



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 10:03 PM UTC

PDB ID : 7DOP / pdb_00007dop
EMDB ID : EMD-30796
Title : Structural insights into viral RNA capping and plasma membrane targeting
by Chikungunya virus nonstructural protein 1
Authors : Zhang, K.; Law, Y.S.; Law, M.C.Y.; Tan, Y.B.; Wirawan, M.; Luo, D.H.
Deposited on : 2020-12-15
Resolution : 2.38 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:

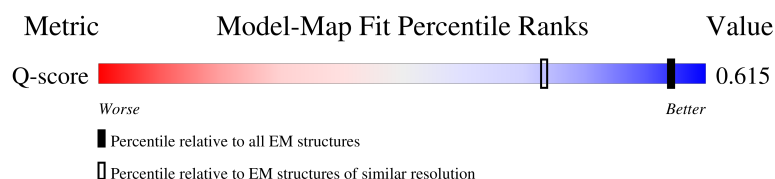
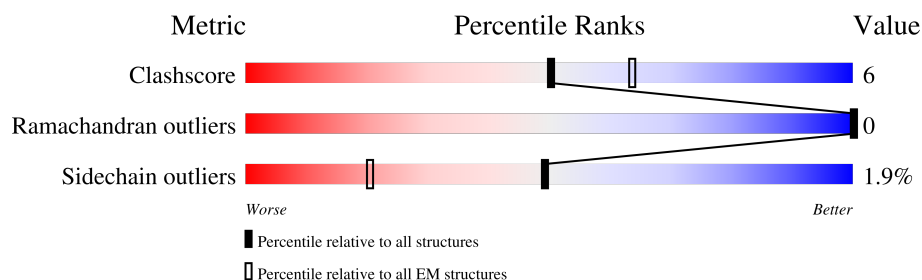
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

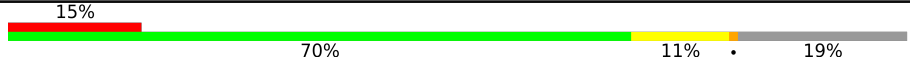
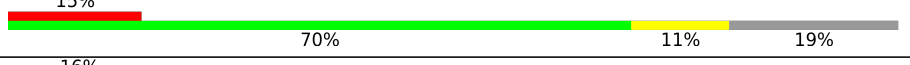
The reported resolution of this entry is 2.38 Å.

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	4811 (1.88 - 2.88)

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	552	
1	B	552	
1	C	552	
1	D	552	

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Mol	Chain	Length	Quality of chain
1	E	552	
1	F	552	
1	G	552	
1	H	552	
1	I	552	
1	J	552	
1	K	552	
1	L	552	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 41700 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 Nonstructural Protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	B	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	C	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	D	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	E	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	F	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	G	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	H	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	I	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	J	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	K	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		
1	L	446	Total	C	N	O	S	1	0
			3474	2200	600	645	29		

There are 432 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	517	GLY	-	expression tag	UNP Q8JUX6
A	518	GLY	-	expression tag	UNP Q8JUX6
A	519	GLY	-	expression tag	UNP Q8JUX6
A	520	GLY	-	expression tag	UNP Q8JUX6
A	521	SER	-	expression tag	UNP Q8JUX6
A	522	TRP	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	-	expression tag	UNP Q8JUX6
A	524	HIS	-	expression tag	UNP Q8JUX6
A	525	PRO	-	expression tag	UNP Q8JUX6
A	526	GLN	-	expression tag	UNP Q8JUX6
A	527	PHE	-	expression tag	UNP Q8JUX6
A	528	GLU	-	expression tag	UNP Q8JUX6
A	529	LYS	-	expression tag	UNP Q8JUX6
A	530	MET	-	expression tag	UNP Q8JUX6
A	531	ASP	-	expression tag	UNP Q8JUX6
A	532	TYR	-	expression tag	UNP Q8JUX6
A	533	LYS	-	expression tag	UNP Q8JUX6
A	534	ASP	-	expression tag	UNP Q8JUX6
A	535	HIS	-	expression tag	UNP Q8JUX6
A	536	ASP	-	expression tag	UNP Q8JUX6
A	537	GLY	-	expression tag	UNP Q8JUX6
A	538	ASP	-	expression tag	UNP Q8JUX6
A	539	TYR	-	expression tag	UNP Q8JUX6
A	540	LYS	-	expression tag	UNP Q8JUX6
A	541	ASP	-	expression tag	UNP Q8JUX6
A	542	HIS	-	expression tag	UNP Q8JUX6
A	543	ASP	-	expression tag	UNP Q8JUX6
A	544	ILE	-	expression tag	UNP Q8JUX6
A	545	ASP	-	expression tag	UNP Q8JUX6
A	546	TYR	-	expression tag	UNP Q8JUX6
A	547	LYS	-	expression tag	UNP Q8JUX6
A	548	ASP	-	expression tag	UNP Q8JUX6
A	549	ASP	-	expression tag	UNP Q8JUX6
A	550	ASP	-	expression tag	UNP Q8JUX6
A	551	ASP	-	expression tag	UNP Q8JUX6
A	552	LYS	-	expression tag	UNP Q8JUX6
B	517	GLY	-	expression tag	UNP Q8JUX6
B	518	GLY	-	expression tag	UNP Q8JUX6
B	519	GLY	-	expression tag	UNP Q8JUX6
B	520	GLY	-	expression tag	UNP Q8JUX6
B	521	SER	-	expression tag	UNP Q8JUX6
B	522	TRP	-	expression tag	UNP Q8JUX6
B	523	SER	-	expression tag	UNP Q8JUX6
B	524	HIS	-	expression tag	UNP Q8JUX6
B	525	PRO	-	expression tag	UNP Q8JUX6
B	526	GLN	-	expression tag	UNP Q8JUX6
B	527	PHE	-	expression tag	UNP Q8JUX6
B	528	GLU	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	529	LYS	-	expression tag	UNP Q8JUX6
B	530	MET	-	expression tag	UNP Q8JUX6
B	531	ASP	-	expression tag	UNP Q8JUX6
B	532	TYR	-	expression tag	UNP Q8JUX6
B	533	LYS	-	expression tag	UNP Q8JUX6
B	534	ASP	-	expression tag	UNP Q8JUX6
B	535	HIS	-	expression tag	UNP Q8JUX6
B	536	ASP	-	expression tag	UNP Q8JUX6
B	537	GLY	-	expression tag	UNP Q8JUX6
B	538	ASP	-	expression tag	UNP Q8JUX6
B	539	TYR	-	expression tag	UNP Q8JUX6
B	540	LYS	-	expression tag	UNP Q8JUX6
B	541	ASP	-	expression tag	UNP Q8JUX6
B	542	HIS	-	expression tag	UNP Q8JUX6
B	543	ASP	-	expression tag	UNP Q8JUX6
B	544	ILE	-	expression tag	UNP Q8JUX6
B	545	ASP	-	expression tag	UNP Q8JUX6
B	546	TYR	-	expression tag	UNP Q8JUX6
B	547	LYS	-	expression tag	UNP Q8JUX6
B	548	ASP	-	expression tag	UNP Q8JUX6
B	549	ASP	-	expression tag	UNP Q8JUX6
B	550	ASP	-	expression tag	UNP Q8JUX6
B	551	ASP	-	expression tag	UNP Q8JUX6
B	552	LYS	-	expression tag	UNP Q8JUX6
C	517	GLY	-	expression tag	UNP Q8JUX6
C	518	GLY	-	expression tag	UNP Q8JUX6
C	519	GLY	-	expression tag	UNP Q8JUX6
C	520	GLY	-	expression tag	UNP Q8JUX6
C	521	SER	-	expression tag	UNP Q8JUX6
C	522	TRP	-	expression tag	UNP Q8JUX6
C	523	SER	-	expression tag	UNP Q8JUX6
C	524	HIS	-	expression tag	UNP Q8JUX6
C	525	PRO	-	expression tag	UNP Q8JUX6
C	526	GLN	-	expression tag	UNP Q8JUX6
C	527	PHE	-	expression tag	UNP Q8JUX6
C	528	GLU	-	expression tag	UNP Q8JUX6
C	529	LYS	-	expression tag	UNP Q8JUX6
C	530	MET	-	expression tag	UNP Q8JUX6
C	531	ASP	-	expression tag	UNP Q8JUX6
C	532	TYR	-	expression tag	UNP Q8JUX6
C	533	LYS	-	expression tag	UNP Q8JUX6
C	534	ASP	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	535	HIS	-	expression tag	UNP Q8JUX6
C	536	ASP	-	expression tag	UNP Q8JUX6
C	537	GLY	-	expression tag	UNP Q8JUX6
C	538	ASP	-	expression tag	UNP Q8JUX6
C	539	TYR	-	expression tag	UNP Q8JUX6
C	540	LYS	-	expression tag	UNP Q8JUX6
C	541	ASP	-	expression tag	UNP Q8JUX6
C	542	HIS	-	expression tag	UNP Q8JUX6
C	543	ASP	-	expression tag	UNP Q8JUX6
C	544	ILE	-	expression tag	UNP Q8JUX6
C	545	ASP	-	expression tag	UNP Q8JUX6
C	546	TYR	-	expression tag	UNP Q8JUX6
C	547	LYS	-	expression tag	UNP Q8JUX6
C	548	ASP	-	expression tag	UNP Q8JUX6
C	549	ASP	-	expression tag	UNP Q8JUX6
C	550	ASP	-	expression tag	UNP Q8JUX6
C	551	ASP	-	expression tag	UNP Q8JUX6
C	552	LYS	-	expression tag	UNP Q8JUX6
D	517	GLY	-	expression tag	UNP Q8JUX6
D	518	GLY	-	expression tag	UNP Q8JUX6
D	519	GLY	-	expression tag	UNP Q8JUX6
D	520	GLY	-	expression tag	UNP Q8JUX6
D	521	SER	-	expression tag	UNP Q8JUX6
D	522	TRP	-	expression tag	UNP Q8JUX6
D	523	SER	-	expression tag	UNP Q8JUX6
D	524	HIS	-	expression tag	UNP Q8JUX6
D	525	PRO	-	expression tag	UNP Q8JUX6
D	526	GLN	-	expression tag	UNP Q8JUX6
D	527	PHE	-	expression tag	UNP Q8JUX6
D	528	GLU	-	expression tag	UNP Q8JUX6
D	529	LYS	-	expression tag	UNP Q8JUX6
D	530	MET	-	expression tag	UNP Q8JUX6
D	531	ASP	-	expression tag	UNP Q8JUX6
D	532	TYR	-	expression tag	UNP Q8JUX6
D	533	LYS	-	expression tag	UNP Q8JUX6
D	534	ASP	-	expression tag	UNP Q8JUX6
D	535	HIS	-	expression tag	UNP Q8JUX6
D	536	ASP	-	expression tag	UNP Q8JUX6
D	537	GLY	-	expression tag	UNP Q8JUX6
D	538	ASP	-	expression tag	UNP Q8JUX6
D	539	TYR	-	expression tag	UNP Q8JUX6
D	540	LYS	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	541	ASP	-	expression tag	UNP Q8JUX6
D	542	HIS	-	expression tag	UNP Q8JUX6
D	543	ASP	-	expression tag	UNP Q8JUX6
D	544	ILE	-	expression tag	UNP Q8JUX6
D	545	ASP	-	expression tag	UNP Q8JUX6
D	546	TYR	-	expression tag	UNP Q8JUX6
D	547	LYS	-	expression tag	UNP Q8JUX6
D	548	ASP	-	expression tag	UNP Q8JUX6
D	549	ASP	-	expression tag	UNP Q8JUX6
D	550	ASP	-	expression tag	UNP Q8JUX6
D	551	ASP	-	expression tag	UNP Q8JUX6
D	552	LYS	-	expression tag	UNP Q8JUX6
E	517	GLY	-	expression tag	UNP Q8JUX6
E	518	GLY	-	expression tag	UNP Q8JUX6
E	519	GLY	-	expression tag	UNP Q8JUX6
E	520	GLY	-	expression tag	UNP Q8JUX6
E	521	SER	-	expression tag	UNP Q8JUX6
E	522	TRP	-	expression tag	UNP Q8JUX6
E	523	SER	-	expression tag	UNP Q8JUX6
E	524	HIS	-	expression tag	UNP Q8JUX6
E	525	PRO	-	expression tag	UNP Q8JUX6
E	526	GLN	-	expression tag	UNP Q8JUX6
E	527	PHE	-	expression tag	UNP Q8JUX6
E	528	GLU	-	expression tag	UNP Q8JUX6
E	529	LYS	-	expression tag	UNP Q8JUX6
E	530	MET	-	expression tag	UNP Q8JUX6
E	531	ASP	-	expression tag	UNP Q8JUX6
E	532	TYR	-	expression tag	UNP Q8JUX6
E	533	LYS	-	expression tag	UNP Q8JUX6
E	534	ASP	-	expression tag	UNP Q8JUX6
E	535	HIS	-	expression tag	UNP Q8JUX6
E	536	ASP	-	expression tag	UNP Q8JUX6
E	537	GLY	-	expression tag	UNP Q8JUX6
E	538	ASP	-	expression tag	UNP Q8JUX6
E	539	TYR	-	expression tag	UNP Q8JUX6
E	540	LYS	-	expression tag	UNP Q8JUX6
E	541	ASP	-	expression tag	UNP Q8JUX6
E	542	HIS	-	expression tag	UNP Q8JUX6
E	543	ASP	-	expression tag	UNP Q8JUX6
E	544	ILE	-	expression tag	UNP Q8JUX6
E	545	ASP	-	expression tag	UNP Q8JUX6
E	546	TYR	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	547	LYS	-	expression tag	UNP Q8JUX6
E	548	ASP	-	expression tag	UNP Q8JUX6
E	549	ASP	-	expression tag	UNP Q8JUX6
E	550	ASP	-	expression tag	UNP Q8JUX6
E	551	ASP	-	expression tag	UNP Q8JUX6
E	552	LYS	-	expression tag	UNP Q8JUX6
F	517	GLY	-	expression tag	UNP Q8JUX6
F	518	GLY	-	expression tag	UNP Q8JUX6
F	519	GLY	-	expression tag	UNP Q8JUX6
F	520	GLY	-	expression tag	UNP Q8JUX6
F	521	SER	-	expression tag	UNP Q8JUX6
F	522	TRP	-	expression tag	UNP Q8JUX6
F	523	SER	-	expression tag	UNP Q8JUX6
F	524	HIS	-	expression tag	UNP Q8JUX6
F	525	PRO	-	expression tag	UNP Q8JUX6
F	526	GLN	-	expression tag	UNP Q8JUX6
F	527	PHE	-	expression tag	UNP Q8JUX6
F	528	GLU	-	expression tag	UNP Q8JUX6
F	529	LYS	-	expression tag	UNP Q8JUX6
F	530	MET	-	expression tag	UNP Q8JUX6
F	531	ASP	-	expression tag	UNP Q8JUX6
F	532	TYR	-	expression tag	UNP Q8JUX6
F	533	LYS	-	expression tag	UNP Q8JUX6
F	534	ASP	-	expression tag	UNP Q8JUX6
F	535	HIS	-	expression tag	UNP Q8JUX6
F	536	ASP	-	expression tag	UNP Q8JUX6
F	537	GLY	-	expression tag	UNP Q8JUX6
F	538	ASP	-	expression tag	UNP Q8JUX6
F	539	TYR	-	expression tag	UNP Q8JUX6
F	540	LYS	-	expression tag	UNP Q8JUX6
F	541	ASP	-	expression tag	UNP Q8JUX6
F	542	HIS	-	expression tag	UNP Q8JUX6
F	543	ASP	-	expression tag	UNP Q8JUX6
F	544	ILE	-	expression tag	UNP Q8JUX6
F	545	ASP	-	expression tag	UNP Q8JUX6
F	546	TYR	-	expression tag	UNP Q8JUX6
F	547	LYS	-	expression tag	UNP Q8JUX6
F	548	ASP	-	expression tag	UNP Q8JUX6
F	549	ASP	-	expression tag	UNP Q8JUX6
F	550	ASP	-	expression tag	UNP Q8JUX6
F	551	ASP	-	expression tag	UNP Q8JUX6
F	552	LYS	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	517	GLY	-	expression tag	UNP Q8JUX6
G	518	GLY	-	expression tag	UNP Q8JUX6
G	519	GLY	-	expression tag	UNP Q8JUX6
G	520	GLY	-	expression tag	UNP Q8JUX6
G	521	SER	-	expression tag	UNP Q8JUX6
G	522	TRP	-	expression tag	UNP Q8JUX6
G	523	SER	-	expression tag	UNP Q8JUX6
G	524	HIS	-	expression tag	UNP Q8JUX6
G	525	PRO	-	expression tag	UNP Q8JUX6
G	526	GLN	-	expression tag	UNP Q8JUX6
G	527	PHE	-	expression tag	UNP Q8JUX6
G	528	GLU	-	expression tag	UNP Q8JUX6
G	529	LYS	-	expression tag	UNP Q8JUX6
G	530	MET	-	expression tag	UNP Q8JUX6
G	531	ASP	-	expression tag	UNP Q8JUX6
G	532	TYR	-	expression tag	UNP Q8JUX6
G	533	LYS	-	expression tag	UNP Q8JUX6
G	534	ASP	-	expression tag	UNP Q8JUX6
G	535	HIS	-	expression tag	UNP Q8JUX6
G	536	ASP	-	expression tag	UNP Q8JUX6
G	537	GLY	-	expression tag	UNP Q8JUX6
G	538	ASP	-	expression tag	UNP Q8JUX6
G	539	TYR	-	expression tag	UNP Q8JUX6
G	540	LYS	-	expression tag	UNP Q8JUX6
G	541	ASP	-	expression tag	UNP Q8JUX6
G	542	HIS	-	expression tag	UNP Q8JUX6
G	543	ASP	-	expression tag	UNP Q8JUX6
G	544	ILE	-	expression tag	UNP Q8JUX6
G	545	ASP	-	expression tag	UNP Q8JUX6
G	546	TYR	-	expression tag	UNP Q8JUX6
G	547	LYS	-	expression tag	UNP Q8JUX6
G	548	ASP	-	expression tag	UNP Q8JUX6
G	549	ASP	-	expression tag	UNP Q8JUX6
G	550	ASP	-	expression tag	UNP Q8JUX6
G	551	ASP	-	expression tag	UNP Q8JUX6
G	552	LYS	-	expression tag	UNP Q8JUX6
H	517	GLY	-	expression tag	UNP Q8JUX6
H	518	GLY	-	expression tag	UNP Q8JUX6
H	519	GLY	-	expression tag	UNP Q8JUX6
H	520	GLY	-	expression tag	UNP Q8JUX6
H	521	SER	-	expression tag	UNP Q8JUX6
H	522	TRP	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	523	SER	-	expression tag	UNP Q8JUX6
H	524	HIS	-	expression tag	UNP Q8JUX6
H	525	PRO	-	expression tag	UNP Q8JUX6
H	526	GLN	-	expression tag	UNP Q8JUX6
H	527	PHE	-	expression tag	UNP Q8JUX6
H	528	GLU	-	expression tag	UNP Q8JUX6
H	529	LYS	-	expression tag	UNP Q8JUX6
H	530	MET	-	expression tag	UNP Q8JUX6
H	531	ASP	-	expression tag	UNP Q8JUX6
H	532	TYR	-	expression tag	UNP Q8JUX6
H	533	LYS	-	expression tag	UNP Q8JUX6
H	534	ASP	-	expression tag	UNP Q8JUX6
H	535	HIS	-	expression tag	UNP Q8JUX6
H	536	ASP	-	expression tag	UNP Q8JUX6
H	537	GLY	-	expression tag	UNP Q8JUX6
H	538	ASP	-	expression tag	UNP Q8JUX6
H	539	TYR	-	expression tag	UNP Q8JUX6
H	540	LYS	-	expression tag	UNP Q8JUX6
H	541	ASP	-	expression tag	UNP Q8JUX6
H	542	HIS	-	expression tag	UNP Q8JUX6
H	543	ASP	-	expression tag	UNP Q8JUX6
H	544	ILE	-	expression tag	UNP Q8JUX6
H	545	ASP	-	expression tag	UNP Q8JUX6
H	546	TYR	-	expression tag	UNP Q8JUX6
H	547	LYS	-	expression tag	UNP Q8JUX6
H	548	ASP	-	expression tag	UNP Q8JUX6
H	549	ASP	-	expression tag	UNP Q8JUX6
H	550	ASP	-	expression tag	UNP Q8JUX6
H	551	ASP	-	expression tag	UNP Q8JUX6
H	552	LYS	-	expression tag	UNP Q8JUX6
I	517	GLY	-	expression tag	UNP Q8JUX6
I	518	GLY	-	expression tag	UNP Q8JUX6
I	519	GLY	-	expression tag	UNP Q8JUX6
I	520	GLY	-	expression tag	UNP Q8JUX6
I	521	SER	-	expression tag	UNP Q8JUX6
I	522	TRP	-	expression tag	UNP Q8JUX6
I	523	SER	-	expression tag	UNP Q8JUX6
I	524	HIS	-	expression tag	UNP Q8JUX6
I	525	PRO	-	expression tag	UNP Q8JUX6
I	526	GLN	-	expression tag	UNP Q8JUX6
I	527	PHE	-	expression tag	UNP Q8JUX6
I	528	GLU	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	529	LYS	-	expression tag	UNP Q8JUX6
I	530	MET	-	expression tag	UNP Q8JUX6
I	531	ASP	-	expression tag	UNP Q8JUX6
I	532	TYR	-	expression tag	UNP Q8JUX6
I	533	LYS	-	expression tag	UNP Q8JUX6
I	534	ASP	-	expression tag	UNP Q8JUX6
I	535	HIS	-	expression tag	UNP Q8JUX6
I	536	ASP	-	expression tag	UNP Q8JUX6
I	537	GLY	-	expression tag	UNP Q8JUX6
I	538	ASP	-	expression tag	UNP Q8JUX6
I	539	TYR	-	expression tag	UNP Q8JUX6
I	540	LYS	-	expression tag	UNP Q8JUX6
I	541	ASP	-	expression tag	UNP Q8JUX6
I	542	HIS	-	expression tag	UNP Q8JUX6
I	543	ASP	-	expression tag	UNP Q8JUX6
I	544	ILE	-	expression tag	UNP Q8JUX6
I	545	ASP	-	expression tag	UNP Q8JUX6
I	546	TYR	-	expression tag	UNP Q8JUX6
I	547	LYS	-	expression tag	UNP Q8JUX6
I	548	ASP	-	expression tag	UNP Q8JUX6
I	549	ASP	-	expression tag	UNP Q8JUX6
I	550	ASP	-	expression tag	UNP Q8JUX6
I	551	ASP	-	expression tag	UNP Q8JUX6
I	552	LYS	-	expression tag	UNP Q8JUX6
J	517	GLY	-	expression tag	UNP Q8JUX6
J	518	GLY	-	expression tag	UNP Q8JUX6
J	519	GLY	-	expression tag	UNP Q8JUX6
J	520	GLY	-	expression tag	UNP Q8JUX6
J	521	SER	-	expression tag	UNP Q8JUX6
J	522	TRP	-	expression tag	UNP Q8JUX6
J	523	SER	-	expression tag	UNP Q8JUX6
J	524	HIS	-	expression tag	UNP Q8JUX6
J	525	PRO	-	expression tag	UNP Q8JUX6
J	526	GLN	-	expression tag	UNP Q8JUX6
J	527	PHE	-	expression tag	UNP Q8JUX6
J	528	GLU	-	expression tag	UNP Q8JUX6
J	529	LYS	-	expression tag	UNP Q8JUX6
J	530	MET	-	expression tag	UNP Q8JUX6
J	531	ASP	-	expression tag	UNP Q8JUX6
J	532	TYR	-	expression tag	UNP Q8JUX6
J	533	LYS	-	expression tag	UNP Q8JUX6
J	534	ASP	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	535	HIS	-	expression tag	UNP Q8JUX6
J	536	ASP	-	expression tag	UNP Q8JUX6
J	537	GLY	-	expression tag	UNP Q8JUX6
J	538	ASP	-	expression tag	UNP Q8JUX6
J	539	TYR	-	expression tag	UNP Q8JUX6
J	540	LYS	-	expression tag	UNP Q8JUX6
J	541	ASP	-	expression tag	UNP Q8JUX6
J	542	HIS	-	expression tag	UNP Q8JUX6
J	543	ASP	-	expression tag	UNP Q8JUX6
J	544	ILE	-	expression tag	UNP Q8JUX6
J	545	ASP	-	expression tag	UNP Q8JUX6
J	546	TYR	-	expression tag	UNP Q8JUX6
J	547	LYS	-	expression tag	UNP Q8JUX6
J	548	ASP	-	expression tag	UNP Q8JUX6
J	549	ASP	-	expression tag	UNP Q8JUX6
J	550	ASP	-	expression tag	UNP Q8JUX6
J	551	ASP	-	expression tag	UNP Q8JUX6
J	552	LYS	-	expression tag	UNP Q8JUX6
K	517	GLY	-	expression tag	UNP Q8JUX6
K	518	GLY	-	expression tag	UNP Q8JUX6
K	519	GLY	-	expression tag	UNP Q8JUX6
K	520	GLY	-	expression tag	UNP Q8JUX6
K	521	SER	-	expression tag	UNP Q8JUX6
K	522	TRP	-	expression tag	UNP Q8JUX6
K	523	SER	-	expression tag	UNP Q8JUX6
K	524	HIS	-	expression tag	UNP Q8JUX6
K	525	PRO	-	expression tag	UNP Q8JUX6
K	526	GLN	-	expression tag	UNP Q8JUX6
K	527	PHE	-	expression tag	UNP Q8JUX6
K	528	GLU	-	expression tag	UNP Q8JUX6
K	529	LYS	-	expression tag	UNP Q8JUX6
K	530	MET	-	expression tag	UNP Q8JUX6
K	531	ASP	-	expression tag	UNP Q8JUX6
K	532	TYR	-	expression tag	UNP Q8JUX6
K	533	LYS	-	expression tag	UNP Q8JUX6
K	534	ASP	-	expression tag	UNP Q8JUX6
K	535	HIS	-	expression tag	UNP Q8JUX6
K	536	ASP	-	expression tag	UNP Q8JUX6
K	537	GLY	-	expression tag	UNP Q8JUX6
K	538	ASP	-	expression tag	UNP Q8JUX6
K	539	TYR	-	expression tag	UNP Q8JUX6
K	540	LYS	-	expression tag	UNP Q8JUX6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	541	ASP	-	expression tag	UNP Q8JUX6
K	542	HIS	-	expression tag	UNP Q8JUX6
K	543	ASP	-	expression tag	UNP Q8JUX6
K	544	ILE	-	expression tag	UNP Q8JUX6
K	545	ASP	-	expression tag	UNP Q8JUX6
K	546	TYR	-	expression tag	UNP Q8JUX6
K	547	LYS	-	expression tag	UNP Q8JUX6
K	548	ASP	-	expression tag	UNP Q8JUX6
K	549	ASP	-	expression tag	UNP Q8JUX6
K	550	ASP	-	expression tag	UNP Q8JUX6
K	551	ASP	-	expression tag	UNP Q8JUX6
K	552	LYS	-	expression tag	UNP Q8JUX6
L	517	GLY	-	expression tag	UNP Q8JUX6
L	518	GLY	-	expression tag	UNP Q8JUX6
L	519	GLY	-	expression tag	UNP Q8JUX6
L	520	GLY	-	expression tag	UNP Q8JUX6
L	521	SER	-	expression tag	UNP Q8JUX6
L	522	TRP	-	expression tag	UNP Q8JUX6
L	523	SER	-	expression tag	UNP Q8JUX6
L	524	HIS	-	expression tag	UNP Q8JUX6
L	525	PRO	-	expression tag	UNP Q8JUX6
L	526	GLN	-	expression tag	UNP Q8JUX6
L	527	PHE	-	expression tag	UNP Q8JUX6
L	528	GLU	-	expression tag	UNP Q8JUX6
L	529	LYS	-	expression tag	UNP Q8JUX6
L	530	MET	-	expression tag	UNP Q8JUX6
L	531	ASP	-	expression tag	UNP Q8JUX6
L	532	TYR	-	expression tag	UNP Q8JUX6
L	533	LYS	-	expression tag	UNP Q8JUX6
L	534	ASP	-	expression tag	UNP Q8JUX6
L	535	HIS	-	expression tag	UNP Q8JUX6
L	536	ASP	-	expression tag	UNP Q8JUX6
L	537	GLY	-	expression tag	UNP Q8JUX6
L	538	ASP	-	expression tag	UNP Q8JUX6
L	539	TYR	-	expression tag	UNP Q8JUX6
L	540	LYS	-	expression tag	UNP Q8JUX6
L	541	ASP	-	expression tag	UNP Q8JUX6
L	542	HIS	-	expression tag	UNP Q8JUX6
L	543	ASP	-	expression tag	UNP Q8JUX6
L	544	ILE	-	expression tag	UNP Q8JUX6
L	545	ASP	-	expression tag	UNP Q8JUX6
L	546	TYR	-	expression tag	UNP Q8JUX6

