



## Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 05:09 AM JST

PDB ID : 7FES  
EMDB ID : EMD-31562  
Title : Cryo-EM structure of apo BsClpP at pH 4.2  
Authors : Kim, L.; Lee, B.-G.; Kim, M.K.; Kwon, D.H.; Kim, H.; Brotz-Oesterhelt, H.; Roh, S.-H.; Song, H.K.  
Deposited on : 2021-07-21  
Resolution : 3.40 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

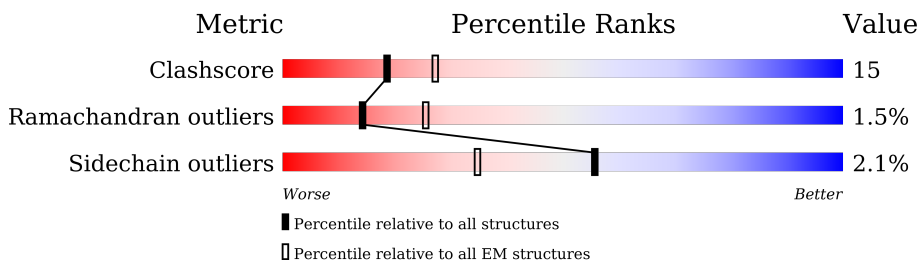
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	202	
1	B	202	
1	C	202	
1	D	202	
1	E	202	
1	F	202	
1	G	202	
1	H	202	

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Mol	Chain	Length	Quality of chain
1	I	202	<p>44% 61% 16% 22%</p>
1	J	202	<p>40% 61% 12% 22%</p>
1	K	202	<p>39% 55% 21% 22%</p>
1	L	202	<p>42% 61% 15% 22%</p>
1	M	202	<p>40% 47% 25% 6% 22%</p>
1	N	202	<p>40% 59% 15% 22%</p>

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 33873 atoms, of which 17095 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	157	2402	759	1205	201	230	7	0	0
1	B	157	2422	759	1225	201	230	7	0	0
1	C	157	2411	759	1214	201	230	7	0	0
1	D	157	2426	762	1225	202	230	7	0	0
1	E	157	2419	762	1218	202	230	7	0	0
1	F	157	2422	759	1225	201	230	7	0	0
1	G	157	2422	759	1225	201	230	7	0	0
1	H	157	2422	759	1225	201	230	7	0	0
1	I	157	2418	759	1221	201	230	7	0	0
1	J	157	2380	759	1183	201	230	7	0	0
1	K	157	2422	759	1225	201	230	7	0	0
1	L	157	2422	759	1225	201	230	7	0	0
1	M	157	2463	768	1254	204	230	7	0	0
1	N	157	2422	759	1225	201	230	7	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	HIS	-	expression tag	UNP P80244
A	198	HIS	-	expression tag	UNP P80244

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Chain	Residue	Modelled	Actual	Comment	Reference
A	199	HIS	-	expression tag	UNP P80244
A	200	HIS	-	expression tag	UNP P80244
A	201	HIS	-	expression tag	UNP P80244
A	202	HIS	-	expression tag	UNP P80244
B	197	HIS	-	expression tag	UNP P80244
B	198	HIS	-	expression tag	UNP P80244
B	199	HIS	-	expression tag	UNP P80244
B	200	HIS	-	expression tag	UNP P80244
B	201	HIS	-	expression tag	UNP P80244
B	202	HIS	-	expression tag	UNP P80244
C	197	HIS	-	expression tag	UNP P80244
C	198	HIS	-	expression tag	UNP P80244
C	199	HIS	-	expression tag	UNP P80244
C	200	HIS	-	expression tag	UNP P80244
C	201	HIS	-	expression tag	UNP P80244
C	202	HIS	-	expression tag	UNP P80244
D	197	HIS	-	expression tag	UNP P80244
D	198	HIS	-	expression tag	UNP P80244
D	199	HIS	-	expression tag	UNP P80244
D	200	HIS	-	expression tag	UNP P80244
D	201	HIS	-	expression tag	UNP P80244
D	202	HIS	-	expression tag	UNP P80244
E	197	HIS	-	expression tag	UNP P80244
E	198	HIS	-	expression tag	UNP P80244
E	199	HIS	-	expression tag	UNP P80244
E	200	HIS	-	expression tag	UNP P80244
E	201	HIS	-	expression tag	UNP P80244
E	202	HIS	-	expression tag	UNP P80244
F	197	HIS	-	expression tag	UNP P80244
F	198	HIS	-	expression tag	UNP P80244
F	199	HIS	-	expression tag	UNP P80244
F	200	HIS	-	expression tag	UNP P80244
F	201	HIS	-	expression tag	UNP P80244
F	202	HIS	-	expression tag	UNP P80244
G	197	HIS	-	expression tag	UNP P80244
G	198	HIS	-	expression tag	UNP P80244
G	199	HIS	-	expression tag	UNP P80244
G	200	HIS	-	expression tag	UNP P80244
G	201	HIS	-	expression tag	UNP P80244
G	202	HIS	-	expression tag	UNP P80244
H	197	HIS	-	expression tag	UNP P80244
H	198	HIS	-	expression tag	UNP P80244

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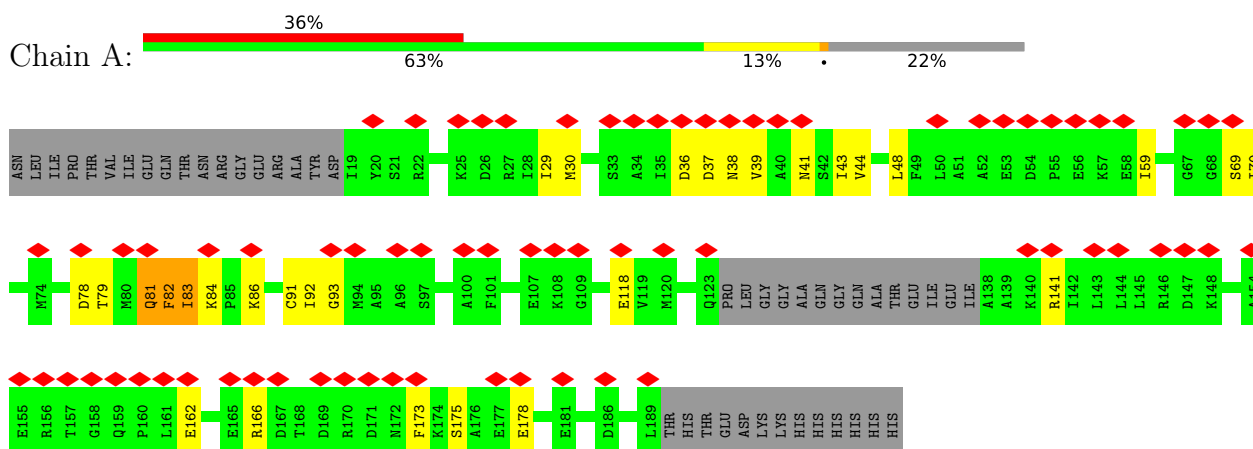
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Chain	Residue	Modelled	Actual	Comment	Reference
H	199	HIS	-	expression tag	UNP P80244
H	200	HIS	-	expression tag	UNP P80244
H	201	HIS	-	expression tag	UNP P80244
H	202	HIS	-	expression tag	UNP P80244
I	197	HIS	-	expression tag	UNP P80244
I	198	HIS	-	expression tag	UNP P80244
I	199	HIS	-	expression tag	UNP P80244
I	200	HIS	-	expression tag	UNP P80244
I	201	HIS	-	expression tag	UNP P80244
I	202	HIS	-	expression tag	UNP P80244
J	197	HIS	-	expression tag	UNP P80244
J	198	HIS	-	expression tag	UNP P80244
J	199	HIS	-	expression tag	UNP P80244
J	200	HIS	-	expression tag	UNP P80244
J	201	HIS	-	expression tag	UNP P80244
J	202	HIS	-	expression tag	UNP P80244
K	197	HIS	-	expression tag	UNP P80244
K	198	HIS	-	expression tag	UNP P80244
K	199	HIS	-	expression tag	UNP P80244
K	200	HIS	-	expression tag	UNP P80244
K	201	HIS	-	expression tag	UNP P80244
K	202	HIS	-	expression tag	UNP P80244
L	197	HIS	-	expression tag	UNP P80244
L	198	HIS	-	expression tag	UNP P80244
L	199	HIS	-	expression tag	UNP P80244
L	200	HIS	-	expression tag	UNP P80244
L	201	HIS	-	expression tag	UNP P80244
L	202	HIS	-	expression tag	UNP P80244
M	197	HIS	-	expression tag	UNP P80244
M	198	HIS	-	expression tag	UNP P80244
M	199	HIS	-	expression tag	UNP P80244
M	200	HIS	-	expression tag	UNP P80244
M	201	HIS	-	expression tag	UNP P80244
M	202	HIS	-	expression tag	UNP P80244
N	197	HIS	-	expression tag	UNP P80244
N	198	HIS	-	expression tag	UNP P80244
N	199	HIS	-	expression tag	UNP P80244
N	200	HIS	-	expression tag	UNP P80244
N	201	HIS	-	expression tag	UNP P80244
N	202	HIS	-	expression tag	UNP P80244

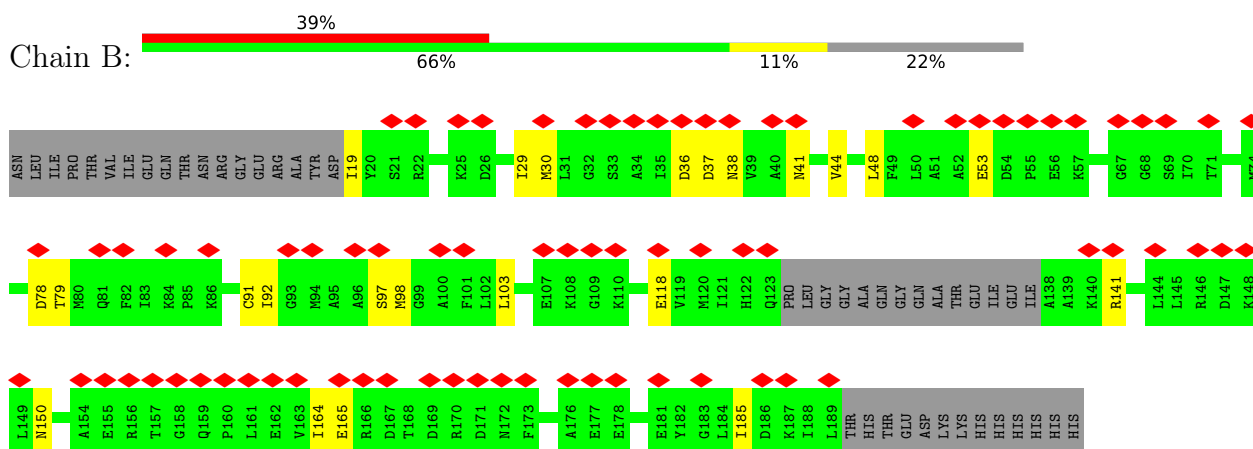
### 3 Residue-property plots [i](#)

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

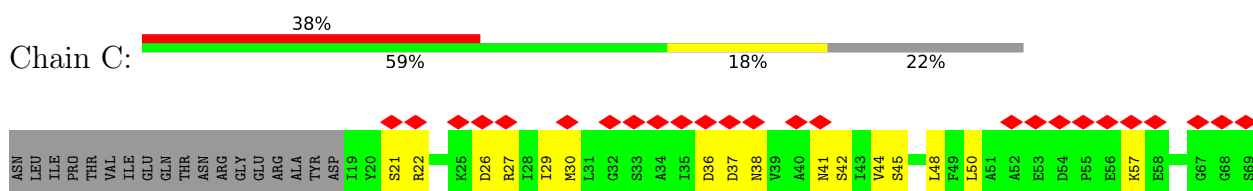
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

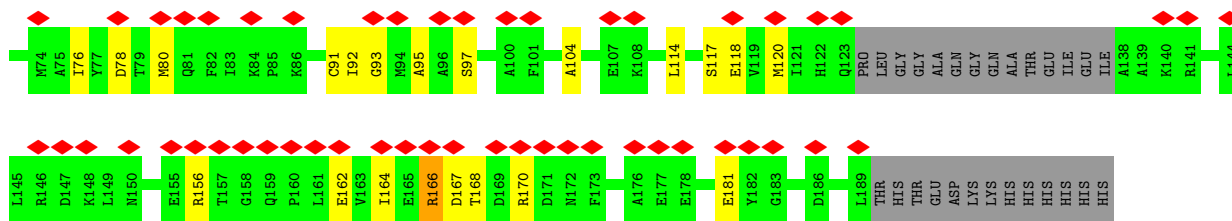


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

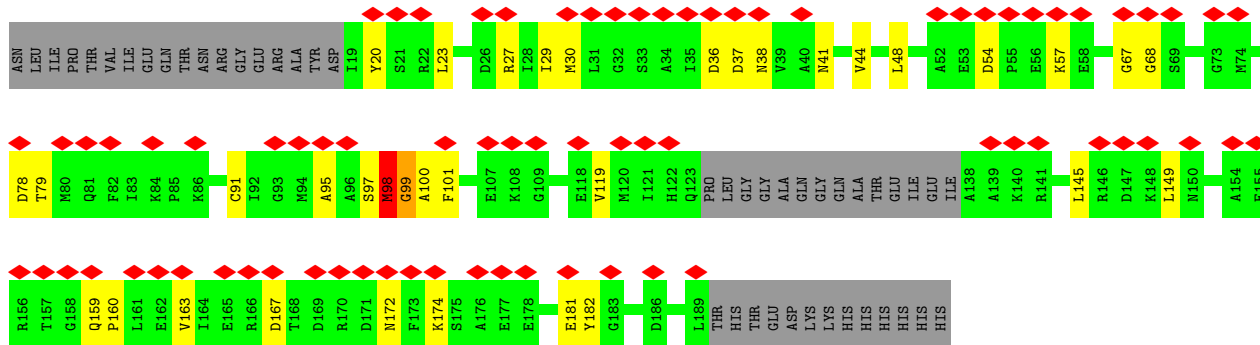
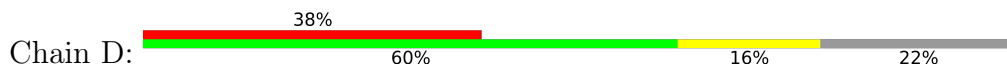


