



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:06 PM UTC

PDB ID : 6BGO / pdb_00006bgo
EMDB ID : EMD-7098
Title : Singly PafE-capped 20S CP in Mycobacterium tuberculosis
Authors : Li, H.; Hu, K.
Deposited on : 2017-10-29
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

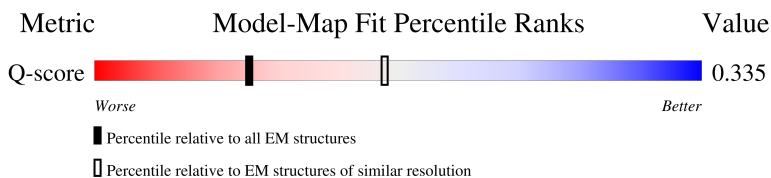
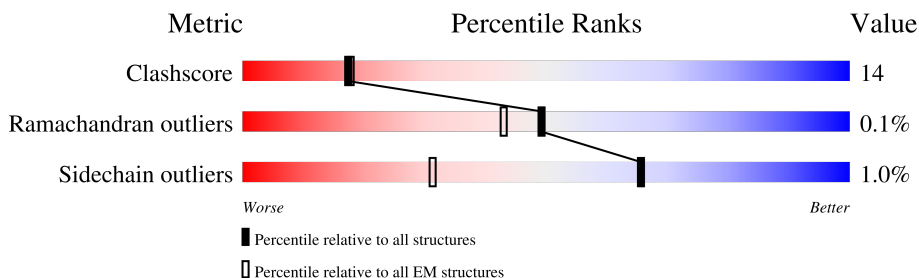
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



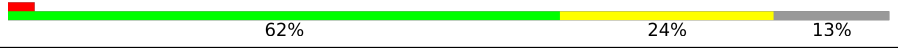
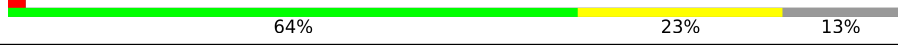
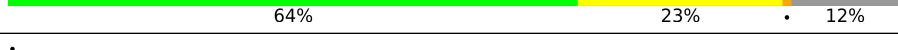
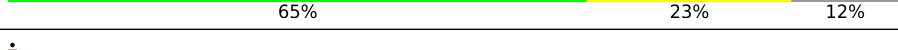
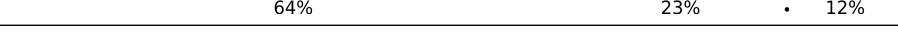
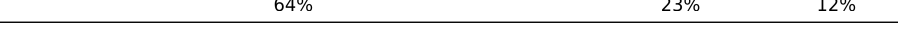
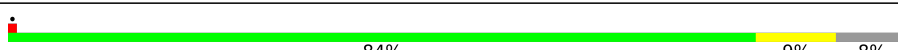
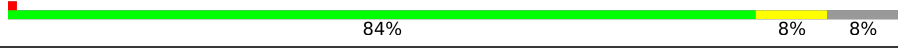
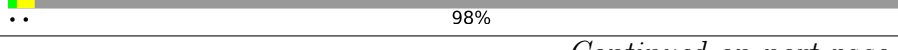
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	A	248	
1	C	248	
1	D	248	
1	E	248	

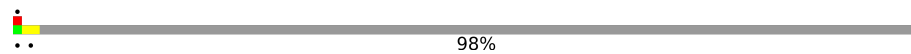
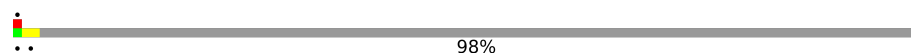
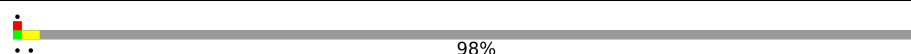
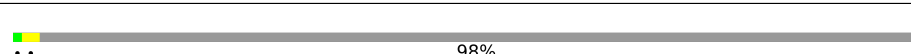
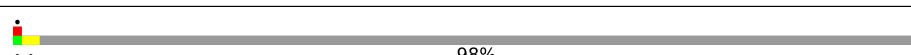
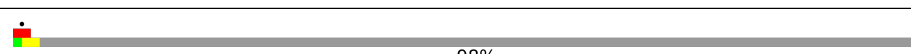
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Mol	Chain	Length	Quality of chain
1	F	248	
1	G	248	
1	H	248	
1	I	248	
1	J	248	
1	K	248	
1	L	248	
1	M	248	
1	N	248	
1	O	248	
2	P	240	
2	Q	240	
2	R	240	
2	S	240	
2	T	240	
2	U	240	
2	V	240	
2	W	240	
2	X	240	
2	Y	240	
2	Z	240	
2	a	240	
2	b	240	
2	c	240	
3	d	174	

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Mol	Chain	Length	Quality of chain
3	e	174	 98%
3	f	174	 98%
3	g	174	 98%
3	h	174	 98%
3	i	174	 98%
3	j	174	 98%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 46500 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	A	218	Total	C	N	O	S	0	0
			1673	1048	306	316	3		
1	C	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	D	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	E	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	F	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	G	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	H	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	I	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
1	J	219	Total	C	N	O	S	0	0
			1678	1051	307	317	3		
1	K	219	Total	C	N	O	S	0	0
			1678	1051	307	317	3		
1	L	218	Total	C	N	O	S	0	0
			1673	1048	306	316	3		
1	M	219	Total	C	N	O	S	0	0
			1678	1051	307	317	3		
1	N	219	Total	C	N	O	S	0	0
			1678	1051	307	317	3		
1	O	217	Total	C	N	O	S	0	0
			1668	1045	305	315	3		

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	R	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	S	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	T	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
2	U	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	V	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	W	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	X	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	Y	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	Z	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	a	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	b	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
2	c	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	535	HIS	-	expression tag	UNP A5U4D6
P	536	HIS	-	expression tag	UNP A5U4D6
P	537	HIS	-	expression tag	UNP A5U4D6
P	538	HIS	-	expression tag	UNP A5U4D6
P	539	HIS	-	expression tag	UNP A5U4D6
P	540	HIS	-	expression tag	UNP A5U4D6
Q	535	HIS	-	expression tag	UNP A5U4D6
Q	536	HIS	-	expression tag	UNP A5U4D6
Q	537	HIS	-	expression tag	UNP A5U4D6
Q	538	HIS	-	expression tag	UNP A5U4D6
Q	539	HIS	-	expression tag	UNP A5U4D6
Q	540	HIS	-	expression tag	UNP A5U4D6
R	535	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
R	536	HIS	-	expression tag	UNP A5U4D6
R	537	HIS	-	expression tag	UNP A5U4D6
R	538	HIS	-	expression tag	UNP A5U4D6
R	539	HIS	-	expression tag	UNP A5U4D6
R	540	HIS	-	expression tag	UNP A5U4D6
S	535	HIS	-	expression tag	UNP A5U4D6
S	536	HIS	-	expression tag	UNP A5U4D6
S	537	HIS	-	expression tag	UNP A5U4D6
S	538	HIS	-	expression tag	UNP A5U4D6
S	539	HIS	-	expression tag	UNP A5U4D6
S	540	HIS	-	expression tag	UNP A5U4D6
T	535	HIS	-	expression tag	UNP A5U4D6
T	536	HIS	-	expression tag	UNP A5U4D6
T	537	HIS	-	expression tag	UNP A5U4D6
T	538	HIS	-	expression tag	UNP A5U4D6
T	539	HIS	-	expression tag	UNP A5U4D6
T	540	HIS	-	expression tag	UNP A5U4D6
U	535	HIS	-	expression tag	UNP A5U4D6
U	536	HIS	-	expression tag	UNP A5U4D6
U	537	HIS	-	expression tag	UNP A5U4D6
U	538	HIS	-	expression tag	UNP A5U4D6
U	539	HIS	-	expression tag	UNP A5U4D6
U	540	HIS	-	expression tag	UNP A5U4D6
V	535	HIS	-	expression tag	UNP A5U4D6
V	536	HIS	-	expression tag	UNP A5U4D6
V	537	HIS	-	expression tag	UNP A5U4D6
V	538	HIS	-	expression tag	UNP A5U4D6
V	539	HIS	-	expression tag	UNP A5U4D6
V	540	HIS	-	expression tag	UNP A5U4D6
W	535	HIS	-	expression tag	UNP A5U4D6
W	536	HIS	-	expression tag	UNP A5U4D6
W	537	HIS	-	expression tag	UNP A5U4D6
W	538	HIS	-	expression tag	UNP A5U4D6
W	539	HIS	-	expression tag	UNP A5U4D6
W	540	HIS	-	expression tag	UNP A5U4D6
X	535	HIS	-	expression tag	UNP A5U4D6
X	536	HIS	-	expression tag	UNP A5U4D6
X	537	HIS	-	expression tag	UNP A5U4D6
X	538	HIS	-	expression tag	UNP A5U4D6
X	539	HIS	-	expression tag	UNP A5U4D6
X	540	HIS	-	expression tag	UNP A5U4D6
Y	535	HIS	-	expression tag	UNP A5U4D6

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	536	HIS	-	expression tag	UNP A5U4D6
Y	537	HIS	-	expression tag	UNP A5U4D6
Y	538	HIS	-	expression tag	UNP A5U4D6
Y	539	HIS	-	expression tag	UNP A5U4D6
Y	540	HIS	-	expression tag	UNP A5U4D6
Z	535	HIS	-	expression tag	UNP A5U4D6
Z	536	HIS	-	expression tag	UNP A5U4D6
Z	537	HIS	-	expression tag	UNP A5U4D6
Z	538	HIS	-	expression tag	UNP A5U4D6
Z	539	HIS	-	expression tag	UNP A5U4D6
Z	540	HIS	-	expression tag	UNP A5U4D6
a	535	HIS	-	expression tag	UNP A5U4D6
a	536	HIS	-	expression tag	UNP A5U4D6
a	537	HIS	-	expression tag	UNP A5U4D6
a	538	HIS	-	expression tag	UNP A5U4D6
a	539	HIS	-	expression tag	UNP A5U4D6
a	540	HIS	-	expression tag	UNP A5U4D6
b	535	HIS	-	expression tag	UNP A5U4D6
b	536	HIS	-	expression tag	UNP A5U4D6
b	537	HIS	-	expression tag	UNP A5U4D6
b	538	HIS	-	expression tag	UNP A5U4D6
b	539	HIS	-	expression tag	UNP A5U4D6
b	540	HIS	-	expression tag	UNP A5U4D6
c	535	HIS	-	expression tag	UNP A5U4D6
c	536	HIS	-	expression tag	UNP A5U4D6
c	537	HIS	-	expression tag	UNP A5U4D6
c	538	HIS	-	expression tag	UNP A5U4D6
c	539	HIS	-	expression tag	UNP A5U4D6
c	540	HIS	-	expression tag	UNP A5U4D6

- Molecule 3 is a protein called Bacterial proteasome activator.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	d	4	Total	C	N	O	0	0
			34	22	5	7		
3	e	4	Total	C	N	O	0	0
			34	22	5	7		
3	f	4	Total	C	N	O	0	0
			34	22	5	7		
3	g	4	Total	C	N	O	0	0
			34	22	5	7		
3	h	4	Total	C	N	O	0	0
			34	22	5	7		

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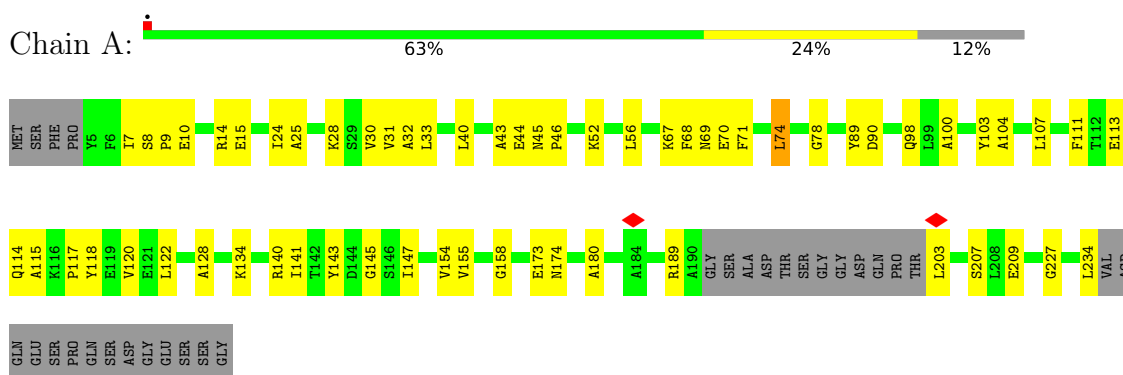
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Mol	Chain	Residues	Atoms				AltConf	Trace
3	i	4	Total	C	N	O	0	0
			34	22	5	7		
3	j	4	Total	C	N	O	0	0
			34	22	5	7		

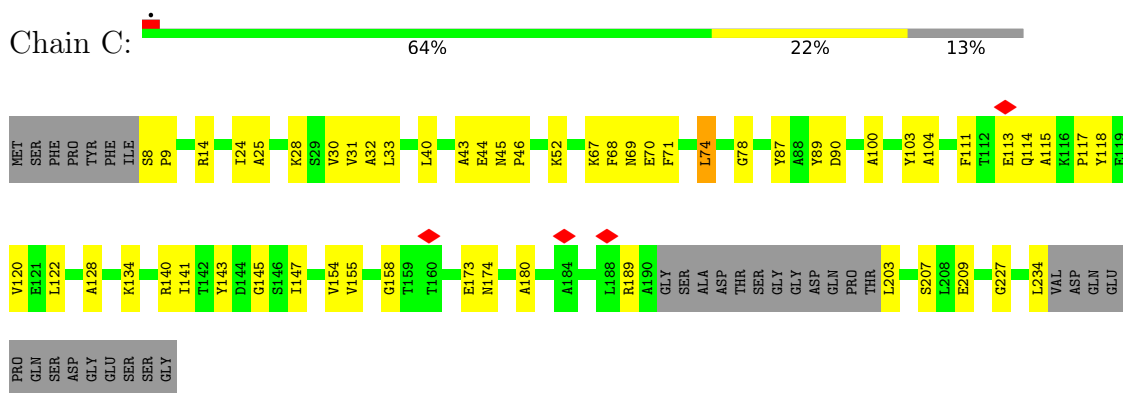
3 Residue-property plots [i](#)

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.

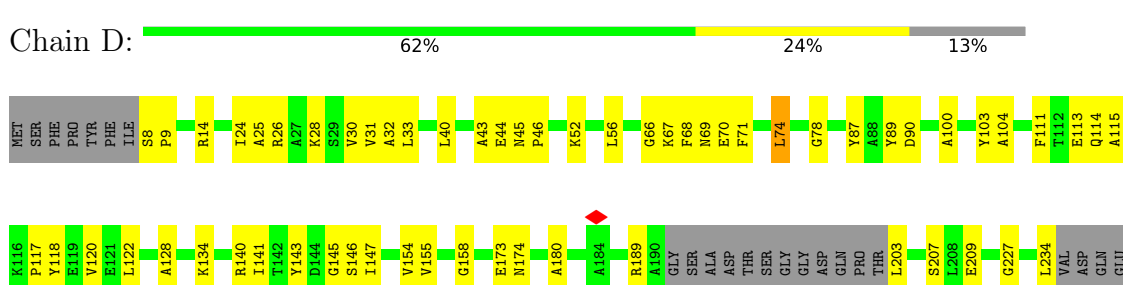
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha



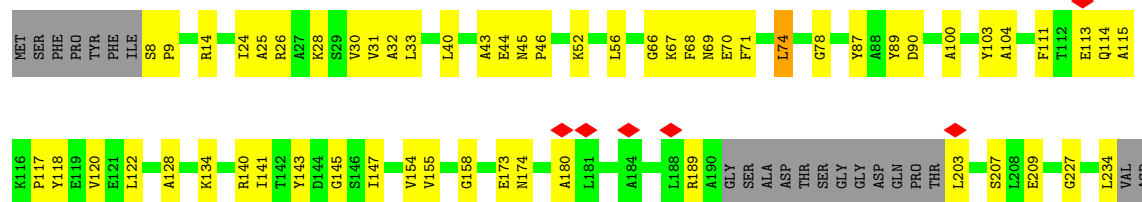
- Molecule 1: Proteasome subunit alpha



SER
PRO
SER
GLN
PHE
SER
ASP
GLY
GLU
SER
SER
GLY

• Molecule 1: Proteasome subunit alpha

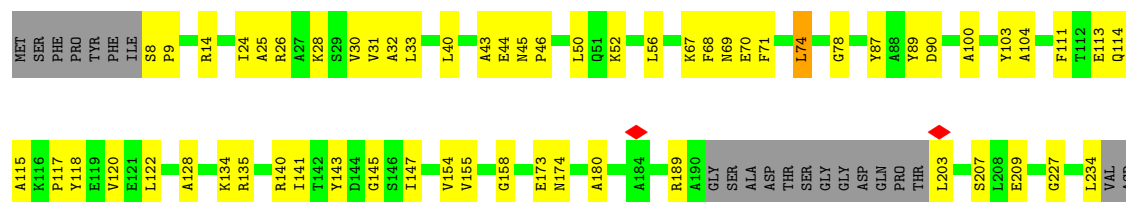
Chain E:



GLN
GLU
SER
PRO
GLN
SER
ASP
GLY
SER
SER
GLY

• Molecule 1: Proteasome subunit alpha

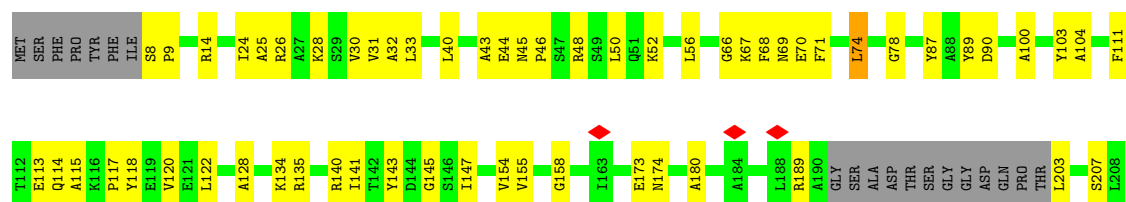
Chain F:



GLN
GLU
SER
PRO
GLN
SER
ASP
GLY
SER
SER
GLY

• Molecule 1: Proteasome subunit alpha

Chain G:

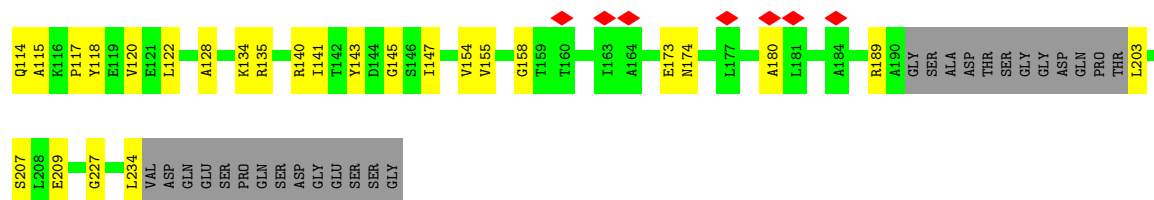


T112
E113
Q114
A115
K116
X117
P118
Y119
E120
V121
L122
A128
K134
R135
R140
K141
R142
T143
Y144
D145
S146
I147
V154
V155
G158
E173
N174
E175
Q176
A180
R189
A190
GLY
SER
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L203
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L208
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L234
VAL
E209

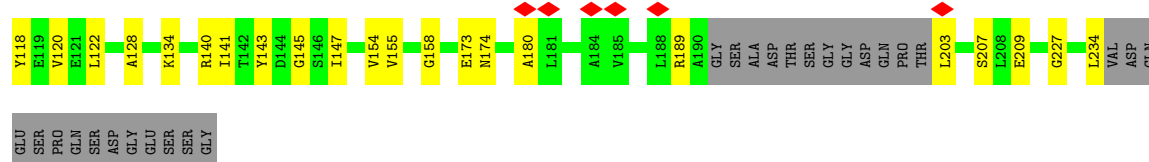
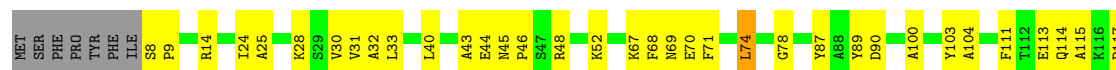
• Molecule 1: Proteasome subunit alpha

Chain H:

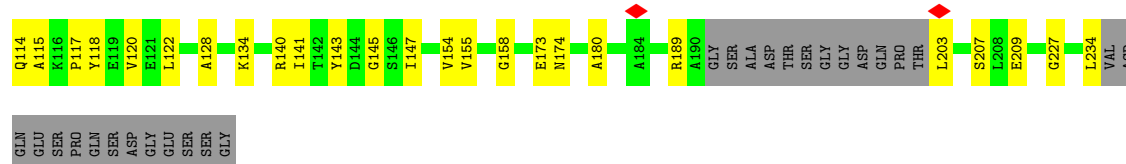
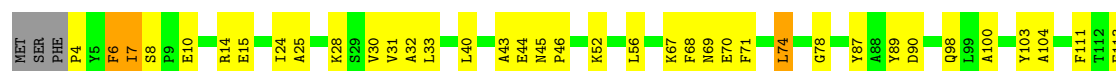




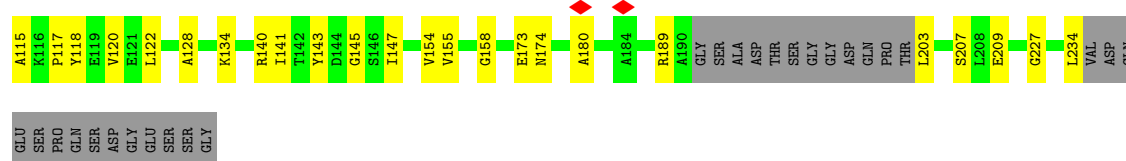
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

