



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:25 AM UTC

PDB ID : 7DDE / pdb\_00007dde  
EMDB ID : EMD-30652  
Title : Cryo-EM structure of the Ape4 and Nbr1 complex  
Authors : Zhang, J.; Ye, K.  
Deposited on : 2020-10-28  
Resolution : 2.26 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

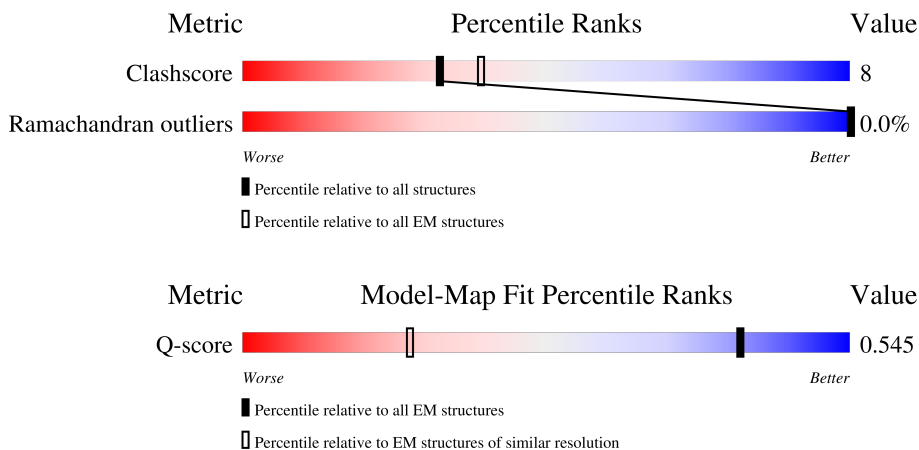
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.26 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.



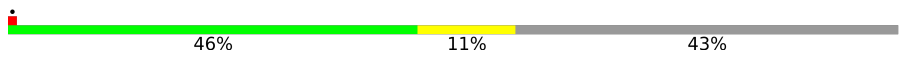
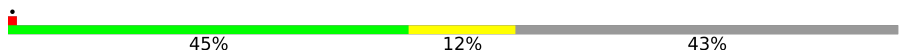
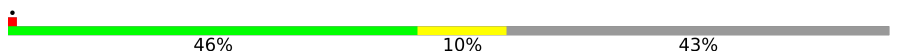
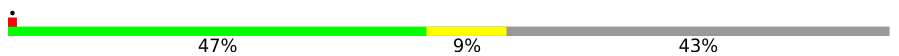
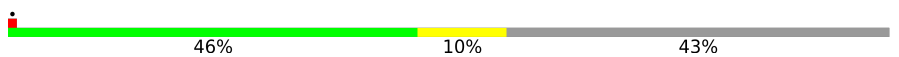
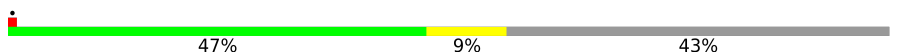
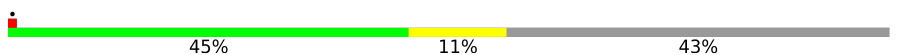
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	3535 ( 1.76 - 2.76 )

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

Mol	Chain	Length	Quality of chain
1	A	929	<span style="color: red;">■</span> <span style="color: orange;">■</span> <span style="color: yellow;">■</span> <span style="color: green;">■</span> <span style="color: grey;">■</span> 46% 10% 43%
1	C	929	<span style="color: red;">■</span> <span style="color: orange;">■</span> <span style="color: yellow;">■</span> <span style="color: green;">■</span> <span style="color: grey;">■</span> 47% 9% 43%
1	E	929	<span style="color: red;">■</span> <span style="color: orange;">■</span> <span style="color: yellow;">■</span> <span style="color: green;">■</span> <span style="color: grey;">■</span> 46% 11% 43%
1	G	929	<span style="color: red;">■</span> <span style="color: orange;">■</span> <span style="color: yellow;">■</span> <span style="color: green;">■</span> <span style="color: grey;">■</span> 45% 11% 43%
1	I	929	<span style="color: red;">■</span> <span style="color: orange;">■</span> <span style="color: yellow;">■</span> <span style="color: green;">■</span> <span style="color: grey;">■</span> 47% 9% 43%

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Mol	Chain	Length	Quality of chain
1	K	929	
1	M	929	
1	O	929	
1	Q	929	
1	S	929	
1	V	929	
1	X	929	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51171 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 Aspartyl aminopeptidase 1,ZZ-type zinc finger-containing protein P35G2.11c,Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	525	4101	2598	696	779	28	0	0
1	C	525	4101	2598	696	779	28	0	0
1	E	525	4101	2598	696	779	28	0	0
1	G	525	4101	2598	696	779	28	0	0
1	I	525	4101	2598	696	779	28	0	0
1	K	525	4101	2598	696	779	28	0	0
1	M	525	4101	2598	696	779	28	0	0
1	O	525	4101	2598	696	779	28	0	0
1	Q	525	4101	2598	696	779	28	0	0
1	S	525	4101	2598	696	779	28	0	0
1	V	525	4101	2598	696	779	28	0	0
1	X	525	4101	2598	696	779	28	0	0

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O36014
A	2	GLN	-	expression tag	UNP O36014
A	3	LEU	-	expression tag	UNP O36014
A	4	HIS	-	expression tag	UNP O36014
A	5	GLY	-	expression tag	UNP O36014

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Chain	Residue	Modelled	Actual	Comment	Reference
A	6	LYS	-	expression tag	UNP O36014
A	474	GLY	-	linker	UNP O36014
A	475	PHE	-	linker	UNP O36014
A	476	LYS	-	linker	UNP O36014
A	477	LYS	-	linker	UNP O36014
A	478	ALA	-	linker	UNP O36014
A	479	SER	-	linker	UNP O36014
A	480	SER	-	linker	UNP O36014
A	481	SER	-	linker	UNP O36014
A	482	ASP	-	linker	UNP O36014
A	483	ASN	-	linker	UNP O36014
A	484	LYS	-	linker	UNP O36014
A	485	GLU	-	linker	UNP O36014
A	486	GLN	-	linker	UNP O36014
C	1	MET	-	initiating methionine	UNP O36014
C	2	GLN	-	expression tag	UNP O36014
C	3	LEU	-	expression tag	UNP O36014
C	4	HIS	-	expression tag	UNP O36014
C	5	GLY	-	expression tag	UNP O36014
C	6	LYS	-	expression tag	UNP O36014
C	474	GLY	-	linker	UNP O36014
C	475	PHE	-	linker	UNP O36014
C	476	LYS	-	linker	UNP O36014
C	477	LYS	-	linker	UNP O36014
C	478	ALA	-	linker	UNP O36014
C	479	SER	-	linker	UNP O36014
C	480	SER	-	linker	UNP O36014
C	481	SER	-	linker	UNP O36014
C	482	ASP	-	linker	UNP O36014
C	483	ASN	-	linker	UNP O36014
C	484	LYS	-	linker	UNP O36014
C	485	GLU	-	linker	UNP O36014
C	486	GLN	-	linker	UNP O36014
E	1	MET	-	initiating methionine	UNP O36014
E	2	GLN	-	expression tag	UNP O36014
E	3	LEU	-	expression tag	UNP O36014
E	4	HIS	-	expression tag	UNP O36014
E	5	GLY	-	expression tag	UNP O36014
E	6	LYS	-	expression tag	UNP O36014
E	474	GLY	-	linker	UNP O36014
E	475	PHE	-	linker	UNP O36014
E	476	LYS	-	linker	UNP O36014

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Chain	Residue	Modelled	Actual	Comment	Reference
E	477	LYS	-	linker	UNP O36014
E	478	ALA	-	linker	UNP O36014
E	479	SER	-	linker	UNP O36014
E	480	SER	-	linker	UNP O36014
E	481	SER	-	linker	UNP O36014
E	482	ASP	-	linker	UNP O36014
E	483	ASN	-	linker	UNP O36014
E	484	LYS	-	linker	UNP O36014
E	485	GLU	-	linker	UNP O36014
E	486	GLN	-	linker	UNP O36014
G	1	MET	-	initiating methionine	UNP O36014
G	2	GLN	-	expression tag	UNP O36014
G	3	LEU	-	expression tag	UNP O36014
G	4	HIS	-	expression tag	UNP O36014
G	5	GLY	-	expression tag	UNP O36014
G	6	LYS	-	expression tag	UNP O36014
G	474	GLY	-	linker	UNP O36014
G	475	PHE	-	linker	UNP O36014
G	476	LYS	-	linker	UNP O36014
G	477	LYS	-	linker	UNP O36014
G	478	ALA	-	linker	UNP O36014
G	479	SER	-	linker	UNP O36014
G	480	SER	-	linker	UNP O36014
G	481	SER	-	linker	UNP O36014
G	482	ASP	-	linker	UNP O36014
G	483	ASN	-	linker	UNP O36014
G	484	LYS	-	linker	UNP O36014
G	485	GLU	-	linker	UNP O36014
G	486	GLN	-	linker	UNP O36014
I	1	MET	-	initiating methionine	UNP O36014
I	2	GLN	-	expression tag	UNP O36014
I	3	LEU	-	expression tag	UNP O36014
I	4	HIS	-	expression tag	UNP O36014
I	5	GLY	-	expression tag	UNP O36014
I	6	LYS	-	expression tag	UNP O36014
I	474	GLY	-	linker	UNP O36014
I	475	PHE	-	linker	UNP O36014
I	476	LYS	-	linker	UNP O36014
I	477	LYS	-	linker	UNP O36014
I	478	ALA	-	linker	UNP O36014
I	479	SER	-	linker	UNP O36014
I	480	SER	-	linker	UNP O36014

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Chain	Residue	Modelled	Actual	Comment	Reference
I	481	SER	-	linker	UNP O36014
I	482	ASP	-	linker	UNP O36014
I	483	ASN	-	linker	UNP O36014
I	484	LYS	-	linker	UNP O36014
I	485	GLU	-	linker	UNP O36014
I	486	GLN	-	linker	UNP O36014
K	1	MET	-	initiating methionine	UNP O36014
K	2	GLN	-	expression tag	UNP O36014
K	3	LEU	-	expression tag	UNP O36014
K	4	HIS	-	expression tag	UNP O36014
K	5	GLY	-	expression tag	UNP O36014
K	6	LYS	-	expression tag	UNP O36014
K	474	GLY	-	linker	UNP O36014
K	475	PHE	-	linker	UNP O36014
K	476	LYS	-	linker	UNP O36014
K	477	LYS	-	linker	UNP O36014
K	478	ALA	-	linker	UNP O36014
K	479	SER	-	linker	UNP O36014
K	480	SER	-	linker	UNP O36014
K	481	SER	-	linker	UNP O36014
K	482	ASP	-	linker	UNP O36014
K	483	ASN	-	linker	UNP O36014
K	484	LYS	-	linker	UNP O36014
K	485	GLU	-	linker	UNP O36014
K	486	GLN	-	linker	UNP O36014
M	1	MET	-	initiating methionine	UNP O36014
M	2	GLN	-	expression tag	UNP O36014
M	3	LEU	-	expression tag	UNP O36014
M	4	HIS	-	expression tag	UNP O36014
M	5	GLY	-	expression tag	UNP O36014
M	6	LYS	-	expression tag	UNP O36014
M	474	GLY	-	linker	UNP O36014
M	475	PHE	-	linker	UNP O36014
M	476	LYS	-	linker	UNP O36014
M	477	LYS	-	linker	UNP O36014
M	478	ALA	-	linker	UNP O36014
M	479	SER	-	linker	UNP O36014
M	480	SER	-	linker	UNP O36014
M	481	SER	-	linker	UNP O36014
M	482	ASP	-	linker	UNP O36014
M	483	ASN	-	linker	UNP O36014
M	484	LYS	-	linker	UNP O36014

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Chain	Residue	Modelled	Actual	Comment	Reference
M	485	GLU	-	linker	UNP O36014
M	486	GLN	-	linker	UNP O36014
O	1	MET	-	initiating methionine	UNP O36014
O	2	GLN	-	expression tag	UNP O36014
O	3	LEU	-	expression tag	UNP O36014
O	4	HIS	-	expression tag	UNP O36014
O	5	GLY	-	expression tag	UNP O36014
O	6	LYS	-	expression tag	UNP O36014
O	474	GLY	-	linker	UNP O36014
O	475	PHE	-	linker	UNP O36014
O	476	LYS	-	linker	UNP O36014
O	477	LYS	-	linker	UNP O36014
O	478	ALA	-	linker	UNP O36014
O	479	SER	-	linker	UNP O36014
O	480	SER	-	linker	UNP O36014
O	481	SER	-	linker	UNP O36014
O	482	ASP	-	linker	UNP O36014
O	483	ASN	-	linker	UNP O36014
O	484	LYS	-	linker	UNP O36014
O	485	GLU	-	linker	UNP O36014
O	486	GLN	-	linker	UNP O36014
Q	1	MET	-	initiating methionine	UNP O36014
Q	2	GLN	-	expression tag	UNP O36014
Q	3	LEU	-	expression tag	UNP O36014
Q	4	HIS	-	expression tag	UNP O36014
Q	5	GLY	-	expression tag	UNP O36014
Q	6	LYS	-	expression tag	UNP O36014
Q	474	GLY	-	linker	UNP O36014
Q	475	PHE	-	linker	UNP O36014
Q	476	LYS	-	linker	UNP O36014
Q	477	LYS	-	linker	UNP O36014
Q	478	ALA	-	linker	UNP O36014
Q	479	SER	-	linker	UNP O36014
Q	480	SER	-	linker	UNP O36014
Q	481	SER	-	linker	UNP O36014
Q	482	ASP	-	linker	UNP O36014
Q	483	ASN	-	linker	UNP O36014
Q	484	LYS	-	linker	UNP O36014
Q	485	GLU	-	linker	UNP O36014
Q	486	GLN	-	linker	UNP O36014
S	1	MET	-	initiating methionine	UNP O36014
S	2	GLN	-	expression tag	UNP O36014

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Chain	Residue	Modelled	Actual	Comment	Reference
S	3	LEU	-	expression tag	UNP O36014
S	4	HIS	-	expression tag	UNP O36014
S	5	GLY	-	expression tag	UNP O36014
S	6	LYS	-	expression tag	UNP O36014
S	474	GLY	-	linker	UNP O36014
S	475	PHE	-	linker	UNP O36014
S	476	LYS	-	linker	UNP O36014
S	477	LYS	-	linker	UNP O36014
S	478	ALA	-	linker	UNP O36014
S	479	SER	-	linker	UNP O36014
S	480	SER	-	linker	UNP O36014
S	481	SER	-	linker	UNP O36014
S	482	ASP	-	linker	UNP O36014
S	483	ASN	-	linker	UNP O36014
S	484	LYS	-	linker	UNP O36014
S	485	GLU	-	linker	UNP O36014
S	486	GLN	-	linker	UNP O36014
V	1	MET	-	initiating methionine	UNP O36014
V	2	GLN	-	expression tag	UNP O36014
V	3	LEU	-	expression tag	UNP O36014
V	4	HIS	-	expression tag	UNP O36014
V	5	GLY	-	expression tag	UNP O36014
V	6	LYS	-	expression tag	UNP O36014
V	474	GLY	-	linker	UNP O36014
V	475	PHE	-	linker	UNP O36014
V	476	LYS	-	linker	UNP O36014
V	477	LYS	-	linker	UNP O36014
V	478	ALA	-	linker	UNP O36014
V	479	SER	-	linker	UNP O36014
V	480	SER	-	linker	UNP O36014
V	481	SER	-	linker	UNP O36014
V	482	ASP	-	linker	UNP O36014
V	483	ASN	-	linker	UNP O36014
V	484	LYS	-	linker	UNP O36014
V	485	GLU	-	linker	UNP O36014
V	486	GLN	-	linker	UNP O36014
X	1	MET	-	initiating methionine	UNP O36014
X	2	GLN	-	expression tag	UNP O36014
X	3	LEU	-	expression tag	UNP O36014
X	4	HIS	-	expression tag	UNP O36014
X	5	GLY	-	expression tag	UNP O36014
X	6	LYS	-	expression tag	UNP O36014

