



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:56 PM UTC

PDB ID : 3IZI / pdb_00003izi
EMDB ID : EMD-5245
Title : Mm-cpn rls with ATP
Authors : Douglas, N.R.; Reissmann, S.; Zhang, J.; Chen, B.; Jakana, J.; Kumar, R.;
Chiu, W.; Frydman, J.
Deposited on : 2010-10-29
Resolution : 6.70 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:

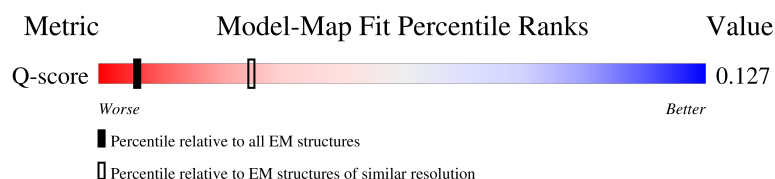
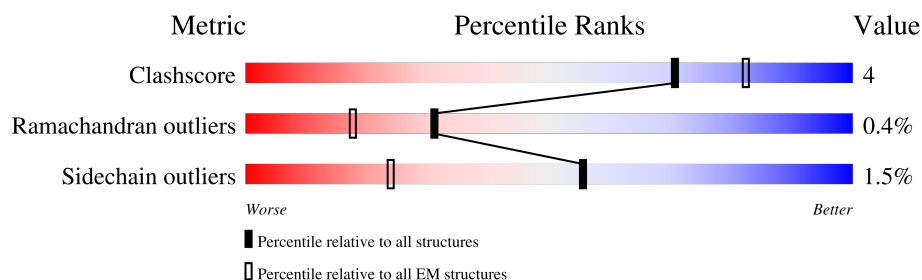
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.70 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	523 (6.20 - 7.20)

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	38% 89% 10%
1	B	513	38% 90% 9%
1	C	513	38% 90% 9%
1	D	513	38% 89% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	513	
1	F	513	
1	G	513	
1	H	513	
1	I	513	
1	J	513	
1	K	513	
1	L	513	
1	M	513	
1	N	513	
1	O	513	
1	P	513	

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

Continued on next page...

Continued from previous page...

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

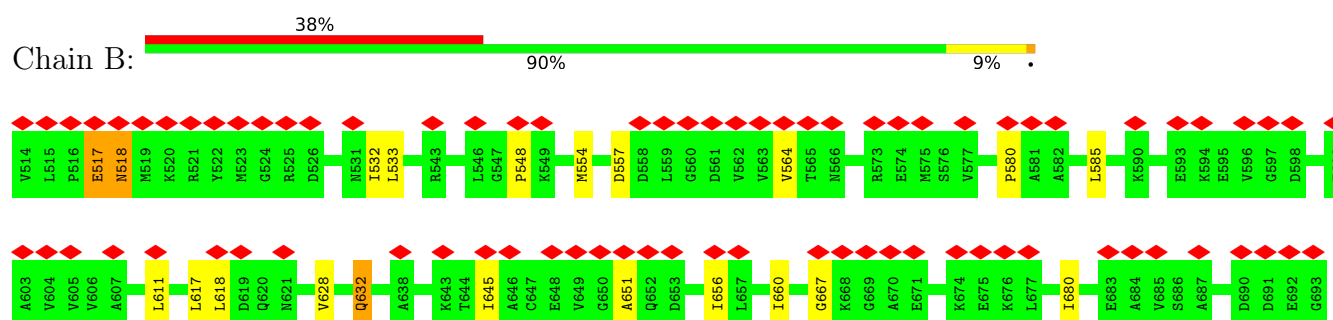
3 Residue-property plots

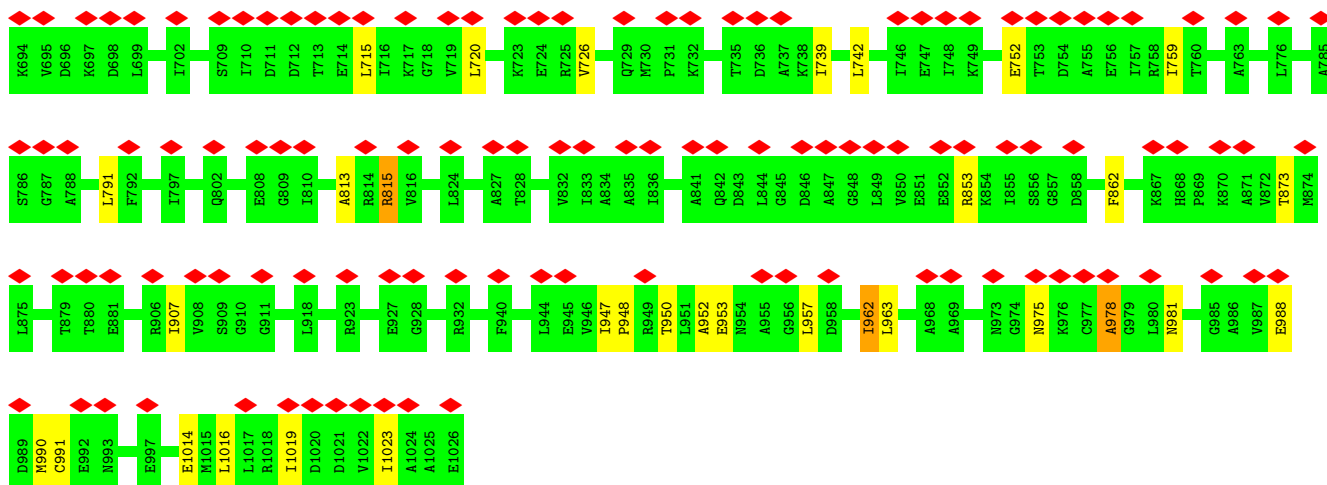
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

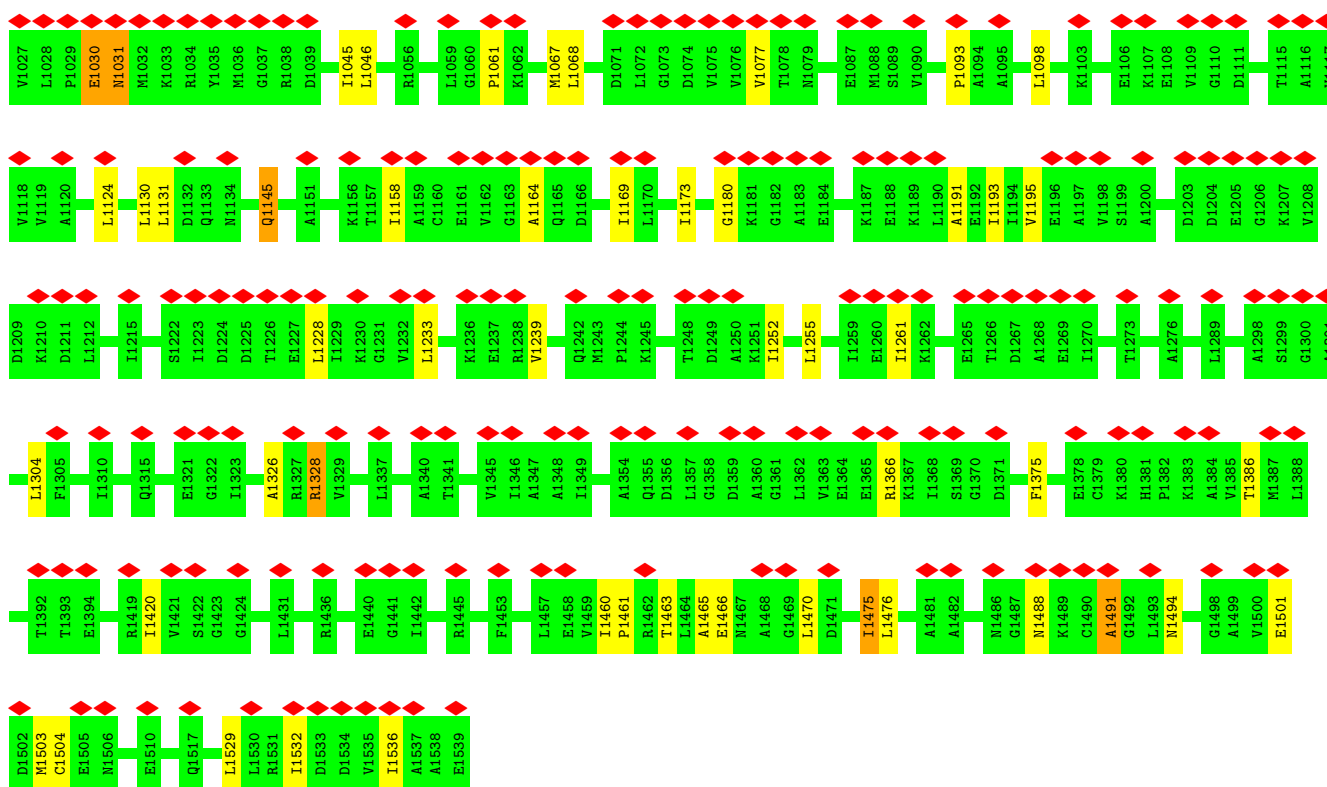
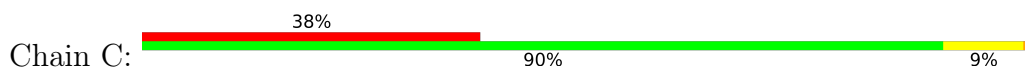


• Molecule 1: Chaperonin

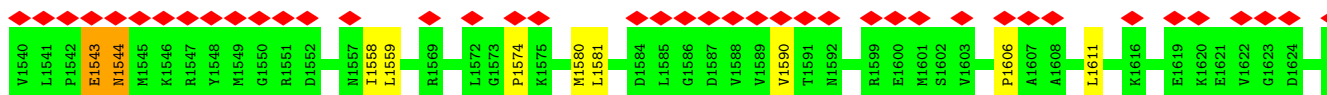
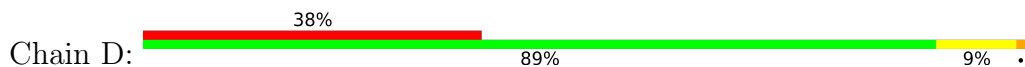


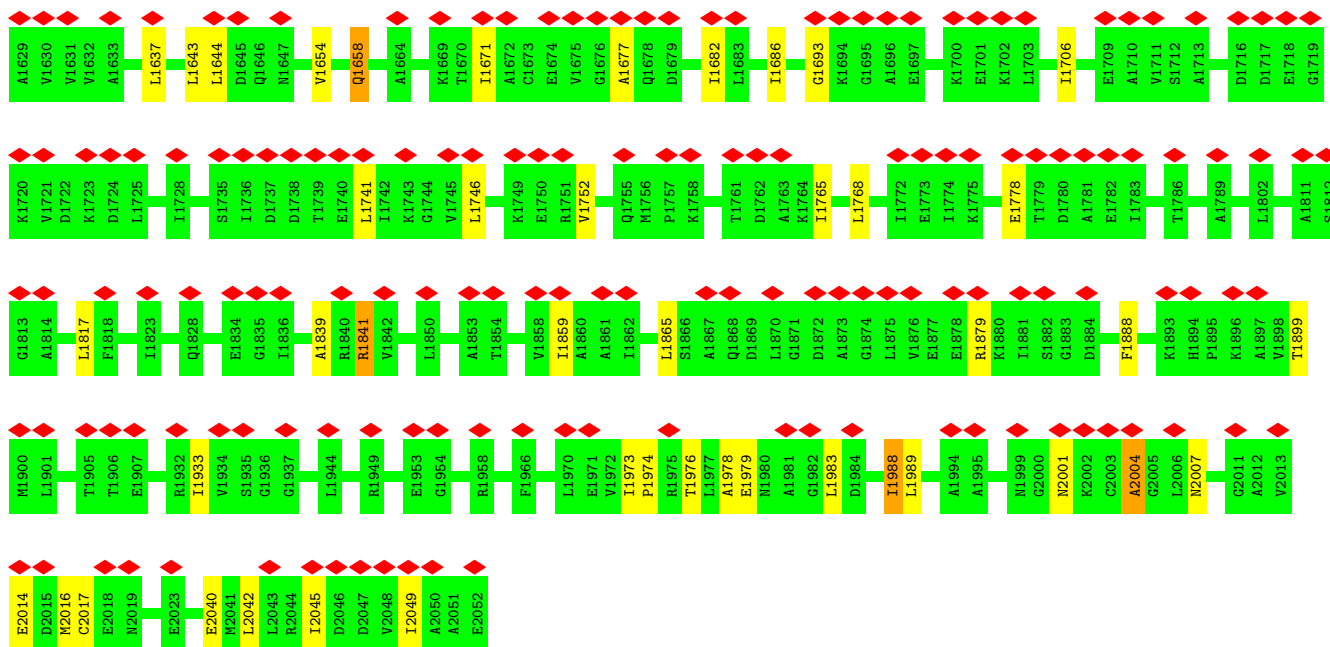


• Molecule 1: Chaperonin

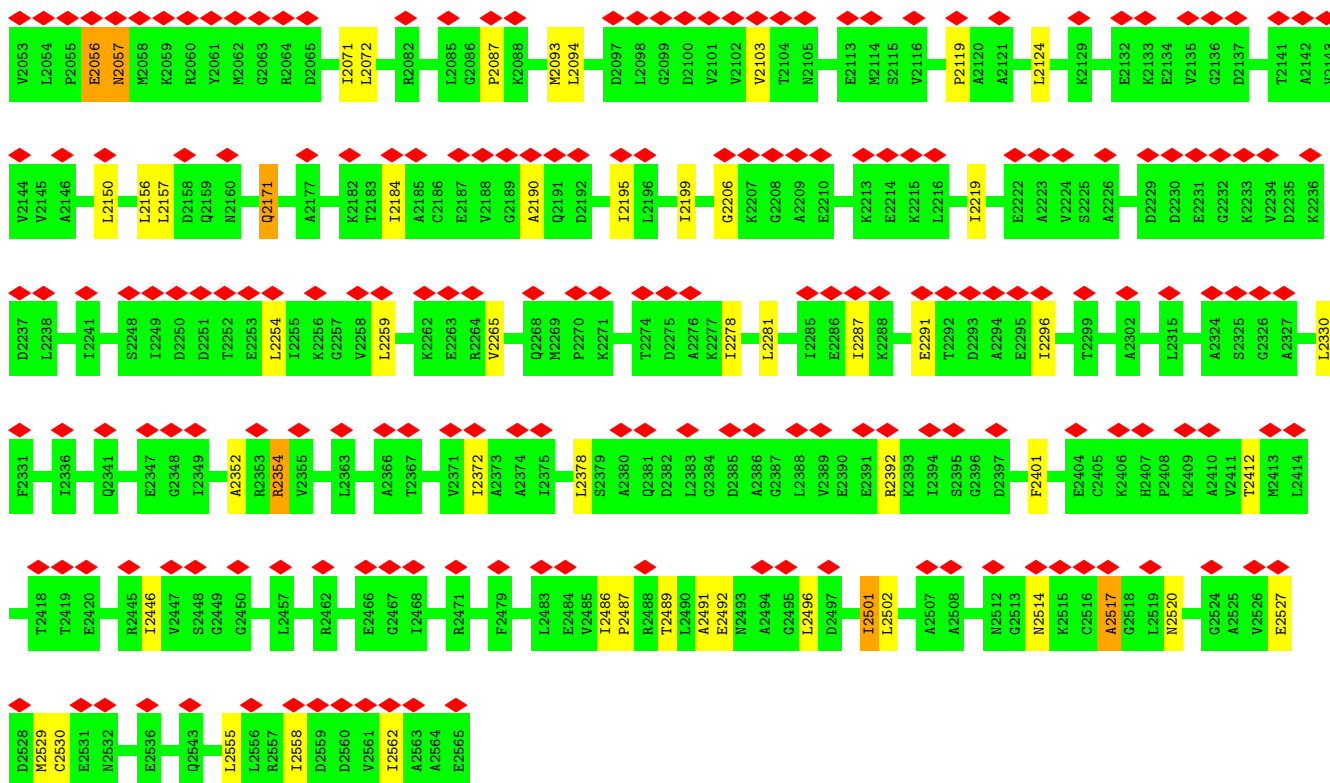
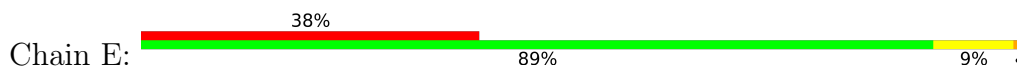


