



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:29 PM UTC

PDB ID : 9K2V / pdb_00009k2v
EMDB ID : EMD-61998
Title : Cyanophage A4 pre-ejectosome
Authors : Hou, P.; Li, Q.; Zhou, C.Z.
Deposited on : 2024-10-18
Resolution : 3.40 Å(reported)

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

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

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:

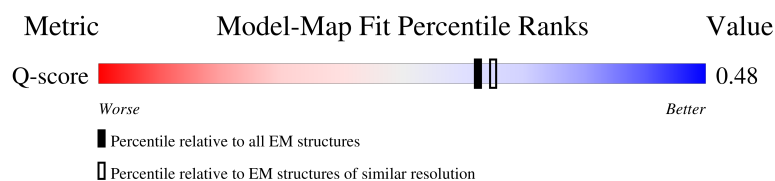
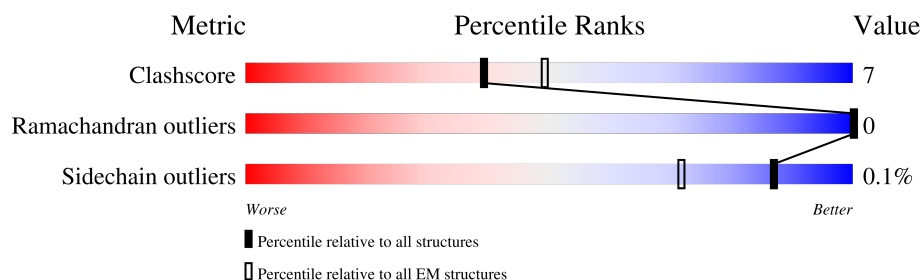
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.40 Å.

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



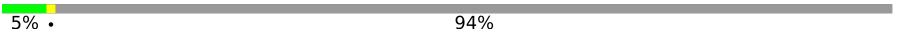
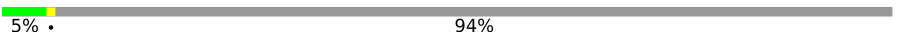
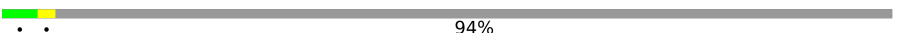
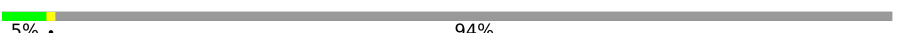
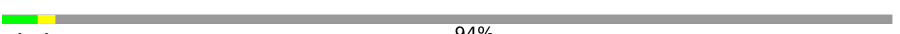
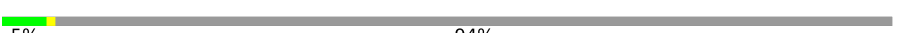
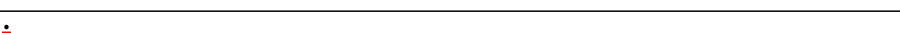
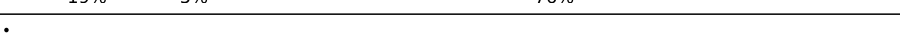
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	F	653	
1	G	653	
1	H	653	
1	I	653	

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Mol	Chain	Length	Quality of chain
1	J	653	 5% • 94%
1	K	653	 5% • 94%
1	L	653	 • • 94%
1	M	653	 5% • 94%
1	N	653	 • • 94%
1	O	653	 5% • 94%
2	V	380	 19% 5% 76%
2	W	380	 19% 5% 76%
2	X	380	 19% 6% 76%
2	Y	380	 19% 6% 76%
2	Z	380	 19% 5% 76%
2	v	380	 20% • 76%
2	w	380	 20% • 76%
2	x	380	 19% 6% 76%
2	y	380	 19% 5% 76%
2	z	380	 21% • 76%
3	A	1058	 5% 72% 14% 14%
3	B	1058	 5% 70% 16% 14%
3	C	1058	 5% 72% 14% 14%
3	D	1058	 • 70% 15% 14%
3	E	1058	 5% 72% 13% 14%
3	a	1058	 • 35% 9% 56%
3	b	1058	 • 34% 10% 56%
3	c	1058	 • 34% 9% 56%
3	d	1058	 • 34% 10% 56%

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Mol	Chain	Length	Quality of chain
3	e	1058	 A horizontal bar chart showing the quality of chain 3e. The bar is divided into three segments: a small red segment at the beginning, a green segment labeled '36%', a yellow segment labeled '7%', and a large grey segment labeled '56%'.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 63405 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 Portal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	K	40	Total	C	N	O	0	0
			290	178	50	62		
1	M	40	Total	C	N	O	0	0
			290	178	50	62		
1	O	40	Total	C	N	O	0	0
			290	178	50	62		
1	G	40	Total	C	N	O	0	0
			290	178	50	62		
1	I	40	Total	C	N	O	0	0
			290	178	50	62		
1	F	40	Total	C	N	O	0	0
			290	178	50	62		
1	H	40	Total	C	N	O	0	0
			290	178	50	62		
1	J	40	Total	C	N	O	0	0
			290	178	50	62		
1	L	40	Total	C	N	O	0	0
			290	178	50	62		
1	N	40	Total	C	N	O	0	0
			290	178	50	62		

- Molecule 2 is a protein called Internal virion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	W	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	X	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	Y	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	Z	92	Total	C	N	O	S	0	0
			706	422	138	142	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	w	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	x	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	y	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	z	92	Total	C	N	O	S	0	0
			706	422	138	142	4		

- Molecule 3 is a protein called Internal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	d	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		
3	A	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	e	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		
3	B	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	a	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		
3	C	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	b	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		
3	D	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	c	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total	Zn	0
			1	1	
4	A	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0

GLU	PRO	GLN	THR	GLY	GLN	ALA	PRO	PRO	ASP	GLU	Q612	T613	N614	P615	F616	Y617	D618	I619	S623	L624	Q625	A651	ASP	GLN
MET	TYR	VAL	ARG	ILE	GLN	ARG	VAL	TYR	THR	ALA	GLN	GLY	PHE	VAL	THR	GLU	PRO	GLU	ILE	ARG	LEU	GLY	ALA	LYS
TYR	VAL	ARG	ILE	GLN	ARG	MET	ASP	PHE	THR	ILE	PHE	GLY	SER	GLN	ILE	PRO	GLN	THR	MET	PRO	GLU	GLY	ALA	LYS

● Molecule 1: Portal protein

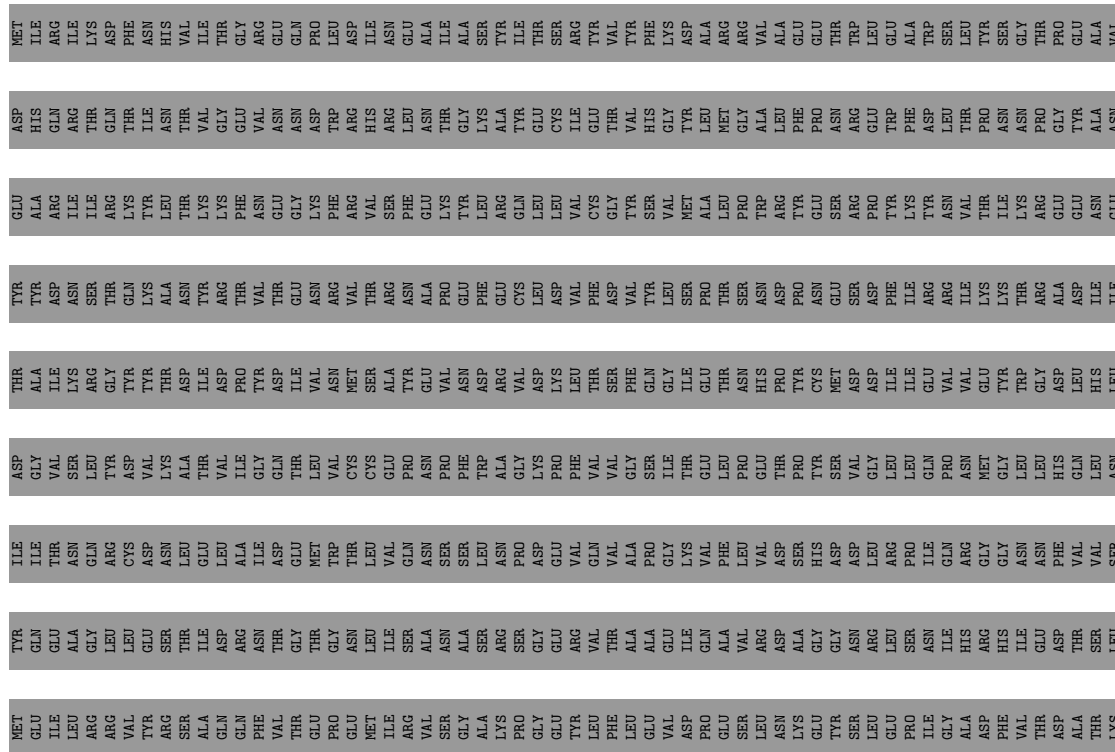
Chain G: 5% 94%

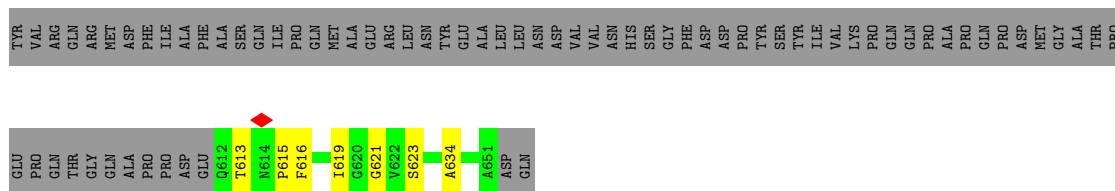
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● Molecule 1: Portal protein

Chain I: 5% 94%

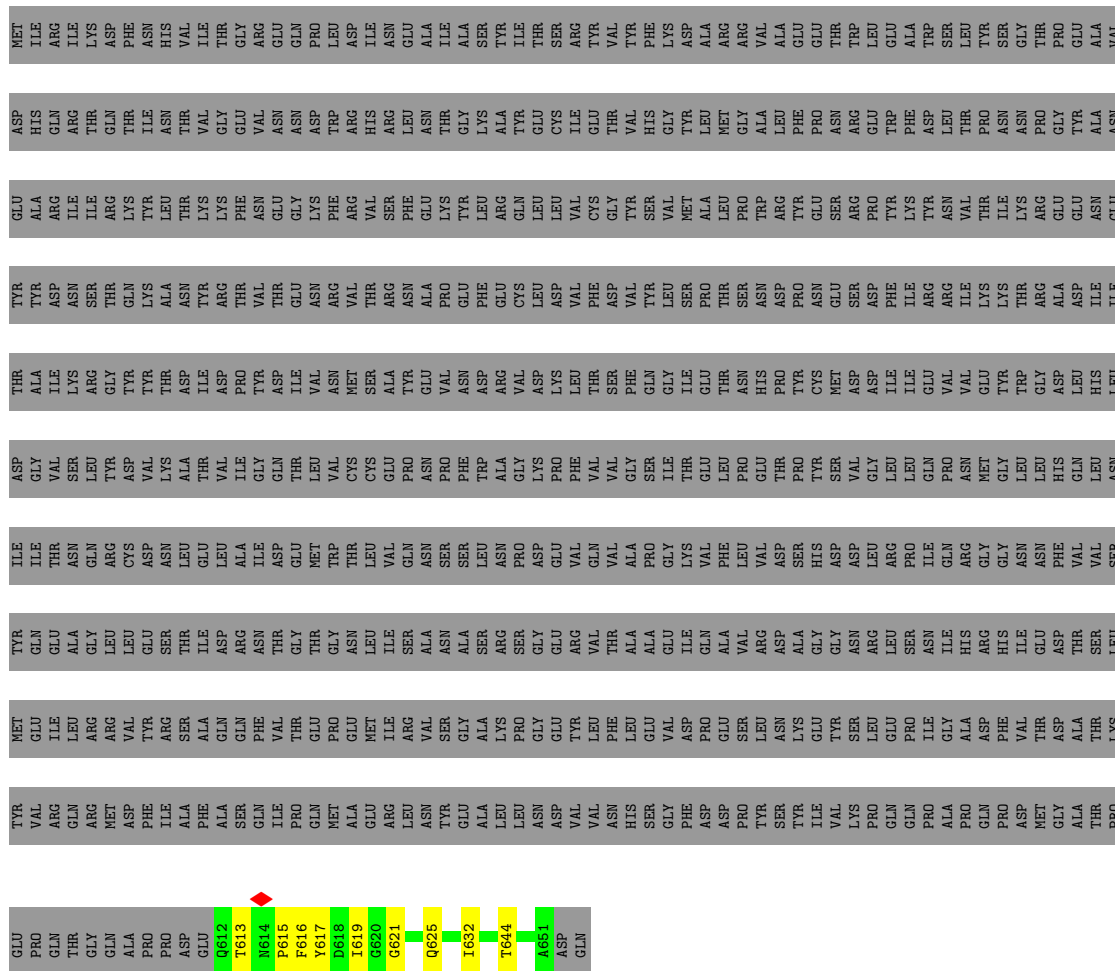
MET	ILE	ARG	ILE	LYS	PHE	ASN	HIS	VAL	THR	ILE	GLY	ARG	GLU	ASN	PRO	LEU	ASP	ASP	ILE	ASN	GLU	SER	TYR	VAL
ASP	HIS	GLN	ARG	THR	GLN	THR	ILE	VAL	GLY	VAL	VAL	VAL	ASN	ASN	ASP	TRP	ARG	HIS	GLY	LYS	ALA	SER	TYR	ILE
ASP	HIS	GLN	ARG	THR	GLN	THR	ILE	VAL	GLY	VAL	VAL	VAL	ASN	ASN	ASP	TRP	ARG	HIS	GLY	LYS	ALA	SER	TYR	ILE





