Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:44 am GMT

PDB ID	:	5LZP
EMDB ID	:	EMD-4128
Title	:	Binding of the C-terminal GQYL motif of the bacterial proteasome activator Bpa to the 20S proteasome
Authors	:	Bolten, M.; Delley, C.L.; Leibundgut, M.; Boehringer, D.; Ban, N.; Weber-Ban, E.
Deposited on	:	2016-09-30
Resolution	:	3.45 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:

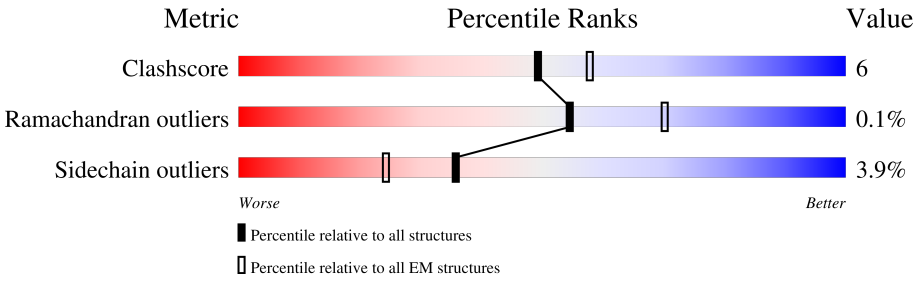
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.45 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	241	71% 16% • 11%
1	2	241	71% 16% • 11%
1	4	241	71% 16% • 11%
1	6	241	72% 15% • 11%
1	8	241	71% 15% • 11%
1	B	241	65% 21% • 11%
1	D	241	69% 19% • 10%
1	H	241	71% 17% • 11%

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Mol	Chain	Length	Quality of chain
1	J	241	69% 17% 11%
1	M	241	68% 19% 11%
1	Q	241	71% 17% 11%
1	S	241	67% 20% 11%
1	W	241	72% 15% 11%
1	Y	241	71% 16% 11%
2	1	180	97%
2	3	180	97%
2	5	180	97%
2	7	180	97%
2	V	180	97%
2	X	180	97%
2	Z	180	97%
3	A	242	85% 6% 8%
3	C	242	80% 12% 8%
3	E	242	81% 10% 8%
3	F	242	83% 8% 8%
3	G	242	84% 7% 8%
3	I	242	81% 11% 8%
3	K	242	81% 11% 8%
3	L	242	83% 7% 8%
3	N	242	84% 12%
3	O	242	84% 8% 8%
3	P	242	90% 7%
3	R	242	82% 10% 8%

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Mol	Chain	Length	Quality of chain
3	T	242	
3	U	242	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 46557 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	2	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	4	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	6	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	8	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	B	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	D	217	Total	C	N	O	S	0	0
			1668	1044	305	316	3		
1	H	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	J	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	M	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	Q	214	Total	C	N	O	S	0	0
			1650	1033	302	312	3		
1	S	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	W	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	Y	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		

- Molecule 2 is a protein called Bacterial proteasome activator.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	5	Total	C	N	O	0	0
			39	25	6	8		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	5	Total	C	N	O	0	0
			39	25	6	8		
2	5	5	Total	C	N	O	0	0
			39	25	6	8		
2	7	5	Total	C	N	O	0	0
			39	25	6	8		
2	V	5	Total	C	N	O	0	0
			39	25	6	8		
2	X	5	Total	C	N	O	0	0
			39	25	6	8		
2	Z	5	Total	C	N	O	0	0
			39	25	6	8		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-5	MET	-	initiating methionine	UNP P9WKX3
1	-4	HIS	-	expression tag	UNP P9WKX3
1	-3	HIS	-	expression tag	UNP P9WKX3
1	-2	HIS	-	expression tag	UNP P9WKX3
1	-1	HIS	-	expression tag	UNP P9WKX3
1	0	HIS	-	expression tag	UNP P9WKX3
1	1	HIS	-	expression tag	UNP P9WKX3
3	-5	MET	-	initiating methionine	UNP P9WKX3
3	-4	HIS	-	expression tag	UNP P9WKX3
3	-3	HIS	-	expression tag	UNP P9WKX3
3	-2	HIS	-	expression tag	UNP P9WKX3
3	-1	HIS	-	expression tag	UNP P9WKX3
3	0	HIS	-	expression tag	UNP P9WKX3
3	1	HIS	-	expression tag	UNP P9WKX3
5	-5	MET	-	initiating methionine	UNP P9WKX3
5	-4	HIS	-	expression tag	UNP P9WKX3
5	-3	HIS	-	expression tag	UNP P9WKX3
5	-2	HIS	-	expression tag	UNP P9WKX3
5	-1	HIS	-	expression tag	UNP P9WKX3
5	0	HIS	-	expression tag	UNP P9WKX3
5	1	HIS	-	expression tag	UNP P9WKX3
7	-5	MET	-	initiating methionine	UNP P9WKX3
7	-4	HIS	-	expression tag	UNP P9WKX3
7	-3	HIS	-	expression tag	UNP P9WKX3
7	-2	HIS	-	expression tag	UNP P9WKX3
7	-1	HIS	-	expression tag	UNP P9WKX3
7	0	HIS	-	expression tag	UNP P9WKX3

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Chain	Residue	Modelled	Actual	Comment	Reference
7	1	HIS	-	expression tag	UNP P9WKX3
V	-5	MET	-	initiating methionine	UNP P9WKX3
V	-4	HIS	-	expression tag	UNP P9WKX3
V	-3	HIS	-	expression tag	UNP P9WKX3
V	-2	HIS	-	expression tag	UNP P9WKX3
V	-1	HIS	-	expression tag	UNP P9WKX3
V	0	HIS	-	expression tag	UNP P9WKX3
V	1	HIS	-	expression tag	UNP P9WKX3
X	-5	MET	-	initiating methionine	UNP P9WKX3
X	-4	HIS	-	expression tag	UNP P9WKX3
X	-3	HIS	-	expression tag	UNP P9WKX3
X	-2	HIS	-	expression tag	UNP P9WKX3
X	-1	HIS	-	expression tag	UNP P9WKX3
X	0	HIS	-	expression tag	UNP P9WKX3
X	1	HIS	-	expression tag	UNP P9WKX3
Z	-5	MET	-	initiating methionine	UNP P9WKX3
Z	-4	HIS	-	expression tag	UNP P9WKX3
Z	-3	HIS	-	expression tag	UNP P9WKX3
Z	-2	HIS	-	expression tag	UNP P9WKX3
Z	-1	HIS	-	expression tag	UNP P9WKX3
Z	0	HIS	-	expression tag	UNP P9WKX3
Z	1	HIS	-	expression tag	UNP P9WKX3

- Molecule 3 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	C	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	E	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	F	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	G	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	I	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	K	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	L	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	234	Total	C	N	O	S	0	0
			1715	1072	295	343	5		
3	O	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	P	234	Total	C	N	O	S	0	0
			1715	1072	295	343	5		
3	R	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	T	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		
3	U	223	Total	C	N	O	S	0	0
			1640	1028	283	324	5		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	ALA	-	expression tag	UNP P9WHT9
A	535	TRP	-	expression tag	UNP P9WHT9
A	536	SER	-	expression tag	UNP P9WHT9
A	537	HIS	-	expression tag	UNP P9WHT9
A	538	PRO	-	expression tag	UNP P9WHT9
A	539	GLN	-	expression tag	UNP P9WHT9
A	540	PHE	-	expression tag	UNP P9WHT9
A	541	GLU	-	expression tag	UNP P9WHT9
A	542	LYS	-	expression tag	UNP P9WHT9
C	301	ALA	-	expression tag	UNP P9WHT9
C	535	TRP	-	expression tag	UNP P9WHT9
C	536	SER	-	expression tag	UNP P9WHT9
C	537	HIS	-	expression tag	UNP P9WHT9
C	538	PRO	-	expression tag	UNP P9WHT9
C	539	GLN	-	expression tag	UNP P9WHT9
C	540	PHE	-	expression tag	UNP P9WHT9
C	541	GLU	-	expression tag	UNP P9WHT9
C	542	LYS	-	expression tag	UNP P9WHT9
E	301	ALA	-	expression tag	UNP P9WHT9
E	535	TRP	-	expression tag	UNP P9WHT9
E	536	SER	-	expression tag	UNP P9WHT9
E	537	HIS	-	expression tag	UNP P9WHT9
E	538	PRO	-	expression tag	UNP P9WHT9
E	539	GLN	-	expression tag	UNP P9WHT9
E	540	PHE	-	expression tag	UNP P9WHT9
E	541	GLU	-	expression tag	UNP P9WHT9
E	542	LYS	-	expression tag	UNP P9WHT9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	301	ALA	-	expression tag	UNP P9WHT9
F	535	TRP	-	expression tag	UNP P9WHT9
F	536	SER	-	expression tag	UNP P9WHT9
F	537	HIS	-	expression tag	UNP P9WHT9
F	538	PRO	-	expression tag	UNP P9WHT9
F	539	GLN	-	expression tag	UNP P9WHT9
F	540	PHE	-	expression tag	UNP P9WHT9
F	541	GLU	-	expression tag	UNP P9WHT9
F	542	LYS	-	expression tag	UNP P9WHT9
G	301	ALA	-	expression tag	UNP P9WHT9
G	535	TRP	-	expression tag	UNP P9WHT9
G	536	SER	-	expression tag	UNP P9WHT9
G	537	HIS	-	expression tag	UNP P9WHT9
G	538	PRO	-	expression tag	UNP P9WHT9
G	539	GLN	-	expression tag	UNP P9WHT9
G	540	PHE	-	expression tag	UNP P9WHT9
G	541	GLU	-	expression tag	UNP P9WHT9
G	542	LYS	-	expression tag	UNP P9WHT9
I	301	ALA	-	expression tag	UNP P9WHT9
I	535	TRP	-	expression tag	UNP P9WHT9
I	536	SER	-	expression tag	UNP P9WHT9
I	537	HIS	-	expression tag	UNP P9WHT9
I	538	PRO	-	expression tag	UNP P9WHT9
I	539	GLN	-	expression tag	UNP P9WHT9
I	540	PHE	-	expression tag	UNP P9WHT9
I	541	GLU	-	expression tag	UNP P9WHT9
I	542	LYS	-	expression tag	UNP P9WHT9
K	301	ALA	-	expression tag	UNP P9WHT9
K	535	TRP	-	expression tag	UNP P9WHT9
K	536	SER	-	expression tag	UNP P9WHT9
K	537	HIS	-	expression tag	UNP P9WHT9
K	538	PRO	-	expression tag	UNP P9WHT9
K	539	GLN	-	expression tag	UNP P9WHT9
K	540	PHE	-	expression tag	UNP P9WHT9
K	541	GLU	-	expression tag	UNP P9WHT9
K	542	LYS	-	expression tag	UNP P9WHT9
L	301	ALA	-	expression tag	UNP P9WHT9
L	535	TRP	-	expression tag	UNP P9WHT9
L	536	SER	-	expression tag	UNP P9WHT9
L	537	HIS	-	expression tag	UNP P9WHT9
L	538	PRO	-	expression tag	UNP P9WHT9
L	539	GLN	-	expression tag	UNP P9WHT9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	540	PHE	-	expression tag	UNP P9WHT9
L	541	GLU	-	expression tag	UNP P9WHT9
L	542	LYS	-	expression tag	UNP P9WHT9
N	301	ALA	-	expression tag	UNP P9WHT9
N	535	TRP	-	expression tag	UNP P9WHT9
N	536	SER	-	expression tag	UNP P9WHT9
N	537	HIS	-	expression tag	UNP P9WHT9
N	538	PRO	-	expression tag	UNP P9WHT9
N	539	GLN	-	expression tag	UNP P9WHT9
N	540	PHE	-	expression tag	UNP P9WHT9
N	541	GLU	-	expression tag	UNP P9WHT9
N	542	LYS	-	expression tag	UNP P9WHT9
O	301	ALA	-	expression tag	UNP P9WHT9
O	535	TRP	-	expression tag	UNP P9WHT9
O	536	SER	-	expression tag	UNP P9WHT9
O	537	HIS	-	expression tag	UNP P9WHT9
O	538	PRO	-	expression tag	UNP P9WHT9
O	539	GLN	-	expression tag	UNP P9WHT9
O	540	PHE	-	expression tag	UNP P9WHT9
O	541	GLU	-	expression tag	UNP P9WHT9
O	542	LYS	-	expression tag	UNP P9WHT9
P	301	ALA	-	expression tag	UNP P9WHT9
P	535	TRP	-	expression tag	UNP P9WHT9
P	536	SER	-	expression tag	UNP P9WHT9
P	537	HIS	-	expression tag	UNP P9WHT9
P	538	PRO	-	expression tag	UNP P9WHT9
P	539	GLN	-	expression tag	UNP P9WHT9
P	540	PHE	-	expression tag	UNP P9WHT9
P	541	GLU	-	expression tag	UNP P9WHT9
P	542	LYS	-	expression tag	UNP P9WHT9
R	301	ALA	-	expression tag	UNP P9WHT9
R	535	TRP	-	expression tag	UNP P9WHT9
R	536	SER	-	expression tag	UNP P9WHT9
R	537	HIS	-	expression tag	UNP P9WHT9
R	538	PRO	-	expression tag	UNP P9WHT9
R	539	GLN	-	expression tag	UNP P9WHT9
R	540	PHE	-	expression tag	UNP P9WHT9
R	541	GLU	-	expression tag	UNP P9WHT9
R	542	LYS	-	expression tag	UNP P9WHT9
T	301	ALA	-	expression tag	UNP P9WHT9
T	535	TRP	-	expression tag	UNP P9WHT9
T	536	SER	-	expression tag	UNP P9WHT9

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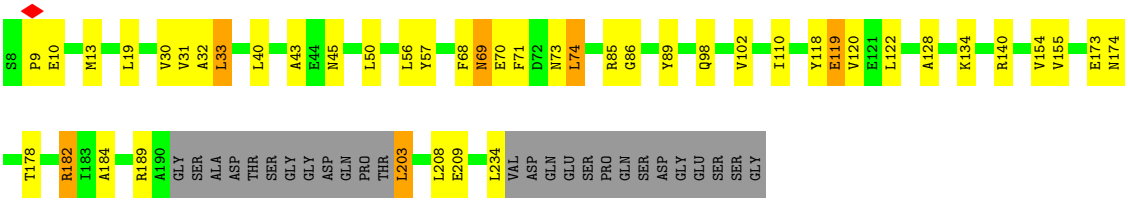
Chain	Residue	Modelled	Actual	Comment	Reference
T	537	HIS	-	expression tag	UNP P9WHT9
T	538	PRO	-	expression tag	UNP P9WHT9
T	539	GLN	-	expression tag	UNP P9WHT9
T	540	PHE	-	expression tag	UNP P9WHT9
T	541	GLU	-	expression tag	UNP P9WHT9
T	542	LYS	-	expression tag	UNP P9WHT9
U	301	ALA	-	expression tag	UNP P9WHT9
U	535	TRP	-	expression tag	UNP P9WHT9
U	536	SER	-	expression tag	UNP P9WHT9
U	537	HIS	-	expression tag	UNP P9WHT9
U	538	PRO	-	expression tag	UNP P9WHT9
U	539	GLN	-	expression tag	UNP P9WHT9
U	540	PHE	-	expression tag	UNP P9WHT9
U	541	GLU	-	expression tag	UNP P9WHT9
U	542	LYS	-	expression tag	UNP P9WHT9

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.

