Full wwPDB EM Validation Report (i)

Feb 12, 2024 – 05:44 PM EST

PDB ID	:	3IZN
EMDB ID	:	EMD-5250
Title	:	Mm-cpn deltalid with ATP
Authors	:	Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.; Chiu, W.; Frydman, J.
Deposited on	:	2010-10-30
Resolution	:	6.40 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

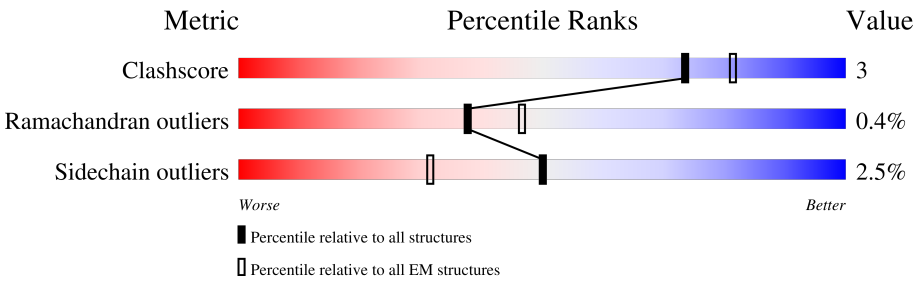
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.40 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)
Clashscore	158937	4297
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	491	40% 90% 9% •
1	B	491	40% 90% 9% •
1	C	491	40% 89% 10% •
1	D	491	40% 90% 9% •
1	E	491	40% 90% 9% •
1	F	491	40% 90% 9% •
1	G	491	40% 90% 9% •
1	H	491	40% 90% 9% •

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Mol	Chain	Length	Quality of chain
1	I	491	41% 90% 9%
1	J	491	40% 90% 9%
1	K	491	41% 90% 10%
1	L	491	40% 90% 10%
1	M	491	41% 90% 9%
1	N	491	40% 90% 9%
1	O	491	41% 90% 9%
1	P	491	40% 90% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 58640 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 Chaperonin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	491	3665	2272	635	734	24	0	0
1	B	491	3665	2272	635	734	24	0	0
1	C	491	3665	2272	635	734	24	0	0
1	D	491	3665	2272	635	734	24	0	0
1	E	491	3665	2272	635	734	24	0	0
1	F	491	3665	2272	635	734	24	0	0
1	G	491	3665	2272	635	734	24	0	0
1	H	491	3665	2272	635	734	24	0	0
1	I	491	3665	2272	635	734	24	0	0
1	J	491	3665	2272	635	734	24	0	0
1	K	491	3665	2272	635	734	24	0	0
1	L	491	3665	2272	635	734	24	0	0
1	M	491	3665	2272	635	734	24	0	0
1	N	491	3665	2272	635	734	24	0	0
1	O	491	3665	2272	635	734	24	0	0
1	P	491	3665	2272	635	734	24	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP Q877G8
A	236	THR	-	expression tag	UNP Q877G8
A	237	ALA	-	expression tag	UNP Q877G8
A	238	SER	-	expression tag	UNP Q877G8
A	239	GLU	-	expression tag	UNP Q877G8
B	726	GLU	-	expression tag	UNP Q877G8
B	727	THR	-	expression tag	UNP Q877G8
B	728	ALA	-	expression tag	UNP Q877G8
B	729	SER	-	expression tag	UNP Q877G8
B	730	GLU	-	expression tag	UNP Q877G8
C	1217	GLU	-	expression tag	UNP Q877G8
C	1218	THR	-	expression tag	UNP Q877G8
C	1219	ALA	-	expression tag	UNP Q877G8
C	1220	SER	-	expression tag	UNP Q877G8
C	1221	GLU	-	expression tag	UNP Q877G8
D	1708	GLU	-	expression tag	UNP Q877G8
D	1709	THR	-	expression tag	UNP Q877G8
D	1710	ALA	-	expression tag	UNP Q877G8
D	1711	SER	-	expression tag	UNP Q877G8
D	1712	GLU	-	expression tag	UNP Q877G8
E	2199	GLU	-	expression tag	UNP Q877G8
E	2200	THR	-	expression tag	UNP Q877G8
E	2201	ALA	-	expression tag	UNP Q877G8
E	2202	SER	-	expression tag	UNP Q877G8
E	2203	GLU	-	expression tag	UNP Q877G8
F	2690	GLU	-	expression tag	UNP Q877G8
F	2691	THR	-	expression tag	UNP Q877G8
F	2692	ALA	-	expression tag	UNP Q877G8
F	2693	SER	-	expression tag	UNP Q877G8
F	2694	GLU	-	expression tag	UNP Q877G8
G	3181	GLU	-	expression tag	UNP Q877G8
G	3182	THR	-	expression tag	UNP Q877G8
G	3183	ALA	-	expression tag	UNP Q877G8
G	3184	SER	-	expression tag	UNP Q877G8
G	3185	GLU	-	expression tag	UNP Q877G8
H	3672	GLU	-	expression tag	UNP Q877G8
H	3673	THR	-	expression tag	UNP Q877G8
H	3674	ALA	-	expression tag	UNP Q877G8
H	3675	SER	-	expression tag	UNP Q877G8
H	3676	GLU	-	expression tag	UNP Q877G8
I	4163	GLU	-	expression tag	UNP Q877G8
I	4164	THR	-	expression tag	UNP Q877G8
I	4165	ALA	-	expression tag	UNP Q877G8

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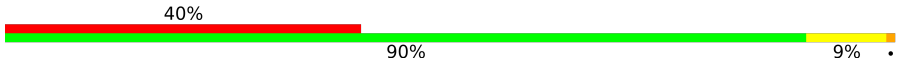
Chain	Residue	Modelled	Actual	Comment	Reference
I	4166	SER	-	expression tag	UNP Q877G8
I	4167	GLU	-	expression tag	UNP Q877G8
J	4654	GLU	-	expression tag	UNP Q877G8
J	4655	THR	-	expression tag	UNP Q877G8
J	4656	ALA	-	expression tag	UNP Q877G8
J	4657	SER	-	expression tag	UNP Q877G8
J	4658	GLU	-	expression tag	UNP Q877G8
K	5145	GLU	-	expression tag	UNP Q877G8
K	5146	THR	-	expression tag	UNP Q877G8
K	5147	ALA	-	expression tag	UNP Q877G8
K	5148	SER	-	expression tag	UNP Q877G8
K	5149	GLU	-	expression tag	UNP Q877G8
L	5636	GLU	-	expression tag	UNP Q877G8
L	5637	THR	-	expression tag	UNP Q877G8
L	5638	ALA	-	expression tag	UNP Q877G8
L	5639	SER	-	expression tag	UNP Q877G8
L	5640	GLU	-	expression tag	UNP Q877G8
M	6127	GLU	-	expression tag	UNP Q877G8
M	6128	THR	-	expression tag	UNP Q877G8
M	6129	ALA	-	expression tag	UNP Q877G8
M	6130	SER	-	expression tag	UNP Q877G8
M	6131	GLU	-	expression tag	UNP Q877G8
N	6618	GLU	-	expression tag	UNP Q877G8
N	6619	THR	-	expression tag	UNP Q877G8
N	6620	ALA	-	expression tag	UNP Q877G8
N	6621	SER	-	expression tag	UNP Q877G8
N	6622	GLU	-	expression tag	UNP Q877G8
O	7109	GLU	-	expression tag	UNP Q877G8
O	7110	THR	-	expression tag	UNP Q877G8
O	7111	ALA	-	expression tag	UNP Q877G8
O	7112	SER	-	expression tag	UNP Q877G8
O	7113	GLU	-	expression tag	UNP Q877G8
P	7600	GLU	-	expression tag	UNP Q877G8
P	7601	THR	-	expression tag	UNP Q877G8
P	7602	ALA	-	expression tag	UNP Q877G8
P	7603	SER	-	expression tag	UNP Q877G8
P	7604	GLU	-	expression tag	UNP Q877G8

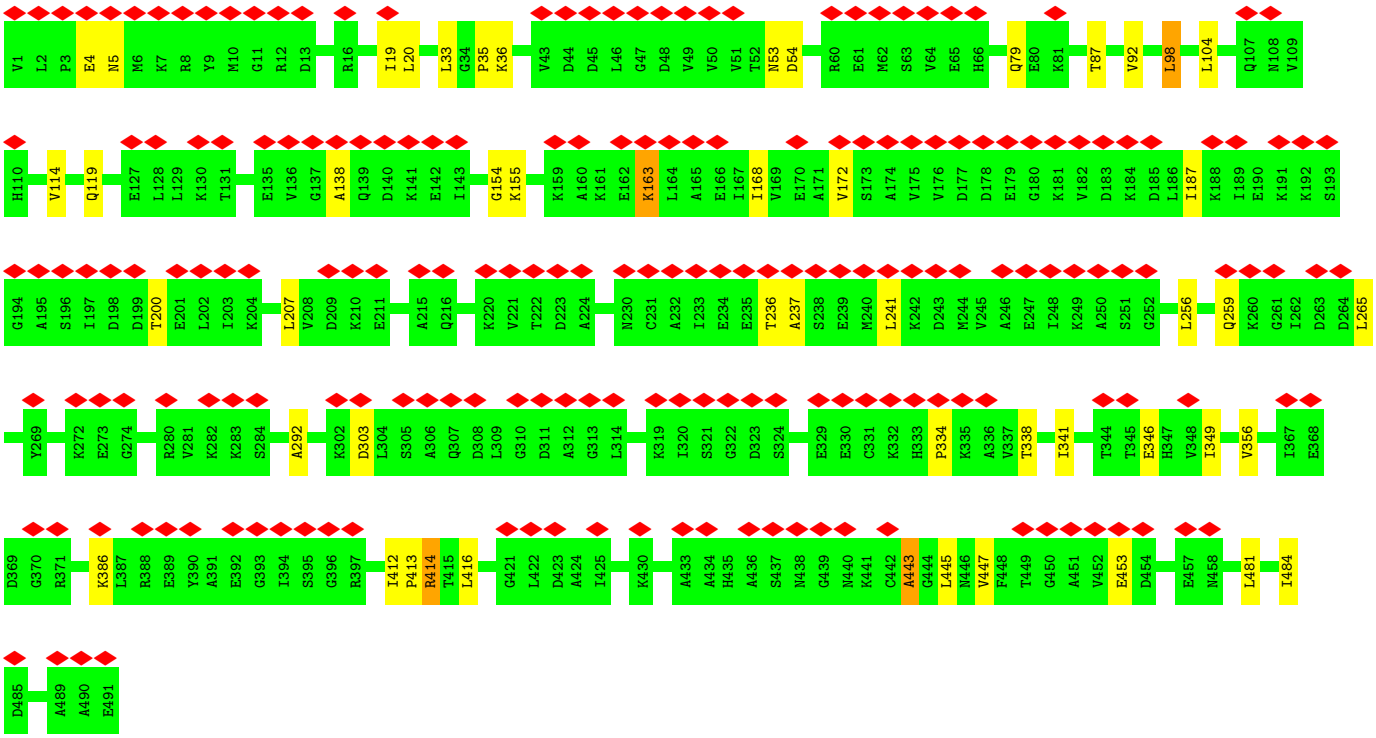
3 Residue-property plots (i)

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: Chaperonin

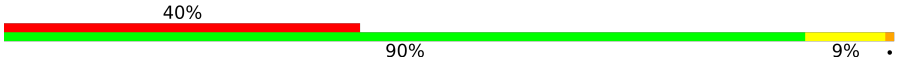
Chain A:

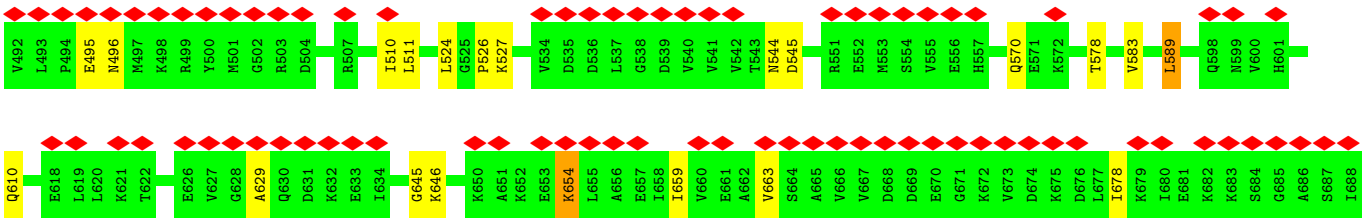


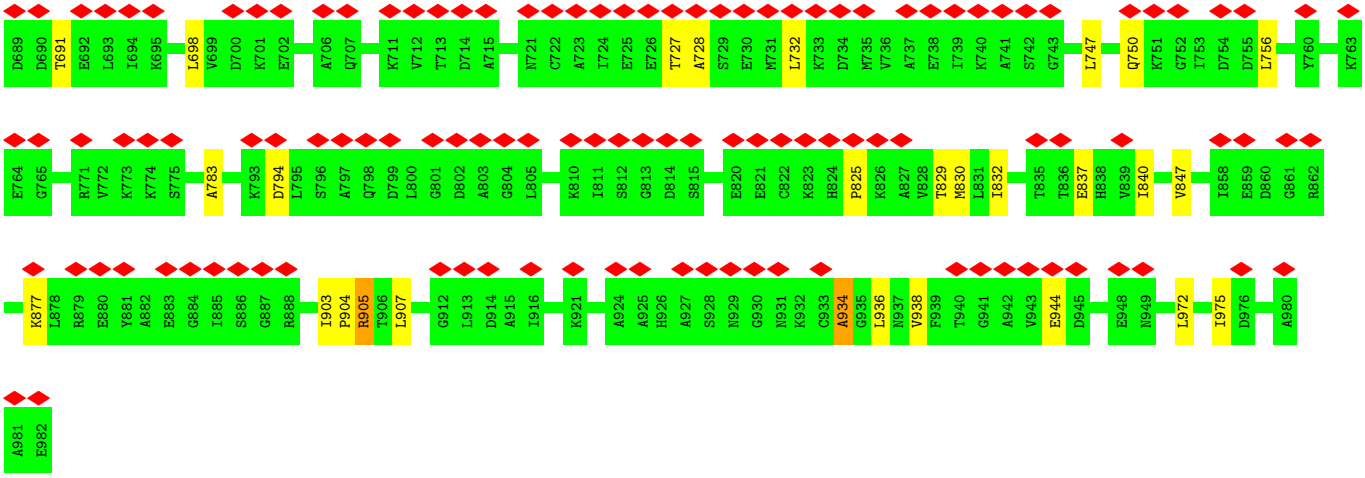


- Molecule 1: Chaperonin

Chain B:

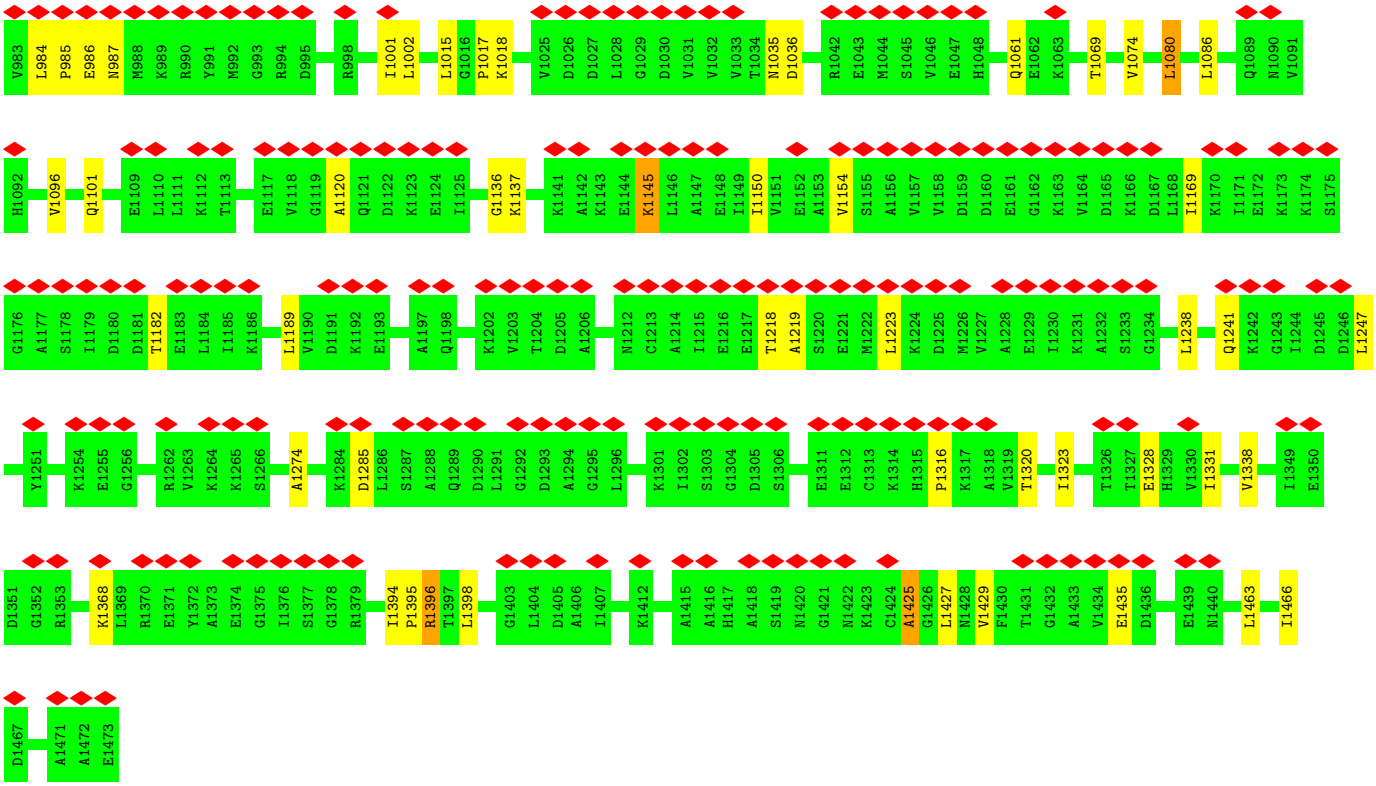






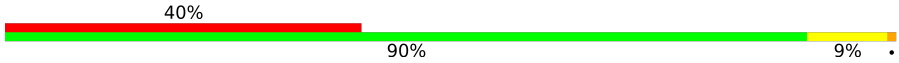
- Molecule 1: Chaperonin

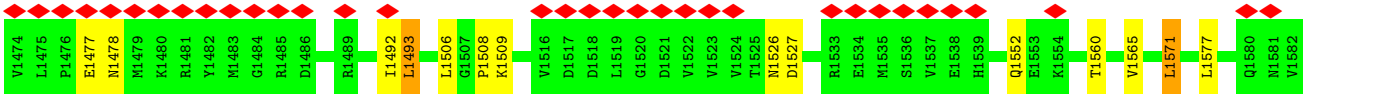
Chain C:

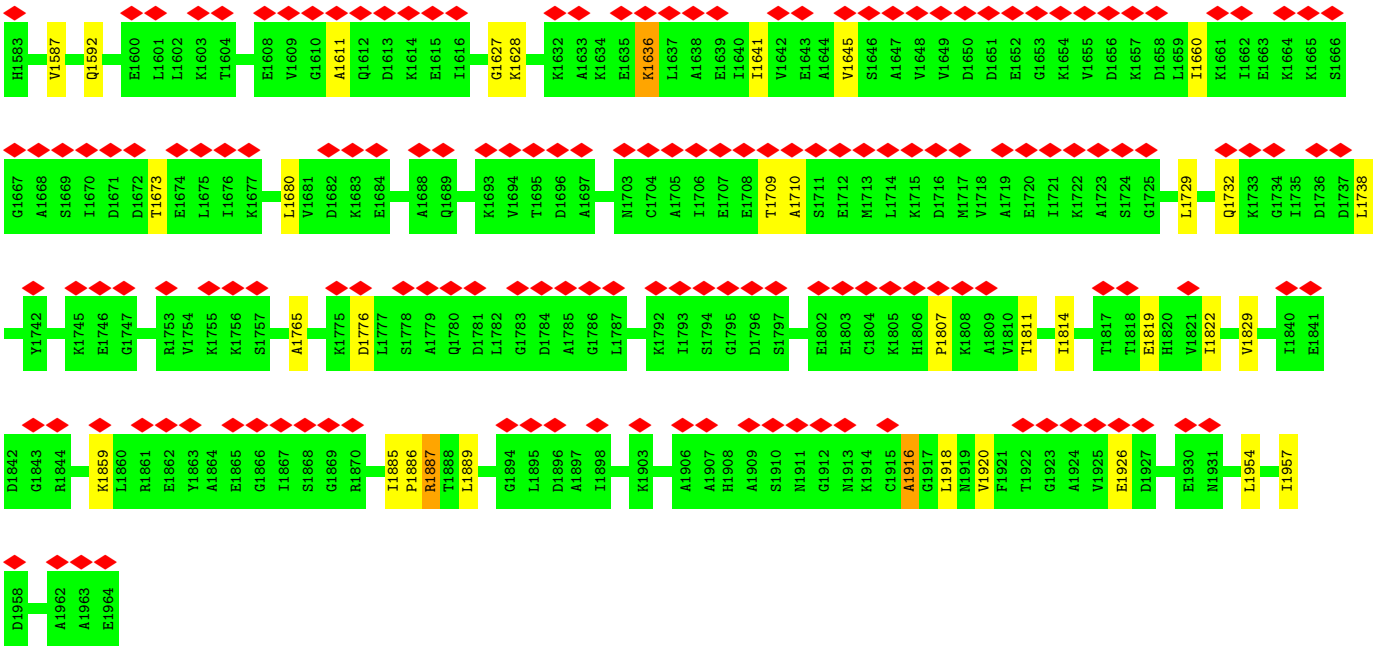


- Molecule 1: Chaperonin

Chain D:

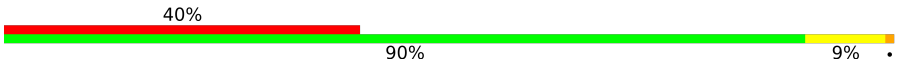


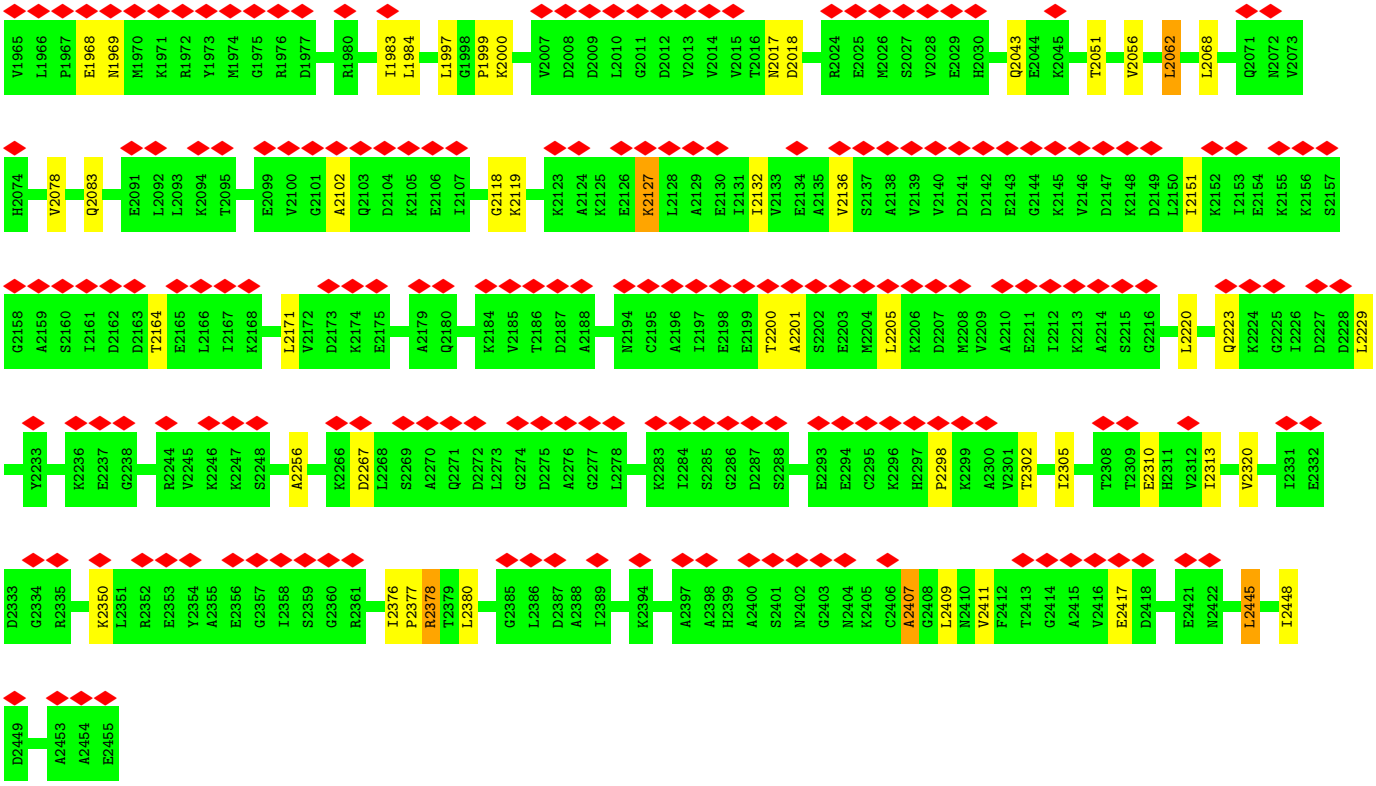




- Molecule 1: Chaperonin

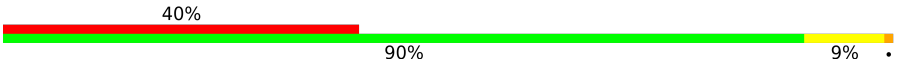
Chain E:

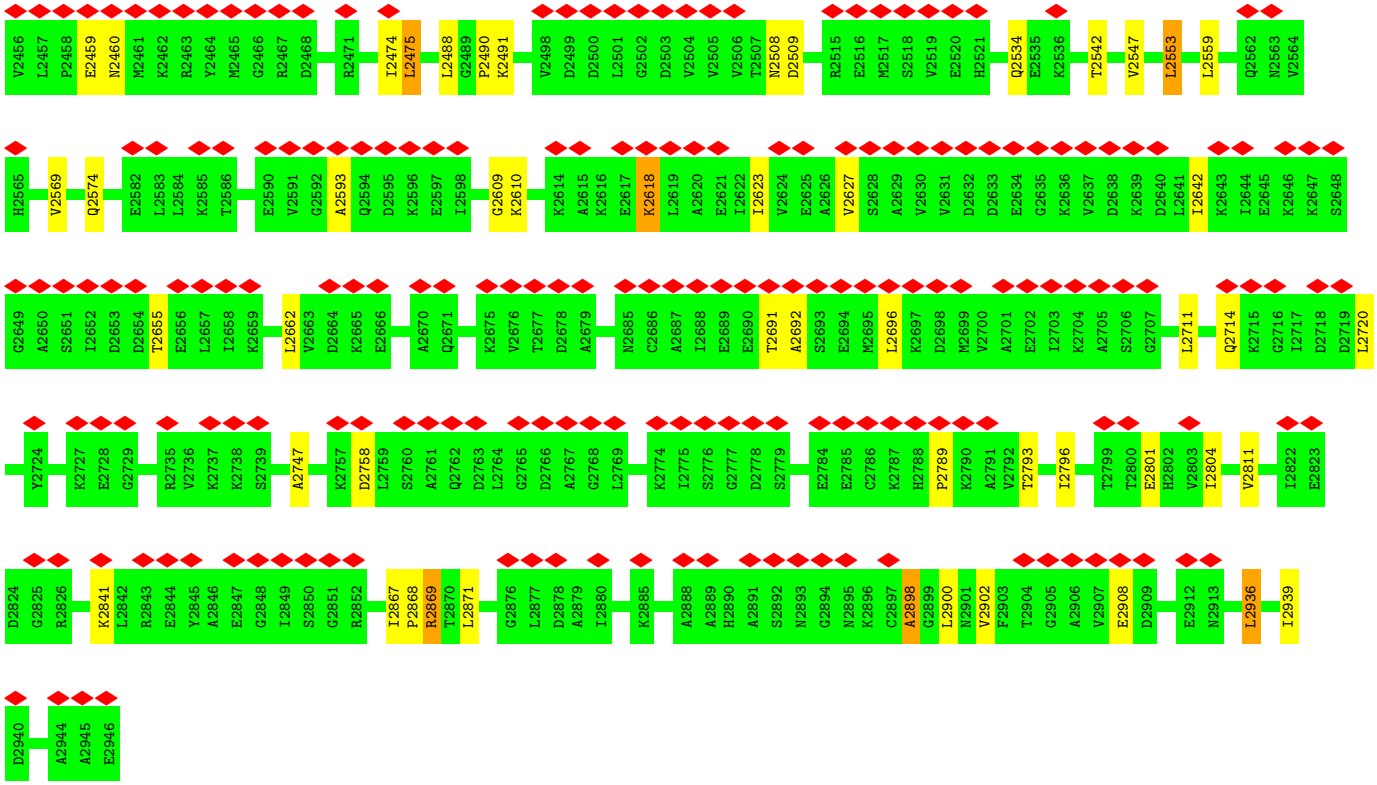




- Molecule 1: Chaperonin

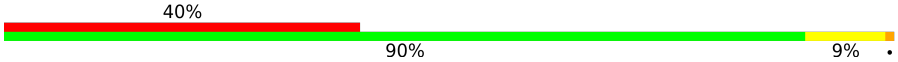
Chain F:

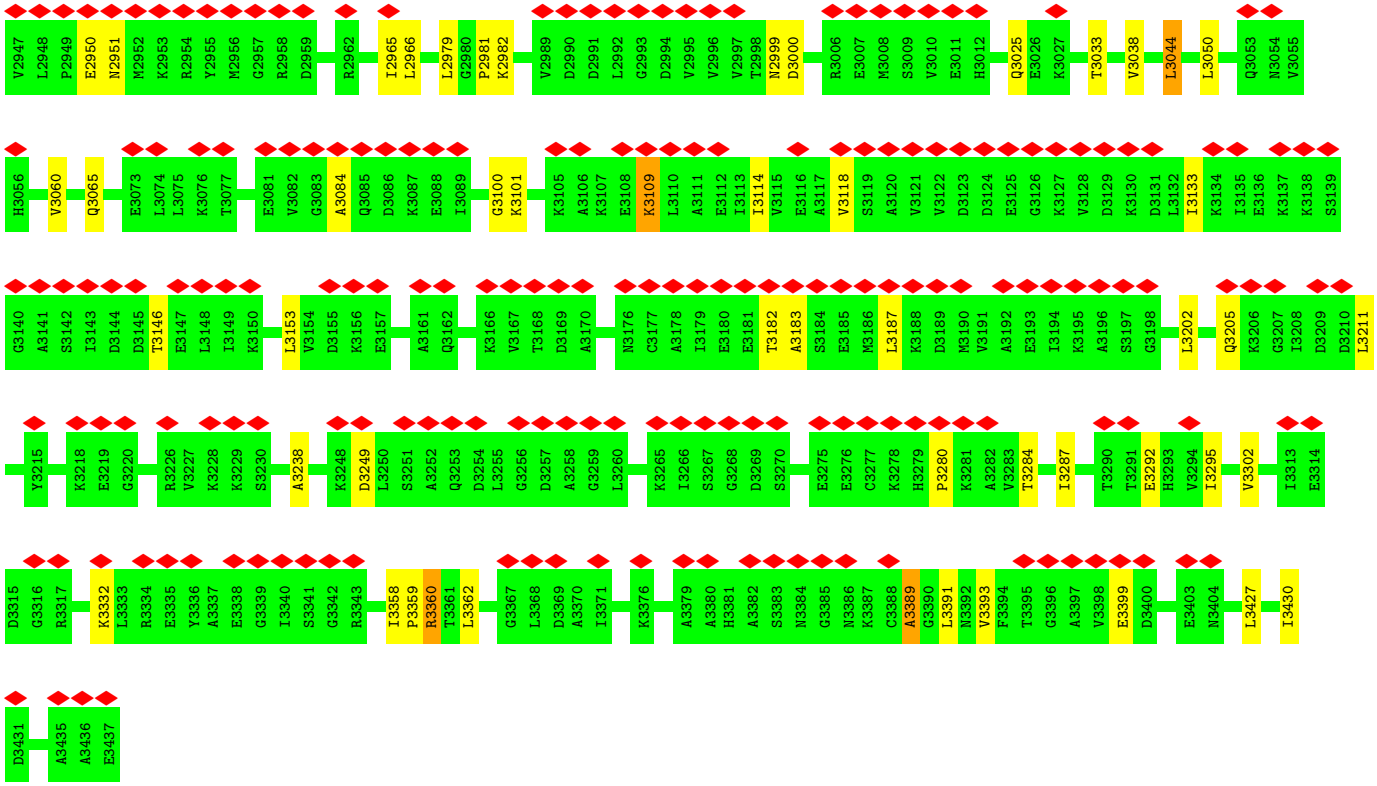




- Molecule 1: Chaperonin

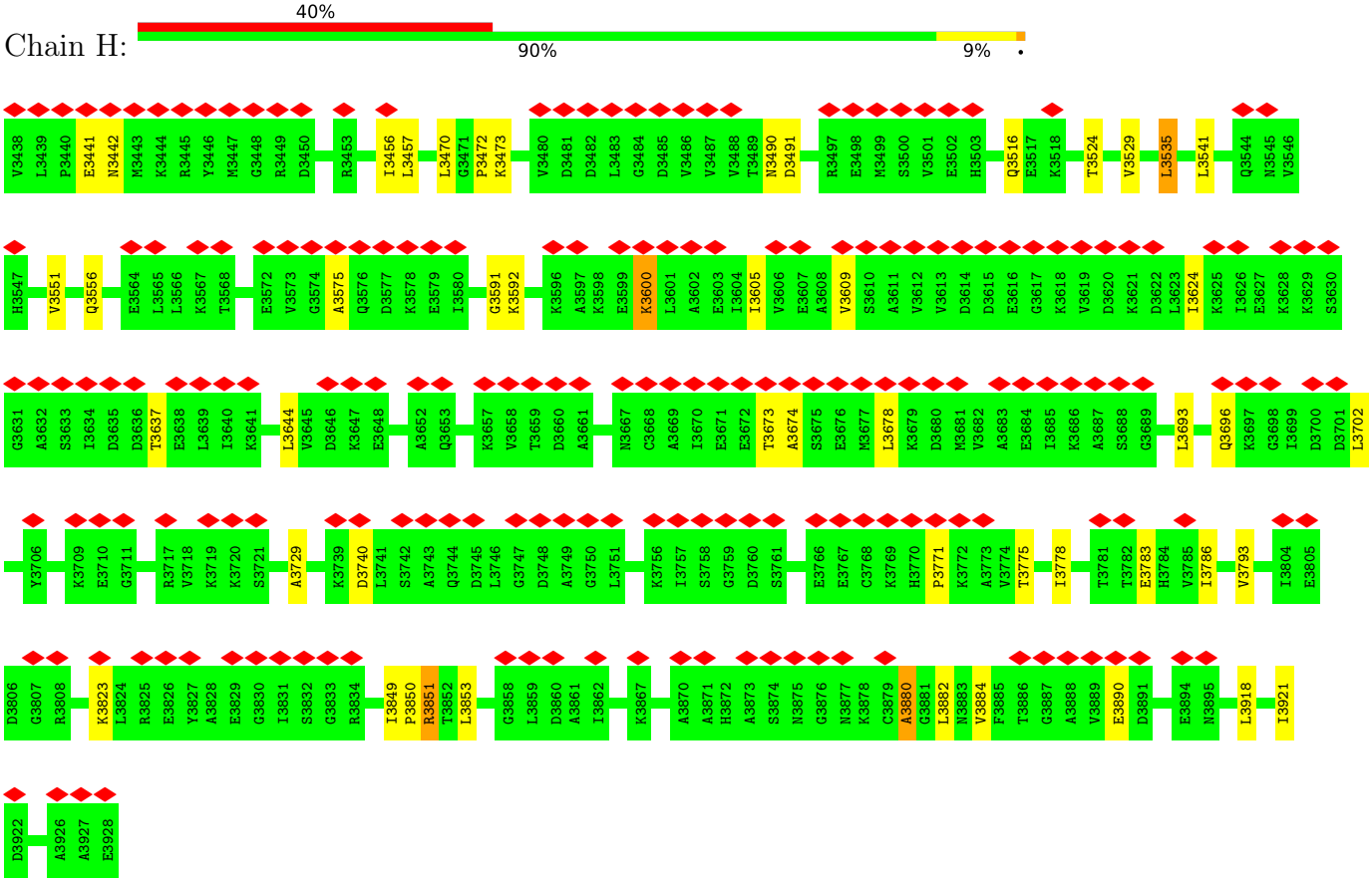
Chain G:





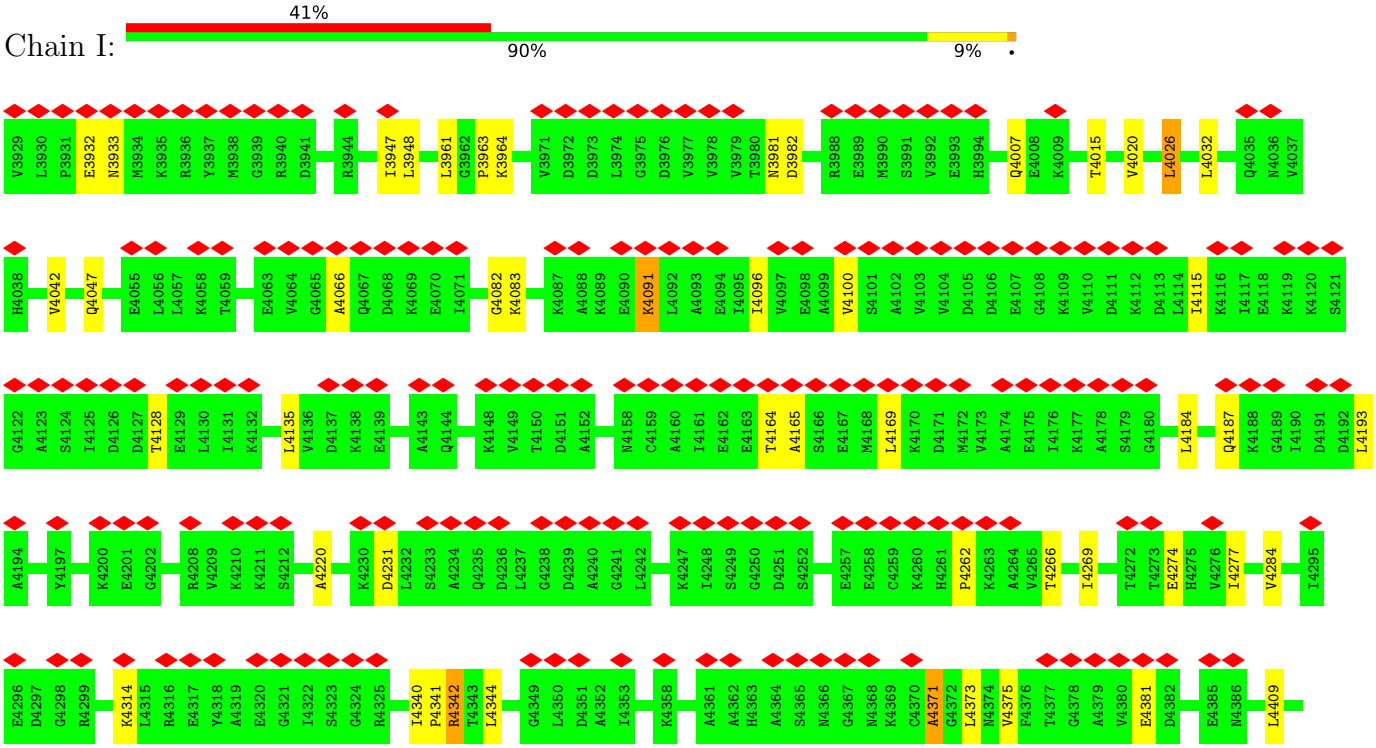
- Molecule 1: Chaperonin

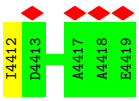
Chain H:



- Molecule 1: Chaperonin

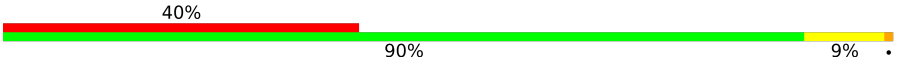
Chain I:

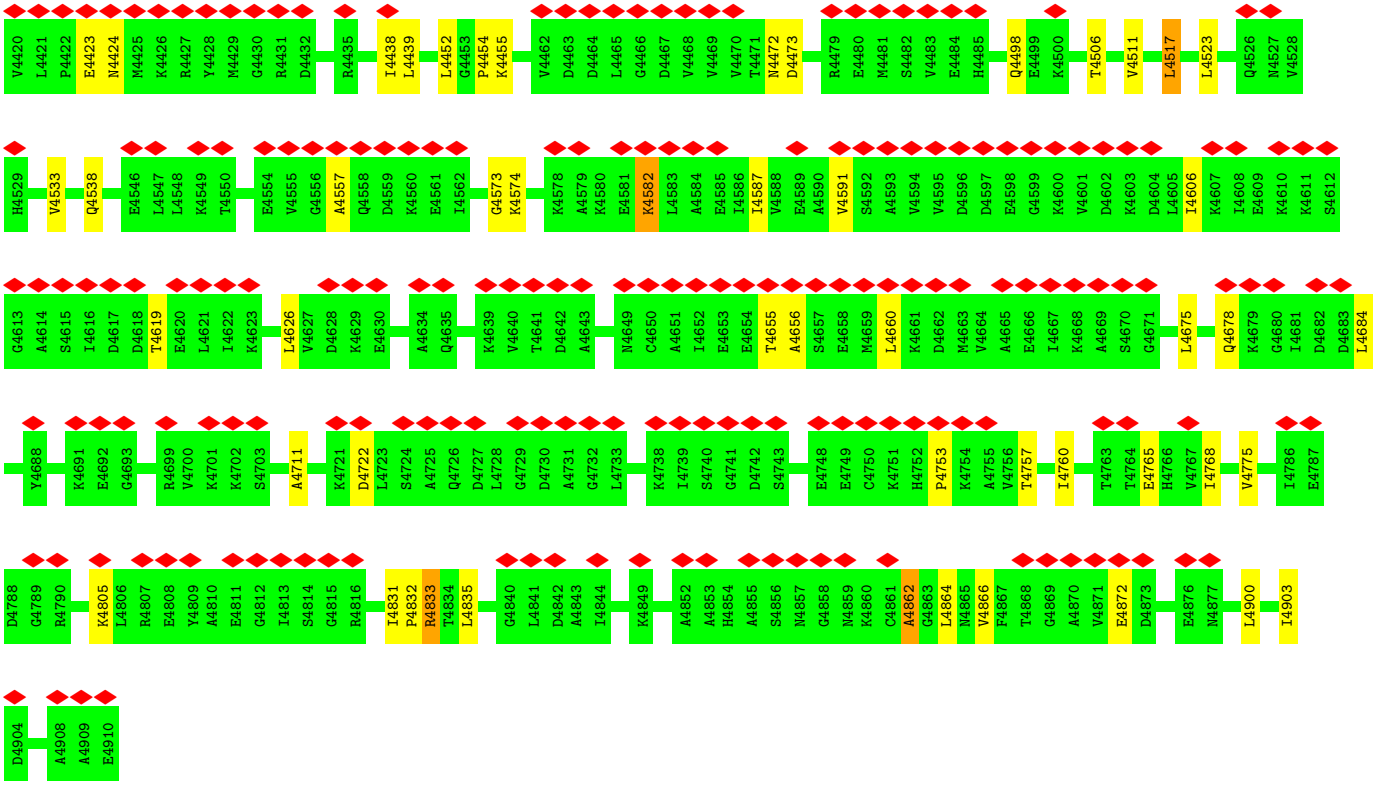




• Molecule 1: Chaperonin

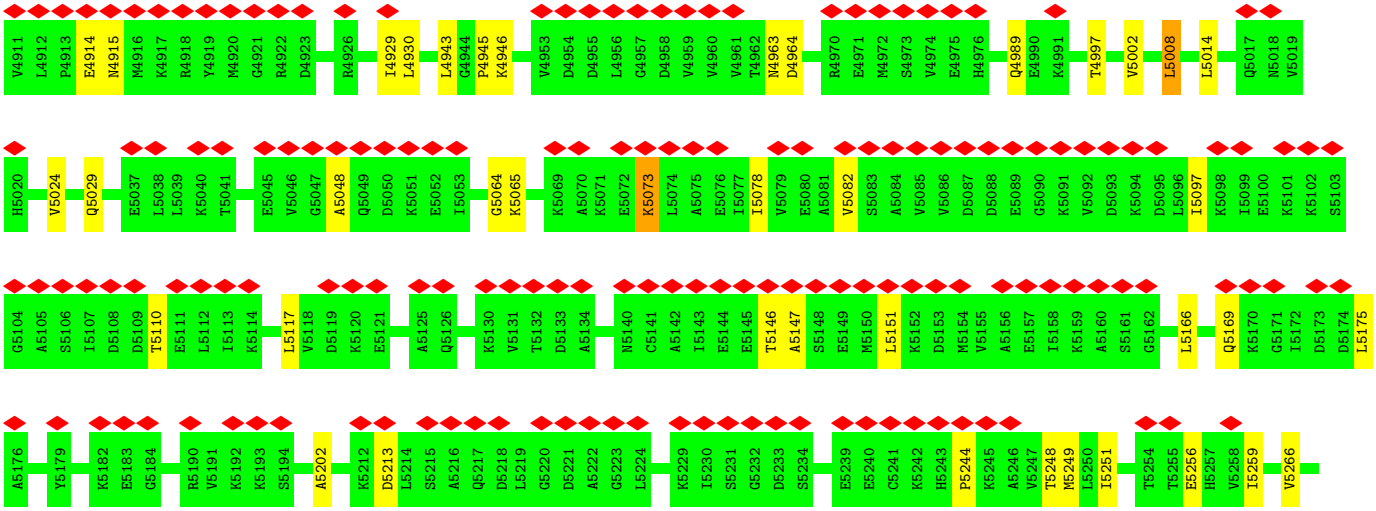
Chain J:

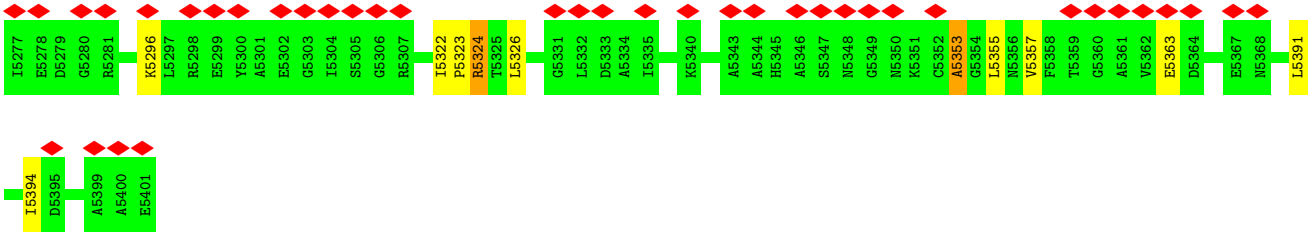




• Molecule 1: Chaperonin

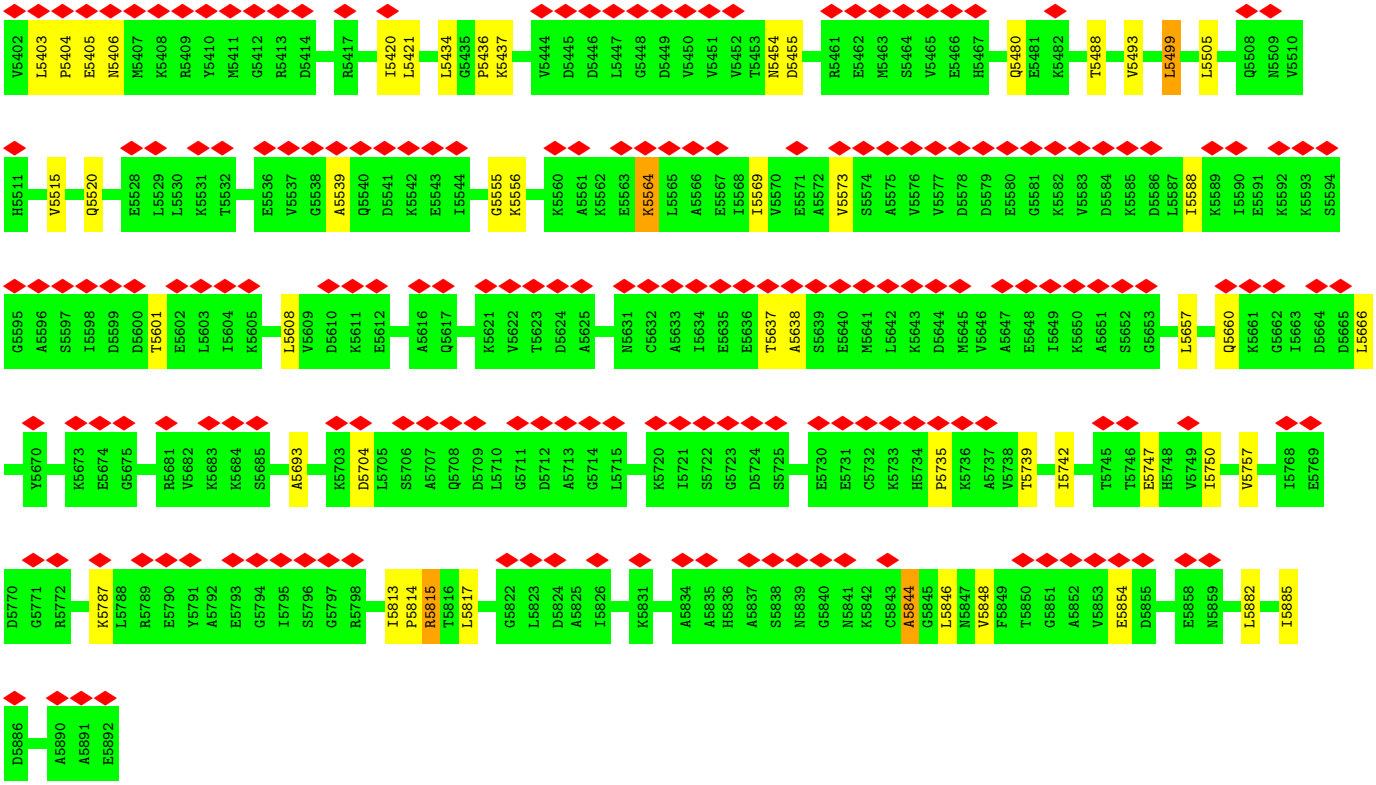
Chain K:





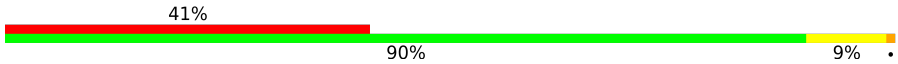
• Molecule 1: Chaperonin

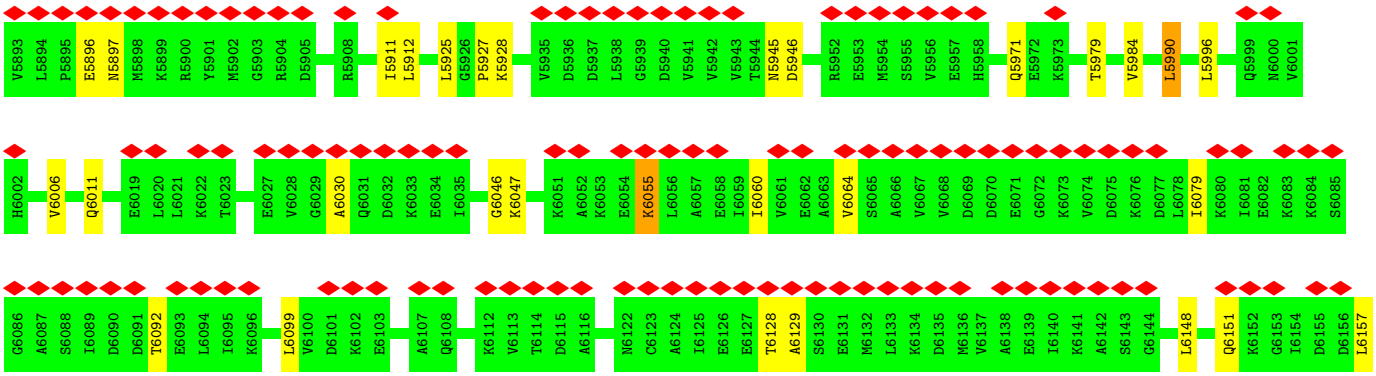
Chain L:

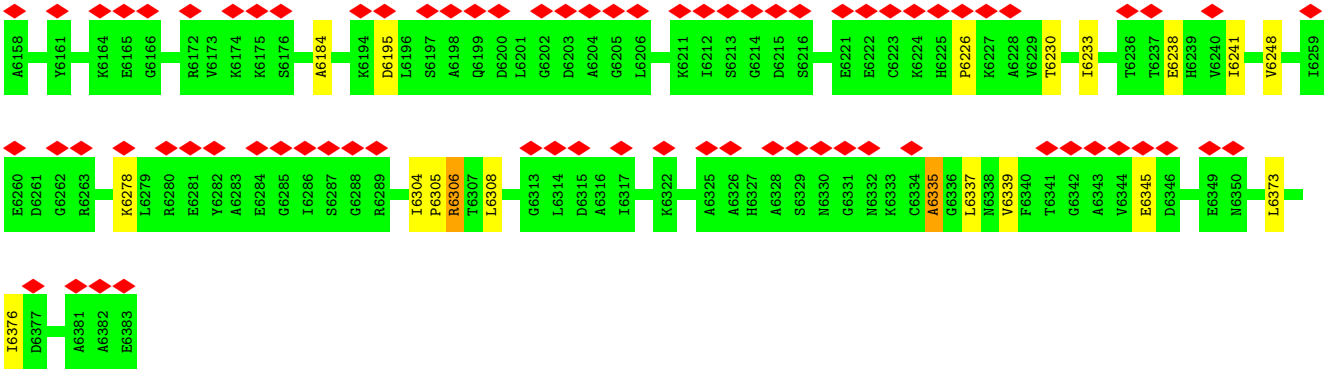


• Molecule 1: Chaperonin

Chain M:

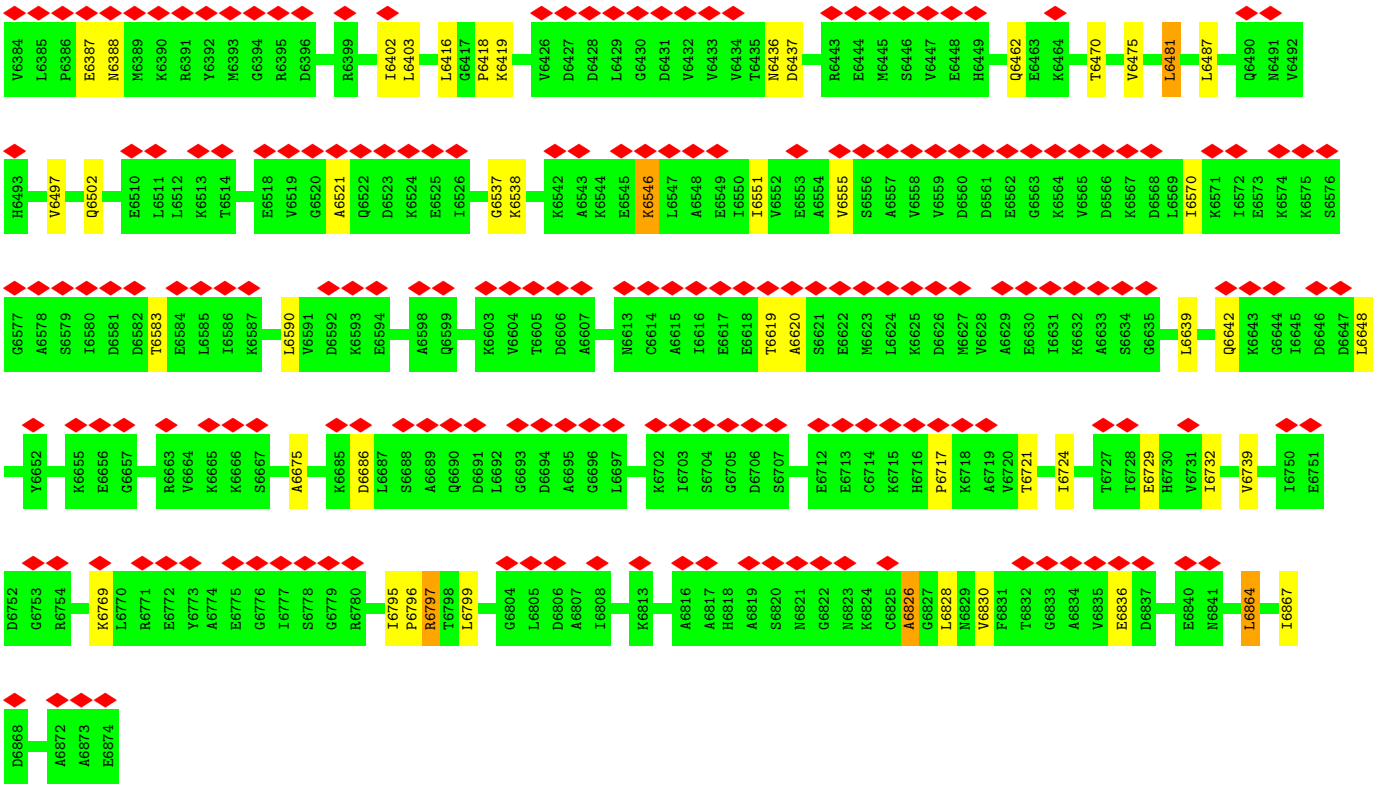






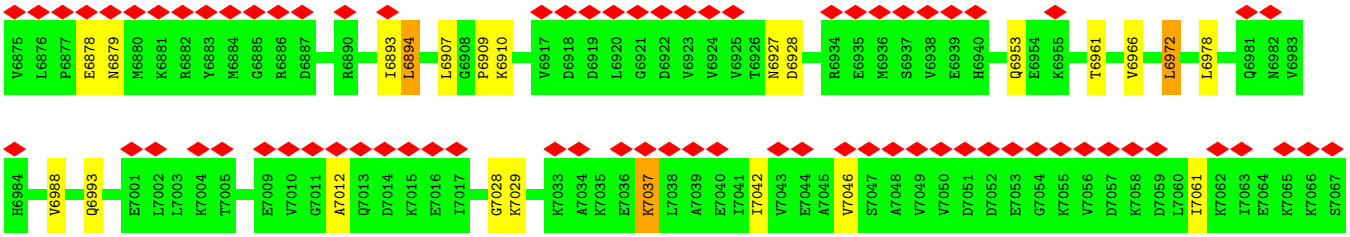
• Molecule 1: Chaperonin

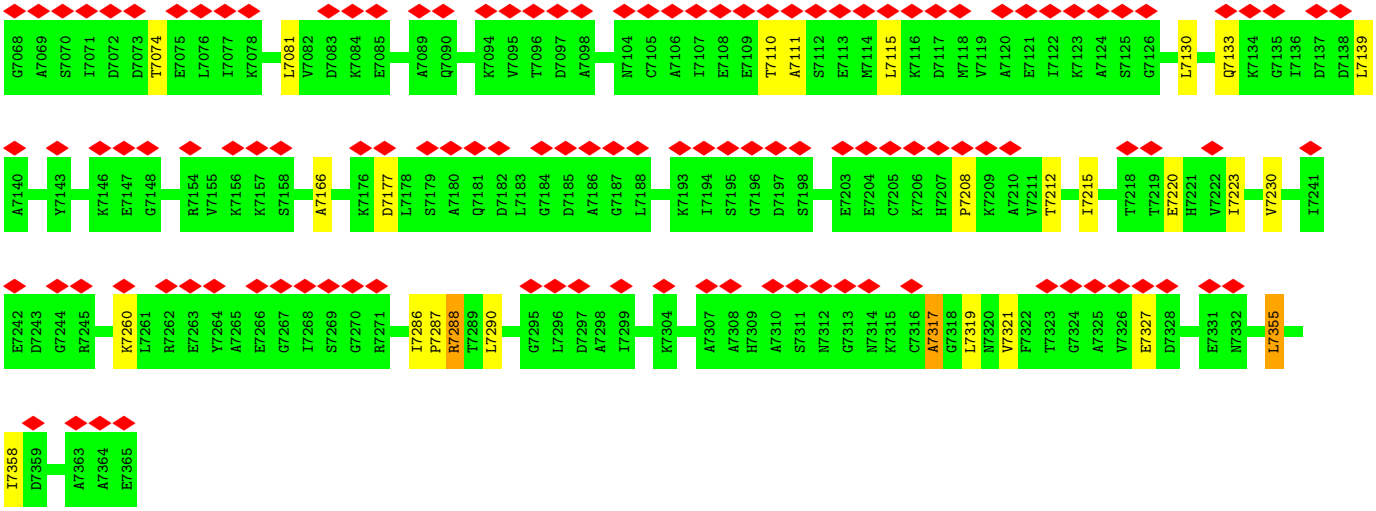
Chain N: 40% 90% 9%



• Molecule 1: Chaperonin

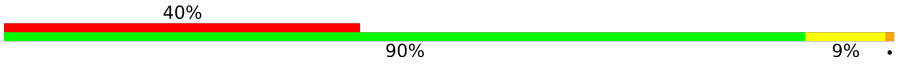
Chain O: 41% 90% 9%

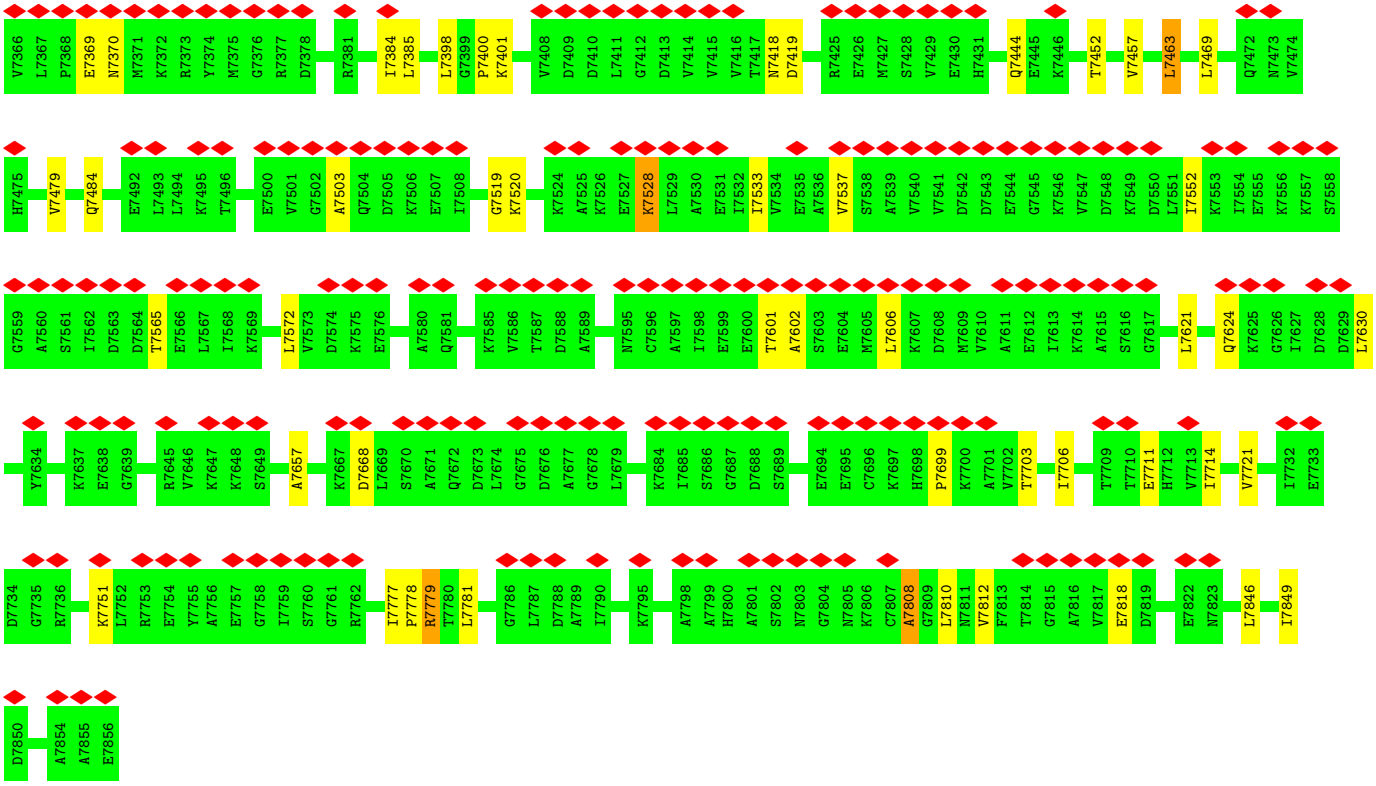




- Molecule 1: Chaperonin

Chain P:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D8	Depositor
Number of particles used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 10000 (10k x 10k)	Depositor
Maximum map value	2.733	Depositor
Minimum map value	-0.479	Depositor
Average map value	0.087	Depositor
Map value standard deviation	0.353	Depositor
Recommended contour level	1.58	Depositor
Map size (Å)	289.44, 289.44, 289.44	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.01, 2.01, 2.01	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	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	B	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	C	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	D	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	E	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	F	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	G	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	H	0.88	1/3686 (0.0%)	0.75	1/4961 (0.0%)
1	I	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	J	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	K	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	L	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	M	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	N	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	O	0.88	1/3686 (0.0%)	0.76	1/4961 (0.0%)
1	P	0.88	1/3686 (0.0%)	0.75	1/4961 (0.0%)
All	All	0.88	16/58976 (0.0%)	0.76	16/79376 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	3
1	K	0	3
1	L	0	3
1	M	0	3
1	N	0	3
1	O	0	3
1	P	0	3
All	All	0	48

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1916	ALA	C-O	5.10	1.33	1.23
1	F	2898	ALA	C-O	5.07	1.32	1.23
1	H	3880	ALA	C-O	5.07	1.32	1.23
1	K	5353	ALA	C-O	5.07	1.32	1.23
1	N	6826	ALA	C-O	5.07	1.32	1.23
1	P	7808	ALA	C-O	5.07	1.32	1.23
1	I	4371	ALA	C-O	5.06	1.32	1.23
1	A	443	ALA	C-O	5.05	1.32	1.23
1	C	1425	ALA	C-O	5.05	1.32	1.23
1	E	2407	ALA	C-O	5.05	1.32	1.23
1	G	3389	ALA	C-O	5.05	1.32	1.23
1	J	4862	ALA	C-O	5.05	1.32	1.23
1	L	5844	ALA	C-O	5.05	1.32	1.23
1	B	934	ALA	C-O	5.03	1.32	1.23
1	M	6335	ALA	C-O	5.03	1.32	1.23
1	O	7317	ALA	C-O	5.02	1.32	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1477	GLU	CA-C-O	-6.63	106.17	120.10
1	O	6878	GLU	CA-C-O	-6.63	106.17	120.10
1	A	4	GLU	CA-C-O	-6.62	106.20	120.10
1	B	495	GLU	CA-C-O	-6.62	106.20	120.10
1	I	3932	GLU	CA-C-O	-6.62	106.20	120.10
1	C	986	GLU	CA-C-O	-6.61	106.22	120.10
1	E	1968	GLU	CA-C-O	-6.61	106.22	120.10
1	F	2459	GLU	CA-C-O	-6.61	106.22	120.10
1	G	2950	GLU	CA-C-O	-6.61	106.22	120.10
1	J	4423	GLU	CA-C-O	-6.61	106.23	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	5405	GLU	CA-C-O	-6.61	106.23	120.10
1	N	6387	GLU	CA-C-O	-6.61	106.23	120.10
1	P	7369	GLU	CA-C-O	-6.61	106.23	120.10
1	K	4914	GLU	CA-C-O	-6.60	106.24	120.10
1	M	5896	GLU	CA-C-O	-6.60	106.24	120.10
1	H	3441	GLU	CA-C-O	-6.59	106.27	120.10