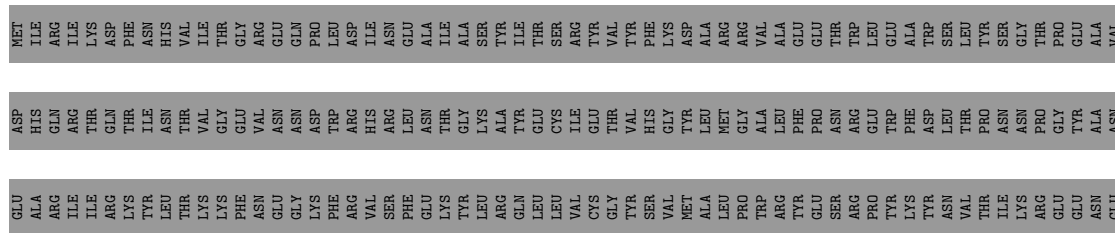
- Molecule 1: Portal protein

Chain H: 5% . 94%



- Molecule 1: Portal protein

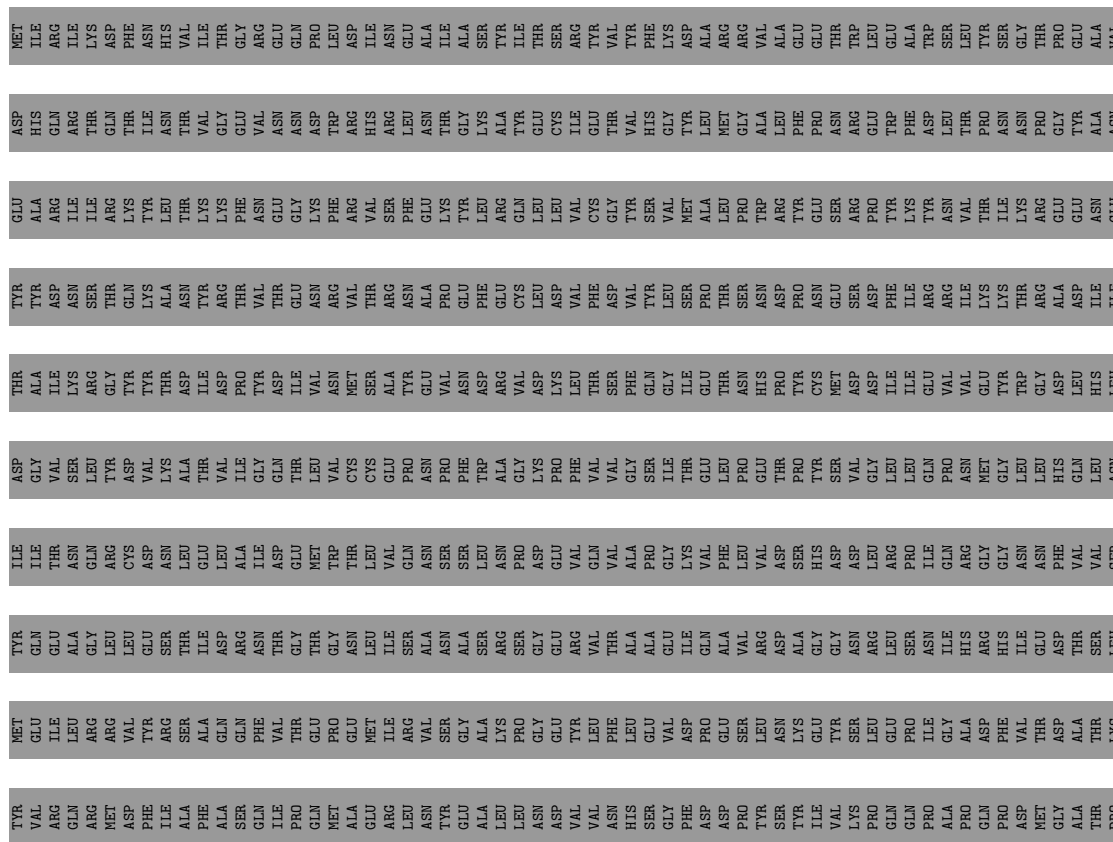
Chain J: 5% . 94%





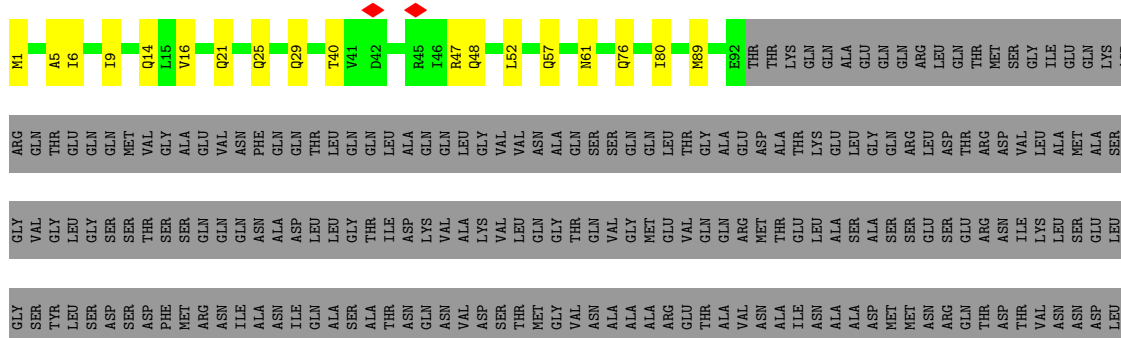
• Molecule 1: Portal protein

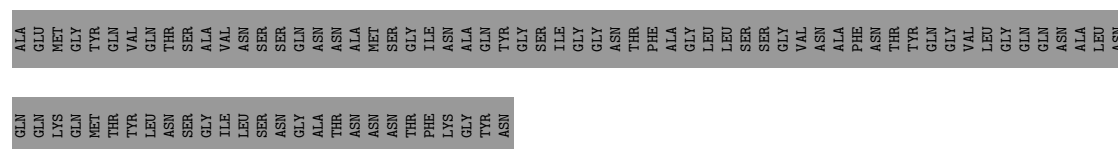
Chain N: 94%



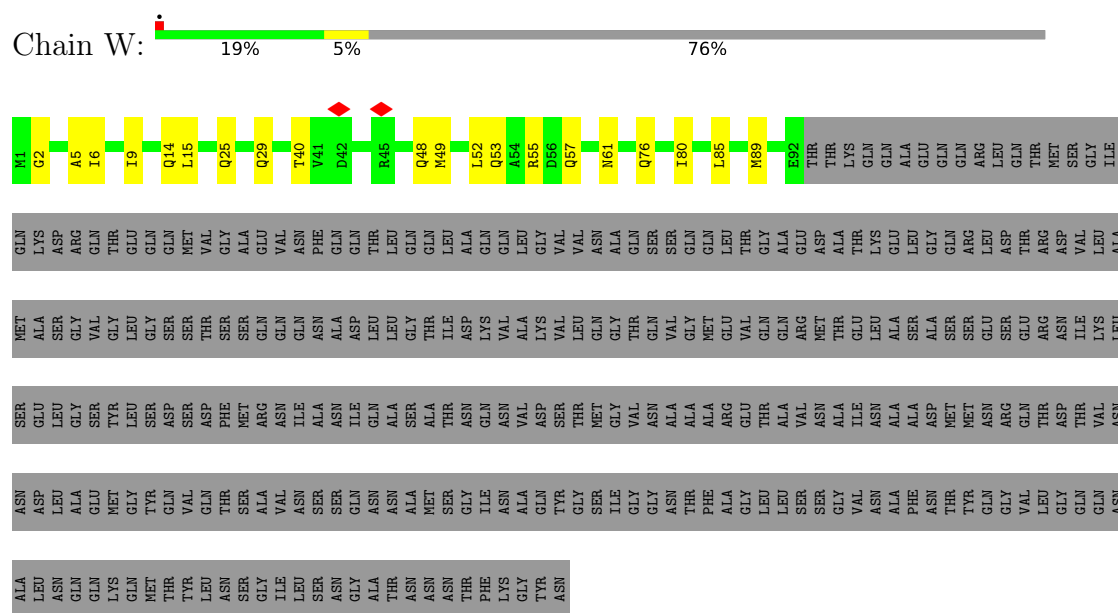
• Molecule 2: Internal virion protein

Chain V: 19% 5% 76%

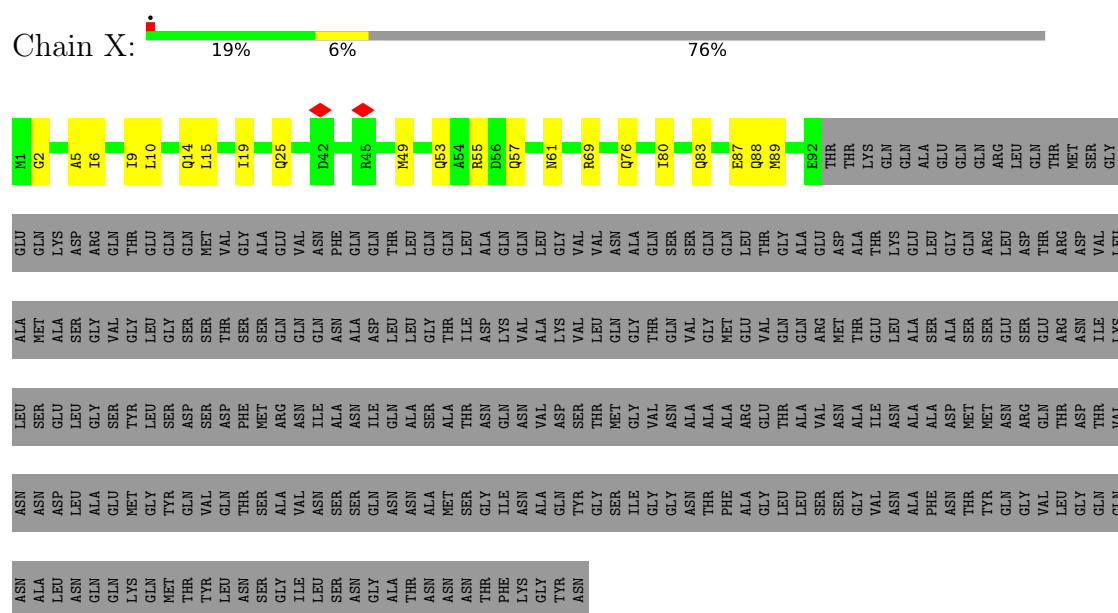




• Molecule 2: Internal virion protein

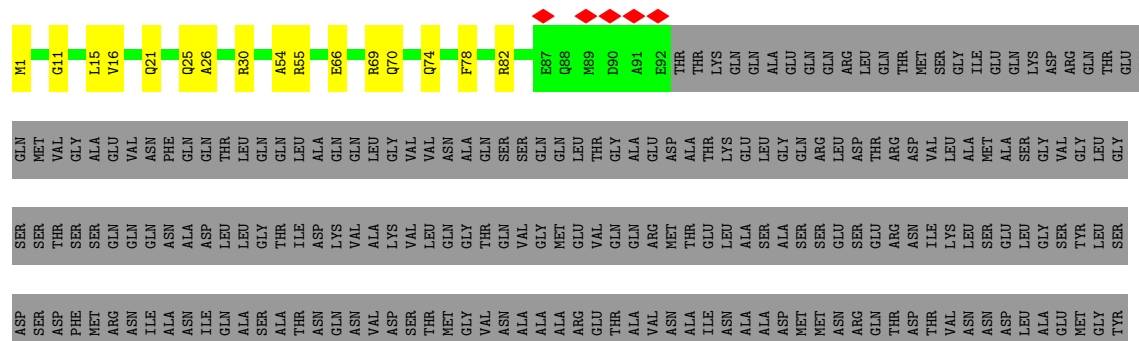


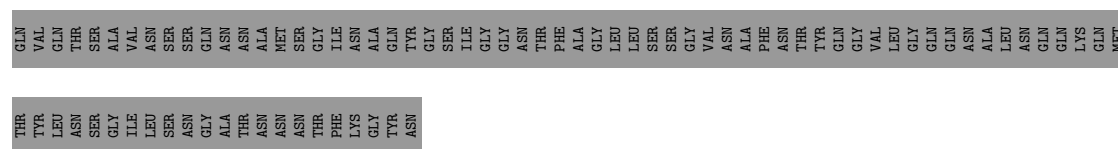
• Molecule 2: Internal virion protein



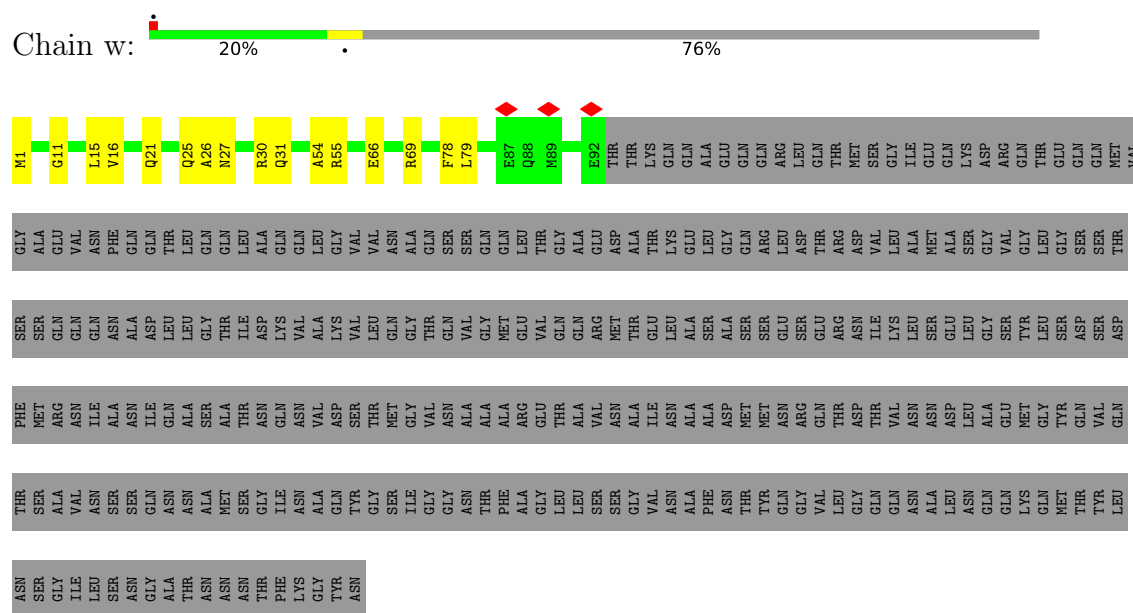
• Molecule 2: Internal virion protein



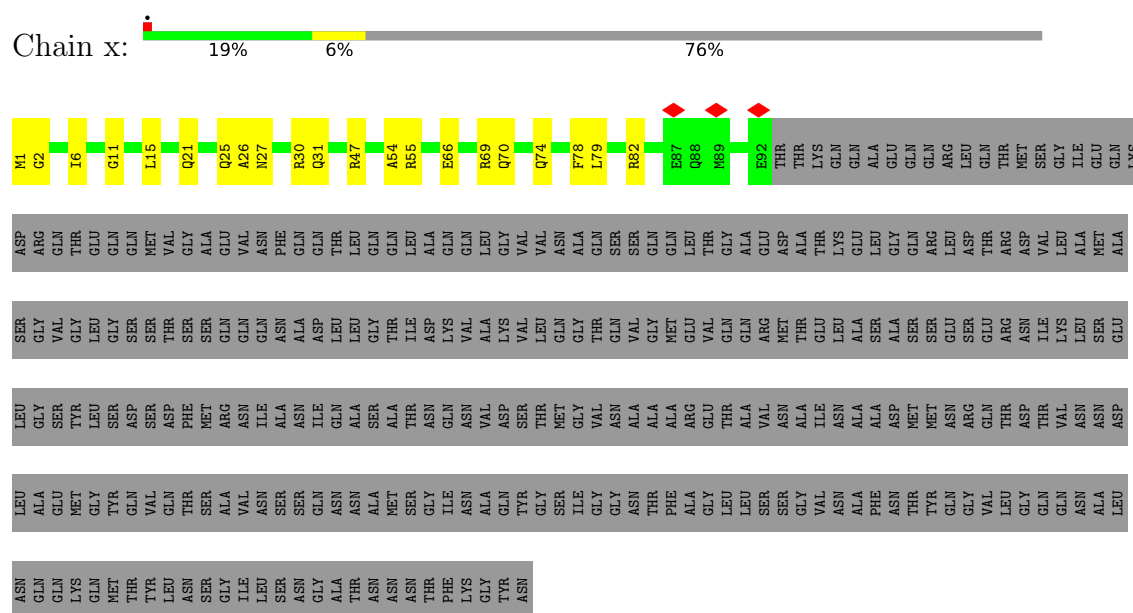




- Molecule 2: Internal virion protein

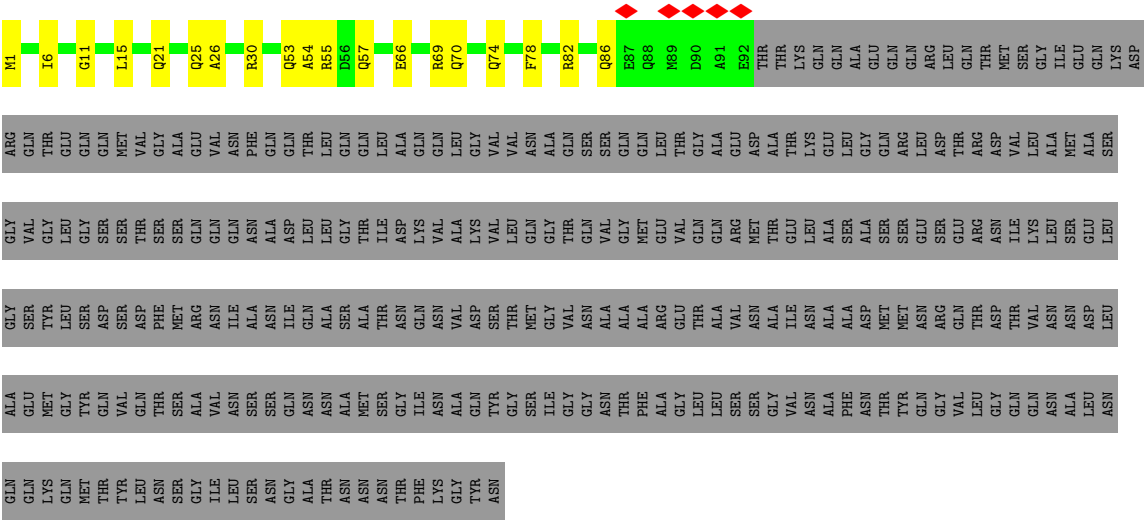


- Molecule 2: Internal virion protein

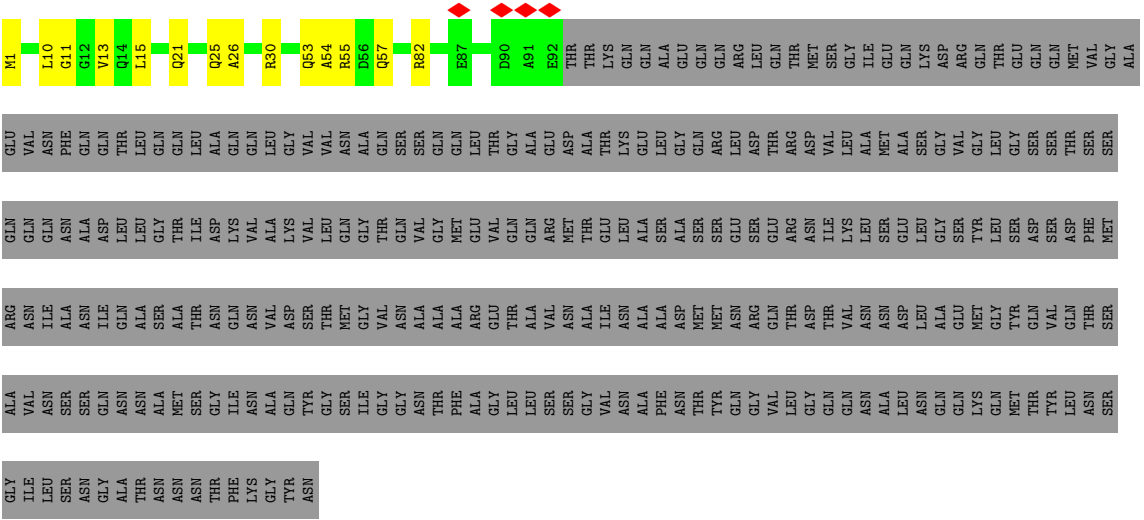


- Molecule 2: Internal virion protein

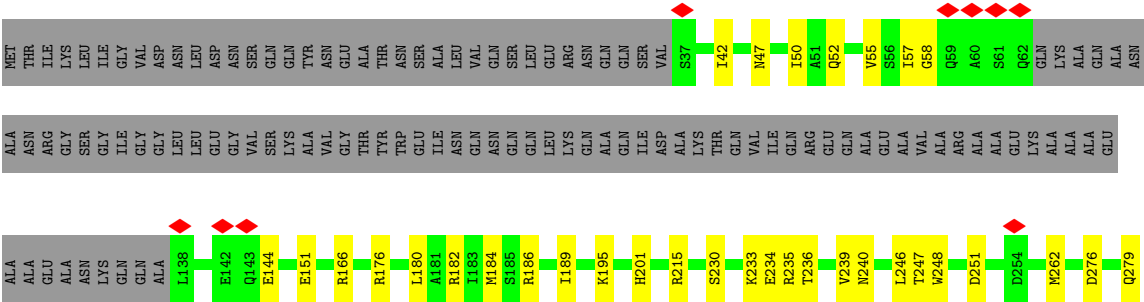


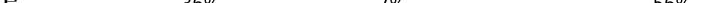


● Molecule 2: Internal virion protein



● Molecule 3: Internal protein



Chain e: 

ASP	PRO	MET	GLN	THR	GLN	ASN	PHE	LYS	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY
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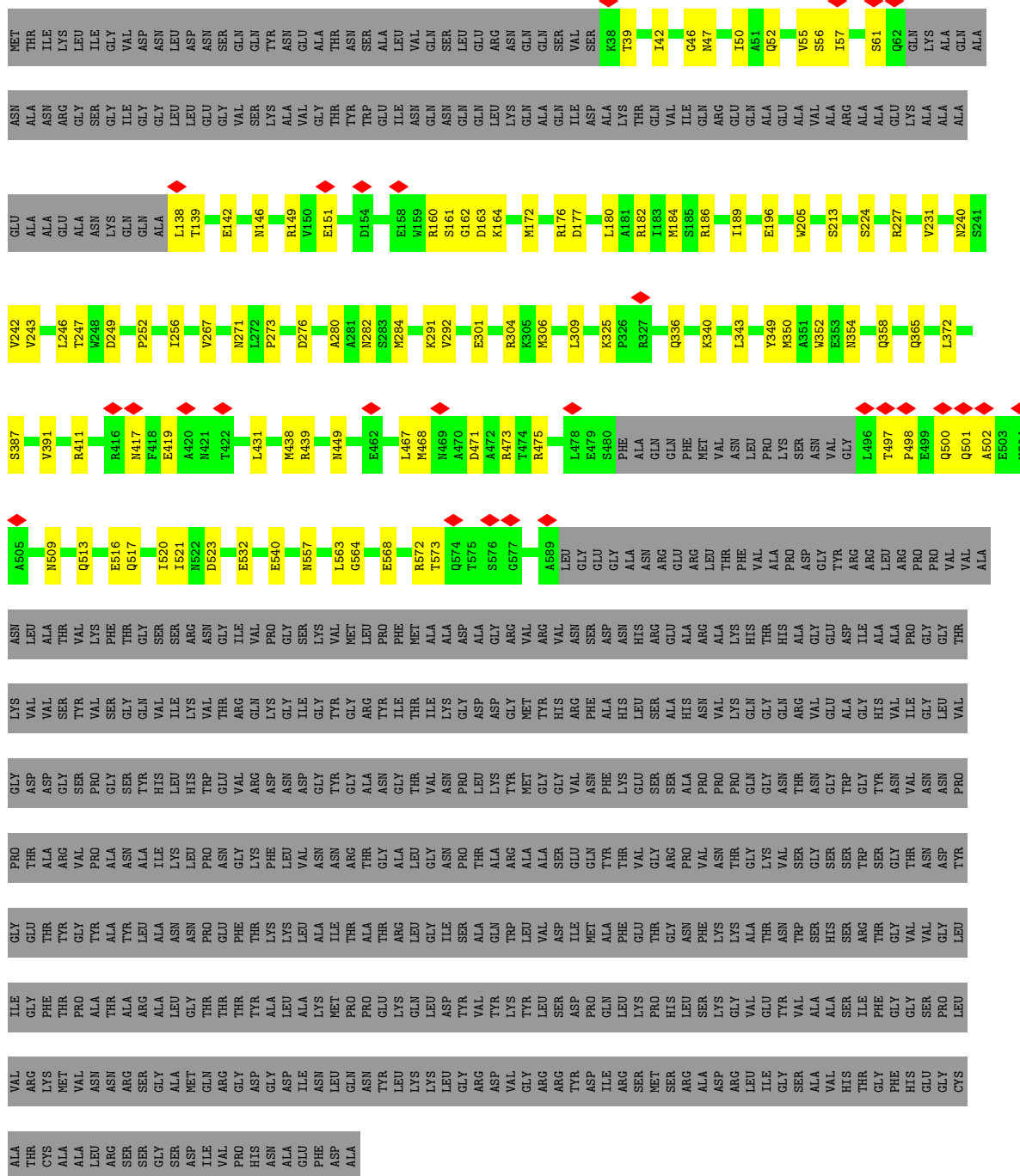
● Molecule 3: Internal protein



MET	THR	ILE	LYS	LEU	ILE	GLY	VAL	ASP	ASN	LEU	ASP	ASN	SER	GLN	GLN	TYR	ASN	ASN	GLU	ALA	THR	THR	SER	ASN	ASN	GLN	GLN	GLN	VAL	S37	L43	N47	Q52	V55	S56	I57	G58	Q59	A60	S61	Q62	GLN	LYS	ALA	ALA	GLN	ALA	ASN	ALA	ASN
ARG	GLY	SER	GLY	ILE	GLY	GLY	LEU	GLY	GLY	LEU	GLY	GLY	VAL	LYS	ALA	VAL	GLY	THR	TRP	ALA	THR	GLU	ILE	ASN	GLN	GLN	GLN	ILE	ASP	LYS	THR	GLN	VAL	ILE	GLN	ARG	ALA	ARG	ALA	ALA	GLU	LYS	ALA	ALA	ALA	GLU	ALA	ALA	ALA	
GLU	ALA	ASN	LYS	GLN	GLN	ALA	L138	E142	Q143	E144	R166	K174	F175	R176	L180	A181	M184	S185	R186	I189	T190	E191	K195	R215	S230	K233	R238	V239	N240	S241	V242	L246	T247	W248	D251	P252	T253	K258	V259	V263	P273	D276								

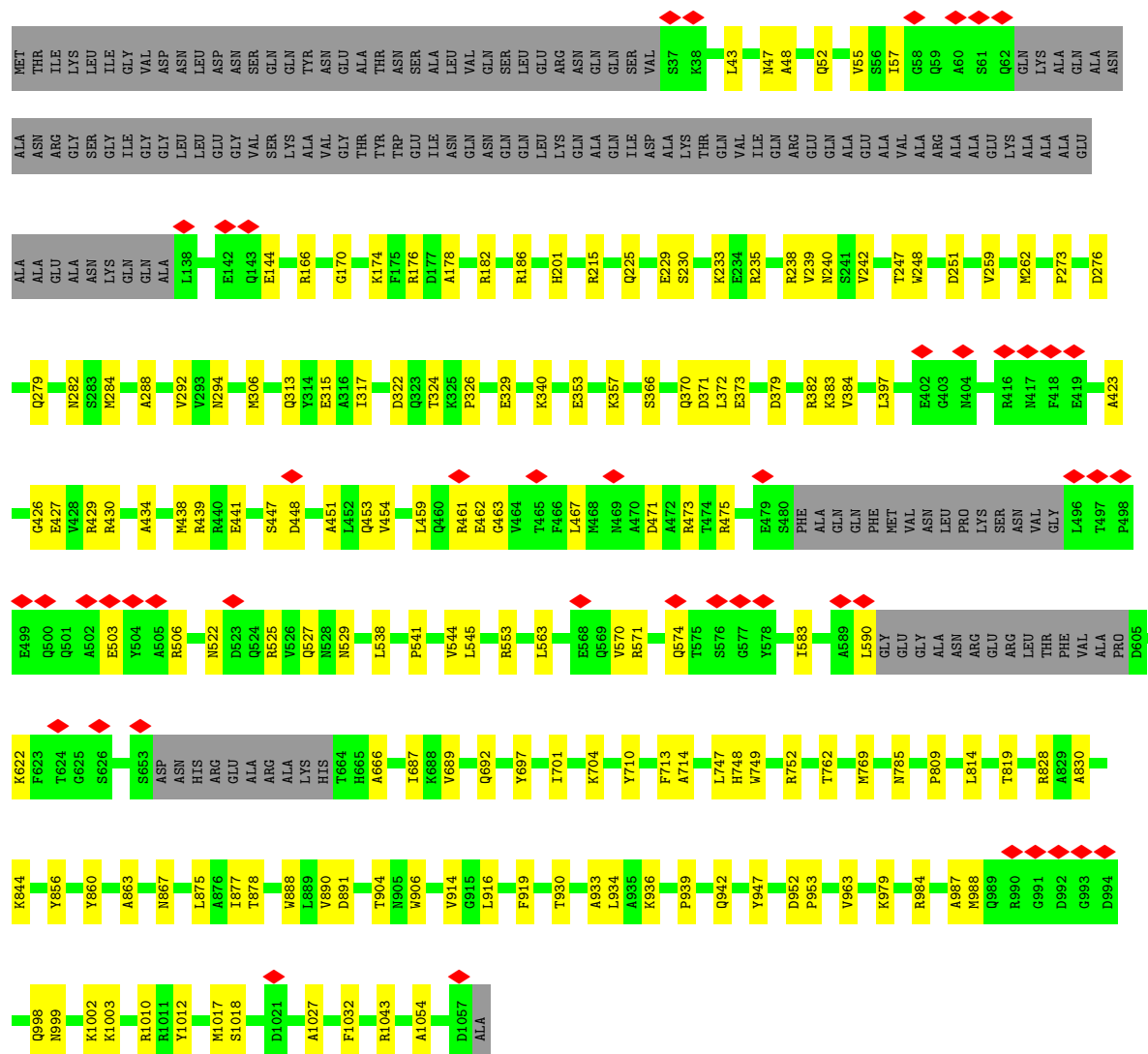


Chain b:

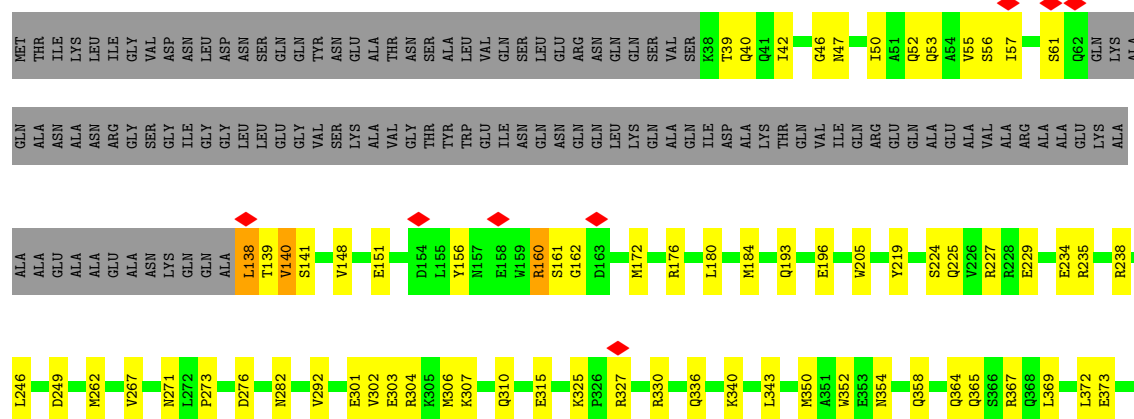
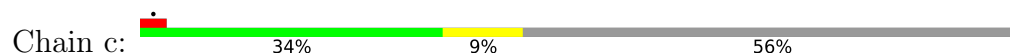


Chain D:





• Molecule 3: Internal protein



ALA	THR	THR	CYS	ALA	ALA	LEU	LEU	ARG	SER	SER	SER	GLY	ALA	ALA	LEU	GLY	ASP	ASP	ILE	GLN	VAL	VAL	PRO	HIS	ASN	ALA	ALA	GLN	GLN	THR	THR	GLY	ASP	ASP	GLN	GLY	THR	THR	GLY	THR	THR	GLY	THR	THR	GLY	THR	THR	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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	F	0.10	0/293	0.36	0/400
1	G	0.11	0/293	0.29	0/400
1	H	0.10	0/293	0.35	0/400
1	I	0.11	0/293	0.31	0/400
1	J	0.10	0/293	0.38	0/400
1	K	0.12	0/293	0.42	1/400 (0.2%)
1	L	0.09	0/293	0.36	0/400
1	M	0.10	0/293	0.27	0/400
1	N	0.10	0/293	0.35	0/400
1	O	0.11	0/293	0.28	0/400
2	V	0.09	0/708	0.22	0/949
2	W	0.09	0/708	0.24	0/949
2	X	0.10	0/708	0.24	0/949
2	Y	0.10	0/708	0.24	0/949
2	Z	0.10	0/708	0.27	0/949
2	v	0.14	0/708	0.26	0/949
2	w	0.16	0/708	0.34	0/949
2	x	0.14	0/708	0.27	0/949
2	y	0.14	0/708	0.25	0/949
2	z	0.16	0/708	0.33	0/949
3	A	0.11	0/7146	0.33	3/9662 (0.0%)
3	B	0.12	0/7146	0.34	4/9662 (0.0%)
3	C	0.11	0/7146	0.28	0/9662
3	D	0.11	0/7146	0.28	0/9662
3	E	0.11	0/7146	0.33	3/9662 (0.0%)
3	a	0.17	0/3701	0.34	3/4993 (0.1%)
3	b	0.17	0/3701	0.37	4/4993 (0.1%)
3	c	0.17	0/3701	0.53	5/4993 (0.1%)
3	d	0.16	0/3701	0.30	0/4993
3	e	0.17	0/3701	0.32	0/4993
All	All	0.13	0/64245	0.33	23/86765 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	a	0	1
3	b	0	1
3	c	0	1
3	d	0	1
3	e	0	1
All	All	0	5

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	162	GLY	N-CA-C	-22.71	74.37	111.38
3	A	579	GLY	N-CA-C	-16.20	88.35	111.03
3	B	579	GLY	N-CA-C	-15.28	89.64	111.03
3	E	579	GLY	N-CA-C	-15.21	89.73	111.03
3	c	161	SER	CB-CA-C	13.87	133.76	110.74
3	b	162	GLY	N-CA-C	-10.54	92.97	111.62
3	c	139	THR	N-CA-CB	9.42	125.76	111.35
3	A	580	GLN	N-CA-CB	7.43	122.13	110.84
3	A	580	GLN	N-CA-C	-6.89	95.75	108.02
3	c	138	LEU	CB-CA-C	-6.81	97.17	110.10
3	B	580	GLN	N-CA-C	-6.54	96.58	108.02
3	E	580	GLN	N-CA-CB	6.52	120.95	110.65
3	E	580	GLN	N-CA-C	-6.52	96.62	108.02
3	B	580	GLN	N-CA-CB	6.49	120.90	110.65
3	a	162	GLY	N-CA-C	-6.12	102.91	112.58
3	c	139	THR	N-CA-C	-5.97	99.73	107.73
3	a	163	ASP	N-CA-C	-5.63	105.07	112.72
3	B	633	PRO	CA-N-CD	-5.60	104.17	112.00
3	b	164	LYS	N-CA-C	-5.38	107.27	113.88
3	a	161	SER	CB-CA-C	-5.15	101.92	110.68
1	K	622	VAL	N-CA-C	-5.14	107.82	112.96
3	b	161	SER	CB-CA-C	-5.06	102.25	110.85
3	b	163	ASP	N-CA-C	-5.02	99.15	107.99

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	a	160	ARG	Sidechain
3	b	160	ARG	Sidechain
3	c	160	ARG	Sidechain
3	d	160	ARG	Sidechain
3	e	160	ARG	Sidechain

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	F	290	0	270	6	0
1	G	290	0	270	10	0
1	H	290	0	270	7	0
1	I	290	0	270	10	0
1	J	290	0	270	7	0
1	K	290	0	270	8	0
1	L	290	0	270	7	0
1	M	290	0	270	7	0
1	N	290	0	270	7	0
1	O	290	0	270	8	0
2	V	706	0	698	17	0
2	W	706	0	698	17	0
2	X	706	0	698	20	0
2	Y	706	0	698	19	0
2	Z	706	0	698	18	0
2	v	706	0	698	14	0
2	w	706	0	698	12	0
2	x	706	0	698	16	0
2	y	706	0	698	14	0
2	z	706	0	698	10	0
3	A	7028	0	6915	106	0
3	B	7028	0	6915	111	0
3	C	7028	0	6915	107	0
3	D	7028	0	6915	108	0
3	E	7028	0	6915	100	0
3	a	3660	0	3597	68	0
3	b	3660	0	3597	74	0
3	c	3660	0	3597	76	0
3	d	3660	0	3597	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	e	3660	0	3597	63	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	63405	0	62240	910	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 7.