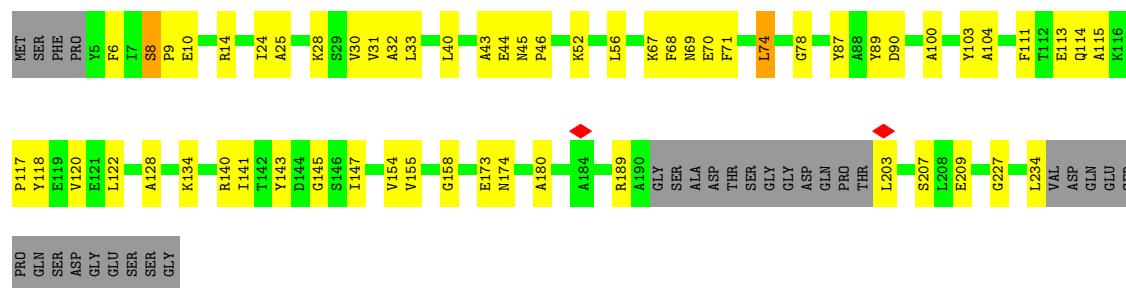


• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha





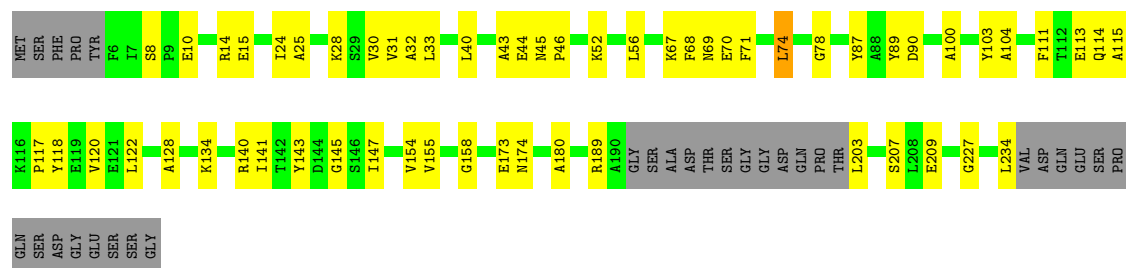
- Molecule 1: Proteasome subunit alpha



- Molecule 1: Proteasome subunit alpha

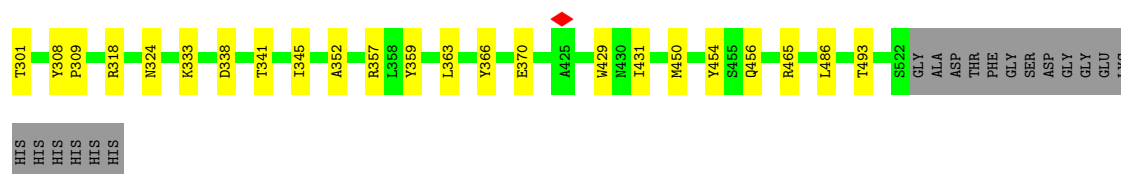


- Molecule 2: Proteasome subunit beta



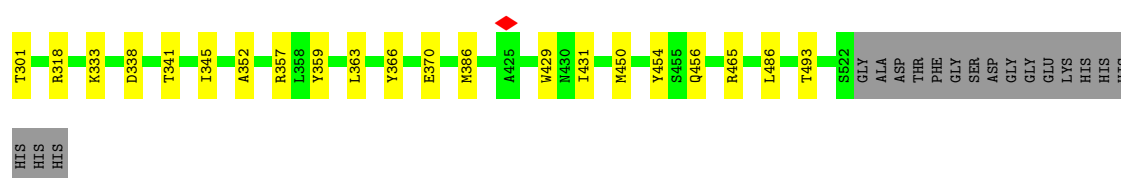
- Molecule 2: Proteasome subunit beta

Chain P:  83% 10% 8%



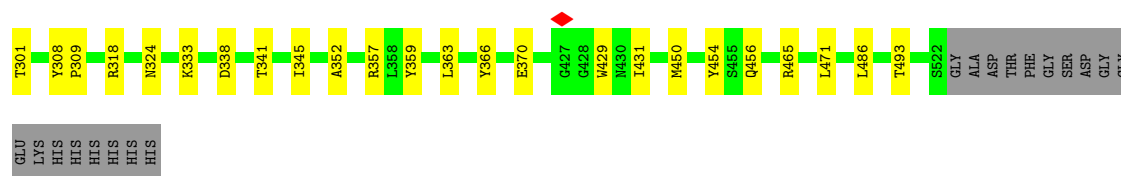
- Molecule 2: Proteasome subunit beta

Chain Q:  84% 9% 8%



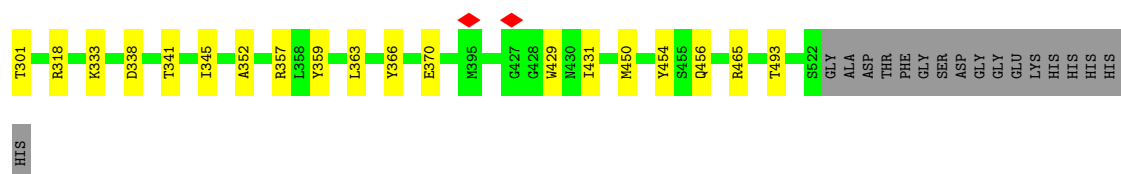
- Molecule 2: Proteasome subunit beta

Chain R:  82% 10% 8%



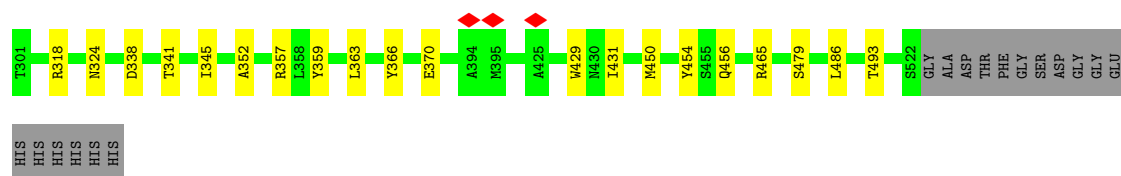
- Molecule 2: Proteasome subunit beta

Chain S:  85% 8% 8%

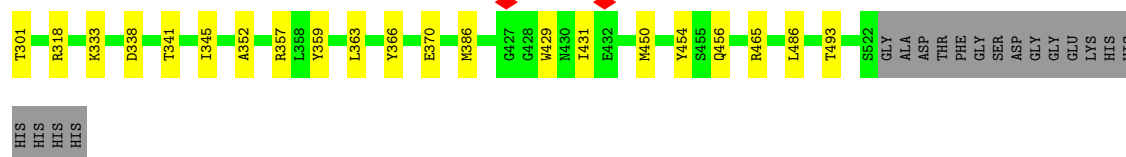
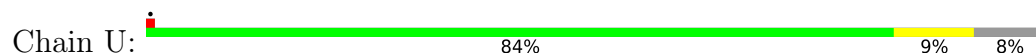


- Molecule 2: Proteasome subunit beta

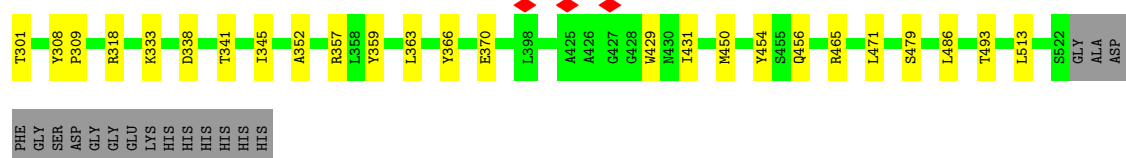
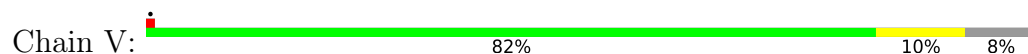
Chain T:  84% 8% 8%



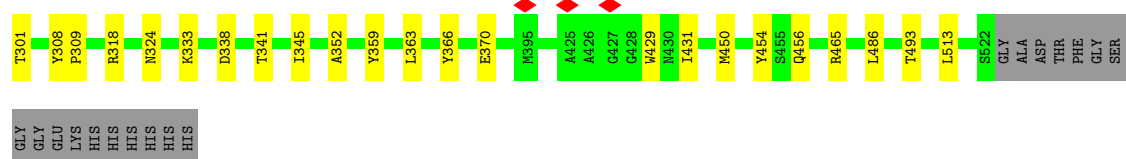
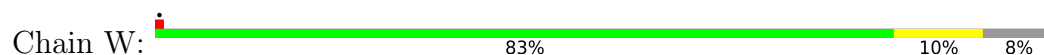
- Molecule 2: Proteasome subunit beta



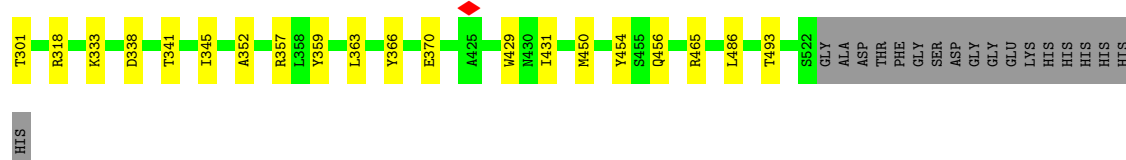
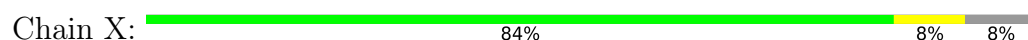
- Molecule 2: Proteasome subunit beta



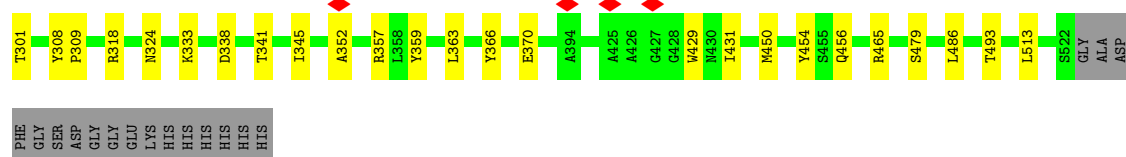
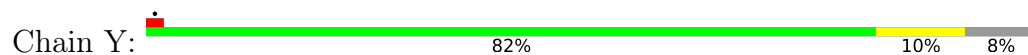
- Molecule 2: Proteasome subunit beta



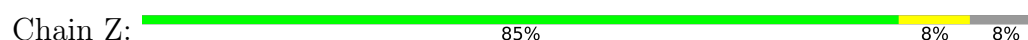
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta



GLN	LEU	VAL	GLY	TRP	LEU	GLU	GLY	LEU	PHE	HIS	GLY	ILE	GLN	THR	ALA	ASP	VAL	ILE	PHE	GLN	GLN	MET	ALA	ALA	ARG	GLN	LEU	GLN	GLN	MET	ARG	GLY	GLY	VAL	LYS	SER	GLY	GLN	HIS	GLY	HIS	GLY	THR	THR	Q172	Y173	L174																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
VAL	ARG	ALA	GLY	PRO	LEU	ASP	GLU	ALA	SER	ARG	ASN	ARG	LEU	ARG	ASP	ASP	VAL	ILE	HIS	ALA	THR	ILE	GLU	GLU	LEU	GLU	LEU	ARG	GLY	GLY	ARG	LEU	THR	LEU	PRO	PHE	ASN	GLU	ASP	ALA	VAL	SER	ASP	ALA	GLU	LEU	ILE	ALA	ALA	GLN	LEU	LEU	GLU	ALA	GLN	GLY	THR	MET	ILE	THR	GLY	ILE	ARG	MET	LYS	GLN	LEU	LEU	GLN	GLY	VAL	GLU	ASN	ASP	SER	GLY	ALA	ARG	VAL	GLN	GLY	VAL	LEU	THR	ASP	GLY	ASP	GLY	LEU	THR	SER	SER	GLY	ASN	ASN	GLY	GLU	LEU	GLY	GLY	VAL	ASP	GLY	GLY	VAL	LEU	GLY	GLY	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	

- Molecule 3: Bacterial proteasome activator

Chain f:  98%

GLN	LEU	VAL	GLY	TRP	LEU	GLU	GLY	LEU	PHE	HIS	GLY	ILE	GLN	THR	ALA	ASP	VAL	ILE	PHE	GLN	GLN	MET	GLN	ALA	ALA	ARG	GLN	GLN	GLN	MET	ARG	GLN	GLY	GLY	VAL	LYS	SER	GLY	GLN	HIS	GLY	HIS	GLY	THR	THR	GLN	LEU	GLN	GLY	THR	GLN	GLY	VAL	ASP	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY
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- Molecule 3: Bacterial proteasome activator

Chain g:  98%

GLN	LEU	VAL	GLY	TRP	LEU	GLU	GLY	LEU	PHE	HIS	GLY	ILE	GLN	THR	ALA	ASP	VAL	ILE	PHE	GLN	GLN	GLN	MET	ALA	ALA	ALA	GLU	GLN	GLY	GLY	VAL	LYS	SER	GLY	GLY	THR	Q172	Y173	L174																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
MET	VAL	ILE	GLY	LEU	SER	THR	GLY	ASP	SER	ASP	ASP	ASP	VAL	VAL	GLU	ASP	VAL	ILE	HIS	GLY	GLY	VAL	ASP	ILE	GLU	LEU	GLU	ASN	ASP	GLU	SER	LEU	THR	ASP	LEU	VAL	GLU	PRO	ALA	GLY	THR	MET	ILE	LYS	LEU	GLU	THR	VAL	GLN	GLY	ASP	ALA	GLY	VAL	ARG	ILE	THR	GLY	GLY	ASP	ARG	VAL	GLN	GLY	ASP	GLY	THR	ASP	GLY	VAL	ALA	GLY	ASP	ALA	GLY	VAL	ARG	ALA	GLY	ASP	GLY	THR	ASP	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	

- Molecule 3: Bacterial proteasome activator

Chain h:  98%

MET	VAL	ILE	GLY	LEU	SER	THR	GLY	ASP	SER	ASP	ASP	ASP	VAL	VAL	GLU	ASP	VAL	ILE	ILE	GLY	GLY	VAL	THR	ALA	ILE	PRO	ARG	LEU	ILE	ALA	VAL	GLN	GLY	THR	ASP	GLY	THR	ILE	LYS	GLN	LEU	LEU	GLU	ALA														
VAL	ARG	ALA	GLY	PRO	LEU	ASP	GLY	ALA	SER	ASP	ASP	ASN	ASP	VAL	THR	ARG	ASP	VAL	ILE	HIS	GLY	ALA	THR	ILE	PRO	ARG	LEU	ILE	ALA	VAL	GLN	GLY	ARG	LEU	PRO	GLY	THR	ASP	GLY	VAL	LYS	SER	GLY	GLN	HIS	LYS	VAL	ASP	ALA	MET	ARG	THR	GLY	THR	ASP	ALA	Y173	L174
GLN	LEU	VAL	TRP	LEU	LEU	GLY	GLY	LEU	LEU	HIS	ASP	GLY	ILE	GLN	THR	ALA	ASP	VAL	ILE	PHE	GLY	ALA	GLN	GLN	MET	ILE	ARG	LEU	ALA	VAL	GLN	GLY	ARG	LEU	PRO	PRO	GLY	VAL	LYS	SER	GLY	GLN	HIS	LYS	VAL	ASP	ALA	MET	ARG	THR	GLY	THR	ASP	ALA	Y173	L174		

- Molecule 3: Bacterial proteasome activator

Chain i:  98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60034	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 ($e^-/\text{\AA}^2$)	1.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00952	Depositor
Map size (Å)	436.0, 436.0, 436.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/1698	0.71	1/2295 (0.0%)
1	C	0.39	0/1683	0.71	1/2274 (0.0%)
1	D	0.40	0/1683	0.71	1/2274 (0.0%)
1	E	0.39	0/1683	0.71	1/2274 (0.0%)
1	F	0.40	0/1683	0.71	1/2274 (0.0%)
1	G	0.39	0/1683	0.71	1/2274 (0.0%)
1	H	0.40	0/1683	0.71	1/2274 (0.0%)
1	I	0.39	0/1683	0.71	1/2274 (0.0%)
1	J	0.40	0/1703	0.72	2/2302 (0.1%)
1	K	0.40	0/1703	0.73	2/2302 (0.1%)
1	L	0.39	0/1698	0.72	1/2295 (0.0%)
1	M	0.39	0/1703	0.72	2/2302 (0.1%)
1	N	0.39	0/1703	0.72	2/2302 (0.1%)
1	O	0.40	0/1693	0.71	1/2288 (0.0%)
2	P	0.34	0/1662	0.57	0/2254
2	Q	0.34	0/1662	0.57	0/2254
2	R	0.34	0/1662	0.57	0/2254
2	S	0.34	0/1662	0.57	0/2254
2	T	0.34	0/1660	0.57	0/2251
2	U	0.34	0/1662	0.57	0/2254
2	V	0.34	0/1662	0.57	0/2254
2	W	0.34	0/1662	0.57	0/2254
2	X	0.34	0/1662	0.57	0/2254
2	Y	0.34	0/1662	0.57	0/2254
2	Z	0.34	0/1662	0.57	0/2254
2	a	0.34	0/1662	0.57	0/2254
2	b	0.34	0/1662	0.57	0/2254
2	c	0.34	0/1662	0.57	0/2254
3	d	0.18	0/34	0.39	0/43
3	e	0.16	0/34	0.38	0/43
3	f	0.17	0/34	0.39	0/43
3	g	0.17	0/34	0.38	0/43
3	h	0.17	0/34	0.38	0/43
3	i	0.18	0/34	0.39	0/43

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	j	0.17	0/34	0.38	0/43
All	All	0.37	0/47186	0.65	18/63858 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	4	PRO	N-CA-CB	6.76	110.44	103.00
1	J	4	PRO	N-CA-CB	6.74	110.41	103.00
1	O	227	GLY	N-CA-C	6.72	123.19	111.50
1	J	227	GLY	N-CA-C	6.71	123.18	111.50
1	M	227	GLY	N-CA-C	6.71	123.18	111.50
1	H	227	GLY	N-CA-C	6.71	123.17	111.50
1	D	227	GLY	N-CA-C	6.71	123.17	111.50
1	G	227	GLY	N-CA-C	6.70	123.16	111.50
1	M	4	PRO	N-CA-CB	6.70	110.37	103.00
1	N	4	PRO	N-CA-CB	6.70	110.36	103.00
1	A	227	GLY	N-CA-C	6.69	123.14	111.50
1	K	227	GLY	N-CA-C	6.69	123.14	111.50
1	L	227	GLY	N-CA-C	6.69	123.14	111.50
1	N	227	GLY	N-CA-C	6.69	123.13	111.50
1	F	227	GLY	N-CA-C	6.68	123.13	111.50
1	E	227	GLY	N-CA-C	6.68	123.12	111.50
1	I	227	GLY	N-CA-C	6.67	123.10	111.50
1	C	227	GLY	N-CA-C	6.65	123.07	111.50

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	1673	0	1665	70	0
1	C	1658	0	1656	75	0
1	D	1658	0	1656	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1658	0	1655	80	0
1	F	1658	0	1657	92	0
1	G	1658	0	1659	106	0
1	H	1658	0	1658	89	0
1	I	1658	0	1656	76	0
1	J	1678	0	1667	76	0
1	K	1678	0	1667	79	0
1	L	1673	0	1665	69	0
1	M	1678	0	1667	72	0
1	N	1678	0	1667	72	0
1	O	1668	0	1663	71	0
2	P	1638	0	1630	18	0
2	Q	1638	0	1630	14	0
2	R	1638	0	1630	14	0
2	S	1638	0	1630	15	0
2	T	1636	0	1625	11	0
2	U	1638	0	1630	13	0
2	V	1638	0	1630	17	0
2	W	1638	0	1630	14	0
2	X	1638	0	1630	15	0
2	Y	1638	0	1630	19	0
2	Z	1638	0	1630	15	0
2	a	1638	0	1630	12	0
2	b	1638	0	1630	13	0
2	c	1638	0	1630	16	0
3	d	34	0	30	24	0
3	e	34	0	30	23	0
3	f	34	0	30	31	0
3	g	34	0	30	13	0
3	h	34	0	30	12	0
3	i	34	0	30	12	0
3	j	34	0	30	8	0
All	All	46500	0	46283	1261	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 14.