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLN	Mainchain
1	A	138	ALA	Mainchain
1	A	453	GLU	Mainchain
1	B	610	GLN	Mainchain
1	B	629	ALA	Mainchain
1	B	944	GLU	Mainchain
1	C	1101	GLN	Mainchain
1	C	1120	ALA	Mainchain
1	C	1435	GLU	Mainchain
1	D	1592	GLN	Mainchain
1	D	1611	ALA	Mainchain
1	D	1926	GLU	Mainchain
1	E	2083	GLN	Mainchain
1	E	2102	ALA	Mainchain
1	E	2417	GLU	Mainchain
1	F	2574	GLN	Mainchain
1	F	2593	ALA	Mainchain
1	F	2908	GLU	Mainchain
1	G	3065	GLN	Mainchain
1	G	3084	ALA	Mainchain
1	G	3399	GLU	Mainchain
1	H	3556	GLN	Mainchain
1	H	3575	ALA	Mainchain
1	H	3890	GLU	Mainchain
1	I	4047	GLN	Mainchain
1	I	4066	ALA	Mainchain
1	I	4381	GLU	Mainchain
1	J	4538	GLN	Mainchain
1	J	4557	ALA	Mainchain
1	J	4872	GLU	Mainchain
1	K	5029	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	K	5048	ALA	Mainchain
1	K	5363	GLU	Mainchain
1	L	5520	GLN	Mainchain
1	L	5539	ALA	Mainchain
1	L	5854	GLU	Mainchain
1	M	6011	GLN	Mainchain
1	M	6030	ALA	Mainchain
1	M	6345	GLU	Mainchain
1	N	6502	GLN	Mainchain
1	N	6521	ALA	Mainchain
1	N	6836	GLU	Mainchain
1	O	6993	GLN	Mainchain
1	O	7012	ALA	Mainchain
1	O	7327	GLU	Mainchain
1	P	7484	GLN	Mainchain
1	P	7503	ALA	Mainchain
1	P	7818	GLU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3665	0	3804	24	0
1	B	3665	0	3801	24	0
1	C	3665	0	3801	25	0
1	D	3665	0	3801	24	0
1	E	3665	0	3801	25	0
1	F	3665	0	3801	26	0
1	G	3665	0	3801	24	0
1	H	3665	0	3801	24	0
1	I	3665	0	3801	24	0
1	J	3665	0	3801	24	0
1	K	3665	0	3801	25	0
1	L	3665	0	3801	24	0
1	M	3665	0	3801	23	0
1	N	3665	0	3801	24	0
1	O	3665	0	3801	26	0
1	P	3665	0	3801	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	58640	0	60819	390	0