All (910) 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)
3:E:578:TYR:CD2	3:E:579:GLY:O	1.92	1.23
3:c:138:LEU:O	3:c:138:LEU:HG	1.65	0.96
3:E:578:TYR:CE2	3:E:579:GLY:O	2.18	0.96
3:b:138:LEU:HD12	3:b:146:ASN:ND2	1.84	0.92
1:O:613:THR:HG22	1:O:615:PRO:HD2	1.52	0.90
1:K:613:THR:HG22	1:K:615:PRO:HD2	1.54	0.90
3:A:577:GLY:O	3:A:578:TYR:CD1	2.26	0.88
1:I:613:THR:HG22	1:I:615:PRO:HD2	1.56	0.85
3:d:47:ASN:HB3	3:d:184:MET:HE1	1.58	0.83
3:c:156:TYR:CZ	3:c:160:ARG:HD2	2.13	0.83
3:E:276:ASP:OD1	3:e:176:ARG:NH2	2.12	0.83
3:d:151:GLU:HG2	3:d:182:ARG:HD3	1.60	0.81
3:A:441:GLU:OE2	3:A:525:ARG:NH2	2.15	0.80
3:d:464:VAL:HG21	3:d:504:TYR:HB3	1.65	0.79
3:e:325:LYS:NZ	3:e:329:GLU:OE1	2.16	0.77
3:a:221:GLU:HG2	3:a:225:GLN:HE21	1.51	0.75
3:b:138:LEU:HD12	3:b:146:ASN:HD21	1.51	0.74
3:B:55:VAL:HG22	3:a:282:ASN:HD22	1.53	0.74
3:B:282:ASN:HB2	3:b:57:ILE:HD13	1.70	0.74
2:v:21:GLN:NE2	2:v:25:GLN:OE1	2.22	0.73
1:F:613:THR:HG22	1:F:615:PRO:HD2	1.72	0.72
1:H:613:THR:HG22	1:H:615:PRO:HD2	1.70	0.71
1:N:613:THR:HG22	1:N:615:PRO:HD2	1.72	0.71
2:V:40:THR:OG1	3:A:382:ARG:NH2	2.23	0.71
2:z:21:GLN:NE2	2:z:25:GLN:OE1	2.22	0.71
3:E:860:TYR:HB3	3:E:1010:ARG:HH12	1.56	0.71
3:b:138:LEU:CD1	3:b:146:ASN:HD21	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:613:THR:HG22	1:L:615:PRO:HD2	1.74	0.70
3:C:251:ASP:OD2	3:c:330:ARG:NH2	2.25	0.69
3:B:441:GLU:OE2	3:B:525:ARG:NH2	2.25	0.69
3:D:451:ALA:HA	3:c:340:LYS:HG3	1.75	0.69
3:c:140:VAL:O	3:c:141:SER:OG	2.08	0.69
3:B:978:ARG:O	3:B:982:ASN:ND2	2.25	0.69
3:d:249:ASP:OD2	3:e:52:GLN:NE2	2.24	0.69
3:B:340:LYS:O	3:b:473:ARG:NH1	2.24	0.69
3:a:464:VAL:HG21	3:a:504:TYR:HB3	1.73	0.69
1:J:613:THR:HG22	1:J:615:PRO:HD2	1.75	0.68
3:e:249:ASP:OD2	3:a:52:GLN:NE2	2.26	0.68
3:e:47:ASN:HB3	3:e:184:MET:HE1	1.76	0.68
3:E:453:GLN:OE1	3:d:336:GLN:NE2	2.27	0.68
3:B:43:LEU:HD21	3:B:184:MET:HG3	1.75	0.68
3:B:860:TYR:HB3	3:B:1010:ARG:HH12	1.58	0.68
3:E:1006:ARG:NH1	3:d:588:THR:O	2.26	0.68
3:e:497:THR:OG1	3:e:500:GLN:OE1	2.12	0.68
3:d:497:THR:OG1	3:d:500:GLN:OE1	2.11	0.68
3:C:451:ALA:HA	3:b:340:LYS:HG3	1.76	0.68
3:d:52:GLN:NE2	3:c:249:ASP:OD2	2.26	0.68
2:y:55:ARG:NH1	3:d:573:THR:OG1	2.27	0.67
3:A:251:ASP:OD2	3:a:330:ARG:NH2	2.28	0.67
3:A:453:GLN:OE1	3:e:336:GLN:NE2	2.27	0.67
3:E:978:ARG:O	3:E:982:ASN:ND2	2.28	0.67
3:E:251:ASP:OD2	3:e:330:ARG:NH2	2.27	0.67
3:d:330:ARG:NH2	3:D:251:ASP:OD2	2.28	0.67
3:D:453:GLN:OE1	3:c:336:GLN:NE2	2.27	0.67
3:C:978:ARG:O	3:C:982:ASN:ND2	2.28	0.67
3:C:43:LEU:HD21	3:C:184:MET:HG3	1.74	0.67
2:Y:40:THR:OG1	3:D:382:ARG:NH2	2.27	0.67
3:b:246:LEU:HD13	3:c:42:ILE:HD11	1.76	0.66
2:w:66:GLU:OE1	2:w:69:ARG:NH2	2.28	0.66
3:b:497:THR:OG1	3:b:500:GLN:OE1	2.12	0.66
3:e:246:LEU:HD13	3:a:42:ILE:HD11	1.76	0.66
2:x:21:GLN:NE2	2:x:25:GLN:OE1	2.27	0.66
2:W:14:GLN:OE1	3:a:271:ASN:ND2	2.29	0.66
2:x:55:ARG:NH1	3:c:573:THR:OG1	2.28	0.66
3:a:497:THR:OG1	3:a:500:GLN:OE1	2.12	0.66
3:E:451:ALA:HA	3:d:340:LYS:HG3	1.79	0.65
3:E:279:GLN:OE1	3:e:176:ARG:NH1	2.30	0.65
3:d:42:ILE:HD11	3:c:246:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:860:TYR:HB3	3:A:1010:ARG:HH12	1.61	0.65
3:B:397:LEU:HD22	3:B:553:ARG:HG2	1.77	0.65
3:B:453:GLN:OE1	3:a:336:GLN:NE2	2.30	0.65
3:c:497:THR:OG1	3:c:500:GLN:OE1	2.12	0.65
2:X:14:GLN:OE1	3:b:271:ASN:ND2	2.30	0.64
2:Z:14:GLN:OE1	3:d:271:ASN:ND2	2.30	0.64
1:O:617:TYR:HB2	1:O:625:GLN:NE2	2.11	0.64
3:D:247:THR:HG22	3:D:248:TRP:H	1.61	0.64
3:D:860:TYR:HB3	3:D:1010:ARG:HH12	1.62	0.64
3:d:246:LEU:HD13	3:e:42:ILE:HD11	1.80	0.64
2:V:89:MET:HE3	2:v:78:PHE:HB3	1.79	0.64
3:A:451:ALA:HA	3:e:340:LYS:HG3	1.80	0.64
3:a:249:ASP:OD2	3:b:52:GLN:NE2	2.31	0.64
3:C:860:TYR:HB3	3:C:1010:ARG:HH12	1.62	0.64
3:E:371:ASP:OD2	3:E:571:ARG:NH2	2.31	0.63
3:E:714:ALA:HB3	3:E:748:HIS:HB3	1.80	0.63
3:D:856:TYR:HE1	3:D:877:ILE:HG13	1.61	0.63
3:E:280:ALA:O	3:E:284:MET:HG3	1.97	0.63
3:C:689:VAL:HG12	3:C:701:ILE:HG12	1.80	0.63
3:C:353:GLU:OE2	3:C:357:LYS:NZ	2.31	0.63
3:C:714:ALA:HB3	3:C:748:HIS:HB3	1.80	0.63
3:b:249:ASP:OD2	3:c:52:GLN:NE2	2.31	0.63
3:D:371:ASP:OD2	3:D:571:ARG:NH2	2.32	0.63
2:V:14:GLN:OE1	3:e:271:ASN:ND2	2.32	0.63
3:C:785:ASN:HB3	3:C:809:PRO:HB3	1.80	0.63
3:B:714:ALA:HB3	3:B:748:HIS:HB3	1.80	0.63
3:E:689:VAL:HG12	3:E:701:ILE:HG12	1.80	0.63
3:A:397:LEU:HD22	3:A:553:ARG:HG2	1.80	0.63
3:A:714:ALA:HB3	3:A:748:HIS:HB3	1.81	0.63
2:X:89:MET:HE3	2:x:78:PHE:HB3	1.80	0.62
2:v:11:GLY:O	2:v:15:LEU:HG	1.98	0.62
2:y:66:GLU:CD	2:y:69:ARG:HH21	2.07	0.62
3:E:687:ILE:HD11	3:E:704:LYS:HB2	1.81	0.62
3:C:453:GLN:OE1	3:b:336:GLN:NE2	2.32	0.62
3:D:441:GLU:OE2	3:D:525:ARG:NH1	2.33	0.62
2:w:11:GLY:O	2:w:15:LEU:HG	1.99	0.62
3:A:438:MET:HE1	3:A:532:GLU:HG2	1.82	0.62
3:D:979:LYS:HG3	3:D:987:ALA:HB2	1.82	0.62
2:Y:14:GLN:OE1	3:c:271:ASN:ND2	2.33	0.62
3:E:459:LEU:HA	3:E:463:GLY:HA2	1.82	0.62
3:A:55:VAL:HG12	3:e:282:ASN:HD22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:785:ASN:HB3	3:A:809:PRO:HB3	1.81	0.62
2:z:11:GLY:O	2:z:15:LEU:HG	2.00	0.61
3:C:282:ASN:HB2	3:c:57:ILE:HD13	1.81	0.61
3:B:689:VAL:HG12	3:B:701:ILE:HG12	1.81	0.61
3:D:353:GLU:OE2	3:D:357:LYS:NZ	2.32	0.61
3:E:247:THR:HG22	3:E:248:TRP:H	1.64	0.61
3:B:439:ARG:NH2	3:B:538:LEU:O	2.33	0.61
3:C:687:ILE:HD11	3:C:704:LYS:HB2	1.81	0.61
3:c:47:ASN:HB3	3:c:184:MET:HE1	1.83	0.61
3:C:340:LYS:O	3:c:473:ARG:NH1	2.25	0.61
3:c:156:TYR:CE2	3:c:160:ARG:HD2	2.35	0.61
3:C:417:ASN:OD1	3:c:524:GLN:NE2	2.34	0.61
2:x:11:GLY:O	2:x:15:LEU:HG	1.99	0.61
3:B:461:ARG:HG2	3:B:462:GLU:HG3	1.82	0.61
3:B:239:VAL:HG13	3:B:259:VAL:HG22	1.81	0.61
3:d:57:ILE:HD13	3:D:282:ASN:HB2	1.82	0.60
3:A:459:LEU:HD12	3:A:467:LEU:HD21	1.83	0.60
3:D:459:LEU:HD12	3:D:467:LEU:HD21	1.83	0.60
1:G:613:THR:HG22	1:G:615:PRO:HD2	1.81	0.60
3:E:397:LEU:HD22	3:E:553:ARG:HG2	1.83	0.60
3:C:461:ARG:HG2	3:C:462:GLU:HG3	1.83	0.60
3:D:714:ALA:HB3	3:D:748:HIS:HB3	1.81	0.60
2:w:55:ARG:NH1	3:b:573:THR:OG1	2.34	0.60
1:M:613:THR:HG22	1:M:615:PRO:HD2	1.82	0.60
2:y:11:GLY:O	2:y:15:LEU:HG	2.01	0.60
3:A:689:VAL:HG12	3:A:701:ILE:HG12	1.83	0.60
3:b:498:PRO:HA	3:b:501:GLN:HB2	1.84	0.60
3:D:785:ASN:HB3	3:D:809:PRO:HB3	1.82	0.60
3:B:144:GLU:HG2	3:B:189:ILE:HD11	1.84	0.60
3:D:984:ARG:NH1	3:D:988:MET:SD	2.73	0.60
3:c:140:VAL:C	3:c:141:SER:HG	2.08	0.60
2:y:66:GLU:OE2	2:y:69:ARG:NH2	2.35	0.60
3:E:246:LEU:HD13	3:A:42:ILE:HD11	1.84	0.60
3:d:458:ARG:NH1	3:D:315:GLU:OE2	2.34	0.60
3:B:785:ASN:HB3	3:B:809:PRO:HB3	1.83	0.60
3:c:302:VAL:HG12	3:c:306:MET:HE2	1.83	0.60
3:A:459:LEU:HA	3:A:463:GLY:HA2	1.83	0.59
3:a:498:PRO:HA	3:a:501:GLN:HB2	1.84	0.59
3:C:276:ASP:OD1	3:c:176:ARG:NH1	2.33	0.59
3:b:517:GLN:O	3:b:521:ILE:HG12	2.02	0.59
3:D:891:ASP:OD1	3:D:1010:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:49:MET:O	2:Z:53:GLN:HG3	2.03	0.59
2:v:66:GLU:CD	2:v:69:ARG:HH21	2.10	0.59
3:A:276:ASP:OD1	3:a:176:ARG:NH1	2.35	0.59
3:A:247:THR:HG22	3:A:248:TRP:H	1.66	0.59
3:e:498:PRO:HA	3:e:501:GLN:HB2	1.84	0.59
3:D:461:ARG:HG2	3:D:462:GLU:HG3	1.84	0.59
2:X:89:MET:HE2	2:x:82:ARG:HB2	1.85	0.59
3:d:280:ALA:O	3:d:284:MET:HG3	2.03	0.59
3:e:172:MET:HE3	3:e:172:MET:HA	1.85	0.59
3:D:459:LEU:HA	3:D:463:GLY:HA2	1.85	0.59
3:b:47:ASN:HB3	3:b:184:MET:HE1	1.85	0.59
3:C:447:SER:OG	3:C:473:ARG:NH2	2.36	0.59
3:E:55:VAL:HG12	3:d:282:ASN:HD22	1.68	0.59
3:E:461:ARG:HG2	3:E:462:GLU:HG3	1.83	0.59
3:B:176:ARG:NH2	3:a:276:ASP:OD1	2.36	0.59
3:C:459:LEU:HA	3:C:463:GLY:HA2	1.85	0.59
3:c:373:GLU:HB2	3:c:383:LYS:HD3	1.85	0.58
3:c:498:PRO:HA	3:c:501:GLN:HB2	1.84	0.58
3:B:240:ASN:ND2	3:b:213:SER:HA	2.18	0.58
3:a:246:LEU:HD13	3:b:42:ILE:HD11	1.84	0.58
2:v:55:ARG:NH1	3:a:573:THR:OG1	2.36	0.58
1:H:619:ILE:O	3:B:215:ARG:NE	2.35	0.58
3:A:439:ARG:NH2	3:A:538:LEU:O	2.36	0.58
3:C:58:GLY:HA2	3:b:306:MET:HE2	1.86	0.58
1:L:619:ILE:O	3:D:215:ARG:NE	2.37	0.58
3:d:498:PRO:HA	3:d:501:GLN:HB2	1.83	0.58
3:E:666:ALA:HB1	3:E:762:THR:HG21	1.85	0.58
3:E:785:ASN:HB3	3:E:809:PRO:HB3	1.84	0.58
3:a:291:LYS:NZ	3:b:39:THR:OG1	2.37	0.58
3:D:397:LEU:HD22	3:D:553:ARG:HG2	1.85	0.58
3:A:313:GLN:O	3:A:317:ILE:HG12	2.04	0.58
3:A:447:SER:OG	3:A:473:ARG:NH2	2.36	0.58
3:A:461:ARG:HG2	3:A:462:GLU:HG3	1.84	0.58
3:C:176:ARG:NH2	3:b:276:ASP:OD1	2.37	0.58
3:B:451:ALA:HA	3:a:340:LYS:HG3	1.85	0.58
3:A:353:GLU:OE2	3:A:357:LYS:NZ	2.37	0.57
3:c:517:GLN:O	3:c:521:ILE:HG12	2.03	0.57
3:A:688:LYS:HE2	3:A:700:TYR:HE1	1.69	0.57
3:A:988:MET:O	3:A:998:GLN:NE2	2.36	0.57
1:N:619:ILE:O	3:E:215:ARG:NE	2.36	0.57
3:d:315:GLU:OE1	3:d:340:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:998:GLN:O	3:D:1002:LYS:HG2	2.04	0.57
3:c:315:GLU:OE2	3:c:340:LYS:NZ	2.38	0.57
3:A:666:ALA:HB1	3:A:762:THR:HG21	1.87	0.57
3:B:246:LEU:HD13	3:C:42:ILE:HD11	1.86	0.57
3:C:397:LEU:HD22	3:C:553:ARG:HG2	1.85	0.57
2:Z:25:GLN:HE21	3:E:544:VAL:HG21	1.69	0.57
1:F:619:ILE:O	3:A:215:ARG:NE	2.36	0.57
3:A:384:VAL:HG13	3:A:936:LYS:HD2	1.86	0.57
3:a:315:GLU:OE2	3:a:340:LYS:NZ	2.38	0.57
3:D:441:GLU:OE1	3:D:529:ASN:ND2	2.31	0.57
2:Z:89:MET:HE2	2:z:82:ARG:HB2	1.87	0.57
3:a:473:ARG:O	3:a:477:LEU:HG	2.05	0.57
2:z:55:ARG:NH1	3:e:573:THR:OG1	2.37	0.57
3:C:247:THR:HG21	3:c:273:PRO:HG3	1.86	0.56
3:A:340:LYS:O	3:a:473:ARG:NH1	2.26	0.56
3:D:988:MET:HE1	3:D:1017:MET:HB2	1.86	0.56
3:E:151:GLU:OE2	3:E:182:ARG:NH1	2.38	0.56
3:C:439:ARG:NH2	3:C:538:LEU:O	2.38	0.56
3:C:988:MET:O	3:C:998:GLN:NE2	2.37	0.56
3:D:666:ALA:HB1	3:D:762:THR:HG21	1.88	0.56
3:D:930:THR:HG23	3:D:933:ALA:H	1.70	0.56
1:N:621:GLY:HA2	3:E:166:ARG:HA	1.87	0.56
3:d:473:ARG:NH1	3:D:340:LYS:O	2.25	0.56
3:D:439:ARG:NH2	3:D:538:LEU:O	2.39	0.56
3:B:934:LEU:O	3:B:942:GLN:NE2	2.38	0.56
3:a:466:PHE:HZ	3:a:474:THR:HG21	1.69	0.56
1:F:621:GLY:HA2	3:A:166:ARG:HA	1.88	0.56
1:J:619:ILE:O	3:C:215:ARG:NE	2.38	0.56
3:E:313:GLN:O	3:E:317:ILE:HG12	2.06	0.56
3:C:448:ASP:OD2	3:C:522:ASN:ND2	2.38	0.56
3:c:224:SER:OG	3:c:227:ARG:NH2	2.38	0.56
1:J:621:GLY:HA2	3:C:166:ARG:HA	1.87	0.56
3:E:248:TRP:HE3	3:A:43:LEU:HD11	1.70	0.56
2:W:49:MET:O	2:W:53:GLN:HG3	2.06	0.56
3:E:439:ARG:NH2	3:E:538:LEU:O	2.38	0.56
3:B:251:ASP:OD2	3:B:253:THR:OG1	2.21	0.56
3:B:930:THR:HG23	3:B:933:ALA:H	1.71	0.56
3:b:516:GLU:O	3:b:520:ILE:HG12	2.06	0.56
3:d:517:GLN:O	3:d:521:ILE:HG12	2.05	0.55
3:B:247:THR:HG22	3:B:248:TRP:H	1.71	0.55
3:d:50:ILE:HD12	3:d:195:LYS:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:471:ASP:O	3:B:475:ARG:HG2	2.06	0.55
3:b:176:ARG:NH2	3:b:177:ASP:OD1	2.39	0.55
3:B:359:TYR:HE1	3:B:363:GLN:HE21	1.53	0.55
3:C:239:VAL:HG21	3:C:284:MET:SD	2.47	0.55
3:C:251:ASP:HB3	3:c:327:ARG:HH11	1.71	0.55
3:C:441:GLU:OE1	3:C:529:ASN:ND2	2.33	0.55
2:W:25:GLN:HE22	3:B:541:PRO:HG2	1.70	0.55
2:w:27:ASN:O	2:w:31:GLN:HG2	2.06	0.55
3:E:988:MET:O	3:E:998:GLN:NE2	2.38	0.55
2:Y:15:LEU:O	2:Y:19:ILE:HG13	2.07	0.55
2:v:70:GLN:O	2:v:74:GLN:HG2	2.07	0.55
3:C:666:ALA:HB1	3:C:762:THR:HG21	1.88	0.55
3:E:58:GLY:HA2	3:d:306:MET:HE2	1.89	0.55
3:A:914:VAL:O	3:A:919:PHE:N	2.39	0.55
3:B:666:ALA:HB1	3:B:762:THR:HG21	1.88	0.55
3:C:55:VAL:HG12	3:b:282:ASN:HD22	1.72	0.55
3:D:687:ILE:HD11	3:D:704:LYS:HB2	1.89	0.55
3:d:213:SER:HA	3:D:240:ASN:ND2	2.22	0.54
3:B:56:SER:C	3:a:282:ASN:HD21	2.15	0.54
3:B:391:VAL:O	3:B:395:VAL:HG23	2.07	0.54
3:a:516:GLU:O	3:a:520:ILE:HG12	2.08	0.54
3:b:280:ALA:O	3:b:284:MET:HG3	2.08	0.54
3:c:138:LEU:O	3:c:138:LEU:CG	2.37	0.54
3:B:57:ILE:HD13	3:a:282:ASN:ND2	2.23	0.54
3:E:282:ASN:HB2	3:e:57:ILE:HD13	1.89	0.54
3:A:930:THR:HG23	3:A:933:ALA:H	1.73	0.54
2:V:89:MET:HE2	2:v:82:ARG:HB2	1.88	0.54
3:E:247:THR:HG21	3:e:273:PRO:HG3	1.89	0.54
3:E:930:THR:HG23	3:E:933:ALA:H	1.72	0.54
3:a:239:VAL:HG21	3:a:284:MET:HG2	1.89	0.54
3:D:43:LEU:HD23	3:D:47:ASN:HB3	1.89	0.54
3:d:149:ARG:NH2	3:d:196:GLU:OE2	2.38	0.54
3:d:176:ARG:NH1	3:D:276:ASP:OD1	2.40	0.54
3:D:57:ILE:HB	3:c:310:GLN:OE1	2.08	0.54
3:c:516:GLU:O	3:c:520:ILE:HG12	2.07	0.54
3:B:280:ALA:O	3:B:284:MET:HG3	2.08	0.54
1:L:641:ILE:O	1:L:645:THR:OG1	2.22	0.54
2:W:6:ILE:HA	2:W:9:ILE:HG12	1.90	0.54
3:b:572:ARG:HG2	3:b:572:ARG:HH11	1.72	0.54
2:x:66:GLU:CD	2:x:69:ARG:HH21	2.14	0.54
3:E:934:LEU:O	3:E:942:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:ALA:O	3:D:182:ARG:HG2	2.08	0.54
1:J:644:THR:HA	3:b:242:VAL:HG22	1.90	0.53
3:D:891:ASP:OD2	3:D:1012:TYR:OH	2.25	0.53
2:Y:83:GLN:O	2:Y:87:GLU:HG2	2.09	0.53
3:B:248:TRP:HE3	3:C:43:LEU:HD11	1.73	0.53
3:b:186:ARG:HB2	3:b:189:ILE:HD12	1.90	0.53
3:B:459:LEU:HA	3:B:463:GLY:HA2	1.89	0.53
3:B:891:ASP:OD1	3:B:1010:ARG:NH2	2.41	0.53
3:b:138:LEU:HD12	3:b:146:ASN:HD22	1.69	0.53
3:D:914:VAL:O	3:D:919:PHE:N	2.40	0.53
1:L:621:GLY:HA2	3:D:166:ARG:HA	1.89	0.53
3:e:280:ALA:O	3:e:284:MET:HG3	2.08	0.53
3:C:280:ALA:O	3:C:284:MET:HG3	2.08	0.53
1:I:617:TYR:HB2	1:I:625:GLN:NE2	2.23	0.53
3:B:687:ILE:HD11	3:B:704:LYS:HB2	1.90	0.53
3:D:875:LEU:HD21	3:D:890:VAL:HG22	1.91	0.53
2:v:66:GLU:OE2	2:v:69:ARG:NH2	2.41	0.53
3:d:292:VAL:HG12	3:e:42:ILE:HD12	1.90	0.53
3:E:315:GLU:OE2	3:e:458:ARG:NH1	2.39	0.53
1:H:621:GLY:HA2	3:B:166:ARG:HA	1.89	0.52
2:Y:47:ARG:HH12	3:D:379:ASP:HB3	1.73	0.52
3:d:301:GLU:OE1	3:d:304:ARG:NH2	2.42	0.52
3:B:43:LEU:HD23	3:B:47:ASN:HB3	1.91	0.52
3:A:179:GLY:O	3:A:183:ILE:HG13	2.08	0.52
3:e:301:GLU:OE1	3:e:304:ARG:NH2	2.42	0.52
2:Y:89:MET:HE3	2:y:78:PHE:HB3	1.91	0.52
3:C:236:THR:HG22	3:C:240:ASN:HD21	1.74	0.52
3:c:234:GLU:OE2	3:c:238:ARG:NH2	2.42	0.52
3:A:248:TRP:HE3	3:B:43:LEU:HD11	1.74	0.52
3:A:448:ASP:OD2	3:A:522:ASN:ND2	2.43	0.52
3:A:934:LEU:O	3:A:942:GLN:NE2	2.43	0.52
3:C:934:LEU:O	3:C:942:GLN:NE2	2.42	0.52
3:D:366:SER:O	3:D:370:GLN:HG2	2.10	0.52
3:d:406:ALA:O	3:d:410:GLU:HG3	2.09	0.52
3:a:55:VAL:HG13	3:a:57:ILE:HG12	1.91	0.52
3:C:263:VAL:HG21	3:C:285:TYR:CE1	2.45	0.52
3:D:235:ARG:HH11	3:D:262:MET:HE1	1.74	0.52
1:J:615:PRO:O	1:J:619:ILE:HG13	2.10	0.51
3:B:263:VAL:HG21	3:B:285:TYR:CE1	2.45	0.51
3:B:459:LEU:HD12	3:B:467:LEU:HD21	1.92	0.51
3:b:449:ASN:ND2	3:b:523:ASP:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:999:ASN:O	3:D:1003:LYS:HG3	2.10	0.51
3:E:448:ASP:OD2	3:E:522:ASN:ND2	2.43	0.51
3:A:628:ARG:NH1	3:A:633:PRO:HG3	2.25	0.51
3:A:893:MET:HG2	3:A:916:LEU:HB3	1.92	0.51
3:c:172:MET:HB3	3:c:205:TRP:HE1	1.75	0.51
3:A:999:ASN:O	3:A:1003:LYS:HG3	2.11	0.51
3:a:172:MET:HB3	3:a:205:TRP:HE1	1.74	0.51
3:a:224:SER:OG	3:a:227:ARG:NH2	2.43	0.51
3:C:317:ILE:HG13	3:c:53:GLN:HG2	1.92	0.51
3:C:697:TYR:HB3	3:C:700:TYR:CD2	2.45	0.51
3:C:930:THR:HG23	3:C:933:ALA:H	1.74	0.51
3:b:301:GLU:OE1	3:b:304:ARG:NH2	2.43	0.51
