



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:46 PM UTC

PDB ID : 3IZN / pdb_00003izn
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 ⓘ 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:

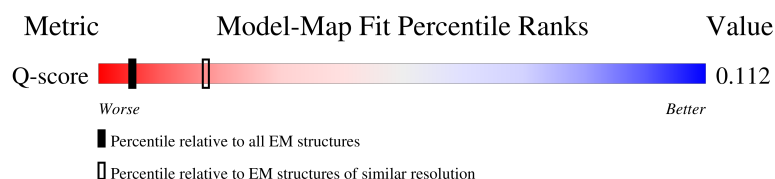
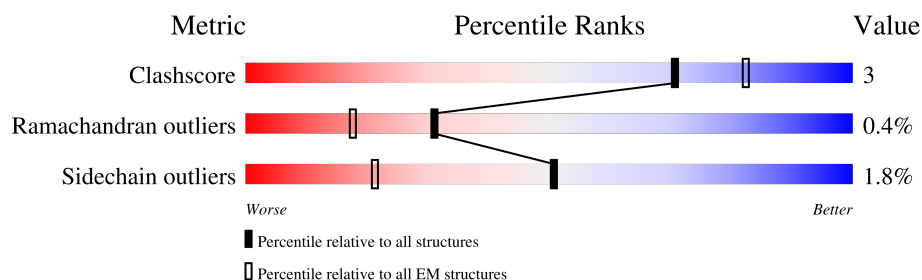
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	544 (5.90 - 6.90)

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	491	
1	B	491	
1	C	491	
1	D	491	

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Mol	Chain	Length	Quality of chain
1	E	491	40% 89% 9%
1	F	491	40% 90% 9%
1	G	491	40% 89% 9%
1	H	491	40% 90% 9%
1	I	491	41% 89% 9%
1	J	491	40% 89% 9%
1	K	491	41% 89% 9%
1	L	491	40% 89% 10%
1	M	491	41% 90% 9%
1	N	491	40% 89% 9%
1	O	491	41% 90% 9%
1	P	491	40% 89% 9%

2 Entry composition

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

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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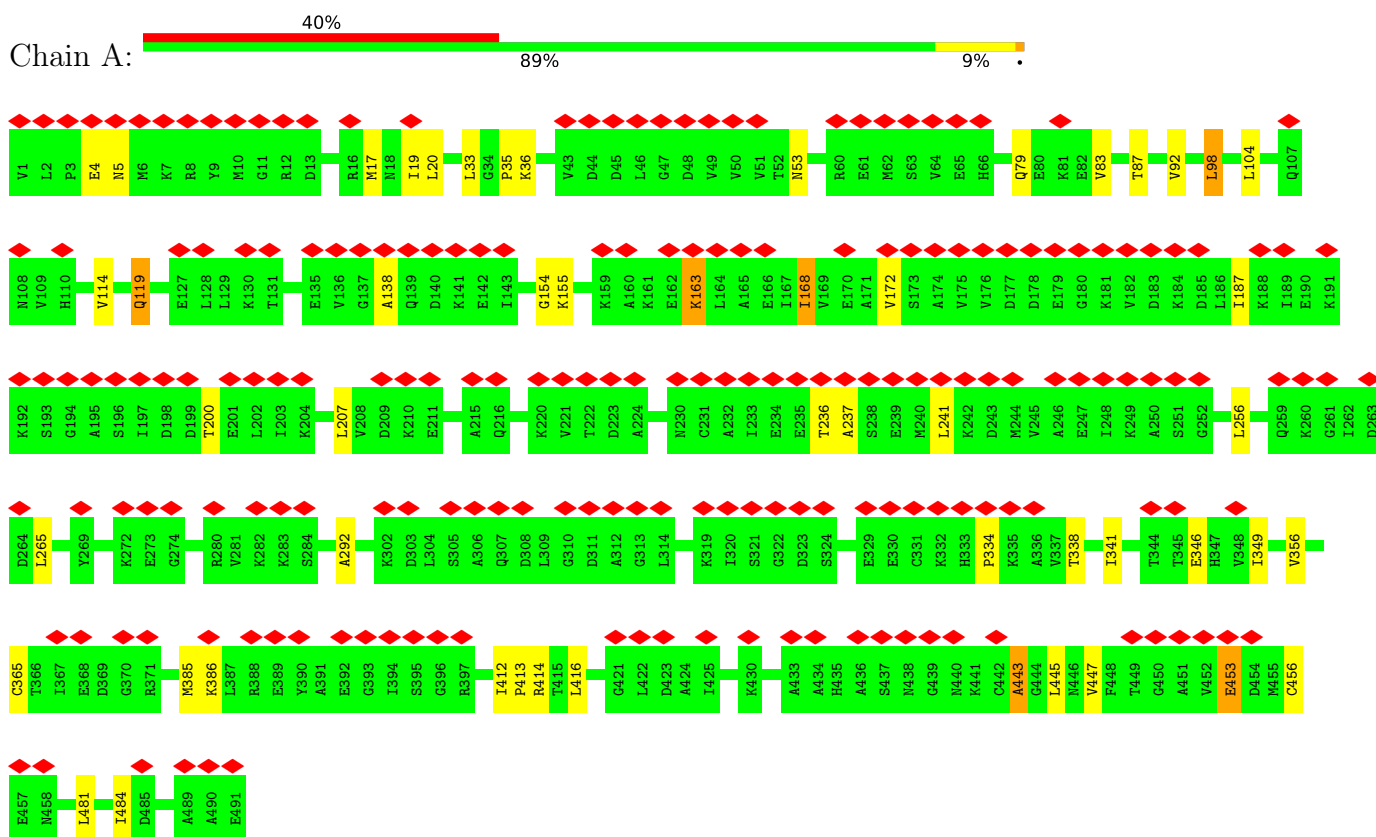
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Chain	Residue	Modelled	Actual	Comment	Reference
I	4166	SER	-	expression tag	UNP Q877G8
I	4167	GLU	-	expression tag	UNP Q877G8
J	4654	GLU	-	expression tag	UNP Q877G8
J	4655	THR	-	expression tag	UNP Q877G8
J	4656	ALA	-	expression tag	UNP Q877G8
J	4657	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

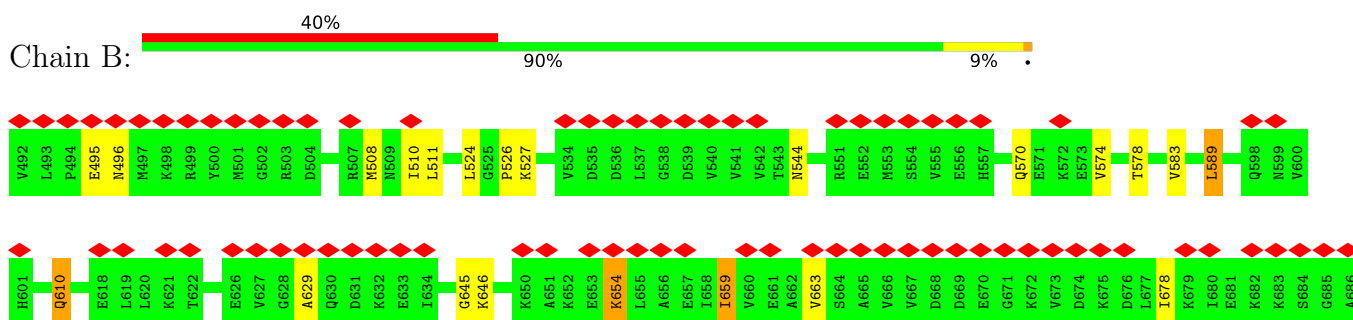
3 Residue-property plots

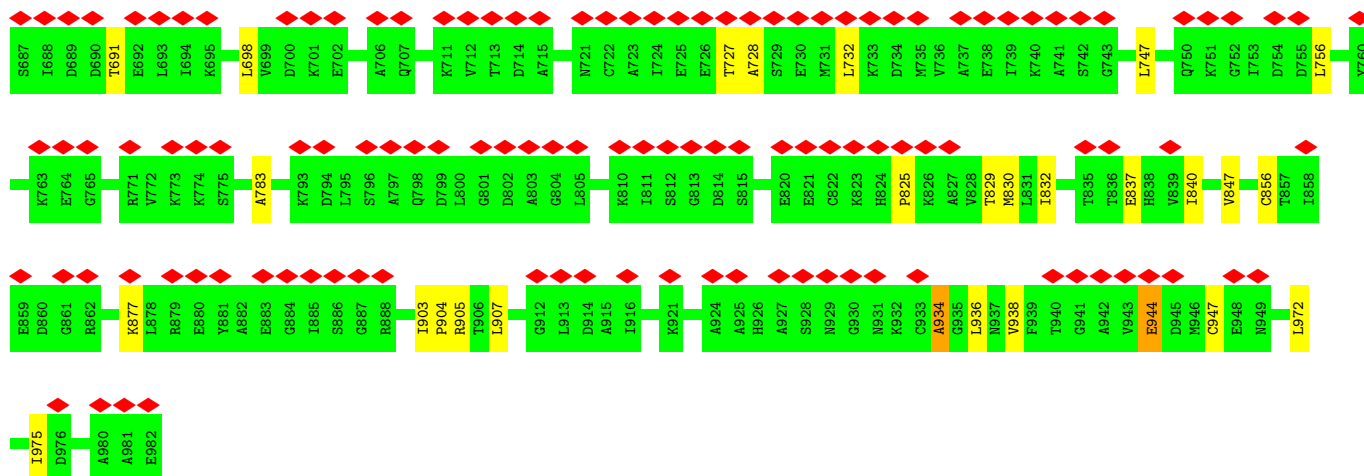
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

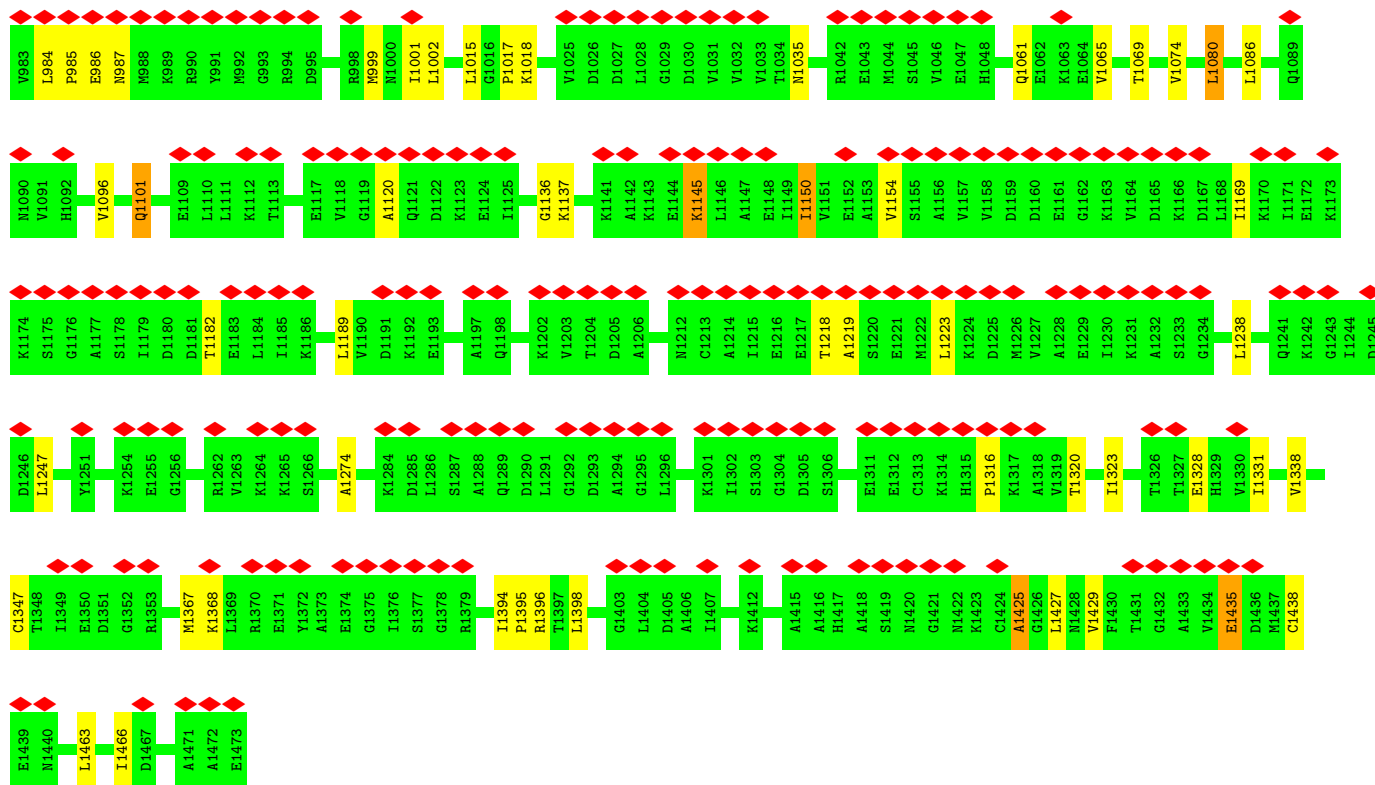
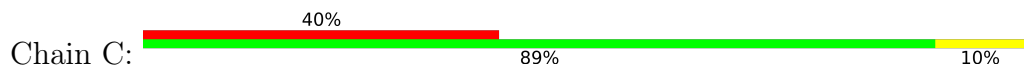


• Molecule 1: Chaperonin

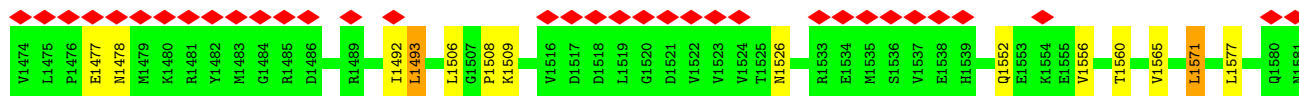
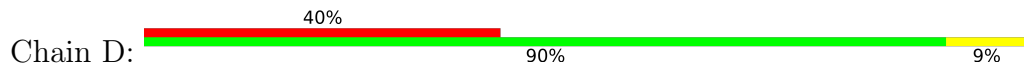