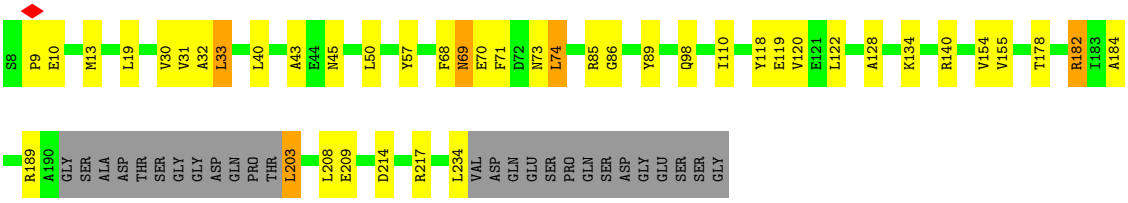
• Molecule 1: Proteasome subunit alpha

Chain 0:



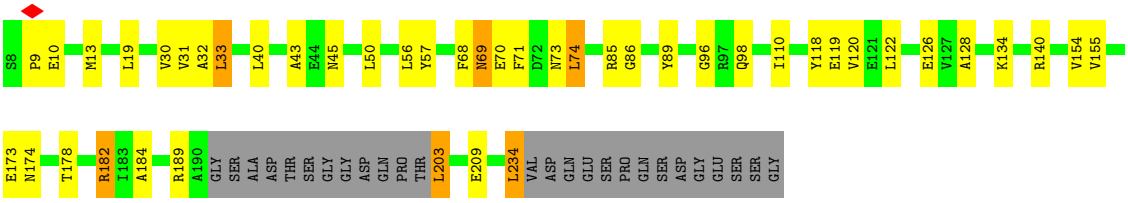
• Molecule 1: Proteasome subunit alpha

Chain 2:



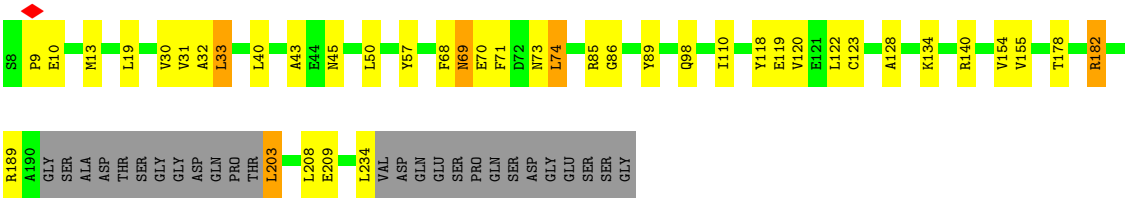
• Molecule 1: Proteasome subunit alpha

Chain 4:



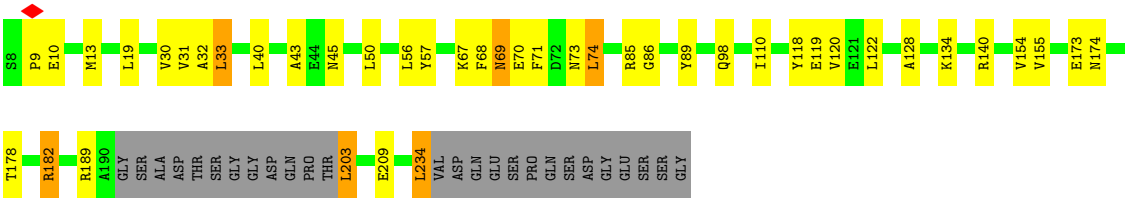
• Molecule 1: Proteasome subunit alpha

Chain 6:



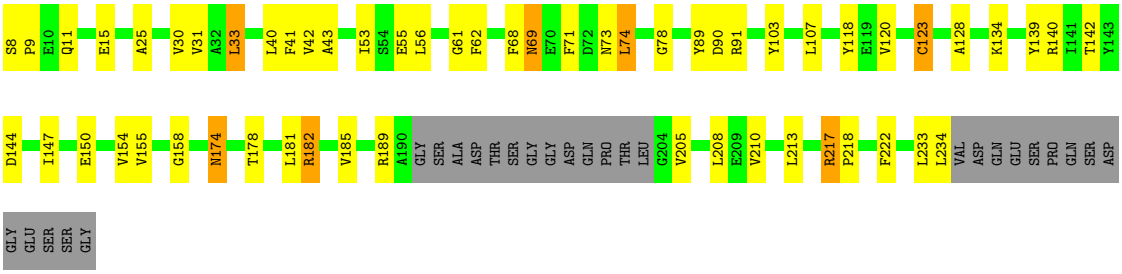
• Molecule 1: Proteasome subunit alpha

Chain 8:



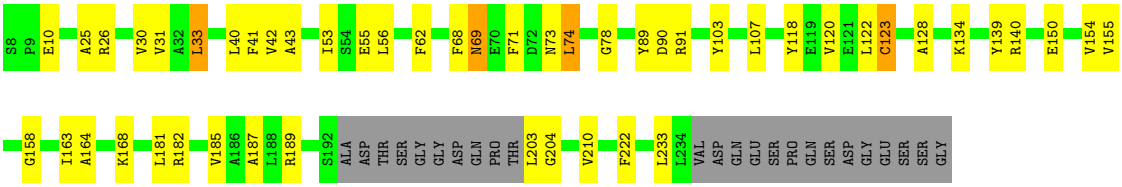
• Molecule 1: Proteasome subunit alpha

Chain B:



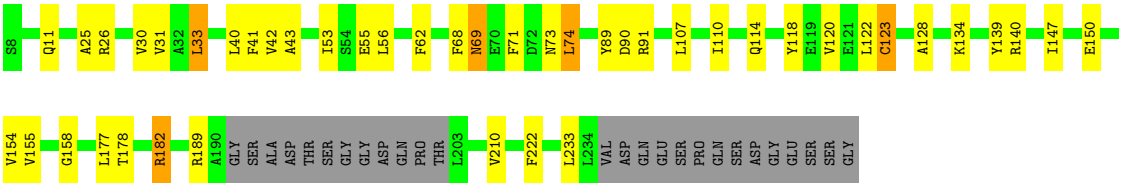
• Molecule 1: Proteasome subunit alpha

Chain D:



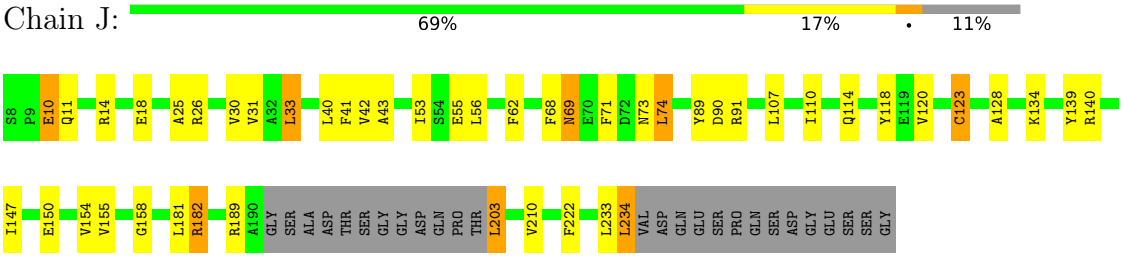
• Molecule 1: Proteasome subunit alpha

Chain H:



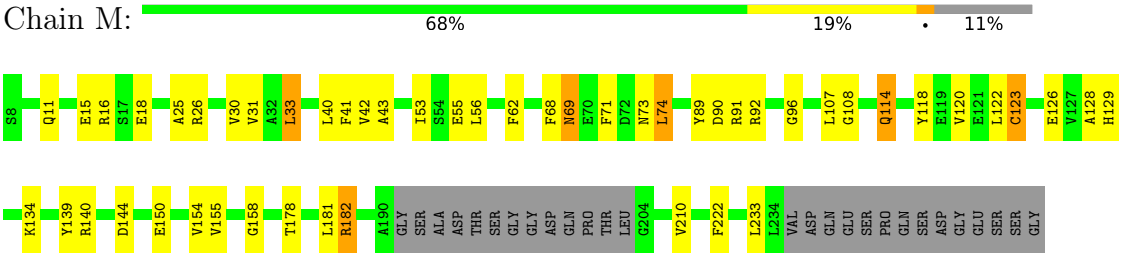
• Molecule 1: Proteasome subunit alpha

Chain J:



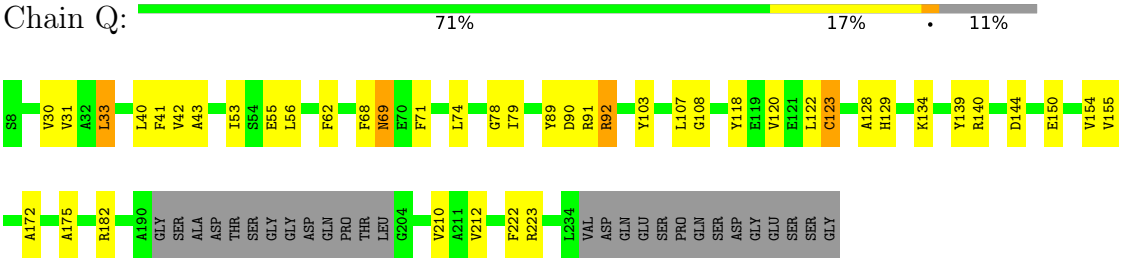
• Molecule 1: Proteasome subunit alpha

Chain M:



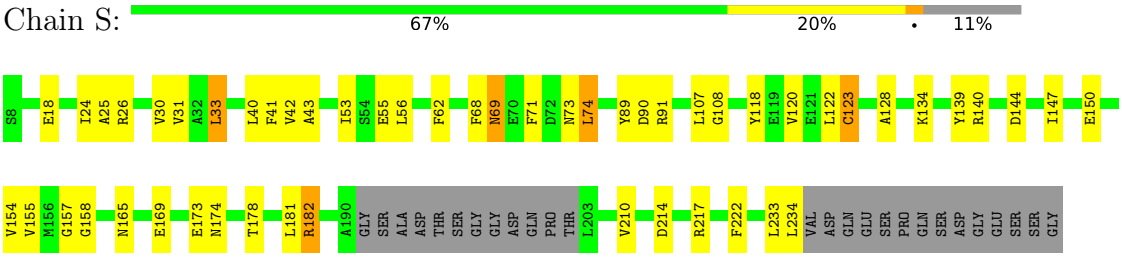
• Molecule 1: Proteasome subunit alpha

Chain Q:



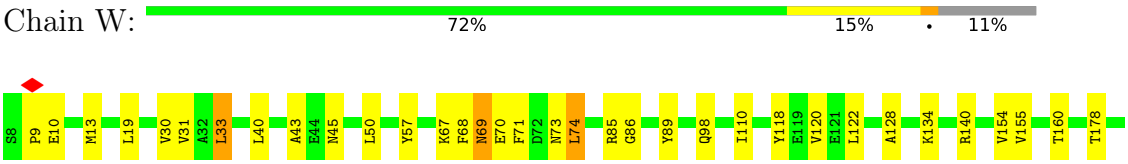
• Molecule 1: Proteasome subunit alpha

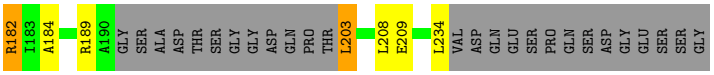
Chain S:



• Molecule 1: Proteasome subunit alpha

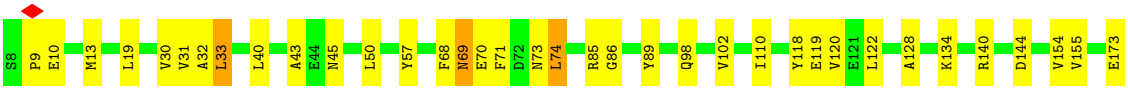
Chain W:





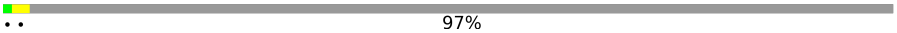
• Molecule 1: Proteasome subunit alpha

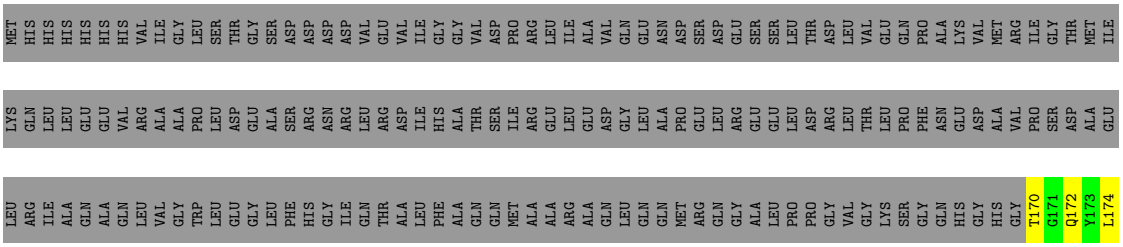
Chain Y:



• Molecule 2: Bacterial proteasome activator

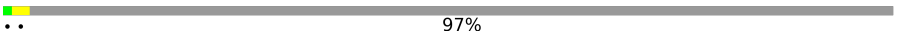
Chain 1:

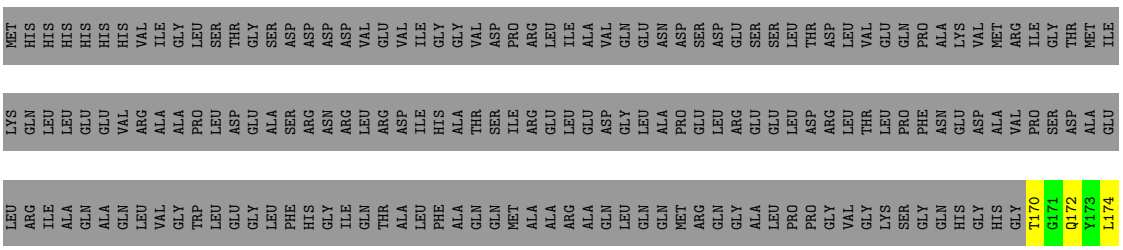




• Molecule 2: Bacterial proteasome activator

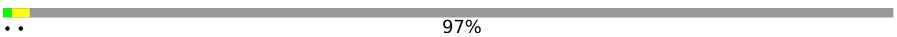
Chain 3:

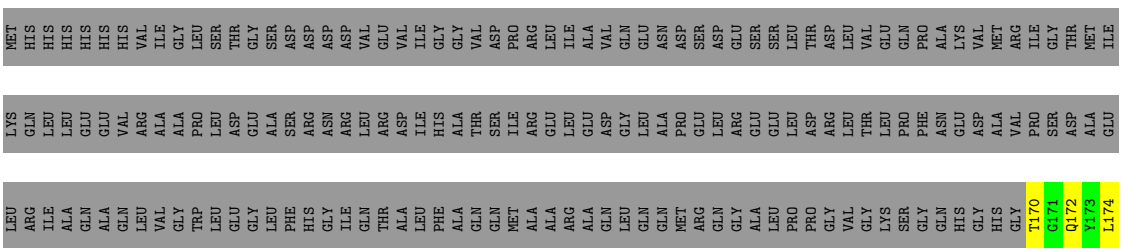




• Molecule 2: Bacterial proteasome activator

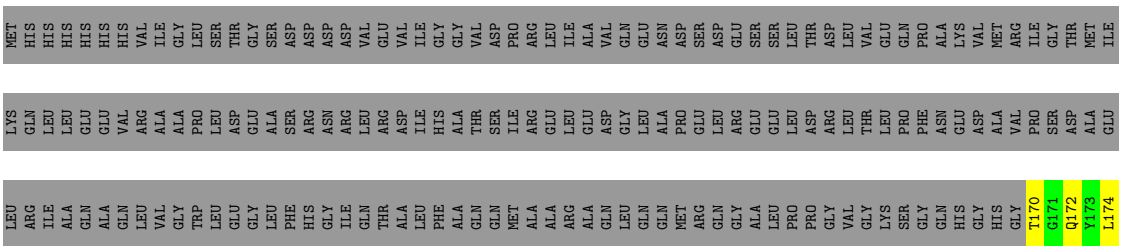
Chain 5:





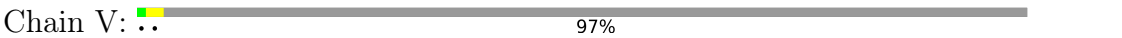
• Molecule 2: Bacterial proteasome activator

Chain 7:



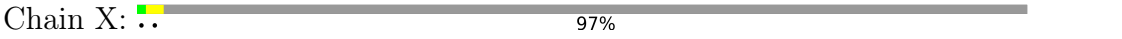
• Molecule 2: Bacterial proteasome activator

Chain V:



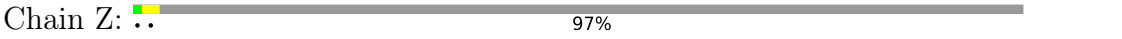
• Molecule 2: Bacterial proteasome activator

Chain X:



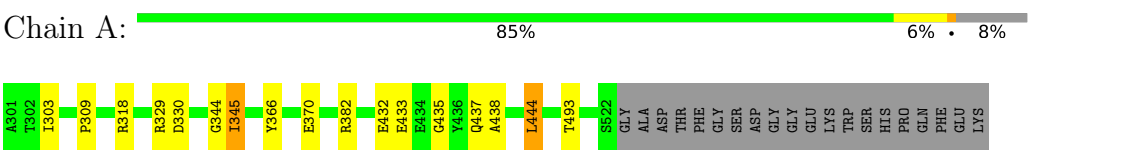
• Molecule 2: Bacterial proteasome activator

Chain Z:



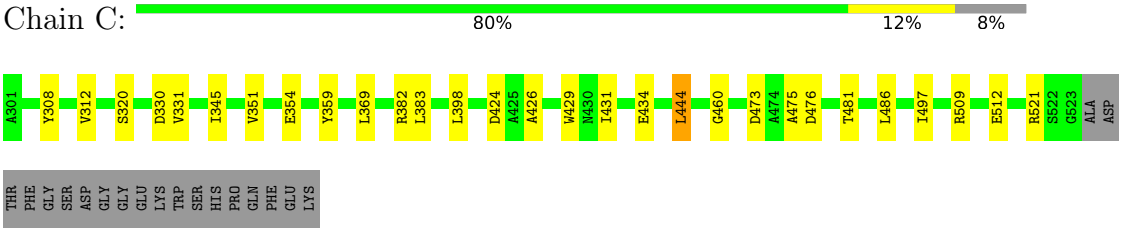
• Molecule 3: Proteasome subunit beta

Chain A:



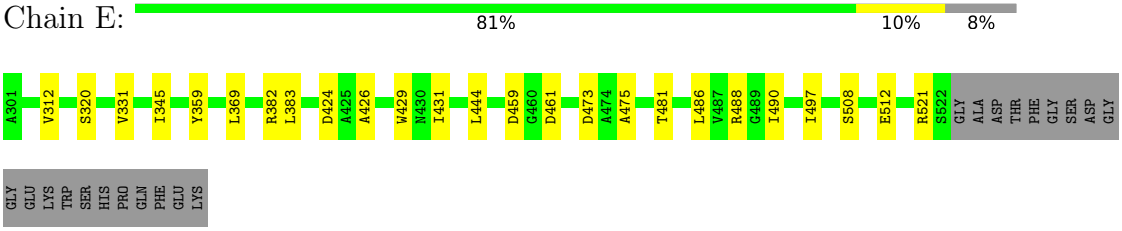
• Molecule 3: Proteasome subunit beta

Chain C:



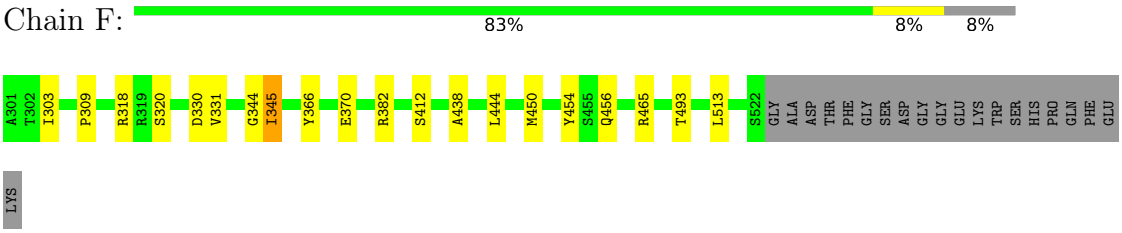
• Molecule 3: Proteasome subunit beta

Chain E:



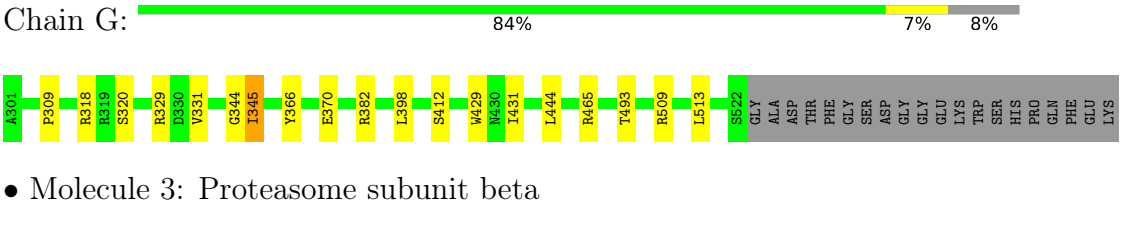
• Molecule 3: Proteasome subunit beta

Chain F:



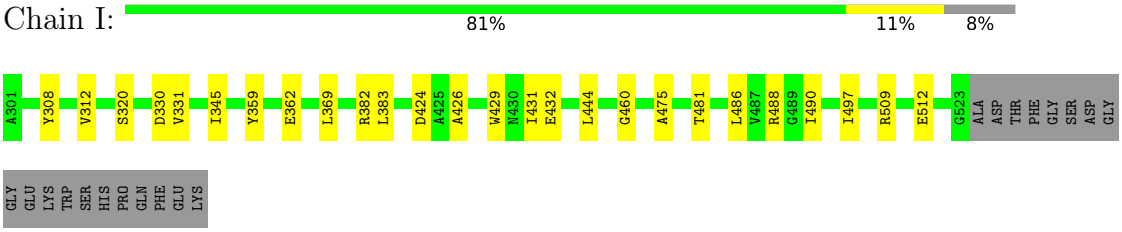
• Molecule 3: Proteasome subunit beta

Chain G:



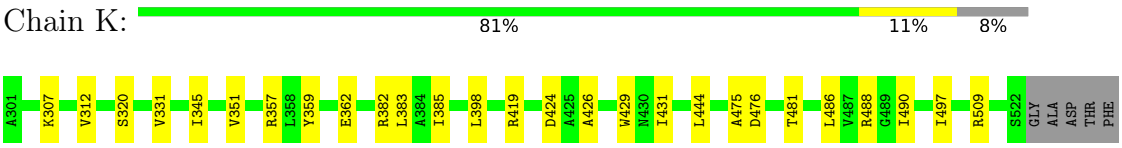
• Molecule 3: Proteasome subunit beta

Chain I:



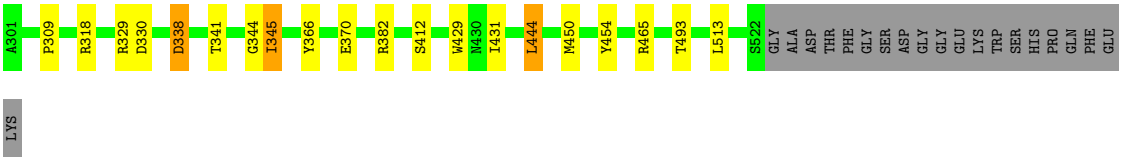
• Molecule 3: Proteasome subunit beta

Chain K:



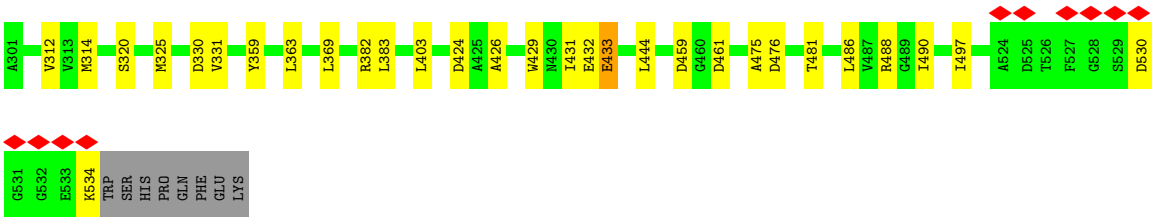
• Molecule 3: Proteasome subunit beta

Chain L:



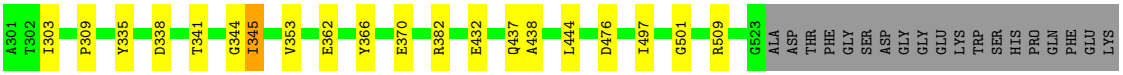
• Molecule 3: Proteasome subunit beta

Chain N:



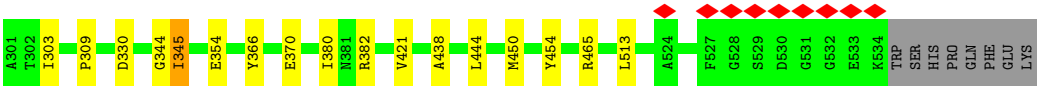
• Molecule 3: Proteasome subunit beta

Chain O:



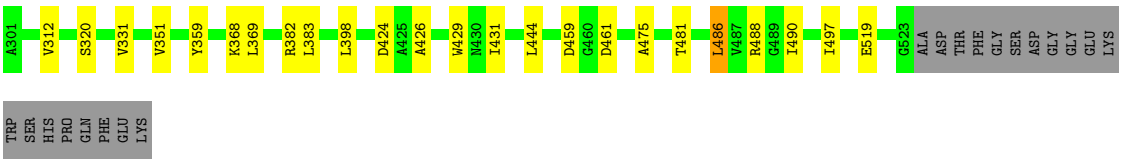
• Molecule 3: Proteasome subunit beta

Chain P:



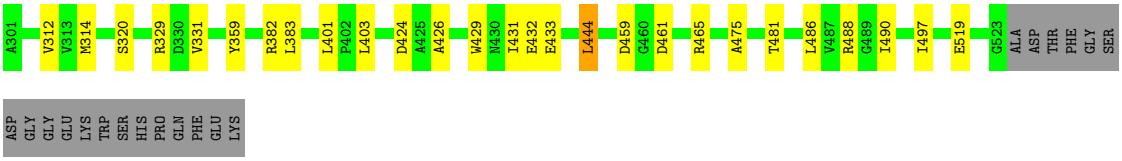
• Molecule 3: Proteasome subunit beta

Chain R:

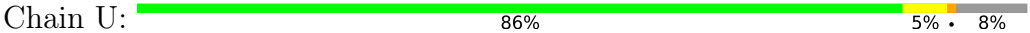


• Molecule 3: Proteasome subunit beta

Chain T:



• Molecule 3: Proteasome subunit beta



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	48799	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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.395	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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	0	0.39	0/1683	0.57	0/2274
1	2	0.39	0/1683	0.57	0/2274
1	4	0.39	0/1683	0.57	0/2274
1	6	0.39	0/1683	0.56	0/2274
1	8	0.39	0/1683	0.57	0/2274
1	B	0.36	0/1675	0.53	0/2263
1	D	0.35	0/1693	0.51	0/2287
1	H	0.35	0/1683	0.53	0/2274
1	J	0.37	0/1683	0.53	0/2274
1	M	0.36	0/1675	0.52	0/2263
1	Q	0.35	0/1675	0.52	0/2263
1	S	0.38	0/1683	0.54	0/2274
1	W	0.39	0/1683	0.57	0/2274
1	Y	0.41	0/1683	0.57	0/2274
2	1	0.78	0/39	1.18	0/50
2	3	0.74	0/39	1.07	0/50
2	5	0.62	0/39	0.99	0/50
2	7	0.65	0/39	1.00	0/50
2	V	0.68	0/39	1.14	0/50
2	X	0.70	0/39	1.13	0/50
2	Z	0.77	0/39	1.17	0/50
3	A	0.38	0/1660	0.58	0/2251
3	C	0.39	0/1664	0.58	0/2256
3	E	0.40	0/1660	0.58	0/2251
3	F	0.38	0/1660	0.57	0/2251
3	G	0.39	0/1660	0.58	0/2251
3	I	0.39	0/1664	0.59	0/2256
3	K	0.39	0/1660	0.58	0/2251
3	L	0.38	0/1660	0.58	0/2251
3	N	0.40	0/1740	0.58	0/2357
3	O	0.39	0/1664	0.58	0/2256
3	P	0.38	0/1740	0.56	0/2357
3	R	0.39	0/1664	0.60	0/2256
3	T	0.40	0/1664	0.59	0/2256

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	U	0.38	0/1664	0.57	0/2256
All	All	0.39	0/47245	0.57	0/63922

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1658	0	1659	33	0
1	2	1658	0	1659	31	0
1	4	1658	0	1659	33	0
1	6	1658	0	1659	28	0
1	8	1658	0	1659	33	0
1	B	1650	0	1648	35	0
1	D	1668	0	1667	27	0
1	H	1658	0	1659	24	0
1	J	1658	0	1659	27	0
1	M	1650	0	1648	31	0
1	Q	1650	0	1648	26	0
1	S	1658	0	1659	30	0
1	W	1658	0	1659	33	0
1	Y	1658	0	1659	34	0
2	1	39	0	32	5	0
2	3	39	0	32	5	0
2	5	39	0	32	5	0
2	7	39	0	32	5	0
2	V	39	0	32	7	0
2	X	39	0	32	5	0
2	Z	39	0	32	5	0
3	A	1636	0	1628	10	0
3	C	1640	0	1631	16	0
3	E	1636	0	1628	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1636	0	1628	11	0
3	G	1636	0	1628	9	0
3	I	1640	0	1631	13	0
3	K	1636	0	1628	15	0
3	L	1636	0	1628	11	0
3	N	1715	0	1693	18	0
3	O	1640	0	1631	12	0
3	P	1715	0	1693	7	0
3	R	1640	0	1631	13	0
3	T	1640	0	1631	17	0
3	U	1640	0	1631	6	0
All	All	46557	0	46365	565	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 6.