3:D:471:ASP:O	3:D:475:ARG:HG3	2.10	0.51
2:w:21:GLN:NE2	2:w:25:GLN:OE1	2.44	0.51
3:E:471:ASP:O	3:E:475:ARG:HG2	2.10	0.51
3:d:239:VAL:HG21	3:d:284:MET:SD	2.50	0.51
3:A:247:THR:HG22	3:A:248:TRP:N	2.26	0.51
2:Z:6:ILE:HA	2:Z:9:ILE:HG12	1.92	0.51
3:C:236:THR:O	3:C:240:ASN:ND2	2.43	0.51
1:H:644:THR:HA	3:a:242:VAL:HG22	1.91	0.51
2:V:21:GLN:NE2	3:e:350:MET:SD	2.68	0.51
2:X:6:ILE:HA	2:X:9:ILE:HG12	1.93	0.51
2:y:54:ALA:HB2	3:D:590:LEU:HD21	1.93	0.51
3:E:447:SER:OG	3:E:473:ARG:NH2	2.44	0.51
3:C:916:LEU:HD21	3:C:939:PRO:HB3	1.93	0.51
3:c:301:GLU:OE1	3:c:304:ARG:NH2	2.44	0.51
3:E:247:THR:HG22	3:E:248:TRP:N	2.25	0.51
3:E:916:LEU:HD21	3:E:939:PRO:HB3	1.92	0.51
3:E:956:LYS:HA	3:E:959:LEU:HD13	1.93	0.51
3:A:583:ILE:HD11	3:A:769:MET:HE1	1.92	0.51
3:e:239:VAL:HG21	3:e:284:MET:SD	2.50	0.51
3:D:856:TYR:CE1	3:D:877:ILE:HG13	2.44	0.51
1:N:641:ILE:O	1:N:645:THR:OG1	2.28	0.51
2:Y:6:ILE:HA	2:Y:9:ILE:HG12	1.92	0.51
3:E:933:ALA:O	3:E:937:MET:HG3	2.11	0.51
3:e:449:ASN:ND2	3:e:523:ASP:OD1	2.44	0.51
3:B:447:SER:OG	3:B:473:ARG:NH2	2.43	0.51
2:x:66:GLU:OE2	2:x:69:ARG:NH2	2.44	0.50
3:d:365:GLN:NE2	3:d:557:ASN:OD1	2.40	0.50
3:a:301:GLU:OE1	3:a:304:ARG:NH2	2.44	0.50
3:b:438:MET:HE1	3:b:532:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:54:ALA:HB2	3:E:590:LEU:HD21	1.93	0.50
3:b:498:PRO:O	3:b:502:ALA:N	2.44	0.50
1:O:615:PRO:O	1:O:619:ILE:HG12	2.11	0.50
3:B:445:LEU:HD11	3:B:525:ARG:HH21	1.77	0.50
3:B:577:GLY:O	3:B:578:TYR:CG	2.63	0.50
3:C:937:MET:O	3:C:942:GLN:NE2	2.44	0.50
3:B:863:ALA:O	3:B:867:ASN:ND2	2.44	0.50
3:D:239:VAL:HG21	3:D:284:MET:SD	2.51	0.50
1:M:617:TYR:HB2	1:M:625:GLN:OE1	2.11	0.50
2:Y:89:MET:HE2	2:y:82:ARG:HB2	1.94	0.50
3:E:1006:ARG:HH12	3:d:589:ALA:HA	1.76	0.50
3:d:449:ASN:ND2	3:d:523:ASP:OD1	2.44	0.50
3:B:856:TYR:HE1	3:B:877:ILE:HG13	1.77	0.50
3:C:247:THR:HG22	3:C:248:TRP:H	1.76	0.50
3:C:856:TYR:HE1	3:C:877:ILE:HG13	1.77	0.50
3:E:340:LYS:O	3:e:473:ARG:NH1	2.45	0.50
3:e:509:ASN:O	3:e:513:GLN:HG2	2.12	0.50
3:c:55:VAL:HG13	3:c:57:ILE:HG12	1.94	0.50
3:E:628:ARG:NH1	3:E:633:PRO:HG3	2.27	0.50
3:B:577:GLY:O	3:B:578:TYR:CD2	2.65	0.50
2:v:54:ALA:HB2	3:A:590:LEU:HD21	1.94	0.50
2:z:15:LEU:HD13	3:E:234:GLU:OE1	2.12	0.50
3:A:688:LYS:HE2	3:A:700:TYR:CE1	2.47	0.50
3:D:426:GLY:HA2	3:D:429:ARG:HE	1.76	0.49
3:c:498:PRO:O	3:c:502:ALA:N	2.44	0.49
3:E:459:LEU:HD12	3:E:467:LEU:HD21	1.94	0.49
3:A:366:SER:O	3:A:370:GLN:HG2	2.11	0.49
3:e:163:ASP:C	3:e:165:PHE:N	2.67	0.49
3:B:916:LEU:HD21	3:B:939:PRO:HB3	1.94	0.49
3:C:43:LEU:HD23	3:C:47:ASN:HB3	1.94	0.49
3:C:172:MET:HB3	3:C:205:TRP:HE1	1.76	0.49
3:D:48:ALA:O	3:D:52:GLN:HG3	2.12	0.49
3:D:689:VAL:HG12	3:D:701:ILE:HG12	1.94	0.49
1:I:643:PHE:CZ	3:B:258:LYS:HB3	2.48	0.49
2:Y:25:GLN:CD	3:c:350:MET:HE3	2.36	0.49
3:E:423:ALA:HB3	3:E:906:TRP:HB2	1.94	0.49
3:d:288:ALA:O	3:d:292:VAL:HG22	2.12	0.49
3:A:247:THR:HG21	3:a:273:PRO:HG3	1.94	0.49
3:a:498:PRO:O	3:a:502:ALA:N	2.45	0.49
3:D:448:ASP:OD2	3:D:522:ASN:ND2	2.45	0.49
1:M:644:THR:HA	3:D:242:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:6:ILE:HA	2:V:9:ILE:HG12	1.93	0.49
3:A:235:ARG:HH11	3:A:262:MET:HE1	1.77	0.49
3:A:263:VAL:HG21	3:A:285:TYR:CE1	2.47	0.49
3:A:856:TYR:HE1	3:A:877:ILE:HG13	1.76	0.49
3:B:247:THR:HG22	3:B:248:TRP:N	2.27	0.49
3:B:426:GLY:HA2	3:B:429:ARG:HE	1.77	0.49
3:a:447:SER:OG	3:a:473:ARG:NH2	2.43	0.49
3:C:366:SER:O	3:C:370:GLN:HG2	2.12	0.49
3:b:267:VAL:HG21	3:b:343:LEU:HD23	1.94	0.49
3:D:934:LEU:O	3:D:942:GLN:NE2	2.45	0.49
1:G:617:TYR:HB2	1:G:625:GLN:OE1	2.12	0.49
3:A:833:GLN:HG3	3:A:838:ARG:NH2	2.28	0.49
3:e:55:VAL:HG13	3:e:57:ILE:HG12	1.93	0.49
3:e:498:PRO:O	3:e:502:ALA:N	2.44	0.49
3:C:326:PRO:HG2	3:C:329:GLU:HB3	1.95	0.49
3:C:426:GLY:HA2	3:C:429:ARG:HE	1.77	0.49
3:c:447:SER:OG	3:c:473:ARG:NH2	2.43	0.49
3:d:40:GLN:NE2	3:d:177:ASP:OD2	2.45	0.49
3:A:43:LEU:HD21	3:A:184:MET:HG3	1.93	0.49
3:B:458:ARG:HG2	3:B:466:PHE:CD1	2.47	0.49
1:I:644:THR:HA	3:B:242:VAL:HG22	1.93	0.49
2:W:25:GLN:NE2	3:a:350:MET:HE3	2.27	0.49
2:x:26:ALA:O	2:x:30:ARG:HG2	2.12	0.49
3:E:366:SER:O	3:E:370:GLN:HG2	2.13	0.49
3:d:162:GLY:C	3:d:164:LYS:N	2.70	0.49
3:B:439:ARG:HH12	3:B:545:LEU:HD12	1.78	0.49
3:b:468:MET:N	3:b:468:MET:HE2	2.28	0.49
2:y:21:GLN:NE2	2:y:25:GLN:OE1	2.46	0.49
3:E:914:VAL:O	3:E:919:PHE:N	2.42	0.49
3:e:417:ASN:HD21	3:e:419:GLU:HB2	1.78	0.49
2:y:26:ALA:O	2:y:30:ARG:HG2	2.13	0.49
3:E:426:GLY:HA2	3:E:429:ARG:HE	1.78	0.49
3:a:50:ILE:HD12	3:a:195:LYS:HE3	1.94	0.49
3:a:56:SER:OG	3:a:61:SER:O	2.26	0.49
3:a:378:ILE:HG23	3:a:382:ARG:HB3	1.95	0.49
2:W:52:LEU:HD13	3:B:573:THR:HG21	1.95	0.48
3:d:176:ARG:NH2	3:d:177:ASP:OD1	2.45	0.48
3:B:144:GLU:OE2	3:B:186:ARG:HB3	2.13	0.48
3:B:313:GLN:O	3:B:317:ILE:HG12	2.13	0.48
2:Y:25:GLN:HE22	3:D:541:PRO:HG2	1.78	0.48
3:E:815:VAL:HG12	3:E:816:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:THR:HG22	3:C:248:TRP:N	2.28	0.48
2:X:25:GLN:CD	3:b:350:MET:HE3	2.38	0.48
2:x:70:GLN:O	2:x:74:GLN:HG2	2.13	0.48
2:y:66:GLU:CD	2:y:69:ARG:NH2	2.71	0.48
3:A:423:ALA:HB3	3:A:906:TRP:HB2	1.95	0.48
3:C:144:GLU:OE2	3:C:186:ARG:HB3	2.14	0.48
3:E:427:GLU:OE2	3:E:430:ARG:NH2	2.43	0.48
3:d:498:PRO:O	3:d:502:ALA:N	2.44	0.48
3:A:426:GLY:HA2	3:A:429:ARG:HE	1.78	0.48
1:N:629:GLY:O	1:N:633:GLN:HG3	2.12	0.48
2:x:54:ALA:HB2	3:C:590:LEU:HD21	1.96	0.48
3:a:417:ASN:HD21	3:a:419:GLU:HB2	1.79	0.48
3:b:291:LYS:NZ	3:c:39:THR:OG1	2.46	0.48
3:D:451:ALA:CA	3:c:340:LYS:HG3	2.43	0.48
2:Y:48:GLN:O	2:Y:52:LEU:HD23	2.14	0.48
2:y:70:GLN:O	2:y:74:GLN:HG2	2.13	0.48
3:A:184:MET:HE2	3:A:198:ILE:HD11	1.93	0.48
2:Z:52:LEU:HD13	3:E:573:THR:HG21	1.96	0.48
3:A:172:MET:HE1	3:e:233:LYS:NZ	2.29	0.48
3:c:267:VAL:HG21	3:c:343:LEU:HD23	1.96	0.48
2:W:57:GLN:HE21	2:W:61:ASN:HD21	1.62	0.48
3:d:417:ASN:HD21	3:d:419:GLU:HB2	1.79	0.48
3:B:239:VAL:HG21	3:B:284:MET:SD	2.53	0.48
3:B:625:GLY:O	3:B:628:ARG:NH2	2.47	0.48
3:a:186:ARG:HG3	3:a:186:ARG:HH11	1.78	0.48
3:C:423:ALA:HB3	3:C:906:TRP:HB2	1.95	0.48
2:V:25:GLN:NE2	3:e:350:MET:HE2	2.29	0.48
2:w:54:ALA:HB2	3:B:590:LEU:HD21	1.95	0.48
3:d:163:ASP:C	3:d:165:PHE:N	2.71	0.48
3:A:280:ALA:O	3:A:284:MET:HG3	2.13	0.48
3:C:459:LEU:HD12	3:C:467:LEU:HD21	1.96	0.48
3:E:288:ALA:O	3:E:292:VAL:HG22	2.14	0.47
3:d:447:SER:OG	3:d:473:ARG:NH2	2.42	0.47
3:e:382:ARG:HG3	3:e:382:ARG:HH11	1.78	0.47
3:B:889:LEU:HG	3:B:893:MET:SD	2.54	0.47
2:Y:57:GLN:HE21	2:Y:61:ASN:HD21	1.62	0.47
3:B:174:LYS:HA	3:a:225:GLN:OE1	2.14	0.47
3:B:366:SER:O	3:B:370:GLN:HG2	2.14	0.47
3:C:236:THR:HG22	3:C:240:ASN:ND2	2.29	0.47
3:D:144:GLU:OE2	3:D:186:ARG:HB3	2.14	0.47
3:D:322:ASP:OD1	3:D:324:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:710:TYR:N	3:D:752:ARG:O	2.41	0.47
3:D:916:LEU:HD21	3:D:939:PRO:HB3	1.96	0.47
2:v:26:ALA:O	2:v:30:ARG:HG2	2.13	0.47
2:w:26:ALA:O	2:w:30:ARG:HG2	2.13	0.47
3:B:423:ALA:HB3	3:B:906:TRP:HB2	1.95	0.47
3:B:914:VAL:O	3:B:919:PHE:N	2.42	0.47
3:c:373:GLU:OE1	3:c:383:LYS:NZ	2.31	0.47
3:d:325:LYS:NZ	3:d:329:GLU:OE1	2.33	0.47
3:e:547:LYS:C	3:e:548:ASN:HD22	2.22	0.47
3:B:988:MET:O	3:B:998:GLN:NE2	2.40	0.47
3:C:874:LYS:NZ	3:C:944:ASP:OD1	2.46	0.47
3:D:583:ILE:HD11	3:D:769:MET:HE1	1.95	0.47
2:Z:11:GLY:O	2:Z:15:LEU:HG	2.15	0.47
3:E:561:TYR:O	3:E:565:THR:HG23	2.14	0.47
3:A:888:TRP:HB3	3:A:963:VAL:HG23	1.97	0.47
3:B:445:LEU:HD11	3:B:525:ARG:NH2	2.30	0.47
3:C:988:MET:SD	3:C:1017:MET:HB2	2.55	0.47
2:X:57:GLN:HE21	2:X:61:ASN:HD21	1.63	0.47
3:E:373:GLU:HB2	3:E:383:LYS:HG3	1.97	0.47
3:B:276:ASP:OD1	3:b:176:ARG:NH1	2.47	0.47
3:B:427:GLU:OE2	3:B:430:ARG:NH2	2.44	0.47
3:D:326:PRO:HG2	3:D:329:GLU:HB3	1.96	0.47
3:c:417:ASN:HD21	3:c:419:GLU:HB2	1.79	0.47
1:I:634:ALA:HB2	2:w:16:VAL:HG22	1.97	0.47
1:L:640:LEU:O	1:L:644:THR:HG23	2.15	0.47
2:V:57:GLN:HE21	2:V:61:ASN:HD21	1.61	0.47
2:Y:25:GLN:HE21	3:D:544:VAL:HG21	1.80	0.47
2:x:27:ASN:O	2:x:31:GLN:HG2	2.15	0.47
2:z:26:ALA:O	2:z:30:ARG:HG2	2.14	0.47
3:E:856:TYR:HE1	3:E:877:ILE:HG13	1.79	0.47
3:d:55:VAL:HG22	3:D:282:ASN:HD22	1.80	0.47
3:A:43:LEU:HD23	3:A:47:ASN:HB3	1.96	0.47
3:e:267:VAL:HG21	3:e:343:LEU:HD23	1.95	0.47
3:B:288:ALA:O	3:B:292:VAL:HG22	2.15	0.47
3:a:151:GLU:OE2	3:a:182:ARG:HD3	2.15	0.47
3:a:239:VAL:HG11	3:a:284:MET:HG2	1.97	0.47
3:b:172:MET:HB3	3:b:205:TRP:HE1	1.80	0.47
3:b:417:ASN:HD21	3:b:419:GLU:HB2	1.78	0.47
3:c:56:SER:OG	3:c:61:SER:O	2.32	0.47
1:F:623:SER:OG	3:e:233:LYS:HG3	2.14	0.47
3:E:236:THR:HG22	3:E:240:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:372:LEU:HD11	3:d:563:LEU:HB3	1.96	0.47
3:d:471:ASP:OD1	3:d:471:ASP:N	2.47	0.47
3:A:814:LEU:HD13	3:A:819:THR:HB	1.97	0.47
3:A:1032:PHE:CE2	3:A:1043:ARG:HG3	2.50	0.47
3:e:365:GLN:NE2	3:e:557:ASN:OD1	2.38	0.47
3:e:473:ARG:O	3:e:477:LEU:HG	2.15	0.47
3:a:238:ARG:O	3:a:242:VAL:HG23	2.15	0.47
1:I:643:PHE:CE1	3:B:242:VAL:HG21	2.50	0.47
3:B:1032:PHE:CE2	3:B:1043:ARG:HG3	2.50	0.47
3:C:914:VAL:O	3:C:919:PHE:N	2.41	0.47
1:F:616:PHE:HE2	2:v:1:MET:HG3	1.79	0.46
3:E:884:ILE:HG21	3:E:959:LEU:HB3	1.96	0.46
3:d:509:ASN:O	3:d:513:GLN:HG2	2.16	0.46
3:e:163:ASP:C	3:e:165:PHE:H	2.23	0.46
3:c:235:ARG:HD3	3:c:262:MET:HE1	1.96	0.46
2:Z:57:GLN:HE21	2:Z:61:ASN:HD21	1.62	0.46
2:v:66:GLU:CD	2:v:69:ARG:NH2	2.73	0.46
3:e:159:TRP:HB3	3:e:165:PHE:CE2	2.50	0.46
3:e:372:LEU:HD11	3:e:563:LEU:HB3	1.96	0.46
3:C:893:MET:HG2	3:C:916:LEU:HB3	1.96	0.46
3:b:509:ASN:O	3:b:513:GLN:HG2	2.16	0.46
3:B:238:ARG:O	3:B:242:VAL:HG23	2.16	0.46
3:b:224:SER:OG	3:b:227:ARG:NH2	2.49	0.46
3:D:55:VAL:HG12	3:c:282:ASN:HD22	1.80	0.46
3:D:313:GLN:O	3:D:317:ILE:HG12	2.15	0.46
3:D:427:GLU:OE2	3:D:430:ARG:NH2	2.46	0.46
3:c:378:ILE:HG23	3:c:382:ARG:HB3	1.97	0.46
2:V:48:GLN:O	2:V:52:LEU:HD23	2.15	0.46
2:X:25:GLN:HE22	3:C:541:PRO:HG2	1.80	0.46
3:a:449:ASN:ND2	3:a:523:ASP:OD1	2.48	0.46
3:b:149:ARG:HH12	3:b:196:GLU:CD	2.23	0.46
3:d:327:ARG:HH11	3:D:251:ASP:HB3	1.80	0.46
3:C:451:ALA:CA	3:b:340:LYS:HG3	2.42	0.46
3:D:863:ALA:O	3:D:867:ASN:ND2	2.49	0.46
1:K:623:SER:HB2	3:C:230:SER:HA	1.98	0.46
3:A:451:ALA:CA	3:e:340:LYS:HG3	2.45	0.46
3:A:916:LEU:HD21	3:A:939:PRO:HB3	1.97	0.46
3:D:888:TRP:HB3	3:D:963:VAL:HG23	1.98	0.46
3:c:438:MET:HE1	3:c:532:GLU:OE2	2.15	0.46
3:d:378:ILE:HG23	3:d:382:ARG:HB3	1.97	0.46
3:A:288:ALA:O	3:A:292:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:888:TRP:HB3	3:B:963:VAL:HG23	1.97	0.46
3:b:471:ASP:N	3:b:471:ASP:OD1	2.48	0.46
3:D:423:ALA:HB3	3:D:906:TRP:HB2	1.97	0.46
3:D:814:LEU:HD11	3:D:830:ALA:HB2	1.98	0.46
2:y:82:ARG:O	2:y:86:GLN:HG3	2.16	0.46
3:E:1032:PHE:CE2	3:E:1043:ARG:HG3	2.50	0.46
3:A:239:VAL:HG11	3:A:284:MET:HB3	1.97	0.46
3:A:282:ASN:OD1	3:a:57:ILE:HA	2.16	0.46
3:a:369:LEU:HG	3:a:383:LYS:HG3	1.98	0.46
3:D:273:PRO:HD2	3:D:276:ASP:HB2	1.98	0.46
3:D:1032:PHE:CE2	3:D:1043:ARG:HG3	2.51	0.46
1:K:617:TYR:HB2	1:K:625:GLN:OE1	2.16	0.46
3:E:888:TRP:HB3	3:E:963:VAL:HG23	1.98	0.46
3:b:46:GLY:O	3:b:50:ILE:HG12	2.16	0.46
3:b:176:ARG:O	3:b:180:LEU:HG	2.16	0.46
1:K:635:ASP:OD1	1:K:635:ASP:N	2.49	0.45
1:H:632:ILE:HD11	2:w:1:MET:HE2	1.97	0.45
3:A:326:PRO:HG2	3:A:329:GLU:HB3	1.98	0.45
3:B:247:THR:HG21	3:b:273:PRO:HG3	1.98	0.45
3:C:632:VAL:HG23	3:C:635:SER:HB3	1.98	0.45
3:D:239:VAL:HG13	3:D:259:VAL:HG22	1.99	0.45
1:M:615:PRO:HG2	2:Z:2:GLY:HA2	1.98	0.45
1:J:643:PHE:CE2	3:b:242:VAL:HG21	2.51	0.45
2:Z:25:GLN:CD	3:d:350:MET:HE3	2.40	0.45
3:C:710:TYR:N	3:C:752:ARG:O	2.44	0.45
3:C:814:LEU:HD13	3:C:819:THR:HB	1.97	0.45
3:E:451:ALA:CA	3:d:340:LYS:HG3	2.45	0.45
3:E:999:ASN:O	3:E:1003:LYS:HG3	2.16	0.45
3:A:814:LEU:HD11	3:A:830:ALA:HB2	1.98	0.45
3:B:964:GLU:HG3	3:B:984:ARG:HH12	1.81	0.45
3:C:1032:PHE:CE2	3:C:1043:ARG:HG3	2.51	0.45
3:A:971:PHE:HB2	3:A:1000:TYR:CE2	2.52	0.45
3:B:791:TYR:O	3:B:859:THR:OG1	2.32	0.45
3:B:878:THR:HG23	3:B:947:TYR:HB2	1.98	0.45
3:B:952:ASP:OD1	3:B:953:PRO:HD2	2.16	0.45
2:V:48:GLN:HG2	2:V:52:LEU:HD23	1.98	0.45
2:x:1:MET:HB2	2:x:2:GLY:H	1.61	0.45
3:d:238:ARG:HD2	3:d:262:MET:SD	2.57	0.45
3:d:572:ARG:HG2	3:d:572:ARG:HH11	1.82	0.45
3:B:326:PRO:HG2	3:B:329:GLU:HB3	1.99	0.45
3:a:509:ASN:O	3:a:513:GLN:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:752:ARG:NH1	3:C:758:GLY:O	2.37	0.45
3:c:364:GLN:OE1	3:c:367:ARG:NH2	2.49	0.45
3:c:373:GLU:HB2	3:c:383:LYS:CD	2.47	0.45
1:I:623:SER:HB2	3:B:230:SER:HA	1.99	0.45
2:X:49:MET:O	2:X:53:GLN:HG3	2.17	0.45
3:E:57:ILE:HB	3:d:310:GLN:OE1	2.15	0.45
3:A:577:GLY:O	3:A:578:TYR:CG	2.69	0.45
3:A:878:THR:HG23	3:A:947:TYR:HB2	1.99	0.45
3:b:467:LEU:O	3:b:475:ARG:NH2	2.49	0.45
3:D:170:GLY:HA2	3:c:229:GLU:HG2	1.99	0.45
3:D:288:ALA:O	3:D:292:VAL:HG22	2.16	0.45
3:c:509:ASN:O	3:c:513:GLN:HG2	2.16	0.45
1:K:643:PHE:CE1	3:C:242:VAL:HG21	2.52	0.45
3:A:833:GLN:HG3	3:A:838:ARG:HH21	1.80	0.45
3:A:44:GLU:OE1	3:A:47:ASN:ND2	2.50	0.45
3:D:749:TRP:HH2	3:D:769:MET:HG3	1.82	0.45
3:c:560:MET:HE3	3:c:560:MET:HB3	1.83	0.45
1:J:641:ILE:O	1:J:645:THR:OG1	2.30	0.45
3:d:239:VAL:HG13	3:d:259:VAL:HG22	1.99	0.45
3:D:372:LEU:HD11	3:D:563:LEU:HB3	1.98	0.45
1:G:619:ILE:O	3:a:215:ARG:NE	2.34	0.45
3:E:236:THR:HG22	3:E:240:ASN:ND2	2.32	0.45
3:e:471:ASP:OD1	3:e:471:ASP:N	2.50	0.45
3:C:288:ALA:O	3:C:292:VAL:HG22	2.17	0.45
3:C:713:PHE:HB3	3:C:747:LEU:HD11	1.99	0.45
3:e:516:GLU:O	3:e:520:ILE:HG12	2.17	0.44
3:B:806:ILE:HD12	3:B:814:LEU:HD23	1.97	0.44
3:a:159:TRP:HA	3:a:164:LYS:HE3	1.99	0.44
3:d:56:SER:OG	3:d:61:SER:O	2.34	0.44
3:A:251:ASP:HB3	3:a:327:ARG:HH11	1.82	0.44
3:e:224:SER:OG	3:e:227:ARG:NH2	2.50	0.44
3:D:689:VAL:O	3:D:689:VAL:HG23	2.18	0.44
3:d:172:MET:HB2	3:D:229:GLU:OE1	2.17	0.44
3:a:307:LYS:HA	3:a:307:LYS:HD3	1.77	0.44
3:a:572:ARG:HH11	3:a:572:ARG:HG2	1.82	0.44
3:C:439:ARG:HH12	3:C:545:LEU:HD12	1.83	0.44
2:X:25:GLN:HE21	3:C:544:VAL:HG21	1.83	0.44
3:d:163:ASP:C	3:d:165:PHE:H	2.26	0.44
3:D:238:ARG:O	3:D:242:VAL:HG23	2.17	0.44
1:O:623:SER:HB2	3:E:230:SER:HA	2.00	0.44
2:Y:49:MET:O	2:Y:53:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:364:GLN:OE1	3:a:367:ARG:NH2	2.50	0.44
3:a:517:GLN:O	3:a:521:ILE:HG12	2.17	0.44
3:E:878:THR:HG23	3:E:947:TYR:HB2	1.99	0.44
3:B:273:PRO:HD2	3:B:276:ASP:HB2	2.00	0.44
3:C:814:LEU:HD11	3:C:830:ALA:HB2	1.98	0.44
3:C:878:THR:HG23	3:C:947:TYR:HB2	1.98	0.44
3:c:193:GLN:HA	3:c:196:GLU:HG2	1.99	0.44
2:W:40:THR:HG23	3:B:382:ARG:HD3	1.99	0.44
3:e:382:ARG:HG3	3:e:382:ARG:NH1	2.32	0.44
3:a:46:GLY:O	3:a:50:ILE:HG12	2.18	0.44
3:C:372:LEU:HD11	3:C:563:LEU:HB3	2.00	0.44
3:d:55:VAL:HG13	3:d:57:ILE:HG12	1.99	0.44
3:A:874:LYS:NZ	3:A:944:ASP:OD1	2.42	0.44
