



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:33 PM UTC

PDB ID : 3IZJ / pdb_00003izj
EMDB ID : EMD-5246
Title : Mm-cpn rls with ATP and AlFx
Authors : Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.;
Chiu, W.; Frydman, J.
Deposited on : 2010-10-29
Resolution : 6.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

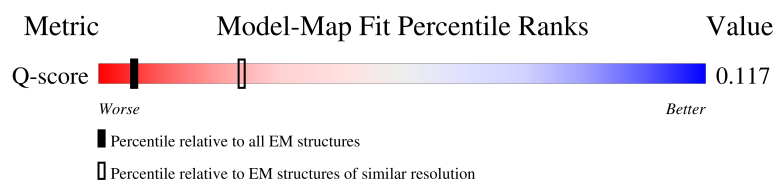
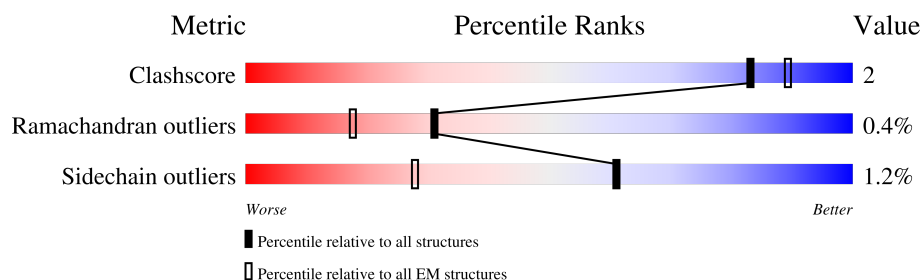
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 6.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	479 (6.40 - 7.40)

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

Mol	Chain	Length	Quality of chain
1	A	513	39% 93% 6%
1	B	513	39% 93% 6%
1	C	513	39% 92% 6%
1	D	513	39% 92% 7%

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Mol	Chain	Length	Quality of chain
1	E	513	39% 92% 6%
1	F	513	39% 92% 6%
1	G	513	39% 93% 6%
1	H	513	39% 92% 6%
1	I	513	39% 93% 6%
1	J	513	39% 92% 6%
1	K	513	39% 93% 6%
1	L	513	39% 92% 6%
1	M	513	39% 92% 6%
1	N	513	39% 92% 7%
1	O	513	39% 92% 6%
1	P	513	39% 92% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 61440 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
1	A	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	B	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	C	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	D	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	E	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	F	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	G	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	H	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	I	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	J	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	K	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	L	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	M	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	N	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	O	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		
1	P	513	Total	C	N	O	S	0	0
			3840	2385	662	768	25		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	321	ALA	THR	engineered mutation	UNP Q877G8
A	322	ALA	ASN	engineered mutation	UNP Q877G8
A	324	ALA	LYS	engineered mutation	UNP Q877G8
A	325	ALA	ASP	engineered mutation	UNP Q877G8
B	834	ALA	THR	engineered mutation	UNP Q877G8
B	835	ALA	ASN	engineered mutation	UNP Q877G8
B	837	ALA	LYS	engineered mutation	UNP Q877G8
B	838	ALA	ASP	engineered mutation	UNP Q877G8
C	1347	ALA	THR	engineered mutation	UNP Q877G8
C	1348	ALA	ASN	engineered mutation	UNP Q877G8
C	1350	ALA	LYS	engineered mutation	UNP Q877G8
C	1351	ALA	ASP	engineered mutation	UNP Q877G8
D	1860	ALA	THR	engineered mutation	UNP Q877G8
D	1861	ALA	ASN	engineered mutation	UNP Q877G8
D	1863	ALA	LYS	engineered mutation	UNP Q877G8
D	1864	ALA	ASP	engineered mutation	UNP Q877G8
E	2373	ALA	THR	engineered mutation	UNP Q877G8
E	2374	ALA	ASN	engineered mutation	UNP Q877G8
E	2376	ALA	LYS	engineered mutation	UNP Q877G8
E	2377	ALA	ASP	engineered mutation	UNP Q877G8
F	2886	ALA	THR	engineered mutation	UNP Q877G8
F	2887	ALA	ASN	engineered mutation	UNP Q877G8
F	2889	ALA	LYS	engineered mutation	UNP Q877G8
F	2890	ALA	ASP	engineered mutation	UNP Q877G8
G	3399	ALA	THR	engineered mutation	UNP Q877G8
G	3400	ALA	ASN	engineered mutation	UNP Q877G8
G	3402	ALA	LYS	engineered mutation	UNP Q877G8
G	3403	ALA	ASP	engineered mutation	UNP Q877G8
H	3912	ALA	THR	engineered mutation	UNP Q877G8
H	3913	ALA	ASN	engineered mutation	UNP Q877G8
H	3915	ALA	LYS	engineered mutation	UNP Q877G8
H	3916	ALA	ASP	engineered mutation	UNP Q877G8
I	4425	ALA	THR	engineered mutation	UNP Q877G8
I	4426	ALA	ASN	engineered mutation	UNP Q877G8
I	4428	ALA	LYS	engineered mutation	UNP Q877G8
I	4429	ALA	ASP	engineered mutation	UNP Q877G8
J	4938	ALA	THR	engineered mutation	UNP Q877G8
J	4939	ALA	ASN	engineered mutation	UNP Q877G8
J	4941	ALA	LYS	engineered mutation	UNP Q877G8
J	4942	ALA	ASP	engineered mutation	UNP Q877G8
K	5451	ALA	THR	engineered mutation	UNP Q877G8
K	5452	ALA	ASN	engineered mutation	UNP Q877G8
K	5454	ALA	LYS	engineered mutation	UNP Q877G8

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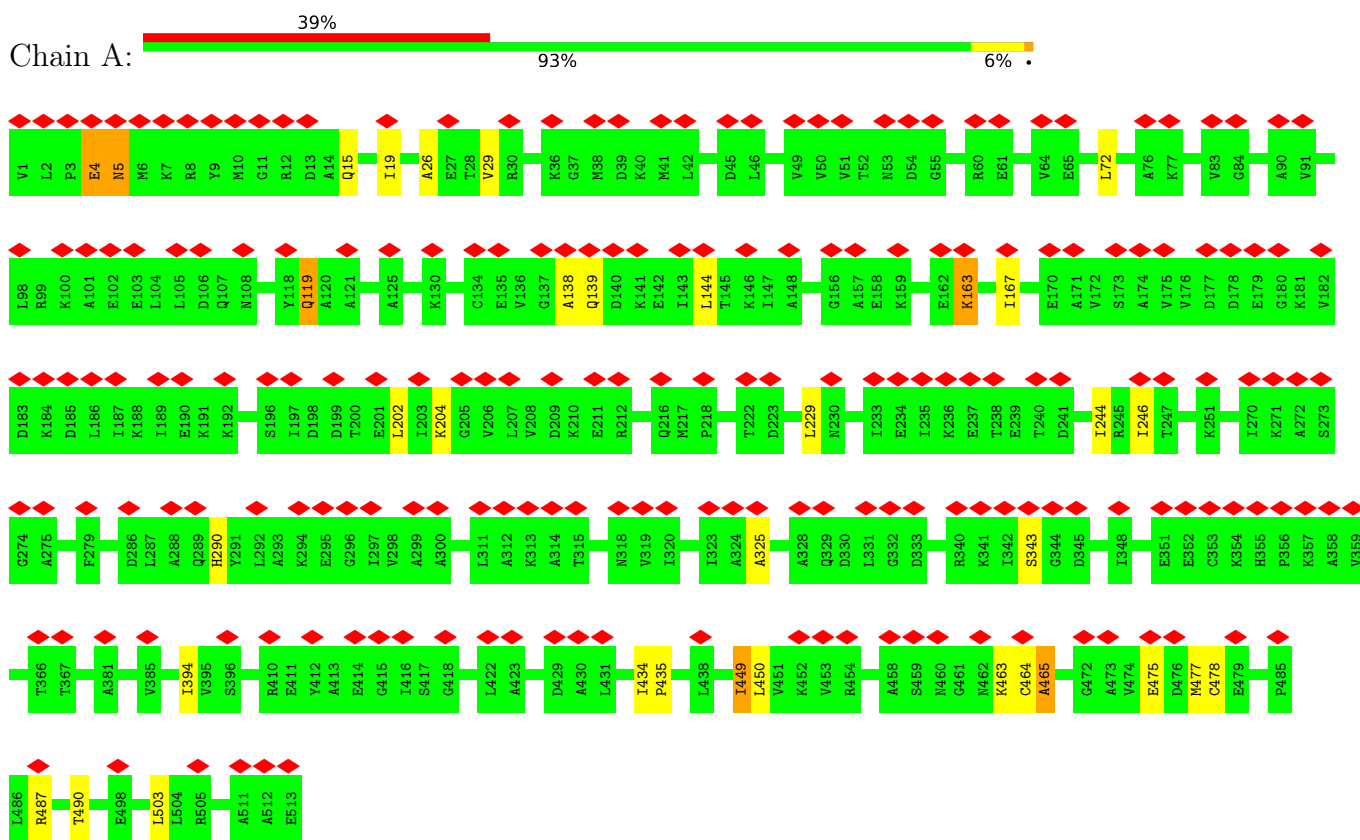
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Chain	Residue	Modelled	Actual	Comment	Reference
K	5455	ALA	ASP	engineered mutation	UNP Q877G8
L	5964	ALA	THR	engineered mutation	UNP Q877G8
L	5965	ALA	ASN	engineered mutation	UNP Q877G8
L	5967	ALA	LYS	engineered mutation	UNP Q877G8
L	5968	ALA	ASP	engineered mutation	UNP Q877G8
M	6477	ALA	THR	engineered mutation	UNP Q877G8
M	6478	ALA	ASN	engineered mutation	UNP Q877G8
M	6480	ALA	LYS	engineered mutation	UNP Q877G8
M	6481	ALA	ASP	engineered mutation	UNP Q877G8
N	6990	ALA	THR	engineered mutation	UNP Q877G8
N	6991	ALA	ASN	engineered mutation	UNP Q877G8
N	6993	ALA	LYS	engineered mutation	UNP Q877G8
N	6994	ALA	ASP	engineered mutation	UNP Q877G8
O	7503	ALA	THR	engineered mutation	UNP Q877G8
O	7504	ALA	ASN	engineered mutation	UNP Q877G8
O	7506	ALA	LYS	engineered mutation	UNP Q877G8
O	7507	ALA	ASP	engineered mutation	UNP Q877G8
P	8016	ALA	THR	engineered mutation	UNP Q877G8
P	8017	ALA	ASN	engineered mutation	UNP Q877G8
P	8019	ALA	LYS	engineered mutation	UNP Q877G8
P	8020	ALA	ASP	engineered mutation	UNP Q877G8

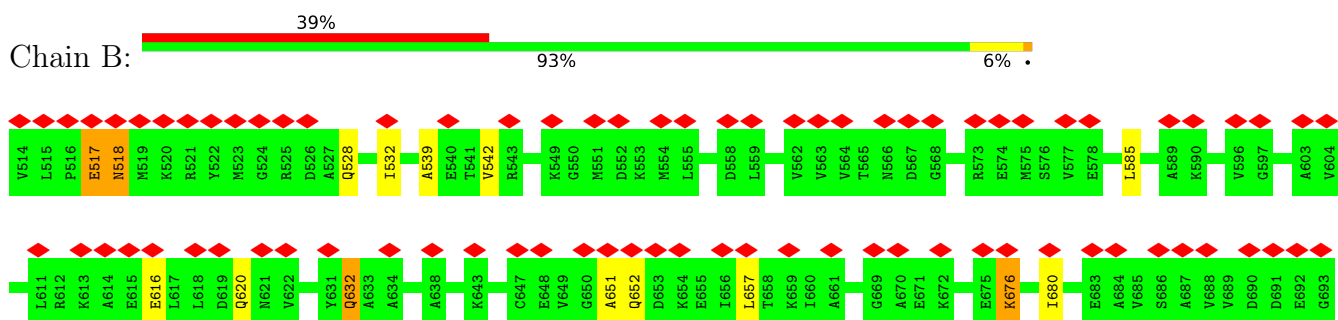
3 Residue-property plots

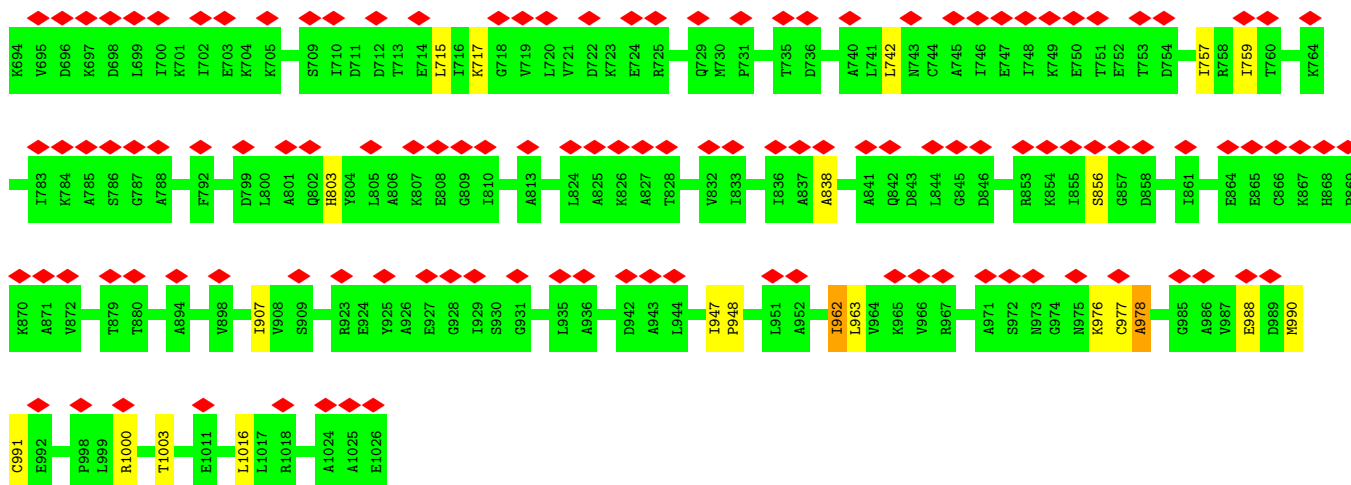
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Chaperonin