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

All (390) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1247:LEU:HD23	1:C:1247:LEU:C	2.17	0.65
1:J:4684:LEU:C	1:J:4684:LEU:HD23	2.17	0.65
1:P:7630:LEU:C	1:P:7630:LEU:HD23	2.17	0.65
1:A:265:LEU:C	1:A:265:LEU:HD23	2.17	0.65
1:G:3211:LEU:C	1:G:3211:LEU:HD23	2.17	0.65
1:M:6157:LEU:HD23	1:M:6157:LEU:C	2.17	0.65
1:D:1738:LEU:C	1:D:1738:LEU:HD23	2.17	0.65
1:F:2720:LEU:C	1:F:2720:LEU:HD23	2.17	0.65
1:O:7139:LEU:C	1:O:7139:LEU:HD23	2.17	0.65
1:H:3702:LEU:C	1:H:3702:LEU:HD23	2.17	0.65
1:L:5666:LEU:HD23	1:L:5666:LEU:C	2.17	0.65
1:I:4193:LEU:C	1:I:4193:LEU:HD23	2.17	0.64
1:E:2229:LEU:C	1:E:2229:LEU:HD23	2.17	0.64
1:N:6648:LEU:HD23	1:N:6648:LEU:C	2.17	0.64
1:B:756:LEU:C	1:B:756:LEU:HD23	2.17	0.64
1:K:5175:LEU:C	1:K:5175:LEU:HD23	2.17	0.63
1:K:5322:ILE:HB	1:K:5323:PRO:HD3	1.84	0.59
1:B:903:ILE:HB	1:B:904:PRO:HD3	1.84	0.59
1:C:1394:ILE:HB	1:C:1395:PRO:HD3	1.84	0.59
1:L:5813:ILE:HB	1:L:5814:PRO:HD3	1.84	0.59
1:J:4831:ILE:HB	1:J:4832:PRO:HD3	1.84	0.59
1:E:2376:ILE:HB	1:E:2377:PRO:HD3	1.84	0.58
1:H:3849:ILE:HB	1:H:3850:PRO:HD3	1.84	0.58
1:A:412:ILE:HB	1:A:413:PRO:HD3	1.84	0.58
1:I:4340:ILE:HB	1:I:4341:PRO:HD3	1.84	0.58
1:D:1885:ILE:HB	1:D:1886:PRO:HD3	1.84	0.58
1:N:6795:ILE:HB	1:N:6796:PRO:HD3	1.84	0.58
1:P:7777:ILE:HB	1:P:7778:PRO:HD3	1.84	0.58
1:G:3358:ILE:HB	1:G:3359:PRO:HD3	1.84	0.58
1:M:6304:ILE:HB	1:M:6305:PRO:HD3	1.84	0.58
1:F:2867:ILE:HB	1:F:2868:PRO:HD3	1.84	0.58
1:J:4684:LEU:HD23	1:J:4684:LEU:O	2.04	0.58
1:M:6157:LEU:HD23	1:M:6157:LEU:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD23	1:A:265:LEU:O	2.04	0.58
1:B:756:LEU:HD23	1:B:756:LEU:O	2.04	0.58
1:D:1738:LEU:HD23	1:D:1738:LEU:O	2.04	0.58
1:E:2229:LEU:HD23	1:E:2229:LEU:O	2.04	0.58
1:O:7286:ILE:HB	1:O:7287:PRO:HD3	1.84	0.58
1:K:5175:LEU:HD23	1:K:5175:LEU:O	2.04	0.58
1:N:6648:LEU:HD23	1:N:6648:LEU:O	2.04	0.58
1:G:3211:LEU:HD23	1:G:3211:LEU:O	2.04	0.57
1:P:7630:LEU:HD23	1:P:7630:LEU:O	2.04	0.57
1:F:2720:LEU:HD23	1:F:2720:LEU:O	2.04	0.57
1:H:3702:LEU:HD23	1:H:3702:LEU:O	2.04	0.57
1:I:4193:LEU:HD23	1:I:4193:LEU:O	2.04	0.57
1:O:7139:LEU:HD23	1:O:7139:LEU:O	2.04	0.57
1:C:1247:LEU:HD23	1:C:1247:LEU:O	2.04	0.57
1:L:5666:LEU:HD23	1:L:5666:LEU:O	2.04	0.57
1:B:747:LEU:C	1:B:747:LEU:HD13	2.28	0.54
1:K:5166:LEU:C	1:K:5166:LEU:HD13	2.28	0.54
1:M:6148:LEU:HD13	1:M:6148:LEU:C	2.28	0.54
1:D:1729:LEU:HD13	1:D:1729:LEU:C	2.28	0.54
1:A:256:LEU:HD13	1:A:256:LEU:C	2.28	0.54
1:J:4675:LEU:C	1:J:4675:LEU:HD13	2.28	0.54
1:C:1238:LEU:HD13	1:C:1238:LEU:C	2.28	0.54
1:L:5657:LEU:HD13	1:L:5657:LEU:C	2.28	0.54
1:E:2220:LEU:HD13	1:E:2220:LEU:C	2.28	0.53
1:I:4184:LEU:C	1:I:4184:LEU:HD13	2.28	0.53
1:N:6639:LEU:HD13	1:N:6639:LEU:C	2.28	0.53
1:H:3693:LEU:HD13	1:H:3693:LEU:C	2.28	0.53
1:G:3202:LEU:HD13	1:G:3202:LEU:C	2.28	0.53
1:P:7621:LEU:HD13	1:P:7621:LEU:C	2.28	0.53
1:F:2711:LEU:HD13	1:F:2711:LEU:C	2.28	0.53
1:O:7130:LEU:HD13	1:O:7130:LEU:C	2.28	0.52
1:B:936:LEU:N	1:B:936:LEU:HD12	2.26	0.51
1:K:5355:LEU:N	1:K:5355:LEU:HD12	2.26	0.51
1:C:1427:LEU:HD12	1:C:1427:LEU:N	2.26	0.51
1:L:5846:LEU:N	1:L:5846:LEU:HD12	2.26	0.51
1:D:1918:LEU:HD12	1:D:1918:LEU:N	2.26	0.51
1:M:6337:LEU:N	1:M:6337:LEU:HD12	2.26	0.51
1:P:7810:LEU:HD12	1:P:7810:LEU:N	2.26	0.51
1:G:3391:LEU:HD12	1:G:3391:LEU:N	2.26	0.51
1:N:6828:LEU:HD12	1:N:6828:LEU:N	2.26	0.51
1:E:2409:LEU:HD12	1:E:2409:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7319:LEU:HD12	1:O:7319:LEU:N	2.26	0.50
1:F:2900:LEU:HD12	1:F:2900:LEU:N	2.26	0.50
1:J:4864:LEU:N	1:J:4864:LEU:HD12	2.26	0.50
1:A:445:LEU:HD12	1:A:445:LEU:N	2.26	0.50
1:H:3882:LEU:HD12	1:H:3882:LEU:N	2.26	0.50
1:I:4373:LEU:N	1:I:4373:LEU:HD12	2.26	0.50
1:I:4091:LYS:HA	1:I:4091:LYS:HE3	1.96	0.48
1:A:79:GLN:HG2	1:A:87:THR:HA	1.96	0.48
1:K:4989:GLN:HG2	1:K:4997:THR:HA	1.96	0.48
1:B:570:GLN:HG2	1:B:578:THR:HA	1.96	0.48
1:H:3600:LYS:HA	1:H:3600:LYS:HE3	1.96	0.48
1:J:4498:GLN:HG2	1:J:4506:THR:HA	1.96	0.48
1:J:4582:LYS:HE3	1:J:4582:LYS:HA	1.96	0.47
1:C:1061:GLN:HG2	1:C:1069:THR:HA	1.96	0.47
1:H:3516:GLN:HG2	1:H:3524:THR:HA	1.96	0.47
1:I:4007:GLN:HG2	1:I:4015:THR:HA	1.96	0.47
1:L:5480:GLN:HG2	1:L:5488:THR:HA	1.96	0.47
1:A:163:LYS:HA	1:A:163:LYS:HE3	1.96	0.47
1:G:3109:LYS:HE3	1:G:3109:LYS:HA	1.96	0.47
1:P:7444:GLN:HG2	1:P:7452:THR:HA	1.96	0.47
1:P:7528:LYS:HA	1:P:7528:LYS:HE3	1.96	0.47
1:G:3025:GLN:HG2	1:G:3033:THR:HA	1.96	0.47
1:C:1189:LEU:HB3	1:C:1320:THR:HG21	1.97	0.47
1:D:1552:GLN:HG2	1:D:1560:THR:HA	1.96	0.47
1:L:5608:LEU:HB3	1:L:5739:THR:HG21	1.97	0.47
1:B:654:LYS:HE3	1:B:654:LYS:HA	1.96	0.46
1:F:2618:LYS:HA	1:F:2618:LYS:HE3	1.96	0.46
1:M:5971:GLN:HG2	1:M:5979:THR:HA	1.96	0.46
1:O:6953:GLN:HG2	1:O:6961:THR:HA	1.96	0.46
1:O:7037:LYS:HE3	1:O:7037:LYS:HA	1.96	0.46
1:D:1680:LEU:HB3	1:D:1811:THR:HG21	1.97	0.46
1:F:2534:GLN:HG2	1:F:2542:THR:HA	1.96	0.46
1:H:3644:LEU:HB3	1:H:3775:THR:HG21	1.97	0.46
1:K:5073:LYS:HE3	1:K:5073:LYS:HA	1.96	0.46
1:I:4135:LEU:HB3	1:I:4266:THR:HG21	1.98	0.46
1:D:1509:LYS:HG2	1:D:1920:VAL:HG23	1.98	0.46
1:F:2491:LYS:HG2	1:F:2902:VAL:HG23	1.98	0.46
1:M:5928:LYS:HG2	1:M:6339:VAL:HG23	1.98	0.46
1:M:6099:LEU:HB3	1:M:6230:THR:HG21	1.98	0.46
1:N:6546:LYS:HE3	1:N:6546:LYS:HA	1.96	0.46
1:O:6910:LYS:HG2	1:O:7321:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:7401:LYS:HG2	1:P:7812:VAL:HG23	1.98	0.46
1:C:1145:LYS:HE3	1:C:1145:LYS:HA	1.96	0.46
1:E:2171:LEU:HB3	1:E:2302:THR:HG21	1.98	0.46
1:G:2982:LYS:HG2	1:G:3393:VAL:HG23	1.98	0.46
1:N:6590:LEU:HB3	1:N:6721:THR:HG21	1.97	0.46
1:P:7572:LEU:HB3	1:P:7703:THR:HG21	1.97	0.46
1:B:698:LEU:HB3	1:B:829:THR:HG21	1.97	0.46
1:E:2043:GLN:HG2	1:E:2051:THR:HA	1.96	0.46
1:E:2127:LYS:HE3	1:E:2127:LYS:HA	1.96	0.46
1:K:5117:LEU:HB3	1:K:5248:THR:HG21	1.98	0.46
1:L:5437:LYS:HG2	1:L:5848:VAL:HG23	1.98	0.46
1:N:6462:GLN:HG2	1:N:6470:THR:HA	1.96	0.46
1:C:1018:LYS:HG2	1:C:1429:VAL:HG23	1.98	0.46
1:E:2000:LYS:HG2	1:E:2411:VAL:HG23	1.98	0.46
1:G:3153:LEU:HB3	1:G:3284:THR:HG21	1.97	0.46
1:N:6419:LYS:HG2	1:N:6830:VAL:HG23	1.98	0.46
1:L:5564:LYS:HE3	1:L:5564:LYS:HA	1.96	0.46
1:A:207:LEU:HB3	1:A:338:THR:HG21	1.97	0.46
1:F:2662:LEU:HB3	1:F:2793:THR:HG21	1.97	0.46
1:O:7081:LEU:HB3	1:O:7212:THR:HG21	1.97	0.45
1:H:3473:LYS:HG2	1:H:3884:VAL:HG23	1.98	0.45
1:I:3964:LYS:HG2	1:I:4375:VAL:HG23	1.98	0.45
1:J:4626:LEU:HB3	1:J:4757:THR:HG21	1.97	0.45
1:J:4903:ILE:HD12	1:J:4903:ILE:N	2.32	0.45
1:M:6055:LYS:HE3	1:M:6055:LYS:HA	1.96	0.45
1:A:484:ILE:N	1:A:484:ILE:HD12	2.32	0.45
1:B:527:LYS:HG2	1:B:938:VAL:HG23	1.98	0.45
1:D:1636:LYS:HE3	1:D:1636:LYS:HA	1.96	0.45
1:F:2939:ILE:N	1:F:2939:ILE:HD12	2.32	0.45
1:O:7358:ILE:HD12	1:O:7358:ILE:N	2.32	0.45
1:K:4946:LYS:HG2	1:K:5357:VAL:HG23	1.98	0.45
1:E:2448:ILE:N	1:E:2448:ILE:HD12	2.32	0.45
1:M:6376:ILE:HD12	1:M:6376:ILE:N	2.32	0.45
1:N:6867:ILE:HD12	1:N:6867:ILE:N	2.32	0.45
1:D:1957:ILE:N	1:D:1957:ILE:HD12	2.32	0.45
1:G:3430:ILE:N	1:G:3430:ILE:HD12	2.32	0.45
1:M:5927:PRO:O	1:M:6046:GLY:N	2.50	0.45
1:D:1508:PRO:O	1:D:1627:GLY:N	2.50	0.45
1:E:1999:PRO:O	1:E:2118:GLY:N	2.50	0.45
1:J:4455:LYS:HG2	1:J:4866:VAL:HG23	1.98	0.45
1:L:5885:ILE:HD12	1:L:5885:ILE:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:HG2	1:A:447:VAL:HG23	1.98	0.45
1:F:2655:THR:HG23	1:F:2796:ILE:HA	1.99	0.45
1:N:6418:PRO:O	1:N:6537:GLY:N	2.50	0.45
1:O:7074:THR:HG23	1:O:7215:ILE:HA	1.99	0.45
1:P:7849:ILE:N	1:P:7849:ILE:HD12	2.32	0.45
1:A:35:PRO:O	1:A:154:GLY:N	2.50	0.45
1:C:1466:ILE:HD12	1:C:1466:ILE:N	2.32	0.45
1:H:3472:PRO:O	1:H:3591:GLY:N	2.50	0.45
1:I:3963:PRO:O	1:I:4082:GLY:N	2.50	0.45
1:I:4412:ILE:N	1:I:4412:ILE:HD12	2.32	0.45
1:J:4454:PRO:O	1:J:4573:GLY:N	2.50	0.45
1:H:3921:ILE:N	1:H:3921:ILE:HD12	2.32	0.44
1:F:2490:PRO:O	1:F:2609:GLY:N	2.50	0.44
1:G:2981:PRO:O	1:G:3100:GLY:N	2.50	0.44
1:K:5146:THR:O	1:K:5147:ALA:HB3	2.18	0.44
1:K:5394:ILE:HD12	1:K:5394:ILE:N	2.32	0.44
1:O:6909:PRO:O	1:O:7028:GLY:N	2.50	0.44
1:B:975:ILE:N	1:B:975:ILE:HD12	2.32	0.44
1:H:3637:THR:HG23	1:H:3778:ILE:HA	1.99	0.44
1:I:4128:THR:HG23	1:I:4269:ILE:HA	1.99	0.44
1:I:4164:THR:O	1:I:4165:ALA:HB3	2.18	0.44
1:J:4655:THR:O	1:J:4656:ALA:HB3	2.18	0.44
1:L:5436:PRO:O	1:L:5555:GLY:N	2.50	0.44
1:P:7400:PRO:O	1:P:7519:GLY:N	2.50	0.44
1:A:236:THR:O	1:A:237:ALA:HB3	2.18	0.44
1:B:727:THR:O	1:B:728:ALA:HB3	2.18	0.44
1:E:2164:THR:HG23	1:E:2305:ILE:HA	1.99	0.44
1:H:3673:THR:O	1:H:3674:ALA:HB3	2.18	0.44
1:C:1017:PRO:O	1:C:1136:GLY:N	2.50	0.44
1:M:6092:THR:HG23	1:M:6233:ILE:HA	1.99	0.44
1:C:1247:LEU:C	1:C:1247:LEU:CD2	2.86	0.44
1:D:1492:ILE:HG23	1:D:1571:LEU:HB3	2.00	0.44
1:D:1673:THR:HG23	1:D:1814:ILE:HA	1.99	0.44
1:L:5666:LEU:C	1:L:5666:LEU:CD2	2.86	0.44
1:N:6583:THR:HG23	1:N:6724:ILE:HA	1.99	0.44
1:A:19:ILE:HG23	1:A:98:LEU:HB3	2.00	0.44
1:J:4438:ILE:HG23	1:J:4517:LEU:HB3	2.00	0.44
1:L:5637:THR:O	1:L:5638:ALA:HB3	2.18	0.44
1:N:6402:ILE:HG23	1:N:6481:LEU:HB3	2.00	0.44
1:B:510:ILE:HG23	1:B:589:LEU:HB3	2.00	0.44
1:B:526:PRO:O	1:B:645:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1983:ILE:HG23	1:E:2062:LEU:HB3	2.00	0.44
1:K:4929:ILE:HG23	1:K:5008:LEU:HB3	2.00	0.44
1:M:5911:ILE:HG23	1:M:5990:LEU:HB3	2.00	0.44
1:B:691:THR:HG23	1:B:832:ILE:HA	1.99	0.44
1:C:1218:THR:O	1:C:1219:ALA:HB3	2.18	0.44
1:G:3146:THR:HG23	1:G:3287:ILE:HA	1.99	0.44
1:K:4945:PRO:O	1:K:5064:GLY:N	2.50	0.44
1:D:1738:LEU:C	1:D:1738:LEU:CD2	2.86	0.43
1:G:3182:THR:O	1:G:3183:ALA:HB3	2.18	0.43
1:K:5110:THR:HG23	1:K:5251:ILE:HA	1.99	0.43
1:O:6893:ILE:HG23	1:O:6972:LEU:HB3	2.00	0.43
1:M:6157:LEU:C	1:M:6157:LEU:CD2	2.86	0.43
1:P:7565:THR:HG23	1:P:7706:ILE:HA	1.99	0.43
1:C:1001:ILE:HG23	1:C:1080:LEU:HB3	2.00	0.43
1:D:1709:THR:O	1:D:1710:ALA:HB3	2.18	0.43
1:E:2200:THR:O	1:E:2201:ALA:HB3	2.18	0.43
1:F:2474:ILE:HG23	1:F:2553:LEU:HB3	2.00	0.43
1:H:3456:ILE:HG23	1:H:3535:LEU:HB3	2.00	0.43
1:I:3947:ILE:HG23	1:I:4026:LEU:HB3	2.00	0.43
1:N:6619:THR:O	1:N:6620:ALA:HB3	2.18	0.43
1:P:7601:THR:O	1:P:7602:ALA:HB3	2.18	0.43
1:K:5175:LEU:C	1:K:5175:LEU:CD2	2.86	0.43
1:M:6128:THR:O	1:M:6129:ALA:HB3	2.18	0.43
1:B:756:LEU:C	1:B:756:LEU:CD2	2.86	0.43
1:G:2965:ILE:HG23	1:G:3044:LEU:HB3	2.00	0.43
1:L:5420:ILE:HG23	1:L:5499:LEU:HB3	2.00	0.43
1:L:5601:THR:HG23	1:L:5742:ILE:HA	1.99	0.43
1:O:7110:THR:O	1:O:7111:ALA:HB3	2.18	0.43
1:F:2691:THR:O	1:F:2692:ALA:HB3	2.18	0.43
1:A:33:LEU:HD11	1:A:92:VAL:HG11	2.01	0.43
1:A:200:THR:HG23	1:A:341:ILE:HA	1.99	0.43
1:A:265:LEU:C	1:A:265:LEU:CD2	2.86	0.43
1:C:1182:THR:HG23	1:C:1323:ILE:HA	1.99	0.43
1:J:4619:THR:HG23	1:J:4760:ILE:HA	1.99	0.43
1:P:7384:ILE:HG23	1:P:7463:LEU:HB3	2.00	0.43
1:J:4452:LEU:HD11	1:J:4511:VAL:HG11	2.01	0.43
1:J:4684:LEU:C	1:J:4684:LEU:CD2	2.86	0.43
1:G:3360:ARG:HD3	1:G:3360:ARG:C	2.40	0.43
1:I:3981:ASN:HB3	1:I:4083:LYS:HG2	2.01	0.43
1:P:7398:LEU:HD11	1:P:7457:VAL:HG11	2.01	0.43
1:P:7779:ARG:HD3	1:P:7779:ARG:C	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ARG:HD3	1:A:414:ARG:C	2.40	0.42
1:E:2017:ASN:HB3	1:E:2119:LYS:HG2	2.01	0.42
1:G:2979:LEU:HD11	1:G:3038:VAL:HG11	2.01	0.42
1:H:3490:ASN:HB3	1:H:3592:LYS:HG2	2.01	0.42
1:B:663:VAL:HA	1:B:678:ILE:HD11	2.01	0.42
1:K:4963:ASN:HB3	1:K:5065:LYS:HG2	2.01	0.42
1:K:5082:VAL:HA	1:K:5097:ILE:HD11	2.01	0.42
1:B:544:ASN:HB3	1:B:646:LYS:HG2	2.01	0.42
1:B:905:ARG:HD3	1:B:905:ARG:C	2.40	0.42
1:D:1526:ASN:HB3	1:D:1628:LYS:HG2	2.01	0.42
1:J:4833:ARG:HD3	1:J:4833:ARG:C	2.40	0.42
1:K:5324:ARG:HD3	1:K:5324:ARG:C	2.40	0.42
1:M:5945:ASN:HB3	1:M:6047:LYS:HG2	2.01	0.42
1:O:6927:ASN:HB3	1:O:7029:LYS:HG2	2.01	0.42
1:E:2229:LEU:C	1:E:2229:LEU:CD2	2.86	0.42
1:F:2508:ASN:HB3	1:F:2610:LYS:HG2	2.01	0.42
1:F:2869:ARG:HD3	1:F:2869:ARG:C	2.40	0.42
1:H:3851:ARG:HD3	1:H:3851:ARG:C	2.40	0.42
1:L:5815:ARG:HD3	1:L:5815:ARG:C	2.40	0.42
1:N:6436:ASN:HB3	1:N:6538:LYS:HG2	2.01	0.42
1:O:7288:ARG:C	1:O:7288:ARG:HD3	2.40	0.42
1:A:172:VAL:HA	1:A:187:ILE:HD11	2.01	0.42
1:C:1154:VAL:HA	1:C:1169:ILE:HD11	2.01	0.42
1:C:1396:ARG:C	1:C:1396:ARG:HD3	2.40	0.42
1:L:5573:VAL:HA	1:L:5588:ILE:HD11	2.01	0.42
1:C:1035:ASN:HB3	1:C:1137:LYS:HG2	2.01	0.42
1:H:3702:LEU:C	1:H:3702:LEU:CD2	2.86	0.42
1:I:4342:ARG:HD3	1:I:4342:ARG:C	2.40	0.42
1:J:4591:VAL:HA	1:J:4606:ILE:HD11	2.01	0.42
1:K:5202:ALA:HA	1:K:5244:PRO:HA	2.02	0.42
1:A:53:ASN:HB3	1:A:155:LYS:HG2	2.01	0.42
1:B:783:ALA:HA	1:B:825:PRO:HA	2.01	0.42
1:C:1015:LEU:HD11	1:C:1074:VAL:HG11	2.01	0.42
1:C:1274:ALA:HA	1:C:1316:PRO:HA	2.01	0.42
1:F:2627:VAL:HA	1:F:2642:ILE:HD11	2.01	0.42
1:L:5403:LEU:HA	1:L:5404:PRO:HD3	1.91	0.42
1:N:6648:LEU:C	1:N:6648:LEU:CD2	2.86	0.42
1:P:7418:ASN:HB3	1:P:7520:LYS:HG2	2.01	0.42
1:F:2801:GLU:O	1:F:2804:ILE:HG12	2.20	0.42
1:G:2999:ASN:HB3	1:G:3101:LYS:HG2	2.01	0.42
1:I:4193:LEU:C	1:I:4193:LEU:CD2	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5434:LEU:HD11	1:L:5493:VAL:HG11	2.01	0.42
1:L:5454:ASN:HB3	1:L:5556:LYS:HG2	2.01	0.42
1:M:6306:ARG:C	1:M:6306:ARG:HD3	2.40	0.42
1:O:7046:VAL:HA	1:O:7061:ILE:HD11	2.01	0.42
1:D:1641:ILE:HD11	1:D:1829:VAL:HB	2.02	0.42
1:J:4472:ASN:HB3	1:J:4574:LYS:HG2	2.01	0.42
1:L:5693:ALA:HA	1:L:5735:PRO:HA	2.02	0.42
1:M:6060:ILE:HD11	1:M:6248:VAL:HB	2.02	0.42
1:O:7220:GLU:O	1:O:7223:ILE:HG12	2.20	0.42
1:B:659:ILE:HD11	1:B:847:VAL:HB	2.02	0.42
1:D:1577:LEU:HD23	1:D:1587:VAL:HG23	2.02	0.42
1:D:1887:ARG:C	1:D:1887:ARG:HD3	2.40	0.42
1:M:5996:LEU:HD23	1:M:6006:VAL:HG23	2.02	0.42
1:P:7537:VAL:HA	1:P:7552:ILE:HD11	2.01	0.42
1:E:2068:LEU:HD23	1:E:2078:VAL:HG23	2.02	0.41
1:F:2936:LEU:HD12	1:F:2936:LEU:HA	1.87	0.41
1:K:5078:ILE:HD11	1:K:5266:VAL:HB	2.03	0.41
1:L:5569:ILE:HD11	1:L:5757:VAL:HB	2.02	0.41
1:N:6551:ILE:HD11	1:N:6739:VAL:HB	2.02	0.41
1:N:6555:VAL:HA	1:N:6570:ILE:HD11	2.01	0.41
1:O:7166:ALA:HA	1:O:7208:PRO:HA	2.01	0.41
1:P:7711:GLU:O	1:P:7714:ILE:HG12	2.20	0.41
1:A:168:ILE:HD11	1:A:356:VAL:HB	2.02	0.41
1:A:292:ALA:HA	1:A:334:PRO:HA	2.02	0.41
1:A:346:GLU:O	1:A:349:ILE:HG12	2.20	0.41
1:C:984:LEU:HA	1:C:985:PRO:HD3	1.91	0.41
1:E:2132:ILE:HD11	1:E:2320:VAL:HB	2.02	0.41
1:E:2136:VAL:HA	1:E:2151:ILE:HD11	2.01	0.41
1:G:3118:VAL:HA	1:G:3133:ILE:HD11	2.01	0.41
1:G:3292:GLU:O	1:G:3295:ILE:HG12	2.20	0.41
1:I:3961:LEU:HD11	1:I:4020:VAL:HG11	2.01	0.41
1:J:4711:ALA:HA	1:J:4753:PRO:HA	2.01	0.41
1:J:4765:GLU:O	1:J:4768:ILE:HG12	2.20	0.41
1:E:1997:LEU:HD11	1:E:2056:VAL:HG11	2.01	0.41
1:E:2378:ARG:HD3	1:E:2378:ARG:C	2.40	0.41
1:F:2747:ALA:HA	1:F:2789:PRO:HA	2.02	0.41
1:H:3470:LEU:HD11	1:H:3529:VAL:HG11	2.01	0.41
1:J:4587:ILE:HD11	1:J:4775:VAL:HB	2.02	0.41
1:N:6416:LEU:HD11	1:N:6475:VAL:HG11	2.01	0.41
1:N:6487:LEU:HD23	1:N:6497:VAL:HG23	2.02	0.41
1:B:524:LEU:HD11	1:B:583:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1150:ILE:HD11	1:C:1338:VAL:HB	2.02	0.41
1:F:2559:LEU:HD23	1:F:2569:VAL:HG23	2.02	0.41
1:H:3678:LEU:HD23	1:H:3702:LEU:HB3	2.02	0.41
1:M:6184:ALA:HA	1:M:6226:PRO:HA	2.01	0.41
1:M:6238:GLU:O	1:M:6241:ILE:HG12	2.20	0.41
1:N:6729:GLU:O	1:N:6732:ILE:HG12	2.20	0.41
1:N:6797:ARG:C	1:N:6797:ARG:HD3	2.40	0.41
1:P:7606:LEU:HD23	1:P:7630:LEU:HB3	2.02	0.41
1:P:7657:ALA:HA	1:P:7699:PRO:HA	2.02	0.41
1:A:241:LEU:HD23	1:A:265:LEU:HB3	2.02	0.41
1:D:1765:ALA:HA	1:D:1807:PRO:HA	2.01	0.41
1:D:1819:GLU:O	1:D:1822:ILE:HG12	2.20	0.41
1:E:2310:GLU:O	1:E:2313:ILE:HG12	2.20	0.41
1:F:2475:LEU:HD12	1:F:2475:LEU:HA	1.86	0.41
1:F:2720:LEU:C	1:F:2720:LEU:CD2	2.86	0.41
1:G:3187:LEU:HD23	1:G:3211:LEU:HB3	2.03	0.41
1:G:3238:ALA:HA	1:G:3280:PRO:HA	2.02	0.41
1:I:4169:LEU:HD23	1:I:4193:LEU:HB3	2.03	0.41
1:K:4943:LEU:HD11	1:K:5002:VAL:HG11	2.01	0.41
1:K:5256:GLU:O	1:K:5259:ILE:HG12	2.20	0.41
1:M:6064:VAL:HA	1:M:6079:ILE:HD11	2.01	0.41
1:B:837:GLU:O	1:B:840:ILE:HG12	2.20	0.41
1:D:1506:LEU:HD11	1:D:1565:VAL:HG11	2.01	0.41
1:D:1645:VAL:HA	1:D:1660:ILE:HD11	2.01	0.41
1:H:3609:VAL:HA	1:H:3624:ILE:HD11	2.01	0.41
1:H:3729:ALA:HA	1:H:3771:PRO:HA	2.01	0.41
1:I:4100:VAL:HA	1:I:4115:ILE:HD11	2.01	0.41
1:I:4220:ALA:HA	1:I:4262:PRO:HA	2.02	0.41
1:J:4660:LEU:HD23	1:J:4684:LEU:HB3	2.02	0.41
1:M:5925:LEU:HD11	1:M:5984:VAL:HG11	2.01	0.41
1:N:6864:LEU:HA	1:N:6864:LEU:HD12	1.87	0.41
1:O:7355:LEU:HD12	1:O:7355:LEU:HA	1.87	0.41
1:G:3211:LEU:C	1:G:3211:LEU:CD2	2.86	0.41
1:I:4032:LEU:HD23	1:I:4042:VAL:HG23	2.02	0.41
1:O:6978:LEU:HD23	1:O:6988:VAL:HG23	2.02	0.41
1:O:7139:LEU:C	1:O:7139:LEU:CD2	2.86	0.41
1:B:732:LEU:HD23	1:B:756:LEU:HB3	2.02	0.41
1:E:2256:ALA:HA	1:E:2298:PRO:HA	2.02	0.41
1:H:3605:ILE:HD11	1:H:3793:VAL:HB	2.02	0.41
1:K:5151:LEU:HD23	1:K:5175:LEU:HB3	2.02	0.41
1:N:6675:ALA:HA	1:N:6717:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7042:ILE:HD11	1:O:7230:VAL:HB	2.02	0.41
1:P:7630:LEU:C	1:P:7630:LEU:CD2	2.86	0.41
1:A:104:LEU:HD23	1:A:114:VAL:HG23	2.02	0.41
1:F:2623:ILE:HD11	1:F:2811:VAL:HB	2.02	0.41
1:H:3541:LEU:HD23	1:H:3551:VAL:HG23	2.02	0.41
1:I:4096:ILE:HD11	1:I:4284:VAL:HB	2.02	0.41
1:I:4274:GLU:O	1:I:4277:ILE:HG12	2.20	0.41
1:J:4523:LEU:HD23	1:J:4533:VAL:HG23	2.02	0.41
1:L:5747:GLU:O	1:L:5750:ILE:HG12	2.20	0.41
1:O:6894:LEU:HD12	1:O:6894:LEU:HA	1.86	0.41
1:O:6907:LEU:HD11	1:O:6966:VAL:HG11	2.01	0.41
1:C:1328:GLU:O	1:C:1331:ILE:HG12	2.20	0.41
1:F:2488:LEU:HD11	1:F:2547:VAL:HG11	2.01	0.41
1:E:2445:LEU:HA	1:E:2445:LEU:HD12	1.87	0.40
1:F:2696:LEU:HD23	1:F:2720:LEU:HB3	2.02	0.40
1:H:3783:GLU:O	1:H:3786:ILE:HG12	2.20	0.40
1:L:5505:LEU:HD23	1:L:5515:VAL:HG23	2.02	0.40
1:P:7533:ILE:HD11	1:P:7721:VAL:HB	2.02	0.40
1:C:1086:LEU:HD23	1:C:1096:VAL:HG23	2.02	0.40
1:D:1493:LEU:HD12	1:D:1493:LEU:HA	1.86	0.40
1:G:3114:ILE:HD11	1:G:3302:VAL:HB	2.02	0.40
1:O:7115:LEU:HD23	1:O:7139:LEU:HB3	2.03	0.40
1:B:659:ILE:HD12	1:B:830:MET:SD	2.62	0.40
1:P:7469:LEU:HD23	1:P:7479:VAL:HG23	2.02	0.40
1:C:1223:LEU:HD23	1:C:1247:LEU:HB3	2.02	0.40
1:E:2205:LEU:HD23	1:E:2229:LEU:HB3	2.02	0.40
1:G:3050:LEU:HD23	1:G:3060:VAL:HG23	2.02	0.40
1:K:5014:LEU:HD23	1:K:5024:VAL:HG23	2.02	0.40
1:K:5078:ILE:HD12	1:K:5249:MET:SD	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	B	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	C	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	D	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	E	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	F	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	G	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	H	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	I	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	J	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	K	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	L	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	M	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	N	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	O	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
1	P	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	34	72
All	All	7824/7856 (100%)	7488 (96%)	304 (4%)	32 (0%)	38	72