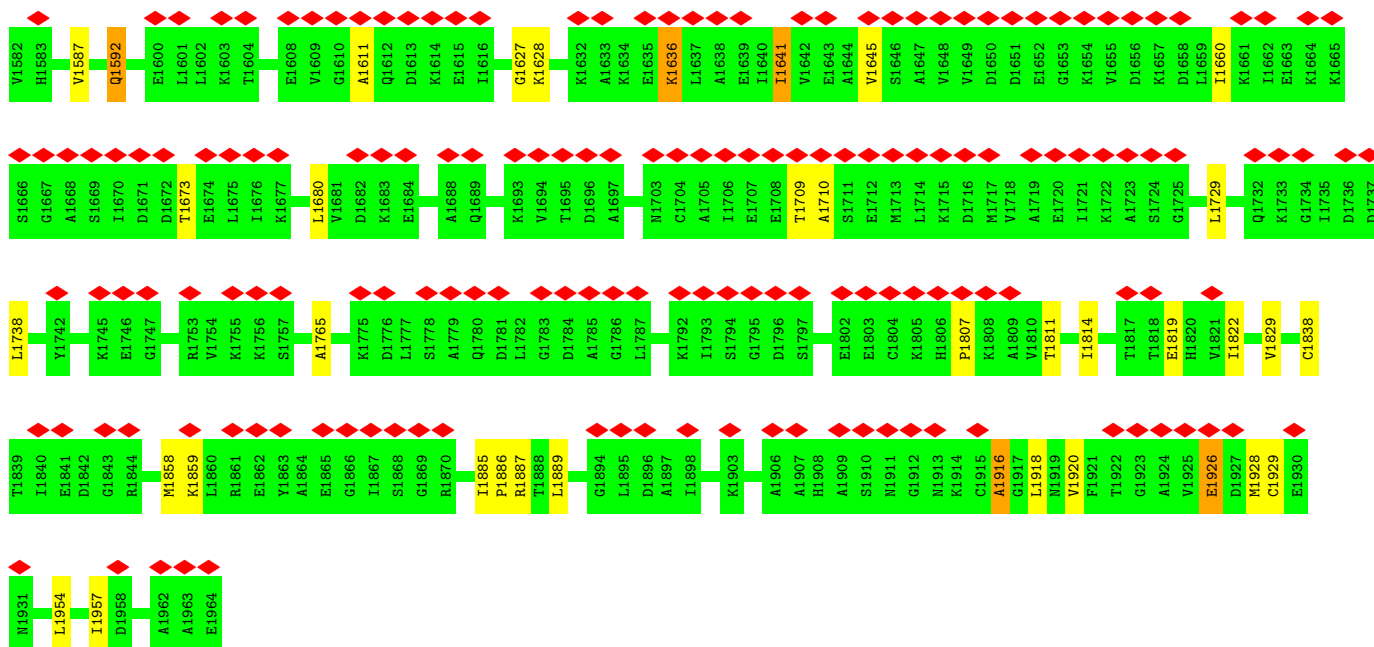


• Molecule 1: Chaperonin

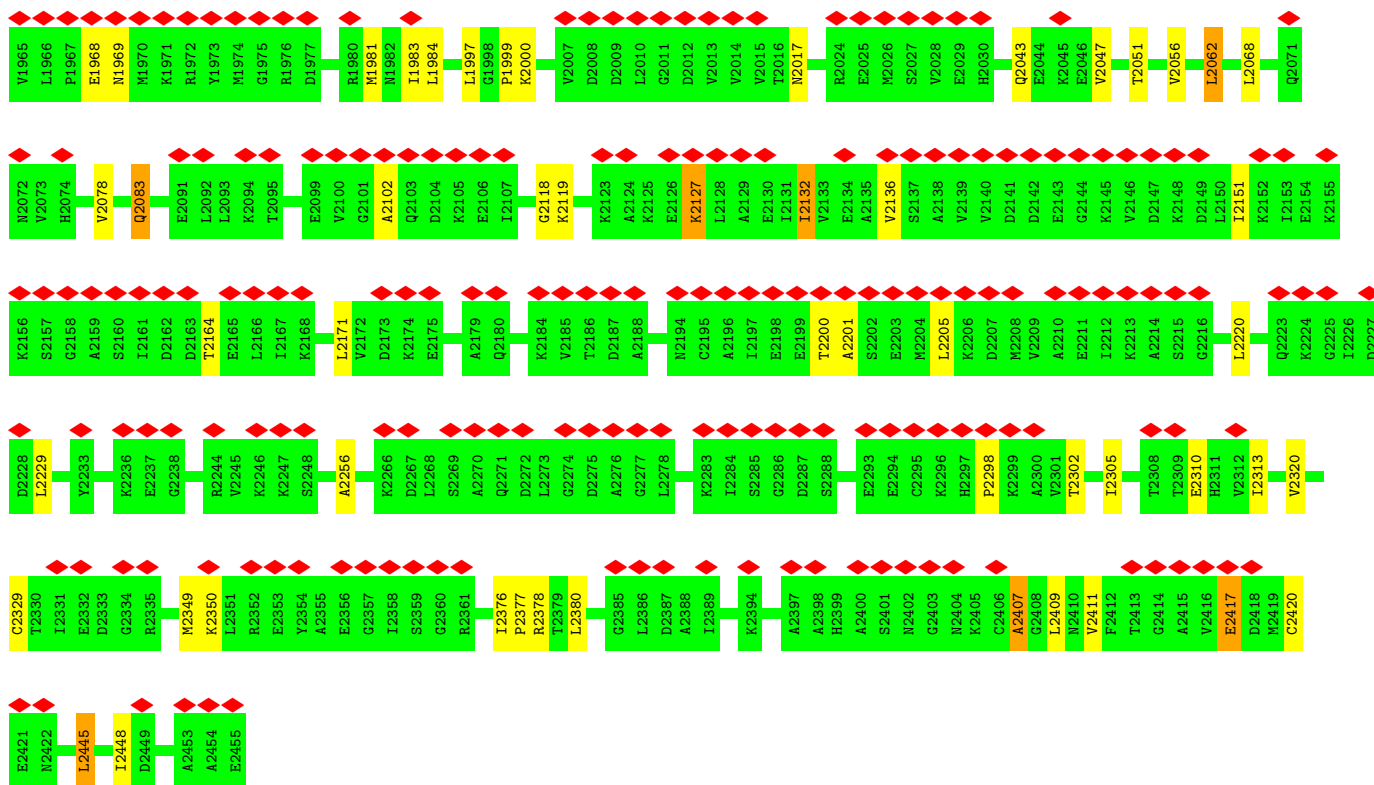
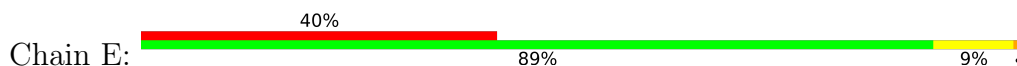


• Molecule 1: Chaperonin

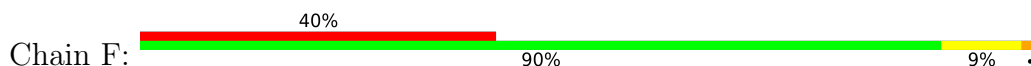


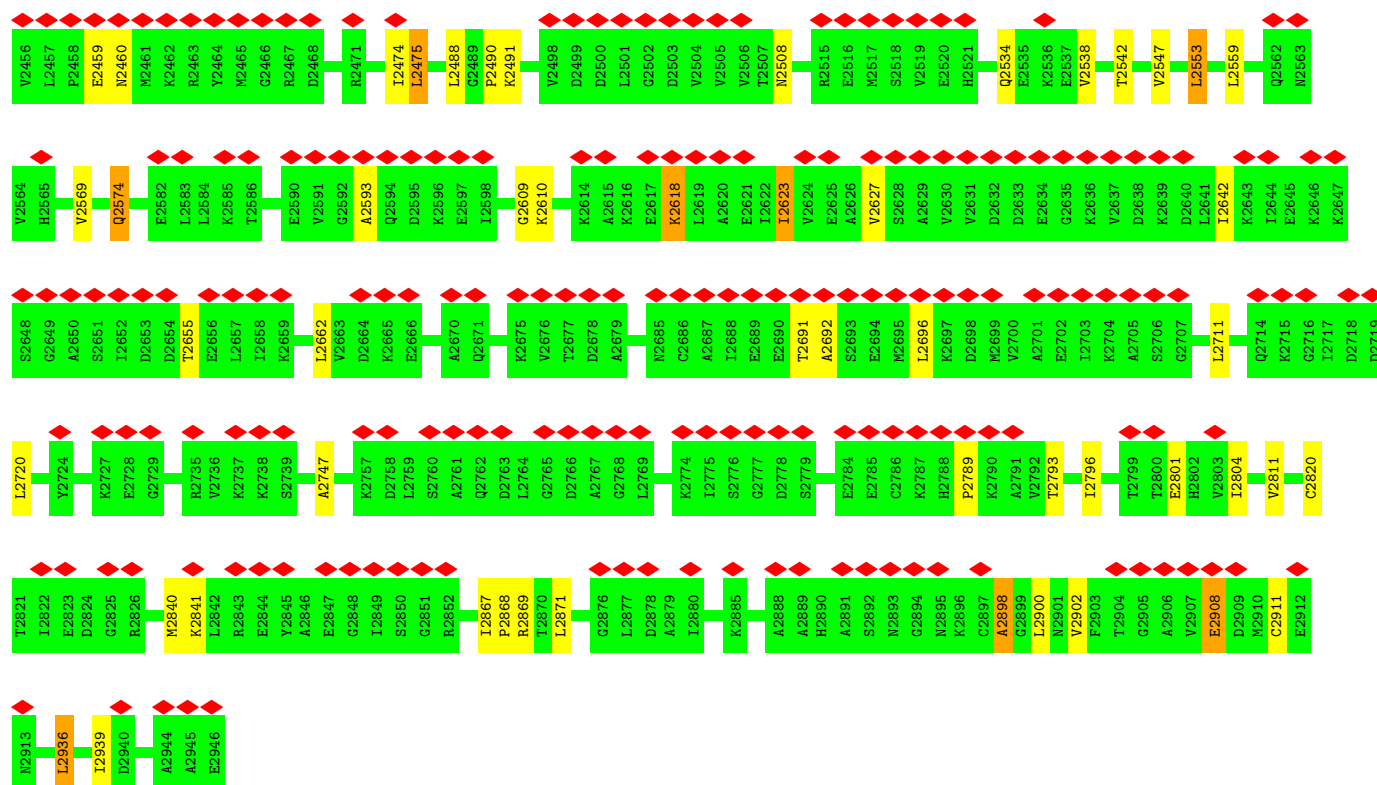


• Molecule 1: Chaperonin

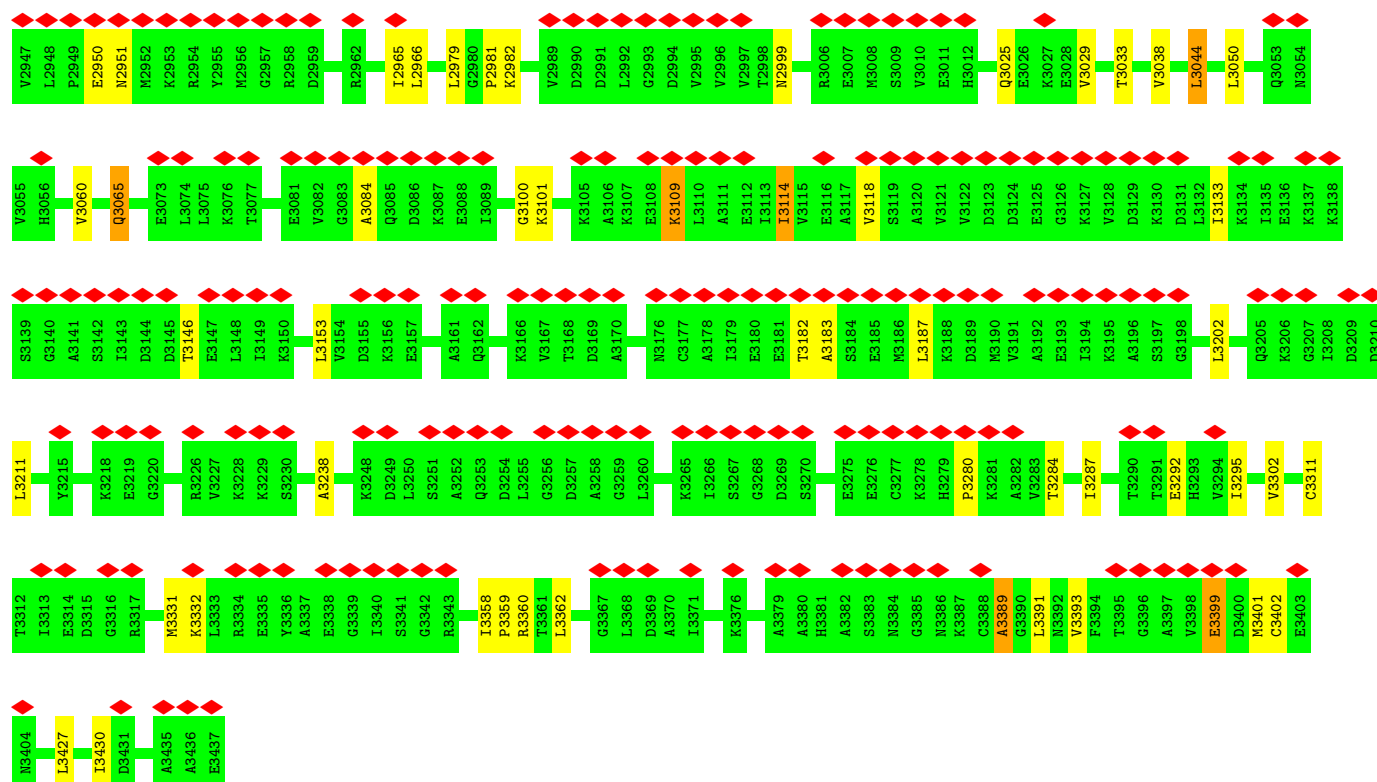
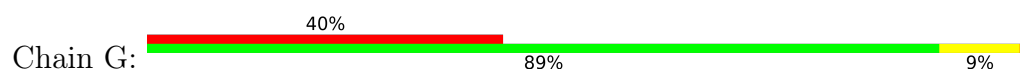