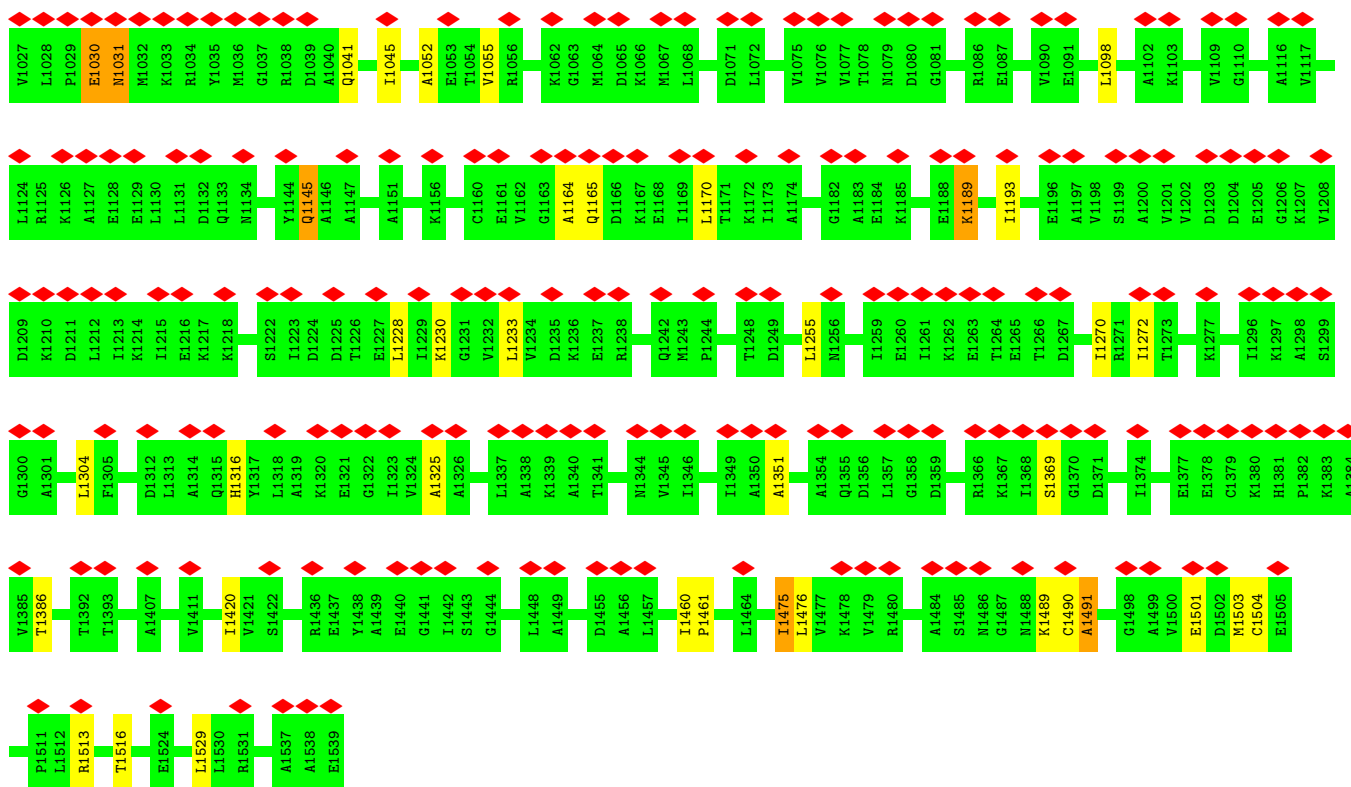
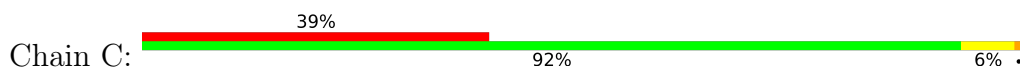


• Molecule 1: Chaperonin

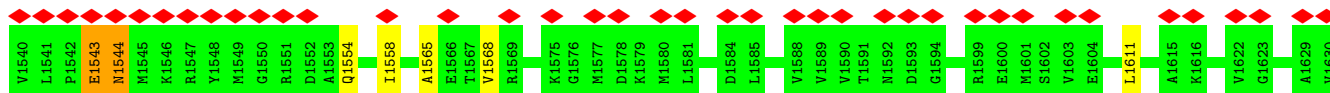
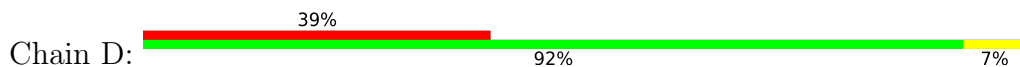


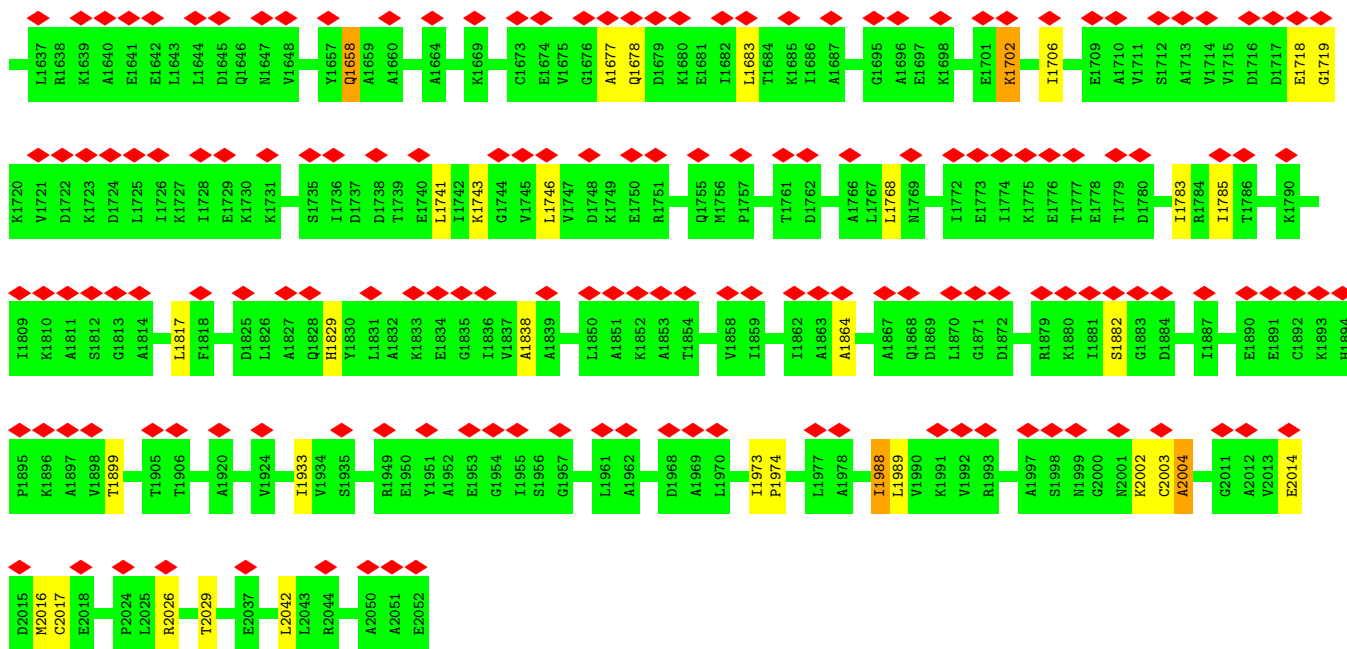


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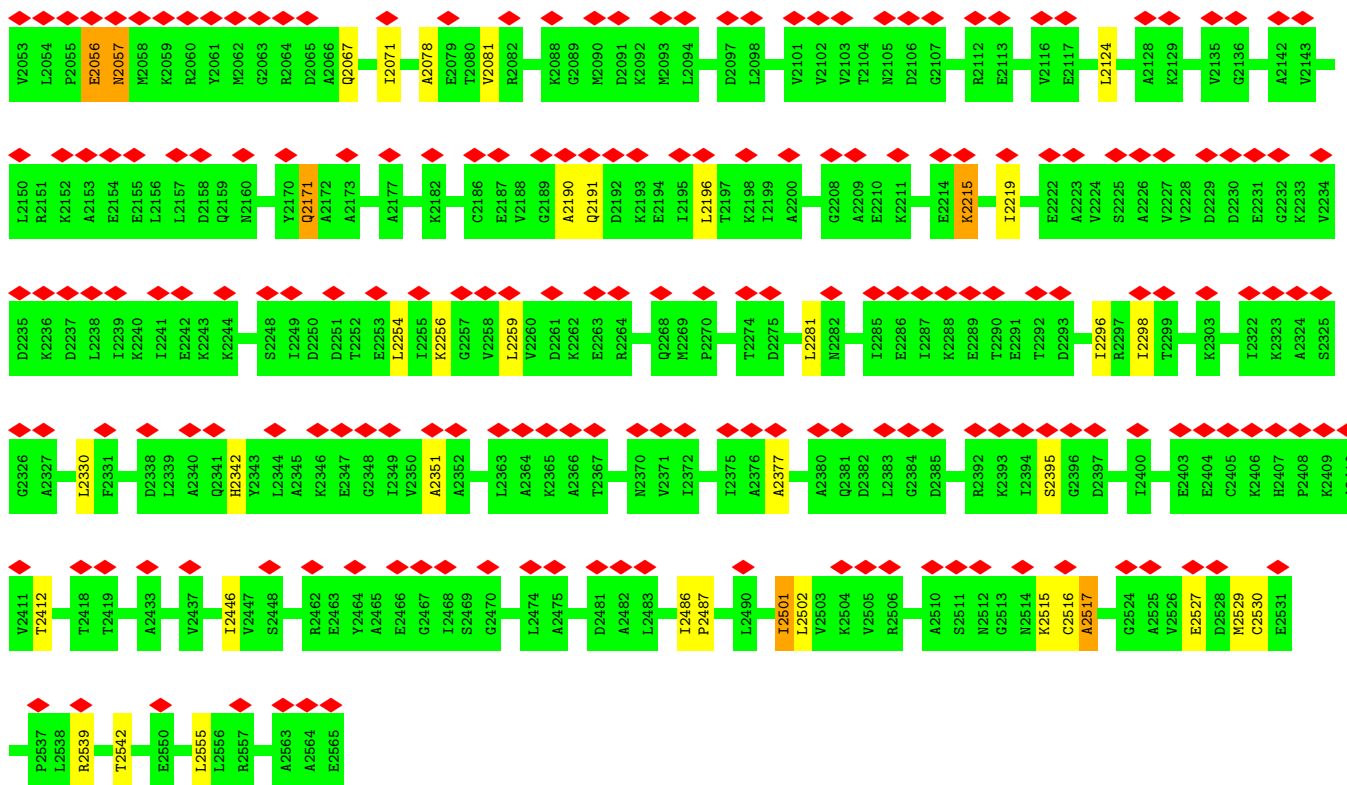
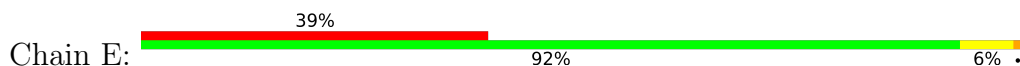


• Molecule 1: Chaperonin



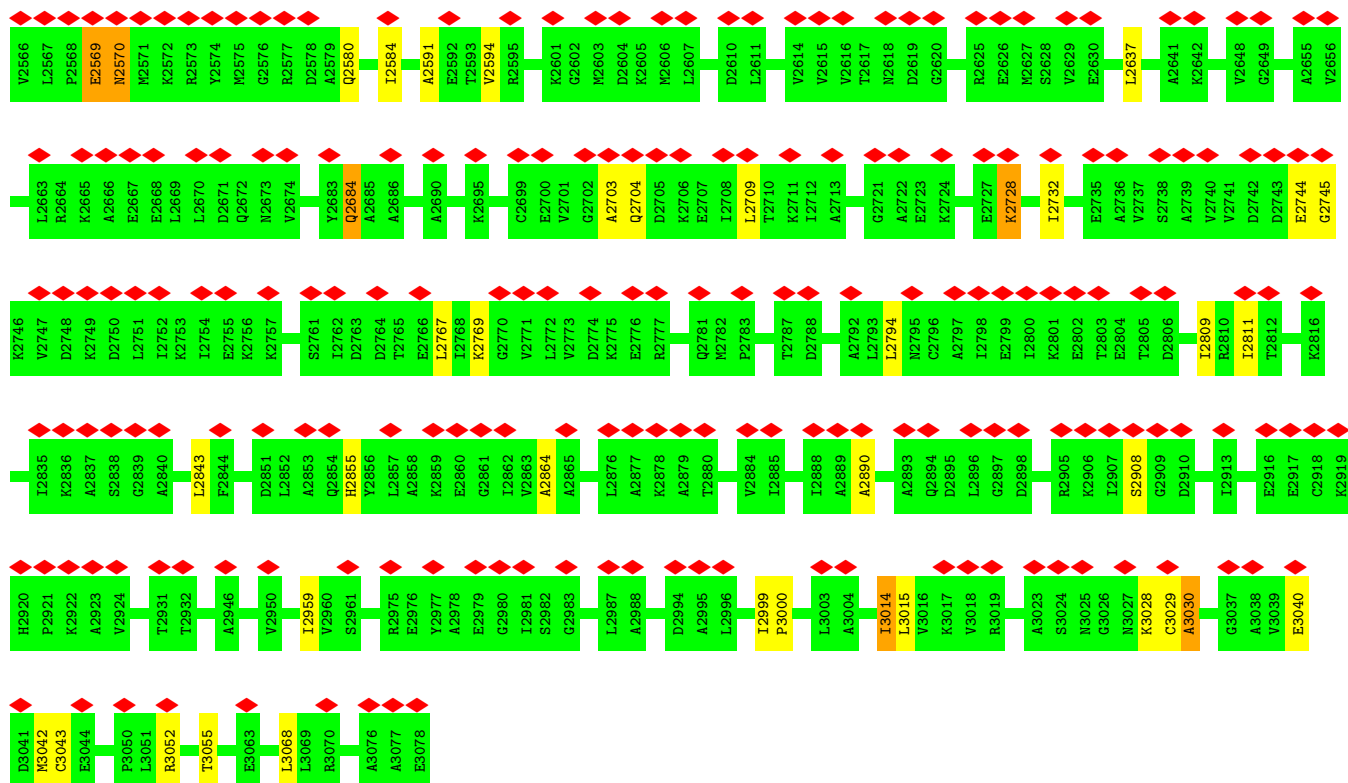


• Molecule 1: Chaperonin

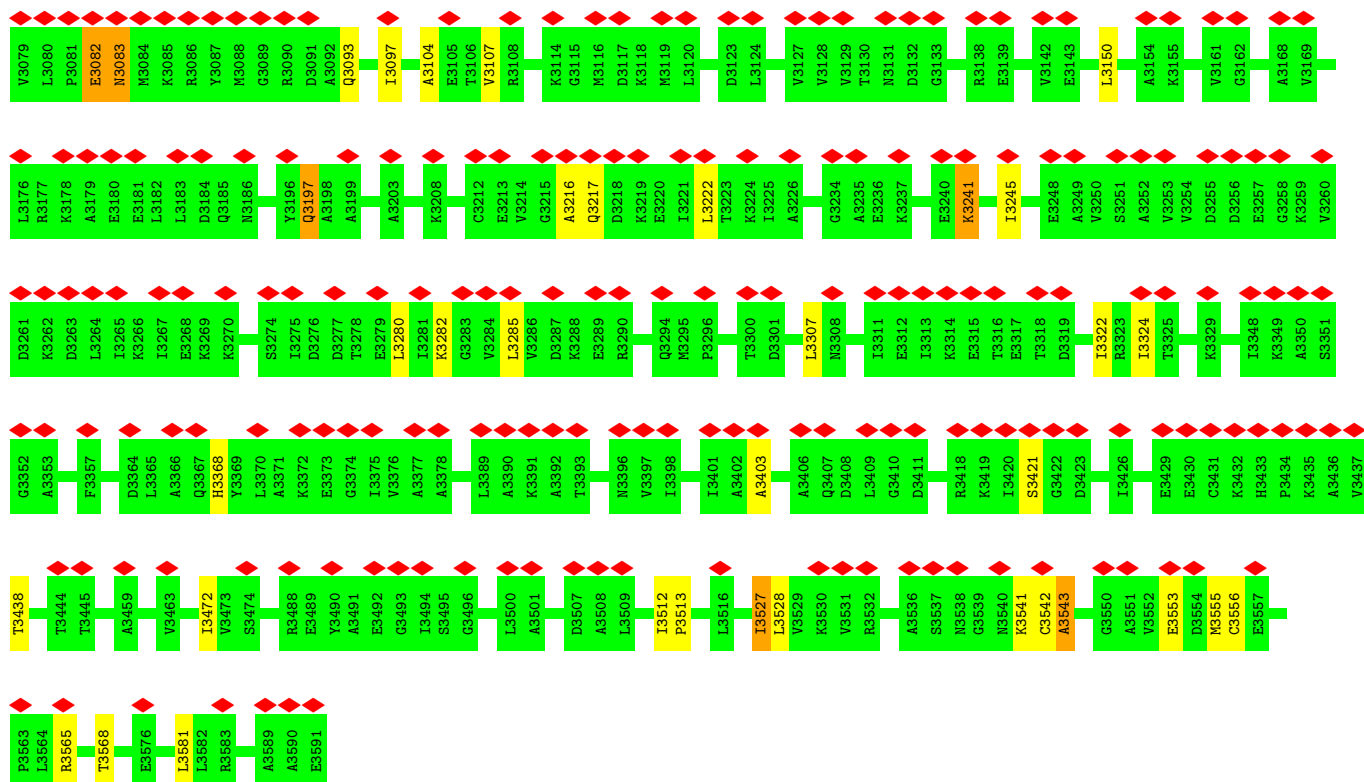
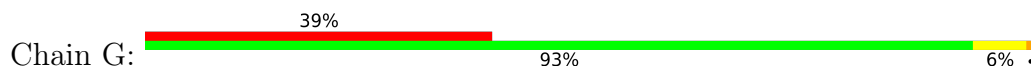


