



Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 05:27 PM JST

PDB ID : 8GZN
EMDB ID : EMD-34399
Title : IgM-var2CSA complex
Authors : Akhouri, R.R.; Goel, S.; Skoglund, U.
Deposited on : 2022-09-27
Resolution : 3.60 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

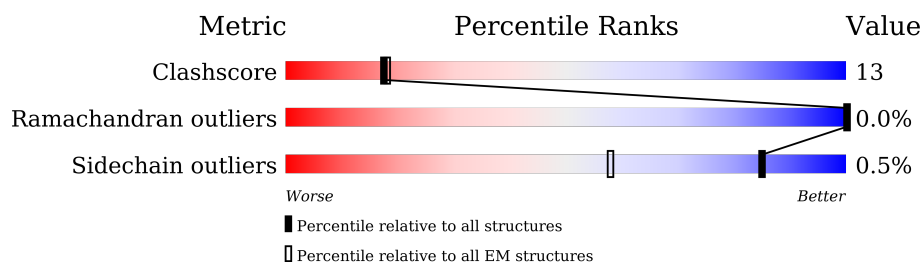
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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





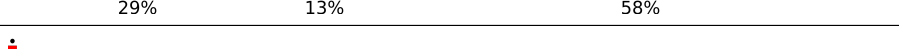


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	453	 19% 10% 71%
1	B	453	 33% 17% 50%
1	C	453	 34% 16% 50%
1	D	453	 35% 14% 51%
1	E	453	 33% 17% 51%
1	F	453	 35% 14% 51%
1	G	453	 31% 18% 51%
1	H	453	 38% 13% 49%

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Mol	Chain	Length	Quality of chain
1	K	453	
1	L	453	
2	I	2680	
2	M	2680	
3	J	136	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35322 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 Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1026	648	174	198	6		
1	B	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
1	C	225	Total	C	N	O	S	0	0
			1749	1103	297	341	8		
1	D	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	E	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	F	221	Total	C	N	O	S	0	0
			1723	1087	292	336	8		
1	G	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
1	H	230	Total	C	N	O	S	0	0
			1785	1124	301	351	9		
1	K	230	Total	C	N	O	S	0	0
			1786	1124	302	351	9		
1	L	127	Total	C	N	O	S	0	0
			993	626	168	193	6		

- Molecule 2 is a protein called Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1115	Total	C	N	O	S	0	0
			9208	5813	1571	1758	66		
2	M	1115	Total	C	N	O	S	0	0
			9208	5813	1571	1758	66		

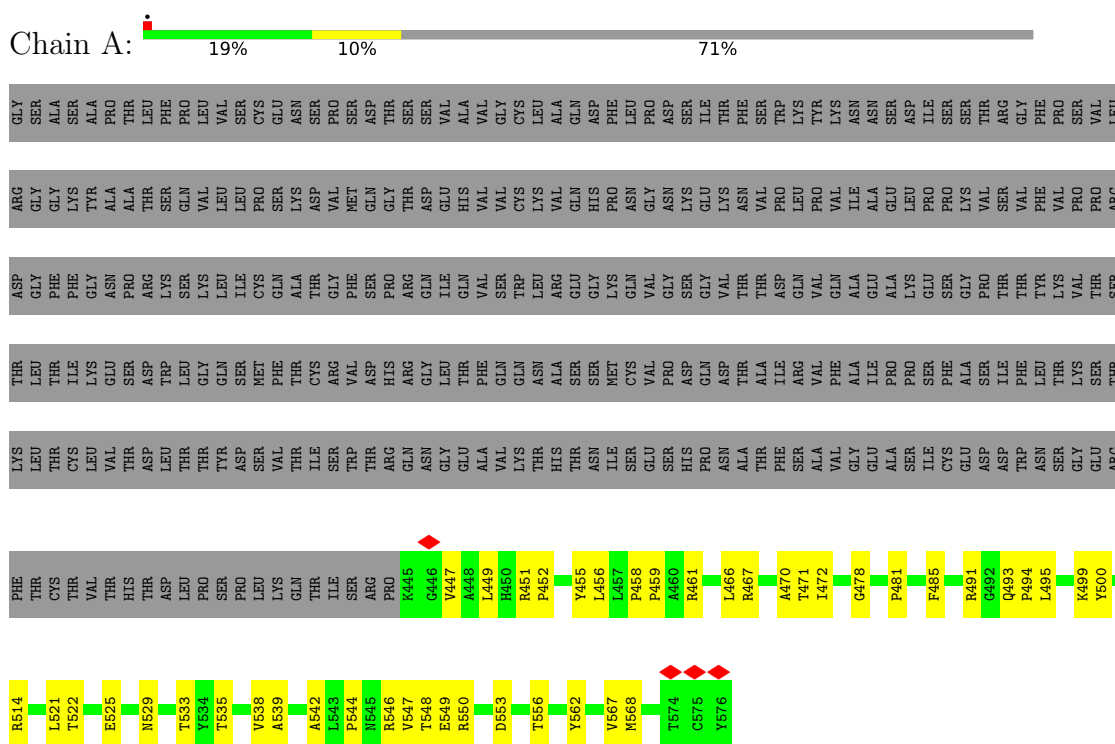
- Molecule 3 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	106	Total	C	N	O	S	0	0
			851	528	150	166	7		