• Molecule 1: Chaperonin



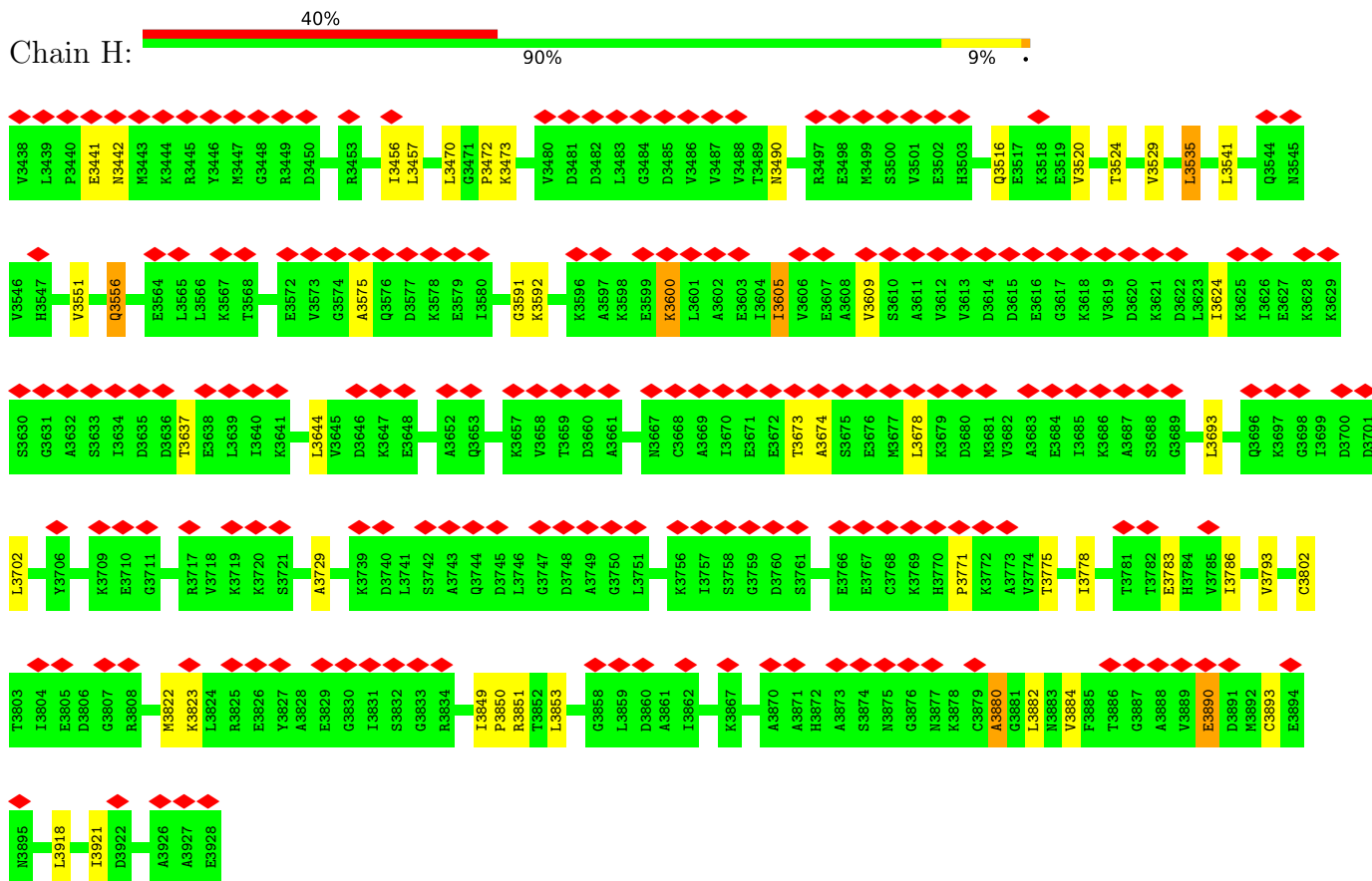


• Molecule 1: Chaperonin



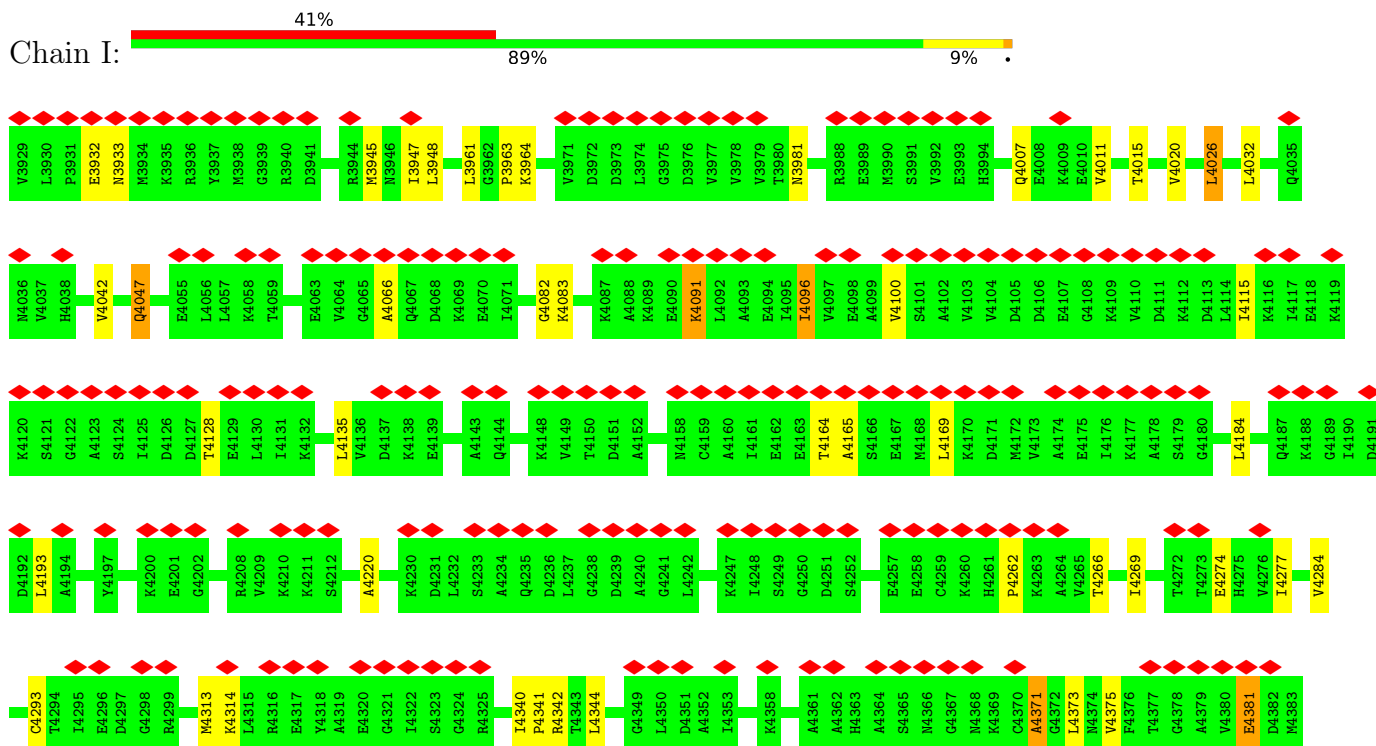
- Molecule 1: Chaperonin

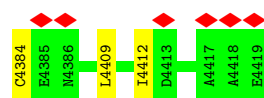
Chain H:



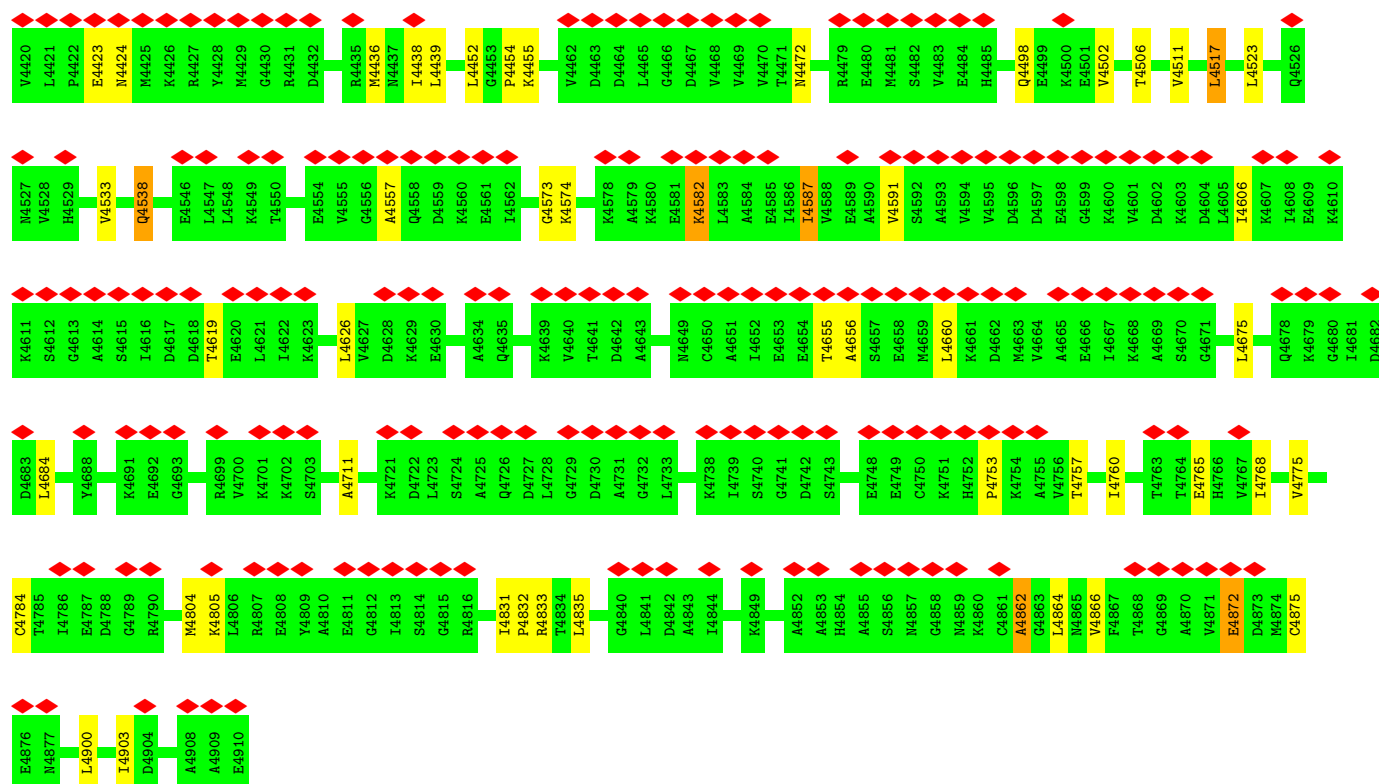
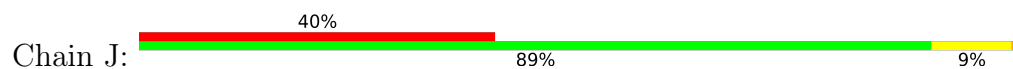
- Molecule 1: Chaperonin

Chain I:

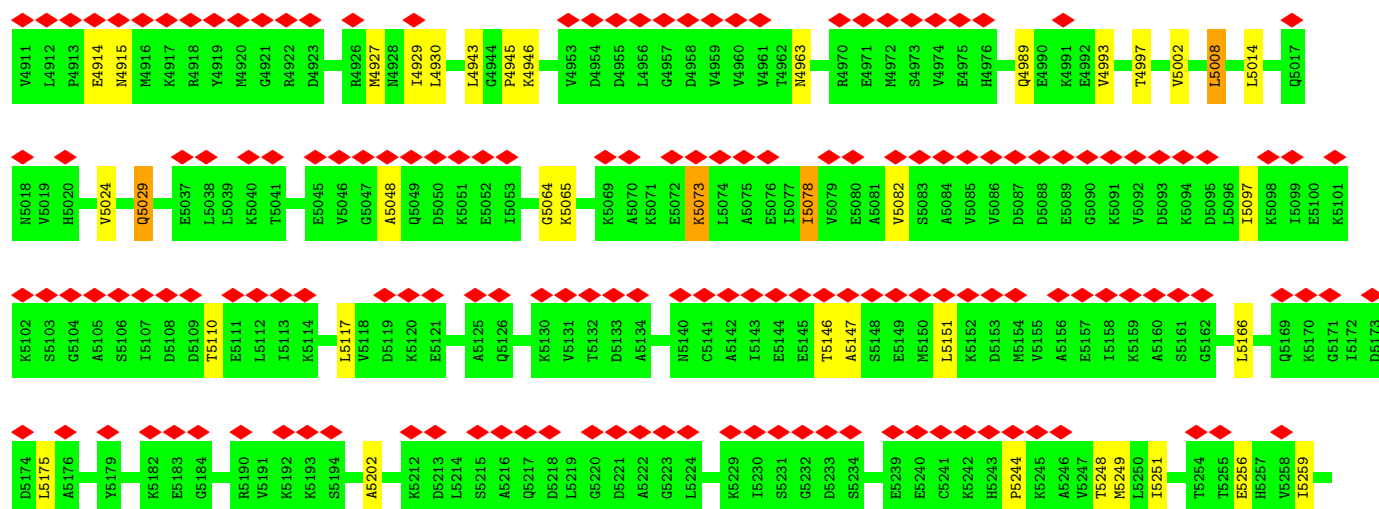
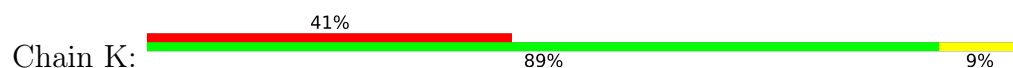