- Molecule 1: ATP-dependent Clp protease proteolytic subunit

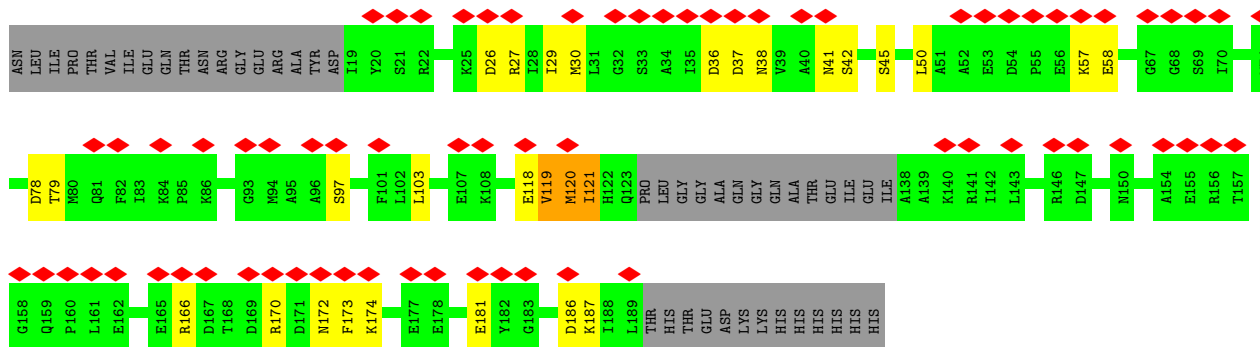




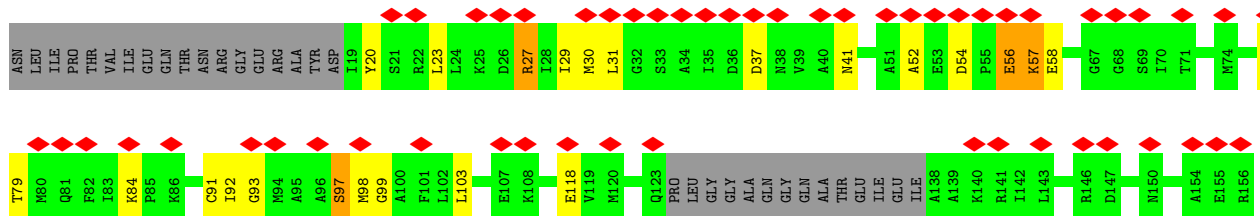
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



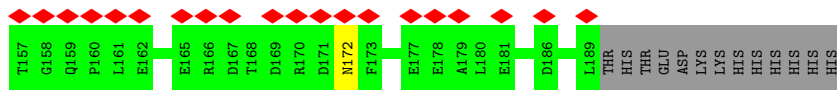
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



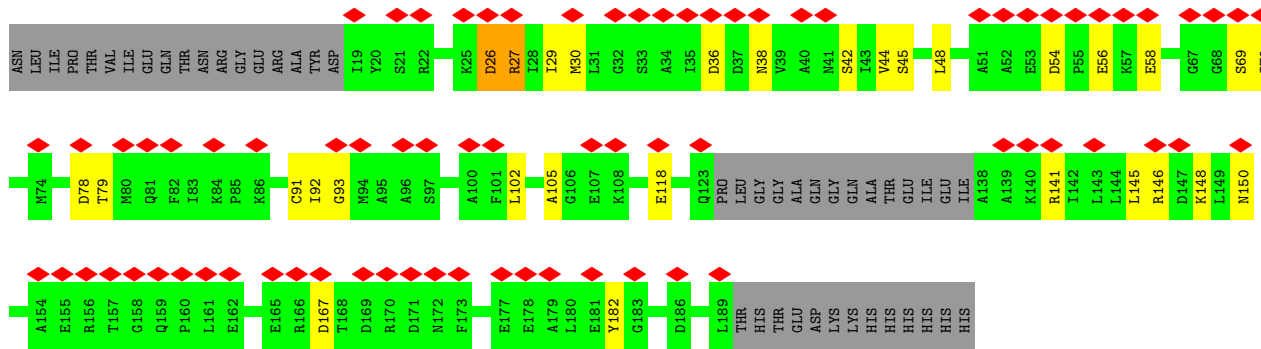
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



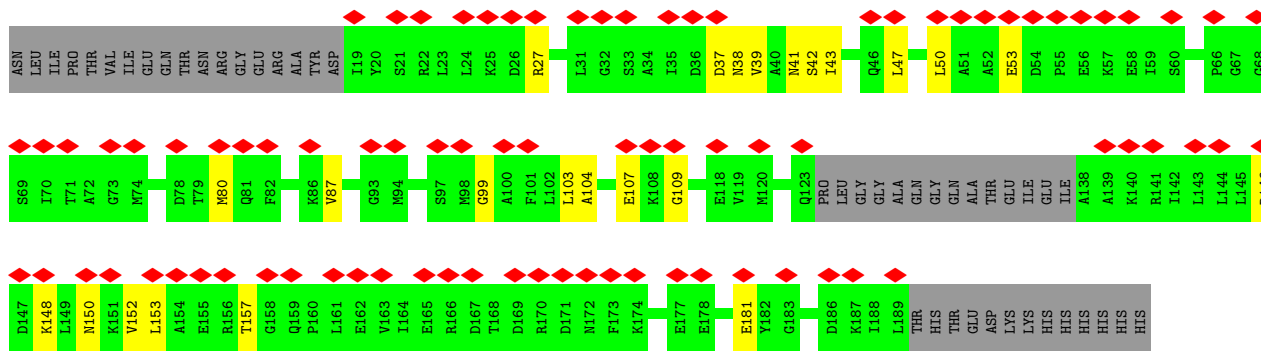
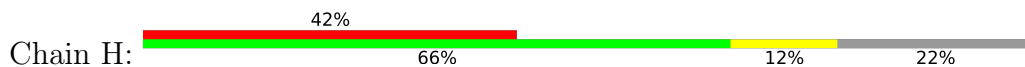




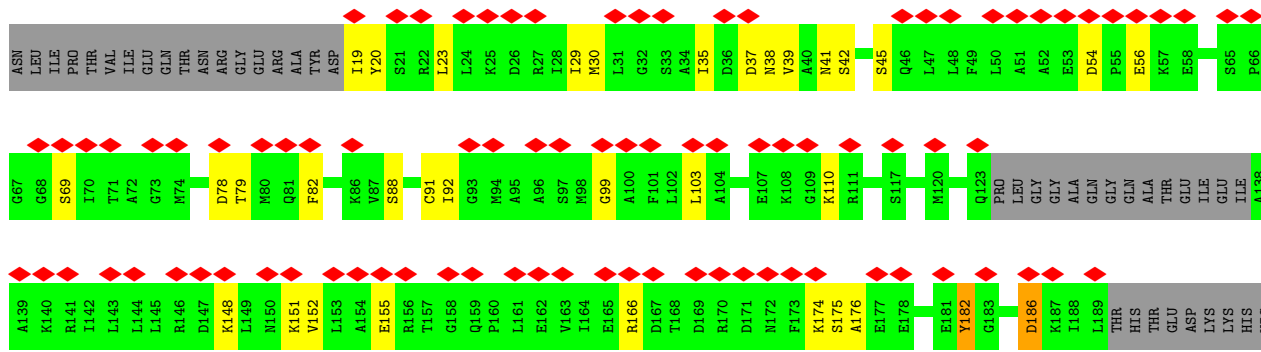
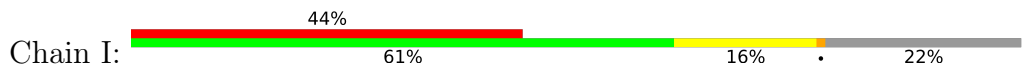
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



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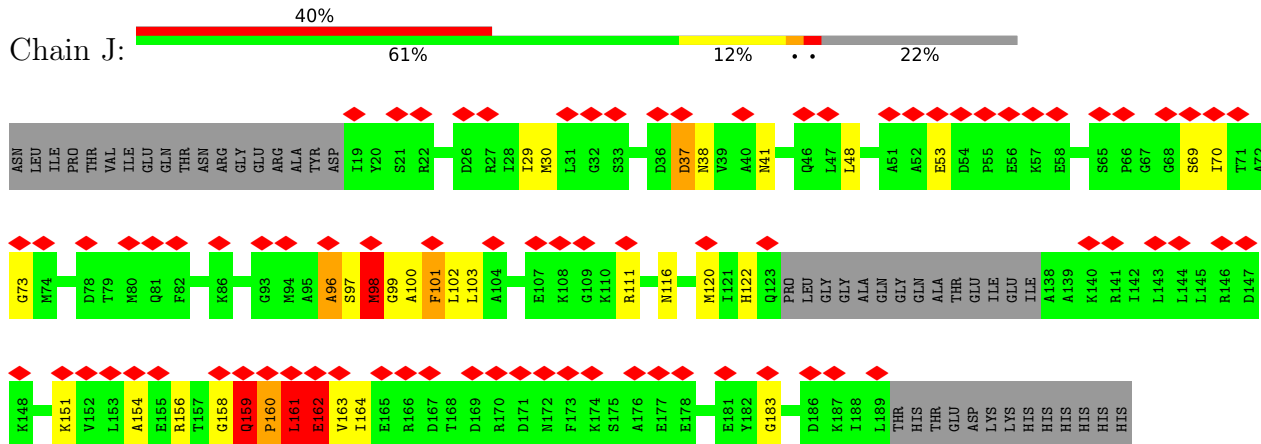


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

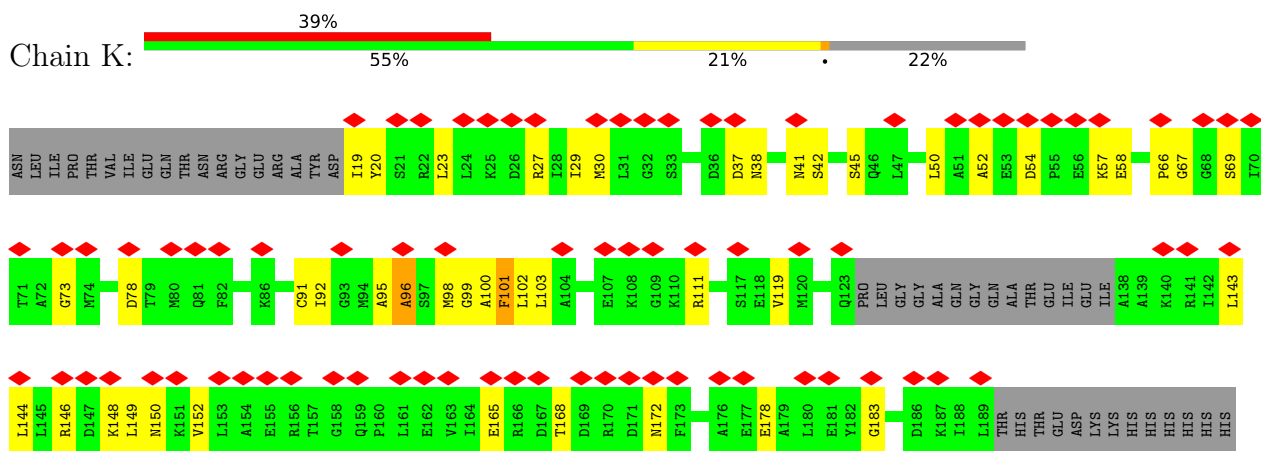


HIS  
HIS

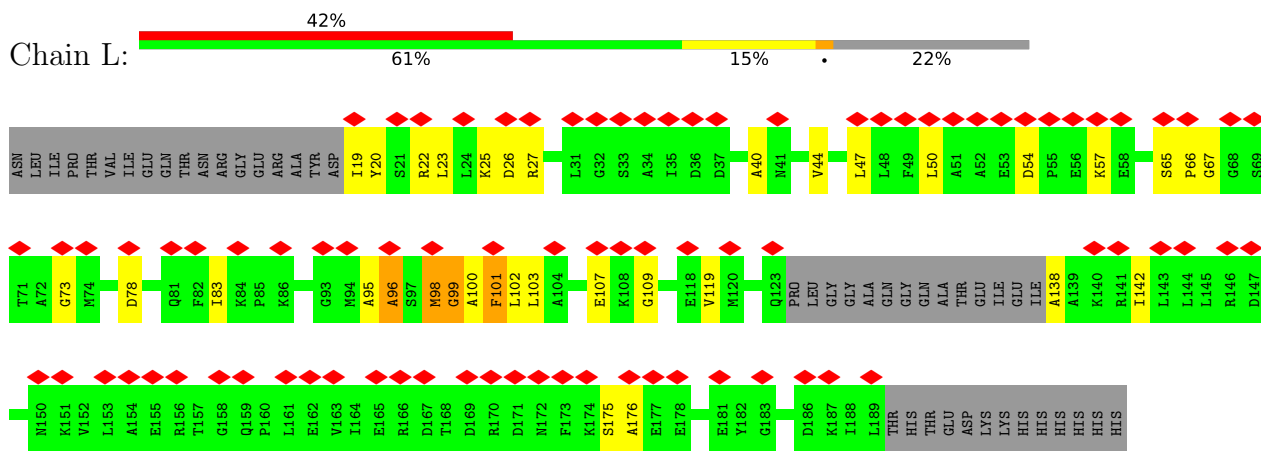
• Molecule 1: ATP-dependent Clp protease proteolytic subunit