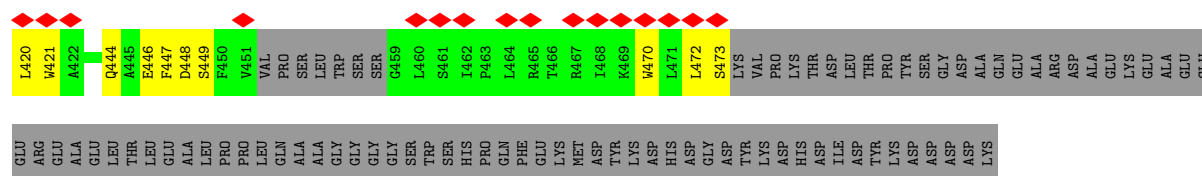
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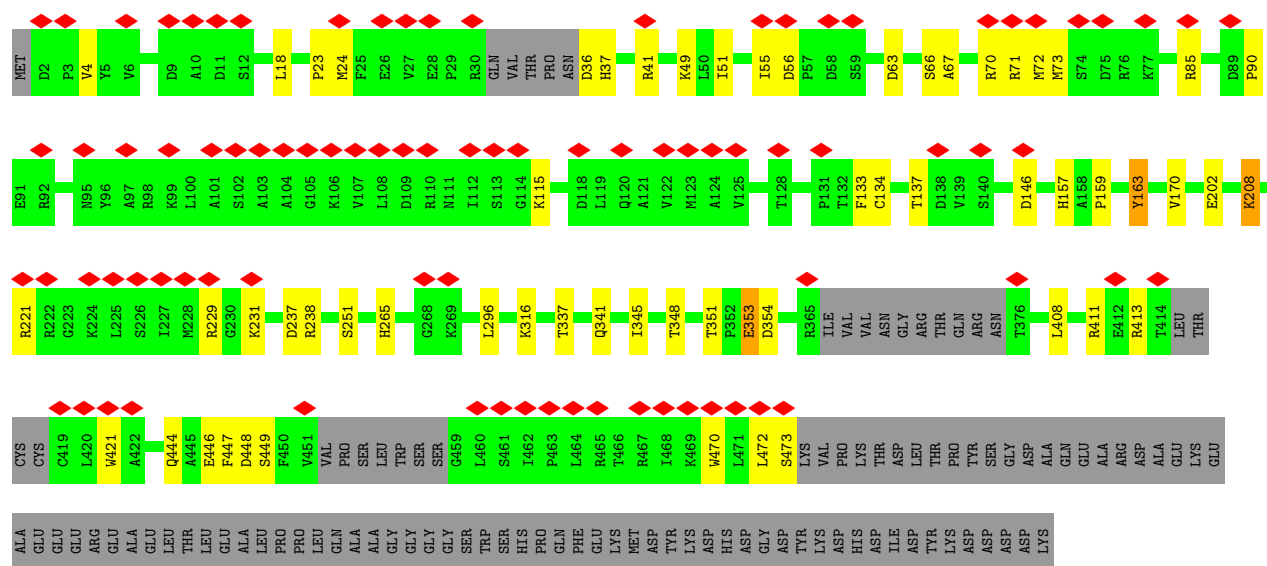
Chain	Residue	Modelled	Actual	Comment	Reference
L	547	LYS	-	expression tag	UNP Q8JUX6
L	548	ASP	-	expression tag	UNP Q8JUX6
L	549	ASP	-	expression tag	UNP Q8JUX6
L	550	ASP	-	expression tag	UNP Q8JUX6
L	551	ASP	-	expression tag	UNP Q8JUX6
L	552	LYS	-	expression tag	UNP Q8JUX6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