All (1261) 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:H:26:ARG:NH2	3:g:173:TYR:CE2	1.74	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:ARG:NH2	1:I:48:ARG:NH1	1.62	1.45
1:C:52:LYS:CE	3:i:174:LEU:OXT	1.67	1.39
1:G:135:ARG:NH2	1:H:48:ARG:NH1	1.70	1.39
1:G:135:ARG:NH2	1:H:48:ARG:HH12	1.17	1.37
1:I:111:PHE:CE1	1:I:117:PRO:HB3	1.65	1.32
1:L:111:PHE:CE1	1:L:117:PRO:HB3	1.64	1.32
1:A:111:PHE:CE1	1:A:117:PRO:HB3	1.65	1.32
1:J:111:PHE:CE1	1:J:117:PRO:HB3	1.65	1.32
1:E:68:PHE:HA	1:E:71:PHE:CE2	1.65	1.32
1:M:111:PHE:CE1	1:M:117:PRO:HB3	1.65	1.32
1:A:68:PHE:HA	1:A:71:PHE:CE2	1.65	1.32
1:D:68:PHE:HA	1:D:71:PHE:CE2	1.65	1.32
1:G:111:PHE:CE1	1:G:117:PRO:HB3	1.65	1.32
1:K:68:PHE:HA	1:K:71:PHE:CE2	1.65	1.31
1:F:68:PHE:HA	1:F:71:PHE:CE2	1.65	1.31
1:J:68:PHE:HA	1:J:71:PHE:CE2	1.65	1.31
1:J:111:PHE:CD1	1:J:117:PRO:HB3	1.66	1.31
1:O:68:PHE:HA	1:O:71:PHE:CE2	1.65	1.31
1:A:111:PHE:CD1	1:A:117:PRO:HB3	1.66	1.31
1:D:111:PHE:CD1	1:D:117:PRO:HB3	1.66	1.31
1:G:111:PHE:CD1	1:G:117:PRO:HB3	1.66	1.31
1:L:111:PHE:CD1	1:L:117:PRO:HB3	1.66	1.31
1:C:111:PHE:CE1	1:C:117:PRO:HB3	1.65	1.31
1:G:68:PHE:HA	1:G:71:PHE:CE2	1.65	1.31
1:I:111:PHE:CD1	1:I:117:PRO:HB3	1.66	1.31
1:D:111:PHE:CE1	1:D:117:PRO:HB3	1.65	1.31
1:F:111:PHE:CE1	1:F:117:PRO:HB3	1.64	1.31
1:N:68:PHE:HA	1:N:71:PHE:CE2	1.65	1.31
1:N:111:PHE:CE1	1:N:117:PRO:HB3	1.65	1.31
1:C:68:PHE:HA	1:C:71:PHE:CE2	1.65	1.30
1:C:111:PHE:CD1	1:C:117:PRO:HB3	1.66	1.30
1:E:26:ARG:NH2	3:d:173:TYR:CE2	1.95	1.30
1:I:68:PHE:HA	1:I:71:PHE:CE2	1.65	1.30
1:M:111:PHE:CD1	1:M:117:PRO:HB3	1.66	1.30
1:O:111:PHE:CE1	1:O:117:PRO:HB3	1.65	1.30
1:E:26:ARG:NH2	3:d:173:TYR:OH	1.63	1.30
1:E:111:PHE:CE1	1:E:117:PRO:HB3	1.65	1.30
1:E:111:PHE:CD1	1:E:117:PRO:HB3	1.66	1.30
1:H:68:PHE:HA	1:H:71:PHE:CE2	1.65	1.30
1:F:111:PHE:CD1	1:F:117:PRO:HB3	1.66	1.30
1:L:68:PHE:HA	1:L:71:PHE:CE2	1.65	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:PHE:CE1	1:H:117:PRO:HB3	1.65	1.29
1:K:111:PHE:CD1	1:K:117:PRO:HB3	1.66	1.29
1:M:68:PHE:HA	1:M:71:PHE:CE2	1.65	1.29
1:N:111:PHE:CD1	1:N:117:PRO:HB3	1.66	1.29
1:I:52:LYS:NZ	3:h:174:LEU:OXT	1.63	1.29
1:H:111:PHE:CD1	1:H:117:PRO:HB3	1.66	1.29
1:K:111:PHE:CE1	1:K:117:PRO:HB3	1.65	1.29
1:O:111:PHE:CD1	1:O:117:PRO:HB3	1.66	1.28
1:G:50:LEU:CD1	3:f:172:GLN:HE21	1.48	1.27
1:G:50:LEU:HD12	3:f:172:GLN:NE2	1.54	1.22
1:E:26:ARG:NH2	3:d:173:TYR:CZ	2.00	1.22
1:E:26:ARG:NE	3:d:173:TYR:CE2	2.08	1.20
1:G:52:LYS:CE	3:f:174:LEU:HB3	1.70	1.20
1:G:50:LEU:CD1	3:f:172:GLN:NE2	2.03	1.20
1:J:114:GLN:HG3	1:J:115:ALA:H	1.06	1.19
1:F:135:ARG:NH2	1:G:48:ARG:HH12	1.39	1.19
1:G:66:GLY:O	3:f:174:LEU:O	1.53	1.19
1:F:26:ARG:NH2	3:e:173:TYR:OH	1.73	1.19
1:F:135:ARG:NH2	1:G:48:ARG:NH1	1.91	1.19
1:E:66:GLY:O	3:d:174:LEU:O	1.58	1.18
1:D:66:GLY:O	3:j:174:LEU:O	1.61	1.18
1:C:52:LYS:HE2	3:i:174:LEU:OXT	1.03	1.18
1:G:114:GLN:HG3	1:G:115:ALA:H	1.05	1.18
1:F:114:GLN:HG3	1:F:115:ALA:H	1.05	1.15
1:E:26:ARG:CZ	3:d:173:TYR:CE2	2.29	1.15
1:I:114:GLN:HG3	1:I:115:ALA:H	1.05	1.15
1:C:114:GLN:HG3	1:C:115:ALA:H	1.05	1.15
1:H:66:GLY:O	3:g:174:LEU:O	1.65	1.15
1:J:10:GLU:OE2	1:K:15:GLU:CG	1.95	1.15
1:A:114:GLN:HG3	1:A:115:ALA:H	1.05	1.14
1:J:10:GLU:OE2	1:K:15:GLU:HG3	1.51	1.10
1:D:114:GLN:HG3	1:D:115:ALA:H	1.05	1.10
1:E:114:GLN:HG3	1:E:115:ALA:H	1.05	1.10
1:L:114:GLN:HG3	1:L:115:ALA:H	1.05	1.10
1:G:52:LYS:NZ	3:f:174:LEU:OXT	1.85	1.10
1:K:114:GLN:HG3	1:K:115:ALA:H	1.05	1.10
1:G:135:ARG:HH21	1:H:48:ARG:NH1	1.32	1.09
1:N:114:GLN:HG3	1:N:115:ALA:H	1.05	1.09
1:O:114:GLN:HG3	1:O:115:ALA:H	1.05	1.09
1:J:6:PHE:CB	1:K:4:PRO:N	2.15	1.09
1:F:52:LYS:NZ	3:e:174:LEU:OXT	1.85	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:GLN:HG3	1:H:115:ALA:H	1.05	1.07
1:M:114:GLN:HG3	1:M:115:ALA:H	1.05	1.07
1:C:141:ILE:HG12	1:C:147:ILE:HG22	1.37	1.06
1:F:52:LYS:CE	3:e:174:LEU:OXT	2.03	1.06
1:M:141:ILE:HG12	1:M:147:ILE:HG22	1.37	1.06
1:F:141:ILE:HG12	1:F:147:ILE:HG22	1.37	1.06
1:N:10:GLU:OE2	1:O:15:GLU:CG	2.03	1.06
1:J:6:PHE:CB	1:K:4:PRO:O	2.04	1.05
1:D:141:ILE:HG12	1:D:147:ILE:HG22	1.38	1.05
1:O:141:ILE:HG12	1:O:147:ILE:HG22	1.37	1.05
1:A:141:ILE:HG12	1:A:147:ILE:HG22	1.37	1.05
1:F:135:ARG:HH21	1:G:48:ARG:NH1	1.53	1.04
1:G:141:ILE:HG12	1:G:147:ILE:HG22	1.37	1.04
1:N:141:ILE:HG12	1:N:147:ILE:HG22	1.37	1.03
1:H:141:ILE:HG12	1:H:147:ILE:HG22	1.37	1.03
1:L:141:ILE:HG12	1:L:147:ILE:HG22	1.37	1.03
2:V:301:THR:HG22	2:V:333:LYS:HZ1	1.18	1.03
1:F:52:LYS:HE2	3:e:174:LEU:OXT	1.58	1.02
1:E:141:ILE:HG12	1:E:147:ILE:HG22	1.37	1.02
1:J:141:ILE:HG12	1:J:147:ILE:HG22	1.37	1.02
1:K:141:ILE:HG12	1:K:147:ILE:HG22	1.38	1.02
1:L:6:PHE:CB	1:M:6:PHE:CB	2.37	1.02
1:C:52:LYS:NZ	3:i:174:LEU:OXT	1.93	1.01
1:A:15:GLU:CG	1:O:10:GLU:OE2	2.08	1.01
1:I:141:ILE:HG12	1:I:147:ILE:HG22	1.37	1.00
1:G:52:LYS:CE	3:f:174:LEU:OXT	2.09	1.00
1:E:26:ARG:NH2	3:d:173:TYR:HE2	1.55	0.99
1:D:146:SER:OG	3:d:172:GLN:HB3	1.62	0.98
2:Y:301:THR:HG22	2:Y:333:LYS:HZ3	1.28	0.98
1:G:52:LYS:HE3	3:f:174:LEU:HB3	1.43	0.98
1:L:10:GLU:OE2	1:M:15:GLU:CG	2.11	0.98
1:E:114:GLN:HG3	1:E:115:ALA:N	1.79	0.98
1:L:10:GLU:OE2	1:M:15:GLU:HG3	1.62	0.98
1:H:26:ARG:NH2	3:g:173:TYR:CZ	2.13	0.97
1:N:114:GLN:HG3	1:N:115:ALA:N	1.79	0.97
2:b:301:THR:HG22	2:b:333:LYS:HZ3	1.26	0.97
1:F:114:GLN:HG3	1:F:115:ALA:N	1.79	0.97
1:K:114:GLN:HG3	1:K:115:ALA:N	1.79	0.96
2:W:301:THR:HG22	2:W:333:LYS:HZ1	1.29	0.96
1:G:114:GLN:HG3	1:G:115:ALA:N	1.79	0.96
1:H:114:GLN:HG3	1:H:115:ALA:N	1.78	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:SER:OG	1:K:11:GLN:HG2	1.64	0.96
1:D:114:GLN:HG3	1:D:115:ALA:N	1.79	0.96
1:G:52:LYS:HE2	3:f:174:LEU:HB3	1.46	0.96
1:N:10:GLU:OE2	1:O:15:GLU:HG2	1.64	0.96
1:K:8:SER:OG	1:K:11:GLN:CG	2.13	0.95
1:O:114:GLN:HG3	1:O:115:ALA:N	1.79	0.95
1:E:46:PRO:HA	1:E:207:SER:HB2	1.48	0.95
1:L:114:GLN:HG3	1:L:115:ALA:N	1.79	0.95
1:M:114:GLN:HG3	1:M:115:ALA:N	1.78	0.95
1:J:114:GLN:HG3	1:J:115:ALA:N	1.79	0.94
1:I:114:GLN:HG3	1:I:115:ALA:N	1.79	0.94
2:U:301:THR:HG22	2:U:333:LYS:HZ3	1.29	0.94
1:C:46:PRO:HA	1:C:207:SER:HB2	1.47	0.94
1:M:10:GLU:OE2	1:N:15:GLU:CG	2.15	0.94
1:H:26:ARG:CZ	3:g:173:TYR:CE2	2.51	0.94
1:A:114:GLN:HG3	1:A:115:ALA:N	1.79	0.94
2:R:301:THR:HG22	2:R:333:LYS:HZ3	1.33	0.93
1:D:46:PRO:HA	1:D:207:SER:HB2	1.47	0.93
1:D:111:PHE:CE1	1:D:117:PRO:CB	2.52	0.93
1:M:111:PHE:CE1	1:M:117:PRO:CB	2.52	0.93
1:G:114:GLN:CG	1:G:115:ALA:H	1.82	0.93
1:L:111:PHE:CE1	1:L:117:PRO:CB	2.52	0.93
1:O:111:PHE:CE1	1:O:117:PRO:CB	2.52	0.93
1:C:111:PHE:CE1	1:C:117:PRO:CB	2.52	0.92
1:A:15:GLU:HG2	1:O:10:GLU:OE2	1.67	0.92
1:C:114:GLN:CG	1:C:115:ALA:H	1.82	0.92
1:F:111:PHE:CE1	1:F:117:PRO:CB	2.52	0.92
1:K:111:PHE:CE1	1:K:117:PRO:CB	2.52	0.92
1:L:114:GLN:CG	1:L:115:ALA:H	1.82	0.92
1:C:114:GLN:HG3	1:C:115:ALA:N	1.79	0.92
1:K:114:GLN:CG	1:K:115:ALA:H	1.82	0.92
1:N:10:GLU:OE2	1:O:15:GLU:HG3	1.69	0.92
1:G:50:LEU:HD11	3:f:172:GLN:HE21	1.34	0.92
1:H:111:PHE:CE1	1:H:117:PRO:CB	2.52	0.92
1:J:114:GLN:CG	1:J:115:ALA:H	1.82	0.92
1:O:114:GLN:CG	1:O:115:ALA:H	1.82	0.92
1:D:146:SER:OG	3:d:172:GLN:CB	2.18	0.92
1:E:111:PHE:CE1	1:E:117:PRO:CB	2.52	0.92
1:J:10:GLU:OE2	1:K:15:GLU:HG2	1.67	0.92
1:N:114:GLN:CG	1:N:115:ALA:H	1.82	0.92
2:a:301:THR:HG22	2:a:333:LYS:HZ3	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:GLN:CG	1:H:115:ALA:H	1.82	0.91
1:I:114:GLN:CG	1:I:115:ALA:H	1.82	0.91
1:E:114:GLN:CG	1:E:115:ALA:H	1.82	0.91
1:M:114:GLN:CG	1:M:115:ALA:H	1.82	0.91
2:Q:301:THR:HG22	2:Q:333:LYS:HZ1	1.32	0.91
1:A:111:PHE:CE1	1:A:117:PRO:CB	2.52	0.91
1:J:111:PHE:CE1	1:J:117:PRO:CB	2.52	0.91
1:N:111:PHE:CE1	1:N:117:PRO:CB	2.52	0.91
1:A:114:GLN:CG	1:A:115:ALA:H	1.82	0.91
2:c:301:THR:HG22	2:c:333:LYS:HZ1	1.36	0.91
1:D:114:GLN:CG	1:D:115:ALA:H	1.82	0.90
1:F:26:ARG:NH2	3:e:173:TYR:CZ	2.32	0.90
1:F:111:PHE:HE1	1:F:117:PRO:HB3	1.36	0.90
1:H:26:ARG:NH2	3:g:173:TYR:HE2	1.43	0.90
1:D:78:GLY:HA3	1:D:103:TYR:OH	1.72	0.90
1:J:111:PHE:HE1	1:J:117:PRO:HB3	1.36	0.90
1:F:114:GLN:CG	1:F:115:ALA:H	1.82	0.90
1:O:78:GLY:HA3	1:O:103:TYR:OH	1.72	0.90
1:G:111:PHE:CE1	1:G:117:PRO:CB	2.52	0.90
1:G:111:PHE:HE1	1:G:117:PRO:HB3	1.36	0.90
1:M:78:GLY:HA3	1:M:103:TYR:OH	1.72	0.90
1:A:78:GLY:HA3	1:A:103:TYR:OH	1.72	0.90
1:I:111:PHE:CE1	1:I:117:PRO:CB	2.52	0.90
1:M:46:PRO:HA	1:M:207:SER:HB2	1.52	0.90
1:E:111:PHE:HE1	1:E:117:PRO:HB3	1.37	0.90
1:I:46:PRO:HA	1:I:207:SER:HB2	1.52	0.90
1:F:78:GLY:HA3	1:F:103:TYR:OH	1.72	0.89
1:O:111:PHE:HE1	1:O:117:PRO:HB3	1.36	0.89
1:C:68:PHE:HD1	1:C:71:PHE:CZ	1.91	0.89
1:J:78:GLY:HA3	1:J:103:TYR:OH	1.72	0.89
1:L:111:PHE:HE1	1:L:117:PRO:HB3	1.36	0.89
1:O:68:PHE:HD1	1:O:71:PHE:CZ	1.91	0.89
1:I:78:GLY:HA3	1:I:103:TYR:OH	1.72	0.89
1:C:111:PHE:HE1	1:C:117:PRO:HB3	1.37	0.89
1:E:78:GLY:HA3	1:E:103:TYR:OH	1.72	0.89
1:F:46:PRO:HA	1:F:207:SER:HB2	1.54	0.89
1:K:78:GLY:HA3	1:K:103:TYR:OH	1.72	0.89
1:E:68:PHE:HD1	1:E:71:PHE:CZ	1.91	0.89
1:L:78:GLY:HA3	1:L:103:TYR:OH	1.72	0.89
1:N:111:PHE:HD1	1:N:117:PRO:HB3	1.38	0.89
1:G:78:GLY:HA3	1:G:103:TYR:OH	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:LYS:HZ3	3:f:174:LEU:C	1.81	0.89
1:H:111:PHE:HD1	1:H:117:PRO:HB3	1.38	0.89
1:M:68:PHE:HD1	1:M:71:PHE:CZ	1.91	0.89
1:J:68:PHE:HD1	1:J:71:PHE:CZ	1.91	0.88
1:K:68:PHE:HD1	1:K:71:PHE:CZ	1.91	0.88
1:N:78:GLY:HA3	1:N:103:TYR:OH	1.72	0.88
1:G:135:ARG:HH22	1:H:48:ARG:NH1	1.71	0.88
1:G:68:PHE:HD1	1:G:71:PHE:CZ	1.91	0.88
1:H:46:PRO:HA	1:H:207:SER:HB2	1.55	0.88
1:K:46:PRO:HA	1:K:207:SER:HB2	1.53	0.88
1:M:111:PHE:HE1	1:M:117:PRO:HB3	1.36	0.88
1:L:68:PHE:HD1	1:L:71:PHE:CZ	1.91	0.88
1:C:78:GLY:HA3	1:C:103:TYR:OH	1.72	0.88
1:A:111:PHE:HE1	1:A:117:PRO:HB3	1.37	0.88
1:I:68:PHE:HD1	1:I:71:PHE:CZ	1.91	0.88
1:H:78:GLY:HA3	1:H:103:TYR:OH	1.72	0.88
1:N:111:PHE:HE1	1:N:117:PRO:HB3	1.36	0.88
1:G:52:LYS:HE2	3:f:174:LEU:OXT	1.72	0.87
1:A:68:PHE:HD1	1:A:71:PHE:CZ	1.91	0.87
1:D:68:PHE:HD1	1:D:71:PHE:CZ	1.91	0.87
1:F:68:PHE:HD1	1:F:71:PHE:CZ	1.91	0.87
1:H:68:PHE:HD1	1:H:71:PHE:CZ	1.91	0.87
1:D:111:PHE:HE1	1:D:117:PRO:HB3	1.36	0.87
1:N:68:PHE:HD1	1:N:71:PHE:CZ	1.91	0.87
1:L:46:PRO:HA	1:L:207:SER:HB2	1.55	0.87
1:G:50:LEU:HD12	3:f:172:GLN:HE22	1.34	0.87
1:M:111:PHE:HD1	1:M:117:PRO:HB3	1.38	0.87
1:I:111:PHE:HE1	1:I:117:PRO:HB3	1.36	0.86
1:L:111:PHE:HD1	1:L:117:PRO:HB3	1.38	0.86
1:E:111:PHE:HD1	1:E:117:PRO:HB3	1.38	0.86
1:K:111:PHE:HD1	1:K:117:PRO:HB3	1.38	0.86
1:A:111:PHE:HD1	1:A:117:PRO:HB3	1.38	0.85
1:I:111:PHE:HD1	1:I:117:PRO:HB3	1.38	0.85
1:N:46:PRO:HA	1:N:207:SER:HB2	1.58	0.85
1:I:189:ARG:HD3	1:I:203:LEU:HD23	1.58	0.85
1:L:189:ARG:HD3	1:L:203:LEU:HD23	1.59	0.85
1:D:146:SER:CB	3:d:172:GLN:HB2	2.06	0.85
1:H:135:ARG:HH22	1:I:48:ARG:NH1	1.74	0.85
1:F:189:ARG:HD3	1:F:203:LEU:HD23	1.58	0.85
1:M:10:GLU:OE2	1:N:15:GLU:HG3	1.75	0.84
2:W:301:THR:HG22	2:W:333:LYS:NZ	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:301:THR:HG22	2:c:333:LYS:NZ	1.92	0.84
1:C:189:ARG:HD3	1:C:203:LEU:HD23	1.59	0.84
2:P:301:THR:HG22	2:P:333:LYS:NZ	1.92	0.84
2:V:301:THR:HG22	2:V:333:LYS:NZ	1.92	0.84
2:a:301:THR:HG22	2:a:333:LYS:NZ	1.92	0.84
1:O:189:ARG:HD3	1:O:203:LEU:HD23	1.59	0.84
1:K:189:ARG:HD3	1:K:203:LEU:HD23	1.59	0.84
2:Z:301:THR:HG22	2:Z:333:LYS:NZ	1.92	0.84
2:Y:301:THR:HG22	2:Y:333:LYS:NZ	1.92	0.83
1:E:26:ARG:CZ	3:d:173:TYR:CZ	2.58	0.83
1:E:189:ARG:HD3	1:E:203:LEU:HD23	1.59	0.83
1:A:189:ARG:HD3	1:A:203:LEU:HD23	1.59	0.83
1:K:111:PHE:HE1	1:K:117:PRO:HB3	1.37	0.83
1:G:46:PRO:HA	1:G:207:SER:HB2	1.59	0.83
2:Q:301:THR:HG22	2:Q:333:LYS:NZ	1.92	0.83
2:S:301:THR:HG22	2:S:333:LYS:HZ3	1.41	0.83
2:U:301:THR:HG22	2:U:333:LYS:NZ	1.92	0.83
1:J:189:ARG:HD3	1:J:203:LEU:HD23	1.58	0.83
2:S:301:THR:HG22	2:S:333:LYS:NZ	1.92	0.83
1:D:189:ARG:HD3	1:D:203:LEU:HD23	1.59	0.83
1:I:52:LYS:CE	3:h:174:LEU:OXT	2.26	0.83
1:N:189:ARG:HD3	1:N:203:LEU:HD23	1.59	0.83
1:M:10:GLU:OE2	1:N:15:GLU:HG2	1.79	0.83
2:P:301:THR:HG22	2:P:333:LYS:HZ1	1.44	0.83
1:G:189:ARG:HD3	1:G:203:LEU:HD23	1.59	0.82
2:X:301:THR:HG22	2:X:333:LYS:HZ1	1.43	0.82
1:M:189:ARG:HD3	1:M:203:LEU:HD23	1.59	0.82
2:R:301:THR:HG22	2:R:333:LYS:NZ	1.92	0.82
1:J:111:PHE:HD1	1:J:117:PRO:HB3	1.38	0.82
2:b:301:THR:HG22	2:b:333:LYS:NZ	1.92	0.82
1:F:52:LYS:HZ3	3:e:174:LEU:C	1.86	0.82
1:H:189:ARG:HD3	1:H:203:LEU:HD23	1.59	0.82
2:X:301:THR:HG22	2:X:333:LYS:NZ	1.92	0.82
1:H:111:PHE:HE1	1:H:117:PRO:HB3	1.37	0.82
1:D:111:PHE:HD1	1:D:117:PRO:HB3	1.38	0.82
1:O:111:PHE:HD1	1:O:117:PRO:HB3	1.38	0.82
1:C:111:PHE:HD1	1:C:117:PRO:HB3	1.38	0.81
1:L:111:PHE:CD1	1:L:117:PRO:CB	2.60	0.81
1:D:146:SER:HB3	3:d:172:GLN:HB2	1.61	0.81
1:F:111:PHE:HD1	1:F:117:PRO:HB3	1.38	0.81
1:A:10:GLU:OE2	1:J:15:GLU:CG	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:PHE:CD1	1:H:117:PRO:CB	2.60	0.81
1:F:111:PHE:CD1	1:F:117:PRO:CB	2.60	0.80
1:G:111:PHE:HD1	1:G:117:PRO:HB3	1.38	0.80
1:C:68:PHE:HA	1:C:71:PHE:CD2	2.17	0.79
1:D:68:PHE:HA	1:D:71:PHE:CD2	2.18	0.79
1:I:111:PHE:CD1	1:I:117:PRO:CB	2.60	0.79
1:O:111:PHE:CD1	1:O:117:PRO:CB	2.60	0.79
2:Z:301:THR:HG22	2:Z:333:LYS:HZ1	1.44	0.79
1:I:68:PHE:CA	1:I:71:PHE:CE2	2.60	0.79
1:O:68:PHE:HA	1:O:71:PHE:CD2	2.18	0.79
1:A:15:GLU:HG3	1:O:10:GLU:OE2	1.81	0.79
1:N:68:PHE:HA	1:N:71:PHE:CD2	2.18	0.79
1:O:46:PRO:HA	1:O:207:SER:HB2	1.63	0.79
1:G:111:PHE:CD1	1:G:117:PRO:CB	2.60	0.79
1:J:46:PRO:HA	1:J:207:SER:HB2	1.63	0.79
1:F:52:LYS:CE	3:e:174:LEU:HB3	2.13	0.79
1:J:68:PHE:HA	1:J:71:PHE:CD2	2.18	0.79
1:M:68:PHE:HA	1:M:71:PHE:CD2	2.18	0.79
1:N:111:PHE:CD1	1:N:117:PRO:CB	2.60	0.79
1:A:68:PHE:HA	1:A:71:PHE:CD2	2.18	0.79
1:E:68:PHE:HA	1:E:71:PHE:CD2	2.18	0.79
1:N:189:ARG:HD3	1:N:203:LEU:CD2	2.13	0.79
1:G:68:PHE:CA	1:G:71:PHE:CE2	2.60	0.79
1:H:68:PHE:HA	1:H:71:PHE:CD2	2.18	0.79
1:I:68:PHE:HA	1:I:71:PHE:CD2	2.18	0.79
1:N:68:PHE:CA	1:N:71:PHE:CE2	2.60	0.78
1:D:189:ARG:HD3	1:D:203:LEU:CD2	2.13	0.78
1:E:189:ARG:HD3	1:E:203:LEU:CD2	2.13	0.78
1:G:189:ARG:HD3	1:G:203:LEU:CD2	2.13	0.78
1:M:189:ARG:HD3	1:M:203:LEU:CD2	2.13	0.78
1:O:68:PHE:CA	1:O:71:PHE:CE2	2.60	0.78
1:J:189:ARG:HD3	1:J:203:LEU:CD2	2.13	0.78
1:O:189:ARG:HD3	1:O:203:LEU:CD2	2.13	0.78
1:L:189:ARG:HD3	1:L:203:LEU:CD2	2.14	0.78
1:F:68:PHE:HA	1:F:71:PHE:CD2	2.17	0.78
1:H:189:ARG:HD3	1:H:203:LEU:CD2	2.13	0.78
1:F:189:ARG:HD3	1:F:203:LEU:CD2	2.13	0.78
1:M:111:PHE:CD1	1:M:117:PRO:CB	2.60	0.78
1:A:189:ARG:HD3	1:A:203:LEU:CD2	2.13	0.77
1:D:26:ARG:NH2	3:j:173:TYR:OH	2.16	0.77
1:I:189:ARG:HD3	1:I:203:LEU:CD2	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HA	1:A:207:SER:HB2	1.66	0.77
1:G:68:PHE:HA	1:G:71:PHE:CD2	2.18	0.77
1:J:111:PHE:CD1	1:J:117:PRO:CB	2.60	0.77
1:K:68:PHE:HA	1:K:71:PHE:CD2	2.17	0.77
1:L:68:PHE:HA	1:L:71:PHE:CD2	2.18	0.77
1:K:189:ARG:HD3	1:K:203:LEU:CD2	2.13	0.77
1:D:68:PHE:CA	1:D:71:PHE:CE2	2.59	0.77
1:E:52:LYS:NZ	3:d:174:LEU:OXT	2.16	0.77
1:C:189:ARG:HD3	1:C:203:LEU:CD2	2.13	0.76
1:A:111:PHE:CD1	1:A:117:PRO:CB	2.60	0.76
1:E:87:TYR:CE1	2:S:357:ARG:NH1	2.54	0.76
1:E:26:ARG:NE	3:d:173:TYR:CZ	2.54	0.76
1:H:135:ARG:NH2	1:I:48:ARG:HH11	1.83	0.76
1:E:111:PHE:CD1	1:E:117:PRO:CB	2.60	0.76
1:F:26:ARG:NH2	3:e:173:TYR:CE2	2.53	0.76
1:G:52:LYS:CE	3:f:174:LEU:CB	2.59	0.76
1:J:68:PHE:CA	1:J:71:PHE:CE2	2.60	0.76
1:K:68:PHE:CA	1:K:71:PHE:CE2	2.60	0.76
1:F:68:PHE:CA	1:F:71:PHE:CE2	2.60	0.76
2:V:338:ASP:OD1	2:V:341:THR:OG1	2.05	0.75
1:H:68:PHE:CA	1:H:71:PHE:CE2	2.60	0.75
1:C:52:LYS:HE2	3:i:174:LEU:C	2.05	0.75
1:K:111:PHE:CD1	1:K:117:PRO:CB	2.60	0.75
2:P:338:ASP:OD1	2:P:341:THR:OG1	2.05	0.75
1:A:68:PHE:CA	1:A:71:PHE:CE2	2.60	0.75
1:C:68:PHE:CA	1:C:71:PHE:CE2	2.60	0.75
1:O:111:PHE:HE1	1:O:117:PRO:CB	1.97	0.74
1:E:68:PHE:CA	1:E:71:PHE:CE2	2.60	0.74
2:S:338:ASP:OD1	2:S:341:THR:OG1	2.05	0.74
2:c:338:ASP:OD1	2:c:341:THR:OG1	2.05	0.74
1:O:68:PHE:HA	1:O:71:PHE:HE2	1.51	0.74
1:C:111:PHE:HE1	1:C:117:PRO:CB	1.97	0.74
2:Y:338:ASP:OD1	2:Y:341:THR:OG1	2.05	0.74
1:D:111:PHE:CD1	1:D:117:PRO:CB	2.60	0.73
1:H:111:PHE:HE1	1:H:117:PRO:CB	1.97	0.73
1:N:68:PHE:CD1	1:N:71:PHE:CZ	2.77	0.73
1:G:26:ARG:NH2	3:f:173:TYR:OH	2.22	0.73
2:U:338:ASP:OD1	2:U:341:THR:OG1	2.05	0.73
1:D:68:PHE:CD1	1:D:71:PHE:CZ	2.77	0.73
1:K:68:PHE:HA	1:K:71:PHE:HE2	1.51	0.73
2:X:338:ASP:OD1	2:X:341:THR:OG1	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASN:OD1	1:C:70:GLU:HG3	1.89	0.73
2:a:338:ASP:OD1	2:a:341:THR:OG1	2.05	0.73
1:A:10:GLU:OE2	1:J:15:GLU:HG2	1.88	0.73
1:L:68:PHE:CA	1:L:71:PHE:CE2	2.60	0.73
1:K:111:PHE:HE1	1:K:117:PRO:CB	1.97	0.72
1:D:111:PHE:HE1	1:D:117:PRO:CB	1.97	0.72
1:M:69:ASN:OD1	1:M:70:GLU:HG3	1.89	0.72
1:F:69:ASN:OD1	1:F:70:GLU:HG3	1.89	0.72
1:D:69:ASN:OD1	1:D:70:GLU:HG3	1.89	0.72
1:F:68:PHE:CD1	1:F:71:PHE:CZ	2.77	0.72
1:H:68:PHE:CD1	1:H:71:PHE:CZ	2.77	0.72
1:I:68:PHE:CD1	1:I:71:PHE:CZ	2.77	0.72
1:A:68:PHE:CD1	1:A:71:PHE:CZ	2.77	0.72
1:C:111:PHE:CD1	1:C:117:PRO:CB	2.60	0.72
1:N:69:ASN:OD1	1:N:70:GLU:HG3	1.89	0.72
1:C:68:PHE:HA	1:C:71:PHE:HE2	1.51	0.72
1:M:68:PHE:CD1	1:M:71:PHE:CZ	2.77	0.72
1:M:68:PHE:CA	1:M:71:PHE:CE2	2.60	0.72
1:N:111:PHE:HE1	1:N:117:PRO:CB	1.97	0.72
1:E:69:ASN:OD1	1:E:70:GLU:HG3	1.89	0.72
1:G:69:ASN:OD1	1:G:70:GLU:HG3	1.89	0.72
1:K:68:PHE:CD1	1:K:71:PHE:CZ	2.77	0.72
1:L:69:ASN:OD1	1:L:70:GLU:HG3	1.89	0.72
1:F:111:PHE:HE1	1:F:117:PRO:CB	1.97	0.72
1:N:74:LEU:HD23	1:N:122:LEU:HD11	1.72	0.72
1:O:74:LEU:HD23	1:O:122:LEU:HD11	1.72	0.72
1:K:74:LEU:HD23	1:K:122:LEU:HD11	1.72	0.71
1:E:74:LEU:HD23	1:E:122:LEU:HD11	1.72	0.71
1:I:69:ASN:OD1	1:I:70:GLU:HG3	1.89	0.71
1:J:74:LEU:HD23	1:J:122:LEU:HD11	1.73	0.71
1:J:69:ASN:OD1	1:J:70:GLU:HG3	1.89	0.71
1:G:52:LYS:NZ	3:f:174:LEU:C	2.45	0.71
1:G:74:LEU:HD23	1:G:122:LEU:HD11	1.72	0.71
1:H:69:ASN:OD1	1:H:70:GLU:HG3	1.89	0.71
1:I:74:LEU:HD23	1:I:122:LEU:HD11	1.72	0.71
1:J:68:PHE:CD1	1:J:71:PHE:CZ	2.77	0.71
1:J:111:PHE:HE1	1:J:117:PRO:CB	1.97	0.71
1:A:69:ASN:OD1	1:A:70:GLU:HG3	1.90	0.71
1:E:68:PHE:HA	1:E:71:PHE:HE2	1.51	0.71
1:G:68:PHE:CD1	1:G:71:PHE:CZ	2.77	0.71
1:D:74:LEU:HD23	1:D:122:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:74:LEU:HD23	1:L:122:LEU:HD11	1.72	0.71
1:O:68:PHE:CD1	1:O:71:PHE:CZ	2.77	0.71
1:O:69:ASN:OD1	1:O:70:GLU:HG3	1.89	0.71
1:C:74:LEU:HD23	1:C:122:LEU:HD11	1.72	0.71
1:F:135:ARG:HH22	1:G:48:ARG:NH1	1.88	0.71
1:A:234:LEU:O	1:A:234:LEU:HG	1.91	0.71
1:K:10:GLU:OE1	1:K:10:GLU:N	2.20	0.71
1:G:234:LEU:O	1:G:234:LEU:HG	1.91	0.70
1:D:68:PHE:HA	1:D:71:PHE:HE2	1.51	0.70
1:E:111:PHE:HE1	1:E:117:PRO:CB	1.97	0.70
1:K:69:ASN:OD1	1:K:70:GLU:HG3	1.90	0.70
1:K:234:LEU:O	1:K:234:LEU:HG	1.91	0.70
1:N:234:LEU:O	1:N:234:LEU:HG	1.91	0.70
1:M:74:LEU:HD23	1:M:122:LEU:HD11	1.73	0.70
2:R:338:ASP:OD1	2:R:341:THR:OG1	2.05	0.70
1:E:68:PHE:CD1	1:E:71:PHE:CZ	2.77	0.70
1:H:74:LEU:HD23	1:H:122:LEU:HD11	1.73	0.70
1:I:234:LEU:O	1:I:234:LEU:HG	1.91	0.70
1:D:234:LEU:O	1:D:234:LEU:HG	1.91	0.70
1:L:68:PHE:HA	1:L:71:PHE:HE2	1.51	0.70
1:C:234:LEU:HG	1:C:234:LEU:O	1.91	0.70
1:H:234:LEU:HG	1:H:234:LEU:O	1.91	0.70
1:E:234:LEU:HG	1:E:234:LEU:O	1.91	0.70
1:G:111:PHE:HE1	1:G:117:PRO:CB	1.97	0.70
1:C:68:PHE:CD1	1:C:71:PHE:CZ	2.77	0.69
1:F:74:LEU:HD23	1:F:122:LEU:HD11	1.72	0.69
1:A:74:LEU:HD23	1:A:122:LEU:HD11	1.72	0.69
1:J:234:LEU:HG	1:J:234:LEU:O	1.91	0.69
1:J:68:PHE:HA	1:J:71:PHE:HE2	1.51	0.69
1:L:234:LEU:O	1:L:234:LEU:HG	1.91	0.69
1:D:146:SER:CB	3:d:172:GLN:CB	2.70	0.69
1:O:234:LEU:HG	1:O:234:LEU:O	1.91	0.69
2:W:338:ASP:OD1	2:W:341:THR:OG1	2.05	0.69
1:H:68:PHE:HA	1:H:71:PHE:HE2	1.51	0.69
1:L:68:PHE:CD1	1:L:71:PHE:CZ	2.77	0.69
1:M:234:LEU:HG	1:M:234:LEU:O	1.91	0.69
1:I:111:PHE:HE1	1:I:117:PRO:CB	1.97	0.68
1:F:234:LEU:O	1:F:234:LEU:HG	1.91	0.68