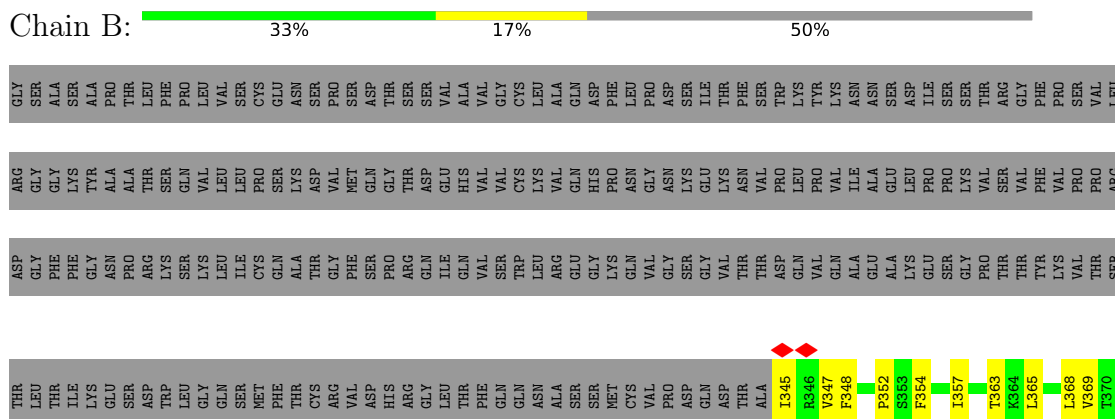
3 Residue-property plots

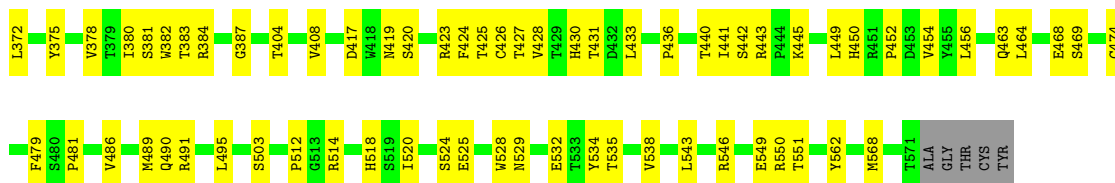
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Immunoglobulin heavy constant mu