• Molecule 1: Chaperonin

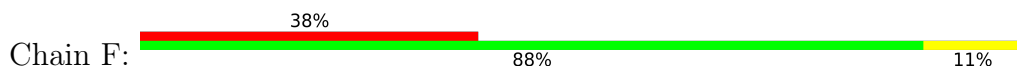


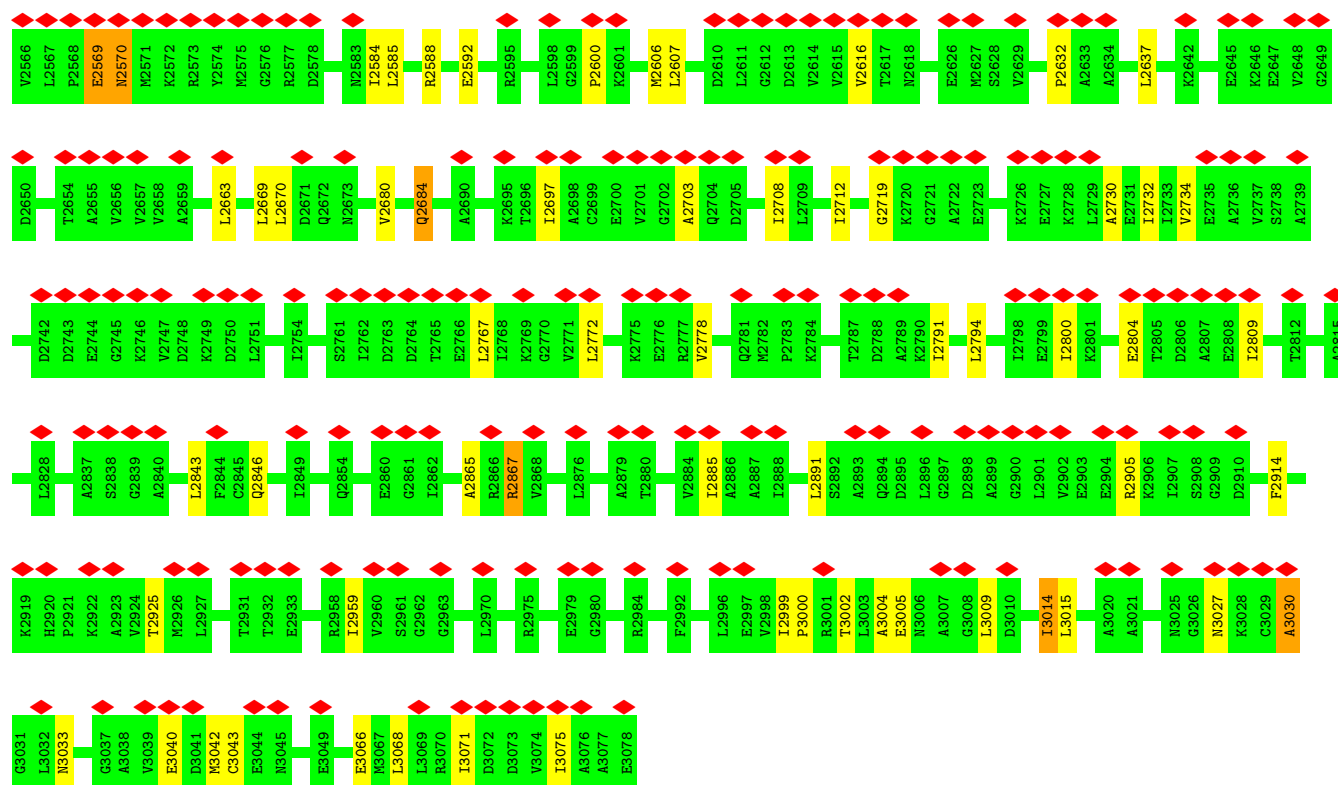


- Molecule 1: Chaperonin

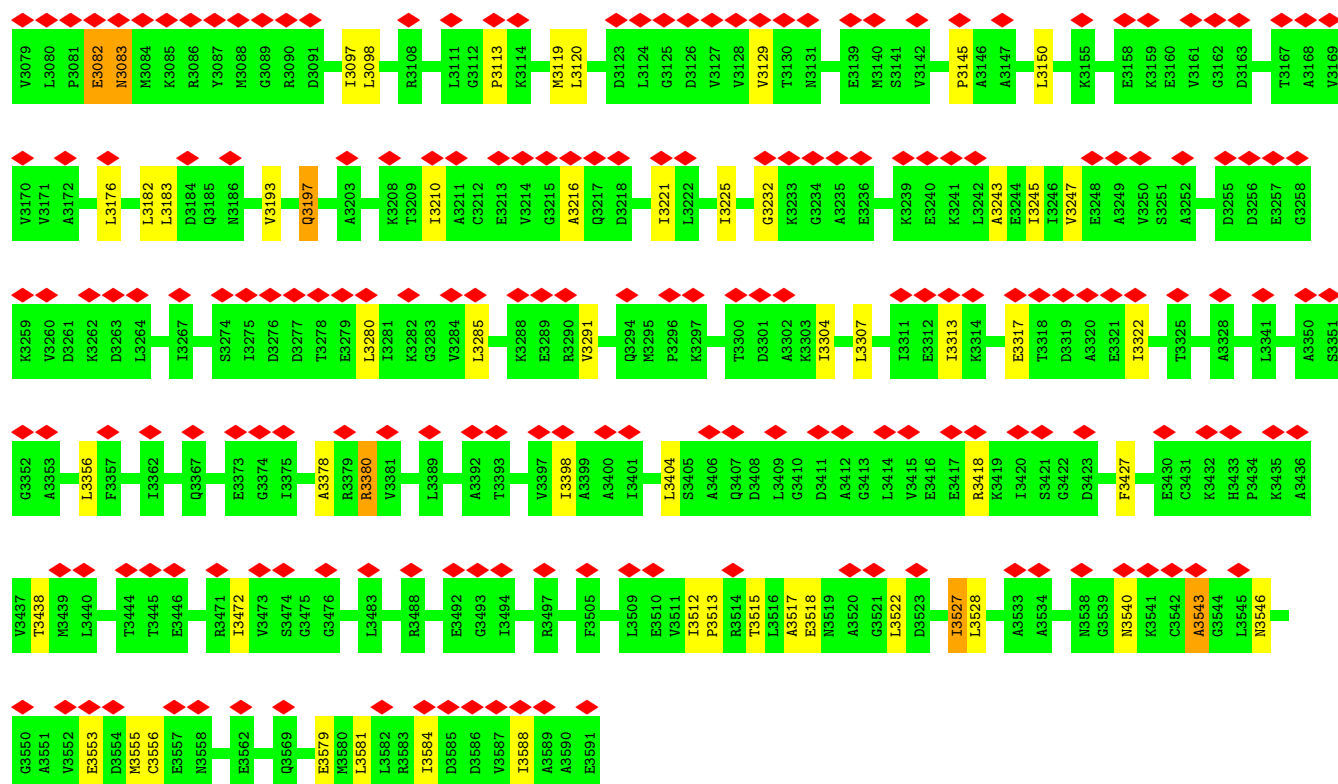
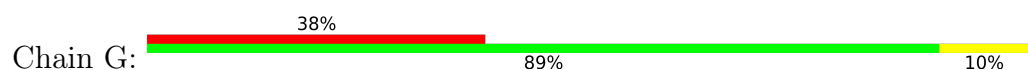


- Molecule 1: Chaperonin

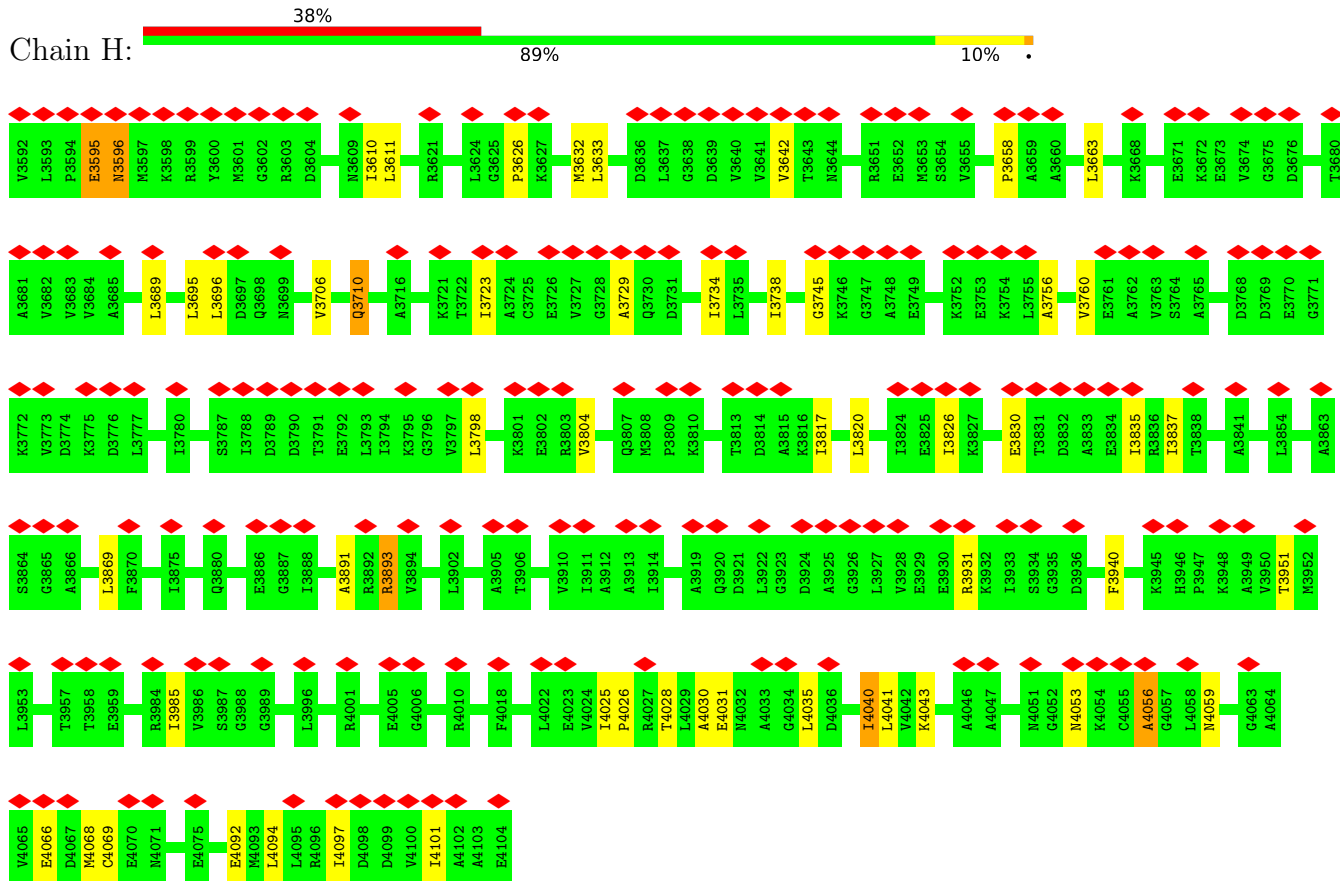




• Molecule 1: Chaperonin

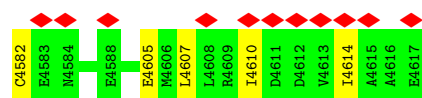


• Molecule 1: Chaperonin

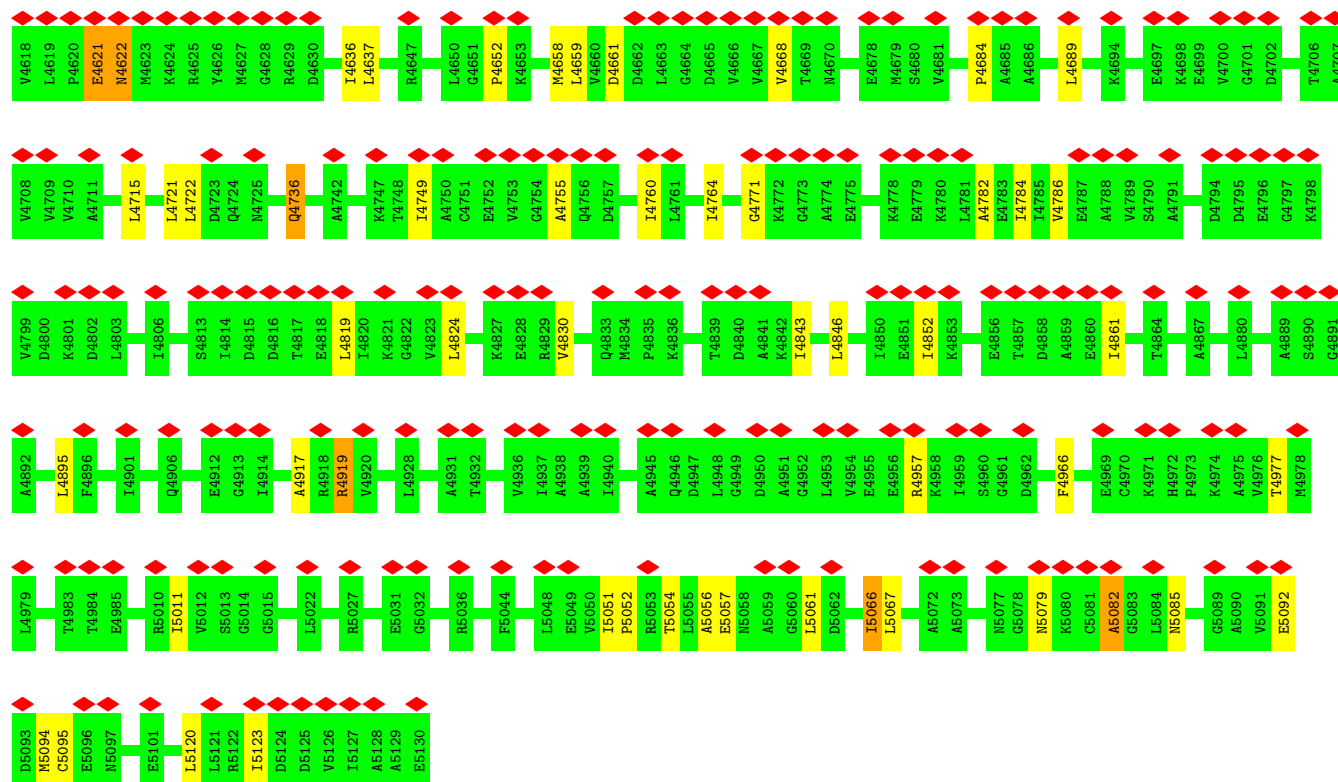
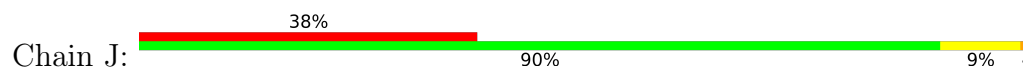


• Molecule 1: Chaperonin

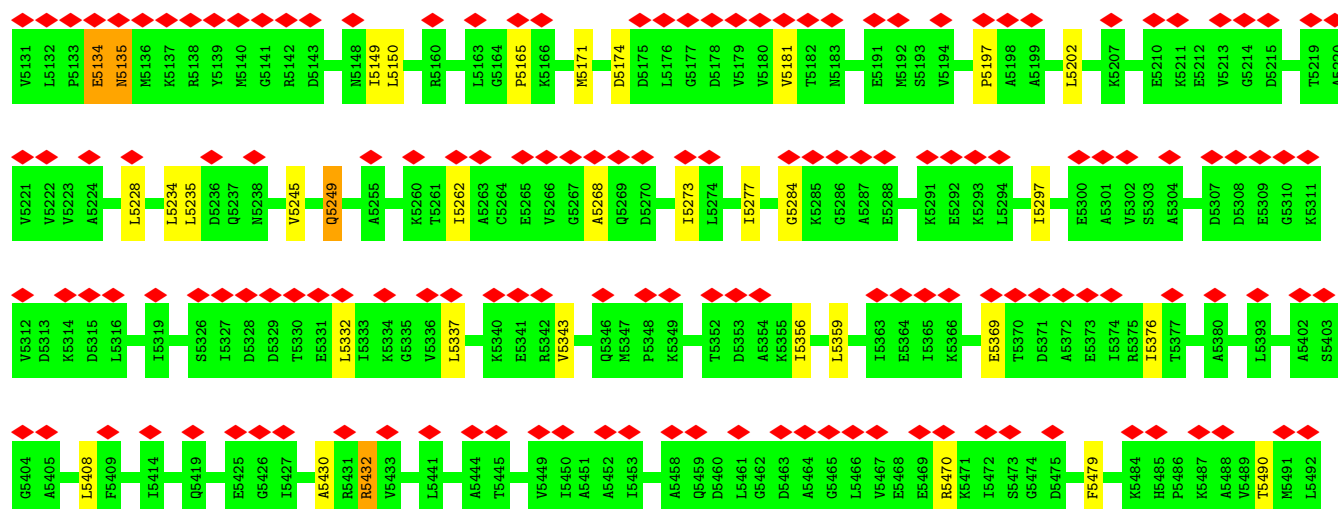
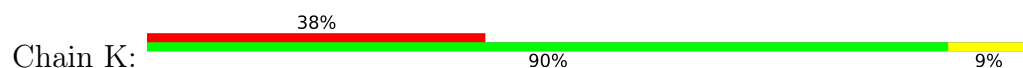