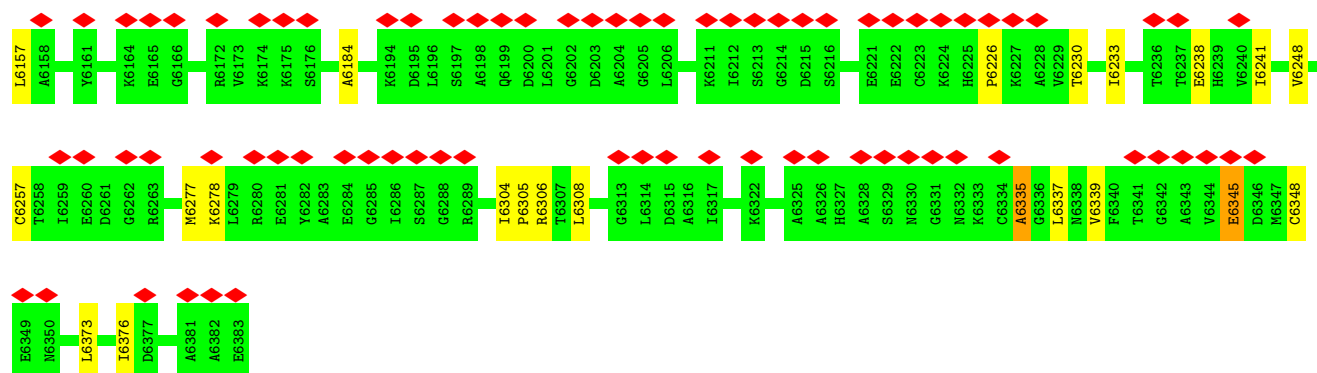


• Molecule 1: Chaperonin

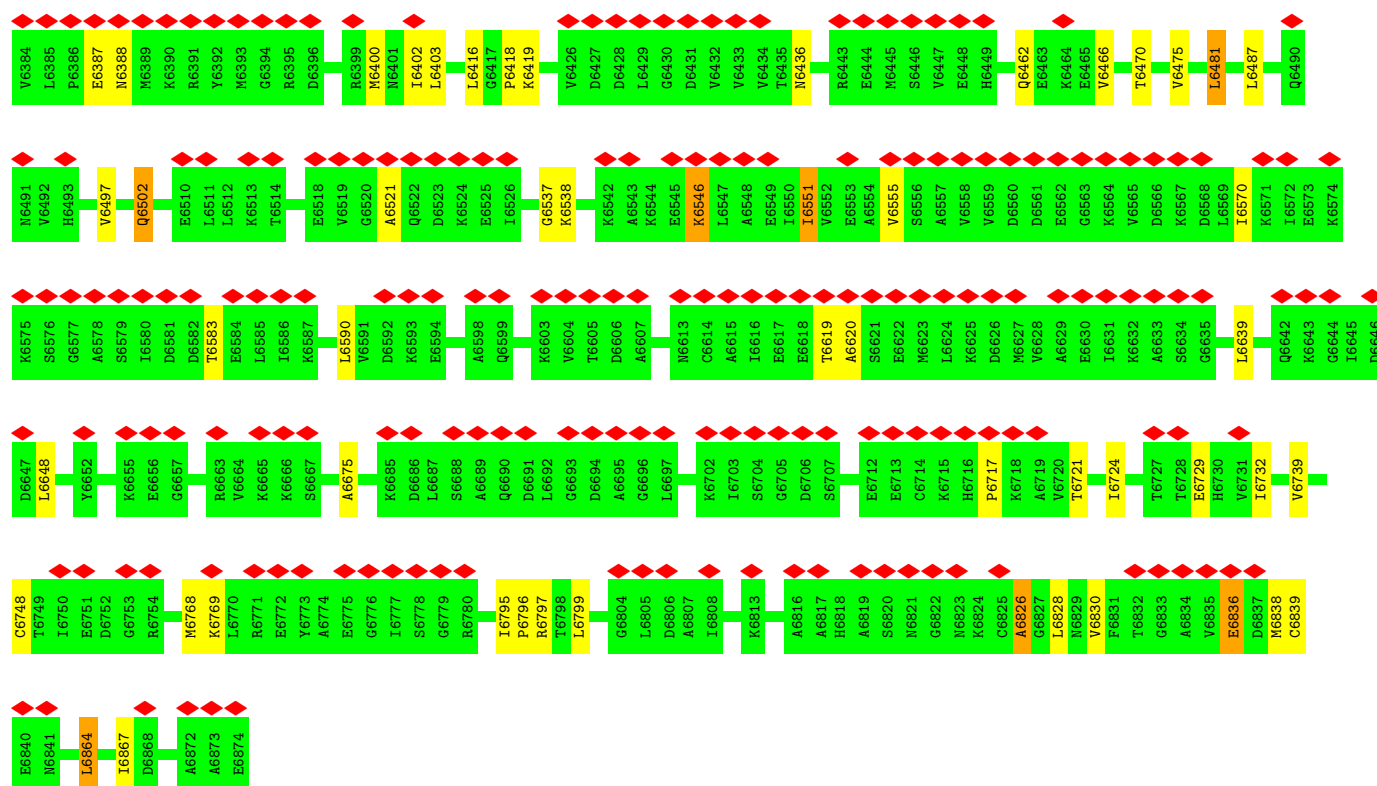
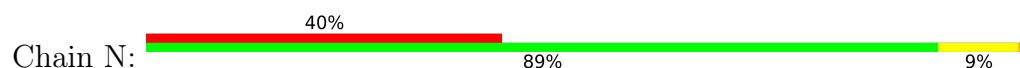


• Molecule 1: Chaperonin

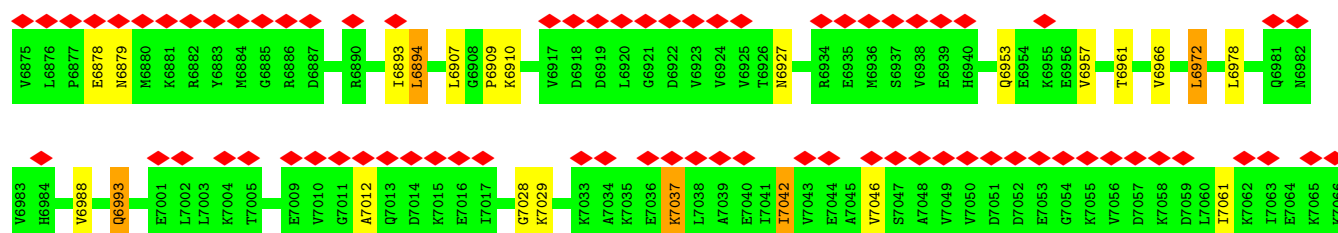
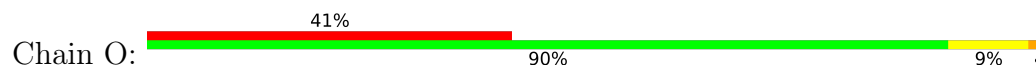


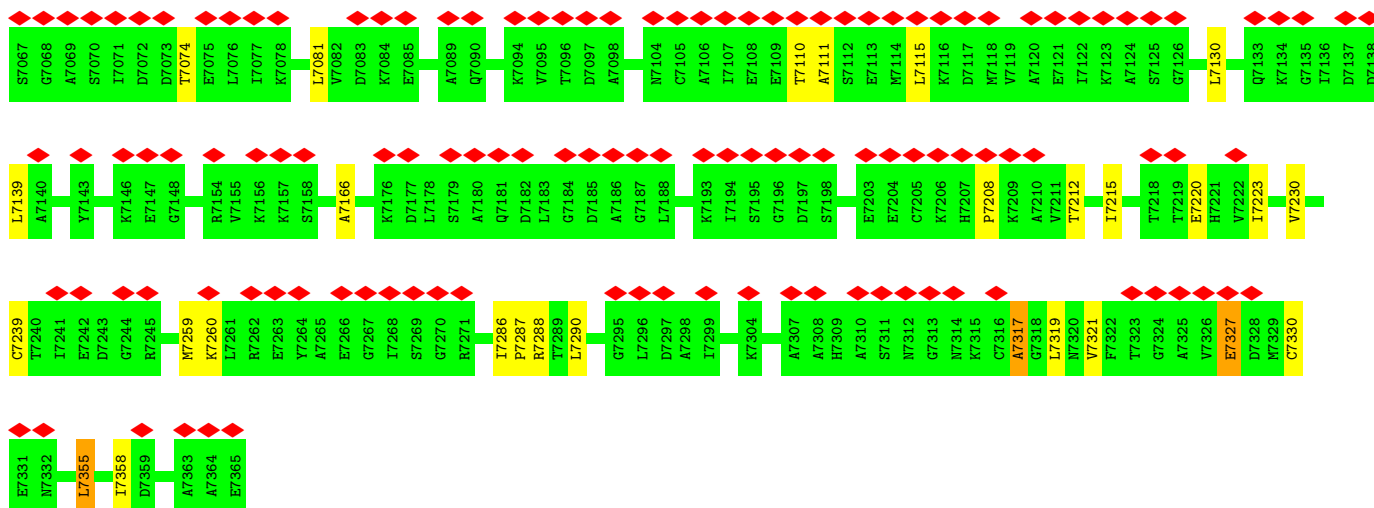


• Molecule 1: Chaperonin

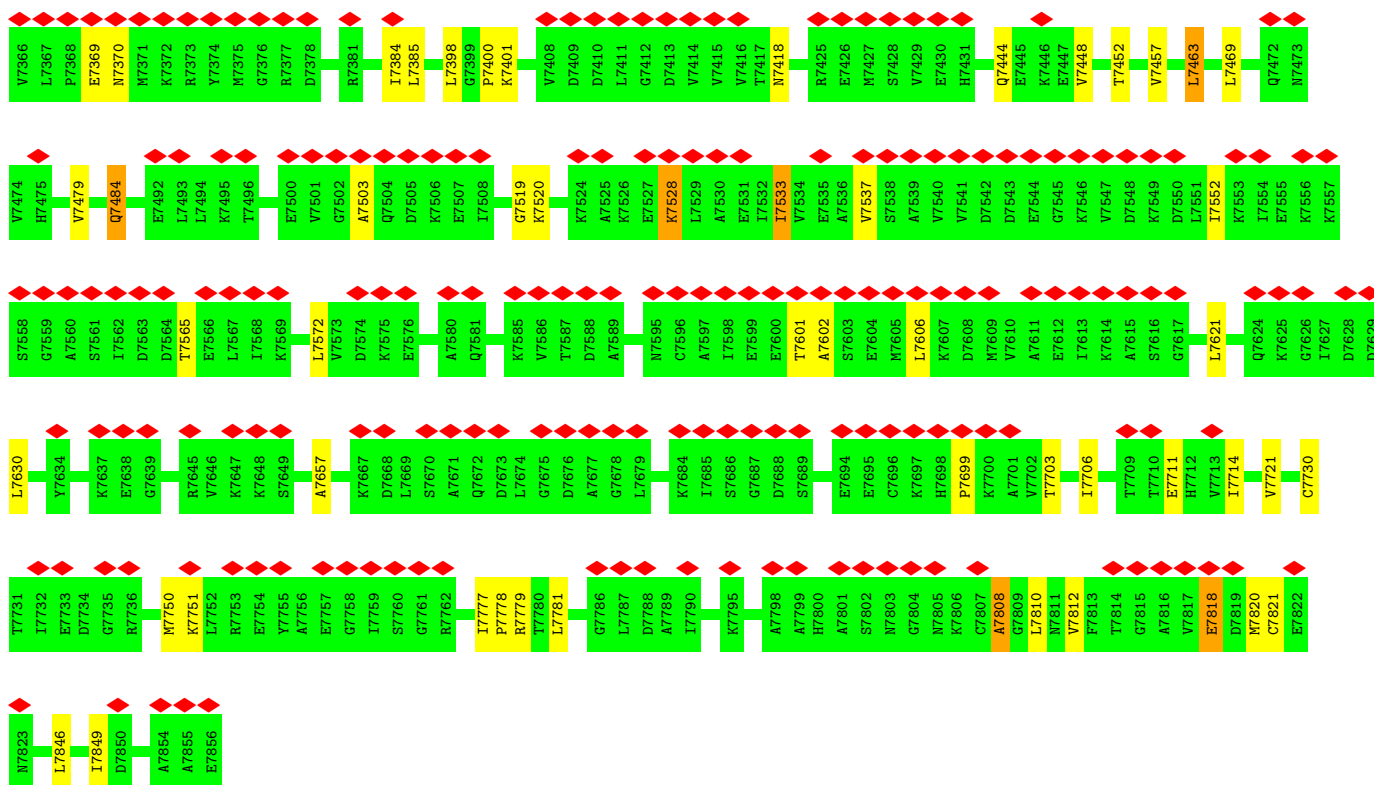
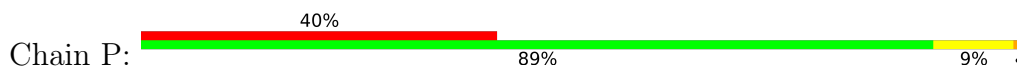


• Molecule 1: Chaperonin





• 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 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 ($\text{\AA}$)	289.44, 289.44, 289.44	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.01, 2.01, 2.01	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	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	B	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	C	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	D	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	E	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	F	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	G	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	H	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	I	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	J	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	K	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	L	0.93	3/3686 (0.1%)	1.07	7/4961 (0.1%)
1	M	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	N	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
1	O	0.93	3/3686 (0.1%)	1.07	7/4961 (0.1%)
1	P	0.93	3/3686 (0.1%)	1.07	9/4961 (0.2%)
All	All	0.93	48/58976 (0.1%)	1.07	140/79376 (0.2%)