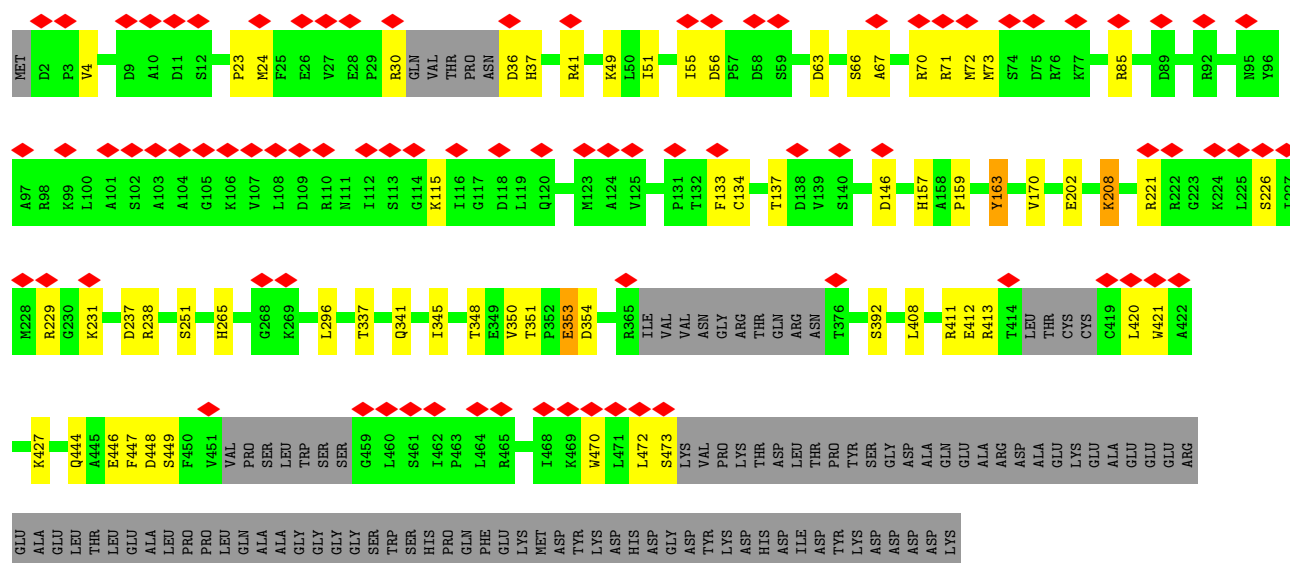
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Zn 1 1	0
2	B	1	Total Zn 1 1	0
2	C	1	Total Zn 1 1	0
2	D	1	Total Zn 1 1	0
2	E	1	Total Zn 1 1	0
2	F	1	Total Zn 1 1	0
2	G	1	Total Zn 1 1	0
2	H	1	Total Zn 1 1	0
2	I	1	Total Zn 1 1	0
2	J	1	Total Zn 1 1	0
2	K	1	Total Zn 1 1	0
2	L	1	Total Zn 1 1	0