1:H:26:ARG:NH2	3:g:173:TYR:OH	2.26	0.68
1:L:111:PHE:HE1	1:L:117:PRO:CB	1.97	0.68
1:G:52:LYS:HE2	3:f:174:LEU:CB	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:PRO:HA	1:E:207:SER:CB	2.24	0.68
1:A:68:PHE:HA	1:A:71:PHE:HE2	1.51	0.68
1:G:68:PHE:HA	1:G:71:PHE:HE2	1.51	0.67
1:A:10:GLU:OE2	1:J:15:GLU:HG3	1.93	0.67
1:F:33:LEU:HD11	1:F:180:ALA:HB1	1.77	0.67
1:E:33:LEU:HD11	1:E:180:ALA:HB1	1.77	0.67
1:M:111:PHE:HE1	1:M:117:PRO:CB	1.97	0.67
1:D:26:ARG:NH2	3:j:173:TYR:CZ	2.61	0.67
1:G:33:LEU:HD11	1:G:180:ALA:HB1	1.77	0.67
1:J:33:LEU:HD11	1:J:180:ALA:HB1	1.77	0.67
1:E:52:LYS:CE	3:d:174:LEU:OXT	2.43	0.67
1:N:33:LEU:HD11	1:N:180:ALA:HB1	1.77	0.67
2:b:338:ASP:OD1	2:b:341:THR:OG1	2.05	0.67
1:C:33:LEU:HD11	1:C:180:ALA:HB1	1.77	0.67
1:C:46:PRO:HA	1:C:207:SER:CB	2.23	0.66
1:O:33:LEU:HD11	1:O:180:ALA:HB1	1.77	0.66
1:D:46:PRO:HA	1:D:207:SER:CB	2.24	0.66
1:D:33:LEU:HD11	1:D:180:ALA:HB1	1.77	0.66
1:F:52:LYS:HE3	3:e:174:LEU:HB3	1.78	0.66
1:M:68:PHE:HA	1:M:71:PHE:HE2	1.51	0.66
1:A:33:LEU:HD11	1:A:180:ALA:HB1	1.77	0.66
1:A:111:PHE:HE1	1:A:117:PRO:CB	1.97	0.66
1:L:10:GLU:OE2	1:M:15:GLU:HG2	1.94	0.66
1:H:26:ARG:NE	3:g:173:TYR:CD2	2.64	0.66
1:I:33:LEU:HD11	1:I:180:ALA:HB1	1.77	0.66
2:T:338:ASP:OD1	2:T:341:THR:OG1	2.05	0.66
1:F:68:PHE:HA	1:F:71:PHE:HE2	1.51	0.65
1:F:111:PHE:HE1	1:F:117:PRO:CG	2.09	0.65
1:I:111:PHE:HE1	1:I:117:PRO:CG	2.09	0.65
1:K:111:PHE:HE1	1:K:117:PRO:CG	2.09	0.65
1:K:87:TYR:CE1	2:Y:357:ARG:NH1	2.64	0.65
1:L:33:LEU:HD11	1:L:180:ALA:HB1	1.77	0.65
1:G:52:LYS:NZ	3:f:174:LEU:CA	2.59	0.65
1:N:111:PHE:HE1	1:N:117:PRO:CG	2.09	0.65
1:D:146:SER:OG	3:d:172:GLN:HB2	1.96	0.65
1:E:111:PHE:HE1	1:E:117:PRO:CG	2.09	0.65
1:O:111:PHE:HE1	1:O:117:PRO:CG	2.09	0.65
1:A:111:PHE:HE1	1:A:117:PRO:CG	2.09	0.65
1:G:111:PHE:HE1	1:G:117:PRO:CG	2.09	0.65
1:H:111:PHE:HE1	1:H:117:PRO:CG	2.09	0.64
1:M:33:LEU:HD11	1:M:180:ALA:HB1	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:68:PHE:HA	1:N:71:PHE:HE2	1.51	0.64
1:D:111:PHE:HE1	1:D:117:PRO:CG	2.09	0.64
1:L:111:PHE:HE1	1:L:117:PRO:CG	2.09	0.64
1:H:33:LEU:HD11	1:H:180:ALA:HB1	1.77	0.64
1:K:33:LEU:HD11	1:K:180:ALA:HB1	1.77	0.64
2:R:324:ASN:O	2:a:479:SER:OG	2.14	0.64
1:F:26:ARG:NH2	3:e:173:TYR:HH	1.94	0.64
1:I:46:PRO:HA	1:I:207:SER:CB	2.26	0.64
1:J:111:PHE:HE1	1:J:117:PRO:CG	2.09	0.64
1:K:68:PHE:HD1	1:K:71:PHE:HZ	1.46	0.64
1:F:46:PRO:HA	1:F:207:SER:CB	2.28	0.64
1:K:46:PRO:HA	1:K:207:SER:CB	2.27	0.64
1:M:111:PHE:HE1	1:M:117:PRO:CG	2.09	0.64
1:C:111:PHE:HE1	1:C:117:PRO:CG	2.09	0.63
1:I:52:LYS:HZ3	3:h:174:LEU:C	1.92	0.63
1:F:50:LEU:CD1	3:e:172:GLN:NE2	2.61	0.63
1:H:26:ARG:NE	3:g:173:TYR:CE2	2.66	0.63
1:L:87:TYR:CE1	2:Z:357:ARG:NH1	2.66	0.63
1:I:100:ALA:O	1:I:141:ILE:HD11	1.99	0.63
1:G:100:ALA:O	1:G:141:ILE:HD11	1.99	0.63
1:A:100:ALA:O	1:A:141:ILE:HD11	1.99	0.62
1:E:100:ALA:O	1:E:141:ILE:HD11	1.99	0.62
1:L:68:PHE:HD1	1:L:71:PHE:HZ	1.46	0.62
1:M:100:ALA:O	1:M:141:ILE:HD11	1.99	0.62
1:E:52:LYS:HE2	3:d:174:LEU:OXT	1.99	0.62
1:F:100:ALA:O	1:F:141:ILE:HD11	1.99	0.62
1:G:135:ARG:HH21	1:H:48:ARG:CZ	2.08	0.62
1:H:52:LYS:NZ	3:g:174:LEU:OXT	2.19	0.62
1:N:68:PHE:HD1	1:N:71:PHE:HZ	1.46	0.62
1:G:50:LEU:HD11	3:f:172:GLN:NE2	1.98	0.62
1:I:68:PHE:HA	1:I:71:PHE:HE2	1.51	0.62
1:L:100:ALA:O	1:L:141:ILE:HD11	1.99	0.62
1:M:46:PRO:HA	1:M:207:SER:CB	2.26	0.62
1:H:100:ALA:O	1:H:141:ILE:HD11	1.99	0.62
1:J:100:ALA:O	1:J:141:ILE:HD11	1.99	0.62
1:C:100:ALA:O	1:C:141:ILE:HD11	1.99	0.62
1:K:100:ALA:O	1:K:141:ILE:HD11	1.99	0.62
1:L:46:PRO:HA	1:L:207:SER:CB	2.29	0.62
1:O:100:ALA:O	1:O:141:ILE:HD11	1.99	0.62
1:D:100:ALA:O	1:D:141:ILE:HD11	1.99	0.62
1:H:68:PHE:HD1	1:H:71:PHE:HZ	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:100:ALA:O	1:N:141:ILE:HD11	1.99	0.62
1:H:46:PRO:HA	1:H:207:SER:CB	2.29	0.61
1:M:68:PHE:HD1	1:M:71:PHE:HZ	1.46	0.61
1:N:46:PRO:HA	1:N:207:SER:CB	2.31	0.61
1:F:68:PHE:HD1	1:F:71:PHE:HZ	1.46	0.61
1:A:68:PHE:HD1	1:A:71:PHE:HZ	1.46	0.61
1:F:50:LEU:CD1	3:e:172:GLN:HE21	2.13	0.61
1:G:52:LYS:HZ1	3:f:174:LEU:HA	1.65	0.61
1:J:189:ARG:CD	1:J:203:LEU:CD2	2.79	0.60
1:O:68:PHE:HD1	1:O:71:PHE:HZ	1.46	0.60
1:F:189:ARG:CD	1:F:203:LEU:CD2	2.79	0.60
1:I:52:LYS:CE	3:h:174:LEU:HB3	2.30	0.60
1:D:147:ILE:O	3:d:172:GLN:NE2	2.34	0.60
1:G:189:ARG:CD	1:G:203:LEU:CD2	2.80	0.60
1:H:189:ARG:CD	1:H:203:LEU:CD2	2.80	0.60
1:D:68:PHE:HD1	1:D:71:PHE:HZ	1.46	0.60
1:C:140:ARG:NH1	1:C:154:VAL:HG13	2.17	0.60
1:C:189:ARG:CD	1:C:203:LEU:CD2	2.79	0.60
1:I:68:PHE:HD1	1:I:71:PHE:HZ	1.46	0.60
1:I:140:ARG:NH1	1:I:154:VAL:HG13	2.17	0.60
1:K:140:ARG:NH1	1:K:154:VAL:HG13	2.17	0.60
1:G:189:ARG:CD	1:G:203:LEU:HD21	2.32	0.60
1:H:140:ARG:NH1	1:H:154:VAL:HG13	2.17	0.60
1:I:189:ARG:CD	1:I:203:LEU:HD21	2.32	0.60
1:D:189:ARG:CD	1:D:203:LEU:HD21	2.32	0.60
1:H:189:ARG:CD	1:H:203:LEU:HD21	2.32	0.60
1:I:189:ARG:CD	1:I:203:LEU:CD2	2.79	0.60
1:K:8:SER:OG	1:K:11:GLN:HG3	2.01	0.60
1:K:189:ARG:CD	1:K:203:LEU:HD21	2.32	0.60
1:A:189:ARG:CD	1:A:203:LEU:CD2	2.80	0.60
1:J:189:ARG:CD	1:J:203:LEU:HD21	2.32	0.60
1:L:189:ARG:CD	1:L:203:LEU:CD2	2.80	0.60
1:M:189:ARG:CD	1:M:203:LEU:HD21	2.32	0.60
1:N:140:ARG:NH1	1:N:154:VAL:HG13	2.17	0.60
1:D:140:ARG:NH1	1:D:154:VAL:HG13	2.17	0.59
1:E:68:PHE:HD1	1:E:71:PHE:HZ	1.46	0.59
1:L:140:ARG:NH1	1:L:154:VAL:HG13	2.17	0.59
1:F:189:ARG:CD	1:F:203:LEU:HD21	2.32	0.59
1:A:189:ARG:CD	1:A:203:LEU:HD21	2.32	0.59
1:E:140:ARG:NH1	1:E:154:VAL:HG13	2.17	0.59
1:K:189:ARG:CD	1:K:203:LEU:CD2	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ARG:NH1	1:A:154:VAL:HG13	2.17	0.59
1:G:46:PRO:HA	1:G:207:SER:CB	2.31	0.59
1:N:189:ARG:CD	1:N:203:LEU:HD21	2.32	0.59
1:E:189:ARG:CD	1:E:203:LEU:CD2	2.80	0.59
1:E:189:ARG:CD	1:E:203:LEU:HD21	2.32	0.59
1:M:189:ARG:CD	1:M:203:LEU:CD2	2.80	0.59
1:C:189:ARG:CD	1:C:203:LEU:HD21	2.32	0.59
1:N:189:ARG:CD	1:N:203:LEU:CD2	2.80	0.59
1:O:189:ARG:CD	1:O:203:LEU:HD21	2.32	0.59
1:F:50:LEU:HD12	3:e:172:GLN:NE2	2.17	0.59
1:M:140:ARG:NH1	1:M:154:VAL:HG13	2.17	0.59
3:e:172:GLN:HA	3:e:172:GLN:OE1	2.03	0.59
1:G:140:ARG:NH1	1:G:154:VAL:HG13	2.17	0.58
3:f:172:GLN:HA	3:f:172:GLN:OE1	2.03	0.58
1:D:189:ARG:CD	1:D:203:LEU:CD2	2.80	0.58
1:O:189:ARG:CD	1:O:203:LEU:CD2	2.80	0.58
1:F:140:ARG:NH1	1:F:154:VAL:HG13	2.17	0.58
1:J:140:ARG:NH1	1:J:154:VAL:HG13	2.17	0.58
3:j:172:GLN:HA	3:j:172:GLN:OE1	2.03	0.58
3:h:172:GLN:HA	3:h:172:GLN:OE1	2.03	0.58
3:i:172:GLN:OE1	3:i:172:GLN:HA	2.03	0.58
1:G:28:LYS:HB2	1:G:52:LYS:HZ2	1.68	0.58
1:O:140:ARG:NH1	1:O:154:VAL:HG13	2.17	0.58
1:L:189:ARG:CD	1:L:203:LEU:HD21	2.32	0.58
2:T:345:ILE:HG21	2:T:352:ALA:HA	1.86	0.58
2:Q:345:ILE:HG21	2:Q:352:ALA:HA	1.86	0.58
1:J:46:PRO:HA	1:J:207:SER:CB	2.33	0.58
2:Z:345:ILE:HG21	2:Z:352:ALA:HA	1.86	0.57
3:g:172:GLN:OE1	3:g:172:GLN:HA	2.03	0.57
3:d:172:GLN:OE1	3:d:172:GLN:HA	2.03	0.57
2:R:345:ILE:HG21	2:R:352:ALA:HA	1.86	0.57
2:U:345:ILE:HG21	2:U:352:ALA:HA	1.86	0.57
2:X:345:ILE:HG21	2:X:352:ALA:HA	1.86	0.57
2:a:345:ILE:HG21	2:a:352:ALA:HA	1.86	0.57
2:b:345:ILE:HG21	2:b:352:ALA:HA	1.86	0.57
1:E:111:PHE:HD1	1:E:117:PRO:CB	2.12	0.57
1:J:68:PHE:HD1	1:J:71:PHE:HZ	1.46	0.57
2:P:345:ILE:HG21	2:P:352:ALA:HA	1.86	0.57
1:C:31:VAL:HG12	1:C:155:VAL:HG22	1.87	0.56
2:Y:345:ILE:HG21	2:Y:352:ALA:HA	1.86	0.56
1:C:28:LYS:HB2	1:C:52:LYS:HZ2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:VAL:HG12	1:H:155:VAL:HG22	1.87	0.56
1:J:31:VAL:HG12	1:J:155:VAL:HG22	1.88	0.56
1:E:31:VAL:HG12	1:E:155:VAL:HG22	1.88	0.56
1:G:31:VAL:HG12	1:G:155:VAL:HG22	1.88	0.56
1:M:31:VAL:HG12	1:M:155:VAL:HG22	1.88	0.56
2:S:345:ILE:HG21	2:S:352:ALA:HA	1.86	0.56
2:V:345:ILE:HG21	2:V:352:ALA:HA	1.86	0.56
2:W:345:ILE:HG21	2:W:352:ALA:HA	1.86	0.56
1:A:31:VAL:HG12	1:A:155:VAL:HG22	1.88	0.56
1:F:26:ARG:NE	3:e:173:TYR:CE2	2.74	0.56
1:N:31:VAL:HG12	1:N:155:VAL:HG22	1.88	0.56
1:C:8:SER:OG	1:C:9:PRO:HD2	2.06	0.56
1:O:69:ASN:OD1	1:O:70:GLU:N	2.39	0.56
1:C:87:TYR:CE1	2:Q:357:ARG:NH1	2.74	0.56
1:D:31:VAL:HG12	1:D:155:VAL:HG22	1.88	0.56
1:I:28:LYS:HB2	1:I:52:LYS:HZ2	1.71	0.56
2:c:345:ILE:HG21	2:c:352:ALA:HA	1.87	0.56
1:D:69:ASN:OD1	1:D:70:GLU:N	2.39	0.56
1:C:68:PHE:HD1	1:C:71:PHE:HZ	1.46	0.56
1:E:69:ASN:OD1	1:E:70:GLU:N	2.39	0.56
1:J:6:PHE:CB	1:K:4:PRO:C	2.77	0.56
1:J:69:ASN:OD1	1:J:70:GLU:N	2.39	0.56
1:K:31:VAL:HG12	1:K:155:VAL:HG22	1.87	0.56
1:L:31:VAL:HG12	1:L:155:VAL:HG22	1.88	0.56
1:M:128:ALA:HB2	1:M:134:LYS:HB3	1.88	0.56
1:O:46:PRO:HA	1:O:207:SER:CB	2.34	0.56
1:A:69:ASN:OD1	1:A:70:GLU:N	2.39	0.56
1:C:69:ASN:OD1	1:C:70:GLU:N	2.39	0.56
1:E:8:SER:OG	1:E:9:PRO:HD2	2.06	0.56
1:I:52:LYS:HE2	3:h:174:LEU:OXT	2.02	0.56
1:D:8:SER:OG	1:D:9:PRO:HD2	2.06	0.55
1:G:68:PHE:HD1	1:G:71:PHE:HZ	1.46	0.55
1:H:69:ASN:OD1	1:H:70:GLU:N	2.39	0.55
1:H:128:ALA:HB2	1:H:134:LYS:HB3	1.89	0.55
1:K:69:ASN:OD1	1:K:70:GLU:N	2.39	0.55
1:K:111:PHE:HD1	1:K:117:PRO:CB	2.12	0.55
1:K:128:ALA:HB2	1:K:134:LYS:HB3	1.88	0.55
1:C:128:ALA:HB2	1:C:134:LYS:HB3	1.88	0.55
1:G:69:ASN:OD1	1:G:70:GLU:N	2.39	0.55
1:D:128:ALA:HB2	1:D:134:LYS:HB3	1.88	0.55
1:G:45:ASN:ND2	1:G:209:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:128:ALA:HB2	1:G:134:LYS:HB3	1.88	0.55
1:H:66:GLY:O	3:g:174:LEU:C	2.46	0.55
1:J:128:ALA:HB2	1:J:134:LYS:HB3	1.88	0.55
1:M:45:ASN:ND2	1:M:209:GLU:OE1	2.40	0.55
1:M:69:ASN:OD1	1:M:70:GLU:N	2.39	0.55
3:j:172:GLN:O	3:j:172:GLN:HG3	2.07	0.55
1:A:45:ASN:ND2	1:A:209:GLU:OE1	2.40	0.55
1:C:45:ASN:ND2	1:C:209:GLU:OE1	2.40	0.55
1:E:45:ASN:ND2	1:E:209:GLU:OE1	2.40	0.55
1:E:69:ASN:OD1	1:E:70:GLU:CG	2.55	0.55
1:E:114:GLN:CG	1:E:115:ALA:N	2.49	0.55
1:F:69:ASN:OD1	1:F:70:GLU:N	2.39	0.55
1:H:45:ASN:ND2	1:H:209:GLU:OE1	2.40	0.55
1:O:45:ASN:ND2	1:O:209:GLU:OE1	2.40	0.55
1:A:128:ALA:HB2	1:A:134:LYS:HB3	1.89	0.55
1:F:31:VAL:HG12	1:F:155:VAL:HG22	1.88	0.55
1:H:8:SER:OG	1:H:9:PRO:HD2	2.06	0.55
1:J:69:ASN:OD1	1:J:70:GLU:CG	2.55	0.55
1:L:69:ASN:OD1	1:L:70:GLU:CG	2.55	0.55
1:E:26:ARG:NE	3:d:173:TYR:CD2	2.59	0.55
1:L:69:ASN:OD1	1:L:70:GLU:N	2.39	0.55
1:N:69:ASN:OD1	1:N:70:GLU:N	2.39	0.55
1:O:31:VAL:HG12	1:O:155:VAL:HG22	1.88	0.55
3:d:172:GLN:O	3:d:172:GLN:HG3	2.07	0.55
3:e:172:GLN:O	3:e:172:GLN:HG3	2.07	0.55
1:F:8:SER:OG	1:F:9:PRO:HD2	2.06	0.55
1:F:52:LYS:HE2	3:e:174:LEU:HB3	1.88	0.55
1:I:8:SER:OG	1:I:9:PRO:HD2	2.06	0.55
1:I:31:VAL:HG12	1:I:155:VAL:HG22	1.88	0.55
1:I:69:ASN:OD1	1:I:70:GLU:N	2.39	0.55
1:N:128:ALA:HB2	1:N:134:LYS:HB3	1.89	0.55
1:O:69:ASN:OD1	1:O:70:GLU:CG	2.55	0.55
3:g:172:GLN:O	3:g:172:GLN:HG3	2.06	0.55
1:F:128:ALA:HB2	1:F:134:LYS:HB3	1.89	0.55
1:H:69:ASN:OD1	1:H:70:GLU:CG	2.55	0.55
1:C:69:ASN:OD1	1:C:70:GLU:CG	2.55	0.55
1:G:8:SER:OG	1:G:9:PRO:HD2	2.06	0.55
1:L:45:ASN:ND2	1:L:209:GLU:OE1	2.40	0.55
1:N:69:ASN:OD1	1:N:70:GLU:CG	2.55	0.55
1:F:45:ASN:ND2	1:F:209:GLU:OE1	2.40	0.54
1:I:128:ALA:HB2	1:I:134:LYS:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:45:ASN:ND2	1:J:209:GLU:OE1	2.40	0.54
1:N:45:ASN:ND2	1:N:209:GLU:OE1	2.40	0.54
1:E:128:ALA:HB2	1:E:134:LYS:HB3	1.88	0.54
1:G:69:ASN:OD1	1:G:70:GLU:CG	2.55	0.54
2:Y:456:GLN:NE2	2:Y:465:ARG:HH22	2.06	0.54
1:A:46:PRO:HA	1:A:207:SER:CB	2.36	0.54
1:D:69:ASN:OD1	1:D:70:GLU:CG	2.55	0.54
1:F:114:GLN:CG	1:F:115:ALA:N	2.49	0.54
3:h:172:GLN:HG3	3:h:172:GLN:O	2.07	0.54
2:a:456:GLN:NE2	2:a:465:ARG:HH22	2.06	0.54
1:L:128:ALA:HB2	1:L:134:LYS:HB3	1.88	0.54
1:M:69:ASN:OD1	1:M:70:GLU:CG	2.55	0.54
3:f:172:GLN:HG3	3:f:172:GLN:O	2.07	0.54
2:W:456:GLN:NE2	2:W:465:ARG:HH22	2.06	0.54
3:i:172:GLN:O	3:i:172:GLN:HG3	2.07	0.54
1:C:46:PRO:CA	1:C:207:SER:HB2	2.30	0.54
1:I:87:TYR:CE1	2:P:357:ARG:NH1	2.76	0.54
1:O:128:ALA:HB2	1:O:134:LYS:HB3	1.89	0.54
2:X:456:GLN:NE2	2:X:465:ARG:HH22	2.06	0.54
1:D:45:ASN:ND2	1:D:209:GLU:OE1	2.40	0.54
1:I:45:ASN:ND2	1:I:209:GLU:OE1	2.40	0.54
1:A:69:ASN:OD1	1:A:70:GLU:CG	2.55	0.54
1:K:10:GLU:H	1:K:10:GLU:CD	2.13	0.54
2:T:456:GLN:NE2	2:T:465:ARG:HH22	2.06	0.54
1:K:69:ASN:OD1	1:K:70:GLU:CG	2.55	0.54
2:P:456:GLN:NE2	2:P:465:ARG:HH22	2.06	0.54
1:G:52:LYS:HE2	3:f:174:LEU:C	2.32	0.53
1:K:45:ASN:ND2	1:K:209:GLU:OE1	2.40	0.53
2:Q:456:GLN:NE2	2:Q:465:ARG:HH22	2.06	0.53
2:Z:456:GLN:NE2	2:Z:465:ARG:HH22	2.06	0.53
1:G:66:GLY:C	3:f:174:LEU:O	2.43	0.53
2:R:456:GLN:NE2	2:R:465:ARG:HH22	2.06	0.53
2:U:456:GLN:NE2	2:U:465:ARG:HH22	2.06	0.53
2:Q:359:TYR:CE2	2:Q:363:LEU:HD11	2.44	0.53
2:U:359:TYR:CE2	2:U:363:LEU:HD11	2.44	0.53
1:D:67:LYS:HZ1	1:D:69:ASN:HD21	1.56	0.53
1:I:69:ASN:OD1	1:I:70:GLU:CG	2.55	0.53
2:P:359:TYR:CE2	2:P:363:LEU:HD11	2.44	0.53
2:W:359:TYR:CE2	2:W:363:LEU:HD11	2.44	0.53
1:D:28:LYS:HB2	1:D:52:LYS:NZ	2.24	0.53
1:F:69:ASN:OD1	1:F:70:GLU:CG	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:46:PRO:CA	1:I:207:SER:HB2	2.34	0.53
1:O:28:LYS:HB2	1:O:52:LYS:NZ	2.24	0.53
2:T:359:TYR:CE2	2:T:363:LEU:HD11	2.44	0.53
2:V:456:GLN:NE2	2:V:465:ARG:HH22	2.06	0.53
2:b:456:GLN:NE2	2:b:465:ARG:HH22	2.06	0.53
1:G:28:LYS:HB2	1:G:52:LYS:NZ	2.24	0.53
1:H:111:PHE:HD1	1:H:117:PRO:CB	2.12	0.53
1:J:28:LYS:HB2	1:J:52:LYS:NZ	2.24	0.53
1:K:28:LYS:HB2	1:K:52:LYS:NZ	2.24	0.53
2:S:359:TYR:CE2	2:S:363:LEU:HD11	2.44	0.53
2:c:359:TYR:CE2	2:c:363:LEU:HD11	2.44	0.53
2:c:456:GLN:NE2	2:c:465:ARG:HH22	2.06	0.53
1:A:28:LYS:HB2	1:A:52:LYS:NZ	2.24	0.53
1:M:28:LYS:HB2	1:M:52:LYS:NZ	2.24	0.53
2:b:359:TYR:CE2	2:b:363:LEU:HD11	2.44	0.53
1:L:28:LYS:HB2	1:L:52:LYS:NZ	2.24	0.53
1:O:111:PHE:HD1	1:O:117:PRO:CB	2.12	0.53
1:G:52:LYS:NZ	3:f:174:LEU:HA	2.24	0.52
2:Q:338:ASP:OD1	2:Q:341:THR:OG1	2.05	0.52
1:E:28:LYS:HB2	1:E:52:LYS:NZ	2.24	0.52
2:X:359:TYR:CE2	2:X:363:LEU:HD11	2.44	0.52
2:Z:359:TYR:CE2	2:Z:363:LEU:HD11	2.44	0.52
1:F:28:LYS:HB2	1:F:52:LYS:HZ2	1.74	0.52
1:K:111:PHE:HE1	1:K:117:PRO:HG3	1.75	0.52
2:R:359:TYR:CE2	2:R:363:LEU:HD11	2.44	0.52
2:S:456:GLN:NE2	2:S:465:ARG:HH22	2.06	0.52
2:V:359:TYR:CE2	2:V:363:LEU:HD11	2.44	0.52
2:Y:359:TYR:CE2	2:Y:363:LEU:HD11	2.44	0.52
1:C:28:LYS:HB2	1:C:52:LYS:NZ	2.24	0.52
1:F:111:PHE:HD1	1:F:117:PRO:CB	2.12	0.52
1:G:111:PHE:HD1	1:G:117:PRO:CB	2.12	0.52
2:a:359:TYR:CE2	2:a:363:LEU:HD11	2.44	0.52
1:D:52:LYS:HE3	3:j:174:LEU:HB3	1.92	0.52
1:D:67:LYS:NZ	1:D:69:ASN:HD21	2.08	0.52
1:F:111:PHE:HE1	1:F:117:PRO:HG3	1.75	0.52
1:H:28:LYS:HB2	1:H:52:LYS:NZ	2.24	0.52
1:J:6:PHE:CA	1:K:4:PRO:O	2.57	0.52
1:O:67:LYS:NZ	1:O:69:ASN:HD21	2.08	0.52
1:F:28:LYS:HB2	1:F:52:LYS:NZ	2.24	0.52
1:G:111:PHE:HE1	1:G:117:PRO:HG3	1.75	0.52
1:H:111:PHE:HE1	1:H:117:PRO:HG3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:LYS:HB2	1:N:52:LYS:NZ	2.24	0.52
1:K:114:GLN:CG	1:K:115:ALA:N	2.49	0.52
1:E:67:LYS:NZ	1:E:69:ASN:HD21	2.08	0.51
1:E:111:PHE:HE1	1:E:117:PRO:HG3	1.75	0.51
1:J:67:LYS:NZ	1:J:69:ASN:HD21	2.08	0.51
1:J:111:PHE:HE1	1:J:117:PRO:HG3	1.75	0.51
1:L:67:LYS:NZ	1:L:69:ASN:HD21	2.08	0.51
1:G:67:LYS:NZ	1:G:69:ASN:HD21	2.08	0.51
1:M:67:LYS:NZ	1:M:69:ASN:HD21	2.08	0.51
1:C:111:PHE:HE1	1:C:117:PRO:HG3	1.75	0.51
1:I:28:LYS:HB2	1:I:52:LYS:NZ	2.24	0.51
1:N:67:LYS:NZ	1:N:69:ASN:HD21	2.08	0.51
1:E:46:PRO:CA	1:E:207:SER:HB2	2.31	0.51
1:H:67:LYS:NZ	1:H:69:ASN:HD21	2.08	0.51
1:H:87:TYR:CE1	2:V:357:ARG:NH1	2.78	0.51
1:J:6:PHE:O	1:J:7:ILE:C	2.53	0.51
1:J:10:GLU:CD	1:K:15:GLU:HG2	2.33	0.51
1:K:67:LYS:NZ	1:K:69:ASN:HD21	2.08	0.51
1:G:26:ARG:NH2	3:f:173:TYR:CE2	2.78	0.51
1:J:98:GLN:NE2	2:Y:370:GLU:OE1	2.44	0.51
1:D:24:ILE:HD11	1:D:143:TYR:CD2	2.46	0.51
1:L:114:GLN:CG	1:L:115:ALA:N	2.49	0.51
1:N:8:SER:HB3	1:N:11:GLN:HB2	1.93	0.51
1:A:8:SER:OG	1:A:9:PRO:HD2	2.10	0.51
1:C:24:ILE:HD11	1:C:143:TYR:CD2	2.46	0.51
1:F:50:LEU:HD11	3:e:172:GLN:HE21	1.74	0.51
1:O:24:ILE:HD11	1:O:143:TYR:CD2	2.46	0.51
1:O:111:PHE:HE1	1:O:117:PRO:HG3	1.75	0.51
1:A:67:LYS:NZ	1:A:69:ASN:HD21	2.08	0.51
1:I:24:ILE:HD11	1:I:143:TYR:CD2	2.46	0.51
1:I:111:PHE:HE1	1:I:117:PRO:HG3	1.75	0.51
1:J:111:PHE:HD1	1:J:117:PRO:CB	2.12	0.51
1:M:24:ILE:HD11	1:M:143:TYR:CD2	2.46	0.51
1:C:67:LYS:NZ	1:C:69:ASN:HD21	2.08	0.50
1:G:24:ILE:HD11	1:G:143:TYR:CD2	2.46	0.50
1:A:24:ILE:HD11	1:A:143:TYR:CD2	2.46	0.50
1:A:111:PHE:HE1	1:A:117:PRO:HG3	1.75	0.50
1:F:24:ILE:HD11	1:F:143:TYR:CD2	2.46	0.50
1:K:87:TYR:HE1	2:Y:357:ARG:NH1	2.09	0.50
1:L:111:PHE:HE1	1:L:117:PRO:HG3	1.75	0.50
1:F:67:LYS:NZ	1:F:69:ASN:HD21	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:ILE:HD11	1:H:143:TYR:CD2	2.46	0.50
1:N:24:ILE:HD11	1:N:143:TYR:CD2	2.46	0.50
1:E:87:TYR:HE1	2:S:357:ARG:NH1	2.06	0.50
1:G:52:LYS:CE	3:f:174:LEU:C	2.83	0.50
1:N:98:GLN:NE2	2:c:370:GLU:OE1	2.43	0.50
1:A:89:TYR:O	1:A:90:ASP:HB2	2.12	0.50
1:J:24:ILE:HD11	1:J:143:TYR:CD2	2.46	0.50
1:C:111:PHE:HD1	1:C:117:PRO:CB	2.12	0.50
1:L:24:ILE:HD11	1:L:143:TYR:CD2	2.46	0.50
2:P:301:THR:HG22	2:P:333:LYS:HZ3	1.74	0.50
1:F:89:TYR:O	1:F:90:ASP:HB2	2.12	0.50
1:N:111:PHE:HE1	1:N:117:PRO:HG3	1.75	0.50
1:H:89:TYR:O	1:H:90:ASP:HB2	2.12	0.50
1:I:67:LYS:NZ	1:I:69:ASN:HD21	2.08	0.50
1:J:114:GLN:CG	1:J:115:ALA:N	2.49	0.50
1:F:26:ARG:CZ	3:e:173:TYR:CE2	2.94	0.49
2:S:301:THR:HG22	2:S:333:LYS:HZ2	1.77	0.49
1:K:46:PRO:CA	1:K:207:SER:HB2	2.35	0.49
1:K:98:GLN:NE2	2:Z:370:GLU:OE1	2.44	0.49
1:D:111:PHE:HE1	1:D:117:PRO:HG3	1.75	0.49
1:F:78:GLY:CA	1:F:103:TYR:OH	2.55	0.49
1:L:89:TYR:O	1:L:90:ASP:HB2	2.12	0.49
1:E:24:ILE:HD11	1:E:143:TYR:CD2	2.46	0.49
1:F:52:LYS:NZ	3:e:174:LEU:C	2.57	0.49
1:D:24:ILE:HD11	1:D:143:TYR:HD2	1.78	0.49
1:J:24:ILE:HD11	1:J:143:TYR:HD2	1.78	0.49
1:A:24:ILE:HD11	1:A:143:TYR:HD2	1.78	0.49
1:C:89:TYR:O	1:C:90:ASP:HB2	2.12	0.49
1:I:24:ILE:HD11	1:I:143:TYR:HD2	1.78	0.49
1:A:111:PHE:HD1	1:A:117:PRO:CB	2.12	0.49
1:C:24:ILE:HD11	1:C:143:TYR:HD2	1.78	0.49
1:G:24:ILE:HD11	1:G:143:TYR:HD2	1.78	0.49
1:G:52:LYS:HZ1	3:f:174:LEU:CA	2.24	0.49
1:M:111:PHE:HE1	1:M:117:PRO:HG3	1.75	0.49
1:N:24:ILE:HD11	1:N:143:TYR:HD2	1.78	0.49
1:G:89:TYR:O	1:G:90:ASP:HB2	2.12	0.49
1:M:89:TYR:O	1:M:90:ASP:HB2	2.12	0.49
2:X:301:THR:HG22	2:X:333:LYS:HZ3	1.76	0.49
1:D:111:PHE:HD1	1:D:117:PRO:CB	2.12	0.49
1:F:24:ILE:HD11	1:F:143:TYR:HD2	1.78	0.49
1:L:24:ILE:HD11	1:L:143:TYR:HD2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:89:TYR:O	1:N:90:ASP:HB2	2.12	0.49
1:K:24:ILE:HD11	1:K:143:TYR:CD2	2.46	0.48
1:D:89:TYR:O	1:D:90:ASP:HB2	2.12	0.48
1:E:89:TYR:O	1:E:90:ASP:HB2	2.12	0.48
1:I:89:TYR:O	1:I:90:ASP:HB2	2.12	0.48
1:C:78:GLY:CA	1:C:103:TYR:OH	2.55	0.48
1:K:89:TYR:O	1:K:90:ASP:HB2	2.12	0.48
1:H:114:GLN:CG	1:H:115:ALA:N	2.49	0.48
1:J:89:TYR:O	1:J:90:ASP:HB2	2.12	0.48
1:M:67:LYS:HZ1	1:M:69:ASN:HD21	1.59	0.48
1:O:89:TYR:O	1:O:90:ASP:HB2	2.12	0.48
1:E:24:ILE:HD11	1:E:143:TYR:HD2	1.78	0.48
1:M:24:ILE:HD11	1:M:143:TYR:HD2	1.78	0.48
1:M:111:PHE:HD1	1:M:117:PRO:CB	2.12	0.48
1:H:78:GLY:CA	1:H:103:TYR:OH	2.55	0.48
1:H:46:PRO:CA	1:H:207:SER:HB2	2.37	0.48
1:D:104:ALA:HB1	1:D:145:GLY:O	2.14	0.48
1:G:104:ALA:HB1	1:G:145:GLY:O	2.14	0.48
1:M:104:ALA:HB1	1:M:145:GLY:O	2.14	0.48
1:O:24:ILE:HD11	1:O:143:TYR:HD2	1.78	0.48
1:O:104:ALA:HB1	1:O:145:GLY:O	2.14	0.48
1:D:28:LYS:HB2	1:D:52:LYS:HZ2	1.79	0.47
1:H:24:ILE:HD11	1:H:143:TYR:HD2	1.78	0.47
1:J:104:ALA:HB1	1:J:145:GLY:O	2.14	0.47
1:K:24:ILE:HD11	1:K:143:TYR:HD2	1.78	0.47
1:A:78:GLY:CA	1:A:103:TYR:OH	2.55	0.47
1:C:104:ALA:HB1	1:C:145:GLY:O	2.14	0.47
1:D:46:PRO:CA	1:D:207:SER:HB2	2.31	0.47
1:L:46:PRO:CA	1:L:207:SER:HB2	2.37	0.47
1:L:111:PHE:HD1	1:L:117:PRO:CB	2.12	0.47
1:C:52:LYS:CE	3:i:174:LEU:HB3	2.45	0.47
1:C:52:LYS:HE3	3:i:174:LEU:HB3	1.96	0.47
1:D:87:TYR:CE1	2:R:357:ARG:NH1	2.82	0.47
1:H:104:ALA:HB1	1:H:145:GLY:O	2.14	0.47
1:J:30:VAL:HG13	1:J:43:ALA:HB2	1.97	0.47
1:K:104:ALA:HB1	1:K:145:GLY:O	2.14	0.47
1:L:78:GLY:CA	1:L:103:TYR:OH	2.55	0.47
1:L:104:ALA:HB1	1:L:145:GLY:O	2.14	0.47