3:C:791:TYR:O	3:C:859:THR:OG1	2.34	0.44
3:C:937:MET:HE1	3:C:945:TYR:HE2	1.83	0.44
1:O:619:ILE:O	3:e:215:ARG:NE	2.36	0.44
1:N:616:PHE:HE2	2:z:1:MET:HG3	1.82	0.44
3:B:1027:ALA:O	3:B:1054:ALA:N	2.51	0.44
3:C:888:TRP:HB3	3:C:963:VAL:HG23	2.00	0.44
3:b:247:THR:HA	3:c:40:GLN:NE2	2.33	0.44
3:D:176:ARG:NH1	3:c:276:ASP:OD1	2.50	0.44
1:G:615:PRO:HG2	2:W:2:GLY:HA2	2.00	0.43
2:V:29:GLN:OE1	3:A:548:ASN:ND2	2.50	0.43
2:W:76:GLN:O	2:W:80:ILE:HG12	2.18	0.43
3:d:438:MET:HE3	3:d:533:LEU:HD21	1.99	0.43
1:M:623:SER:HB2	3:D:230:SER:HA	2.00	0.43
1:L:627:ALA:O	1:L:631:ASN:ND2	2.51	0.43
2:Z:48:GLN:O	2:Z:52:LEU:HD23	2.18	0.43
2:Z:76:GLN:O	2:Z:80:ILE:HG12	2.19	0.43
2:x:66:GLU:CD	2:x:69:ARG:NH2	2.76	0.43
3:A:57:ILE:HB	3:e:310:GLN:OE1	2.18	0.43
3:A:144:GLU:OE2	3:A:186:ARG:HB3	2.17	0.43
3:C:887:GLN:NE2	3:C:1010:ARG:HD2	2.34	0.43
3:b:55:VAL:HG13	3:b:57:ILE:HG12	2.00	0.43
3:c:354:ASN:O	3:c:358:GLN:HG3	2.18	0.43
3:c:365:GLN:NE2	3:c:557:ASN:OD1	2.40	0.43
2:X:83:GLN:O	2:X:87:GLU:HG2	2.17	0.43
2:y:1:MET:HA	2:y:6:ILE:HD11	2.00	0.43
3:C:933:ALA:O	3:C:937:MET:HG3	2.17	0.43
3:C:998:GLN:HG2	3:C:1017:MET:HG3	2.00	0.43
1:I:615:PRO:O	1:I:619:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:144:GLU:OE1	3:E:186:ARG:HB3	2.18	0.43
3:E:439:ARG:HH12	3:E:545:LEU:HD12	1.83	0.43
3:B:427:GLU:OE2	3:B:536:TYR:OH	2.25	0.43
3:a:307:LYS:O	3:a:310:GLN:HB2	2.19	0.43
3:E:984:ARG:HG3	3:E:984:ARG:HH11	1.81	0.43
3:A:439:ARG:HH12	3:A:545:LEU:HD12	1.83	0.43
3:C:1027:ALA:O	3:C:1054:ALA:N	2.52	0.43
3:D:447:SER:OG	3:D:473:ARG:NH2	2.48	0.43
3:D:878:THR:HG23	3:D:947:TYR:HB2	1.99	0.43
3:c:372:LEU:HD11	3:c:563:LEU:HB3	2.01	0.43
2:V:76:GLN:O	2:V:80:ILE:HG12	2.18	0.43
2:X:15:LEU:O	2:X:19:ILE:HG13	2.18	0.43
2:Y:76:GLN:O	2:Y:80:ILE:HG12	2.18	0.43
3:E:144:GLU:HB3	3:E:189:ILE:HD11	1.99	0.43
3:E:470:ALA:HB3	3:E:475:ARG:HD3	1.99	0.43
3:d:267:VAL:HG21	3:d:343:LEU:HD23	2.00	0.43
3:A:300:ALA:O	3:A:304:ARG:HG3	2.18	0.43
3:e:517:GLN:O	3:e:521:ILE:HG12	2.18	0.43
3:B:52:GLN:O	3:B:55:VAL:HG12	2.19	0.43
3:c:176:ARG:O	3:c:180:LEU:HG	2.19	0.43
1:M:619:ILE:O	3:d:215:ARG:NE	2.38	0.43
2:V:25:GLN:HE22	3:A:541:PRO:HG2	1.84	0.43
2:x:47:ARG:HD2	2:x:47:ARG:HA	1.76	0.43
2:z:53:GLN:O	2:z:57:GLN:HG3	2.19	0.43
3:E:235:ARG:HH11	3:E:262:MET:HE1	1.84	0.43
3:E:937:MET:HE1	3:E:945:TYR:CD2	2.53	0.43
3:B:618:LEU:HD23	3:B:618:LEU:HA	1.87	0.43
3:C:273:PRO:HD2	3:C:276:ASP:HB2	2.01	0.43
3:D:434:ALA:HB1	3:D:438:MET:HE3	1.99	0.43
1:M:623:SER:OG	3:D:233:LYS:HD2	2.18	0.43
1:O:623:SER:OG	3:E:233:LYS:HD2	2.19	0.43
3:E:236:THR:O	3:E:240:ASN:ND2	2.52	0.43
3:E:539:SER:O	3:d:349:TYR:OH	2.31	0.43
3:b:372:LEU:HD11	3:b:563:LEU:HB3	2.00	0.43
3:D:384:VAL:HG23	3:D:936:LYS:HD2	2.00	0.43
2:W:48:GLN:O	2:W:52:LEU:HD23	2.19	0.43
3:A:315:GLU:OE1	3:a:458:ARG:NH2	2.52	0.43
3:A:570:VAL:O	3:A:574:GLN:N	2.52	0.43
3:e:390:PHE:HZ	3:e:560:MET:SD	2.42	0.43
3:a:365:GLN:NE2	3:a:557:ASN:OD1	2.42	0.43
3:b:564:GLY:O	3:b:568:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:454:VAL:HG23	3:c:336:GLN:HG2	2.01	0.43
3:c:148:VAL:HA	3:c:151:GLU:HG2	2.01	0.43
3:c:325:LYS:HB3	3:c:325:LYS:HE3	1.92	0.43
2:X:55:ARG:HD2	3:C:573:THR:HG22	2.01	0.43
2:Z:15:LEU:HD21	3:d:231:VAL:HG22	2.00	0.43
3:d:325:LYS:HB3	3:d:325:LYS:HE3	1.92	0.43
3:A:454:VAL:HG23	3:e:336:GLN:HG2	2.00	0.43
3:B:874:LYS:NZ	3:B:944:ASP:OD1	2.38	0.43
2:X:76:GLN:O	2:X:80:ILE:HG12	2.18	0.42
3:E:1006:ARG:NH1	3:E:1007:ASP:OD1	2.52	0.42
3:E:1006:ARG:NH1	3:d:589:ALA:HA	2.34	0.42
3:d:263:VAL:HG21	3:d:285:TYR:CE1	2.54	0.42
3:a:256:ILE:HD11	3:a:298:ALA:HB1	2.01	0.42
3:a:372:LEU:HD11	3:a:563:LEU:HB3	2.01	0.42
3:C:539:SER:O	3:b:349:TYR:OH	2.30	0.42
1:O:616:PHE:HE2	2:V:1:MET:HB2	1.83	0.42
3:E:384:VAL:HG23	3:E:936:LYS:HD2	2.01	0.42
3:d:46:GLY:O	3:d:50:ILE:HG12	2.19	0.42
3:e:325:LYS:HE3	3:e:325:LYS:HB3	1.82	0.42
3:a:267:VAL:HG21	3:a:343:LEU:HD23	2.01	0.42
3:C:239:VAL:HG13	3:C:259:VAL:HG22	2.00	0.42
3:b:56:SER:OG	3:b:61:SER:O	2.33	0.42
3:b:352:TRP:NE1	3:b:411:ARG:HH21	2.17	0.42
2:Y:48:GLN:HG2	2:Y:52:LEU:HD23	2.00	0.42
2:x:1:MET:HA	2:x:6:ILE:HD11	2.01	0.42
3:E:47:ASN:HB3	3:E:184:MET:HE3	2.01	0.42
3:B:713:PHE:HB3	3:B:747:LEU:HD11	2.01	0.42
3:B:752:ARG:NH1	3:B:758:GLY:O	2.36	0.42
3:a:438:MET:HE3	3:a:533:LEU:HD21	2.01	0.42
3:C:289:TYR:HB2	3:C:302:VAL:HG11	2.01	0.42
3:C:741:SER:OG	3:C:744:SER:OG	2.37	0.42
3:b:252:PRO:O	3:b:256:ILE:HG12	2.18	0.42
3:B:665:HIS:NE2	3:B:669:ASP:OD1	2.48	0.42
3:b:387:SER:O	3:b:391:VAL:HG23	2.19	0.42
3:D:713:PHE:HB3	3:D:747:LEU:HD11	2.01	0.42
1:G:623:SER:HB2	3:A:230:SER:HA	2.01	0.42
3:C:48:ALA:O	3:C:52:GLN:HG3	2.19	0.42
3:C:427:GLU:OE2	3:C:536:TYR:OH	2.23	0.42
3:b:439:ARG:NH2	3:b:540:GLU:O	2.47	0.42
3:c:391:VAL:HG12	3:c:431:LEU:HD12	2.01	0.42
2:Z:5:ALA:O	2:Z:9:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:176:ARG:HA	3:E:201:HIS:NE2	2.35	0.42
3:A:632:VAL:HG23	3:A:635:SER:HB3	2.01	0.42
3:A:889:LEU:HG	3:A:893:MET:SD	2.60	0.42
3:B:294:ASN:ND2	3:C:42:ILE:O	2.48	0.42
3:C:50:ILE:HG23	3:C:195:LYS:HG2	2.01	0.42
3:D:692:GLN:HB2	3:D:697:TYR:O	2.20	0.42
3:c:390:PHE:HZ	3:c:560:MET:SD	2.42	0.42
2:X:25:GLN:NE2	3:b:350:MET:HE3	2.35	0.42
3:E:180:LEU:O	3:E:184:MET:HG2	2.20	0.42
3:d:224:SER:OG	3:d:227:ARG:NH2	2.52	0.42
3:C:322:ASP:OD1	3:C:324:THR:HG22	2.20	0.42
3:C:709:MET:HG3	3:C:752:ARG:O	2.18	0.42
3:b:151:GLU:OE2	3:b:182:ARG:HD3	2.19	0.42
3:b:291:LYS:HD3	3:b:291:LYS:HA	1.91	0.42
1:G:634:ALA:HB2	2:v:16:VAL:HG22	2.02	0.42
3:E:239:VAL:HG21	3:E:284:MET:SD	2.60	0.42
3:d:516:GLU:O	3:d:520:ILE:HG12	2.20	0.42
3:B:315:GLU:OE2	3:B:340:LYS:NZ	2.51	0.42
3:A:176:ARG:NH1	3:e:276:ASP:OD1	2.50	0.42
3:b:365:GLN:NE2	3:b:557:ASN:OD1	2.38	0.42
3:D:439:ARG:HH12	3:D:545:LEU:HD12	1.85	0.42
3:c:46:GLY:O	3:c:50:ILE:HG12	2.19	0.42
1:K:623:SER:OG	3:C:233:LYS:HD2	2.19	0.42
2:X:5:ALA:O	2:X:9:ILE:HG23	2.20	0.42
3:E:50:ILE:HG23	3:E:195:LYS:HG2	2.00	0.42
2:V:5:ALA:O	2:V:9:ILE:HG23	2.20	0.41
2:W:29:GLN:OE1	3:B:548:ASN:ND2	2.53	0.41
3:B:180:LEU:HD23	3:B:180:LEU:HA	1.87	0.41
3:B:570:VAL:O	3:B:574:GLN:N	2.52	0.41
3:C:692:GLN:HB2	3:C:697:TYR:O	2.20	0.41
3:b:309:LEU:HD13	3:b:343:LEU:HD21	2.01	0.41
3:D:174:LYS:HA	3:c:225:GLN:NE2	2.35	0.41
3:D:373:GLU:OE2	3:D:904:THR:OG1	2.36	0.41
1:G:644:THR:HA	3:A:242:VAL:HG22	2.02	0.41
3:d:390:PHE:HZ	3:d:560:MET:SD	2.42	0.41
3:D:844:LYS:HE2	3:D:1018:SER:OG	2.21	0.41
2:V:47:ARG:HH12	3:A:379:ASP:HB3	1.85	0.41
2:W:5:ALA:O	2:W:9:ILE:HG23	2.20	0.41
2:W:15:LEU:HD21	3:a:231:VAL:HG22	2.02	0.41
3:E:42:ILE:O	3:D:294:ASN:ND2	2.45	0.41
3:A:642:MET:HG3	3:A:679:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:56:SER:OG	3:e:61:SER:O	2.34	0.41
3:C:454:VAL:HG23	3:b:336:GLN:HG2	2.01	0.41
3:C:889:LEU:HG	3:C:893:MET:SD	2.61	0.41
3:D:814:LEU:HD13	3:D:819:THR:HB	2.01	0.41
1:K:615:PRO:HG2	2:Y:2:GLY:HA2	2.01	0.41
1:I:623:SER:OG	3:B:233:LYS:HD2	2.19	0.41
1:H:616:PHE:HE2	2:w:1:MET:HG3	1.85	0.41
3:A:356:ARG:HH21	3:A:357:LYS:HZ2	1.68	0.41
3:A:503:GLU:HG2	3:A:506:ARG:HH21	1.86	0.41
2:Y:5:ALA:O	2:Y:9:ILE:HG23	2.20	0.41
3:A:929:THR:OG1	3:A:930:THR:N	2.53	0.41
3:B:1002:LYS:HE3	3:B:1021:ASP:OD2	2.20	0.41
1:G:643:PHE:CE1	3:A:242:VAL:HG21	2.54	0.41
1:H:617:TYR:HB2	1:H:625:GLN:NE2	2.36	0.41
2:Y:2:GLY:O	3:c:219:TYR:OH	2.34	0.41
3:d:40:GLN:HE21	3:D:225:GLN:HE21	1.69	0.41
3:A:707:ASP:OD2	3:A:768:TYR:OH	2.31	0.41
3:e:46:GLY:O	3:e:50:ILE:HG12	2.20	0.41
3:c:406:ALA:O	3:c:410:GLU:HG3	2.21	0.41
3:c:540:GLU:HB2	3:c:545:LEU:HG	2.02	0.41
2:y:53:GLN:O	2:y:57:GLN:HG3	2.21	0.41
3:E:625:GLY:O	3:E:628:ARG:NH2	2.52	0.41
3:E:749:TRP:HH2	3:E:769:MET:HG3	1.86	0.41
3:E:1027:ALA:O	3:E:1054:ALA:N	2.53	0.41
3:d:176:ARG:HD3	3:D:279:GLN:OE1	2.20	0.41
1:F:634:ALA:HB2	2:V:16:VAL:HG23	2.02	0.41
2:X:15:LEU:HD21	3:b:231:VAL:HG22	2.02	0.41
2:Z:25:GLN:NE2	3:d:350:MET:HE3	2.35	0.41
3:E:454:VAL:HG23	3:d:336:GLN:HG2	2.02	0.41
3:b:354:ASN:O	3:b:358:GLN:HG3	2.20	0.41
3:c:352:TRP:NE1	3:c:411:ARG:HH21	2.18	0.41
1:G:623:SER:OG	3:A:233:LYS:HD2	2.21	0.41
1:I:615:PRO:HG2	2:X:2:GLY:HA2	2.01	0.41
2:W:55:ARG:HD2	3:B:573:THR:HG22	2.02	0.41
2:z:10:LEU:O	2:z:13:VAL:HG12	2.21	0.41
3:E:902:LYS:HE3	3:E:908:HIS:CE1	2.56	0.41
3:A:248:TRP:HH2	3:B:181:ALA:HB2	1.86	0.41
3:A:340:LYS:HG3	3:a:451:ALA:HB2	2.02	0.41
3:e:252:PRO:O	3:e:256:ILE:HG12	2.21	0.41
3:e:292:VAL:HG12	3:e:292:VAL:O	2.21	0.41
3:e:315:GLU:OE1	3:e:340:LYS:NZ	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:373:GLU:HB2	3:B:383:LYS:HG3	2.01	0.41
3:C:445:LEU:HD11	3:C:525:ARG:NH1	2.36	0.41
3:C:929:THR:OG1	3:C:930:THR:N	2.54	0.41
3:b:325:LYS:HB3	3:b:325:LYS:HE3	1.87	0.41
3:D:1027:ALA:O	3:D:1054:ALA:N	2.53	0.41
3:c:303:GLU:O	3:c:307:LYS:HG2	2.21	0.41
3:c:369:LEU:HG	3:c:383:LYS:HG2	2.01	0.41
2:W:89:MET:HE3	2:w:78:PHE:HB3	2.03	0.41
2:X:69:ARG:NH1	3:C:773:ASN:OD1	2.43	0.41
2:X:88:GLN:HG2	2:x:79:LEU:HD22	2.03	0.41
2:Z:2:GLY:O	3:d:219:TYR:OH	2.35	0.41
3:E:340:LYS:HG3	3:e:451:ALA:HB2	2.03	0.41
3:a:458:ARG:HD2	3:a:466:PHE:CD1	2.56	0.41
3:a:555:LEU:HD23	3:a:555:LEU:HA	1.97	0.41
3:b:431:LEU:HD23	3:b:431:LEU:HA	1.92	0.41
3:D:176:ARG:HA	3:D:201:HIS:NE2	2.36	0.41
3:D:622:LYS:HB3	3:D:622:LYS:HE2	1.77	0.41
3:D:952:ASP:OD1	3:D:953:PRO:HD2	2.21	0.41
1:N:617:TYR:HB2	1:N:625:GLN:NE2	2.36	0.40
3:E:52:GLN:HA	3:d:275:LEU:HD13	2.03	0.40
3:d:252:PRO:O	3:d:256:ILE:HG12	2.21	0.40
3:d:560:MET:HE3	3:d:560:MET:HB3	1.87	0.40
3:d:568:GLU:HA	3:d:571:ARG:HG2	2.02	0.40
3:A:248:TRP:HB3	3:B:43:LEU:HD13	2.03	0.40
3:A:497:THR:OG1	3:A:500:GLN:HG2	2.21	0.40
3:B:248:TRP:HB3	3:C:43:LEU:HD13	2.03	0.40
3:B:692:GLN:HB2	3:B:697:TYR:O	2.22	0.40
3:b:372:LEU:HD23	3:b:372:LEU:HA	1.89	0.40
1:K:644:THR:HA	3:C:242:VAL:HG22	2.03	0.40
1:G:627:ALA:HB1	3:A:234:GLU:HB2	2.02	0.40
2:W:85:LEU:HD12	2:w:79:LEU:HD21	2.03	0.40
3:E:372:LEU:HD11	3:E:563:LEU:HB3	2.02	0.40
3:A:273:PRO:HD2	3:A:276:ASP:HB2	2.03	0.40
3:A:979:LYS:HE3	3:A:987:ALA:HA	2.04	0.40
3:e:247:THR:HA	3:a:40:GLN:NE2	2.37	0.40
3:B:191:GLU:O	3:B:195:LYS:HG3	2.22	0.40
3:B:506:ARG:NH1	3:B:507:GLN:OE1	2.55	0.40
3:C:285:TYR:HD2	3:C:306:MET:HG2	1.86	0.40
3:C:570:VAL:O	3:C:574:GLN:N	2.55	0.40
2:v:15:LEU:HD13	3:A:234:GLU:OE1	2.22	0.40
3:B:622:LYS:HE2	3:B:622:LYS:HB3	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:749:TRP:HH2	3:B:769:MET:HG3	1.86	0.40
3:b:138:LEU:HB3	3:b:142:GLU:HB2	2.03	0.40
3:b:292:VAL:O	3:b:292:VAL:HG12	2.21	0.40
3:D:503:GLU:HG2	3:D:506:ARG:HH21	1.86	0.40
3:c:292:VAL:HG12	3:c:292:VAL:O	2.21	0.40
2:Z:55:ARG:HD2	3:E:573:THR:HG22	2.04	0.40
3:B:497:THR:OG1	3:B:500:GLN:HG2	2.22	0.40
3:a:342:GLY:HA2	3:a:345:VAL:HG23	2.04	0.40
3:b:240:ASN:HA	3:b:243:VAL:HG12	2.03	0.40
3:D:570:VAL:O	3:D:574:GLN:N	2.54	0.40
3:D:828:ARG:HB2	3:D:828:ARG:NH1	2.36	0.40
1:O:612:GLN:HA	1:O:625:GLN:HG2	2.03	0.40
1:L:617:TYR:HB2	1:L:625:GLN:NE2	2.37	0.40
2:X:9:ILE:HG13	2:X:10:LEU:N	2.37	0.40
2:Z:25:GLN:HE22	3:E:541:PRO:HG2	1.87	0.40
3:d:59:GLN:HB2	3:D:306:MET:SD	2.61	0.40
3:d:159:TRP:HB3	3:d:165:PHE:CE2	2.56	0.40
3:A:622:LYS:HB3	3:A:622:LYS:HE2	1.78	0.40
3:A:713:PHE:HB3	3:A:747:LEU:HD11	2.03	0.40
3:e:364:GLN:OE1	3:e:367:ARG:NH2	2.54	0.40
3:D:373:GLU:HB2	3:D:383:LYS:HG3	2.04	0.40
3:c:52:GLN:O	3:c:55:VAL:HG12	2.21	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	F	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	G	38/653 (6%)	37 (97%)	1 (3%)	0	100	100
1	H	38/653 (6%)	36 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	38/653 (6%)	37 (97%)	1 (3%)	0	100	100
1	J	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	K	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	L	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	M	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	N	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	O	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
2	V	90/380 (24%)	90 (100%)	0	0	100	100
2	W	90/380 (24%)	90 (100%)	0	0	100	100
2	X	90/380 (24%)	90 (100%)	0	0	100	100
2	Y	90/380 (24%)	90 (100%)	0	0	100	100
2	Z	90/380 (24%)	90 (100%)	0	0	100	100
2	v	90/380 (24%)	90 (100%)	0	0	100	100
2	w	90/380 (24%)	90 (100%)	0	0	100	100
2	x	90/380 (24%)	90 (100%)	0	0	100	100
2	y	90/380 (24%)	90 (100%)	0	0	100	100
2	z	90/380 (24%)	90 (100%)	0	0	100	100
3	A	897/1058 (85%)	873 (97%)	24 (3%)	0	100	100
3	B	897/1058 (85%)	870 (97%)	27 (3%)	0	100	100
3	C	897/1058 (85%)	869 (97%)	28 (3%)	0	100	100
3	D	897/1058 (85%)	869 (97%)	28 (3%)	0	100	100
3	E	897/1058 (85%)	868 (97%)	29 (3%)	0	100	100
3	a	456/1058 (43%)	451 (99%)	5 (1%)	0	100	100
3	b	456/1058 (43%)	452 (99%)	4 (1%)	0	100	100
3	c	456/1058 (43%)	451 (99%)	5 (1%)	0	100	100
3	d	456/1058 (43%)	449 (98%)	7 (2%)	0	100	100
3	e	456/1058 (43%)	451 (99%)	5 (1%)	0	100	100
All	All	8045/20910 (38%)	7865 (98%)	180 (2%)	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	F	30/572 (5%)	30 (100%)	0	100	100
1	G	30/572 (5%)	30 (100%)	0	100	100
1	H	30/572 (5%)	30 (100%)	0	100	100
1	I	30/572 (5%)	30 (100%)	0	100	100
1	J	30/572 (5%)	30 (100%)	0	100	100
1	K	30/572 (5%)	30 (100%)	0	100	100
1	L	30/572 (5%)	30 (100%)	0	100	100
1	M	30/572 (5%)	30 (100%)	0	100	100
1	N	30/572 (5%)	30 (100%)	0	100	100
1	O	30/572 (5%)	30 (100%)	0	100	100
2	V	73/306 (24%)	73 (100%)	0	100	100
2	W	73/306 (24%)	73 (100%)	0	100	100
2	X	73/306 (24%)	73 (100%)	0	100	100
2	Y	73/306 (24%)	73 (100%)	0	100	100
2	Z	73/306 (24%)	73 (100%)	0	100	100
2	v	73/306 (24%)	73 (100%)	0	100	100
2	w	73/306 (24%)	73 (100%)	0	100	100
2	x	73/306 (24%)	73 (100%)	0	100	100
2	y	73/306 (24%)	73 (100%)	0	100	100
2	z	73/306 (24%)	73 (100%)	0	100	100
3	A	735/850 (86%)	735 (100%)	0	100	100
3	B	735/850 (86%)	735 (100%)	0	100	100
3	C	735/850 (86%)	735 (100%)	0	100	100
3	D	735/850 (86%)	734 (100%)	1 (0%)	88	89
3	E	735/850 (86%)	735 (100%)	0	100	100
3	a	386/850 (45%)	386 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	b	386/850 (45%)	385 (100%)	1 (0%)	86	84
3	c	386/850 (45%)	385 (100%)	1 (0%)	86	84
3	d	386/850 (45%)	386 (100%)	0	100	100
3	e	386/850 (45%)	385 (100%)	1 (0%)	86	84
All	All	6635/17280 (38%)	6631 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	e	139	THR
3	b	139	THR
3	D	527	GLN
3	c	140	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	648	ASN
1	K	650	ASN
1	M	648	ASN
1	O	625	GLN
1	O	648	ASN
1	O	650	ASN
1	G	648	ASN
1	I	648	ASN
1	F	631	ASN
1	F	648	ASN
1	H	648	ASN
1	J	648	ASN
1	J	650	ASN
1	L	648	ASN
1	L	650	ASN
1	N	648	ASN
2	V	23	ASN
2	V	25	GLN
2	V	57	GLN
2	V	88	GLN
2	W	25	GLN
2	W	36	GLN
2	W	57	GLN