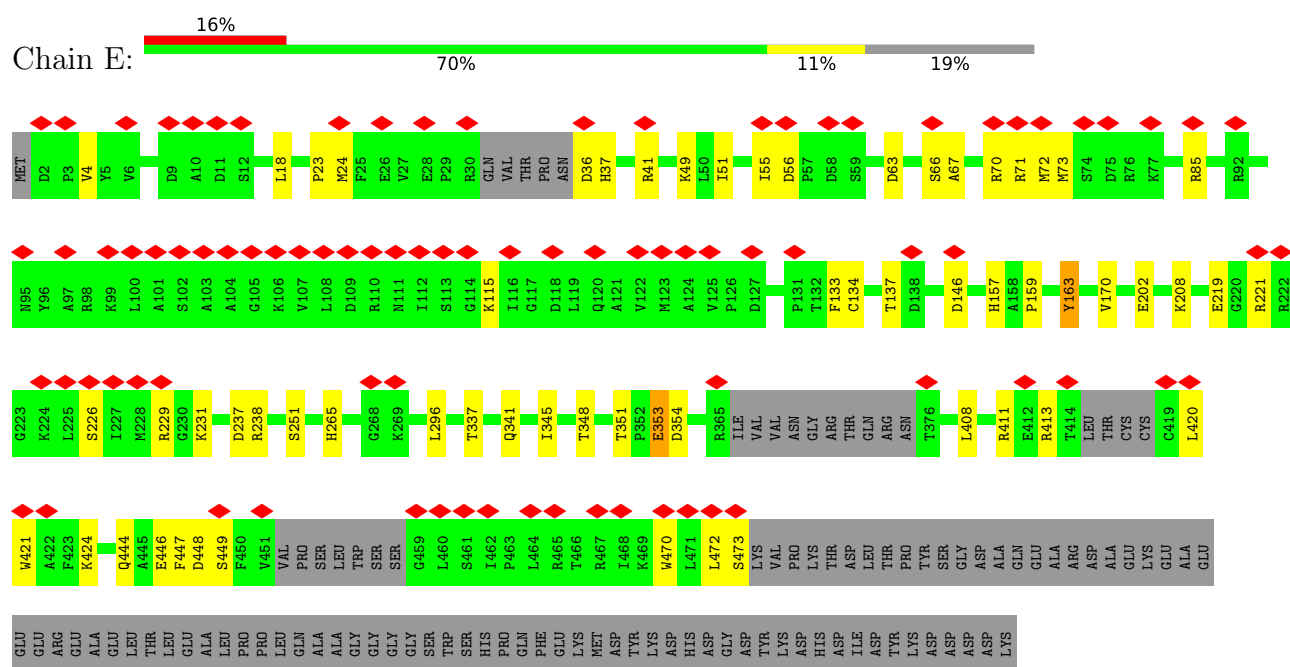
• Molecule 1: Nonstructural Protein 1



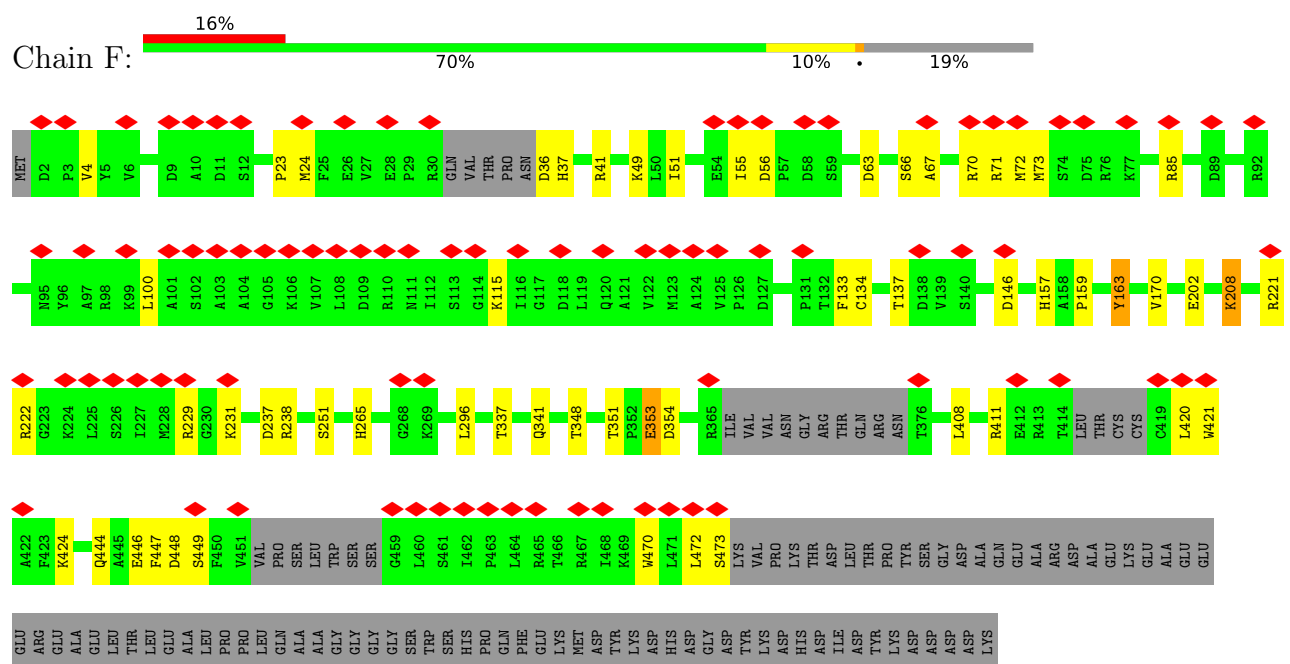
• Molecule 1: Nonstructural Protein 1



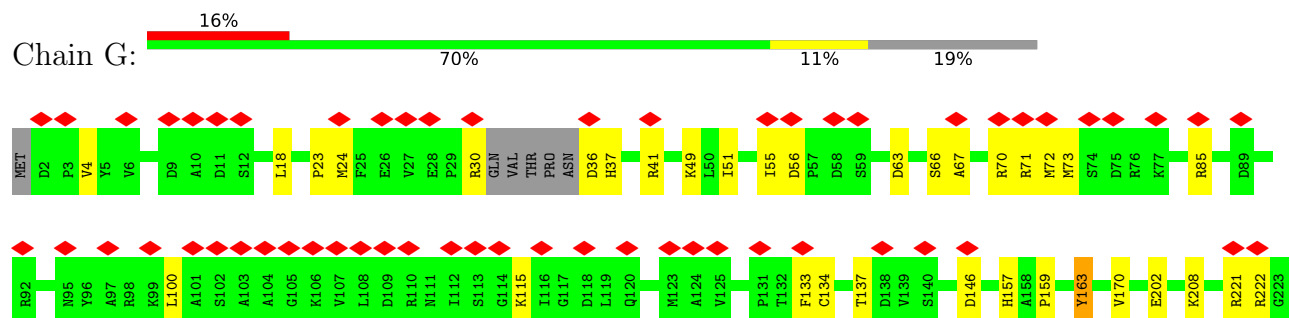
• Molecule 1: Nonstructural Protein 1

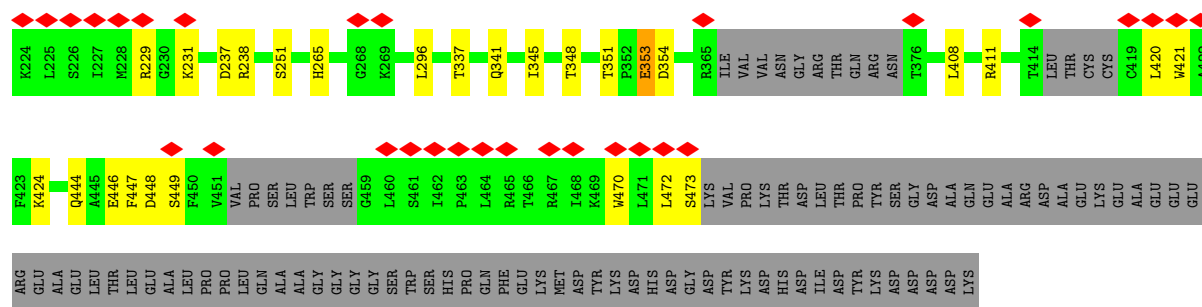


- Molecule 1: Nonstructural Protein 1

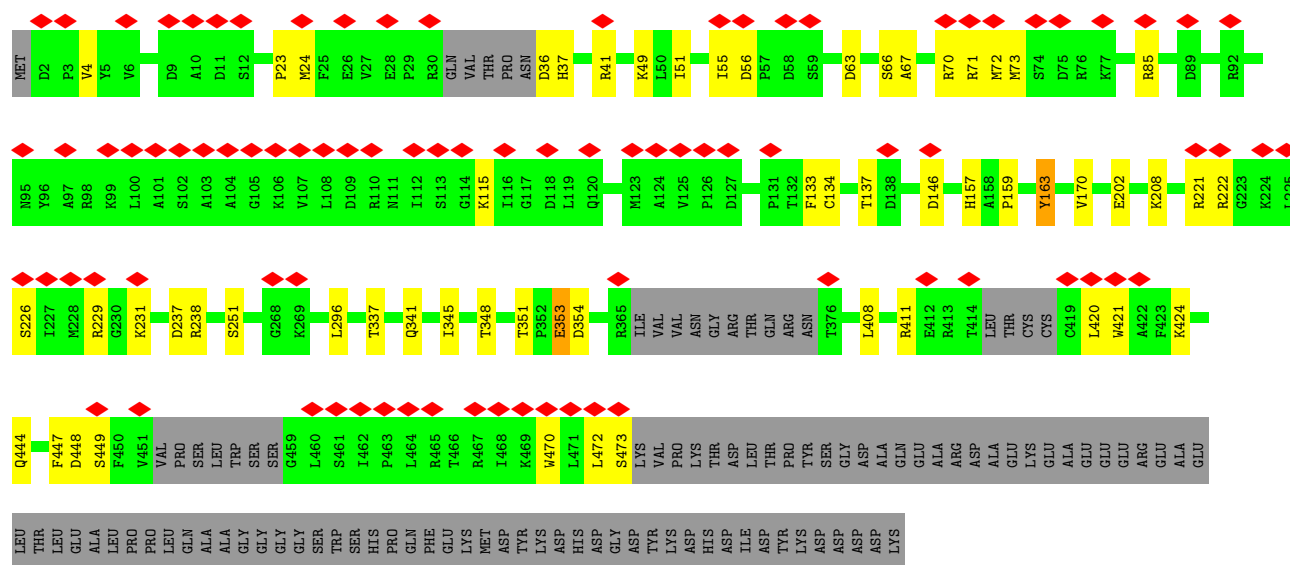


- Molecule 1: Nonstructural Protein 1

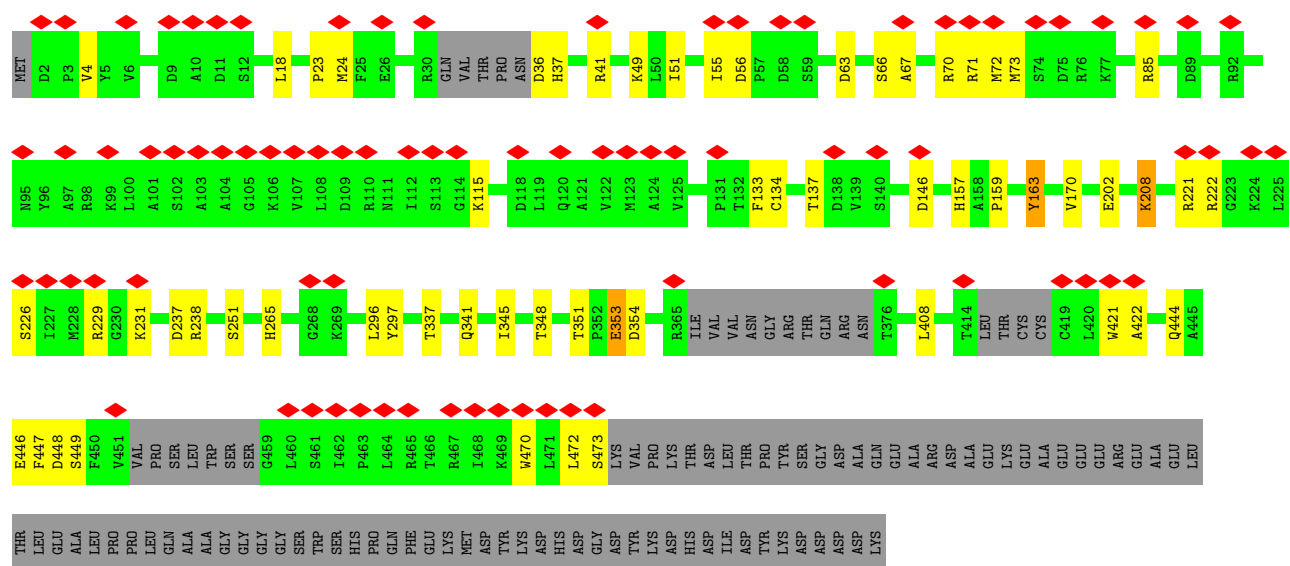




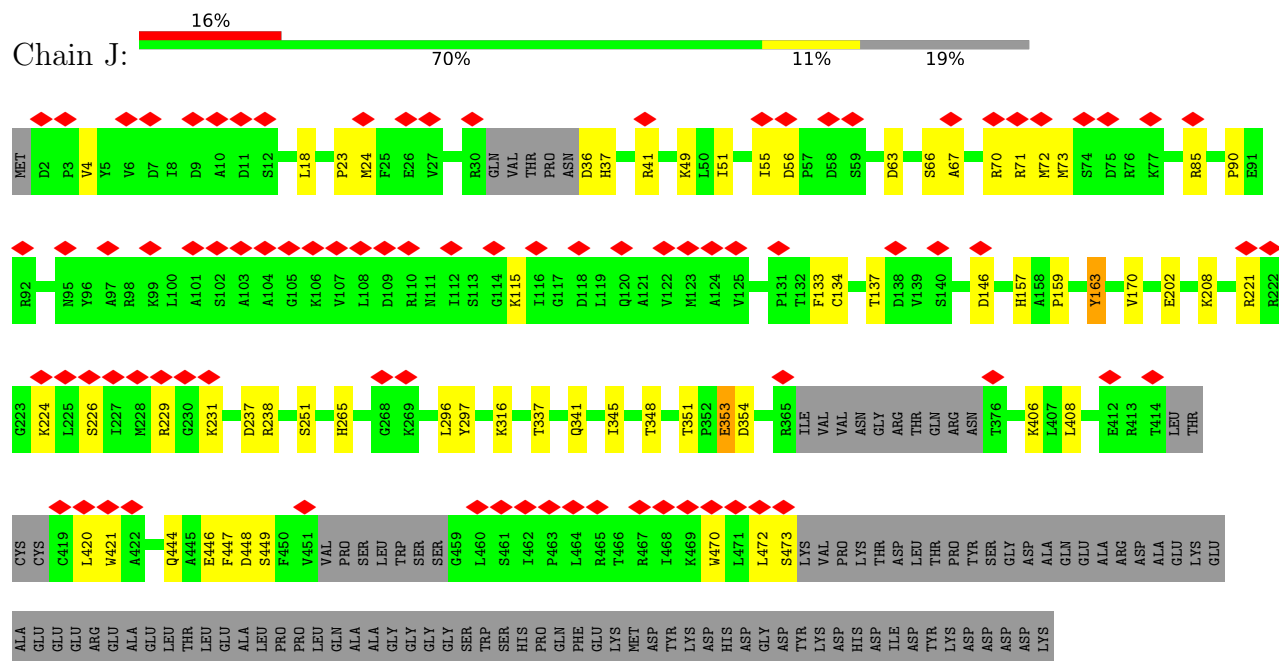
• Molecule 1: Nonstructural Protein 1



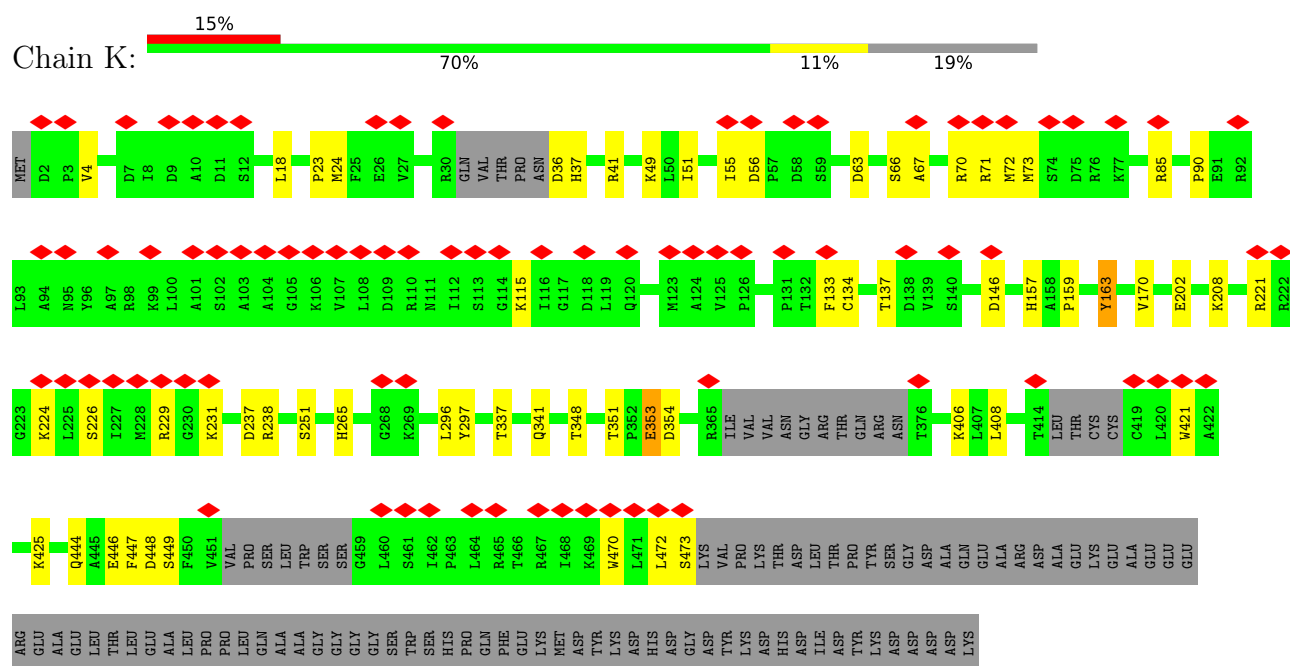
• Molecule 1: Nonstructural Protein 1



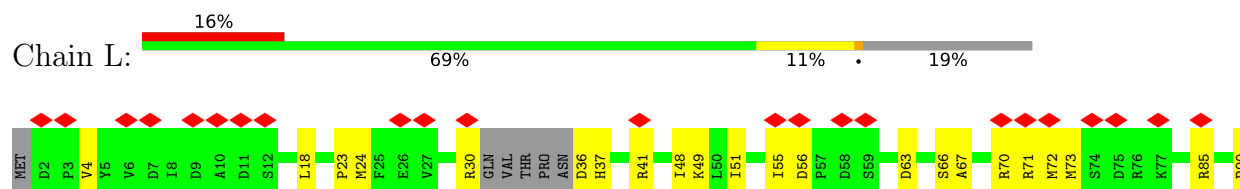
- Molecule 1: Nonstructural Protein 1

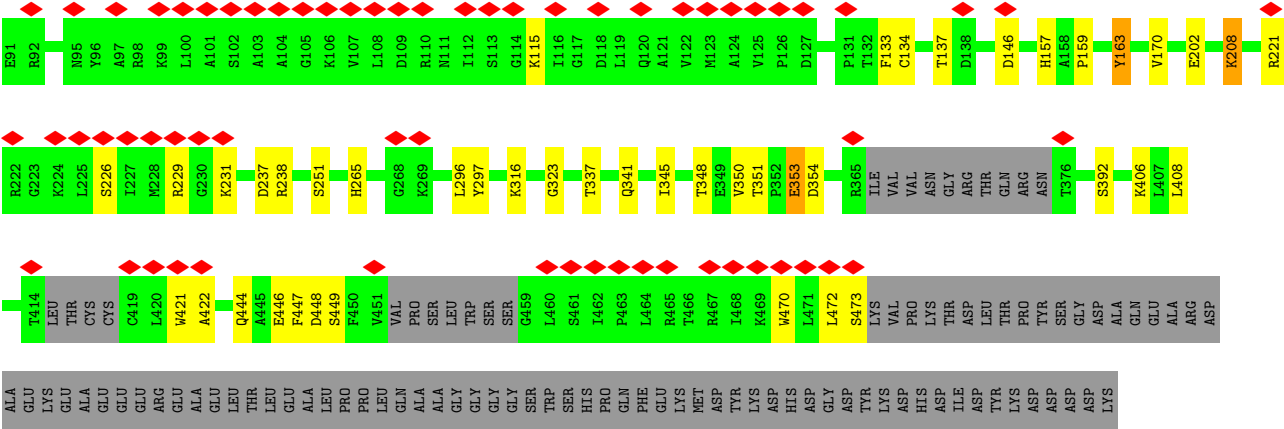


- Molecule 1: Nonstructural Protein 1



- Molecule 1: Nonstructural Protein 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	269498	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.149	Depositor
Minimum map value	-1.874	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	411.84, 411.84, 411.84	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.858, 0.858, 0.858	Depositor