All (565) 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)
2:5:170:THR:N	1:8:13:MET:SD	2.46	0.89
2:3:170:THR:N	1:6:13:MET:SD	2.47	0.87
2:V:170:THR:N	1:Y:13:MET:SD	2.48	0.86
2:1:170:THR:N	1:4:13:MET:SD	2.48	0.86
2:7:170:THR:N	1:W:13:MET:SD	2.51	0.84
1:Q:42:VAL:HG22	1:Q:210:VAL:HG22	1.62	0.82
1:B:185:VAL:HG21	1:B:234:LEU:HD11	1.59	0.81
1:0:13:MET:SD	2:X:170:THR:N	2.53	0.81
3:C:509:ARG:NH1	3:C:512:GLU:OE1	2.14	0.80
1:2:13:MET:SD	2:Z:170:THR:N	2.54	0.80
1:J:42:VAL:HG22	1:J:210:VAL:HG22	1.64	0.79
1:D:140:ARG:NH1	1:D:154:VAL:HG13	1.99	0.78
1:J:31:VAL:HG12	1:J:155:VAL:HG22	1.66	0.77
1:S:31:VAL:HG12	1:S:155:VAL:HG22	1.66	0.77
1:B:31:VAL:HG12	1:B:155:VAL:HG22	1.67	0.76
1:B:140:ARG:NH1	1:B:154:VAL:HG13	2.00	0.76
1:M:140:ARG:NH1	1:M:154:VAL:HG13	2.00	0.76
1:S:140:ARG:NH1	1:S:154:VAL:HG13	2.00	0.76
1:H:140:ARG:NH1	1:H:154:VAL:HG13	2.00	0.76
1:B:42:VAL:HG22	1:B:210:VAL:HG22	1.66	0.76
1:Q:140:ARG:NH1	1:Q:154:VAL:HG13	2.01	0.75
1:Q:31:VAL:HG12	1:Q:155:VAL:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:VAL:HG12	1:H:155:VAL:HG22	1.69	0.75
1:J:140:ARG:NH1	1:J:154:VAL:HG13	2.02	0.75
1:M:31:VAL:HG12	1:M:155:VAL:HG22	1.69	0.75
1:D:42:VAL:HG22	1:D:210:VAL:HG22	1.69	0.74
1:D:31:VAL:HG12	1:D:155:VAL:HG22	1.67	0.74
1:H:42:VAL:HG22	1:H:210:VAL:HG22	1.68	0.74
1:M:42:VAL:HG22	1:M:210:VAL:HG22	1.67	0.74
3:O:362:GLU:OE2	3:O:382:ARG:HD3	1.89	0.72
1:S:42:VAL:HG22	1:S:210:VAL:HG22	1.71	0.70
2:3:172:GLN:HG3	1:4:68:PHE:HB3	1.73	0.69
1:Q:74:LEU:HD23	1:Q:122:LEU:HD11	1.75	0.69
2:1:172:GLN:HG3	1:2:68:PHE:HB3	1.75	0.67
2:5:172:GLN:HG3	1:6:68:PHE:HB3	1.76	0.67
2:7:172:GLN:HG3	1:8:68:PHE:HB3	1.78	0.65
2:X:172:GLN:HG3	1:Y:68:PHE:HB3	1.78	0.65
1:0:68:PHE:HB3	2:Z:172:GLN:HG3	1.79	0.65
1:B:8:SER:HB3	1:B:9:PRO:HD3	1.79	0.65
1:S:181:LEU:HD22	1:S:233:LEU:HD23	1.79	0.65
3:K:362:GLU:OE2	3:K:382:ARG:HD3	1.98	0.64
1:2:74:LEU:HD23	1:2:122:LEU:HD11	1.79	0.64
2:V:172:GLN:HG3	1:W:68:PHE:HB3	1.78	0.64
1:0:85:ARG:HH12	1:0:98:GLN:NE2	1.96	0.63
1:6:74:LEU:HD23	1:6:122:LEU:HD11	1.79	0.63
1:B:217:ARG:HG3	1:B:218:PRO:HD2	1.81	0.63
1:0:74:LEU:HD23	1:0:122:LEU:HD11	1.80	0.63
1:8:140:ARG:NH1	1:8:154:VAL:HG13	2.13	0.62
1:W:140:ARG:NH1	1:W:154:VAL:HG13	2.14	0.62
1:4:140:ARG:NH1	1:4:154:VAL:HG13	2.14	0.62
1:6:140:ARG:NH1	1:6:154:VAL:HG13	2.15	0.62
1:Y:140:ARG:NH1	1:Y:154:VAL:HG13	2.15	0.62
3:N:429:TRP:HZ3	3:N:431:ILE:HG13	1.65	0.62
3:K:382:ARG:HH21	3:K:385:ILE:HD13	1.64	0.62
3:O:382:ARG:HD2	1:W:89:TYR:CE1	2.36	0.61
1:M:92:ARG:HH12	1:M:129:HIS:CG	2.18	0.61
1:S:182:ARG:NH1	1:S:234:LEU:O	2.34	0.61
1:0:68:PHE:HD2	2:Z:172:GLN:HE21	1.49	0.61
3:I:362:GLU:OE2	3:I:382:ARG:HD3	1.99	0.61
1:B:74:LEU:HD21	1:B:107:LEU:HD21	1.82	0.60
1:4:45:ASN:ND2	1:4:209:GLU:OE1	2.35	0.60
2:V:172:GLN:HE21	1:W:68:PHE:HD2	1.50	0.60
1:4:74:LEU:HD23	1:4:122:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:74:LEU:HD23	1:W:122:LEU:HD11	1.83	0.60
1:0:140:ARG:NH1	1:0:154:VAL:HG13	2.17	0.60
3:T:429:TRP:HZ3	3:T:431:ILE:HG13	1.67	0.60
1:Y:74:LEU:HD23	1:Y:122:LEU:HD11	1.83	0.60
1:Q:128:ALA:HB2	1:Q:134:LYS:HB3	1.83	0.60
1:8:74:LEU:HD23	1:8:122:LEU:HD11	1.83	0.60
2:X:172:GLN:HE21	1:Y:68:PHE:HD2	1.49	0.59
1:2:85:ARG:HH12	1:2:98:GLN:NE2	1.99	0.59
1:2:140:ARG:NH1	1:2:154:VAL:HG13	2.17	0.59
1:M:74:LEU:HD21	1:M:107:LEU:HD21	1.85	0.59
1:B:128:ALA:HB2	1:B:134:LYS:HB3	1.84	0.59
3:T:320:SER:HB3	3:T:331:VAL:HG21	1.85	0.59
1:W:31:VAL:HG12	1:W:155:VAL:HG22	1.85	0.59
3:K:382:ARG:NH2	3:K:385:ILE:HD13	2.18	0.59
1:S:128:ALA:HB2	1:S:134:LYS:HB3	1.84	0.58
1:4:189:ARG:NH1	1:4:203:LEU:N	2.52	0.58
1:2:31:VAL:HG12	1:2:155:VAL:HG22	1.84	0.58
1:J:128:ALA:HB2	1:J:134:LYS:HB3	1.85	0.58
1:Y:189:ARG:NH1	1:Y:203:LEU:N	2.52	0.58
1:8:85:ARG:HH12	1:8:98:GLN:NE2	2.01	0.58
1:Q:30:VAL:HG13	1:Q:43:ALA:HB2	1.84	0.58
1:H:128:ALA:HB2	1:H:134:LYS:HB3	1.85	0.58
1:W:189:ARG:NH1	1:W:203:LEU:N	2.52	0.58
2:1:172:GLN:HE21	1:2:68:PHE:HD2	1.50	0.58
1:0:189:ARG:NH1	1:0:203:LEU:N	2.52	0.58
1:6:45:ASN:ND2	1:6:209:GLU:OE1	2.37	0.58
1:4:31:VAL:HG12	1:4:155:VAL:HG22	1.85	0.57
1:2:45:ASN:ND2	1:2:209:GLU:OE1	2.36	0.57
1:6:31:VAL:HG12	1:6:155:VAL:HG22	1.85	0.57
1:6:189:ARG:NH1	1:6:203:LEU:N	2.52	0.57
1:6:128:ALA:HB2	1:6:134:LYS:HB3	1.86	0.57
3:E:429:TRP:HZ3	3:E:431:ILE:HG13	1.70	0.57
3:N:424:ASP:OD1	3:N:426:ALA:N	2.35	0.57
1:S:30:VAL:HG13	1:S:43:ALA:HB2	1.86	0.57
1:8:31:VAL:HG12	1:8:155:VAL:HG22	1.87	0.57
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.85	0.57
1:2:189:ARG:NH1	1:2:203:LEU:N	2.53	0.57
1:M:128:ALA:HB2	1:M:134:LYS:HB3	1.86	0.57
1:Y:85:ARG:HH12	1:Y:98:GLN:NE2	2.02	0.57
1:H:74:LEU:HD21	1:H:107:LEU:HD21	1.86	0.57
1:J:74:LEU:HD21	1:J:107:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:74:LEU:HD21	1:S:107:LEU:HD21	1.87	0.56
3:C:429:TRP:HZ3	3:C:431:ILE:HG13	1.70	0.56
3:R:320:SER:HB3	3:R:331:VAL:HG21	1.88	0.56
1:8:189:ARG:NH1	1:8:203:LEU:N	2.53	0.56
3:N:320:SER:HB3	3:N:331:VAL:HG21	1.88	0.56
1:Q:74:LEU:HD21	1:Q:107:LEU:HD21	1.88	0.56
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.87	0.56
1:D:140:ARG:HH11	1:D:154:VAL:HG13	1.69	0.56
3:R:424:ASP:OD1	3:R:426:ALA:N	2.37	0.56
1:Y:31:VAL:HG12	1:Y:155:VAL:HG22	1.88	0.56
1:D:74:LEU:HD21	1:D:107:LEU:HD21	1.88	0.56
3:C:320:SER:HB3	3:C:331:VAL:HG21	1.87	0.56
1:W:85:ARG:HH12	1:W:98:GLN:NE2	2.03	0.55
1:0:31:VAL:HG12	1:0:155:VAL:HG22	1.88	0.55
2:5:172:GLN:HE21	1:6:68:PHE:HD2	1.53	0.55
1:8:128:ALA:HB2	1:8:134:LYS:HB3	1.87	0.55
3:L:465:ARG:HG3	3:L:513:LEU:HD22	1.87	0.55
1:4:85:ARG:HH12	1:4:98:GLN:NE2	2.05	0.55
1:4:128:ALA:HB2	1:4:134:LYS:HB3	1.89	0.55
3:E:320:SER:HB3	3:E:331:VAL:HG21	1.88	0.55
1:J:189:ARG:NH1	1:J:203:LEU:N	2.54	0.55
3:N:432:GLU:OE2	3:N:433:GLU:N	2.39	0.55
1:Y:128:ALA:HB2	1:Y:134:LYS:HB3	1.88	0.55
1:H:68:PHE:HA	1:H:71:PHE:CE2	2.42	0.55
1:W:128:ALA:HB2	1:W:134:LYS:HB3	1.88	0.55
3:R:429:TRP:HZ3	3:R:431:ILE:HG13	1.72	0.55
1:0:45:ASN:ND2	1:0:209:GLU:OE1	2.40	0.55
1:B:174:ASN:N	1:B:174:ASN:HD22	2.05	0.54
1:M:140:ARG:HH11	1:M:154:VAL:HG13	1.73	0.54
1:S:140:ARG:HH11	1:S:154:VAL:HG13	1.70	0.54
1:2:128:ALA:HB2	1:2:134:LYS:HB3	1.89	0.54
1:H:150:GLU:HG3	1:H:154:VAL:HG22	1.90	0.54
1:M:16:ARG:NH2	1:M:114:GLN:O	2.27	0.54
2:7:172:GLN:HE21	1:8:68:PHE:HD2	1.54	0.54
1:J:30:VAL:HG13	1:J:43:ALA:HB2	1.89	0.54
1:0:128:ALA:HB2	1:0:134:LYS:HB3	1.88	0.54
1:8:45:ASN:ND2	1:8:209:GLU:OE1	2.41	0.54
3:I:320:SER:HB3	3:I:331:VAL:HG21	1.89	0.54
1:M:68:PHE:HA	1:M:71:PHE:CE2	2.43	0.54
1:M:181:LEU:HD23	1:M:233:LEU:HB3	1.89	0.54
1:H:177:LEU:HG	1:H:233:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:424:ASP:OD1	3:C:426:ALA:N	2.41	0.53
3:T:424:ASP:OD1	3:T:426:ALA:N	2.41	0.53
1:D:89:TYR:CE1	3:K:382:ARG:HD2	2.43	0.53
1:M:92:ARG:NH1	1:M:129:HIS:CG	2.77	0.53
1:H:30:VAL:HG13	1:H:43:ALA:HB2	1.89	0.53
1:J:68:PHE:HA	1:J:71:PHE:CE2	2.44	0.53
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.89	0.53
1:8:89:TYR:CD1	3:G:382:ARG:HD3	2.44	0.53
1:B:140:ARG:HH11	1:B:154:VAL:HG13	1.71	0.53
1:H:110:ILE:HA	1:H:114:GLN:HG3	1.91	0.53
2:3:172:GLN:HE21	1:4:68:PHE:HD2	1.54	0.53
1:H:69:ASN:H	1:H:69:ASN:HD22	1.56	0.53
1:B:68:PHE:HA	1:B:71:PHE:CE2	2.44	0.52
3:E:424:ASP:OD1	3:E:426:ALA:N	2.41	0.52
1:B:178:THR:HG22	1:B:182:ARG:HE	1.74	0.52
3:O:382:ARG:HD2	1:W:89:TYR:HE1	1.73	0.52
1:8:70:GLU:HB3	1:8:118:TYR:CD2	2.45	0.52
1:B:30:VAL:HG13	1:B:43:ALA:HB2	1.90	0.52
1:B:8:SER:CB	1:B:9:PRO:HD3	2.39	0.52
1:D:150:GLU:HG3	1:D:154:VAL:HG22	1.92	0.52
1:6:68:PHE:HA	1:6:71:PHE:CE2	2.44	0.52
1:8:68:PHE:HA	1:8:71:PHE:CE2	2.44	0.52
1:B:182:ARG:HH11	1:B:234:LEU:HD23	1.75	0.52
1:M:11:GLN:O	1:M:15:GLU:HG2	2.10	0.52
1:J:18:GLU:OE2	1:J:18:GLU:HA	2.10	0.52
1:S:150:GLU:HG3	1:S:154:VAL:HG22	1.92	0.52
1:Y:45:ASN:ND2	1:Y:209:GLU:OE1	2.43	0.52
1:W:45:ASN:ND2	1:W:209:GLU:OE1	2.44	0.51
1:J:150:GLU:HG3	1:J:154:VAL:HG22	1.92	0.51
1:B:150:GLU:HG3	1:B:154:VAL:HG22	1.93	0.51
3:K:359:TYR:CE1	3:K:383:LEU:HB2	2.45	0.51
1:S:165:ASN:O	1:S:169:GLU:HG2	2.09	0.51
1:6:70:GLU:HB3	1:6:118:TYR:CD2	2.46	0.51
1:B:123:CYS:HA	1:B:139:TYR:O	2.11	0.51
2:3:174:LEU:HD11	1:4:50:LEU:HB3	1.93	0.51
1:S:68:PHE:HA	1:S:71:PHE:CE2	2.46	0.51
1:S:90:ASP:OD2	1:S:91:ARG:N	2.44	0.51
1:4:68:PHE:HA	1:4:71:PHE:CE2	2.45	0.51
1:B:181:LEU:HD23	1:B:233:LEU:HB3	1.92	0.51
1:D:69:ASN:H	1:D:69:ASN:HD22	1.57	0.51
1:D:90:ASP:OD2	1:D:91:ARG:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:CYS:HA	1:J:139:TYR:O	2.11	0.51
1:W:70:GLU:HB3	1:W:118:TYR:CD2	2.46	0.51
1:6:85:ARG:HH12	1:6:98:GLN:NE2	2.08	0.51
1:B:11:GLN:O	1:B:15:GLU:HB2	2.11	0.51
3:K:320:SER:HB3	3:K:331:VAL:HG21	1.92	0.51
1:0:68:PHE:HA	1:0:71:PHE:CE2	2.46	0.50
1:B:69:ASN:HD22	1:B:69:ASN:H	1.58	0.50
3:I:429:TRP:HZ3	3:I:431:ILE:HG13	1.77	0.50
1:2:68:PHE:HA	1:2:71:PHE:CE2	2.45	0.50
3:G:329:ARG:NH2	3:N:476:ASP:O	2.45	0.50
1:S:118:TYR:HB3	1:S:120:VAL:HG22	1.93	0.50
3:T:432:GLU:OE2	3:T:433:GLU:N	2.37	0.50
1:2:19:LEU:HD12	1:4:9:PRO:HG2	1.94	0.50
1:M:150:GLU:HG3	1:M:154:VAL:HG22	1.93	0.50
1:Y:70:GLU:HB3	1:Y:118:TYR:CD2	2.46	0.50
3:I:312:VAL:HG12	3:I:497:ILE:HB	1.92	0.50
3:T:459:ASP:OD1	3:T:461:ASP:N	2.45	0.50
1:Y:68:PHE:HA	1:Y:71:PHE:CE2	2.46	0.50
1:J:69:ASN:HD22	1:J:69:ASN:H	1.59	0.50
1:S:25:ALA:O	1:S:158:GLY:HA2	2.11	0.50
1:W:68:PHE:HA	1:W:71:PHE:CE2	2.46	0.50
1:W:110:ILE:HG21	1:W:118:TYR:CD1	2.47	0.50
1:Q:41:PHE:HB3	1:Q:53:ILE:HD13	1.94	0.50
1:6:89:TYR:CD1	3:A:382:ARG:HD3	2.47	0.49
1:8:69:ASN:HD22	1:8:69:ASN:H	1.59	0.49
1:8:110:ILE:HG21	1:8:118:TYR:CD1	2.47	0.49
1:B:55:GLU:HB2	1:B:222:PHE:CG	2.47	0.49
1:Q:92:ARG:NH1	1:Q:129:HIS:CD2	2.80	0.49
1:S:178:THR:HG22	1:S:182:ARG:HE	1.77	0.49
3:U:382:ARG:HD3	1:Y:89:TYR:CD1	2.47	0.49
1:H:123:CYS:HA	1:H:139:TYR:O	2.13	0.49
3:K:424:ASP:OD1	3:K:426:ALA:N	2.45	0.49
2:1:174:LEU:HD11	1:2:50:LEU:HB3	1.94	0.49
1:2:89:TYR:CD1	3:L:382:ARG:HD3	2.47	0.49
2:5:174:LEU:HD11	1:6:50:LEU:HB3	1.93	0.49
1:B:142:THR:OG1	1:B:144:ASP:OD2	2.29	0.49
3:C:312:VAL:HG12	3:C:497:ILE:HB	1.94	0.49
1:0:89:TYR:CD1	3:P:382:ARG:HD3	2.47	0.49
1:4:89:TYR:CD1	3:F:382:ARG:HD3	2.46	0.49
1:Q:68:PHE:HA	1:Q:71:PHE:CE2	2.48	0.49
1:W:118:TYR:HB3	1:W:120:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:70:GLU:HB3	1:4:118:TYR:CD2	2.48	0.49
1:M:18:GLU:OE2	1:M:18:GLU:HA	2.12	0.49
1:M:69:ASN:H	1:M:69:ASN:HD22	1.59	0.49
3:N:459:ASP:OD1	3:N:461:ASP:N	2.44	0.49
2:V:174:LEU:HD12	1:W:68:PHE:CD1	2.48	0.49
1:D:68:PHE:HA	1:D:71:PHE:CE2	2.47	0.49
2:1:174:LEU:HD12	1:2:68:PHE:CD1	2.48	0.49
1:2:33:LEU:HD12	1:2:40:LEU:HB3	1.94	0.49
3:E:459:ASP:OD1	3:E:461:ASP:N	2.44	0.49
1:6:110:ILE:HG21	1:6:118:TYR:CD1	2.47	0.49
1:D:41:PHE:HB3	1:D:53:ILE:HD13	1.95	0.49
1:M:178:THR:HG22	1:M:182:ARG:HE	1.76	0.49
1:Y:69:ASN:HD22	1:Y:69:ASN:H	1.60	0.49
1:4:33:LEU:HD12	1:4:40:LEU:HB3	1.94	0.49
3:F:465:ARG:HG3	3:F:513:LEU:HD22	1.94	0.49
1:M:55:GLU:HB2	1:M:222:PHE:CG	2.48	0.49
1:Y:110:ILE:HG21	1:Y:118:TYR:CD1	2.48	0.49
3:T:429:TRP:CZ3	3:T:431:ILE:HG13	2.48	0.48
3:E:382:ARG:HD3	1:Q:89:TYR:CD1	2.48	0.48
3:P:465:ARG:HG3	3:P:513:LEU:HD22	1.95	0.48
3:I:359:TYR:CE1	3:I:383:LEU:HB2	2.48	0.48
1:8:33:LEU:HD12	1:8:40:LEU:HB3	1.93	0.48
3:K:312:VAL:HG12	3:K:497:ILE:HB	1.94	0.48
1:S:214:ASP:OD2	1:S:217:ARG:HG2	2.13	0.48
1:W:33:LEU:HD12	1:W:40:LEU:HB3	1.94	0.48
1:0:19:LEU:HD12	1:2:9:PRO:HG2	1.95	0.48
1:0:68:PHE:CD1	2:Z:174:LEU:HD12	2.49	0.48
1:0:178:THR:HG22	1:0:182:ARG:HE	1.79	0.48
2:5:174:LEU:HD12	1:6:68:PHE:CD1	2.48	0.48
1:B:182:ARG:HD2	1:B:234:LEU:HD23	1.94	0.48
2:3:174:LEU:HD12	1:4:68:PHE:CD1	2.49	0.48
1:H:140:ARG:HH11	1:H:154:VAL:HG13	1.75	0.48
1:6:33:LEU:HD12	1:6:40:LEU:HB3	1.94	0.48
2:7:174:LEU:HD12	1:8:68:PHE:CD1	2.49	0.48
1:J:41:PHE:HB3	1:J:53:ILE:HD13	1.96	0.48
2:X:174:LEU:HD12	1:Y:68:PHE:CD1	2.48	0.48
1:H:55:GLU:HB2	1:H:222:PHE:CG	2.49	0.48
1:W:69:ASN:H	1:W:69:ASN:HD22	1.60	0.48
3:N:312:VAL:HG12	3:N:497:ILE:HB	1.96	0.48
1:S:69:ASN:HD22	1:S:69:ASN:H	1.61	0.48
1:J:90:ASP:OD2	1:J:91:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:359:TYR:CE1	3:E:383:LEU:HB2	2.49	0.47
3:K:476:ASP:O	3:L:329:ARG:NH2	2.45	0.47
3:N:325:MET:HE1	3:T:444:LEU:HD11	1.96	0.47
1:Q:92:ARG:HD3	1:Q:129:HIS:CE1	2.49	0.47
1:Q:123:CYS:HA	1:Q:139:TYR:O	2.14	0.47
1:Q:140:ARG:HH11	1:Q:154:VAL:HG13	1.74	0.47
3:T:312:VAL:HG12	3:T:497:ILE:HB	1.96	0.47
3:I:424:ASP:OD1	3:I:426:ALA:N	2.46	0.47
1:0:50:LEU:HB3	2:Z:174:LEU:HD11	1.95	0.47
1:4:110:ILE:HG21	1:4:118:TYR:CD1	2.49	0.47
1:8:118:TYR:HB3	1:8:120:VAL:HG22	1.97	0.47
1:B:185:VAL:O	1:B:189:ARG:HG3	2.14	0.47
1:J:140:ARG:HH11	1:J:154:VAL:HG13	1.75	0.47
3:K:429:TRP:HZ3	3:K:431:ILE:HG13	1.79	0.47
3:K:475:ALA:HA	3:K:481:THR:HB	1.95	0.47
1:Y:118:TYR:HB3	1:Y:120:VAL:HG22	1.97	0.47
1:0:33:LEU:HD12	1:0:40:LEU:HB3	1.95	0.47
3:E:312:VAL:HG12	3:E:497:ILE:HB	1.96	0.47
1:S:123:CYS:HA	1:S:139:TYR:O	2.15	0.47
1:Y:33:LEU:HD12	1:Y:40:LEU:HB3	1.95	0.47
1:2:178:THR:HG22	1:2:182:ARG:HE	1.80	0.47
1:B:89:TYR:CD1	3:N:382:ARG:HD3	2.49	0.47
1:D:123:CYS:HA	1:D:139:TYR:O	2.14	0.47
3:R:312:VAL:HG12	3:R:497:ILE:HB	1.96	0.47
3:A:344:GLY:C	3:A:345:ILE:HG12	2.35	0.47
1:J:110:ILE:HA	1:J:114:GLN:HG3	1.96	0.47
1:S:55:GLU:HB2	1:S:222:PHE:CG	2.50	0.47
1:8:182:ARG:NH1	1:8:234:LEU:O	2.48	0.47
1:W:178:THR:HG22	1:W:182:ARG:HE	1.79	0.47
1:2:70:GLU:HB3	1:2:118:TYR:CD2	2.50	0.47
1:6:69:ASN:HD22	1:6:69:ASN:H	1.62	0.47
3:C:382:ARG:HD3	1:H:89:TYR:CD1	2.49	0.47
1:M:123:CYS:HA	1:M:139:TYR:O	2.15	0.47