1:M:46:PRO:CA	1:M:207:SER:HB2	2.34	0.47
1:N:78:GLY:CA	1:N:103:TYR:OH	2.55	0.47
1:C:30:VAL:HG13	1:C:43:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:GLU:HB3	1:I:118:TYR:CD2	2.50	0.47
1:I:111:PHE:HD1	1:I:117:PRO:CB	2.12	0.47
1:A:30:VAL:HG13	1:A:43:ALA:HB2	1.97	0.47
1:A:70:GLU:HB3	1:A:118:TYR:CD2	2.50	0.47
1:D:30:VAL:HG13	1:D:43:ALA:HB2	1.97	0.47
1:E:67:LYS:HZ2	1:E:69:ASN:HD21	1.61	0.47
1:E:70:GLU:HB3	1:E:118:TYR:CD2	2.50	0.47
1:E:78:GLY:CA	1:E:103:TYR:OH	2.55	0.47
1:F:104:ALA:HB1	1:F:145:GLY:O	2.14	0.47
1:I:52:LYS:NZ	3:h:174:LEU:HB3	2.29	0.47
1:I:104:ALA:HB1	1:I:145:GLY:O	2.14	0.47
1:J:70:GLU:HB3	1:J:118:TYR:CD2	2.50	0.47
1:A:104:ALA:HB1	1:A:145:GLY:O	2.14	0.47
1:G:30:VAL:HG13	1:G:43:ALA:HB2	1.97	0.47
1:N:30:VAL:HG13	1:N:43:ALA:HB2	1.97	0.47
1:E:30:VAL:HG13	1:E:43:ALA:HB2	1.97	0.46
1:G:70:GLU:HB3	1:G:118:TYR:CD2	2.50	0.46
1:N:104:ALA:HB1	1:N:145:GLY:O	2.14	0.46
1:K:78:GLY:CA	1:K:103:TYR:OH	2.55	0.46
1:C:87:TYR:HE1	2:Q:357:ARG:NH1	2.12	0.46
1:E:104:ALA:HB1	1:E:145:GLY:O	2.14	0.46
1:H:30:VAL:HG13	1:H:43:ALA:HB2	1.97	0.46
1:I:52:LYS:NZ	3:h:174:LEU:C	2.60	0.46
1:I:87:TYR:HE1	2:P:357:ARG:NH1	2.13	0.46
1:K:30:VAL:HG13	1:K:43:ALA:HB2	1.97	0.46
1:M:30:VAL:HG13	1:M:43:ALA:HB2	1.97	0.46
1:K:10:GLU:N	1:K:10:GLU:CD	2.73	0.46
1:K:70:GLU:HB3	1:K:118:TYR:CD2	2.50	0.46
1:L:70:GLU:HB3	1:L:118:TYR:CD2	2.50	0.46
1:O:70:GLU:HB3	1:O:118:TYR:CD2	2.50	0.46
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.77	0.46
1:F:30:VAL:HG13	1:F:43:ALA:HB2	1.97	0.46
1:F:70:GLU:HB3	1:F:118:TYR:CD2	2.50	0.46
1:H:70:GLU:HB3	1:H:118:TYR:CD2	2.50	0.46
1:N:70:GLU:HB3	1:N:118:TYR:CD2	2.50	0.46
1:O:30:VAL:HG13	1:O:43:ALA:HB2	1.97	0.46
1:G:104:ALA:HB2	1:G:147:ILE:CG2	2.46	0.46
1:O:104:ALA:HB2	1:O:147:ILE:CG2	2.46	0.46
1:I:104:ALA:HB2	1:I:147:ILE:CG2	2.46	0.46
2:Z:301:THR:HG22	2:Z:333:LYS:HZ3	1.74	0.46
1:D:70:GLU:HB3	1:D:118:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ALA:HB2	1:D:147:ILE:CG2	2.46	0.46
1:F:46:PRO:CA	1:F:207:SER:HB2	2.36	0.46
1:J:104:ALA:HB2	1:J:147:ILE:CG2	2.46	0.46
1:K:113:GLU:HA	1:K:113:GLU:OE1	2.16	0.46
1:O:113:GLU:OE1	1:O:113:GLU:HA	2.16	0.46
1:C:52:LYS:NZ	3:i:174:LEU:C	2.70	0.45
1:C:70:GLU:HB3	1:C:118:TYR:CD2	2.50	0.45
1:M:104:ALA:HB2	1:M:147:ILE:CG2	2.46	0.45
2:T:429:TRP:HZ3	2:T:431:ILE:HG13	1.82	0.45
2:V:479:SER:OG	2:W:324:ASN:O	2.22	0.45
1:C:113:GLU:HA	1:C:113:GLU:OE1	2.17	0.45
1:E:104:ALA:HB2	1:E:147:ILE:CG2	2.46	0.45
1:F:173:GLU:O	1:F:174:ASN:HB2	2.17	0.45
1:L:30:VAL:HG13	1:L:43:ALA:HB2	1.97	0.45
1:O:118:TYR:HB3	1:O:120:VAL:HG22	1.99	0.45
1:A:113:GLU:HA	1:A:113:GLU:OE1	2.16	0.45
1:D:113:GLU:HA	1:D:113:GLU:OE1	2.16	0.45
1:H:113:GLU:HA	1:H:113:GLU:OE1	2.16	0.45
1:M:113:GLU:HA	1:M:113:GLU:OE1	2.16	0.45
1:A:141:ILE:HG12	1:A:147:ILE:CG2	2.28	0.45
1:E:26:ARG:CZ	3:d:173:TYR:HE2	1.97	0.45
1:H:104:ALA:HB2	1:H:147:ILE:CG2	2.46	0.45
1:J:118:TYR:HB3	1:J:120:VAL:HG22	1.99	0.45
1:L:141:ILE:HG12	1:L:147:ILE:CG2	2.28	0.45
1:N:118:TYR:HB3	1:N:120:VAL:HG22	1.98	0.45
2:Q:429:TRP:HZ3	2:Q:431:ILE:HG13	1.82	0.45
1:C:118:TYR:HB3	1:C:120:VAL:HG22	1.99	0.45
1:F:113:GLU:HA	1:F:113:GLU:OE1	2.17	0.45
1:G:87:TYR:CE1	2:U:357:ARG:NH1	2.85	0.45
1:G:118:TYR:HB3	1:G:120:VAL:HG22	1.99	0.45
1:I:30:VAL:HG13	1:I:43:ALA:HB2	1.97	0.45
2:S:429:TRP:HZ3	2:S:431:ILE:HG13	1.82	0.45
2:b:429:TRP:HZ3	2:b:431:ILE:HG13	1.82	0.45
1:C:104:ALA:HB2	1:C:147:ILE:CG2	2.46	0.45
1:J:113:GLU:OE1	1:J:113:GLU:HA	2.16	0.45
1:K:104:ALA:HB2	1:K:147:ILE:CG2	2.46	0.45
1:M:70:GLU:HB3	1:M:118:TYR:CD2	2.50	0.45
2:Y:429:TRP:HZ3	2:Y:431:ILE:HG13	1.82	0.45
2:c:429:TRP:HZ3	2:c:431:ILE:HG13	1.82	0.45
1:E:113:GLU:OE1	1:E:113:GLU:HA	2.16	0.45
1:J:6:PHE:CB	1:K:4:PRO:CA	2.92	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:ALA:HB2	1:L:147:ILE:CG2	2.46	0.45
1:L:118:TYR:HB3	1:L:120:VAL:HG22	1.99	0.45
1:N:104:ALA:HB2	1:N:147:ILE:CG2	2.46	0.45
1:N:173:GLU:O	1:N:174:ASN:HB2	2.17	0.45
2:Z:429:TRP:HZ3	2:Z:431:ILE:HG13	1.82	0.45
1:A:104:ALA:HB2	1:A:147:ILE:CG2	2.46	0.45
1:C:173:GLU:O	1:C:174:ASN:HB2	2.17	0.45
1:F:135:ARG:HH21	1:G:48:ARG:HH12	1.23	0.45
1:H:173:GLU:O	1:H:174:ASN:HB2	2.17	0.45
2:W:429:TRP:HZ3	2:W:431:ILE:HG13	1.82	0.45
1:C:114:GLN:CG	1:C:115:ALA:N	2.49	0.45
1:G:113:GLU:OE1	1:G:113:GLU:HA	2.16	0.45
1:G:114:GLN:CG	1:G:115:ALA:N	2.49	0.45
1:M:28:LYS:HB2	1:M:52:LYS:HZ2	1.81	0.45
1:M:118:TYR:HB3	1:M:120:VAL:HG22	1.99	0.45
2:T:479:SER:OG	2:Y:324:ASN:O	2.27	0.45
1:F:67:LYS:HZ2	1:F:69:ASN:HD21	1.63	0.45
1:F:104:ALA:HB2	1:F:147:ILE:CG2	2.46	0.45
1:K:118:TYR:HB3	1:K:120:VAL:HG22	1.99	0.45
2:V:308:TYR:CD1	2:V:309:PRO:O	2.70	0.45
2:c:308:TYR:CD1	2:c:309:PRO:O	2.70	0.45
1:D:118:TYR:HB3	1:D:120:VAL:HG22	1.99	0.44
1:G:25:ALA:O	1:G:158:GLY:HA2	2.17	0.44
1:N:113:GLU:OE1	1:N:113:GLU:HA	2.17	0.44
1:O:114:GLN:CG	1:O:115:ALA:N	2.49	0.44
1:A:173:GLU:O	1:A:174:ASN:HB2	2.17	0.44
1:D:25:ALA:O	1:D:158:GLY:HA2	2.18	0.44
1:E:25:ALA:O	1:E:158:GLY:HA2	2.17	0.44
1:E:173:GLU:O	1:E:174:ASN:HB2	2.17	0.44
1:L:113:GLU:OE1	1:L:113:GLU:HA	2.17	0.44
1:O:173:GLU:O	1:O:174:ASN:HB2	2.17	0.44
2:P:429:TRP:HZ3	2:P:431:ILE:HG13	1.82	0.44
2:a:429:TRP:HZ3	2:a:431:ILE:HG13	1.82	0.44
1:E:118:TYR:HB3	1:E:120:VAL:HG22	1.99	0.44
1:I:113:GLU:OE1	1:I:113:GLU:HA	2.17	0.44
1:I:173:GLU:O	1:I:174:ASN:HB2	2.17	0.44
1:L:8:SER:HA	1:L:9:PRO:HD3	1.70	0.44
1:L:173:GLU:O	1:L:174:ASN:HB2	2.17	0.44
1:N:140:ARG:HH11	1:N:154:VAL:HG13	1.83	0.44
1:C:25:ALA:O	1:C:158:GLY:HA2	2.18	0.44
1:C:140:ARG:HH11	1:C:154:VAL:HG13	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:ARG:HH22	1:I:48:ARG:HH11	1.56	0.44
1:I:140:ARG:HH11	1:I:154:VAL:HG13	1.83	0.44
1:J:173:GLU:O	1:J:174:ASN:HB2	2.17	0.44
2:U:429:TRP:HZ3	2:U:431:ILE:HG13	1.82	0.44
1:G:173:GLU:O	1:G:174:ASN:HB2	2.17	0.44
1:H:118:TYR:HB3	1:H:120:VAL:HG22	1.99	0.44
1:I:52:LYS:HZ1	3:h:174:LEU:HB3	1.81	0.44
1:J:25:ALA:O	1:J:158:GLY:HA2	2.17	0.44
1:M:173:GLU:O	1:M:174:ASN:HB2	2.17	0.44
1:O:87:TYR:CE1	2:c:357:ARG:NH1	2.85	0.44
1:O:234:LEU:O	1:O:234:LEU:CG	2.63	0.44
2:P:450:MET:O	2:P:454:TYR:HB2	2.18	0.44
2:b:450:MET:O	2:b:454:TYR:HB2	2.18	0.44
1:A:118:TYR:HB3	1:A:120:VAL:HG22	1.99	0.44
1:M:25:ALA:O	1:M:158:GLY:HA2	2.18	0.44
1:N:25:ALA:O	1:N:158:GLY:HA2	2.18	0.44
1:O:25:ALA:O	1:O:158:GLY:HA2	2.18	0.44
2:X:429:TRP:HZ3	2:X:431:ILE:HG13	1.82	0.44
2:Z:450:MET:O	2:Z:454:TYR:HB2	2.18	0.44
2:c:318:ARG:HD3	2:c:493:THR:HG23	2.00	0.44
3:e:173:TYR:O	3:e:174:LEU:HG	2.18	0.44
1:F:56:LEU:HD23	1:F:56:LEU:HA	1.77	0.44
1:G:141:ILE:HG12	1:G:147:ILE:CG2	2.28	0.44
2:V:429:TRP:HZ3	2:V:431:ILE:HG13	1.82	0.44
1:F:118:TYR:HB3	1:F:120:VAL:HG22	1.99	0.44
1:I:118:TYR:HB3	1:I:120:VAL:HG22	1.99	0.44
1:J:28:LYS:HD2	1:J:44:GLU:CD	2.43	0.44
2:Q:450:MET:O	2:Q:454:TYR:HB2	2.18	0.44
2:V:450:MET:O	2:V:454:TYR:HB2	2.18	0.44
2:c:450:MET:O	2:c:454:TYR:HB2	2.18	0.44
3:d:173:TYR:O	3:d:174:LEU:HG	2.18	0.44
1:D:28:LYS:HD2	1:D:44:GLU:CD	2.43	0.44
1:D:173:GLU:O	1:D:174:ASN:HB2	2.17	0.44
1:G:100:ALA:O	1:G:141:ILE:CD1	2.66	0.44
1:K:173:GLU:O	1:K:174:ASN:HB2	2.17	0.44
1:L:25:ALA:O	1:L:158:GLY:HA2	2.18	0.44
2:W:450:MET:O	2:W:454:TYR:HB2	2.18	0.44
2:a:450:MET:O	2:a:454:TYR:HB2	2.18	0.44
1:A:98:GLN:NE2	2:X:370:GLU:OE1	2.50	0.43
1:C:52:LYS:CE	3:i:174:LEU:C	2.73	0.43
1:G:28:LYS:HD2	1:G:44:GLU:CD	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:ARG:HH11	1:H:154:VAL:HG13	1.83	0.43
1:N:46:PRO:CA	1:N:207:SER:HB2	2.39	0.43
1:O:28:LYS:HD2	1:O:44:GLU:CD	2.43	0.43
2:R:450:MET:O	2:R:454:TYR:HB2	2.18	0.43
2:S:318:ARG:HD3	2:S:493:THR:HG23	2.00	0.43
2:X:450:MET:O	2:X:454:TYR:HB2	2.18	0.43
3:f:173:TYR:O	3:f:174:LEU:HG	2.18	0.43
3:j:173:TYR:O	3:j:174:LEU:HG	2.18	0.43
1:C:100:ALA:O	1:C:141:ILE:CD1	2.66	0.43
1:I:28:LYS:HD2	1:I:44:GLU:CD	2.43	0.43
2:V:318:ARG:HD3	2:V:493:THR:HG23	2.00	0.43
2:Y:450:MET:O	2:Y:454:TYR:HB2	2.18	0.43
1:E:28:LYS:HD2	1:E:44:GLU:CD	2.43	0.43
1:K:25:ALA:O	1:K:158:GLY:HA2	2.17	0.43
1:N:100:ALA:O	1:N:141:ILE:CD1	2.66	0.43
2:T:318:ARG:HD3	2:T:493:THR:HG23	2.00	0.43
2:T:450:MET:O	2:T:454:TYR:HB2	2.18	0.43
2:U:450:MET:O	2:U:454:TYR:HB2	2.18	0.43
2:Y:318:ARG:HD3	2:Y:493:THR:HG23	2.00	0.43
1:C:28:LYS:HD2	1:C:44:GLU:CD	2.43	0.43
1:H:25:ALA:O	1:H:158:GLY:HA2	2.18	0.43
1:J:28:LYS:HB2	1:J:52:LYS:HZ2	1.83	0.43
2:Q:318:ARG:HD3	2:Q:493:THR:HG23	2.00	0.43
2:R:429:TRP:HZ3	2:R:431:ILE:HG13	1.82	0.43
2:X:318:ARG:HD3	2:X:493:THR:HG23	2.00	0.43
3:h:173:TYR:O	3:h:174:LEU:HG	2.18	0.43
1:A:25:ALA:O	1:A:158:GLY:HA2	2.17	0.43
1:D:141:ILE:HG12	1:D:147:ILE:CG2	2.28	0.43
1:E:56:LEU:HD23	1:E:56:LEU:HA	1.77	0.43
1:F:25:ALA:O	1:F:158:GLY:HA2	2.17	0.43
3:i:173:TYR:O	3:i:174:LEU:HG	2.18	0.43
1:A:100:ALA:O	1:A:141:ILE:CD1	2.66	0.43
1:F:28:LYS:HD2	1:F:44:GLU:CD	2.43	0.43
1:K:28:LYS:HD2	1:K:44:GLU:CD	2.43	0.43
1:M:28:LYS:HD2	1:M:44:GLU:CD	2.43	0.43
1:N:111:PHE:HD1	1:N:117:PRO:CB	2.12	0.43
1:O:78:GLY:CA	1:O:103:TYR:OH	2.55	0.43
2:Z:301:THR:CG2	2:Z:333:LYS:HZ3	2.32	0.43
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.77	0.43
1:I:114:GLN:CG	1:I:115:ALA:N	2.49	0.43
2:P:301:THR:CB	2:P:333:LYS:HZ3	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:450:MET:O	2:S:454:TYR:HB2	2.18	0.43
2:W:318:ARG:HD3	2:W:493:THR:HG23	2.00	0.43
2:Z:318:ARG:HD3	2:Z:493:THR:HG23	2.00	0.43
2:a:318:ARG:HD3	2:a:493:THR:HG23	2.00	0.43
1:G:33:LEU:C	1:G:33:LEU:HD12	2.44	0.43
1:L:28:LYS:HD2	1:L:44:GLU:CD	2.43	0.43
1:N:28:LYS:HD2	1:N:44:GLU:CD	2.43	0.43
2:W:513:LEU:HD23	2:W:513:LEU:HA	1.90	0.43
1:A:28:LYS:HD2	1:A:44:GLU:CD	2.43	0.43
1:H:33:LEU:C	1:H:33:LEU:HD12	2.44	0.43
1:I:33:LEU:C	1:I:33:LEU:HD12	2.44	0.43
1:J:33:LEU:C	1:J:33:LEU:HD12	2.44	0.43
1:M:141:ILE:HG12	1:M:147:ILE:CG2	2.28	0.43
1:N:33:LEU:C	1:N:33:LEU:HD12	2.44	0.43
2:R:318:ARG:HD3	2:R:493:THR:HG23	2.00	0.43
1:A:33:LEU:HD12	1:A:33:LEU:C	2.44	0.43
1:I:25:ALA:O	1:I:158:GLY:HA2	2.18	0.43
1:I:52:LYS:HE3	3:h:174:LEU:HB3	1.99	0.43
1:I:100:ALA:O	1:I:141:ILE:CD1	2.66	0.43
2:R:366:TYR:CZ	2:R:370:GLU:HG3	2.54	0.43
2:S:366:TYR:CZ	2:S:370:GLU:HG3	2.54	0.43
2:b:366:TYR:CZ	2:b:370:GLU:HG3	2.54	0.43
2:c:366:TYR:CZ	2:c:370:GLU:HG3	2.54	0.43
1:C:141:ILE:HG12	1:C:147:ILE:CG2	2.28	0.42
1:E:100:ALA:O	1:E:141:ILE:CD1	2.66	0.42
1:F:100:ALA:O	1:F:141:ILE:CD1	2.66	0.42
1:H:28:LYS:HD2	1:H:44:GLU:CD	2.43	0.42
1:H:32:ALA:HA	1:H:40:LEU:O	2.19	0.42
1:I:32:ALA:HA	1:I:40:LEU:O	2.19	0.42
1:J:32:ALA:HA	1:J:40:LEU:O	2.19	0.42
1:K:32:ALA:HA	1:K:40:LEU:O	2.19	0.42
1:L:32:ALA:HA	1:L:40:LEU:O	2.19	0.42
1:M:32:ALA:HA	1:M:40:LEU:O	2.19	0.42
2:U:318:ARG:HD3	2:U:493:THR:HG23	2.00	0.42
1:D:140:ARG:HH11	1:D:154:VAL:HG13	1.83	0.42
1:E:32:ALA:HA	1:E:40:LEU:O	2.20	0.42
1:M:33:LEU:HD12	1:M:33:LEU:C	2.44	0.42
1:M:100:ALA:O	1:M:141:ILE:CD1	2.66	0.42
1:M:140:ARG:HH11	1:M:154:VAL:HG13	1.83	0.42
1:N:134:LYS:HB3	1:N:134:LYS:HE2	1.89	0.42
2:P:366:TYR:CZ	2:P:370:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:301:THR:CB	2:X:333:LYS:HZ3	2.32	0.42
2:Z:301:THR:CB	2:Z:333:LYS:HZ3	2.32	0.42
3:g:173:TYR:O	3:g:174:LEU:HG	2.18	0.42
1:F:134:LYS:HB3	1:F:134:LYS:HE2	1.90	0.42
1:G:32:ALA:HA	1:G:40:LEU:O	2.20	0.42
2:P:318:ARG:HD3	2:P:493:THR:HG23	2.00	0.42
1:D:32:ALA:HA	1:D:40:LEU:O	2.19	0.42
1:E:33:LEU:C	1:E:33:LEU:HD12	2.44	0.42
1:G:78:GLY:CA	1:G:103:TYR:OH	2.55	0.42
1:K:33:LEU:HD12	1:K:33:LEU:C	2.44	0.42
1:L:87:TYR:HE1	2:Z:357:ARG:NH1	2.14	0.42
1:O:28:LYS:HB2	1:O:52:LYS:HZ3	1.83	0.42
1:O:32:ALA:HA	1:O:40:LEU:O	2.19	0.42
1:O:33:LEU:C	1:O:33:LEU:HD12	2.44	0.42
2:P:324:ASN:O	2:c:479:SER:OG	2.28	0.42
2:Y:366:TYR:CZ	2:Y:370:GLU:HG3	2.54	0.42
1:D:33:LEU:HD12	1:D:33:LEU:C	2.44	0.42
1:E:140:ARG:HH11	1:E:154:VAL:HG13	1.82	0.42
1:K:56:LEU:HD23	1:K:56:LEU:HA	1.77	0.42
1:M:56:LEU:HD23	1:M:56:LEU:HA	1.77	0.42
1:N:32:ALA:HA	1:N:40:LEU:O	2.20	0.42
1:A:32:ALA:HA	1:A:40:LEU:O	2.19	0.42
1:C:33:LEU:C	1:C:33:LEU:HD12	2.44	0.42
1:C:67:LYS:HZ1	1:C:69:ASN:HD21	1.66	0.42
1:L:33:LEU:C	1:L:33:LEU:HD12	2.44	0.42
2:V:513:LEU:HD23	2:V:513:LEU:HA	1.91	0.42
2:Z:366:TYR:CZ	2:Z:370:GLU:HG3	2.54	0.42
1:C:32:ALA:HA	1:C:40:LEU:O	2.19	0.42
1:D:100:ALA:O	1:D:141:ILE:CD1	2.66	0.42
1:F:33:LEU:HD12	1:F:33:LEU:C	2.44	0.42
1:G:140:ARG:HH11	1:G:154:VAL:HG13	1.83	0.42
1:H:67:LYS:HZ2	1:H:69:ASN:HD21	1.66	0.42
1:K:100:ALA:O	1:K:141:ILE:CD1	2.66	0.42
2:P:301:THR:CG2	2:P:333:LYS:HZ3	2.32	0.42
2:T:366:TYR:CZ	2:T:370:GLU:HG3	2.54	0.42
2:W:366:TYR:CZ	2:W:370:GLU:HG3	2.54	0.42
1:D:78:GLY:CA	1:D:103:TYR:OH	2.55	0.42
2:U:366:TYR:CZ	2:U:370:GLU:HG3	2.54	0.42
1:G:135:ARG:NH2	1:H:48:ARG:HH11	1.97	0.42
1:L:6:PHE:CB	1:M:6:PHE:CA	2.98	0.42
2:V:471:LEU:HD23	2:V:471:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:513:LEU:HD23	2:Y:513:LEU:HA	1.91	0.42
1:F:140:ARG:HH11	1:F:154:VAL:HG13	1.83	0.42
1:G:46:PRO:CA	1:G:207:SER:HB2	2.40	0.42
1:G:87:TYR:HE1	2:U:357:ARG:NH1	2.18	0.42
1:H:28:LYS:HB2	1:H:52:LYS:HZ2	1.84	0.42
2:R:308:TYR:O	2:R:309:PRO:C	2.62	0.42
2:a:366:TYR:CZ	2:a:370:GLU:HG3	2.54	0.42
1:J:78:GLY:CA	1:J:103:TYR:OH	2.55	0.41
1:J:140:ARG:HH11	1:J:154:VAL:HG13	1.83	0.41
1:N:10:GLU:CD	1:O:15:GLU:HG2	2.39	0.41
2:R:471:LEU:HD23	2:R:471:LEU:HA	1.89	0.41
2:X:301:THR:CG2	2:X:333:LYS:HZ3	2.33	0.41
2:X:366:TYR:CZ	2:X:370:GLU:HG3	2.54	0.41
2:b:318:ARG:HD3	2:b:493:THR:HG23	2.00	0.41
1:O:56:LEU:HA	1:O:56:LEU:HD23	1.77	0.41
1:D:52:LYS:CE	3:j:174:LEU:HB3	2.49	0.41
1:K:140:ARG:HH11	1:K:154:VAL:HG13	1.83	0.41
2:P:308:TYR:CD1	2:P:309:PRO:O	2.73	0.41
2:P:308:TYR:O	2:P:309:PRO:C	2.63	0.41
2:Q:366:TYR:CZ	2:Q:370:GLU:HG3	2.54	0.41
2:Q:386:MET:HE3	2:Q:386:MET:HB2	1.95	0.41
2:W:301:THR:CG2	2:W:333:LYS:NZ	2.75	0.41
1:A:114:GLN:CG	1:A:115:ALA:N	2.49	0.41
1:F:87:TYR:CE1	2:T:357:ARG:NH1	2.88	0.41
1:J:56:LEU:HD23	1:J:56:LEU:HA	1.77	0.41
1:L:134:LYS:HB3	1:L:134:LYS:HE2	1.89	0.41
1:F:32:ALA:HA	1:F:40:LEU:O	2.19	0.41
1:N:67:LYS:HZ2	1:N:69:ASN:HD21	1.68	0.41
2:b:513:LEU:HD23	2:b:513:LEU:HA	1.90	0.41
1:C:52:LYS:HZ3	3:i:174:LEU:C	2.23	0.41
1:G:135:ARG:HH22	1:H:48:ARG:HH11	1.61	0.41
1:O:140:ARG:HH11	1:O:154:VAL:HG13	1.83	0.41
2:V:308:TYR:O	2:V:309:PRO:C	2.62	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.96	0.41
1:J:87:TYR:CE1	2:X:357:ARG:NH1	2.89	0.41
2:V:366:TYR:CZ	2:V:370:GLU:HG3	2.54	0.41
2:W:308:TYR:CD1	2:W:309:PRO:O	2.74	0.41
2:Y:308:TYR:O	2:Y:309:PRO:C	2.62	0.41
1:O:100:ALA:O	1:O:141:ILE:CD1	2.66	0.41
2:S:301:THR:CB	2:S:333:LYS:HZ2	2.33	0.41
2:b:471:LEU:HD23	2:b:471:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LYS:HB2	1:E:52:LYS:HZ2	1.86	0.41
1:F:26:ARG:CZ	3:e:173:TYR:CZ	3.00	0.41
1:H:56:LEU:HD23	1:H:56:LEU:HA	1.77	0.41
1:H:87:TYR:HE1	2:V:357:ARG:NH1	2.18	0.41
1:M:114:GLN:CG	1:M:115:ALA:N	2.49	0.41
1:N:141:ILE:HG12	1:N:147:ILE:CG2	2.28	0.41
2:c:301:THR:CG2	2:c:333:LYS:NZ	2.75	0.41
1:A:140:ARG:HH11	1:A:154:VAL:HG13	1.83	0.41
1:G:52:LYS:CE	3:f:174:LEU:CA	2.99	0.41
1:H:141:ILE:HG12	1:H:147:ILE:CG2	2.28	0.41
1:O:134:LYS:HB3	1:O:134:LYS:HE2	1.89	0.41
2:U:386:MET:HE3	2:U:386:MET:HB2	1.95	0.41
2:c:513:LEU:HD23	2:c:513:LEU:HA	1.90	0.41
1:G:50:LEU:HD13	3:f:172:GLN:HE21	1.65	0.40
1:G:56:LEU:HD23	1:G:56:LEU:HA	1.77	0.40
1:H:100:ALA:O	1:H:141:ILE:CD1	2.66	0.40
2:Y:308:TYR:CD1	2:Y:309:PRO:O	2.74	0.40
2:Y:301:THR:CG2	2:Y:333:LYS:NZ	2.75	0.40
1:F:141:ILE:HG12	1:F:147:ILE:CG2	2.28	0.40
1:H:134:LYS:HB3	1:H:134:LYS:HE2	1.90	0.40
1:M:78:GLY:CA	1:M:103:TYR:OH	2.55	0.40
2:T:324:ASN:O	2:Y:479:SER:OG	2.20	0.40
2:Q:301:THR:CG2	2:Q:333:LYS:NZ	2.75	0.40
2:S:301:THR:CG2	2:S:333:LYS:HZ2	2.34	0.40
1:F:52:LYS:NZ	3:e:174:LEU:CA	2.85	0.40
1:J:134:LYS:HB3	1:J:134:LYS:HE2	1.90	0.40
1:L:56:LEU:HD23	1:L:56:LEU:HA	1.77	0.40
1:N:56:LEU:HD23	1:N:56:LEU:HA	1.76	0.40
2:a:301:THR:CG2	2:a:333:LYS:NZ	2.75	0.40
2:b:301:THR:CG2	2:b:333:LYS:NZ	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/248 (86%)	206 (96%)	7 (3%)	1 (0%)	24	62
1	C	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	D	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	E	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	F	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	G	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	H	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
1	I	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	J	215/248 (87%)	207 (96%)	6 (3%)	2 (1%)	14	49
1	K	51/248 (21%)	47 (92%)	4 (8%)	0	100	100
1	L	5/248 (2%)	5 (100%)	0	0	100	100
1	M	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
1	N	215/248 (87%)	206 (96%)	9 (4%)	0	100	100
1	O	213/248 (86%)	204 (96%)	9 (4%)	0	100	100
2	P	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	Q	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	R	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	S	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	T	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	U	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	V	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	W	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	X	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	Y	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	Z	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	a	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	b	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
2	c	220/240 (92%)	214 (97%)	6 (3%)	0	100	100
3	d	2/174 (1%)	2 (100%)	0	0	100	100
3	e	2/174 (1%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	f	2/174 (1%)	2 (100%)	0	0	100	100
3	g	2/174 (1%)	2 (100%)	0	0	100	100
3	h	2/174 (1%)	2 (100%)	0	0	100	100
3	i	2/174 (1%)	2 (100%)	0	0	100	100
3	j	2/174 (1%)	2 (100%)	0	0	100	100
All	All	5695/8050 (71%)	5521 (97%)	171 (3%)	3 (0%)	49	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	J	6	PHE
1	J	7	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	C	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	D	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	E	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	F	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	G	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	H	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	I	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	J	165/192 (86%)	162 (98%)	3 (2%)	51	66
1	K	165/192 (86%)	163 (99%)	2 (1%)	63	73
1	L	165/192 (86%)	162 (98%)	3 (2%)	51	66
1	M	165/192 (86%)	162 (98%)	3 (2%)	51	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	165/192 (86%)	162 (98%)	3 (2%)	51	66
1	O	165/192 (86%)	162 (98%)	3 (2%)	51	66
2	P	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	Q	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	R	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	S	36/178 (20%)	36 (100%)	0	100	100
2	T	157/178 (88%)	156 (99%)	1 (1%)	78	80
2	U	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	V	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	W	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	X	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	Y	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	Z	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	a	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	b	165/178 (93%)	164 (99%)	1 (1%)	78	80
2	c	165/178 (93%)	164 (99%)	1 (1%)	78	80
3	d	3/141 (2%)	3 (100%)	0	100	100
3	e	3/141 (2%)	3 (100%)	0	100	100
3	f	3/141 (2%)	3 (100%)	0	100	100
3	g	3/141 (2%)	3 (100%)	0	100	100
3	h	3/141 (2%)	3 (100%)	0	100	100
3	i	3/141 (2%)	3 (100%)	0	100	100
3	j	3/141 (2%)	3 (100%)	0	100	100
All	All	4504/6167 (73%)	4458 (99%)	46 (1%)	65	75

