204	6477	1842	1831	54		
1	K	1362	Total	C	N	O	S	0	0
			10253	6502	1857	1839	55		
1	L	1362	Total	C	N	O	S	0	0
			10242	6493	1851	1843	55		
1	M	1365	Total	C	N	O	S	0	0
			10275	6515	1859	1846	55		
1	N	1362	Total	C	N	O	S	0	0
			10254	6499	1857	1843	55		
1	O	1362	Total	C	N	O	S	0	0
			10251	6500	1859	1837	55		
1	P	1362	Total	C	N	O	S	0	0
			10256	6502	1855	1844	55		

- Molecule 2 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
2	R	307	Total	C	N	O	S	0	0
			2175	1405	392	370	8		
2	T	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
2	U	307	Total	C	N	O	S	0	0
			2179	1407	393	371	8		
2	W	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
2	X	308	Total	C	N	O	S	0	0
			2187	1411	394	374	8		
2	Z	299	Total	C	N	O	S	0	0
			2063	1334	366	356	7		
2	a	307	Total	C	N	O	S	0	0
			2169	1402	389	370	8		
2	c	299	Total	C	N	O	S	0	0
			2078	1341	373	357	7		
2	d	308	Total	C	N	O	S	0	0
			2187	1411	394	374	8		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	329	Total	C	N	O	S	0	0
			2267	1437	411	402	17		
3	V	346	Total	C	N	O	S	0	0
			2365	1500	432	416	17		
3	Y	347	Total	C	N	O	S	0	0
			2386	1512	437	420	17		
3	b	343	Total	C	N	O	S	0	0
			2331	1478	421	416	16		
3	e	343	Total	C	N	O	S	0	0
			2364	1497	435	415	17		

- Molecule 4 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	g	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	h	107	Total	C	N	O	S	0	0
			628	387	119	120	2		

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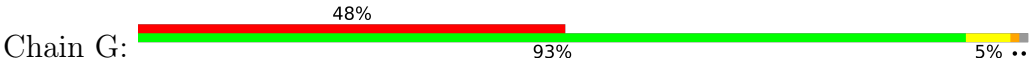
Mol	Chain	Residues	Atoms					AltConf	Trace
4	i	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	j	107	Total	C	N	O	S	0	0
			632	390	120	120	2		
4	k	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	l	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	m	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	n	107	Total	C	N	O	S	0	0
			625	385	119	120	1		
4	o	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	p	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	q	107	Total	C	N	O	S	0	0
			628	387	119	120	2		
4	r	107	Total	C	N	O	S	0	0
			632	390	120	120	2		
4	s	107	Total	C	N	O	S	0	0
			634	390	122	120	2		
4	t	107	Total	C	N	O	S	0	0
			628	387	119	120	2		

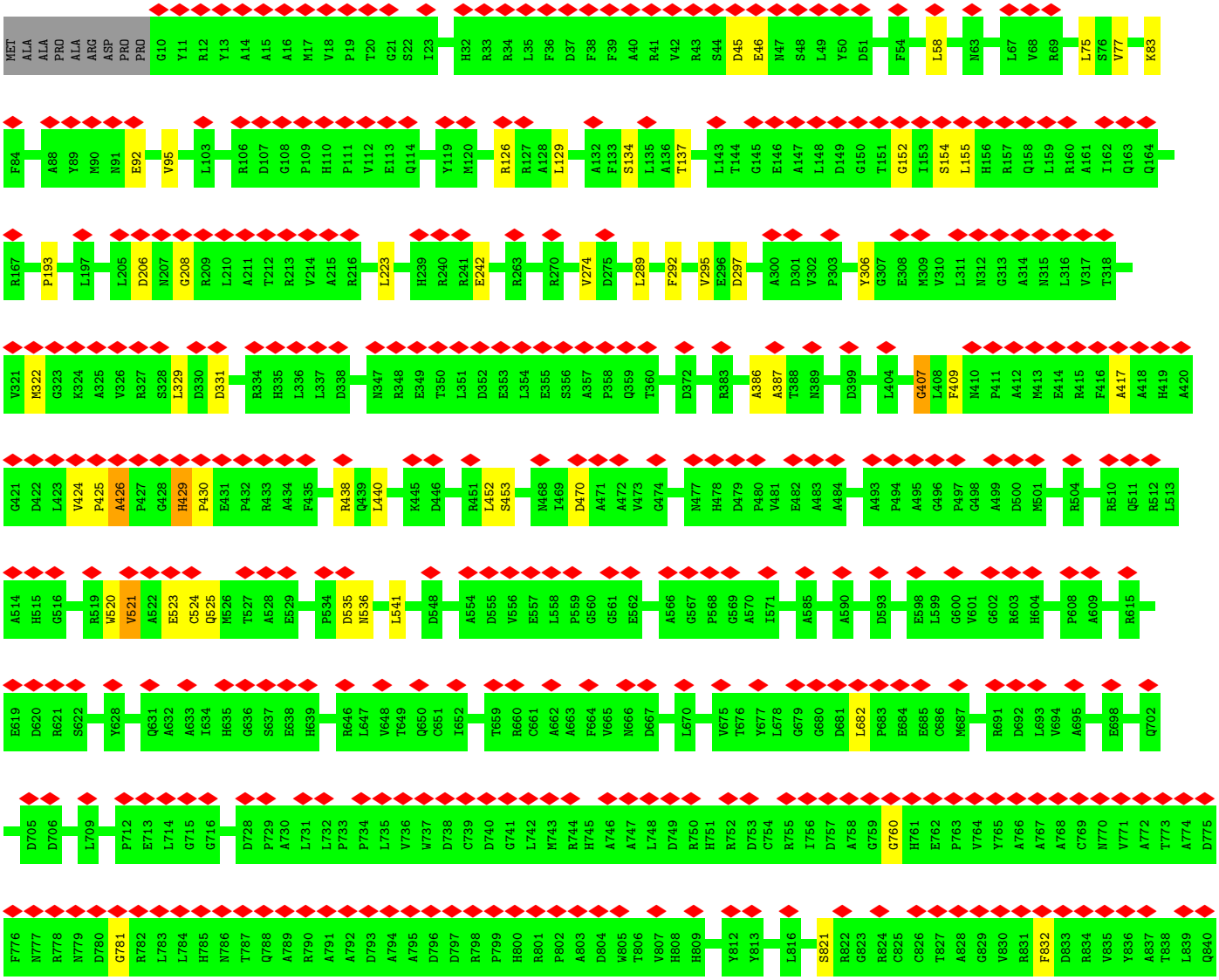
3 Residue-property plots (i)

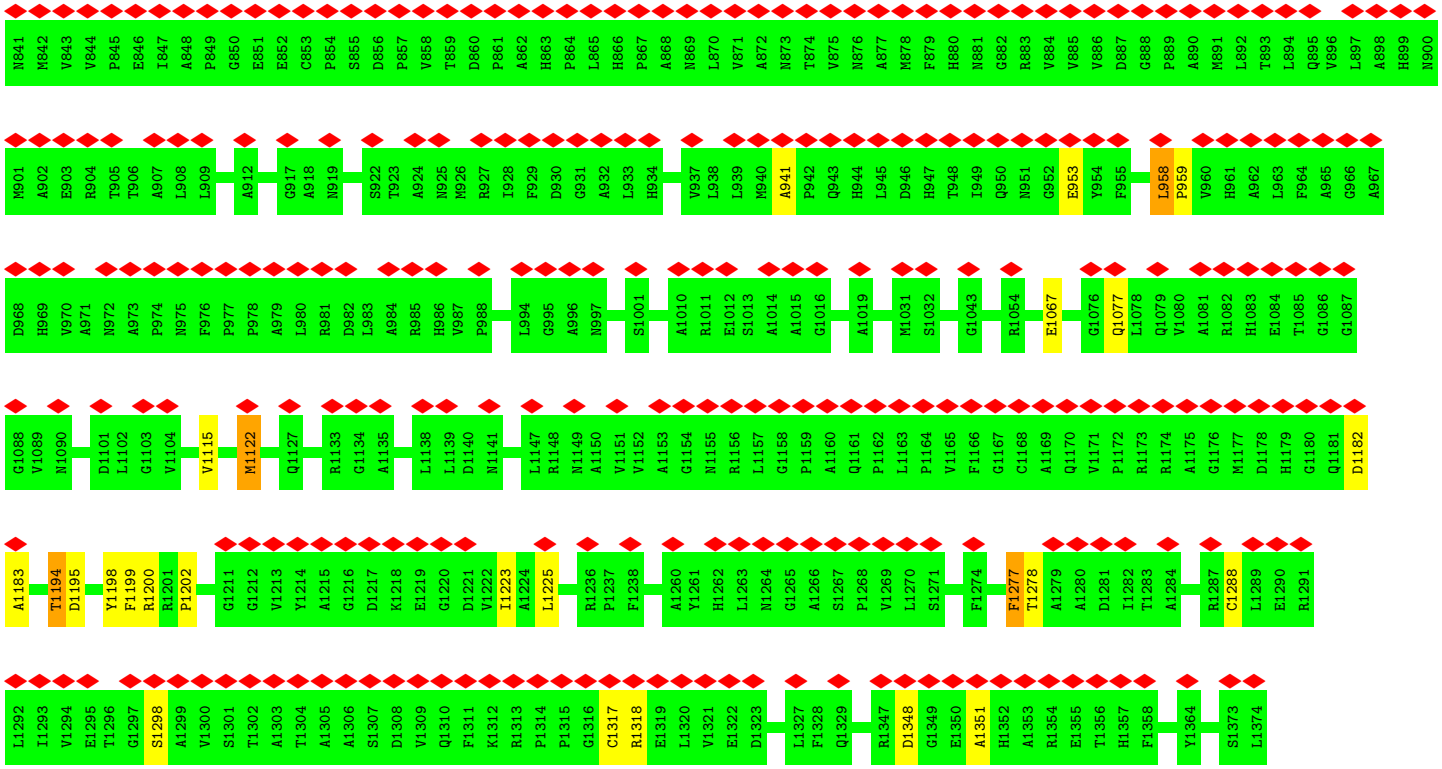
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Major capsid protein

Chain G:

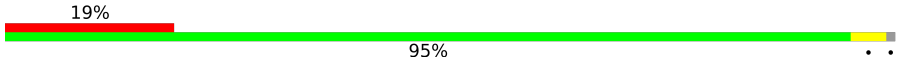


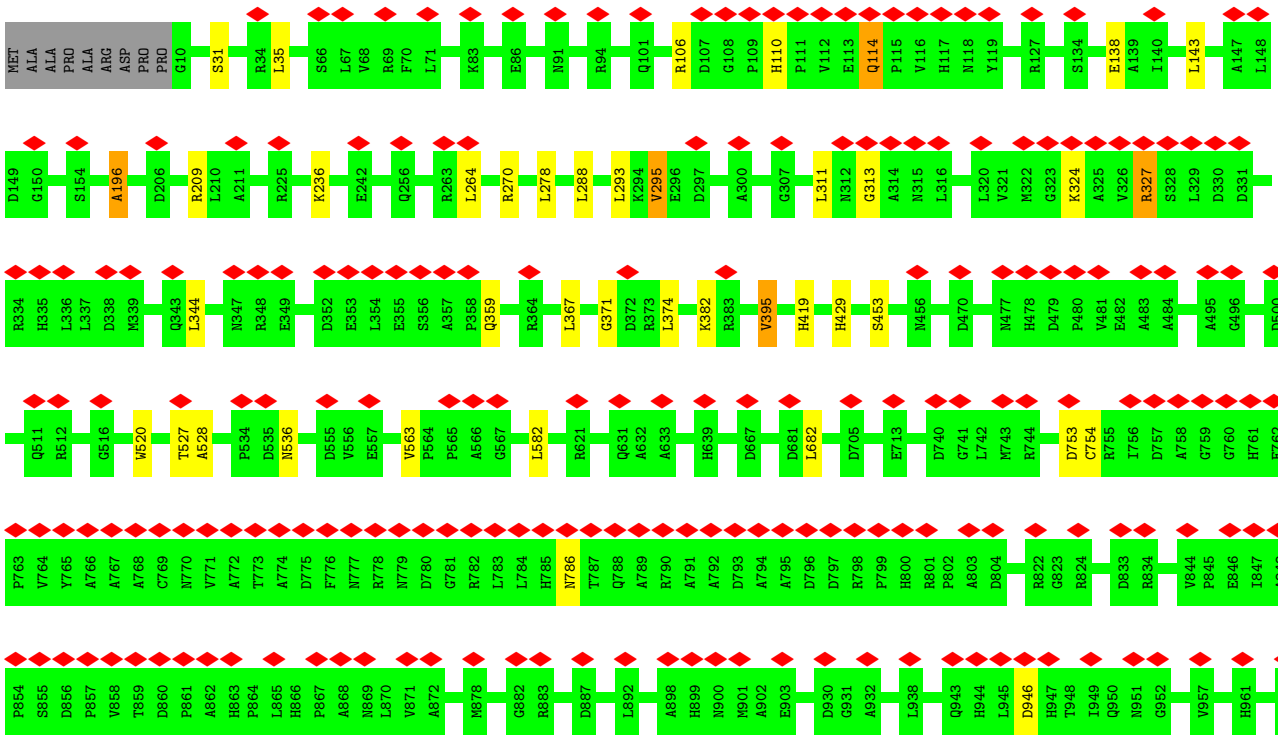


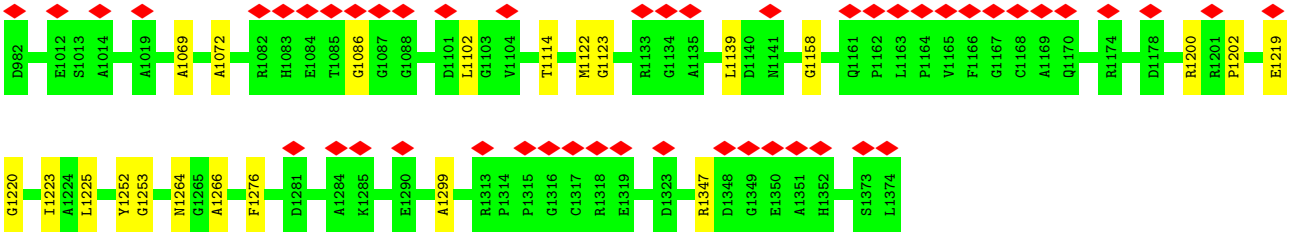


• Molecule 1: Major capsid protein

Chain A:

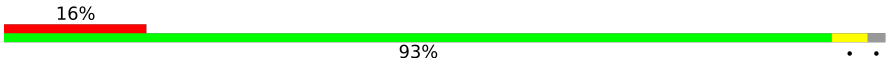


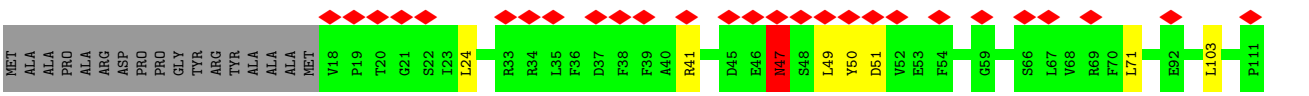


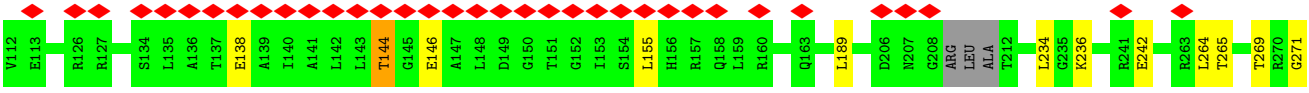


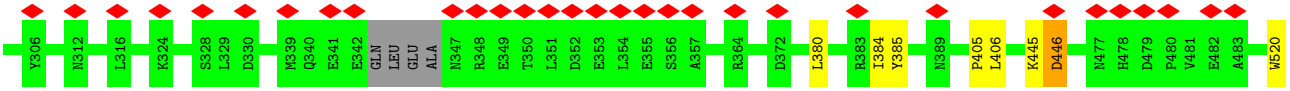
• Molecule 1: Major capsid protein

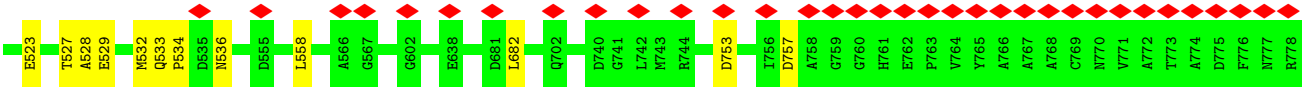
Chain B:

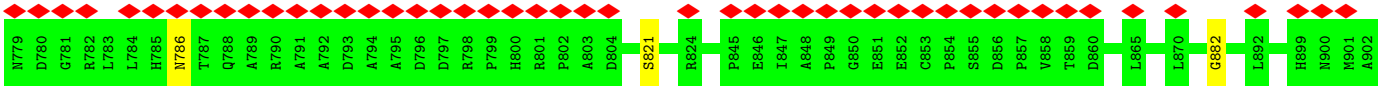


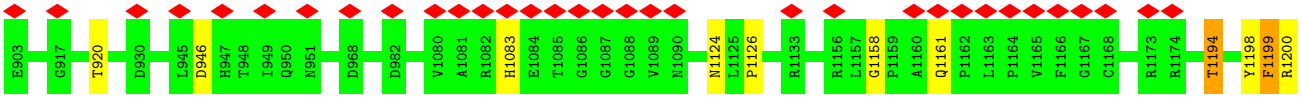


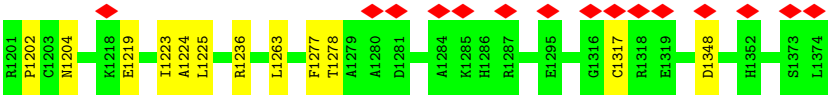






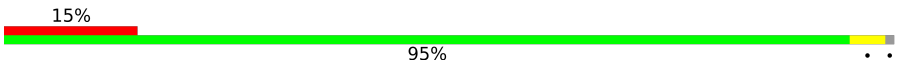


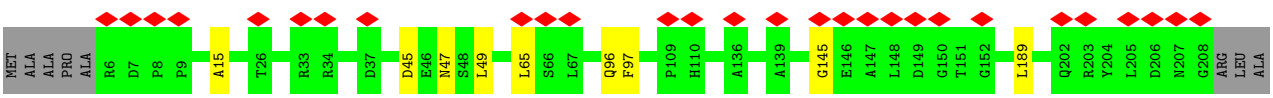


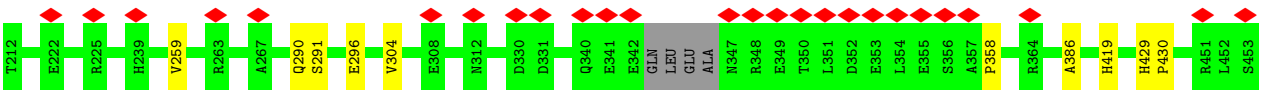


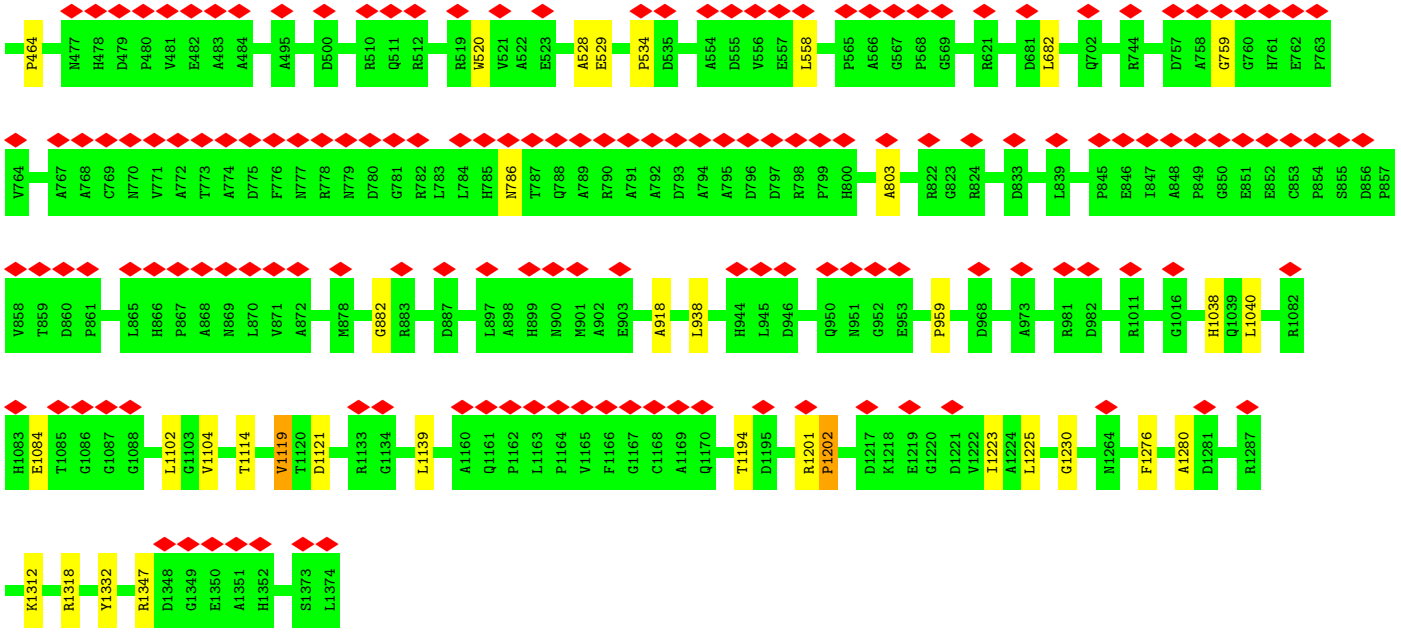
• Molecule 1: Major capsid protein

Chain C:



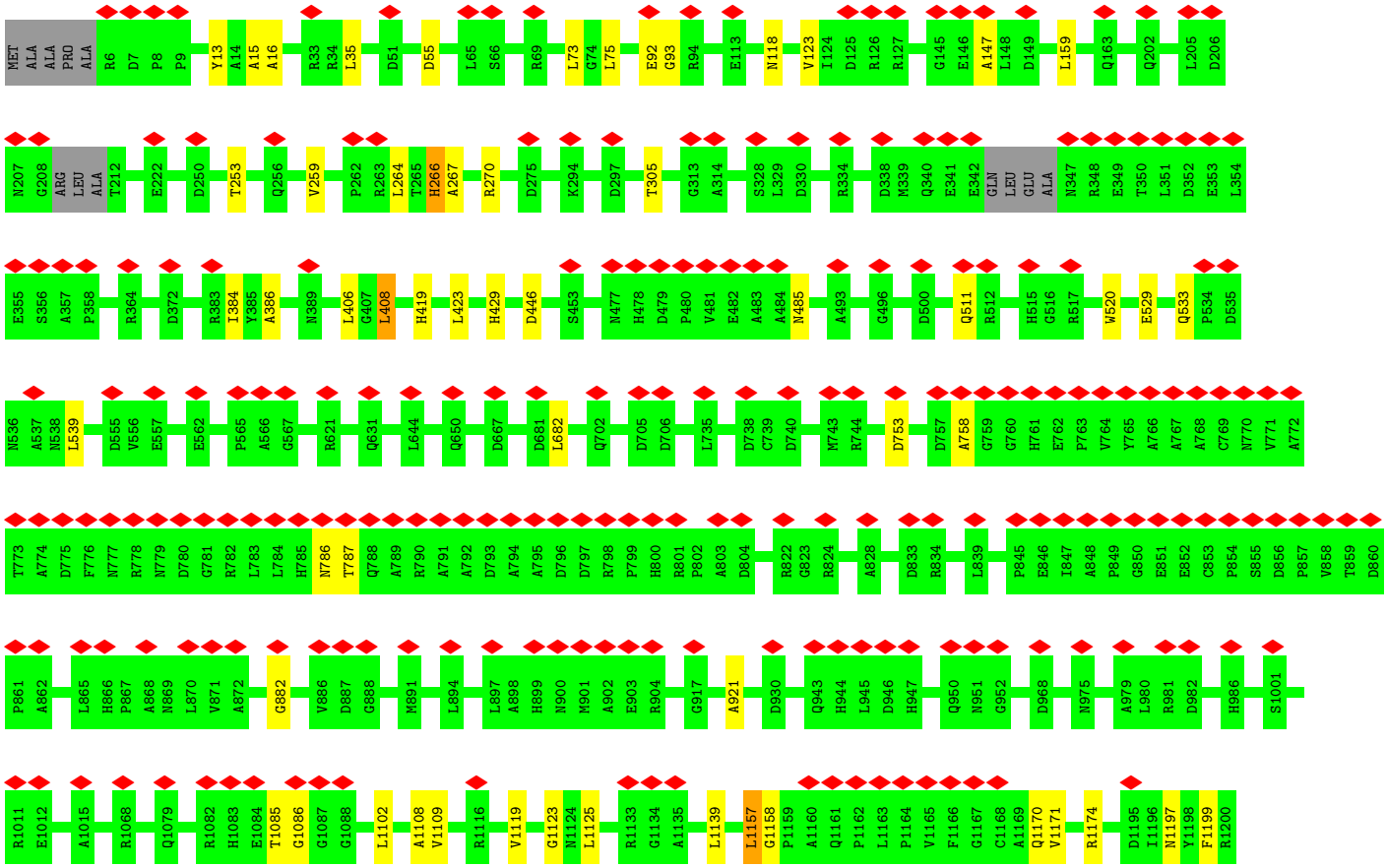


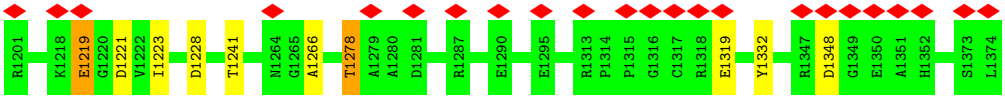




- Molecule 1: Major capsid protein

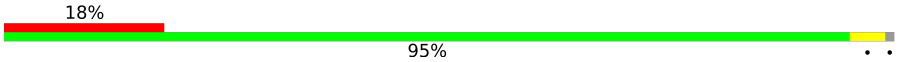
Chain D:

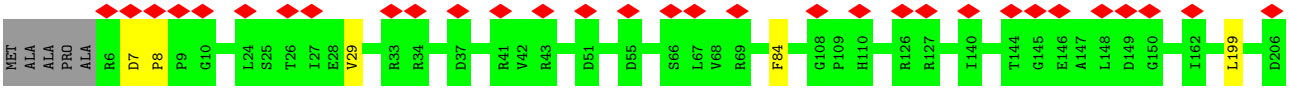


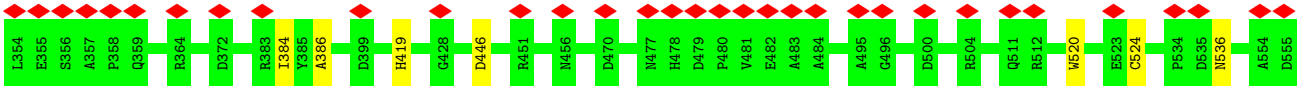


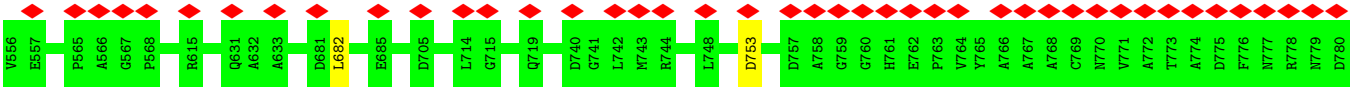
• Molecule 1: Major capsid protein

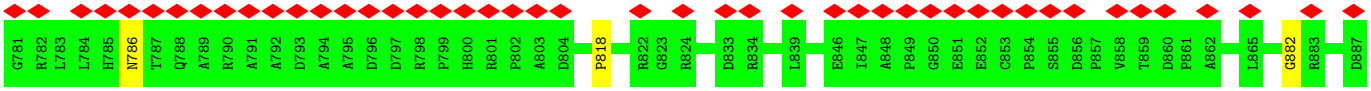
Chain E:

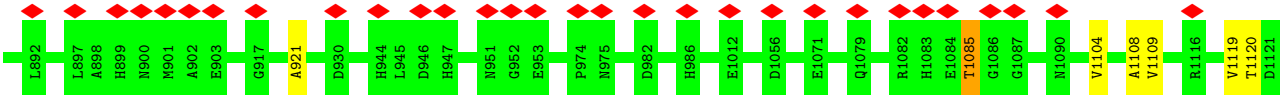


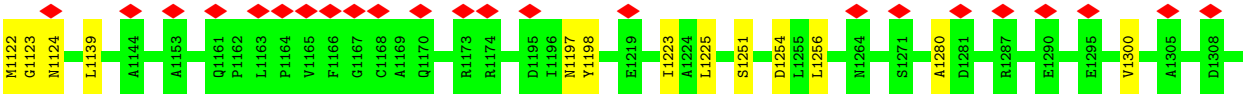


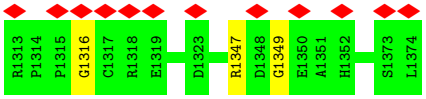






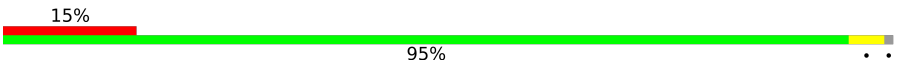


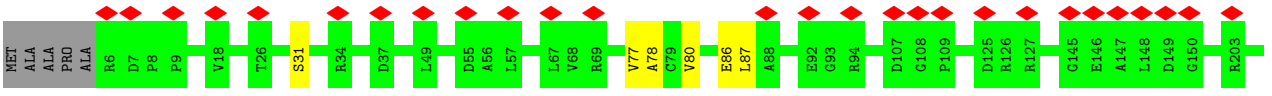


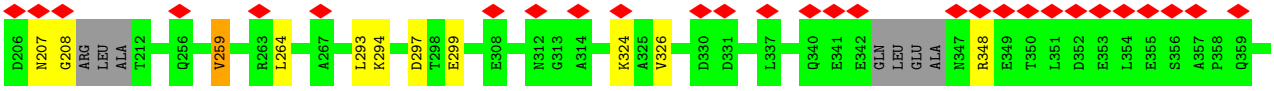


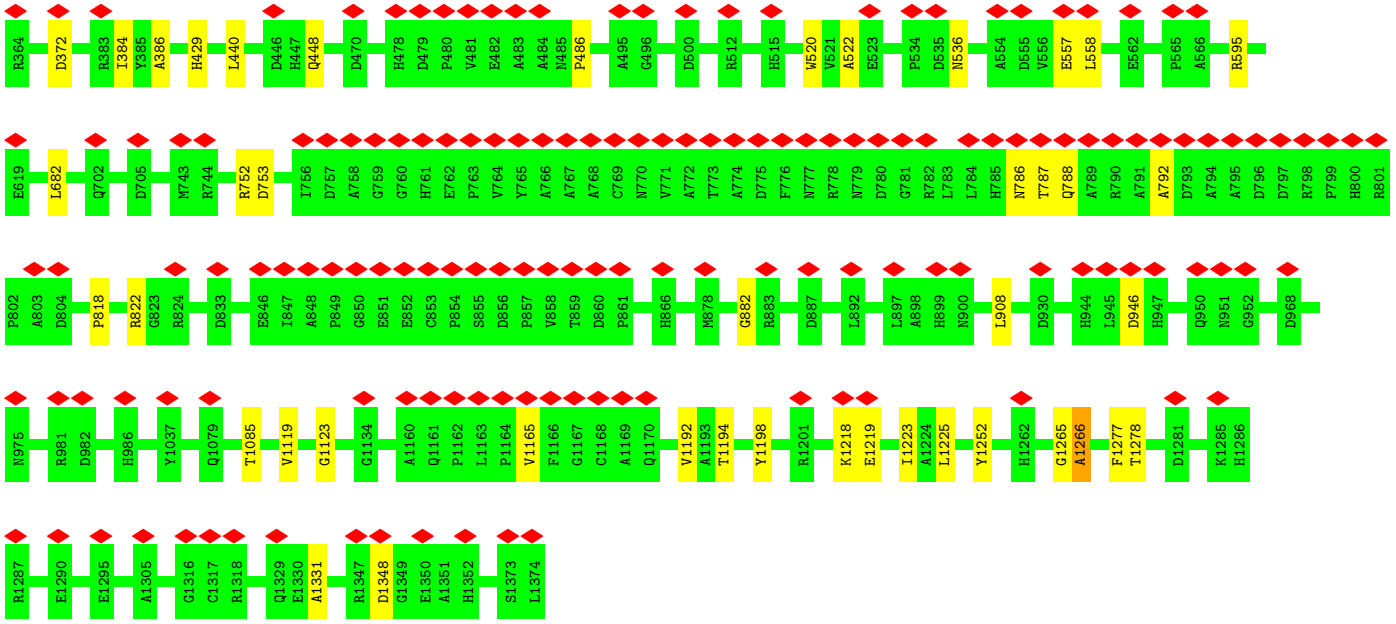
• Molecule 1: Major capsid protein

Chain F:



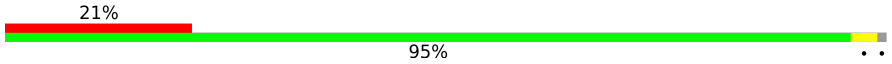


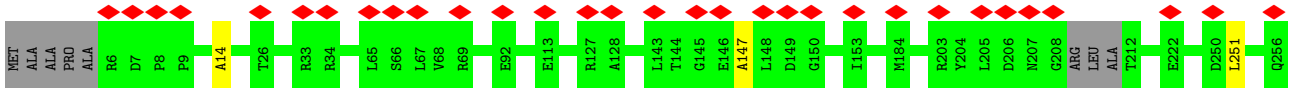


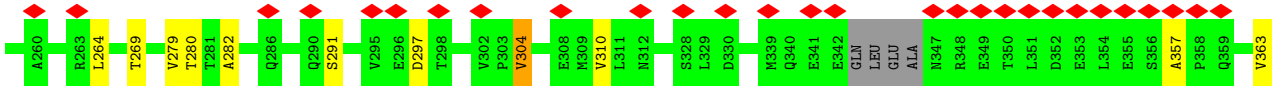


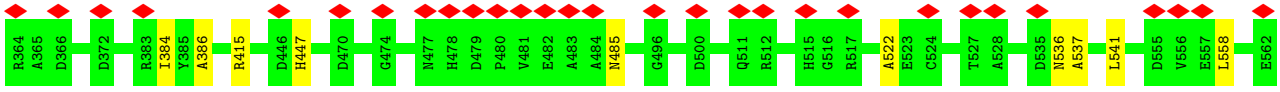
• Molecule 1: Major capsid protein

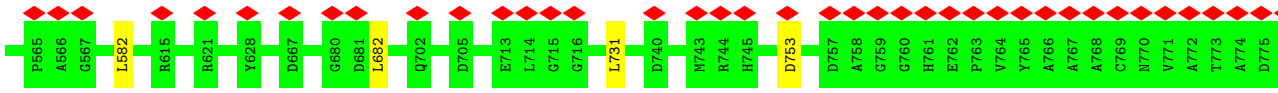
Chain H:

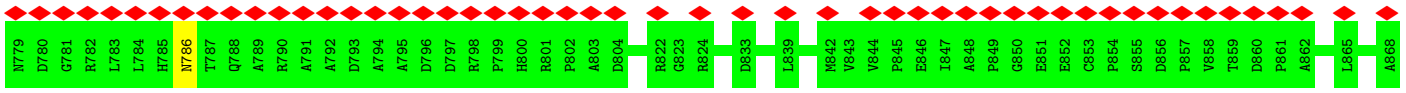


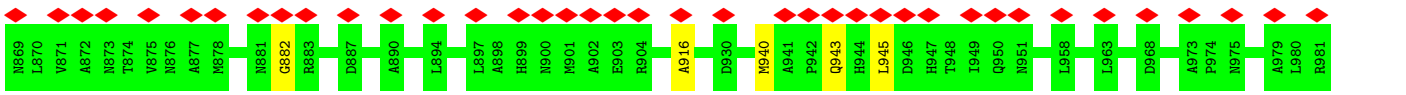


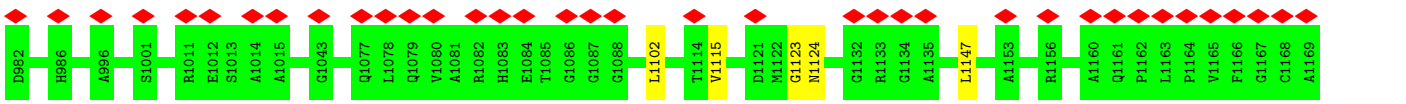


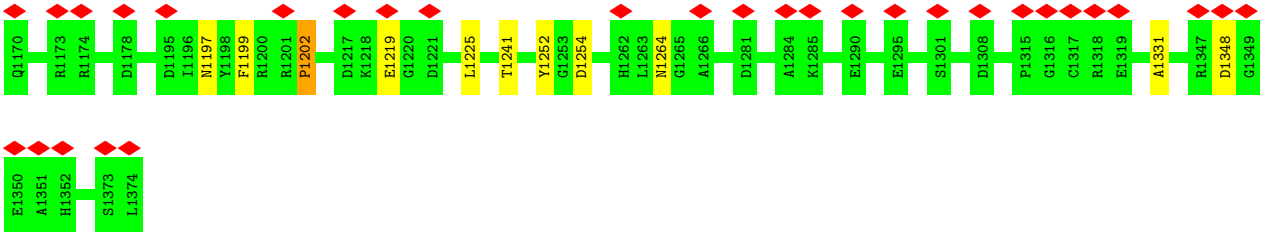






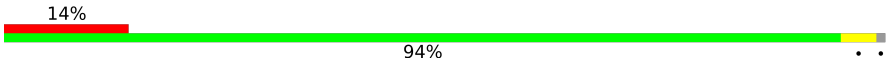


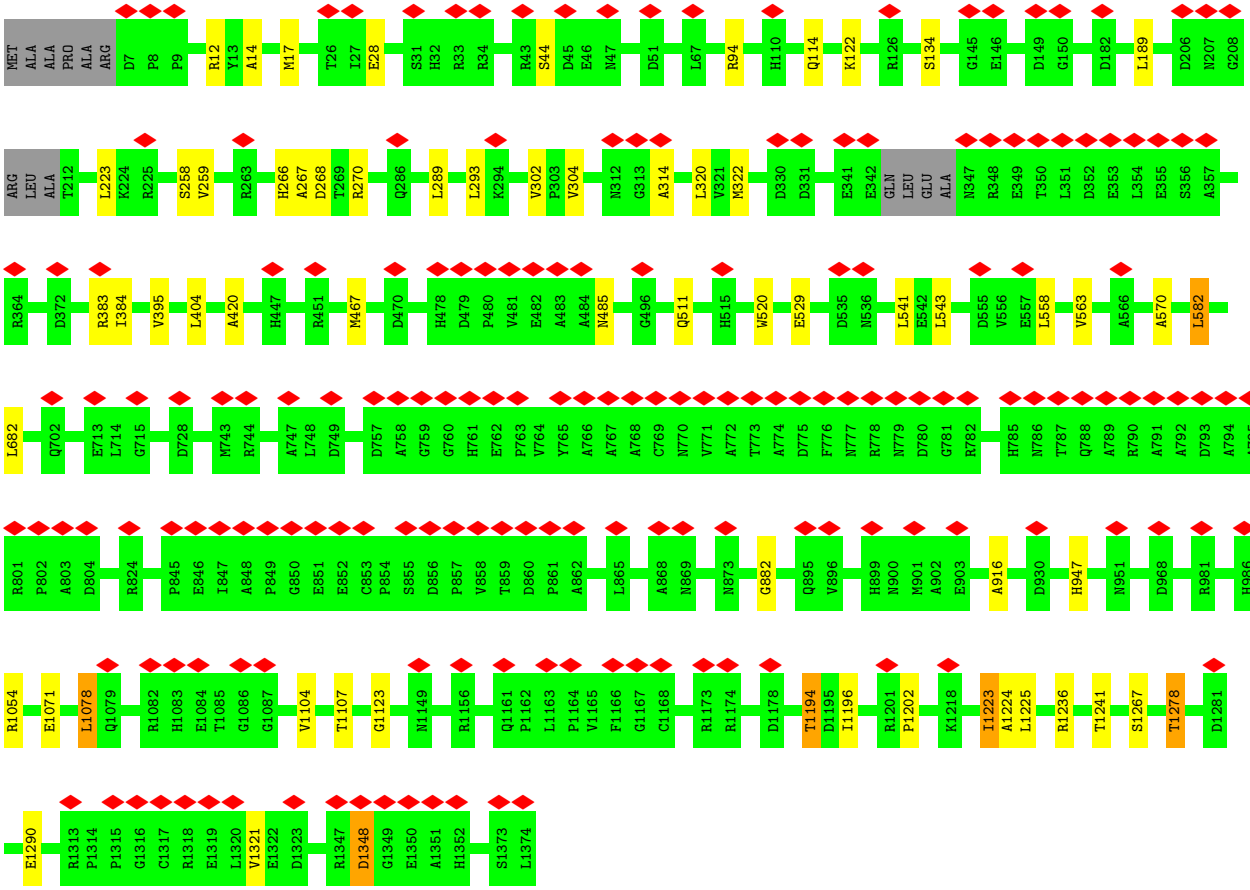




• Molecule 1: Major capsid protein

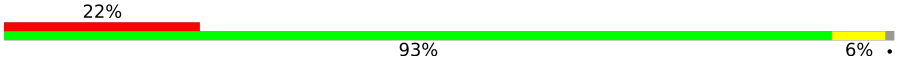
Chain I:

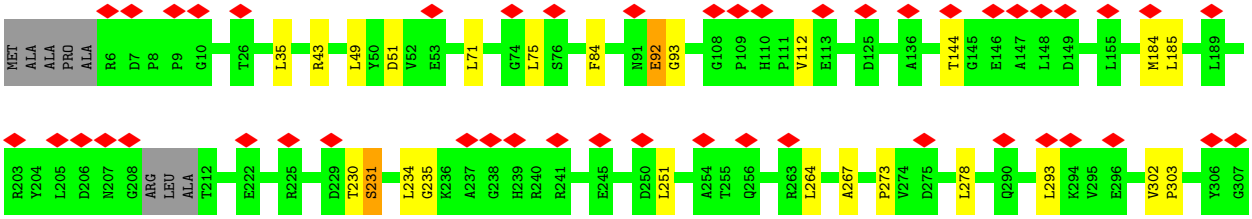


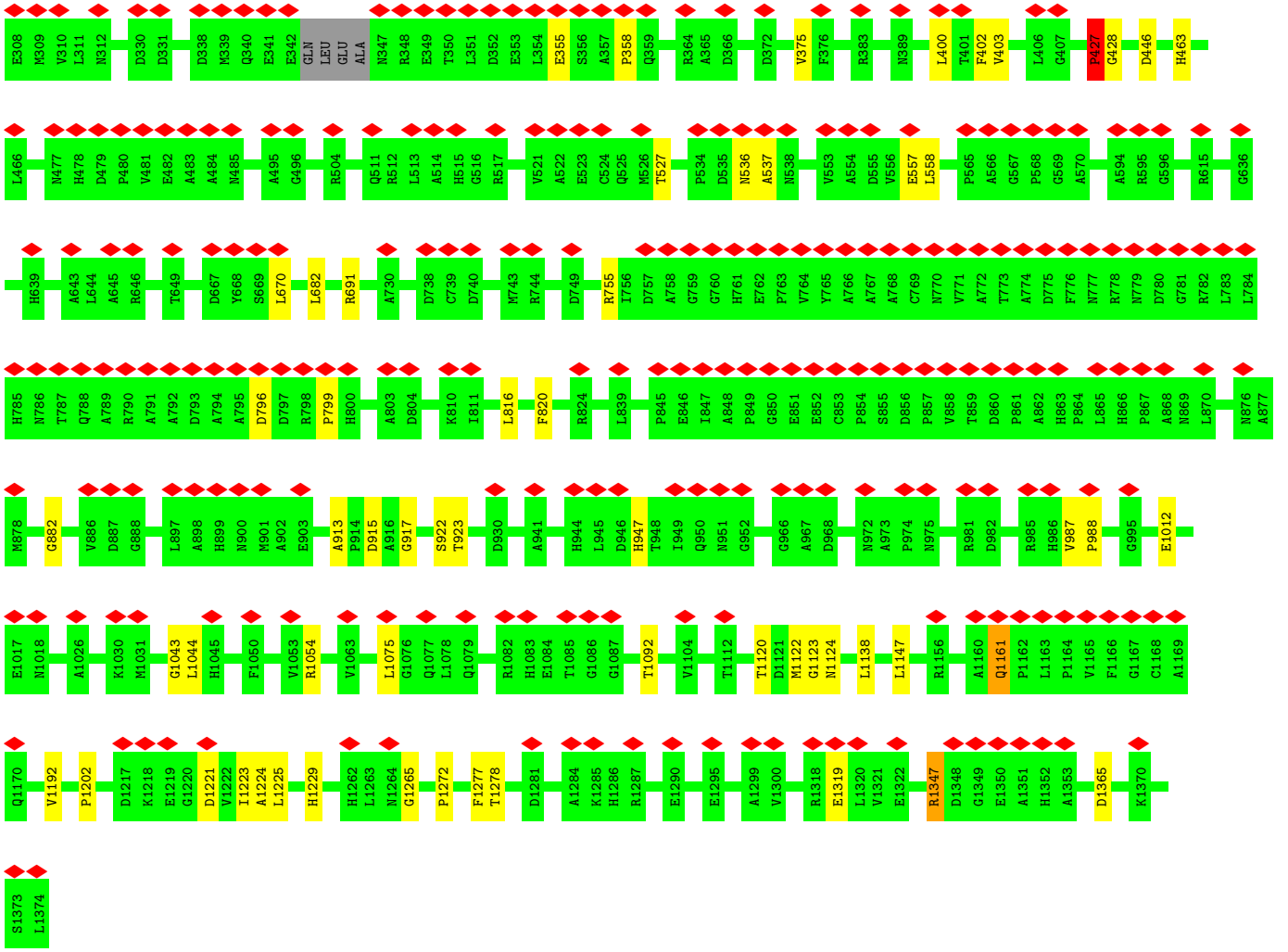


• Molecule 1: Major capsid protein

Chain J:

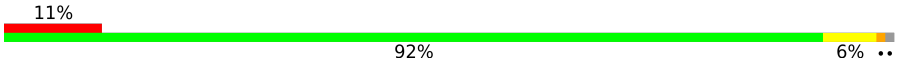


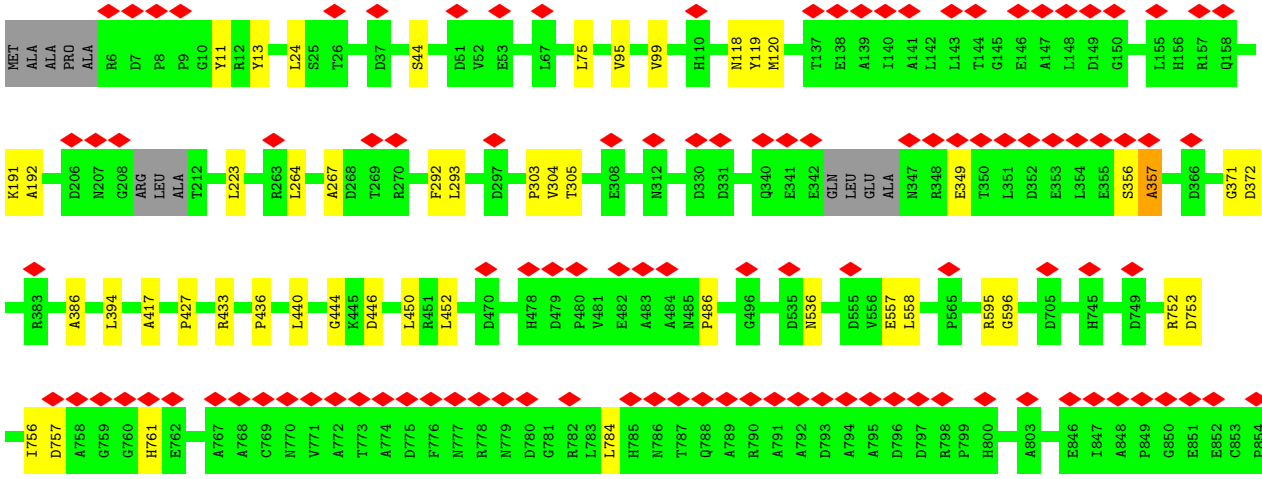


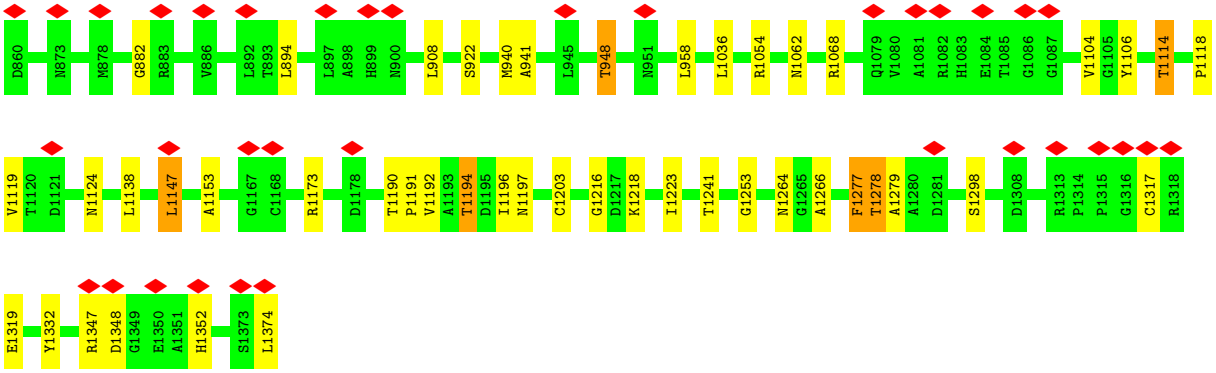


• Molecule 1: Major capsid protein

Chain K:

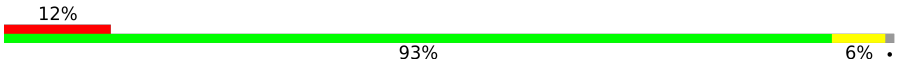


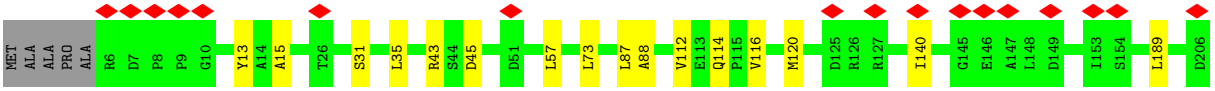


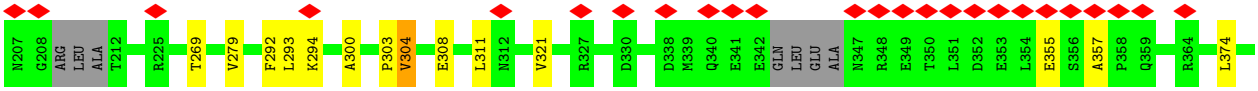


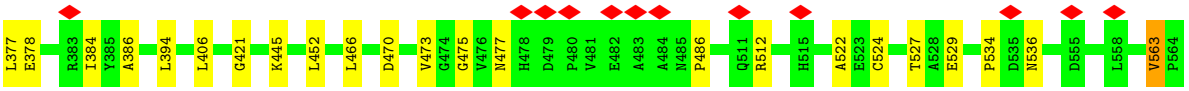
• Molecule 1: Major capsid protein

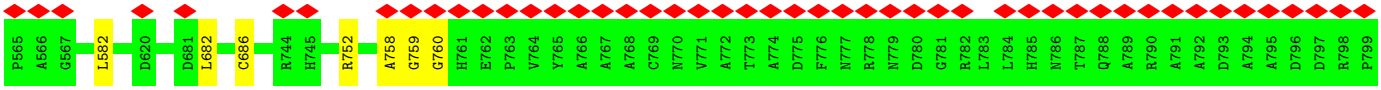
Chain L:

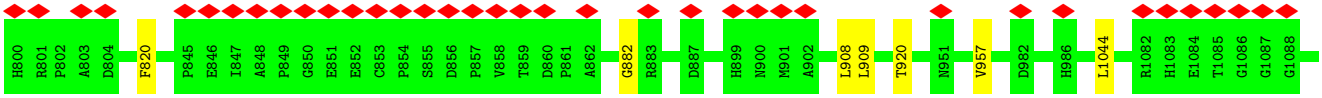


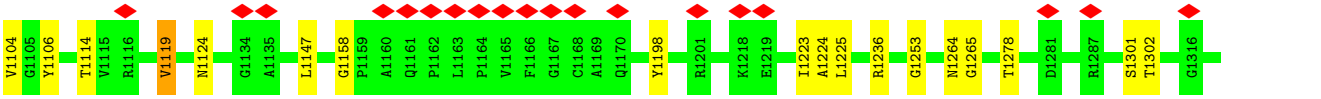


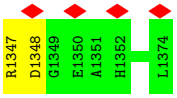






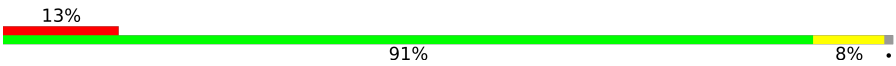


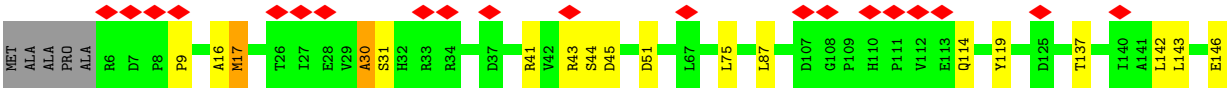




• Molecule 1: Major capsid protein

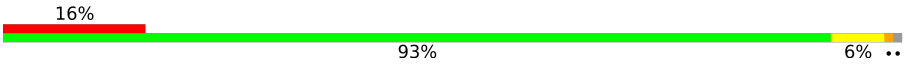
Chain M:

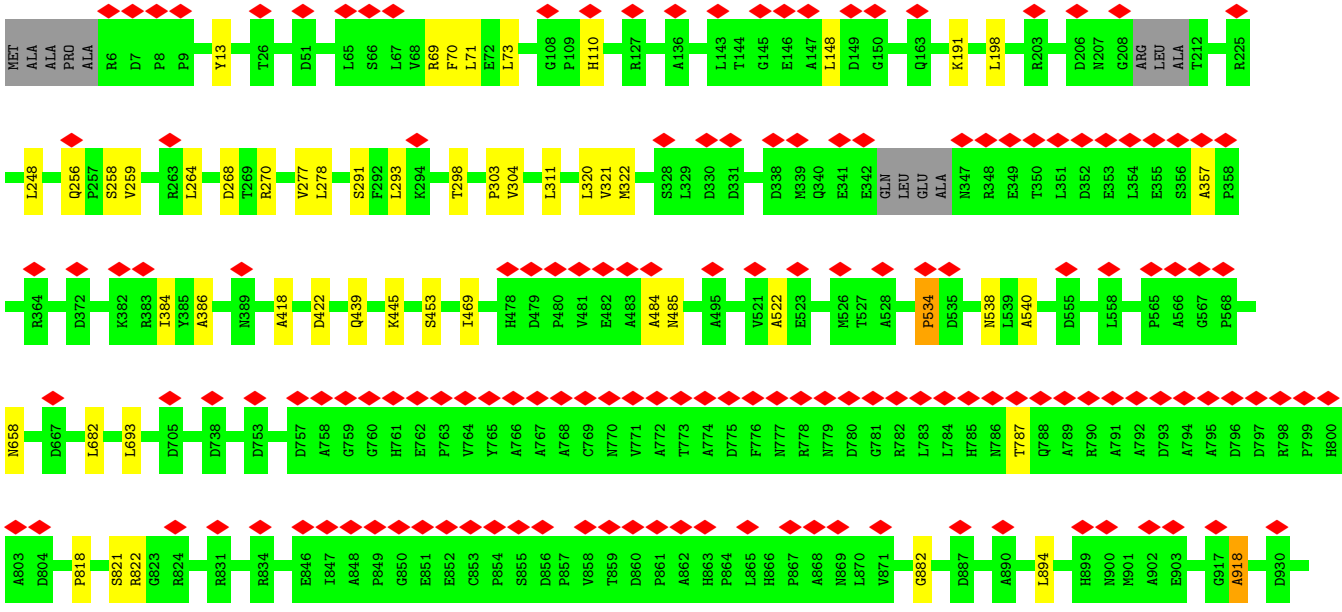


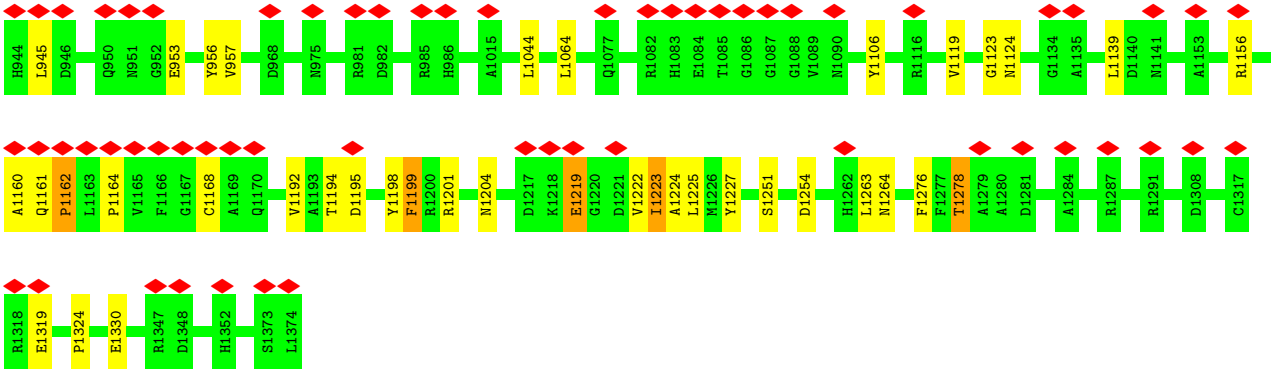


- Molecule 1: Major capsid protein

Chain N:

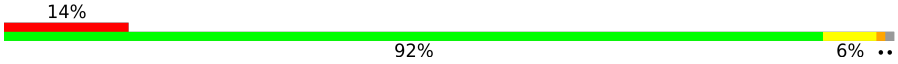


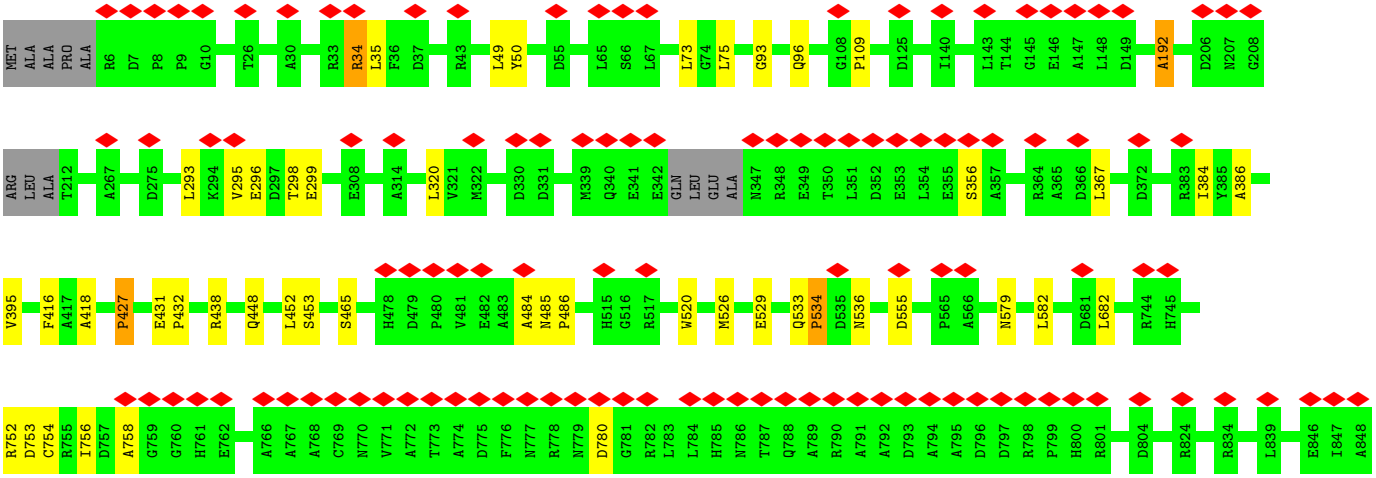




• Molecule 1: Major capsid protein

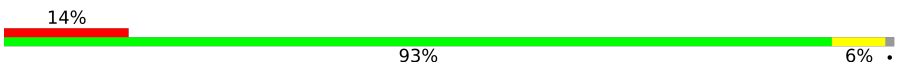
Chain O:

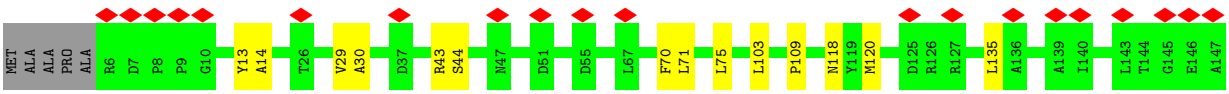


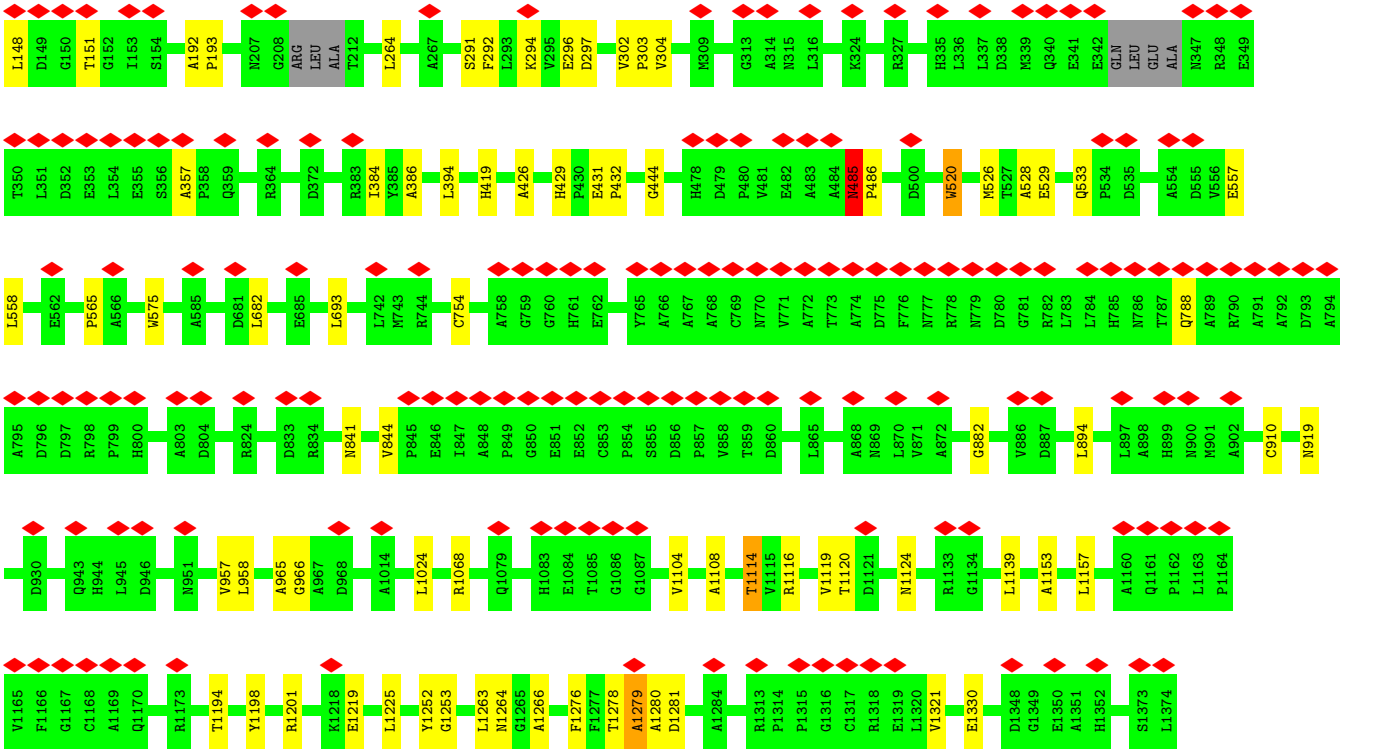


• Molecule 1: Major capsid protein

Chain P:

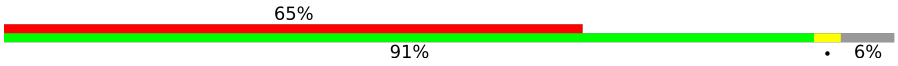


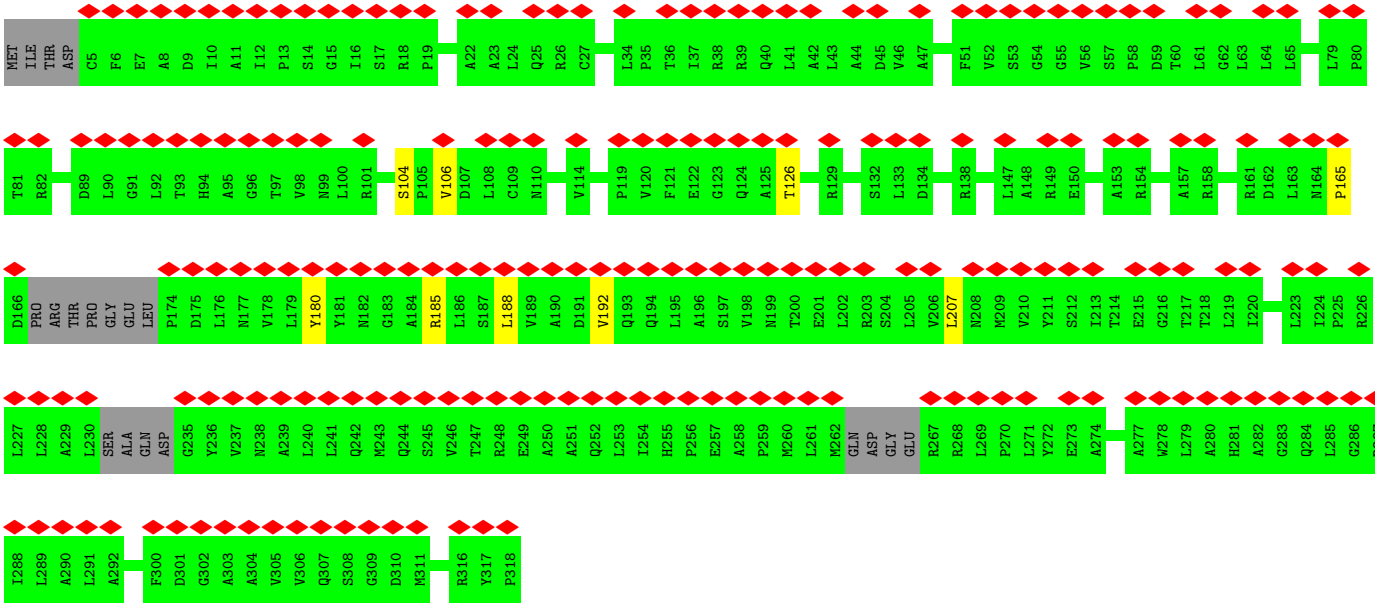




• Molecule 2: Triplex capsid protein 2

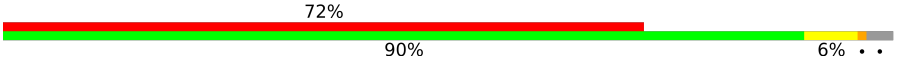
Chain Q:

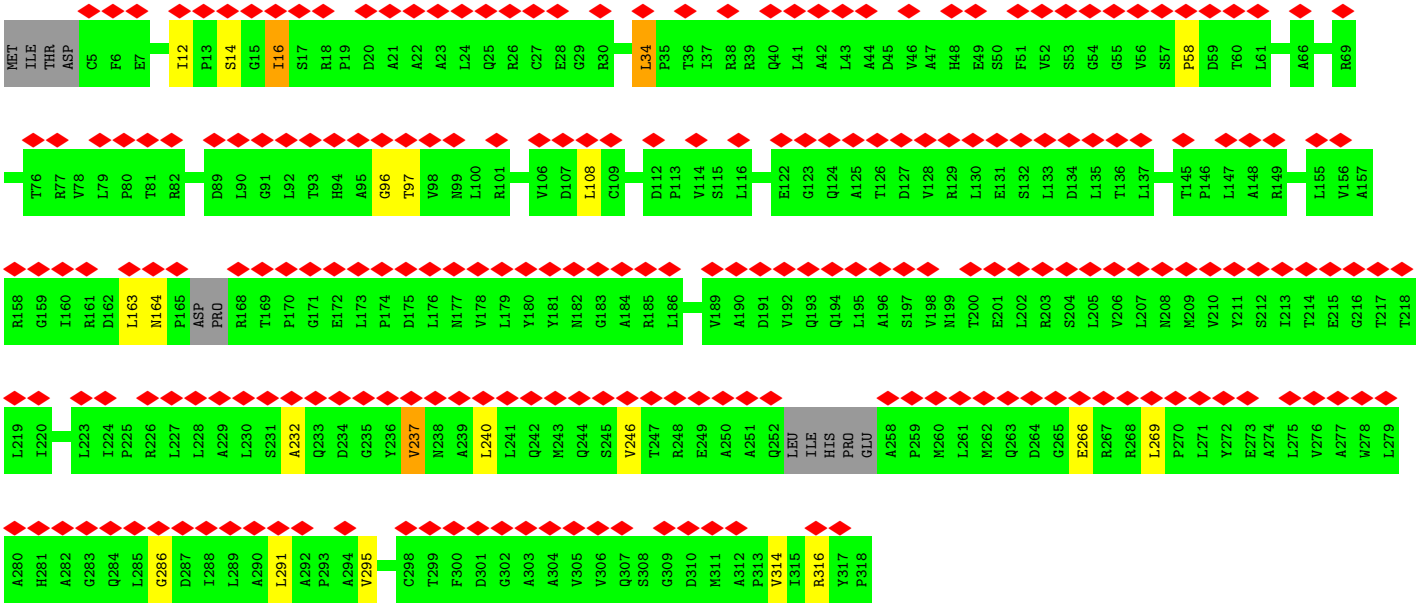




• Molecule 2: Triplex capsid protein 2

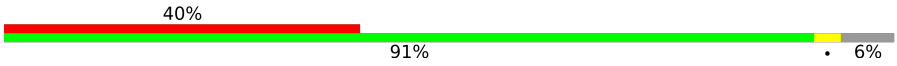
Chain R:

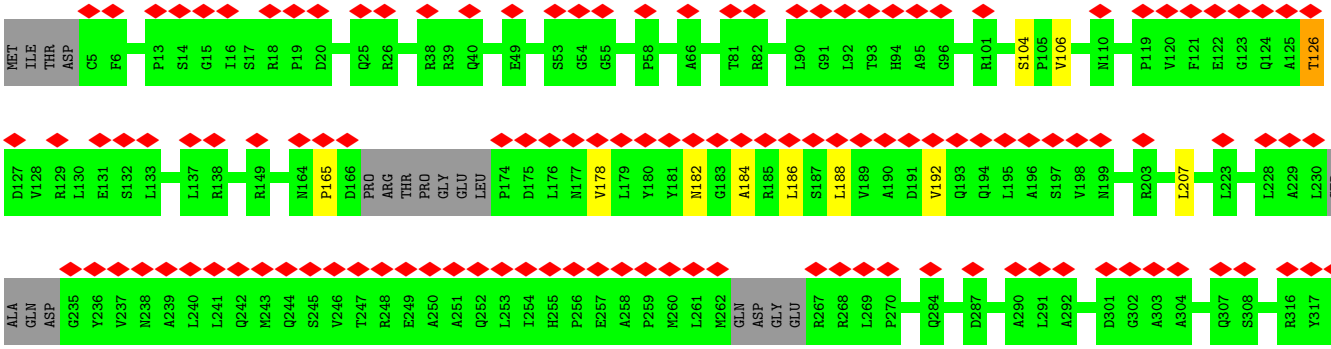




• Molecule 2: Triplex capsid protein 2

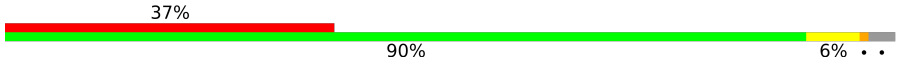
Chain T:

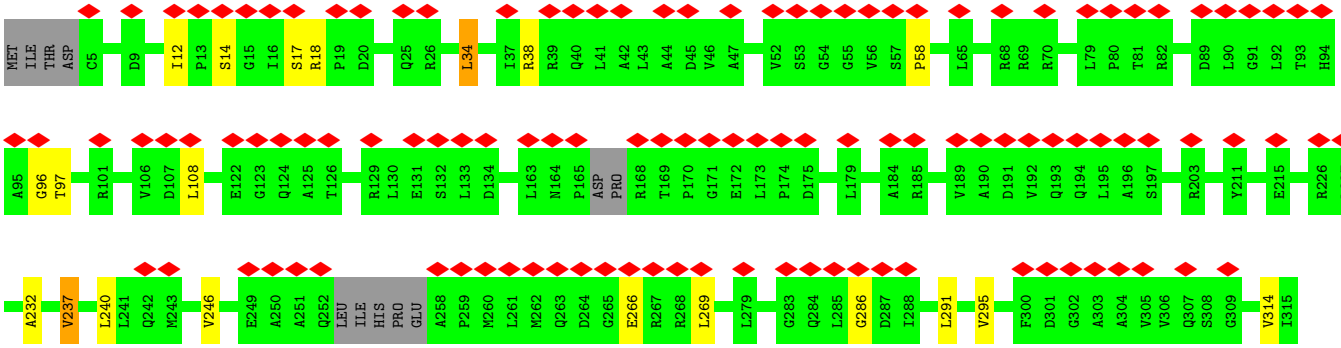




• Molecule 2: Triplex capsid protein 2

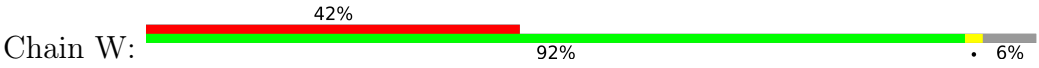
Chain U:

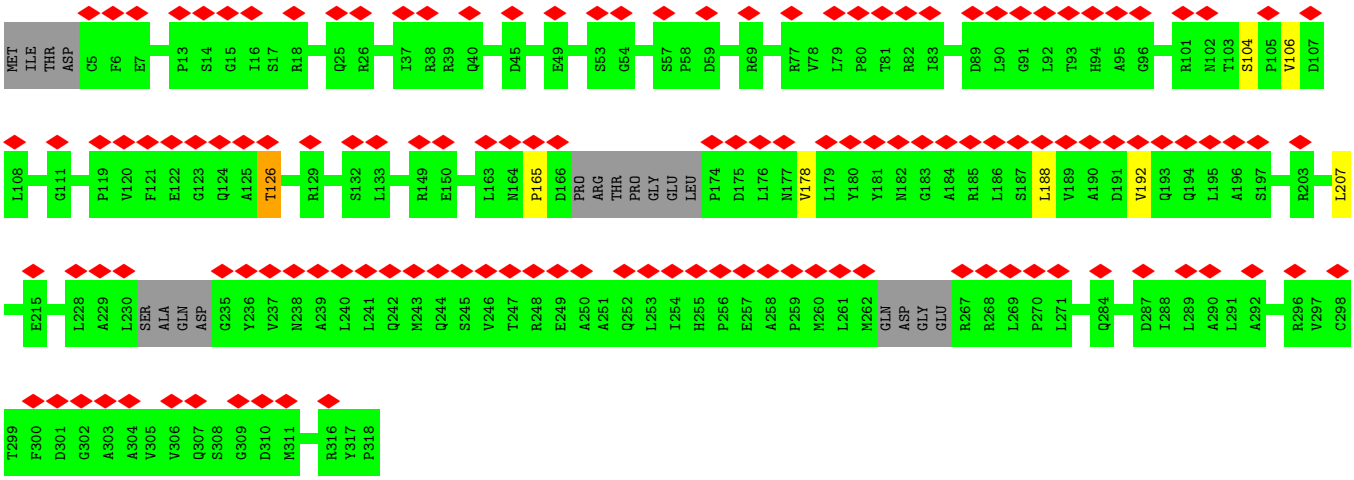




• Molecule 2: Triplex capsid protein 2

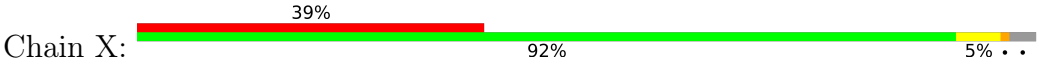
Chain W:

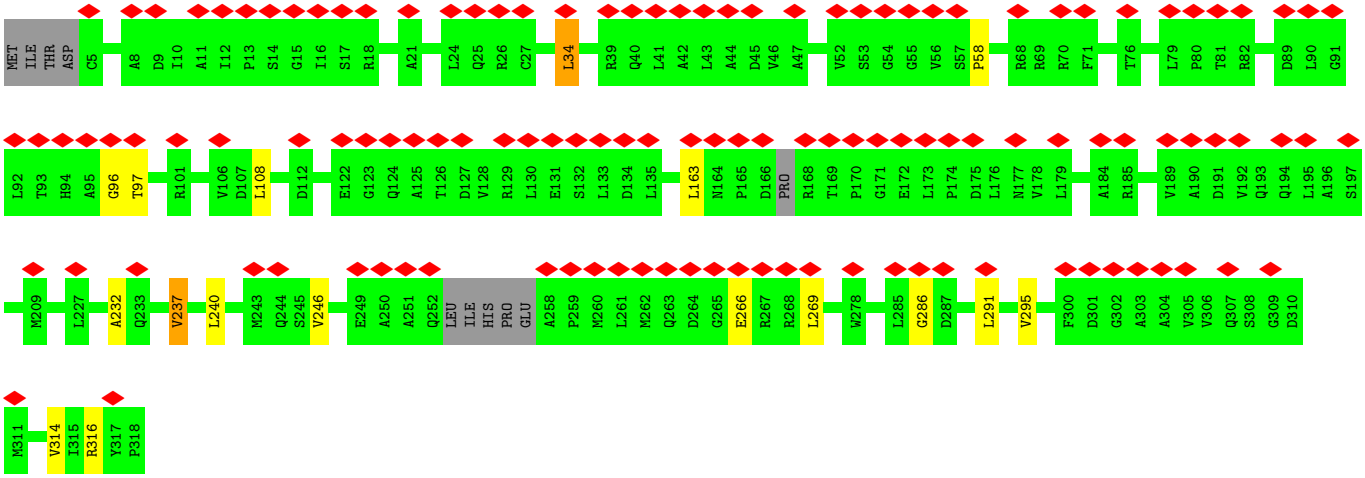




• Molecule 2: Triplex capsid protein 2

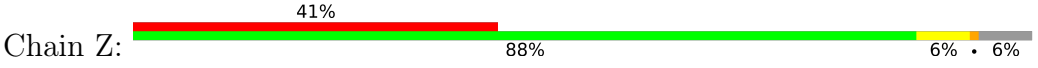
Chain X:

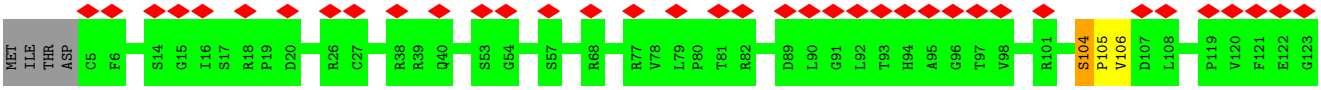


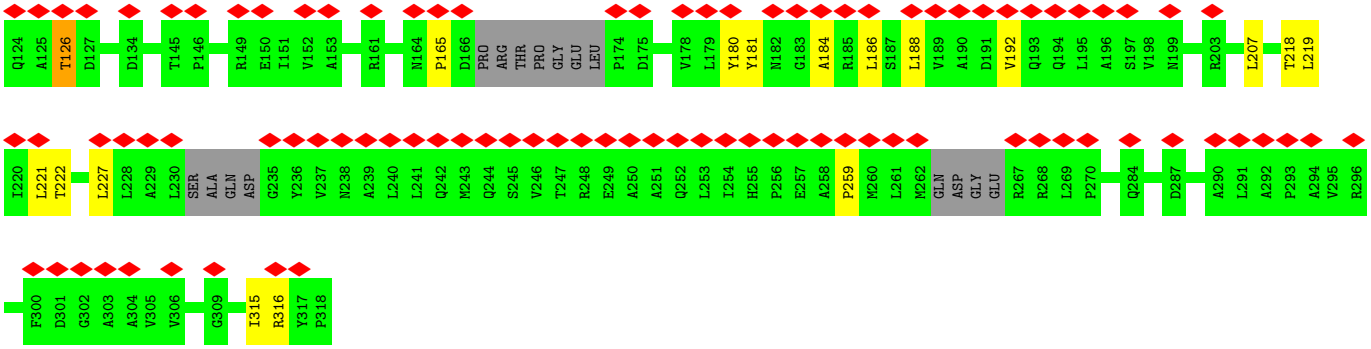


• Molecule 2: Triplex capsid protein 2

Chain Z:

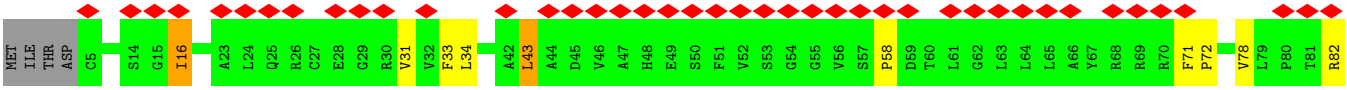


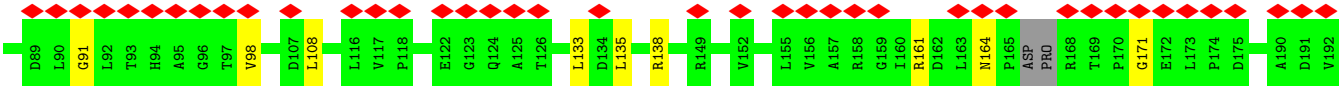


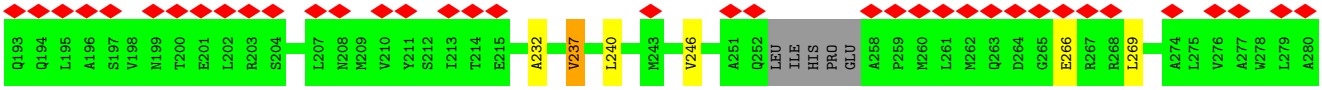


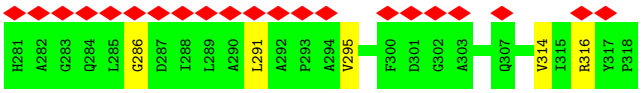
• Molecule 2: Triplex capsid protein 2

Chain a:



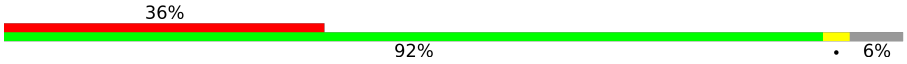


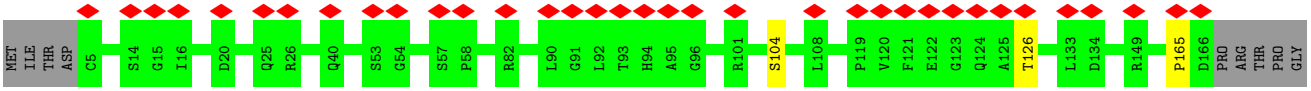


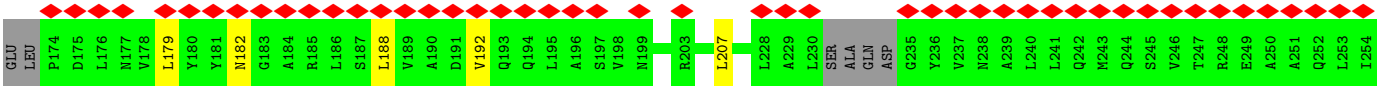


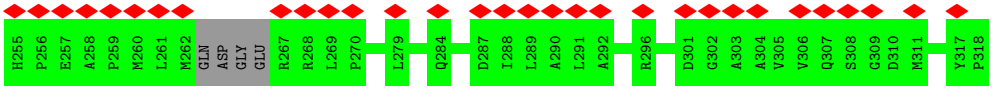
• Molecule 2: Triplex capsid protein 2

Chain c:



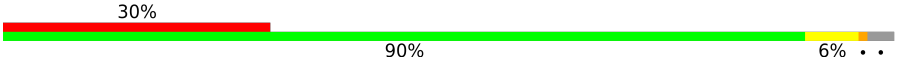


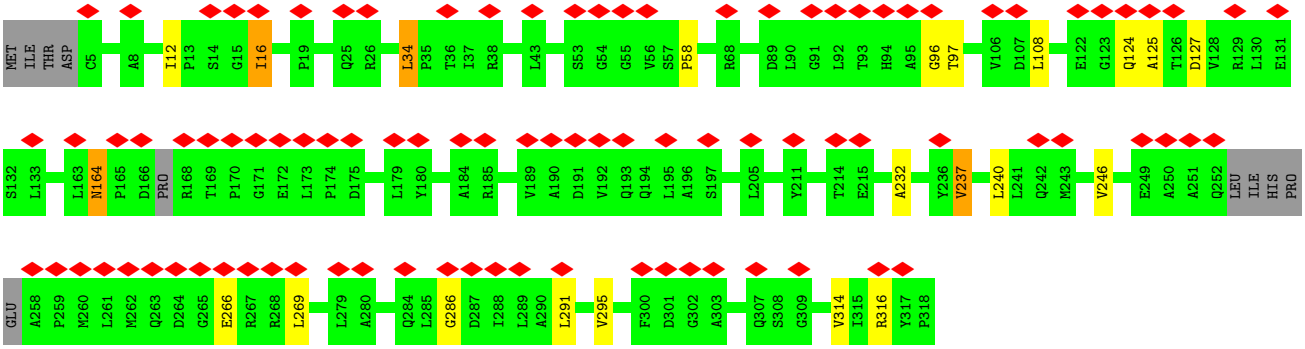




• Molecule 2: Triplex capsid protein 2

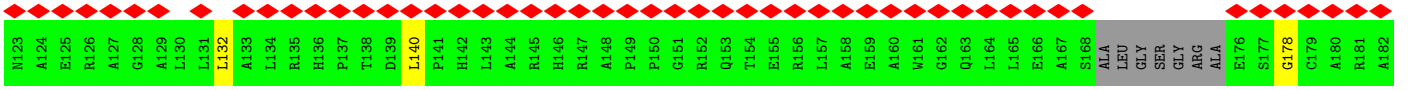
Chain d:

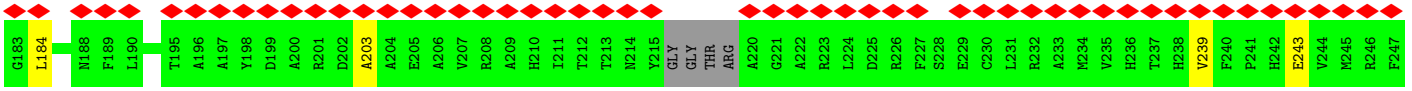


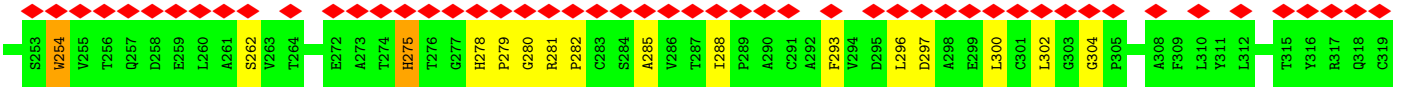


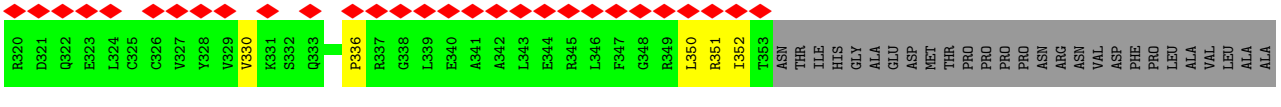
• Molecule 3: Triplex capsid protein 1

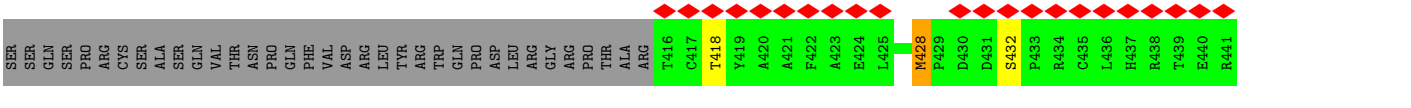
Chain S:

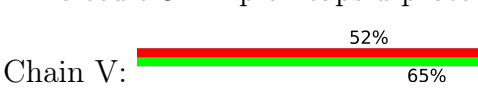






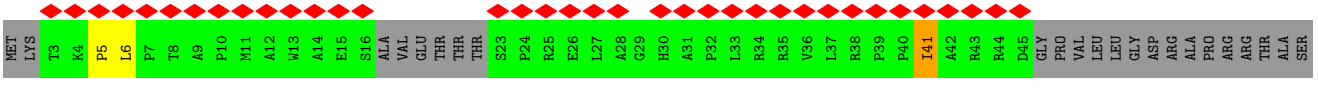


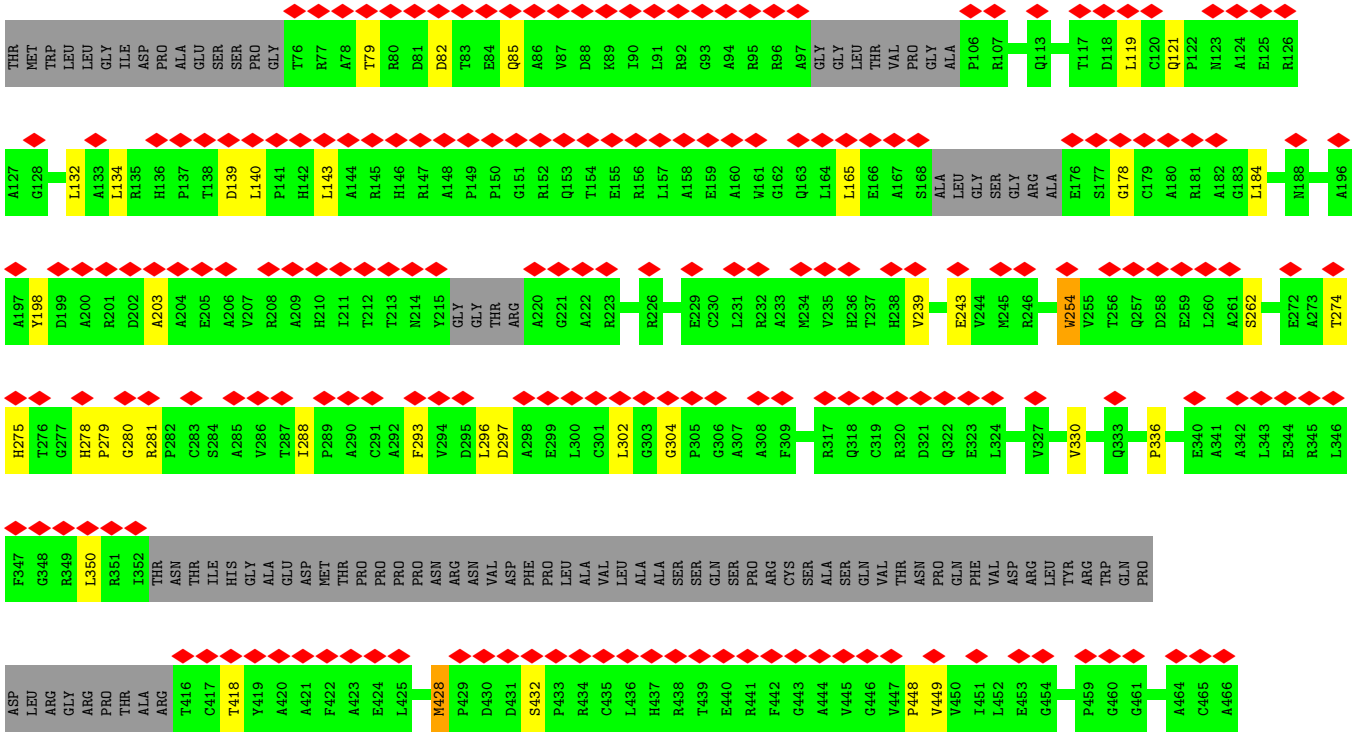




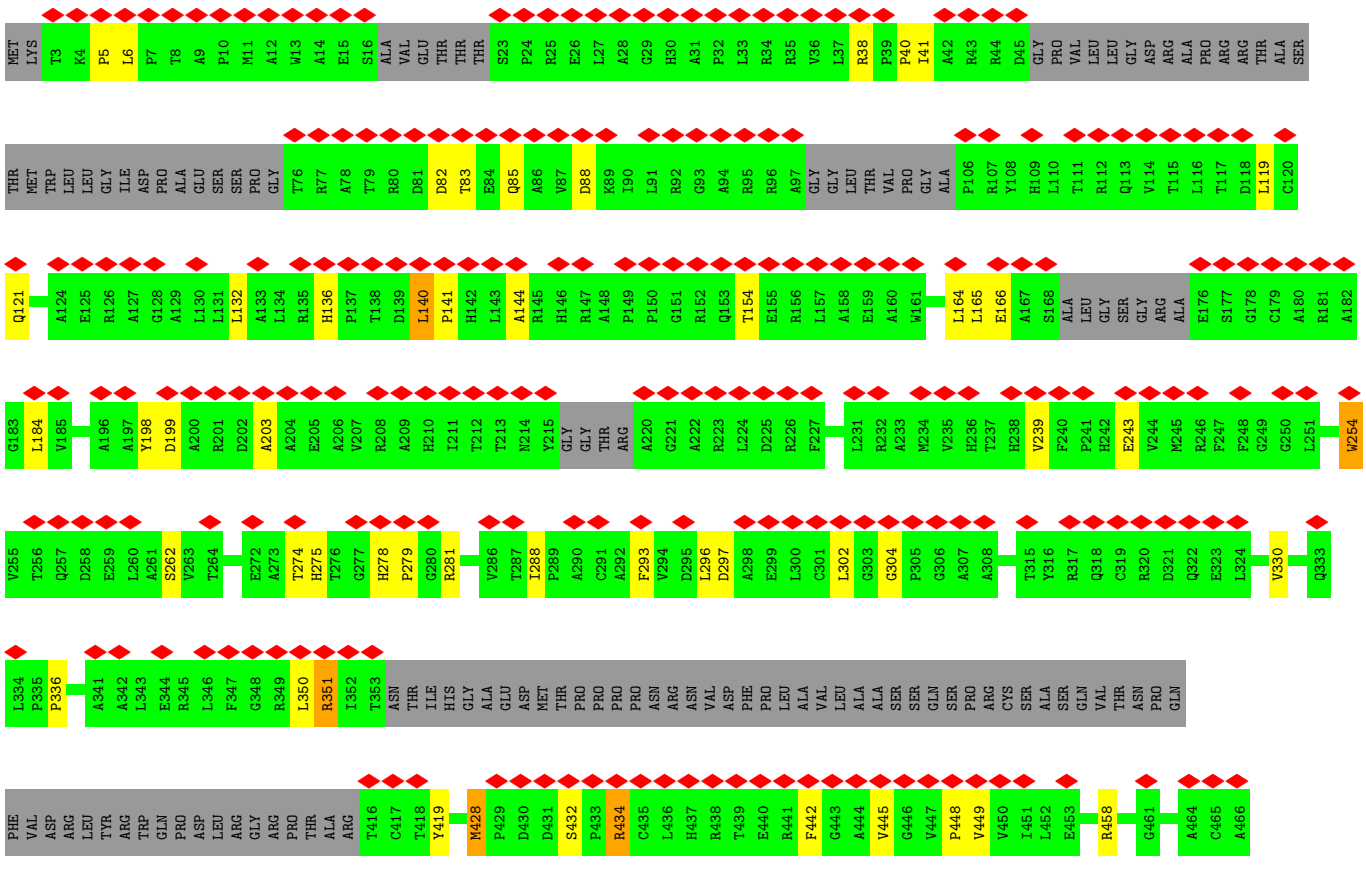
• Molecule 3: Triplex capsid protein 1

Chain V:



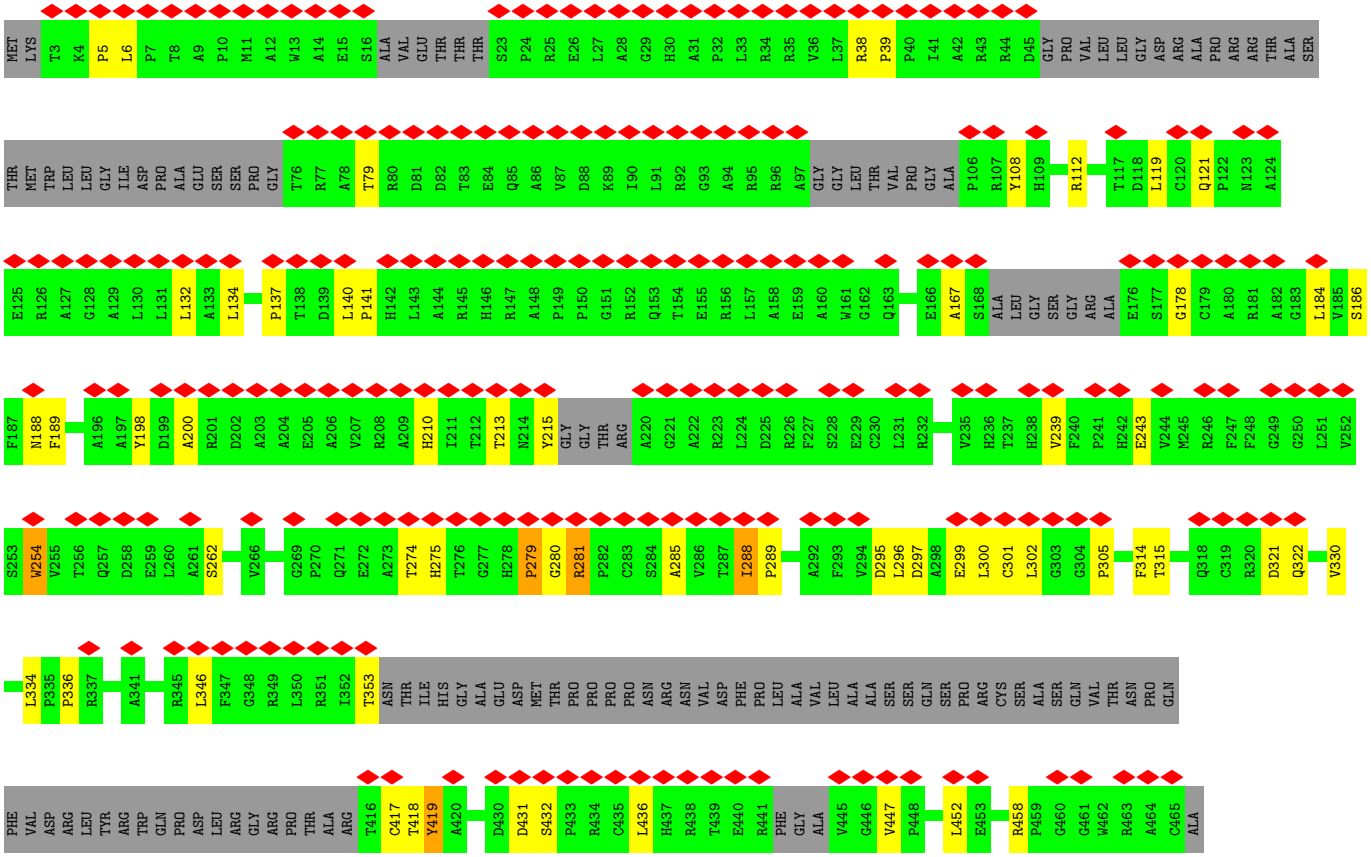


• Molecule 3: Triplex capsid protein 1



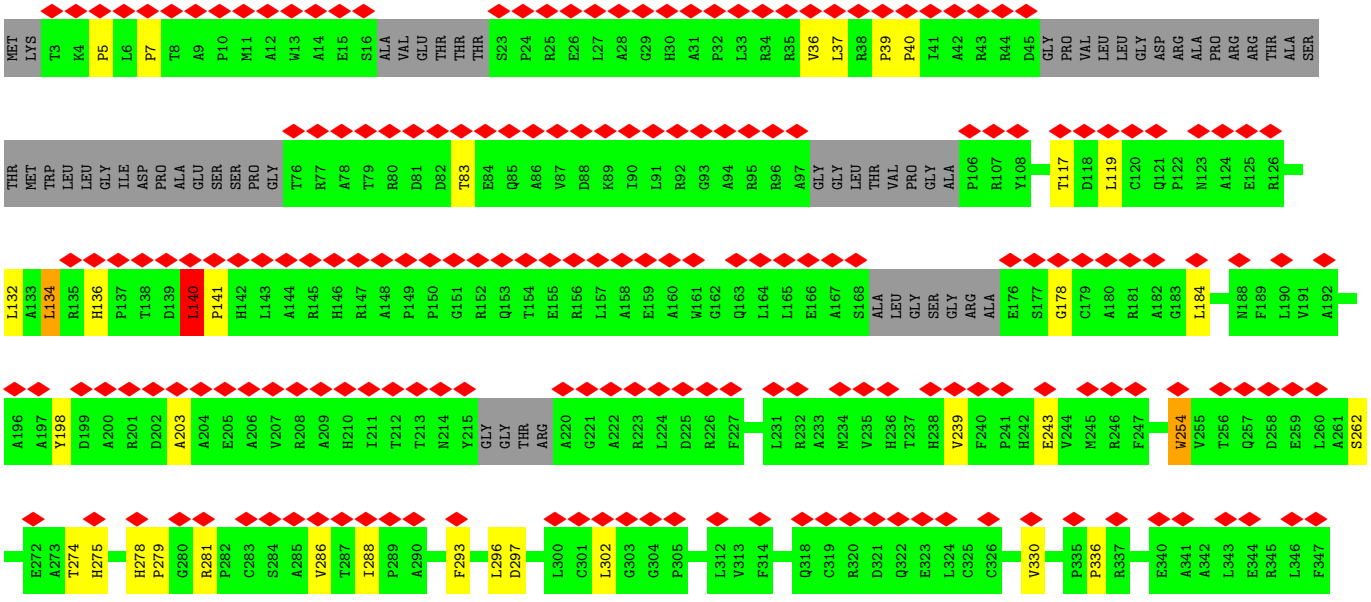
• Molecule 3: Triplex capsid protein 1

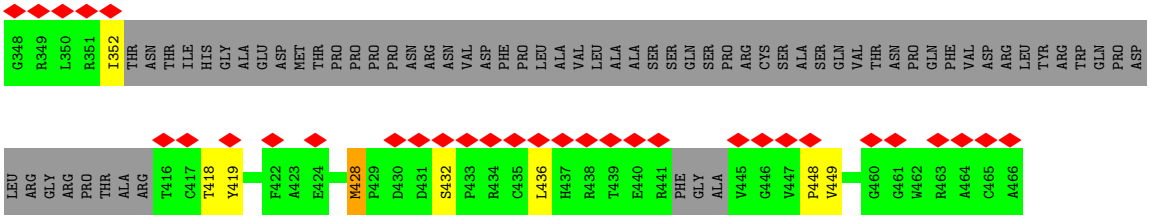
Chain b:



• Molecule 3: Triplex capsid protein 1

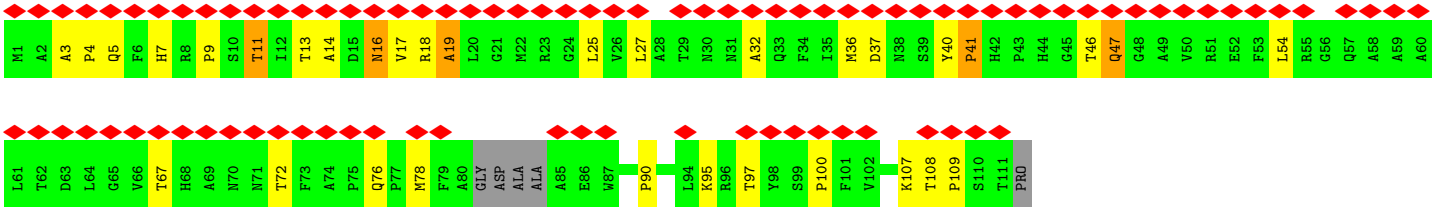
Chain e:





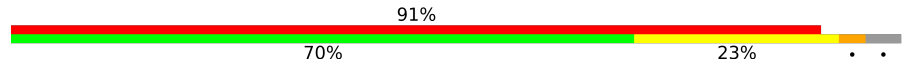
• Molecule 4: Small capsomere-interacting protein

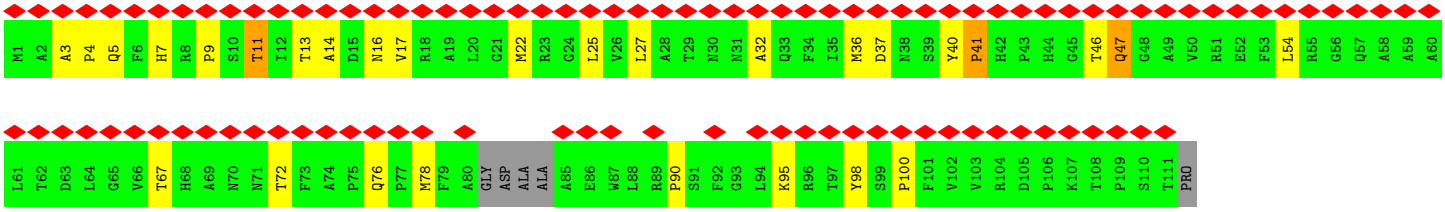
Chain f:



• Molecule 4: Small capsomere-interacting protein

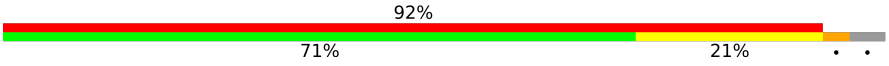
Chain g:

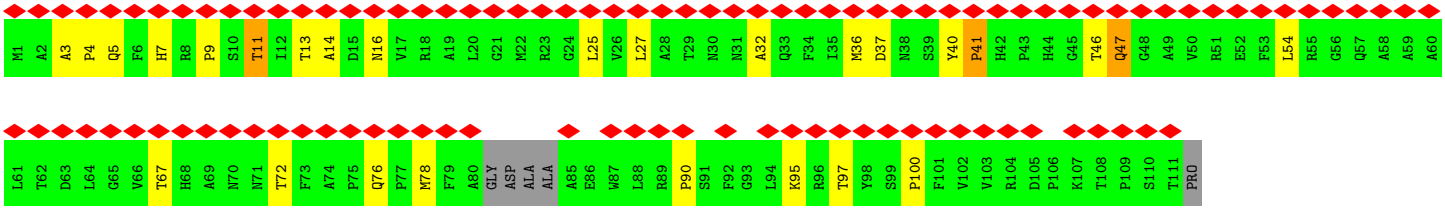




• Molecule 4: Small capsomere-interacting protein

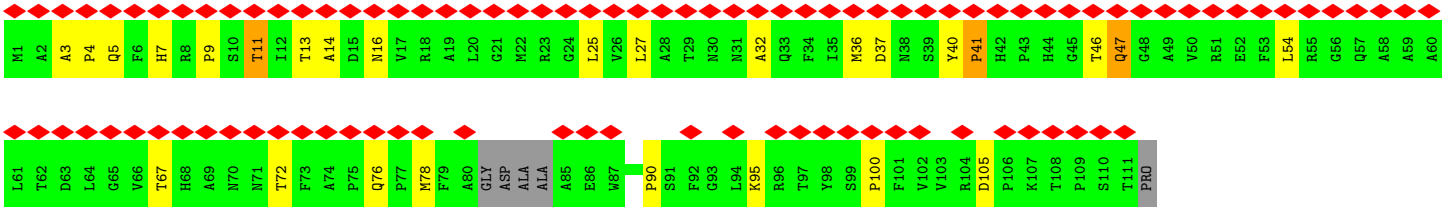
Chain h:





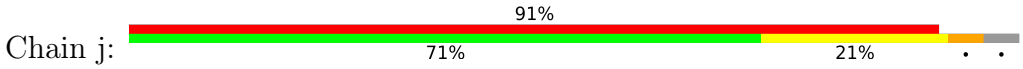
• Molecule 4: Small capsomere-interacting protein

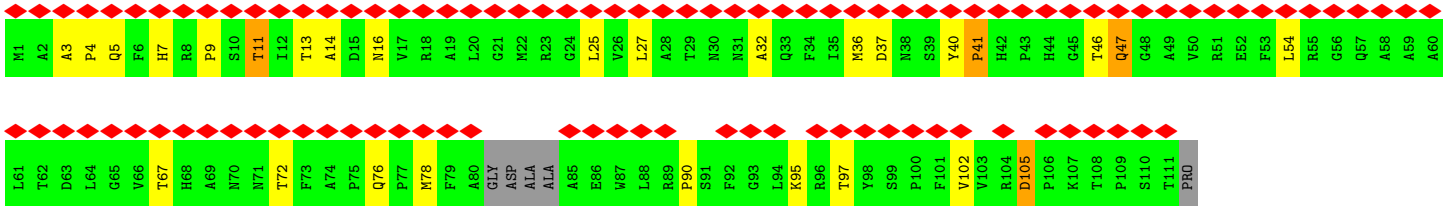
Chain i:



• Molecule 4: Small capsomere-interacting protein

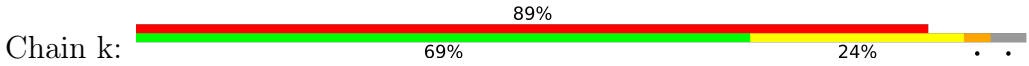
Chain j:

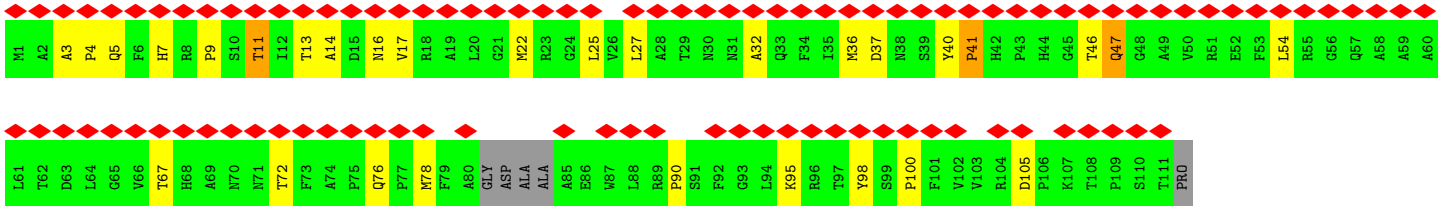




• Molecule 4: Small capsomere-interacting protein

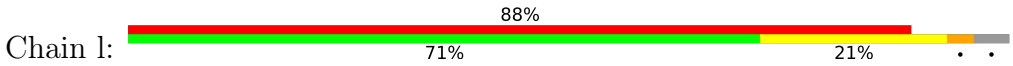
Chain k:

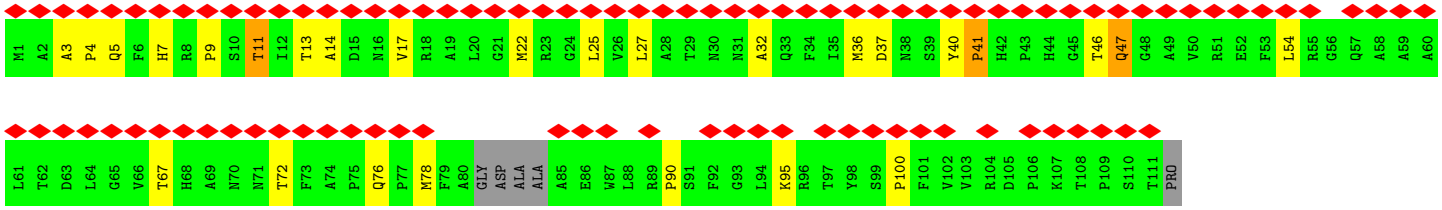




• Molecule 4: Small capsomere-interacting protein

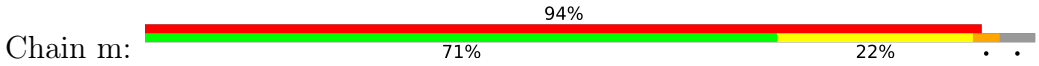
Chain l:

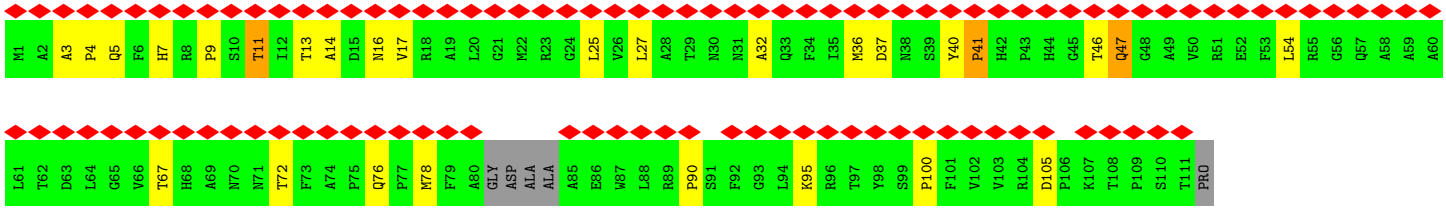




• Molecule 4: Small capsomere-interacting protein

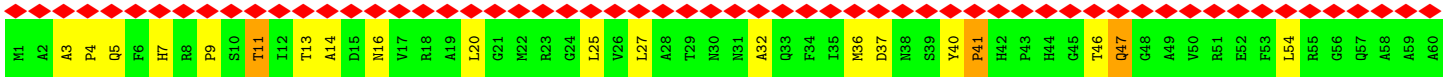
Chain m:

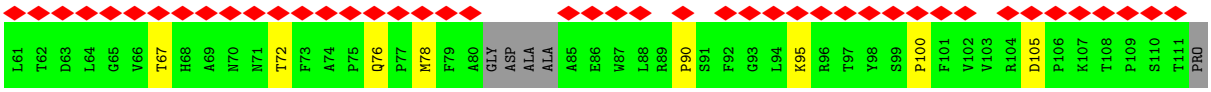




• Molecule 4: Small capsomere-interacting protein

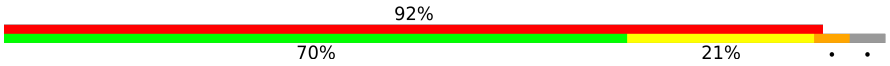
Chain n:

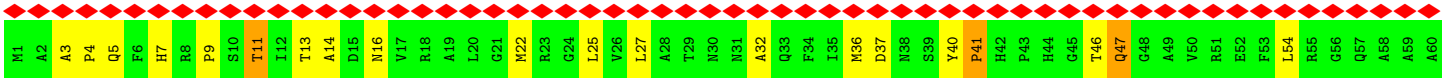


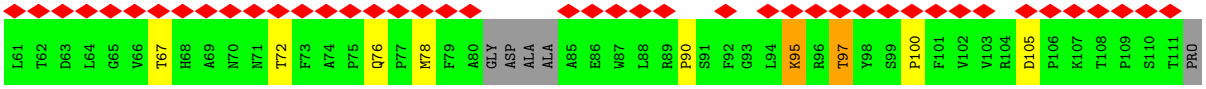


• Molecule 4: Small capsomere-interacting protein

Chain o:

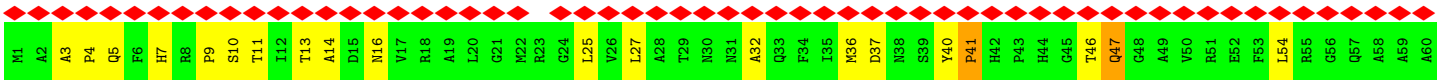


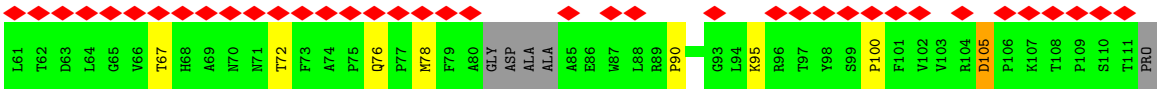




• Molecule 4: Small capsomere-interacting protein

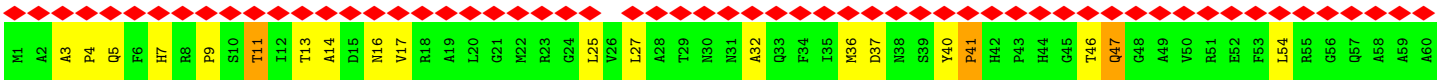
Chain p:

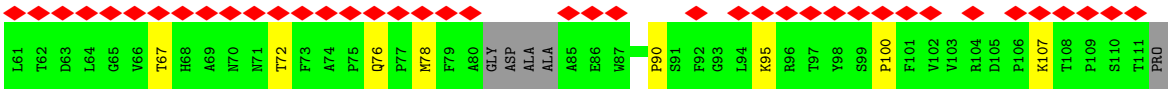




• Molecule 4: Small capsomere-interacting protein

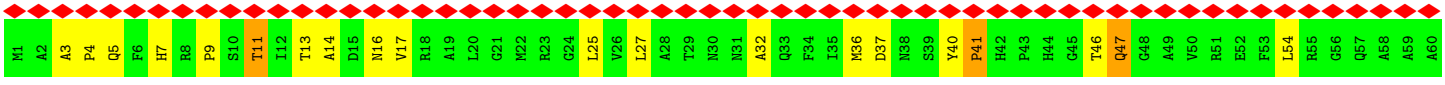
Chain q:

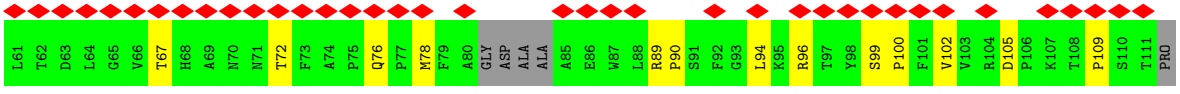




• Molecule 4: Small capsomere-interacting protein

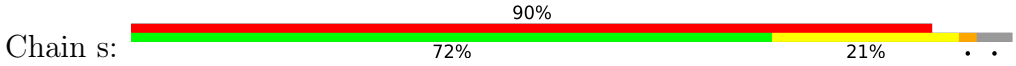
Chain r:

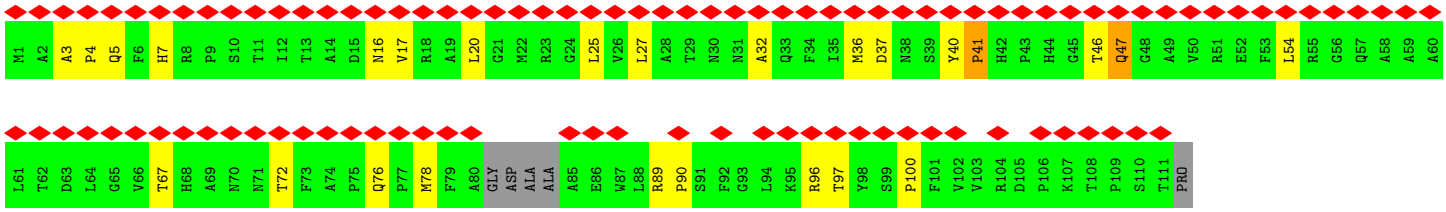




• Molecule 4: Small capsomere-interacting protein

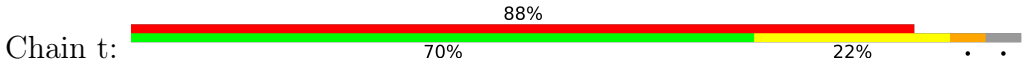
Chain s:

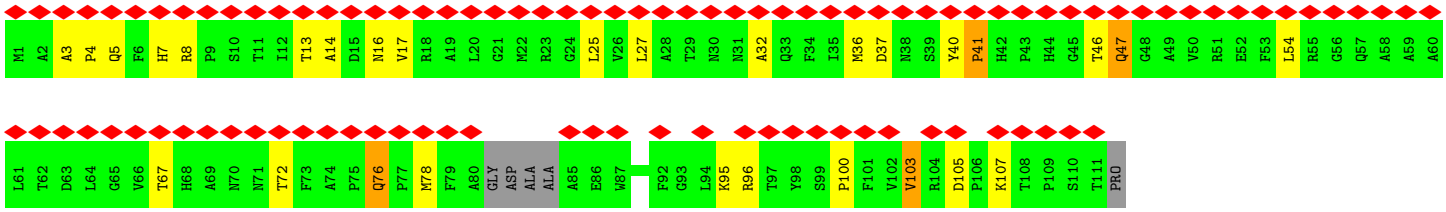




• Molecule 4: Small capsomere-interacting protein

Chain t:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	121.639	Depositor
Minimum map value	-84.361	Depositor
Average map value	0.001	Depositor
Map value standard deviation	3.240	Depositor
Recommended contour level	12.0	Depositor
Map size (Å)	1656.0, 1656.0, 1656.0	wwPDB
Map dimensions	1200, 1200, 1200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.65	1/10414 (0.0%)	0.85	33/14248 (0.2%)
1	B	0.68	0/10355	0.84	32/14158 (0.2%)
1	C	0.69	0/10476	0.84	27/14321 (0.2%)
1	D	0.63	1/10485 (0.0%)	0.81	28/14333 (0.2%)
1	E	0.61	0/10488	0.80	27/14335 (0.2%)
1	F	0.69	3/10494 (0.0%)	0.81	20/14341 (0.1%)
1	G	0.59	1/10355 (0.0%)	0.87	43/14175 (0.3%)
1	H	0.60	1/10501 (0.0%)	0.79	20/14351 (0.1%)
1	I	0.72	0/10495	0.87	30/14343 (0.2%)
1	J	0.79	1/10460 (0.0%)	0.97	53/14301 (0.4%)
1	K	1.01	6/10509 (0.1%)	1.00	58/14360 (0.4%)
1	L	0.99	8/10497 (0.1%)	1.00	50/14346 (0.3%)
1	M	0.93	11/10532 (0.1%)	0.99	68/14394 (0.5%)
1	N	0.90	9/10509 (0.1%)	0.98	59/14360 (0.4%)
1	O	1.00	7/10507 (0.1%)	1.00	58/14358 (0.4%)
1	P	0.96	7/10512 (0.1%)	0.97	54/14365 (0.4%)
2	Q	0.67	0/2114	0.84	3/2909 (0.1%)
2	R	0.65	0/2215	0.94	10/3047 (0.3%)
2	T	0.69	0/2114	0.84	3/2909 (0.1%)
2	U	0.65	0/2219	0.93	10/3052 (0.3%)
2	W	0.68	0/2114	0.84	3/2909 (0.1%)
2	X	0.64	0/2227	0.92	9/3063 (0.3%)
2	Z	0.69	0/2099	0.86	5/2891 (0.2%)
2	a	0.69	0/2209	1.04	14/3040 (0.5%)
2	c	0.69	0/2114	0.84	1/2909 (0.0%)
2	d	0.65	0/2227	0.96	14/3063 (0.5%)
3	S	0.67	0/2311	1.09	20/3167 (0.6%)
3	V	0.67	0/2413	1.11	24/3309 (0.7%)
3	Y	0.69	0/2433	1.23	27/3334 (0.8%)
3	b	0.64	0/2376	1.06	18/3261 (0.6%)
3	e	0.67	0/2410	1.08	20/3301 (0.6%)
4	f	0.83	1/635 (0.2%)	1.51	14/877 (1.6%)
4	g	0.83	1/635 (0.2%)	1.42	11/877 (1.3%)
4	h	0.81	1/635 (0.2%)	1.40	10/877 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	i	0.82	1/635 (0.2%)	1.41	11/877 (1.3%)
4	j	0.81	1/639 (0.2%)	1.40	11/881 (1.2%)
4	k	0.83	1/635 (0.2%)	1.42	11/877 (1.3%)
4	l	0.82	1/635 (0.2%)	1.40	10/877 (1.1%)
4	m	0.82	1/635 (0.2%)	1.41	11/877 (1.3%)
4	n	0.82	1/632 (0.2%)	1.42	11/874 (1.3%)
4	o	0.82	1/635 (0.2%)	1.43	11/877 (1.3%)
4	p	0.83	1/635 (0.2%)	1.39	11/877 (1.3%)
4	q	0.84	1/635 (0.2%)	1.43	10/877 (1.1%)
4	r	0.77	1/639 (0.2%)	1.45	13/881 (1.5%)
4	s	0.75	1/641 (0.2%)	1.39	8/884 (0.9%)
4	t	0.77	1/635 (0.2%)	1.36	11/877 (1.3%)
All	All	0.77	71/210720 (0.0%)	0.95	1005/288420 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
2	R	0	1
2	U	0	1
2	X	0	1
2	a	0	1
2	d	0	1
3	S	0	1
3	V	0	1
3	Y	0	1
3	e	0	1
4	f	0	1
4	g	0	1
4	h	0	1
4	i	0	1
4	j	0	1
4	k	0	1
4	l	0	1
4	m	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	n	0	1
4	o	0	1
4	p	0	1
4	q	0	1
4	r	0	1
4	s	0	1
4	t	0	1
All	All	0	30

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	818	PRO	N-CD	-8.60	1.35	1.47
1	L	1253	GLY	C-O	-8.07	1.10	1.23
1	P	1198	TYR	CE1-CZ	-7.96	1.28	1.38
1	J	273	PRO	N-CD	-7.86	1.36	1.47
1	F	818	PRO	N-CD	-7.84	1.36	1.47
1	L	486	PRO	N-CD	-7.83	1.36	1.47
1	M	818	PRO	N-CD	-7.48	1.37	1.47
1	N	1324	PRO	N-CD	-7.44	1.37	1.47
1	L	475	GLY	C-O	-7.24	1.12	1.23
1	P	1252	TYR	CE1-CZ	-7.11	1.29	1.38
1	K	1253	GLY	C-O	-6.95	1.12	1.23
1	P	1330	GLU	CD-OE1	-6.92	1.18	1.25
1	P	109	PRO	N-CD	-6.80	1.38	1.47
1	N	1227	TYR	CE1-CZ	-6.69	1.29	1.38
1	O	1202	PRO	N-CD	-6.63	1.38	1.47
1	K	1203	CYS	C-O	-6.16	1.11	1.23
1	L	1106	TYR	CE1-CZ	-6.13	1.30	1.38
1	O	964	PHE	CA-CB	-6.04	1.40	1.53
1	N	1106	TYR	CE1-CZ	-6.04	1.30	1.38
1	F	1331	ALA	C-N	-5.85	1.20	1.34
1	A	1252	TYR	CE1-CZ	-5.82	1.30	1.38
1	N	821	SER	CA-CB	-5.82	1.44	1.52
1	K	303	PRO	N-CD	-5.79	1.39	1.47
1	M	416	PHE	CG-CD2	-5.76	1.30	1.38
1	N	1251	SER	CB-OG	-5.72	1.34	1.42
1	M	1037	TYR	CB-CG	-5.69	1.43	1.51
1	N	1198	TYR	CE2-CZ	-5.62	1.31	1.38
1	M	1202	PRO	N-CD	-5.61	1.40	1.47
1	M	492	ALA	C-N	-5.60	1.21	1.34
4	l	32	ALA	CA-C	5.59	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	n	32	ALA	CA-C	5.58	1.67	1.52
4	r	32	ALA	CA-C	5.57	1.67	1.52
4	g	32	ALA	CA-C	5.57	1.67	1.52
4	h	32	ALA	CA-C	5.57	1.67	1.52
4	t	32	ALA	CA-C	5.56	1.67	1.52
4	i	32	ALA	CA-C	5.56	1.67	1.52
4	j	32	ALA	CA-C	5.55	1.67	1.52
4	k	32	ALA	CA-C	5.55	1.67	1.52
4	o	32	ALA	CA-C	5.55	1.67	1.52
4	q	32	ALA	CA-C	5.55	1.67	1.52
4	s	32	ALA	CA-C	5.54	1.67	1.52
4	f	32	ALA	CA-C	5.54	1.67	1.52
4	p	32	ALA	CA-C	5.54	1.67	1.52
4	m	32	ALA	CA-C	5.53	1.67	1.52
1	P	13	TYR	CE1-CZ	-5.48	1.31	1.38
1	L	534	PRO	N-CD	-5.46	1.40	1.47
1	P	1253	GLY	C-O	-5.46	1.15	1.23
1	K	119	TYR	CB-CG	-5.45	1.43	1.51
1	F	1198	TYR	CB-CG	-5.43	1.43	1.51
1	H	1331	ALA	C-N	-5.37	1.21	1.34
1	P	575	TRP	CB-CG	-5.37	1.40	1.50
1	D	13	TYR	CE1-CZ	-5.28	1.31	1.38
1	O	1253	GLY	C-O	-5.28	1.15	1.23
1	M	1253	GLY	C-O	-5.25	1.15	1.23
1	G	274	VAL	CB-CG1	-5.22	1.41	1.52
1	M	1227	TYR	CE1-CZ	-5.21	1.31	1.38
1	N	303	PRO	N-CD	-5.20	1.40	1.47
1	N	956	TYR	CE2-CZ	-5.18	1.31	1.38
1	K	596	GLY	C-O	-5.17	1.15	1.23
1	M	416	PHE	CG-CD1	-5.17	1.30	1.38
1	O	109	PRO	C-N	-5.17	1.22	1.34
1	O	50	TYR	CE1-CZ	-5.11	1.31	1.38
1	K	1106	TYR	CE1-CZ	-5.09	1.31	1.38
1	L	1158	GLY	CA-C	-5.09	1.43	1.51
1	M	1252	TYR	CG-CD2	-5.06	1.32	1.39
1	O	416	PHE	CG-CD2	-5.05	1.31	1.38
1	L	120	MET	C-O	-5.05	1.13	1.23
1	L	686	CYS	CB-SG	-5.04	1.73	1.81
1	M	385	TYR	CD2-CE2	-5.03	1.31	1.39
1	O	1198	TYR	CE1-CZ	-5.01	1.32	1.38
1	M	119	TYR	CE1-CZ	-5.01	1.32	1.38