5 Model quality

5.1 Standard geometry

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	0.22	0/3546	0.44	0/4802
1	B	0.22	0/3546	0.44	0/4802
1	C	0.22	0/3546	0.44	0/4802
1	D	0.22	0/3546	0.44	0/4802
1	E	0.22	0/3546	0.44	0/4802
1	F	0.22	0/3546	0.44	0/4802
1	G	0.22	0/3546	0.44	0/4802
1	H	0.22	0/3546	0.44	0/4802
1	I	0.22	0/3546	0.44	0/4802
1	J	0.22	0/3546	0.44	0/4802
1	K	0.22	0/3546	0.44	0/4802
1	L	0.22	0/3546	0.44	0/4802
All	All	0.22	0/42552	0.44	0/57624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3474	0	3437	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3474	0	3437	41	0
1	C	3474	0	3437	42	0
1	D	3474	0	3437	48	0
1	E	3474	0	3437	45	0
1	F	3474	0	3437	41	0
1	G	3474	0	3437	44	0
1	H	3474	0	3437	41	0
1	I	3474	0	3437	41	0
1	J	3474	0	3437	42	0
1	K	3474	0	3437	41	0
1	L	3474	0	3437	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
All	All	41700	0	41244	465	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:411:ARG:O	1:H:231:LYS:HD2	1.95	0.66
1:E:353:GLU:N	1:E:353:GLU:OE1	2.29	0.66
1:F:353:GLU:OE1	1:F:353:GLU:N	2.29	0.66
1:D:353:GLU:N	1:D:353:GLU:OE1	2.29	0.66
1:L:353:GLU:N	1:L:353:GLU:OE1	2.29	0.66
1:G:353:GLU:N	1:G:353:GLU:OE1	2.29	0.66
1:K:353:GLU:OE1	1:K:353:GLU:N	2.29	0.66
1:I:353:GLU:N	1:I:353:GLU:OE1	2.29	0.65
1:J:353:GLU:N	1:J:353:GLU:OE1	2.29	0.65
1:H:353:GLU:OE1	1:H:353:GLU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:GLU:OE1	1:C:353:GLU:N	2.29	0.65
1:A:353:GLU:OE1	1:A:353:GLU:N	2.29	0.65
1:D:411:ARG:O	1:E:231:LYS:HD2	1.97	0.65
1:B:353:GLU:N	1:B:353:GLU:OE1	2.29	0.65
1:G:421:TRP:O	1:H:226:SER:N	2.27	0.63
1:I:421:TRP:O	1:K:226:SER:N	2.34	0.61
1:D:36:ASP:O	1:D:37:HIS:ND1	2.30	0.61
1:K:36:ASP:O	1:K:37:HIS:ND1	2.30	0.61
1:C:36:ASP:O	1:C:37:HIS:ND1	2.30	0.60
1:L:36:ASP:O	1:L:37:HIS:ND1	2.30	0.60
1:I:36:ASP:O	1:I:37:HIS:ND1	2.30	0.59
1:L:353:GLU:H	1:L:353:GLU:CD	2.11	0.59
1:F:353:GLU:CD	1:F:353:GLU:H	2.11	0.59
1:I:353:GLU:CD	1:I:353:GLU:H	2.11	0.59
1:A:353:GLU:CD	1:A:353:GLU:H	2.11	0.59
1:B:36:ASP:O	1:B:37:HIS:ND1	2.30	0.59
1:B:353:GLU:H	1:B:353:GLU:CD	2.11	0.59
1:G:353:GLU:H	1:G:353:GLU:CD	2.11	0.58
1:D:353:GLU:CD	1:D:353:GLU:H	2.11	0.58
1:D:421:TRP:O	1:E:226:SER:N	2.31	0.58
1:E:353:GLU:H	1:E:353:GLU:CD	2.11	0.58
1:C:353:GLU:CD	1:C:353:GLU:H	2.11	0.58
1:H:36:ASP:O	1:H:37:HIS:ND1	2.30	0.58
1:J:226:SER:N	1:L:421:TRP:O	2.36	0.58
1:J:353:GLU:H	1:J:353:GLU:CD	2.11	0.57
1:H:353:GLU:CD	1:H:353:GLU:H	2.11	0.57
1:K:353:GLU:CD	1:K:353:GLU:H	2.11	0.57
1:H:421:TRP:O	1:I:226:SER:N	2.36	0.57
1:G:470:TRP:O	1:G:473:SER:OG	2.21	0.57
1:G:36:ASP:O	1:G:37:HIS:ND1	2.30	0.57
1:E:411:ARG:O	1:F:231:LYS:HD2	2.04	0.56
1:A:36:ASP:O	1:A:37:HIS:ND1	2.30	0.56
1:A:470:TRP:O	1:A:473:SER:OG	2.21	0.56
1:C:470:TRP:O	1:C:473:SER:OG	2.21	0.56
1:F:470:TRP:O	1:F:473:SER:OG	2.21	0.56
1:D:411:ARG:HB2	1:E:231:LYS:HA	1.87	0.55
1:I:237:ASP:OD2	1:I:251:SER:OG	2.25	0.55
1:F:36:ASP:O	1:F:37:HIS:ND1	2.30	0.55
1:J:470:TRP:O	1:J:473:SER:OG	2.21	0.55
1:L:237:ASP:OD2	1:L:251:SER:OG	2.25	0.55
1:B:470:TRP:O	1:B:473:SER:OG	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:TRP:O	1:E:473:SER:OG	2.21	0.54
1:B:237:ASP:OD2	1:B:251:SER:OG	2.25	0.54
1:A:237:ASP:OD2	1:A:251:SER:OG	2.25	0.54
1:C:237:ASP:OD2	1:C:251:SER:OG	2.25	0.54
1:E:36:ASP:O	1:E:37:HIS:ND1	2.30	0.54
1:E:411:ARG:HB2	1:F:231:LYS:HA	1.90	0.54
1:H:237:ASP:OD2	1:H:251:SER:OG	2.25	0.54
1:D:470:TRP:O	1:D:473:SER:OG	2.21	0.53
1:J:41:ARG:HB3	1:J:41:ARG:CZ	2.39	0.53
1:L:41:ARG:HB3	1:L:41:ARG:CZ	2.39	0.53
1:E:237:ASP:OD2	1:E:251:SER:OG	2.25	0.53
1:D:237:ASP:OD2	1:D:251:SER:OG	2.25	0.53
1:B:72:MET:O	1:B:115:LYS:NZ	2.42	0.53
1:F:237:ASP:OD2	1:F:251:SER:OG	2.25	0.53
1:L:470:TRP:O	1:L:473:SER:OG	2.21	0.53
1:A:72:MET:O	1:A:115:LYS:NZ	2.42	0.53
1:G:146:ASP:HA	1:G:170:VAL:HA	1.91	0.53
1:K:470:TRP:O	1:K:473:SER:OG	2.21	0.53
1:J:36:ASP:O	1:J:37:HIS:ND1	2.30	0.53
1:K:72:MET:O	1:K:115:LYS:NZ	2.42	0.53
1:K:146:ASP:HA	1:K:170:VAL:HA	1.91	0.53
1:K:297:TYR:OH	1:L:90:PRO:HG2	2.09	0.53
1:H:67:ALA:O	1:H:70:ARG:HG2	2.09	0.52
1:I:67:ALA:O	1:I:70:ARG:HG2	2.09	0.52
1:I:146:ASP:HA	1:I:170:VAL:HA	1.91	0.52
1:C:72:MET:O	1:C:115:LYS:NZ	2.42	0.52
1:K:41:ARG:HB3	1:K:41:ARG:CZ	2.39	0.52
1:K:406:LYS:O	1:L:316:LYS:NZ	2.41	0.52
1:L:72:MET:O	1:L:115:LYS:NZ	2.42	0.52
1:G:421:TRP:HB2	1:H:226:SER:O	2.09	0.52
1:H:72:MET:HE2	1:H:73:MET:HG2	1.92	0.52
1:K:237:ASP:OD2	1:K:251:SER:OG	2.25	0.52
1:B:41:ARG:CZ	1:B:41:ARG:HB3	2.38	0.52
1:E:229:ARG:NE	1:E:231:LYS:HG3	2.25	0.52
1:G:67:ALA:O	1:G:70:ARG:HG2	2.09	0.52
1:I:72:MET:O	1:I:115:LYS:NZ	2.42	0.52
1:H:229:ARG:NE	1:H:231:LYS:HG3	2.25	0.52
1:K:67:ALA:O	1:K:70:ARG:HG2	2.09	0.52
1:D:229:ARG:NE	1:D:231:LYS:HG3	2.25	0.52
1:F:229:ARG:NE	1:F:231:LYS:HG3	2.25	0.52
1:J:72:MET:O	1:J:115:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:MET:HE2	1:K:73:MET:HG2	1.92	0.52
1:B:146:ASP:HA	1:B:170:VAL:HA	1.91	0.52
1:E:146:ASP:HA	1:E:170:VAL:HA	1.91	0.52
1:F:146:ASP:HA	1:F:170:VAL:HA	1.91	0.52
1:G:229:ARG:NE	1:G:231:LYS:HG3	2.25	0.52
1:L:72:MET:HE2	1:L:73:MET:HG2	1.92	0.52
1:B:67:ALA:O	1:B:70:ARG:HG2	2.09	0.52
1:C:67:ALA:O	1:C:70:ARG:HG2	2.09	0.52
1:H:146:ASP:HA	1:H:170:VAL:HA	1.91	0.52
1:J:90:PRO:HG2	1:L:297:TYR:OH	2.09	0.52
1:L:67:ALA:O	1:L:70:ARG:HG2	2.09	0.52
1:C:146:ASP:HA	1:C:170:VAL:HA	1.91	0.52
1:F:41:ARG:CZ	1:F:41:ARG:HB3	2.39	0.52
1:G:237:ASP:OD2	1:G:251:SER:OG	2.24	0.52
1:J:146:ASP:HA	1:J:170:VAL:HA	1.91	0.52
1:K:229:ARG:NE	1:K:231:LYS:HG3	2.25	0.52
1:A:146:ASP:HA	1:A:170:VAL:HA	1.91	0.52
1:G:41:ARG:CZ	1:G:41:ARG:HB3	2.38	0.52
1:I:470:TRP:O	1:I:473:SER:OG	2.21	0.52
1:J:229:ARG:NE	1:J:231:LYS:HG3	2.25	0.52
1:L:229:ARG:NE	1:L:231:LYS:HG3	2.25	0.52
1:E:72:MET:O	1:E:115:LYS:NZ	2.42	0.51
1:D:67:ALA:O	1:D:70:ARG:HG2	2.09	0.51
1:E:41:ARG:CZ	1:E:41:ARG:HB3	2.39	0.51
1:F:67:ALA:O	1:F:70:ARG:HG2	2.09	0.51
1:F:72:MET:O	1:F:115:LYS:NZ	2.42	0.51
1:L:146:ASP:HA	1:L:170:VAL:HA	1.91	0.51
1:A:229:ARG:NE	1:A:231:LYS:HG3	2.25	0.51
1:D:72:MET:O	1:D:115:LYS:NZ	2.42	0.51
1:G:72:MET:HE2	1:G:73:MET:HG2	1.92	0.51
1:A:72:MET:HE2	1:A:73:MET:HG2	1.92	0.51
1:D:146:ASP:HA	1:D:170:VAL:HA	1.91	0.51
1:I:229:ARG:NE	1:I:231:LYS:HG3	2.25	0.51
1:J:67:ALA:O	1:J:70:ARG:HG2	2.09	0.51
1:A:67:ALA:O	1:A:70:ARG:HG2	2.09	0.51
1:I:72:MET:HE2	1:I:73:MET:HG2	1.92	0.51
1:C:229:ARG:NE	1:C:231:LYS:HG3	2.25	0.51
1:E:67:ALA:O	1:E:70:ARG:HG2	2.09	0.51
1:E:72:MET:HE2	1:E:73:MET:HG2	1.92	0.51
1:G:72:MET:O	1:G:115:LYS:NZ	2.42	0.51
1:H:41:ARG:HB3	1:H:41:ARG:CZ	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:MET:O	1:H:115:LYS:NZ	2.42	0.51
1:J:237:ASP:OD2	1:J:251:SER:OG	2.25	0.51
1:F:72:MET:HE2	1:F:73:MET:HG2	1.92	0.51
1:B:72:MET:HE2	1:B:73:MET:HG2	1.92	0.51
1:C:72:MET:HE2	1:C:73:MET:HG2	1.92	0.51
1:D:72:MET:HE2	1:D:73:MET:HG2	1.92	0.51
1:B:229:ARG:NE	1:B:231:LYS:HG3	2.25	0.50
1:A:41:ARG:HB3	1:A:41:ARG:CZ	2.39	0.50
1:A:90:PRO:HG2	1:J:297:TYR:OH	2.11	0.50
1:D:41:ARG:CZ	1:D:41:ARG:HB3	2.38	0.50
1:H:470:TRP:O	1:H:473:SER:OG	2.21	0.50
1:J:72:MET:HE2	1:J:73:MET:HG2	1.92	0.50
1:C:411:ARG:HB2	1:D:231:LYS:HA	1.93	0.50
1:I:41:ARG:HB3	1:I:41:ARG:CZ	2.39	0.49
1:A:421:TRP:O	1:B:226:SER:N	2.42	0.49
1:H:70:ARG:HG3	1:H:71:ARG:HG2	1.95	0.49
1:D:70:ARG:HG3	1:D:71:ARG:HG2	1.95	0.49
1:L:51:ILE:O	1:L:55:ILE:HG12	2.13	0.49
1:D:51:ILE:O	1:D:55:ILE:HG12	2.13	0.49
1:E:70:ARG:HG3	1:E:71:ARG:HG2	1.95	0.49
1:F:424:LYS:HE3	1:G:222:ARG:HE	1.78	0.49
1:G:70:ARG:HG3	1:G:71:ARG:HG2	1.95	0.49
1:G:157:HIS:CE1	1:G:159:PRO:HG2	2.48	0.49
1:B:51:ILE:O	1:B:55:ILE:HG12	2.13	0.49
1:C:413:ARG:HB2	1:D:231:LYS:HD3	1.94	0.49
1:D:157:HIS:CE1	1:D:159:PRO:HG2	2.48	0.49
1:H:157:HIS:CE1	1:H:159:PRO:HG2	2.48	0.49
1:J:51:ILE:O	1:J:55:ILE:HG12	2.13	0.49
1:A:51:ILE:O	1:A:55:ILE:HG12	2.13	0.48
1:A:70:ARG:HG3	1:A:71:ARG:HG2	1.95	0.48
1:B:157:HIS:CE1	1:B:159:PRO:HG2	2.48	0.48
1:C:157:HIS:CE1	1:C:159:PRO:HG2	2.48	0.48
1:K:70:ARG:HG3	1:K:71:ARG:HG2	1.95	0.48
1:F:157:HIS:CE1	1:F:159:PRO:HG2	2.48	0.48
1:I:157:HIS:CE1	1:I:159:PRO:HG2	2.48	0.48
1:L:70:ARG:HG3	1:L:71:ARG:HG2	1.95	0.48
1:I:297:TYR:OH	1:K:90:PRO:HG2	2.13	0.48
1:B:70:ARG:HG3	1:B:71:ARG:HG2	1.95	0.48
1:K:51:ILE:O	1:K:55:ILE:HG12	2.13	0.48
1:A:157:HIS:CE1	1:A:159:PRO:HG2	2.48	0.48
1:C:411:ARG:O	1:D:231:LYS:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:ILE:O	1:I:55:ILE:HG12	2.13	0.48
1:A:226:SER:N	1:J:421:TRP:O	2.45	0.48
1:H:51:ILE:O	1:H:55:ILE:HG12	2.13	0.48
1:H:163:TYR:C	1:H:163:TYR:CD2	2.92	0.48
1:K:157:HIS:CE1	1:K:159:PRO:HG2	2.48	0.48
1:L:157:HIS:CE1	1:L:159:PRO:HG2	2.48	0.48
1:C:70:ARG:HG3	1:C:71:ARG:HG2	1.95	0.48
1:E:157:HIS:CE1	1:E:159:PRO:HG2	2.48	0.48
1:F:51:ILE:O	1:F:55:ILE:HG12	2.13	0.48
1:G:163:TYR:C	1:G:163:TYR:CD2	2.92	0.48
1:C:51:ILE:O	1:C:55:ILE:HG12	2.13	0.48
1:F:411:ARG:O	1:G:231:LYS:HD2	2.13	0.48
1:I:163:TYR:C	1:I:163:TYR:CD2	2.92	0.48
1:A:316:LYS:NZ	1:J:406:LYS:O	2.46	0.47
1:C:41:ARG:HB3	1:C:41:ARG:CZ	2.39	0.47
1:G:411:ARG:HB2	1:H:231:LYS:HA	1.95	0.47
1:I:70:ARG:HG3	1:I:71:ARG:HG2	1.95	0.47
1:K:163:TYR:C	1:K:163:TYR:CD2	2.92	0.47
1:G:51:ILE:O	1:G:55:ILE:HG12	2.13	0.47
1:J:157:HIS:CE1	1:J:159:PRO:HG2	2.48	0.47
1:F:163:TYR:C	1:F:163:TYR:CD2	2.92	0.47
1:D:163:TYR:C	1:D:163:TYR:CD2	2.92	0.47
1:D:421:TRP:HB2	1:E:226:SER:O	2.14	0.47
1:F:70:ARG:HG3	1:F:71:ARG:HG2	1.95	0.47
1:C:163:TYR:C	1:C:163:TYR:CD2	2.92	0.47
1:D:413:ARG:H	1:E:231:LYS:CD	2.26	0.47
1:E:51:ILE:O	1:E:55:ILE:HG12	2.13	0.47
1:B:163:TYR:C	1:B:163:TYR:CD2	2.92	0.47
1:E:163:TYR:C	1:E:163:TYR:CD2	2.92	0.47
1:J:70:ARG:HG3	1:J:71:ARG:HG2	1.95	0.47
1:A:163:TYR:C	1:A:163:TYR:CD2	2.92	0.47
1:L:163:TYR:C	1:L:163:TYR:CD2	2.92	0.47
1:A:229:ARG:HG3	1:A:231:LYS:HG2	1.97	0.47
1:D:229:ARG:HG3	1:D:231:LYS:HG2	1.97	0.47
1:H:24:MET:SD	1:H:24:MET:N	2.87	0.47
1:K:353:GLU:N	1:K:353:GLU:CD	2.73	0.47
1:E:229:ARG:HG3	1:E:231:LYS:HG2	1.97	0.46
1:J:316:LYS:NZ	1:L:406:LYS:O	2.48	0.46
1:J:163:TYR:C	1:J:163:TYR:CD2	2.92	0.46
1:K:229:ARG:HG3	1:K:231:LYS:HG2	1.97	0.46
1:H:353:GLU:N	1:H:353:GLU:CD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:229:ARG:HG3	1:J:231:LYS:HG2	1.98	0.46
1:A:353:GLU:N	1:A:353:GLU:CD	2.73	0.46
1:A:297:TYR:OH	1:B:90:PRO:HG2	2.15	0.46
1:D:208:LYS:HB3	1:D:208:LYS:HE3	1.76	0.46
1:G:229:ARG:HG3	1:G:231:LYS:HG2	1.97	0.46
1:K:421:TRP:O	1:L:226:SER:N	2.47	0.46
1:B:229:ARG:HG3	1:B:231:LYS:HG2	1.98	0.46
1:H:63:ASP:HB3	1:H:66:SER:HB2	1.98	0.46
1:I:448:ASP:OD2	1:I:449:SER:N	2.49	0.46
1:J:63:ASP:HB3	1:J:66:SER:HB2	1.98	0.46
1:L:63:ASP:HB3	1:L:66:SER:HB2	1.98	0.46
1:L:353:GLU:N	1:L:353:GLU:CD	2.73	0.46
1:G:63:ASP:HB3	1:G:66:SER:HB2	1.98	0.46
1:H:448:ASP:OD2	1:H:449:SER:N	2.49	0.46
1:I:63:ASP:HB3	1:I:66:SER:HB2	1.98	0.46
1:C:229:ARG:HG3	1:C:231:LYS:HG2	1.98	0.46
1:G:448:ASP:OD2	1:G:449:SER:N	2.49	0.46
1:H:411:ARG:O	1:I:231:LYS:HD2	2.16	0.46
1:K:63:ASP:HB3	1:K:66:SER:HB2	1.98	0.46
1:A:63:ASP:HB3	1:A:66:SER:HB2	1.98	0.45
1:A:448:ASP:OD2	1:A:449:SER:N	2.49	0.45
1:C:448:ASP:OD2	1:C:449:SER:N	2.49	0.45
1:D:448:ASP:OD2	1:D:449:SER:N	2.49	0.45
1:F:448:ASP:OD2	1:F:449:SER:N	2.49	0.45