3:G:465:ARG:HG3	3:G:513:LEU:HD22	1.97	0.46
3:R:459:ASP:OD1	3:R:461:ASP:N	2.48	0.46
1:0:33:LEU:HD21	1:0:184:ALA:HB2	1.96	0.46
1:D:55:GLU:HB2	1:D:222:PHE:CG	2.50	0.46
1:M:90:ASP:OD2	1:M:91:ARG:N	2.47	0.46
1:Q:212:VAL:HG21	1:Q:223:ARG:HH21	1.80	0.46
2:V:174:LEU:HD11	1:W:50:LEU:HB3	1.95	0.46
1:Y:178:THR:HG22	1:Y:182:ARG:HE	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:19:LEU:HD12	1:W:9:PRO:HG2	1.96	0.46
3:G:344:GLY:C	3:G:345:ILE:HG12	2.36	0.46
1:J:33:LEU:HD12	1:J:40:LEU:HB3	1.96	0.46
1:S:18:GLU:OE2	1:S:18:GLU:HA	2.16	0.46
1:6:178:THR:HG22	1:6:182:ARG:HE	1.80	0.46
1:8:178:THR:HG22	1:8:182:ARG:HE	1.80	0.46
1:0:9:PRO:HG2	1:Y:19:LEU:HD12	1.96	0.46
1:0:70:GLU:HB3	1:0:118:TYR:CD2	2.50	0.46
1:4:57:TYR:OH	1:4:86:GLY:HA3	2.16	0.46
1:6:19:LEU:HD12	1:8:9:PRO:HG2	1.96	0.46
2:7:174:LEU:HD11	1:8:50:LEU:HB3	1.96	0.46
3:E:429:TRP:CZ3	3:E:431:ILE:HG13	2.51	0.46
3:U:465:ARG:HG3	3:U:465:ARG:HH11	1.81	0.46
1:Y:69:ASN:HD22	1:Y:69:ASN:N	2.13	0.46
1:2:57:TYR:OH	1:2:86:GLY:HA3	2.15	0.46
1:4:19:LEU:HD12	1:6:9:PRO:HG2	1.97	0.46
1:6:118:TYR:HB3	1:6:120:VAL:HG22	1.98	0.46
1:2:33:LEU:HD21	1:2:184:ALA:HB2	1.97	0.46
3:E:508:SER:O	3:E:512:GLU:HG3	2.16	0.46
1:W:19:LEU:HD12	1:Y:9:PRO:HG2	1.97	0.46
1:6:57:TYR:OH	1:6:86:GLY:HA3	2.16	0.46
3:A:366:TYR:CZ	3:A:370:GLU:HG3	2.51	0.46
3:C:429:TRP:CZ3	3:C:431:ILE:HG13	2.51	0.46
1:D:185:VAL:O	1:D:189:ARG:HB2	2.15	0.46
3:E:475:ALA:HA	3:E:481:THR:HB	1.97	0.46
1:M:25:ALA:O	1:M:158:GLY:HA2	2.16	0.46
1:Q:55:GLU:HB2	1:Q:222:PHE:CG	2.51	0.46
3:C:359:TYR:CE1	3:C:383:LEU:HB2	2.51	0.45
1:S:33:LEU:HD12	1:S:40:LEU:HB3	1.97	0.45
1:H:90:ASP:OD2	1:H:91:ARG:N	2.50	0.45
3:L:429:TRP:HZ3	3:L:431:ILE:HG13	1.82	0.45
3:U:366:TYR:CZ	3:U:370:GLU:HG3	2.51	0.45
1:Y:30:VAL:HG13	1:Y:43:ALA:HB2	1.97	0.45
3:N:475:ALA:HA	3:N:481:THR:HB	1.96	0.45
1:W:57:TYR:OH	1:W:86:GLY:HA3	2.17	0.45
1:8:56:LEU:HD23	1:8:56:LEU:HA	1.71	0.45
3:G:398:LEU:N	3:G:398:LEU:HD12	2.32	0.45
1:J:11:GLN:HG2	1:J:14:ARG:HH22	1.81	0.45
1:W:69:ASN:HD22	1:W:69:ASN:N	2.14	0.45
1:Y:140:ARG:HH11	1:Y:154:VAL:HG13	1.81	0.45
1:0:30:VAL:HG13	1:0:43:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:69:ASN:HD22	1:8:69:ASN:N	2.15	0.45
3:I:509:ARG:HA	3:I:512:GLU:OE2	2.17	0.45
3:R:475:ALA:HA	3:R:481:THR:HB	1.98	0.45
2:X:174:LEU:HD11	1:Y:50:LEU:HB3	1.98	0.45
1:0:57:TYR:OH	1:0:86:GLY:HA3	2.16	0.45
1:8:57:TYR:OH	1:8:86:GLY:HA3	2.17	0.45
1:Q:33:LEU:HD12	1:Q:40:LEU:HB3	1.99	0.45
1:2:30:VAL:HG13	1:2:43:ALA:HB2	1.98	0.45
1:4:33:LEU:HD21	1:4:184:ALA:HB2	1.98	0.45
1:4:118:TYR:HB3	1:4:120:VAL:HG22	1.99	0.45
1:4:178:THR:HG22	1:4:182:ARG:HE	1.82	0.45
1:B:56:LEU:HG	1:B:62:PHE:HB2	1.99	0.45
1:H:69:ASN:HD22	1:H:69:ASN:N	2.15	0.45
1:0:118:TYR:HB3	1:0:120:VAL:HG22	1.99	0.45
1:8:67:LYS:HG2	1:8:69:ASN:HD21	1.81	0.45
1:B:90:ASP:OD2	1:B:91:ARG:N	2.50	0.45
1:J:10:GLU:HG3	1:J:11:GLN:N	2.32	0.45
1:Q:150:GLU:HG3	1:Q:154:VAL:HG22	1.98	0.45
1:H:41:PHE:HB3	1:H:53:ILE:HD13	1.99	0.44
3:I:308:TYR:CD2	3:I:460:GLY:HA2	2.51	0.44
3:K:307:LYS:NZ	3:K:419:ARG:HA	2.32	0.44
1:0:140:ARG:HH11	1:0:154:VAL:HG13	1.83	0.44
1:B:41:PHE:HB3	1:B:53:ILE:HD13	1.99	0.44
1:D:33:LEU:HD12	1:D:40:LEU:HB3	1.99	0.44
1:D:69:ASN:HD22	1:D:69:ASN:N	2.16	0.44
1:J:118:TYR:HB3	1:J:120:VAL:HG22	1.99	0.44
1:Q:69:ASN:HD22	1:Q:69:ASN:H	1.64	0.44
3:K:488:ARG:HB2	3:K:490:ILE:HG13	1.99	0.44
1:M:89:TYR:CD1	3:T:382:ARG:HD3	2.52	0.44
3:O:366:TYR:CZ	3:O:370:GLU:HG3	2.52	0.44
3:N:359:TYR:CE1	3:N:383:LEU:HB2	2.52	0.44
1:W:33:LEU:HD21	1:W:184:ALA:HB2	1.99	0.44
3:C:444:LEU:HD12	3:C:444:LEU:HA	1.80	0.44
1:Q:172:ALA:HB3	1:Q:175:ALA:HB2	1.98	0.44
1:0:69:ASN:N	1:0:69:ASN:HD22	2.15	0.44
1:M:69:ASN:HD22	1:M:69:ASN:N	2.15	0.44
1:W:30:VAL:HG13	1:W:43:ALA:HB2	1.99	0.44
1:Y:57:TYR:OH	1:Y:86:GLY:HA3	2.17	0.44
3:C:308:TYR:CE2	3:C:460:GLY:HA2	2.53	0.44
1:D:74:LEU:HD23	1:D:122:LEU:HD11	1.99	0.44
1:S:56:LEU:HG	1:S:62:PHE:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:173:GLU:O	1:8:174:ASN:HB2	2.18	0.44
3:F:318:ARG:HD3	3:F:493:THR:HG23	2.00	0.44
1:J:56:LEU:HG	1:J:62:PHE:HB2	2.00	0.44
3:T:465:ARG:HG2	3:T:465:ARG:HH11	1.82	0.44
1:Y:182:ARG:NH1	1:Y:234:LEU:O	2.51	0.44
1:0:110:ILE:HG21	1:0:118:TYR:CD1	2.53	0.44
1:4:56:LEU:HD23	1:4:56:LEU:HA	1.73	0.44
1:4:173:GLU:O	1:4:174:ASN:HB2	2.16	0.44
1:D:25:ALA:O	1:D:158:GLY:HA2	2.18	0.44
3:G:366:TYR:CZ	3:G:370:GLU:HG3	2.53	0.44
3:N:429:TRP:CZ3	3:N:431:ILE:HG13	2.48	0.44
1:0:203:LEU:HD12	1:0:208:LEU:HD21	2.00	0.43
3:A:329:ARG:NH2	3:C:476:ASP:O	2.48	0.43
3:E:369:LEU:HD23	3:E:369:LEU:HA	1.84	0.43
3:F:344:GLY:C	3:F:345:ILE:HG12	2.37	0.43
3:L:450:MET:O	3:L:454:TYR:HB2	2.18	0.43
1:S:41:PHE:HB3	1:S:53:ILE:HD13	1.99	0.43
1:0:56:LEU:HD23	1:0:56:LEU:HA	1.77	0.43
1:0:69:ASN:HD22	1:0:69:ASN:H	1.65	0.43
1:2:110:ILE:HG21	1:2:118:TYR:CD1	2.53	0.43
3:O:344:GLY:C	3:O:345:ILE:HG12	2.38	0.43
3:P:344:GLY:C	3:P:345:ILE:HG12	2.37	0.43
1:Q:79:ILE:HD13	3:R:368:LYS:HB3	1.99	0.43
3:R:359:TYR:CE1	3:R:383:LEU:HB2	2.53	0.43
1:8:140:ARG:HH11	1:8:154:VAL:HG13	1.82	0.43
1:W:67:LYS:HG2	1:W:69:ASN:HD21	1.83	0.43
1:Y:33:LEU:HD21	1:Y:184:ALA:HB2	2.01	0.43
1:4:140:ARG:HH11	1:4:154:VAL:HG13	1.80	0.43
3:O:335:TYR:OH	3:O:353:VAL:HG22	2.19	0.43
3:R:382:ARG:HD3	1:S:89:TYR:CD1	2.53	0.43
3:T:475:ALA:HA	3:T:481:THR:HB	2.00	0.43
1:4:69:ASN:HD22	1:4:69:ASN:H	1.66	0.43
1:B:69:ASN:HD22	1:B:69:ASN:N	2.17	0.43
1:D:56:LEU:HG	1:D:62:PHE:HB2	2.00	0.43
3:G:318:ARG:HD3	3:G:493:THR:HG23	2.00	0.43
1:W:140:ARG:HH11	1:W:154:VAL:HG13	1.81	0.43
1:8:67:LYS:HG2	1:8:69:ASN:ND2	2.33	0.43
1:H:74:LEU:HD23	1:H:122:LEU:HD11	1.99	0.43
1:J:182:ARG:NH1	1:J:234:LEU:O	2.51	0.43
1:2:203:LEU:HD12	1:2:208:LEU:HD21	2.01	0.43
3:A:433:GLU:HA	3:N:530:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:LEU:HD12	1:H:40:LEU:HB3	2.00	0.43
1:H:56:LEU:HG	1:H:62:PHE:HB2	2.01	0.43
1:H:118:TYR:HB3	1:H:120:VAL:HG22	2.01	0.43
3:P:366:TYR:CZ	3:P:370:GLU:HG3	2.54	0.43
1:0:173:GLU:O	1:0:174:ASN:HB2	2.17	0.43
1:J:25:ALA:O	1:J:158:GLY:HA2	2.19	0.43
3:L:366:TYR:CZ	3:L:370:GLU:HG3	2.54	0.43
1:Q:90:ASP:OD2	1:Q:91:ARG:N	2.52	0.43
3:R:351:VAL:HG21	3:R:398:LEU:HB3	2.01	0.43
1:4:30:VAL:HG13	1:4:43:ALA:HB2	2.00	0.43
1:B:25:ALA:O	1:B:158:GLY:HA2	2.18	0.43
3:C:308:TYR:CD2	3:C:460:GLY:HA2	2.54	0.43
3:I:382:ARG:HD2	1:J:89:TYR:CE1	2.54	0.43
3:I:488:ARG:HB2	3:I:490:ILE:HG13	2.01	0.43
3:U:344:GLY:C	3:U:345:ILE:HG12	2.36	0.43
1:0:32:ALA:HA	1:0:40:LEU:O	2.19	0.43
3:C:473:ASP:OD1	3:C:521:ARG:NH1	2.39	0.43
3:U:465:ARG:HG2	3:U:513:LEU:HD22	2.01	0.43
1:2:69:ASN:N	1:2:69:ASN:HD22	2.16	0.42
1:M:56:LEU:HG	1:M:62:PHE:HB2	2.00	0.42
3:F:450:MET:O	3:F:454:TYR:HB2	2.19	0.42
3:G:429:TRP:HZ3	3:G:431:ILE:HG13	1.84	0.42
1:0:119:GLU:H	1:0:119:GLU:HG3	1.66	0.42
1:J:55:GLU:HB2	1:J:222:PHE:CG	2.54	0.42
1:J:69:ASN:HD22	1:J:69:ASN:N	2.17	0.42
3:L:318:ARG:HD3	3:L:493:THR:HG23	2.00	0.42
3:N:314:MET:HE2	3:N:403:LEU:HG	2.00	0.42
3:C:351:VAL:HG21	3:C:398:LEU:HB3	2.01	0.42
3:I:369:LEU:HD23	3:I:369:LEU:HA	1.81	0.42
3:K:509:ARG:HA	3:K:509:ARG:HD2	1.83	0.42
1:M:74:LEU:HD23	1:M:122:LEU:HD11	2.01	0.42
3:O:303:ILE:O	3:O:438:ALA:HA	2.19	0.42
1:Q:56:LEU:HG	1:Q:62:PHE:HB2	2.00	0.42
3:R:486:LEU:HD12	3:R:486:LEU:HA	1.86	0.42
3:R:488:ARG:HB2	3:R:490:ILE:HG13	2.02	0.42
1:W:67:LYS:HG2	1:W:69:ASN:ND2	2.34	0.42
1:Y:32:ALA:HA	1:Y:40:LEU:O	2.19	0.42
3:A:432:GLU:CD	3:A:437:GLN:HE21	2.22	0.42
1:Q:108:GLY:HA2	1:Q:144:ASP:O	2.19	0.42
3:T:359:TYR:CE1	3:T:383:LEU:HB2	2.55	0.42
2:V:171:GLY:HA3	1:Y:144:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:30:VAL:HG13	1:8:43:ALA:HB2	2.01	0.42
3:A:435:GLY:HA2	3:N:530:ASP:OD1	2.19	0.42
1:D:118:TYR:HB3	1:D:120:VAL:HG22	2.02	0.42
3:T:329:ARG:O	3:T:490:ILE:HG21	2.20	0.42
1:B:33:LEU:HD12	1:B:40:LEU:HB3	2.02	0.42
1:B:118:TYR:HB3	1:B:120:VAL:HG22	2.02	0.42
1:6:32:ALA:HA	1:6:40:LEU:O	2.20	0.42
1:6:69:ASN:HD22	1:6:69:ASN:N	2.17	0.42
3:C:369:LEU:HD23	3:C:369:LEU:HA	1.83	0.42
1:D:203:LEU:HB3	1:D:204:GLY:H	1.50	0.42
1:2:134:LYS:HB3	1:2:134:LYS:HE2	1.87	0.42
1:B:61:GLY:N	1:B:213:LEU:HD11	2.35	0.42
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.89	0.42
1:M:41:PHE:HB3	1:M:53:ILE:HD13	2.01	0.42
3:O:432:GLU:HG3	3:O:437:GLN:HB2	2.02	0.42
1:S:69:ASN:HD22	1:S:69:ASN:N	2.18	0.42
1:Y:173:GLU:O	1:Y:174:ASN:HB2	2.19	0.42
3:E:488:ARG:HB2	3:E:490:ILE:HG13	2.02	0.42
3:I:475:ALA:HA	3:I:481:THR:HB	2.01	0.42
3:L:344:GLY:C	3:L:345:ILE:HG12	2.38	0.42
1:M:92:ARG:HH22	1:M:129:HIS:HB3	1.85	0.42
1:S:174:ASN:HD22	1:S:174:ASN:HA	1.59	0.42
1:4:69:ASN:HD22	1:4:69:ASN:N	2.18	0.41
1:D:181:LEU:HD23	1:D:233:LEU:HB3	2.01	0.41
3:N:488:ARG:HB2	3:N:490:ILE:HG13	2.02	0.41
1:2:118:TYR:HB3	1:2:120:VAL:HG22	2.02	0.41
3:O:338:ASP:OD1	3:O:341:THR:N	2.53	0.41
1:Y:134:LYS:HB3	1:Y:134:LYS:HE2	1.86	0.41
1:2:32:ALA:HA	1:2:40:LEU:O	2.20	0.41
1:4:89:TYR:CE1	3:F:382:ARG:HD3	2.55	0.41
1:6:140:ARG:HH11	1:6:154:VAL:HG13	1.83	0.41
1:8:32:ALA:HA	1:8:40:LEU:O	2.21	0.41
3:A:303:ILE:O	3:A:438:ALA:HA	2.20	0.41
3:R:369:LEU:HA	3:R:369:LEU:HD23	1.84	0.41
3:U:303:ILE:O	3:U:438:ALA:HA	2.21	0.41
1:0:98:GLN:O	1:0:102:VAL:HG23	2.21	0.41
1:6:30:VAL:HG13	1:6:43:ALA:HB2	2.01	0.41
1:S:24:ILE:HG22	1:S:157:GLY:HA2	2.01	0.41
1:W:70:GLU:HB3	1:W:118:TYR:CE2	2.55	0.41
1:D:78:GLY:HA3	1:D:103:TYR:OH	2.20	0.41
3:E:473:ASP:OD1	3:E:521:ARG:NH1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:155:VAL:HG12	1:W:160:THR:HG22	2.03	0.41
1:J:181:LEU:HD23	1:J:233:LEU:HB3	2.03	0.41
3:O:432:GLU:CD	3:O:437:GLN:HE21	2.24	0.41
3:O:476:ASP:O	3:T:329:ARG:NH2	2.51	0.41
3:P:380:ILE:HD11	3:P:421:VAL:HG21	2.01	0.41
1:S:74:LEU:HD23	1:S:122:LEU:HD11	2.02	0.41
1:2:89:TYR:CE1	3:L:382:ARG:HD3	2.56	0.41
1:D:164:ALA:O	1:D:168:LYS:HG3	2.20	0.41
3:N:369:LEU:HD23	3:N:369:LEU:HA	1.83	0.41
3:P:450:MET:O	3:P:454:TYR:HB2	2.21	0.41
1:4:32:ALA:HA	1:4:40:LEU:O	2.21	0.41
1:4:182:ARG:NH1	1:4:234:LEU:O	2.54	0.41
1:8:70:GLU:HB3	1:8:118:TYR:CE2	2.56	0.41
3:C:475:ALA:HA	3:C:481:THR:HB	2.01	0.41
1:D:163:ILE:HG23	1:D:187:ALA:C	2.41	0.41
1:M:118:TYR:HB3	1:M:120:VAL:HG22	2.02	0.41
3:T:488:ARG:HB2	3:T:490:ILE:HG13	2.03	0.41
1:Y:98:GLN:O	1:Y:102:VAL:HG23	2.20	0.41
3:F:303:ILE:O	3:F:438:ALA:HA	2.20	0.41
3:K:351:VAL:HG21	3:K:398:LEU:HB3	2.02	0.41
1:M:33:LEU:HD12	1:M:40:LEU:HB3	2.03	0.41
1:M:96:GLY:H	1:M:126:GLU:CD	2.25	0.41
1:Q:118:TYR:HB3	1:Q:120:VAL:HG22	2.03	0.41
1:Y:208:LEU:HD23	1:Y:208:LEU:HA	1.91	0.41
1:2:69:ASN:HD22	1:2:69:ASN:H	1.68	0.40
3:F:320:SER:HB3	3:F:331:VAL:HG21	2.03	0.40
3:F:456:GLN:HE21	3:F:465:ARG:HH21	1.68	0.40
3:F:513:LEU:HD23	3:F:513:LEU:HA	1.92	0.40
3:N:534:LYS:HE3	3:N:534:LYS:HB3	1.91	0.40
3:P:303:ILE:O	3:P:438:ALA:HA	2.22	0.40
3:A:444:LEU:HD12	3:A:444:LEU:HA	1.82	0.40
1:B:78:GLY:HA3	1:B:103:TYR:OH	2.22	0.40
3:G:320:SER:HB3	3:G:331:VAL:HG21	2.03	0.40
3:L:444:LEU:HA	3:L:444:LEU:HD12	1.83	0.40
1:M:108:GLY:HA2	1:M:144:ASP:O	2.22	0.40
2:V:174:LEU:HD23	2:V:174:LEU:HA	1.89	0.40
1:2:214:ASP:OD2	1:2:217:ARG:HG2	2.22	0.40
3:F:366:TYR:CZ	3:F:370:GLU:HG3	2.56	0.40
1:H:25:ALA:O	1:H:158:GLY:HA2	2.21	0.40
1:Q:78:GLY:HA3	1:Q:103:TYR:OH	2.22	0.40
3:T:401:LEU:HD23	3:T:401:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:THR:HG22	1:H:182:ARG:HE	1.87	0.40
3:I:509:ARG:HA	3:I:512:GLU:CD	2.41	0.40
1:W:208:LEU:HD23	1:W:208:LEU:HA	1.91	0.40
1:4:96:GLY:H	1:4:126:GLU:CD	2.25	0.40
1:6:208:LEU:HD23	1:6:208:LEU:HA	1.90	0.40
3:A:318:ARG:HD3	3:A:493:THR:HG23	2.04	0.40
3:L:338:ASP:OD1	3:L:341:THR:N	2.55	0.40
3:O:497:ILE:HA	3:O:501:GLY:O	2.21	0.40
1:S:108:GLY:HA2	1:S:144:ASP:O	2.21	0.40
3:T:314:MET:HE2	3:T:403:LEU:HG	2.03	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	0	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
1	2	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
1	4	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
1	6	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
1	8	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
1	B	210/241 (87%)	203 (97%)	7 (3%)	0	100	100
1	D	213/241 (88%)	205 (96%)	8 (4%)	0	100	100
1	H	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
1	J	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
1	M	210/241 (87%)	202 (96%)	8 (4%)	0	100	100
1	Q	210/241 (87%)	204 (97%)	6 (3%)	0	100	100
1	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
1	Y	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
2	1	3/180 (2%)	3 (100%)	0	0	100	100
2	3	3/180 (2%)	3 (100%)	0	0	100	100
2	5	3/180 (2%)	3 (100%)	0	0	100	100
2	7	3/180 (2%)	2 (67%)	1 (33%)	0	100	100
2	V	3/180 (2%)	3 (100%)	0	0	100	100
2	X	3/180 (2%)	3 (100%)	0	0	100	100
2	Z	3/180 (2%)	3 (100%)	0	0	100	100
3	A	220/242 (91%)	211 (96%)	8 (4%)	1 (0%)	29	66
3	C	221/242 (91%)	211 (96%)	10 (4%)	0	100	100
3	E	220/242 (91%)	209 (95%)	11 (5%)	0	100	100
3	F	220/242 (91%)	211 (96%)	8 (4%)	1 (0%)	29	66
3	G	220/242 (91%)	212 (96%)	7 (3%)	1 (0%)	29	66
3	I	221/242 (91%)	210 (95%)	11 (5%)	0	100	100
3	K	220/242 (91%)	210 (96%)	10 (4%)	0	100	100
3	L	220/242 (91%)	213 (97%)	6 (3%)	1 (0%)	29	66
3	N	232/242 (96%)	221 (95%)	11 (5%)	0	100	100
3	O	221/242 (91%)	214 (97%)	6 (3%)	1 (0%)	29	66
3	P	232/242 (96%)	225 (97%)	6 (3%)	1 (0%)	34	70
3	R	221/242 (91%)	210 (95%)	11 (5%)	0	100	100
3	T	221/242 (91%)	210 (95%)	11 (5%)	0	100	100
3	U	221/242 (91%)	214 (97%)	6 (3%)	1 (0%)	29	66
All	All	6084/8022 (76%)	5843 (96%)	234 (4%)	7 (0%)	54	84