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Mol	Chain	Res	Type
2	X	25	GLN
2	X	36	GLN
2	X	57	GLN
2	Y	25	GLN
2	Y	36	GLN
2	Y	57	GLN
2	Z	25	GLN
2	Z	57	GLN
2	w	21	GLN
2	w	48	GLN
2	x	21	GLN
2	x	25	GLN
2	x	72	ASN
2	y	21	GLN
3	E	146	ASN
3	E	157	ASN
3	E	188	ASN
3	E	335	GLN
3	E	453	GLN
3	E	460	GLN
3	E	500	GLN
3	E	512	GLN
3	E	527	GLN
3	E	685	GLN
3	E	725	GLN
3	E	982	ASN
3	d	40	GLN
3	d	52	GLN
3	d	282	ASN
3	d	323	GLN
3	d	336	GLN
3	d	363	GLN
3	d	404	ASN
3	A	146	ASN
3	A	157	ASN
3	A	294	ASN
3	A	335	GLN
3	A	453	GLN
3	A	500	GLN
3	A	692	GLN
3	A	794	ASN
3	e	40	GLN

Continued on next page...

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Mol	Chain	Res	Type
3	e	52	GLN
3	e	282	ASN
3	e	336	GLN
3	e	363	GLN
3	e	404	ASN
3	e	548	ASN
3	B	40	GLN
3	B	41	GLN
3	B	146	ASN
3	B	157	ASN
3	B	417	ASN
3	B	453	GLN
3	B	460	GLN
3	B	500	GLN
3	B	512	GLN
3	B	685	GLN
3	B	725	GLN
3	B	794	ASN
3	B	867	ASN
3	B	887	GLN
3	a	40	GLN
3	a	204	ASN
3	a	225	GLN
3	a	282	ASN
3	a	336	GLN
3	a	404	ASN
3	C	146	ASN
3	C	157	ASN
3	C	294	ASN
3	C	335	GLN
3	C	417	ASN
3	C	453	GLN
3	C	500	GLN
3	C	527	GLN
3	C	725	GLN
3	C	867	ASN
3	b	146	ASN
3	b	225	GLN
3	b	313	GLN
3	b	336	GLN
3	b	404	ASN
3	D	146	ASN

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Mol	Chain	Res	Type
3	D	282	ASN
3	D	335	GLN
3	D	415	ASN
3	D	417	ASN
3	D	500	GLN
3	D	665	HIS
3	D	685	GLN
3	D	725	GLN
3	c	40	GLN
3	c	282	ASN
3	c	336	GLN
3	c	363	GLN
3	c	368	GLN
3	c	404	ASN
3	c	524	GLN
3	c	562	GLN

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 5 ligands modelled in this entry, 5 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.

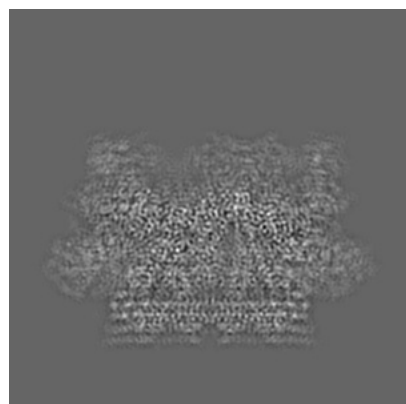
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61998. These allow visual inspection of the internal detail of the map and identification of artifacts.

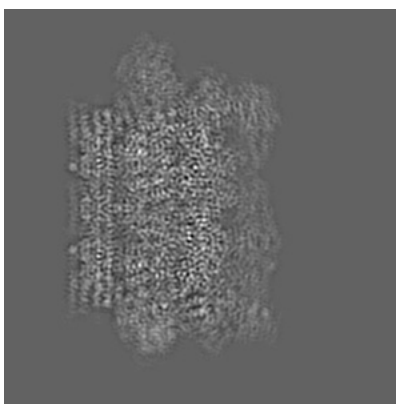
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

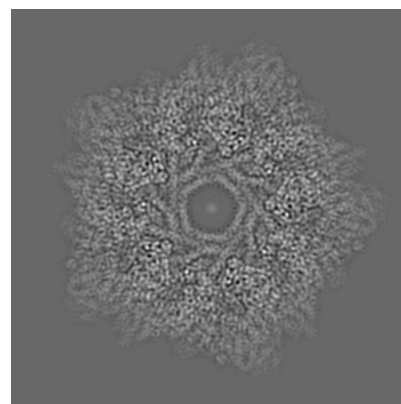
6.1.1 Primary map



X

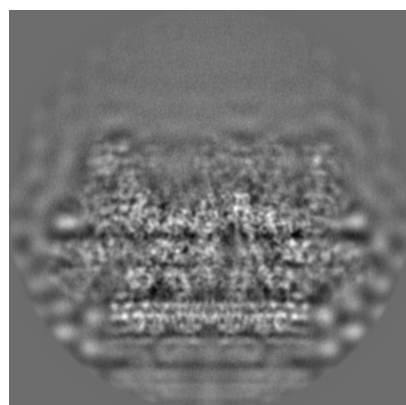


Y

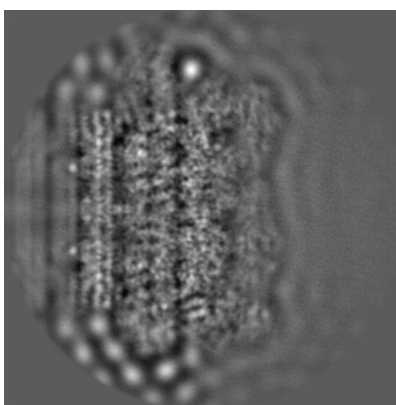


Z

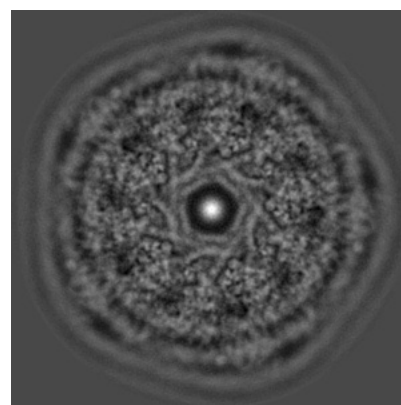
6.1.2 Raw map



X



Y

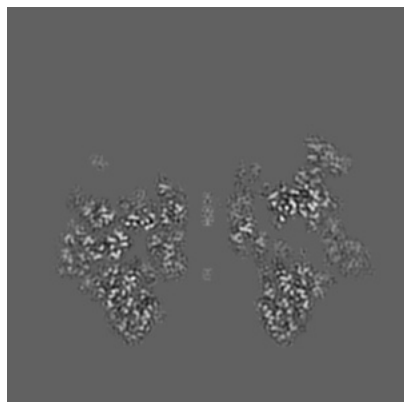


Z

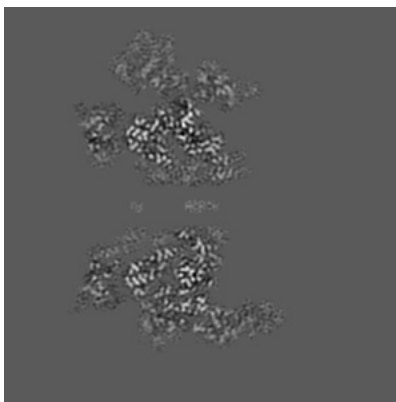
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

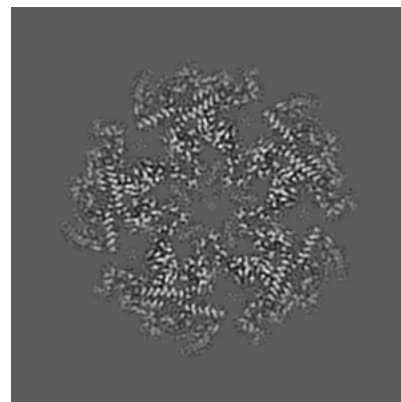
6.2.1 Primary map



X Index: 150

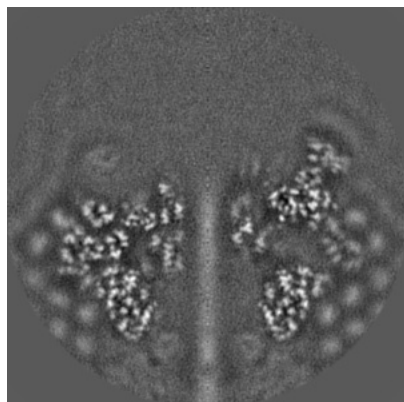


Y Index: 150

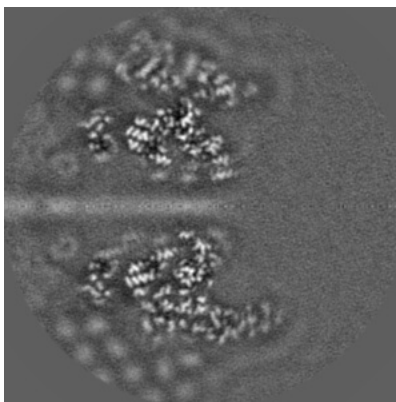


Z Index: 150

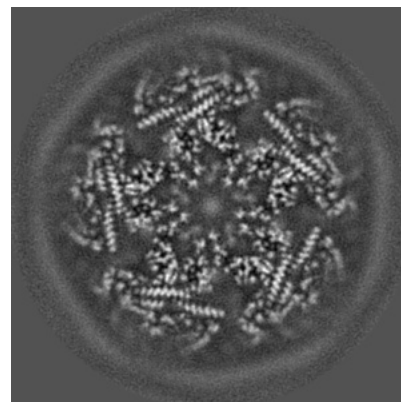
6.2.2 Raw map



X Index: 150



Y Index: 150

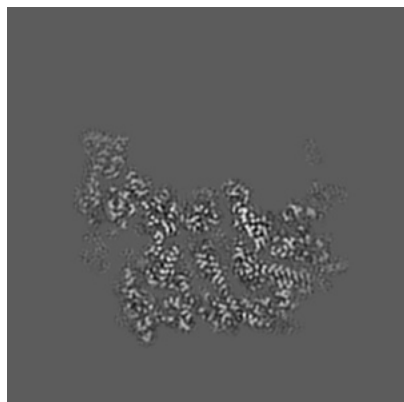


Z Index: 150

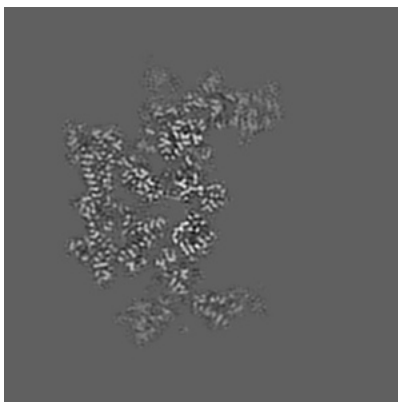
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

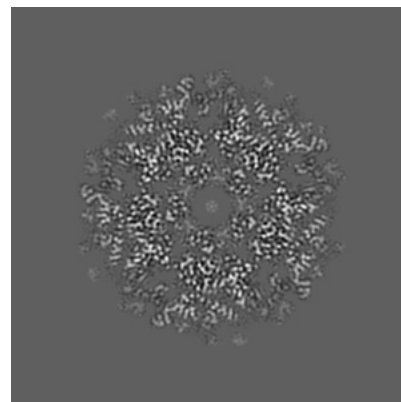
6.3.1 Primary map



X Index: 108

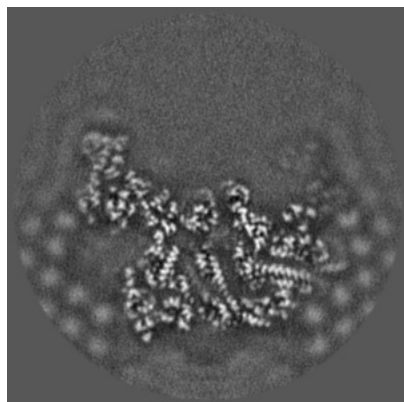


Y Index: 199

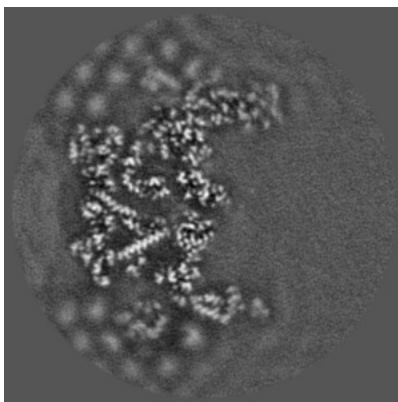


Z Index: 139

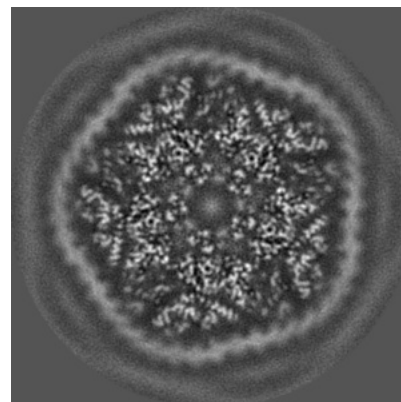
6.3.2 Raw map



X Index: 108



Y Index: 196

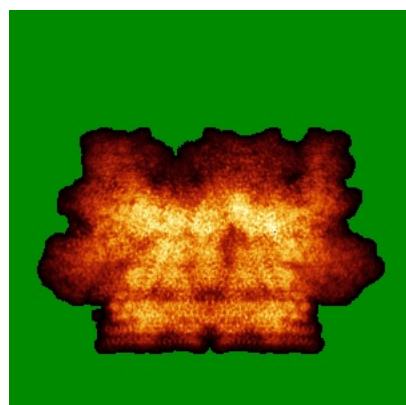


Z Index: 139

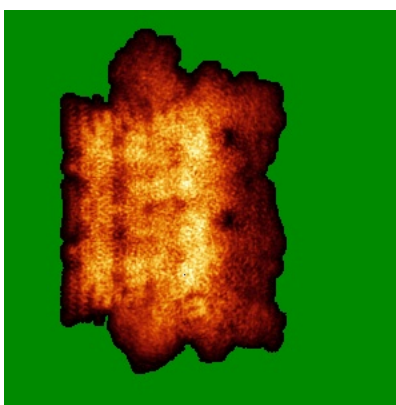
The images above show the largest variance slices of the map in three orthogonal directions.

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

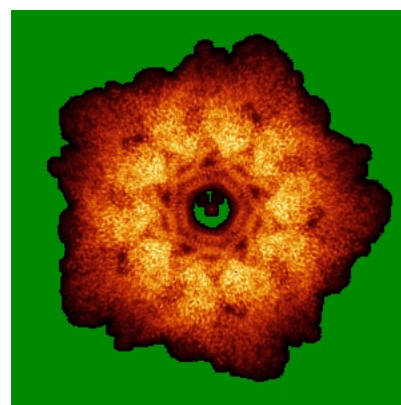
6.4.1 Primary map



X

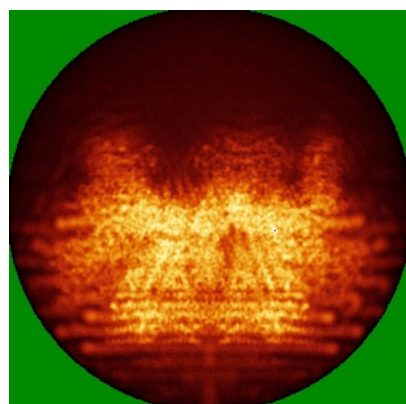


Y

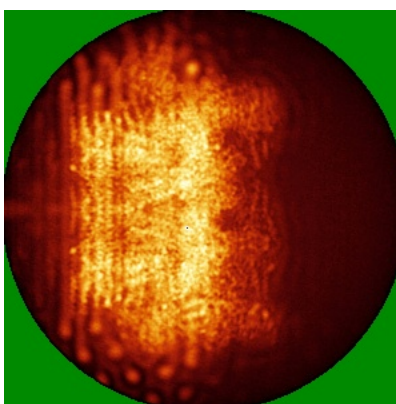


Z

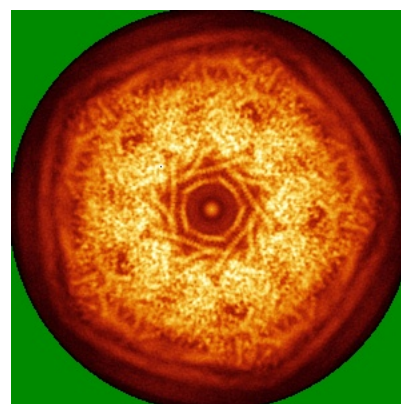
6.4.2 Raw map



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](#)

This section was not generated.

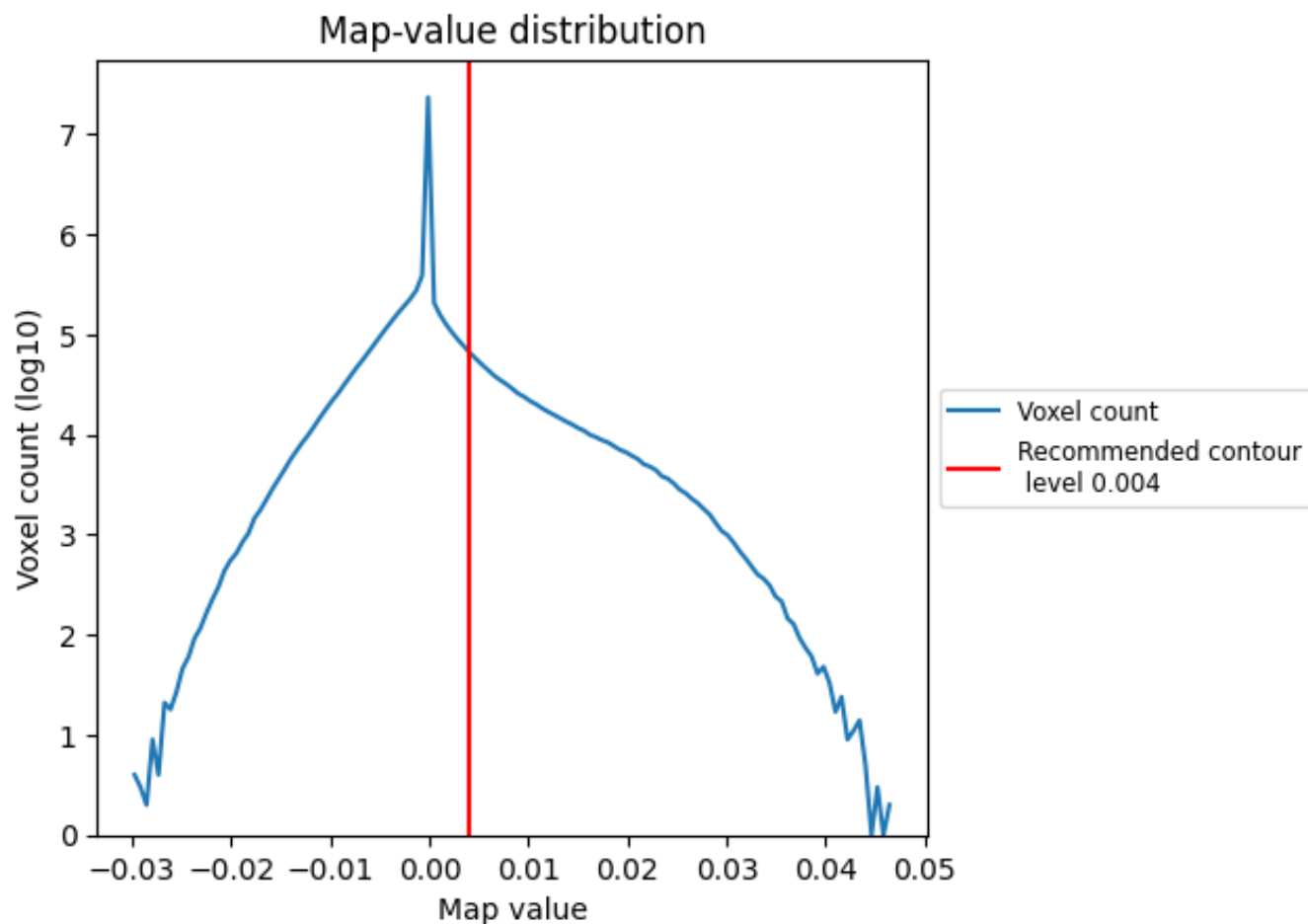
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