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Chain	Residue	Modelled	Actual	Comment	Reference
X	474	GLY	-	linker	UNP O36014
X	475	PHE	-	linker	UNP O36014
X	476	LYS	-	linker	UNP O36014
X	477	LYS	-	linker	UNP O36014
X	478	ALA	-	linker	UNP O36014
X	479	SER	-	linker	UNP O36014
X	480	SER	-	linker	UNP O36014
X	481	SER	-	linker	UNP O36014
X	482	ASP	-	linker	UNP O36014
X	483	ASN	-	linker	UNP O36014
X	484	LYS	-	linker	UNP O36014
X	485	GLU	-	linker	UNP O36014
X	486	GLN	-	linker	UNP O36014

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	4	Total Zn 4 4	0
2	C	4	Total Zn 4 4	0
2	E	4	Total Zn 4 4	0
2	G	4	Total Zn 4 4	0
2	I	4	Total Zn 4 4	0
2	K	4	Total Zn 4 4	0
2	M	4	Total Zn 4 4	0
2	O	4	Total Zn 4 4	0
2	Q	4	Total Zn 4 4	0
2	S	4	Total Zn 4 4	0
2	V	4	Total Zn 4 4	0
2	X	4	Total Zn 4 4	0

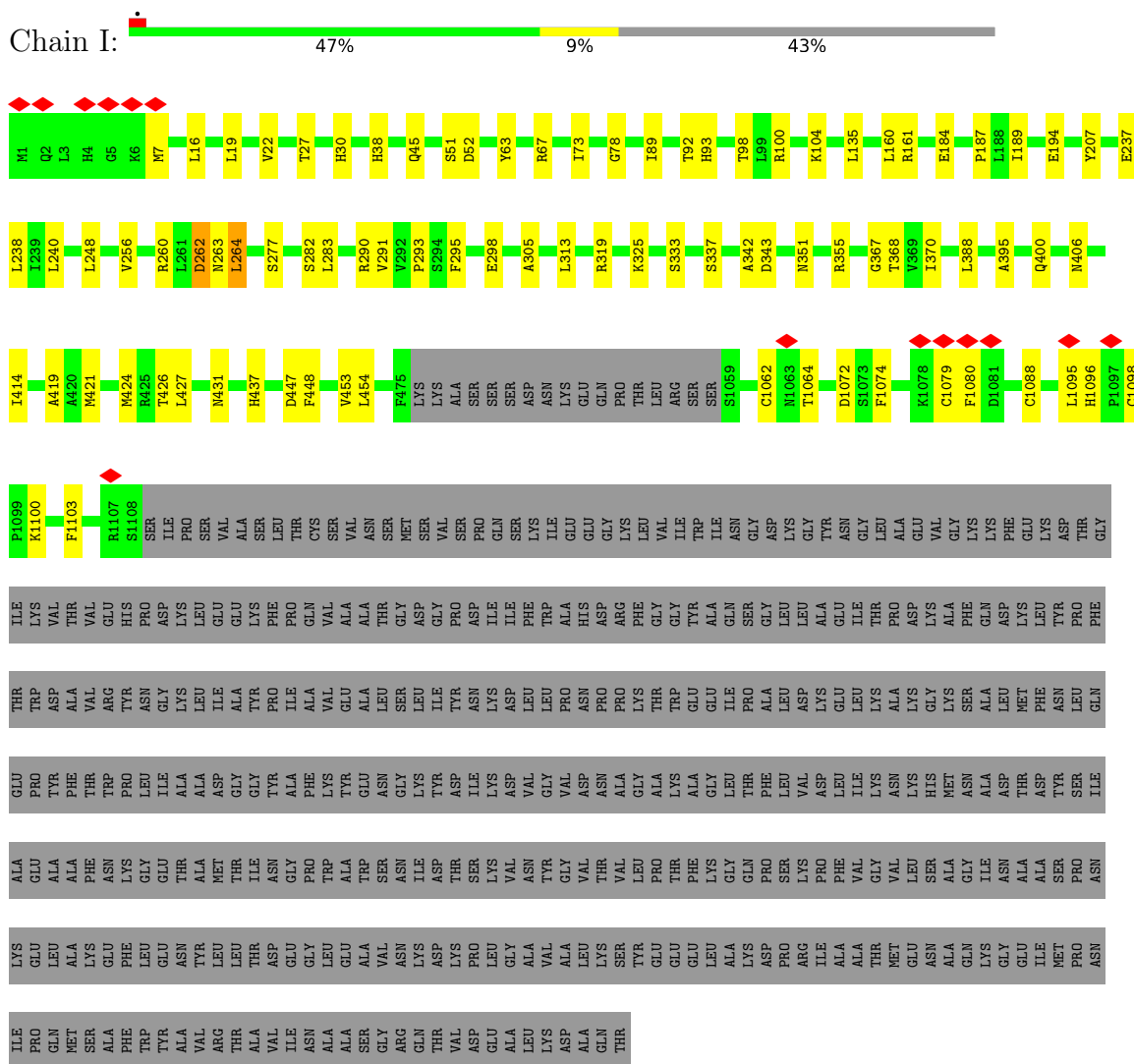
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	166	Total 166	O 166	0
3	C	152	Total 152	O 152	0
3	E	164	Total 164	O 164	0
3	G	151	Total 151	O 151	0
3	I	158	Total 158	O 158	0
3	K	167	Total 167	O 167	0
3	M	162	Total 162	O 162	0
3	O	160	Total 160	O 160	0
3	Q	153	Total 153	O 153	0
3	S	165	Total 165	O 165	0
3	V	151	Total 151	O 151	0
3	X	162	Total 162	O 162	0

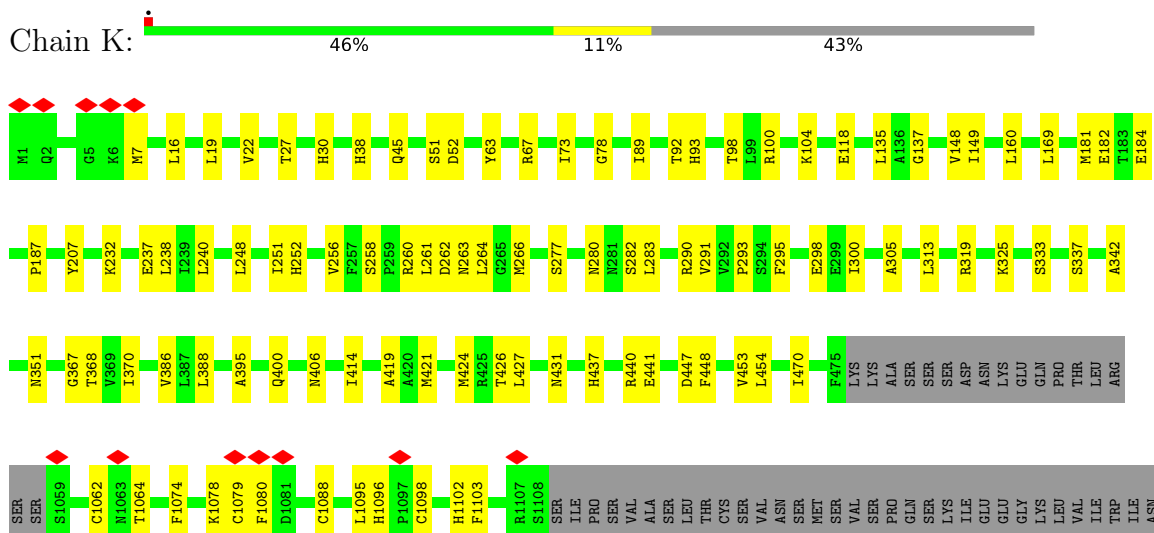








- Molecule 1: Aspartyl aminopeptidase 1,ZZ-type zinc finger-containing protein P35G2.11c,Malto se/maltodextrin-binding periplasmic protein













## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, T	Depositor
Number of particles used	414202	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	41.296	Depositor
Minimum map value	-16.670	Depositor
Average map value	0.055	Depositor
Map value standard deviation	1.605	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	0.38	0/4194	0.68	5/5674 (0.1%)
1	C	0.38	0/4194	0.66	3/5674 (0.1%)
1	E	0.38	0/4194	0.67	4/5674 (0.1%)
1	G	0.38	0/4194	0.68	4/5674 (0.1%)
1	I	0.38	0/4194	0.68	5/5674 (0.1%)
1	K	0.37	0/4194	0.65	2/5674 (0.0%)
1	M	0.38	0/4194	0.66	3/5674 (0.1%)
1	O	0.38	0/4194	0.67	3/5674 (0.1%)
1	Q	0.38	0/4194	0.69	5/5674 (0.1%)
1	S	0.38	0/4194	0.68	4/5674 (0.1%)
1	V	0.38	0/4194	0.69	5/5674 (0.1%)
1	X	0.38	0/4194	0.68	3/5674 (0.1%)
All	All	0.38	0/50328	0.67	46/68088 (0.1%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	264	LEU	N-CA-C	-12.46	98.73	114.56
1	Q	264	LEU	N-CA-C	-12.17	97.90	113.12
1	X	264	LEU	N-CA-C	-11.57	98.04	114.12
1	G	264	LEU	N-CA-C	-9.92	101.18	113.38
1	S	264	LEU	N-CA-C	-9.06	100.54	111.69
1	A	264	LEU	N-CA-C	-8.91	101.48	111.82
1	I	264	LEU	N-CA-C	-8.82	101.75	111.36
1	O	264	LEU	N-CA-C	-8.68	102.13	112.89
1	V	263	ASN	N-CA-C	8.67	123.65	111.52
1	Q	263	ASN	N-CA-C	8.18	122.79	111.74
1	C	264	LEU	N-CA-C	-7.59	103.02	111.82
1	E	265	GLY	N-CA-C	-7.28	103.45	112.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	263	ASN	N-CA-C	7.12	121.92	113.23
1	E	264	LEU	N-CA-C	-6.78	103.96	111.82
1	G	263	ASN	N-CA-C	6.70	122.87	113.56
1	Q	263	ASN	CB-CA-C	-6.24	102.86	111.73
1	V	264	LEU	CA-C-O	6.02	125.41	118.55
1	I	262	ASP	CA-C-N	5.90	132.81	121.54
1	I	262	ASP	C-N-CA	5.90	132.81	121.54
1	A	261	LEU	N-CA-C	5.70	120.23	113.16
1	G	7	MET	CA-C-N	5.39	131.84	121.54
1	G	7	MET	C-N-CA	5.39	131.84	121.54
1	I	7	MET	CA-C-N	5.39	131.84	121.54
1	I	7	MET	C-N-CA	5.39	131.84	121.54
1	E	7	MET	CA-C-N	5.38	131.82	121.54
1	E	7	MET	C-N-CA	5.38	131.82	121.54
1	Q	7	MET	CA-C-N	5.38	131.81	121.54
1	Q	7	MET	C-N-CA	5.38	131.81	121.54
1	V	7	MET	CA-C-N	5.38	131.81	121.54
1	V	7	MET	C-N-CA	5.38	131.81	121.54
1	X	7	MET	CA-C-N	5.37	131.80	121.54
1	X	7	MET	C-N-CA	5.37	131.80	121.54
1	O	7	MET	CA-C-N	5.37	131.80	121.54
1	O	7	MET	C-N-CA	5.37	131.80	121.54
1	A	7	MET	CA-C-N	5.37	131.80	121.54
1	A	7	MET	C-N-CA	5.37	131.80	121.54
1	A	263	ASN	N-CA-C	5.36	121.70	113.28
1	C	7	MET	CA-C-N	5.36	131.78	121.54
1	C	7	MET	C-N-CA	5.36	131.78	121.54
1	K	7	MET	CA-C-N	5.36	131.78	121.54
1	K	7	MET	C-N-CA	5.36	131.78	121.54
1	S	7	MET	CA-C-N	5.36	131.78	121.54
1	S	7	MET	C-N-CA	5.36	131.78	121.54
1	M	7	MET	CA-C-N	5.35	131.75	121.54
1	M	7	MET	C-N-CA	5.35	131.75	121.54
1	M	264	LEU	N-CA-C	-5.32	105.57	111.36

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	4101	0	4022	80	0
1	C	4101	0	4022	65	0
1	E	4101	0	4022	82	0
1	G	4101	0	4022	86	0
1	I	4101	0	4022	63	0
1	K	4101	0	4022	92	0
1	M	4101	0	4022	94	0
1	O	4101	0	4022	70	0
1	Q	4101	0	4022	73	0
1	S	4101	0	4022	75	0
1	V	4101	0	4022	75	0
1	X	4101	0	4022	81	0
2	A	4	0	0	0	0
2	C	4	0	0	0	0
2	E	4	0	0	0	0
2	G	4	0	0	0	0
2	I	4	0	0	0	0
2	K	4	0	0	0	0
2	M	4	0	0	0	0
2	O	4	0	0	0	0
2	Q	4	0	0	0	0
2	S	4	0	0	0	0
2	V	4	0	0	0	0
2	X	4	0	0	0	0
3	A	166	0	0	1	0
3	C	152	0	0	0	0
3	E	164	0	0	2	0
3	G	151	0	0	4	0
3	I	158	0	0	2	0
3	K	167	0	0	3	0
3	M	162	0	0	1	0
3	O	160	0	0	0	0
3	Q	153	0	0	1	0
3	S	165	0	0	0	0
3	V	151	0	0	1	0
3	X	162	0	0	3	0
All	All	51171	0	48264	826	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 8.