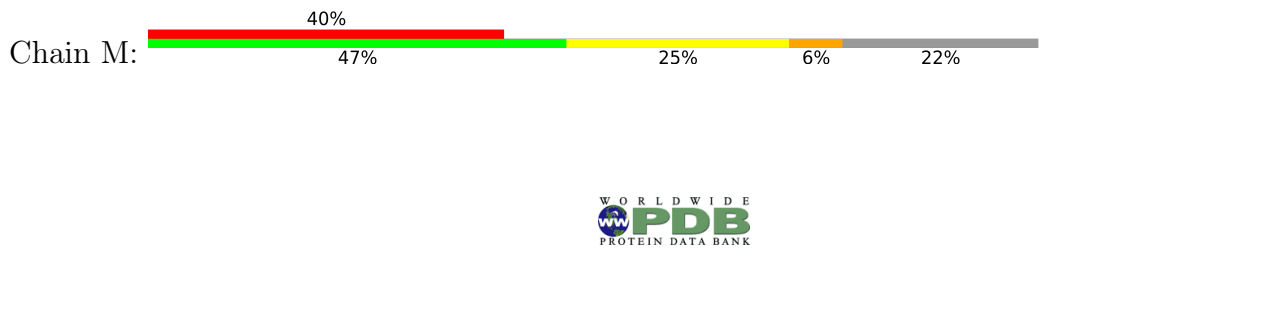
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

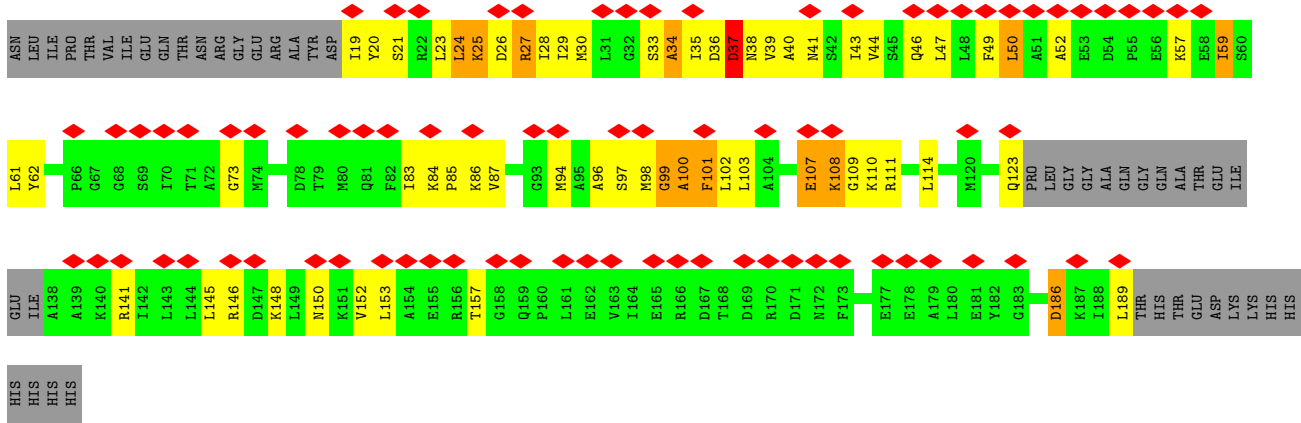


• Molecule 1: ATP-dependent Clp protease proteolytic subunit

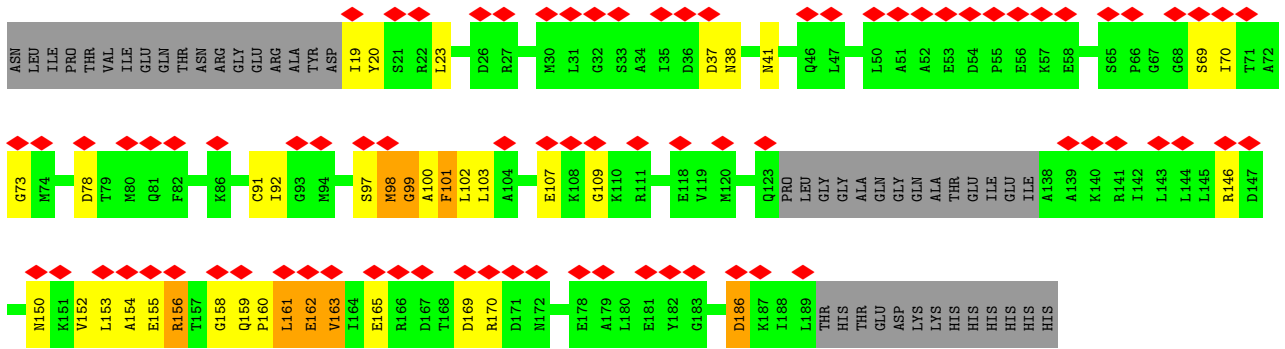


• Molecule 1: ATP-dependent Clp protease proteolytic subunit





• Molecule 1: ATP-dependent Clp protease proteolytic subunit



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.572	Depositor
Minimum map value	-0.883	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.6	Depositor
Map size ( $\text{\AA}$ )	172.0, 172.0, 172.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.86, 0.86, 0.86	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.44	0/1210	0.66	0/1631
1	B	0.45	0/1210	0.60	0/1631
1	C	0.44	0/1210	0.65	0/1631
1	D	0.46	0/1214	0.67	0/1635
1	E	0.43	0/1214	0.60	0/1635
1	F	0.45	0/1210	0.73	2/1631 (0.1%)
1	G	0.45	0/1210	0.63	0/1631
1	H	0.42	0/1210	0.61	0/1631
1	I	0.43	0/1210	0.61	0/1631
1	J	0.47	0/1210	0.82	3/1631 (0.2%)
1	K	0.45	0/1210	0.70	0/1631
1	L	0.45	0/1210	0.71	0/1631
1	M	0.48	0/1222	0.83	5/1643 (0.3%)
1	N	0.51	0/1210	0.71	0/1631
All	All	0.45	0/16960	0.68	10/22854 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	37	ASP	CB-CG-OD2	8.01	125.51	118.30
1	J	116	ASN	C-N-CA	7.14	139.55	121.70
1	F	103	LEU	CB-CG-CD2	6.87	122.68	111.00
1	M	59	ILE	CG1-CB-CG2	6.48	125.65	111.40
1	F	31	LEU	CB-CG-CD2	6.21	121.55	111.00
1	M	50	LEU	CB-CG-CD2	5.94	121.09	111.00
1	M	50	LEU	CB-CG-CD1	5.46	120.28	111.00
1	M	37	ASP	CB-CA-C	-5.41	99.59	110.40
1	M	100	ALA	C-N-CA	-5.33	108.39	121.70
1	J	162	GLU	C-N-CA	-5.09	108.96	121.70

There are no chirality outliers.

There are no planarity outliers.

## 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	1197	1205	1223	22	0
1	B	1197	1225	1223	15	0
1	C	1197	1214	1223	25	0
1	D	1201	1225	1234	37	0
1	E	1201	1218	1234	27	0
1	F	1197	1225	1223	22	0
1	G	1197	1225	1223	19	0
1	H	1197	1225	1223	15	0
1	I	1197	1221	1223	30	0
1	J	1197	1183	1223	56	0
1	K	1197	1225	1223	52	0
1	L	1197	1225	1223	50	0
1	M	1209	1254	1256	96	0
1	N	1197	1225	1223	33	0
All	All	16778	17095	17177	493	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 15.