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	P	309	PRO
3	U	309	PRO
3	F	309	PRO
3	G	309	PRO
3	L	309	PRO
3	O	309	PRO

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Mol	Chain	Res	Type
3	A	309	PRO

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	0	165/185 (89%)	156 (94%)	9 (6%)	21	53
1	2	165/185 (89%)	156 (94%)	9 (6%)	21	53
1	4	165/185 (89%)	156 (94%)	9 (6%)	21	53
1	6	165/185 (89%)	155 (94%)	10 (6%)	18	51
1	8	165/185 (89%)	156 (94%)	9 (6%)	21	53
1	B	164/185 (89%)	154 (94%)	10 (6%)	18	51
1	D	166/185 (90%)	158 (95%)	8 (5%)	25	58
1	H	165/185 (89%)	155 (94%)	10 (6%)	18	51
1	J	165/185 (89%)	154 (93%)	11 (7%)	16	48
1	M	164/185 (89%)	156 (95%)	8 (5%)	25	57
1	Q	164/185 (89%)	159 (97%)	5 (3%)	41	70
1	S	165/185 (89%)	156 (94%)	9 (6%)	21	53
1	W	165/185 (89%)	157 (95%)	8 (5%)	25	58
1	Y	165/185 (89%)	156 (94%)	9 (6%)	21	53
2	1	3/147 (2%)	3 (100%)	0	100	100
2	3	3/147 (2%)	3 (100%)	0	100	100
2	5	3/147 (2%)	3 (100%)	0	100	100
2	7	3/147 (2%)	3 (100%)	0	100	100
2	V	3/147 (2%)	3 (100%)	0	100	100
2	X	3/147 (2%)	3 (100%)	0	100	100
2	Z	3/147 (2%)	3 (100%)	0	100	100
3	A	164/179 (92%)	161 (98%)	3 (2%)	59	81
3	C	164/179 (92%)	158 (96%)	6 (4%)	34	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	164/179 (92%)	161 (98%)	3 (2%)	59	81
3	F	164/179 (92%)	160 (98%)	4 (2%)	49	76
3	G	164/179 (92%)	160 (98%)	4 (2%)	49	76
3	I	164/179 (92%)	159 (97%)	5 (3%)	41	70
3	K	164/179 (92%)	160 (98%)	4 (2%)	49	76
3	L	164/179 (92%)	159 (97%)	5 (3%)	41	70
3	N	171/179 (96%)	166 (97%)	5 (3%)	42	71
3	O	164/179 (92%)	161 (98%)	3 (2%)	59	81
3	P	171/179 (96%)	167 (98%)	4 (2%)	50	76
3	R	164/179 (92%)	161 (98%)	3 (2%)	59	81
3	T	164/179 (92%)	161 (98%)	3 (2%)	59	81
3	U	164/179 (92%)	158 (96%)	6 (4%)	34	64
All	All	4639/6125 (76%)	4457 (96%)	182 (4%)	36	64

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	10	GLU
1	0	33	LEU
1	0	69	ASN
1	0	73	ASN
1	0	74	LEU
1	0	119	GLU
1	0	182	ARG
1	0	203	LEU
1	0	234	LEU
1	2	10	GLU
1	2	33	LEU
1	2	69	ASN
1	2	73	ASN
1	2	74	LEU
1	2	119	GLU
1	2	182	ARG
1	2	203	LEU
1	2	234	LEU
1	4	10	GLU
1	4	33	LEU
1	4	69	ASN

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Mol	Chain	Res	Type
1	4	73	ASN
1	4	74	LEU
1	4	119	GLU
1	4	182	ARG
1	4	203	LEU
1	4	234	LEU
1	6	10	GLU
1	6	33	LEU
1	6	69	ASN
1	6	73	ASN
1	6	74	LEU
1	6	119	GLU
1	6	123	CYS
1	6	182	ARG
1	6	203	LEU
1	6	234	LEU
1	8	10	GLU
1	8	33	LEU
1	8	69	ASN
1	8	73	ASN
1	8	74	LEU
1	8	119	GLU
1	8	182	ARG
1	8	203	LEU
1	8	234	LEU
3	A	330	ASP
3	A	345	ILE
3	A	444	LEU
1	B	33	LEU
1	B	69	ASN
1	B	73	ASN
1	B	74	LEU
1	B	123	CYS
1	B	147	ILE
1	B	174	ASN
1	B	182	ARG
1	B	205	VAL
1	B	217	ARG
3	C	330	ASP
3	C	345	ILE
3	C	354	GLU
3	C	434	GLU

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Mol	Chain	Res	Type
3	C	444	LEU
3	C	486	LEU
1	D	10	GLU
1	D	26	ARG
1	D	33	LEU
1	D	69	ASN
1	D	73	ASN
1	D	74	LEU
1	D	123	CYS
1	D	182	ARG
3	E	345	ILE
3	E	444	LEU
3	E	486	LEU
3	F	330	ASP
3	F	345	ILE
3	F	412	SER
3	F	444	LEU
3	G	345	ILE
3	G	412	SER
3	G	444	LEU
3	G	509	ARG
1	H	11	GLN
1	H	26	ARG
1	H	33	LEU
1	H	69	ASN
1	H	73	ASN
1	H	74	LEU
1	H	123	CYS
1	H	147	ILE
1	H	182	ARG
1	H	189	ARG
3	I	330	ASP
3	I	345	ILE
3	I	432	GLU
3	I	444	LEU
3	I	486	LEU
1	J	10	GLU
1	J	26	ARG
1	J	33	LEU
1	J	69	ASN
1	J	73	ASN
1	J	74	LEU