All (826) 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:E:263:ASN:ND2	1:E:266:MET:HB2	1.32	1.41
1:V:93:HIS:CG	1:V:298:GLU:HG2	1.65	1.32
1:S:22:VAL:HG23	1:S:264:LEU:HD23	1.20	1.15
1:K:261:LEU:HD12	1:K:441:GLU:CB	1.78	1.14
1:K:258:SER:HB3	1:K:261:LEU:HD21	1.30	1.14
1:Q:93:HIS:CD2	1:Q:263:ASN:HD22	1.68	1.11
1:I:263:ASN:HD21	1:I:343:ASP:HA	1.15	1.10
1:M:22:VAL:HG23	1:M:264:LEU:HD23	1.12	1.08
1:X:22:VAL:HG23	1:X:264:LEU:HD23	1.25	1.08
1:Q:22:VAL:HG23	1:Q:264:LEU:HD23	1.34	1.08
1:K:261:LEU:HD12	1:K:441:GLU:HB3	1.36	1.03
1:E:263:ASN:ND2	1:E:266:MET:CB	2.26	0.98
1:G:1095:LEU:HD23	1:G:1095:LEU:H	1.30	0.97
1:G:21:PHE:CE2	1:G:264:LEU:HD23	2.01	0.96
1:M:22:VAL:HG23	1:M:264:LEU:CD2	1.96	0.95
1:M:1095:LEU:HD23	1:M:1095:LEU:H	1.31	0.94
1:I:1095:LEU:H	1:I:1095:LEU:HD23	1.32	0.94
1:C:1095:LEU:HD23	1:C:1095:LEU:H	1.31	0.94
1:O:1095:LEU:HD23	1:O:1095:LEU:H	1.31	0.94
1:O:22:VAL:HG23	1:O:264:LEU:HD23	1.46	0.93
1:E:1095:LEU:HD23	1:E:1095:LEU:H	1.34	0.93
1:A:258:SER:HB3	1:A:261:LEU:HD21	1.50	0.93
1:A:1095:LEU:H	1:A:1095:LEU:HD23	1.34	0.91
1:Q:1095:LEU:HD23	1:Q:1095:LEU:H	1.34	0.91
1:K:1095:LEU:H	1:K:1095:LEU:HD23	1.33	0.91
1:K:262:ASP:OD2	1:K:437:HIS:CD2	2.24	0.91
1:V:1095:LEU:HD23	1:V:1095:LEU:H	1.35	0.90
1:M:22:VAL:CG2	1:M:264:LEU:HD23	2.00	0.90
1:C:263:ASN:HD21	1:C:343:ASP:HA	1.36	0.89
1:V:93:HIS:CG	1:V:298:GLU:CG	2.55	0.89
1:S:1095:LEU:HD23	1:S:1095:LEU:H	1.33	0.89
1:X:1095:LEU:HD23	1:X:1095:LEU:H	1.35	0.87
1:E:263:ASN:HD22	1:E:266:MET:HB2	1.08	0.87
1:E:263:ASN:HD21	1:E:266:MET:HB2	1.38	0.85
1:A:93:HIS:CD2	1:A:263:ASN:OD1	2.31	0.83
1:G:21:PHE:HE2	1:G:264:LEU:HD23	1.44	0.83
1:G:21:PHE:CE2	1:G:264:LEU:CD2	2.62	0.81
1:Q:93:HIS:CD2	1:Q:263:ASN:ND2	2.46	0.81
1:S:22:VAL:CG2	1:S:264:LEU:HD23	2.08	0.81
1:K:22:VAL:HG23	1:K:264:LEU:HD23	1.60	0.80
1:V:93:HIS:CD2	1:V:298:GLU:HG2	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:HD12	1:A:441:GLU:CB	2.12	0.80
1:I:263:ASN:ND2	1:I:343:ASP:HA	1.97	0.80
1:E:263:ASN:ND2	1:E:263:ASN:O	2.16	0.79
1:K:261:LEU:CD1	1:K:441:GLU:C	2.56	0.78
1:Q:184:GLU:HA	1:S:351:ASN:HB3	1.65	0.77
1:V:93:HIS:CB	1:V:298:GLU:HG2	2.14	0.77
1:K:261:LEU:CD1	1:K:441:GLU:CB	2.62	0.76
1:M:263:ASN:OD1	1:M:343:ASP:HA	1.87	0.75
1:A:27:THR:HG1	1:A:30:HIS:HD1	1.35	0.75
1:E:27:THR:HG1	1:E:30:HIS:HD1	1.35	0.75
1:O:27:THR:HG1	1:O:30:HIS:HD1	1.35	0.74
1:M:27:THR:HG1	1:M:30:HIS:HD1	1.35	0.74
1:K:27:THR:HG1	1:K:30:HIS:HD1	1.35	0.74
1:A:261:LEU:HD12	1:A:441:GLU:C	2.14	0.73
1:A:263:ASN:HD21	1:A:343:ASP:HA	1.54	0.73
1:K:262:ASP:OD2	1:K:437:HIS:NE2	2.20	0.73
1:V:27:THR:HG1	1:V:30:HIS:HD1	1.35	0.73
1:S:27:THR:HG1	1:S:30:HIS:HD1	1.35	0.73
1:K:261:LEU:HD11	1:K:441:GLU:O	1.88	0.73
1:K:261:LEU:HD12	1:K:441:GLU:C	2.14	0.72
1:O:1095:LEU:H	1:O:1095:LEU:CD2	2.01	0.72
1:Q:27:THR:HG1	1:Q:30:HIS:HD1	1.35	0.72
1:G:1095:LEU:H	1:G:1095:LEU:CD2	2.01	0.72
1:I:27:THR:HG1	1:I:30:HIS:HD1	1.35	0.72
1:X:27:THR:HG1	1:X:30:HIS:HD1	1.35	0.72
1:K:263:ASN:OD1	1:K:266:MET:HB2	1.91	0.71
1:C:263:ASN:ND2	1:C:343:ASP:HA	2.04	0.71
1:G:27:THR:HG1	1:G:30:HIS:HD1	1.35	0.71
1:Q:22:VAL:CG2	1:Q:264:LEU:HD23	2.16	0.71
1:X:1095:LEU:H	1:X:1095:LEU:CD2	2.04	0.71
1:E:1095:LEU:H	1:E:1095:LEU:CD2	2.03	0.71
1:M:1095:LEU:H	1:M:1095:LEU:CD2	2.01	0.71
1:S:1095:LEU:H	1:S:1095:LEU:CD2	2.03	0.71
1:V:1095:LEU:H	1:V:1095:LEU:CD2	2.03	0.71
1:C:262:ASP:OD2	1:C:437:HIS:CD2	2.44	0.70
1:K:261:LEU:HD12	1:K:441:GLU:HB2	1.72	0.70
1:Q:260:ARG:O	1:Q:264:LEU:HB2	1.90	0.70
1:C:1095:LEU:H	1:C:1095:LEU:CD2	2.02	0.70
1:Q:260:ARG:CB	1:Q:264:LEU:HD22	2.22	0.70
1:X:22:VAL:CG2	1:X:264:LEU:HD23	2.12	0.70
1:A:1095:LEU:H	1:A:1095:LEU:CD2	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:258:SER:HB3	1:K:261:LEU:CD2	2.18	0.69
1:I:1095:LEU:H	1:I:1095:LEU:CD2	2.03	0.69
1:Q:1095:LEU:H	1:Q:1095:LEU:CD2	2.03	0.69
1:K:1095:LEU:H	1:K:1095:LEU:CD2	2.03	0.69
1:O:260:ARG:O	1:O:264:LEU:HB2	1.92	0.69
1:S:4:HIS:HE1	1:S:253:GLU:OE1	1.76	0.69
1:X:18:PHE:HE1	1:X:264:LEU:O	1.77	0.68
1:I:1100:LYS:HE3	1:K:1102:HIS:HB2	1.75	0.68
1:E:169:LEU:O	1:X:355:ARG:NH2	2.26	0.67
1:Q:189:ILE:HG13	1:S:251:ILE:HB	1.76	0.67
1:Q:431:ASN:HD22	1:Q:447:ASP:HB3	1.60	0.67
1:C:431:ASN:HD22	1:C:447:ASP:HB3	1.60	0.67
1:O:431:ASN:HD22	1:O:447:ASP:HB3	1.60	0.67
1:A:431:ASN:HD22	1:A:447:ASP:HB3	1.60	0.67
1:M:431:ASN:HD22	1:M:447:ASP:HB3	1.60	0.67
1:G:431:ASN:HD22	1:G:447:ASP:HB3	1.60	0.67
1:I:431:ASN:HD22	1:I:447:ASP:HB3	1.60	0.67
1:M:260:ARG:O	1:M:264:LEU:HB2	1.95	0.67
1:V:431:ASN:HD22	1:V:447:ASP:HB3	1.60	0.66
1:X:431:ASN:HD22	1:X:447:ASP:HB3	1.60	0.66
1:K:431:ASN:HD22	1:K:447:ASP:HB3	1.60	0.66
1:A:260:ARG:O	1:A:264:LEU:HB2	1.95	0.66
1:K:261:LEU:HD11	1:K:441:GLU:C	2.20	0.66
1:S:431:ASN:HD22	1:S:447:ASP:HB3	1.60	0.65
1:K:261:LEU:CD1	1:K:441:GLU:HB2	2.26	0.65
1:A:261:LEU:HD12	1:A:441:GLU:HB2	1.77	0.65
1:E:431:ASN:HD22	1:E:447:ASP:HB3	1.60	0.65
1:K:182:GLU:CD	1:M:406:ASN:H	2.05	0.65
1:M:1095:LEU:HD23	1:M:1095:LEU:N	2.10	0.64
1:E:263:ASN:HD22	1:E:266:MET:CB	2.00	0.64
1:S:1095:LEU:HD23	1:S:1095:LEU:N	2.11	0.64
1:A:263:ASN:ND2	1:A:343:ASP:OD1	2.31	0.64
1:C:100:ARG:HH21	1:C:237:GLU:HG3	1.63	0.64
1:E:100:ARG:HH21	1:E:237:GLU:HG3	1.63	0.64
1:Q:100:ARG:HH21	1:Q:237:GLU:HG3	1.63	0.64
1:G:184:GLU:HA	1:M:351:ASN:HB3	1.80	0.63
1:Q:260:ARG:HB2	1:Q:264:LEU:HD22	1.79	0.63
1:A:100:ARG:HH21	1:A:237:GLU:HG3	1.63	0.63
1:S:260:ARG:HB2	1:S:264:LEU:HD22	1.79	0.63
1:K:260:ARG:O	1:K:264:LEU:HB2	1.98	0.63
1:X:1095:LEU:HD23	1:X:1095:LEU:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:100:ARG:HH21	1:X:237:GLU:HG3	1.63	0.63
1:V:100:ARG:HH21	1:V:237:GLU:HG3	1.63	0.63
1:A:1095:LEU:HD23	1:A:1095:LEU:N	2.11	0.62
1:X:260:ARG:O	1:X:264:LEU:HB2	1.98	0.62
1:I:262:ASP:OD1	1:I:437:HIS:CD2	2.52	0.62
1:S:100:ARG:HH21	1:S:237:GLU:HG3	1.63	0.62
1:M:100:ARG:HH21	1:M:237:GLU:HG3	1.63	0.62
1:O:100:ARG:HH21	1:O:237:GLU:HG3	1.63	0.62
1:Q:355:ARG:NH2	1:S:169:LEU:O	2.33	0.62
1:S:260:ARG:O	1:S:264:LEU:HB2	2.00	0.62
1:C:260:ARG:O	1:C:264:LEU:HB2	2.00	0.62
1:I:100:ARG:HH21	1:I:237:GLU:HG3	1.63	0.62
1:E:100:ARG:NH2	3:E:1604:HOH:O	2.34	0.61
1:G:100:ARG:HH21	1:G:237:GLU:HG3	1.63	0.61
1:X:22:VAL:HG23	1:X:264:LEU:CD2	2.16	0.61
1:K:100:ARG:HH21	1:K:237:GLU:HG3	1.63	0.61
1:S:260:ARG:CB	1:S:264:LEU:HD22	2.31	0.61
1:G:100:ARG:NH2	3:G:1609:HOH:O	2.34	0.61
1:E:21:PHE:CE2	1:E:264:LEU:HD21	2.36	0.60
1:Q:100:ARG:NH2	3:Q:1606:HOH:O	2.33	0.60
1:G:1100:LYS:HE3	1:M:1102:HIS:HB2	1.82	0.60
1:G:351:ASN:HB3	1:M:184:GLU:HA	1.82	0.60
1:M:100:ARG:NH2	3:M:1604:HOH:O	2.34	0.60
1:E:351:ASN:HB3	1:X:184:GLU:HA	1.82	0.60
1:V:149:ILE:HG22	1:X:470:ILE:HB	1.84	0.60
1:A:258:SER:CB	1:A:261:LEU:HD21	2.29	0.59
1:I:260:ARG:O	1:I:264:LEU:HB2	2.03	0.59
1:I:100:ARG:NH2	3:I:1606:HOH:O	2.34	0.59
1:V:1095:LEU:HD23	1:V:1095:LEU:N	2.12	0.59
1:V:182:GLU:CD	1:X:406:ASN:H	2.10	0.59
1:E:1095:LEU:HD23	1:E:1095:LEU:N	2.11	0.59
1:K:261:LEU:HG	1:K:441:GLU:HB2	1.85	0.59
1:A:95:ASP:OD2	1:A:298:GLU:N	2.35	0.59
1:K:148:VAL:HG11	1:M:386:VAL:HG11	1.85	0.59
1:Q:1095:LEU:HD23	1:Q:1095:LEU:N	2.11	0.59
1:I:1095:LEU:HD23	1:I:1095:LEU:N	2.11	0.59
1:K:261:LEU:CG	1:K:441:GLU:HB2	2.31	0.59
1:O:282:SER:HB3	1:O:290:ARG:HH22	1.68	0.58
1:G:282:SER:HB3	1:G:290:ARG:HH22	1.68	0.58
1:K:1079:CYS:SG	1:K:1080:PHE:N	2.77	0.58
1:C:282:SER:HB3	1:C:290:ARG:HH22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:260:ARG:HB3	1:Q:264:LEU:HD22	1.85	0.58
1:S:1079:CYS:SG	1:S:1080:PHE:N	2.77	0.58
1:X:282:SER:HB3	1:X:290:ARG:HH22	1.68	0.58
1:Q:282:SER:HB3	1:Q:290:ARG:HH22	1.68	0.58
1:I:1079:CYS:SG	1:I:1080:PHE:N	2.77	0.58
1:M:319:ARG:NH1	1:O:331:SER:OG	2.37	0.58
1:G:22:VAL:HG23	1:G:264:LEU:HD13	1.84	0.58
1:X:1079:CYS:SG	1:X:1080:PHE:N	2.77	0.58
1:S:282:SER:HB3	1:S:290:ARG:HH22	1.68	0.58
1:K:282:SER:HB3	1:K:290:ARG:HH22	1.68	0.58
1:A:282:SER:HB3	1:A:290:ARG:HH22	1.68	0.57
1:I:282:SER:HB3	1:I:290:ARG:HH22	1.68	0.57
1:K:277:SER:O	1:K:290:ARG:NH1	2.37	0.57
1:O:1079:CYS:SG	1:O:1080:PHE:N	2.77	0.57
1:Q:277:SER:O	1:Q:290:ARG:NH1	2.37	0.57
1:S:277:SER:O	1:S:290:ARG:NH1	2.37	0.57
1:O:1064:THR:OG1	1:O:1088:CYS:SG	2.62	0.57
1:E:1079:CYS:SG	1:E:1080:PHE:N	2.77	0.57
1:I:277:SER:O	1:I:290:ARG:NH1	2.37	0.57
1:M:282:SER:HB3	1:M:290:ARG:HH22	1.68	0.57
1:O:277:SER:O	1:O:290:ARG:NH1	2.37	0.57
1:V:282:SER:HB3	1:V:290:ARG:HH22	1.68	0.57
1:V:1064:THR:OG1	1:V:1088:CYS:SG	2.62	0.57
1:X:1064:THR:OG1	1:X:1088:CYS:SG	2.62	0.57
1:A:263:ASN:ND2	1:A:343:ASP:HA	2.18	0.57
1:Q:1064:THR:OG1	1:Q:1088:CYS:SG	2.62	0.57
1:M:277:SER:O	1:M:290:ARG:NH1	2.37	0.57
1:C:277:SER:O	1:C:290:ARG:NH1	2.37	0.57
1:G:277:SER:O	1:G:290:ARG:NH1	2.37	0.57
1:K:1064:THR:OG1	1:K:1088:CYS:SG	2.62	0.57
1:A:298:GLU:HG3	1:A:414:ILE:HG23	1.87	0.57
1:E:277:SER:O	1:E:290:ARG:NH1	2.37	0.57
1:E:282:SER:HB3	1:E:290:ARG:HH22	1.68	0.57
1:X:277:SER:O	1:X:290:ARG:NH1	2.37	0.57
1:A:1079:CYS:SG	1:A:1080:PHE:N	2.77	0.57
1:K:1095:LEU:HD23	1:K:1095:LEU:N	2.11	0.57
1:A:258:SER:HB3	1:A:261:LEU:CD2	2.32	0.56
1:Q:355:ARG:NH1	1:S:170:ASP:OD1	2.30	0.56
1:E:21:PHE:CE2	1:E:264:LEU:CD2	2.87	0.56
1:K:298:GLU:HG3	1:K:414:ILE:HG23	1.87	0.56
1:O:1095:LEU:HD23	1:O:1095:LEU:N	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:277:SER:O	1:V:290:ARG:NH1	2.37	0.56
1:A:277:SER:O	1:A:290:ARG:NH1	2.37	0.56
1:G:1079:CYS:SG	1:G:1080:PHE:N	2.77	0.56
1:Q:298:GLU:HG3	1:Q:414:ILE:HG23	1.88	0.56
1:Q:1079:CYS:SG	1:Q:1080:PHE:N	2.77	0.56
1:S:388:LEU:HD12	1:S:427:LEU:HD13	1.88	0.56
1:E:1064:THR:OG1	1:E:1088:CYS:SG	2.62	0.56
1:C:1095:LEU:HD23	1:C:1095:LEU:N	2.10	0.56
1:G:93:HIS:CD2	1:G:263:ASN:HD22	2.23	0.56
1:K:388:LEU:HD12	1:K:427:LEU:HD13	1.88	0.56
1:A:1064:THR:OG1	1:A:1088:CYS:SG	2.62	0.56
1:Q:1:MET:N	1:Q:1083:ASP:HB2	2.21	0.56
1:E:440:ARG:HG2	1:X:161:ARG:HH12	1.69	0.56
1:V:388:LEU:HD12	1:V:427:LEU:HD13	1.88	0.56
1:I:388:LEU:HD12	1:I:427:LEU:HD13	1.88	0.55
1:Q:388:LEU:HD12	1:Q:427:LEU:HD13	1.88	0.55
1:A:263:ASN:HD21	1:A:344:MET:H	1.54	0.55
1:E:251:ILE:HB	1:X:189:ILE:HG13	1.89	0.55
1:O:388:LEU:HD12	1:O:427:LEU:HD13	1.88	0.55
1:C:1079:CYS:SG	1:C:1080:PHE:N	2.77	0.55
1:Q:1100:LYS:HE3	1:S:1102:HIS:HB2	1.89	0.55
1:X:262:ASP:OD2	1:X:437:HIS:CD2	2.60	0.55
1:G:298:GLU:HG3	1:G:414:ILE:HG23	1.87	0.55
1:C:406:ASN:H	1:G:182:GLU:CD	2.14	0.55
1:G:78:GLY:HA2	1:G:283:LEU:HG	1.89	0.55
1:E:388:LEU:HD12	1:E:427:LEU:HD13	1.88	0.55
1:O:78:GLY:HA2	1:O:283:LEU:HG	1.89	0.55
1:A:78:GLY:HA2	1:A:283:LEU:HG	1.89	0.55
1:I:298:GLU:HG3	1:I:414:ILE:HG23	1.88	0.55
1:Q:170:ASP:OD1	1:S:355:ARG:NH1	2.35	0.55
1:C:388:LEU:HD12	1:C:427:LEU:HD13	1.88	0.54
1:G:388:LEU:HD12	1:G:427:LEU:HD13	1.88	0.54
1:X:98:THR:OG1	1:X:240:LEU:O	2.26	0.54
1:M:388:LEU:HD12	1:M:427:LEU:HD13	1.88	0.54
1:A:388:LEU:HD12	1:A:427:LEU:HD13	1.88	0.54
1:E:98:THR:OG1	1:E:240:LEU:O	2.26	0.54
1:K:98:THR:OG1	1:K:240:LEU:O	2.26	0.54
1:S:78:GLY:HA2	1:S:283:LEU:HG	1.89	0.54
1:I:98:THR:OG1	1:I:240:LEU:O	2.26	0.54
1:I:184:GLU:HA	1:K:351:ASN:HB3	1.90	0.54
1:S:298:GLU:HG3	1:S:414:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:GLY:HA2	1:M:283:LEU:HG	1.89	0.54
1:V:98:THR:OG1	1:V:240:LEU:O	2.25	0.54
1:X:298:GLU:HG3	1:X:414:ILE:HG23	1.90	0.54
1:C:98:THR:OG1	1:C:240:LEU:O	2.26	0.54
1:Q:98:THR:OG1	1:Q:240:LEU:O	2.26	0.54
1:V:1079:CYS:SG	1:V:1080:PHE:N	2.77	0.54
1:E:78:GLY:HA2	1:E:283:LEU:HG	1.89	0.54
1:M:98:THR:OG1	1:M:240:LEU:O	2.26	0.54
1:G:1095:LEU:HD23	1:G:1095:LEU:N	2.09	0.54
1:I:22:VAL:HG23	1:I:264:LEU:HD13	1.89	0.54
1:X:388:LEU:HD12	1:X:427:LEU:HD13	1.88	0.54
1:C:78:GLY:HA2	1:C:283:LEU:HG	1.89	0.54
1:G:35:LEU:HD11	1:G:267:THR:HG21	1.90	0.54
1:G:189:ILE:HG13	1:M:251:ILE:HB	1.90	0.53
1:K:261:LEU:HD12	1:K:441:GLU:CA	2.36	0.53
1:C:298:GLU:HG3	1:C:414:ILE:HG23	1.89	0.53
1:G:98:THR:OG1	1:G:240:LEU:O	2.26	0.53
1:E:148:VAL:HG11	1:G:386:VAL:HG11	1.90	0.53
1:K:78:GLY:HA2	1:K:283:LEU:HG	1.89	0.53
1:M:298:GLU:HG3	1:M:414:ILE:HG23	1.89	0.53
1:Q:78:GLY:HA2	1:Q:283:LEU:HG	1.89	0.53
1:V:78:GLY:HA2	1:V:283:LEU:HG	1.89	0.53
1:C:149:ILE:HG22	1:E:470:ILE:HB	1.90	0.53
1:O:98:THR:OG1	1:O:240:LEU:O	2.26	0.53
1:X:261:LEU:HD13	3:X:1666:HOH:O	2.08	0.53
1:A:355:ARG:NH2	1:C:169:LEU:O	2.40	0.53
1:S:386:VAL:HG11	1:X:148:VAL:HG11	1.91	0.53
1:E:298:GLU:HG3	1:E:414:ILE:HG23	1.91	0.53
1:S:1064:THR:OG1	1:S:1088:CYS:SG	2.62	0.53
1:E:262:ASP:OD2	1:E:299:GLU:OE2	2.27	0.53
1:E:1074:PHE:HB3	1:E:1103:PHE:HB3	1.91	0.53
1:S:98:THR:OG1	1:S:240:LEU:O	2.26	0.53
1:G:1074:PHE:HB3	1:G:1103:PHE:HB3	1.91	0.53