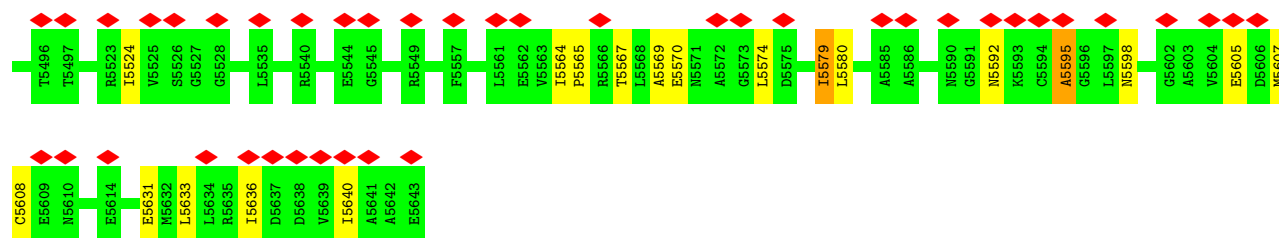


• Molecule 1: Chaperonin

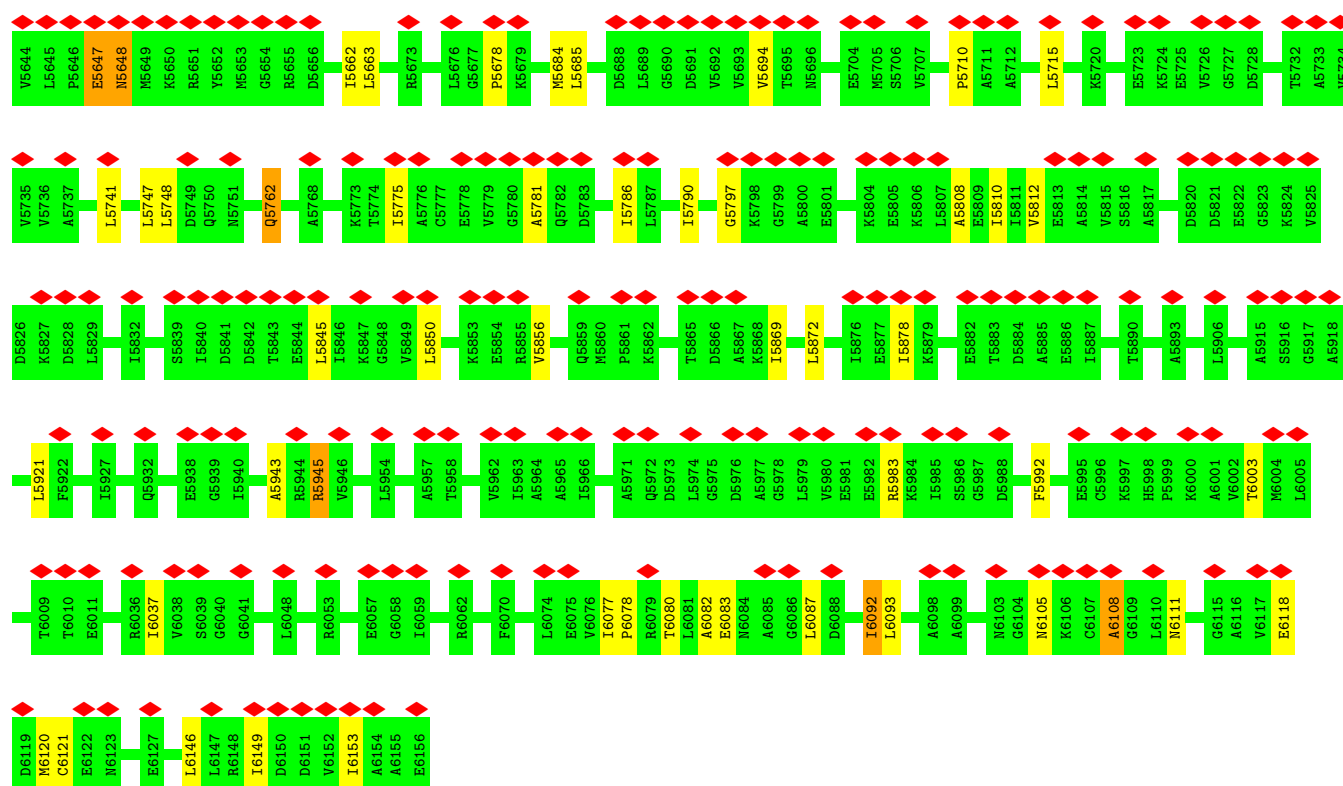
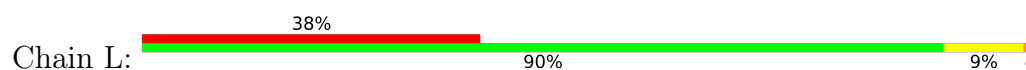


• Molecule 1: Chaperonin

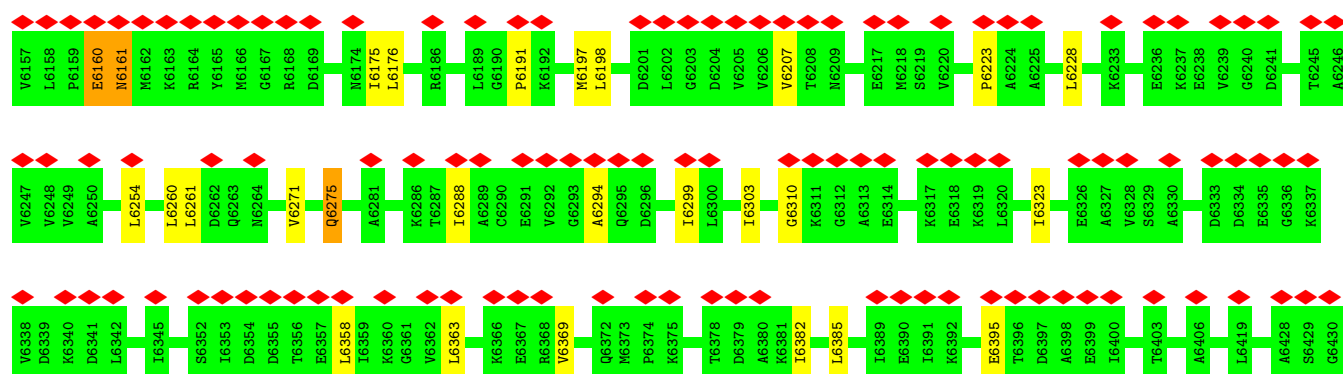
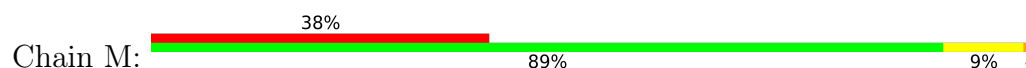


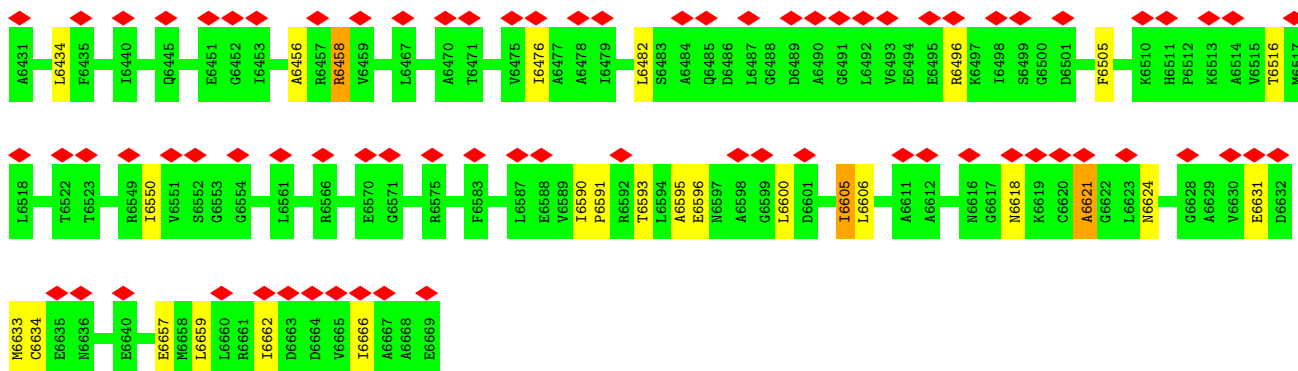


• Molecule 1: Chaperonin

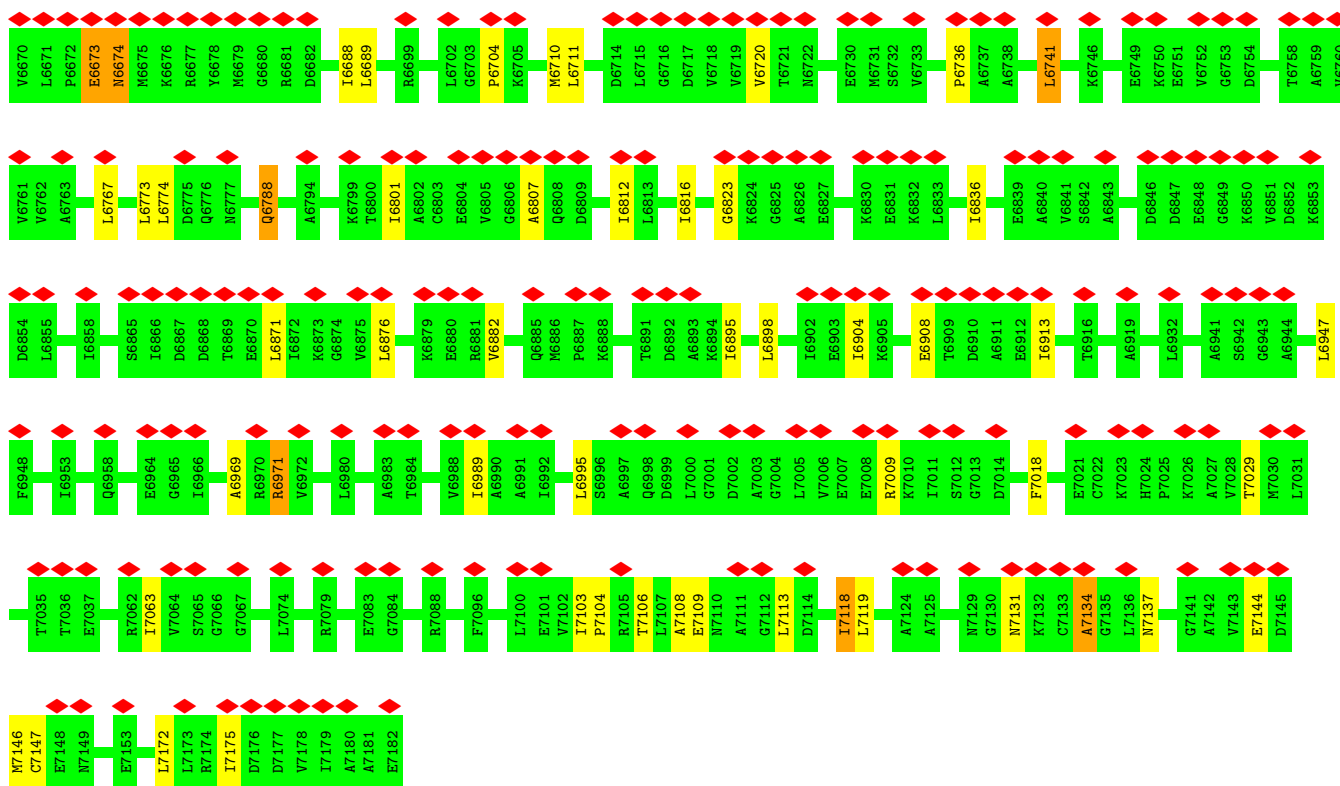
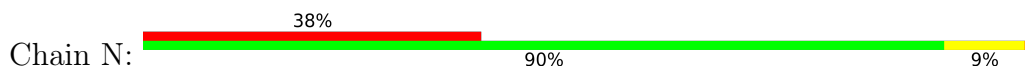


• Molecule 1: Chaperonin

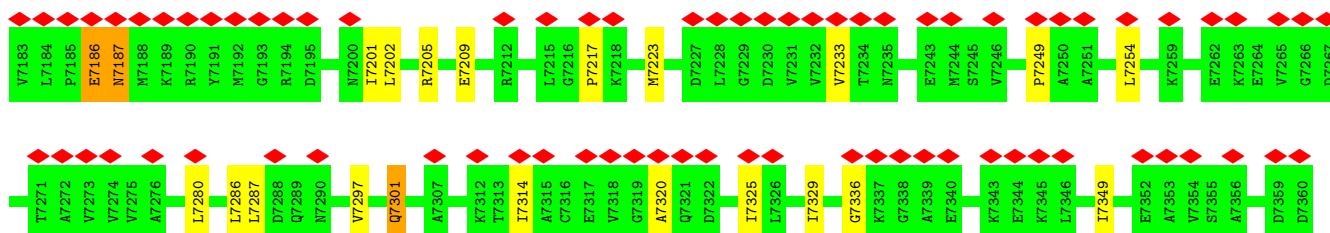
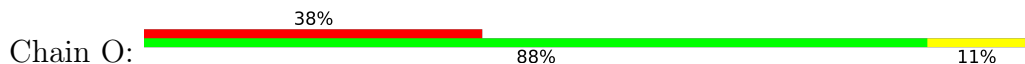


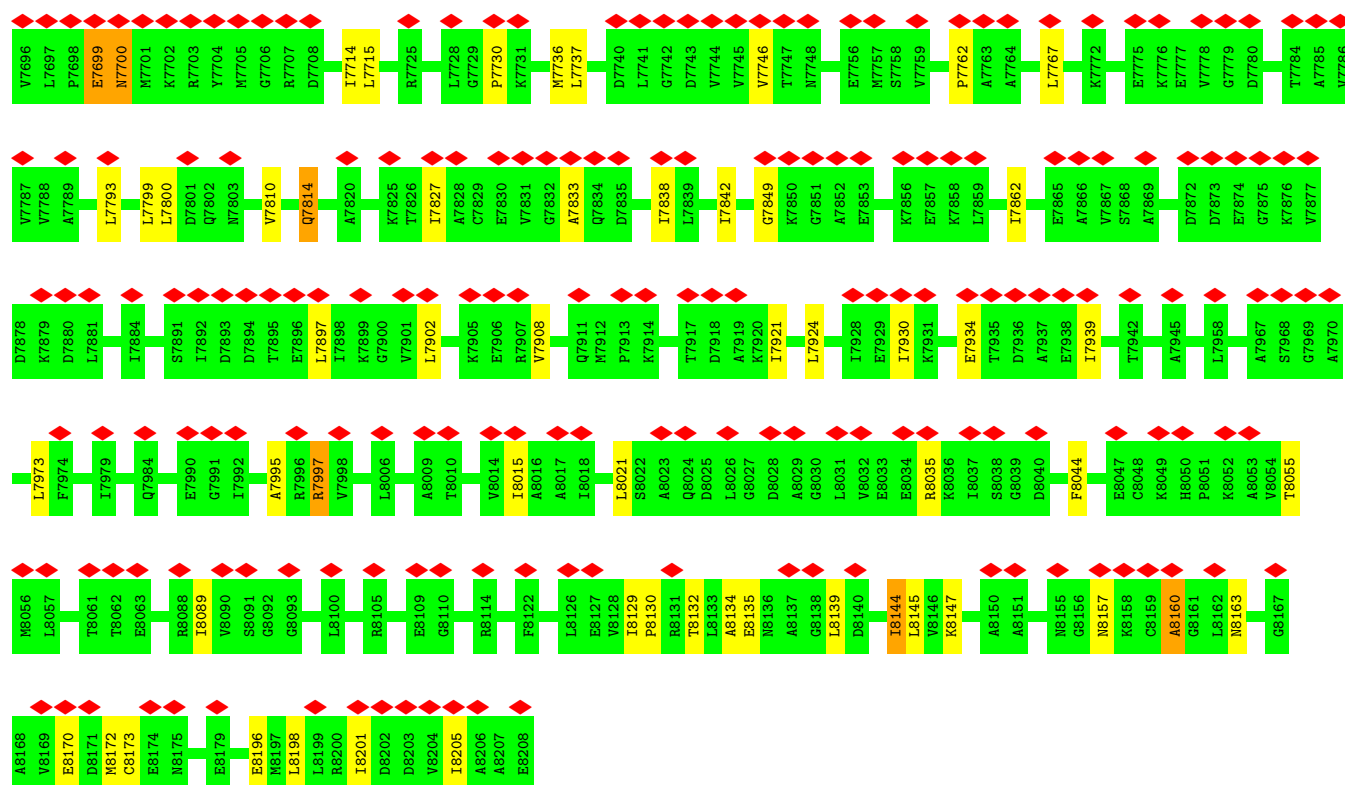


• Molecule 1: Chaperonin



• 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 4000 (4k x 4k)	Depositor
Maximum map value	0.744	Depositor
Minimum map value	-0.366	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.28	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	0.95	6/3863 (0.2%)	1.04	5/5199 (0.1%)
1	B	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	C	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	D	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	E	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	F	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	G	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	H	0.95	6/3863 (0.2%)	1.04	5/5199 (0.1%)
1	I	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	J	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	K	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	L	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	M	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	N	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	O	0.95	5/3863 (0.1%)	1.04	5/5199 (0.1%)
1	P	0.95	6/3863 (0.2%)	1.04	5/5199 (0.1%)
All	All	0.95	83/61808 (0.1%)	1.04	80/83184 (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

Continued on next page...