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 (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1916	ALA	C-O	7.19	1.33	1.24
1	F	2898	ALA	C-O	7.14	1.32	1.24
1	H	3880	ALA	C-O	7.14	1.32	1.24
1	K	5353	ALA	C-O	7.14	1.32	1.24
1	N	6826	ALA	C-O	7.14	1.32	1.24
1	P	7808	ALA	C-O	7.14	1.32	1.24
1	I	4371	ALA	C-O	7.13	1.32	1.24
1	A	443	ALA	C-O	7.11	1.32	1.24
1	C	1425	ALA	C-O	7.11	1.32	1.24
1	E	2407	ALA	C-O	7.11	1.32	1.24
1	G	3389	ALA	C-O	7.11	1.32	1.24
1	J	4862	ALA	C-O	7.11	1.32	1.24
1	L	5844	ALA	C-O	7.11	1.32	1.24
1	B	934	ALA	C-O	7.08	1.32	1.24
1	M	6335	ALA	C-O	7.08	1.32	1.24
1	O	7317	ALA	C-O	7.07	1.32	1.24
1	L	5405	GLU	C-O	5.64	1.30	1.23
1	K	4914	GLU	C-O	5.64	1.30	1.23
1	M	5896	GLU	C-O	5.64	1.30	1.23
1	B	495	GLU	C-O	5.63	1.30	1.23
1	D	1477	GLU	C-O	5.63	1.30	1.23
1	I	3932	GLU	C-O	5.63	1.30	1.23
1	O	6878	GLU	C-O	5.63	1.30	1.23
1	A	4	GLU	C-O	5.59	1.30	1.23
1	J	4423	GLU	C-O	5.59	1.30	1.23
1	N	6387	GLU	C-O	5.59	1.30	1.23
1	P	7369	GLU	C-O	5.59	1.30	1.23
1	G	2950	GLU	C-O	5.58	1.30	1.23
1	H	3441	GLU	C-O	5.58	1.30	1.23
1	F	2459	GLU	C-O	5.57	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	986	GLU	C-O	5.53	1.30	1.23
1	E	1968	GLU	C-O	5.53	1.30	1.23
1	J	4423	GLU	C-N	-5.32	1.26	1.33
1	D	1477	GLU	C-N	-5.32	1.26	1.33
1	A	4	GLU	C-N	-5.31	1.26	1.33
1	L	5405	GLU	C-N	-5.31	1.26	1.33
1	G	2950	GLU	C-N	-5.28	1.26	1.33
1	B	495	GLU	C-N	-5.28	1.26	1.33
1	I	3932	GLU	C-N	-5.28	1.26	1.33
1	M	5896	GLU	C-N	-5.28	1.26	1.33
1	O	6878	GLU	C-N	-5.28	1.26	1.33
1	N	6387	GLU	C-N	-5.26	1.26	1.33
1	P	7369	GLU	C-N	-5.26	1.26	1.33
1	F	2459	GLU	C-N	-5.25	1.26	1.33
1	H	3441	GLU	C-N	-5.25	1.26	1.33
1	K	4914	GLU	C-N	-5.25	1.26	1.33
1	C	986	GLU	C-N	-5.22	1.26	1.33
1	E	1968	GLU	C-N	-5.22	1.26	1.33

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1477	GLU	CA-C-O	-13.38	106.17	121.16
1	O	6878	GLU	CA-C-O	-13.38	106.17	121.16
1	A	4	GLU	CA-C-O	-13.36	106.20	121.16
1	B	495	GLU	CA-C-O	-13.36	106.20	121.16
1	I	3932	GLU	CA-C-O	-13.36	106.20	121.16
1	C	986	GLU	CA-C-O	-13.34	106.22	121.16
1	E	1968	GLU	CA-C-O	-13.34	106.22	121.16
1	F	2459	GLU	CA-C-O	-13.34	106.22	121.16
1	G	2950	GLU	CA-C-O	-13.34	106.22	121.16
1	J	4423	GLU	CA-C-O	-13.33	106.23	121.16
1	L	5405	GLU	CA-C-O	-13.33	106.23	121.16
1	N	6387	GLU	CA-C-O	-13.33	106.23	121.16
1	P	7369	GLU	CA-C-O	-13.33	106.23	121.16
1	K	4914	GLU	CA-C-O	-13.32	106.24	121.16
1	M	5896	GLU	CA-C-O	-13.32	106.24	121.16
1	H	3441	GLU	CA-C-O	-13.30	106.27	121.16
1	O	6993	GLN	CA-C-O	-8.14	112.32	120.70
1	A	119	GLN	CA-C-O	-8.13	112.32	120.70
1	F	2574	GLN	CA-C-O	-8.12	112.34	120.70
1	I	4047	GLN	CA-C-O	-8.11	112.34	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	5520	GLN	CA-C-O	-8.11	112.35	120.70
1	N	6502	GLN	CA-C-O	-8.10	112.36	120.70
1	P	7484	GLN	CA-C-O	-8.10	112.36	120.70
1	C	1101	GLN	CA-C-O	-8.09	112.36	120.70
1	M	6011	GLN	CA-C-O	-8.09	112.36	120.70
1	K	5029	GLN	CA-C-O	-8.09	112.37	120.70
1	E	2083	GLN	CA-C-O	-8.08	112.38	120.70
1	H	3556	GLN	CA-C-O	-8.08	112.38	120.70
1	J	4538	GLN	CA-C-O	-8.07	112.39	120.70
1	D	1592	GLN	CA-C-O	-8.07	112.39	120.70
1	B	610	GLN	CA-C-O	-8.06	112.39	120.70
1	G	3065	GLN	CA-C-O	-8.05	112.41	120.70
1	B	574	VAL	N-CA-C	5.96	116.69	111.56
1	D	1556	VAL	N-CA-C	5.96	116.69	111.56
1	F	2538	VAL	N-CA-C	5.96	116.69	111.56
1	A	83	VAL	N-CA-C	5.95	116.68	111.56
1	E	2047	VAL	N-CA-C	5.95	116.67	111.56
1	P	7448	VAL	N-CA-C	5.95	116.67	111.56
1	J	4502	VAL	N-CA-C	5.94	116.67	111.56
1	G	3029	VAL	N-CA-C	5.93	116.66	111.56
1	H	3520	VAL	N-CA-C	5.92	116.65	111.56
1	I	4011	VAL	N-CA-C	5.92	116.65	111.56
1	N	6466	VAL	N-CA-C	5.92	116.66	111.56
1	K	4993	VAL	N-CA-C	5.92	116.65	111.56
1	O	6957	VAL	N-CA-C	5.91	116.64	111.56
1	M	5975	VAL	N-CA-C	5.90	116.64	111.56
1	L	5484	VAL	N-CA-C	5.90	116.64	111.56
1	C	1065	VAL	N-CA-C	5.89	116.62	111.56
1	C	1435	GLU	CA-C-O	-5.64	114.88	120.80
1	J	4872	GLU	CA-C-O	-5.64	114.88	120.80
1	B	944	GLU	CA-C-O	-5.63	114.89	120.80
1	D	1926	GLU	CA-C-O	-5.63	114.89	120.80
1	I	4381	GLU	CA-C-O	-5.63	114.89	120.80
1	K	5363	GLU	CA-C-O	-5.62	114.89	120.80
1	M	6345	GLU	CA-C-O	-5.62	114.89	120.80
1	A	453	GLU	CA-C-O	-5.62	114.90	120.80
1	N	6836	GLU	CA-C-O	-5.62	114.90	120.80
1	O	7327	GLU	CA-C-O	-5.62	114.90	120.80
1	G	3399	GLU	CA-C-O	-5.60	114.92	120.80
1	L	5854	GLU	CA-C-O	-5.60	114.92	120.80
1	P	7818	GLU	CA-C-O	-5.60	114.92	120.80
1	H	3890	GLU	CA-C-O	-5.59	114.93	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2908	GLU	CA-C-O	-5.57	114.95	120.80
1	E	2417	GLU	CA-C-O	-5.54	114.99	120.80
1	L	5857	CYS	N-CA-CB	-5.33	102.28	110.12
1	A	456	CYS	N-CA-CB	-5.33	102.29	110.12
1	J	4875	CYS	N-CA-CB	-5.31	102.31	110.12
1	E	2420	CYS	N-CA-CB	-5.30	102.32	110.12
1	G	3402	CYS	N-CA-CB	-5.30	102.33	110.12
1	P	7821	CYS	N-CA-CB	-5.30	102.33	110.12
1	M	6348	CYS	N-CA-CB	-5.30	102.33	110.12
1	B	947	CYS	N-CA-CB	-5.29	102.34	110.12
1	D	1929	CYS	N-CA-CB	-5.29	102.34	110.12
1	F	2911	CYS	N-CA-CB	-5.29	102.34	110.12
1	H	3893	CYS	N-CA-CB	-5.29	102.34	110.12
1	I	4384	CYS	N-CA-CB	-5.29	102.34	110.12
1	K	5366	CYS	N-CA-CB	-5.29	102.34	110.12
1	C	1438	CYS	N-CA-CB	-5.28	102.36	110.12
1	N	6839	CYS	N-CA-CB	-5.28	102.36	110.12
1	O	7330	CYS	N-CA-CB	-5.27	102.37	110.12
1	J	4538	GLN	N-CA-C	-5.26	105.45	111.14
1	M	6011	GLN	N-CA-C	-5.26	105.46	111.14
1	L	5520	GLN	N-CA-C	-5.25	105.47	111.14
1	K	5029	GLN	N-CA-C	-5.22	105.50	111.14
1	O	6993	GLN	N-CA-C	-5.22	105.50	111.14
1	A	119	GLN	N-CA-C	-5.22	105.51	111.14
1	N	6502	GLN	N-CA-C	-5.22	105.51	111.14
1	C	1101	GLN	N-CA-C	-5.21	105.51	111.14
1	P	7484	GLN	N-CA-C	-5.21	105.52	111.14
1	H	3556	GLN	N-CA-C	-5.20	105.52	111.14
1	E	2083	GLN	N-CA-C	-5.19	105.53	111.14
1	G	3065	GLN	N-CA-C	-5.19	105.53	111.14
1	F	2574	GLN	N-CA-C	-5.18	105.55	111.14
1	I	4047	GLN	N-CA-C	-5.18	105.55	111.14
1	B	610	GLN	N-CA-C	-5.18	105.55	111.14
1	D	1592	GLN	N-CA-C	-5.18	105.55	111.14
1	J	4784	CYS	N-CA-CB	-5.08	102.64	110.12
1	A	365	CYS	N-CA-CB	-5.08	102.66	110.12
1	F	2820	CYS	N-CA-CB	-5.08	102.65	110.12
1	I	4293	CYS	N-CA-CB	-5.08	102.65	110.12
1	M	6257	CYS	N-CA-CB	-5.07	102.66	110.12
1	B	610	GLN	CA-C-N	5.06	127.01	120.44
1	B	610	GLN	C-N-CA	5.06	127.01	120.44
1	B	856	CYS	N-CA-CB	-5.06	102.69	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1347	CYS	N-CA-CB	-5.06	102.69	110.12
1	D	1592	GLN	CA-C-N	5.06	127.01	120.44
1	D	1592	GLN	C-N-CA	5.06	127.01	120.44
1	D	1838	CYS	N-CA-CB	-5.06	102.69	110.12
1	H	3802	CYS	N-CA-CB	-5.06	102.69	110.12
1	K	5275	CYS	N-CA-CB	-5.06	102.69	110.12
1	E	2329	CYS	N-CA-CB	-5.05	102.69	110.12
1	G	3311	CYS	N-CA-CB	-5.05	102.69	110.12
1	P	7730	CYS	N-CA-CB	-5.05	102.69	110.12
1	O	7239	CYS	N-CA-CB	-5.05	102.69	110.12
1	N	6748	CYS	N-CA-CB	-5.05	102.70	110.12
1	K	5029	GLN	CA-C-N	5.05	127.00	120.44
1	K	5029	GLN	C-N-CA	5.05	127.00	120.44
1	P	7484	GLN	CA-C-N	5.05	127.00	120.44
1	P	7484	GLN	C-N-CA	5.05	127.00	120.44
1	L	5766	CYS	N-CA-CB	-5.04	102.71	110.12
1	M	6011	GLN	CA-C-N	5.04	127.00	120.44
1	M	6011	GLN	C-N-CA	5.04	127.00	120.44
1	E	2083	GLN	CA-C-N	5.04	126.99	120.44
1	E	2083	GLN	C-N-CA	5.04	126.99	120.44
1	A	119	GLN	CA-C-N	5.04	126.99	120.44
1	A	119	GLN	C-N-CA	5.04	126.99	120.44
1	C	1101	GLN	CA-C-N	5.04	126.99	120.44
1	C	1101	GLN	C-N-CA	5.04	126.99	120.44
1	G	3065	GLN	CA-C-N	5.04	126.98	120.44
1	G	3065	GLN	C-N-CA	5.04	126.98	120.44
1	F	2574	GLN	CA-C-N	5.03	126.98	120.44
1	F	2574	GLN	C-N-CA	5.03	126.98	120.44
1	N	6502	GLN	CA-C-N	5.02	126.97	120.44
1	N	6502	GLN	C-N-CA	5.02	126.97	120.44
1	H	3556	GLN	CA-C-N	5.02	126.97	120.44
1	H	3556	GLN	C-N-CA	5.02	126.97	120.44
1	I	4047	GLN	CA-C-N	5.02	126.97	120.44
1	I	4047	GLN	C-N-CA	5.02	126.97	120.44
1	J	4538	GLN	CA-C-N	5.01	126.95	120.44
1	J	4538	GLN	C-N-CA	5.01	126.95	120.44