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	74	LEU
1	C	14	ARG
1	C	74	LEU
1	D	14	ARG
1	D	74	LEU

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Mol	Chain	Res	Type
1	E	14	ARG
1	E	74	LEU
1	F	14	ARG
1	F	74	LEU
1	G	14	ARG
1	G	74	LEU
1	H	14	ARG
1	H	74	LEU
1	I	14	ARG
1	I	74	LEU
1	J	8	SER
1	J	14	ARG
1	J	74	LEU
1	K	14	ARG
1	K	74	LEU
1	L	8	SER
1	L	14	ARG
1	L	74	LEU
1	M	8	SER
1	M	14	ARG
1	M	74	LEU
1	N	8	SER
1	N	14	ARG
1	N	74	LEU
1	O	8	SER
1	O	14	ARG
1	O	74	LEU
2	P	486	LEU
2	Q	486	LEU
2	R	486	LEU
2	T	486	LEU
2	U	486	LEU
2	V	486	LEU
2	W	486	LEU
2	X	486	LEU
2	Y	486	LEU
2	Z	486	LEU
2	a	486	LEU
2	b	486	LEU
2	c	486	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	80	GLN
1	C	11	GLN
1	C	80	GLN
1	D	11	GLN
1	D	80	GLN
1	E	11	GLN
1	E	80	GLN
1	F	11	GLN
1	F	80	GLN
1	G	11	GLN
1	G	80	GLN
1	H	11	GLN
1	H	80	GLN
1	I	11	GLN
1	I	80	GLN
1	J	11	GLN
1	J	80	GLN
1	K	11	GLN
1	K	80	GLN
1	L	11	GLN
1	L	80	GLN
1	M	11	GLN
1	M	80	GLN
1	N	11	GLN
1	N	80	GLN
1	O	11	GLN
1	O	80	GLN
2	P	456	GLN
2	Q	415	GLN
2	Q	456	GLN
2	R	415	GLN
2	R	456	GLN
2	T	456	GLN
2	U	456	GLN
2	V	456	GLN
2	W	456	GLN
2	X	456	GLN
2	Y	415	GLN
2	Y	456	GLN
2	Z	415	GLN
2	Z	456	GLN
2	a	456	GLN