• Molecule 1: Chaperonin



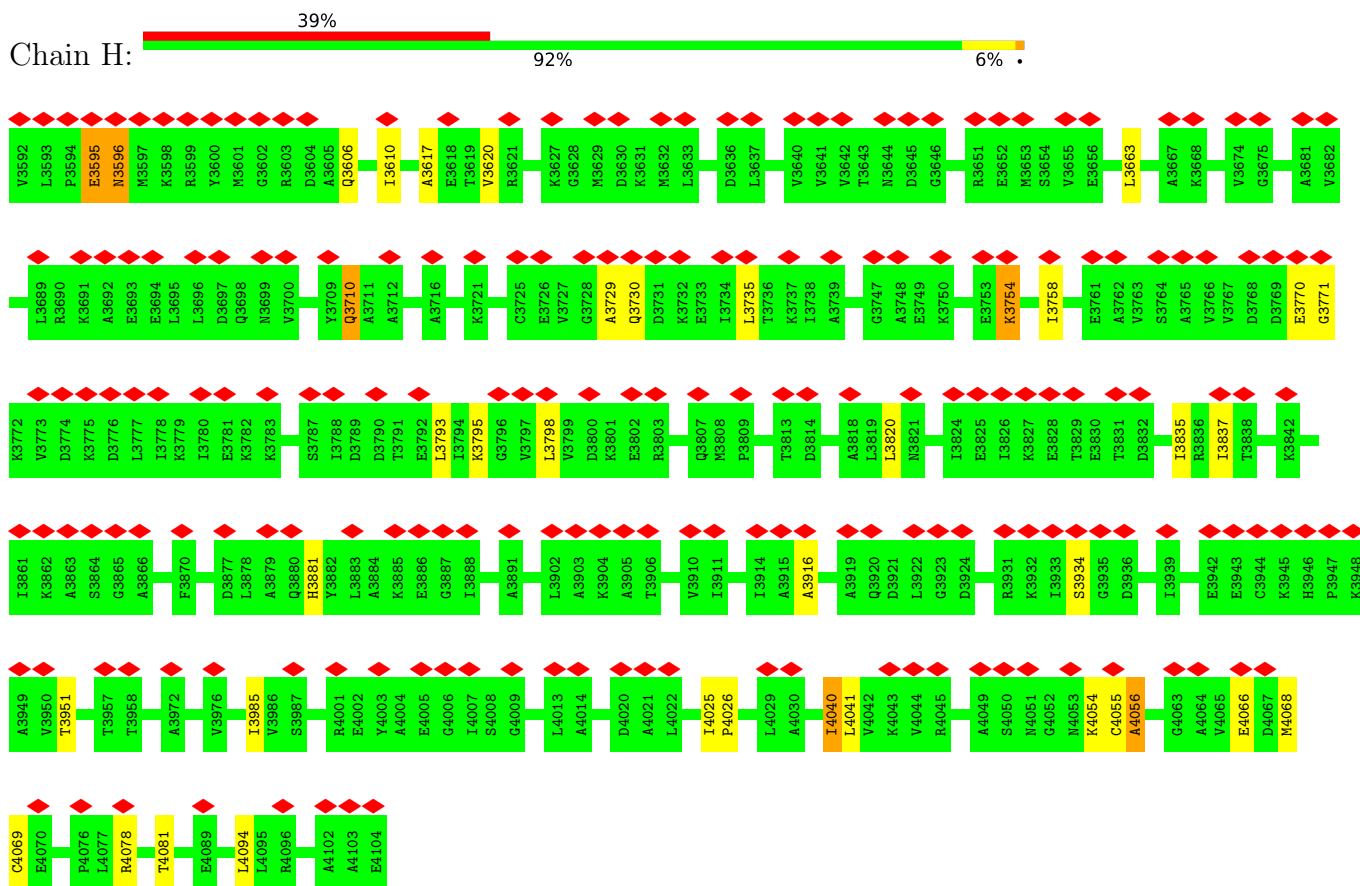


• Molecule 1: Chaperonin



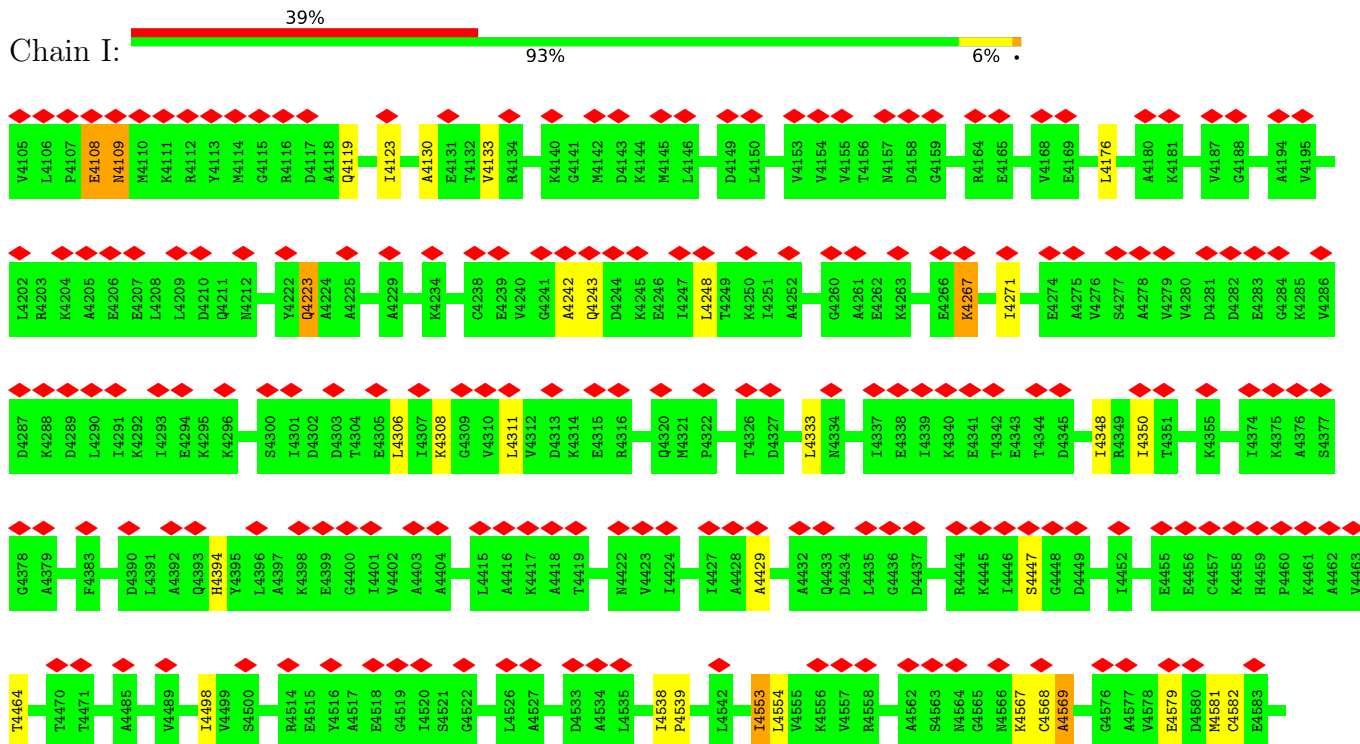
• Molecule 1: Chaperonin

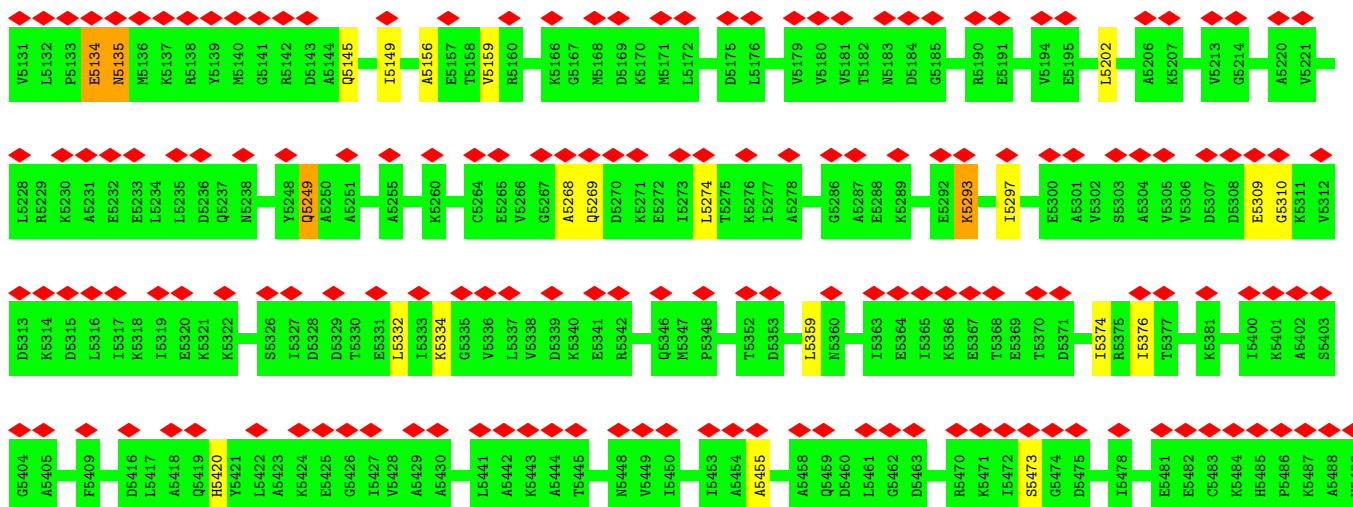
Chain H:

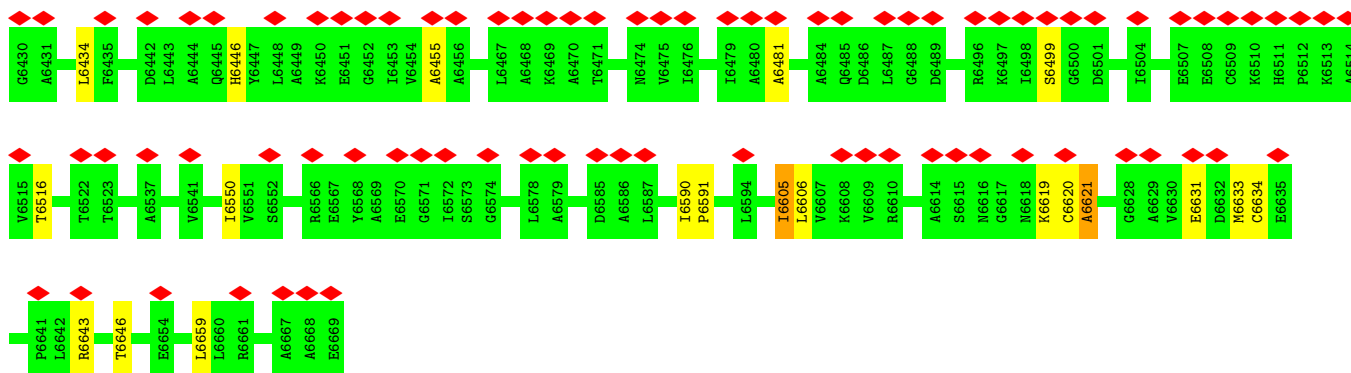


• Molecule 1: Chaperonin

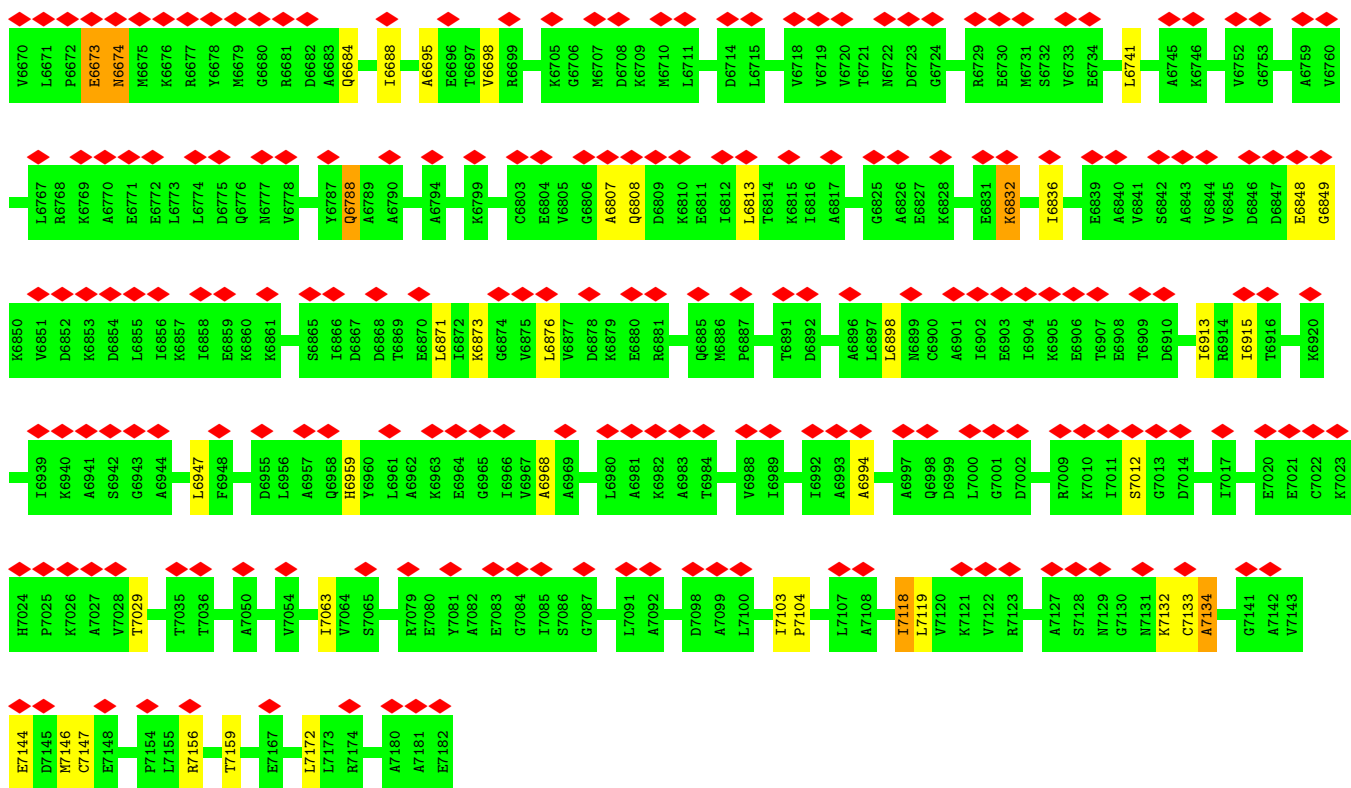
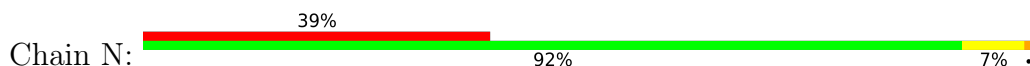
Chain I:



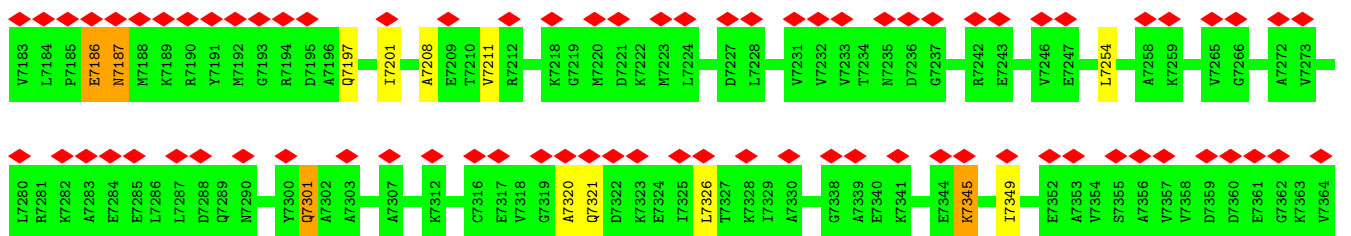
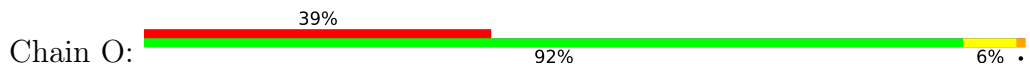