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Mol	Chain	Res	Type
1	J	123	CYS
1	J	147	ILE
1	J	182	ARG
1	J	203	LEU
1	J	234	LEU
3	K	345	ILE
3	K	357	ARG
3	K	444	LEU
3	K	486	LEU
3	L	330	ASP
3	L	338	ASP
3	L	345	ILE
3	L	412	SER
3	L	444	LEU
1	M	26	ARG
1	M	33	LEU
1	M	69	ASN
1	M	73	ASN
1	M	74	LEU
1	M	114	GLN
1	M	123	CYS
1	M	182	ARG
3	N	330	ASP
3	N	363	LEU
3	N	433	GLU
3	N	444	LEU
3	N	486	LEU
3	O	345	ILE
3	O	444	LEU
3	O	509	ARG
3	P	330	ASP
3	P	345	ILE
3	P	354	GLU
3	P	444	LEU
1	Q	33	LEU
1	Q	69	ASN
1	Q	92	ARG
1	Q	123	CYS
1	Q	182	ARG
3	R	444	LEU
3	R	486	LEU
3	R	519	GLU

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Mol	Chain	Res	Type
1	S	26	ARG
1	S	33	LEU
1	S	69	ASN
1	S	73	ASN
1	S	74	LEU
1	S	123	CYS
1	S	147	ILE
1	S	173	GLU
1	S	182	ARG
3	T	444	LEU
3	T	486	LEU
3	T	519	GLU
3	U	345	ILE
3	U	412	SER
3	U	433	GLU
3	U	444	LEU
3	U	465	ARG
3	U	512	GLU
1	W	10	GLU
1	W	33	LEU
1	W	69	ASN
1	W	73	ASN
1	W	74	LEU
1	W	182	ARG
1	W	203	LEU
1	W	234	LEU
1	Y	10	GLU
1	Y	33	LEU
1	Y	69	ASN
1	Y	73	ASN
1	Y	74	LEU
1	Y	119	GLU
1	Y	182	ARG
1	Y	203	LEU
1	Y	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	11	GLN
1	0	69	ASN
1	0	80	GLN

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Mol	Chain	Res	Type
1	0	98	GLN
1	0	114	GLN
1	2	11	GLN
1	2	69	ASN
1	2	80	GLN
1	2	98	GLN
1	2	114	GLN
1	4	11	GLN
1	4	69	ASN
1	4	80	GLN
1	4	98	GLN
1	4	114	GLN
1	6	11	GLN
1	6	69	ASN
1	6	80	GLN
1	6	114	GLN
1	8	11	GLN
1	8	69	ASN
1	8	80	GLN
1	8	114	GLN
3	A	456	GLN
1	B	69	ASN
1	B	80	GLN
1	B	98	GLN
1	B	114	GLN
1	B	152	HIS
1	B	174	ASN
3	C	456	GLN
1	D	69	ASN
1	D	80	GLN
1	D	114	GLN
3	E	456	GLN
3	F	456	GLN
3	G	456	GLN
1	H	69	ASN
1	H	80	GLN
1	H	114	GLN
3	I	430	ASN
3	I	456	GLN
1	J	11	GLN
1	J	69	ASN
1	J	80	GLN

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Mol	Chain	Res	Type
1	J	114	GLN
3	K	430	ASN
3	K	456	GLN
3	L	456	GLN
1	M	69	ASN
1	M	80	GLN
3	N	456	GLN
3	O	456	GLN
3	P	456	GLN
1	Q	11	GLN
1	Q	69	ASN
1	Q	80	GLN
1	Q	114	GLN
1	Q	129	HIS
3	R	456	GLN
1	S	69	ASN
1	S	80	GLN
1	S	114	GLN
1	S	174	ASN
3	T	430	ASN
3	T	456	GLN
3	U	456	GLN
1	W	11	GLN
1	W	69	ASN
1	W	80	GLN
1	W	114	GLN
1	Y	11	GLN
1	Y	69	ASN
1	Y	80	GLN
1	Y	114	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

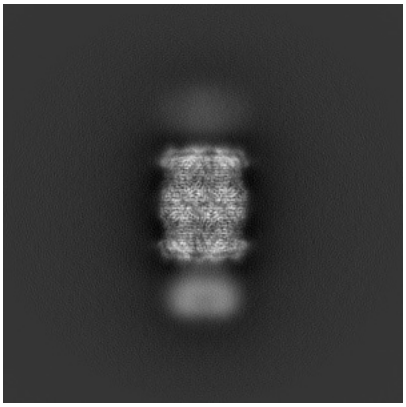
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4128. These allow visual inspection of the internal detail of the map and identification of artifacts.

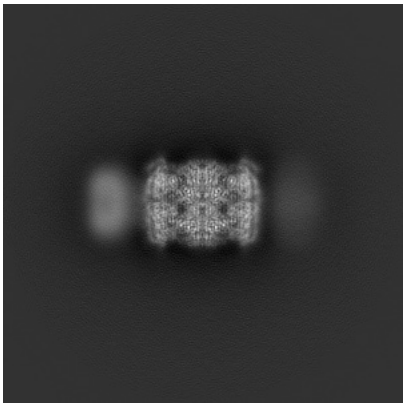
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

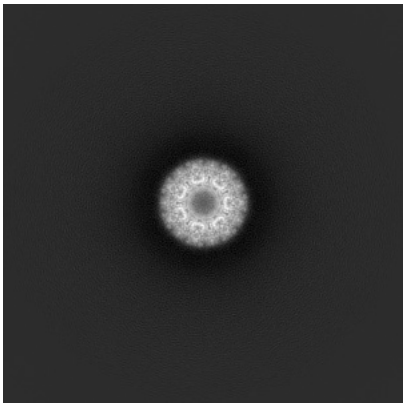
6.1.1 Primary map



X



Y

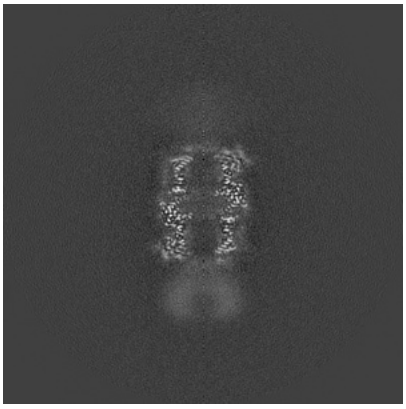


Z

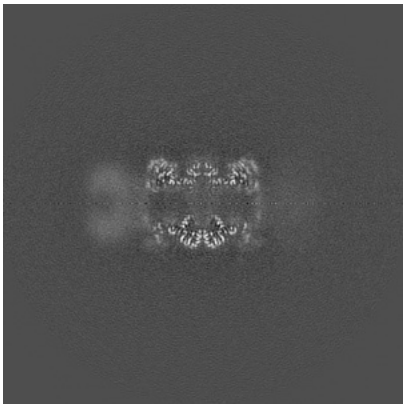
The images above show the map projected in three orthogonal directions.

6.2 Central slices

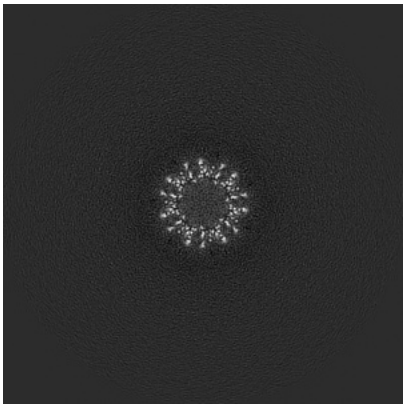
6.2.1 Primary map



X Index: 192



Y Index: 192

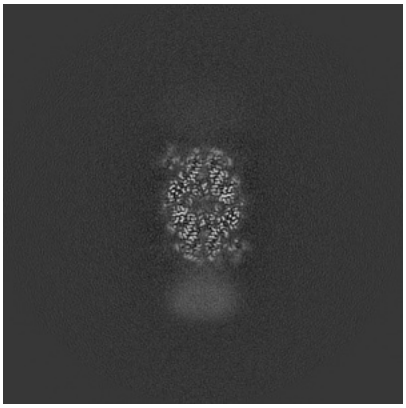


Z Index: 192

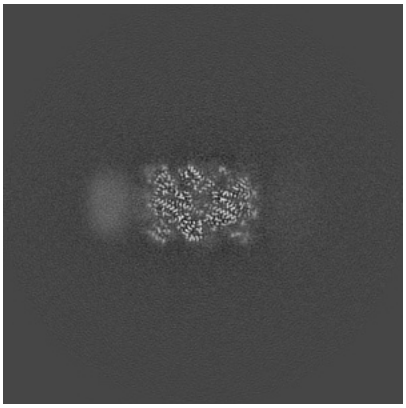
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

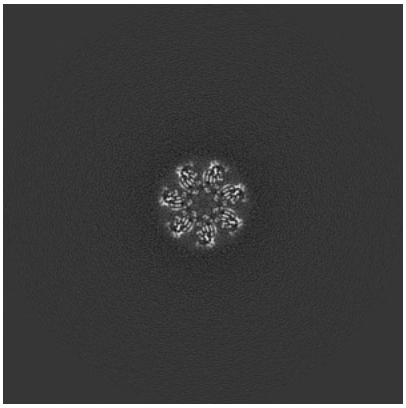
6.3.1 Primary map



X Index: 174



Y Index: 171

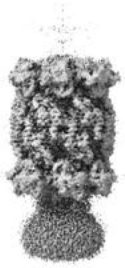


Z Index: 178

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 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

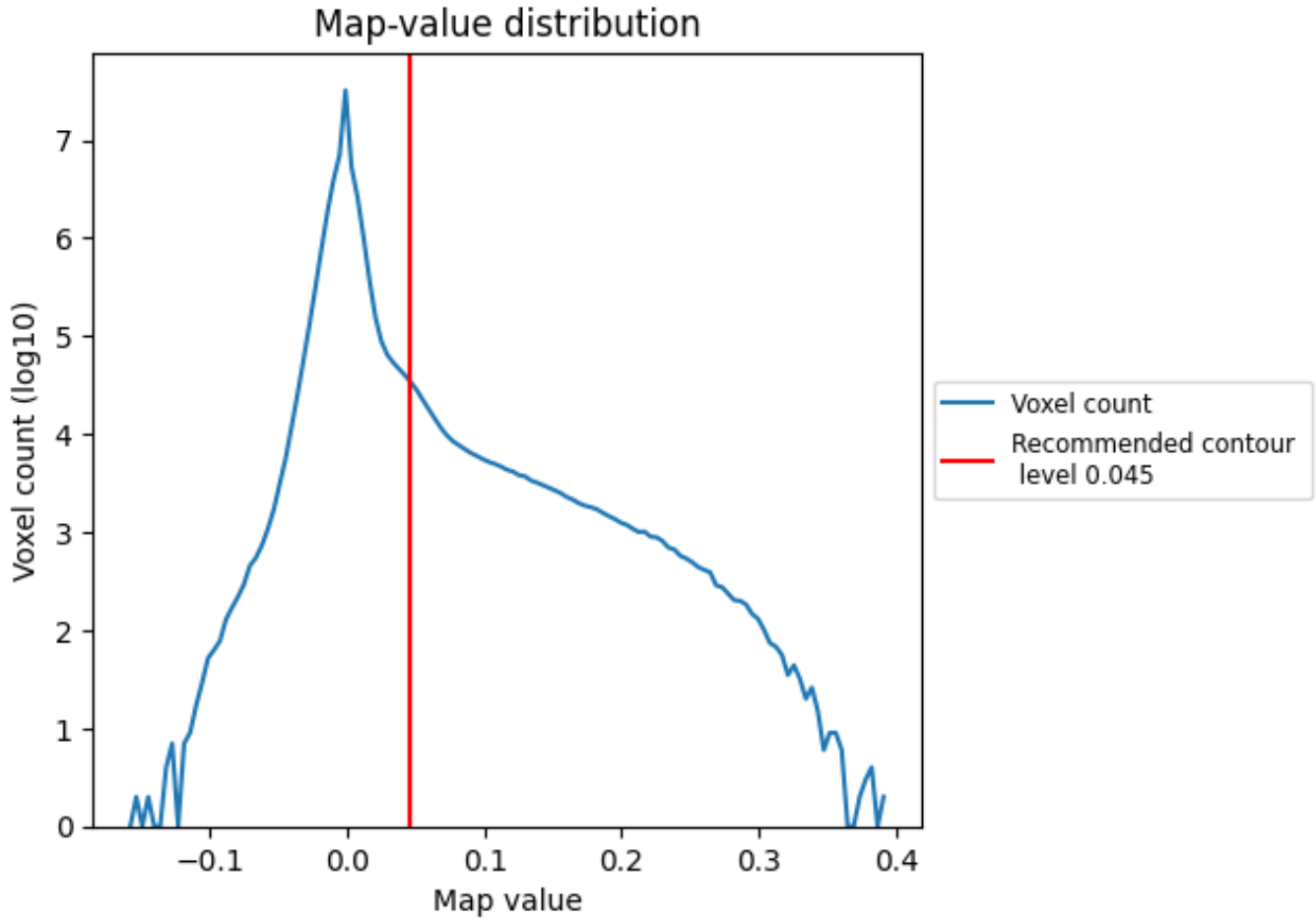
6.5 Mask visualisation (i)

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

7 Map analysis

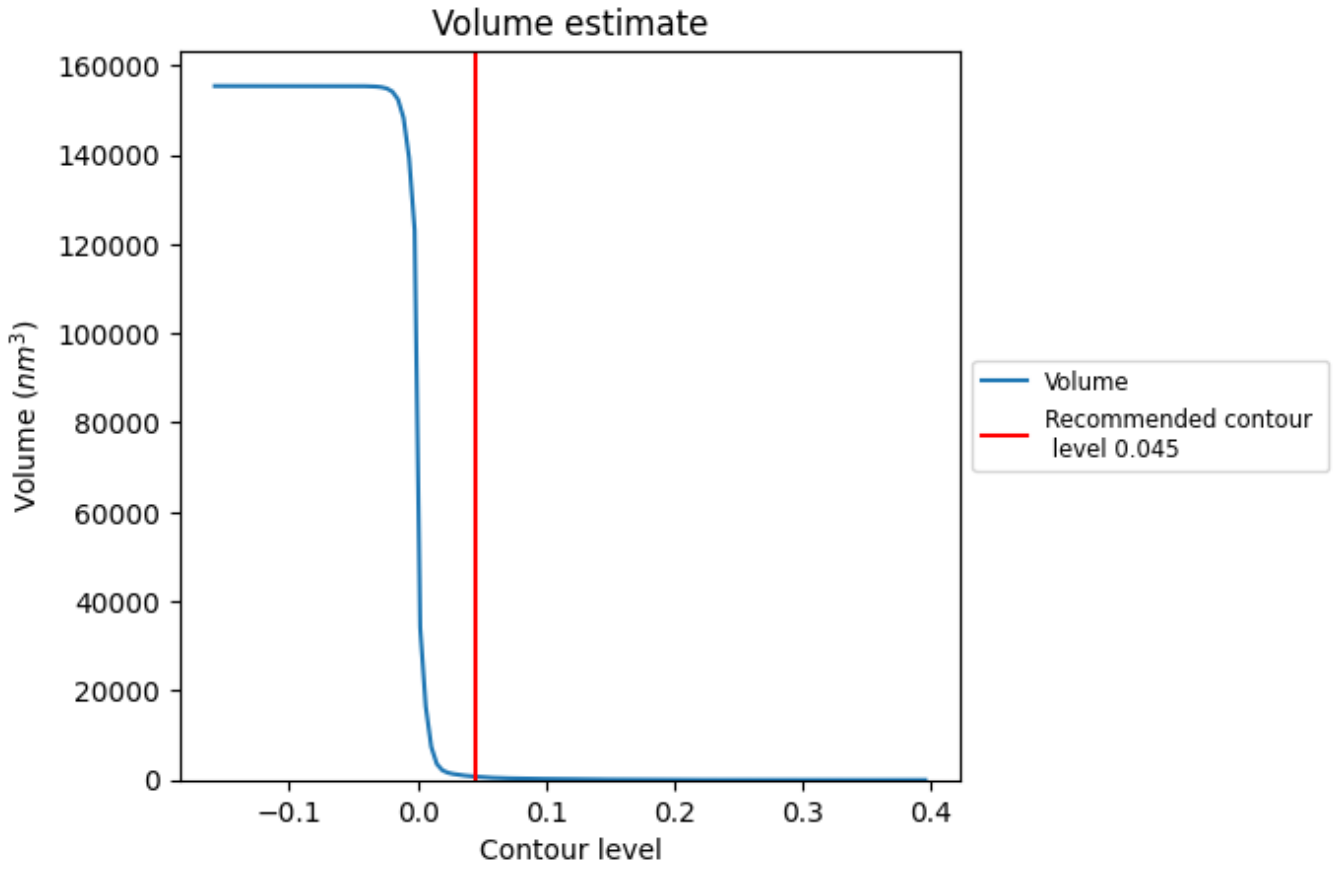
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