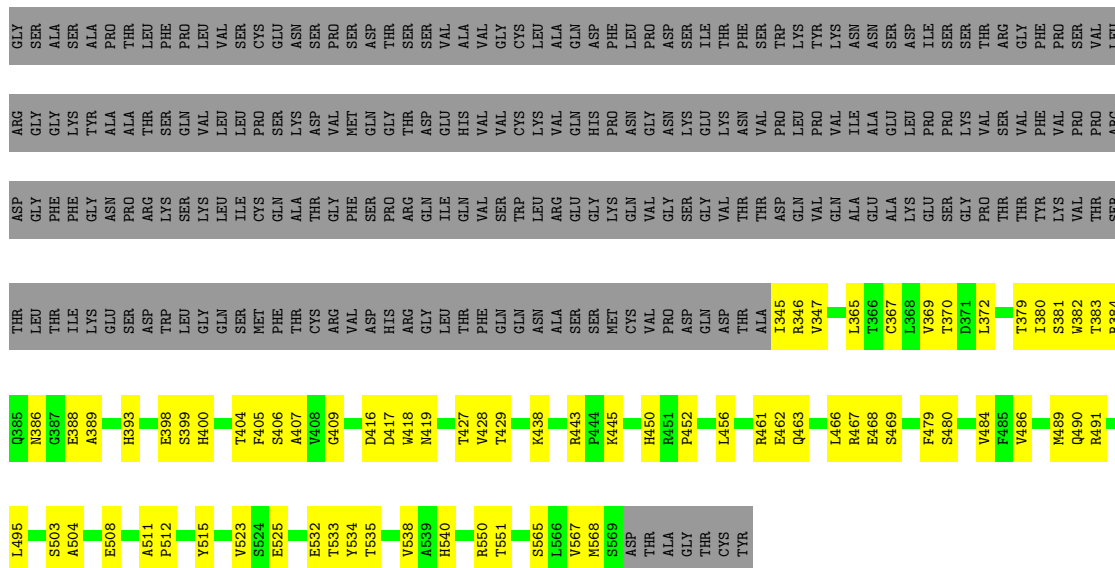
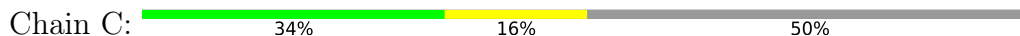


• Molecule 1: Immunoglobulin heavy constant mu

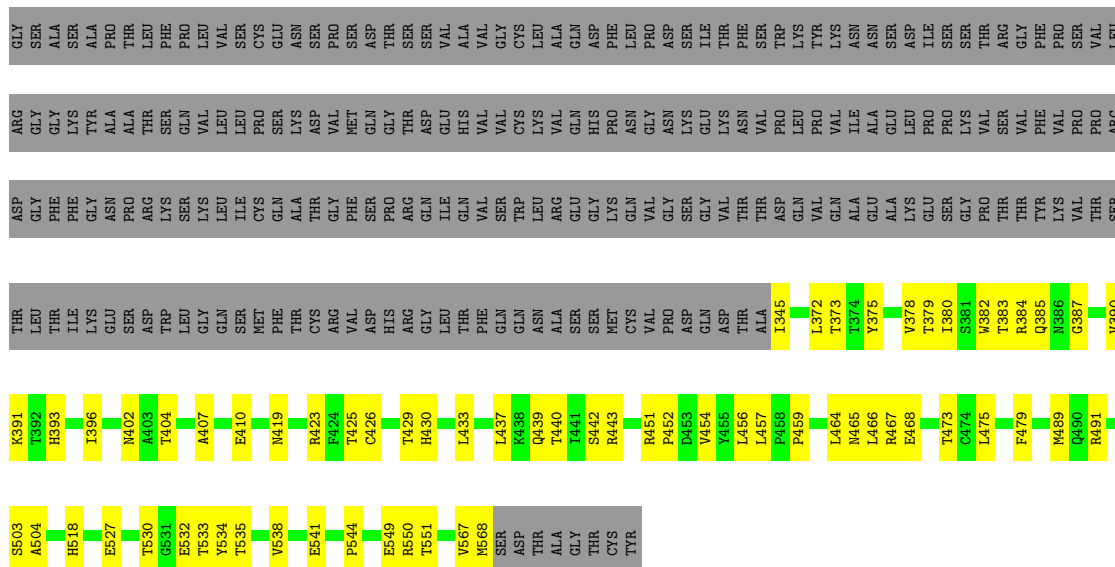
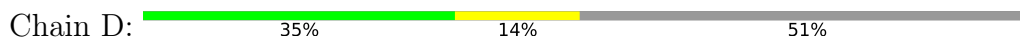





- Molecule 1: Immunoglobulin heavy constant mu



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- Molecule 1: Immunoglobulin heavy constant mu

Chain E:  33% 17% 51%


R461		V378		T379		I380		T383		R384		Q385		E388		A389		V390		K391		T392		H393		I396		E397		S399		H400		A403		T404		F405		S406		A407		V408		G409		E410		D416		D417		W418		N419		S420		G421		E422		R423		F424		T425		V428		T429		H430		T440		I441		S442		R443		P444		K445		P452		D453		V454		L457		P458		A460		R461																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
GLY	SER	ALA	SER	ALA	PRO	THR	LEU	PHE	PRO	GLN	VAL	SER	CYS	GLU	ASN	SER	PRO	SER	ASP	THR	SER	VAL	ALA	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP	THR	SER	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	ALA	GLN	ASP</