Continued from previous page...

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 (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2056	GLU	C-O	-10.04	1.11	1.24
1	D	1543	GLU	C-O	-9.97	1.11	1.24
1	P	7699	GLU	C-O	-9.96	1.12	1.24
1	J	4621	GLU	C-O	-9.95	1.12	1.24
1	O	7186	GLU	C-O	-9.94	1.12	1.24
1	C	1030	GLU	C-O	-9.94	1.12	1.24
1	B	517	GLU	C-O	-9.93	1.12	1.24
1	K	5134	GLU	C-O	-9.93	1.12	1.24
1	A	4	GLU	C-O	-9.90	1.12	1.24
1	G	3082	GLU	C-O	-9.90	1.12	1.24
1	L	5647	GLU	C-O	-9.90	1.12	1.24
1	N	6673	GLU	C-O	-9.90	1.12	1.24
1	M	6160	GLU	C-O	-9.87	1.12	1.24
1	F	2569	GLU	C-O	-9.86	1.12	1.24
1	H	3595	GLU	C-O	-9.86	1.12	1.24
1	I	4108	GLU	C-O	-9.86	1.12	1.24
1	E	2056	GLU	C-N	9.63	1.47	1.33
1	J	4621	GLU	C-N	9.63	1.47	1.33
1	B	517	GLU	C-N	9.61	1.47	1.33
1	D	1543	GLU	C-N	9.60	1.47	1.33
1	C	1030	GLU	C-N	9.59	1.47	1.33
1	L	5647	GLU	C-N	9.59	1.47	1.33
1	P	7699	GLU	C-N	9.59	1.47	1.33
1	F	2569	GLU	C-N	9.56	1.47	1.33
1	H	3595	GLU	C-N	9.56	1.47	1.33
1	I	4108	GLU	C-N	9.56	1.47	1.33
1	K	5134	GLU	C-N	9.56	1.47	1.33
1	M	6160	GLU	C-N	9.56	1.47	1.33
1	O	7186	GLU	C-N	9.56	1.47	1.33
1	A	4	GLU	C-N	9.53	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	3082	GLU	C-N	9.53	1.47	1.33
1	N	6673	GLU	C-N	9.53	1.47	1.33
1	J	5082	ALA	C-O	-6.84	1.15	1.24
1	N	7134	ALA	C-O	-6.84	1.15	1.24
1	I	4569	ALA	C-O	-6.82	1.15	1.24
1	B	978	ALA	C-O	-6.80	1.15	1.24
1	D	2004	ALA	C-O	-6.80	1.15	1.24
1	M	6621	ALA	C-O	-6.80	1.15	1.24
1	E	2517	ALA	C-O	-6.78	1.15	1.24
1	G	3543	ALA	C-O	-6.78	1.15	1.24
1	P	8160	ALA	C-O	-6.78	1.15	1.24
1	L	6108	ALA	C-O	-6.78	1.15	1.24
1	K	5595	ALA	C-O	-6.78	1.15	1.24
1	F	3030	ALA	C-O	-6.76	1.15	1.24
1	H	4056	ALA	C-O	-6.76	1.15	1.24
1	O	7647	ALA	C-O	-6.76	1.15	1.24
1	A	465	ALA	C-O	-6.73	1.15	1.24
1	C	1491	ALA	C-O	-6.73	1.15	1.24
1	L	5762	GLN	C-O	-6.39	1.16	1.24
1	K	5249	GLN	C-O	-6.38	1.16	1.24
1	E	2171	GLN	C-O	-6.34	1.16	1.24
1	G	3197	GLN	C-O	-6.34	1.16	1.24
1	O	7301	GLN	C-O	-6.34	1.16	1.24
1	D	1658	GLN	C-O	-6.31	1.16	1.24
1	B	632	GLN	C-O	-6.31	1.16	1.24
1	A	119	GLN	C-O	-6.30	1.16	1.24
1	C	1145	GLN	C-O	-6.30	1.16	1.24
1	P	7814	GLN	C-O	-6.30	1.16	1.24
1	F	2684	GLN	C-O	-6.26	1.16	1.24
1	H	3710	GLN	C-O	-6.26	1.16	1.24
1	I	4223	GLN	C-O	-6.26	1.16	1.24
1	M	6275	GLN	C-O	-6.26	1.16	1.24
1	J	4736	GLN	C-O	-6.25	1.16	1.24
1	N	6788	GLN	C-O	-6.25	1.16	1.24
1	G	3197	GLN	C-N	5.11	1.40	1.33
1	L	5762	GLN	C-N	5.11	1.40	1.33
1	K	5249	GLN	C-N	5.09	1.40	1.33
1	B	632	GLN	C-N	5.08	1.40	1.33
1	D	1658	GLN	C-N	5.08	1.40	1.33
1	F	2684	GLN	C-N	5.08	1.40	1.33
1	H	3710	GLN	C-N	5.08	1.40	1.33
1	M	6275	GLN	C-N	5.08	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	7301	GLN	C-N	5.08	1.40	1.33
1	A	119	GLN	C-N	5.07	1.40	1.33
1	E	2171	GLN	C-N	5.07	1.40	1.33
1	J	4736	GLN	C-N	5.07	1.40	1.33
1	P	7814	GLN	C-N	5.04	1.40	1.33
1	H	4043	LYS	C-O	-5.02	1.18	1.24
1	I	4223	GLN	C-N	5.02	1.40	1.33
1	C	1145	GLN	C-N	5.01	1.40	1.33
1	N	6788	GLN	C-N	5.01	1.40	1.33
1	A	452	LYS	C-O	-5.01	1.18	1.24
1	P	8147	LYS	C-O	-5.01	1.18	1.24

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1768	LEU	CD1-CG-CD2	-6.28	96.97	110.80
1	I	4333	LEU	CD1-CG-CD2	-6.28	96.97	110.80
1	B	742	LEU	CD1-CG-CD2	-6.28	96.98	110.80
1	M	6385	LEU	CD1-CG-CD2	-6.28	96.98	110.80
1	N	6898	LEU	CD1-CG-CD2	-6.28	96.98	110.80
1	J	4846	LEU	CD1-CG-CD2	-6.28	96.98	110.80
1	O	7411	LEU	CD1-CG-CD2	-6.27	97.00	110.80
1	E	2281	LEU	CD1-CG-CD2	-6.27	97.00	110.80
1	G	3307	LEU	CD1-CG-CD2	-6.27	97.00	110.80
1	L	5872	LEU	CD1-CG-CD2	-6.27	97.01	110.80
1	P	7924	LEU	CD1-CG-CD2	-6.27	97.00	110.80
1	F	2794	LEU	CD1-CG-CD2	-6.26	97.02	110.80
1	K	5359	LEU	CD1-CG-CD2	-6.26	97.02	110.80
1	H	3820	LEU	CD1-CG-CD2	-6.26	97.02	110.80
1	A	229	LEU	CD1-CG-CD2	-6.25	97.05	110.80
1	C	1255	LEU	CD1-CG-CD2	-6.25	97.05	110.80
1	D	1543	GLU	N-CA-C	-6.00	101.02	109.96
1	J	4621	GLU	N-CA-C	-5.99	101.03	109.96
1	F	2569	GLU	N-CA-C	-5.99	101.03	109.96
1	E	2056	GLU	N-CA-C	-5.99	101.03	109.96
1	A	4	GLU	N-CA-C	-5.99	101.04	109.96
1	L	5647	GLU	N-CA-C	-5.98	101.05	109.96
1	B	517	GLU	N-CA-C	-5.98	101.06	109.96
1	H	3595	GLU	N-CA-C	-5.98	101.06	109.96
1	I	4108	GLU	N-CA-C	-5.97	101.06	109.96
1	K	5134	GLU	N-CA-C	-5.97	101.06	109.96
1	P	7699	GLU	N-CA-C	-5.97	101.06	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	7186	GLU	N-CA-C	-5.97	101.07	109.96
1	G	3082	GLU	N-CA-C	-5.97	101.07	109.96
1	C	1030	GLU	N-CA-C	-5.96	101.07	109.96
1	M	6160	GLU	N-CA-C	-5.96	101.07	109.96
1	N	6673	GLU	N-CA-C	-5.96	101.08	109.96
1	M	6160	GLU	CA-C-O	-5.68	114.17	120.70
1	O	7186	GLU	CA-C-O	-5.65	114.20	120.70
1	P	7699	GLU	CA-C-O	-5.65	114.21	120.70
1	G	3082	GLU	CA-C-O	-5.64	114.22	120.70
1	N	6673	GLU	CA-C-O	-5.63	114.23	120.70
1	H	4040	ILE	CB-CG1-CD1	5.62	125.61	113.80
1	A	4	GLU	CA-C-O	-5.62	114.24	120.70
1	L	5647	GLU	CA-C-O	-5.62	114.24	120.70
1	A	449	ILE	CB-CG1-CD1	5.61	125.59	113.80
1	F	3014	ILE	CB-CG1-CD1	5.61	125.58	113.80
1	J	4621	GLU	CA-C-O	-5.61	114.25	120.70
1	M	6605	ILE	CB-CG1-CD1	5.61	125.58	113.80
1	C	1475	ILE	CB-CG1-CD1	5.61	125.58	113.80
1	F	2569	GLU	CA-C-O	-5.61	114.25	120.70
1	I	4108	GLU	CA-C-O	-5.61	114.25	120.70
1	B	962	ILE	CB-CG1-CD1	5.61	125.57	113.80
1	G	3527	ILE	CB-CG1-CD1	5.60	125.57	113.80
1	K	5134	GLU	CA-C-O	-5.60	114.25	120.70
1	L	6092	ILE	CB-CG1-CD1	5.60	125.57	113.80
1	D	1988	ILE	CB-CG1-CD1	5.60	125.56	113.80
1	H	3595	GLU	CA-C-O	-5.60	114.26	120.70
1	J	5066	ILE	CB-CG1-CD1	5.60	125.56	113.80
1	O	7631	ILE	CB-CG1-CD1	5.60	125.56	113.80
1	I	4553	ILE	CB-CG1-CD1	5.60	125.55	113.80
1	K	5579	ILE	CB-CG1-CD1	5.60	125.55	113.80
1	B	517	GLU	CA-C-O	-5.59	114.27	120.70
1	N	7118	ILE	CB-CG1-CD1	5.59	125.55	113.80
1	E	2501	ILE	CB-CG1-CD1	5.59	125.54	113.80
1	P	8144	ILE	CB-CG1-CD1	5.59	125.53	113.80
1	D	1543	GLU	CA-C-O	-5.57	114.30	120.70
1	E	2056	GLU	CA-C-O	-5.56	114.30	120.70
1	C	1030	GLU	CA-C-O	-5.56	114.31	120.70
1	N	7147	CYS	N-CA-CB	-5.29	102.33	110.01
1	L	6121	CYS	N-CA-CB	-5.29	102.34	110.01
1	E	2530	CYS	N-CA-CB	-5.29	102.34	110.01
1	D	2017	CYS	N-CA-CB	-5.28	102.35	110.01
1	H	4069	CYS	N-CA-CB	-5.28	102.35	110.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	CYS	N-CA-CB	-5.28	102.35	110.01
1	G	3556	CYS	N-CA-CB	-5.28	102.35	110.01
1	J	5095	CYS	N-CA-CB	-5.28	102.35	110.01
1	P	8173	CYS	N-CA-CB	-5.28	102.35	110.01
1	C	1504	CYS	N-CA-CB	-5.27	102.36	110.01
1	I	4582	CYS	N-CA-CB	-5.27	102.37	110.01
1	B	991	CYS	N-CA-CB	-5.27	102.37	110.01
1	F	3043	CYS	N-CA-CB	-5.26	102.38	110.01
1	M	6634	CYS	N-CA-CB	-5.26	102.38	110.01
1	O	7660	CYS	N-CA-CB	-5.26	102.39	110.01
1	K	5608	CYS	N-CA-CB	-5.23	102.42	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	32	0
1	B	3840	0	3983	31	0
1	C	3840	0	3983	30	0
1	D	3840	0	3983	31	0
1	E	3840	0	3983	32	0
1	F	3840	0	3983	35	0
1	G	3840	0	3983	34	0
1	H	3840	0	3983	33	0
1	I	3840	0	3983	33	0
1	J	3840	0	3983	31	0
1	K	3840	0	3983	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3840	0	3983	30	0
1	M	3840	0	3983	31	0
1	N	3840	0	3983	32	0
1	O	3840	0	3983	34	0
1	P	3840	0	3983	33	0
All	All	61440	0	63731	438	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 4.