All (493) 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:M:83:ILE:CD1	1:M:85:PRO:HG2	1.37	1.52
1:J:73:GLY:HA3	1:J:98:MET:CE	1.41	1.47
1:I:174:LYS:CE	1:I:182:TYR:CE1	1.99	1.44
1:I:174:LYS:HE2	1:I:182:TYR:CE1	1.52	1.42
1:M:27:ARG:HH21	1:M:57:LYS:CE	1.31	1.41
1:M:27:ARG:NH2	1:M:57:LYS:HE2	1.37	1.37
1:M:83:ILE:HD12	1:M:85:PRO:CG	1.55	1.34
1:I:174:LYS:CE	1:I:182:TYR:HE1	1.37	1.33
1:I:174:LYS:NZ	1:I:182:TYR:HE1	1.30	1.29
1:M:25:LYS:CD	1:M:26:ASP:H	1.48	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:GLY:CA	1:K:102:LEU:HD13	1.66	1.24
1:J:161:LEU:O	1:J:163:VAL:N	1.72	1.23
1:L:73:GLY:HA3	1:L:98:MET:CE	1.69	1.21
1:M:27:ARG:NH2	1:M:57:LYS:CE	1.98	1.21
1:D:68:GLY:N	1:D:98:MET:HE1	1.54	1.19
1:N:99:GLY:O	1:N:102:LEU:HG	1.42	1.18
1:M:109:GLY:O	1:M:186:ASP:OD2	1.62	1.17
1:J:160:PRO:O	1:J:163:VAL:HG22	1.44	1.17
1:J:73:GLY:CA	1:J:98:MET:CE	2.22	1.16
1:L:73:GLY:HA3	1:L:98:MET:HE2	1.21	1.14
1:M:109:GLY:HA2	1:M:186:ASP:OD2	1.45	1.14
1:L:27:ARG:HH21	1:L:57:LYS:HD2	0.97	1.13
1:M:86:LYS:HD2	1:M:107:GLU:OE1	1.48	1.12
1:J:99:GLY:O	1:J:102:LEU:HG	1.49	1.12
1:D:68:GLY:CA	1:D:98:MET:HE1	1.81	1.11
1:M:25:LYS:CD	1:M:26:ASP:N	2.14	1.10
1:M:36:ASP:O	1:M:38:ASN:N	1.84	1.10
1:L:27:ARG:NH2	1:L:57:LYS:HD2	1.68	1.08
1:K:99:GLY:HA2	1:K:102:LEU:CD1	1.84	1.06
1:M:27:ARG:HH21	1:M:57:LYS:HE3	1.16	1.06
1:A:83:ILE:HD12	1:A:84:LYS:N	1.70	1.05
1:M:25:LYS:HD3	1:M:26:ASP:H	0.96	1.05
1:M:25:LYS:HD2	1:M:26:ASP:N	1.73	1.04
1:M:109:GLY:CA	1:M:186:ASP:OD2	2.06	1.04
1:J:73:GLY:CA	1:J:98:MET:HE2	1.85	1.02
1:M:99:GLY:O	1:M:102:LEU:HG	1.58	1.02
1:F:27:ARG:NH2	1:F:58:GLU:HG2	1.75	1.01
1:J:159:GLN:HB2	1:J:160:PRO:HD3	1.40	1.00
1:M:27:ARG:HD2	1:M:50:LEU:HD21	1.43	1.00
1:K:99:GLY:O	1:K:102:LEU:HB2	1.59	1.00
1:M:83:ILE:CG1	1:M:85:PRO:HG2	1.91	0.99
1:N:100:ALA:O	1:N:102:LEU:N	1.95	0.99
1:D:91:CYS:SG	1:D:95:ALA:HB2	2.03	0.99
1:M:27:ARG:HG3	1:M:50:LEU:HD11	1.46	0.97
1:M:83:ILE:HD12	1:M:85:PRO:HG2	1.03	0.96
1:M:100:ALA:O	1:M:103:LEU:N	1.98	0.96
1:K:99:GLY:HA2	1:K:102:LEU:HD13	0.98	0.96
1:I:174:LYS:HZ1	1:I:182:TYR:HE1	1.08	0.95
1:M:100:ALA:O	1:M:102:LEU:N	2.00	0.95
1:L:100:ALA:O	1:L:102:LEU:N	2.00	0.94
1:L:66:PRO:C	1:L:96:ALA:HB1	1.87	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:24:LEU:HG	1:M:46:GLN:NE2	1.81	0.94
1:M:83:ILE:HD12	1:M:85:PRO:HG3	1.46	0.94
1:L:100:ALA:O	1:L:103:LEU:N	2.00	0.93
1:I:174:LYS:HE2	1:I:182:TYR:CZ	2.04	0.93
1:N:100:ALA:O	1:N:103:LEU:N	2.01	0.93
1:M:100:ALA:O	1:M:101:PHE:C	2.05	0.93
1:N:100:ALA:O	1:N:101:PHE:C	2.05	0.92
1:L:66:PRO:C	1:L:96:ALA:CB	2.36	0.92
1:M:109:GLY:C	1:M:186:ASP:OD2	2.07	0.92
1:L:99:GLY:HA2	1:L:102:LEU:HD13	1.50	0.91
1:J:161:LEU:O	1:J:164:ILE:N	2.04	0.91
1:J:161:LEU:C	1:J:163:VAL:N	2.23	0.91
1:M:25:LYS:HD3	1:M:26:ASP:N	1.79	0.91
1:M:83:ILE:CD1	1:M:85:PRO:CG	2.24	0.91
1:L:99:GLY:O	1:L:102:LEU:HD13	1.69	0.91
1:M:27:ARG:HH22	1:M:57:LYS:HE2	1.33	0.91
1:G:26:ASP:O	1:G:27:ARG:HB3	1.71	0.90
1:J:99:GLY:O	1:J:102:LEU:CG	2.19	0.90
1:D:98:MET:O	1:D:101:PHE:N	2.04	0.89
1:L:100:ALA:O	1:L:101:PHE:C	2.08	0.89
1:K:100:ALA:O	1:K:103:LEU:N	2.06	0.89
1:M:83:ILE:HD11	1:M:85:PRO:HG2	1.52	0.88
1:F:54:ASP:OD2	1:F:56:GLU:O	1.92	0.87
1:L:99:GLY:O	1:L:102:LEU:HB2	1.73	0.87
1:I:174:LYS:NZ	1:I:182:TYR:CE1	2.21	0.87
1:K:67:GLY:N	1:K:96:ALA:CB	2.38	0.87
1:F:27:ARG:HH21	1:F:58:GLU:HG2	1.36	0.86
1:N:99:GLY:O	1:N:102:LEU:CG	2.24	0.86
1:J:161:LEU:O	1:J:162:GLU:C	2.07	0.85
1:J:73:GLY:HA3	1:J:98:MET:HE2	0.88	0.85
1:M:186:ASP:N	1:M:186:ASP:OD1	2.07	0.85
1:L:99:GLY:O	1:L:102:LEU:CD1	2.25	0.85
1:J:96:ALA:O	1:J:120:MET:CE	2.26	0.84
1:G:26:ASP:O	1:G:27:ARG:CB	2.26	0.84
1:K:99:GLY:O	1:K:102:LEU:CB	2.25	0.84
1:L:73:GLY:CA	1:L:98:MET:CE	2.56	0.84
1:M:99:GLY:O	1:M:102:LEU:CG	2.25	0.84
1:K:67:GLY:HA2	1:K:96:ALA:HB1	1.60	0.83
1:D:98:MET:O	1:D:100:ALA:N	2.12	0.82
1:I:174:LYS:HE3	1:I:182:TYR:CE1	2.13	0.82
1:M:84:LYS:N	1:M:85:PRO:HD2	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:GLY:CA	1:D:98:MET:CE	2.57	0.82
1:M:27:ARG:HD2	1:M:50:LEU:CD2	2.10	0.81
1:M:36:ASP:C	1:M:38:ASN:H	1.79	0.81
1:E:120:MET:HG2	1:E:173:PHE:CD1	2.16	0.81
1:E:27:ARG:NH1	1:E:58:GLU:O	2.13	0.80
1:L:66:PRO:O	1:L:96:ALA:HB1	1.81	0.80
1:L:99:GLY:CA	1:L:102:LEU:HD13	2.10	0.80
1:K:66:PRO:C	1:K:96:ALA:HB2	2.02	0.79
1:L:47:LEU:HD13	1:L:83:ILE:HG21	1.64	0.78
1:N:160:PRO:O	1:N:163:VAL:HG23	1.83	0.78
1:C:37:ASP:O	1:C:41:ASN:ND2	2.15	0.78
1:K:101:PHE:HE1	1:K:149:LEU:HG	1.48	0.78
1:D:37:ASP:O	1:D:41:ASN:ND2	2.17	0.78
1:K:27:ARG:NH2	1:K:57:LYS:O	2.17	0.77
1:J:159:GLN:HB2	1:J:160:PRO:CD	2.15	0.77
1:A:78:ASP:O	1:A:81:GLN:O	2.02	0.77
1:K:99:GLY:C	1:K:102:LEU:HD13	2.06	0.77
1:B:37:ASP:O	1:B:41:ASN:ND2	2.18	0.76
1:D:68:GLY:HA3	1:D:98:MET:CE	2.16	0.75
1:D:172:ASN:O	1:D:174:LYS:NZ	2.19	0.75
1:J:100:ALA:O	1:J:103:LEU:N	2.18	0.75
1:K:100:ALA:O	1:K:103:LEU:CB	2.33	0.75
1:J:99:GLY:O	1:J:102:LEU:CB	2.34	0.75
1:L:99:GLY:O	1:L:102:LEU:CB	2.34	0.75
1:A:83:ILE:HD12	1:A:84:LYS:CA	2.03	0.74
1:M:86:LYS:CD	1:M:107:GLU:OE1	2.32	0.74
1:J:73:GLY:HA3	1:J:98:MET:HE3	1.66	0.74
1:K:99:GLY:O	1:K:102:LEU:N	2.21	0.74
1:J:100:ALA:O	1:J:102:LEU:N	2.21	0.74
1:K:67:GLY:CA	1:K:96:ALA:HB1	2.17	0.74
1:L:27:ARG:HD2	1:L:50:LEU:HD21	1.70	0.73
1:I:37:ASP:O	1:I:41:ASN:ND2	2.22	0.72
1:H:39:VAL:O	1:H:42:SER:OG	2.07	0.72
1:J:73:GLY:CA	1:J:98:MET:HE3	2.19	0.72
1:J:100:ALA:O	1:J:101:PHE:C	2.24	0.72
1:K:37:ASP:O	1:K:41:ASN:ND2	2.23	0.71
1:I:39:VAL:O	1:I:42:SER:OG	2.08	0.71
1:K:66:PRO:C	1:K:96:ALA:CB	2.59	0.71
1:J:161:LEU:C	1:J:163:VAL:H	1.91	0.71
1:F:27:ARG:HG3	1:F:57:LYS:HD3	1.72	0.70
1:E:121:ILE:HG12	1:E:121:ILE:O	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:ARG:NH1	1:G:58:GLU:O	2.24	0.70
1:H:37:ASP:O	1:H:41:ASN:ND2	2.24	0.70
1:G:167:ASP:OD2	1:G:182:TYR:OH	2.10	0.70
1:L:27:ARG:NH2	1:L:57:LYS:CD	2.53	0.70
1:M:109:GLY:O	1:M:111:ARG:N	2.24	0.70
1:F:58:GLU:HG2	1:F:58:GLU:O	1.93	0.69
1:K:20:TYR:HA	1:K:23:LEU:HD12	1.73	0.69
1:M:27:ARG:NH2	1:M:57:LYS:HE3	1.89	0.69
1:K:98:MET:O	1:K:102:LEU:HD12	1.93	0.68
1:K:101:PHE:CE1	1:K:149:LEU:HG	2.27	0.68
1:I:20:TYR:HA	1:I:23:LEU:HD12	1.76	0.68
1:J:161:LEU:C	1:J:161:LEU:HD12	2.14	0.68
1:N:186:ASP:OD1	1:N:186:ASP:N	2.26	0.68
1:D:98:MET:O	1:D:99:GLY:C	2.28	0.68
1:K:99:GLY:O	1:K:102:LEU:CD1	2.42	0.68
1:J:98:MET:O	1:J:101:PHE:N	2.26	0.68
1:F:27:ARG:NH2	1:F:58:GLU:CG	2.53	0.68
1:L:99:GLY:C	1:L:102:LEU:HD13	2.14	0.68
1:I:186:ASP:OD1	1:I:186:ASP:N	2.24	0.68
1:M:73:GLY:HA3	1:M:98:MET:CE	2.24	0.68
1:D:68:GLY:HA3	1:D:98:MET:HE1	1.70	0.67
1:J:99:GLY:O	1:J:102:LEU:N	2.27	0.67
1:L:19:ILE:O	1:L:23:LEU:N	2.27	0.67
1:B:150:ASN:ND2	1:B:165:GLU:OE1	2.27	0.67
1:F:27:ARG:NH2	1:F:58:GLU:OE1	2.27	0.67
1:M:146:ARG:O	1:M:150:ASN:ND2	2.27	0.67
1:J:96:ALA:O	1:J:120:MET:HE2	1.94	0.67
1:L:50:LEU:O	1:L:54:ASP:N	2.26	0.67
1:D:20:TYR:HA	1:D:23:LEU:HD12	1.77	0.67
1:J:53:GLU:N	1:J:53:GLU:OE1	2.28	0.67
1:A:173:PHE:O	1:G:141:ARG:NH2	2.28	0.66
1:K:42:SER:O	1:K:45:SER:OG	2.11	0.66
1:M:43:ILE:HG23	1:M:47:LEU:HD12	1.76	0.66
1:J:99:GLY:C	1:J:102:LEU:HG	2.15	0.66
1:K:99:GLY:O	1:K:102:LEU:HD13	1.95	0.66
1:K:91:CYS:SG	1:K:92:ILE:N	2.69	0.66
1:D:160:PRO:O	1:D:163:VAL:HG22	1.95	0.65
1:L:100:ALA:C	1:L:102:LEU:N	2.46	0.65
1:C:164:ILE:O	1:C:168:THR:OG1	2.15	0.65
1:N:20:TYR:HA	1:N:23:LEU:HD12	1.79	0.65
1:D:67:GLY:C	1:D:98:MET:HE1	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:151:LYS:O	1:I:151:LYS:NZ	2.23	0.65
1:B:36:ASP:OD2	1:B:38:ASN:N	2.30	0.65
1:J:161:LEU:HG	1:J:162:GLU:N	2.11	0.65
1:L:99:GLY:O	1:L:102:LEU:N	2.28	0.65
1:J:99:GLY:HA2	1:J:102:LEU:HG	1.79	0.65
1:M:99:GLY:O	1:M:102:LEU:CB	2.44	0.65
1:M:100:ALA:C	1:M:102:LEU:N	2.50	0.65
1:N:37:ASP:O	1:N:41:ASN:ND2	2.30	0.64
1:K:98:MET:O	1:K:102:LEU:CD1	2.45	0.64
1:L:20:TYR:HA	1:L:23:LEU:HD12	1.79	0.64
1:M:83:ILE:HG13	1:M:85:PRO:HG2	1.76	0.64
1:D:54:ASP:O	1:D:57:LYS:HG2	1.98	0.64
1:N:73:GLY:HA3	1:N:98:MET:CE	2.27	0.64
1:K:100:ALA:O	1:K:103:LEU:HB3	1.97	0.64
1:N:100:ALA:C	1:N:102:LEU:N	2.48	0.64
1:L:66:PRO:C	1:L:96:ALA:HB2	2.18	0.63
1:E:97:SER:HB2	1:E:121:ILE:HB	1.78	0.63
1:M:27:ARG:CG	1:M:50:LEU:HD11	2.25	0.63
1:M:27:ARG:HG3	1:M:50:LEU:CD1	2.23	0.63
1:E:172:ASN:O	1:E:174:LYS:NZ	2.31	0.63
1:A:37:ASP:O	1:A:41:ASN:ND2	2.32	0.63
1:E:120:MET:HG2	1:E:173:PHE:CG	2.34	0.63
1:I:35:ILE:O	1:I:69:SER:OG	2.17	0.63
1:L:40:ALA:O	1:L:44:VAL:HG23	1.99	0.62
1:M:83:ILE:CG1	1:M:85:PRO:CG	2.70	0.62
1:M:24:LEU:HG	1:M:46:GLN:HE22	1.64	0.62
1:L:67:GLY:N	1:L:96:ALA:CB	2.61	0.62
1:M:153:LEU:O	1:M:157:THR:OG1	2.13	0.62
1:C:166:ARG:O	1:C:170:ARG:NH1	2.33	0.62
1:J:38:ASN:O	1:J:41:ASN:ND2	2.33	0.62
1:B:53:GLU:OE1	1:B:53:GLU:N	2.33	0.62
1:L:47:LEU:CD1	1:L:83:ILE:HG21	2.30	0.62
1:G:54:ASP:OD1	1:G:56:GLU:N	2.33	0.62
1:J:161:LEU:HG	1:J:162:GLU:H	1.63	0.62
1:L:95:ALA:HB3	1:L:119:VAL:HG23	1.82	0.61
1:M:36:ASP:OD2	1:M:38:ASN:ND2	2.33	0.61
1:H:146:ARG:O	1:H:150:ASN:ND2	2.32	0.61
1:E:42:SER:O	1:E:45:SER:OG	2.18	0.61
1:E:120:MET:HG2	1:E:173:PHE:HA	1.82	0.61
1:C:97:SER:N	1:C:120:MET:SD	2.74	0.61
1:F:27:ARG:NH2	1:F:58:GLU:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:178:GLU:N	1:K:178:GLU:OE1	2.34	0.61
1:C:36:ASP:OD1	1:C:38:ASN:N	2.33	0.61
1:E:119:VAL:HG22	1:E:119:VAL:O	2.01	0.61
1:F:27:ARG:HH21	1:F:58:GLU:CG	2.11	0.61
1:M:35:ILE:HD12	1:M:35:ILE:O	2.00	0.61
1:F:97:SER:O	1:F:99:GLY:N	2.34	0.61
1:G:78:ASP:OD1	1:G:79:THR:N	2.34	0.61
1:H:153:LEU:O	1:H:157:THR:OG1	2.12	0.60
1:A:83:ILE:HD12	1:A:83:ILE:C	2.22	0.60
1:D:78:ASP:OD1	1:D:79:THR:N	2.34	0.60
1:L:65:SER:O	1:L:96:ALA:HB2	2.01	0.60
1:M:84:LYS:H	1:M:85:PRO:HD2	1.65	0.60
1:A:83:ILE:CD1	1:A:84:LYS:N	2.57	0.60
1:K:111:ARG:NH2	1:K:183:GLY:O	2.34	0.60
1:M:20:TYR:HA	1:M:23:LEU:HD12	1.82	0.59
1:L:67:GLY:N	1:L:96:ALA:HB1	2.16	0.59
1:A:36:ASP:OD1	1:A:38:ASN:N	2.35	0.59
1:J:161:LEU:CG	1:J:162:GLU:N	2.65	0.59
1:L:27:ARG:HD2	1:L:50:LEU:CD2	2.32	0.59
1:N:19:ILE:O	1:N:23:LEU:N	2.36	0.59
1:D:95:ALA:O	1:D:119:VAL:HA	2.01	0.59
1:N:98:MET:O	1:N:101:PHE:N	2.30	0.59
1:D:27:ARG:CZ	1:D:57:LYS:HB2	2.32	0.59
1:M:47:LEU:HD13	1:M:83:ILE:HD13	1.83	0.59
1:C:26:ASP:O	1:C:27:ARG:HG2	2.03	0.58
1:J:99:GLY:CA	1:J:102:LEU:HG	2.32	0.58
1:M:27:ARG:CG	1:M:50:LEU:CD1	2.81	0.58
1:J:98:MET:O	1:J:101:PHE:HB3	2.02	0.58
1:N:91:CYS:SG	1:N:92:ILE:N	2.75	0.58
1:I:99:GLY:O	1:I:103:LEU:N	2.35	0.58
1:J:96:ALA:O	1:J:120:MET:HG3	2.03	0.57
1:K:19:ILE:HG23	1:K:20:TYR:CD1	2.39	0.57
1:G:93:GLY:O	1:G:118:GLU:N	2.38	0.57
1:J:100:ALA:C	1:J:102:LEU:N	2.58	0.57
1:K:67:GLY:CA	1:K:96:ALA:CB	2.80	0.57
1:L:66:PRO:CA	1:L:96:ALA:HB2	2.35	0.57
1:K:99:GLY:CA	1:K:102:LEU:CD1	2.59	0.57
1:D:54:ASP:OD1	1:D:57:LYS:HD3	2.04	0.57
1:C:162:GLU:O	1:C:166:ARG:N	2.37	0.57
1:M:39:VAL:O	1:M:43:ILE:N	2.37	0.57