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	496	ASN
1	C	987	ASN
1	D	1478	ASN
1	E	1969	ASN
1	F	2460	ASN
1	G	2951	ASN
1	H	3442	ASN
1	I	3933	ASN
1	J	4424	ASN
1	K	4915	ASN
1	L	5406	ASN
1	M	5897	ASN
1	N	6388	ASN
1	O	6879	ASN
1	P	7370	ASN

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Mol	Chain	Res	Type
1	A	443	ALA
1	B	934	ALA
1	C	1425	ALA
1	D	1916	ALA
1	E	2407	ALA
1	F	2898	ALA
1	G	3389	ALA
1	H	3880	ALA
1	I	4371	ALA
1	J	4862	ALA
1	K	5353	ALA
1	L	5844	ALA
1	M	6335	ALA
1	N	6826	ALA
1	O	7317	ALA
1	P	7808	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	B	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	C	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	D	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	E	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	F	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	G	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	H	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	I	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	J	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	K	393/393 (100%)	383 (98%)	10 (2%)	47	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	M	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	N	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	O	393/393 (100%)	383 (98%)	10 (2%)	47	68
1	P	393/393 (100%)	383 (98%)	10 (2%)	47	68
All	All	6288/6288 (100%)	6128 (98%)	160 (2%)	50	68

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	54	ASP
1	A	98	LEU
1	A	163	LYS
1	A	259	GLN
1	A	303	ASP
1	A	386	LYS
1	A	414	ARG
1	A	416	LEU
1	A	481	LEU
1	B	511	LEU
1	B	545	ASP
1	B	589	LEU
1	B	654	LYS
1	B	750	GLN
1	B	794	ASP
1	B	877	LYS
1	B	905	ARG
1	B	907	LEU
1	B	972	LEU
1	C	1002	LEU
1	C	1036	ASP
1	C	1080	LEU
1	C	1145	LYS
1	C	1241	GLN
1	C	1285	ASP
1	C	1368	LYS
1	C	1396	ARG
1	C	1398	LEU
1	C	1463	LEU

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Mol	Chain	Res	Type
1	D	1493	LEU
1	D	1527	ASP
1	D	1571	LEU
1	D	1636	LYS
1	D	1732	GLN
1	D	1776	ASP
1	D	1859	LYS
1	D	1887	ARG
1	D	1889	LEU
1	D	1954	LEU
1	E	1984	LEU
1	E	2018	ASP
1	E	2062	LEU
1	E	2127	LYS
1	E	2223	GLN
1	E	2267	ASP
1	E	2350	LYS
1	E	2378	ARG
1	E	2380	LEU
1	E	2445	LEU
1	F	2475	LEU
1	F	2509	ASP
1	F	2553	LEU
1	F	2618	LYS
1	F	2714	GLN
1	F	2758	ASP
1	F	2841	LYS
1	F	2869	ARG
1	F	2871	LEU
1	F	2936	LEU
1	G	2966	LEU
1	G	3000	ASP
1	G	3044	LEU
1	G	3109	LYS
1	G	3205	GLN
1	G	3249	ASP
1	G	3332	LYS
1	G	3360	ARG
1	G	3362	LEU
1	G	3427	LEU
1	H	3457	LEU
1	H	3491	ASP

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Mol	Chain	Res	Type
1	H	3535	LEU
1	H	3600	LYS
1	H	3696	GLN
1	H	3740	ASP
1	H	3823	LYS
1	H	3851	ARG
1	H	3853	LEU
1	H	3918	LEU
1	I	3948	LEU
1	I	3982	ASP
1	I	4026	LEU
1	I	4091	LYS
1	I	4187	GLN
1	I	4231	ASP
1	I	4314	LYS
1	I	4342	ARG
1	I	4344	LEU
1	I	4409	LEU
1	J	4439	LEU
1	J	4473	ASP
1	J	4517	LEU
1	J	4582	LYS
1	J	4678	GLN
1	J	4722	ASP
1	J	4805	LYS
1	J	4833	ARG
1	J	4835	LEU
1	J	4900	LEU
1	K	4930	LEU
1	K	4964	ASP
1	K	5008	LEU
1	K	5073	LYS
1	K	5169	GLN
1	K	5213	ASP
1	K	5296	LYS
1	K	5324	ARG
1	K	5326	LEU
1	K	5391	LEU
1	L	5421	LEU
1	L	5455	ASP
1	L	5499	LEU
1	L	5564	LYS

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Mol	Chain	Res	Type
1	L	5660	GLN
1	L	5704	ASP
1	L	5787	LYS
1	L	5815	ARG
1	L	5817	LEU
1	L	5882	LEU
1	M	5912	LEU
1	M	5946	ASP
1	M	5990	LEU
1	M	6055	LYS
1	M	6151	GLN
1	M	6195	ASP
1	M	6278	LYS
1	M	6306	ARG
1	M	6308	LEU
1	M	6373	LEU
1	N	6403	LEU
1	N	6437	ASP
1	N	6481	LEU
1	N	6546	LYS
1	N	6642	GLN
1	N	6686	ASP
1	N	6769	LYS
1	N	6797	ARG
1	N	6799	LEU
1	N	6864	LEU
1	O	6894	LEU
1	O	6928	ASP
1	O	6972	LEU
1	O	7037	LYS
1	O	7133	GLN
1	O	7177	ASP
1	O	7260	LYS
1	O	7288	ARG
1	O	7290	LEU
1	O	7355	LEU
1	P	7385	LEU
1	P	7419	ASP
1	P	7463	LEU
1	P	7528	LYS
1	P	7624	GLN
1	P	7668	ASP

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Mol	Chain	Res	Type
1	P	7751	LYS
1	P	7779	ARG
1	P	7781	LEU
1	P	7846	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	B	960	GLN
1	C	1451	GLN
1	D	1942	GLN
1	E	2433	GLN
1	H	3906	GLN
1	I	4397	GLN
1	J	4888	GLN
1	K	5379	GLN
1	L	5870	GLN
1	M	6361	GLN
1	P	7834	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

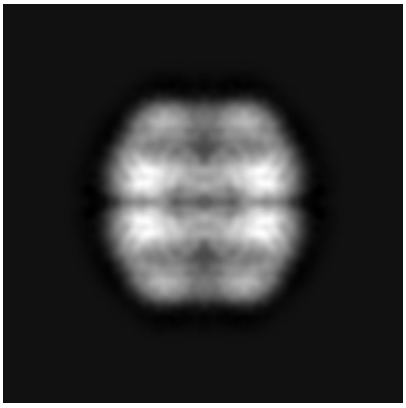
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5250. These allow visual inspection of the internal detail of the map and identification of artifacts.

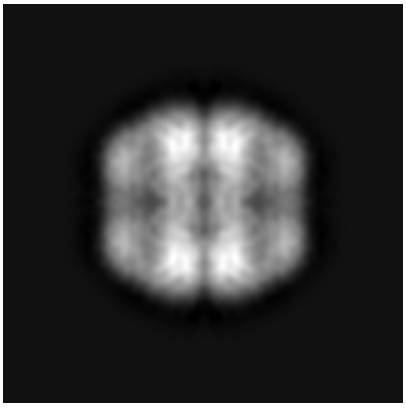
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



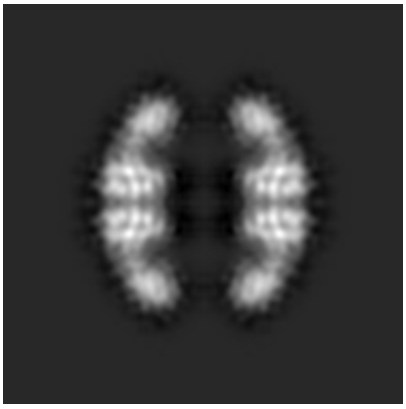
Y

Z

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

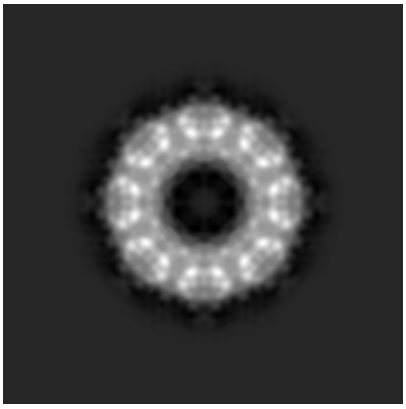
6.2 Central slices (i)

6.2.1 Primary map



X Index: 72

Y Index: 72

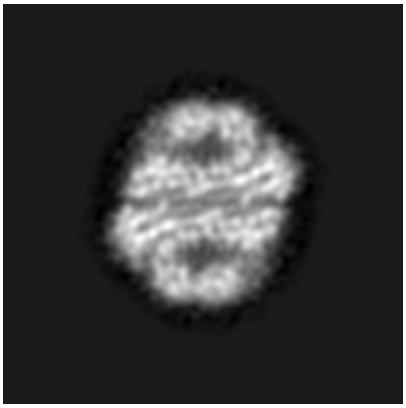


Z Index: 72

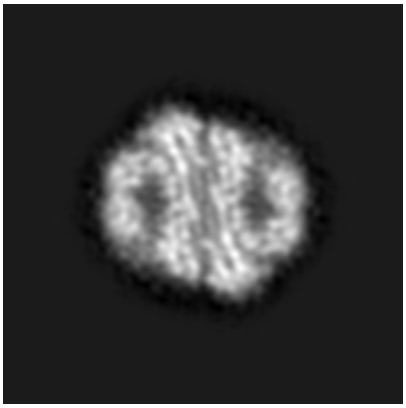
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 92



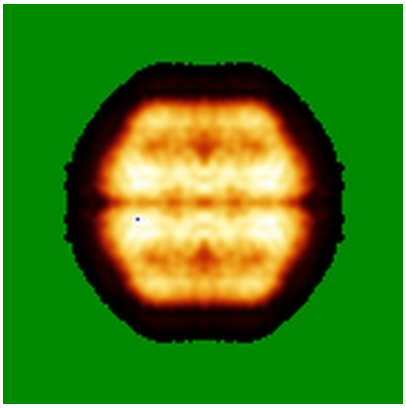
Y Index: 92

Z Index: 61

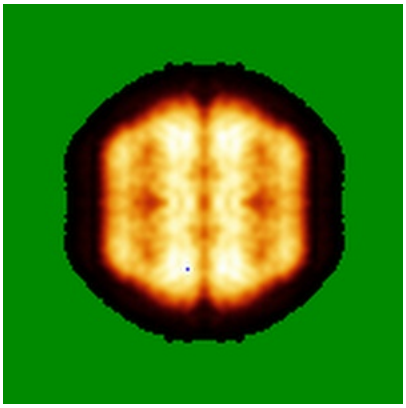
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

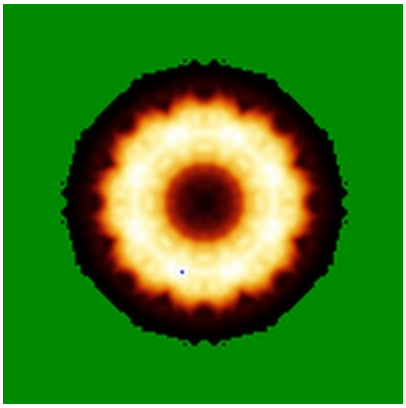
6.4.1 Primary map



X



Y

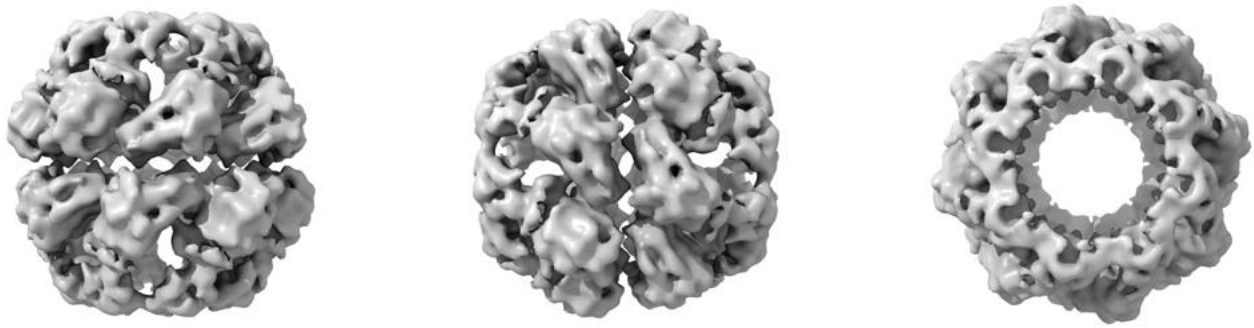


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.58. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

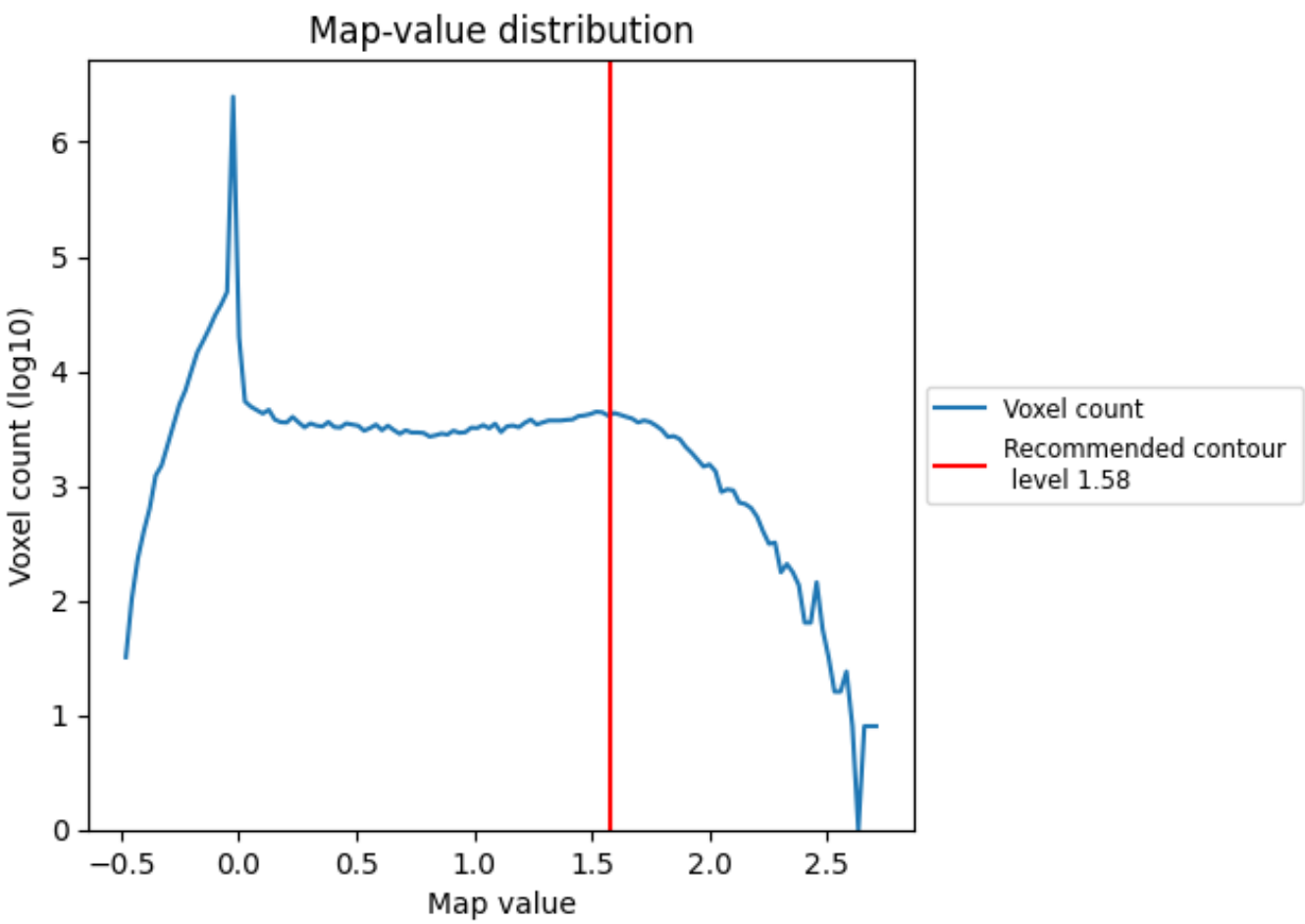
6.6 Mask visualisation (i)