- Molecule 1: Immunoglobulin heavy constant mu

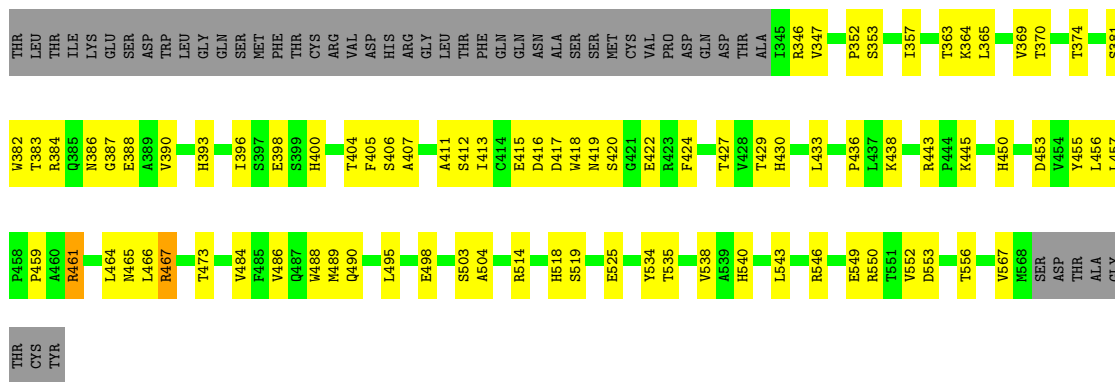
Chain F:  35% 14% 51%

GLY	SER	ALA	SER	ALA	PRO	THR	LEU	PHE	PRO	GLN	VAL	SER	CYS	GLU	ASN	SER	PRO	SER	ASP	THR	SER	VAL	ALA	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU	
ARG	GLY	LYS	TYR	ALA	ALA	THR	THR	SER	GLN	VAL	LEU	LEU	PRO	SER	GLU	ASP	VAL	MET	GLN	GLY	THR	GLY	ASP	HIS	VAL	VAL	GLN	CYS	VAL	GLY	THR	ASP	PRO	THR	VAL	PRO	ASP	GLN	ASP	THR	VAL	PRO	VAL	THR	THR	VAL	THR	THR	THR	THR	THR
ASP	GLY	PHE	GLY	ASN	PRO	ARG	ARG	LYS	LYS	VAL	LEU	ILE	CYS	GLN	ALA	THR	GLY	PHE	SER	PRO	ARG	GLN	ILE	THR	VAL	VAL	SER	ARG	GLN	ASP	GLY	THR	ASP	PRO	THR	VAL	PRO	ASP	GLN	ASP	THR	VAL	PRO	VAL	THR	THR	THR	THR	THR	THR	
THR	LEU	THR	ILE	GLY	GLY	SER	ASP	TRP	GLY	GLN	SER	MET	PHE	THR	CYS	ARG	VAL	ASP	HIS	THR	GLY	ASP	GLN	THR	PHE	GLN	GLN	ASN	ALA	SER	SER	SER	GLY	ASP	GLN	VAL	VAL	GLN	VAL	GLU	ALA	ILE	VAL	PRO	VAL	THR	THR	THR	THR	THR	
K382	T383	R384	E388	H393	H400	F405	S406	A407	V408	G409	E410	A411	S412	D416	D417	W418	N419	C426	H430	T431	D432	Q439	R443	P444	LYS	GLY	VAL	A448	P452	V454	L455	L457	P459	R467	S469	A470	T471	L472	T473	C474	L475	V476	F479	T480	S481	T482	S483				
V484	M489	V501	E508	P509	Q510	A511	B514	H518	N529	T530	G531	E532	T533	T535	C536	V537	V538	A539	H540	T551	V552	D553	S555	T556	M568	SER	ASP	THR	THR	ALA	GLY	THR	CYS	TYR																	