1:M:73:GLY:HA3	1:M:98:MET:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:CYS:SG	1:F:92:ILE:N	2.77	0.57
1:M:49:PHE:O	1:M:52:ALA:HB3	2.04	0.57
1:D:36:ASP:OD1	1:D:38:ASN:N	2.38	0.57
1:H:99:GLY:O	1:H:103:LEU:N	2.38	0.57
1:H:148:LYS:O	1:H:152:VAL:HG23	2.05	0.56
1:B:98:MET:SD	1:B:98:MET:N	2.79	0.56
1:D:159:GLN:HB3	1:D:163:VAL:HG21	1.87	0.56
1:F:20:TYR:HA	1:F:23:LEU:HD12	1.86	0.56
1:I:148:LYS:O	1:I:152:VAL:HG23	2.05	0.56
1:K:95:ALA:HB3	1:K:119:VAL:HG23	1.86	0.56
1:M:27:ARG:HH21	1:M:57:LYS:CD	2.12	0.56
1:F:54:ASP:OD2	1:F:56:GLU:C	2.44	0.56
1:C:166:ARG:NH1	1:C:167:ASP:OD1	2.38	0.56
1:E:97:SER:HB2	1:E:121:ILE:CB	2.36	0.56
1:A:141:ARG:NH1	1:B:118:GLU:OE2	2.39	0.56
1:M:40:ALA:O	1:M:44:VAL:HG23	2.06	0.56
1:H:107:GLU:OE1	1:H:109:GLY:N	2.37	0.56
1:M:84:LYS:N	1:M:85:PRO:CD	2.68	0.56
1:G:145:LEU:O	1:G:148:LYS:N	2.39	0.55
1:L:98:MET:O	1:L:101:PHE:N	2.39	0.55
1:N:160:PRO:O	1:N:163:VAL:CG2	2.53	0.55
1:L:22:ARG:HA	1:L:25:LYS:HB2	1.87	0.55
1:B:44:VAL:O	1:B:48:LEU:HD12	2.06	0.55
1:B:91:CYS:SG	1:B:92:ILE:N	2.79	0.55
1:D:167:ASP:OD2	1:D:182:TYR:OH	2.25	0.55
1:C:181:GLU:OE1	1:C:181:GLU:N	2.38	0.55
1:H:181:GLU:OE1	1:H:181:GLU:N	2.40	0.55
1:E:166:ARG:O	1:E:170:ARG:NH1	2.41	0.54
1:K:73:GLY:HA3	1:K:98:MET:SD	2.48	0.54
1:A:69:SER:OG	1:A:70:ILE:N	2.37	0.54
1:J:111:ARG:NH2	1:J:183:GLY:O	2.40	0.54
1:D:97:SER:O	1:D:99:GLY:N	2.41	0.54
1:M:123:GLN:OE1	1:M:146:ARG:NH2	2.41	0.54
1:E:97:SER:HB2	1:E:121:ILE:CA	2.38	0.54
1:K:67:GLY:N	1:K:96:ALA:HB1	2.17	0.54
1:D:27:ARG:CD	1:D:57:LYS:HD2	2.38	0.54
1:A:175:SER:N	1:A:178:GLU:OE2	2.41	0.53
1:C:42:SER:O	1:C:45:SER:OG	2.25	0.53
1:C:104:ALA:O	1:C:156:ARG:NH1	2.40	0.53
1:J:73:GLY:CA	1:J:98:MET:HE1	2.29	0.53
1:J:160:PRO:O	1:J:163:VAL:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:19:ILE:O	1:M:23:LEU:N	2.38	0.53
1:F:78:ASP:OD1	1:F:79:THR:N	2.41	0.53
1:L:47:LEU:HD13	1:L:83:ILE:HD13	1.89	0.53
1:E:121:ILE:HD13	1:E:121:ILE:H	1.73	0.53
1:N:73:GLY:HA3	1:N:98:MET:HE3	1.90	0.53
1:J:96:ALA:O	1:J:120:MET:SD	2.67	0.53
1:N:107:GLU:OE1	1:N:109:GLY:N	2.40	0.53
1:G:91:CYS:SG	1:G:92:ILE:N	2.81	0.53
1:E:120:MET:CG	1:E:173:PHE:CD1	2.92	0.53
1:E:186:ASP:OD1	1:E:187:LYS:N	2.42	0.53
1:M:83:ILE:HG13	1:M:85:PRO:CD	2.39	0.53
1:I:88:SER:OG	1:I:110:LYS:O	2.23	0.52
1:J:160:PRO:O	1:J:163:VAL:N	2.37	0.52
1:M:24:LEU:CG	1:M:46:GLN:NE2	2.65	0.52
1:M:73:GLY:HA3	1:M:98:MET:HE3	1.91	0.52
1:B:103:LEU:HD21	1:B:185:ILE:HD13	1.91	0.52
1:G:42:SER:O	1:G:45:SER:OG	2.23	0.52
1:D:54:ASP:OD1	1:D:54:ASP:N	2.42	0.52
1:K:146:ARG:O	1:K:150:ASN:ND2	2.42	0.52
1:N:152:VAL:O	1:N:155:GLU:HB2	2.09	0.52
1:F:54:ASP:OD2	1:F:56:GLU:N	2.39	0.52
1:N:101:PHE:CE1	1:N:153:LEU:HD21	2.44	0.52
1:A:78:ASP:OD1	1:A:79:THR:N	2.43	0.52
1:D:27:ARG:NE	1:D:57:LYS:HB2	2.24	0.52
1:J:120:MET:HE3	1:J:122:HIS:HB2	1.92	0.51
1:D:27:ARG:NH2	1:D:57:LYS:HB2	2.25	0.51
1:G:36:ASP:OD1	1:G:38:ASN:N	2.44	0.51
1:M:111:ARG:HB2	1:M:186:ASP:OD1	2.10	0.51
1:M:83:ILE:HG13	1:M:85:PRO:CG	2.39	0.51
1:C:21:SER:OG	1:C:22:ARG:N	2.44	0.51
1:H:53:GLU:N	1:H:53:GLU:OE1	2.43	0.51
1:I:174:LYS:CE	1:I:182:TYR:CD1	2.85	0.51
1:I:175:SER:OG	1:I:176:ALA:N	2.43	0.51
1:A:39:VAL:O	1:A:43:ILE:HD12	2.11	0.51
1:M:43:ILE:CG2	1:M:47:LEU:HD12	2.41	0.51
1:M:109:GLY:O	1:M:186:ASP:CG	2.45	0.51
1:M:36:ASP:C	1:M:38:ASN:HD22	2.14	0.51
1:K:102:LEU:HD12	1:K:102:LEU:H	1.74	0.50
1:D:54:ASP:OD2	1:D:57:LYS:HB3	2.11	0.50
1:F:52:ALA:CB	1:G:26:ASP:OD2	2.59	0.50
1:E:26:ASP:OD1	1:E:26:ASP:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:SER:OG	1:J:70:ILE:N	2.43	0.50
1:A:91:CYS:SG	1:A:92:ILE:N	2.84	0.50
1:F:37:ASP:O	1:F:41:ASN:ND2	2.38	0.50
1:M:33:SER:O	1:M:34:ALA:HB2	2.12	0.50
1:D:68:GLY:HA3	1:D:98:MET:HE3	1.89	0.50
1:N:73:GLY:HA3	1:N:98:MET:HE2	1.91	0.49
1:A:162:GLU:O	1:A:166:ARG:NH1	2.45	0.49
1:M:94:MET:SD	1:M:94:MET:N	2.85	0.49
1:H:80:MET:HE3	1:H:87:VAL:HG11	1.94	0.49
1:N:146:ARG:O	1:N:150:ASN:ND2	2.46	0.49
1:K:52:ALA:CB	1:L:26:ASP:OD1	2.61	0.49
1:K:98:MET:HA	1:K:98:MET:CE	2.43	0.49
1:I:91:CYS:SG	1:I:92:ILE:N	2.85	0.49
1:J:48:LEU:HD23	1:J:48:LEU:H	1.78	0.49
1:N:99:GLY:O	1:N:102:LEU:CB	2.60	0.49
1:C:44:VAL:O	1:C:48:LEU:HD12	2.12	0.49
1:J:99:GLY:O	1:J:102:LEU:HB2	2.12	0.49
1:G:69:SER:OG	1:G:70:ILE:N	2.44	0.48
1:M:27:ARG:HD3	1:M:27:ARG:N	2.28	0.48
1:L:73:GLY:HA3	1:L:98:MET:HE3	1.78	0.48
1:D:181:GLU:OE1	1:D:181:GLU:N	2.45	0.48
1:E:103:LEU:HD12	1:E:103:LEU:O	2.12	0.48
1:K:100:ALA:O	1:K:103:LEU:HB2	2.13	0.48
1:B:141:ARG:NE	1:C:118:GLU:OE2	2.42	0.48
1:D:44:VAL:O	1:D:48:LEU:HD12	2.13	0.48
1:J:29:ILE:HG22	1:J:30:MET:N	2.28	0.48
1:F:52:ALA:HB1	1:G:26:ASP:OD2	2.14	0.48
1:I:78:ASP:O	1:I:82:PHE:N	2.45	0.48
1:K:148:LYS:O	1:K:152:VAL:HG23	2.14	0.48
1:C:92:ILE:HG22	1:C:114:LEU:HD11	1.96	0.47
1:K:165:GLU:HA	1:K:168:THR:HG22	1.95	0.47
1:L:175:SER:OG	1:L:176:ALA:N	2.46	0.47
1:M:47:LEU:HD22	1:M:83:ILE:CD1	2.44	0.47
1:M:36:ASP:O	1:M:38:ASN:ND2	2.41	0.47
1:M:148:LYS:O	1:M:152:VAL:HG23	2.14	0.47
1:E:181:GLU:N	1:E:181:GLU:OE1	2.46	0.47
1:N:154:ALA:O	1:N:158:GLY:HA2	2.13	0.47
1:C:29:ILE:HG22	1:C:30:MET:N	2.30	0.47
1:C:50:LEU:HD21	1:C:57:LYS:HB3	1.97	0.47
1:G:44:VAL:O	1:G:48:LEU:HD12	2.13	0.47
1:K:99:GLY:O	1:K:102:LEU:CA	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:100:ALA:C	1:L:102:LEU:H	2.19	0.47
1:J:159:GLN:CD	1:J:159:GLN:H	2.16	0.46
1:A:118:GLU:N	1:A:118:GLU:OE1	2.48	0.46
1:M:99:GLY:O	1:M:102:LEU:HB2	2.13	0.46
1:I:174:LYS:HE3	1:I:182:TYR:CD1	2.50	0.46
1:E:121:ILE:HD13	1:E:121:ILE:N	2.30	0.46
1:C:91:CYS:SG	1:C:92:ILE:N	2.88	0.46
1:L:27:ARG:HD3	1:L:27:ARG:N	2.30	0.46
1:B:29:ILE:HG22	1:B:30:MET:N	2.31	0.46
1:A:93:GLY:O	1:A:118:GLU:N	2.47	0.45
1:B:97:SER:OG	1:B:98:MET:SD	2.63	0.45
1:L:47:LEU:HD22	1:L:83:ILE:HD13	1.98	0.45
1:M:141:ARG:HH12	1:M:145:LEU:HD21	1.81	0.45
1:A:29:ILE:HG22	1:A:30:MET:N	2.32	0.45
1:A:82:PHE:CD2	1:A:82:PHE:O	2.70	0.45
1:B:150:ASN:OD1	1:B:164:ILE:HG21	2.15	0.45
1:J:98:MET:O	1:J:101:PHE:CB	2.65	0.45
1:M:46:GLN:O	1:M:50:LEU:HG	2.17	0.45
1:F:27:ARG:NH2	1:F:58:GLU:CD	2.69	0.45
1:N:162:GLU:N	1:N:162:GLU:CD	2.70	0.45
1:E:78:ASP:OD2	1:E:79:THR:N	2.50	0.45
1:A:82:PHE:CD2	1:A:82:PHE:C	2.90	0.44
1:H:37:ASP:OD1	1:H:38:ASN:N	2.50	0.44
1:H:103:LEU:HD23	1:H:104:ALA:N	2.32	0.44
1:I:19:ILE:O	1:I:23:LEU:N	2.49	0.44
1:M:29:ILE:HG22	1:M:30:MET:N	2.33	0.44
1:D:145:LEU:O	1:D:149:LEU:N	2.44	0.44
1:C:93:GLY:N	1:C:117:SER:OG	2.48	0.44
1:D:98:MET:C	1:D:100:ALA:N	2.70	0.44
1:I:37:ASP:OD1	1:I:38:ASN:N	2.51	0.44
1:J:73:GLY:HA2	1:J:98:MET:HE3	1.97	0.44
1:N:69:SER:OG	1:N:70:ILE:N	2.50	0.44
1:D:29:ILE:HG22	1:D:30:MET:N	2.32	0.44
1:K:37:ASP:OD1	1:K:38:ASN:N	2.51	0.44
1:N:161:LEU:CD1	1:N:161:LEU:C	2.85	0.44
1:N:78:ASP:OD1	1:N:78:ASP:N	2.49	0.44
1:M:114:LEU:HD23	1:M:189:LEU:HD11	1.99	0.44
1:A:44:VAL:O	1:A:48:LEU:HD12	2.17	0.43
1:M:73:GLY:CA	1:M:98:MET:HE3	2.48	0.43
1:D:57:LYS:O	1:D:57:LYS:HG3	2.18	0.43
1:E:50:LEU:HD23	1:E:57:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:96:ALA:O	1:J:120:MET:HE1	2.16	0.43
1:M:20:TYR:O	1:M:24:LEU:HB2	2.19	0.43
1:E:36:ASP:OD2	1:E:38:ASN:N	2.51	0.43
1:E:37:ASP:O	1:E:41:ASN:ND2	2.43	0.43
1:K:58:GLU:OE1	1:K:58:GLU:N	2.48	0.43
1:J:73:GLY:C	1:J:98:MET:HE1	2.39	0.43
1:B:37:ASP:OD1	1:B:38:ASN:N	2.51	0.43
1:L:107:GLU:OE1	1:L:109:GLY:N	2.47	0.43
1:E:29:ILE:HG22	1:E:30:MET:N	2.32	0.43
1:G:102:LEU:O	1:G:105:ALA:HB3	2.19	0.43
1:K:172:ASN:OD1	1:K:172:ASN:N	2.51	0.43
1:C:91:CYS:SG	1:C:95:ALA:HB2	2.59	0.43
1:K:29:ILE:HG22	1:K:30:MET:N	2.34	0.43
1:N:37:ASP:OD1	1:N:38:ASN:N	2.51	0.43
1:D:29:ILE:HG22	1:D:30:MET:H	1.83	0.42
1:E:118:GLU:N	1:E:118:GLU:OE2	2.52	0.42
1:F:93:GLY:O	1:F:118:GLU:N	2.47	0.42
1:J:151:LYS:O	1:J:154:ALA:HB3	2.19	0.42
1:K:69:SER:O	1:K:98:MET:HG2	2.19	0.42
1:F:29:ILE:HG22	1:F:30:MET:N	2.34	0.42
1:N:100:ALA:C	1:N:102:LEU:H	2.21	0.42
1:M:27:ARG:CD	1:M:50:LEU:CD2	2.92	0.42
1:I:152:VAL:O	1:I:155:GLU:N	2.49	0.42
1:M:21:SER:O	1:M:25:LYS:N	2.53	0.42
1:M:59:ILE:HG23	1:M:87:VAL:HG22	1.99	0.42
1:J:159:GLN:CD	1:J:159:GLN:N	2.73	0.42
1:L:67:GLY:CA	1:L:96:ALA:HB1	2.49	0.42
1:C:78:ASP:OD2	1:C:78:ASP:N	2.51	0.42
1:D:27:ARG:HD2	1:D:57:LYS:HD2	2.01	0.42
1:J:161:LEU:C	1:J:161:LEU:CD1	2.83	0.42
1:K:27:ARG:NH1	1:K:54:ASP:OD2	2.53	0.42
1:C:50:LEU:O	1:C:50:LEU:HD23	2.20	0.42
1:M:47:LEU:HD13	1:M:83:ILE:CD1	2.49	0.42
1:M:47:LEU:HD22	1:M:85:PRO:CG	2.49	0.42
1:M:83:ILE:HB	1:M:85:PRO:HD2	2.00	0.42
1:N:159:GLN:CD	1:N:159:GLN:N	2.72	0.41
1:F:172:ASN:OD1	1:F:172:ASN:N	2.54	0.41
1:K:143:LEU:HD12	1:K:144:LEU:N	2.35	0.41
1:B:78:ASP:OD1	1:B:79:THR:N	2.53	0.41
1:G:29:ILE:HG22	1:G:30:MET:N	2.35	0.41
1:G:146:ARG:O	1:G:150:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:138:ALA:O	1:L:142:ILE:HD12	2.21	0.41
1:K:78:ASP:N	1:K:78:ASP:OD2	2.53	0.41
1:M:61:LEU:HD12	1:M:62:TYR:N	2.35	0.41
1:M:107:GLU:O	1:M:107:GLU:HG3	2.21	0.41
1:E:120:MET:SD	1:E:120:MET:O	2.78	0.41
1:I:78:ASP:OD2	1:I:79:THR:HG23	2.21	0.41
1:N:69:SER:O	1:N:98:MET:HG2	2.21	0.41
1:A:59:ILE:HG22	1:A:86:LYS:O	2.21	0.41
1:H:43:ILE:O	1:H:47:LEU:N	2.54	0.41
1:I:29:ILE:HG22	1:I:30:MET:N	2.35	0.41
1:M:37:ASP:C	1:M:39:VAL:H	2.24	0.41
1:N:159:GLN:OE1	1:N:159:GLN:CA	2.69	0.41
1:E:97:SER:HB2	1:E:121:ILE:HA	2.03	0.41
1:M:28:ILE:HG22	1:M:29:ILE:N	2.36	0.40
1:M:37:ASP:O	1:M:41:ASN:ND2	2.54	0.40
1:N:152:VAL:HG12	1:N:156:ARG:HG2	2.03	0.40
1:C:76:ILE:HG22	1:C:80:MET:HG3	2.03	0.40
1:H:50:LEU:N	1:H:50:LEU:HD12	2.36	0.40
1:I:54:ASP:OD1	1:I:56:GLU:N	2.49	0.40
1:K:27:ARG:CD	1:K:50:LEU:HD21	2.51	0.40
1:L:66:PRO:HA	1:L:96:ALA:HB2	2.03	0.40
1:C:29:ILE:HG22	1:C:30:MET:H	1.86	0.40
1:C:50:LEU:HD21	1:C:57:LYS:HD2	2.04	0.40
1:H:80:MET:CE	1:H:87:VAL:HG11	2.51	0.40
1:I:78:ASP:OD2	1:I:79:THR:N	2.55	0.40
1:K:101:PHE:CD1	1:K:149:LEU:HD23	2.57	0.40
1:I:42:SER:O	1:I:45:SER:OG	2.38	0.40
1:J:96:ALA:O	1:J:120:MET:CG	2.67	0.40
1:J:161:LEU:O	1:J:163:VAL:CA	2.63	0.40
1:L:27:ARG:HG3	1:L:50:LEU:HD11	2.03	0.40
1:L:78:ASP:OD1	1:L:78:ASP:N	2.52	0.40
1:M:83:ILE:HG13	1:M:85:PRO:HD2	2.02	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	153/202 (76%)	128 (84%)	24 (16%)	1 (1%)	22	55
1	B	153/202 (76%)	125 (82%)	28 (18%)	0	100	100
1	C	153/202 (76%)	130 (85%)	23 (15%)	0	100	100
1	D	153/202 (76%)	123 (80%)	28 (18%)	2 (1%)	12	39
1	E	153/202 (76%)	126 (82%)	27 (18%)	0	100	100
1	F	153/202 (76%)	125 (82%)	25 (16%)	3 (2%)	7	30
1	G	153/202 (76%)	124 (81%)	28 (18%)	1 (1%)	22	55
1	H	153/202 (76%)	126 (82%)	27 (18%)	0	100	100
1	I	153/202 (76%)	121 (79%)	32 (21%)	0	100	100
1	J	153/202 (76%)	121 (79%)	24 (16%)	8 (5%)	2	13
1	K	153/202 (76%)	119 (78%)	33 (22%)	1 (1%)	22	55
1	L	153/202 (76%)	123 (80%)	26 (17%)	4 (3%)	5	26
1	M	153/202 (76%)	116 (76%)	28 (18%)	9 (6%)	1	11
1	N	153/202 (76%)	124 (81%)	26 (17%)	3 (2%)	7	30
All	All	2142/2828 (76%)	1731 (81%)	379 (18%)	32 (2%)	14	36