1:S:263:ASN:OD1	1:S:343:ASP:OD1	2.27	0.53
1:O:298:GLU:HG3	1:O:414:ILE:HG23	1.90	0.53
1:S:1074:PHE:HB3	1:S:1103:PHE:HB3	1.91	0.53
1:A:98:THR:OG1	1:A:240:LEU:O	2.26	0.52
1:I:355:ARG:NH2	1:K:169:LEU:O	2.42	0.52
1:S:470:ILE:HB	1:X:149:ILE:HG22	1.91	0.52
1:I:78:GLY:HA2	1:I:283:LEU:HG	1.89	0.52
1:E:300:ILE:HG21	1:G:375:ASN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:118:GLU:HG3	1:M:374:ALA:HB2	1.90	0.52
1:M:1074:PHE:HB3	1:M:1103:PHE:HB3	1.91	0.52
1:Q:1074:PHE:HB3	1:Q:1103:PHE:HB3	1.91	0.52
1:X:78:GLY:HA2	1:X:283:LEU:HG	1.89	0.52
1:A:1074:PHE:HB3	1:A:1103:PHE:HB3	1.91	0.52
1:G:21:PHE:CE2	1:G:264:LEU:HD21	2.43	0.52
1:I:1074:PHE:HB3	1:I:1103:PHE:HB3	1.91	0.52
1:O:1100:LYS:HE3	1:V:1102:HIS:HB2	1.91	0.52
1:Q:1096:HIS:NE2	1:Q:1098:CYS:HB2	2.25	0.52
1:V:1096:HIS:NE2	1:V:1098:CYS:HB2	2.25	0.52
1:K:181:MET:HG3	1:M:406:ASN:HB3	1.91	0.52
1:V:1074:PHE:HB3	1:V:1103:PHE:HB3	1.91	0.52
1:C:1074:PHE:HB3	1:C:1103:PHE:HB3	1.91	0.52
1:C:1096:HIS:NE2	1:C:1098:CYS:HB2	2.25	0.52
1:O:1074:PHE:HB3	1:O:1103:PHE:HB3	1.91	0.52
1:A:1096:HIS:NE2	1:A:1098:CYS:HB2	2.25	0.52
1:C:1064:THR:OG1	1:C:1088:CYS:SG	2.62	0.52
1:M:1064:THR:OG1	1:M:1088:CYS:SG	2.62	0.52
1:S:1096:HIS:NE2	1:S:1098:CYS:HB2	2.25	0.52
1:G:1096:HIS:NE2	1:G:1098:CYS:HB2	2.25	0.52
1:M:1079:CYS:SG	1:M:1080:PHE:N	2.77	0.52
1:G:251:ILE:HB	1:M:189:ILE:HG13	1.91	0.51
1:K:1074:PHE:HB3	1:K:1103:PHE:HB3	1.91	0.51
1:O:355:ARG:NH2	1:V:169:LEU:O	2.43	0.51
1:C:104:LYS:HD2	1:C:207:TYR:HA	1.93	0.51
1:E:1096:HIS:NE2	1:E:1098:CYS:HB2	2.25	0.51
1:M:1096:HIS:NE2	1:M:1098:CYS:HB2	2.25	0.51
1:S:4:HIS:HE1	1:S:253:GLU:CD	2.18	0.51
1:X:1096:HIS:NE2	1:X:1098:CYS:HB2	2.25	0.51
1:M:93:HIS:H	1:M:263:ASN:HD22	1.57	0.51
1:O:169:LEU:O	1:V:355:ARG:NH2	2.43	0.51
1:V:93:HIS:CD2	1:V:298:GLU:CG	2.89	0.51
1:O:104:LYS:HD2	1:O:207:TYR:HA	1.93	0.51
1:X:1074:PHE:HB3	1:X:1103:PHE:HB3	1.91	0.51
1:A:22:VAL:HG23	1:A:264:LEU:HD13	1.92	0.51
1:A:104:LYS:HD2	1:A:207:TYR:HA	1.93	0.51
1:E:104:LYS:HD2	1:E:207:TYR:HA	1.93	0.51
1:K:1096:HIS:NE2	1:K:1098:CYS:HB2	2.25	0.51
1:O:184:GLU:HA	1:V:351:ASN:HB3	1.93	0.51
1:Q:190:GLY:HA3	1:S:251:ILE:HG22	1.93	0.51
1:E:263:ASN:HD21	1:E:266:MET:CB	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1102:HIS:HB2	1:X:1100:LYS:HE3	1.93	0.51
1:O:1096:HIS:NE2	1:O:1098:CYS:HB2	2.25	0.51
1:E:264:LEU:O	1:E:264:LEU:HD23	2.11	0.50
1:M:104:LYS:HD2	1:M:207:TYR:HA	1.93	0.50
1:O:252:HIS:HD1	1:V:194:GLU:CD	2.19	0.50
1:A:22:VAL:HG23	1:A:264:LEU:CD1	2.40	0.50
1:I:1096:HIS:NE2	1:I:1098:CYS:HB2	2.25	0.50
1:M:262:ASP:OD2	1:M:437:HIS:CD2	2.65	0.50
1:G:242:ASP:OD1	3:G:1601:HOH:O	2.20	0.50
1:G:104:LYS:HD2	1:G:207:TYR:HA	1.93	0.50
1:K:262:ASP:OD2	1:K:437:HIS:HD2	1.89	0.50
1:K:406:ASN:H	1:O:182:GLU:CD	2.20	0.50
1:G:188:LEU:HD12	1:M:442:MET:HE1	1.92	0.50
1:I:1064:THR:OG1	1:I:1088:CYS:SG	2.62	0.50
1:K:104:LYS:HD2	1:K:207:TYR:HA	1.93	0.50
1:X:104:LYS:HD2	1:X:207:TYR:HA	1.93	0.50
1:I:22:VAL:HG23	1:I:264:LEU:CD1	2.42	0.50
1:S:263:ASN:ND2	1:S:342:ALA:O	2.45	0.50
1:G:93:HIS:CD2	1:G:263:ASN:ND2	2.79	0.50
1:M:148:VAL:HG11	1:O:386:VAL:HG11	1.94	0.50
1:O:351:ASN:HB3	1:V:184:GLU:HA	1.94	0.50
1:Q:104:LYS:HD2	1:Q:207:TYR:HA	1.93	0.50
1:E:280:ASN:N	3:E:1612:HOH:O	2.39	0.49
1:Q:161:ARG:HH12	1:S:440:ARG:HG2	1.76	0.49
1:S:104:LYS:HD2	1:S:207:TYR:HA	1.93	0.49
1:E:333:SER:O	1:E:337:SER:OG	2.27	0.49
1:G:1064:THR:OG1	1:G:1088:CYS:SG	2.62	0.49
1:S:4:HIS:CE1	1:S:253:GLU:OE1	2.61	0.49
1:V:93:HIS:CE1	1:V:263:ASN:HB2	2.47	0.49
1:I:27:THR:OG1	1:I:30:HIS:ND1	2.38	0.49
1:V:92:THR:HG22	1:V:342:ALA:HB3	1.95	0.49
1:V:118:GLU:HG3	1:X:374:ALA:HB2	1.93	0.49
1:Q:92:THR:HG22	1:Q:342:ALA:HB3	1.95	0.49
1:V:104:LYS:HD2	1:V:207:TYR:HA	1.93	0.49
1:X:92:THR:HG22	1:X:342:ALA:HB3	1.95	0.49
1:A:280:ASN:N	3:A:1615:HOH:O	2.39	0.49
1:I:51:SER:OG	1:I:52:ASP:N	2.46	0.49
1:I:104:LYS:HD2	1:I:207:TYR:HA	1.93	0.49
1:A:92:THR:HG22	1:A:342:ALA:HB3	1.95	0.49
1:I:1062:CYS:SG	1:I:1064:THR:OG1	2.71	0.49
1:Q:51:SER:OG	1:Q:52:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:92:THR:HG22	1:S:342:ALA:HB3	1.95	0.49
1:C:22:VAL:HG23	1:C:264:LEU:CD1	2.42	0.49
1:K:182:GLU:OE1	1:M:406:ASN:N	2.46	0.49
1:X:51:SER:OG	1:X:52:ASP:N	2.46	0.49
1:C:51:SER:OG	1:C:52:ASP:N	2.46	0.49
1:C:92:THR:HG22	1:C:342:ALA:HB3	1.95	0.49
1:C:1062:CYS:SG	1:C:1064:THR:OG1	2.71	0.49
1:G:92:THR:HG22	1:G:342:ALA:HB3	1.95	0.49
1:M:51:SER:OG	1:M:52:ASP:N	2.46	0.49
1:E:261:LEU:HD12	1:E:441:GLU:C	2.38	0.49
1:G:157:ARG:HH12	1:M:4:HIS:CE1	2.31	0.49
1:G:1062:CYS:SG	1:G:1064:THR:OG1	2.71	0.49
1:C:182:GLU:CD	1:E:406:ASN:H	2.20	0.48
1:E:1062:CYS:SG	1:E:1064:THR:OG1	2.71	0.48
1:S:1062:CYS:SG	1:S:1064:THR:OG1	2.71	0.48
1:V:93:HIS:NE2	1:V:263:ASN:HB2	2.28	0.48
1:A:1062:CYS:SG	1:A:1064:THR:OG1	2.71	0.48
1:E:92:THR:HG22	1:E:342:ALA:HB3	1.95	0.48
3:G:1606:HOH:O	1:M:440:ARG:NH2	2.46	0.48
1:K:300:ILE:HD12	1:M:376:GLN:HB2	1.95	0.48
1:K:1062:CYS:SG	1:K:1064:THR:OG1	2.71	0.48
1:X:433:MET:HE3	3:X:1666:HOH:O	2.13	0.48
1:M:92:THR:HG22	1:M:342:ALA:HB3	1.95	0.48
1:O:73:ILE:HG12	1:O:293:PRO:HB3	1.96	0.48
1:E:73:ILE:HG12	1:E:293:PRO:HB3	1.96	0.48
1:K:73:ILE:HG12	1:K:293:PRO:HB3	1.96	0.48
1:O:1102:HIS:HB2	1:V:1100:LYS:HE3	1.94	0.48
1:S:263:ASN:HD21	1:S:343:ASP:HA	1.79	0.48
1:A:89:ILE:HD12	1:A:424:MET:HE1	1.96	0.48
1:A:295:PHE:HZ	1:A:313:LEU:HB2	1.79	0.48
1:C:93:HIS:NE2	1:C:263:ASN:HB2	2.28	0.48
1:G:19:LEU:HD11	1:G:248:LEU:HG	1.96	0.48
1:M:1062:CYS:SG	1:M:1064:THR:OG1	2.71	0.48
1:O:92:THR:HG22	1:O:342:ALA:HB3	1.95	0.48
1:Q:19:LEU:HD11	1:Q:248:LEU:HG	1.96	0.48
1:S:295:PHE:HZ	1:S:313:LEU:HB2	1.79	0.48
1:V:93:HIS:CD2	1:V:298:GLU:CD	2.92	0.48
1:C:19:LEU:HD11	1:C:248:LEU:HG	1.96	0.48
1:G:295:PHE:HZ	1:G:313:LEU:HB2	1.79	0.48
1:I:92:THR:HG22	1:I:342:ALA:HB3	1.95	0.48
1:K:89:ILE:HD12	1:K:424:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:19:LEU:HD11	1:M:248:LEU:HG	1.96	0.48
1:A:19:LEU:HD11	1:A:248:LEU:HG	1.96	0.48
1:E:19:LEU:HD11	1:E:248:LEU:HG	1.96	0.48
1:G:442:MET:HE1	1:M:188:LEU:HD12	1.96	0.48
1:I:295:PHE:HZ	1:I:313:LEU:HB2	1.79	0.48
1:Q:419:ALA:HB2	1:Q:426:THR:HG21	1.96	0.48
1:V:19:LEU:HD11	1:V:248:LEU:HG	1.96	0.48
1:C:73:ILE:HG12	1:C:293:PRO:HB3	1.96	0.48
1:C:89:ILE:HD12	1:C:424:MET:HE1	1.96	0.48
1:E:51:SER:OG	1:E:52:ASP:N	2.46	0.48
1:G:1102:HIS:HB2	1:M:1100:LYS:HE3	1.96	0.48
1:I:367:GLY:O	1:I:400:GLN:NE2	2.47	0.48
1:O:89:ILE:HD12	1:O:424:MET:HE1	1.96	0.48
1:V:27:THR:OG1	1:V:30:HIS:ND1	2.38	0.48
1:V:419:ALA:HB2	1:V:426:THR:HG21	1.96	0.48
1:A:261:LEU:CD1	1:A:441:GLU:C	2.85	0.47
1:C:295:PHE:HZ	1:C:313:LEU:HB2	1.79	0.47
1:Q:89:ILE:HD12	1:Q:424:MET:HE1	1.96	0.47
1:Q:351:ASN:HB3	1:S:184:GLU:HA	1.96	0.47
1:V:148:VAL:HG11	1:X:386:VAL:HG11	1.96	0.47
1:X:73:ILE:HG12	1:X:293:PRO:HB3	1.96	0.47
1:A:51:SER:OG	1:A:52:ASP:N	2.46	0.47
1:C:148:VAL:HG11	1:E:386:VAL:HG11	1.96	0.47
1:K:92:THR:HG22	1:K:342:ALA:HB3	1.95	0.47
1:V:295:PHE:HZ	1:V:313:LEU:HB2	1.79	0.47
1:K:51:SER:OG	1:K:52:ASP:N	2.46	0.47
1:X:367:GLY:O	1:X:400:GLN:NE2	2.47	0.47
1:I:19:LEU:HD11	1:I:248:LEU:HG	1.96	0.47
1:M:295:PHE:HZ	1:M:313:LEU:HB2	1.79	0.47
1:Q:295:PHE:HZ	1:Q:313:LEU:HB2	1.79	0.47
1:S:370:ILE:HG23	1:S:427:LEU:HD21	1.96	0.47
1:V:51:SER:OG	1:V:52:ASP:N	2.46	0.47
1:X:89:ILE:HD12	1:X:424:MET:HE1	1.96	0.47
1:C:264:LEU:HD23	1:C:264:LEU:HA	1.69	0.47
1:E:295:PHE:HZ	1:E:313:LEU:HB2	1.79	0.47
1:E:419:ALA:HB2	1:E:426:THR:HG21	1.96	0.47
1:I:73:ILE:HG12	1:I:293:PRO:HB3	1.96	0.47
1:S:51:SER:OG	1:S:52:ASP:N	2.46	0.47
1:S:73:ILE:HG12	1:S:293:PRO:HB3	1.96	0.47
1:E:89:ILE:HD12	1:E:424:MET:HE1	1.96	0.47
1:I:419:ALA:HB2	1:I:426:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:419:ALA:HB2	1:K:426:THR:HG21	1.96	0.47
1:M:325:LYS:HA	1:M:325:LYS:HD3	1.70	0.47
1:S:419:ALA:HB2	1:S:426:THR:HG21	1.96	0.47
1:V:368:THR:HG21	1:V:454:LEU:HD22	1.97	0.47
1:E:163:PRO:HG2	1:X:349:HIS:CE1	2.49	0.47
1:G:73:ILE:HG12	1:G:293:PRO:HB3	1.96	0.47
1:G:89:ILE:HD12	1:G:424:MET:HE1	1.96	0.47
1:G:370:ILE:HG23	1:G:427:LEU:HD21	1.96	0.47
1:I:370:ILE:HG23	1:I:427:LEU:HD21	1.96	0.47
1:M:73:ILE:HG12	1:M:293:PRO:HB3	1.96	0.47
1:M:333:SER:O	1:M:337:SER:OG	2.27	0.47
1:O:295:PHE:HZ	1:O:313:LEU:HB2	1.79	0.47
1:O:367:GLY:O	1:O:400:GLN:NE2	2.47	0.47
1:O:370:ILE:HG23	1:O:427:LEU:HD21	1.96	0.47
1:Q:73:ILE:HG12	1:Q:293:PRO:HB3	1.96	0.47
1:V:303:VAL:N	3:V:1621:HOH:O	2.47	0.47
1:V:370:ILE:HG23	1:V:427:LEU:HD21	1.96	0.47
1:X:419:ALA:HB2	1:X:426:THR:HG21	1.96	0.47
1:K:295:PHE:HZ	1:K:313:LEU:HB2	1.79	0.47
1:S:367:GLY:O	1:S:400:GLN:NE2	2.47	0.47
1:V:73:ILE:HG12	1:V:293:PRO:HB3	1.96	0.47
1:G:419:ALA:HB2	1:G:426:THR:HG21	1.96	0.47
1:M:89:ILE:HD12	1:M:424:MET:HE1	1.96	0.47
1:M:368:THR:HG21	1:M:454:LEU:HD22	1.97	0.47
1:X:19:LEU:HD11	1:X:248:LEU:HG	1.96	0.47
1:A:419:ALA:HB2	1:A:426:THR:HG21	1.96	0.46
1:I:89:ILE:HD12	1:I:424:MET:HE1	1.96	0.46
1:V:89:ILE:HD12	1:V:424:MET:HE1	1.96	0.46
1:X:160:LEU:HG	1:X:240:LEU:HD21	1.98	0.46
1:A:367:GLY:O	1:A:400:GLN:NE2	2.47	0.46
1:A:370:ILE:HG23	1:A:427:LEU:HD21	1.96	0.46
1:G:1095:LEU:CD2	1:G:1095:LEU:N	2.75	0.46
1:I:333:SER:O	1:I:337:SER:OG	2.27	0.46
1:K:19:LEU:HD11	1:K:248:LEU:HG	1.96	0.46
1:M:147:ARG:NH2	1:O:470:ILE:HG13	2.31	0.46
1:M:305:ALA:HB2	1:O:419:ALA:HB1	1.96	0.46
1:Q:370:ILE:HG23	1:Q:427:LEU:HD21	1.96	0.46
1:E:370:ILE:HG23	1:E:427:LEU:HD21	1.96	0.46
1:G:51:SER:OG	1:G:52:ASP:N	2.46	0.46
1:M:370:ILE:HG23	1:M:427:LEU:HD21	1.96	0.46
1:S:19:LEU:HD11	1:S:248:LEU:HG	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HG	1:A:240:LEU:HD21	1.98	0.46
1:E:160:LEU:HG	1:E:240:LEU:HD21	1.98	0.46
1:G:93:HIS:CE1	1:G:263:ASN:HB2	2.51	0.46
1:G:368:THR:HG21	1:G:454:LEU:HD22	1.97	0.46
1:K:370:ILE:HG23	1:K:427:LEU:HD21	1.96	0.46
1:O:19:LEU:HD11	1:O:248:LEU:HG	1.96	0.46
1:Q:333:SER:O	1:Q:337:SER:OG	2.27	0.46
1:E:368:THR:HG21	1:E:454:LEU:HD22	1.97	0.46
1:K:368:THR:HG21	1:K:454:LEU:HD22	1.97	0.46
1:M:160:LEU:HG	1:M:240:LEU:HD21	1.98	0.46
1:Q:367:GLY:O	1:Q:400:GLN:NE2	2.47	0.46
1:X:370:ILE:HG23	1:X:427:LEU:HD21	1.96	0.46
1:A:368:THR:HG21	1:A:454:LEU:HD22	1.97	0.46
1:C:419:ALA:HB2	1:C:426:THR:HG21	1.96	0.46
1:M:367:GLY:O	1:M:400:GLN:NE2	2.47	0.46
1:O:51:SER:OG	1:O:52:ASP:N	2.46	0.46
1:O:93:HIS:H	1:O:263:ASN:HD22	1.62	0.46
1:A:73:ILE:HG12	1:A:293:PRO:HB3	1.96	0.46
1:C:370:ILE:HG23	1:C:427:LEU:HD21	1.96	0.46
1:G:333:SER:O	1:G:337:SER:OG	2.27	0.46
1:S:368:THR:HG21	1:S:454:LEU:HD22	1.97	0.46
1:C:160:LEU:HG	1:C:240:LEU:HD21	1.98	0.46
1:C:367:GLY:O	1:C:400:GLN:NE2	2.47	0.46
1:G:367:GLY:O	1:G:400:GLN:NE2	2.47	0.46
1:M:419:ALA:HB2	1:M:426:THR:HG21	1.96	0.46
1:S:89:ILE:HD12	1:S:424:MET:HE1	1.96	0.46
1:V:160:LEU:HG	1:V:240:LEU:HD21	1.98	0.46
1:X:16:LEU:HD23	1:X:19:LEU:HD12	1.98	0.46
1:X:18:PHE:CE1	1:X:264:LEU:O	2.65	0.46
1:C:368:THR:HG21	1:C:454:LEU:HD22	1.97	0.46
1:G:93:HIS:NE2	1:G:263:ASN:HB2	2.31	0.46
1:Q:368:THR:HG21	1:Q:454:LEU:HD22	1.97	0.46
1:K:333:SER:O	1:K:337:SER:OG	2.26	0.46
1:M:16:LEU:HD23	1:M:19:LEU:HD12	1.98	0.46
1:M:311:THR:HG23	1:O:420:ALA:O	2.16	0.46
1:V:325:LYS:HA	1:V:325:LYS:HD3	1.70	0.46
1:A:169:LEU:O	1:C:355:ARG:NH2	2.48	0.45
1:C:22:VAL:HG23	1:C:264:LEU:HD13	1.99	0.45
1:K:160:LEU:HG	1:K:240:LEU:HD21	1.98	0.45
1:K:261:LEU:N	1:K:441:GLU:OE1	2.48	0.45
1:X:295:PHE:HZ	1:X:313:LEU:HB2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:16:LEU:HD23	1:Q:19:LEU:HD12	1.98	0.45
1:V:367:GLY:O	1:V:400:GLN:NE2	2.47	0.45
1:X:368:THR:HG21	1:X:454:LEU:HD22	1.97	0.45
1:E:4:HIS:CE1	1:X:157:ARG:HH12	2.34	0.45
1:E:16:LEU:HD23	1:E:19:LEU:HD12	1.98	0.45
1:I:16:LEU:HD23	1:I:19:LEU:HD12	1.98	0.45
1:I:368:THR:HG21	1:I:454:LEU:HD22	1.97	0.45
1:O:368:THR:HG21	1:O:454:LEU:HD22	1.97	0.45
1:O:419:ALA:HB2	1:O:426:THR:HG21	1.96	0.45
1:O:16:LEU:HD23	1:O:19:LEU:HD12	1.98	0.45
1:A:260:ARG:HB2	1:A:264:LEU:HD12	1.97	0.45
1:C:27:THR:OG1	1:C:30:HIS:ND1	2.38	0.45
1:G:160:LEU:HG	1:G:240:LEU:HD21	1.97	0.45
1:O:160:LEU:HG	1:O:240:LEU:HD21	1.98	0.45
1:G:4:HIS:CE1	1:M:157:ARG:HH12	2.34	0.45
1:G:16:LEU:HD23	1:G:19:LEU:HD12	1.98	0.45
1:Q:22:VAL:HG23	1:Q:264:LEU:CD2	2.25	0.45
1:Q:160:LEU:HG	1:Q:240:LEU:HD21	1.98	0.45
1:A:16:LEU:HD23	1:A:19:LEU:HD12	1.98	0.45
1:A:325:LYS:HA	1:A:325:LYS:HD3	1.70	0.45
1:C:27:THR:HG1	1:C:30:HIS:HD1	1.60	0.45
1:O:35:LEU:HD11	1:O:267:THR:HG21	1.99	0.45
1:C:16:LEU:HD23	1:C:19:LEU:HD12	1.98	0.45
1:K:93:HIS:NE2	1:K:263:ASN:HB2	2.32	0.45
1:M:118:GLU:HA	1:O:406:ASN:HD21	1.80	0.45
1:I:160:LEU:HG	1:I:240:LEU:HD21	1.98	0.45
1:V:16:LEU:HD23	1:V:19:LEU:HD12	1.98	0.45