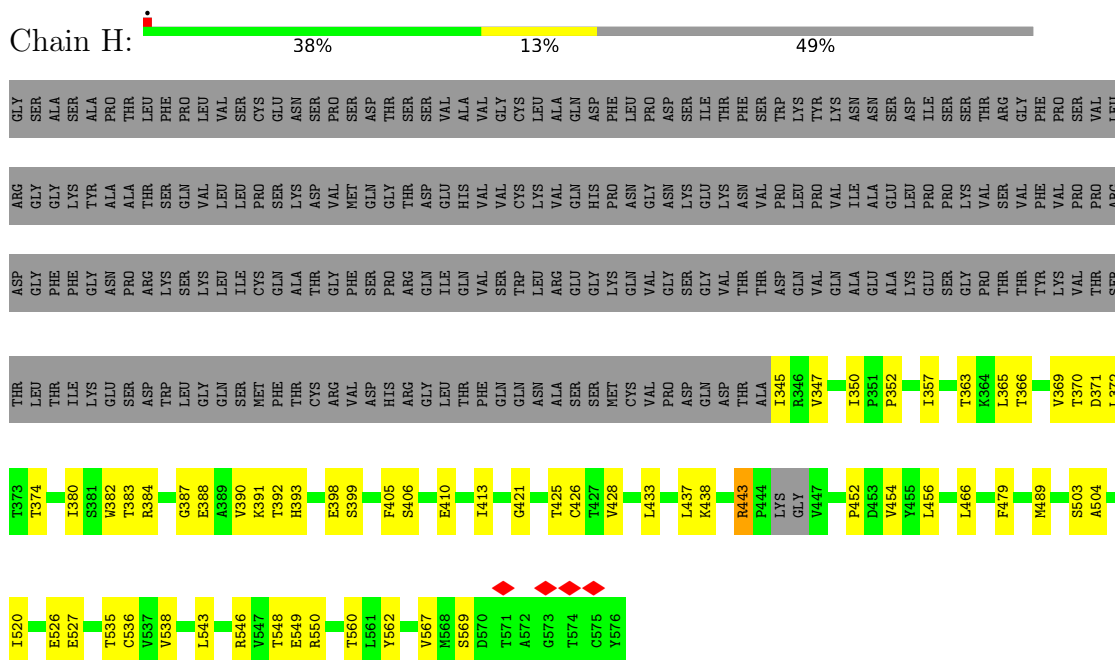
- Molecule 1: Immunoglobulin heavy constant mu

Chain G:  31% 18% 51%

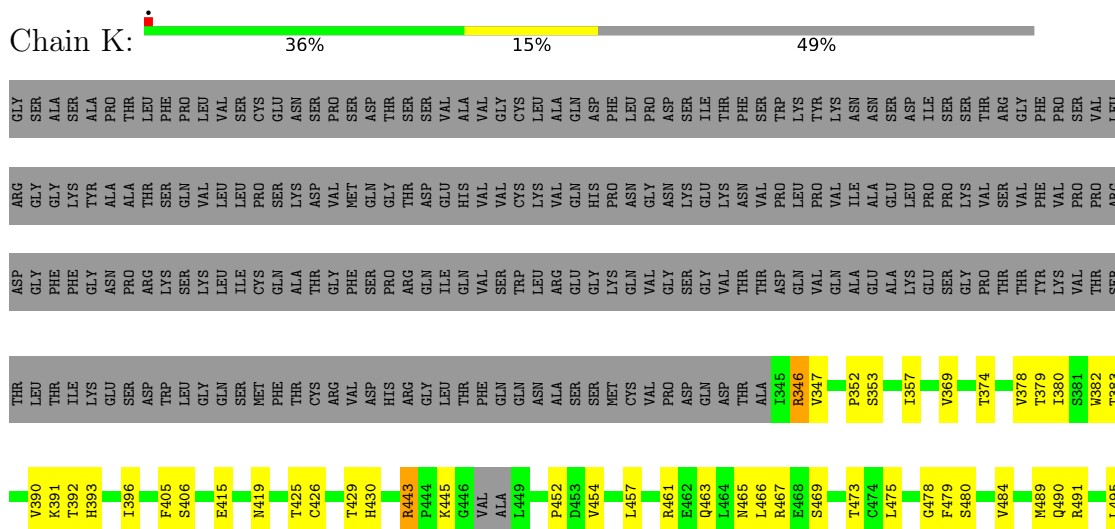
GLY	SER	ALA	SER	ALA	PRO	THR	LEU	PHE	PRO	GLN	VAL	SER	CYS	GLU	ASN	SER	PRO	SER	ASP	THR	SER	VAL	ALA	VAL	GLY	CYS	LEU	ALA	GLN	ASP	PHE	GLN	LEU	PRO	LYS	TYR	LYS	ASN	GLU	SER	ASP	ILE	SER	PRO	GLY	PHE	PRO	VAL	SER	LEU																																																																																																	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