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	27	ARG
1	J	158	GLY
1	J	159	GLN
1	J	162	GLU
1	M	37	ASP
1	M	96	ALA
1	M	99	GLY
1	M	110	LYS
1	A	82	PHE
1	D	98	MET
1	D	99	GLY
1	F	98	MET
1	J	160	PRO
1	L	96	ALA
1	L	99	GLY

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Mol	Chain	Res	Type
1	L	101	PHE
1	M	34	ALA
1	M	101	PHE
1	M	107	GLU
1	N	99	GLY
1	N	101	PHE
1	F	97	SER
1	J	96	ALA
1	J	98	MET
1	J	101	PHE
1	L	98	MET
1	M	108	LYS
1	F	84	LYS
1	J	161	LEU
1	K	96	ALA
1	M	27	ARG
1	N	98	MET

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/168 (76%)	125 (98%)	2 (2%)	62	81
1	B	127/168 (76%)	126 (99%)	1 (1%)	81	91
1	C	127/168 (76%)	126 (99%)	1 (1%)	81	91
1	D	128/168 (76%)	127 (99%)	1 (1%)	81	91
1	E	128/168 (76%)	125 (98%)	3 (2%)	50	74
1	F	127/168 (76%)	124 (98%)	3 (2%)	49	74
1	G	127/168 (76%)	126 (99%)	1 (1%)	81	91
1	H	127/168 (76%)	126 (99%)	1 (1%)	81	91
1	I	127/168 (76%)	124 (98%)	3 (2%)	49	74
1	J	127/168 (76%)	120 (94%)	7 (6%)	21	51
1	K	127/168 (76%)	126 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	127/168 (76%)	127 (100%)	0	100	100
1	M	130/168 (77%)	125 (96%)	5 (4%)	33	61
1	N	127/168 (76%)	118 (93%)	9 (7%)	14	44
All	All	1783/2352 (76%)	1745 (98%)	38 (2%)	56	76

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	83	ILE
1	B	19	ILE
1	C	166	ARG
1	D	98	MET
1	E	119	VAL
1	E	120	MET
1	E	121	ILE
1	F	27	ARG
1	F	56	GLU
1	F	57	LYS
1	G	26	ASP
1	H	27	ARG
1	I	166	ARG
1	I	182	TYR
1	I	186	ASP
1	J	37	ASP
1	J	97	SER
1	J	98	MET
1	J	156	ARG
1	J	159	GLN
1	J	161	LEU
1	J	162	GLU
1	K	101	PHE
1	M	24	LEU
1	M	25	LYS
1	M	97	SER
1	M	108	LYS
1	M	186	ASP
1	N	97	SER
1	N	156	ARG
1	N	161	LEU
1	N	162	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	N	163	VAL
1	N	165	GLU
1	N	169	ASP
1	N	170	ARG
1	N	186	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	ASN
1	C	41	ASN
1	C	159	GLN
1	D	41	ASN
1	D	116	ASN
1	G	150	ASN
1	H	150	ASN
1	J	41	ASN
1	K	150	ASN
1	M	38	ASN
1	M	41	ASN
1	M	46	GLN
1	M	81	GLN
1	N	41	ASN
1	N	150	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