1:A:470:ILE:HB	1:Q:149:ILE:HG22	2.00	0.44
1:C:325:LYS:HA	1:C:325:LYS:HD3	1.70	0.44
1:S:333:SER:O	1:S:337:SER:OG	2.26	0.44
1:A:161:ARG:HH12	1:C:440:ARG:HG2	1.80	0.44
1:K:16:LEU:HD23	1:K:19:LEU:HD12	1.98	0.44
1:Q:189:ILE:O	1:S:251:ILE:N	2.48	0.44
1:A:261:LEU:CD1	1:A:441:GLU:O	2.65	0.44
1:C:406:ASN:HB3	1:G:181:MET:HG3	1.99	0.44
1:G:161:ARG:HH12	1:M:440:ARG:HG2	1.83	0.44
1:K:238:LEU:HD23	1:K:238:LEU:HA	1.85	0.44
1:S:160:LEU:HG	1:S:240:LEU:HD21	1.97	0.44
1:M:1095:LEU:CD2	1:M:1095:LEU:N	2.75	0.44
1:O:194:GLU:CD	1:V:252:HIS:HD1	2.25	0.44
1:O:325:LYS:HA	1:O:325:LYS:HD3	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:238:LEU:HD23	1:Q:238:LEU:HA	1.85	0.44
1:S:16:LEU:HD23	1:S:19:LEU:HD12	1.98	0.44
1:V:421:MET:HE3	1:V:421:MET:HB2	1.85	0.44
1:E:112:TYR:CE1	1:X:350:PRO:HD3	2.52	0.44
1:E:114:GLN:NE2	1:X:351:ASN:OD1	2.50	0.44
1:I:238:LEU:HD23	1:I:238:LEU:HA	1.85	0.44
1:I:421:MET:HE3	1:I:421:MET:HB2	1.86	0.44
1:K:367:GLY:O	1:K:400:GLN:NE2	2.47	0.44
1:V:93:HIS:CD2	1:V:263:ASN:HD22	2.36	0.44
1:X:263:ASN:ND2	1:X:342:ALA:O	2.50	0.44
1:A:261:LEU:N	1:A:441:GLU:OE1	2.46	0.44
1:I:351:ASN:HB3	1:K:184:GLU:HA	1.99	0.44
1:G:238:LEU:HD23	1:G:238:LEU:HA	1.85	0.44
1:A:51:SER:O	1:A:319:ARG:NH2	2.51	0.44
1:E:258:SER:HB3	1:E:261:LEU:HG	2.00	0.44
1:K:386:VAL:HG11	1:O:148:VAL:HG11	1.99	0.44
1:M:300:ILE:HG21	1:O:375:ASN:HA	2.00	0.44
1:G:355:ARG:NH2	1:M:169:LEU:O	2.50	0.43
1:I:161:ARG:HH12	1:K:440:ARG:HG2	1.81	0.43
1:I:1100:LYS:H	1:K:1078:LYS:NZ	2.15	0.43
1:V:51:SER:O	1:V:319:ARG:NH2	2.51	0.43
1:G:158:PRO:HG2	1:M:247:ARG:HG3	2.00	0.43
1:I:51:SER:O	1:I:319:ARG:NH2	2.51	0.43
1:M:51:SER:O	1:M:319:ARG:NH2	2.51	0.43
1:O:51:SER:O	1:O:319:ARG:NH2	2.51	0.43
1:O:1095:LEU:CD2	1:O:1095:LEU:N	2.75	0.43
1:A:184:GLU:HA	1:C:351:ASN:HB3	2.00	0.43
1:C:51:SER:O	1:C:319:ARG:NH2	2.51	0.43
1:Q:325:LYS:HA	1:Q:325:LYS:HD3	1.70	0.43
1:V:93:HIS:ND1	1:V:298:GLU:CG	2.81	0.43
1:A:261:LEU:HD12	1:A:441:GLU:HB3	1.96	0.43
1:C:160:LEU:HD12	1:C:187:PRO:HB2	2.01	0.43
1:E:238:LEU:HD23	1:E:238:LEU:HA	1.85	0.43
1:E:367:GLY:O	1:E:400:GLN:NE2	2.47	0.43
1:E:122:GLY:O	1:X:167:ILE:HG21	2.19	0.43
1:G:170:ASP:OD1	1:M:355:ARG:NH1	2.42	0.43
1:G:440:ARG:HG2	1:M:161:ARG:HH12	1.83	0.43
1:K:149:ILE:HG22	1:M:470:ILE:HB	1.99	0.43
1:Q:260:ARG:HB2	1:Q:264:LEU:CD2	2.47	0.43
1:S:181:MET:HG3	1:V:406:ASN:HB3	2.00	0.43
1:K:45:GLN:HB2	1:K:63:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:35:LEU:HD11	1:S:267:THR:HG21	2.00	0.43
1:X:325:LYS:HD3	1:X:325:LYS:HA	1.70	0.43
1:I:38:HIS:ND1	3:I:1613:HOH:O	2.37	0.43
1:K:160:LEU:HD12	1:K:187:PRO:HB2	2.01	0.43
1:K:264:LEU:HD12	1:K:264:LEU:HA	1.71	0.43
1:O:160:LEU:HD12	1:O:187:PRO:HB2	2.01	0.43
1:O:232:LYS:HD3	1:O:232:LYS:HA	1.86	0.43
1:A:172:SER:O	1:A:175:SER:OG	2.35	0.43
1:A:263:ASN:CG	1:A:343:ASP:OD1	2.62	0.43
1:E:45:GLN:HB2	1:E:63:TYR:HD1	1.84	0.43
1:G:51:SER:O	1:G:319:ARG:NH2	2.51	0.43
1:G:169:LEU:O	1:M:355:ARG:NH2	2.51	0.43
1:V:263:ASN:C	1:V:264:LEU:HD12	2.44	0.43
1:X:1:MET:N	1:X:1083:ASP:HB2	2.33	0.43
1:X:51:SER:O	1:X:319:ARG:NH2	2.51	0.43
1:C:45:GLN:HB2	1:C:63:TYR:HD1	1.84	0.43
1:C:135:LEU:HD11	1:C:238:LEU:HB3	2.01	0.43
1:E:51:SER:O	1:E:319:ARG:NH2	2.51	0.43
1:G:45:GLN:HB2	1:G:63:TYR:HD1	1.84	0.43
1:G:67:ARG:NH1	1:G:305:ALA:O	2.52	0.43
1:G:196:ALA:HB3	1:M:6:LYS:NZ	2.34	0.43
1:K:1078:LYS:HA	1:K:1078:LYS:HD3	1.87	0.43
1:M:67:ARG:NH1	1:M:305:ALA:O	2.52	0.43
1:M:238:LEU:HD23	1:M:238:LEU:HA	1.84	0.43
1:S:51:SER:O	1:S:319:ARG:NH2	2.51	0.43
1:V:45:GLN:HB2	1:V:63:TYR:HD1	1.84	0.43
1:X:45:GLN:HB2	1:X:63:TYR:HD1	1.84	0.43
1:A:160:LEU:HD12	1:A:187:PRO:HB2	2.01	0.42
1:G:21:PHE:CD2	1:G:264:LEU:CD2	3.01	0.42
1:K:232:LYS:HD3	1:K:232:LYS:HA	1.86	0.42
1:Q:51:SER:O	1:Q:319:ARG:NH2	2.51	0.42
1:X:67:ARG:NH1	1:X:305:ALA:O	2.52	0.42
1:X:333:SER:O	1:X:337:SER:OG	2.27	0.42
1:C:67:ARG:NH1	1:C:305:ALA:O	2.52	0.42
1:E:135:LEU:HD11	1:E:238:LEU:HB3	2.01	0.42
1:E:442:MET:HE1	1:X:188:LEU:HD12	2.00	0.42
1:G:93:HIS:O	1:G:263:ASN:HB3	2.19	0.42
1:I:45:GLN:HB2	1:I:63:TYR:HD1	1.84	0.42
1:K:280:ASN:N	3:K:1618:HOH:O	2.40	0.42
1:Q:135:LEU:HD11	1:Q:238:LEU:HB3	2.01	0.42
1:Q:189:ILE:HD11	1:S:251:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:45:GLN:HB2	1:S:63:TYR:HD1	1.84	0.42
1:X:135:LEU:HD11	1:X:238:LEU:HB3	2.01	0.42
1:I:67:ARG:NH1	1:I:305:ALA:O	2.52	0.42
1:I:194:GLU:CD	1:K:252:HIS:HD1	2.27	0.42
1:I:325:LYS:HA	1:I:325:LYS:HD3	1.70	0.42
1:K:470:ILE:HB	1:O:149:ILE:HG22	2.02	0.42
1:M:27:THR:OG1	1:M:30:HIS:ND1	2.38	0.42
1:M:104:LYS:HG2	1:O:359:SER:HB2	2.00	0.42
1:M:256:VAL:HG21	1:M:448:PHE:HE1	1.85	0.42
1:S:182:GLU:CD	1:V:406:ASN:H	2.28	0.42
1:V:67:ARG:NH1	1:V:305:ALA:O	2.52	0.42
1:V:135:LEU:HD11	1:V:238:LEU:HB3	2.01	0.42
1:V:160:LEU:HD12	1:V:187:PRO:HB2	2.01	0.42
1:A:93:HIS:ND1	1:A:95:ASP:OD1	2.51	0.42
1:G:261:LEU:N	1:G:441:GLU:OE1	2.51	0.42
1:K:325:LYS:HA	1:K:325:LYS:HD3	1.70	0.42
1:O:67:ARG:NH1	1:O:305:ALA:O	2.52	0.42
1:Q:67:ARG:NH1	1:Q:305:ALA:O	2.52	0.42
1:E:27:THR:OG1	1:E:30:HIS:ND1	2.37	0.42
1:G:325:LYS:HA	1:G:325:LYS:HD3	1.70	0.42
1:I:135:LEU:HD11	1:I:238:LEU:HB3	2.01	0.42
1:M:160:LEU:HD12	1:M:187:PRO:HB2	2.01	0.42
1:Q:256:VAL:HG21	1:Q:448:PHE:HE1	1.85	0.42
1:S:67:ARG:NH1	1:S:305:ALA:O	2.52	0.42
1:A:182:GLU:CD	1:I:406:ASN:H	2.27	0.42
1:C:256:VAL:HG21	1:C:448:PHE:HE1	1.85	0.42
1:M:93:HIS:NE2	1:M:263:ASN:HB2	2.34	0.42
1:M:232:LYS:HD3	1:M:232:LYS:HA	1.86	0.42
1:M:1078:LYS:HD3	1:M:1078:LYS:HA	1.87	0.42
1:O:395:ALA:HB1	1:O:453:VAL:HG12	2.02	0.42
1:Q:291:VAL:HG12	1:Q:293:PRO:HD3	2.02	0.42
1:S:232:LYS:HD3	1:S:232:LYS:HA	1.86	0.42
1:A:291:VAL:HG12	1:A:293:PRO:HD3	2.02	0.42
1:E:67:ARG:NH1	1:E:305:ALA:O	2.52	0.42
1:K:51:SER:O	1:K:319:ARG:NH2	2.51	0.42
1:K:67:ARG:NH1	1:K:305:ALA:O	2.52	0.42
1:K:237:GLU:OE2	1:M:382:SER:N	2.42	0.42
1:M:172:SER:O	1:M:175:SER:OG	2.35	0.42
1:M:395:ALA:HB1	1:M:453:VAL:HG12	2.02	0.42
1:S:135:LEU:HD11	1:S:238:LEU:HB3	2.01	0.42
1:V:232:LYS:HA	1:V:232:LYS:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:256:VAL:HG21	1:V:448:PHE:HE1	1.85	0.42
1:V:395:ALA:HB1	1:V:453:VAL:HG12	2.02	0.42
1:A:256:VAL:HG21	1:A:448:PHE:HE1	1.85	0.42
1:E:291:VAL:HG12	1:E:293:PRO:HD3	2.02	0.42
1:G:110:TYR:CE2	1:M:348:MET:HE2	2.55	0.42
1:K:135:LEU:HD11	1:K:238:LEU:HB3	2.01	0.42
1:K:298:GLU:HG3	1:K:414:ILE:CG2	2.49	0.42
1:O:256:VAL:HG21	1:O:448:PHE:HE1	1.85	0.42
1:Q:160:LEU:HD12	1:Q:187:PRO:HB2	2.01	0.42
1:Q:172:SER:O	1:Q:175:SER:OG	2.35	0.42
1:S:291:VAL:HG12	1:S:293:PRO:HD3	2.02	0.42
1:X:232:LYS:HD3	1:X:232:LYS:HA	1.86	0.42
1:X:291:VAL:HG12	1:X:293:PRO:HD3	2.02	0.42
1:A:418:LEU:HD23	1:A:418:LEU:HA	1.90	0.42
1:C:376:GLN:HB2	1:G:300:ILE:HD12	2.00	0.42
1:G:160:LEU:HD12	1:G:187:PRO:HB2	2.01	0.42
1:G:395:ALA:HB1	1:G:453:VAL:HG12	2.02	0.42
1:G:1078:LYS:HA	1:G:1078:LYS:HD3	1.87	0.42
1:K:38:HIS:ND1	3:K:1614:HOH:O	2.37	0.42
1:M:135:LEU:HD11	1:M:238:LEU:HB3	2.01	0.42
1:O:261:LEU:N	1:O:441:GLU:OE1	2.51	0.42
1:O:1100:LYS:H	1:V:1078:LYS:HZ1	1.67	0.42
1:Q:395:ALA:HB1	1:Q:453:VAL:HG12	2.02	0.42
1:S:256:VAL:HG21	1:S:448:PHE:HE1	1.85	0.42
1:V:1078:LYS:HD3	1:V:1078:LYS:HA	1.87	0.42
1:E:325:LYS:HA	1:E:325:LYS:HD3	1.70	0.42
1:E:348:MET:HE2	1:X:110:TYR:CE2	2.55	0.42
1:I:256:VAL:HG21	1:I:448:PHE:HE1	1.85	0.42
1:Q:45:GLN:HB2	1:Q:63:TYR:HD1	1.84	0.42
1:Q:1078:LYS:HA	1:Q:1078:LYS:HD3	1.87	0.42
1:G:135:LEU:HD11	1:G:238:LEU:HB3	2.01	0.41
1:M:45:GLN:HB2	1:M:63:TYR:HD1	1.84	0.41
1:M:291:VAL:HG12	1:M:293:PRO:HD3	2.02	0.41
1:O:291:VAL:HG12	1:O:293:PRO:HD3	2.02	0.41
1:X:238:LEU:HD23	1:X:238:LEU:HA	1.84	0.41
1:A:395:ALA:HB1	1:A:453:VAL:HG12	2.02	0.41
1:E:160:LEU:HD12	1:E:187:PRO:HB2	2.01	0.41
1:O:135:LEU:HD11	1:O:238:LEU:HB3	2.01	0.41
1:S:395:ALA:HB1	1:S:453:VAL:HG12	2.02	0.41
1:X:160:LEU:HD12	1:X:187:PRO:HB2	2.01	0.41
1:X:172:SER:O	1:X:175:SER:OG	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:256:VAL:HG21	1:X:448:PHE:HE1	1.85	0.41
1:A:135:LEU:HD11	1:A:238:LEU:HB3	2.01	0.41
1:E:232:LYS:HA	1:E:232:LYS:HD3	1.86	0.41
1:G:256:VAL:HG21	1:G:448:PHE:HE1	1.85	0.41
1:I:291:VAL:HG12	1:I:293:PRO:HD3	2.02	0.41
1:O:45:GLN:HB2	1:O:63:TYR:HD1	1.84	0.41
1:O:93:HIS:NE2	1:O:263:ASN:HB2	2.36	0.41
1:V:291:VAL:HG12	1:V:293:PRO:HD3	2.02	0.41
1:A:386:VAL:HG11	1:Q:148:VAL:HG11	2.03	0.41
1:O:421:MET:HB2	1:O:421:MET:HE3	1.86	0.41
1:S:160:LEU:HD12	1:S:187:PRO:HB2	2.01	0.41
1:V:93:HIS:CD2	1:V:263:ASN:ND2	2.88	0.41
1:V:333:SER:O	1:V:337:SER:OG	2.27	0.41
1:C:93:HIS:CE1	1:C:263:ASN:HB2	2.55	0.41
1:C:291:VAL:HG12	1:C:293:PRO:HD3	2.02	0.41
1:E:395:ALA:HB1	1:E:453:VAL:HG12	2.02	0.41
1:G:21:PHE:CD2	1:G:264:LEU:HD23	2.52	0.41
1:Q:27:THR:OG1	1:Q:30:HIS:ND1	2.38	0.41
1:Q:298:GLU:HG3	1:Q:414:ILE:CG2	2.51	0.41
1:S:331:SER:OG	1:X:319:ARG:NH1	2.54	0.41
1:X:413:THR:O	3:X:1601:HOH:O	2.22	0.41
1:A:67:ARG:NH1	1:A:305:ALA:O	2.52	0.41
1:A:93:HIS:NE2	1:A:263:ASN:OD1	2.51	0.41
1:A:194:GLU:CD	1:C:252:HIS:HD1	2.28	0.41
1:C:374:ALA:HB2	1:G:118:GLU:HG3	2.03	0.41
1:G:280:ASN:N	3:G:1622:HOH:O	2.41	0.41
1:K:421:MET:HE3	1:K:421:MET:HB2	1.86	0.41
1:Q:261:LEU:N	1:Q:441:GLU:OE1	2.51	0.41
1:S:261:LEU:N	1:S:441:GLU:OE1	2.51	0.41
1:C:395:ALA:HB1	1:C:453:VAL:HG12	2.02	0.41
1:I:160:LEU:HD12	1:I:187:PRO:HB2	2.01	0.41
1:A:45:GLN:HB2	1:A:63:TYR:HD1	1.84	0.41
1:A:263:ASN:ND2	1:A:344:MET:H	2.18	0.41
1:E:1078:LYS:HD2	1:X:1078:LYS:HD2	2.03	0.41
1:I:298:GLU:HG3	1:I:414:ILE:CG2	2.51	0.41
1:K:256:VAL:HG21	1:K:448:PHE:HE1	1.85	0.41
1:K:262:ASP:HB2	3:K:1631:HOH:O	2.20	0.41
1:K:395:ALA:HB1	1:K:453:VAL:HG12	2.02	0.41
1:Q:264:LEU:HD12	1:Q:264:LEU:HA	1.65	0.41
1:S:300:ILE:HD12	1:V:376:GLN:HB2	2.02	0.41
1:V:93:HIS:O	1:V:263:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASP:OD2	1:A:437:HIS:CD2	2.73	0.41
1:A:298:GLU:HG3	1:A:414:ILE:CG2	2.50	0.40
1:C:1078:LYS:HD3	1:C:1078:LYS:HA	1.87	0.40
1:E:27:THR:HG21	1:E:137:GLY:HA2	2.03	0.40
1:E:421:MET:HB2	1:E:421:MET:HE3	1.86	0.40
1:E:437:HIS:CE1	1:X:168:HIS:HE1	2.38	0.40
1:K:263:ASN:ND2	1:K:342:ALA:O	2.48	0.40
1:K:291:VAL:HG12	1:K:293:PRO:HD3	2.02	0.40
1:M:298:GLU:HG3	1:M:414:ILE:CG2	2.51	0.40
1:S:325:LYS:HA	1:S:325:LYS:HD3	1.70	0.40
1:V:27:THR:HG21	1:V:137:GLY:HA2	2.04	0.40
1:A:333:SER:O	1:A:337:SER:OG	2.27	0.40
1:E:21:PHE:HE2	1:E:264:LEU:CD2	2.33	0.40
1:E:256:VAL:HG21	1:E:448:PHE:HE1	1.85	0.40
1:G:27:THR:HG21	1:G:137:GLY:HA2	2.04	0.40
1:G:247:ARG:HG3	1:M:158:PRO:HG2	2.02	0.40
1:K:27:THR:HG21	1:K:137:GLY:HA2	2.04	0.40
1:S:238:LEU:HD23	1:S:238:LEU:HA	1.84	0.40
1:X:1072:ASP:OD1	1:X:1072:ASP:N	2.55	0.40
1:X:1078:LYS:HD3	1:X:1078:LYS:HA	1.87	0.40
1:A:298:GLU:CG	1:A:414:ILE:HG23	2.51	0.40
1:E:110:TYR:CD2	1:X:348:MET:HE2	2.57	0.40
1:E:251:ILE:HG22	1:X:190:GLY:HA3	2.03	0.40
1:I:189:ILE:HG13	1:K:251:ILE:HB	2.03	0.40
1:I:1072:ASP:OD1	1:I:1072:ASP:N	2.55	0.40
1:S:1072:ASP:OD1	1:S:1072:ASP:N	2.55	0.40
1:X:27:THR:HG21	1:X:137:GLY:HA2	2.03	0.40
1:C:135:LEU:HD21	1:C:238:LEU:HD13	2.04	0.40
1:C:347:ALA:HB2	1:C:432:PRO:HB2	2.04	0.40
1:C:421:MET:HE3	1:C:421:MET:HB2	1.86	0.40
1:I:395:ALA:HB1	1:I:453:VAL:HG12	2.02	0.40
1:Q:135:LEU:HD21	1:Q:238:LEU:HD13	2.04	0.40
1:Q:347:ALA:HB2	1:Q:432:PRO:HB2	2.04	0.40
1:S:262:ASP:OD2	1:S:437:HIS:CD2	2.74	0.40
1:V:347:ALA:HB2	1:V:432:PRO:HB2	2.04	0.40
1:X:135:LEU:HD21	1:X:238:LEU:HD13	2.04	0.40
1:X:395:ALA:HB1	1:X:453:VAL:HG12	2.02	0.40
1:A:307:GLY:O	1:A:310:SER:OG	2.36	0.40
1:A:377:ARG:HG3	1:A:410:CYS:HB3	2.04	0.40
1:G:291:VAL:HG12	1:G:293:PRO:HD3	2.02	0.40
1:I:93:HIS:NE2	1:I:263:ASN:HB2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:118:GLU:HA	1:O:406:ASN:ND2	2.36	0.40
1:M:347:ALA:HB2	1:M:432:PRO:HB2	2.04	0.40
1:O:347:ALA:HB2	1:O:432:PRO:HB2	2.04	0.40
1:O:1072:ASP:OD1	1:O:1072:ASP:N	2.55	0.40
1:S:377:ARG:HG3	1:S:410:CYS:HB3	2.04	0.40
1:V:135:LEU:HD21	1:V:238:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/929 (56%)	495 (95%)	26 (5%)	0	100	100
1	C	521/929 (56%)	494 (95%)	27 (5%)	0	100	100
1	E	521/929 (56%)	495 (95%)	26 (5%)	0	100	100
1	G	521/929 (56%)	495 (95%)	26 (5%)	0	100	100
1	I	521/929 (56%)	494 (95%)	27 (5%)	0	100	100
1	K	521/929 (56%)	494 (95%)	27 (5%)	0	100	100
1	M	521/929 (56%)	495 (95%)	25 (5%)	1 (0%)	43	50
1	O	521/929 (56%)	495 (95%)	26 (5%)	0	100	100
1	Q	521/929 (56%)	495 (95%)	26 (5%)	0	100	100
1	S	521/929 (56%)	495 (95%)	26 (5%)	0	100	100
1	V	521/929 (56%)	495 (95%)	26 (5%)	0	100	100
1	X	521/929 (56%)	494 (95%)	27 (5%)	0	100	100
All	All	6252/11148 (56%)	5936 (95%)	315 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	262	ASP