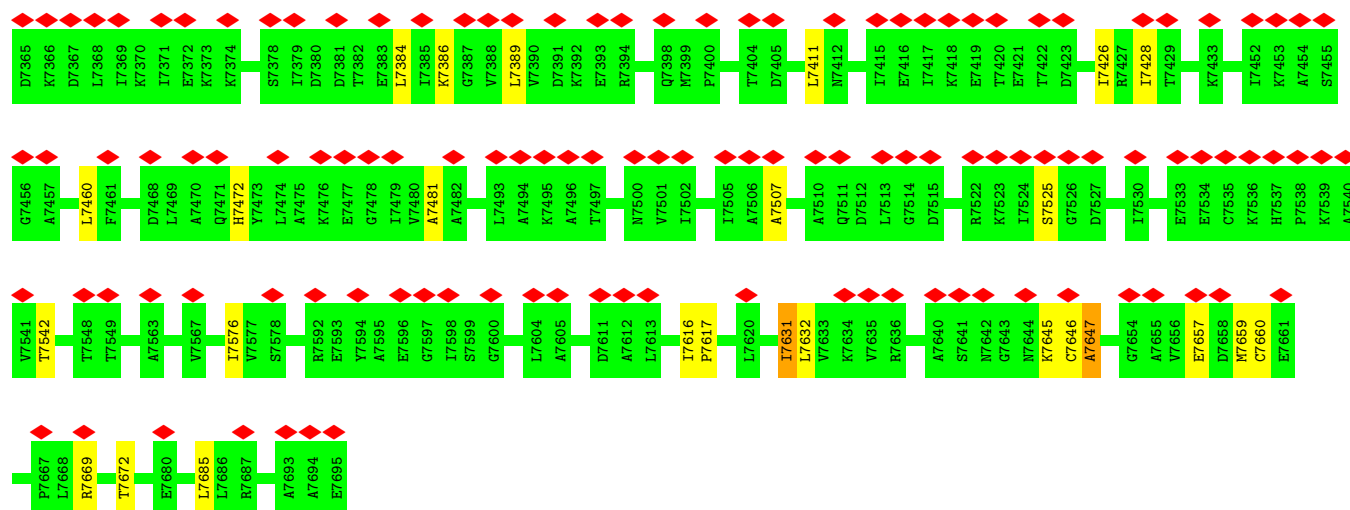


• Molecule 1: Chaperonin

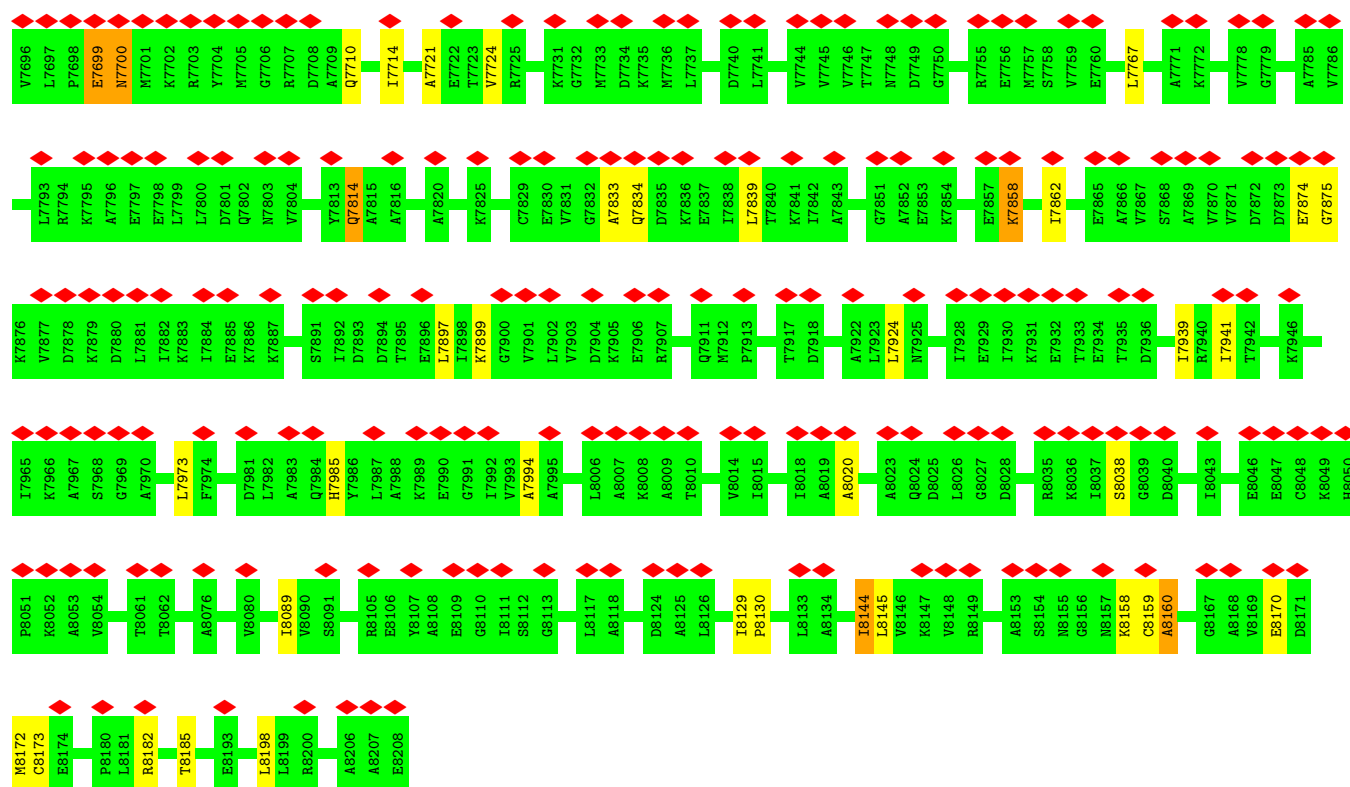
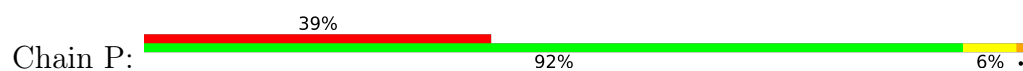


• Molecule 1: Chaperonin





• Molecule 1: Chaperonin



4 Experimental information

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 ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	1.021	Depositor
Minimum map value	-0.478	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.35	Depositor
Map size ($\text{\AA}$)	255.36002, 255.36002, 255.36002	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	B	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	C	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	D	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	E	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	F	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	G	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	H	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	I	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	J	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	K	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	L	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	M	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	N	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	O	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
1	P	0.96	5/3863 (0.1%)	1.05	6/5199 (0.1%)
All	All	0.96	80/61808 (0.1%)	1.05	96/83184 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	4108	GLU	C-O	-9.94	1.11	1.23
1	K	5134	GLU	C-O	-9.94	1.11	1.23
1	J	4621	GLU	C-O	-9.90	1.12	1.23
1	L	5647	GLU	C-O	-9.90	1.12	1.23
1	A	4	GLU	C-O	-9.88	1.12	1.23
1	C	1030	GLU	C-O	-9.88	1.12	1.23
1	E	2056	GLU	C-O	-9.88	1.12	1.23
1	G	3082	GLU	C-O	-9.88	1.12	1.23
1	M	6160	GLU	C-O	-9.88	1.12	1.23
1	O	7186	GLU	C-O	-9.88	1.12	1.23
1	B	517	GLU	C-O	-9.84	1.12	1.23
1	D	1543	GLU	C-O	-9.84	1.12	1.23
1	F	2569	GLU	C-O	-9.84	1.12	1.23
1	H	3595	GLU	C-O	-9.84	1.12	1.23
1	N	6673	GLU	C-O	-9.84	1.12	1.23
1	P	7699	GLU	C-O	-9.84	1.12	1.23
1	J	4621	GLU	C-N	9.57	1.47	1.33
1	L	5647	GLU	C-N	9.57	1.47	1.33
1	I	4108	GLU	C-N	9.53	1.47	1.33
1	K	5134	GLU	C-N	9.53	1.47	1.33
1	A	4	GLU	C-N	9.53	1.47	1.33
1	C	1030	GLU	C-N	9.53	1.47	1.33
1	E	2056	GLU	C-N	9.53	1.47	1.33
1	G	3082	GLU	C-N	9.53	1.47	1.33
1	M	6160	GLU	C-N	9.53	1.47	1.33
1	O	7186	GLU	C-N	9.53	1.47	1.33
1	B	517	GLU	C-N	9.52	1.47	1.33
1	D	1543	GLU	C-N	9.52	1.47	1.33
1	F	2569	GLU	C-N	9.52	1.47	1.33
1	H	3595	GLU	C-N	9.52	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	6673	GLU	C-N	9.52	1.47	1.33
1	P	7699	GLU	C-N	9.52	1.47	1.33
1	M	6621	ALA	C-O	-6.78	1.15	1.24
1	B	978	ALA	C-O	-6.78	1.15	1.24
1	D	2004	ALA	C-O	-6.78	1.15	1.24
1	F	3030	ALA	C-O	-6.78	1.15	1.24
1	H	4056	ALA	C-O	-6.78	1.15	1.24
1	O	7647	ALA	C-O	-6.76	1.15	1.24
1	L	6108	ALA	C-O	-6.75	1.15	1.24
1	N	7134	ALA	C-O	-6.75	1.15	1.24
1	K	5595	ALA	C-O	-6.72	1.15	1.24
1	A	465	ALA	C-O	-6.70	1.15	1.24
1	C	1491	ALA	C-O	-6.70	1.15	1.24
1	E	2517	ALA	C-O	-6.70	1.15	1.24
1	G	3543	ALA	C-O	-6.70	1.15	1.24
1	I	4569	ALA	C-O	-6.70	1.15	1.24
1	J	5082	ALA	C-O	-6.69	1.15	1.24
1	P	8160	ALA	C-O	-6.69	1.15	1.24
1	J	4736	GLN	C-O	-6.31	1.16	1.24
1	P	7814	GLN	C-O	-6.31	1.16	1.24
1	A	119	GLN	C-O	-6.28	1.16	1.24
1	C	1145	GLN	C-O	-6.28	1.16	1.24
1	E	2171	GLN	C-O	-6.28	1.16	1.24
1	G	3197	GLN	C-O	-6.28	1.16	1.24
1	M	6275	GLN	C-O	-6.28	1.16	1.24
1	O	7301	GLN	C-O	-6.28	1.16	1.24
1	I	4223	GLN	C-O	-6.25	1.16	1.24
1	K	5249	GLN	C-O	-6.25	1.16	1.24
1	B	632	GLN	C-O	-6.25	1.16	1.24
1	D	1658	GLN	C-O	-6.25	1.16	1.24
1	F	2684	GLN	C-O	-6.25	1.16	1.24
1	H	3710	GLN	C-O	-6.25	1.16	1.24
1	L	5762	GLN	C-O	-6.25	1.16	1.24
1	N	6788	GLN	C-O	-6.25	1.16	1.24
1	J	4736	GLN	C-N	5.07	1.40	1.33
1	P	7814	GLN	C-N	5.07	1.40	1.33
1	I	4223	GLN	C-N	5.05	1.40	1.33
1	O	7301	GLN	C-N	5.05	1.40	1.33
1	B	632	GLN	C-N	5.04	1.40	1.33
1	D	1658	GLN	C-N	5.04	1.40	1.33
1	F	2684	GLN	C-N	5.04	1.40	1.33
1	H	3710	GLN	C-N	5.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	5762	GLN	C-N	5.04	1.40	1.33
1	N	6788	GLN	C-N	5.04	1.40	1.33
1	A	119	GLN	C-N	5.04	1.40	1.33
1	C	1145	GLN	C-N	5.04	1.40	1.33
1	E	2171	GLN	C-N	5.04	1.40	1.33
1	G	3197	GLN	C-N	5.04	1.40	1.33
1	K	5249	GLN	C-N	5.04	1.40	1.33
1	M	6275	GLN	C-N	5.04	1.40	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	7411	LEU	CD1-CG-CD2	-6.29	96.95	110.80
1	A	229	LEU	CD1-CG-CD2	-6.29	96.97	110.80
1	B	742	LEU	CD1-CG-CD2	-6.29	96.97	110.80
1	C	1255	LEU	CD1-CG-CD2	-6.29	96.97	110.80
1	D	1768	LEU	CD1-CG-CD2	-6.29	96.97	110.80
1	E	2281	LEU	CD1-CG-CD2	-6.29	96.97	110.80
1	F	2794	LEU	CD1-CG-CD2	-6.29	96.97	110.80
1	G	3307	LEU	CD1-CG-CD2	-6.29	96.97	110.80
1	H	3820	LEU	CD1-CG-CD2	-6.29	96.97	110.80
1	J	4846	LEU	CD1-CG-CD2	-6.28	96.98	110.80
1	I	4333	LEU	CD1-CG-CD2	-6.28	96.99	110.80
1	M	6385	LEU	CD1-CG-CD2	-6.28	96.99	110.80
1	L	5872	LEU	CD1-CG-CD2	-6.27	97.00	110.80
1	P	7924	LEU	CD1-CG-CD2	-6.27	97.01	110.80
1	K	5359	LEU	CD1-CG-CD2	-6.26	97.02	110.80
1	N	6898	LEU	CD1-CG-CD2	-6.26	97.03	110.80
1	B	517	GLU	N-CA-C	-6.09	101.03	110.10
1	D	1543	GLU	N-CA-C	-6.09	101.03	110.10
1	F	2569	GLU	N-CA-C	-6.09	101.03	110.10
1	H	3595	GLU	N-CA-C	-6.09	101.03	110.10
1	A	4	GLU	N-CA-C	-6.07	101.05	110.10
1	C	1030	GLU	N-CA-C	-6.07	101.05	110.10
1	E	2056	GLU	N-CA-C	-6.07	101.05	110.10
1	G	3082	GLU	N-CA-C	-6.07	101.05	110.10
1	I	4108	GLU	N-CA-C	-6.07	101.06	110.10
1	O	7186	GLU	N-CA-C	-6.05	101.08	110.10
1	J	4621	GLU	N-CA-C	-6.05	101.08	110.10
1	L	5647	GLU	N-CA-C	-6.05	101.08	110.10
1	N	6673	GLU	N-CA-C	-6.05	101.08	110.10
1	P	7699	GLU	N-CA-C	-6.05	101.08	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	5134	GLU	N-CA-C	-6.05	101.09	110.10
1	M	6160	GLU	N-CA-C	-6.04	101.10	110.10
1	I	4108	GLU	CA-C-O	-5.89	114.20	120.92
1	K	5134	GLU	CA-C-O	-5.89	114.20	120.92
1	M	6160	GLU	CA-C-O	-5.89	114.21	120.92
1	O	7186	GLU	CA-C-O	-5.89	114.21	120.92
1	A	4	GLU	CA-C-O	-5.87	114.23	120.92
1	C	1030	GLU	CA-C-O	-5.87	114.23	120.92
1	E	2056	GLU	CA-C-O	-5.87	114.23	120.92
1	G	3082	GLU	CA-C-O	-5.87	114.23	120.92
1	N	6673	GLU	CA-C-O	-5.86	114.24	120.92
1	P	7699	GLU	CA-C-O	-5.86	114.24	120.92
1	B	517	GLU	CA-C-O	-5.84	114.26	120.92
1	D	1543	GLU	CA-C-O	-5.84	114.26	120.92
1	F	2569	GLU	CA-C-O	-5.84	114.26	120.92
1	H	3595	GLU	CA-C-O	-5.84	114.26	120.92
1	J	4621	GLU	CA-C-O	-5.82	114.29	120.92
1	L	5647	GLU	CA-C-O	-5.82	114.29	120.92
1	I	4568	CYS	N-CA-CB	-5.76	102.83	111.64
1	K	5594	CYS	N-CA-CB	-5.76	102.83	111.64
1	N	7133	CYS	N-CA-CB	-5.76	102.83	111.64
1	P	8159	CYS	N-CA-CB	-5.76	102.83	111.64
1	A	464	CYS	N-CA-CB	-5.75	102.85	111.64
1	C	1490	CYS	N-CA-CB	-5.75	102.85	111.64
1	E	2516	CYS	N-CA-CB	-5.75	102.85	111.64
1	G	3542	CYS	N-CA-CB	-5.75	102.85	111.64
1	B	977	CYS	N-CA-CB	-5.74	102.86	111.64
1	D	2003	CYS	N-CA-CB	-5.74	102.86	111.64
1	F	3029	CYS	N-CA-CB	-5.74	102.86	111.64
1	H	4055	CYS	N-CA-CB	-5.74	102.86	111.64
1	J	5081	CYS	N-CA-CB	-5.73	102.87	111.64
1	L	6107	CYS	N-CA-CB	-5.73	102.87	111.64
1	M	6620	CYS	N-CA-CB	-5.73	102.88	111.64
1	O	7646	CYS	N-CA-CB	-5.73	102.88	111.64
1	A	449	ILE	CB-CG1-CD1	5.63	125.63	113.80
1	C	1475	ILE	CB-CG1-CD1	5.63	125.63	113.80
1	E	2501	ILE	CB-CG1-CD1	5.63	125.63	113.80
1	G	3527	ILE	CB-CG1-CD1	5.63	125.63	113.80
1	I	4553	ILE	CB-CG1-CD1	5.63	125.63	113.80
1	K	5579	ILE	CB-CG1-CD1	5.63	125.63	113.80
1	M	6605	ILE	CB-CG1-CD1	5.63	125.63	113.80
1	O	7631	ILE	CB-CG1-CD1	5.63	125.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	962	ILE	CB-CG1-CD1	5.63	125.62	113.80
1	D	1988	ILE	CB-CG1-CD1	5.63	125.62	113.80
1	F	3014	ILE	CB-CG1-CD1	5.63	125.62	113.80
1	H	4040	ILE	CB-CG1-CD1	5.63	125.62	113.80
1	N	7118	ILE	CB-CG1-CD1	5.63	125.62	113.80
1	P	8144	ILE	CB-CG1-CD1	5.63	125.62	113.80
1	J	5066	ILE	CB-CG1-CD1	5.62	125.61	113.80
1	L	6092	ILE	CB-CG1-CD1	5.62	125.61	113.80
1	L	6121	CYS	N-CA-CB	-5.28	102.36	110.01
1	J	5095	CYS	N-CA-CB	-5.28	102.36	110.01
1	N	7147	CYS	N-CA-CB	-5.27	102.36	110.01
1	P	8173	CYS	N-CA-CB	-5.27	102.37	110.01
1	K	5608	CYS	N-CA-CB	-5.27	102.37	110.01
1	M	6634	CYS	N-CA-CB	-5.27	102.37	110.01
1	A	478	CYS	N-CA-CB	-5.26	102.38	110.01
1	C	1504	CYS	N-CA-CB	-5.26	102.38	110.01
1	E	2530	CYS	N-CA-CB	-5.26	102.38	110.01
1	G	3556	CYS	N-CA-CB	-5.26	102.38	110.01
1	I	4582	CYS	N-CA-CB	-5.26	102.38	110.01
1	O	7660	CYS	N-CA-CB	-5.26	102.38	110.01
1	B	991	CYS	N-CA-CB	-5.26	102.39	110.01
1	D	2017	CYS	N-CA-CB	-5.26	102.39	110.01
1	F	3043	CYS	N-CA-CB	-5.26	102.39	110.01
1	H	4069	CYS	N-CA-CB	-5.26	102.39	110.01