All (1005) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	140	LEU	C-N-CD	-29.80	55.04	120.60
1	M	1161	GLN	C-N-CD	-13.85	90.14	120.60
3	e	140	LEU	C-N-CD	-11.74	94.77	120.60
3	b	281	ARG	C-N-CD	-11.72	94.82	120.60
1	L	1265	GLY	N-CA-C	-11.18	85.14	113.10
1	I	302	VAL	C-N-CD	-10.95	96.50	120.60
1	K	433	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	K	557	GLU	N-CA-C	-10.62	82.33	111.00
1	O	1265	GLY	N-CA-C	-10.26	87.45	113.10
1	J	302	VAL	C-N-CD	-10.19	98.19	120.60
1	K	371	GLY	N-CA-C	-10.11	87.84	113.10
1	A	1086	GLY	N-CA-C	-10.10	87.85	113.10
1	P	528	ALA	N-CA-C	-9.88	84.31	111.00
1	A	1158	GLY	N-CA-C	-9.79	88.63	113.10
1	E	29	VAL	CB-CA-C	-9.66	93.04	111.40
1	F	882	GLY	N-CA-C	-9.54	89.24	113.10
1	F	1265	GLY	N-CA-C	-9.53	89.28	113.10
1	K	882	GLY	N-CA-C	-9.48	89.39	113.10
1	E	882	GLY	N-CA-C	-9.48	89.40	113.10
4	o	97	THR	N-CA-C	-9.42	85.57	111.00
1	N	1219	GLU	CB-CA-C	-9.42	91.57	110.40
1	H	1147	LEU	CA-CB-CG	9.33	136.76	115.30
1	I	882	GLY	N-CA-C	-9.19	90.12	113.10
1	J	235	GLY	N-CA-C	-9.18	90.15	113.10
1	L	1224	ALA	N-CA-C	-9.04	86.59	111.00
1	P	965	ALA	N-CA-C	-9.00	86.70	111.00
1	M	302	VAL	C-N-CD	-8.99	100.82	120.60
1	K	536	ASN	N-CA-C	-8.89	86.99	111.00
1	J	527	THR	N-CA-C	-8.88	87.02	111.00
1	M	945	LEU	CB-CA-C	-8.87	93.35	110.20
1	M	527	THR	CB-CA-C	-8.86	87.69	111.60
1	D	529	GLU	N-CA-C	-8.78	87.31	111.00
1	L	1147	LEU	CB-CG-CD1	-8.76	96.12	111.00
1	M	917	GLY	N-CA-C	-8.75	91.21	113.10
1	C	529	GLU	N-CA-C	-8.73	87.44	111.00
1	J	234	LEU	CB-CA-C	-8.71	93.65	110.20
1	B	882	GLY	N-CA-C	-8.70	91.34	113.10
1	E	1316	GLY	N-CA-C	8.69	134.82	113.10
1	A	1253	GLY	N-CA-C	-8.69	91.38	113.10
1	P	1279	ALA	CB-CA-C	-8.65	97.13	110.10
1	P	882	GLY	N-CA-C	-8.63	91.52	113.10
1	M	381	GLU	N-CA-C	-8.62	87.73	111.00
1	L	882	GLY	N-CA-C	-8.59	91.63	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	f	19	ALA	N-CA-C	-8.57	87.86	111.00
1	O	1226	MET	CG-SD-CE	8.45	113.72	100.20
1	I	404	LEU	CA-CB-CG	8.39	134.60	115.30
1	C	145	GLY	N-CA-C	-8.37	92.18	113.10
1	N	264	LEU	CA-CB-CG	8.34	134.47	115.30
4	j	97	THR	N-CA-C	-8.33	88.52	111.00
1	L	1198	TYR	N-CA-C	-8.32	88.52	111.00
1	O	917	GLY	N-CA-C	-8.31	92.32	113.10
1	E	921	ALA	N-CA-CB	8.31	121.73	110.10
1	H	1199	PHE	N-CA-C	-8.31	88.57	111.00
1	K	433	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	I	529	GLU	N-CA-C	-8.30	88.59	111.00
1	I	1123	GLY	N-CA-C	8.28	133.81	113.10
1	N	70	PHE	CB-CA-C	-8.26	93.88	110.40
1	C	1119	VAL	CB-CA-C	-8.23	95.76	111.40
1	J	446	ASP	N-CA-C	-8.22	88.81	111.00
1	K	1196	ILE	N-CA-C	-8.21	88.84	111.00
1	O	438	ARG	NE-CZ-NH2	8.19	124.40	120.30
1	O	1347	ARG	N-CA-C	-8.19	88.88	111.00
1	G	536	ASN	N-CA-C	-8.17	88.95	111.00
1	M	882	GLY	N-CA-C	-8.16	92.69	113.10
1	M	536	ASN	N-CA-C	-8.13	89.04	111.00
1	A	295	VAL	N-CA-C	8.12	132.93	111.00
1	O	920	THR	N-CA-C	-8.11	89.11	111.00
1	N	293	LEU	CB-CG-CD2	-8.09	97.25	111.00
4	s	97	THR	N-CA-C	-8.08	89.19	111.00
3	b	280	GLY	N-CA-C	-8.07	92.91	113.10
1	N	258	SER	N-CA-C	8.07	132.78	111.00
1	A	270	ARG	N-CA-C	-8.03	89.33	111.00
1	D	1219	GLU	CB-CA-C	-8.02	94.36	110.40
1	E	1120	THR	N-CA-C	-8.02	89.35	111.00
1	J	1075	LEU	CA-CB-CG	8.01	133.73	115.30
1	N	110	HIS	N-CA-C	-8.01	89.37	111.00
1	C	882	GLY	N-CA-C	-8.00	93.09	113.10
1	C	1194	THR	N-CA-C	-7.95	89.54	111.00
4	q	11	THR	N-CA-C	7.94	132.45	111.00
1	L	536	ASN	N-CA-C	-7.94	89.57	111.00
1	D	882	GLY	N-CA-C	-7.92	93.31	113.10
1	P	304	VAL	CB-CA-C	-7.92	96.36	111.40
1	E	786	ASN	N-CA-C	7.88	132.29	111.00
1	D	1158	GLY	N-CA-C	-7.83	93.52	113.10
1	E	304	VAL	CB-CA-C	-7.83	96.52	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1219	GLU	CB-CA-C	-7.81	94.78	110.40
1	N	277	VAL	N-CA-C	-7.76	90.05	111.00
1	H	536	ASN	N-CA-C	-7.74	90.12	111.00
4	k	76	GLN	N-CA-C	-7.70	90.21	111.00
1	J	400	LEU	N-CA-C	-7.70	90.22	111.00
4	t	76	GLN	N-CA-C	-7.70	90.22	111.00
4	j	76	GLN	N-CA-C	-7.69	90.24	111.00
4	q	76	GLN	N-CA-C	-7.69	90.24	111.00
4	r	76	GLN	N-CA-C	-7.69	90.24	111.00
4	s	76	GLN	N-CA-C	-7.69	90.25	111.00
4	h	76	GLN	N-CA-C	-7.69	90.25	111.00
4	o	76	GLN	N-CA-C	-7.68	90.25	111.00
1	O	1138	LEU	CB-CG-CD1	-7.68	97.94	111.00
4	g	76	GLN	N-CA-C	-7.68	90.25	111.00
4	i	76	GLN	N-CA-C	-7.68	90.26	111.00
4	l	76	GLN	N-CA-C	-7.68	90.26	111.00
4	m	76	GLN	N-CA-C	-7.68	90.26	111.00
4	f	76	GLN	N-CA-C	-7.68	90.26	111.00
4	p	76	GLN	N-CA-C	-7.68	90.27	111.00
4	n	76	GLN	N-CA-C	-7.67	90.30	111.00
1	M	1086	GLY	N-CA-C	-7.66	93.94	113.10
1	D	1199	PHE	N-CA-C	-7.64	90.36	111.00
1	L	73	LEU	CA-CB-CG	7.64	132.88	115.30
2	a	43	LEU	C-N-CA	-7.64	102.60	121.70
4	r	94	LEU	N-CA-C	-7.62	90.41	111.00
3	V	278	HIS	C-N-CD	-7.62	103.84	120.60
1	E	1123	GLY	N-CA-C	7.61	132.12	113.10
1	F	557	GLU	N-CA-C	-7.60	90.48	111.00
1	J	1054	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	E	1124	ASN	N-CA-C	7.50	131.26	111.00
1	B	786	ASN	N-CA-C	7.50	131.25	111.00
2	a	71	PHE	C-N-CD	-7.49	104.11	120.60
1	I	682	LEU	CA-CB-CG	7.47	132.47	115.30
1	O	93	GLY	N-CA-C	-7.47	94.44	113.10
1	K	1138	LEU	CB-CG-CD1	-7.45	98.33	111.00
1	P	1194	THR	N-CA-C	-7.45	90.89	111.00
1	I	1194	THR	N-CA-C	-7.44	90.91	111.00
1	J	355	GLU	N-CA-C	-7.43	90.94	111.00
1	J	882	GLY	N-CA-C	-7.43	94.52	113.10
1	P	70	PHE	CB-CA-C	-7.42	95.56	110.40
1	M	1225	LEU	CA-CB-CG	7.41	132.33	115.30
4	n	11	THR	N-CA-C	7.39	130.95	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	h	11	THR	N-CA-C	7.38	130.93	111.00
4	o	11	THR	N-CA-C	7.38	130.93	111.00
4	l	11	THR	N-CA-C	7.38	130.92	111.00
3	S	278	HIS	C-N-CD	-7.38	104.38	120.60
4	i	11	THR	N-CA-C	7.37	130.91	111.00
4	g	11	THR	N-CA-C	7.37	130.90	111.00
4	j	11	THR	N-CA-C	7.37	130.89	111.00
4	k	11	THR	N-CA-C	7.37	130.90	111.00
4	f	11	THR	N-CA-C	7.36	130.88	111.00
4	m	11	THR	N-CA-C	7.36	130.88	111.00
1	L	1347	ARG	N-CA-C	-7.33	91.21	111.00
1	M	44	SER	N-CA-C	-7.31	91.25	111.00
1	J	51	ASP	N-CA-C	-7.30	91.29	111.00
1	P	966	GLY	N-CA-C	-7.29	94.87	113.10
1	O	1108	ALA	N-CA-C	7.28	130.65	111.00
3	b	279	PRO	N-CA-C	-7.28	93.18	112.10
3	b	274	THR	N-CA-C	7.27	130.62	111.00
3	e	274	THR	N-CA-C	7.25	130.59	111.00
1	O	293	LEU	CA-CB-CG	7.25	131.98	115.30
1	N	1224	ALA	N-CA-C	-7.24	91.44	111.00
1	N	71	LEU	N-CA-C	-7.24	91.45	111.00
1	B	1224	ALA	N-CA-C	-7.24	91.46	111.00
3	Y	274	THR	N-CA-C	7.23	130.53	111.00
1	H	682	LEU	CA-CB-CG	7.23	131.93	115.30
3	V	274	THR	N-CA-C	7.22	130.50	111.00
3	V	6	LEU	CB-CA-C	7.21	123.90	110.20
1	M	528	ALA	N-CA-C	-7.21	91.53	111.00
1	J	267	ALA	C-N-CA	-7.21	103.68	121.70
3	b	6	LEU	CB-CA-C	7.20	123.88	110.20
1	B	1194	THR	N-CA-C	-7.20	91.57	111.00
1	L	445	LYS	N-CA-C	-7.19	91.58	111.00
1	N	918	ALA	N-CA-C	-7.19	91.59	111.00
1	B	1083	HIS	N-CA-C	-7.18	91.61	111.00
1	H	916	ALA	N-CA-C	-7.17	91.63	111.00
3	Y	6	LEU	CB-CA-C	7.17	123.83	110.20
1	H	786	ASN	N-CA-C	7.15	130.30	111.00
1	J	1138	LEU	CB-CG-CD2	-7.14	98.86	111.00
1	N	13	TYR	N-CA-C	-7.14	91.73	111.00
1	P	682	LEU	CA-CB-CG	7.13	131.70	115.30
1	B	1200	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	G	387	ALA	N-CA-CB	7.11	120.06	110.10
1	K	595	ARG	NE-CZ-NH2	-7.10	116.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	682	LEU	CA-CB-CG	7.08	131.59	115.30
1	K	1266	ALA	N-CA-C	-7.08	91.87	111.00
1	M	528	ALA	C-N-CA	7.08	139.39	121.70
1	I	1224	ALA	N-CA-C	-7.07	91.90	111.00
3	S	282	PRO	N-CA-C	7.07	130.48	112.10
1	L	87	LEU	N-CA-C	-7.06	91.94	111.00
1	H	753	ASP	N-CA-CB	7.06	123.31	110.60
3	S	293	PHE	N-CA-C	-7.06	91.95	111.00
3	e	293	PHE	N-CA-C	-7.05	91.96	111.00
4	l	7	HIS	N-CA-C	-7.05	91.97	111.00
1	A	419	HIS	N-CA-CB	7.05	123.28	110.60
1	H	363	VAL	N-CA-C	7.05	130.02	111.00
3	Y	293	PHE	N-CA-C	-7.05	91.98	111.00
4	n	7	HIS	N-CA-C	-7.04	91.98	111.00
4	r	7	HIS	N-CA-C	-7.04	91.98	111.00
4	k	7	HIS	N-CA-C	-7.04	91.99	111.00
4	p	7	HIS	N-CA-C	-7.04	91.99	111.00
1	K	1147	LEU	CA-CB-CG	7.04	131.49	115.30
4	g	7	HIS	N-CA-C	-7.04	92.00	111.00
4	s	7	HIS	N-CA-C	-7.04	91.99	111.00
3	V	293	PHE	N-CA-C	-7.03	92.01	111.00
4	m	7	HIS	N-CA-C	-7.03	92.01	111.00
1	N	1124	ASN	N-CA-C	7.03	129.98	111.00
1	O	35	LEU	CA-CB-CG	7.03	131.47	115.30
4	f	7	HIS	N-CA-C	-7.03	92.02	111.00
4	j	7	HIS	N-CA-C	-7.03	92.03	111.00
4	o	7	HIS	N-CA-C	-7.03	92.03	111.00
1	K	293	LEU	CA-CB-CG	7.03	131.46	115.30
4	h	7	HIS	N-CA-C	-7.03	92.03	111.00
4	i	7	HIS	N-CA-C	-7.03	92.03	111.00
1	M	31	SER	N-CA-C	-7.02	92.03	111.00
4	q	7	HIS	N-CA-C	-7.02	92.04	111.00
4	t	7	HIS	N-CA-C	-7.02	92.06	111.00
1	K	1264	ASN	N-CA-C	-7.00	92.10	111.00
3	Y	140	LEU	N-CA-C	-6.98	92.14	111.00
1	G	821	SER	N-CA-C	-6.98	92.15	111.00
3	Y	448	PRO	N-CA-C	-6.97	93.98	112.10
3	V	448	PRO	N-CA-C	-6.96	94.00	112.10
1	M	1147	LEU	CB-CG-CD1	-6.95	99.18	111.00
1	N	1198	TYR	N-CA-C	-6.95	92.23	111.00
3	e	448	PRO	N-CA-C	-6.95	94.03	112.10
1	P	526	MET	N-CA-C	-6.94	92.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	1224	ALA	N-CA-C	-6.94	92.26	111.00
3	S	448	PRO	N-CA-C	-6.94	94.06	112.10
1	C	419	HIS	N-CA-CB	6.93	123.08	110.60
1	O	452	LEU	CA-CB-CG	6.93	131.24	115.30
1	A	367	LEU	CB-CG-CD1	-6.92	99.24	111.00
1	P	1280	ALA	N-CA-C	-6.92	92.33	111.00
1	N	1222	VAL	N-CA-C	-6.92	92.33	111.00
3	V	41	ILE	N-CA-C	-6.89	92.40	111.00
1	N	1201	ARG	N-CA-C	-6.88	92.42	111.00
1	C	1280	ALA	N-CA-C	-6.86	92.48	111.00
1	P	357	ALA	N-CA-C	-6.85	92.50	111.00
1	J	427	PRO	N-CA-C	6.84	129.89	112.10
1	N	304	VAL	CB-CA-C	-6.83	98.42	111.40
1	P	1225	LEU	CA-CB-CG	6.82	130.98	115.30
1	H	1124	ASN	N-CA-C	6.81	129.38	111.00
1	O	1253	GLY	N-CA-C	-6.81	96.08	113.10
3	Y	288	ILE	C-N-CD	-6.80	105.64	120.60
4	r	11	THR	N-CA-C	6.80	129.36	111.00
1	L	45	ASP	N-CA-CB	-6.80	98.36	110.60
3	V	288	ILE	C-N-CD	-6.79	105.65	120.60
3	S	288	ILE	C-N-CD	-6.79	105.66	120.60
1	O	49	LEU	CA-CB-CG	6.78	130.90	115.30
3	e	288	ILE	C-N-CD	-6.78	105.68	120.60
1	E	1198	TYR	N-CA-C	-6.78	92.70	111.00
1	P	754	CYS	N-CA-C	-6.76	92.74	111.00
1	D	682	LEU	CA-CB-CG	6.76	130.85	115.30
2	d	96	GLY	N-CA-C	6.76	129.99	113.10
2	X	96	GLY	N-CA-C	6.75	129.99	113.10
1	O	536	ASN	N-CA-C	-6.75	92.78	111.00
2	U	96	GLY	N-CA-C	6.75	129.98	113.10
2	R	96	GLY	N-CA-C	6.75	129.97	113.10
1	N	945	LEU	CA-CB-CG	6.75	130.81	115.30
1	M	293	LEU	CA-CB-CG	6.74	130.79	115.30
1	M	30	ALA	CB-CA-C	-6.72	100.01	110.10
1	I	1078	LEU	CA-CB-CG	6.72	130.76	115.30
1	K	24	LEU	CA-CB-CG	6.72	130.76	115.30
1	J	1347	ARG	N-CA-C	-6.72	92.86	111.00
1	O	1348	ASP	N-CA-C	-6.72	92.86	111.00
1	G	126	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	D	429	HIS	N-CA-C	6.72	129.13	111.00
2	Z	316	ARG	N-CA-C	6.72	129.13	111.00
2	d	164	ASN	N-CA-C	-6.72	92.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	921	ALA	N-CA-C	6.71	129.12	111.00
1	G	760	GLY	N-CA-C	6.70	129.85	113.10
1	O	73	LEU	CA-CB-CG	6.70	130.71	115.30
2	Z	207	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	L	682	LEU	CA-CB-CG	6.70	130.70	115.30
1	G	520	TRP	N-CA-C	-6.69	92.92	111.00
2	Q	207	LEU	CB-CG-CD1	-6.69	99.63	111.00
1	N	484	ALA	N-CA-C	-6.68	92.97	111.00
1	L	294	LYS	N-CA-C	-6.67	93.00	111.00
1	O	395	VAL	N-CA-C	-6.67	92.99	111.00
1	L	466	LEU	N-CA-C	-6.66	93.01	111.00
2	T	207	LEU	CB-CG-CD1	-6.66	99.68	111.00
1	B	682	LEU	CA-CB-CG	6.66	130.61	115.30
2	W	207	LEU	CB-CG-CD1	-6.65	99.69	111.00
2	c	207	LEU	CB-CG-CD1	-6.65	99.69	111.00
1	J	1224	ALA	N-CA-C	-6.65	93.05	111.00
1	K	304	VAL	CB-CA-C	-6.64	98.79	111.40
1	O	1123	GLY	N-CA-C	6.64	129.69	113.10
1	K	1279	ALA	C-N-CA	6.62	138.25	121.70
3	b	458	ARG	N-CA-C	-6.61	93.15	111.00
3	e	432	SER	N-CA-C	6.61	128.84	111.00
1	A	682	LEU	CA-CB-CG	6.60	130.48	115.30
1	I	541	LEU	CA-CB-CG	-6.60	100.12	115.30
1	J	463	HIS	N-CA-C	-6.60	93.19	111.00
3	S	432	SER	N-CA-C	6.59	128.80	111.00
3	V	432	SER	N-CA-C	6.59	128.78	111.00
1	O	945	LEU	CA-CB-CG	6.58	130.44	115.30
1	C	938	LEU	CA-CB-CG	6.58	130.43	115.30
1	K	940	MET	N-CA-C	6.58	128.76	111.00
1	N	882	GLY	N-CA-C	-6.58	96.66	113.10
1	D	1123	GLY	N-CA-C	6.57	129.53	113.10
3	e	239	VAL	N-CA-C	-6.57	93.25	111.00
3	b	239	VAL	N-CA-C	-6.57	93.26	111.00
3	V	239	VAL	N-CA-C	-6.57	93.27	111.00
3	S	239	VAL	N-CA-C	-6.56	93.28	111.00
1	M	682	LEU	CA-CB-CG	6.56	130.39	115.30
3	Y	432	SER	N-CA-C	6.56	128.71	111.00
1	E	682	LEU	CA-CB-CG	6.56	130.38	115.30
1	N	73	LEU	CA-CB-CG	6.56	130.38	115.30
1	M	87	LEU	CA-CB-CG	6.55	130.37	115.30
1	O	1267	SER	N-CA-C	-6.55	93.31	111.00
1	N	311	LEU	CB-CG-CD1	-6.55	99.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	239	VAL	N-CA-C	-6.55	93.32	111.00
1	L	1119	VAL	CB-CA-C	-6.54	98.97	111.40
1	F	1225	LEU	CA-CB-CG	6.54	130.34	115.30
1	L	527	THR	N-CA-C	-6.52	93.39	111.00
1	A	1219	GLU	N-CA-C	6.52	128.60	111.00
1	B	1124	ASN	N-CA-C	6.52	128.61	111.00
1	N	682	LEU	CA-CB-CG	6.51	130.28	115.30
2	d	16	ILE	N-CA-C	-6.51	93.43	111.00
4	r	96	ARG	N-CA-C	-6.50	93.44	111.00
1	G	541	LEU	CA-CB-CG	-6.50	100.35	115.30
1	A	536	ASN	N-CA-C	-6.50	93.45	111.00
1	A	786	ASN	N-CA-C	6.48	128.50	111.00
1	K	1194	THR	N-CA-C	-6.48	93.50	111.00
1	A	1266	ALA	N-CA-C	-6.48	93.51	111.00
1	N	268	ASP	N-CA-C	6.46	128.44	111.00
1	N	259	VAL	N-CA-CB	6.45	125.70	111.50
3	b	300	LEU	N-CA-C	-6.45	93.58	111.00
1	F	429	HIS	N-CA-C	6.44	128.40	111.00
1	K	440	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	K	1216	GLY	N-CA-C	6.43	129.18	113.10
1	I	267	ALA	N-CA-C	-6.43	93.64	111.00
1	G	682	LEU	CA-CB-CG	6.43	130.08	115.30
1	M	1198	TYR	N-CA-C	-6.42	93.65	111.00
1	J	1123	GLY	N-CA-C	6.42	129.15	113.10
1	K	444	GLY	N-CA-C	-6.42	97.05	113.10
1	J	403	VAL	N-CA-C	-6.41	93.69	111.00
1	O	1125	LEU	CA-CB-CG	6.40	130.01	115.30
1	E	536	ASN	N-CA-C	-6.39	93.74	111.00
1	I	258	SER	CB-CA-C	-6.38	97.97	110.10
1	L	466	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	236	LYS	N-CA-C	-6.37	93.80	111.00
1	G	521	VAL	N-CA-C	-6.37	93.81	111.00
1	B	529	GLU	N-CA-C	-6.37	93.81	111.00
1	J	947	HIS	N-CA-C	6.36	128.16	111.00
1	O	883	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	371	GLY	N-CA-C	-6.35	97.22	113.10
1	B	757	ASP	N-CA-C	6.35	128.15	111.00
1	C	558	LEU	CB-CG-CD2	-6.35	100.20	111.00
1	N	1319	GLU	N-CA-C	-6.35	93.85	111.00
3	e	203	ALA	N-CA-C	-6.35	93.86	111.00
1	C	296	GLU	N-CA-C	6.35	128.14	111.00
1	G	1225	LEU	CA-CB-CG	6.34	129.89	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	203	ALA	N-CA-C	-6.34	93.89	111.00
1	L	957	VAL	N-CA-C	6.33	128.10	111.00
3	V	203	ALA	N-CA-C	-6.33	93.91	111.00
3	Y	203	ALA	N-CA-C	-6.33	93.92	111.00
1	H	882	GLY	N-CA-C	-6.32	97.29	113.10
1	L	140	ILE	CB-CA-C	-6.32	98.97	111.60
1	D	267	ALA	N-CA-CB	6.31	118.94	110.10
1	C	15	ALA	N-CA-C	-6.31	93.96	111.00
1	J	231	SER	N-CA-C	-6.31	93.96	111.00
1	K	1054	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	F	1194	THR	N-CA-C	-6.30	93.99	111.00
1	B	1225	LEU	CA-CB-CG	6.29	129.77	115.30
1	L	293	LEU	CA-CB-CG	6.28	129.73	115.30
1	I	28	GLU	N-CA-C	-6.27	94.08	111.00
1	A	1220	GLY	N-CA-C	-6.27	97.43	113.10
1	J	1225	LEU	CA-CB-CG	6.27	129.71	115.30
3	S	280	GLY	N-CA-C	-6.26	97.44	113.10
1	J	682	LEU	CA-CB-CG	6.26	129.69	115.30
1	M	946	ASP	N-CA-C	-6.25	94.12	111.00
3	V	280	GLY	N-CA-C	-6.25	97.47	113.10
1	D	266	HIS	N-CA-C	-6.25	94.12	111.00
1	D	15	ALA	N-CA-CB	6.23	118.83	110.10
4	t	8	ARG	C-N-CD	-6.23	106.89	120.60
1	G	386	ALA	CB-CA-C	-6.23	100.75	110.10
4	f	18	ARG	N-CA-C	-6.23	94.19	111.00
3	e	352	ILE	N-CA-C	-6.22	94.20	111.00
1	K	558	LEU	N-CA-C	6.22	127.79	111.00
3	V	275	HIS	N-CA-C	-6.22	94.21	111.00
3	b	275	HIS	N-CA-C	-6.22	94.21	111.00
3	e	275	HIS	N-CA-C	-6.21	94.23	111.00
1	J	93	GLY	N-CA-C	-6.20	97.59	113.10
1	O	520	TRP	C-N-CA	6.20	137.21	121.70
3	Y	275	HIS	N-CA-C	-6.20	94.26	111.00
1	O	682	LEU	CA-CB-CG	6.19	129.54	115.30
1	P	841	ASN	N-CA-C	-6.19	94.28	111.00
3	Y	351	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	L	13	TYR	N-CA-C	-6.18	94.30	111.00
3	Y	199	ASP	N-CA-C	6.18	127.69	111.00
1	D	485	ASN	N-CA-C	-6.18	94.32	111.00
1	P	30	ALA	N-CA-CB	6.16	118.72	110.10
1	K	450	LEU	CB-CG-CD1	-6.15	100.55	111.00
1	N	534	PRO	CA-N-CD	-6.14	102.90	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	444	GLY	N-CA-C	-6.14	97.74	113.10
1	P	419	HIS	N-CA-CB	6.14	121.65	110.60
1	N	1264	ASN	N-CA-C	-6.14	94.42	111.00
4	p	11	THR	N-CA-C	6.14	127.57	111.00
1	K	908	LEU	CA-CB-CG	6.13	129.41	115.30
1	B	103	LEU	CA-CB-CG	6.13	129.40	115.30
1	N	248	LEU	CA-CB-CG	6.13	129.40	115.30
1	C	96	GLN	N-CA-C	6.12	127.54	111.00
3	b	167	ALA	C-N-CA	6.12	137.01	121.70
1	K	1190	THR	C-N-CD	-6.11	107.16	120.60
2	U	12	ILE	C-N-CD	6.10	141.22	128.40
2	d	12	ILE	C-N-CD	6.10	141.22	128.40
1	E	1349	GLY	N-CA-C	6.10	128.36	113.10
1	P	30	ALA	N-CA-C	-6.09	94.55	111.00
1	L	406	LEU	CA-CB-CG	6.09	129.30	115.30
1	N	1123	GLY	N-CA-C	6.08	128.31	113.10
1	O	438	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	M	430	PRO	N-CA-C	6.08	127.90	112.10
1	H	1225	LEU	CA-CB-CG	6.07	129.27	115.30
1	O	34	ARG	CB-CA-C	-6.06	98.28	110.40
1	G	523	GLU	N-CA-C	-6.05	94.66	111.00
1	M	219	LEU	CA-CB-CG	6.04	129.20	115.30
1	P	1124	ASN	N-CA-C	6.04	127.30	111.00
1	O	1124	ASN	N-CA-C	6.03	127.28	111.00
1	K	13	TYR	N-CA-C	-6.03	94.72	111.00
1	L	452	LEU	CA-CB-CG	6.03	129.16	115.30
1	G	1194	THR	N-CA-C	-6.02	94.75	111.00
1	J	1278	THR	N-CA-CB	6.01	121.72	110.30
1	E	1347	ARG	N-CA-C	-5.99	94.83	111.00
1	M	1349	GLY	N-CA-C	-5.99	98.13	113.10
1	N	248	LEU	CB-CG-CD2	-5.98	100.83	111.00
1	N	1044	LEU	CA-CB-CG	5.97	129.04	115.30
1	M	558	LEU	CA-CB-CG	-5.97	101.57	115.30
1	J	917	GLY	N-CA-C	-5.96	98.20	113.10
1	A	196	ALA	N-CA-C	-5.96	94.92	111.00
1	N	1194	THR	N-CA-C	-5.95	94.93	111.00
1	B	236	LYS	N-CA-C	-5.95	94.94	111.00
1	C	290	GLN	N-CA-C	-5.95	94.94	111.00
1	F	293	LEU	CA-CB-CG	5.94	128.97	115.30
1	O	1107	THR	CA-CB-CG2	-5.93	104.10	112.40
1	O	1221	ASP	CB-CG-OD1	5.92	123.63	118.30
1	L	529	GLU	N-CA-CB	5.92	121.25	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	291	SER	N-CA-CB	-5.92	101.62	110.50
1	E	199	LEU	CA-CB-CG	5.91	128.90	115.30
1	N	198	LEU	CA-CB-CG	-5.91	101.71	115.30
1	J	144	THR	N-CA-C	-5.91	95.05	111.00
1	C	1347	ARG	N-CA-C	-5.90	95.06	111.00
1	F	536	ASN	N-CA-C	-5.90	95.07	111.00
1	M	378	GLU	CB-CA-C	-5.90	98.60	110.40
1	K	948	THR	N-CA-C	-5.90	95.07	111.00
1	G	242	GLU	N-CA-CB	5.88	121.19	110.60
1	D	786	ASN	N-CA-C	5.88	126.86	111.00
3	Y	119	LEU	CA-CB-CG	5.87	128.80	115.30
1	G	409	PHE	N-CA-C	-5.87	95.16	111.00
1	K	1173	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	N	693	LEU	CA-CB-CG	5.87	128.79	115.30
3	V	119	LEU	CA-CB-CG	5.87	128.79	115.30
3	b	119	LEU	CA-CB-CG	5.86	128.78	115.30
1	O	957	VAL	N-CA-C	5.86	126.81	111.00
1	L	355	GLU	N-CA-C	5.85	126.80	111.00
1	I	259	VAL	N-CA-CB	-5.84	98.65	111.50
1	P	565	PRO	N-CA-C	-5.84	96.92	112.10
3	S	119	LEU	CA-CB-CG	5.84	128.73	115.30
1	L	759	GLY	N-CA-C	5.83	127.69	113.10
4	o	32	ALA	N-CA-C	5.83	126.75	111.00
1	K	1068	ARG	CB-CA-C	-5.83	98.74	110.40
4	r	32	ALA	N-CA-C	5.83	126.75	111.00
4	s	32	ALA	N-CA-C	5.83	126.74	111.00
2	T	106	VAL	N-CA-C	5.83	126.74	111.00
1	M	189	LEU	CA-CB-CG	5.83	128.70	115.30
4	k	32	ALA	N-CA-C	5.82	126.72	111.00
4	m	32	ALA	N-CA-C	5.82	126.72	111.00
4	h	95	LYS	N-CA-C	-5.82	95.28	111.00
4	l	95	LYS	N-CA-C	-5.82	95.28	111.00
4	o	95	LYS	N-CA-C	-5.82	95.29	111.00
4	p	32	ALA	N-CA-C	5.82	126.72	111.00
2	W	106	VAL	N-CA-C	5.82	126.70	111.00
4	g	32	ALA	N-CA-C	5.82	126.71	111.00
4	g	95	LYS	N-CA-C	-5.82	95.30	111.00
4	q	32	ALA	N-CA-C	5.82	126.70	111.00
1	K	452	LEU	CA-CB-CG	5.82	128.67	115.30
4	i	95	LYS	N-CA-C	-5.82	95.30	111.00
4	j	32	ALA	N-CA-C	5.82	126.70	111.00
4	h	32	ALA	N-CA-C	5.81	126.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	l	32	ALA	N-CA-C	5.81	126.69	111.00
4	n	32	ALA	N-CA-C	5.81	126.69	111.00
4	f	32	ALA	N-CA-C	5.81	126.68	111.00
4	i	32	ALA	N-CA-C	5.81	126.69	111.00
1	M	1124	ASN	N-CA-C	5.81	126.68	111.00
2	Q	106	VAL	N-CA-C	5.81	126.68	111.00
2	Z	106	VAL	N-CA-C	5.81	126.67	111.00
4	t	32	ALA	N-CA-C	5.81	126.68	111.00
4	m	95	LYS	N-CA-C	-5.80	95.33	111.00
4	p	95	LYS	N-CA-C	-5.80	95.33	111.00
4	f	95	LYS	N-CA-C	-5.80	95.33	111.00
1	O	484	ALA	N-CA-C	-5.80	95.34	111.00
4	q	95	LYS	N-CA-C	-5.80	95.34	111.00
1	O	1228	ASP	N-CA-C	-5.79	95.36	111.00
4	n	95	LYS	N-CA-C	-5.79	95.36	111.00
1	P	485	ASN	N-CA-C	-5.79	95.36	111.00
3	V	296	LEU	N-CA-CB	5.79	121.98	110.40
1	O	448	GLN	N-CA-C	-5.79	95.37	111.00
3	e	296	LEU	N-CA-CB	5.79	121.97	110.40
1	G	426	ALA	N-CA-C	-5.78	95.38	111.00
4	k	95	LYS	N-CA-C	-5.78	95.39	111.00
1	L	466	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	B	753	ASP	N-CA-C	5.78	126.60	111.00
3	S	296	LEU	N-CA-CB	5.78	121.96	110.40
1	G	1277	PHE	N-CA-C	-5.77	95.41	111.00
1	M	958	LEU	N-CA-C	-5.77	95.42	111.00
1	N	1223	ILE	CB-CA-C	-5.77	100.06	111.60
1	M	1241	THR	CB-CA-C	-5.77	96.03	111.60
2	X	232	ALA	N-CA-C	5.76	126.55	111.00
2	R	232	ALA	N-CA-C	5.76	126.54	111.00
3	Y	296	LEU	N-CA-CB	5.76	121.91	110.40
1	G	155	LEU	CA-CB-CG	5.74	128.51	115.30
2	a	232	ALA	N-CA-C	5.74	126.50	111.00
1	B	47	ASN	N-CA-C	-5.74	95.50	111.00
1	B	1263	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	234	LEU	N-CA-C	-5.74	95.50	111.00
1	P	303	PRO	CA-N-CD	-5.74	103.47	111.50
2	d	232	ALA	N-CA-C	5.74	126.49	111.00
1	N	445	LYS	N-CA-C	-5.74	95.51	111.00
2	U	232	ALA	N-CA-C	5.73	126.47	111.00
1	P	1330	GLU	CB-CA-C	-5.73	98.94	110.40
3	S	352	ILE	N-CA-C	-5.73	95.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	417	ALA	N-CA-C	5.72	126.46	111.00
1	M	440	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	K	264	LEU	CA-CB-CG	5.72	128.46	115.30
1	L	920	THR	N-CA-C	-5.72	95.55	111.00
1	K	440	LEU	CA-CB-CG	5.72	128.45	115.30
1	P	894	LEU	CA-CB-CG	5.72	128.45	115.30
1	E	1225	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	K	1218	LYS	N-CA-C	-5.72	95.56	111.00
3	Y	351	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	L	57	LEU	N-CA-C	-5.71	95.57	111.00
3	V	184	LEU	N-CA-C	5.71	126.43	111.00
1	D	406	LEU	CA-CB-CG	5.71	128.44	115.30
1	J	670	LEU	CB-CA-C	-5.71	99.35	110.20
1	J	557	GLU	N-CA-C	-5.71	95.58	111.00
1	M	1115	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	O	1344	ARG	NE-CZ-NH2	-5.70	117.45	120.30
3	S	184	LEU	N-CA-C	5.70	126.40	111.00
3	e	184	LEU	N-CA-C	5.70	126.40	111.00
1	O	192	ALA	C-N-CD	5.70	140.37	128.40
3	b	184	LEU	N-CA-C	5.70	126.39	111.00
3	Y	184	LEU	N-CA-C	5.70	126.38	111.00
1	K	1124	ASN	C-N-CA	-5.70	107.46	121.70
1	L	1124	ASN	N-CA-C	5.70	126.38	111.00
1	L	1158	GLY	C-N-CD	5.70	140.36	128.40
1	G	958	LEU	C-N-CD	5.69	140.36	128.40
1	F	682	LEU	CA-CB-CG	5.68	128.37	115.30
1	O	533	GLN	C-N-CD	5.68	140.33	128.40
1	A	1200	ARG	N-CA-CB	5.68	120.82	110.60
1	A	327	ARG	N-CA-C	-5.68	95.67	111.00
1	I	1241	THR	CB-CA-C	-5.67	96.28	111.60
1	F	558	LEU	CB-CG-CD2	-5.67	101.37	111.00
1	I	223	LEU	CA-CB-CG	5.67	128.33	115.30
4	m	5	GLN	CA-C-N	-5.67	104.73	117.20
1	P	292	PHE	N-CA-C	5.67	126.29	111.00
4	q	5	GLN	CA-C-N	-5.66	104.74	117.20
4	g	5	GLN	CA-C-N	-5.66	104.75	117.20
1	M	1348	ASP	CB-CG-OD1	5.66	123.39	118.30
4	j	5	GLN	CA-C-N	-5.66	104.75	117.20
4	i	5	GLN	CA-C-N	-5.66	104.76	117.20
2	d	127	ASP	N-CA-C	-5.65	95.73	111.00
4	f	5	GLN	CA-C-N	-5.65	104.76	117.20
1	M	1326	GLY	N-CA-C	-5.65	98.97	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	1265	GLY	N-CA-C	-5.65	98.97	113.10
1	K	1068	ARG	N-CA-C	5.65	126.26	111.00
4	o	5	GLN	CA-C-N	-5.65	104.77	117.20
1	I	189	LEU	CA-CB-CG	5.65	128.29	115.30
2	R	237	VAL	CB-CA-C	-5.65	100.67	111.40
4	t	5	GLN	CA-C-N	-5.65	104.77	117.20
1	G	208	GLY	N-CA-C	-5.65	98.99	113.10
1	E	419	HIS	N-CA-CB	5.64	120.76	110.60
1	N	320	LEU	N-CA-C	-5.64	95.76	111.00
1	G	152	GLY	N-CA-C	5.64	127.20	113.10
4	r	5	GLN	CA-C-N	-5.64	104.79	117.20
1	C	1312	LYS	N-CA-C	-5.64	95.77	111.00
1	D	73	LEU	CA-CB-CG	5.64	128.27	115.30
3	Y	297	ASP	N-CA-C	-5.64	95.78	111.00
4	k	5	GLN	CA-C-N	-5.64	104.79	117.20
4	l	5	GLN	CA-C-N	-5.64	104.80	117.20
1	L	563	VAL	C-N-CD	5.64	140.24	128.40
2	d	237	VAL	CB-CA-C	-5.64	100.69	111.40
4	p	5	GLN	CA-C-N	-5.64	104.80	117.20
4	s	5	GLN	CA-C-N	-5.64	104.80	117.20
1	M	146	GLU	N-CA-C	5.63	126.22	111.00
1	O	96	GLN	CB-CA-C	-5.63	99.13	110.40
4	h	5	GLN	CA-C-N	-5.63	104.81	117.20
2	X	237	VAL	CB-CA-C	-5.63	100.70	111.40
1	J	49	LEU	N-CA-C	-5.63	95.81	111.00
1	K	894	LEU	CA-CB-CG	5.63	128.24	115.30
1	L	311	LEU	CA-CB-CG	5.63	128.24	115.30
1	N	1263	LEU	CB-CG-CD2	-5.63	101.44	111.00
3	S	297	ASP	N-CA-C	-5.63	95.81	111.00
3	e	297	ASP	N-CA-C	-5.63	95.81	111.00
1	H	558	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	L	35	LEU	CA-CB-CG	5.62	128.24	115.30
1	M	440	LEU	CA-CB-CG	5.62	128.23	115.30
1	D	1266	ALA	N-CA-C	-5.62	95.83	111.00
1	C	1040	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	J	1277	PHE	CB-CA-C	-5.62	99.17	110.40
1	A	359	GLN	N-CA-C	5.61	126.16	111.00
1	B	385	TYR	N-CA-C	5.61	126.16	111.00
1	A	527	THR	N-CA-C	-5.61	95.85	111.00
2	a	237	VAL	CB-CA-C	-5.61	100.74	111.40
1	G	126	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	I	1054	ARG	NE-CZ-NH1	-5.61	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	44	SER	N-CA-CB	5.61	118.92	110.50
3	V	297	ASP	N-CA-C	-5.61	95.85	111.00
4	n	5	GLN	CA-C-N	-5.61	104.86	117.20
1	P	135	LEU	N-CA-C	-5.61	95.86	111.00
1	O	526	MET	N-CA-C	-5.60	95.87	111.00
1	B	558	LEU	CB-CG-CD2	-5.60	101.48	111.00
1	B	533	GLN	C-N-CD	5.60	140.15	128.40
1	N	69	ARG	N-CA-C	5.60	126.11	111.00
1	G	407	GLY	N-CA-C	5.59	127.09	113.10
2	U	237	VAL	CB-CA-C	-5.59	100.77	111.40
1	G	535	ASP	N-CA-C	5.58	126.07	111.00
2	a	16	ILE	N-CA-C	-5.58	95.93	111.00
1	K	372	ASP	C-N-CA	-5.58	107.76	121.70
1	L	1225	LEU	CA-CB-CG	5.58	128.12	115.30
2	R	34	LEU	CA-CB-CG	5.57	128.12	115.30
1	H	14	ALA	CB-CA-C	-5.57	101.74	110.10
1	N	1254	ASP	N-CA-C	-5.57	95.95	111.00
1	E	272	ARG	C-N-CD	5.57	140.10	128.40
2	d	34	LEU	CA-CB-CG	5.57	128.11	115.30
2	U	34	LEU	CA-CB-CG	5.57	128.10	115.30
2	X	34	LEU	CA-CB-CG	5.57	128.10	115.30
1	K	1241	THR	CB-CA-C	-5.56	96.58	111.60
1	N	357	ALA	C-N-CD	5.56	140.08	128.40
1	N	1064	LEU	CB-CG-CD2	-5.56	101.55	111.00
1	M	1087	GLY	N-CA-C	-5.56	99.20	113.10
1	B	536	ASN	N-CA-C	-5.55	96.01	111.00
1	J	251	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	P	693	LEU	CA-CB-CG	5.55	128.06	115.30
1	D	264	LEU	CA-CB-CG	5.55	128.06	115.30
1	M	16	ALA	N-CA-C	-5.55	96.03	111.00
1	A	138	GLU	N-CA-C	-5.54	96.03	111.00
1	N	1225	LEU	CB-CG-CD1	-5.54	101.58	111.00
1	K	1277	PHE	N-CA-C	-5.54	96.04	111.00
2	R	108	LEU	N-CA-C	5.53	125.94	111.00
2	X	108	LEU	N-CA-C	5.53	125.94	111.00
1	M	908	LEU	CA-CB-CG	5.53	128.02	115.30
1	G	1182	ASP	N-CA-C	5.53	125.93	111.00
1	C	1276	PHE	N-CA-C	5.53	125.94	111.00
3	Y	278	HIS	C-N-CD	-5.53	108.44	120.60
2	d	108	LEU	N-CA-C	5.53	125.93	111.00
3	Y	428	MET	N-CA-C	-5.53	96.08	111.00
4	k	98	TYR	N-CA-C	5.53	125.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	278	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	F	448	GLN	CB-CA-C	-5.51	99.37	110.40
1	O	485	ASN	N-CA-C	-5.51	96.11	111.00
3	S	428	MET	N-CA-C	-5.51	96.11	111.00
2	U	108	LEU	N-CA-C	5.51	125.88	111.00
3	e	428	MET	N-CA-C	-5.51	96.12	111.00
1	J	293	LEU	CA-CB-CG	5.51	127.97	115.30
3	V	428	MET	N-CA-C	-5.51	96.13	111.00
2	a	108	LEU	N-CA-C	5.51	125.87	111.00
4	t	47	GLN	N-CA-C	-5.50	96.15	111.00
4	p	47	GLN	N-CA-C	-5.49	96.17	111.00
4	h	47	GLN	N-CA-C	-5.49	96.17	111.00
1	D	533	GLN	C-N-CD	5.49	139.93	128.40
1	M	298	THR	N-CA-C	-5.49	96.18	111.00
1	D	423	LEU	CA-CB-CG	-5.49	102.68	115.30
4	r	47	GLN	N-CA-C	-5.49	96.19	111.00
4	i	47	GLN	N-CA-C	-5.49	96.19	111.00
4	k	47	GLN	N-CA-C	-5.49	96.19	111.00
4	s	47	GLN	N-CA-C	-5.49	96.19	111.00
4	r	99	SER	N-CA-C	5.48	125.81	111.00
1	P	429	HIS	N-CA-C	5.48	125.80	111.00
1	N	148	LEU	CA-CB-CG	5.48	127.90	115.30
1	O	485	ASN	C-N-CD	5.48	139.91	128.40
4	g	47	GLN	N-CA-C	-5.48	96.21	111.00
1	C	1040	LEU	CA-CB-CG	5.47	127.89	115.30
4	f	47	GLN	N-CA-C	-5.47	96.22	111.00
1	M	1218	LYS	N-CA-C	-5.47	96.23	111.00
2	a	33	PHE	N-CA-C	-5.47	96.23	111.00
1	A	382	LYS	N-CA-C	-5.47	96.24	111.00
4	m	47	GLN	N-CA-C	-5.47	96.24	111.00
4	o	47	GLN	N-CA-C	-5.46	96.25	111.00
4	j	47	GLN	N-CA-C	-5.46	96.25	111.00
4	n	47	GLN	N-CA-C	-5.46	96.25	111.00
4	l	47	GLN	N-CA-C	-5.46	96.26	111.00
1	E	271	GLY	N-CA-C	5.46	126.74	113.10
1	H	541	LEU	CA-CB-CG	-5.46	102.75	115.30
1	J	51	ASP	N-CA-CB	5.46	120.42	110.60
3	b	431	ASP	N-CA-C	5.46	125.73	111.00
4	q	47	GLN	N-CA-C	-5.46	96.27	111.00
1	P	386	ALA	N-CA-C	5.45	125.73	111.00
2	R	12	ILE	N-CA-C	-5.45	96.27	111.00
4	h	14	ALA	N-CA-C	-5.45	96.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	o	14	ALA	N-CA-C	-5.45	96.29	111.00
1	H	447	HIS	C-N-CA	-5.45	108.08	121.70
1	J	536	ASN	N-CA-C	5.45	125.71	111.00
4	j	14	ALA	N-CA-C	-5.45	96.29	111.00
1	G	83	LYS	C-N-CA	-5.45	108.08	121.70
1	J	915	ASP	N-CA-C	-5.45	96.30	111.00
1	L	760	GLY	C-N-CA	-5.44	108.09	121.70
4	n	14	ALA	N-CA-C	-5.44	96.30	111.00
4	p	14	ALA	N-CA-C	-5.44	96.31	111.00
1	K	357	ALA	C-N-CD	5.44	139.83	128.40
1	I	1225	LEU	CA-CB-CG	5.44	127.81	115.30
4	m	14	ALA	N-CA-C	-5.44	96.32	111.00
4	g	14	ALA	N-CA-C	-5.43	96.33	111.00
4	l	14	ALA	N-CA-C	-5.43	96.33	111.00
4	f	14	ALA	N-CA-C	-5.43	96.34	111.00
1	C	97	PHE	N-CA-C	5.43	125.66	111.00
4	q	14	ALA	N-CA-C	-5.43	96.34	111.00
1	I	511	GLN	CB-CA-C	-5.43	99.54	110.40
1	O	1107	THR	N-CA-C	-5.43	96.34	111.00
2	a	31	VAL	N-CA-C	5.43	125.65	111.00
4	k	14	ALA	N-CA-C	-5.43	96.35	111.00
1	J	84	PHE	C-N-CD	-5.42	108.67	120.60
3	S	296	LEU	CB-CG-CD2	5.42	120.22	111.00
4	f	97	THR	N-CA-C	-5.42	96.36	111.00
4	i	14	ALA	N-CA-C	-5.42	96.35	111.00
4	t	14	ALA	N-CA-C	-5.42	96.35	111.00
1	N	386	ALA	N-CA-C	5.42	125.64	111.00
4	t	103	VAL	N-CA-C	-5.42	96.37	111.00
1	C	1119	VAL	N-CA-C	5.42	125.62	111.00
1	L	189	LEU	CA-CB-CG	5.42	127.76	115.30
1	E	84	PHE	C-N-CD	5.41	139.77	128.40
1	O	427	PRO	N-CA-C	5.41	126.17	112.10
1	D	1086	GLY	N-CA-C	-5.41	99.58	113.10
1	M	444	GLY	N-CA-C	-5.41	99.58	113.10
3	e	296	LEU	CB-CG-CD2	5.41	120.19	111.00
1	M	1280	ALA	N-CA-C	-5.41	96.41	111.00
4	r	14	ALA	N-CA-C	-5.41	96.41	111.00
1	N	894	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	395	VAL	N-CA-C	-5.40	96.42	111.00
1	K	427	PRO	N-CA-C	5.40	126.14	112.10
1	O	1070	SER	CB-CA-C	-5.40	99.84	110.10
1	L	374	LEU	N-CA-C	-5.40	96.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	435	PHE	C-N-CD	5.40	139.73	128.40
2	X	96	GLY	C-N-CA	-5.40	108.21	121.70
1	D	16	ALA	N-CA-C	-5.40	96.43	111.00
1	P	520	TRP	C-N-CA	5.39	135.18	121.70
3	V	296	LEU	CB-CG-CD2	5.39	120.17	111.00
4	f	16	ASN	C-N-CA	5.39	135.18	121.70
1	G	1183	ALA	N-CA-C	-5.39	96.46	111.00
1	I	258	SER	N-CA-C	-5.39	96.45	111.00
1	M	1109	VAL	N-CA-C	-5.39	96.46	111.00
1	P	558	LEU	N-CA-C	5.39	125.54	111.00
1	G	306	TYR	N-CA-C	5.38	125.54	111.00
1	J	1044	LEU	CA-CB-CG	5.38	127.68	115.30
3	V	304	GLY	C-N-CD	5.38	139.69	128.40
1	J	428	GLY	N-CA-C	-5.38	99.66	113.10
3	Y	296	LEU	CB-CG-CD2	5.37	120.14	111.00
2	d	96	GLY	C-N-CA	-5.37	108.27	121.70
1	M	944	HIS	N-CA-C	-5.37	96.50	111.00
1	P	558	LEU	C-N-CD	5.37	139.68	128.40
2	U	96	GLY	C-N-CA	-5.37	108.28	121.70
3	Y	458	ARG	N-CA-C	-5.37	96.51	111.00
1	D	93	GLY	N-CA-C	-5.36	99.70	113.10
1	P	75	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	E	1085	THR	N-CA-CB	5.36	120.47	110.30
1	L	582	LEU	C-N-CD	5.35	139.64	128.40
1	G	297	ASP	N-CA-C	5.35	125.45	111.00
1	L	15	ALA	N-CA-C	-5.35	96.56	111.00
2	R	96	GLY	C-N-CA	-5.35	108.33	121.70
1	A	288	LEU	CA-CB-CG	5.34	127.58	115.30
1	C	429	HIS	N-CA-C	5.34	125.41	111.00
1	F	1266	ALA	N-CA-C	-5.34	96.59	111.00
3	V	134	LEU	CB-CG-CD2	-5.33	101.93	111.00
3	e	134	LEU	N-CA-C	-5.33	96.61	111.00
1	B	446	ASP	N-CA-CB	5.32	120.18	110.60
1	A	114	GLN	C-N-CD	5.32	139.57	128.40
2	a	72	PRO	N-CA-C	5.32	125.93	112.10
1	C	534	PRO	N-CA-C	-5.32	98.27	112.10
1	D	1157	LEU	CA-CB-CG	5.32	127.53	115.30
1	O	1315	PRO	N-CA-C	5.32	125.92	112.10
3	e	278	HIS	C-N-CD	-5.31	108.91	120.60
1	I	570	ALA	N-CA-C	-5.31	96.66	111.00
1	K	292	PHE	N-CA-C	5.31	125.34	111.00
3	b	134	LEU	CB-CG-CD2	-5.31	101.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	t	40	TYR	C-N-CD	5.31	139.54	128.40
1	I	485	ASN	C-N-CD	5.30	139.54	128.40
1	I	1236	ARG	C-N-CD	5.30	139.54	128.40
1	D	1219	GLU	N-CA-C	5.30	125.31	111.00
1	N	278	LEU	N-CA-C	-5.30	96.68	111.00
4	f	40	TYR	C-N-CD	5.30	139.53	128.40
1	O	356	SER	N-CA-C	5.30	125.31	111.00
1	H	269	THR	N-CA-C	-5.30	96.70	111.00
1	A	264	LEU	N-CA-C	-5.29	96.70	111.00
1	P	957	VAL	N-CA-C	5.29	125.29	111.00
1	J	1043	GLY	N-CA-C	5.29	126.33	113.10
4	k	40	TYR	C-N-CD	5.29	139.51	128.40
1	B	51	ASP	N-CA-C	-5.29	96.72	111.00
1	O	529	GLU	N-CA-C	-5.29	96.72	111.00
1	A	536	ASN	C-N-CA	-5.29	108.48	121.70
1	P	1266	ALA	N-CA-C	-5.29	96.73	111.00
4	r	40	TYR	C-N-CD	5.29	139.50	128.40
4	g	98	TYR	N-CA-C	5.29	125.27	111.00
4	n	40	TYR	C-N-CD	5.29	139.50	128.40
1	F	264	LEU	CA-CB-CG	5.28	127.45	115.30
1	L	1124	ASN	CB-CA-C	-5.28	99.83	110.40
1	N	1156	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	d	164	ASN	C-N-CD	5.28	139.50	128.40
4	g	40	TYR	C-N-CD	5.28	139.50	128.40
4	j	40	TYR	C-N-CD	5.28	139.50	128.40
1	G	429	HIS	C-N-CD	5.28	139.49	128.40
1	G	1077	GLN	O-C-N	5.28	131.15	122.70
4	s	40	TYR	C-N-CD	5.28	139.49	128.40
1	K	11	TYR	N-CA-C	-5.28	96.75	111.00
1	F	299	GLU	N-CA-C	-5.28	96.75	111.00
1	J	913	ALA	C-N-CD	5.28	139.48	128.40
1	O	1112	THR	N-CA-C	-5.28	96.75	111.00
1	P	1104	VAL	CB-CA-C	5.28	121.43	111.40
3	Y	442	PHE	N-CA-C	-5.28	96.75	111.00
1	P	910	CYS	CA-CB-SG	5.27	123.49	114.00
4	o	40	TYR	C-N-CD	5.27	139.47	128.40
1	C	189	LEU	CA-CB-CG	5.27	127.42	115.30
4	l	40	TYR	C-N-CD	5.27	139.46	128.40
1	B	189	LEU	CA-CB-CG	5.27	127.41	115.30
4	i	40	TYR	C-N-CD	5.27	139.46	128.40
1	M	415	ARG	CB-CG-CD	-5.26	97.91	111.60
4	m	40	TYR	C-N-CD	5.26	139.46	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	q	40	TYR	C-N-CD	5.26	139.46	128.40
1	J	1122	MET	N-CA-C	5.26	125.21	111.00
1	F	259	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	N	191	LYS	CB-CA-C	-5.26	99.88	110.40
1	B	271	GLY	N-CA-C	5.26	126.25	113.10
1	B	406	LEU	CB-CG-CD1	-5.26	102.06	111.00
2	a	91	GLY	N-CA-C	-5.26	99.96	113.10
1	I	558	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	K	95	VAL	N-CA-C	-5.25	96.82	111.00
4	h	40	TYR	C-N-CD	5.25	139.43	128.40
1	D	305	THR	N-CA-CB	-5.25	100.33	110.30
2	a	286	GLY	C-N-CA	5.25	134.82	121.70
4	p	40	TYR	C-N-CD	5.25	139.42	128.40
1	N	485	ASN	C-N-CD	5.25	139.41	128.40
1	B	527	THR	N-CA-C	-5.24	96.84	111.00
1	J	1044	LEU	C-N-CA	-5.24	108.60	121.70
1	M	484	ALA	N-CA-C	-5.24	96.85	111.00
1	K	417	ALA	N-CA-C	-5.24	96.86	111.00
1	K	1332	TYR	C-N-CD	5.24	139.40	128.40
1	M	51	ASP	N-CA-C	5.24	125.15	111.00
1	M	1124	ASN	N-CA-CB	-5.24	101.17	110.60
1	N	1199	PHE	CB-CA-C	-5.24	99.92	110.40
1	P	431	GLU	C-N-CD	5.24	139.40	128.40
2	d	286	GLY	C-N-CA	5.24	134.79	121.70
2	R	286	GLY	C-N-CA	5.23	134.79	121.70
1	G	1288	CYS	C-N-CA	-5.23	108.63	121.70
1	P	958	LEU	C-N-CD	5.23	139.38	128.40
3	Y	136	HIS	N-CA-C	5.23	125.12	111.00
1	G	535	ASP	CB-CA-C	-5.23	99.95	110.40
1	L	522	ALA	N-CA-C	-5.23	96.89	111.00
1	B	445	LYS	N-CA-C	-5.23	96.89	111.00
1	F	440	LEU	CB-CG-CD2	-5.23	102.12	111.00
2	X	286	GLY	C-N-CA	5.22	134.76	121.70
1	J	375	VAL	N-CA-C	-5.22	96.90	111.00
1	K	75	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	G	1115	VAL	CB-CA-C	-5.22	101.49	111.40
4	r	5	GLN	O-C-N	5.21	131.04	122.70
1	L	114	GLN	C-N-CD	5.21	139.35	128.40
1	O	367	LEU	CA-CB-CG	-5.21	103.31	115.30
4	p	105	ASP	C-N-CD	5.21	139.34	128.40
2	U	286	GLY	C-N-CA	5.21	134.72	121.70
1	O	320	LEU	CA-CB-CG	5.21	127.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	558	LEU	C-N-CD	5.20	139.33	128.40
1	F	324	LYS	N-CA-C	5.20	125.04	111.00
3	e	254	TRP	N-CA-C	5.20	125.04	111.00
1	P	557	GLU	N-CA-C	-5.20	96.96	111.00
3	V	278	HIS	O-C-N	5.20	130.98	121.10
3	Y	254	TRP	N-CA-C	5.19	125.03	111.00
4	j	5	GLN	O-C-N	5.19	131.01	122.70
1	A	1123	GLY	N-CA-C	5.19	126.08	113.10
4	f	5	GLN	O-C-N	5.19	131.00	122.70
4	m	5	GLN	O-C-N	5.19	131.00	122.70
4	o	5	GLN	O-C-N	5.18	130.99	122.70
1	F	208	GLY	N-CA-C	5.18	126.05	113.10
4	s	5	GLN	O-C-N	5.18	130.99	122.70
4	g	5	GLN	O-C-N	5.18	130.99	122.70
3	S	254	TRP	N-CA-C	5.18	124.98	111.00
1	M	43	ARG	N-CA-C	5.17	124.97	111.00
3	b	254	TRP	N-CA-C	5.17	124.97	111.00
1	A	313	GLY	N-CA-C	5.17	126.03	113.10
4	i	5	GLN	O-C-N	5.17	130.97	122.70
1	O	431	GLU	C-N-CD	5.17	139.26	128.40
1	P	394	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	D	1241	THR	CB-CA-C	-5.17	97.64	111.60
1	K	941	ALA	N-CA-C	-5.17	97.04	111.00
1	A	1069	ALA	N-CA-C	-5.17	97.05	111.00
3	V	254	TRP	N-CA-C	5.17	124.95	111.00
2	a	240	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	P	844	VAL	C-N-CD	5.16	139.24	128.40
4	l	5	GLN	O-C-N	5.16	130.96	122.70
1	F	908	LEU	CA-CB-CG	5.16	127.17	115.30
4	k	5	GLN	O-C-N	5.16	130.96	122.70
4	q	5	GLN	O-C-N	5.16	130.96	122.70
1	M	1163	LEU	CA-CB-CG	5.16	127.16	115.30
4	t	96	ARG	N-CA-C	-5.16	97.08	111.00
1	J	691	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	L	394	LEU	CB-CG-CD1	-5.15	102.24	111.00
1	L	512	ARG	NE-CZ-NH2	-5.15	117.72	120.30
4	t	5	GLN	O-C-N	5.15	130.94	122.70
1	N	485	ASN	N-CA-C	-5.15	97.09	111.00
4	n	5	GLN	O-C-N	5.15	130.94	122.70
4	p	5	GLN	O-C-N	5.15	130.94	122.70
1	E	1120	THR	N-CA-CB	5.15	120.08	110.30
1	J	1124	ASN	N-CA-C	5.15	124.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	d	240	LEU	CB-CG-CD1	-5.15	102.25	111.00
4	h	5	GLN	O-C-N	5.15	130.94	122.70
1	C	1332	TYR	C-N-CD	5.14	139.21	128.40
1	M	1243	ASN	N-CA-C	-5.14	97.11	111.00
2	a	31	VAL	C-N-CA	-5.14	108.84	121.70
1	H	147	ALA	N-CA-C	5.14	124.89	111.00
2	R	240	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	P	1225	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	K	436	PRO	C-N-CD	5.14	139.19	128.40
4	m	105	ASP	C-N-CD	5.14	139.19	128.40
1	M	356	SER	N-CA-C	5.14	124.87	111.00
1	L	421	GLY	N-CA-C	-5.13	100.26	113.10
1	O	432	PRO	CA-N-CD	-5.13	104.31	111.50
1	G	424	VAL	C-N-CD	5.13	139.18	128.40
1	M	1155	ASN	O-C-N	5.13	130.91	122.70
1	P	71	LEU	N-CA-C	-5.13	97.14	111.00
3	V	262	SER	N-CA-C	-5.13	97.15	111.00
1	P	1157	LEU	CB-CG-CD1	-5.13	102.28	111.00
3	S	262	SER	N-CA-C	-5.13	97.15	111.00
2	X	240	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	I	1236	ARG	N-CA-C	-5.13	97.16	111.00
2	d	266	GLU	C-N-CA	-5.13	108.89	121.70
1	N	1330	GLU	CB-CA-C	-5.12	100.15	110.40
1	O	1024	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	I	582	LEU	C-N-CD	5.12	139.16	128.40
2	R	266	GLU	C-N-CA	-5.12	108.90	121.70
2	U	266	GLU	C-N-CA	-5.12	108.89	121.70
1	H	1123	GLY	N-CA-C	5.12	125.90	113.10
3	Y	262	SER	N-CA-C	-5.12	97.18	111.00
3	b	262	SER	N-CA-C	-5.12	97.18	111.00
1	A	1072	ALA	N-CA-C	-5.12	97.19	111.00
2	U	240	LEU	CB-CG-CD1	-5.12	102.30	111.00
2	a	266	GLU	C-N-CA	-5.12	108.91	121.70
3	e	262	SER	N-CA-C	-5.12	97.19	111.00
4	j	105	ASP	C-N-CD	5.12	139.14	128.40
1	P	193	PRO	C-N-CD	5.11	139.14	128.40
1	E	84	PHE	N-CA-C	-5.11	97.20	111.00
1	I	14	ALA	N-CA-CB	5.11	117.25	110.10
1	L	357	ALA	C-N-CD	5.11	139.13	128.40
1	M	940	MET	N-CA-C	5.11	124.80	111.00
1	K	958	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	G	386	ALA	N-CA-C	5.10	124.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	1276	PHE	N-CA-C	5.10	124.77	111.00
1	I	563	VAL	C-N-CD	5.10	139.11	128.40
1	P	533	GLN	C-N-CD	5.10	139.10	128.40
2	X	266	GLU	C-N-CA	-5.09	108.97	121.70
1	M	114	GLN	C-N-CD	5.09	139.09	128.40
1	N	1276	PHE	N-CA-C	5.09	124.74	111.00
1	B	1158	GLY	C-N-CD	5.09	139.08	128.40
1	H	1102	LEU	C-N-CA	-5.08	111.62	122.30
1	M	1024	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	B	528	ALA	N-CA-CB	5.08	117.21	110.10
1	B	1199	PHE	N-CA-CB	5.08	119.74	110.60
1	J	185	LEU	C-N-CA	-5.08	109.00	121.70
1	C	430	PRO	N-CA-C	5.08	125.30	112.10
1	O	908	LEU	CA-CB-CG	5.08	126.97	115.30
1	P	1024	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	D	1171	VAL	C-N-CD	5.07	139.05	128.40
1	J	49	LEU	CA-CB-CG	5.07	126.97	115.30
1	M	623	TYR	C-N-CD	5.07	139.06	128.40
1	K	267	ALA	N-CA-C	-5.07	97.31	111.00
1	E	7	ASP	C-N-CD	5.07	139.05	128.40
1	L	1236	ARG	C-N-CD	5.07	139.05	128.40
1	N	1162	PRO	CA-N-CD	-5.07	104.40	111.50
1	J	1147	LEU	CA-CB-CG	-5.07	103.64	115.30
1	G	941	ALA	N-CA-CB	5.07	117.19	110.10
1	K	1374	LEU	CA-CB-CG	5.07	126.95	115.30
1	N	256	GLN	C-N-CD	5.07	139.04	128.40
1	B	1198	TYR	N-CA-C	-5.06	97.33	111.00
1	J	35	LEU	CA-CB-CG	5.06	126.95	115.30
1	K	446	ASP	N-CA-C	-5.06	97.33	111.00
1	O	1230	GLY	N-CA-C	-5.06	100.44	113.10
4	i	105	ASP	C-N-CD	5.06	139.03	128.40
1	K	1278	THR	CB-CA-C	5.06	125.27	111.60
1	O	75	LEU	CA-CB-CG	5.06	126.94	115.30
1	F	1123	GLY	N-CA-C	5.06	125.75	113.10
1	O	582	LEU	C-N-CD	5.06	139.02	128.40
3	S	275	HIS	N-CA-CB	5.06	119.71	110.60
3	S	304	GLY	C-N-CD	5.06	139.03	128.40
1	P	294	LYS	N-CA-C	-5.06	97.35	111.00
3	b	288	ILE	C-N-CD	5.05	139.01	128.40
1	E	265	THR	N-CA-C	-5.05	97.36	111.00
1	N	1204	ASN	C-N-CD	5.04	139.00	128.40
3	V	140	LEU	C-N-CD	5.04	138.99	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	126	THR	N-CA-CB	5.04	119.88	110.30
1	P	151	THR	C-N-CA	-5.04	111.71	122.30
1	E	1122	MET	N-CA-C	5.04	124.60	111.00
1	M	1078	LEU	CA-CB-CG	-5.04	103.71	115.30
1	G	452	LEU	N-CA-C	-5.04	97.41	111.00
1	H	251	LEU	CA-CB-CG	5.03	126.88	115.30
1	L	1236	ARG	N-CA-C	-5.03	97.41	111.00
1	G	440	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	A	293	LEU	CA-CB-CG	5.03	126.87	115.30
3	b	141	PRO	CA-N-CD	-5.03	104.46	111.50
1	I	916	ALA	N-CA-C	-5.03	97.42	111.00
1	E	306	TYR	CB-CA-C	-5.03	100.34	110.40
1	M	419	HIS	N-CA-CB	5.03	119.64	110.60
1	M	1200	ARG	N-CA-C	-5.02	97.44	111.00
1	P	103	LEU	CA-CB-CG	5.02	126.85	115.30
2	T	126	THR	N-CA-CB	5.02	119.84	110.30
1	C	1121	ASP	CB-CG-OD1	5.02	122.82	118.30
1	N	1160	ALA	N-CA-C	-5.02	97.45	111.00
2	Q	185	ARG	N-CA-C	-5.02	97.45	111.00
1	K	1317	CYS	N-CA-C	-5.02	97.45	111.00
3	e	37	LEU	N-CA-C	5.02	124.55	111.00
1	G	1122	MET	N-CA-C	5.02	124.54	111.00
2	Z	104	SER	C-N-CD	5.02	138.93	128.40
1	K	1348	ASP	N-CA-CB	-5.01	101.58	110.60
1	M	1279	ALA	CB-CA-C	-5.01	102.58	110.10
4	n	105	ASP	C-N-CD	5.01	138.93	128.40
1	J	816	LEU	CA-CB-CG	-5.01	103.77	115.30
1	M	1194	THR	N-CA-C	-5.01	97.48	111.00
1	M	1243	ASN	C-N-CD	5.01	138.92	128.40
1	K	349	GLU	N-CA-C	-5.01	97.48	111.00
1	G	953	GLU	CB-CA-C	-5.00	100.39	110.40
1	L	445	LYS	CD-CE-NZ	-5.00	100.19	111.70
3	Y	304	GLY	C-N-CD	5.00	138.91	128.40
4	r	102	VAL	N-CA-C	5.00	124.51	111.00
1	G	77	VAL	CB-CA-C	-5.00	101.90	111.40
1	M	75	LEU	CA-CB-CG	5.00	126.80	115.30
1	P	426	ALA	N-CA-C	-5.00	97.50	111.00
2	W	126	THR	N-CA-CB	5.00	119.80	110.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1276	PHE	Mainchain
1	A	374	LEU	Mainchain
1	B	265	THR	Mainchain
1	C	464	PRO	Mainchain
1	D	92	GLU	Mainchain
1	F	294	LYS	Mainchain
2	R	58	PRO	Mainchain
3	S	330	VAL	Mainchain
2	U	58	PRO	Mainchain
3	V	330	VAL	Mainchain
2	X	58	PRO	Mainchain
3	Y	330	VAL	Mainchain
2	a	58	PRO	Mainchain
2	d	58	PRO	Mainchain
3	e	330	VAL	Mainchain
4	f	25	LEU	Mainchain
4	g	25	LEU	Mainchain
4	h	25	LEU	Mainchain
4	i	25	LEU	Mainchain
4	j	25	LEU	Mainchain
4	k	25	LEU	Mainchain
4	l	25	LEU	Mainchain
4	m	25	LEU	Mainchain
4	n	25	LEU	Mainchain
4	o	25	LEU	Mainchain
4	p	25	LEU	Mainchain
4	q	25	LEU	Mainchain
4	r	25	LEU	Mainchain
4	s	25	LEU	Mainchain
4	t	25	LEU	Mainchain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1363/1374 (99%)	1209 (89%)	140 (10%)	14 (1%)	15	49
1	B	1344/1374 (98%)	1194 (89%)	129 (10%)	21 (2%)	9	37
1	C	1356/1374 (99%)	1212 (89%)	126 (9%)	18 (1%)	12	42
1	D	1356/1374 (99%)	1212 (89%)	124 (9%)	20 (2%)	10	39
1	E	1356/1374 (99%)	1201 (89%)	143 (10%)	12 (1%)	17	52
1	F	1356/1374 (99%)	1212 (89%)	125 (9%)	19 (1%)	11	40
1	G	1363/1374 (99%)	1193 (88%)	148 (11%)	22 (2%)	9	37
1	H	1356/1374 (99%)	1220 (90%)	123 (9%)	13 (1%)	15	49
1	I	1355/1374 (99%)	1228 (91%)	112 (8%)	15 (1%)	14	46
1	J	1356/1374 (99%)	1206 (89%)	132 (10%)	18 (1%)	12	42
1	K	1356/1374 (99%)	1235 (91%)	107 (8%)	14 (1%)	15	49
1	L	1356/1374 (99%)	1226 (90%)	114 (8%)	16 (1%)	13	44
1	M	1361/1374 (99%)	1228 (90%)	112 (8%)	21 (2%)	10	39
1	N	1356/1374 (99%)	1218 (90%)	118 (9%)	20 (2%)	10	39
1	O	1356/1374 (99%)	1216 (90%)	121 (9%)	19 (1%)	11	40
1	P	1356/1374 (99%)	1227 (90%)	112 (8%)	17 (1%)	12	42
2	Q	291/318 (92%)	254 (87%)	34 (12%)	3 (1%)	15	49
2	R	301/318 (95%)	264 (88%)	32 (11%)	5 (2%)	9	36
2	T	291/318 (92%)	252 (87%)	34 (12%)	5 (2%)	9	36
2	U	301/318 (95%)	262 (87%)	35 (12%)	4 (1%)	12	42
2	W	291/318 (92%)	254 (87%)	34 (12%)	3 (1%)	15	49
2	X	302/318 (95%)	260 (86%)	39 (13%)	3 (1%)	15	49
2	Z	291/318 (92%)	252 (87%)	33 (11%)	6 (2%)	7	30
2	a	301/318 (95%)	273 (91%)	25 (8%)	3 (1%)	15	49
2	c	291/318 (92%)	254 (87%)	34 (12%)	3 (1%)	15	49
2	d	302/318 (95%)	263 (87%)	34 (11%)	5 (2%)	9	36
3	S	313/466 (67%)	268 (86%)	36 (12%)	9 (3%)	4	24
3	V	332/466 (71%)	278 (84%)	46 (14%)	8 (2%)	6	27
3	Y	333/466 (72%)	276 (83%)	43 (13%)	14 (4%)	3	16
3	b	327/466 (70%)	273 (84%)	37 (11%)	17 (5%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	e	327/466 (70%)	265 (81%)	47 (14%)	15 (5%)	2 15
4	f	103/112 (92%)	70 (68%)	15 (15%)	18 (18%)	0 0
4	g	103/112 (92%)	71 (69%)	17 (16%)	15 (15%)	0 1
4	h	103/112 (92%)	73 (71%)	17 (16%)	13 (13%)	0 1
4	i	103/112 (92%)	73 (71%)	17 (16%)	13 (13%)	0 1
4	j	103/112 (92%)	71 (69%)	17 (16%)	15 (15%)	0 1
4	k	103/112 (92%)	71 (69%)	16 (16%)	16 (16%)	0 0
4	l	103/112 (92%)	70 (68%)	19 (18%)	14 (14%)	0 1
4	m	103/112 (92%)	71 (69%)	18 (18%)	14 (14%)	0 1
4	n	103/112 (92%)	71 (69%)	19 (18%)	13 (13%)	0 1
4	o	103/112 (92%)	70 (68%)	17 (16%)	16 (16%)	0 0
4	p	103/112 (92%)	74 (72%)	16 (16%)	13 (13%)	0 1
4	q	103/112 (92%)	71 (69%)	17 (16%)	15 (15%)	0 1
4	r	103/112 (92%)	70 (68%)	16 (16%)	17 (16%)	0 0
4	s	103/112 (92%)	77 (75%)	13 (13%)	13 (13%)	0 1
4	t	103/112 (92%)	75 (73%)	12 (12%)	16 (16%)	0 0
All	All	27841/29174 (95%)	24463 (88%)	2775 (10%)	603 (2%)	10 29