All (438) 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:G:3380:ARG:HE	1:G:3380:ARG:HA	1.60	0.67
1:A:302:ARG:HE	1:A:302:ARG:HA	1.60	0.67
1:P:7997:ARG:HE	1:P:7997:ARG:HA	1.60	0.67
1:J:4919:ARG:HE	1:J:4919:ARG:HA	1.60	0.67
1:H:3893:ARG:HE	1:H:3893:ARG:HA	1.60	0.66
1:B:815:ARG:HE	1:B:815:ARG:HA	1.60	0.66
1:I:4406:ARG:HE	1:I:4406:ARG:HA	1.60	0.66
1:K:5432:ARG:HE	1:K:5432:ARG:HA	1.60	0.66
1:C:1328:ARG:HE	1:C:1328:ARG:HA	1.60	0.66
1:L:5945:ARG:HE	1:L:5945:ARG:HA	1.60	0.66
1:F:2867:ARG:HE	1:F:2867:ARG:HA	1.60	0.65
1:M:6458:ARG:HE	1:M:6458:ARG:HA	1.60	0.65
1:O:7484:ARG:HE	1:O:7484:ARG:HA	1.60	0.65
1:D:1841:ARG:HE	1:D:1841:ARG:HA	1.60	0.65
1:E:2354:ARG:HE	1:E:2354:ARG:HA	1.60	0.65
1:N:6971:ARG:HE	1:N:6971:ARG:HA	1.60	0.65
1:F:2999:ILE:HB	1:F:3000:PRO:HD3	1.84	0.60
1:O:7616:ILE:HB	1:O:7617:PRO:HD3	1.84	0.60
1:I:4538:ILE:HB	1:I:4539:PRO:HD3	1.84	0.60
1:H:4025:ILE:HB	1:H:4026:PRO:HD3	1.84	0.60
1:G:3512:ILE:HB	1:G:3513:PRO:HD3	1.84	0.60
1:P:8129:ILE:HB	1:P:8130:PRO:HD3	1.84	0.60
1:E:2486:ILE:HB	1:E:2487:PRO:HD3	1.84	0.59
1:N:7103:ILE:HB	1:N:7104:PRO:HD3	1.84	0.59
1:J:5051:ILE:HB	1:J:5052:PRO:HD3	1.84	0.59
1:A:434:ILE:HB	1:A:435:PRO:HD3	1.84	0.59
1:B:947:ILE:HB	1:B:948:PRO:HD3	1.84	0.58
1:K:5564:ILE:HB	1:K:5565:PRO:HD3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1973:ILE:HB	1:D:1974:PRO:HD3	1.84	0.58
1:M:6590:ILE:HB	1:M:6591:PRO:HD3	1.84	0.58
1:C:1465:ALA:HB1	1:C:1470:LEU:HB2	1.86	0.58
1:B:952:ALA:HB1	1:B:957:LEU:HB2	1.86	0.58
1:F:3004:ALA:HB1	1:F:3009:LEU:HB2	1.86	0.58
1:L:6082:ALA:HB1	1:L:6087:LEU:HB2	1.86	0.58
1:O:7621:ALA:HB1	1:O:7626:LEU:HB2	1.86	0.58
1:K:5569:ALA:HB1	1:K:5574:LEU:HB2	1.86	0.58
1:E:2491:ALA:HB1	1:E:2496:LEU:HB2	1.86	0.58
1:N:7108:ALA:HB1	1:N:7113:LEU:HB2	1.86	0.58
1:C:1460:ILE:HB	1:C:1461:PRO:HD3	1.84	0.57
1:L:6077:ILE:HB	1:L:6078:PRO:HD3	1.84	0.57
1:A:439:ALA:HB1	1:A:444:LEU:HB2	1.86	0.57
1:J:5056:ALA:HB1	1:J:5061:LEU:HB2	1.86	0.57
1:I:4543:ALA:HB1	1:I:4548:LEU:HB2	1.86	0.57
1:G:3517:ALA:HB1	1:G:3522:LEU:HB2	1.86	0.57
1:H:4030:ALA:HB1	1:H:4035:LEU:HB2	1.86	0.57
1:P:8134:ALA:HB1	1:P:8139:LEU:HB2	1.86	0.56
1:D:1978:ALA:HB1	1:D:1983:LEU:HB2	1.86	0.56
1:M:6595:ALA:HB1	1:M:6600:LEU:HB2	1.86	0.56
1:L:5921:LEU:C	1:L:5921:LEU:HD13	2.32	0.56
1:C:1304:LEU:C	1:C:1304:LEU:HD13	2.32	0.55
1:D:1817:LEU:HD13	1:D:1817:LEU:C	2.32	0.55
1:B:791:LEU:HD13	1:B:791:LEU:C	2.32	0.55
1:K:5408:LEU:HD13	1:K:5408:LEU:C	2.32	0.55
1:M:6434:LEU:HD13	1:M:6434:LEU:C	2.32	0.55
1:E:2330:LEU:C	1:E:2330:LEU:HD13	2.32	0.55
1:H:3869:LEU:HD13	1:H:3869:LEU:C	2.32	0.55
1:N:6947:LEU:HD13	1:N:6947:LEU:C	2.32	0.55
1:I:4382:LEU:C	1:I:4382:LEU:HD13	2.32	0.55
1:P:7973:LEU:HD13	1:P:7973:LEU:C	2.32	0.55
1:G:3356:LEU:C	1:G:3356:LEU:HD13	2.32	0.54
1:J:4895:LEU:C	1:J:4895:LEU:HD13	2.32	0.54
1:A:278:LEU:HD13	1:A:278:LEU:C	2.32	0.54
1:F:2843:LEU:HD13	1:F:2843:LEU:C	2.32	0.54
1:O:7460:LEU:HD13	1:O:7460:LEU:C	2.32	0.54
1:K:5134:GLU:O	1:K:5135:ASN:CB	2.60	0.50
1:B:517:GLU:O	1:B:518:ASN:CB	2.60	0.50
1:C:1030:GLU:O	1:C:1031:ASN:CB	2.60	0.50
1:L:5647:GLU:O	1:L:5648:ASN:CB	2.60	0.50
1:M:6160:GLU:O	1:M:6161:ASN:CB	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:O	1:A:5:ASN:CB	2.60	0.50
1:D:1543:GLU:O	1:D:1544:ASN:CB	2.60	0.50
1:J:4621:GLU:O	1:J:4622:ASN:CB	2.60	0.49
1:N:6673:GLU:O	1:N:6674:ASN:CB	2.60	0.49
1:E:2056:GLU:O	1:E:2057:ASN:CB	2.60	0.49
1:I:4108:GLU:O	1:I:4109:ASN:CB	2.60	0.49
1:G:3082:GLU:O	1:G:3083:ASN:CB	2.60	0.49
1:H:3595:GLU:O	1:H:3596:ASN:CB	2.60	0.49
1:N:6736:PRO:HB2	1:O:7223:MET:SD	2.53	0.49
1:C:1093:PRO:HB2	1:D:1580:MET:SD	2.53	0.49
1:F:2569:GLU:O	1:F:2570:ASN:CB	2.60	0.49
1:L:5710:PRO:HB2	1:M:6197:MET:SD	2.53	0.49
1:E:2119:PRO:HB2	1:F:2606:MET:SD	2.53	0.49
1:M:6223:PRO:HB2	1:N:6710:MET:SD	2.53	0.49
1:O:7186:GLU:O	1:O:7187:ASN:CB	2.60	0.49
1:P:7699:GLU:O	1:P:7700:ASN:CB	2.60	0.49
1:D:1606:PRO:HB2	1:E:2093:MET:SD	2.53	0.49
1:N:7137:ASN:HB2	1:N:7146:MET:HE1	1.95	0.49
1:D:2007:ASN:HB2	1:D:2016:MET:HE1	1.95	0.49
1:E:2520:ASN:HB2	1:E:2529:MET:HE1	1.95	0.49
1:M:6624:ASN:HB2	1:M:6633:MET:HE1	1.95	0.49
1:A:67:PRO:HB2	1:B:554:MET:SD	2.53	0.48
1:B:580:PRO:HB2	1:C:1067:MET:SD	2.53	0.48
1:K:5197:PRO:HB2	1:L:5684:MET:SD	2.53	0.48
1:A:468:ASN:HB2	1:A:477:MET:HE1	1.95	0.48
1:G:3145:PRO:HB2	1:H:3632:MET:SD	2.53	0.48
1:J:4684:PRO:HB2	1:K:5171:MET:SD	2.53	0.48
1:J:5085:ASN:HB2	1:J:5094:MET:HE1	1.95	0.48
1:L:6111:ASN:HB2	1:L:6120:MET:HE1	1.95	0.48
1:A:41:MET:SD	1:H:3658:PRO:HB2	2.53	0.48
1:C:1494:ASN:HB2	1:C:1503:MET:HE1	1.95	0.48
1:O:7650:ASN:HB2	1:O:7659:MET:HE1	1.95	0.48
1:I:4145:MET:SD	1:P:7762:PRO:HB2	2.53	0.48
1:F:2632:PRO:HB2	1:G:3119:MET:SD	2.53	0.48
1:F:3033:ASN:HB2	1:F:3042:MET:HE1	1.95	0.48
1:I:4171:PRO:HB2	1:J:4658:MET:SD	2.53	0.48
1:O:7249:PRO:HB2	1:P:7736:MET:SD	2.53	0.48
1:G:3546:ASN:HB2	1:G:3555:MET:HE1	1.95	0.48
1:P:8163:ASN:HB2	1:P:8172:MET:HE1	1.95	0.48
1:K:5598:ASN:HB2	1:K:5607:MET:HE1	1.95	0.47
1:B:981:ASN:HB2	1:B:990:MET:HE1	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4572:ASN:HB2	1:I:4581:MET:HE1	1.95	0.47
1:H:4059:ASN:HB2	1:H:4068:MET:HE1	1.95	0.47
1:J:4636:ILE:HG12	1:J:4715:LEU:HB3	1.99	0.45
1:A:19:ILE:HG12	1:A:98:LEU:HB3	1.99	0.45
1:G:3097:ILE:HG12	1:G:3176:LEU:HB3	1.99	0.45
1:B:532:ILE:HG12	1:B:611:LEU:HB3	1.99	0.45
1:H:3610:ILE:HG12	1:H:3689:LEU:HB3	1.99	0.45
1:J:4824:LEU:HB3	1:J:4977:THR:HG21	1.98	0.45
1:K:5149:ILE:HG12	1:K:5228:LEU:HB3	1.99	0.45
1:O:7389:LEU:HB3	1:O:7542:THR:HG21	1.98	0.45
1:I:4123:ILE:HG12	1:I:4202:LEU:HB3	1.99	0.45
1:L:5869:ILE:N	1:L:5869:ILE:HD12	2.32	0.45
1:O:7201:ILE:HG12	1:O:7280:LEU:HB3	1.99	0.45
1:P:7714:ILE:HG12	1:P:7793:LEU:HB3	1.99	0.45
1:A:207:LEU:HB3	1:A:360:THR:HG21	1.98	0.45
1:F:2584:ILE:HG12	1:F:2663:LEU:HB3	1.99	0.45
1:F:2772:LEU:HB3	1:F:2925:THR:HG21	1.98	0.45
1:C:1252:ILE:N	1:C:1252:ILE:HD12	2.32	0.45
1:G:3285:LEU:HB3	1:G:3438:THR:HG21	1.98	0.45
1:I:4311:LEU:HB3	1:I:4464:THR:HG21	1.98	0.45
1:D:1765:ILE:HD12	1:D:1765:ILE:N	2.32	0.45
1:K:5337:LEU:HB3	1:K:5490:THR:HG21	1.98	0.45
1:N:6688:ILE:HG12	1:N:6767:LEU:HB3	1.99	0.45
1:P:7902:LEU:HB3	1:P:8055:THR:HG21	1.98	0.45
1:C:1045:ILE:HG12	1:C:1124:LEU:HB3	1.99	0.45
1:E:2071:ILE:HG12	1:E:2150:LEU:HB3	1.99	0.45
1:H:3798:LEU:HB3	1:H:3951:THR:HG21	1.98	0.45
1:L:5662:ILE:HG12	1:L:5741:LEU:HB3	1.99	0.45
1:M:6382:ILE:HD12	1:M:6382:ILE:N	2.32	0.45
1:N:6876:LEU:HB3	1:N:7029:THR:HG21	1.98	0.45
1:B:720:LEU:HB3	1:B:873:THR:HG21	1.98	0.45
1:C:1233:LEU:HB3	1:C:1386:THR:HG21	1.98	0.45
1:D:1746:LEU:HB3	1:D:1899:THR:HG21	1.98	0.45
1:L:5850:LEU:HB3	1:L:6003:THR:HG21	1.98	0.45
1:I:4610:ILE:HD12	1:I:4610:ILE:N	2.33	0.44
1:D:1558:ILE:HG12	1:D:1637:LEU:HB3	1.99	0.44
1:E:2259:LEU:HB3	1:E:2412:THR:HG21	1.98	0.44
1:J:5123:ILE:N	1:J:5123:ILE:HD12	2.33	0.44
1:M:6363:LEU:HB3	1:M:6516:THR:HG21	1.98	0.44
1:M:6662:ILE:N	1:M:6662:ILE:HD12	2.33	0.44
1:A:506:ILE:HD12	1:A:506:ILE:N	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2045:ILE:HD12	1:D:2045:ILE:N	2.33	0.44
1:H:4097:ILE:N	1:H:4097:ILE:HD12	2.33	0.44
1:I:4553:ILE:HG13	1:I:4554:LEU:N	2.33	0.44
1:K:5356:ILE:HD12	1:K:5356:ILE:N	2.32	0.44
1:K:5636:ILE:N	1:K:5636:ILE:HD12	2.33	0.44
1:M:6175:ILE:HG12	1:M:6254:LEU:HB3	1.99	0.44
1:B:739:ILE:N	1:B:739:ILE:HD12	2.32	0.44
1:B:1019:ILE:HD12	1:B:1019:ILE:N	2.33	0.44
1:H:4040:ILE:HG13	1:H:4041:LEU:N	2.33	0.44
1:E:2489:THR:HA	1:E:2492:GLU:HB3	2.00	0.44
1:G:3584:ILE:HD12	1:G:3584:ILE:N	2.33	0.44
1:J:5066:ILE:HG13	1:J:5067:LEU:N	2.33	0.44
1:O:7688:ILE:N	1:O:7688:ILE:HD12	2.33	0.44
1:P:8201:ILE:HD12	1:P:8201:ILE:N	2.33	0.44
1:A:449:ILE:HG13	1:A:450:LEU:N	2.33	0.44
1:E:2278:ILE:N	1:E:2278:ILE:HD12	2.32	0.44
1:L:6149:ILE:HD12	1:L:6149:ILE:N	2.33	0.44
1:N:7106:THR:HA	1:N:7109:GLU:HB3	2.00	0.44
1:A:226:ILE:HD12	1:A:226:ILE:N	2.32	0.44
1:F:3071:ILE:HD12	1:F:3071:ILE:N	2.33	0.44
1:J:4843:ILE:N	1:J:4843:ILE:HD12	2.32	0.44
1:M:6605:ILE:HG13	1:M:6606:LEU:N	2.33	0.44
1:D:1988:ILE:HG13	1:D:1989:LEU:N	2.33	0.44
1:G:3527:ILE:HG13	1:G:3528:LEU:N	2.33	0.44
1:N:6895:ILE:N	1:N:6895:ILE:HD12	2.32	0.44
1:N:7118:ILE:HG13	1:N:7119:LEU:N	2.33	0.44
1:P:8144:ILE:HG13	1:P:8145:LEU:N	2.33	0.44
1:C:1532:ILE:N	1:C:1532:ILE:HD12	2.33	0.44
1:E:2558:ILE:HD12	1:E:2558:ILE:N	2.33	0.44
1:G:3515:THR:HA	1:G:3518:GLU:HB3	2.00	0.44
1:I:4330:ILE:N	1:I:4330:ILE:HD12	2.32	0.44
1:E:2501:ILE:HG13	1:E:2502:LEU:N	2.33	0.43
1:H:3817:ILE:N	1:H:3817:ILE:HD12	2.32	0.43
1:N:7175:ILE:HD12	1:N:7175:ILE:N	2.33	0.43
1:P:8132:THR:HA	1:P:8135:GLU:HB3	2.00	0.43
1:C:1463:THR:HA	1:C:1466:GLU:HB3	2.00	0.43
1:F:3014:ILE:HG13	1:F:3015:LEU:N	2.33	0.43
1:L:6080:THR:HA	1:L:6083:GLU:HB3	2.00	0.43
1:O:7619:THR:HA	1:O:7622:GLU:HB3	2.00	0.43
1:O:7631:ILE:HG13	1:O:7632:LEU:N	2.33	0.43
1:B:962:ILE:HG13	1:B:963:LEU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2791:ILE:HD12	1:F:2791:ILE:N	2.32	0.43
1:L:6092:ILE:HG13	1:L:6093:LEU:N	2.33	0.43
1:A:35:PRO:O	1:A:154:GLY:HA2	2.19	0.43
1:G:3304:ILE:N	1:G:3304:ILE:HD12	2.32	0.43
1:J:4652:PRO:O	1:J:4771:GLY:HA2	2.19	0.43
1:K:5579:ILE:HG13	1:K:5580:LEU:N	2.33	0.43
1:N:6704:PRO:O	1:N:6823:GLY:HA2	2.19	0.43
1:O:7408:ILE:N	1:O:7408:ILE:HD12	2.32	0.43
1:C:1475:ILE:HG13	1:C:1476:LEU:N	2.33	0.43
1:F:3002:THR:HA	1:F:3005:GLU:HB3	2.00	0.43
1:P:7921:ILE:HD12	1:P:7921:ILE:N	2.32	0.43
1:B:548:PRO:O	1:B:667:GLY:HA2	2.19	0.43
1:E:2087:PRO:O	1:E:2206:GLY:HA2	2.19	0.43
1:H:3626:PRO:O	1:H:3745:GLY:HA2	2.19	0.43
1:I:4139:PRO:O	1:I:4258:GLY:HA2	2.19	0.43
1:K:5165:PRO:O	1:K:5284:GLY:HA2	2.19	0.43
1:M:6191:PRO:O	1:M:6310:GLY:HA2	2.19	0.43
1:A:132:ILE:HD11	1:A:462:ASN:HB3	2.01	0.43
1:C:1061:PRO:O	1:C:1180:GLY:HA2	2.19	0.43
1:D:1574:PRO:O	1:D:1693:GLY:HA2	2.19	0.43
1:L:5678:PRO:O	1:L:5797:GLY:HA2	2.19	0.43
1:O:7217:PRO:O	1:O:7336:GLY:HA2	2.19	0.43
1:A:437:THR:HA	1:A:440:GLU:HB3	2.00	0.43
1:F:2600:PRO:O	1:F:2719:GLY:HA2	2.19	0.42
1:J:4749:ILE:HD11	1:J:5079:ASN:HB3	2.01	0.42
1:J:5054:THR:HA	1:J:5057:GLU:HB3	2.00	0.42
1:M:6593:THR:HA	1:M:6596:GLU:HB3	2.00	0.42
1:P:7730:PRO:O	1:P:7849:GLY:HA2	2.19	0.42
1:D:1976:THR:HA	1:D:1979:GLU:HB3	2.00	0.42
1:G:3113:PRO:O	1:G:3232:GLY:HA2	2.19	0.42
1:H:3985:ILE:HD12	1:H:3985:ILE:C	2.45	0.42
1:H:4028:THR:HA	1:H:4031:GLU:HB3	2.00	0.42
1:A:51:VAL:HG11	1:H:4097:ILE:HD11	2.01	0.42
1:I:4498:ILE:C	1:I:4498:ILE:HD12	2.45	0.42
1:I:4541:THR:HA	1:I:4544:GLU:HB3	2.00	0.42
1:A:340:ARG:HD2	1:A:349:PHE:CD1	2.55	0.42
1:E:2392:ARG:HD2	1:E:2401:PHE:CD1	2.55	0.42
1:J:4957:ARG:HD2	1:J:4966:PHE:CD1	2.55	0.42
1:N:7009:ARG:HD2	1:N:7018:PHE:CD1	2.55	0.42
1:C:1366:ARG:HD2	1:C:1375:PHE:CD1	2.55	0.42
1:H:3931:ARG:HD2	1:H:3940:PHE:CD1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4236:ILE:HD11	1:I:4566:ASN:HB3	2.01	0.42
1:I:4610:ILE:HD11	1:J:4668:VAL:HG11	2.02	0.42
1:B:853:ARG:HD2	1:B:862:PHE:CD1	2.55	0.42
1:B:1019:ILE:HD11	1:C:1077:VAL:HG11	2.02	0.42
1:I:4444:ARG:HD2	1:I:4453:PHE:CD1	2.55	0.42
1:K:5470:ARG:HD2	1:K:5479:PHE:CD1	2.55	0.42
1:L:6037:ILE:C	1:L:6037:ILE:HD12	2.45	0.42
1:M:6299:ILE:O	1:M:6303:ILE:HG12	2.20	0.42
1:N:6801:ILE:HD11	1:N:7131:ASN:HB3	2.01	0.42
1:B:726:VAL:HG13	1:B:813:ALA:HA	2.02	0.42
1:B:907:ILE:C	1:B:907:ILE:HD12	2.45	0.42
1:D:1682:ILE:O	1:D:1686:ILE:HG12	2.20	0.42
1:G:3418:ARG:HD2	1:G:3427:PHE:CD1	2.55	0.42
1:H:3723:ILE:HD11	1:H:4053:ASN:HB3	2.01	0.42
1:K:5343:VAL:HG13	1:K:5430:ALA:HA	2.02	0.42
1:K:5524:ILE:C	1:K:5524:ILE:HD12	2.45	0.42
1:K:5636:ILE:HD11	1:L:5694:VAL:HG11	2.02	0.42
1:L:5983:ARG:HD2	1:L:5992:PHE:CD1	2.55	0.42
1:M:6550:ILE:HD12	1:M:6550:ILE:C	2.45	0.42
1:P:7827:ILE:HD11	1:P:8157:ASN:HB3	2.01	0.42
1:P:8089:ILE:C	1:P:8089:ILE:HD12	2.45	0.42
1:B:656:ILE:O	1:B:660:ILE:HG12	2.20	0.42
1:C:1420:ILE:HD12	1:C:1420:ILE:C	2.45	0.42
1:D:1671:ILE:HD11	1:D:2001:ASN:HB3	2.01	0.42
1:E:2184:ILE:HD11	1:E:2514:ASN:HB3	2.01	0.42
1:E:2446:ILE:C	1:E:2446:ILE:HD12	2.45	0.42
1:G:3210:ILE:HD11	1:G:3540:ASN:HB3	2.01	0.42
1:M:6288:ILE:HD11	1:M:6618:ASN:HB3	2.01	0.42
1:N:7063:ILE:C	1:N:7063:ILE:HD12	2.45	0.42
1:A:143:ILE:O	1:A:147:ILE:HG12	2.20	0.42
1:C:1158:ILE:HD11	1:C:1488:ASN:HB3	2.01	0.42
1:D:1933:ILE:C	1:D:1933:ILE:HD12	2.45	0.42
1:G:3472:ILE:C	1:G:3472:ILE:HD12	2.45	0.42
1:P:8035:ARG:HD2	1:P:8044:PHE:CD1	2.55	0.42
1:B:950:THR:HA	1:B:953:GLU:HB3	2.00	0.42
1:D:1879:ARG:HD2	1:D:1888:PHE:CD1	2.55	0.42
1:F:2959:ILE:HD12	1:F:2959:ILE:C	2.45	0.42
1:J:4760:ILE:O	1:J:4764:ILE:HG12	2.20	0.42
1:K:5273:ILE:O	1:K:5277:ILE:HG12	2.20	0.42
1:K:5567:THR:HA	1:K:5570:GLU:HB3	2.00	0.42
1:L:5775:ILE:HD11	1:L:6105:ASN:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:6496:ARG:HD2	1:M:6505:PHE:CD1	2.55	0.42
1:A:394:ILE:C	1:A:394:ILE:HD12	2.45	0.41
1:C:1169:ILE:O	1:C:1173:ILE:HG12	2.20	0.41
1:G:3584:ILE:HD11	1:H:3642:VAL:HG11	2.02	0.41
1:J:5011:ILE:HD12	1:J:5011:ILE:C	2.45	0.41
1:K:5262:ILE:HD11	1:K:5592:ASN:HB3	2.01	0.41
1:O:7576:ILE:HD12	1:O:7576:ILE:C	2.45	0.41
1:B:645:ILE:HD11	1:B:975:ASN:HB3	2.01	0.41
1:B:981:ASN:HB2	1:B:990:MET:CE	2.51	0.41
1:B:1019:ILE:HG12	1:C:1067:MET:HB2	2.02	0.41
1:H:3734:ILE:O	1:H:3738:ILE:HG12	2.20	0.41
1:I:4155:VAL:HG11	1:P:8201:ILE:HD11	2.02	0.41
1:J:5123:ILE:HD11	1:K:5181:VAL:HG11	2.01	0.41
1:K:5598:ASN:HB2	1:K:5607:MET:CE	2.51	0.41
1:K:5636:ILE:HG12	1:L:5684:MET:HB2	2.02	0.41
1:L:5786:ILE:O	1:L:5790:ILE:HG12	2.20	0.41
1:L:6149:ILE:HG12	1:M:6197:MET:HB2	2.02	0.41
1:C:1532:ILE:HG12	1:D:1580:MET:HB2	2.03	0.41
1:D:1778:GLU:HB2	1:E:2287:ILE:HB	2.03	0.41
1:D:2007:ASN:HB2	1:D:2016:MET:CE	2.51	0.41
1:E:2219:ILE:HG23	1:E:2254:LEU:HB2	2.03	0.41
1:E:2520:ASN:HB2	1:E:2529:MET:CE	2.51	0.41
1:F:2708:ILE:O	1:F:2712:ILE:HG12	2.20	0.41
1:F:2804:GLU:HB2	1:G:3313:ILE:HB	2.03	0.41
1:H:4059:ASN:HB2	1:H:4068:MET:CE	2.50	0.41
1:I:4572:ASN:HB2	1:I:4581:MET:CE	2.50	0.41
1:J:4830:VAL:HG13	1:J:4917:ALA:HA	2.02	0.41
1:M:6395:GLU:HB2	1:N:6904:ILE:HB	2.03	0.41
1:M:6624:ASN:HB2	1:M:6633:MET:CE	2.51	0.41
1:N:7137:ASN:HB2	1:N:7146:MET:CE	2.50	0.41
1:O:7522:ARG:HD2	1:O:7531:PHE:CD1	2.55	0.41
1:A:213:VAL:HG13	1:A:300:ALA:HA	2.02	0.41
1:C:1193:ILE:HG23	1:C:1228:LEU:HB2	2.03	0.41
1:F:2697:ILE:HD11	1:F:3027:ASN:HB3	2.01	0.41
1:F:2905:ARG:HD2	1:F:2914:PHE:CD1	2.55	0.41
1:G:3221:ILE:O	1:G:3225:ILE:HG12	2.20	0.41
1:I:4247:ILE:O	1:I:4251:ILE:HG12	2.20	0.41
1:N:6836:ILE:HG23	1:N:6871:LEU:HB2	2.03	0.41
1:O:7314:ILE:HD11	1:O:7644:ASN:HB3	2.01	0.41
1:O:7325:ILE:O	1:O:7329:ILE:HG12	2.20	0.41
1:D:1752:VAL:HG13	1:D:1839:ALA:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2045:ILE:HG12	1:E:2093:MET:HB2	2.02	0.41
1:F:2778:VAL:HG13	1:F:2865:ALA:HA	2.02	0.41
1:I:4317:VAL:HG13	1:I:4404:ALA:HA	2.02	0.41
1:M:6369:VAL:HG13	1:M:6456:ALA:HA	2.02	0.41
1:O:7688:ILE:HD11	1:P:7746:VAL:HG11	2.01	0.41
1:E:2195:ILE:O	1:E:2199:ILE:HG12	2.20	0.41
1:L:5810:ILE:HG23	1:L:5845:LEU:HB2	2.03	0.41
1:M:6662:ILE:HG12	1:N:6710:MET:HB2	2.02	0.41
1:O:7395:VAL:HG13	1:O:7482:ALA:HA	2.02	0.41
1:P:7838:ILE:O	1:P:7842:ILE:HG12	2.20	0.41
1:P:7862:ILE:HG23	1:P:7897:LEU:HB2	2.03	0.41
1:P:8163:ASN:HB2	1:P:8172:MET:CE	2.50	0.41
1:F:3071:ILE:HD11	1:G:3129:VAL:HG11	2.02	0.41
1:G:3245:ILE:HG23	1:G:3280:LEU:HB2	2.03	0.41
1:G:3546:ASN:HB2	1:G:3555:MET:CE	2.51	0.41
1:H:3804:VAL:HG13	1:H:3891:ALA:HA	2.02	0.41
1:I:4339:ILE:HB	1:P:7934:GLU:HB2	2.02	0.41
1:N:6812:ILE:O	1:N:6816:ILE:HG12	2.20	0.41
1:O:7421:GLU:HB2	1:P:7930:ILE:HB	2.03	0.41
1:O:7692:ILE:O	1:P:7737:LEU:HA	2.21	0.41
1:C:1536:ILE:O	1:D:1581:LEU:HA	2.21	0.41
1:D:2045:ILE:HD11	1:E:2103:VAL:HG11	2.02	0.41
1:E:2558:ILE:HD11	1:F:2616:VAL:HG11	2.01	0.41
1:F:3075:ILE:O	1:G:3120:LEU:HA	2.21	0.41
1:H:3835:ILE:HD12	1:H:3835:ILE:N	2.36	0.41
1:I:4348:ILE:HD12	1:I:4348:ILE:N	2.36	0.41
1:K:5245:VAL:HB	1:K:5631:GLU:HG3	2.03	0.41
1:L:6153:ILE:O	1:M:6198:LEU:HA	2.21	0.41
1:M:6662:ILE:HD11	1:N:6720:VAL:HG11	2.02	0.41
1:A:167:ILE:HG23	1:A:202:LEU:HB2	2.03	0.41
1:A:506:ILE:HD11	1:B:564:VAL:HG11	2.02	0.41
1:A:506:ILE:HG12	1:B:554:MET:HB2	2.02	0.41
1:B:628:VAL:HB	1:B:1014:GLU:HG3	2.03	0.41
1:C:1191:ALA:O	1:C:1195:VAL:HG23	2.21	0.41
1:C:1239:VAL:HG13	1:C:1326:ALA:HA	2.02	0.41
1:C:1532:ILE:HD11	1:D:1590:VAL:HG11	2.01	0.41
1:D:2049:ILE:O	1:E:2094:LEU:HA	2.21	0.41
1:E:2296:ILE:HD12	1:E:2296:ILE:N	2.36	0.41
1:G:3291:VAL:HG13	1:G:3378:ALA:HA	2.02	0.41
1:G:3317:GLU:HB2	1:H:3826:ILE:HB	2.02	0.41
1:G:3322:ILE:HD12	1:G:3322:ILE:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3706:VAL:HB	1:H:4092:GLU:HG3	2.03	0.41
1:I:4219:VAL:HB	1:I:4605:GLU:HG3	2.03	0.41
1:J:4784:ILE:HG23	1:J:4819:LEU:HB2	2.03	0.41
1:J:5123:ILE:HG12	1:K:5171:MET:HB2	2.03	0.41
1:L:5856:VAL:HG13	1:L:5943:ALA:HA	2.02	0.41
1:M:6666:ILE:O	1:N:6711:LEU:HA	2.21	0.41
1:N:6882:VAL:HG13	1:N:6969:ALA:HA	2.02	0.41
1:N:6908:GLU:HB2	1:O:7417:ILE:HB	2.02	0.41
1:N:6913:ILE:HD12	1:N:6913:ILE:N	2.36	0.41
1:P:7908:VAL:HG13	1:P:7995:ALA:HA	2.02	0.41
1:P:7939:ILE:N	1:P:7939:ILE:HD12	2.36	0.41
1:E:2265:VAL:HG13	1:E:2352:ALA:HA	2.02	0.41
1:F:2809:ILE:HD12	1:F:2809:ILE:N	2.36	0.41
1:G:3588:ILE:O	1:H:3633:LEU:HA	2.21	0.41
1:I:4343:GLU:HB2	1:J:4852:ILE:HB	2.03	0.41
1:K:5297:ILE:HG23	1:K:5332:LEU:HB2	2.03	0.41
1:O:7650:ASN:HB2	1:O:7659:MET:CE	2.50	0.41
1:A:235:ILE:HB	1:H:3830:GLU:HB2	2.03	0.40
1:B:680:ILE:HG23	1:B:715:LEU:HB2	2.03	0.40
1:F:2732:ILE:HG23	1:F:2767:LEU:HB2	2.03	0.40
1:H:3756:ALA:O	1:H:3760:VAL:HG23	2.22	0.40
1:I:4146:LEU:HA	1:P:8205:ILE:O	2.21	0.40
1:I:4350:ILE:HB	1:P:7939:ILE:HG13	2.04	0.40
1:L:5808:ALA:O	1:L:5812:VAL:HG23	2.22	0.40
1:L:6149:ILE:HD11	1:M:6207:VAL:HG11	2.01	0.40
1:O:7349:ILE:HG23	1:O:7384:LEU:HB2	2.03	0.40
1:A:41:MET:HB2	1:H:4097:ILE:HG12	2.03	0.40
1:A:468:ASN:HB2	1:A:477:MET:CE	2.50	0.40
1:B:1023:ILE:O	1:C:1068:LEU:HA	2.21	0.40
1:F:2588:ARG:O	1:F:2592:GLU:N	2.49	0.40
1:F:3033:ASN:HB2	1:F:3042:MET:CE	2.50	0.40
1:I:4145:MET:HB2	1:P:8201:ILE:HG12	2.02	0.40
1:I:4269:ALA:O	1:I:4273:VAL:HG23	2.22	0.40
1:I:4610:ILE:HG12	1:J:4658:MET:HB2	2.03	0.40
1:M:6323:ILE:HG23	1:M:6358:LEU:HB2	2.03	0.40
1:N:7175:ILE:HD11	1:O:7233:VAL:HG11	2.02	0.40
1:O:7426:ILE:HD12	1:O:7426:ILE:N	2.36	0.40
1:A:42:LEU:HA	1:H:4101:ILE:O	2.21	0.40
1:A:115:VAL:HB	1:A:501:GLU:HG3	2.03	0.40
1:A:244:ILE:HG13	1:B:759:ILE:HB	2.04	0.40
1:B:557:ASP:OD1	1:B:557:ASP:C	2.65	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2558:ILE:HG12	1:F:2606:MET:HB2	2.02	0.40
1:G:3193:VAL:HB	1:G:3579:GLU:HG3	2.03	0.40
1:G:3584:ILE:HG12	1:H:3632:MET:HB2	2.02	0.40
1:J:4661:ASP:OD1	1:J:4661:ASP:C	2.65	0.40
1:J:5085:ASN:HB2	1:J:5094:MET:CE	2.51	0.40
1:K:5369:GLU:HB2	1:L:5878:ILE:HB	2.03	0.40
1:M:6476:ILE:HG13	1:M:6482:LEU:HD23	2.04	0.40
1:N:7175:ILE:HG12	1:O:7223:MET:HB2	2.02	0.40
1:O:7297:VAL:HB	1:O:7683:GLU:HG3	2.03	0.40
1:P:7810:VAL:HB	1:P:8196:GLU:HG3	2.03	0.40
1:A:44:ASP:OD1	1:A:44:ASP:C	2.65	0.40
1:A:165:ALA:O	1:A:169:VAL:HG23	2.22	0.40
1:B:752:GLU:HB2	1:C:1261:ILE:HB	2.03	0.40
1:C:1494:ASN:HB2	1:C:1503:MET:CE	2.51	0.40
1:D:1654:VAL:HB	1:D:2040:GLU:HG3	2.03	0.40
1:D:1706:ILE:HG23	1:D:1741:LEU:HB2	2.03	0.40
1:D:1859:ILE:HG13	1:D:1865:LEU:HD23	2.04	0.40
1:E:2291:GLU:HB2	1:F:2800:ILE:HB	2.03	0.40
1:E:2562:ILE:O	1:F:2607:LEU:HA	2.21	0.40
1:F:2680:VAL:HB	1:F:3066:GLU:HG3	2.03	0.40
1:F:2846:GLN:OE1	1:F:2867:ARG:NH2	2.55	0.40
1:G:3398:ILE:HG13	1:G:3404:LEU:HD23	2.04	0.40
1:I:4614:ILE:O	1:J:4659:LEU:HA	2.21	0.40
1:J:4782:ALA:O	1:J:4786:VAL:HG23	2.21	0.40
1:J:4861:ILE:HG13	1:K:5376:ILE:HB	2.04	0.40
1:K:5174:ASP:OD1	1:K:5174:ASP:C	2.65	0.40
1:K:5640:ILE:O	1:L:5685:LEU:HA	2.21	0.40
1:L:6111:ASN:HB2	1:L:6120:MET:CE	2.51	0.40
1:M:6271:VAL:HB	1:M:6657:GLU:HG3	2.03	0.40
1:N:6989:ILE:HG13	1:N:6995:LEU:HD23	2.04	0.40
1:O:7205:ARG:O	1:O:7209:GLU:N	2.49	0.40
1:O:7463:GLN:OE1	1:O:7484:ARG:NH2	2.55	0.40
1:P:8015:ILE:HG13	1:P:8021:LEU:HD23	2.04	0.40
1:E:2372:ILE:HG13	1:E:2378:LEU:HD23	2.04	0.40
1:F:2730:ALA:O	1:F:2734:VAL:HG23	2.21	0.40
1:F:2885:ILE:HG13	1:F:2891:LEU:HD23	2.04	0.40
1:G:3243:ALA:O	1:G:3247:VAL:HG23	2.21	0.40
1:G:3322:ILE:HG13	1:H:3837:ILE:HB	2.04	0.40
1:N:6741:LEU:HD23	1:N:6741:LEU:O	2.22	0.40
1:O:7394:ARG:HD2	1:O:7480:VAL:HB	2.04	0.40
1:O:7502:ILE:HG13	1:O:7508:LEU:HD23	2.04	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	404 (98%)	6 (2%)	57	72
1	B	410/410 (100%)	404 (98%)	6 (2%)	57	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	D	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	E	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	F	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	G	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	H	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	I	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	J	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	K	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	L	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	M	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	N	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	O	410/410 (100%)	404 (98%)	6 (2%)	57	72
1	P	410/410 (100%)	404 (98%)	6 (2%)	57	72
All	All	6560/6560 (100%)	6464 (98%)	96 (2%)	55	72