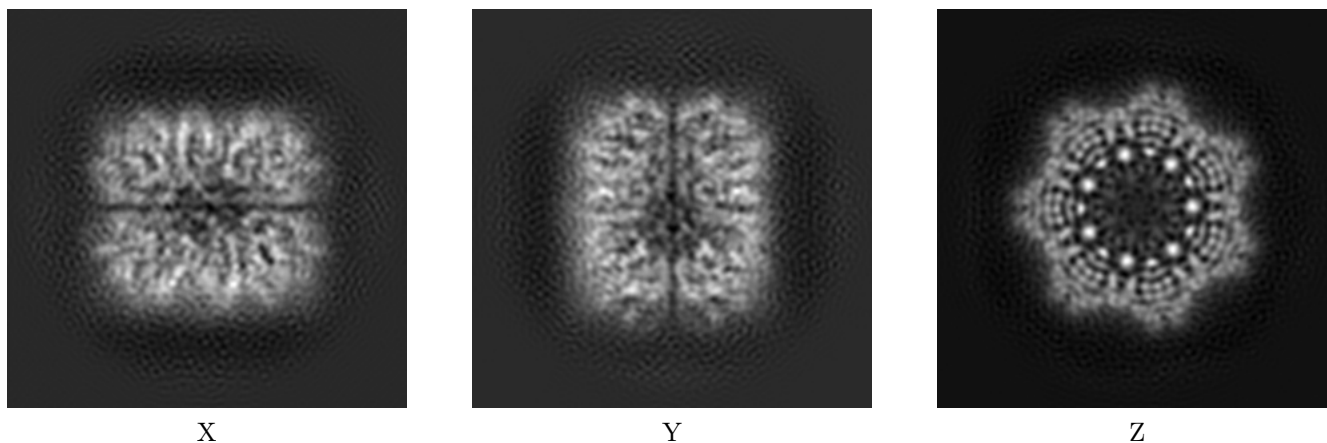
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31562. 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](#)

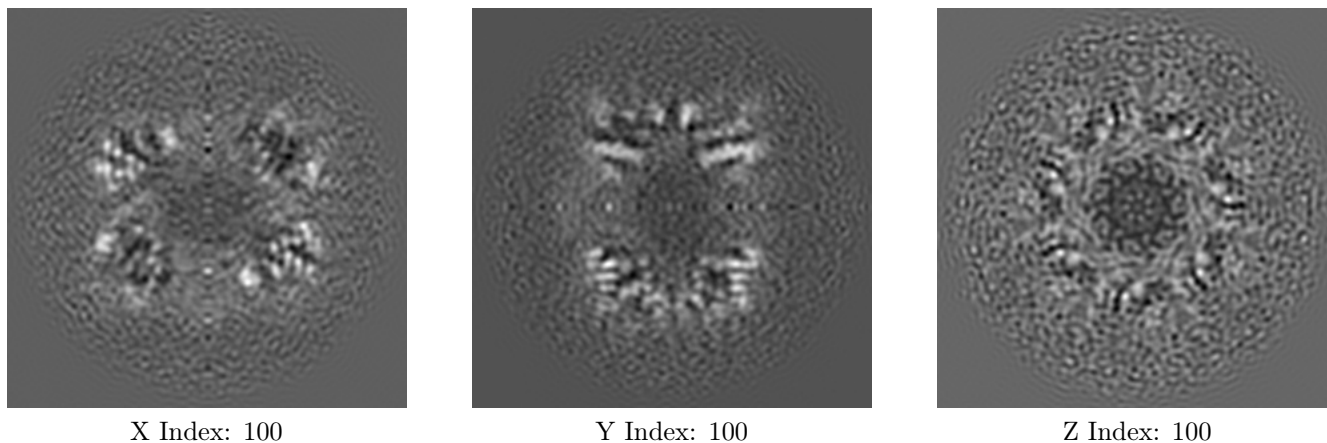
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map

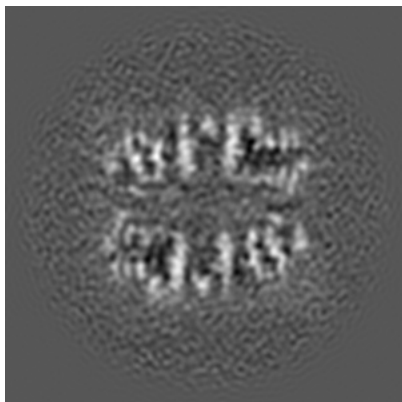




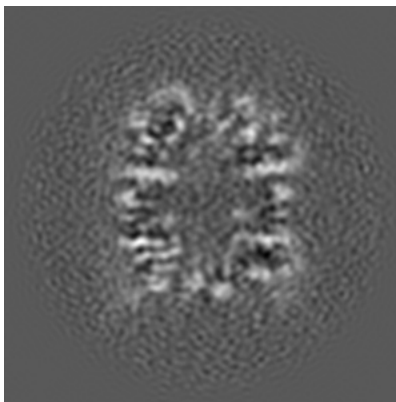
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

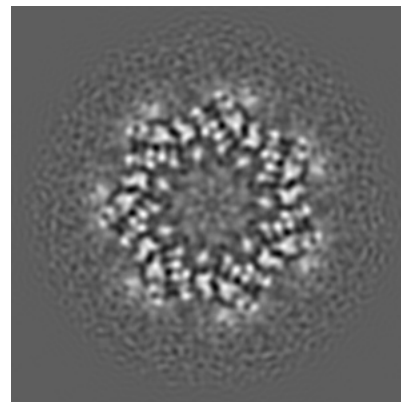
### 6.3.1 Primary map



X Index: 76



Y Index: 122

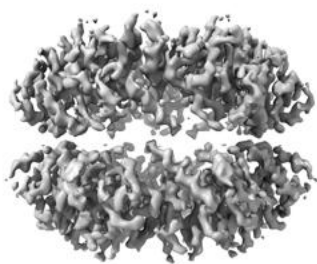


Z Index: 76

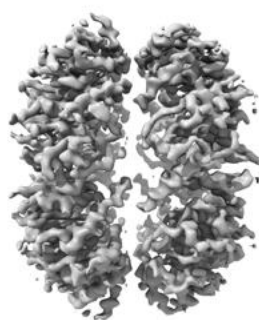
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

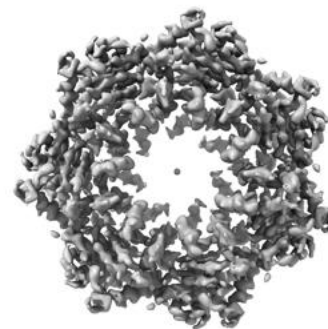
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

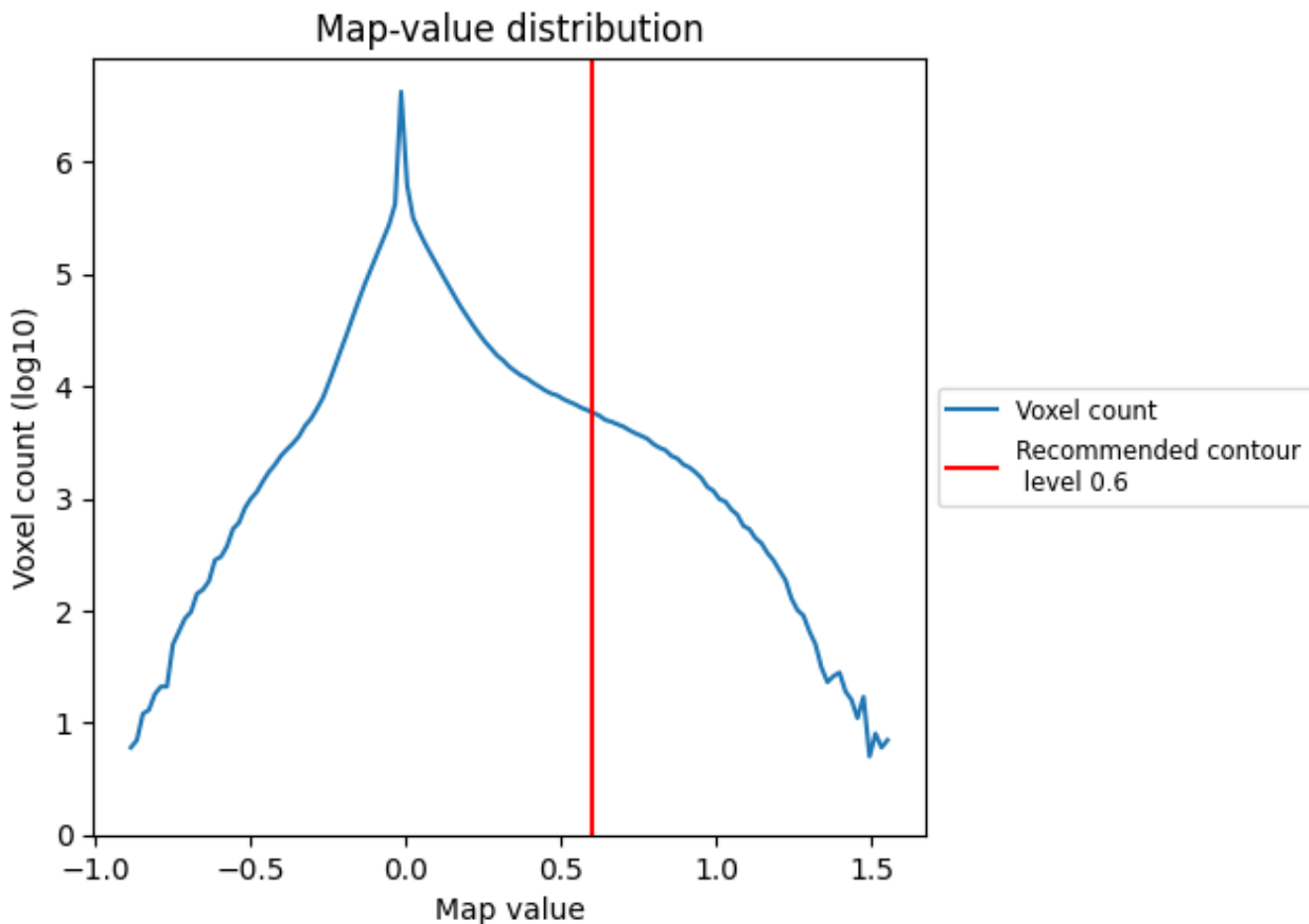
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

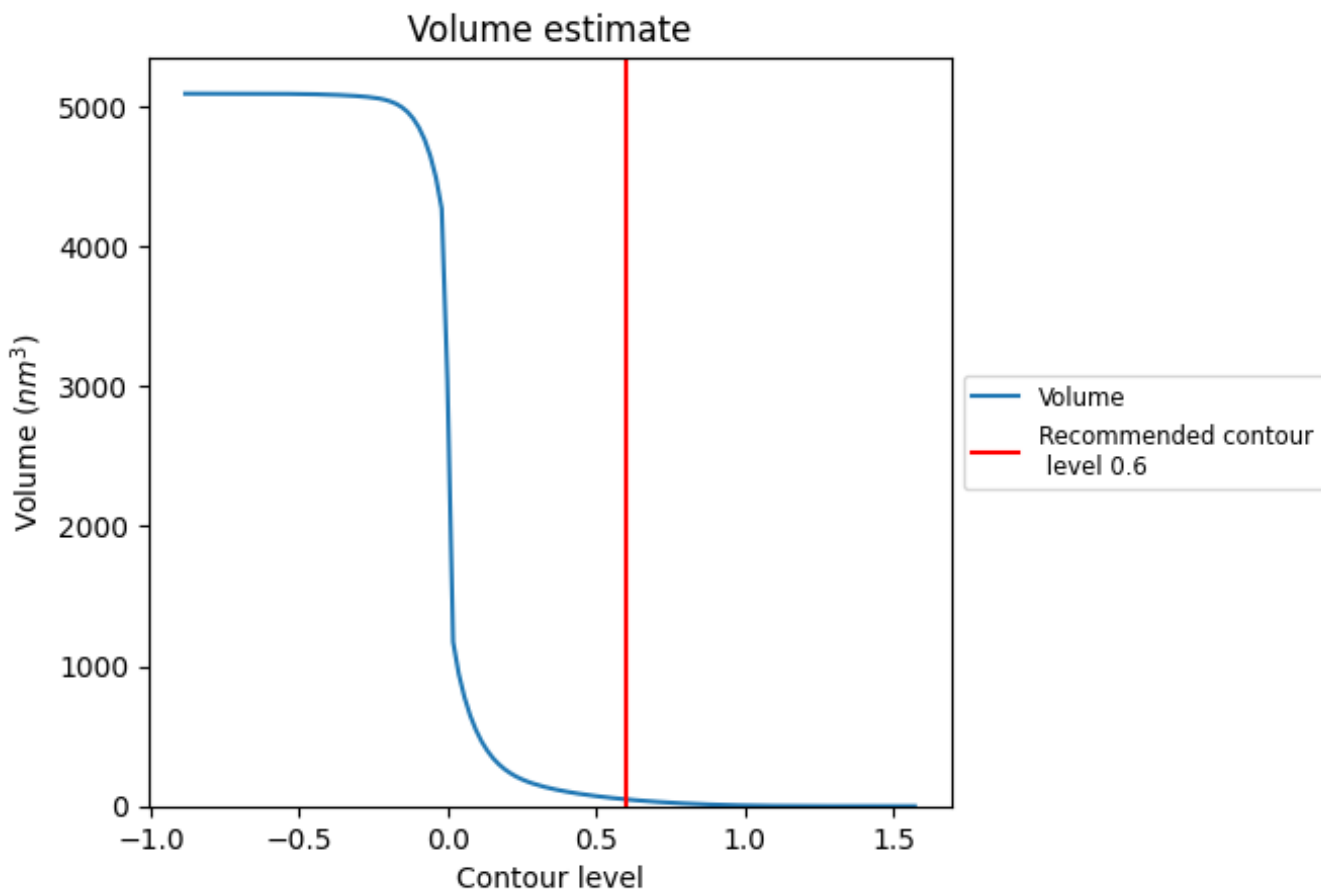
This section contains the results of statistical analysis of the map.