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	475	GLU	Mainchain
1	B	632	GLN	Mainchain
1	B	651	ALA	Mainchain
1	B	988	GLU	Mainchain
1	C	1145	GLN	Mainchain
1	C	1164	ALA	Mainchain
1	C	1501	GLU	Mainchain
1	D	1658	GLN	Mainchain
1	D	1677	ALA	Mainchain
1	D	2014	GLU	Mainchain
1	E	2171	GLN	Mainchain

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Mol	Chain	Res	Type	Group
1	E	2190	ALA	Mainchain
1	E	2527	GLU	Mainchain
1	F	2684	GLN	Mainchain
1	F	2703	ALA	Mainchain
1	F	3040	GLU	Mainchain
1	G	3197	GLN	Mainchain
1	G	3216	ALA	Mainchain
1	G	3553	GLU	Mainchain
1	H	3710	GLN	Mainchain
1	H	3729	ALA	Mainchain
1	H	4066	GLU	Mainchain
1	I	4223	GLN	Mainchain
1	I	4242	ALA	Mainchain
1	I	4579	GLU	Mainchain
1	J	4736	GLN	Mainchain
1	J	4755	ALA	Mainchain
1	J	5092	GLU	Mainchain
1	K	5249	GLN	Mainchain
1	K	5268	ALA	Mainchain
1	K	5605	GLU	Mainchain
1	L	5762	GLN	Mainchain
1	L	5781	ALA	Mainchain
1	L	6118	GLU	Mainchain
1	M	6275	GLN	Mainchain
1	M	6294	ALA	Mainchain
1	M	6631	GLU	Mainchain
1	N	6788	GLN	Mainchain
1	N	6807	ALA	Mainchain
1	N	7144	GLU	Mainchain
1	O	7301	GLN	Mainchain
1	O	7320	ALA	Mainchain
1	O	7657	GLU	Mainchain
1	P	7814	GLN	Mainchain
1	P	7833	ALA	Mainchain
1	P	8170	GLU	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3840	0	3986	19	0
1	B	3840	0	3983	20	0
1	C	3840	0	3983	21	0
1	D	3840	0	3983	22	0
1	E	3840	0	3983	21	0
1	F	3840	0	3983	20	0
1	G	3840	0	3983	19	0
1	H	3840	0	3983	21	0
1	I	3840	0	3983	19	0
1	J	3840	0	3983	21	0
1	K	3840	0	3983	20	0
1	L	3840	0	3983	21	0
1	M	3840	0	3983	21	0
1	N	3840	0	3983	22	0
1	O	3840	0	3983	21	0
1	P	3840	0	3983	20	0
All	All	61440	0	63731	296	0