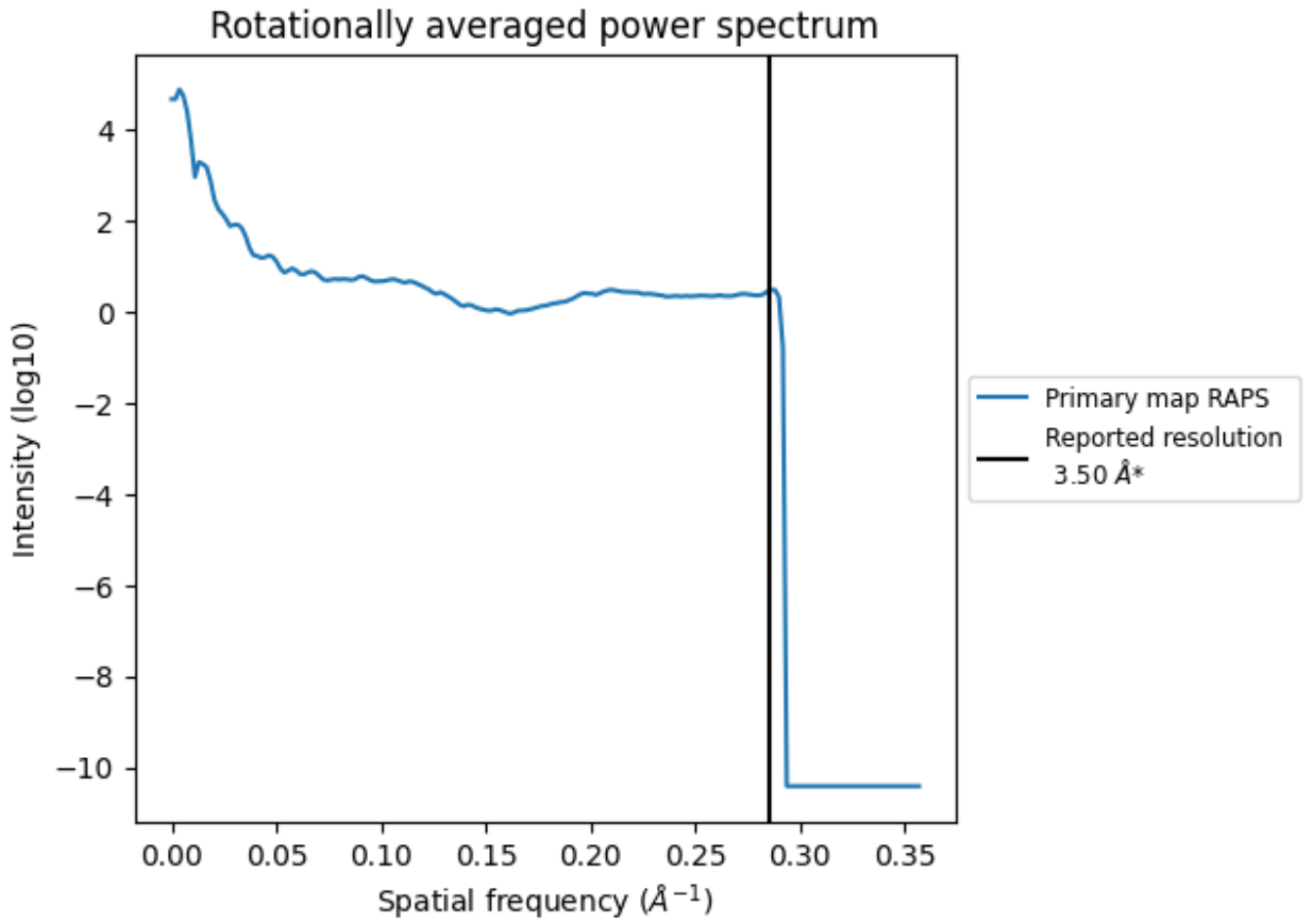
7.2 Volume estimate



The volume at the recommended contour level is 746 nm^3; this corresponds to an approximate mass of 674 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)

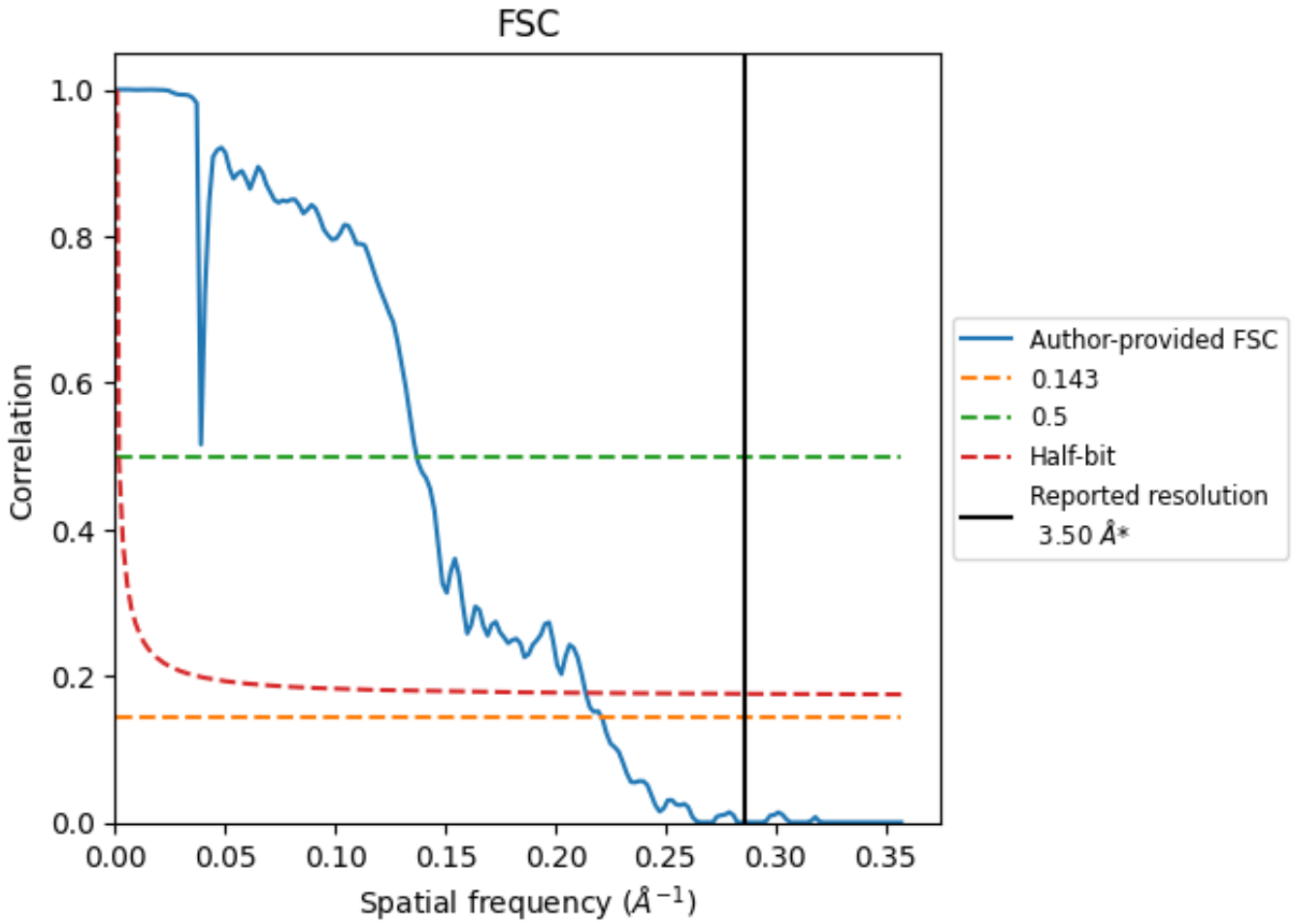


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

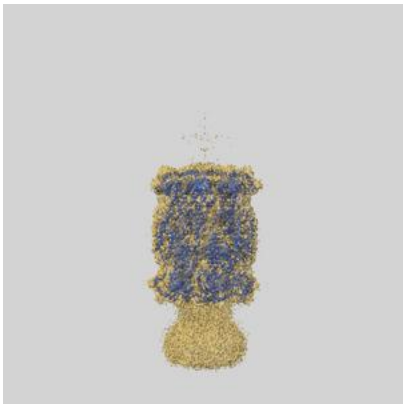
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	4.52	7.29	4.68
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.5 by more than 10 %

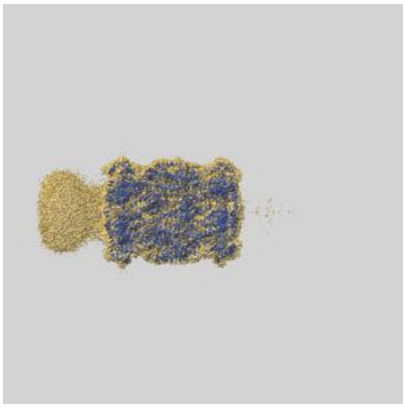
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4128 and PDB model 5LZP. Per-residue inclusion information can be found in section 3 on page 12.

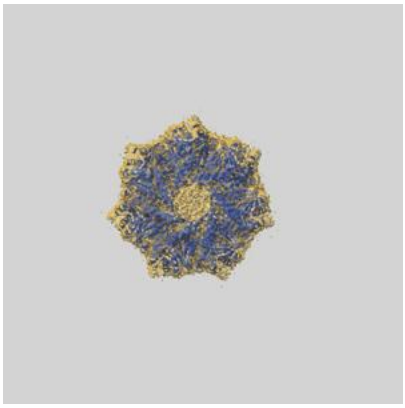
9.1 Map-model overlay



X



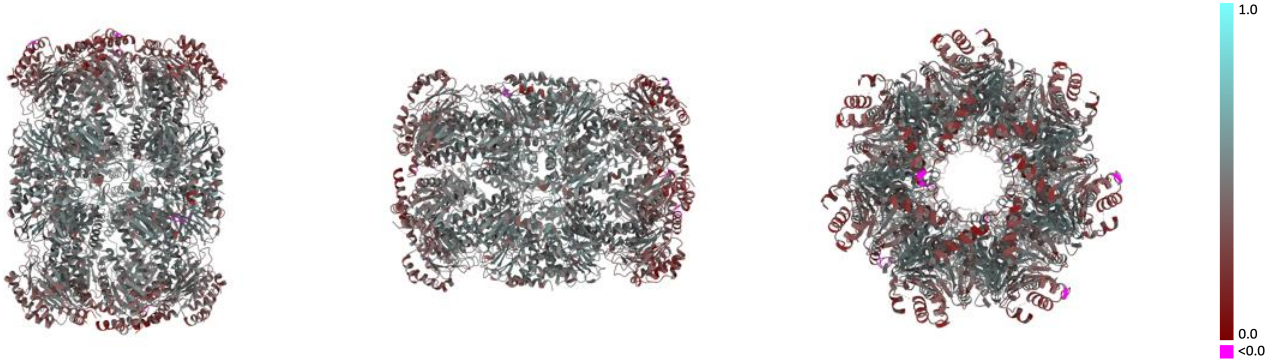
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

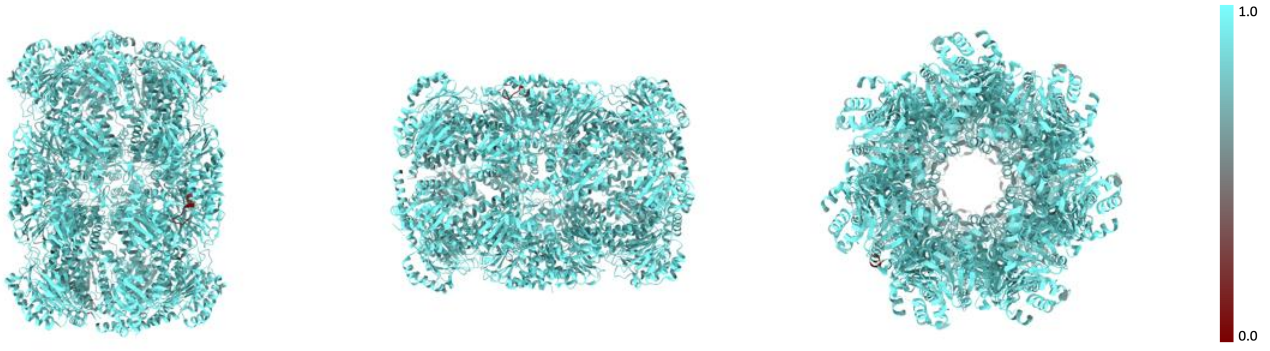
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

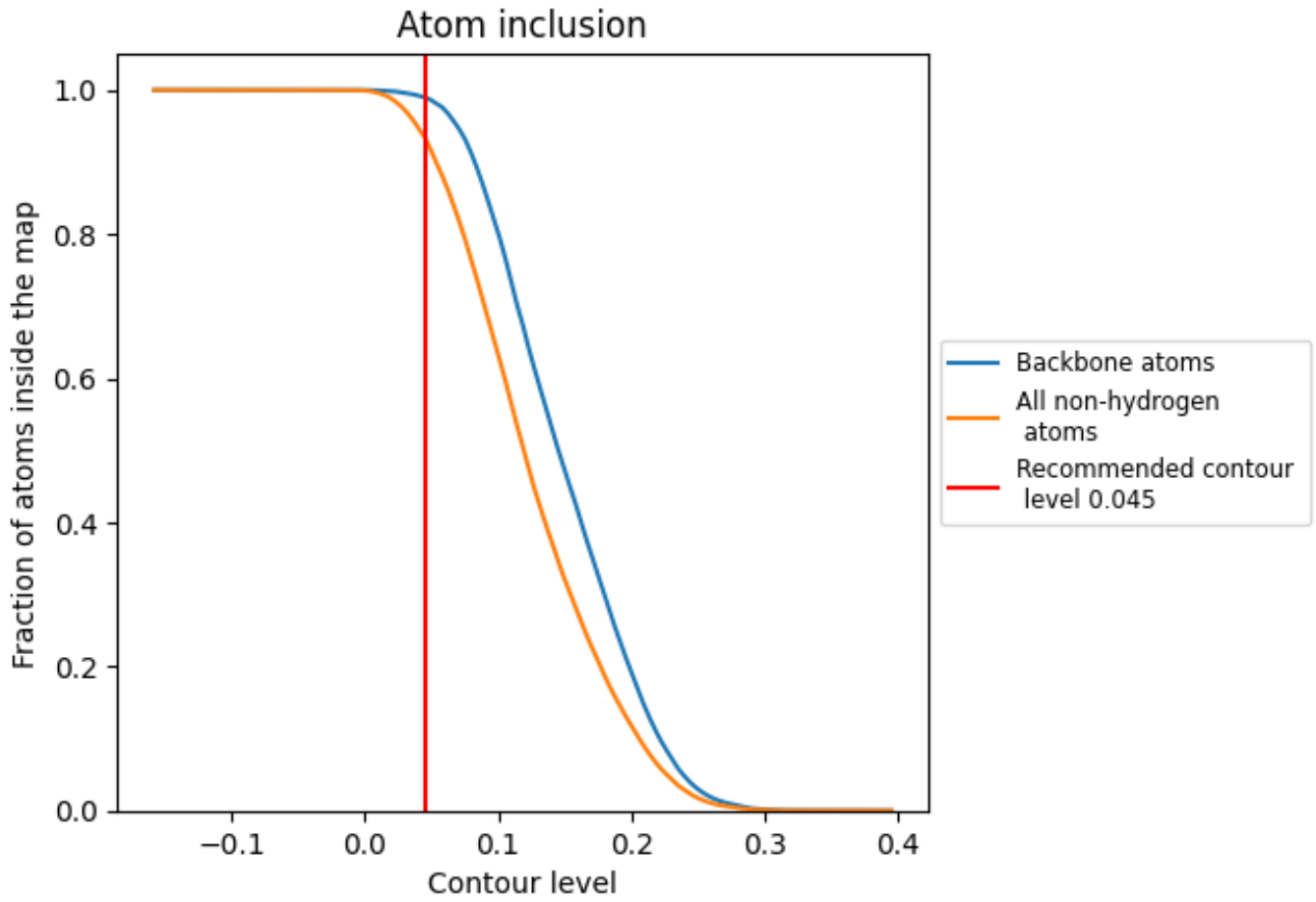
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 93% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9344	0.4400
0	0.9209	0.4130
1	0.8158	0.2610
2	0.9234	0.4130
3	0.7895	0.2580
4	0.9253	0.4120
5	0.7632	0.2420
6	0.9265	0.4120
7	0.7895	0.2550
8	0.9203	0.4130
A	0.9569	0.4930
B	0.9230	0.3700
C	0.9445	0.4910
D	0.9307	0.3760
E	0.9531	0.4880
F	0.9556	0.4930
G	0.9563	0.4930
H	0.9271	0.3760
I	0.9464	0.4890
J	0.9253	0.3720
K	0.9475	0.4910
L	0.9563	0.4960
M	0.9218	0.3790
N	0.9101	0.4710
O	0.9539	0.4930
P	0.9178	0.4690
Q	0.9230	0.3650
R	0.9483	0.4880
S	0.9253	0.3740
T	0.9458	0.4910
U	0.9551	0.4930
V	0.7895	0.2300
W	0.9215	0.4150
X	0.8158	0.2460
Y	0.9265	0.4140
Z	0.7895	0.2280