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	72	LEU
1	A	104	LEU
1	A	105	LEU
1	A	302	ARG
1	A	503	LEU
1	B	533	LEU
1	B	585	LEU
1	B	617	LEU
1	B	618	LEU
1	B	815	ARG
1	B	1016	LEU
1	C	1046	LEU
1	C	1098	LEU
1	C	1130	LEU
1	C	1131	LEU
1	C	1328	ARG
1	C	1529	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1559	LEU
1	D	1611	LEU
1	D	1643	LEU
1	D	1644	LEU
1	D	1841	ARG
1	D	2042	LEU
1	E	2072	LEU
1	E	2124	LEU
1	E	2156	LEU
1	E	2157	LEU
1	E	2354	ARG
1	E	2555	LEU
1	F	2585	LEU
1	F	2637	LEU
1	F	2669	LEU
1	F	2670	LEU
1	F	2867	ARG
1	F	3068	LEU
1	G	3098	LEU
1	G	3150	LEU
1	G	3182	LEU
1	G	3183	LEU
1	G	3380	ARG
1	G	3581	LEU
1	H	3611	LEU
1	H	3663	LEU
1	H	3695	LEU
1	H	3696	LEU
1	H	3893	ARG
1	H	4094	LEU
1	I	4124	LEU
1	I	4176	LEU
1	I	4208	LEU
1	I	4209	LEU
1	I	4406	ARG
1	I	4607	LEU
1	J	4637	LEU
1	J	4689	LEU
1	J	4721	LEU
1	J	4722	LEU
1	J	4919	ARG
1	J	5120	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	5150	LEU
1	K	5202	LEU
1	K	5234	LEU
1	K	5235	LEU
1	K	5432	ARG
1	K	5633	LEU
1	L	5663	LEU
1	L	5715	LEU
1	L	5747	LEU
1	L	5748	LEU
1	L	5945	ARG
1	L	6146	LEU
1	M	6176	LEU
1	M	6228	LEU
1	M	6260	LEU
1	M	6261	LEU
1	M	6458	ARG
1	M	6659	LEU
1	N	6689	LEU
1	N	6741	LEU
1	N	6773	LEU
1	N	6774	LEU
1	N	6971	ARG
1	N	7172	LEU
1	O	7202	LEU
1	O	7254	LEU
1	O	7286	LEU
1	O	7287	LEU
1	O	7484	ARG
1	O	7685	LEU
1	P	7715	LEU
1	P	7767	LEU
1	P	7799	LEU
1	P	7800	LEU
1	P	7997	ARG
1	P	8198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	107	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	119	GLN
1	A	123	GLN
1	A	126	GLN
1	A	468	ASN
1	A	491	GLN
1	A	494	GLN
1	B	579	HIS
1	B	632	GLN
1	B	636	GLN
1	B	639	GLN
1	B	981	ASN
1	B	1004	GLN
1	B	1007	GLN
1	C	1092	HIS
1	C	1145	GLN
1	C	1149	GLN
1	C	1152	GLN
1	C	1494	ASN
1	C	1517	GLN
1	C	1520	GLN
1	D	1605	HIS
1	D	1658	GLN
1	D	1662	GLN
1	D	1665	GLN
1	D	2007	ASN
1	D	2030	GLN
1	D	2033	GLN
1	E	2118	HIS
1	E	2171	GLN
1	E	2175	GLN
1	E	2178	GLN
1	E	2520	ASN
1	E	2543	GLN
1	E	2546	GLN
1	F	2631	HIS
1	F	2684	GLN
1	F	2688	GLN
1	F	2691	GLN
1	F	3033	ASN
1	F	3056	GLN
1	F	3059	GLN
1	G	3144	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	3185	GLN
1	G	3197	GLN
1	G	3201	GLN
1	G	3204	GLN
1	G	3546	ASN
1	G	3569	GLN
1	G	3572	GLN
1	H	3657	HIS
1	H	3698	GLN
1	H	3710	GLN
1	H	3714	GLN
1	H	3717	GLN
1	H	3807	GLN
1	H	4059	ASN
1	H	4082	GLN
1	H	4085	GLN
1	I	4170	HIS
1	I	4211	GLN
1	I	4223	GLN
1	I	4227	GLN
1	I	4230	GLN
1	I	4572	ASN
1	I	4595	GLN
1	I	4598	GLN
1	J	4683	HIS
1	J	4736	GLN
1	J	4740	GLN
1	J	4743	GLN
1	J	5085	ASN
1	J	5108	GLN
1	J	5111	GLN
1	K	5196	HIS
1	K	5249	GLN
1	K	5253	GLN
1	K	5256	GLN
1	K	5598	ASN
1	K	5621	GLN
1	K	5624	GLN
1	L	5709	HIS
1	L	5751	ASN
1	L	5762	GLN
1	L	5766	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	5769	GLN
1	L	6111	ASN
1	L	6134	GLN
1	L	6137	GLN
1	M	6222	HIS
1	M	6275	GLN
1	M	6279	GLN
1	M	6282	GLN
1	M	6624	ASN
1	M	6647	GLN
1	M	6650	GLN
1	N	6735	HIS
1	N	6788	GLN
1	N	6792	GLN
1	N	6795	GLN
1	N	7137	ASN
1	N	7163	GLN
1	O	7248	HIS
1	O	7301	GLN
1	O	7305	GLN
1	O	7308	GLN
1	O	7650	ASN
1	O	7676	GLN
1	P	7761	HIS
1	P	7802	GLN
1	P	7814	GLN
1	P	7818	GLN
1	P	7821	GLN
1	P	8163	ASN
1	P	8186	GLN
1	P	8189	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.