All (603) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	137	THR
1	G	295	VAL
1	G	1223	ILE
1	G	1277	PHE
1	G	1278	THR
1	A	196	ALA
1	A	209	ARG
1	A	327	ARG
1	A	395	VAL
1	A	946	ASP
1	A	1223	ILE
1	B	144	THR
1	B	146	GLU
1	B	446	ASP
1	B	920	THR

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Mol	Chain	Res	Type
1	B	946	ASP
1	B	1219	GLU
1	B	1223	ILE
1	B	1278	THR
1	B	1348	ASP
1	C	358	PRO
1	C	1201	ARG
1	C	1223	ILE
1	D	270	ARG
1	D	419	HIS
1	D	446	ASP
1	D	758	ALA
1	D	1085	THR
1	D	1170	GLN
1	D	1223	ILE
1	D	1278	THR
1	E	259	VAL
1	E	753	ASP
1	E	1085	THR
1	E	1119	VAL
1	E	1223	ILE
1	F	78	ALA
1	F	259	VAL
1	F	372	ASP
1	F	946	ASP
1	F	1119	VAL
1	F	1219	GLU
1	F	1223	ILE
1	F	1252	TYR
1	F	1266	ALA
1	F	1277	PHE
1	H	282	ALA
1	H	357	ALA
1	H	1115	VAL
1	H	1252	TYR
1	I	268	ASP
1	I	314	ALA
1	I	1223	ILE
1	I	1278	THR
1	I	1348	ASP
1	J	92	GLU
1	J	358	PRO

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Mol	Chain	Res	Type
1	J	820	PHE
1	J	987	VAL
1	J	1012	GLU
1	J	1202	PRO
1	J	1223	ILE
1	J	1229	HIS
1	K	192	ALA
1	K	948	THR
1	K	1119	VAL
1	K	1223	ILE
1	K	1278	THR
1	L	112	VAL
1	L	269	THR
1	L	321	VAL
1	L	758	ALA
1	L	1223	ILE
1	L	1278	THR
1	L	1348	ASP
1	M	203	ARG
1	M	321	VAL
1	M	357	ALA
1	M	558	LEU
1	M	820	PHE
1	M	1119	VAL
1	M	1161	GLN
1	M	1162	PRO
1	M	1223	ILE
1	M	1278	THR
1	M	1327	LEU
1	N	298	THR
1	N	534	PRO
1	N	822	ARG
1	N	918	ALA
1	N	1119	VAL
1	N	1161	GLN
1	N	1199	PHE
1	N	1223	ILE
1	N	1278	THR
1	O	418	ALA
1	O	758	ALA
1	O	1114	THR
1	O	1119	VAL

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Mol	Chain	Res	Type
1	O	1223	ILE
1	O	1278	THR
1	O	1348	ASP
1	P	192	ALA
1	P	485	ASN
1	P	1108	ALA
1	P	1119	VAL
1	P	1219	GLU
1	P	1278	THR
2	Q	104	SER
2	R	14	SER
2	R	16	ILE
2	R	97	THR
3	S	140	LEU
3	S	243	GLU
3	S	279	PRO
3	S	285	ALA
2	T	104	SER
2	T	184	ALA
2	U	97	THR
3	V	243	GLU
3	V	279	PRO
2	W	104	SER
2	X	97	THR
3	Y	38	ARG
3	Y	41	ILE
3	Y	140	LEU
3	Y	141	PRO
3	Y	243	GLU
3	Y	279	PRO
2	Z	104	SER
2	Z	184	ALA
3	b	243	GLU
3	b	279	PRO
3	b	285	ALA
3	b	419	TYR
2	c	104	SER
2	d	97	THR
2	d	124	GLN
3	e	5	PRO
3	e	7	PRO
3	e	140	LEU

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Mol	Chain	Res	Type
3	e	141	PRO
3	e	243	GLU
3	e	279	PRO
3	e	281	ARG
3	e	418	THR
4	f	3	ALA
4	f	19	ALA
4	f	47	GLN
4	f	78	MET
4	f	90	PRO
4	f	100	PRO
4	f	108	THR
4	f	109	PRO
4	g	3	ALA
4	g	17	VAL
4	g	47	GLN
4	g	78	MET
4	g	90	PRO
4	g	100	PRO
4	h	3	ALA
4	h	16	ASN
4	h	47	GLN
4	h	78	MET
4	h	90	PRO
4	h	100	PRO
4	i	3	ALA
4	i	47	GLN
4	i	78	MET
4	i	90	PRO
4	i	100	PRO
4	j	3	ALA
4	j	47	GLN
4	j	78	MET
4	j	90	PRO
4	j	102	VAL
4	k	3	ALA
4	k	47	GLN
4	k	78	MET
4	k	90	PRO
4	k	100	PRO
4	l	3	ALA
4	l	17	VAL

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Mol	Chain	Res	Type
4	l	47	GLN
4	l	78	MET
4	l	90	PRO
4	l	100	PRO
4	m	3	ALA
4	m	17	VAL
4	m	47	GLN
4	m	78	MET
4	m	90	PRO
4	m	100	PRO
4	n	3	ALA
4	n	47	GLN
4	n	78	MET
4	n	90	PRO
4	n	100	PRO
4	o	3	ALA
4	o	47	GLN
4	o	78	MET
4	o	90	PRO
4	o	100	PRO
4	p	3	ALA
4	p	47	GLN
4	p	78	MET
4	p	90	PRO
4	p	100	PRO
4	q	3	ALA
4	q	17	VAL
4	q	47	GLN
4	q	78	MET
4	q	90	PRO
4	q	100	PRO
4	q	107	LYS
4	r	3	ALA
4	r	17	VAL
4	r	47	GLN
4	r	78	MET
4	r	90	PRO
4	r	100	PRO
4	r	105	ASP
4	s	3	ALA
4	s	16	ASN
4	s	20	LEU