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLN	Mainchain

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	26	0
1	B	3665	0	3801	25	0
1	C	3665	0	3801	27	0
1	D	3665	0	3801	26	0
1	E	3665	0	3801	27	0
1	F	3665	0	3801	27	0
1	G	3665	0	3801	26	0
1	H	3665	0	3801	25	0
1	I	3665	0	3801	26	0
1	J	3665	0	3801	26	0
1	K	3665	0	3801	26	0
1	L	3665	0	3801	26	0
1	M	3665	0	3801	24	0
1	N	3665	0	3801	27	0
1	O	3665	0	3801	27	0
1	P	3665	0	3801	26	0
All	All	58640	0	60819	417	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 (417) 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	0.70
1:J:4684:LEU:C	1:J:4684:LEU:HD23	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:7630:LEU:C	1:P:7630:LEU:HD23	2.17	0.70
1:F:2720:LEU:C	1:F:2720:LEU:HD23	2.17	0.69
1:G:3211:LEU:C	1:G:3211:LEU:HD23	2.17	0.69
1:M:6157:LEU:HD23	1:M:6157:LEU:C	2.17	0.69
1:O:7139:LEU:C	1:O:7139:LEU:HD23	2.17	0.69
1:A:265:LEU:C	1:A:265:LEU:HD23	2.17	0.69
1:D:1738:LEU:C	1:D:1738:LEU:HD23	2.17	0.69
1:H:3702:LEU:C	1:H:3702:LEU:HD23	2.17	0.69
1:L:5666:LEU:HD23	1:L:5666:LEU:C	2.17	0.69
1:I:4193:LEU:C	1:I:4193:LEU:HD23	2.17	0.69
1:E:2229:LEU:C	1:E:2229:LEU:HD23	2.17	0.68
1:N:6648:LEU:HD23	1:N:6648:LEU:C	2.17	0.68
1:B:756:LEU:C	1:B:756:LEU:HD23	2.17	0.68
1:K:5175:LEU:C	1:K:5175:LEU:HD23	2.17	0.68
1:B:747:LEU:C	1:B:747:LEU:HD13	2.28	0.59
1:K:5166:LEU:C	1:K:5166:LEU:HD13	2.28	0.59
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:M:6148:LEU:HD13	1:M:6148:LEU:C	2.28	0.59
1:D:1729:LEU:HD13	1:D:1729:LEU:C	2.28	0.59
1:J:4831:ILE:HB	1:J:4832:PRO:HD3	1.84	0.59
1:H:3693:LEU:HD13	1:H:3693:LEU:C	2.28	0.58
1:I:4184:LEU:C	1:I:4184:LEU:HD13	2.28	0.58
1:J:4675:LEU:C	1:J:4675:LEU:HD13	2.28	0.58
1:A:256:LEU:HD13	1:A:256:LEU:C	2.28	0.58
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:E:2220:LEU:HD13	1:E:2220:LEU:C	2.28	0.58
1:N:6639:LEU:HD13	1:N:6639:LEU:C	2.28	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:F:2711:LEU:HD13	1:F:2711:LEU:C	2.28	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:G:3202:LEU:HD13	1:G:3202:LEU:C	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:7130:LEU:HD13	1:O:7130:LEU:C	2.28	0.58
1:P:7621:LEU:HD13	1:P:7621:LEU:C	2.28	0.58
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:C:1238:LEU:HD13	1:C:1238:LEU:C	2.28	0.58
1:K:5175:LEU:HD23	1:K:5175:LEU:O	2.04	0.58
1:L:5657:LEU:HD13	1:L:5657:LEU:C	2.28	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:L:5666:LEU:HD23	1:L:5666:LEU:O	2.04	0.56
1:C:1247:LEU:HD23	1:C:1247:LEU:O	2.04	0.56
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
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:C:1247:LEU:C	1:C:1247:LEU:CD2	2.86	0.49
1:B:756:LEU:C	1:B:756:LEU:CD2	2.86	0.48
1:K:5175:LEU:C	1:K:5175:LEU:CD2	2.86	0.48
1:L:5666:LEU:C	1:L:5666:LEU:CD2	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1738:LEU:C	1:D:1738:LEU:CD2	2.86	0.48
1:J:4684:LEU:C	1:J:4684:LEU:CD2	2.86	0.48
1:M:6157:LEU:C	1:M:6157:LEU:CD2	2.86	0.48
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:A:265:LEU:C	1:A:265:LEU:CD2	2.86	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:A:414:ARG:HD3	1:A:414:ARG:C	2.40	0.47
1:F:2869:ARG:HD3	1:F:2869:ARG:C	2.40	0.47
1:O:7288:ARG:C	1:O:7288:ARG:HD3	2.40	0.47
1:B:905:ARG:HD3	1:B:905:ARG:C	2.40	0.47
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:J:4833:ARG:HD3	1:J:4833:ARG:C	2.40	0.47
1:K:5324:ARG:HD3	1:K:5324:ARG:C	2.40	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:C:1396:ARG:C	1:C:1396:ARG:HD3	2.40	0.47
1:E:2229:LEU:C	1:E:2229:LEU:CD2	2.86	0.47
1:G:3109:LYS:HE3	1:G:3109:LYS:HA	1.96	0.47
1:H:3851:ARG:HD3	1:H:3851:ARG:C	2.40	0.47
1:L:5815:ARG:HD3	1:L:5815:ARG:C	2.40	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:I:4342:ARG:HD3	1:I:4342:ARG:C	2.40	0.47
1:G:3360:ARG:HD3	1:G:3360:ARG:C	2.40	0.47
1:I:4193:LEU:C	1:I:4193:LEU:CD2	2.86	0.47
1:N:6648:LEU:C	1:N:6648:LEU:CD2	2.86	0.47
1:P:7779:ARG:HD3	1:P:7779:ARG:C	2.40	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:H:3702:LEU:C	1:H:3702:LEU:CD2	2.86	0.47
1:L:5608:LEU:HB3	1:L:5739:THR:HG21	1.97	0.47
1:M:6306:ARG:C	1:M:6306:ARG:HD3	2.40	0.47
1:B:654:LYS:HE3	1:B:654:LYS:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1887:ARG:C	1:D:1887:ARG:HD3	2.40	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
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:E:2378:ARG:HD3	1:E:2378:ARG:C	2.40	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:F:2720:LEU:C	1:F:2720:LEU:CD2	2.86	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:N:6797:ARG:C	1:N:6797:ARG:HD3	2.40	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:O:7139:LEU:C	1:O:7139:LEU:CD2	2.86	0.46
1:L:5564:LYS:HE3	1:L:5564:LYS:HA	1.96	0.46
1:G:3211:LEU:C	1:G:3211:LEU:CD2	2.86	0.46
1:P:7630:LEU:C	1:P:7630:LEU:CD2	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:1709:THR:O	1:D:1710:ALA:HB3	2.18	0.43
1:J:4452:LEU:HD11	1:J:4511:VAL:HG11	2.01	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: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: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:M:6128:THR:O	1:M:6129:ALA:HB3	2.18	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:D:1526:ASN:HB3	1:D:1628:LYS:HG2	2.01	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:F:2508:ASN:HB3	1:F:2610:LYS:HG2	2.01	0.42
1:N:6436:ASN:HB3	1:N:6538:LYS:HG2	2.01	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N:6768:MET:HA	1:N:6768:MET:HE2	2.02	0.41
1:E:1997:LEU:HD11	1:E:2056:VAL:HG11	2.01	0.41
1:E:2349:MET:HE2	1:E:2349:MET:HA	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:1858:MET:HE2	1:D:1858:MET:HA	2.02	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:2840:MET:HE2	1:F:2840:MET:HA	2.02	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:O:7259:MET:HE2	1:O:7259:MET:HA	2.02	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:I:4032:LEU:HD23	1:I:4042:VAL:HG23	2.02	0.41
1:M:6277:MET:HE2	1:M:6277:MET:HA	2.02	0.41
1:O:6978:LEU:HD23	1:O:6988:VAL:HG23	2.02	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
1:O:7042:ILE:HD11	1:O:7230:VAL:HB	2.02	0.41
1:A:104:LEU:HD23	1:A:114:VAL:HG23	2.02	0.41
1:B:508:MET:HA	1:B:508:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1981:MET:HE2	1:E:1981:MET:HA	2.03	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:H:3822:MET:HE2	1:H:3822:MET:HA	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:I:4313:MET:HE2	1:I:4313:MET:HA	2.02	0.41
1:J:4523:LEU:HD23	1:J:4533:VAL:HG23	2.02	0.41
1:K:4927:MET:HE2	1:K:4927:MET:HA	2.03	0.41
1:L:5747:GLU:O	1:L:5750:ILE:HG12	2.20	0.41
1:N:6400:MET:HE2	1:N:6400:MET:HA	2.03	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:A:385:MET:HA	1:A:385:MET:HE2	2.02	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:P:7750:MET:HE2	1:P:7750:MET:HA	2.02	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:G:3331:MET:HE2	1:G:3331:MET:HA	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:J:4804:MET:HE2	1:J:4804:MET:HA	2.02	0.40
1:P:7533:ILE:HD11	1:P:7721:VAL:HB	2.02	0.40
1:P:7820:MET:HE2	1:P:7820:MET:HA	2.04	0.40
1:A:17:MET:HA	1:A:17:MET:HE2	2.03	0.40
1:C:999:MET:HE2	1:C:999:MET:HA	2.03	0.40
1:C:1086:LEU:HD23	1:C:1096:VAL:HG23	2.02	0.40
1:C:1367:MET:HE2	1:C:1367:MET:HA	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:G:3401:MET:HE2	1:G:3401:MET:HA	2.04	0.40
1:J:4436:MET:HE2	1:J:4436:MET:HA	2.03	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:L:5418:MET:HE2	1:L:5418:MET:HA	2.03	0.40
1:L:5786:MET:HE2	1:L:5786:MET:HA	2.02	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:D:1928:MET:HE2	1:D:1928:MET:HA	2.04	0.40
1:E:2205:LEU:HD23	1:E:2229:LEU:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3050:LEU:HD23	1:G:3060:VAL:HG23	2.02	0.40
1:I:3945:MET:HE2	1:I:3945:MET:HA	2.03	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
1:N:6838:MET:HA	1:N:6838:MET:HE2	2.04	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%)	30	67
1	B	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	C	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	D	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	E	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	F	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	G	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	H	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	I	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	J	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	K	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	L	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	M	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	N	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	O	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67
1	P	489/491 (100%)	468 (96%)	19 (4%)	2 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	7824/7856 (100%)	7488 (96%)	304 (4%)	32 (0%)	31	67

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
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 ⓘ

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%)	386 (98%)	7 (2%)	51	67
1	B	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	C	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	D	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	E	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	F	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	G	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	H	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	I	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	J	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	K	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	L	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	M	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	N	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	O	393/393 (100%)	386 (98%)	7 (2%)	51	67
1	P	393/393 (100%)	386 (98%)	7 (2%)	51	67
All	All	6288/6288 (100%)	6176 (98%)	112 (2%)	51	67

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	98	LEU
1	A	163	LYS
1	A	168	ILE
1	A	386	LYS
1	A	416	LEU
1	A	481	LEU
1	B	511	LEU
1	B	589	LEU
1	B	654	LYS
1	B	659	ILE
1	B	877	LYS

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Mol	Chain	Res	Type
1	B	907	LEU
1	B	972	LEU
1	C	1002	LEU
1	C	1080	LEU
1	C	1145	LYS
1	C	1150	ILE
1	C	1368	LYS
1	C	1398	LEU
1	C	1463	LEU
1	D	1493	LEU
1	D	1571	LEU
1	D	1636	LYS
1	D	1641	ILE
1	D	1859	LYS
1	D	1889	LEU
1	D	1954	LEU
1	E	1984	LEU
1	E	2062	LEU
1	E	2127	LYS
1	E	2132	ILE
1	E	2350	LYS
1	E	2380	LEU
1	E	2445	LEU
1	F	2475	LEU
1	F	2553	LEU
1	F	2618	LYS
1	F	2623	ILE
1	F	2841	LYS
1	F	2871	LEU
1	F	2936	LEU
1	G	2966	LEU
1	G	3044	LEU
1	G	3109	LYS
1	G	3114	ILE
1	G	3332	LYS
1	G	3362	LEU
1	G	3427	LEU
1	H	3457	LEU
1	H	3535	LEU
1	H	3600	LYS
1	H	3605	ILE
1	H	3823	LYS

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Mol	Chain	Res	Type
1	H	3853	LEU
1	H	3918	LEU
1	I	3948	LEU
1	I	4026	LEU
1	I	4091	LYS
1	I	4096	ILE
1	I	4314	LYS
1	I	4344	LEU
1	I	4409	LEU
1	J	4439	LEU
1	J	4517	LEU
1	J	4582	LYS
1	J	4587	ILE
1	J	4805	LYS
1	J	4835	LEU
1	J	4900	LEU
1	K	4930	LEU
1	K	5008	LEU
1	K	5073	LYS
1	K	5078	ILE
1	K	5296	LYS
1	K	5326	LEU
1	K	5391	LEU
1	L	5421	LEU
1	L	5499	LEU
1	L	5564	LYS
1	L	5569	ILE
1	L	5787	LYS
1	L	5817	LEU
1	L	5882	LEU
1	M	5912	LEU
1	M	5990	LEU
1	M	6055	LYS
1	M	6060	ILE
1	M	6278	LYS
1	M	6308	LEU
1	M	6373	LEU
1	N	6403	LEU
1	N	6481	LEU
1	N	6546	LYS
1	N	6551	ILE
1	N	6769	LYS

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Mol	Chain	Res	Type
1	N	6799	LEU
1	N	6864	LEU
1	O	6894	LEU
1	O	6972	LEU
1	O	7037	LYS
1	O	7042	ILE
1	O	7260	LYS
1	O	7290	LEU
1	O	7355	LEU
1	P	7385	LEU
1	P	7463	LEU
1	P	7528	LYS
1	P	7533	ILE
1	P	7751	LYS
1	P	7781	LEU
1	P	7846	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	230	ASN
1	A	259	GLN
1	A	296	ASN
1	A	440	ASN
1	A	472	GLN
1	B	506	GLN
1	B	721	ASN
1	B	750	GLN
1	B	787	ASN
1	B	931	ASN
1	B	963	GLN
1	C	997	GLN
1	C	1212	ASN
1	C	1241	GLN
1	C	1278	ASN
1	C	1422	ASN
1	C	1454	GLN
1	D	1488	GLN
1	D	1703	ASN
1	D	1732	GLN
1	D	1769	ASN