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Mol	Chain	Res	Type
2	b	456	GLN
2	c	456	GLN
3	f	172	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

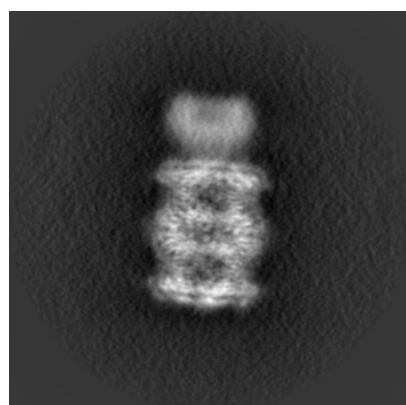
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7098. These allow visual inspection of the internal detail of the map and identification of artifacts.

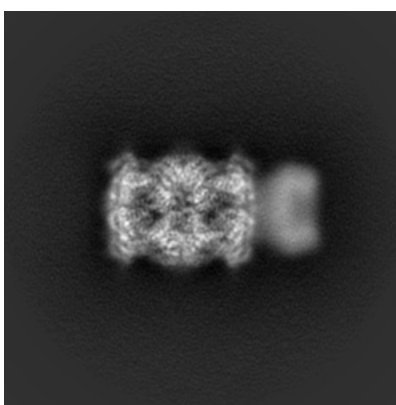
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

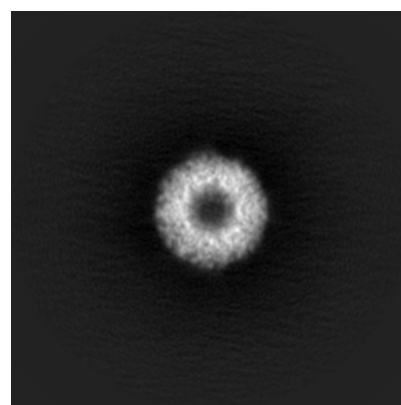
6.1.1 Primary map



X



Y

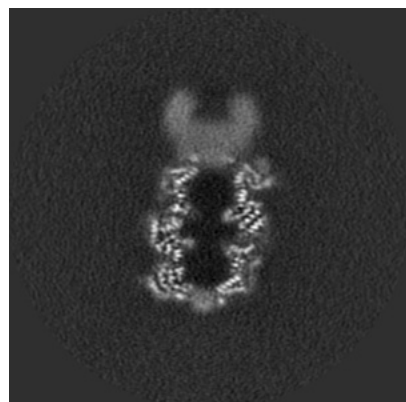


Z

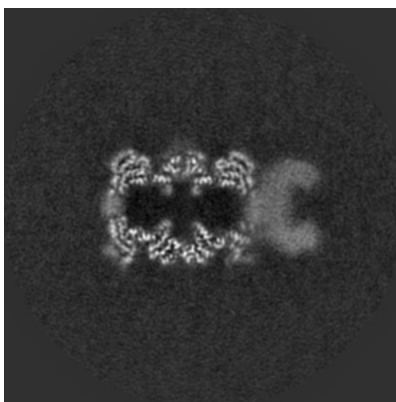
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

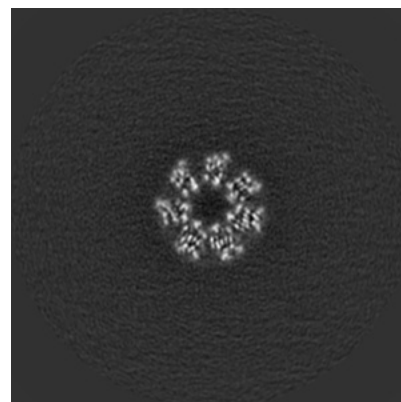
6.2.1 Primary map



X Index: 200



Y Index: 200

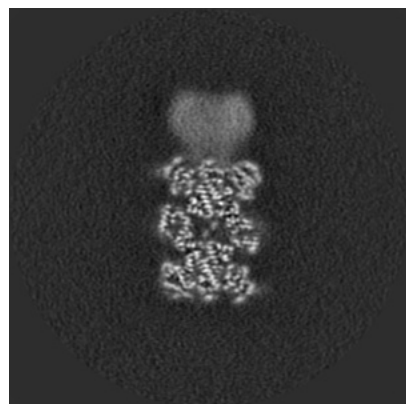


Z Index: 200

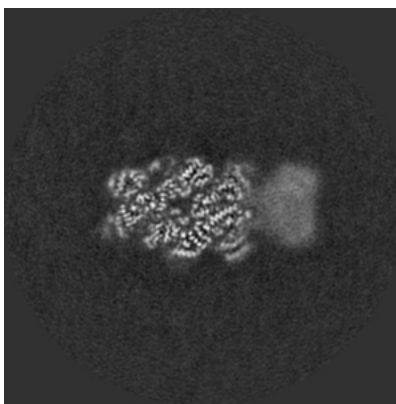
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

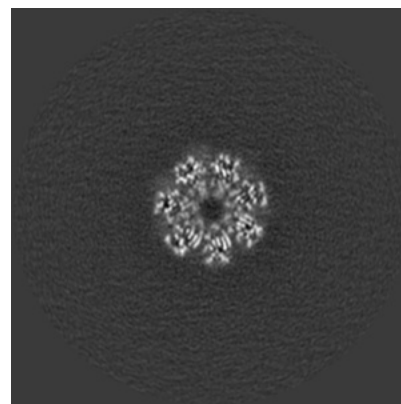
6.3.1 Primary map



X Index: 227



Y Index: 228

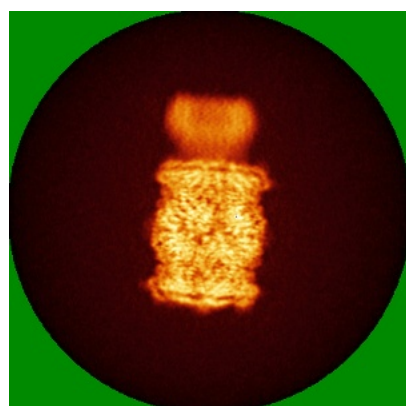


Z Index: 162

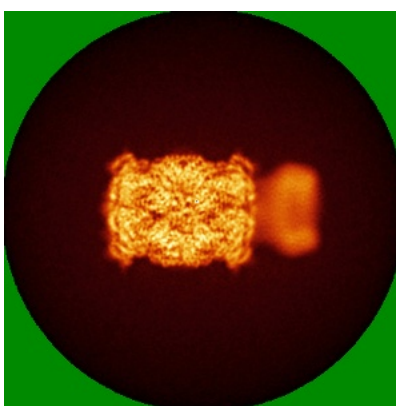
The images above show the largest variance slices of the map in three orthogonal directions.