### 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.

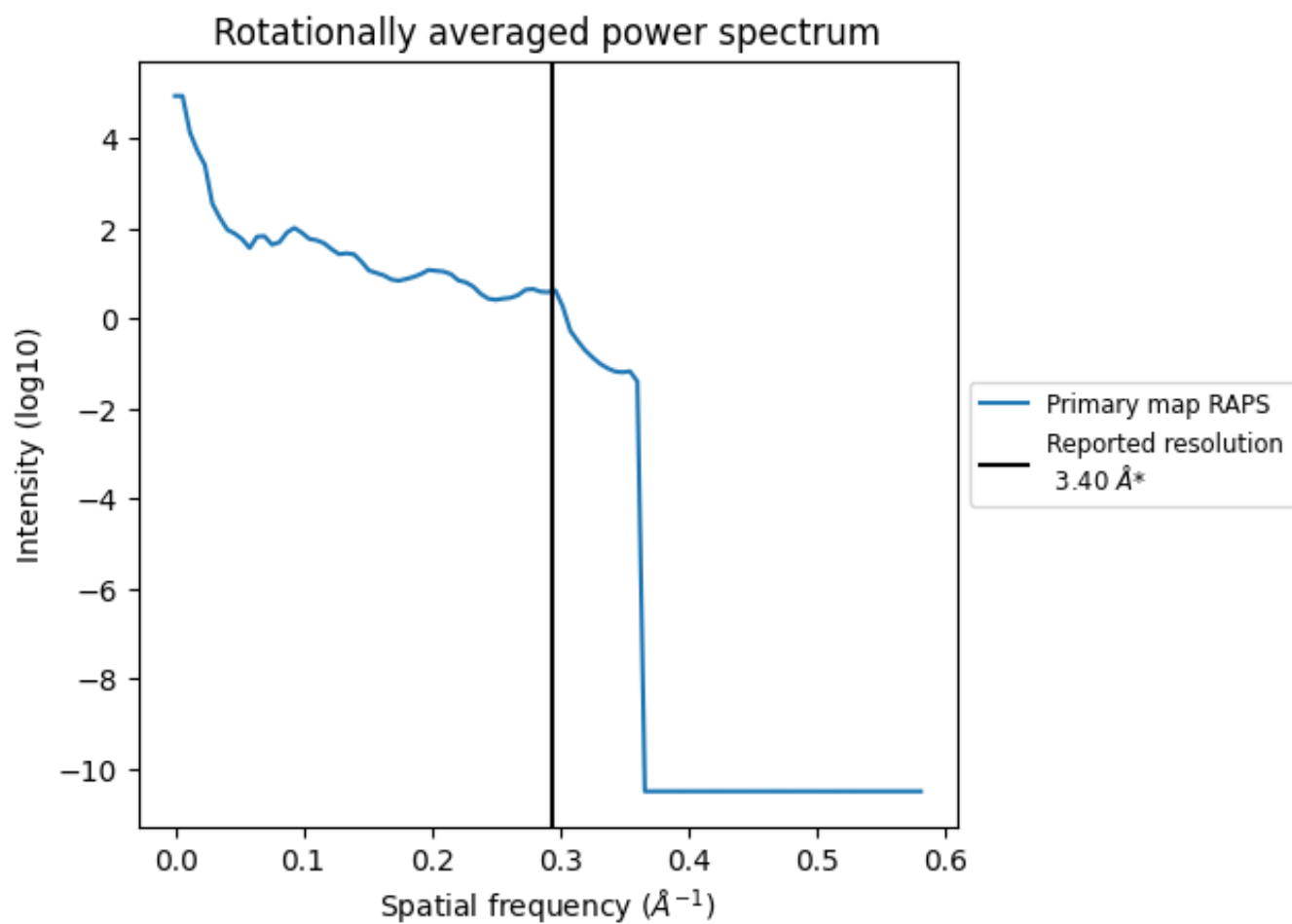
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49  $\text{nm}^3$ ; this corresponds to an approximate mass of 44 kDa.

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

### 7.3 Rotationally averaged power spectrum [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

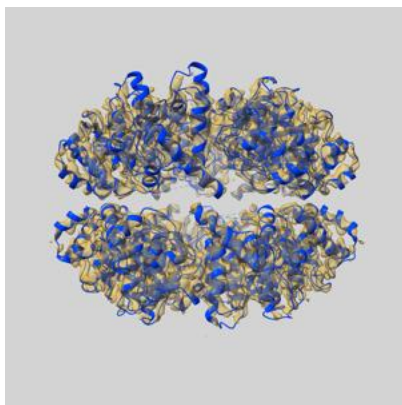
## 8 Fourier-Shell correlation

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

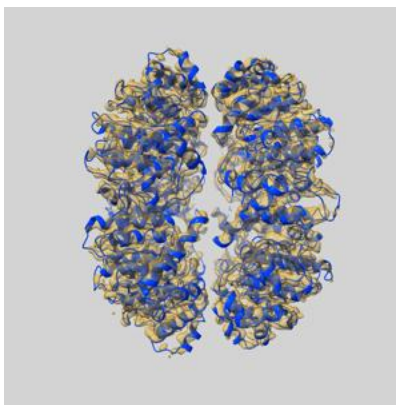
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31562 and PDB model 7FES. Per-residue inclusion information can be found in section 3 on page 7.

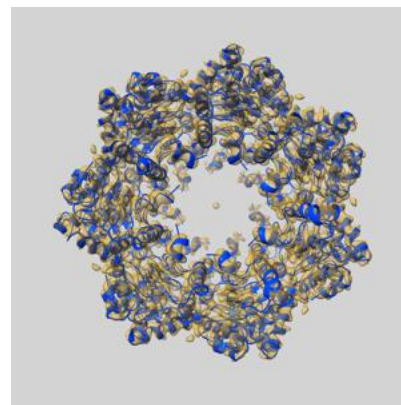
### 9.1 Map-model overlay [i](#)



X



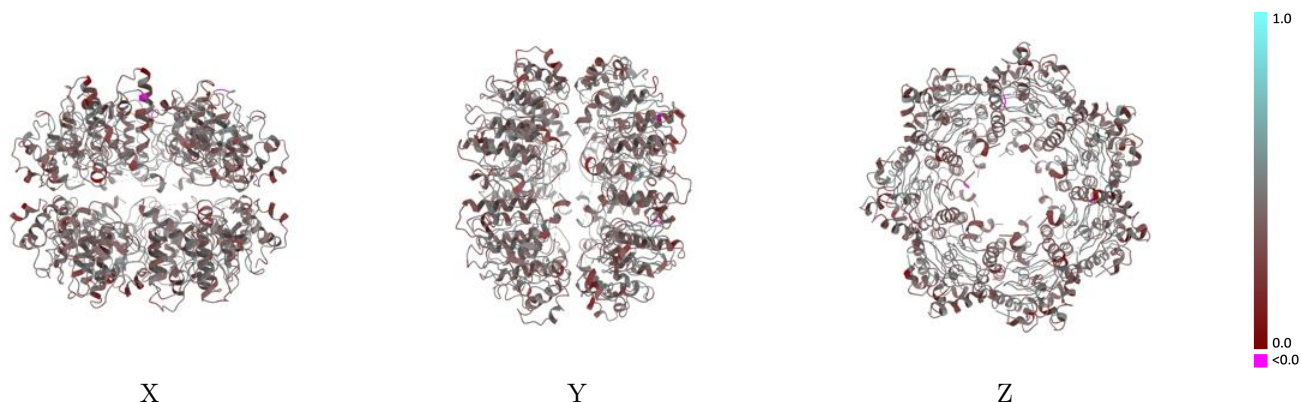
Y



Z

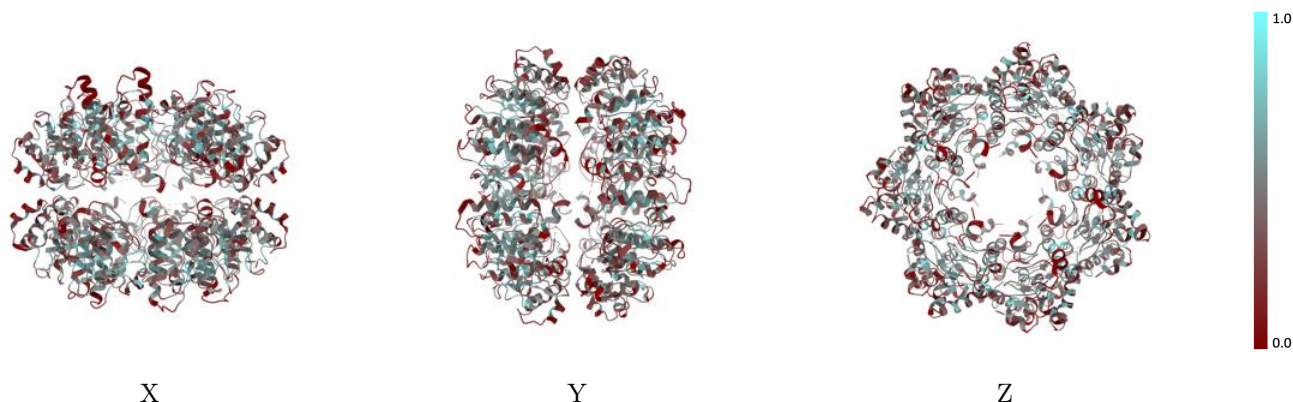
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

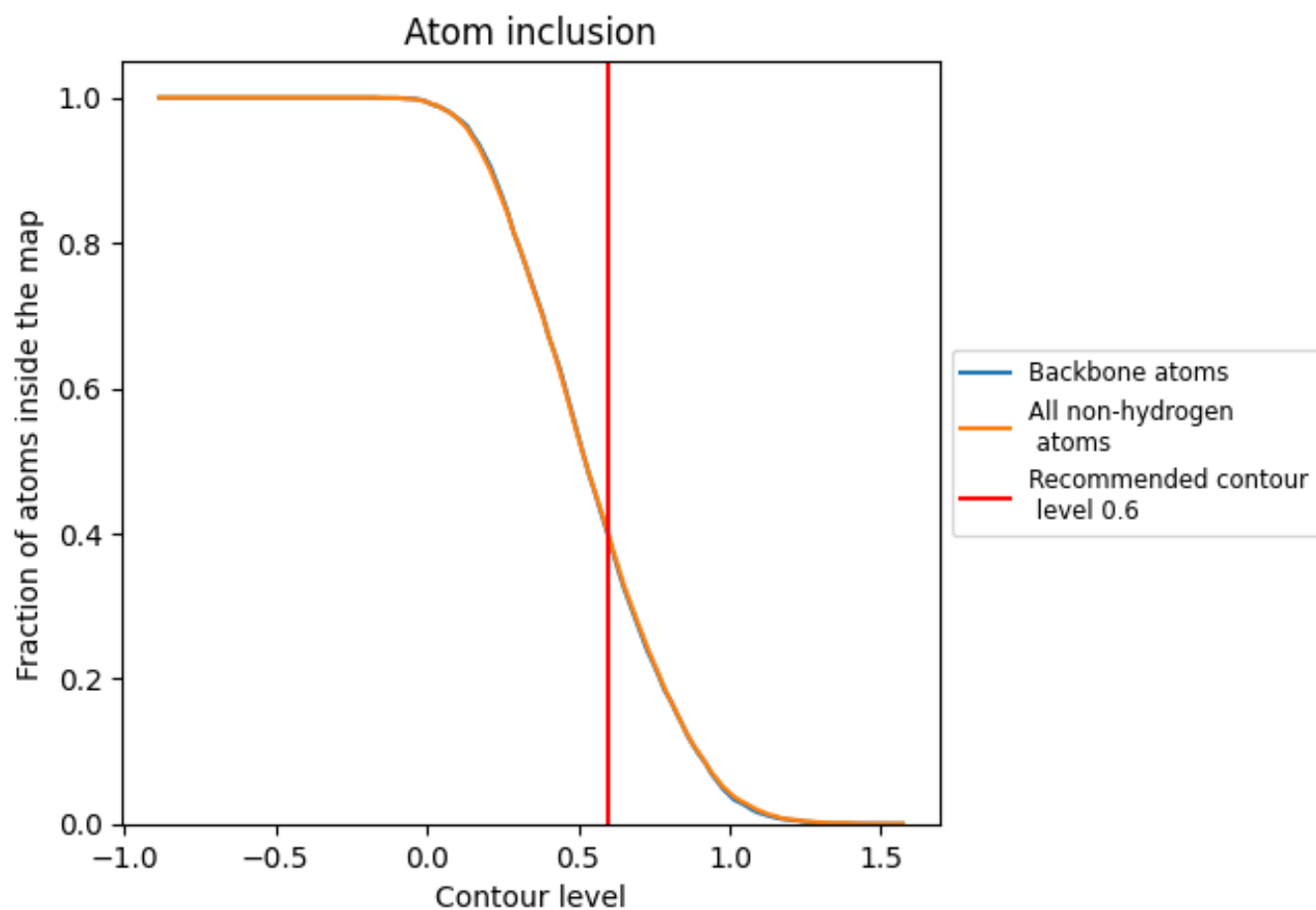
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.6).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3991	0.4080
A	0.4192	0.4130
B	0.4107	0.4110
C	0.4141	0.4030
D	0.4093	0.4080
E	0.4186	0.4090
F	0.4133	0.4090
G	0.4090	0.4070
H	0.3971	0.4050
I	0.3903	0.4070
J	0.3886	0.4120
K	0.3997	0.4070
L	0.3767	0.4060
M	0.3872	0.4030
N	0.4124	0.4160