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Mol	Chain	Res	Type
1	D	1913	ASN
1	D	1945	GLN
1	E	1979	GLN
1	E	2194	ASN
1	E	2223	GLN
1	E	2260	ASN
1	E	2404	ASN
1	E	2436	GLN
1	F	2470	GLN
1	F	2685	ASN
1	F	2714	GLN
1	F	2751	ASN
1	F	2895	ASN
1	F	2927	GLN
1	G	2961	GLN
1	G	3176	ASN
1	G	3205	GLN
1	G	3242	ASN
1	G	3386	ASN
1	G	3418	GLN
1	H	3452	GLN
1	H	3667	ASN
1	H	3696	GLN
1	H	3733	ASN
1	H	3877	ASN
1	H	3909	GLN
1	I	3943	GLN
1	I	4158	ASN
1	I	4187	GLN
1	I	4224	ASN
1	I	4368	ASN
1	I	4400	GLN
1	J	4434	GLN
1	J	4649	ASN
1	J	4678	GLN
1	J	4715	ASN
1	J	4859	ASN
1	J	4891	GLN
1	K	4925	GLN
1	K	5140	ASN
1	K	5169	GLN
1	K	5206	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	K	5350	ASN
1	K	5382	GLN
1	L	5416	GLN
1	L	5631	ASN
1	L	5660	GLN
1	L	5697	ASN
1	L	5841	ASN
1	L	5873	GLN
1	M	5907	GLN
1	M	6122	ASN
1	M	6151	GLN
1	M	6188	ASN
1	M	6332	ASN
1	M	6364	GLN
1	N	6398	GLN
1	N	6613	ASN
1	N	6642	GLN
1	N	6679	ASN
1	N	6823	ASN
1	N	6855	GLN
1	O	6889	GLN
1	O	7104	ASN
1	O	7133	GLN
1	O	7170	ASN
1	O	7314	ASN
1	O	7346	GLN
1	P	7380	GLN
1	P	7595	ASN
1	P	7624	GLN
1	P	7661	ASN
1	P	7805	ASN
1	P	7837	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

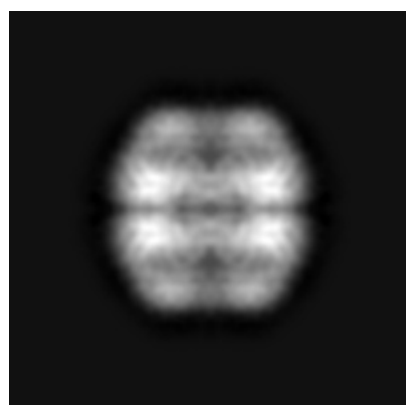
6 Map visualisation [i](#)

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

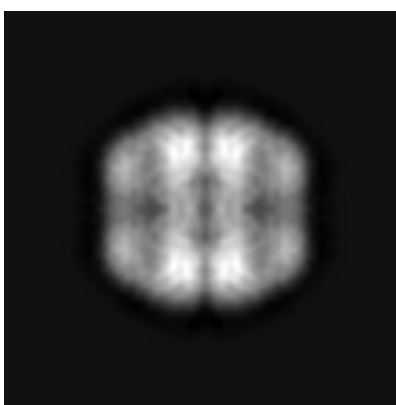
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

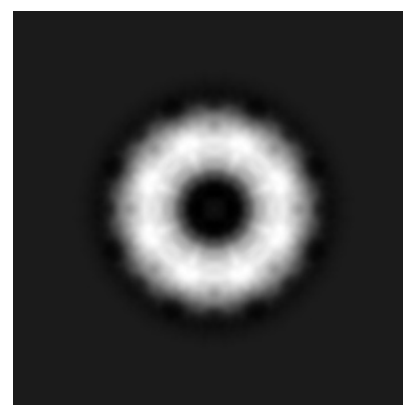
6.1.1 Primary map



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

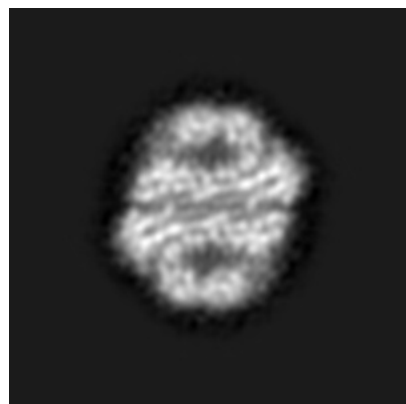


Z Index: 72

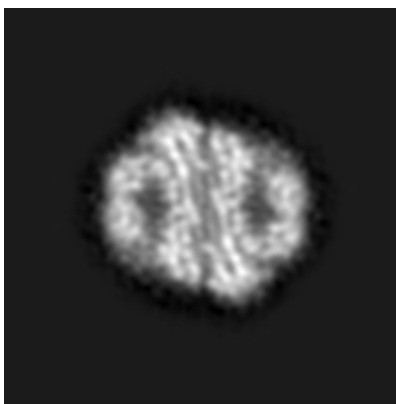
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 92



Y Index: 92

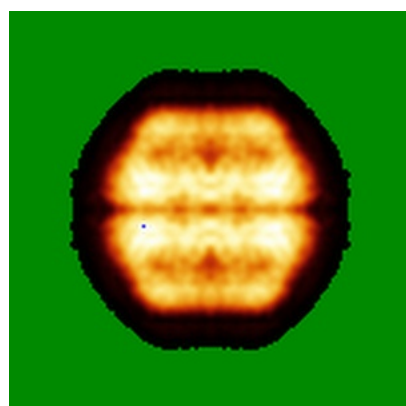


Z Index: 61

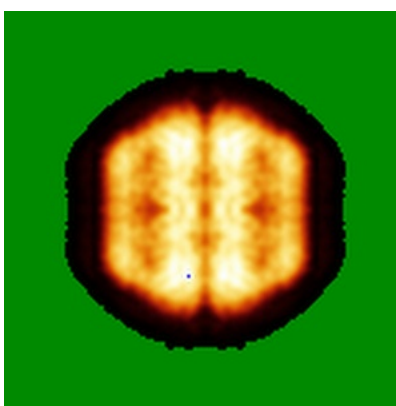
The images above show the largest variance slices of the map in three orthogonal directions.

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

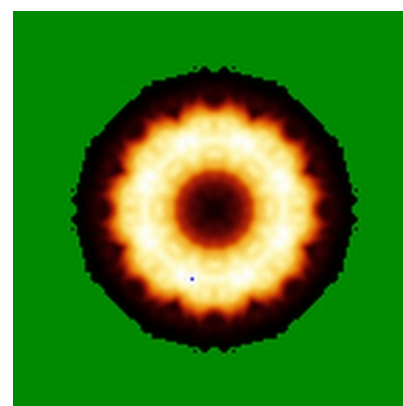
6.4.1 Primary map



X



Y

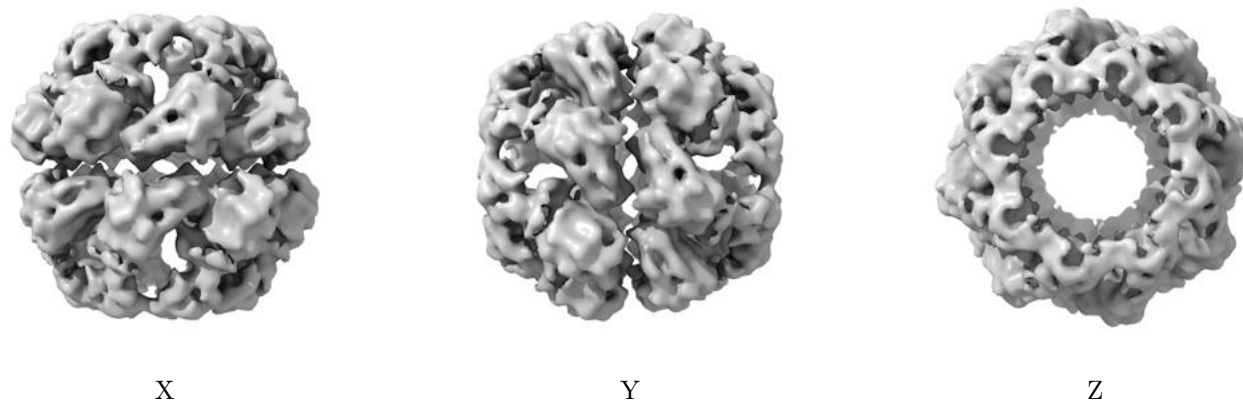


Z

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



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.

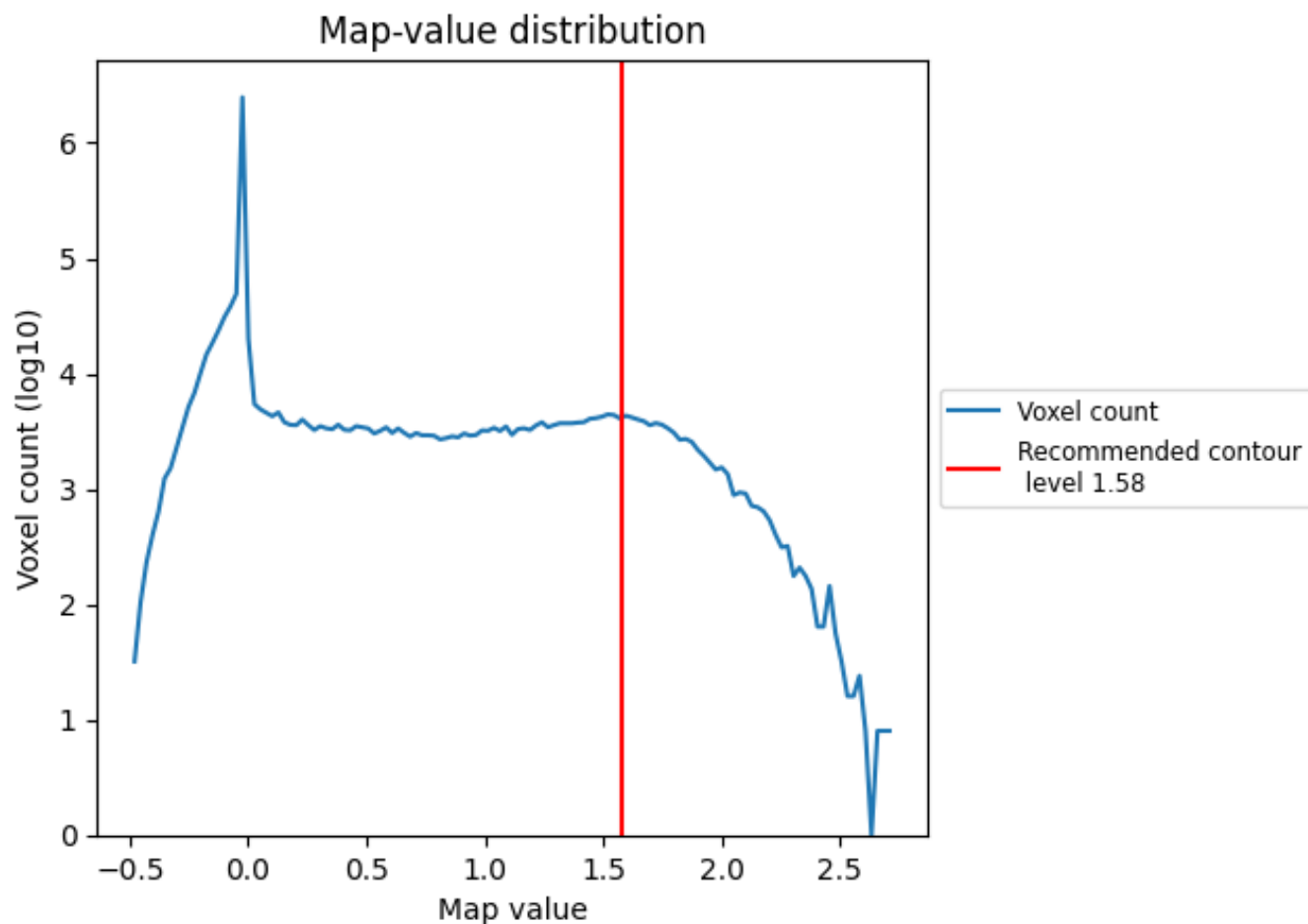
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

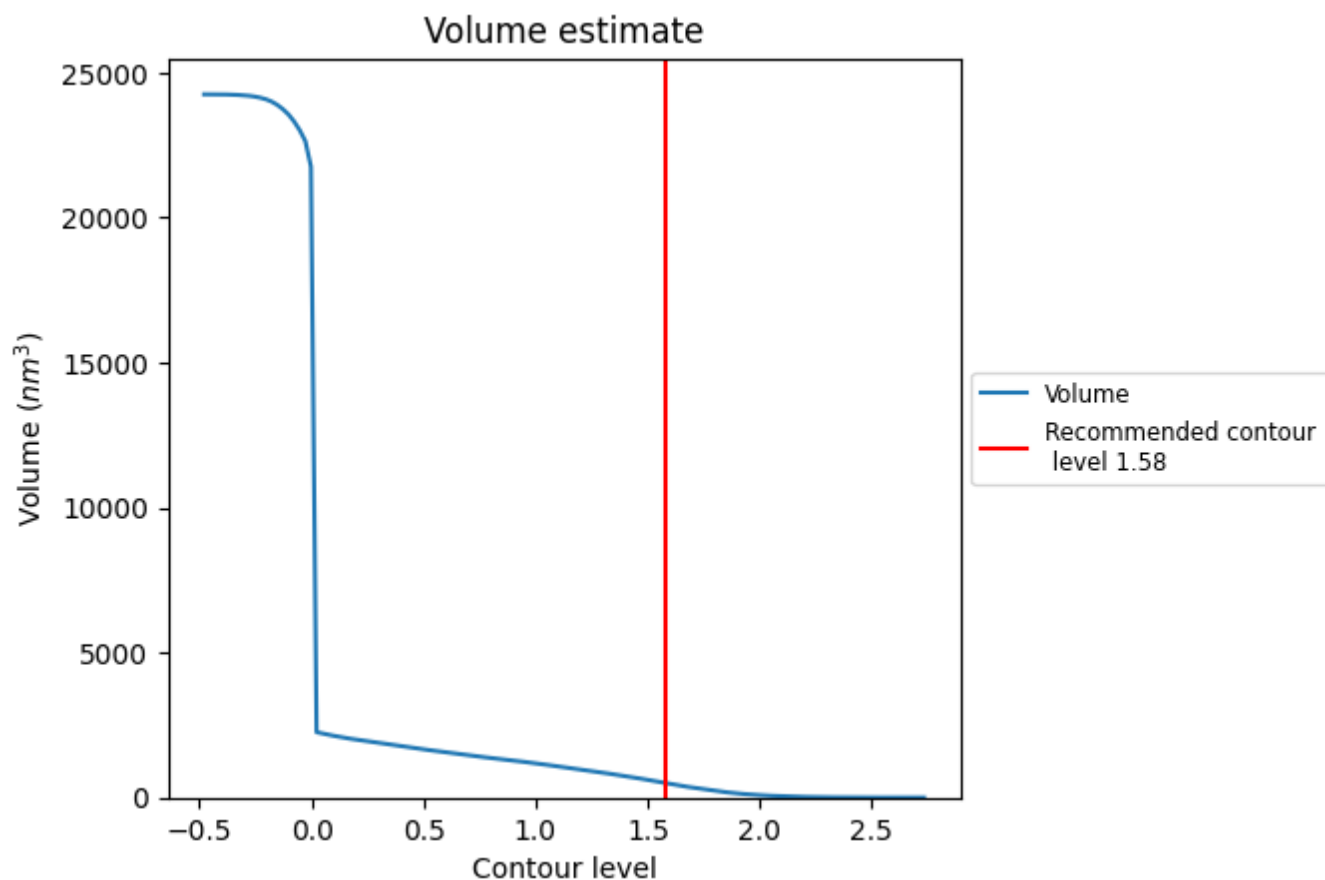
This section contains the results of statistical analysis of the map.