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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.

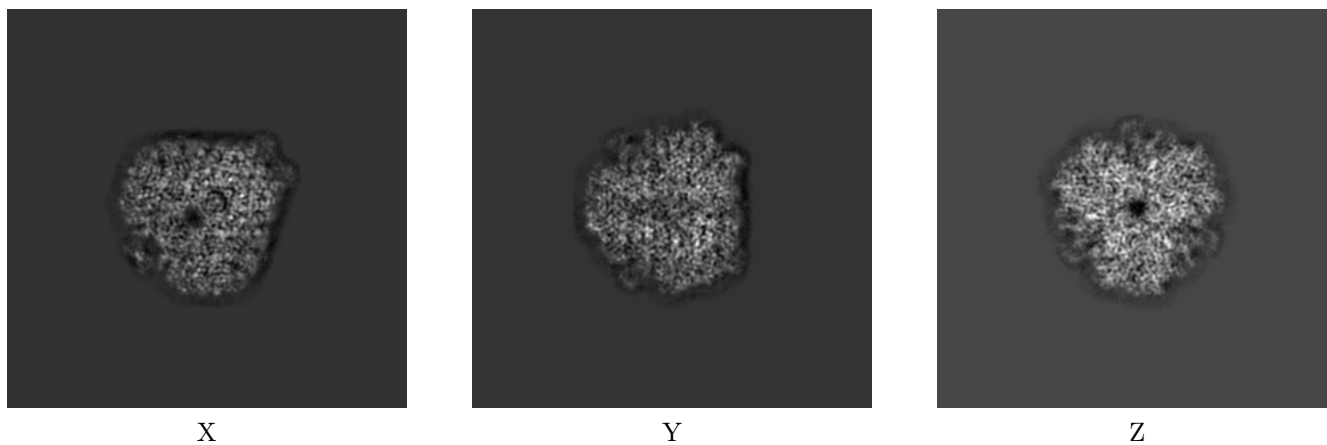
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30652. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