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

All (296) 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:K:5134:GLU:O	1:K:5135:ASN:HB2	2.00	0.61
1:A:4:GLU:O	1:A:5:ASN:HB2	2.00	0.61
1:H:3595:GLU:O	1:H:3596:ASN:HB2	2.00	0.61
1:J:4621:GLU:O	1:J:4622:ASN:HB2	2.00	0.61
1:P:7699:GLU:O	1:P:7700:ASN:HB2	2.00	0.61
1:F:2569:GLU:O	1:F:2570:ASN:HB2	2.00	0.61
1:B:517:GLU:O	1:B:518:ASN:HB2	2.00	0.60
1:L:5647:GLU:O	1:L:5648:ASN:HB2	2.00	0.60
1:I:4108:GLU:O	1:I:4109:ASN:HB2	2.00	0.60
1:M:6160:GLU:O	1:M:6161:ASN:HB2	2.00	0.60
1:O:7186:GLU:O	1:O:7187:ASN:HB2	2.00	0.60
1:E:2056:GLU:O	1:E:2057:ASN:HB2	2.00	0.60
1:G:3082:GLU:O	1:G:3083:ASN:HB2	2.00	0.60
1:C:1030:GLU:O	1:C:1031:ASN:HB2	2.00	0.60
1:N:6673:GLU:O	1:N:6674:ASN:HB2	2.00	0.59
1:D:1543:GLU:O	1:D:1544:ASN:HB2	2.00	0.59
1:H:3595:GLU:O	1:H:3596:ASN:CB	2.60	0.49
1:J:4621:GLU:O	1:J:4622:ASN:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1543:GLU:O	1:D:1544:ASN:CB	2.60	0.49
1:E:2056:GLU:O	1:E:2057:ASN:CB	2.60	0.49
1:H:4054:LYS:N	1:H:4054:LYS:HD2	2.28	0.49
1:J:5080:LYS:N	1:J:5080:LYS:HD2	2.28	0.49
1:O:7186:GLU:O	1:O:7187:ASN:CB	2.60	0.49
1:A:463:LYS:HD2	1:A:463:LYS:N	2.28	0.49
1:G:3541:LYS:HD2	1:G:3541:LYS:N	2.28	0.49
1:I:4567:LYS:HD2	1:I:4567:LYS:N	2.28	0.49
1:K:5593:LYS:HD2	1:K:5593:LYS:N	2.28	0.49
1:N:6673:GLU:O	1:N:6674:ASN:CB	2.60	0.49
1:G:3082:GLU:O	1:G:3083:ASN:CB	2.60	0.49
1:I:4108:GLU:O	1:I:4109:ASN:CB	2.60	0.49
1:K:5134:GLU:O	1:K:5135:ASN:CB	2.60	0.49
1:A:4:GLU:O	1:A:5:ASN:CB	2.60	0.49
1:L:5647:GLU:O	1:L:5648:ASN:CB	2.60	0.49
1:B:517:GLU:O	1:B:518:ASN:CB	2.60	0.49
1:F:3028:LYS:N	1:F:3028:LYS:HD2	2.28	0.48
1:M:6160:GLU:O	1:M:6161:ASN:CB	2.60	0.48
1:P:8158:LYS:HD2	1:P:8158:LYS:N	2.28	0.48
1:B:976:LYS:HD2	1:B:976:LYS:N	2.28	0.48
1:C:1030:GLU:O	1:C:1031:ASN:CB	2.60	0.48
1:L:6106:LYS:HD2	1:L:6106:LYS:N	2.28	0.48
1:C:1489:LYS:HD2	1:C:1489:LYS:N	2.28	0.48
1:F:2569:GLU:O	1:F:2570:ASN:CB	2.60	0.48
1:M:6619:LYS:HD2	1:M:6619:LYS:N	2.28	0.48
1:N:7156:ARG:HA	1:N:7159:THR:HG22	1.96	0.48
1:P:7699:GLU:O	1:P:7700:ASN:CB	2.60	0.48
1:D:2026:ARG:HA	1:D:2029:THR:HG22	1.96	0.48
1:E:2539:ARG:HA	1:E:2542:THR:HG22	1.96	0.48
1:M:6643:ARG:HA	1:M:6646:THR:HG22	1.96	0.48
1:O:7669:ARG:HA	1:O:7672:THR:HG22	1.96	0.48
1:C:1513:ARG:HA	1:C:1516:THR:HG22	1.96	0.48
1:O:7645:LYS:HD2	1:O:7645:LYS:N	2.28	0.48
1:E:2515:LYS:HD2	1:E:2515:LYS:N	2.28	0.48
1:D:2002:LYS:HD2	1:D:2002:LYS:N	2.28	0.47
1:N:7132:LYS:HD2	1:N:7132:LYS:N	2.28	0.47
1:P:8182:ARG:HA	1:P:8185:THR:HG22	1.96	0.47
1:F:3052:ARG:HA	1:F:3055:THR:HG22	1.96	0.47
1:P:8144:ILE:HG13	1:P:8145:LEU:N	2.29	0.47
1:F:3014:ILE:HG13	1:F:3015:LEU:N	2.29	0.47
1:O:7631:ILE:HG13	1:O:7632:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2501:ILE:HG13	1:E:2502:LEU:N	2.29	0.47
1:G:3472:ILE:C	1:G:3472:ILE:HD12	2.40	0.47
1:G:3527:ILE:HG13	1:G:3528:LEU:N	2.29	0.47
1:I:4498:ILE:C	1:I:4498:ILE:HD12	2.40	0.47
1:I:4553:ILE:HG13	1:I:4554:LEU:N	2.29	0.47
1:D:1933:ILE:C	1:D:1933:ILE:HD12	2.40	0.47
1:H:3985:ILE:HD12	1:H:3985:ILE:C	2.40	0.47
1:A:449:ILE:HG13	1:A:450:LEU:N	2.29	0.47
1:B:907:ILE:C	1:B:907:ILE:HD12	2.40	0.47
1:D:1988:ILE:HG13	1:D:1989:LEU:N	2.29	0.47
1:H:4025:ILE:HB	1:H:4026:PRO:CD	2.45	0.47
1:K:5579:ILE:HG13	1:K:5580:LEU:N	2.29	0.47
1:L:6037:ILE:C	1:L:6037:ILE:HD12	2.40	0.47
1:N:7063:ILE:C	1:N:7063:ILE:HD12	2.40	0.47
1:N:7118:ILE:HG13	1:N:7119:LEU:N	2.29	0.47
1:B:1000:ARG:HA	1:B:1003:THR:HG22	1.96	0.47
1:E:2446:ILE:C	1:E:2446:ILE:HD12	2.40	0.47
1:H:4078:ARG:HA	1:H:4081:THR:HG22	1.96	0.47
1:J:5011:ILE:HD12	1:J:5011:ILE:C	2.40	0.47
1:J:5051:ILE:HB	1:J:5052:PRO:CD	2.45	0.47
1:J:5104:ARG:HA	1:J:5107:THR:HG22	1.96	0.47
1:K:5524:ILE:C	1:K:5524:ILE:HD12	2.40	0.47
1:L:6130:ARG:HA	1:L:6133:THR:HG22	1.96	0.47
1:B:962:ILE:HG13	1:B:963:LEU:N	2.29	0.47
1:H:4040:ILE:HG13	1:H:4041:LEU:N	2.29	0.47
1:O:7576:ILE:HD12	1:O:7576:ILE:C	2.40	0.47
1:A:434:ILE:HB	1:A:435:PRO:CD	2.45	0.47
1:G:3512:ILE:HB	1:G:3513:PRO:CD	2.45	0.47
1:I:4591:ARG:HA	1:I:4594:THR:HG22	1.96	0.47
1:J:5066:ILE:HG13	1:J:5067:LEU:N	2.29	0.47
1:K:5564:ILE:HB	1:K:5565:PRO:CD	2.45	0.47
1:L:6092:ILE:HG13	1:L:6093:LEU:N	2.29	0.47
1:A:394:ILE:C	1:A:394:ILE:HD12	2.40	0.46
1:C:1420:ILE:HD12	1:C:1420:ILE:C	2.40	0.46
1:F:2999:ILE:HB	1:F:3000:PRO:CD	2.45	0.46
1:G:3565:ARG:HA	1:G:3568:THR:HG22	1.96	0.46
1:I:4538:ILE:HB	1:I:4539:PRO:CD	2.45	0.46
1:M:6550:ILE:HD12	1:M:6550:ILE:C	2.40	0.46
1:P:7874:GLU:HA	1:P:7875:GLY:HA3	1.78	0.46
1:F:2959:ILE:HD12	1:F:2959:ILE:C	2.40	0.46
1:N:6848:GLU:HA	1:N:6849:GLY:HA3	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:8089:ILE:C	1:P:8089:ILE:HD12	2.40	0.46
1:L:6077:ILE:HB	1:L:6078:PRO:CD	2.45	0.46
1:P:8129:ILE:HB	1:P:8130:PRO:CD	2.45	0.46
1:B:947:ILE:HB	1:B:948:PRO:CD	2.45	0.46
1:C:1460:ILE:HB	1:C:1461:PRO:CD	2.45	0.46
1:K:5617:ARG:HA	1:K:5620:THR:HG22	1.96	0.46
1:D:1973:ILE:HB	1:D:1974:PRO:CD	2.45	0.46
1:E:2486:ILE:HB	1:E:2487:PRO:CD	2.45	0.46
1:M:6590:ILE:HB	1:M:6591:PRO:CD	2.45	0.46
1:N:7103:ILE:HB	1:N:7104:PRO:CD	2.45	0.46
1:O:7616:ILE:HB	1:O:7617:PRO:CD	2.45	0.46
1:D:1718:GLU:HA	1:D:1719:GLY:HA3	1.78	0.46
1:F:2744:GLU:HA	1:F:2745:GLY:HA3	1.78	0.46
1:A:487:ARG:HA	1:A:490:THR:HG22	1.96	0.46
1:M:6605:ILE:HG13	1:M:6606:LEU:N	2.29	0.45
1:C:1475:ILE:HG13	1:C:1476:LEU:N	2.29	0.45
1:I:4243:GLN:O	1:I:4243:GLN:HG2	2.17	0.45
1:G:3217:GLN:O	1:G:3217:GLN:HG2	2.17	0.45
1:J:4756:GLN:HG2	1:J:4756:GLN:O	2.17	0.45
1:H:3730:GLN:O	1:H:3730:GLN:HG2	2.17	0.45
1:L:5658:GLN:O	1:L:5662:ILE:HG12	2.17	0.45
1:L:5782:GLN:HG2	1:L:5782:GLN:O	2.17	0.45
1:A:15:GLN:O	1:A:19:ILE:HG12	2.17	0.45
1:B:528:GLN:O	1:B:532:ILE:HG12	2.17	0.45
1:B:652:GLN:O	1:B:652:GLN:HG2	2.17	0.45
1:H:3754:LYS:HE3	1:H:3754:LYS:HA	1.99	0.45
1:K:5145:GLN:O	1:K:5149:ILE:HG12	2.17	0.45
1:F:2704:GLN:O	1:F:2704:GLN:HG2	2.17	0.45
1:J:4780:LYS:HE3	1:J:4780:LYS:HA	1.99	0.45
1:M:6171:GLN:O	1:M:6175:ILE:HG12	2.17	0.44
1:P:7834:GLN:O	1:P:7834:GLN:HG2	2.17	0.44
1:A:163:LYS:HA	1:A:163:LYS:HE3	1.99	0.44
1:C:1041:GLN:O	1:C:1045:ILE:HG12	2.17	0.44
1:F:2728:LYS:HE3	1:F:2728:LYS:HA	1.99	0.44
1:K:5293:LYS:HE3	1:K:5293:LYS:HA	1.99	0.44
1:N:6684:GLN:O	1:N:6688:ILE:HG12	2.17	0.44
1:P:7858:LYS:HE3	1:P:7858:LYS:HA	1.99	0.44
1:C:1165:GLN:HG2	1:C:1165:GLN:O	2.17	0.44
1:K:5269:GLN:O	1:K:5269:GLN:HG2	2.17	0.44
1:A:139:GLN:O	1:A:139:GLN:HG2	2.17	0.44
1:D:1554:GLN:O	1:D:1558:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3606:GLN:O	1:H:3610:ILE:HG12	2.17	0.44
1:M:6295:GLN:O	1:M:6295:GLN:HG2	2.17	0.44
1:B:676:LYS:HE3	1:B:676:LYS:HA	1.99	0.44
1:J:4632:GLN:O	1:J:4636:ILE:HG12	2.17	0.44
1:N:6808:GLN:O	1:N:6808:GLN:HG2	2.17	0.44
1:O:7321:GLN:O	1:O:7321:GLN:HG2	2.17	0.44
1:C:1189:LYS:HE3	1:C:1189:LYS:HA	1.99	0.44
1:E:2191:GLN:HG2	1:E:2191:GLN:O	2.17	0.44
1:E:2529:MET:HE2	1:E:2529:MET:HA	2.00	0.44
1:I:4429:ALA:HB1	1:J:4907:HIS:CE1	2.53	0.44
1:L:5806:LYS:HA	1:L:5806:LYS:HE3	1.99	0.44
1:M:6319:LYS:HE3	1:M:6319:LYS:HA	1.99	0.44
1:O:7659:MET:HA	1:O:7659:MET:HE2	2.00	0.44
1:D:1678:GLN:O	1:D:1678:GLN:HG2	2.17	0.44
1:D:2016:MET:HE2	1:D:2016:MET:HA	2.00	0.44
1:N:7146:MET:HE2	1:N:7146:MET:HA	2.00	0.44
1:B:757:ILE:HA	1:C:1272:ILE:O	2.19	0.43
1:B:838:ALA:HB1	1:C:1316:HIS:CE1	2.53	0.43
1:D:1702:LYS:HE3	1:D:1702:LYS:HA	1.99	0.43
1:F:2890:ALA:HB1	1:G:3368:HIS:CE1	2.53	0.43
1:F:3042:MET:HE2	1:F:3042:MET:HA	2.00	0.43
1:P:8172:MET:HE2	1:P:8172:MET:HA	2.00	0.43
1:A:167:ILE:HG23	1:A:202:LEU:HB2	2.01	0.43
1:K:5297:ILE:HG23	1:K:5332:LEU:HB2	2.01	0.43
1:K:5455:ALA:HB1	1:L:5933:HIS:CE1	2.53	0.43
1:L:5887:ILE:HA	1:M:6402:ILE:O	2.19	0.43
1:N:6832:LYS:HA	1:N:6832:LYS:HE3	1.99	0.43
1:O:7507:ALA:HB1	1:P:7985:HIS:CE1	2.53	0.43
1:D:1783:ILE:HA	1:E:2298:ILE:O	2.19	0.43
1:E:2067:GLN:O	1:E:2071:ILE:HG12	2.17	0.43
1:E:2296:ILE:HA	1:F:2811:ILE:O	2.19	0.43
1:G:3093:GLN:O	1:G:3097:ILE:HG12	2.17	0.43
1:G:3241:LYS:HE3	1:G:3241:LYS:HA	1.99	0.43
1:N:6913:ILE:HA	1:O:7428:ILE:O	2.19	0.43
1:O:7426:ILE:HA	1:P:7941:ILE:O	2.19	0.43
1:C:1193:ILE:HG23	1:C:1228:LEU:HB2	2.01	0.43
1:D:1864:ALA:HB1	1:E:2342:HIS:CE1	2.53	0.43
1:G:3403:ALA:HB1	1:H:3881:HIS:CE1	2.54	0.43
1:K:5309:GLU:HA	1:K:5310:GLY:HA3	1.78	0.43
1:N:6836:ILE:HG23	1:N:6871:LEU:HB2	2.01	0.43
1:O:7197:GLN:O	1:O:7201:ILE:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:7710:GLN:O	1:P:7714:ILE:HG12	2.17	0.43
1:D:1706:ILE:HG23	1:D:1741:LEU:HB2	2.01	0.43
1:I:4119:GLN:O	1:I:4123:ILE:HG12	2.17	0.43
1:M:6323:ILE:HG23	1:M:6358:LEU:HB2	2.01	0.43
1:E:2377:ALA:HB1	1:F:2855:HIS:CE1	2.54	0.43
1:F:2580:GLN:O	1:F:2584:ILE:HG12	2.17	0.43
1:I:4267:LYS:HE3	1:I:4267:LYS:HA	1.99	0.43
1:I:4394:HIS:CE1	1:P:8020:ALA:HB1	2.54	0.43
1:K:5374:ILE:HA	1:L:5889:ILE:O	2.19	0.43
1:A:325:ALA:HB1	1:B:803:HIS:CE1	2.54	0.43
1:A:477:MET:HE2	1:A:477:MET:HA	2.00	0.43
1:C:1503:MET:HA	1:C:1503:MET:HE2	2.00	0.43
1:G:3555:MET:HE2	1:G:3555:MET:HA	2.00	0.43
1:K:5607:MET:HE2	1:K:5607:MET:HA	2.00	0.43
1:L:5968:ALA:HB1	1:M:6446:HIS:CE1	2.54	0.43
1:A:244:ILE:HA	1:B:759:ILE:O	2.19	0.43
1:I:4581:MET:HE2	1:I:4581:MET:HA	2.00	0.43
1:M:6633:MET:HE2	1:M:6633:MET:HA	2.00	0.43
1:A:290:HIS:CE1	1:H:3916:ALA:HB1	2.53	0.43
1:E:2215:LYS:HE3	1:E:2215:LYS:HA	1.99	0.43
1:J:4796:GLU:HA	1:J:4797:GLY:HA3	1.78	0.43
1:M:6481:ALA:HB1	1:N:6959:HIS:CE1	2.53	0.43
1:N:6994:ALA:HB1	1:O:7472:HIS:CE1	2.54	0.43
1:E:2219:ILE:HG23	1:E:2254:LEU:HB2	2.01	0.43
1:F:2809:ILE:HA	1:G:3324:ILE:O	2.19	0.43
1:G:3245:ILE:HG23	1:G:3280:LEU:HB2	2.01	0.43
1:I:4271:ILE:HG23	1:I:4306:LEU:HB2	2.01	0.43
1:I:4350:ILE:O	1:P:7939:ILE:HA	2.19	0.42
1:O:7345:LYS:HE3	1:O:7345:LYS:HA	1.99	0.42
1:O:7349:ILE:HG23	1:O:7384:LEU:HB2	2.01	0.42
1:G:3322:ILE:HA	1:H:3837:ILE:O	2.19	0.42
1:A:246:ILE:O	1:H:3835:ILE:HA	2.19	0.42
1:B:990:MET:HE2	1:B:990:MET:HA	2.00	0.42
1:H:3758:ILE:HG23	1:H:3793:LEU:HB2	2.01	0.42
1:H:3770:GLU:HA	1:H:3771:GLY:HA3	1.78	0.42
1:I:4348:ILE:HA	1:J:4863:ILE:O	2.19	0.42
1:L:5810:ILE:HG23	1:L:5845:LEU:HB2	2.01	0.42
1:C:1270:ILE:HA	1:D:1785:ILE:O	2.19	0.42
1:L:6120:MET:HA	1:L:6120:MET:HE2	2.00	0.42
1:P:7862:ILE:HG23	1:P:7897:LEU:HB2	2.01	0.42
1:B:680:ILE:HG23	1:B:715:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1351:ALA:HB1	1:D:1829:HIS:CE1	2.54	0.42
1:F:2732:ILE:HG23	1:F:2767:LEU:HB2	2.01	0.42
1:J:4784:ILE:HG23	1:J:4819:LEU:HB2	2.01	0.42
1:J:4861:ILE:HA	1:K:5376:ILE:O	2.19	0.42
1:J:4942:ALA:HB1	1:K:5420:HIS:CE1	2.54	0.42
1:M:6400:ILE:HA	1:N:6915:ILE:O	2.19	0.42
1:J:5094:MET:HA	1:J:5094:MET:HE2	2.00	0.42
1:A:204:LYS:HD2	1:A:204:LYS:N	2.35	0.42
1:B:717:LYS:N	1:B:717:LYS:HD2	2.35	0.42
1:F:2769:LYS:HD2	1:F:2769:LYS:N	2.35	0.42
1:H:4068:MET:HA	1:H:4068:MET:HE2	2.00	0.42
1:K:5334:LYS:HD2	1:K:5334:LYS:N	2.35	0.42
1:L:5847:LYS:HD2	1:L:5847:LYS:N	2.35	0.42
1:M:6360:LYS:HD2	1:M:6360:LYS:N	2.35	0.42
1:P:7899:LYS:HD2	1:P:7899:LYS:N	2.35	0.42
1:C:1230:LYS:HD2	1:C:1230:LYS:N	2.35	0.42
1:I:4308:LYS:HD2	1:I:4308:LYS:N	2.35	0.41
1:G:3282:LYS:N	1:G:3282:LYS:HD2	2.35	0.41
1:N:6873:LYS:HD2	1:N:6873:LYS:N	2.35	0.41
1:D:1743:LYS:HD2	1:D:1743:LYS:N	2.35	0.41
1:E:2256:LYS:N	1:E:2256:LYS:HD2	2.35	0.41
1:L:6077:ILE:HB	1:L:6078:PRO:HD3	2.03	0.41
1:N:6876:LEU:HB3	1:N:7029:THR:HG21	2.02	0.41
1:O:7208:ALA:HA	1:O:7211:VAL:HG12	2.03	0.41
1:A:434:ILE:HB	1:A:435:PRO:HD3	2.03	0.41
1:B:539:ALA:HA	1:B:542:VAL:HG12	2.03	0.41
1:B:947:ILE:HB	1:B:948:PRO:HD3	2.03	0.41
1:C:1460:ILE:HB	1:C:1461:PRO:HD3	2.03	0.41
1:D:1746:LEU:HB3	1:D:1899:THR:HG21	2.03	0.41
1:E:2078:ALA:HA	1:E:2081:VAL:HG12	2.03	0.41
1:L:5669:ALA:HA	1:L:5672:VAL:HG12	2.03	0.41
1:M:6182:ALA:HA	1:M:6185:VAL:HG12	2.03	0.41
1:M:6590:ILE:HB	1:M:6591:PRO:HD3	2.03	0.41
1:N:7103:ILE:HB	1:N:7104:PRO:HD3	2.03	0.41
1:O:7386:LYS:N	1:O:7386:LYS:HD2	2.35	0.41
1:D:1565:ALA:HA	1:D:1568:VAL:HG12	2.03	0.41
1:D:1973:ILE:HB	1:D:1974:PRO:HD3	2.03	0.41
1:H:3795:LYS:HD2	1:H:3795:LYS:N	2.35	0.41
1:K:5564:ILE:HB	1:K:5565:PRO:HD3	2.03	0.41
1:C:1052:ALA:HA	1:C:1055:VAL:HG12	2.03	0.41
1:D:1817:LEU:O	1:D:1838:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2259:LEU:HB3	1:E:2412:THR:HG21	2.02	0.41
1:E:2330:LEU:O	1:E:2351:ALA:HA	2.21	0.41
1:F:2591:ALA:HA	1:F:2594:VAL:HG12	2.03	0.41
1:H:3798:LEU:HB3	1:H:3951:THR:HG21	2.03	0.41
1:J:4821:LYS:N	1:J:4821:LYS:HD2	2.35	0.41
1:J:4824:LEU:HB3	1:J:4977:THR:HG21	2.03	0.41
1:N:6695:ALA:HA	1:N:6698:VAL:HG12	2.03	0.41
1:O:7389:LEU:HB3	1:O:7542:THR:HG21	2.02	0.41
1:P:7721:ALA:HA	1:P:7724:VAL:HG12	2.03	0.41
1:K:5156:ALA:HA	1:K:5159:VAL:HG12	2.03	0.41
1:N:6947:LEU:O	1:N:6968:ALA:HA	2.21	0.41
1:O:7460:LEU:O	1:O:7481:ALA:HA	2.21	0.41
1:O:7616:ILE:HB	1:O:7617:PRO:HD3	2.03	0.41
1:C:1233:LEU:HB3	1:C:1386:THR:HG21	2.02	0.40
1:E:2486:ILE:HB	1:E:2487:PRO:HD3	2.03	0.40
1:M:6363:LEU:HB3	1:M:6516:THR:HG21	2.02	0.40
1:A:26:ALA:HA	1:A:29:VAL:HG12	2.03	0.40
1:C:1304:LEU:O	1:C:1325:ALA:HA	2.21	0.40
1:F:2843:LEU:O	1:F:2864:ALA:HA	2.21	0.40
1:B:616:GLU:O	1:B:620:GLN:HG2	2.22	0.40
1:G:3104:ALA:HA	1:G:3107:VAL:HG12	2.03	0.40
1:H:3617:ALA:HA	1:H:3620:VAL:HG12	2.03	0.40
1:H:4025:ILE:HB	1:H:4026:PRO:HD3	2.03	0.40
1:I:4130:ALA:HA	1:I:4133:VAL:HG12	2.03	0.40
1:L:5746:GLU:O	1:L:5750:GLN:HG2	2.22	0.40
1:M:6434:LEU:O	1:M:6455:ALA:HA	2.21	0.40
1:P:7973:LEU:O	1:P:7994:ALA:HA	2.21	0.40
1:G:3285:LEU:HB3	1:G:3438:THR:HG21	2.02	0.40
1:J:5051:ILE:HB	1:J:5052:PRO:HD3	2.03	0.40
1:I:4311:LEU:HB3	1:I:4464:THR:HG21	2.02	0.40
1:J:4643:ALA:HA	1:J:4646:VAL:HG12	2.03	0.40
1:L:5850:LEU:HB3	1:L:6003:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	B	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	C	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	D	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	E	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	F	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	G	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	H	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	I	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	J	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	K	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	L	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	M	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	N	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	O	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
1	P	511/513 (100%)	493 (96%)	16 (3%)	2 (0%)	30	67
All	All	8176/8208 (100%)	7888 (96%)	256 (3%)	32 (0%)	31	67