- Molecule 1: Immunoglobulin heavy constant mu



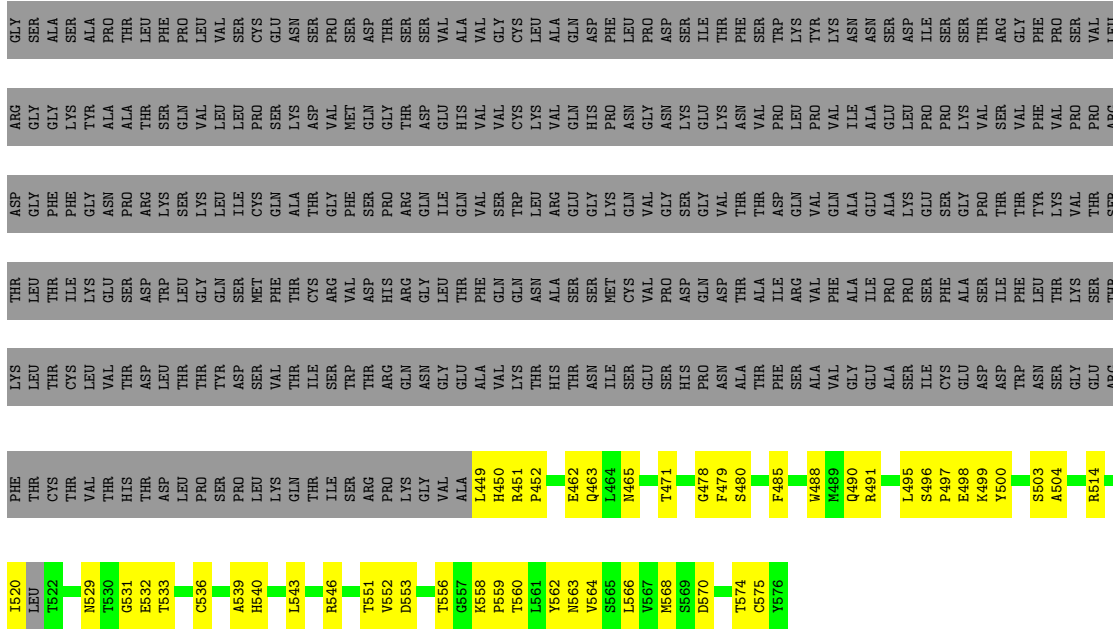
- Molecule 1: Immunoglobulin heavy constant mu





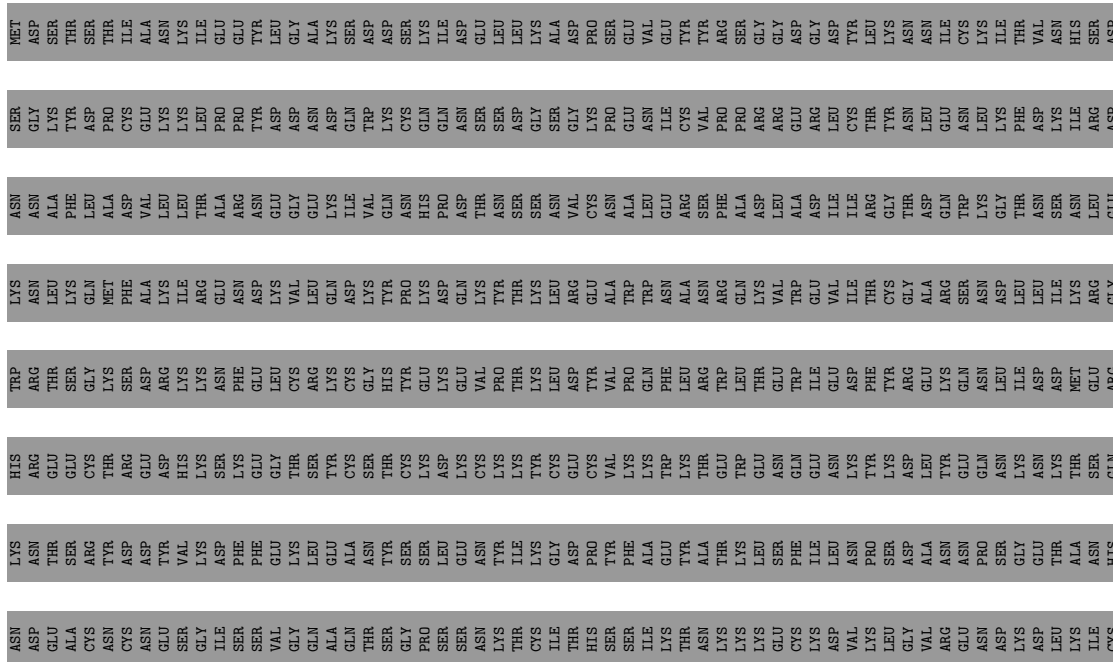
• Molecule 1: Immunoglobulin heavy constant mu