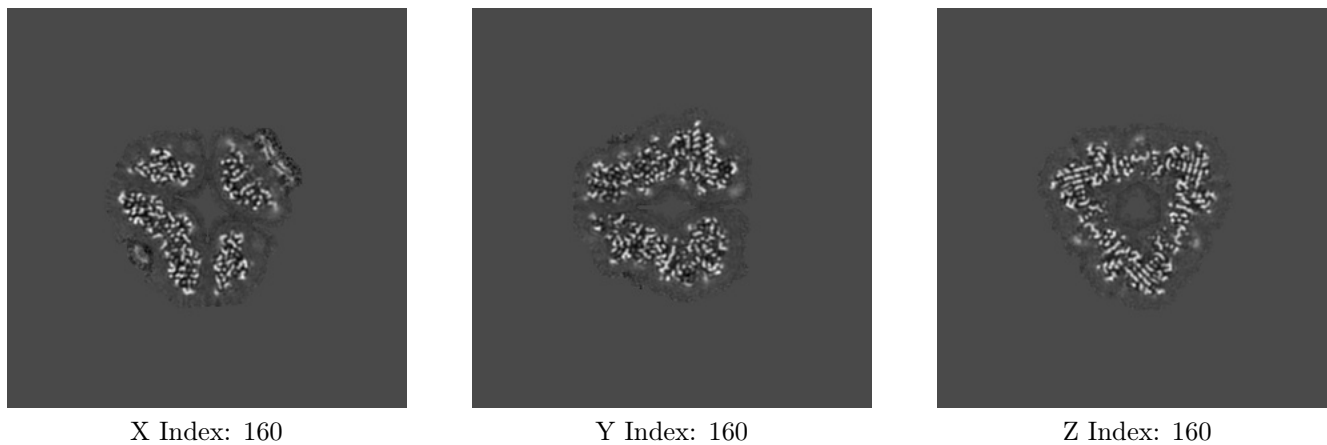
#### 6.1.1 Primary map



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

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

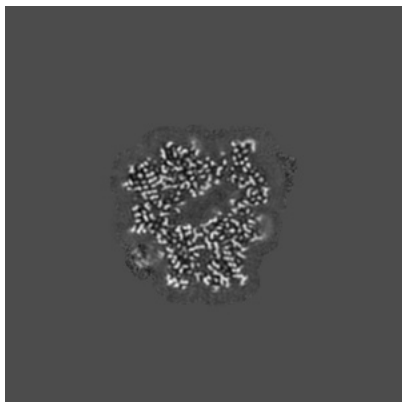
#### 6.2.1 Primary map



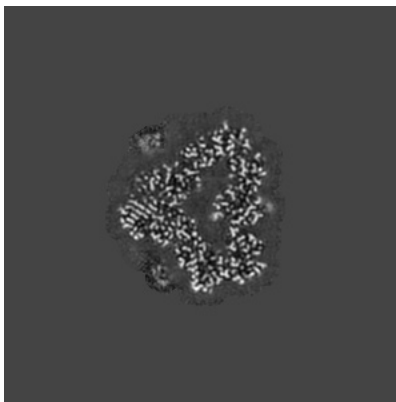
The images above show central slices of the map in three orthogonal directions.

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

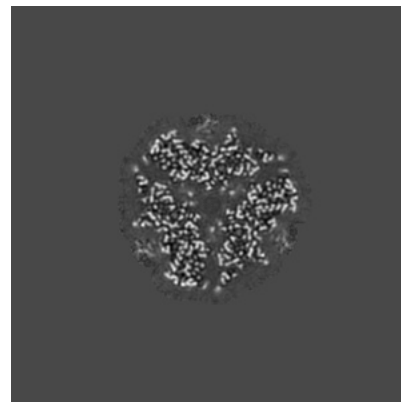
### 6.3.1 Primary map



X Index: 143



Y Index: 178

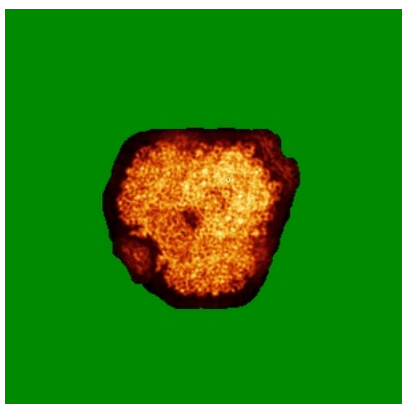


Z Index: 178

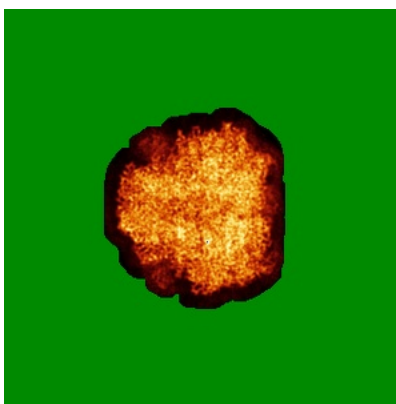
The images above show the largest variance slices of the map in three orthogonal directions.

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

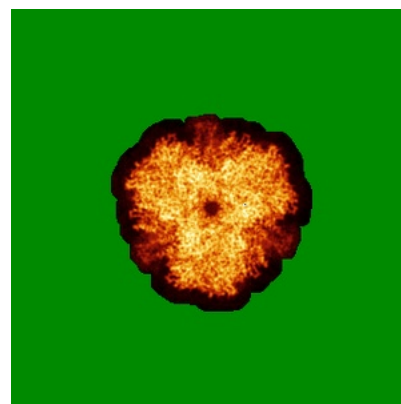
### 6.4.1 Primary map



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

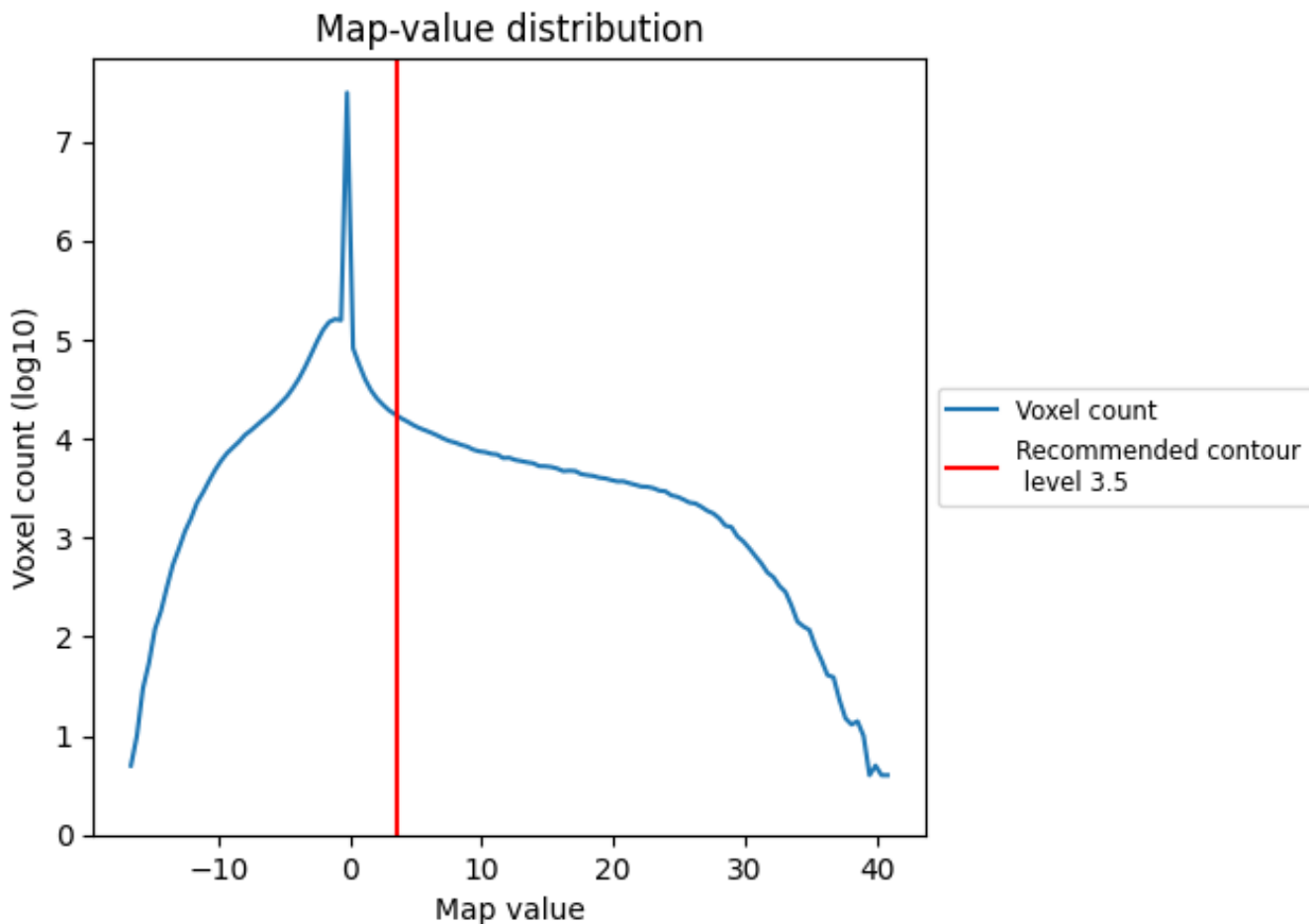
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