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Mol	Chain	Res	Type
4	s	47	GLN
4	s	78	MET
4	s	90	PRO
4	s	100	PRO
4	t	3	ALA
4	t	47	GLN
4	t	72	THR
4	t	76	GLN
4	t	78	MET
4	t	100	PRO
1	G	92	GLU
1	G	521	VAL
1	G	525	GLN
1	G	1199	PHE
1	A	528	ALA
1	B	41	ARG
1	B	242	GLU
1	B	523	GLU
1	B	1199	PHE
1	C	528	ALA
1	C	803	ALA
1	C	918	ALA
1	C	1119	VAL
1	C	1230	GLY
1	D	539	LEU
1	D	753	ASP
1	D	1109	VAL
1	E	1109	VAL
1	F	522	ALA
1	F	753	ASP
1	F	822	ARG
1	H	537	ALA
1	H	945	LEU
1	H	1219	GLU
1	I	17	MET
1	I	270	ARG
1	I	395	VAL
1	I	467	MET
1	I	1107	THR
1	J	537	ALA
1	J	1272	PRO
1	K	757	ASP

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Mol	Chain	Res	Type
1	K	761	HIS
1	K	1197	ASN
1	L	88	ALA
1	L	820	PHE
1	L	1114	THR
1	M	207	ASN
1	N	418	ALA
1	N	522	ALA
1	N	540	ALA
1	N	957	VAL
1	N	1162	PRO
1	O	295	VAL
1	O	298	THR
1	O	1161	GLN
1	O	1202	PRO
1	P	14	ALA
1	P	297	ASP
1	P	529	GLU
2	R	237	VAL
2	R	316	ARG
3	S	121	GLN
3	S	178	GLY
3	S	336	PRO
3	S	418	THR
2	U	237	VAL
2	U	316	ARG
3	V	121	GLN
3	V	178	GLY
3	V	336	PRO
3	V	418	THR
2	X	237	VAL
2	X	316	ARG
3	Y	121	GLN
3	Y	144	ALA
3	Y	154	THR
3	Y	336	PRO
2	a	171	GLY
2	a	237	VAL
2	a	316	ARG
3	b	108	TYR
3	b	121	GLN
3	b	178	GLY

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Mol	Chain	Res	Type
3	b	200	ALA
3	b	281	ARG
3	b	289	PRO
3	b	305	PRO
3	b	418	THR
2	d	237	VAL
2	d	316	ARG
3	e	178	GLY
3	e	336	PRO
3	e	419	TYR
4	f	11	THR
4	f	13	THR
4	f	16	ASN
4	f	17	VAL
4	f	72	THR
4	f	107	LYS
4	g	11	THR
4	g	13	THR
4	g	16	ASN
4	g	72	THR
4	h	11	THR
4	h	13	THR
4	h	72	THR
4	i	11	THR
4	i	13	THR
4	i	16	ASN
4	i	72	THR
4	j	11	THR
4	j	13	THR
4	j	16	ASN
4	j	72	THR
4	k	11	THR
4	k	13	THR
4	k	16	ASN
4	k	72	THR
4	l	11	THR
4	l	13	THR
4	l	72	THR
4	m	11	THR
4	m	13	THR
4	m	16	ASN
4	m	72	THR

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Mol	Chain	Res	Type
4	n	11	THR
4	n	13	THR
4	n	16	ASN
4	n	72	THR
4	o	11	THR
4	o	13	THR
4	o	16	ASN
4	o	22	MET
4	o	72	THR
4	p	13	THR
4	p	16	ASN
4	p	72	THR
4	q	11	THR
4	q	13	THR
4	q	16	ASN
4	q	72	THR
4	r	11	THR
4	r	13	THR
4	r	16	ASN
4	r	72	THR
4	s	72	THR
4	t	13	THR
4	t	16	ASN
4	t	103	VAL
4	t	107	LYS
1	G	154	SER
1	A	753	ASP
1	B	47	ASN
1	C	291	SER
1	C	959	PRO
1	D	147	ALA
1	D	1348	ASP
1	F	1348	ASP
1	H	1348	ASP
1	K	44	SER
1	K	357	ALA
1	K	1114	THR
1	L	300	ALA
1	M	30	ALA
1	M	386	ALA
1	O	192	ALA
1	O	534	PRO

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Mol	Chain	Res	Type
1	O	1203	CYS
1	P	44	SER
1	P	1114	THR
2	Q	165	PRO
2	T	165	PRO
2	W	165	PRO
2	Z	165	PRO
2	c	165	PRO
2	d	125	ALA
4	g	22	MET
4	j	95	LYS
4	j	105	ASP
4	k	22	MET
4	o	105	ASP
4	s	89	ARG
4	t	95	LYS
1	G	46	GLU
1	G	331	ASP
1	G	430	PRO
1	G	470	ASP
1	A	143	LEU
1	A	324	LYS
1	A	1122	MET
1	A	1299	ALA
1	B	1317	CYS
1	C	45	ASP
1	C	386	ALA
1	C	1084	GLU
1	C	1114	THR
1	D	386	ALA
1	D	408	LEU
1	D	1108	ALA
1	D	1119	VAL
1	D	1219	GLU
1	E	446	ASP
1	E	1108	ALA
1	E	1280	ALA
1	F	207	ASN
1	H	522	ALA
1	H	940	MET
1	I	383	ARG
1	I	420	ALA

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Mol	Chain	Res	Type
1	J	923	THR
1	K	386	ALA
1	L	386	ALA
1	M	787	THR
1	N	321	VAL
1	N	1164	PRO
1	N	1219	GLU
1	O	386	ALA
1	P	1068	ARG
1	P	1153	ALA
2	Q	192	VAL
2	T	182	ASN
2	T	192	VAL
2	W	192	VAL
2	Z	192	VAL
3	b	38	ARG
2	c	192	VAL
3	e	136	HIS
4	p	105	ASP
1	G	193	PRO
1	G	425	PRO
1	G	959	PRO
1	A	110	HIS
1	B	138	GLU
1	B	1161	GLN
1	C	304	VAL
1	D	266	HIS
1	E	386	ALA
1	F	386	ALA
1	F	792	ALA
1	H	386	ALA
1	I	293	LEU
1	I	304	VAL
1	I	1202	PRO
1	J	184	MET
1	J	799	PRO
1	K	486	PRO
1	K	1153	ALA
1	M	1202	PRO
1	M	1203	CYS
1	N	953	GLU
1	O	34	ARG

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Mol	Chain	Res	Type
1	P	29	VAL
1	P	296	GLU
1	P	302	VAL
1	P	1279	ALA
3	Y	281	ARG
3	Y	434	ARG
2	Z	259	PRO
3	e	39	PRO
4	f	54	LEU
4	g	54	LEU
4	h	54	LEU
4	i	54	LEU
4	j	54	LEU
4	k	54	LEU
4	k	105	ASP
4	l	54	LEU
4	m	54	LEU
4	n	54	LEU
4	o	54	LEU
4	o	95	LYS
4	p	54	LEU
4	q	54	LEU
4	r	54	LEU
4	r	89	ARG
4	r	109	PRO
4	s	54	LEU
4	t	54	LEU
1	G	45	ASP
1	G	1351	ALA
1	B	534	PRO
1	B	1202	PRO
1	C	759	GLY
1	E	8	PRO
1	E	300	ALA
1	J	112	VAL
1	J	303	PRO
1	J	988	PRO
1	M	17	MET
1	M	273	PRO
1	N	658	ASN
1	O	486	PRO
1	O	997	ASN

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Mol	Chain	Res	Type
3	S	281	ARG
2	U	18	ARG
3	V	281	ARG
2	Z	105	PRO
4	f	4	PRO
4	f	41	PRO
4	g	4	PRO
4	g	41	PRO
4	h	4	PRO
4	h	41	PRO
4	i	4	PRO
4	i	41	PRO
4	j	4	PRO
4	j	41	PRO
4	k	4	PRO
4	k	41	PRO
4	l	4	PRO
4	l	22	MET
4	l	41	PRO
4	m	4	PRO
4	m	41	PRO
4	n	4	PRO
4	n	41	PRO
4	o	4	PRO
4	o	41	PRO
4	p	4	PRO
4	p	41	PRO
4	q	4	PRO
4	q	41	PRO
4	r	4	PRO
4	r	41	PRO
4	s	4	PRO
4	s	41	PRO
4	t	4	PRO
4	t	41	PRO
1	G	426	ALA
1	G	781	GLY
1	B	1126	PRO
1	C	259	VAL
1	F	326	VAL
1	J	1161	GLN
1	L	303	PRO

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Mol	Chain	Res	Type
1	L	1119	VAL
3	V	5	PRO
3	Y	5	PRO
3	b	5	PRO
4	t	17	VAL
1	D	259	VAL
1	M	9	PRO
3	Y	40	PRO
1	B	405	PRO
1	H	304	VAL
1	H	1202	PRO
1	M	304	VAL
1	O	1162	PRO
3	b	39	PRO
1	G	407	GLY
1	A	1202	PRO
1	C	1202	PRO
1	J	427	PRO
1	L	279	VAL
1	N	469	ILE
3	b	336	PRO
3	b	432	SER
3	e	286	VAL
4	k	17	VAL
4	s	17	VAL
4	t	105	ASP
1	F	1165	VAL
1	L	304	VAL
4	f	9	PRO
4	g	9	PRO
4	h	9	PRO
4	i	9	PRO
4	j	9	PRO
4	k	9	PRO
4	l	9	PRO
4	m	9	PRO
4	n	9	PRO
4	q	9	PRO
4	o	9	PRO
4	p	9	PRO
4	r	9	PRO
3	e	40	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1003/1080 (93%)	983 (98%)	20 (2%)	55 80
1	B	1009/1080 (93%)	991 (98%)	18 (2%)	59 82
1	C	1020/1080 (94%)	1008 (99%)	12 (1%)	71 88
1	D	1023/1080 (95%)	1000 (98%)	23 (2%)	52 78
1	E	1023/1080 (95%)	1009 (99%)	14 (1%)	67 86
1	F	1024/1080 (95%)	1005 (98%)	19 (2%)	57 81
1	G	992/1080 (92%)	964 (97%)	28 (3%)	43 73
1	H	1027/1080 (95%)	1009 (98%)	18 (2%)	59 82
1	I	1027/1080 (95%)	1001 (98%)	26 (2%)	47 75
1	J	1016/1080 (94%)	995 (98%)	21 (2%)	53 79
1	K	1028/1080 (95%)	1001 (97%)	27 (3%)	46 74
1	L	1027/1080 (95%)	1005 (98%)	22 (2%)	53 79
1	M	1030/1080 (95%)	1005 (98%)	25 (2%)	49 76
1	N	1029/1080 (95%)	1016 (99%)	13 (1%)	69 87
1	O	1027/1080 (95%)	1006 (98%)	21 (2%)	55 80
1	P	1029/1080 (95%)	1007 (98%)	22 (2%)	53 79
2	Q	195/264 (74%)	192 (98%)	3 (2%)	65 85
2	R	214/264 (81%)	205 (96%)	9 (4%)	30 62
2	T	195/264 (74%)	191 (98%)	4 (2%)	53 79
2	U	215/264 (81%)	206 (96%)	9 (4%)	30 62
2	W	195/264 (74%)	192 (98%)	3 (2%)	65 85
2	X	216/264 (82%)	209 (97%)	7 (3%)	39 69
2	Z	192/264 (73%)	181 (94%)	11 (6%)	20 52
2	a	213/264 (81%)	197 (92%)	16 (8%)	13 42
2	c	195/264 (74%)	191 (98%)	4 (2%)	53 79
2	d	216/264 (82%)	208 (96%)	8 (4%)	34 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	S	198/366 (54%)	189 (96%)	9 (4%)	27 60
3	V	201/366 (55%)	187 (93%)	14 (7%)	15 45
3	Y	205/366 (56%)	187 (91%)	18 (9%)	10 36
3	b	198/366 (54%)	165 (83%)	33 (17%)	2 9
3	e	204/366 (56%)	191 (94%)	13 (6%)	17 48
4	f	35/88 (40%)	29 (83%)	6 (17%)	2 9
4	g	35/88 (40%)	29 (83%)	6 (17%)	2 9
4	h	35/88 (40%)	28 (80%)	7 (20%)	1 5
4	i	35/88 (40%)	29 (83%)	6 (17%)	2 9
4	j	36/88 (41%)	30 (83%)	6 (17%)	2 9
4	k	35/88 (40%)	29 (83%)	6 (17%)	2 9
4	l	35/88 (40%)	29 (83%)	6 (17%)	2 9
4	m	35/88 (40%)	29 (83%)	6 (17%)	2 9
4	n	34/88 (39%)	27 (79%)	7 (21%)	1 5
4	o	35/88 (40%)	28 (80%)	7 (20%)	1 5
4	p	35/88 (40%)	28 (80%)	7 (20%)	1 5
4	q	35/88 (40%)	29 (83%)	6 (17%)	2 9
4	r	36/88 (41%)	30 (83%)	6 (17%)	2 9
4	s	36/88 (41%)	29 (81%)	7 (19%)	1 6
4	t	35/88 (40%)	29 (83%)	6 (17%)	2 9
All	All	19913/23070 (86%)	19328 (97%)	585 (3%)	45 72

All (585) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	58	LEU
1	G	75	LEU
1	G	95	VAL
1	G	129	LEU
1	G	134	SER
1	G	206	ASP
1	G	223	LEU
1	G	289	LEU
1	G	292	PHE
1	G	322	MET

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Mol	Chain	Res	Type
1	G	329	LEU
1	G	429	HIS
1	G	438	ARG
1	G	453	SER
1	G	524	CYS
1	G	832	PHE
1	G	958	LEU
1	G	1067	GLU
1	G	1122	MET
1	G	1194	THR
1	G	1195	ASP
1	G	1198	TYR
1	G	1200	ARG
1	G	1202	PRO
1	G	1298	SER
1	G	1317	CYS
1	G	1318	ARG
1	G	1348	ASP
1	A	31	SER
1	A	35	LEU
1	A	106	ARG
1	A	114	GLN
1	A	278	LEU
1	A	295	VAL
1	A	311	LEU
1	A	344	LEU
1	A	429	HIS
1	A	453	SER
1	A	520	TRP
1	A	563	VAL
1	A	582	LEU
1	A	754	CYS
1	A	1102	LEU
1	A	1114	THR
1	A	1139	LEU
1	A	1225	LEU
1	A	1264	ASN
1	A	1347	ARG
1	B	24	LEU
1	B	47	ASN
1	B	49	LEU
1	B	50	TYR

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Mol	Chain	Res	Type
1	B	71	LEU
1	B	144	THR
1	B	155	LEU
1	B	264	LEU
1	B	269	THR
1	B	380	LEU
1	B	384	ILE
1	B	520	TRP
1	B	532	MET
1	B	821	SER
1	B	1194	THR
1	B	1204	ASN
1	B	1236	ARG
1	B	1277	PHE
1	C	47	ASN
1	C	49	LEU
1	C	65	LEU
1	C	520	TRP
1	C	786	ASN
1	C	1038	HIS
1	C	1102	LEU
1	C	1104	VAL
1	C	1139	LEU
1	C	1202	PRO
1	C	1225	LEU
1	C	1318	ARG
1	D	35	LEU
1	D	55	ASP
1	D	75	LEU
1	D	118	ASN
1	D	123	VAL
1	D	159	LEU
1	D	253	THR
1	D	384	ILE
1	D	408	LEU
1	D	511	GLN
1	D	520	TRP
1	D	787	THR
1	D	1102	LEU
1	D	1125	LEU
1	D	1139	LEU
1	D	1157	LEU

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Mol	Chain	Res	Type
1	D	1174	ARG
1	D	1197	ASN
1	D	1221	ASP
1	D	1228	ASP
1	D	1278	THR
1	D	1319	GLU
1	D	1332	TYR
1	E	264	LEU
1	E	266	HIS
1	E	302	VAL
1	E	384	ILE
1	E	520	TRP
1	E	524	CYS
1	E	818	PRO
1	E	1104	VAL
1	E	1139	LEU
1	E	1197	ASN
1	E	1251	SER
1	E	1254	ASP
1	E	1256	LEU
1	E	1300	VAL
1	F	31	SER
1	F	77	VAL
1	F	80	VAL
1	F	86	GLU
1	F	87	LEU
1	F	297	ASP
1	F	348	ARG
1	F	384	ILE
1	F	486	PRO
1	F	520	TRP
1	F	595	ARG
1	F	752	ARG
1	F	786	ASN
1	F	787	THR
1	F	788	GLN
1	F	1085	THR
1	F	1192	VAL
1	F	1218	LYS
1	F	1278	THR
1	H	264	LEU
1	H	279	VAL

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Mol	Chain	Res	Type
1	H	280	THR
1	H	291	SER
1	H	297	ASP
1	H	304	VAL
1	H	310	VAL
1	H	384	ILE
1	H	415	ARG
1	H	485	ASN
1	H	582	LEU
1	H	731	LEU
1	H	943	GLN
1	H	1197	ASN
1	H	1202	PRO
1	H	1241	THR
1	H	1254	ASP
1	H	1264	ASN
1	I	12	ARG
1	I	44	SER
1	I	94	ARG
1	I	114	GLN
1	I	122	LYS
1	I	134	SER
1	I	266	HIS
1	I	289	LEU
1	I	320	LEU
1	I	322	MET
1	I	384	ILE
1	I	520	TRP
1	I	543	LEU
1	I	582	LEU
1	I	947	HIS
1	I	1071	GLU
1	I	1078	LEU
1	I	1104	VAL
1	I	1194	THR
1	I	1196	ILE
1	I	1223	ILE
1	I	1267	SER
1	I	1278	THR
1	I	1290	GLU
1	I	1321	VAL
1	I	1348	ASP

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Mol	Chain	Res	Type
1	J	43	ARG
1	J	71	LEU
1	J	75	LEU
1	J	92	GLU
1	J	230	THR
1	J	231	SER
1	J	264	LEU
1	J	402	PHE
1	J	427	PRO
1	J	558	LEU
1	J	755	ARG
1	J	796	ASP
1	J	922	SER
1	J	1092	THR
1	J	1120	THR
1	J	1161	GLN
1	J	1192	VAL
1	J	1221	ASP
1	J	1319	GLU
1	J	1347	ARG
1	J	1365	ASP
1	K	99	VAL
1	K	118	ASN
1	K	120	MET
1	K	191	LYS
1	K	223	LEU
1	K	305	THR
1	K	356	SER
1	K	394	LEU
1	K	752	ARG
1	K	753	ASP
1	K	756	ILE
1	K	784	LEU
1	K	922	SER
1	K	1036	LEU
1	K	1062	ASN
1	K	1104	VAL
1	K	1114	THR
1	K	1118	PRO
1	K	1147	LEU
1	K	1191	PRO
1	K	1192	VAL

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Mol	Chain	Res	Type
1	K	1194	THR
1	K	1277	PHE
1	K	1298	SER
1	K	1319	GLU
1	K	1347	ARG
1	K	1352	HIS
1	L	31	SER
1	L	43	ARG
1	L	116	VAL
1	L	292	PHE
1	L	304	VAL
1	L	308	GLU
1	L	377	LEU
1	L	378	GLU
1	L	384	ILE
1	L	470	ASP
1	L	473	VAL
1	L	477	ASN
1	L	524	CYS
1	L	563	VAL
1	L	752	ARG
1	L	908	LEU
1	L	909	LEU
1	L	1044	LEU
1	L	1104	VAL
1	L	1264	ASN
1	L	1301	SER
1	L	1302	THR
1	M	17	MET
1	M	41	ARG
1	M	45	ASP
1	M	137	THR
1	M	142	LEU
1	M	143	LEU
1	M	266	HIS
1	M	299	GLU
1	M	303	PRO
1	M	305	THR
1	M	380	LEU
1	M	381	GLU
1	M	384	ILE
1	M	521	VAL

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Mol	Chain	Res	Type
1	M	524	CYS
1	M	557	GLU
1	M	756	ILE
1	M	780	ASP
1	M	1107	THR
1	M	1195	ASP
1	M	1204	ASN
1	M	1206	ARG
1	M	1221	ASP
1	M	1264	ASN
1	M	1321	VAL
1	N	270	ARG
1	N	322	MET
1	N	384	ILE
1	N	422	ASP
1	N	439	GLN
1	N	453	SER
1	N	538	ASN
1	N	787	THR
1	N	1139	LEU
1	N	1168	CYS
1	N	1192	VAL
1	N	1195	ASP
1	N	1278	THR
1	O	296	GLU
1	O	299	GLU
1	O	384	ILE
1	O	427	PRO
1	O	453	SER
1	O	465	SER
1	O	534	PRO
1	O	555	ASP
1	O	579	ASN
1	O	752	ARG
1	O	753	ASP
1	O	754	CYS
1	O	756	ILE
1	O	780	ASP
1	O	1120	THR
1	O	1125	LEU
1	O	1139	LEU
1	O	1161	GLN

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Mol	Chain	Res	Type
1	O	1206	ARG
1	O	1264	ASN
1	O	1334	ILE
1	P	43	ARG
1	P	118	ASN
1	P	120	MET
1	P	148	LEU
1	P	264	LEU
1	P	291	SER
1	P	384	ILE
1	P	432	PRO
1	P	485	ASN
1	P	486	PRO
1	P	520	TRP
1	P	788	GLN
1	P	919	ASN
1	P	1114	THR
1	P	1116	ARG
1	P	1120	THR
1	P	1139	LEU
1	P	1201	ARG
1	P	1263	LEU
1	P	1264	ASN
1	P	1281	ASP
1	P	1321	VAL
2	Q	126	THR
2	Q	180	TYR
2	Q	188	LEU
2	R	16	ILE
2	R	34	LEU
2	R	163	LEU
2	R	164	ASN
2	R	246	VAL
2	R	269	LEU
2	R	291	LEU
2	R	295	VAL
2	R	314	VAL
3	S	132	LEU
3	S	254	TRP
3	S	275	HIS
3	S	300	LEU
3	S	302	LEU

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Mol	Chain	Res	Type
3	S	350	LEU
3	S	351	ARG
3	S	428	MET
3	S	449	VAL
2	T	126	THR
2	T	178	VAL
2	T	186	LEU
2	T	188	LEU
2	U	14	SER
2	U	17	SER
2	U	34	LEU
2	U	38	ARG
2	U	246	VAL
2	U	269	LEU
2	U	291	LEU
2	U	295	VAL
2	U	314	VAL
3	V	41	ILE
3	V	79	THR
3	V	82	ASP
3	V	85	GLN
3	V	132	LEU
3	V	139	ASP
3	V	143	LEU
3	V	165	LEU
3	V	198	TYR
3	V	254	TRP
3	V	302	LEU
3	V	350	LEU
3	V	428	MET
3	V	449	VAL
2	W	126	THR
2	W	178	VAL
2	W	188	LEU
2	X	34	LEU
2	X	163	LEU
2	X	246	VAL
2	X	269	LEU
2	X	291	LEU
2	X	295	VAL
2	X	314	VAL
3	Y	82	ASP

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Mol	Chain	Res	Type
3	Y	83	THR
3	Y	85	GLN
3	Y	88	ASP
3	Y	132	LEU
3	Y	164	LEU
3	Y	165	LEU
3	Y	166	GLU
3	Y	198	TYR
3	Y	254	TRP
3	Y	302	LEU
3	Y	350	LEU
3	Y	351	ARG
3	Y	419	TYR
3	Y	428	MET
3	Y	434	ARG
3	Y	445	VAL
3	Y	449	VAL
2	Z	126	THR
2	Z	180	TYR
2	Z	181	TYR
2	Z	186	LEU
2	Z	188	LEU
2	Z	218	THR
2	Z	219	LEU
2	Z	221	LEU
2	Z	222	THR
2	Z	227	LEU
2	Z	315	ILE
2	a	16	ILE
2	a	34	LEU
2	a	43	LEU
2	a	78	VAL
2	a	82	ARG
2	a	98	VAL
2	a	133	LEU
2	a	135	LEU
2	a	138	ARG
2	a	161	ARG
2	a	164	ASN
2	a	246	VAL
2	a	269	LEU
2	a	291	LEU

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Mol	Chain	Res	Type
2	a	295	VAL
2	a	314	VAL
3	b	79	THR
3	b	112	ARG
3	b	132	LEU
3	b	137	PRO
3	b	140	LEU
3	b	186	SER
3	b	188	ASN
3	b	189	PHE
3	b	198	TYR
3	b	210	HIS
3	b	213	THR
3	b	215	TYR
3	b	254	TRP
3	b	288	ILE
3	b	295	ASP
3	b	296	LEU
3	b	297	ASP
3	b	299	GLU
3	b	301	CYS
3	b	302	LEU
3	b	314	PHE
3	b	315	THR
3	b	321	ASP
3	b	322	GLN
3	b	330	VAL
3	b	334	LEU
3	b	346	LEU
3	b	353	THR
3	b	417	CYS
3	b	419	TYR
3	b	436	LEU
3	b	447	VAL
3	b	452	LEU
2	c	126	THR
2	c	179	LEU
2	c	182	ASN
2	c	188	LEU
2	d	16	ILE
2	d	34	LEU
2	d	164	ASN

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Mol	Chain	Res	Type
2	d	246	VAL
2	d	269	LEU
2	d	291	LEU
2	d	295	VAL
2	d	314	VAL
3	e	36	VAL
3	e	83	THR
3	e	117	THR
3	e	119	LEU
3	e	132	LEU
3	e	134	LEU
3	e	140	LEU
3	e	198	TYR
3	e	254	TRP
3	e	302	LEU
3	e	428	MET
3	e	436	LEU
3	e	449	VAL
4	f	27	LEU
4	f	36	MET
4	f	37	ASP
4	f	41	PRO
4	f	46	THR
4	f	67	THR
4	g	27	LEU
4	g	36	MET
4	g	37	ASP
4	g	41	PRO
4	g	46	THR
4	g	67	THR
4	h	27	LEU
4	h	36	MET
4	h	37	ASP
4	h	41	PRO
4	h	46	THR
4	h	67	THR
4	h	97	THR
4	i	27	LEU
4	i	36	MET
4	i	37	ASP
4	i	41	PRO
4	i	46	THR

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Mol	Chain	Res	Type
4	i	67	THR
4	j	27	LEU
4	j	36	MET
4	j	37	ASP
4	j	41	PRO
4	j	46	THR
4	j	67	THR
4	k	27	LEU
4	k	36	MET
4	k	37	ASP
4	k	41	PRO
4	k	46	THR
4	k	67	THR
4	l	27	LEU
4	l	36	MET
4	l	37	ASP
4	l	41	PRO
4	l	46	THR
4	l	67	THR
4	m	27	LEU
4	m	36	MET
4	m	37	ASP
4	m	41	PRO
4	m	46	THR
4	m	67	THR
4	n	20	LEU
4	n	27	LEU
4	n	36	MET
4	n	37	ASP
4	n	41	PRO
4	n	46	THR
4	n	67	THR
4	o	27	LEU
4	o	36	MET
4	o	37	ASP
4	o	41	PRO
4	o	46	THR
4	o	67	THR
4	o	97	THR
4	p	10	SER
4	p	27	LEU
4	p	36	MET

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Mol	Chain	Res	Type
4	p	37	ASP
4	p	41	PRO
4	p	46	THR
4	p	67	THR
4	q	27	LEU
4	q	36	MET
4	q	37	ASP
4	q	41	PRO
4	q	46	THR
4	q	67	THR
4	r	27	LEU
4	r	36	MET
4	r	37	ASP
4	r	41	PRO
4	r	46	THR
4	r	67	THR
4	s	27	LEU
4	s	36	MET
4	s	37	ASP
4	s	41	PRO
4	s	46	THR
4	s	67	THR
4	s	96	ARG
4	t	27	LEU
4	t	36	MET
4	t	37	ASP
4	t	41	PRO
4	t	46	THR
4	t	67	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (537) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	100	HIS
1	G	183	GLN
1	G	312	ASN
1	G	419	HIS
1	G	429	HIS
1	G	478	HIS
1	G	485	ASN
1	G	544	HIS
1	G	696	HIS

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Mol	Chain	Res	Type
1	G	724	HIS
1	G	751	HIS
1	G	866	HIS
1	G	869	ASN
1	G	943	GLN
1	G	972	ASN
1	G	1004	GLN
1	G	1008	GLN
1	G	1055	GLN
1	G	1083	HIS
1	G	1090	ASN
1	G	1179	HIS
1	G	1243	ASN
1	G	1310	GLN
1	G	1329	GLN
1	A	100	HIS
1	A	164	GLN
1	A	168	ASN
1	A	207	ASN
1	A	266	HIS
1	A	359	GLN
1	A	536	ASN
1	A	581	ASN
1	A	604	HIS
1	A	639	HIS
1	A	696	HIS
1	A	724	HIS
1	A	785	HIS
1	A	800	HIS
1	A	809	HIS
1	A	866	HIS
1	A	972	ASN
1	A	1008	GLN
1	A	1018	ASN
1	A	1039	GLN
1	A	1062	ASN
1	A	1079	GLN
1	A	1090	ASN
1	A	1124	ASN
1	A	1286	HIS
1	A	1352	HIS
1	A	1357	HIS

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Mol	Chain	Res	Type
1	B	96	GLN
1	B	110	HIS
1	B	164	GLN
1	B	168	ASN
1	B	183	GLN
1	B	266	HIS
1	B	335	HIS
1	B	419	HIS
1	B	456	ASN
1	B	477	ASN
1	B	485	ASN
1	B	536	ASN
1	B	544	HIS
1	B	581	ASN
1	B	658	ASN
1	B	696	HIS
1	B	786	ASN
1	B	880	HIS
1	B	1008	GLN
1	B	1018	ASN
1	B	1204	ASN
1	B	1229	HIS
1	B	1264	ASN
1	B	1286	HIS
1	B	1357	HIS
1	C	101	GLN
1	C	114	GLN
1	C	168	ASN
1	C	183	GLN
1	C	256	GLN
1	C	312	ASN
1	C	335	HIS
1	C	347	ASN
1	C	419	HIS
1	C	448	GLN
1	C	536	ASN
1	C	544	HIS
1	C	581	ASN
1	C	696	HIS
1	C	724	HIS
1	C	745	HIS
1	C	785	HIS

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Mol	Chain	Res	Type
1	C	808	HIS
1	C	866	HIS
1	C	947	HIS
1	C	1004	GLN
1	C	1018	ASN
1	C	1038	HIS
1	C	1045	HIS
1	C	1055	GLN
1	C	1077	GLN
1	C	1079	GLN
1	C	1083	HIS
1	C	1161	GLN
1	C	1286	HIS
1	C	1329	GLN
1	C	1352	HIS
1	C	1357	HIS
1	D	118	ASN
1	D	168	ASN
1	D	266	HIS
1	D	315	ASN
1	D	347	ASN
1	D	429	HIS
1	D	544	HIS
1	D	581	ASN
1	D	639	HIS
1	D	696	HIS
1	D	724	HIS
1	D	745	HIS
1	D	751	HIS
1	D	786	ASN
1	D	866	HIS
1	D	900	ASN
1	D	947	HIS
1	D	986	HIS
1	D	1008	GLN
1	D	1018	ASN
1	D	1039	GLN
1	D	1055	GLN
1	D	1083	HIS
1	D	1286	HIS
1	D	1310	GLN
1	D	1329	GLN

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Mol	Chain	Res	Type
1	D	1357	HIS
1	E	118	ASN
1	E	156	HIS
1	E	168	ASN
1	E	419	HIS
1	E	448	GLN
1	E	544	HIS
1	E	696	HIS
1	E	724	HIS
1	E	866	HIS
1	E	947	HIS
1	E	1008	GLN
1	E	1018	ASN
1	E	1039	GLN
1	E	1055	GLN
1	E	1083	HIS
1	E	1197	ASN
1	E	1264	ASN
1	E	1286	HIS
1	E	1310	GLN
1	E	1329	GLN
1	E	1357	HIS
1	F	164	GLN
1	F	168	ASN
1	F	266	HIS
1	F	315	ASN
1	F	485	ASN
1	F	503	GLN
1	F	536	ASN
1	F	544	HIS
1	F	581	ASN
1	F	639	HIS
1	F	696	HIS
1	F	724	HIS
1	F	785	HIS
1	F	866	HIS
1	F	900	ASN
1	F	1004	GLN
1	F	1008	GLN
1	F	1018	ASN
1	F	1039	GLN
1	F	1055	GLN

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Mol	Chain	Res	Type
1	F	1124	ASN
1	F	1197	ASN
1	F	1286	HIS
1	F	1329	GLN
1	F	1357	HIS
1	H	101	GLN
1	H	156	HIS
1	H	183	GLN
1	H	202	GLN
1	H	312	ASN
1	H	439	GLN
1	H	456	ASN
1	H	485	ASN
1	H	536	ASN
1	H	544	HIS
1	H	581	ASN
1	H	658	ASN
1	H	696	HIS
1	H	724	HIS
1	H	745	HIS
1	H	866	HIS
1	H	1004	GLN
1	H	1008	GLN
1	H	1018	ASN
1	H	1039	GLN
1	H	1055	GLN
1	H	1079	GLN
1	H	1090	ASN
1	H	1095	GLN
1	H	1197	ASN
1	H	1264	ASN
1	H	1286	HIS
1	H	1329	GLN
1	H	1357	HIS
1	I	96	GLN
1	I	114	GLN
1	I	118	ASN
1	I	164	GLN
1	I	168	ASN
1	I	335	HIS
1	I	340	GLN
1	I	347	ASN

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Mol	Chain	Res	Type
1	I	410	ASN
1	I	429	HIS
1	I	448	GLN
1	I	456	ASN
1	I	525	GLN
1	I	544	HIS
1	I	696	HIS
1	I	724	HIS
1	I	745	HIS
1	I	866	HIS
1	I	880	HIS
1	I	944	HIS
1	I	972	ASN
1	I	1008	GLN
1	I	1018	ASN
1	I	1095	GLN
1	I	1248	GLN
1	I	1286	HIS
1	I	1310	GLN
1	I	1329	GLN
1	J	118	ASN
1	J	163	GLN
1	J	266	HIS
1	J	456	ASN
1	J	485	ASN
1	J	544	HIS
1	J	581	ASN
1	J	717	GLN
1	J	724	HIS
1	J	800	HIS
1	J	944	HIS
1	J	951	ASN
1	J	1045	HIS
1	J	1083	HIS
1	J	1095	GLN
1	J	1286	HIS
1	J	1329	GLN
1	K	32	HIS
1	K	118	ASN
1	K	168	ASN
1	K	183	GLN
1	K	266	HIS

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Mol	Chain	Res	Type
1	K	335	HIS
1	K	359	GLN
1	K	439	GLN
1	K	477	ASN
1	K	536	ASN
1	K	544	HIS
1	K	581	ASN
1	K	604	HIS
1	K	639	HIS
1	K	696	HIS
1	K	724	HIS
1	K	785	HIS
1	K	919	ASN
1	K	947	HIS
1	K	1008	GLN
1	K	1009	HIS
1	K	1018	ASN
1	K	1039	GLN
1	K	1045	HIS
1	K	1124	ASN
1	K	1357	HIS
1	L	96	GLN
1	L	156	HIS
1	L	164	GLN
1	L	170	GLN
1	L	202	GLN
1	L	266	HIS
1	L	419	HIS
1	L	429	HIS
1	L	448	GLN
1	L	477	ASN
1	L	536	ASN
1	L	544	HIS
1	L	581	ASN
1	L	639	HIS
1	L	658	ASN
1	L	696	HIS
1	L	724	HIS
1	L	745	HIS
1	L	785	HIS
1	L	786	ASN
1	L	900	ASN