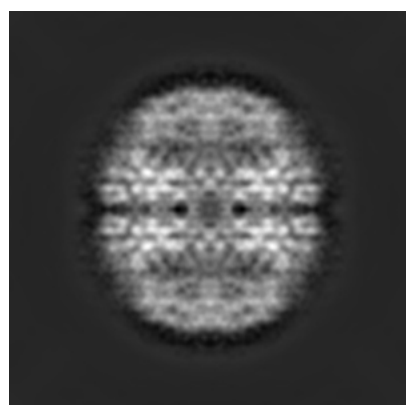
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5245. These allow visual inspection of the internal detail of the map and identification of artifacts.

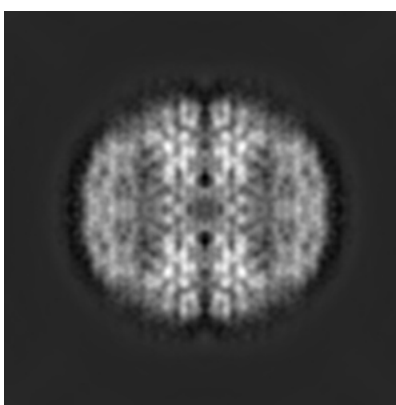
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

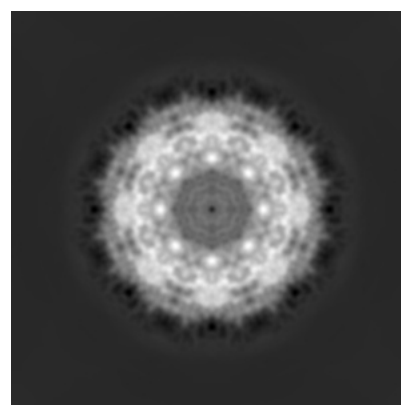
6.1.1 Primary map



X



Y



Z

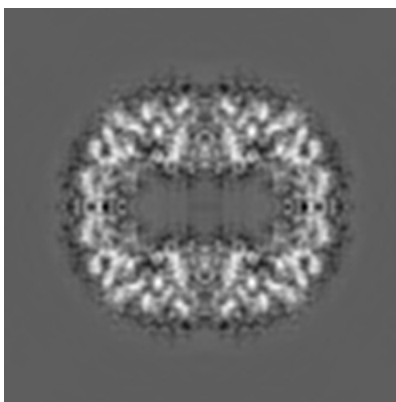
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

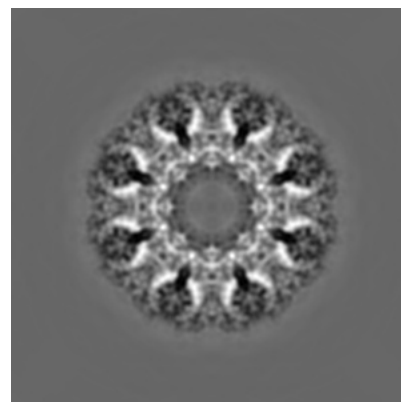
6.2.1 Primary map



X Index: 96



Y Index: 96

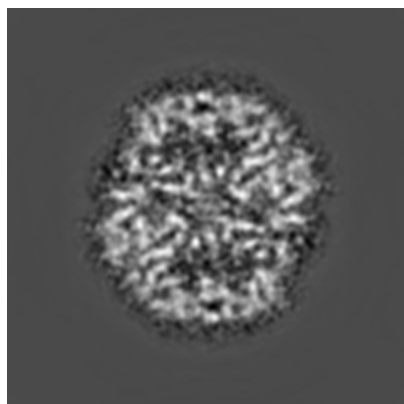


Z Index: 96

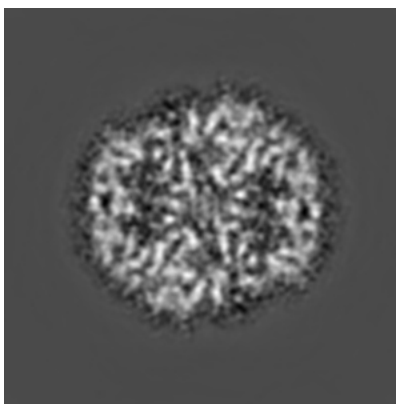
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 69



Y Index: 123

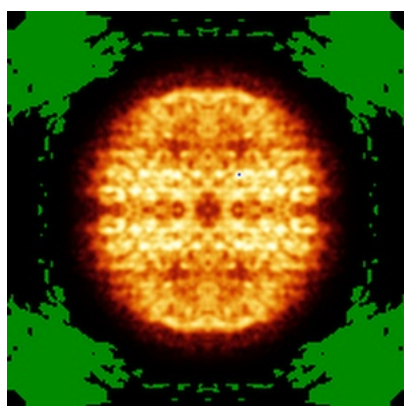


Z Index: 106

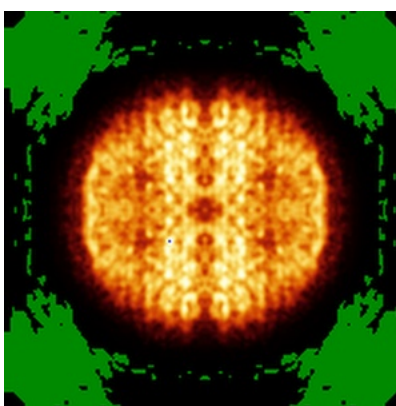
The images above show the largest variance slices of the map in three orthogonal directions.

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

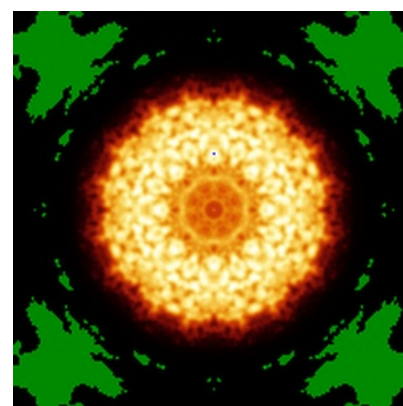
6.4.1 Primary map



X



Y

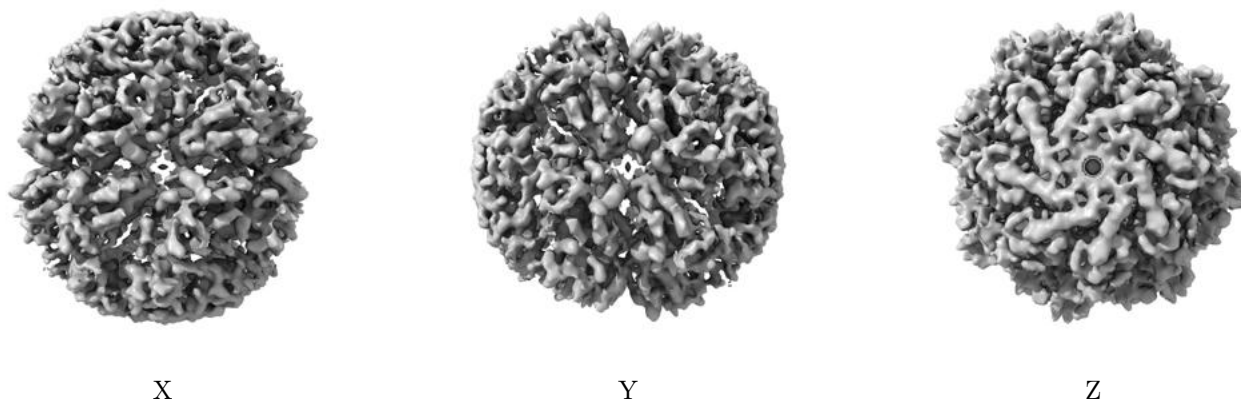


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

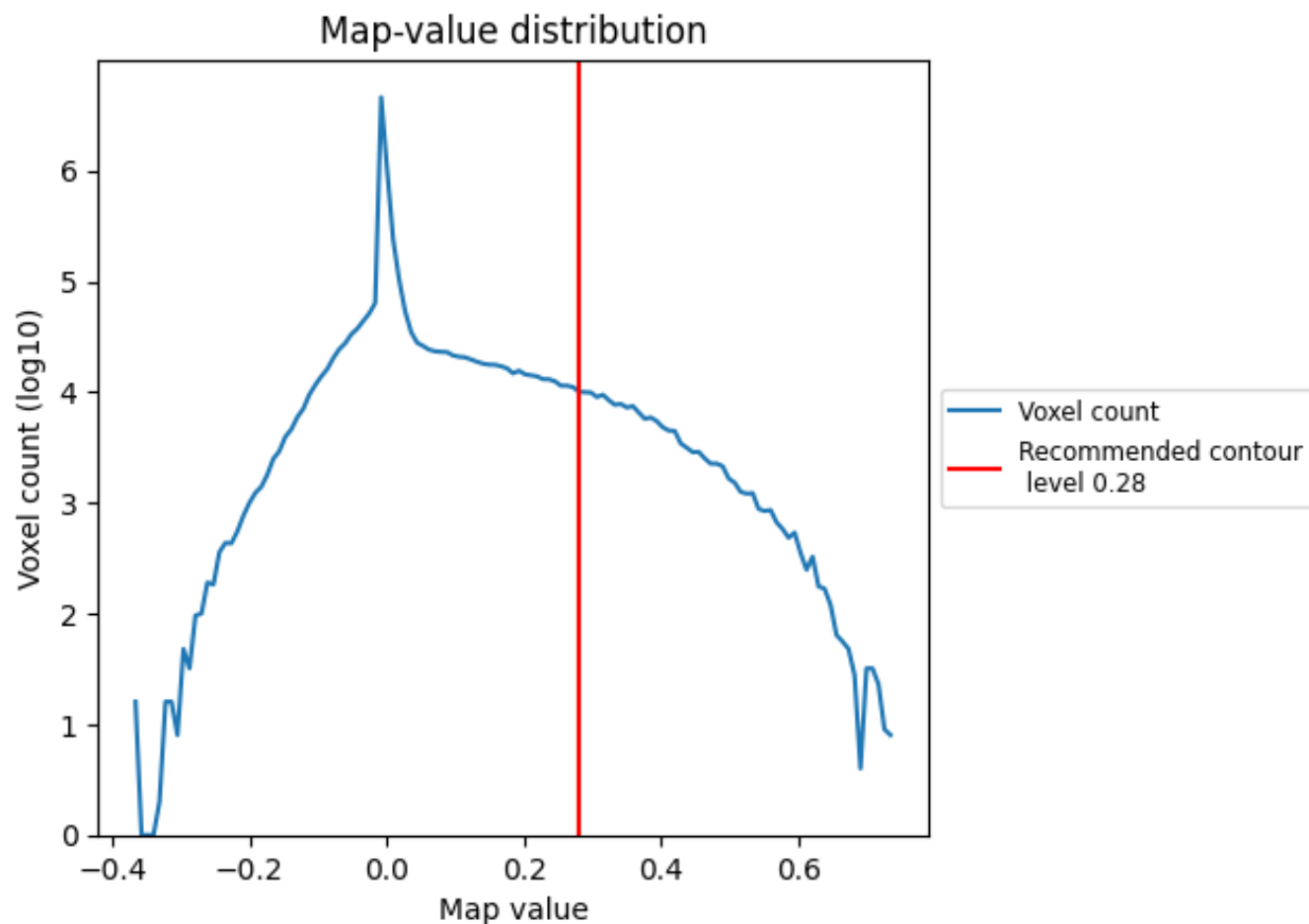
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