1:A:4:VAL:HB	1:A:49:LYS:NZ	2.32	0.45
1:E:448:ASP:OD2	1:E:449:SER:N	2.49	0.45
1:F:353:GLU:N	1:F:353:GLU:CD	2.73	0.45
1:J:448:ASP:OD2	1:J:449:SER:N	2.49	0.45
1:L:229:ARG:HG3	1:L:231:LYS:HG2	1.97	0.45
1:A:296:LEU:HD23	1:A:296:LEU:H	1.82	0.45
1:B:63:ASP:HB3	1:B:66:SER:HB2	1.98	0.45
1:H:229:ARG:HG3	1:H:231:LYS:HG2	1.98	0.45
1:I:229:ARG:HG3	1:I:231:LYS:HG2	1.97	0.45
1:J:4:VAL:HB	1:J:49:LYS:NZ	2.32	0.45
1:K:448:ASP:OD2	1:K:449:SER:N	2.49	0.45
1:B:4:VAL:HB	1:B:49:LYS:NZ	2.32	0.45
1:B:448:ASP:OD2	1:B:449:SER:N	2.49	0.45
1:C:63:ASP:HB3	1:C:66:SER:HB2	1.98	0.45
1:D:427:LYS:HB3	1:E:219:GLU:O	2.16	0.45
1:F:63:ASP:HB3	1:F:66:SER:HB2	1.98	0.45
1:F:208:LYS:HB3	1:F:208:LYS:HE3	1.76	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:LEU:HD23	1:F:296:LEU:H	1.82	0.45
1:H:296:LEU:HD23	1:H:296:LEU:H	1.82	0.45
1:B:296:LEU:H	1:B:296:LEU:HD23	1.82	0.45
1:B:297:TYR:OH	1:C:90:PRO:HG2	2.16	0.45
1:E:4:VAL:HB	1:E:49:LYS:NZ	2.32	0.45
1:F:229:ARG:HG3	1:F:231:LYS:HG2	1.97	0.45
1:L:448:ASP:OD2	1:L:449:SER:N	2.49	0.45
1:D:296:LEU:H	1:D:296:LEU:HD23	1.82	0.45
1:F:411:ARG:HB2	1:G:231:LYS:HA	1.99	0.45
1:D:63:ASP:HB3	1:D:66:SER:HB2	1.98	0.45
1:E:63:ASP:HB3	1:E:66:SER:HB2	1.98	0.45
1:L:4:VAL:HB	1:L:49:LYS:NZ	2.32	0.45
1:C:4:VAL:HB	1:C:49:LYS:NZ	2.32	0.45
1:C:353:GLU:N	1:C:353:GLU:CD	2.73	0.45
1:D:353:GLU:N	1:D:353:GLU:CD	2.73	0.45
1:F:4:VAL:HB	1:F:49:LYS:NZ	2.32	0.45
1:F:163:TYR:C	1:F:163:TYR:HD2	2.25	0.45
1:G:163:TYR:C	1:G:163:TYR:HD2	2.25	0.45
1:H:4:VAL:HB	1:H:49:LYS:NZ	2.32	0.45
1:I:4:VAL:HB	1:I:49:LYS:NZ	2.32	0.45
1:K:296:LEU:H	1:K:296:LEU:HD23	1.82	0.45
1:D:4:VAL:HB	1:D:49:LYS:NZ	2.32	0.45
1:L:296:LEU:HD23	1:L:296:LEU:H	1.82	0.45
1:E:353:GLU:N	1:E:353:GLU:CD	2.73	0.44
1:G:296:LEU:HD23	1:G:296:LEU:H	1.82	0.44
1:J:296:LEU:HD23	1:J:296:LEU:H	1.82	0.44
1:D:133:PHE:HD1	1:D:134:CYS:N	2.16	0.44
1:F:56:ASP:N	1:F:56:ASP:OD1	2.51	0.44
1:C:133:PHE:HD1	1:C:134:CYS:N	2.16	0.44
1:E:133:PHE:HD1	1:E:134:CYS:N	2.16	0.44
1:G:56:ASP:OD1	1:G:56:ASP:N	2.51	0.44
1:I:296:LEU:H	1:I:296:LEU:HD23	1.82	0.44
1:K:4:VAL:HB	1:K:49:LYS:NZ	2.32	0.44
1:E:56:ASP:OD1	1:E:56:ASP:N	2.51	0.44
1:E:163:TYR:C	1:E:163:TYR:HD2	2.25	0.44
1:E:296:LEU:HD23	1:E:296:LEU:H	1.82	0.44
1:F:133:PHE:HD1	1:F:134:CYS:N	2.16	0.44
1:H:56:ASP:OD1	1:H:56:ASP:N	2.51	0.44
1:I:353:GLU:N	1:I:353:GLU:CD	2.73	0.44
1:B:133:PHE:HD1	1:B:134:CYS:N	2.16	0.44
1:C:421:TRP:O	1:D:226:SER:N	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:MET:SD	1:G:24:MET:N	2.87	0.44
1:G:133:PHE:HD1	1:G:134:CYS:N	2.16	0.44
1:H:424:LYS:HE3	1:I:222:ARG:HE	1.81	0.44
1:I:56:ASP:N	1:I:56:ASP:OD1	2.51	0.44
1:L:208:LYS:HB3	1:L:208:LYS:HE3	1.77	0.44
1:A:444:GLN:HG2	1:A:447:PHE:CE1	2.53	0.44
1:B:24:MET:SD	1:B:24:MET:N	2.86	0.44
1:C:208:LYS:HB3	1:C:208:LYS:HE3	1.77	0.44
1:E:18:LEU:HD12	1:E:18:LEU:HA	1.84	0.44
1:G:337:THR:O	1:G:341:GLN:HG3	2.18	0.44
1:I:337:THR:O	1:I:341:GLN:HG3	2.18	0.44
1:J:444:GLN:HG2	1:J:447:PHE:CE1	2.53	0.44
1:A:56:ASP:OD1	1:A:56:ASP:N	2.51	0.44
1:B:444:GLN:HG2	1:B:447:PHE:CE1	2.53	0.44
1:A:133:PHE:HD1	1:A:134:CYS:N	2.16	0.44
1:F:337:THR:O	1:F:341:GLN:HG3	2.18	0.44
1:F:444:GLN:HG2	1:F:447:PHE:CE1	2.53	0.44
1:G:444:GLN:HG2	1:G:447:PHE:CE1	2.53	0.44
1:H:163:TYR:C	1:H:163:TYR:HD2	2.25	0.44
1:I:18:LEU:HD12	1:I:18:LEU:HA	1.84	0.44
1:I:444:GLN:HG2	1:I:447:PHE:CE1	2.53	0.44
1:K:18:LEU:HD12	1:K:18:LEU:HA	1.84	0.44
1:K:163:TYR:C	1:K:163:TYR:HD2	2.25	0.44
1:D:56:ASP:OD1	1:D:56:ASP:N	2.51	0.43
1:D:444:GLN:HG2	1:D:447:PHE:CE1	2.53	0.43
1:G:4:VAL:HB	1:G:49:LYS:NZ	2.32	0.43
1:A:406:LYS:O	1:B:316:LYS:NZ	2.51	0.43
1:C:296:LEU:HD23	1:C:296:LEU:H	1.82	0.43
1:C:444:GLN:HG2	1:C:447:PHE:CE1	2.53	0.43
1:K:444:GLN:HG2	1:K:447:PHE:CE1	2.53	0.43
1:C:413:ARG:H	1:D:231:LYS:CD	2.31	0.43
1:H:133:PHE:HD1	1:H:134:CYS:N	2.16	0.43
1:A:337:THR:O	1:A:341:GLN:HG3	2.18	0.43
1:D:163:TYR:C	1:D:163:TYR:HD2	2.25	0.43
1:E:337:THR:O	1:E:341:GLN:HG3	2.18	0.43
1:F:100:LEU:HD23	1:F:100:LEU:HA	1.84	0.43
1:I:163:TYR:C	1:I:163:TYR:HD2	2.25	0.43
1:K:85:ARG:HH22	1:K:137:THR:HG22	1.84	0.43
1:K:337:THR:O	1:K:341:GLN:HG3	2.18	0.43
1:L:163:TYR:C	1:L:163:TYR:HD2	2.25	0.43
1:L:444:GLN:HG2	1:L:447:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:HG3	1:A:238:ARG:HG3	2.01	0.43
1:D:337:THR:O	1:D:341:GLN:HG3	2.18	0.43
1:I:202:GLU:HG3	1:I:238:ARG:HG3	2.01	0.43
1:J:202:GLU:HG3	1:J:238:ARG:HG3	2.01	0.43
1:L:337:THR:O	1:L:341:GLN:HG3	2.18	0.43
1:A:229:ARG:HB2	1:J:421:TRP:CG	2.54	0.43
1:B:202:GLU:HG3	1:B:238:ARG:HG3	2.01	0.43
1:B:406:LYS:O	1:C:316:LYS:NZ	2.48	0.43
1:E:444:GLN:HG2	1:E:447:PHE:CE1	2.53	0.43
1:I:85:ARG:HH22	1:I:137:THR:HG22	1.84	0.43
1:J:133:PHE:HD1	1:J:134:CYS:N	2.16	0.43
1:K:202:GLU:HG3	1:K:238:ARG:HG3	2.01	0.43
1:K:421:TRP:CG	1:L:229:ARG:HB2	2.54	0.43
1:L:18:LEU:HD12	1:L:18:LEU:HA	1.85	0.43
1:L:85:ARG:HH22	1:L:137:THR:HG22	1.84	0.43
1:E:424:LYS:HE3	1:F:222:ARG:HE	1.82	0.43
1:J:351:THR:OG1	1:J:354:ASP:OD2	2.37	0.43
1:J:353:GLU:N	1:J:353:GLU:CD	2.74	0.43
1:K:56:ASP:N	1:K:56:ASP:OD1	2.51	0.43
1:L:202:GLU:HG3	1:L:238:ARG:HG3	2.01	0.43
1:A:163:TYR:C	1:A:163:TYR:HD2	2.25	0.43
1:B:163:TYR:C	1:B:163:TYR:HD2	2.25	0.43
1:B:337:THR:O	1:B:341:GLN:HG3	2.18	0.43
1:C:351:THR:OG1	1:C:354:ASP:OD2	2.37	0.43
1:G:18:LEU:HD12	1:G:18:LEU:HA	1.84	0.43
1:H:85:ARG:HH22	1:H:137:THR:HG22	1.84	0.43
1:H:337:THR:O	1:H:341:GLN:HG3	2.18	0.43
1:I:133:PHE:HD1	1:I:134:CYS:N	2.16	0.43
1:J:85:ARG:HH22	1:J:137:THR:HG22	1.84	0.43
1:K:133:PHE:HD1	1:K:134:CYS:N	2.16	0.43
1:B:351:THR:OG1	1:B:354:ASP:OD2	2.37	0.43
1:H:351:THR:OG1	1:H:354:ASP:OD2	2.37	0.43
1:L:133:PHE:HD1	1:L:134:CYS:N	2.16	0.43
1:C:202:GLU:HG3	1:C:238:ARG:HG3	2.01	0.43
1:G:353:GLU:N	1:G:353:GLU:CD	2.73	0.43
1:H:202:GLU:HG3	1:H:238:ARG:HG3	2.01	0.43
1:L:351:THR:OG1	1:L:354:ASP:OD2	2.37	0.43
1:A:85:ARG:HH22	1:A:137:THR:HG22	1.84	0.42
1:C:18:LEU:HD12	1:C:18:LEU:HA	1.84	0.42
1:C:163:TYR:C	1:C:163:TYR:HD2	2.25	0.42
1:G:85:ARG:HH22	1:G:137:THR:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:444:GLN:HG2	1:H:447:PHE:CE1	2.53	0.42
1:B:85:ARG:HH22	1:B:137:THR:HG22	1.84	0.42
1:J:163:TYR:C	1:J:163:TYR:HD2	2.25	0.42
1:J:337:THR:O	1:J:341:GLN:HG3	2.18	0.42
1:C:85:ARG:HH22	1:C:137:THR:HG22	1.84	0.42
1:B:353:GLU:N	1:B:353:GLU:CD	2.74	0.42
1:E:85:ARG:HH22	1:E:137:THR:HG22	1.84	0.42
1:F:85:ARG:HH22	1:F:137:THR:HG22	1.84	0.42
1:G:424:LYS:HE3	1:H:222:ARG:HE	1.85	0.42
1:C:337:THR:O	1:C:341:GLN:HG3	2.18	0.42
1:D:85:ARG:HH22	1:D:137:THR:HG22	1.84	0.42
1:E:351:THR:OG1	1:E:354:ASP:OD2	2.37	0.42
1:E:413:ARG:HB2	1:F:231:LYS:HD3	2.02	0.42
1:G:202:GLU:HG3	1:G:238:ARG:HG3	2.01	0.42
1:A:351:THR:OG1	1:A:354:ASP:OD2	2.37	0.42
1:D:202:GLU:HG3	1:D:238:ARG:HG3	2.01	0.42
1:E:202:GLU:HG3	1:E:238:ARG:HG3	2.01	0.42
1:J:56:ASP:OD1	1:J:56:ASP:N	2.50	0.42
1:L:56:ASP:OD1	1:L:56:ASP:N	2.51	0.42
1:F:202:GLU:HG3	1:F:238:ARG:HG3	2.01	0.42
1:K:351:THR:OG1	1:K:354:ASP:OD2	2.37	0.42
1:B:23:PRO:HD2	1:B:24:MET:SD	2.60	0.42
1:D:351:THR:OG1	1:D:354:ASP:OD2	2.37	0.42
1:G:23:PRO:HD2	1:G:24:MET:SD	2.60	0.42
1:G:265:HIS:HB2	1:G:446:GLU:OE1	2.20	0.42
1:J:23:PRO:HD2	1:J:24:MET:SD	2.60	0.42
1:J:224:LYS:O	1:L:422:ALA:HA	2.20	0.42
1:B:56:ASP:OD1	1:B:56:ASP:N	2.51	0.41
1:E:265:HIS:HB2	1:E:446:GLU:OE1	2.20	0.41
1:G:351:THR:OG1	1:G:354:ASP:OD2	2.37	0.41
1:H:23:PRO:HD2	1:H:24:MET:SD	2.60	0.41
1:B:265:HIS:HB2	1:B:446:GLU:OE1	2.20	0.41
1:A:208:LYS:HB3	1:A:208:LYS:HE3	1.77	0.41
1:D:23:PRO:HD2	1:D:24:MET:SD	2.60	0.41
1:I:208:LYS:HB3	1:I:208:LYS:HE3	1.76	0.41
1:K:23:PRO:HD2	1:K:24:MET:SD	2.60	0.41
1:D:265:HIS:HB2	1:D:446:GLU:OE1	2.20	0.41
1:I:265:HIS:HB2	1:I:446:GLU:OE1	2.20	0.41
1:C:23:PRO:HD2	1:C:24:MET:SD	2.60	0.41
1:A:23:PRO:HD2	1:A:24:MET:SD	2.60	0.41
1:B:224:LYS:HE3	1:B:224:LYS:HB3	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:HB2	1:C:231:LYS:HD3	2.01	0.41
1:C:345:ILE:H	1:C:345:ILE:HD12	1.86	0.41
1:D:345:ILE:H	1:D:345:ILE:HD12	1.86	0.41
1:E:23:PRO:HD2	1:E:24:MET:SD	2.60	0.41
1:H:345:ILE:H	1:H:345:ILE:HD12	1.86	0.41
1:I:345:ILE:H	1:I:345:ILE:HD12	1.86	0.41
1:J:265:HIS:HB2	1:J:446:GLU:OE1	2.20	0.41
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.84	0.41
1:C:265:HIS:HB2	1:C:446:GLU:OE1	2.20	0.41
1:F:23:PRO:HD2	1:F:24:MET:SD	2.60	0.41
1:D:24:MET:SD	1:D:24:MET:N	2.87	0.41
1:I:24:MET:SD	1:I:24:MET:N	2.86	0.41
1:J:18:LEU:HD12	1:J:18:LEU:HA	1.84	0.41
1:L:265:HIS:HB2	1:L:446:GLU:OE1	2.20	0.41
1:A:265:HIS:HB2	1:A:446:GLU:OE1	2.20	0.41
1:A:420:LEU:HD12	1:A:421:TRP:H	1.86	0.41
1:F:351:THR:OG1	1:F:354:ASP:OD2	2.37	0.41
1:G:345:ILE:H	1:G:345:ILE:HD12	1.86	0.41
1:I:422:ALA:HA	1:K:224:LYS:O	2.20	0.41
1:J:345:ILE:H	1:J:345:ILE:HD12	1.86	0.41
1:L:23:PRO:HD2	1:L:24:MET:SD	2.60	0.41
1:I:351:THR:OG1	1:I:354:ASP:OD2	2.37	0.41
1:G:100:LEU:HD23	1:G:100:LEU:HA	1.84	0.40
1:I:23:PRO:HD2	1:I:24:MET:SD	2.60	0.40
1:K:425:LYS:HE3	1:L:323:GLY:HA3	2.03	0.40
1:D:412:GLU:HA	1:E:231:LYS:HE3	2.03	0.40
1:E:420:LEU:HD12	1:E:421:TRP:H	1.86	0.40
1:K:421:TRP:CD2	1:L:229:ARG:HB2	2.56	0.40
1:A:24:MET:SD	1:A:24:MET:N	2.86	0.40
1:B:420:LEU:HD12	1:B:421:TRP:H	1.86	0.40
1:D:420:LEU:HD12	1:D:421:TRP:H	1.86	0.40
1:F:265:HIS:HB2	1:F:446:GLU:OE1	2.20	0.40
1:F:420:LEU:HD12	1:F:421:TRP:H	1.86	0.40
1:H:420:LEU:HD12	1:H:421:TRP:H	1.86	0.40
1:J:420:LEU:HD12	1:J:421:TRP:H	1.86	0.40
1:L:48:ILE:HD13	1:L:48:ILE:HA	1.98	0.40
1:L:345:ILE:H	1:L:345:ILE:HD12	1.86	0.40
1:A:345:ILE:H	1:A:345:ILE:HD12	1.86	0.40
1:C:56:ASP:OD1	1:C:56:ASP:N	2.51	0.40
1:D:350:VAL:O	1:D:392:SER:HB2	2.22	0.40
1:K:265:HIS:HB2	1:K:446:GLU:OE1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ILE:H	1:B:345:ILE:HD12	1.86	0.40
1:E:345:ILE:H	1:E:345:ILE:HD12	1.86	0.40
1:G:420:LEU:HD12	1:G:421:TRP:H	1.86	0.40
1:L:350:VAL:O	1:L:392:SER:HB2	2.22	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	437/552 (79%)	420 (96%)	17 (4%)	0	100	100
1	B	437/552 (79%)	421 (96%)	16 (4%)	0	100	100
1	C	437/552 (79%)	420 (96%)	17 (4%)	0	100	100
1	D	437/552 (79%)	421 (96%)	16 (4%)	0	100	100
1	E	437/552 (79%)	421 (96%)	16 (4%)	0	100	100
1	F	437/552 (79%)	421 (96%)	16 (4%)	0	100	100
1	G	437/552 (79%)	420 (96%)	17 (4%)	0	100	100
1	H	437/552 (79%)	421 (96%)	16 (4%)	0	100	100
1	I	437/552 (79%)	421 (96%)	16 (4%)	0	100	100
1	J	437/552 (79%)	420 (96%)	17 (4%)	0	100	100
1	K	437/552 (79%)	421 (96%)	16 (4%)	0	100	100
1	L	437/552 (79%)	421 (96%)	16 (4%)	0	100	100
All	All	5244/6624 (79%)	5048 (96%)	196 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	B	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	C	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	D	374/475 (79%)	366 (98%)	8 (2%)	47	67
1	E	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	F	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	G	374/475 (79%)	366 (98%)	8 (2%)	47	67
1	H	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	I	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	J	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	K	374/475 (79%)	367 (98%)	7 (2%)	50	69
1	L	374/475 (79%)	366 (98%)	8 (2%)	47	67
All	All	4488/5700 (79%)	4401 (98%)	87 (2%)	49	69