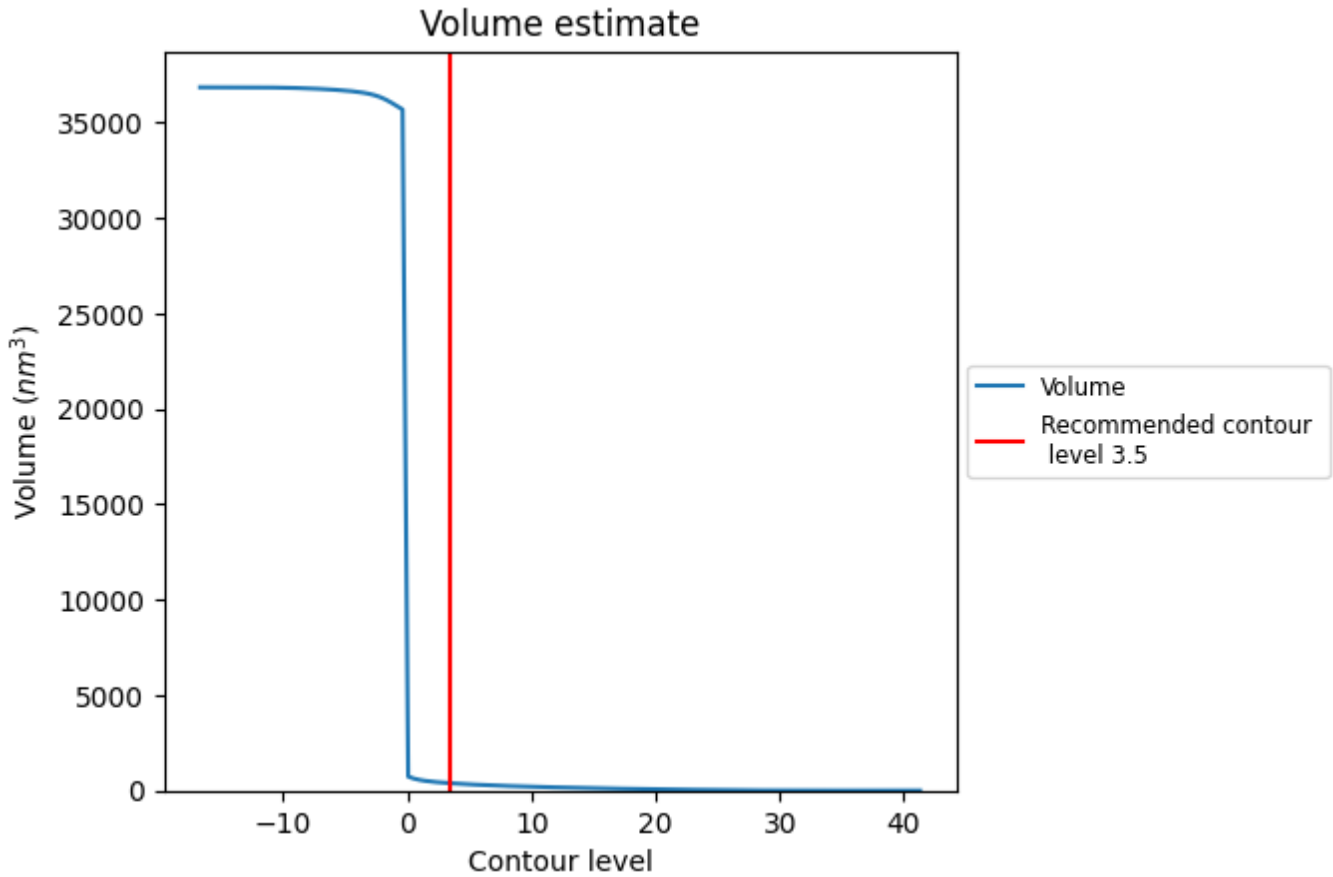
This section contains the results of statistical analysis of the map.

### 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.

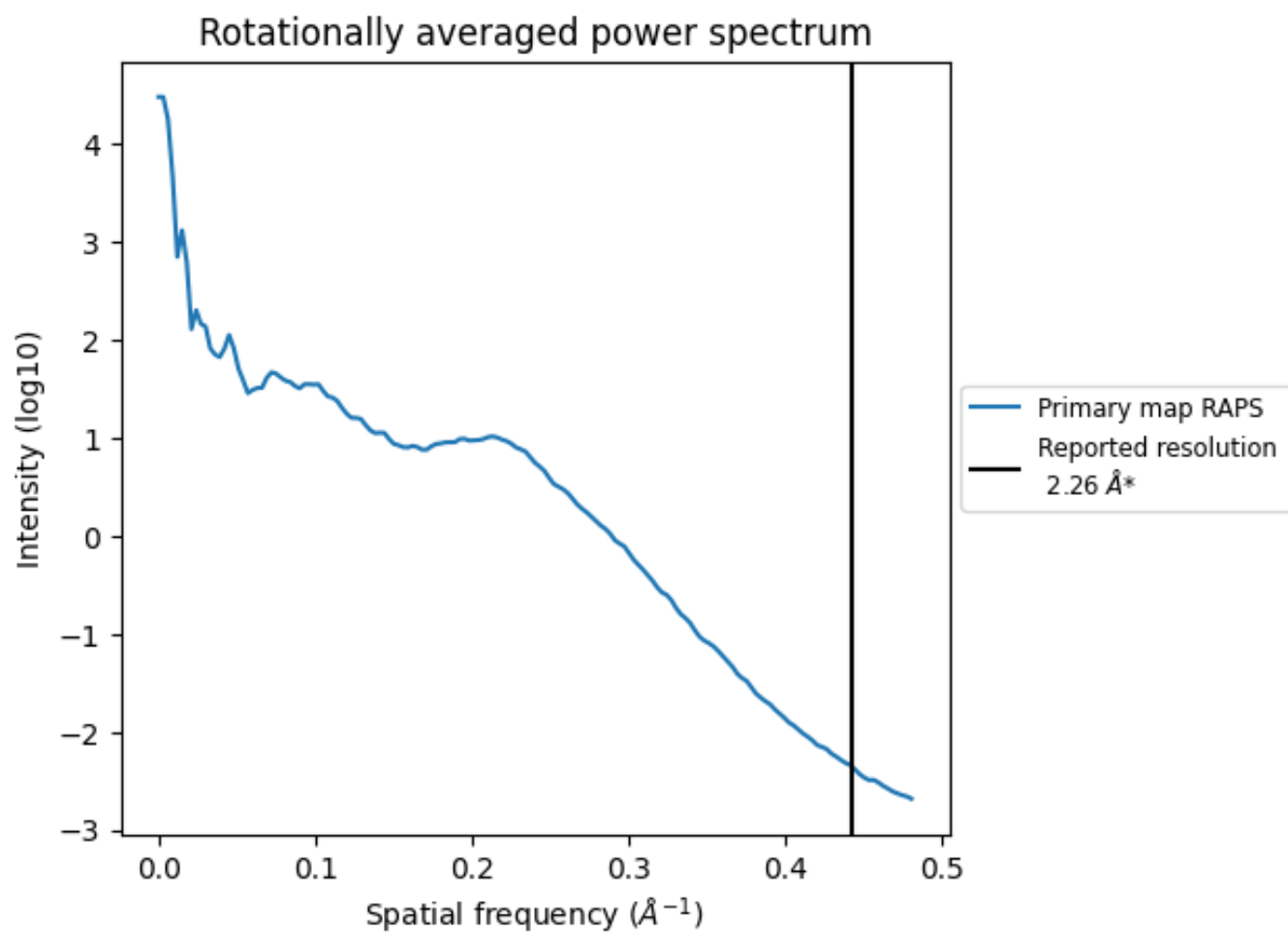
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 385 nm<sup>3</sup>; this corresponds to an approximate mass of 348 kDa.

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

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



\*Reported resolution corresponds to spatial frequency of  $0.442 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation

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

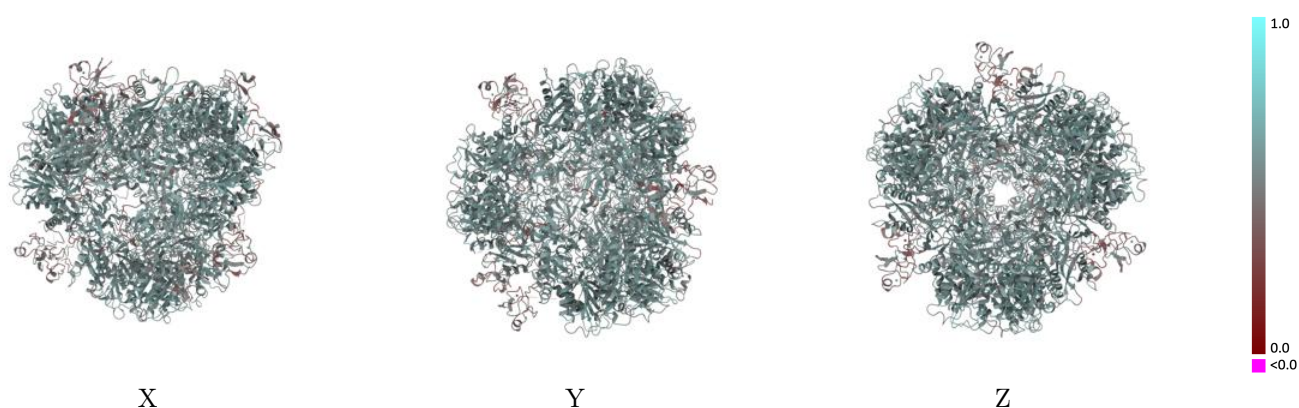
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30652 and PDB model 7DDE. Per-residue inclusion information can be found in section 3 on page 12.

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

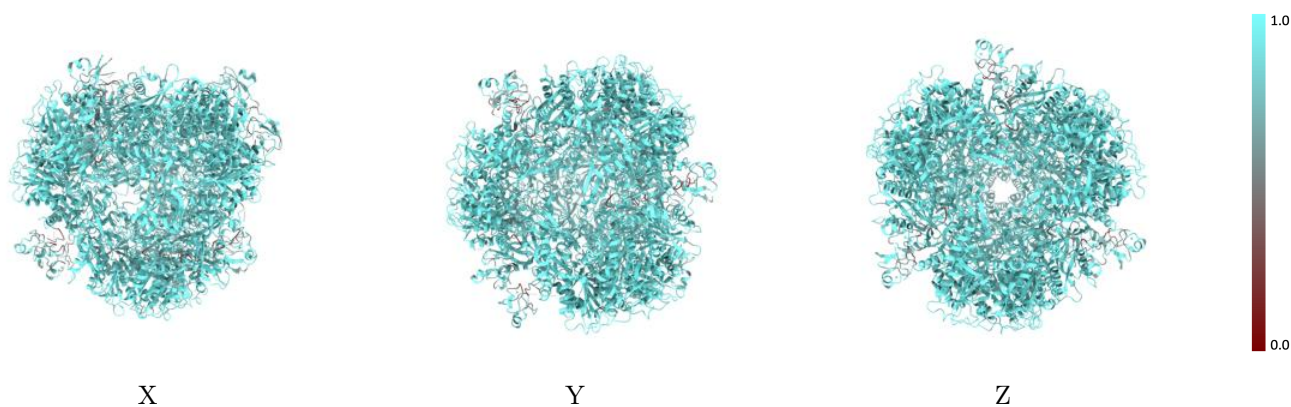
This section was not generated.

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



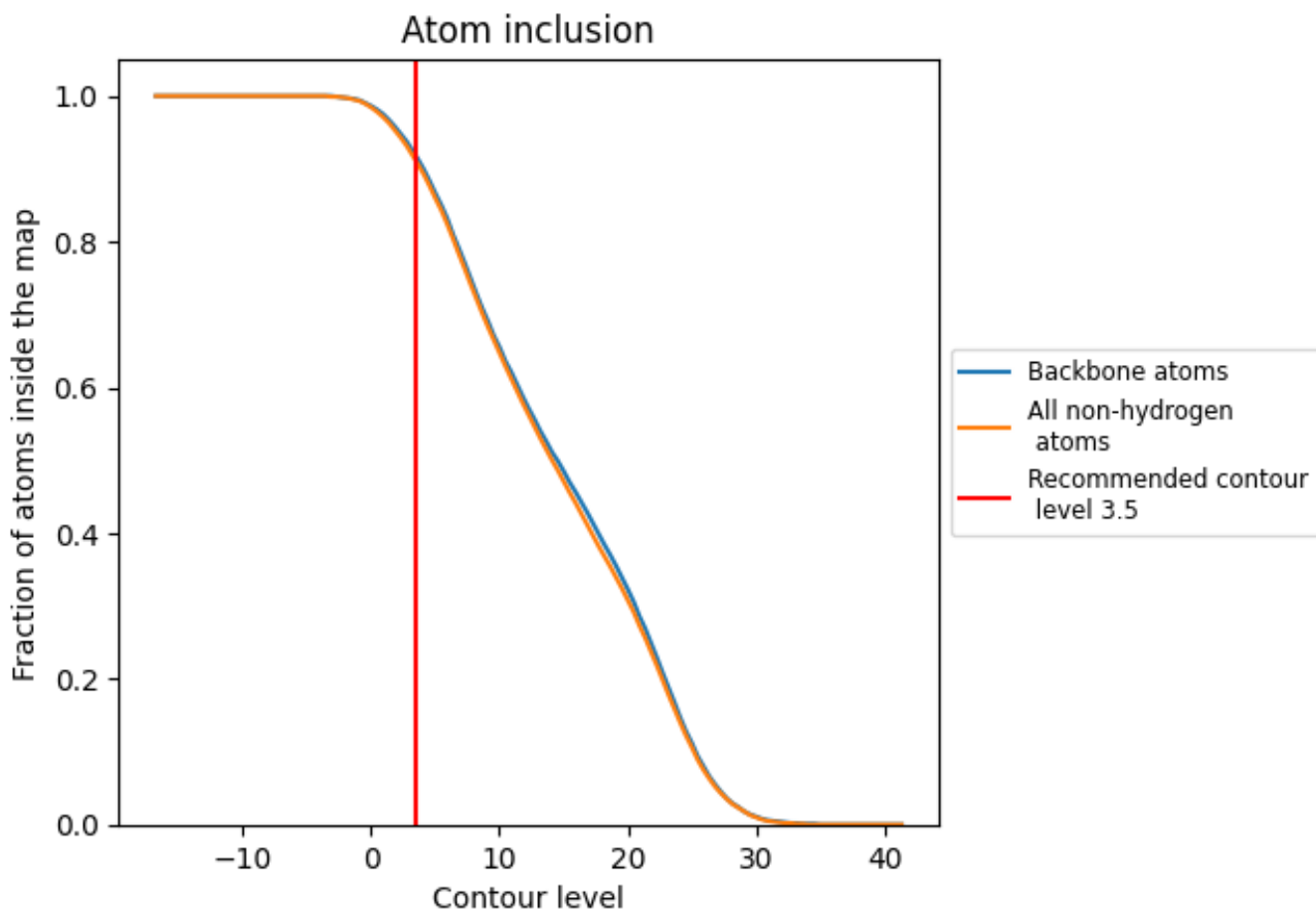
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.5450
A	 0.9170	 0.5440
C	 0.9210	 0.5470
E	 0.9190	 0.5460
G	 0.9150	 0.5440
I	 0.9120	 0.5470
K	 0.9140	 0.5450
M	 0.9080	 0.5400
O	 0.9130	 0.5460
Q	 0.9190	 0.5440
S	 0.9160	 0.5440
V	 0.9120	 0.5460
X	 0.9170	 0.5450