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Mol	Chain	Res	Type
1	L	947	HIS
1	L	1008	GLN
1	L	1018	ASN
1	L	1045	HIS
1	L	1055	GLN
1	L	1077	GLN
1	L	1079	GLN
1	L	1170	GLN
1	L	1286	HIS
1	L	1352	HIS
1	L	1357	HIS
1	M	47	ASN
1	M	130	ASN
1	M	156	HIS
1	M	168	ASN
1	M	170	GLN
1	M	183	GLN
1	M	202	GLN
1	M	429	HIS
1	M	448	GLN
1	M	536	ASN
1	M	544	HIS
1	M	581	ASN
1	M	604	HIS
1	M	639	HIS
1	M	696	HIS
1	M	719	GLN
1	M	724	HIS
1	M	745	HIS
1	M	866	HIS
1	M	880	HIS
1	M	900	ASN
1	M	944	HIS
1	M	972	ASN
1	M	1004	GLN
1	M	1008	GLN
1	M	1018	ASN
1	M	1039	GLN
1	M	1045	HIS
1	M	1079	GLN
1	M	1095	GLN
1	M	1197	ASN

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Mol	Chain	Res	Type
1	M	1204	ASN
1	M	1264	ASN
1	M	1286	HIS
1	M	1357	HIS
1	N	32	HIS
1	N	168	ASN
1	N	207	ASN
1	N	290	GLN
1	N	335	HIS
1	N	347	ASN
1	N	419	HIS
1	N	456	ASN
1	N	581	ASN
1	N	696	HIS
1	N	724	HIS
1	N	947	HIS
1	N	1008	GLN
1	N	1018	ASN
1	N	1077	GLN
1	N	1090	ASN
1	N	1286	HIS
1	N	1329	GLN
1	N	1357	HIS
1	O	32	HIS
1	O	47	ASN
1	O	117	HIS
1	O	156	HIS
1	O	164	GLN
1	O	168	ASN
1	O	170	GLN
1	O	347	ASN
1	O	419	HIS
1	O	429	HIS
1	O	439	GLN
1	O	468	ASN
1	O	536	ASN
1	O	544	HIS
1	O	581	ASN
1	O	639	HIS
1	O	696	HIS
1	O	724	HIS
1	O	866	HIS

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Mol	Chain	Res	Type
1	O	880	HIS
1	O	881	ASN
1	O	900	ASN
1	O	943	GLN
1	O	947	HIS
1	O	1008	GLN
1	O	1018	ASN
1	O	1062	ASN
1	O	1090	ASN
1	O	1124	ASN
1	O	1197	ASN
1	O	1286	HIS
1	O	1329	GLN
1	O	1357	HIS
1	P	32	HIS
1	P	110	HIS
1	P	118	ASN
1	P	130	ASN
1	P	164	GLN
1	P	168	ASN
1	P	183	GLN
1	P	347	ASN
1	P	419	HIS
1	P	429	HIS
1	P	439	GLN
1	P	544	HIS
1	P	581	ASN
1	P	639	HIS
1	P	696	HIS
1	P	719	GLN
1	P	724	HIS
1	P	745	HIS
1	P	785	HIS
1	P	800	HIS
1	P	841	ASN
1	P	866	HIS
1	P	869	ASN
1	P	919	ASN
1	P	925	ASN
1	P	969	HIS
1	P	1008	GLN
1	P	1018	ASN

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Mol	Chain	Res	Type
1	P	1039	GLN
1	P	1045	HIS
1	P	1095	GLN
1	P	1264	ASN
1	P	1286	HIS
1	P	1329	GLN
1	P	1357	HIS
2	Q	48	HIS
2	Q	124	GLN
2	R	94	HIS
2	R	193	GLN
2	R	238	ASN
2	R	281	HIS
3	S	109	HIS
3	S	210	HIS
3	S	214	ASN
3	S	238	HIS
3	S	242	HIS
3	S	271	GLN
2	T	48	HIS
2	T	99	ASN
2	T	124	GLN
2	T	182	ASN
2	U	94	HIS
2	U	193	GLN
2	U	238	ASN
2	U	281	HIS
3	V	85	GLN
3	V	109	HIS
3	V	136	HIS
3	V	142	HIS
3	V	210	HIS
3	V	214	ASN
3	V	238	HIS
3	V	242	HIS
3	V	271	GLN
3	V	275	HIS
3	V	318	GLN
2	W	48	HIS
2	W	99	ASN
2	W	124	GLN
2	W	177	ASN

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Mol	Chain	Res	Type
2	X	94	HIS
2	X	193	GLN
2	X	238	ASN
2	X	281	HIS
3	Y	109	HIS
3	Y	136	HIS
3	Y	214	ASN
3	Y	238	HIS
3	Y	242	HIS
3	Y	271	GLN
3	Y	275	HIS
2	Z	48	HIS
2	Z	124	GLN
2	a	99	ASN
2	a	238	ASN
2	a	281	HIS
3	b	85	GLN
3	b	136	HIS
3	b	163	GLN
3	b	188	ASN
3	b	210	HIS
3	b	214	ASN
3	b	242	HIS
3	b	275	HIS
3	b	318	GLN
3	b	322	GLN
3	b	333	GLN
2	c	40	GLN
2	c	48	HIS
2	c	124	GLN
2	c	284	GLN
2	d	40	GLN
2	d	94	HIS
2	d	193	GLN
2	d	238	ASN
2	d	281	HIS
3	e	109	HIS
3	e	136	HIS
3	e	142	HIS
3	e	210	HIS
3	e	214	ASN
3	e	242	HIS

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Mol	Chain	Res	Type
3	e	271	GLN
3	e	275	HIS
4	f	7	HIS
4	f	57	GLN
4	g	7	HIS
4	h	7	HIS
4	i	7	HIS
4	j	7	HIS
4	k	7	HIS
4	l	7	HIS
4	m	7	HIS
4	m	57	GLN
4	n	7	HIS
4	n	30	ASN
4	o	7	HIS
4	p	7	HIS
4	p	57	GLN
4	q	7	HIS
4	q	57	GLN
4	r	7	HIS
4	s	7	HIS
4	s	57	GLN
4	t	7	HIS
4	t	57	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

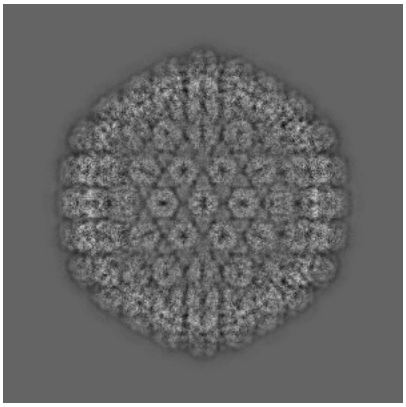
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6907. These allow visual inspection of the internal detail of the map and identification of artifacts.

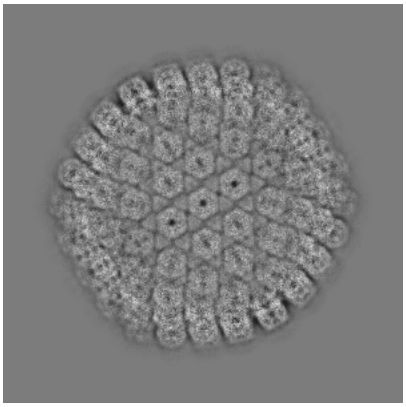
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

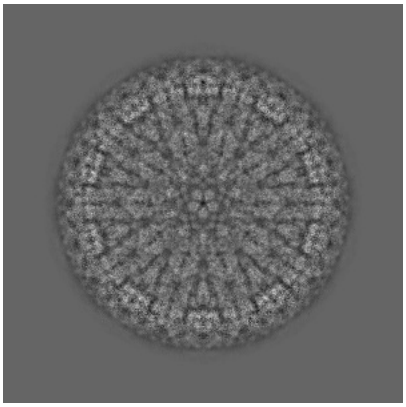
6.1.1 Primary map



X



Y

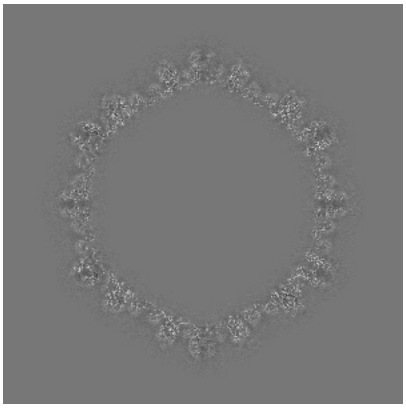


Z

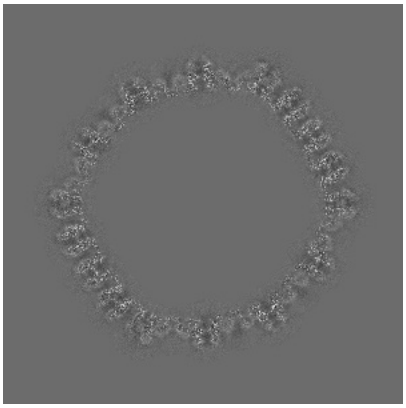
The images above show the map projected in three orthogonal directions.

6.2 Central slices

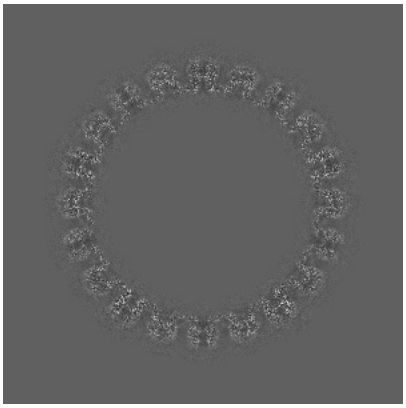
6.2.1 Primary map



X Index: 600



Y Index: 600

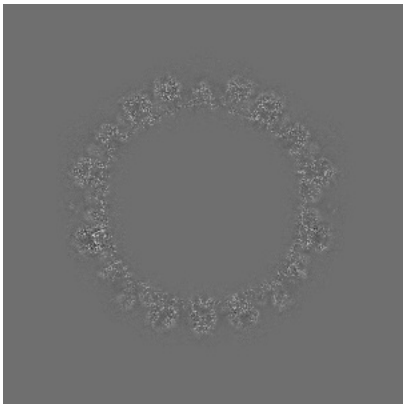


Z Index: 600

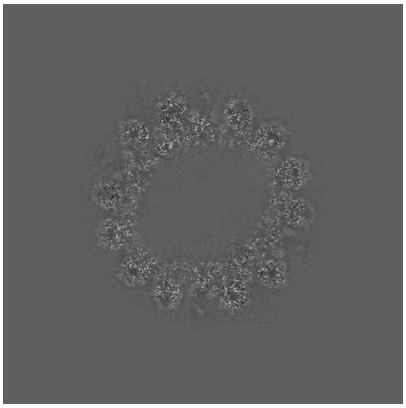
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

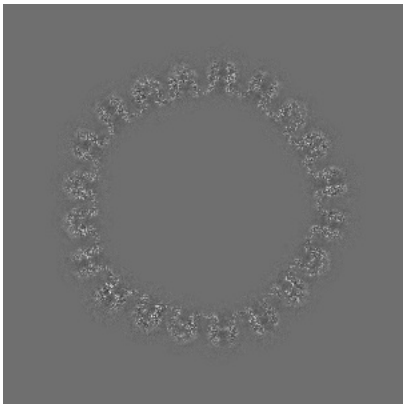
6.3.1 Primary map



X Index: 772



Y Index: 319

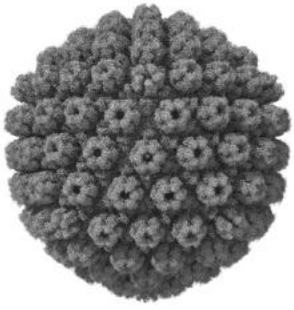


Z Index: 695

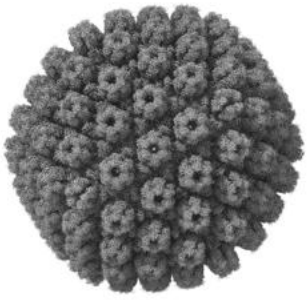
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 12.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

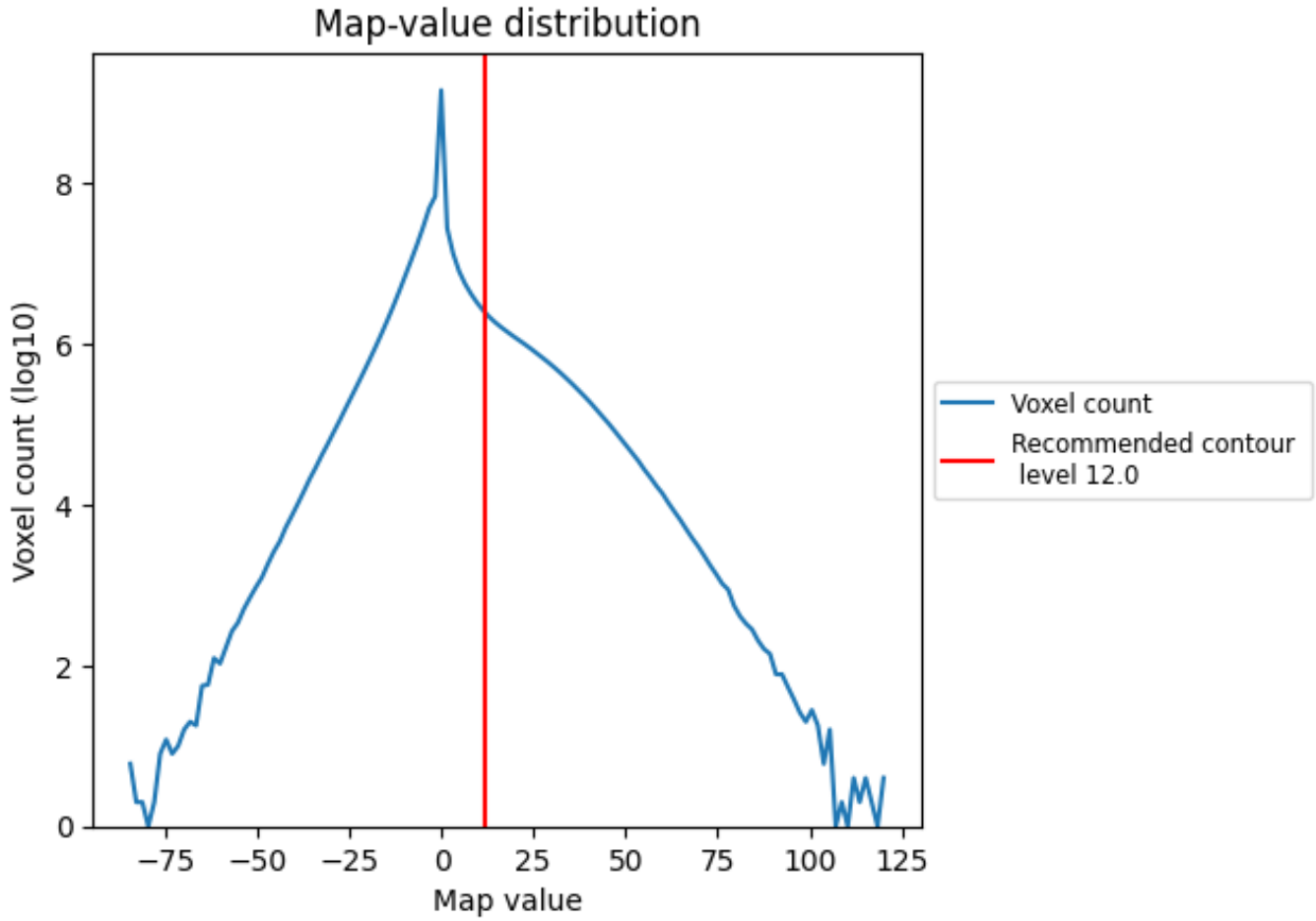
6.5 Mask visualisation (i)

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

7 Map analysis

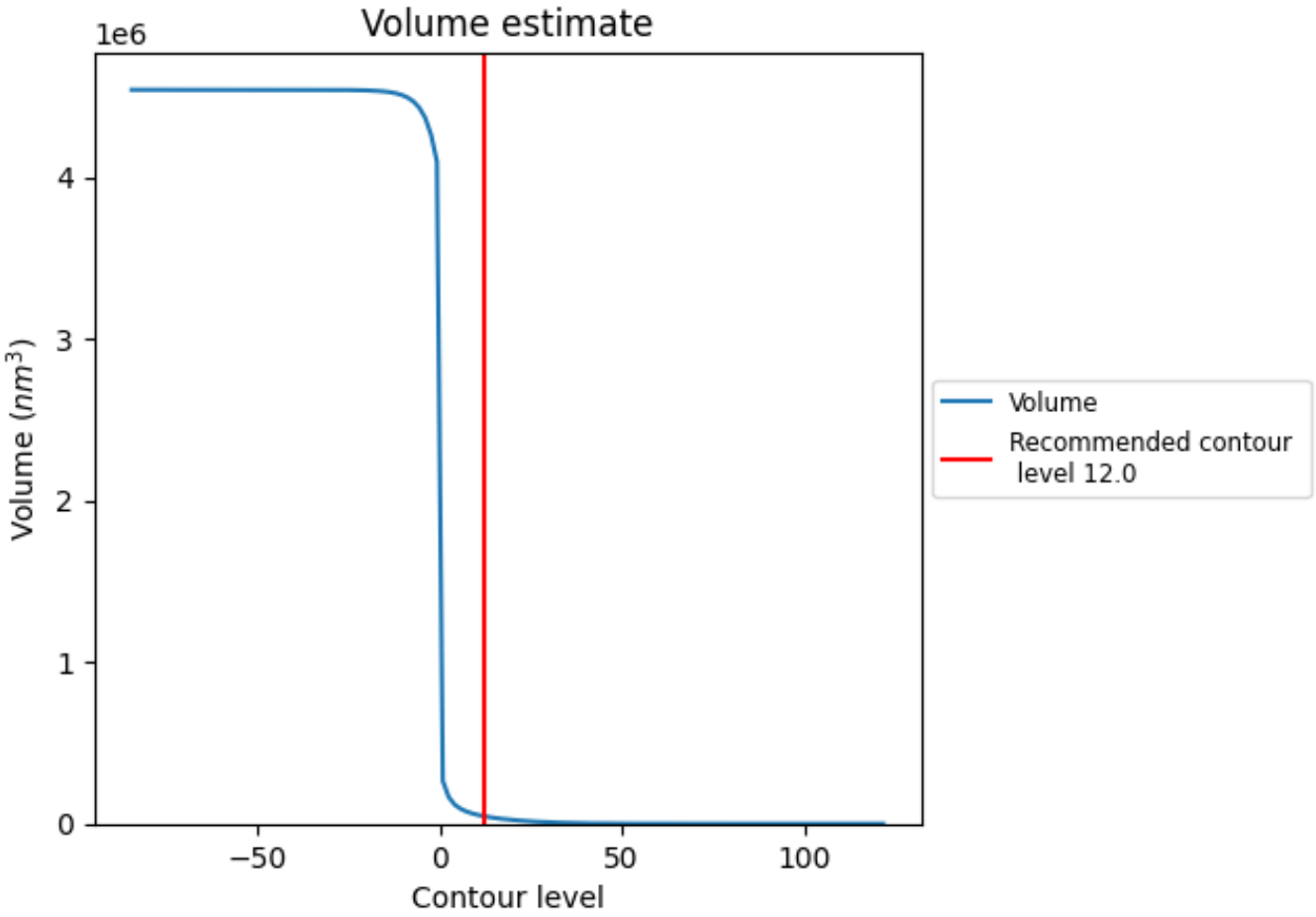
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

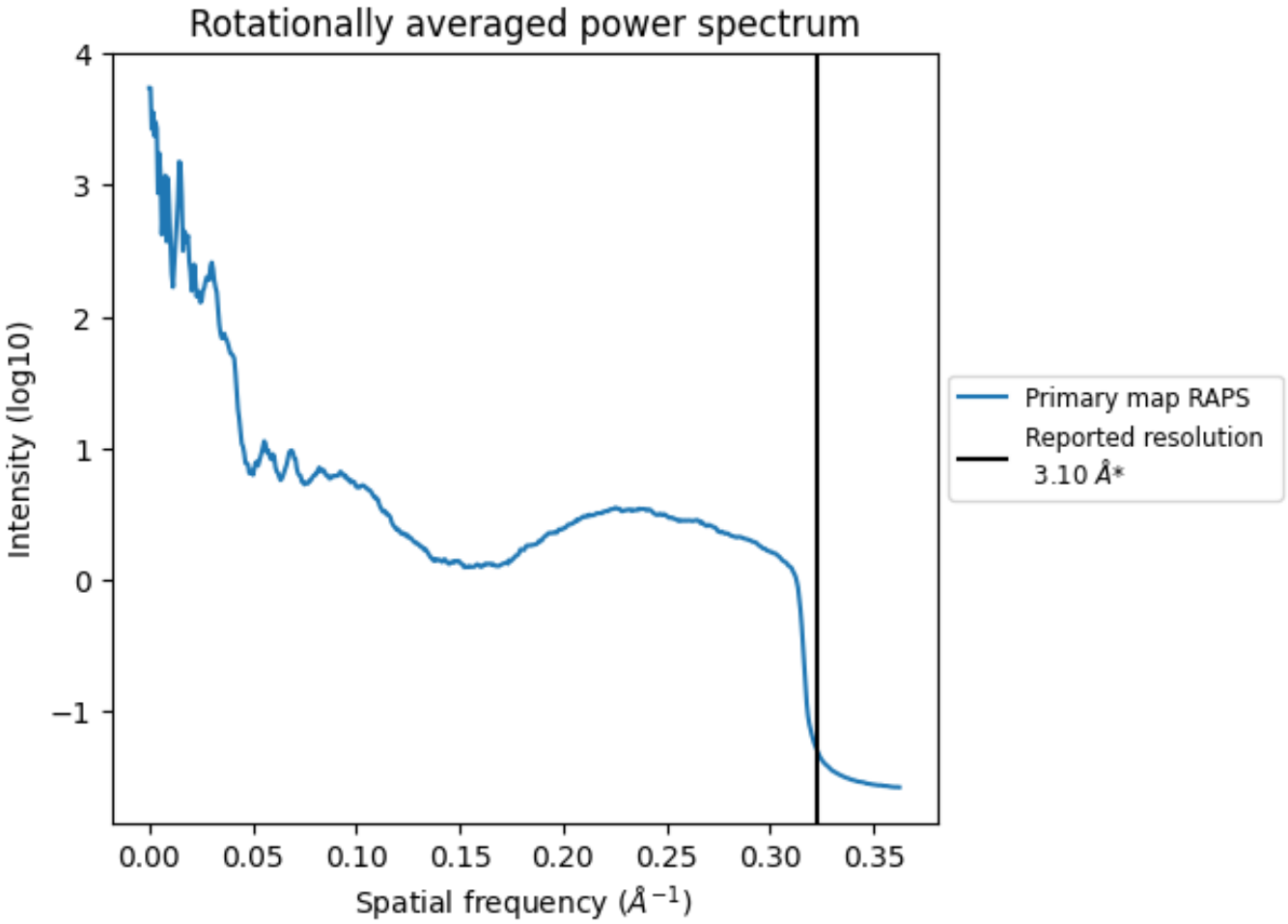
7.2 Volume estimate



The volume at the recommended contour level is 47511 nm^3; this corresponds to an approximate mass of 42918 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.323 $Å^{-1}$

8 Fourier-Shell correlation

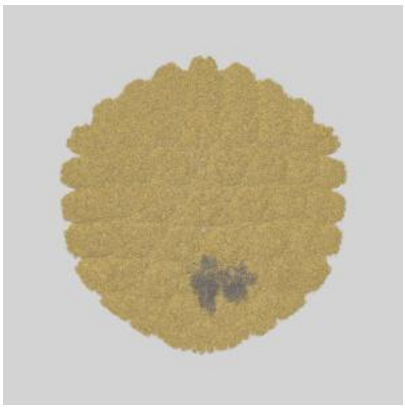
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

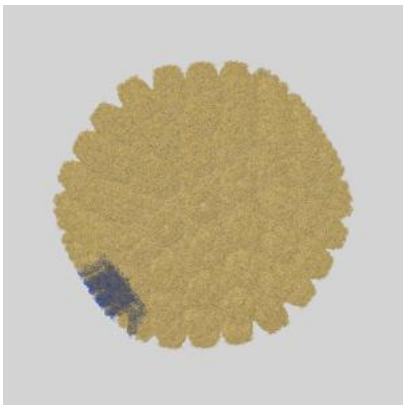
This section contains information regarding the fit between EMDB map EMD-6907 and PDB model 5ZAP. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

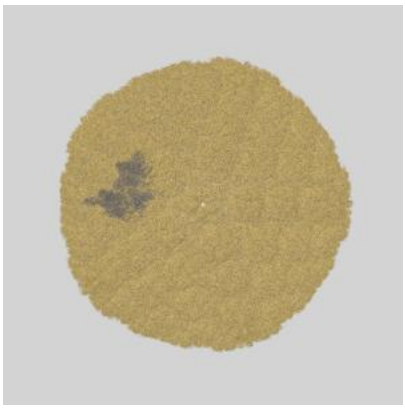
9.1.1 Map-model overlay



X

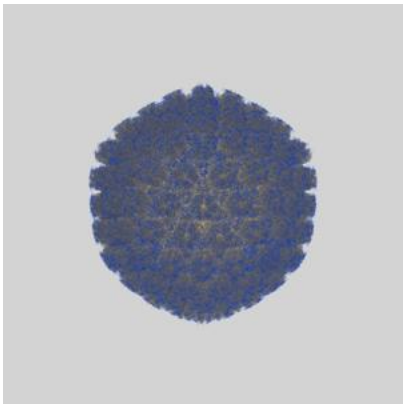


Y

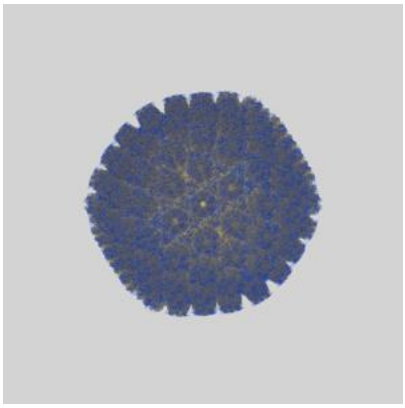


Z

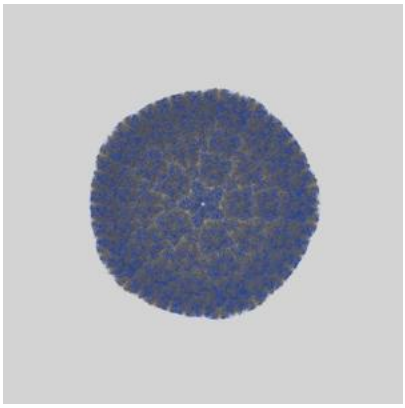
9.1.2 Map-model assembly overlay



X



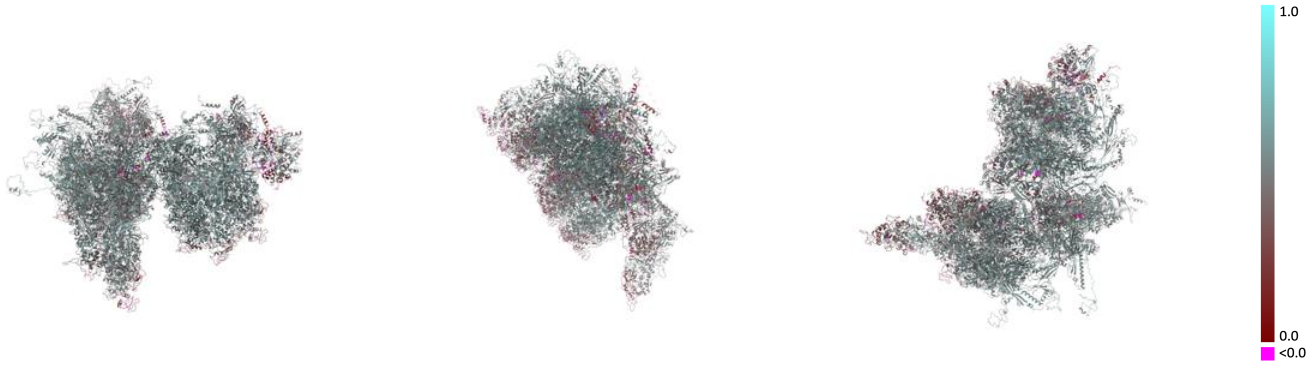
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 12.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

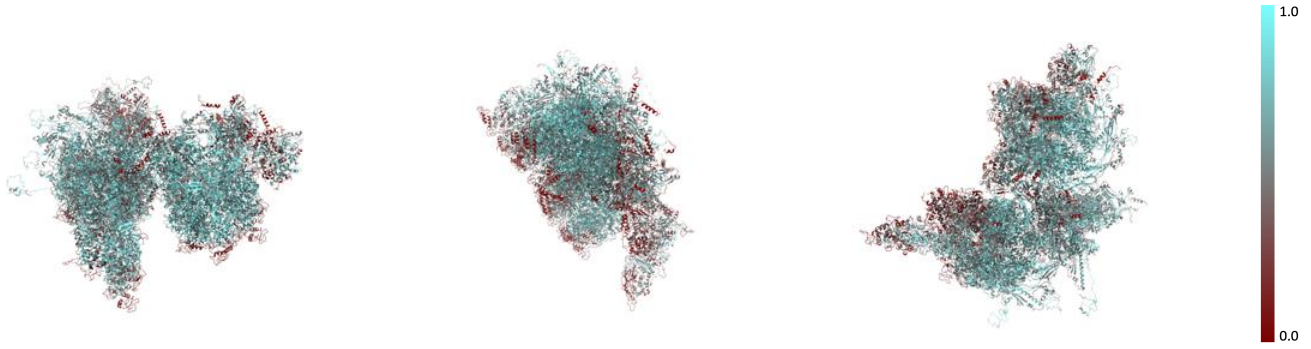
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

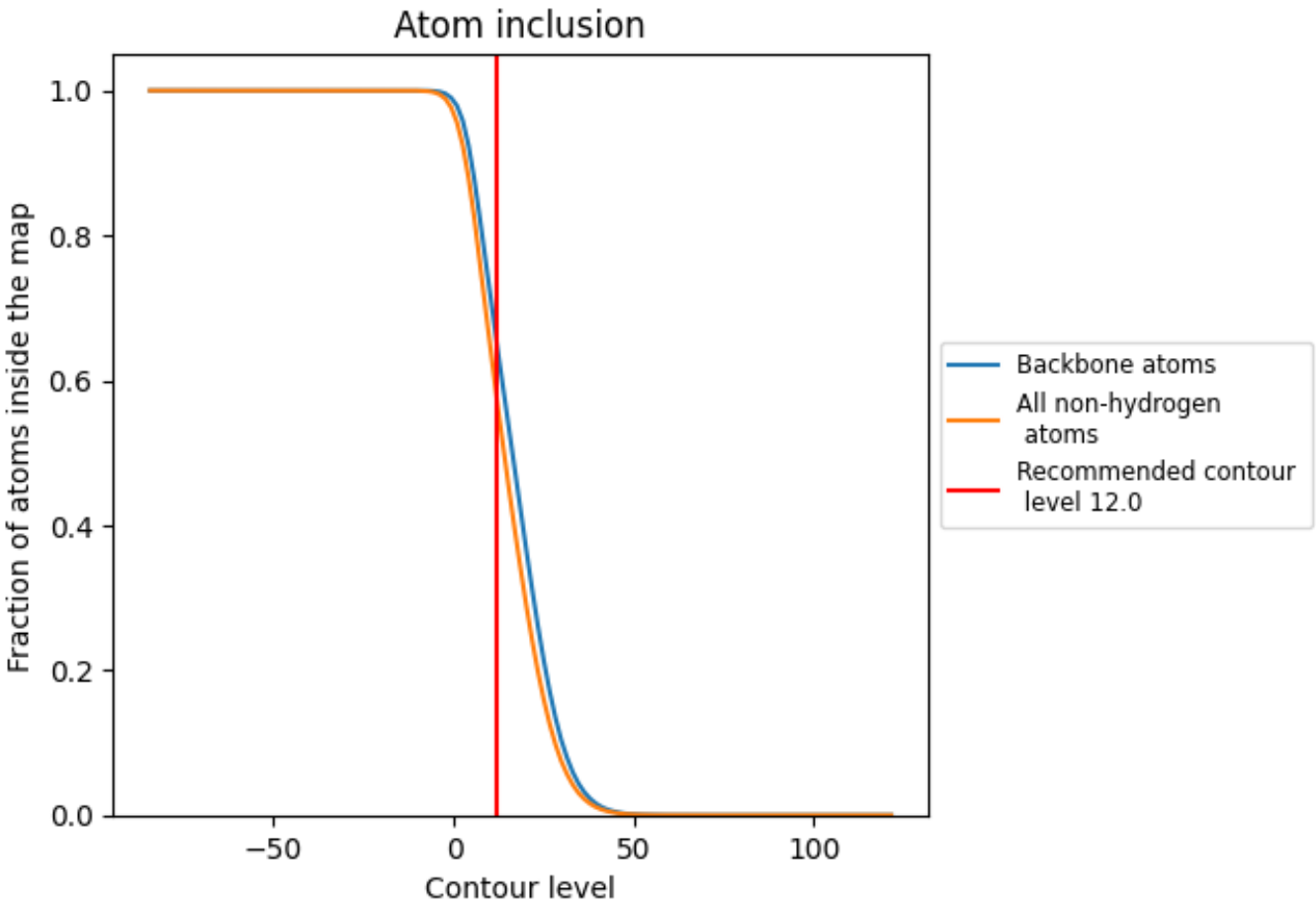
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (12.0).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 57% 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 (12.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5746	0.4880
A	0.6243	0.5110
B	0.6572	0.5130
C	0.6757	0.5170
D	0.6197	0.5140
E	0.6266	0.5230
F	0.6707	0.5210
G	0.4047	0.4200
H	0.5923	0.5030
I	0.6712	0.5120
J	0.6034	0.4880
K	0.7225	0.5420
L	0.7220	0.5370
M	0.6796	0.5410
N	0.6618	0.5310
O	0.6861	0.5300
P	0.6922	0.5270
Q	0.2855	0.3950
R	0.2602	0.3700
S	0.1765	0.3810
T	0.4531	0.4700
U	0.4800	0.4750
V	0.2670	0.3970
W	0.4526	0.4400
X	0.4637	0.4480
Y	0.2967	0.3920
Z	0.4644	0.4230
a	0.4173	0.3570
b	0.2871	0.3550
c	0.4747	0.4860
d	0.5110	0.4820
e	0.2818	0.4150
f	0.1534	0.3980
g	0.0751	0.2750
h	0.0687	0.2780

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Chain	Atom inclusion	Q-score
i	0.1054	0.2800
j	0.0635	0.3190
k	0.1038	0.2930
l	0.1214	0.2810
m	0.0463	0.2520
n	0.1043	0.2720
o	0.0575	0.1720
p	0.1278	0.2930
q	0.1182	0.3040
r	0.0984	0.2730
s	0.0889	0.2860
t	0.0863	0.2950