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

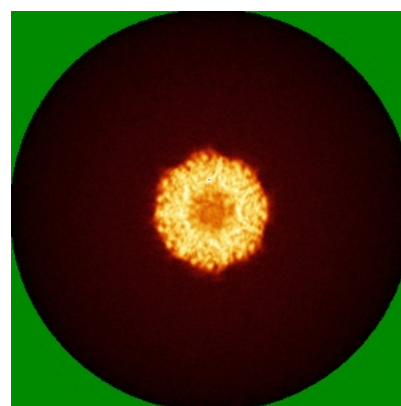
6.4.1 Primary map



X



Y

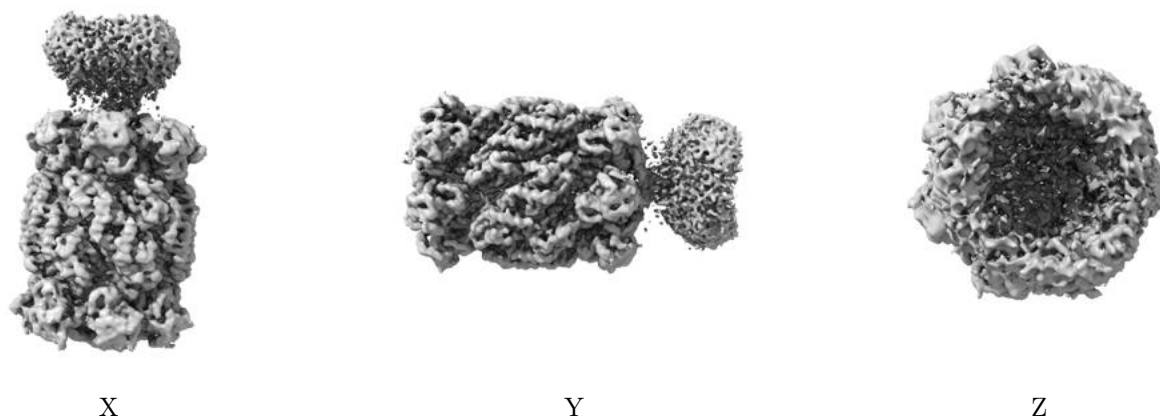


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00952. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

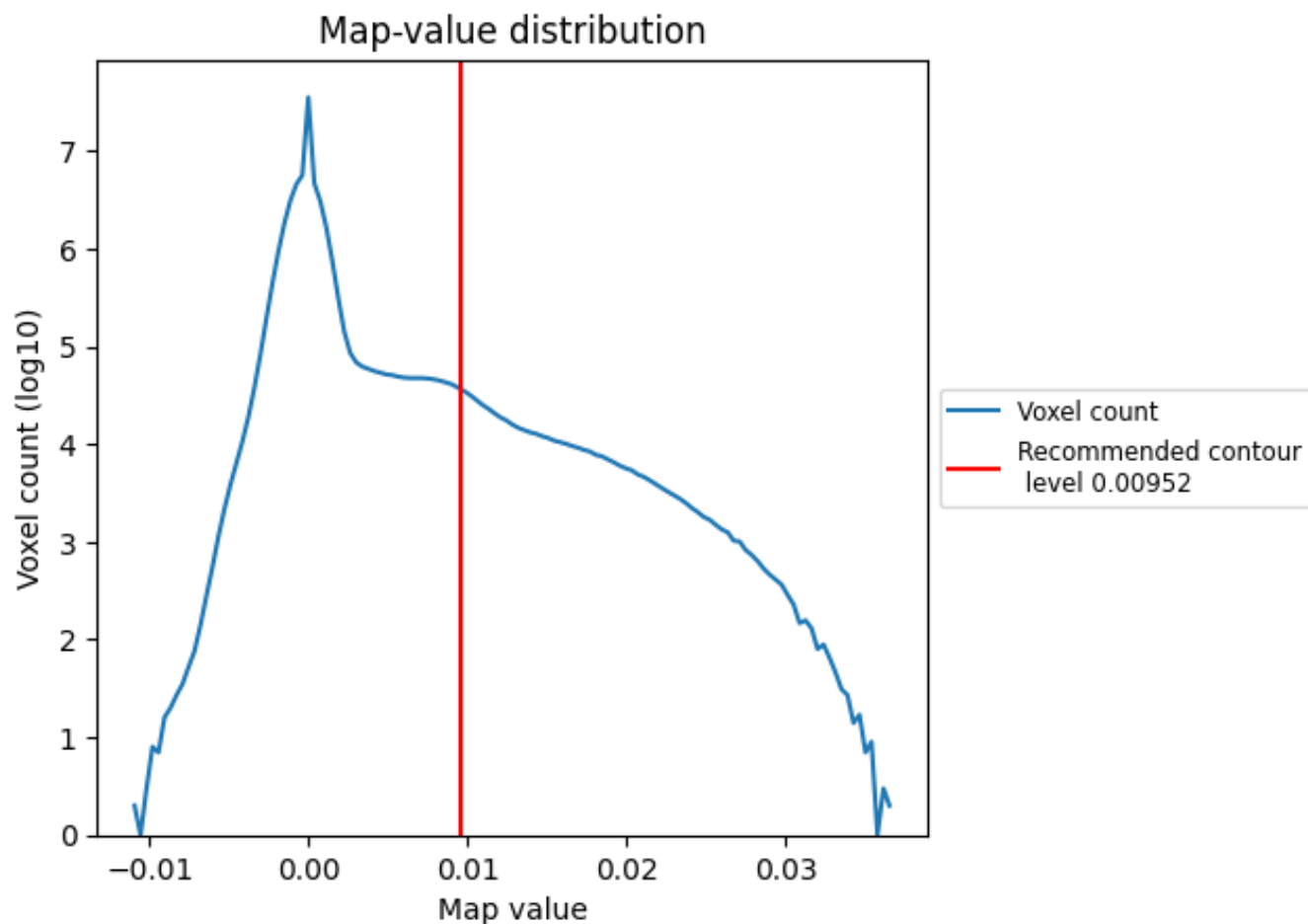
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

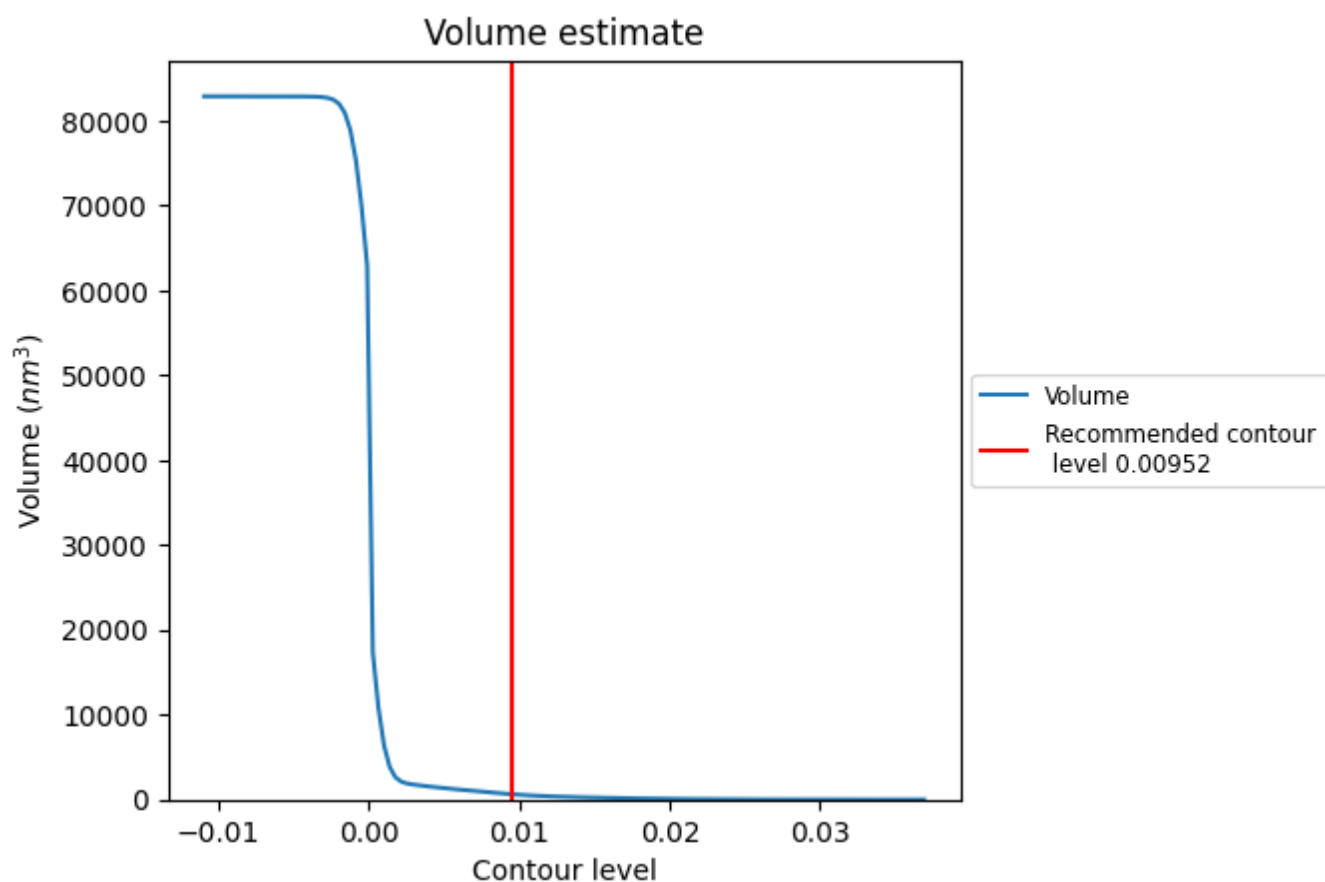
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

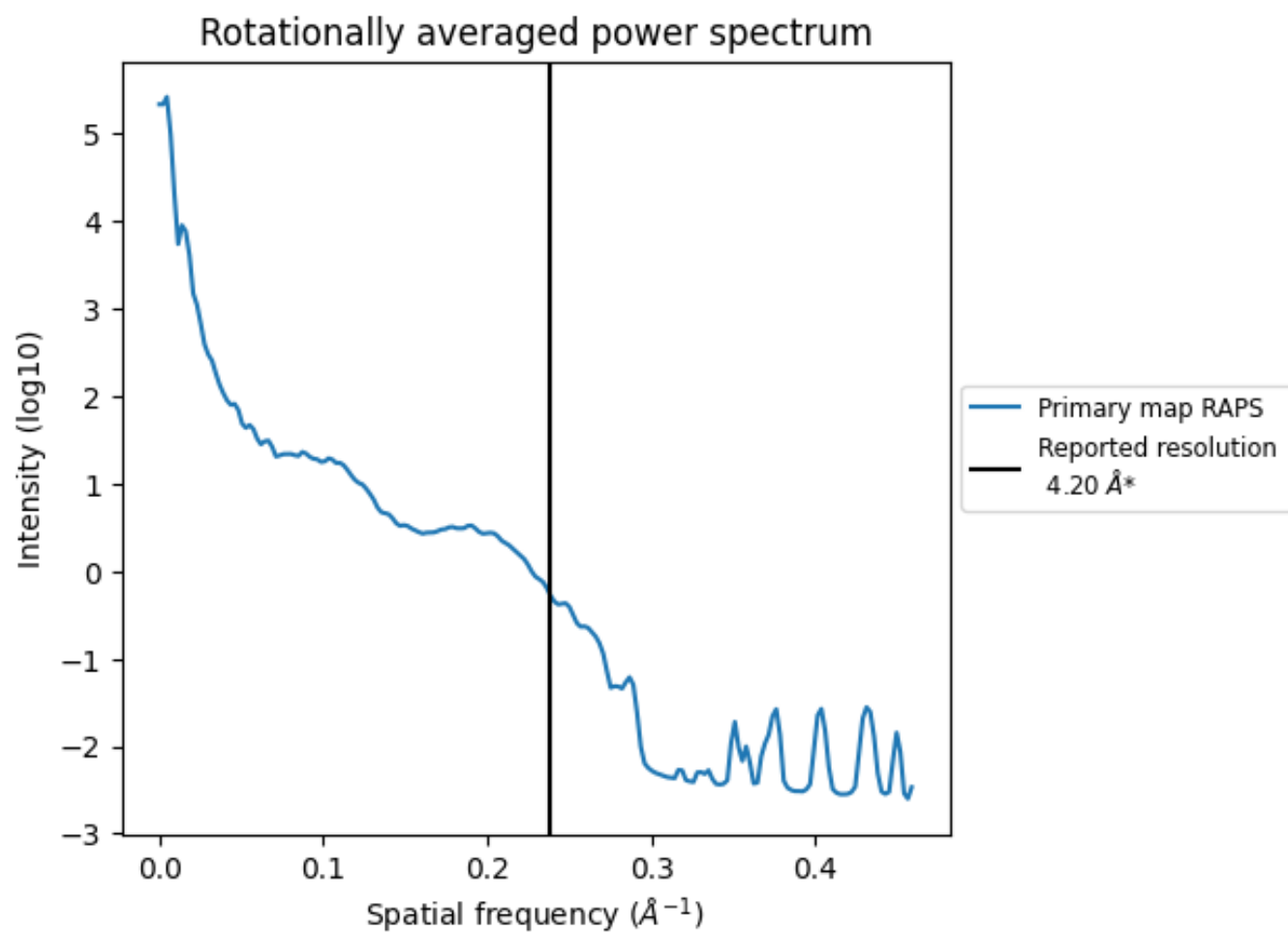
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 628 nm³; this corresponds to an approximate mass of 568 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

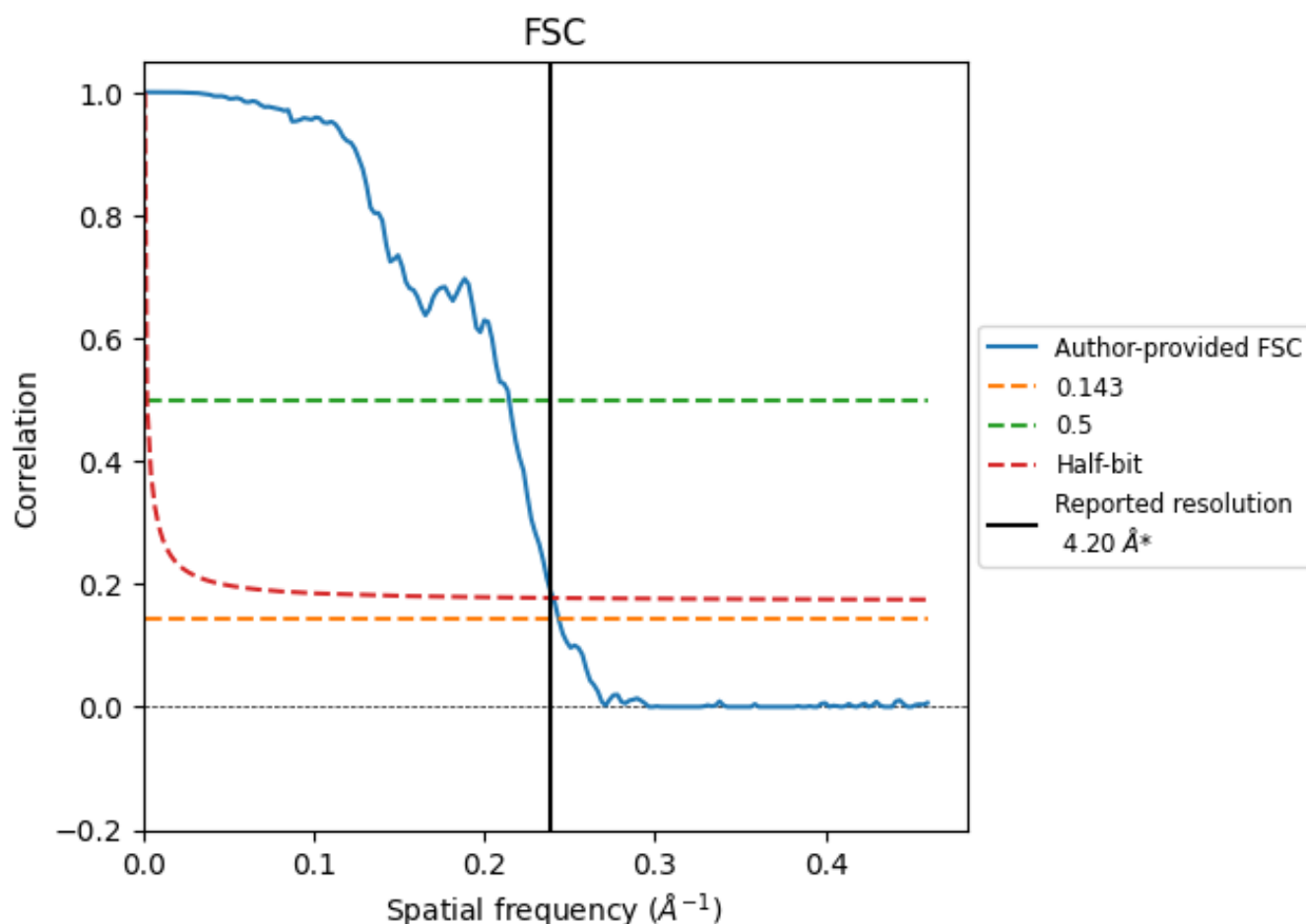


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.11	4.66	4.16
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

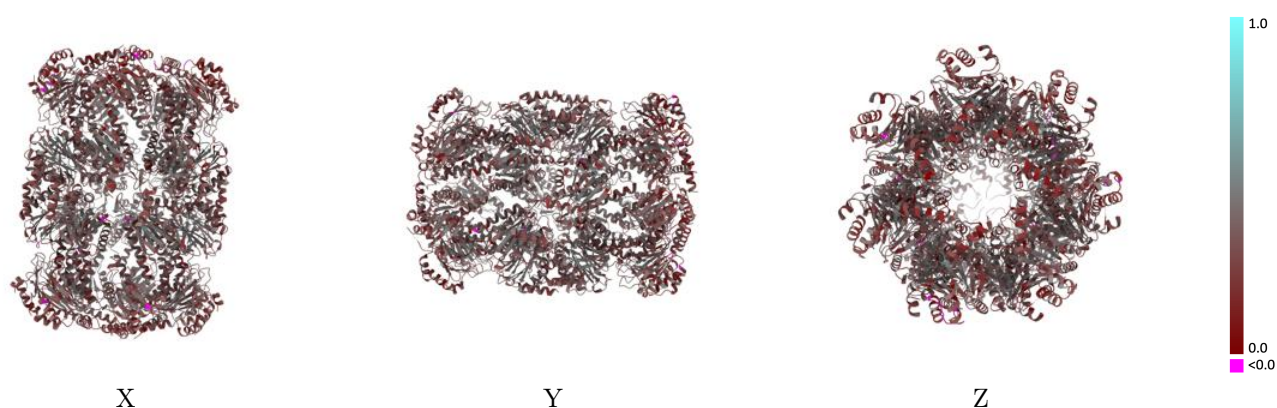
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7098 and PDB model 6BGO. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

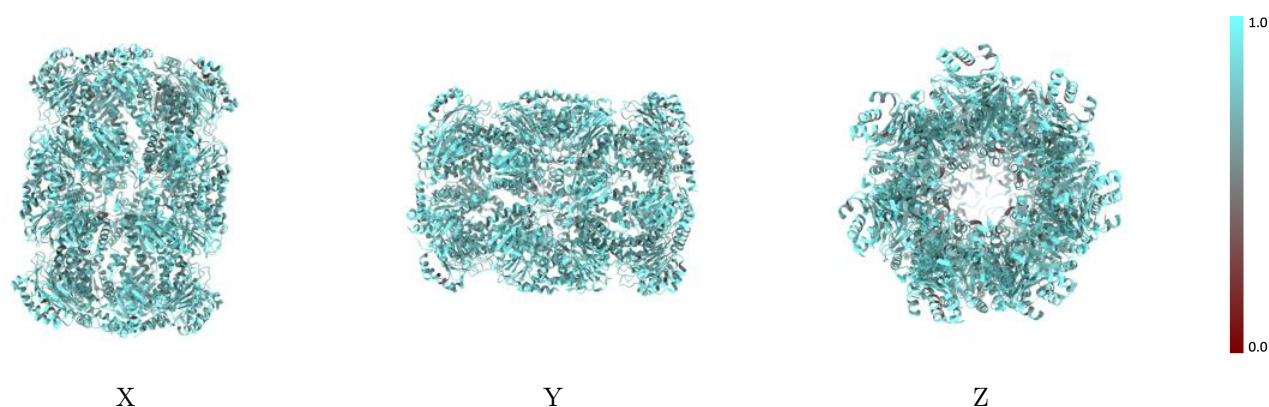
This section was not generated.

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



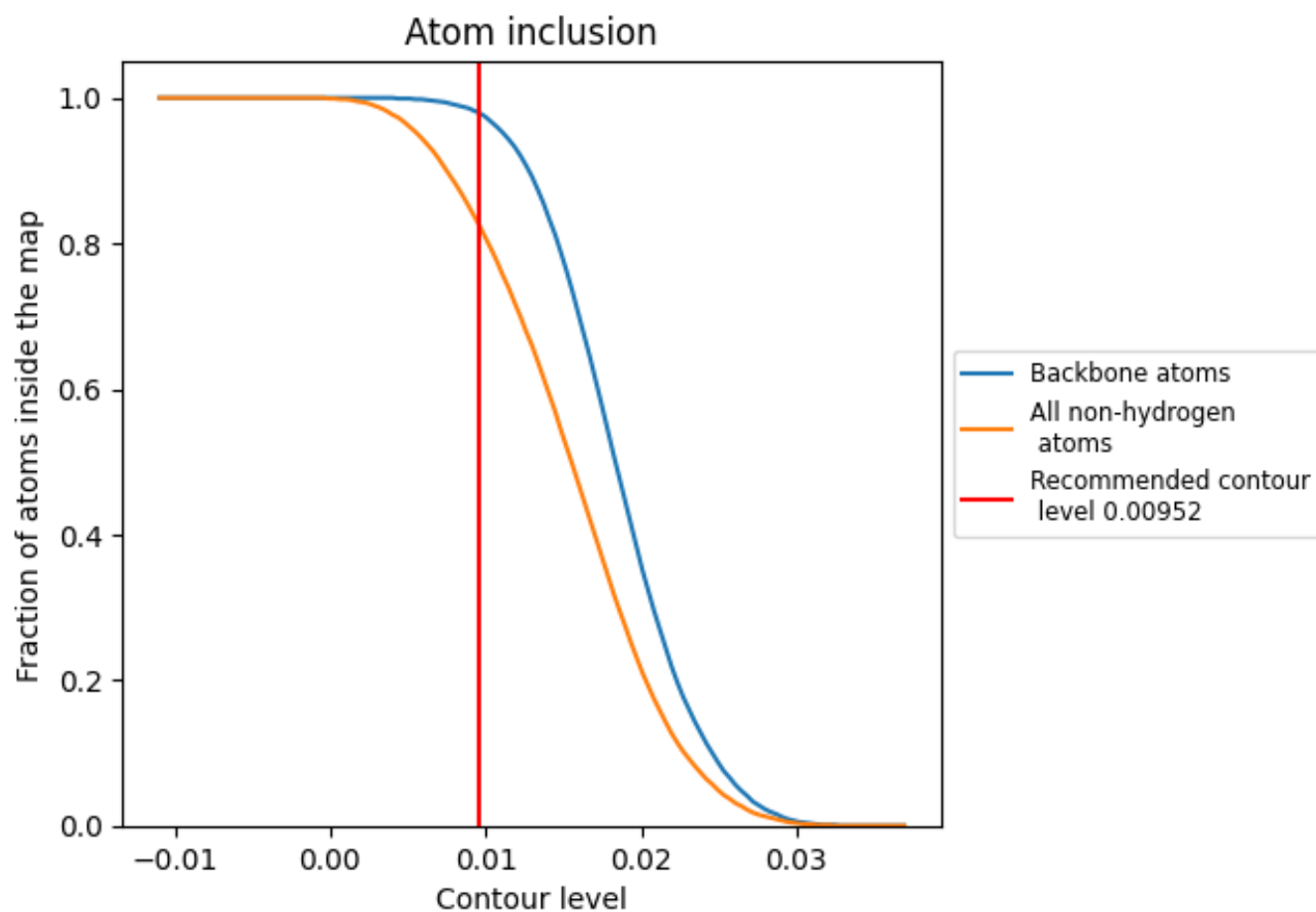
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00952).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 83% 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 (0.00952) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.3350
A	 0.8290	 0.3250
C	 0.7970	 0.3010
D	 0.8150	 0.3120
E	 0.7930	 0.2890
F	 0.8070	 0.3110
G	 0.8190	 0.2930
H	 0.7910	 0.3020
I	 0.8150	 0.3120
J	 0.8330	 0.3240
K	 0.8240	 0.3240
L	 0.8350	 0.3270
M	 0.8260	 0.3270
N	 0.8340	 0.3220
O	 0.8400	 0.3240
P	 0.8430	 0.3590
Q	 0.8500	 0.3630
R	 0.8420	 0.3560
S	 0.8370	 0.3630
T	 0.8320	 0.3600
U	 0.8450	 0.3560
V	 0.8370	 0.3570
W	 0.8430	 0.3620
X	 0.8480	 0.3570
Y	 0.8420	 0.3580
Z	 0.8400	 0.3540
a	 0.8320	 0.3570
b	 0.8460	 0.3610
c	 0.8500	 0.3650
d	 0.3330	 0.0780
e	 0.4850	 0.1820
f	 0.5150	 0.2170
g	 0.3640	 0.0270
h	 0.6360	 0.3120
i	 0.5450	 0.3100
j	 0.5150	 0.1280