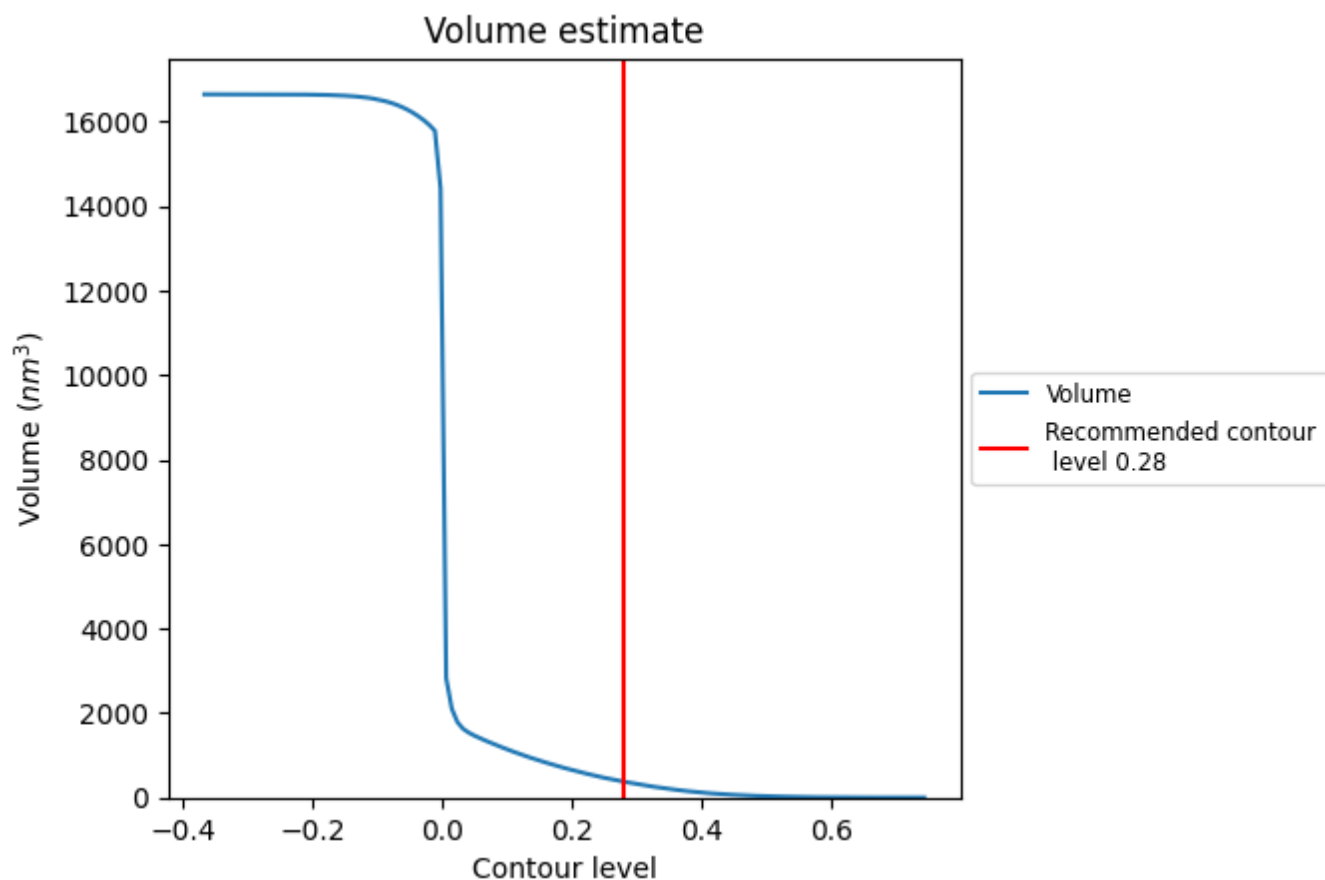
This section contains the results of statistical analysis of the map.

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.

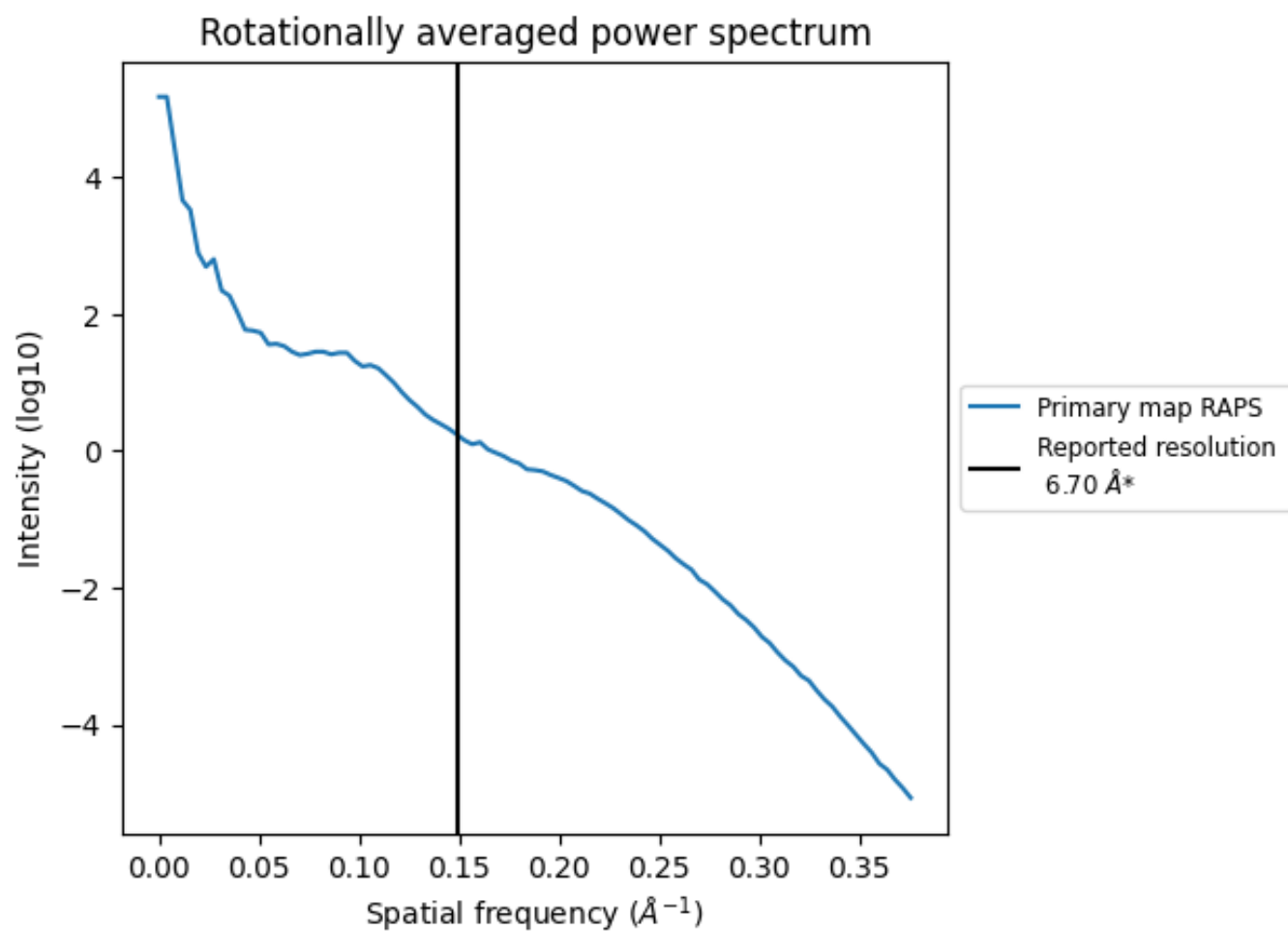
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 379 nm³; this corresponds to an approximate mass of 342 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 0.149 Å⁻¹

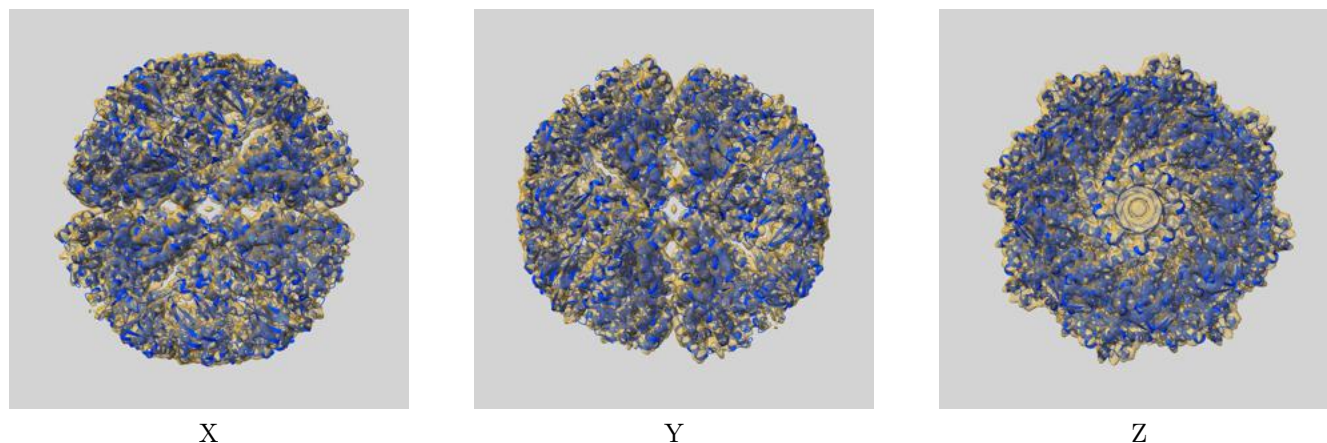
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

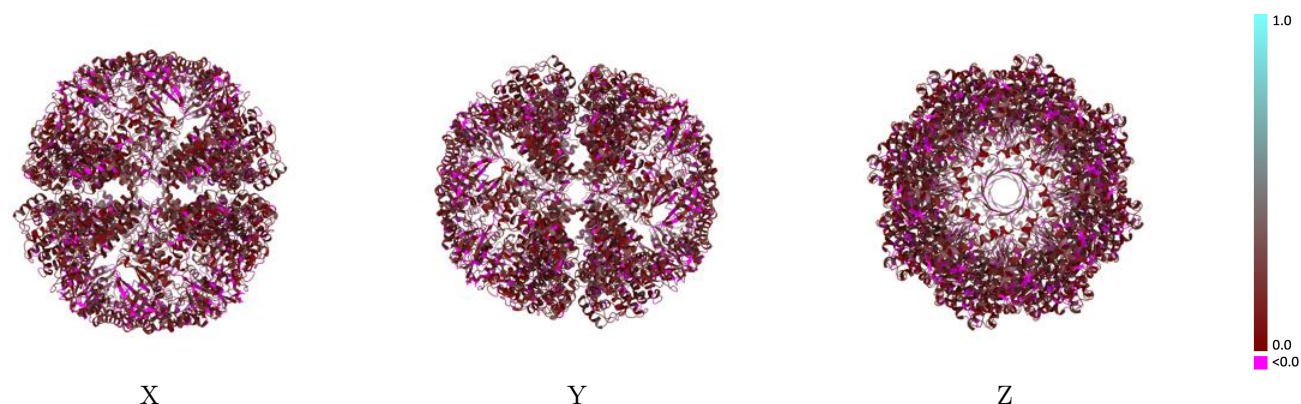
This section contains information regarding the fit between EMDB map EMD-5245 and PDB model 3IZI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



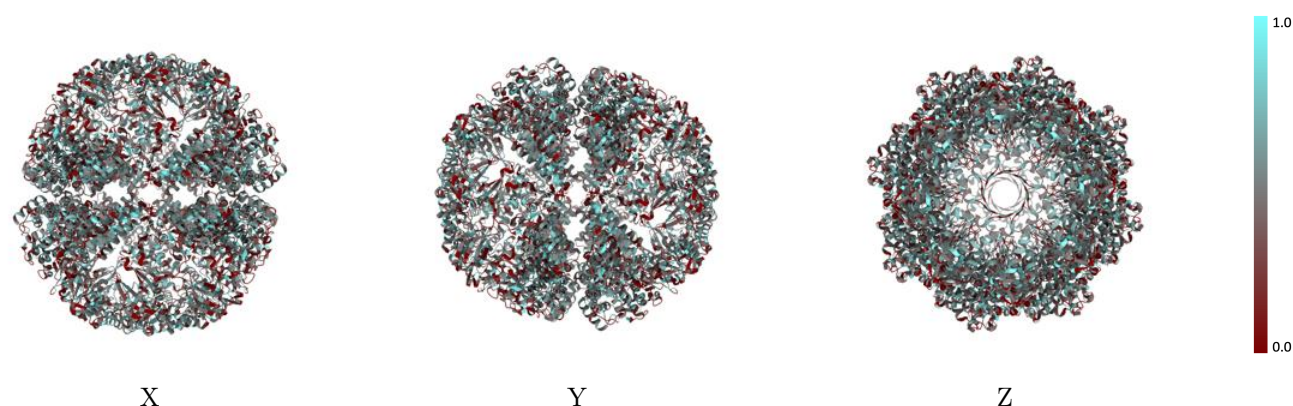
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



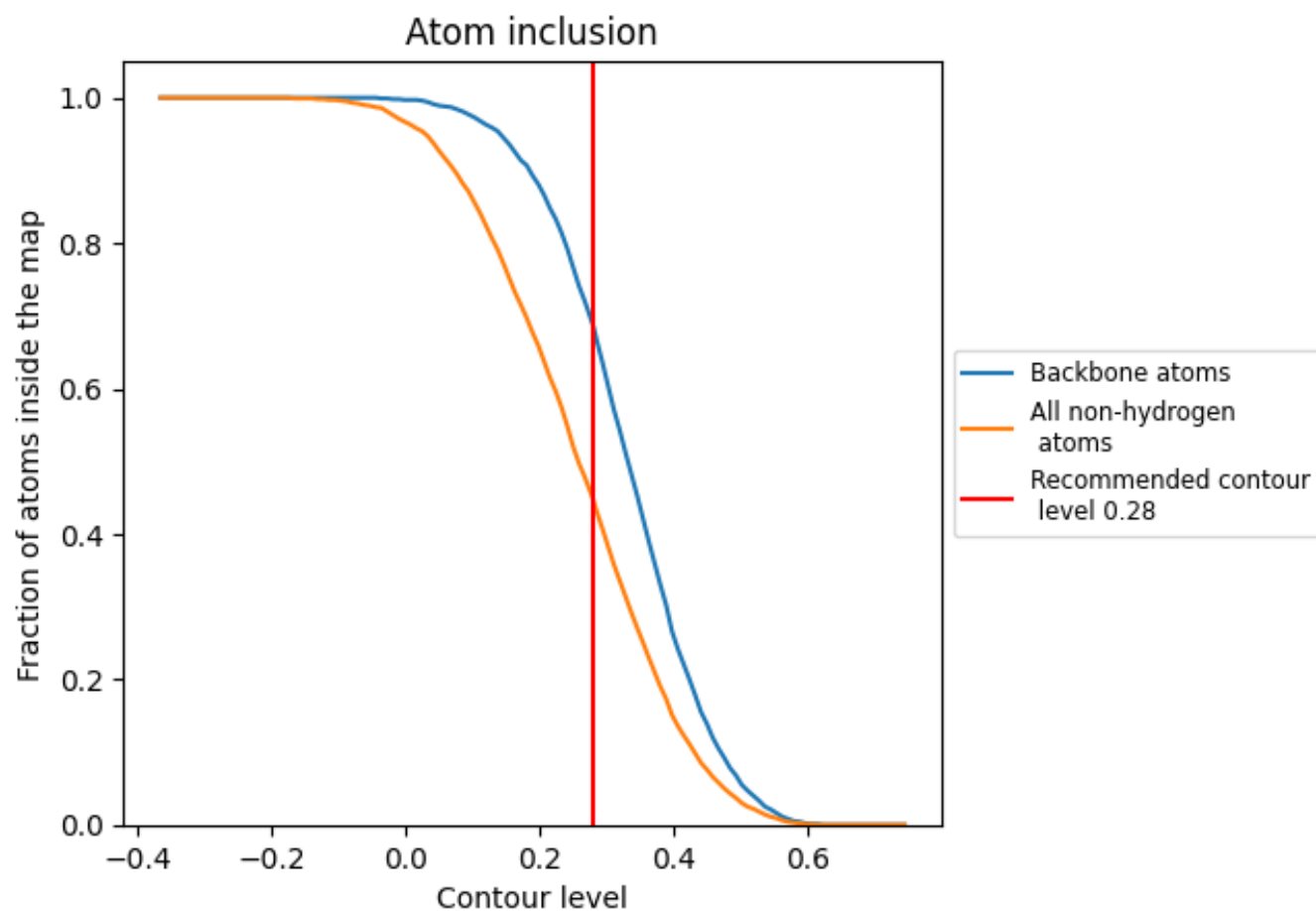
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 45% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4460	0.1270
A	0.4470	0.1260
B	0.4460	0.1270
C	0.4460	0.1260
D	0.4460	0.1270
E	0.4460	0.1270
F	0.4460	0.1280
G	0.4460	0.1270
H	0.4460	0.1270
I	0.4450	0.1260
J	0.4450	0.1260
K	0.4460	0.1270
L	0.4450	0.1270
M	0.4460	0.1270
N	0.4460	0.1270
O	0.4460	0.1260
P	0.4450	0.1260