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

7 Map analysis (i)

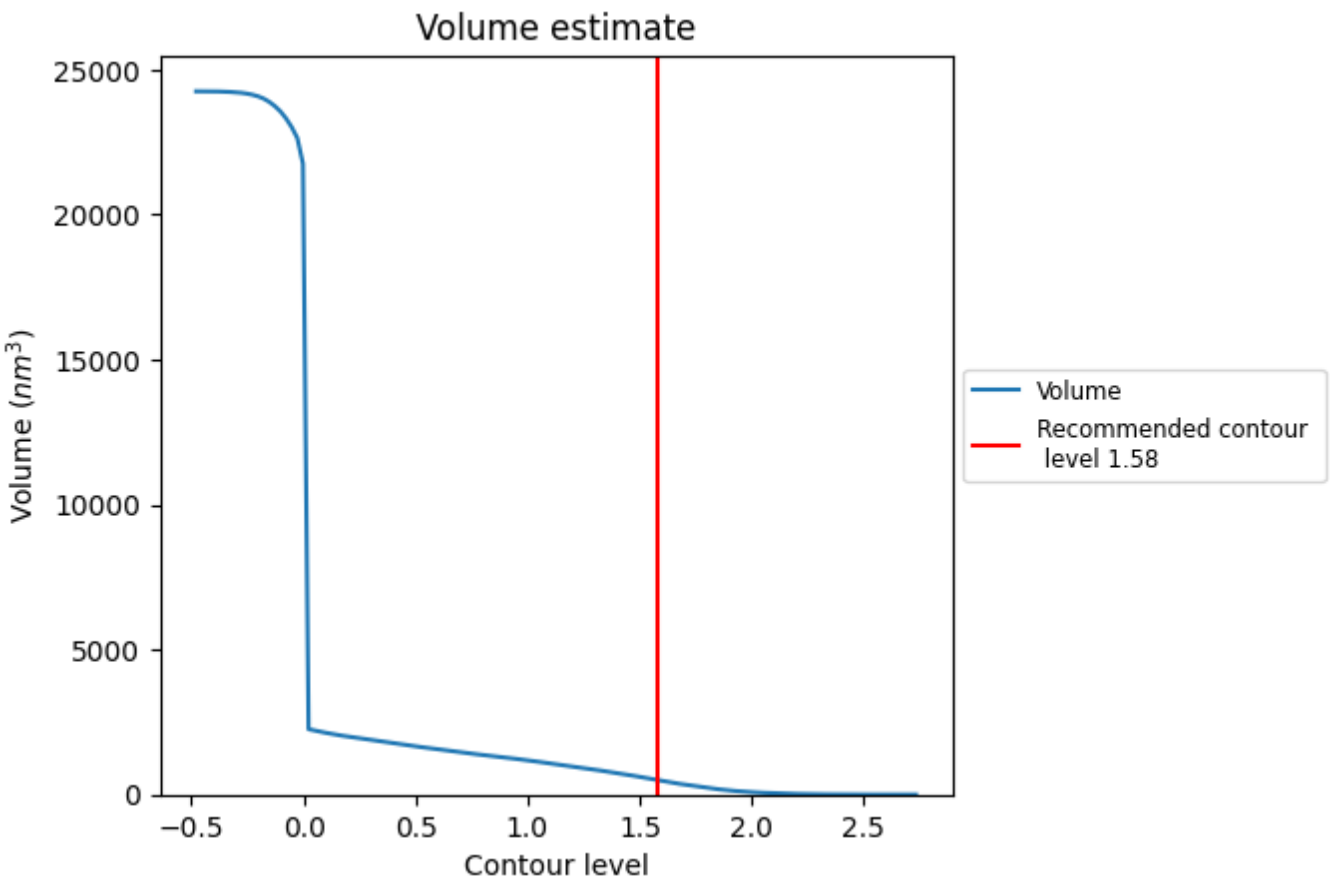
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

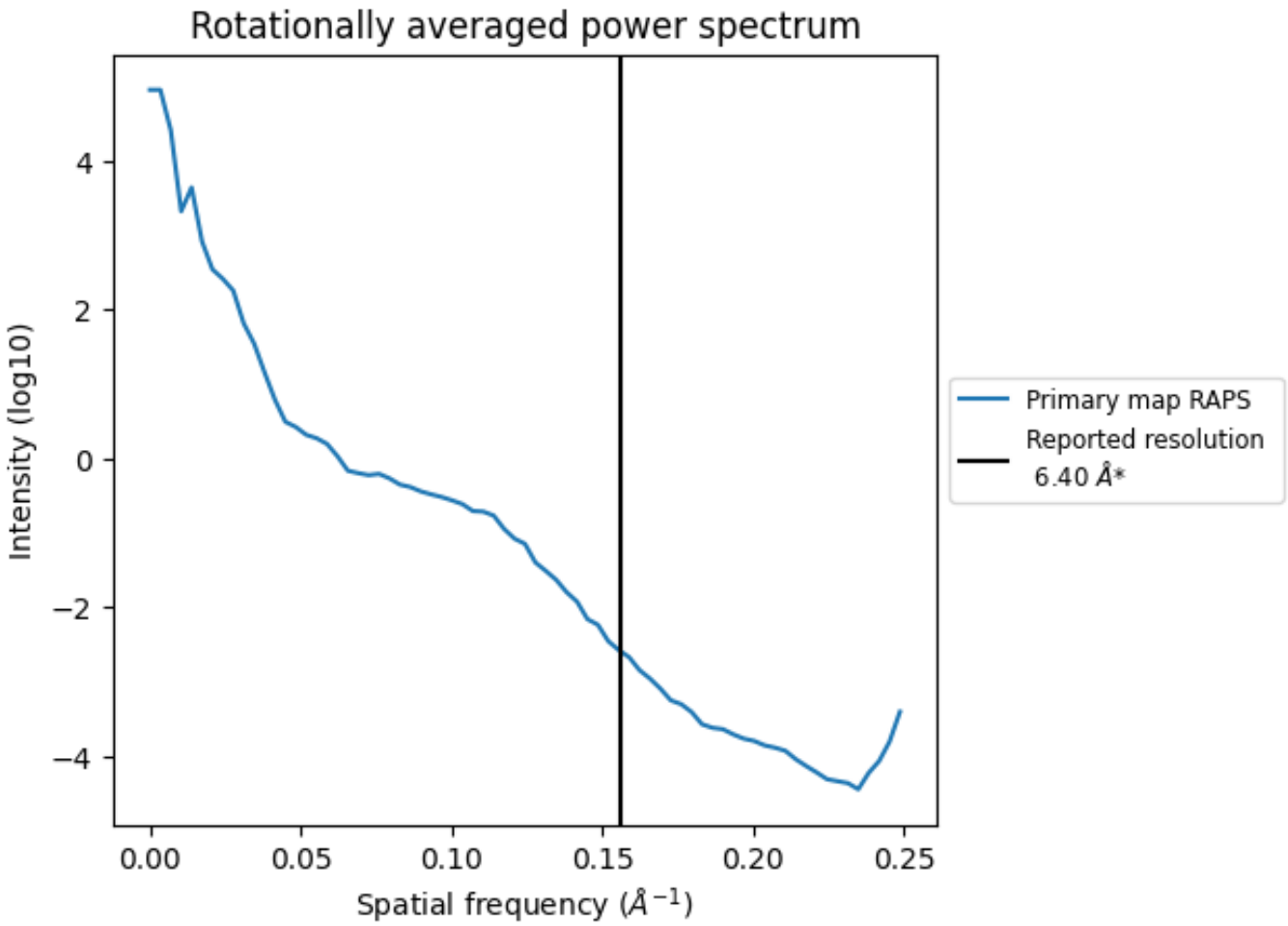
7.2 Volume estimate (i)



The volume at the recommended contour level is 500 nm^3; this corresponds to an approximate mass of 452 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 0.156 Å^{-1}

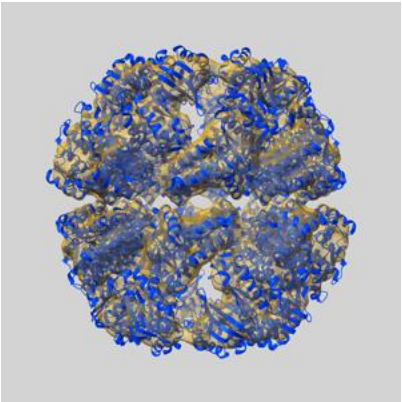
8 Fourier-Shell correlation (i)

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

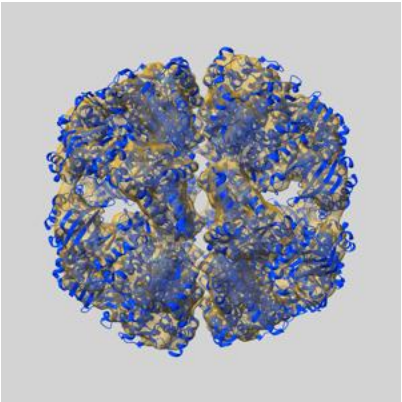
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5250 and PDB model 3IZN. Per-residue inclusion information can be found in section 3 on page 7.

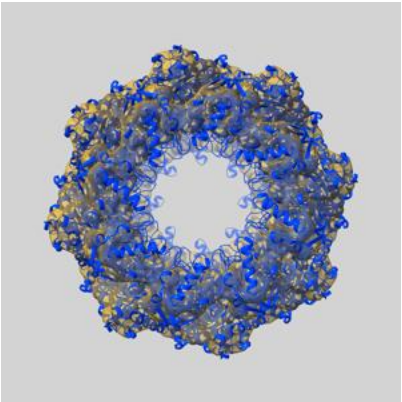
9.1 Map-model overlay (i)



X



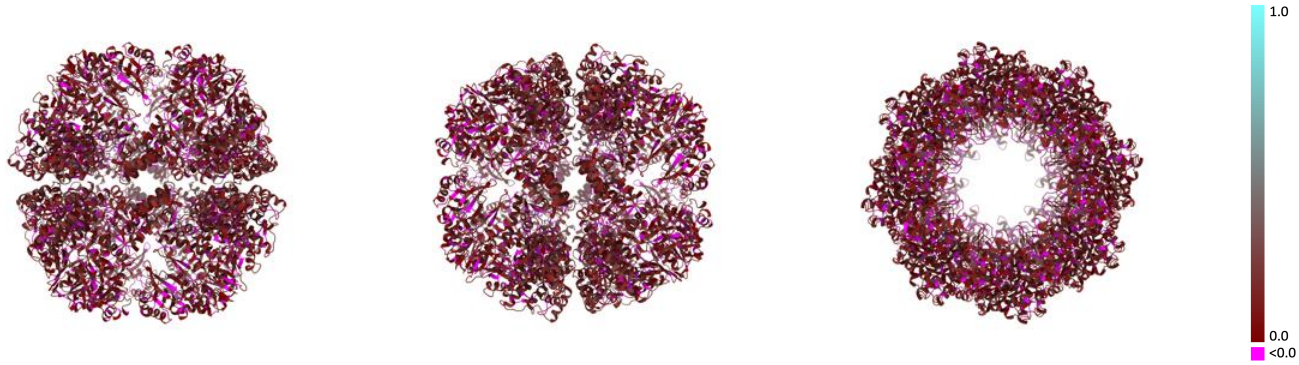
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.58 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.

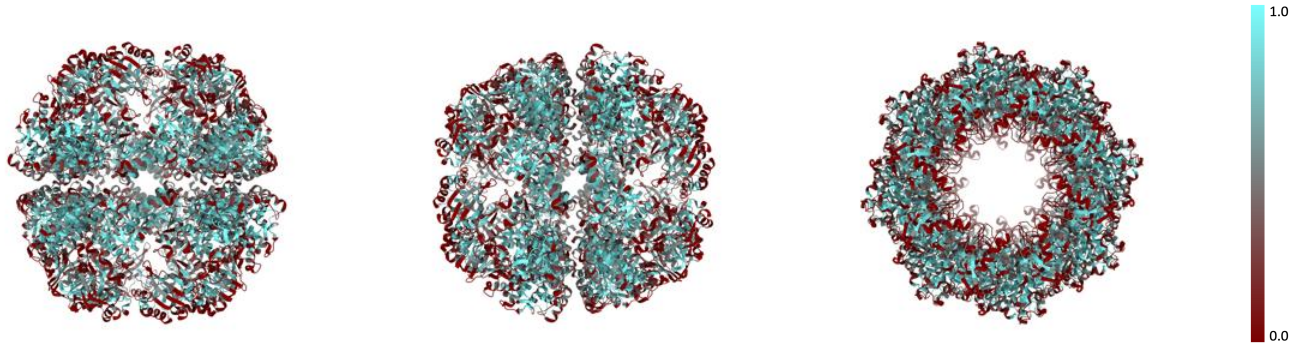
9.2 Q-score mapped to coordinate model (i)



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.

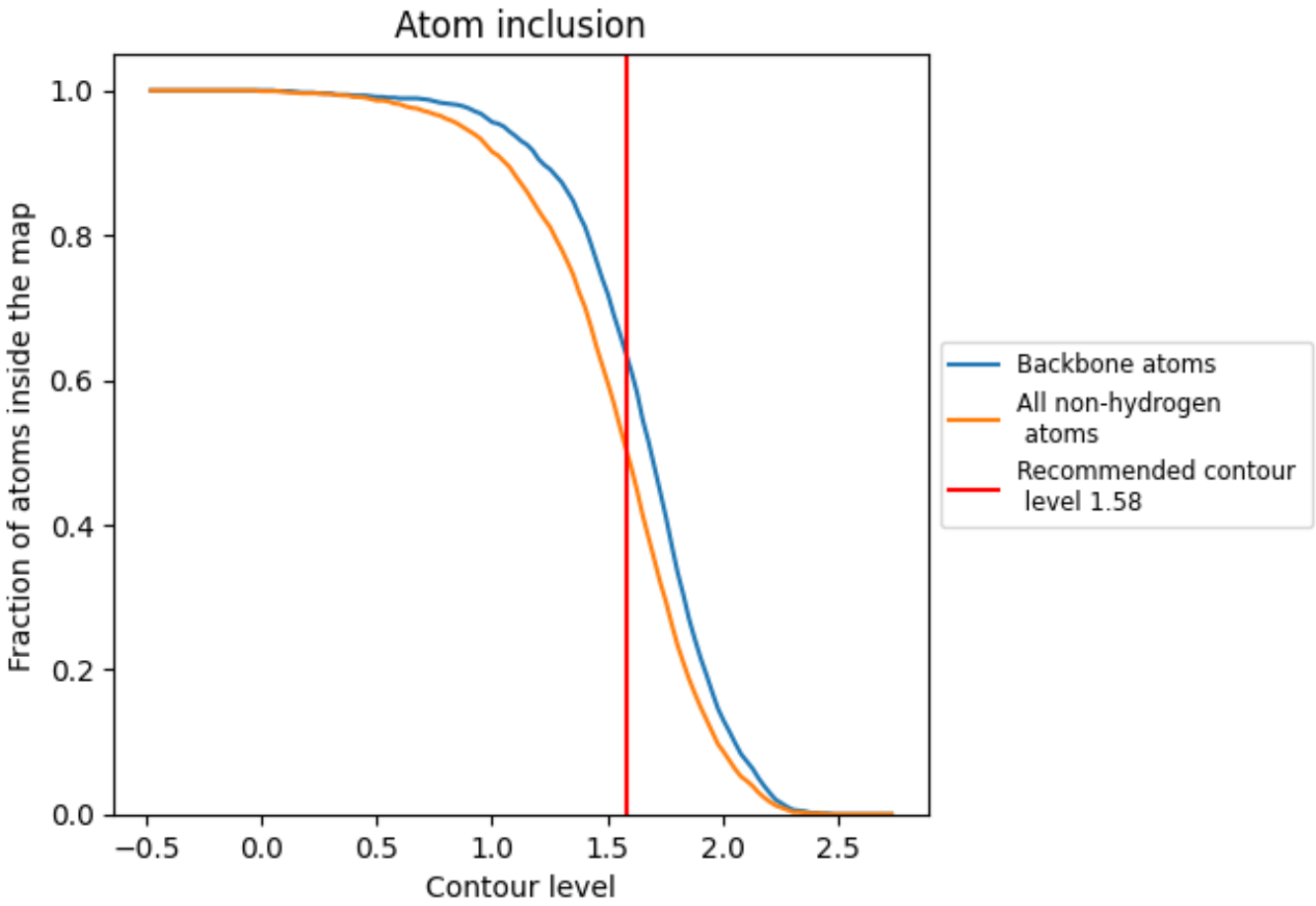
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.58).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.58) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5060	0.1120
A	0.5070	0.1120
B	0.5070	0.1130
C	0.5070	0.1130
D	0.5070	0.1130
E	0.5070	0.1120
F	0.5070	0.1130
G	0.5070	0.1120
H	0.5070	0.1120
I	0.5060	0.1110
J	0.5060	0.1110
K	0.5060	0.1110
L	0.5060	0.1120
M	0.5060	0.1110
N	0.5060	0.1110
O	0.5060	0.1100
P	0.5060	0.1100