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.

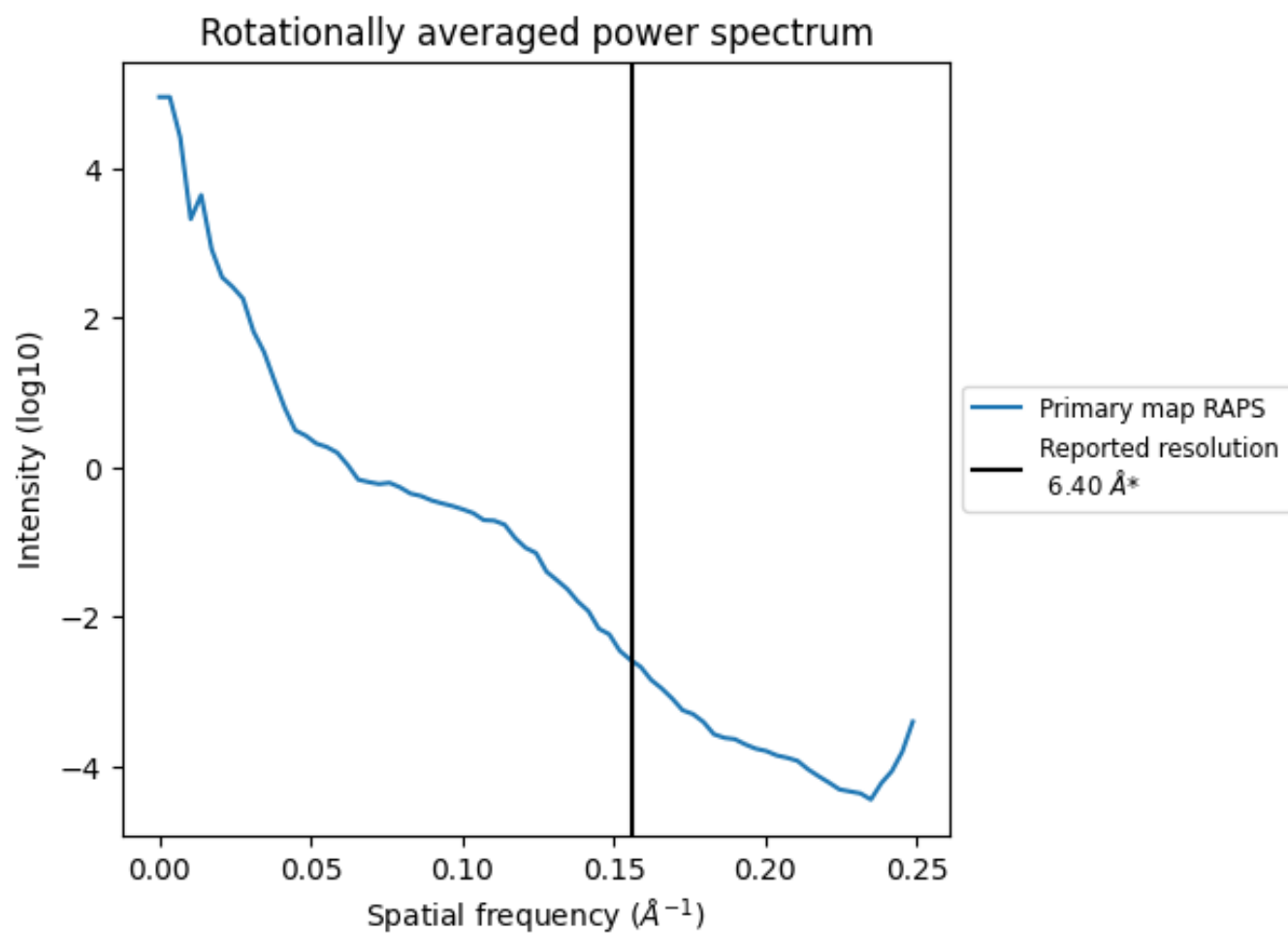
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 500 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.156 Å⁻¹

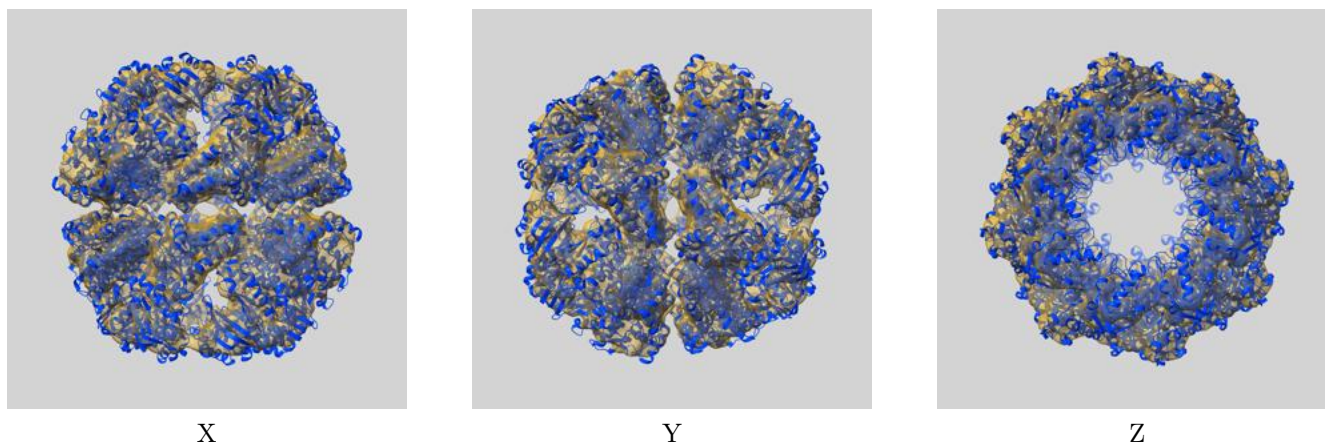
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

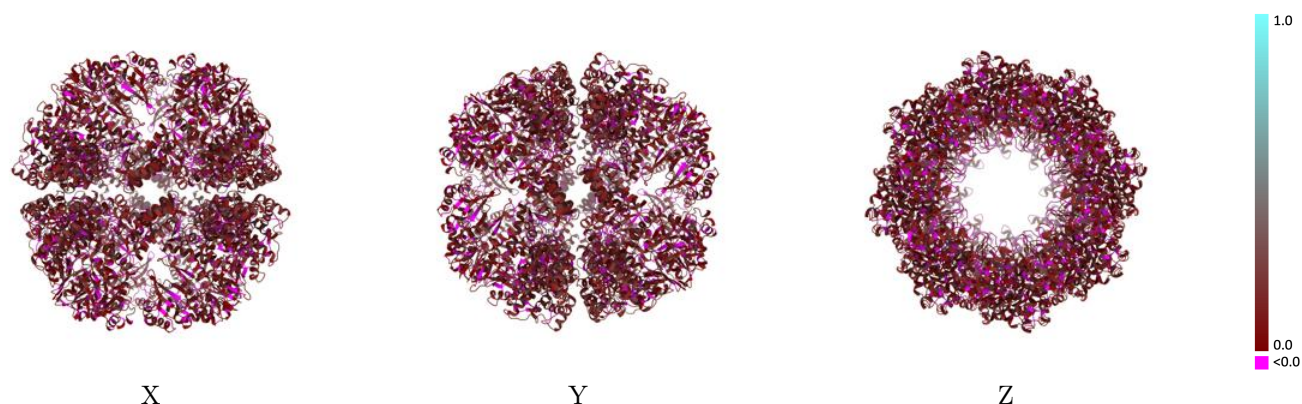
This section contains information regarding the fit between EMDB map EMD-5250 and PDB model 3IZN. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



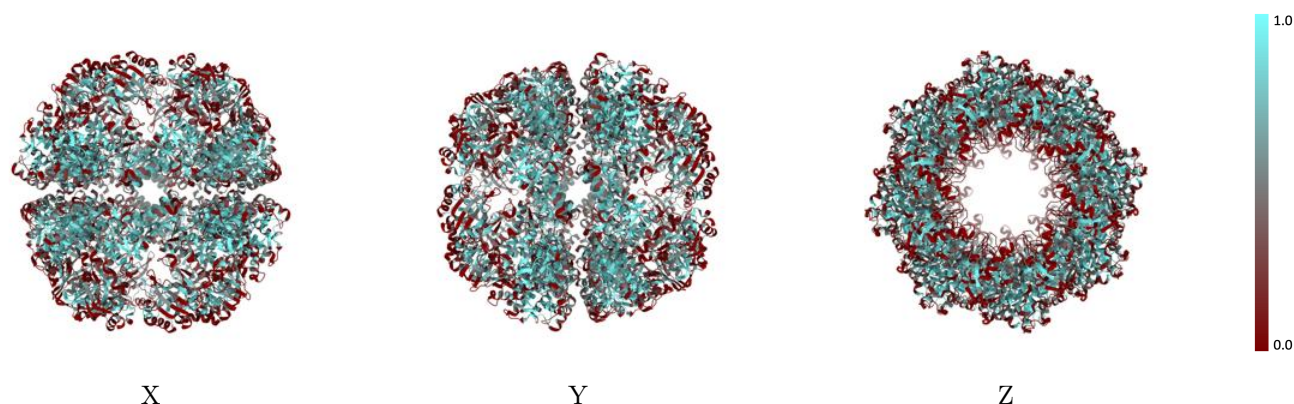
The images above show the 3D surface view of the map at the recommended contour level 1.58 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



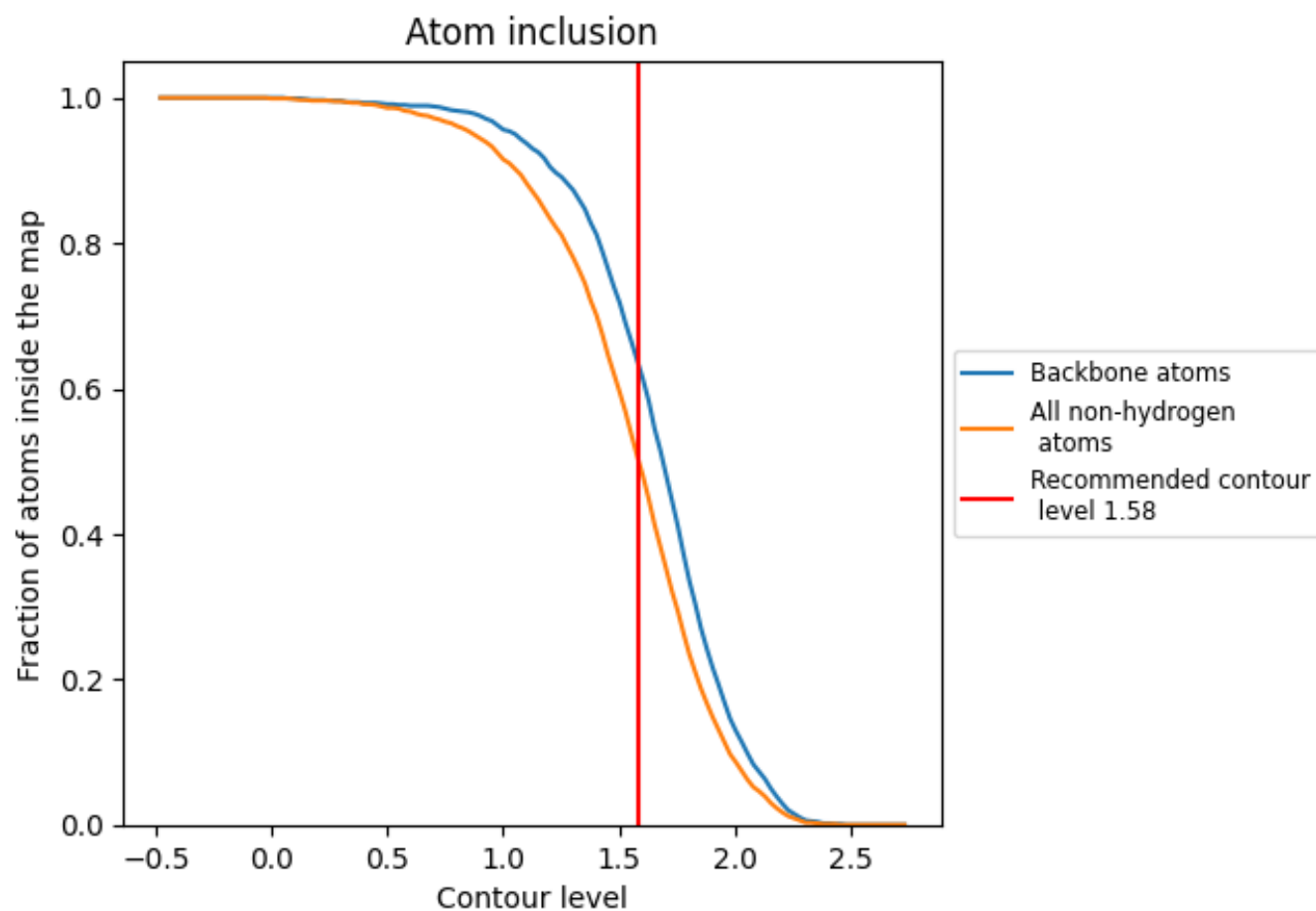
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