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	TYR
1	A	208	LYS
1	A	221	ARG
1	A	348	THR
1	A	353	GLU
1	A	408	LEU
1	A	472	LEU
1	B	163	TYR
1	B	208	LYS
1	B	221	ARG
1	B	348	THR
1	B	353	GLU
1	B	408	LEU
1	B	472	LEU

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Mol	Chain	Res	Type
1	C	163	TYR
1	C	208	LYS
1	C	221	ARG
1	C	348	THR
1	C	353	GLU
1	C	408	LEU
1	C	472	LEU
1	D	30	ARG
1	D	163	TYR
1	D	208	LYS
1	D	221	ARG
1	D	348	THR
1	D	353	GLU
1	D	408	LEU
1	D	472	LEU
1	E	163	TYR
1	E	208	LYS
1	E	221	ARG
1	E	348	THR
1	E	353	GLU
1	E	408	LEU
1	E	472	LEU
1	F	163	TYR
1	F	208	LYS
1	F	221	ARG
1	F	348	THR
1	F	353	GLU
1	F	408	LEU
1	F	472	LEU
1	G	30	ARG
1	G	163	TYR
1	G	208	LYS
1	G	221	ARG
1	G	348	THR
1	G	353	GLU
1	G	408	LEU
1	G	472	LEU
1	H	163	TYR
1	H	208	LYS
1	H	221	ARG
1	H	348	THR
1	H	353	GLU

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Mol	Chain	Res	Type
1	H	408	LEU
1	H	472	LEU
1	I	163	TYR
1	I	208	LYS
1	I	221	ARG
1	I	348	THR
1	I	353	GLU
1	I	408	LEU
1	I	472	LEU
1	J	163	TYR
1	J	208	LYS
1	J	221	ARG
1	J	348	THR
1	J	353	GLU
1	J	408	LEU
1	J	472	LEU
1	K	163	TYR
1	K	208	LYS
1	K	221	ARG
1	K	348	THR
1	K	353	GLU
1	K	408	LEU
1	K	472	LEU
1	L	30	ARG
1	L	163	TYR
1	L	208	LYS
1	L	221	ARG
1	L	348	THR
1	L	353	GLU
1	L	408	LEU
1	L	472	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	198	ASN
1	A	429	HIS
1	B	157	HIS
1	B	198	ASN
1	B	429	HIS
1	C	157	HIS

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Mol	Chain	Res	Type
1	C	198	ASN
1	D	157	HIS
1	D	198	ASN
1	D	429	HIS
1	E	157	HIS
1	E	429	HIS
1	F	157	HIS
1	F	429	HIS
1	G	157	HIS
1	G	198	ASN
1	G	429	HIS
1	H	157	HIS
1	H	429	HIS
1	I	157	HIS
1	I	198	ASN
1	I	429	HIS
1	J	157	HIS
1	J	198	ASN
1	J	429	HIS
1	K	157	HIS
1	K	198	ASN
1	K	429	HIS
1	L	157	HIS
1	L	198	ASN
1	L	429	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

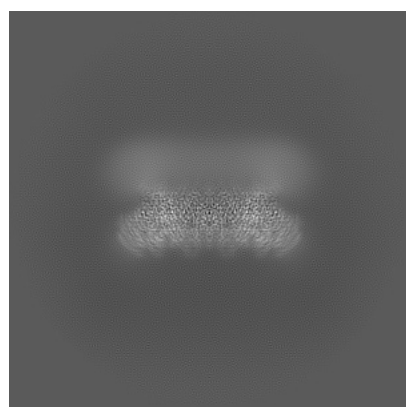
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30796. These allow visual inspection of the internal detail of the map and identification of artifacts.

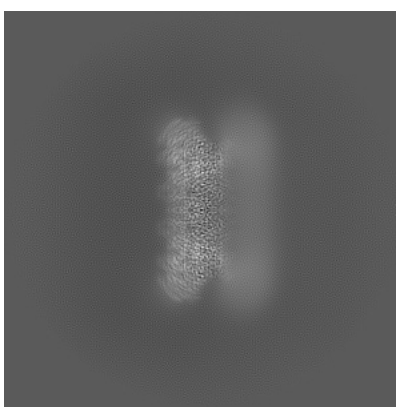
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

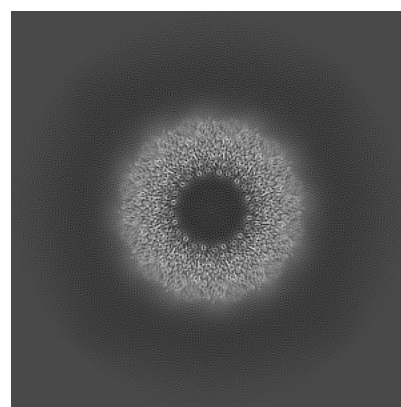
6.1.1 Primary map



X



Y

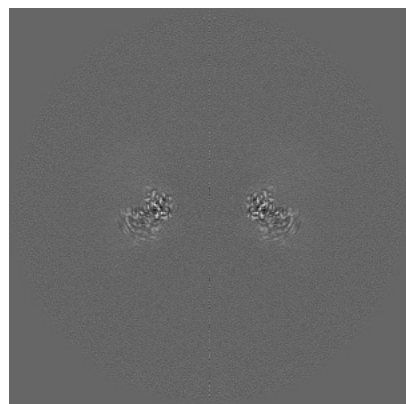


Z

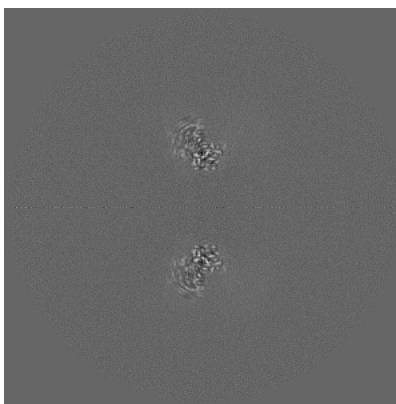
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

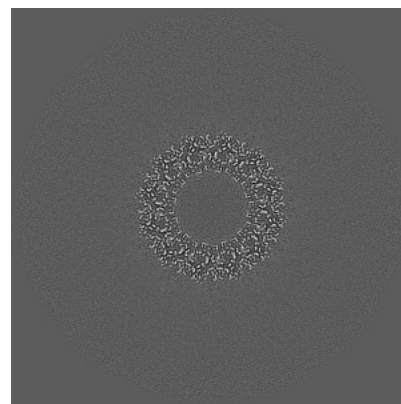
6.2.1 Primary map



X Index: 240



Y Index: 240

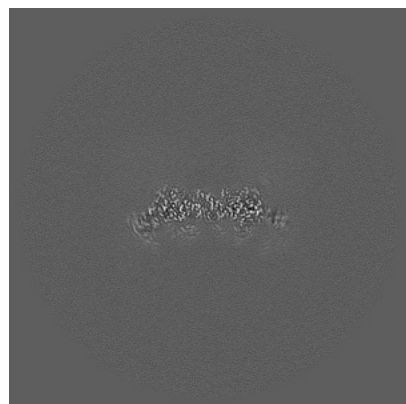


Z Index: 240

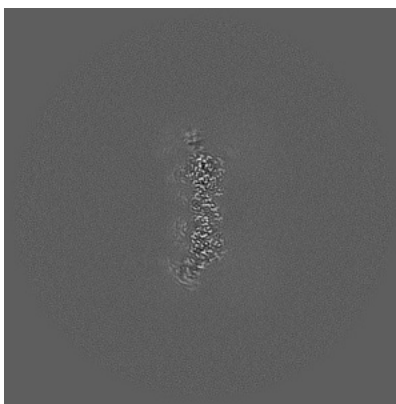
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

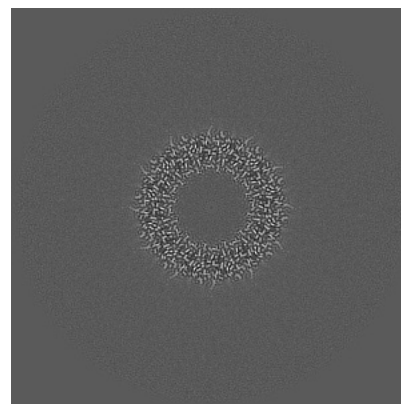
6.3.1 Primary map



X Index: 185



Y Index: 295

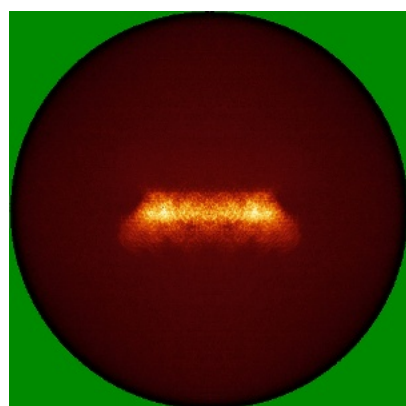


Z Index: 238

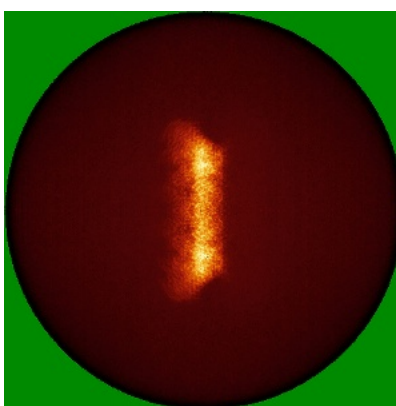
The images above show the largest variance slices of the map in three orthogonal directions.

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

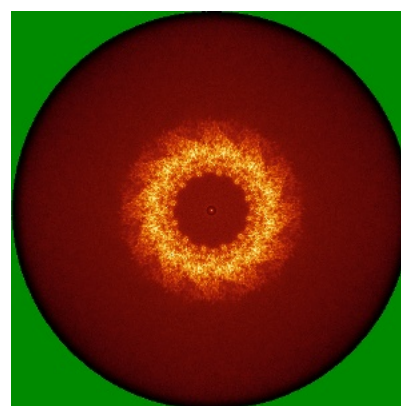
6.4.1 Primary map



X



Y

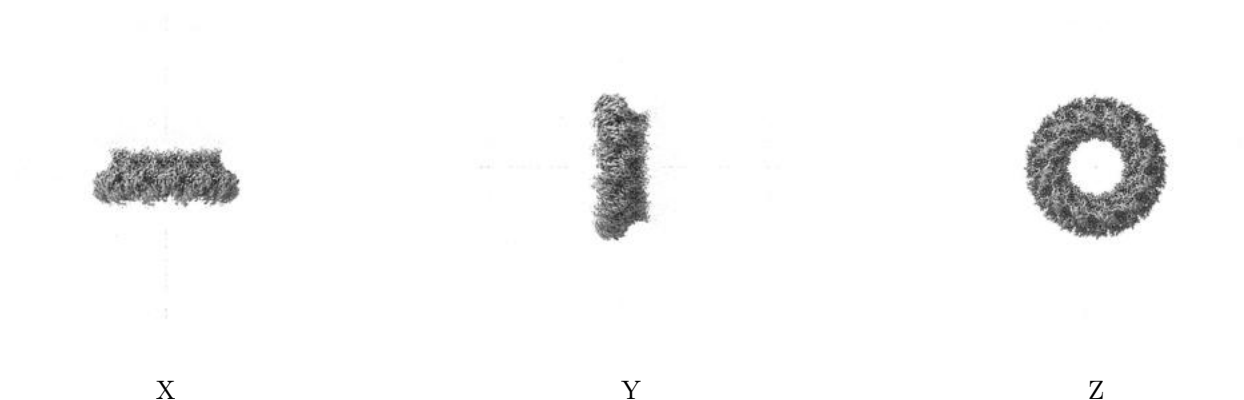


Z

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

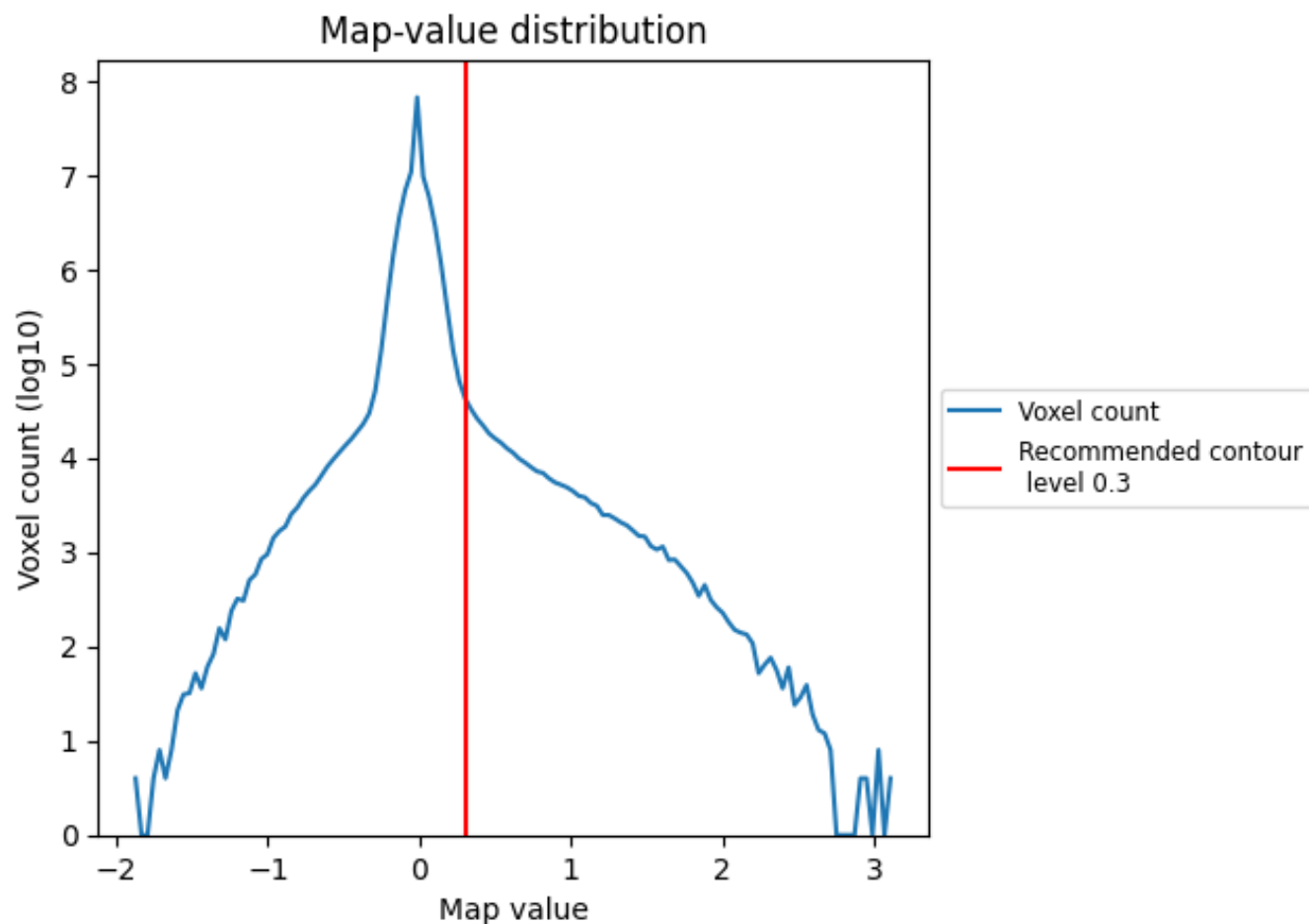
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