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	518	ASN
1	C	1031	ASN
1	D	1544	ASN
1	E	2057	ASN
1	F	2570	ASN
1	G	3083	ASN
1	H	3596	ASN
1	I	4109	ASN
1	J	4622	ASN
1	K	5135	ASN
1	L	5648	ASN

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Mol	Chain	Res	Type
1	M	6161	ASN
1	N	6674	ASN
1	O	7187	ASN
1	P	7700	ASN
1	A	465	ALA
1	B	978	ALA
1	C	1491	ALA
1	D	2004	ALA
1	E	2517	ALA
1	F	3030	ALA
1	G	3543	ALA
1	H	4056	ALA
1	I	4569	ALA
1	J	5082	ALA
1	K	5595	ALA
1	L	6108	ALA
1	M	6621	ALA
1	N	7134	ALA
1	O	7647	ALA
1	P	8160	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	B	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	C	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	D	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	E	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	F	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	G	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	H	410/410 (100%)	405 (99%)	5 (1%)	63	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	J	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	K	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	L	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	M	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	N	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	O	410/410 (100%)	405 (99%)	5 (1%)	63	75
1	P	410/410 (100%)	405 (99%)	5 (1%)	63	75
All	All	6560/6560 (100%)	6480 (99%)	80 (1%)	61	75

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	144	LEU
1	A	163	LYS
1	A	343	SER
1	A	503	LEU
1	B	585	LEU
1	B	657	LEU
1	B	676	LYS
1	B	856	SER
1	B	1016	LEU
1	C	1098	LEU
1	C	1170	LEU
1	C	1189	LYS
1	C	1369	SER
1	C	1529	LEU
1	D	1611	LEU
1	D	1683	LEU
1	D	1702	LYS
1	D	1882	SER
1	D	2042	LEU
1	E	2124	LEU
1	E	2196	LEU
1	E	2215	LYS
1	E	2395	SER
1	E	2555	LEU
1	F	2637	LEU

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Mol	Chain	Res	Type
1	F	2709	LEU
1	F	2728	LYS
1	F	2908	SER
1	F	3068	LEU
1	G	3150	LEU
1	G	3222	LEU
1	G	3241	LYS
1	G	3421	SER
1	G	3581	LEU
1	H	3663	LEU
1	H	3735	LEU
1	H	3754	LYS
1	H	3934	SER
1	H	4094	LEU
1	I	4176	LEU
1	I	4248	LEU
1	I	4267	LYS
1	I	4447	SER
1	I	4607	LEU
1	J	4689	LEU
1	J	4761	LEU
1	J	4780	LYS
1	J	4960	SER
1	J	5120	LEU
1	K	5202	LEU
1	K	5274	LEU
1	K	5293	LYS
1	K	5473	SER
1	K	5633	LEU
1	L	5715	LEU
1	L	5787	LEU
1	L	5806	LYS
1	L	5986	SER
1	L	6146	LEU
1	M	6228	LEU
1	M	6300	LEU
1	M	6319	LYS
1	M	6499	SER
1	M	6659	LEU
1	N	6741	LEU
1	N	6813	LEU
1	N	6832	LYS

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Mol	Chain	Res	Type
1	N	7012	SER
1	N	7172	LEU
1	O	7254	LEU
1	O	7326	LEU
1	O	7345	LYS
1	O	7525	SER
1	O	7685	LEU
1	P	7767	LEU
1	P	7839	LEU
1	P	7858	LYS
1	P	8038	SER
1	P	8198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	281	GLN
1	B	743	ASN
1	B	794	GLN
1	C	1256	ASN
1	C	1307	GLN
1	D	1769	ASN
1	D	1820	GLN
1	E	2282	ASN
1	E	2333	GLN
1	F	2672	GLN
1	F	2795	ASN
1	F	2846	GLN
1	G	3204	GLN
1	G	3308	ASN
1	G	3359	GLN
1	G	3572	GLN
1	H	3821	ASN
1	H	3872	GLN
1	I	4230	GLN
1	I	4334	ASN
1	I	4385	GLN
1	I	4598	GLN
1	J	4847	ASN
1	J	4898	GLN
1	K	5360	ASN

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Mol	Chain	Res	Type
1	K	5411	GLN
1	L	5873	ASN
1	L	5924	GLN
1	M	6386	ASN
1	M	6437	GLN
1	N	6899	ASN
1	N	6950	GLN
1	O	7412	ASN
1	O	7463	GLN
1	P	7925	ASN
1	P	7976	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

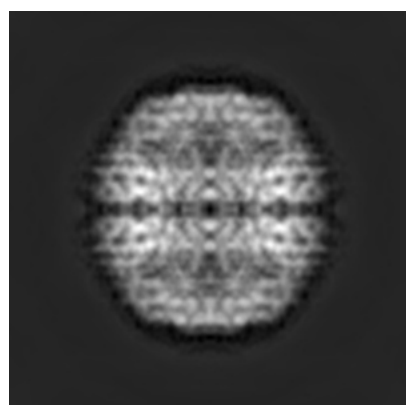
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5246. These allow visual inspection of the internal detail of the map and identification of artifacts.

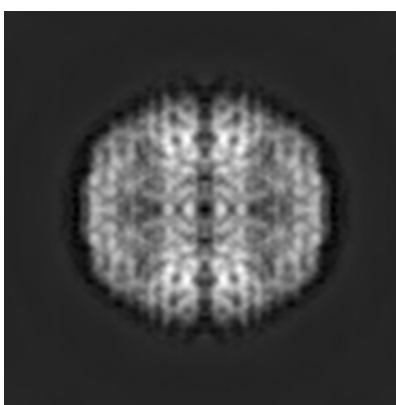
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

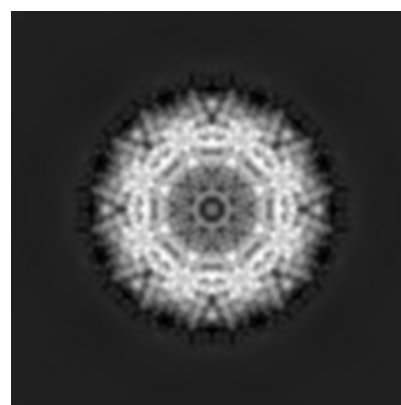
6.1.1 Primary map



X



Y

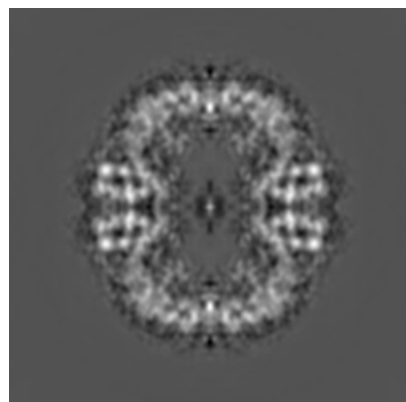


Z

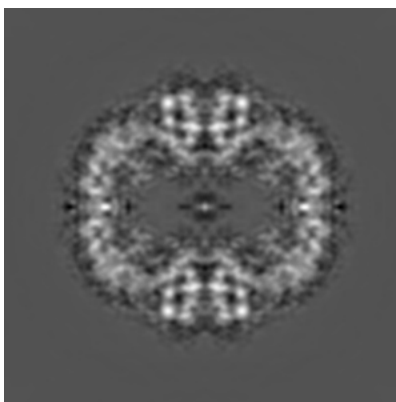
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

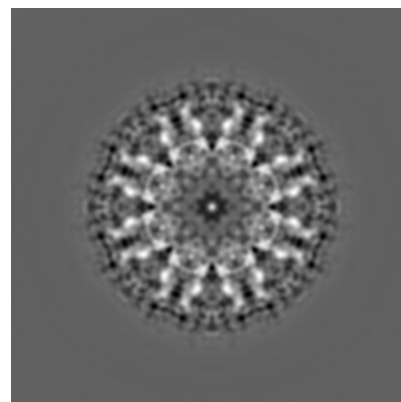
6.2.1 Primary map



X Index: 96



Y Index: 96

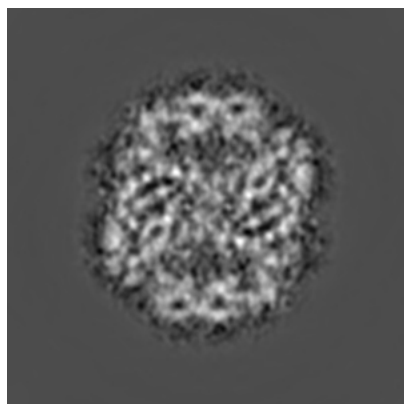


Z Index: 96

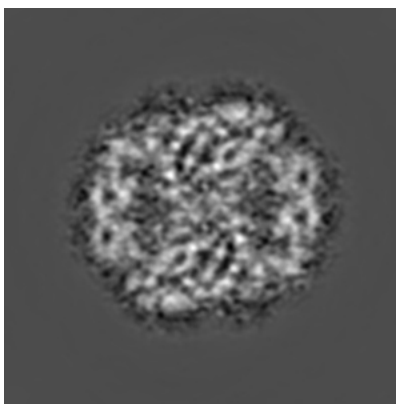
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

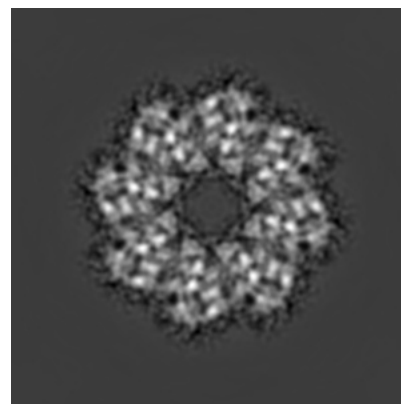
6.3.1 Primary map



X Index: 120



Y Index: 72

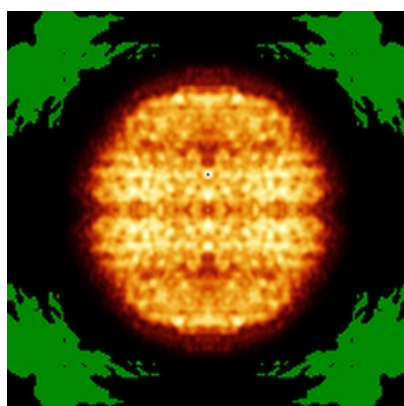


Z Index: 79

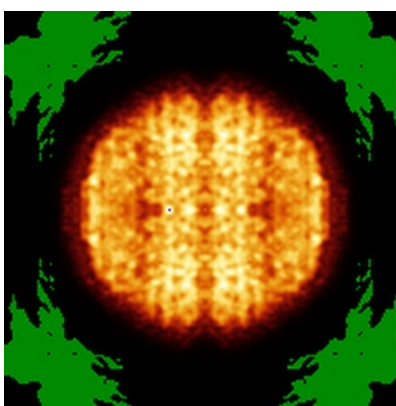
The images above show the largest variance slices of the map in three orthogonal directions.

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

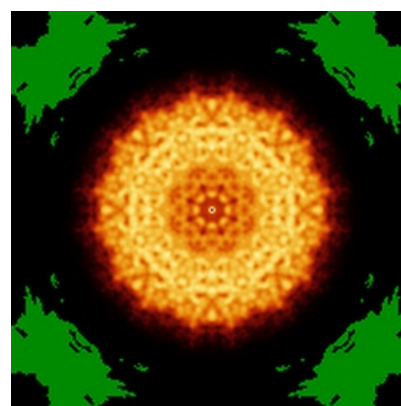
6.4.1 Primary map



X



Y

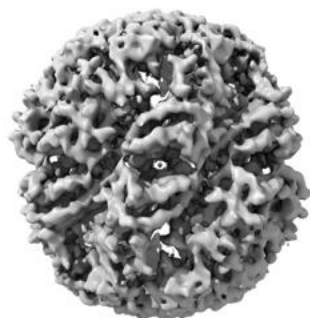


Z

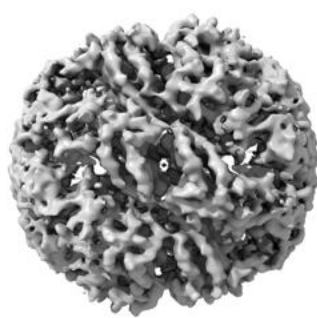
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

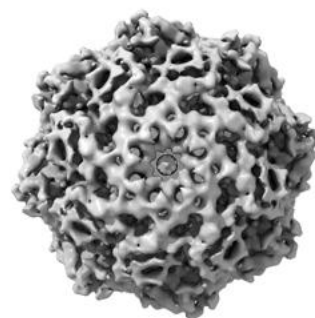
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

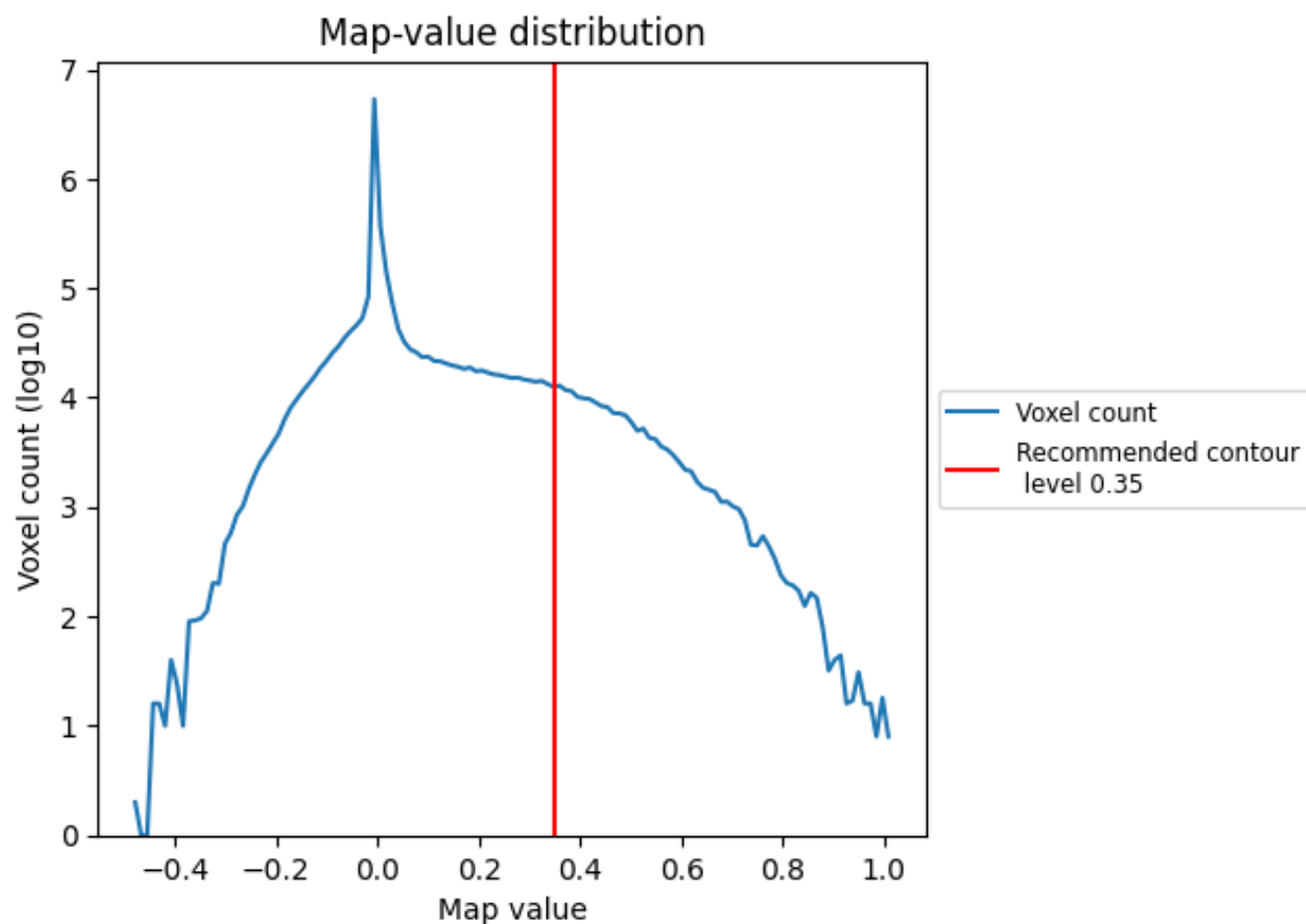
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