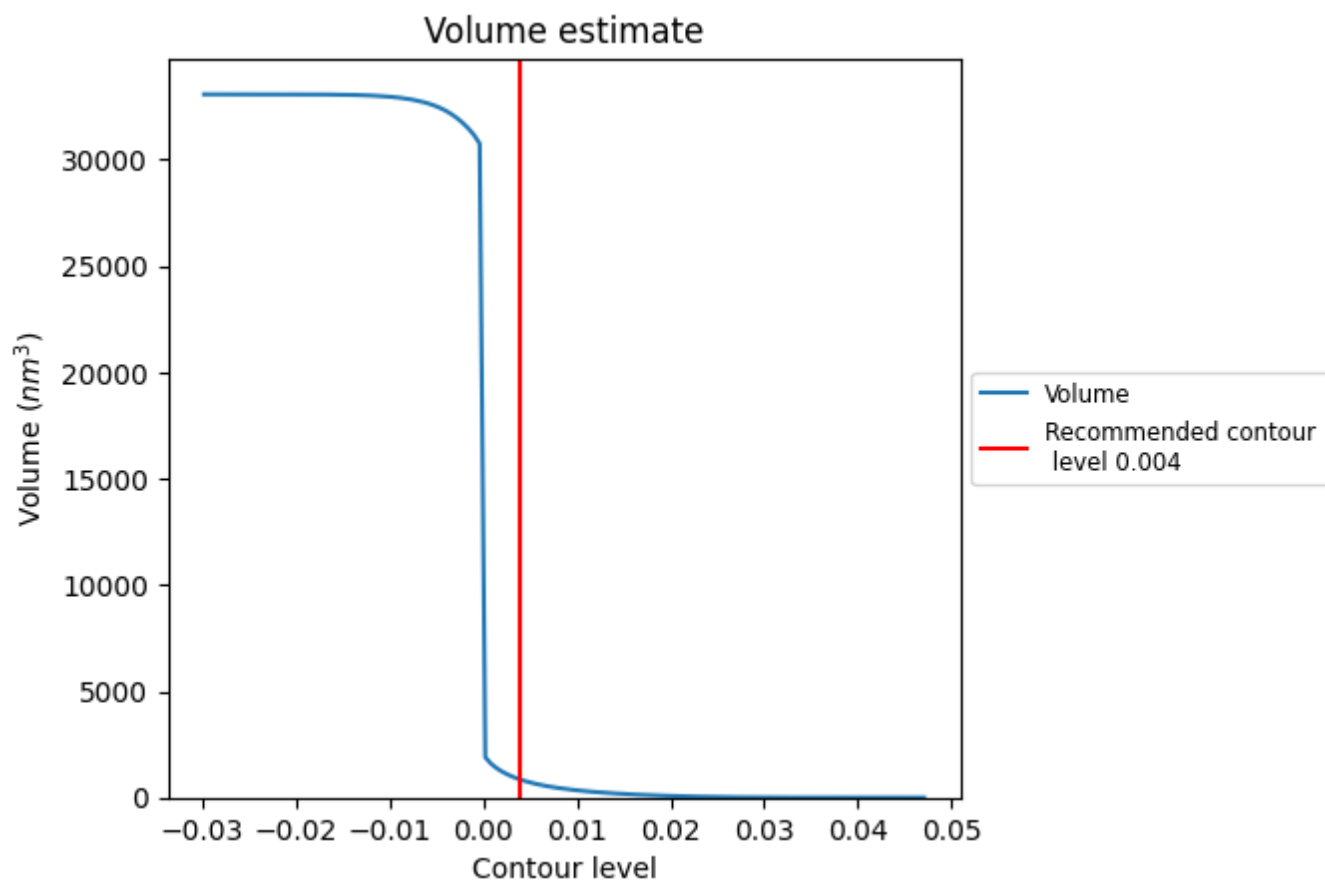
This section contains the results of statistical analysis of the map.

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.

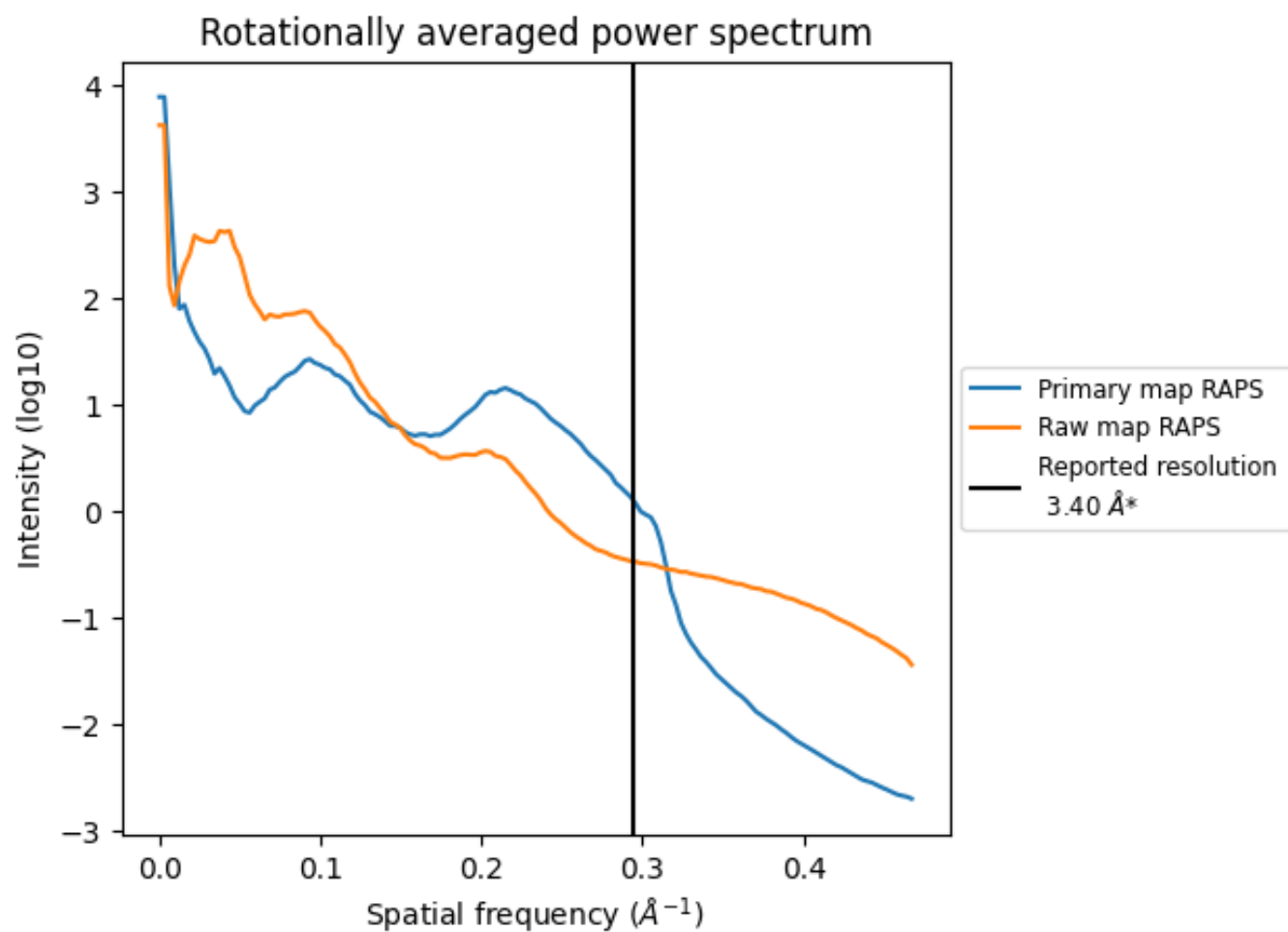
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 843 nm³; this corresponds to an approximate mass of 761 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 ⓘ

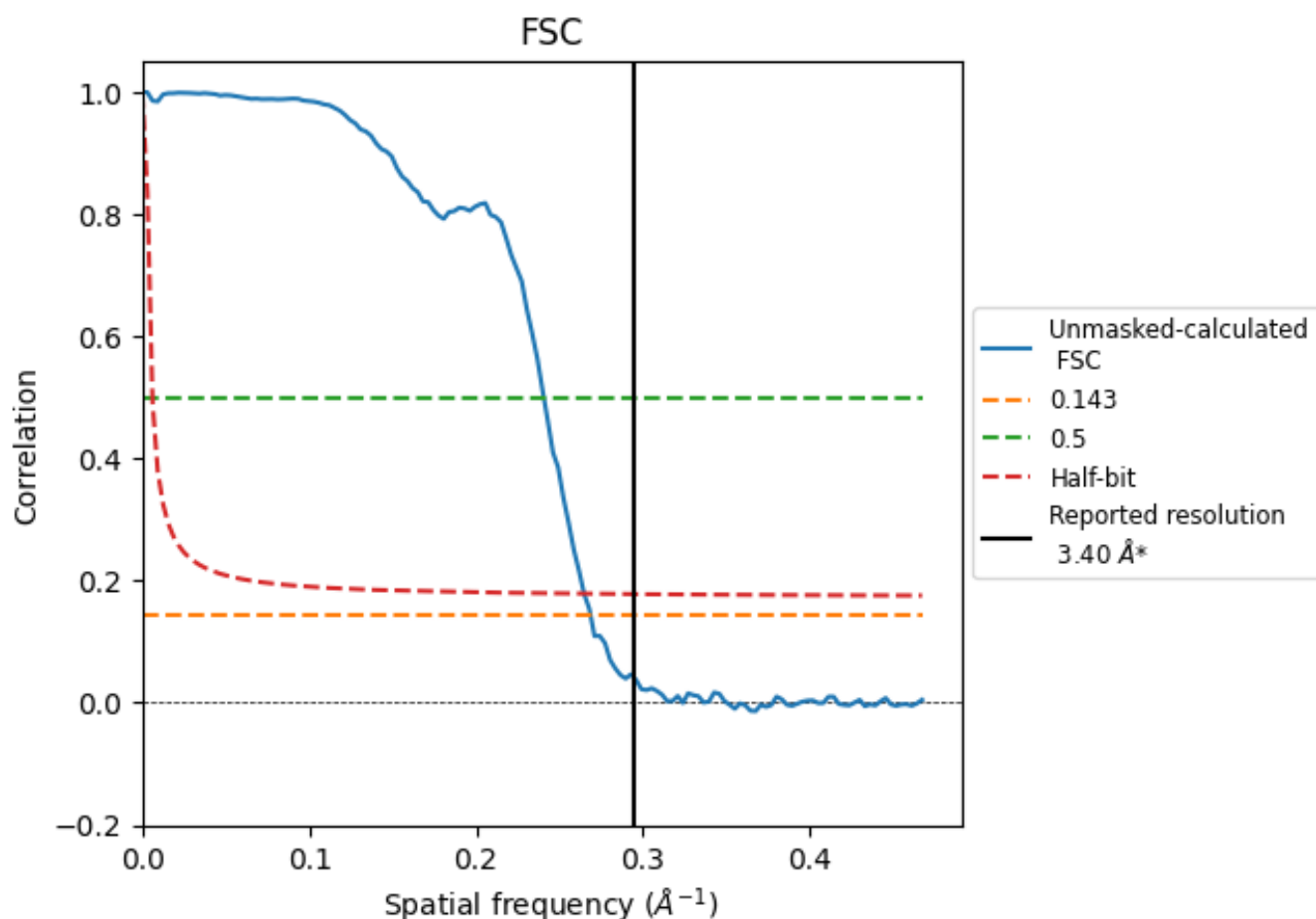


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

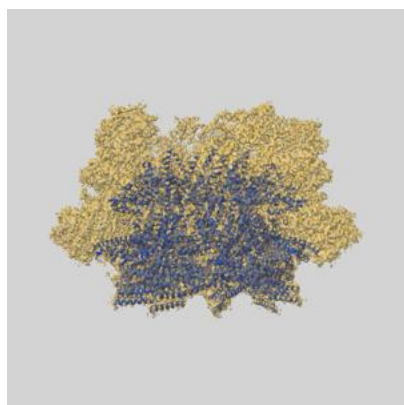
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.16	3.78

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

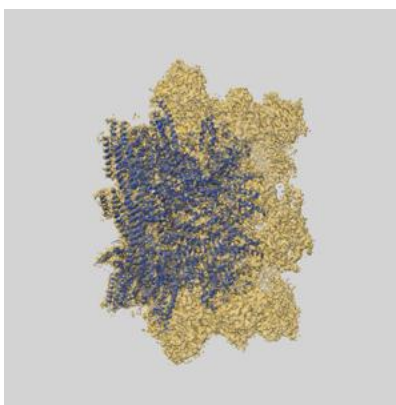
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61998 and PDB model 9K2V. Per-residue inclusion information can be found in section [3](#) on page [8](#).

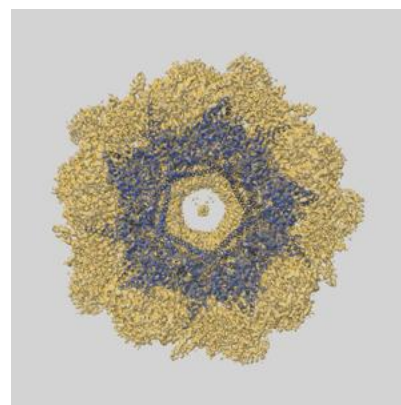
9.1 Map-model overlay [i](#)



X



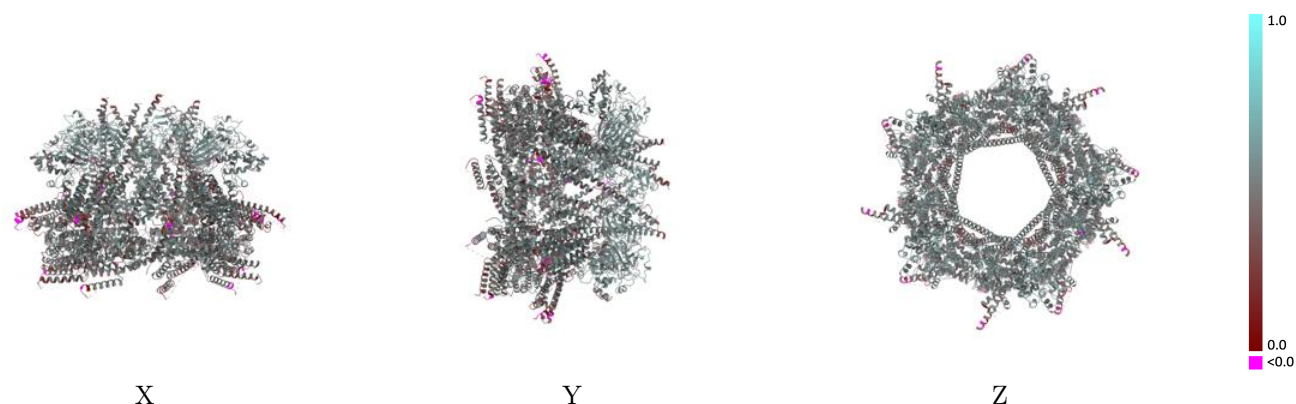
Y



Z

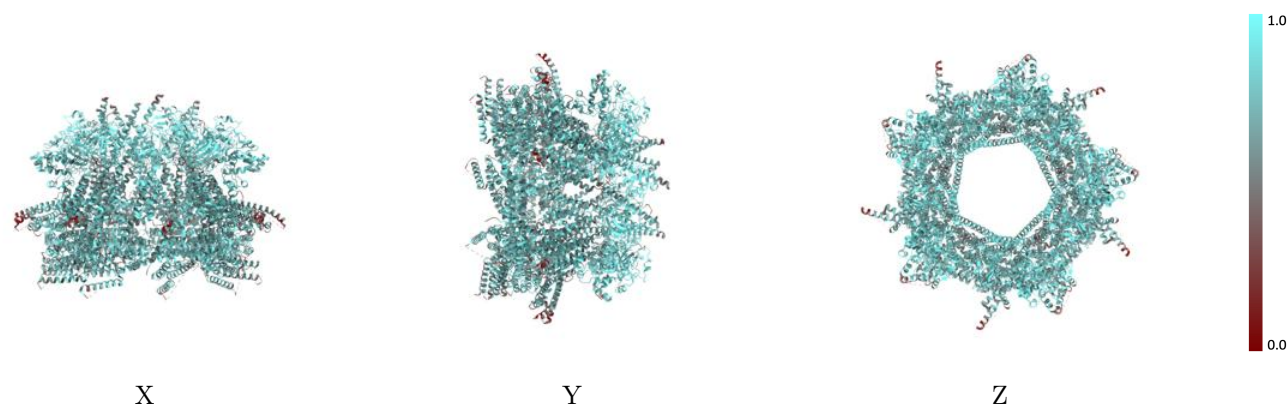
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



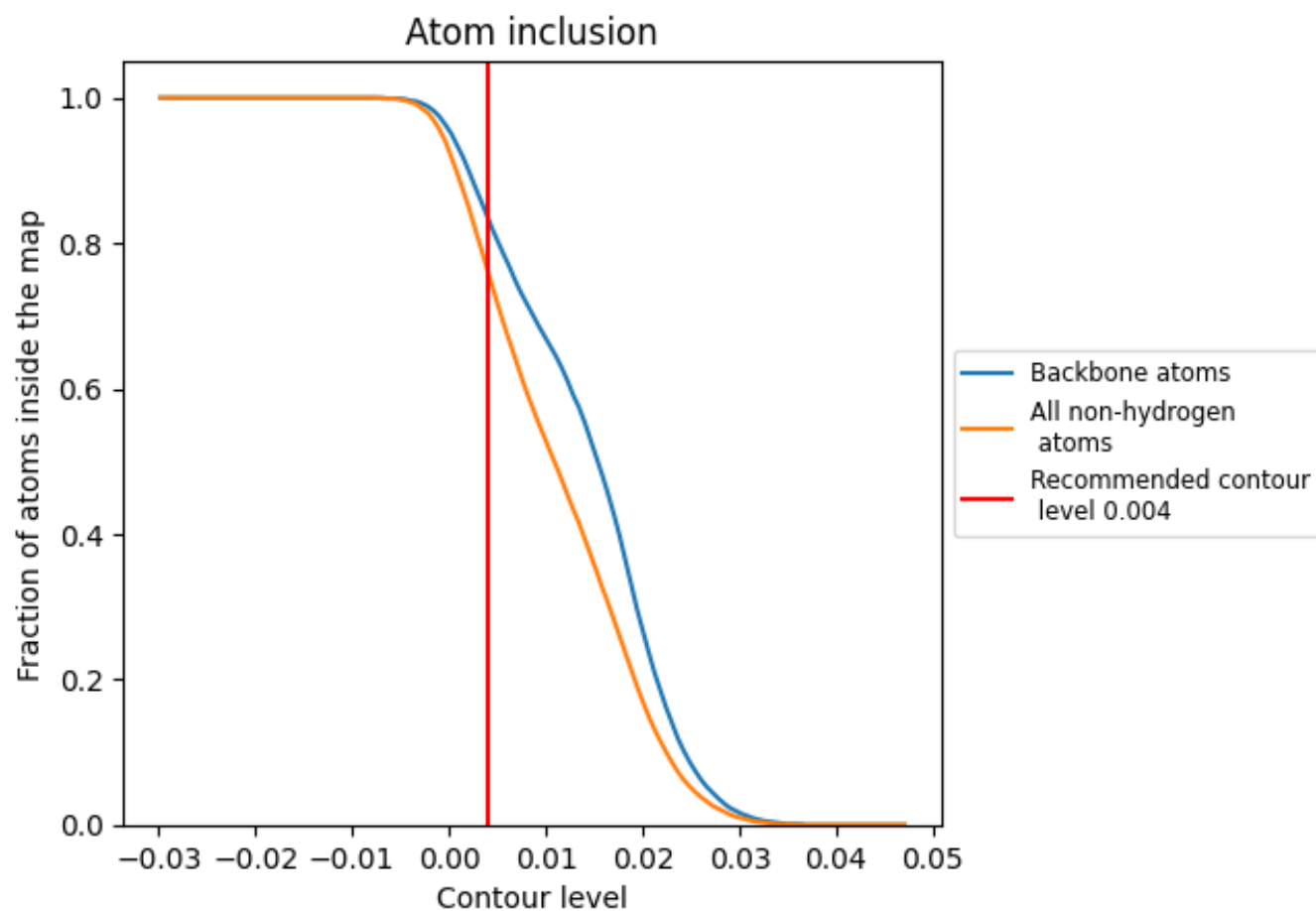
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7620	 0.4800
A	 0.7770	 0.4950
B	 0.7800	 0.4950
C	 0.7780	 0.4940
D	 0.7810	 0.4940
E	 0.7770	 0.4960
F	 0.7680	 0.4950
G	 0.7610	 0.4510
H	 0.7820	 0.4910
I	 0.7580	 0.4570
J	 0.7850	 0.4990
K	 0.7510	 0.4640
L	 0.7850	 0.4980
M	 0.7650	 0.4680
N	 0.7960	 0.4990
O	 0.7470	 0.4550
V	 0.7580	 0.4870
W	 0.7630	 0.4760
X	 0.7510	 0.4750
Y	 0.7700	 0.4780
Z	 0.7630	 0.4830
a	 0.7260	 0.4560
b	 0.7300	 0.4580
c	 0.7350	 0.4610
d	 0.7290	 0.4560
e	 0.7310	 0.4590
v	 0.7510	 0.4550
w	 0.7440	 0.4510
x	 0.7570	 0.4620
y	 0.7440	 0.4520
z	 0.7470	 0.4560