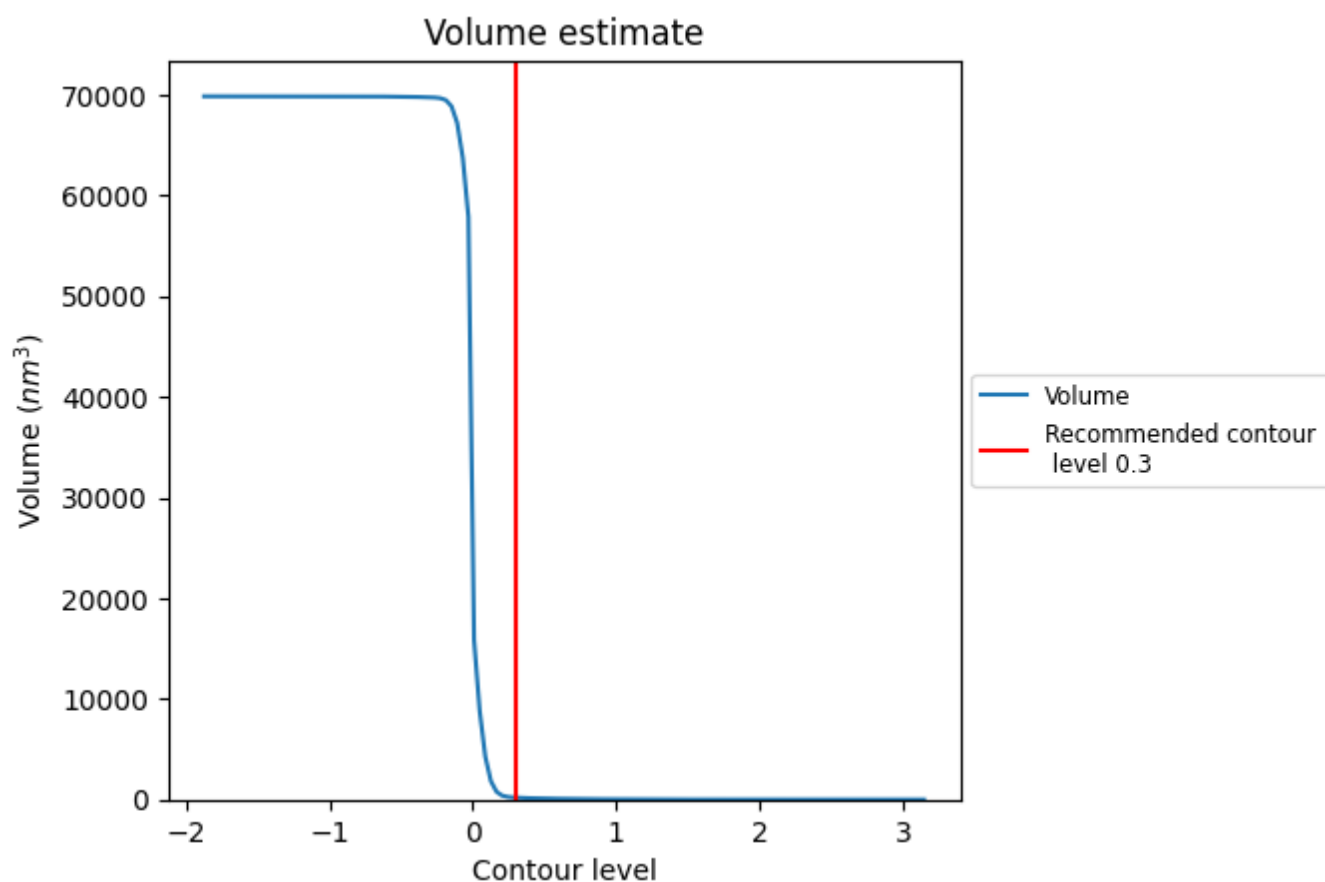
This section contains the results of statistical analysis of the map.

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.

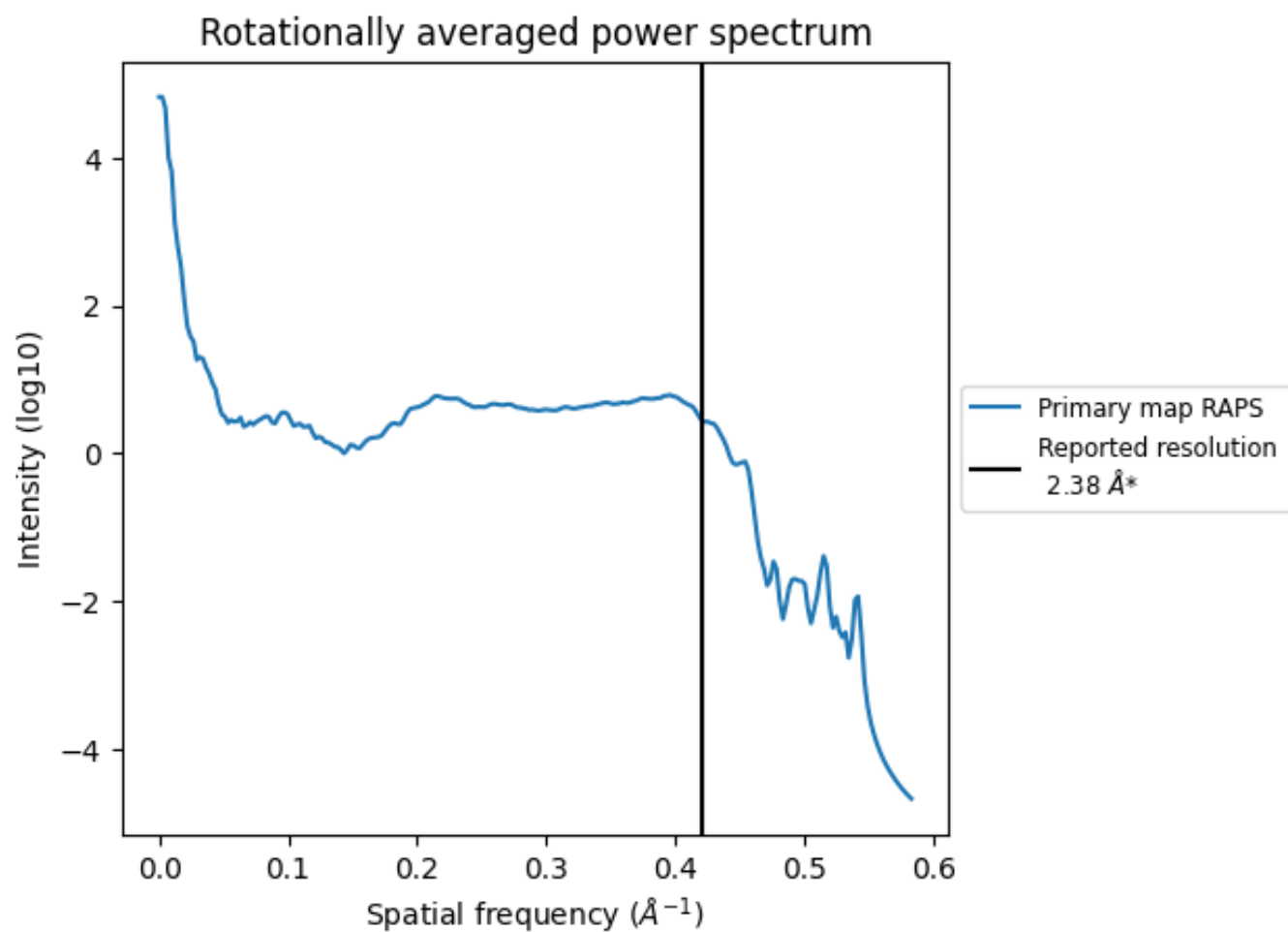
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 176 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 0.420 Å⁻¹

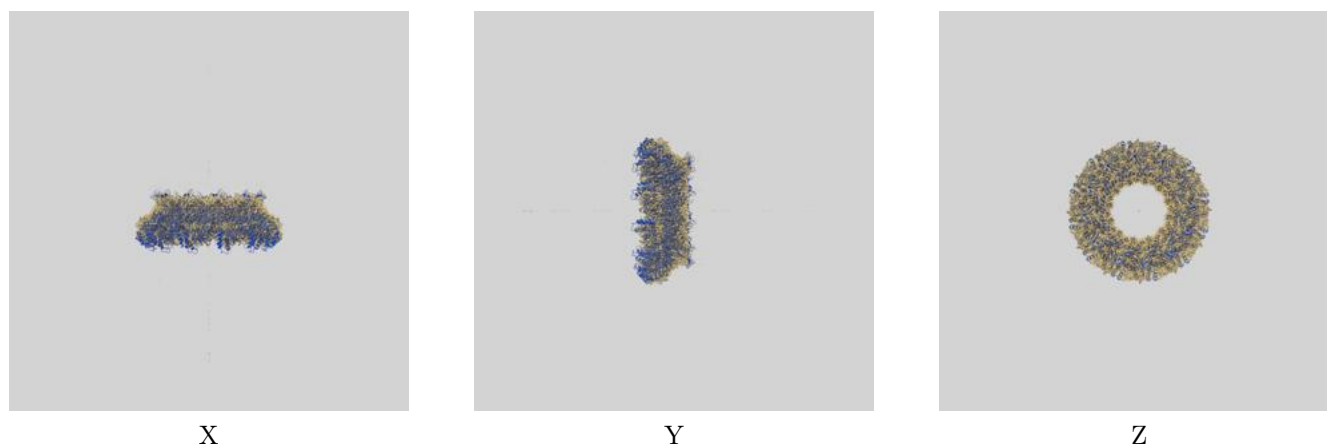
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

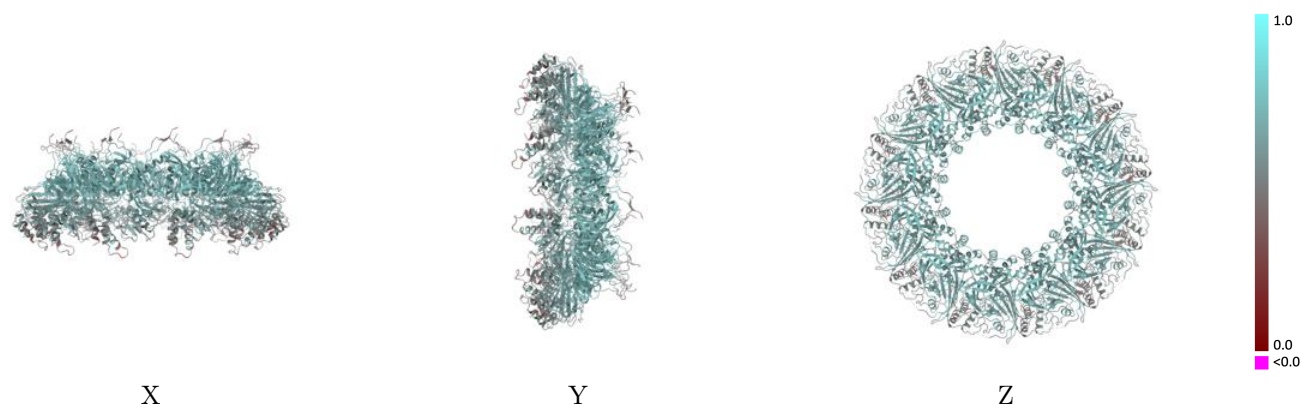
This section contains information regarding the fit between EMDB map EMD-30796 and PDB model 7DOP. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



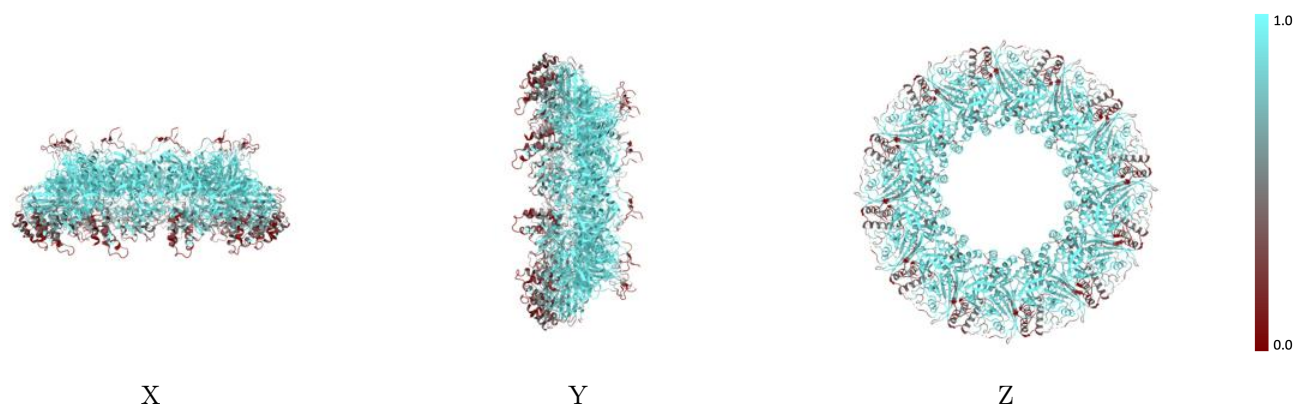
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



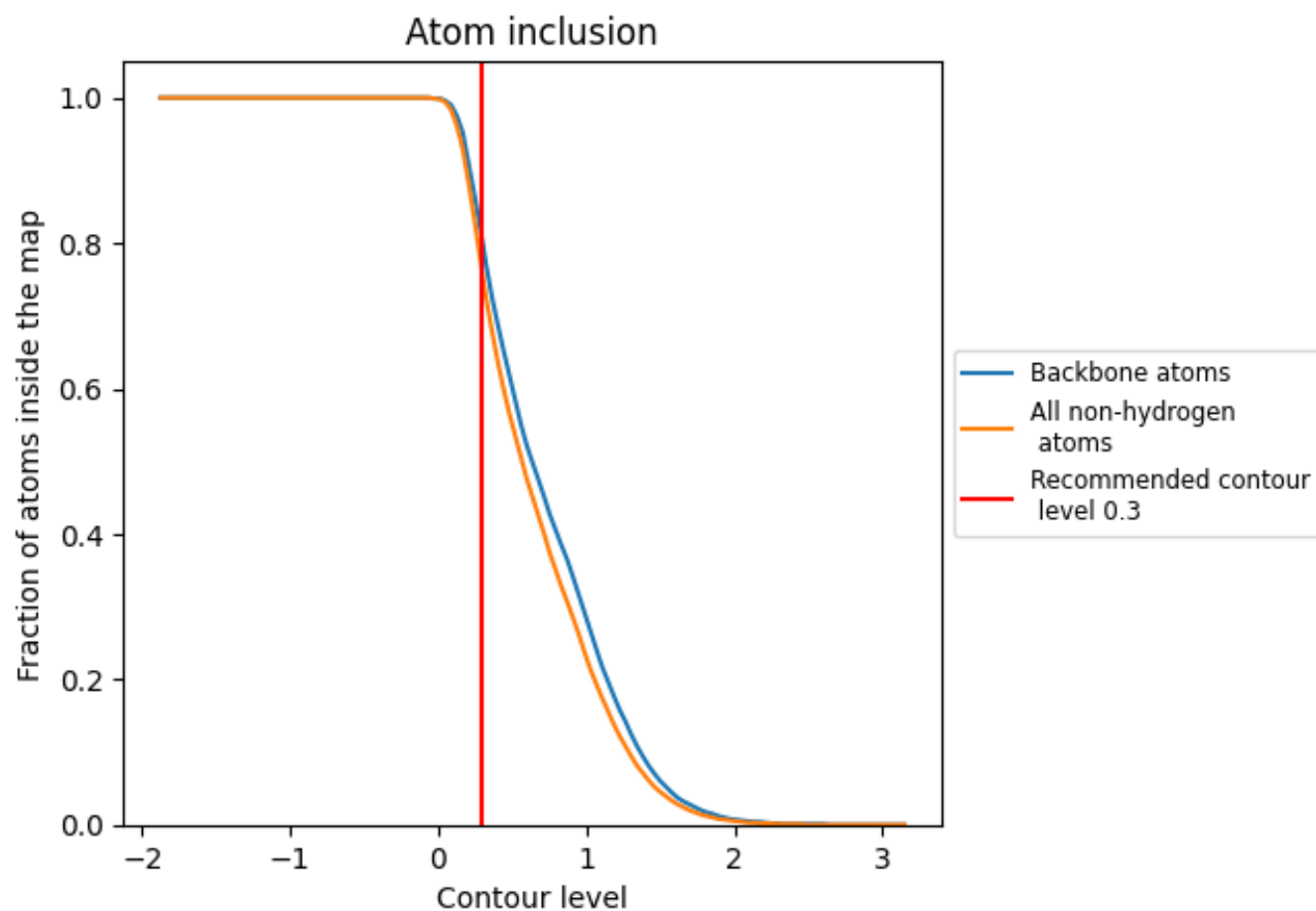
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.6150
A	0.7550	0.6170
B	0.7560	0.6170
C	0.7560	0.6180
D	0.7540	0.6150
E	0.7570	0.6140
F	0.7570	0.6140
G	0.7530	0.6140
H	0.7580	0.6160
I	0.7590	0.6160
J	0.7560	0.6150
K	0.7510	0.6130
L	0.7550	0.6150