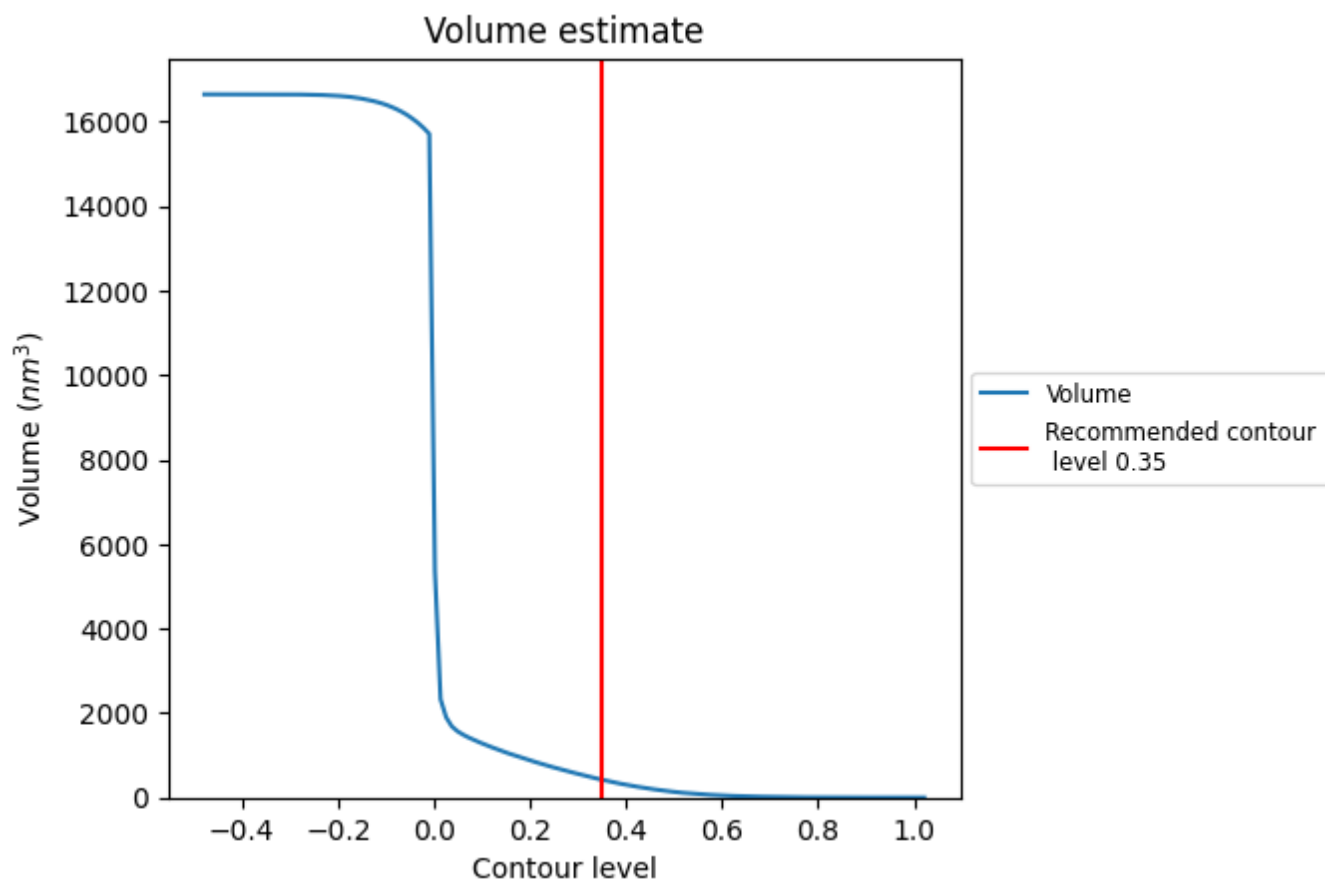
This section contains the results of statistical analysis of the map.

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.

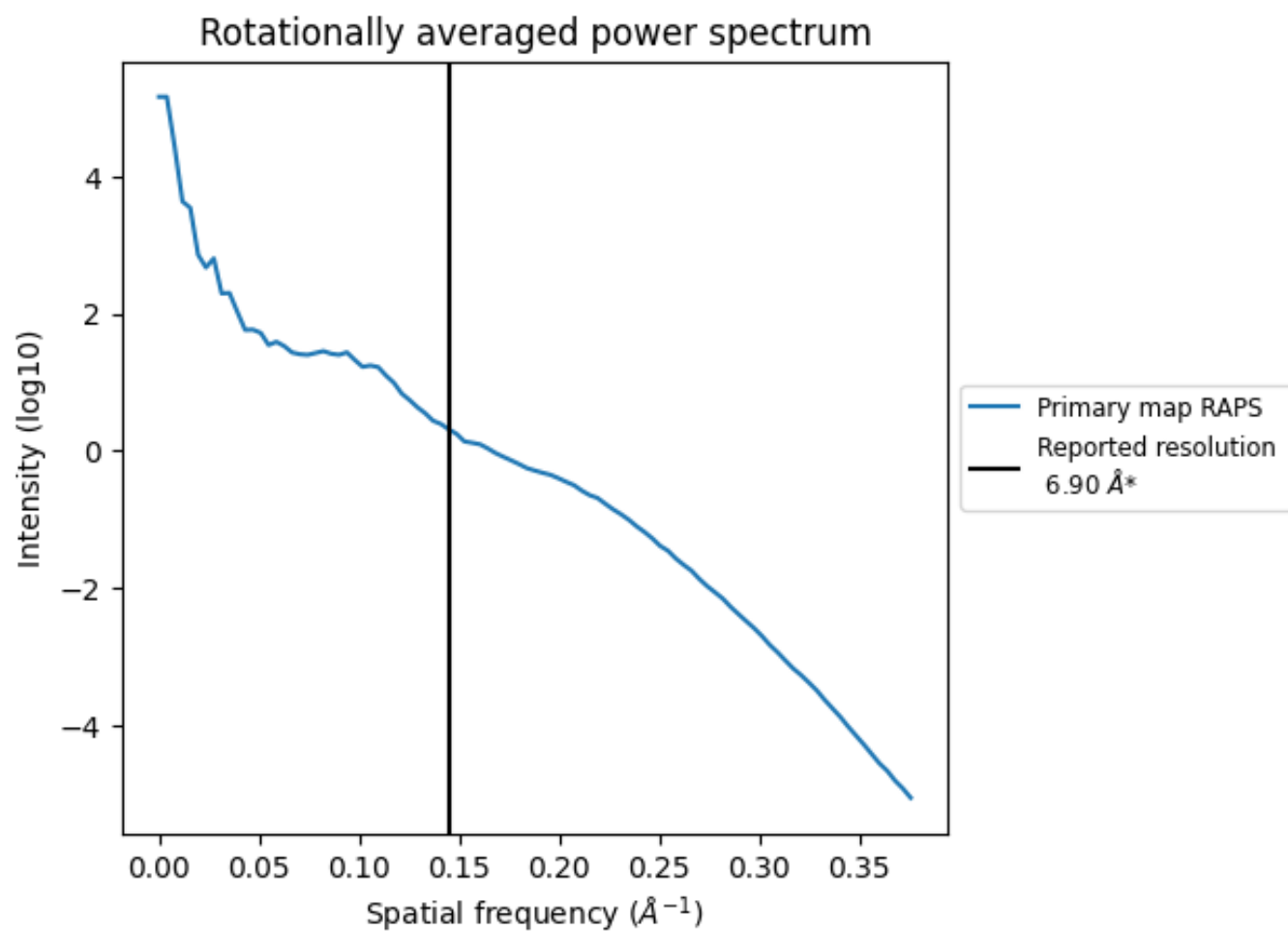
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm³; this corresponds to an approximate mass of 381 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.145 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

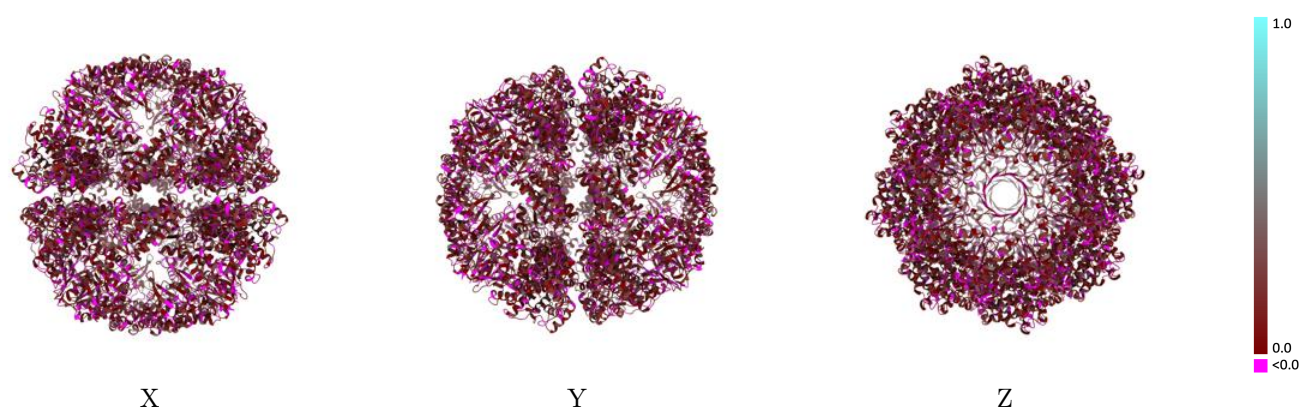
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5246 and PDB model 3IZJ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

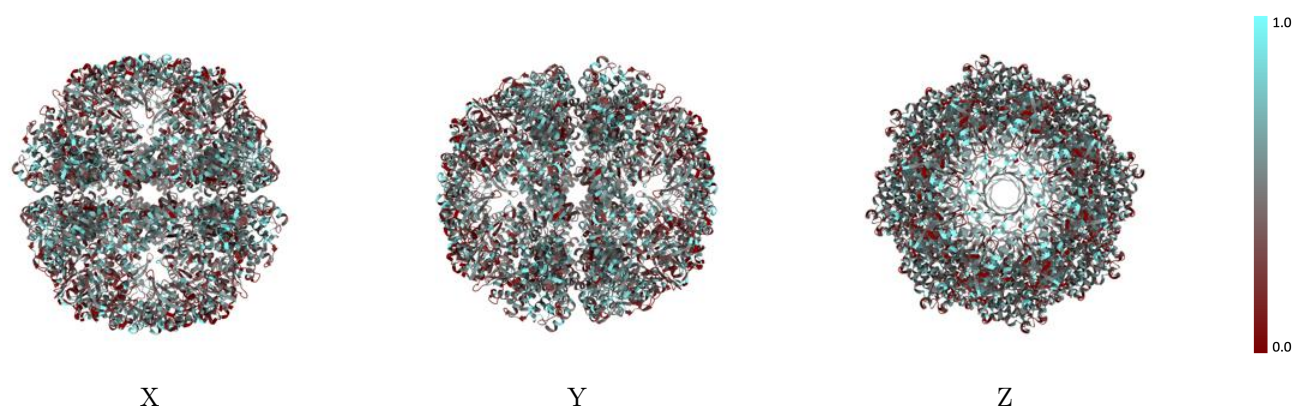
This section was not generated.

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



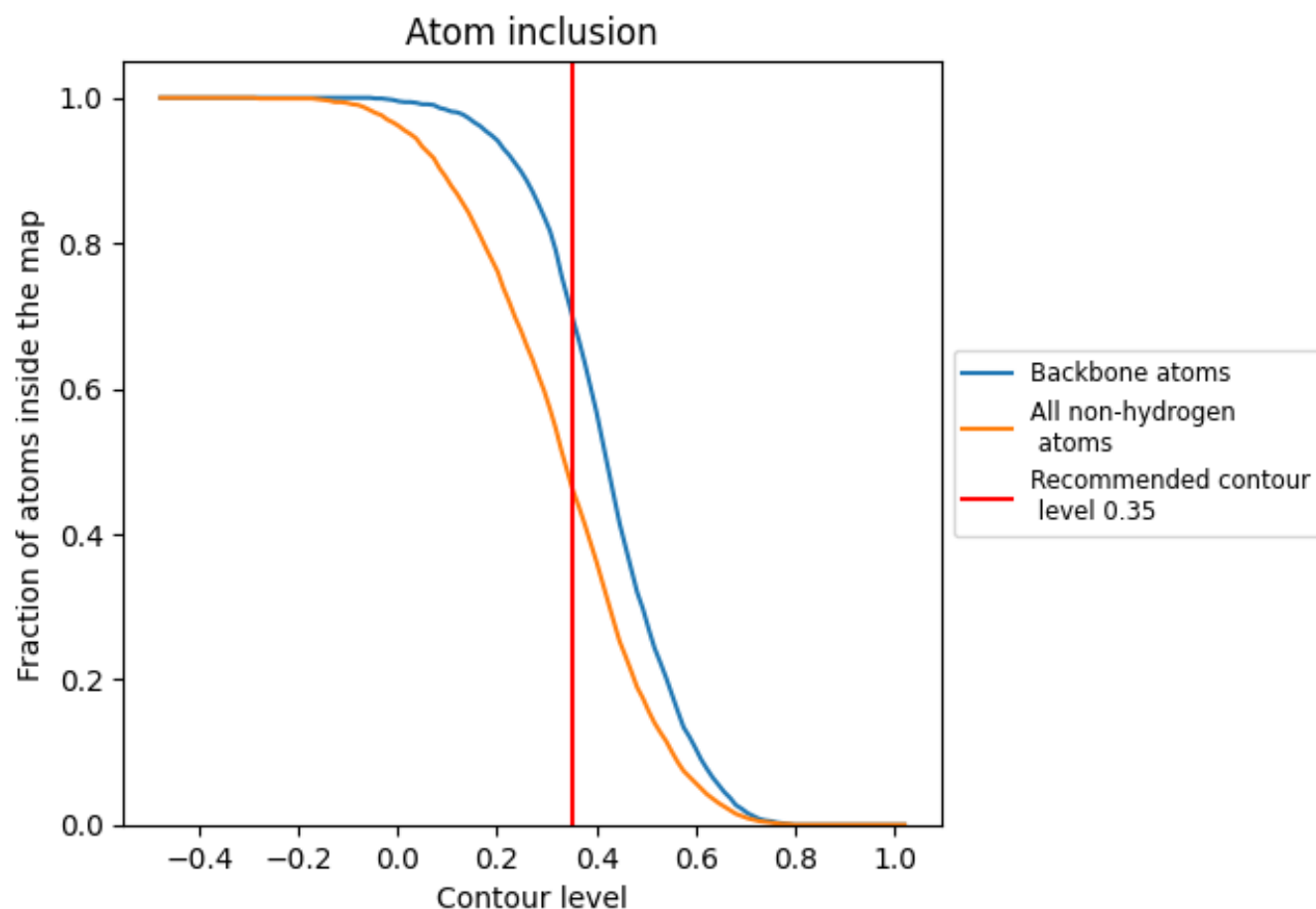
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4660	0.1170
A	0.4660	0.1180
B	0.4670	0.1170
C	0.4650	0.1170
D	0.4670	0.1180
E	0.4660	0.1160
F	0.4670	0.1170
G	0.4660	0.1170
H	0.4670	0.1170
I	0.4650	0.1160
J	0.4670	0.1160
K	0.4660	0.1160
L	0.4670	0.1160
M	0.4650	0.1170
N	0.4670	0.1170
O	0.4660	0.1170
P	0.4680	0.1170

1.0

0.0

<0.0