Chain L: 17% 11% 72%



• Molecule 2: Erythrocyte membrane protein 1

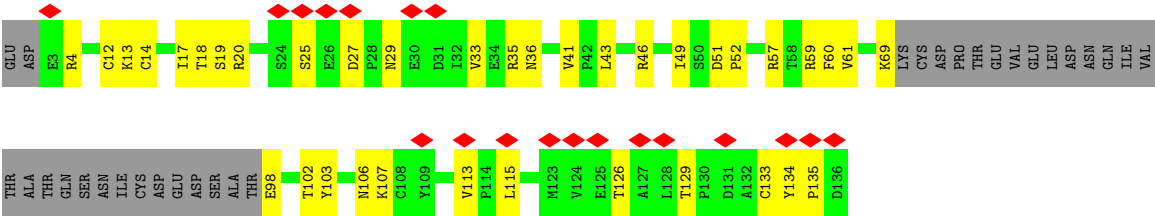
Chain I: 29% 13% 58%



Q1629	P1544	C1437	H1345	G1J	N1117	Y1044	LYS	THR	VAL	THR	GLY	ASP	GLY	VAL
I1639	E1545	P1441	A1346	THR	R1122	Q1045	TTR	ALA	ILE	ALA	THR	VAL	TTR	ILE
N1643	C1546	G1444	V1347	ASP	R1125	Q1048	CYS	GLN	ASN	THR	ILE	ASP	CYS	ASP
E1644	I1547	G1444	R1349	THR	Q1126	A1063	CYS	GLN	ASN	THR	ILE	ASP	ASN	THR
E1645	F1551	E1447	Y1354	ILE	Y1127	ASN	LYS	LYS	ASP	GLU	ASP	PHE	CYS	LYS
G1646	ASP	D1448	K1355	ASN	ASP	ILE	PRO	ILE	ASP	ASP	GLU	ASP	CYS	LYS
K1649	F1553	Q1449	N1356	LYS	ALA	SER	GLY	ALA	ASP	ASN	GLU	THR	GLY	VAL
L1655	F1555	S1452	N1364	THR	GLY	ASP	N970	ARG	ASN	ASN	GLY	THR	ASN	CYS
N1656	N1558	W1453	I1365	S1218	GLN	GLY	N971	ALA	LYS	LYS	LYS	ASP	ARG	CYS
I1657	I1559	F1454	Y1366	GLU	ASN	LYS	E972	PRO	ALA	ALA	CYS	LEU	LEU	CYS
L1658	E1560	K1455	E1367	VAL	ASN	VAL	E973	THR	PRO	GLY	LYS	ASP	GLY	GLN
Q1659	Y1561	W1457	H1368	LEU	LYS	ASP	T974	THR	THR	ASP	CYS	LEU	LEU	ASP
I1660	K1562	F1461	K1371	ASP	VAL	SER	R978	THR	THR	GLY	LYS	LEU	TRP	LEU
V1661	T1563	C1462	I1379	K1238	W1139	VAL	R979	THR	THR	GLN	LYS	LEU	TRP	LEU
R1664	Y1564	I1463	I1380	W1249	S1142	SER	Y981	THR	THR	ASN	CYS	ILE	ILE	GLY
K1671	Y1570	E1464	E1381	K1252	N1143	GLU	C987	THR	THR	GLY	LYS	VAL	TRP	GLY
Q1672	S1571	I1478	K1382	D1253	F1147	THR	G988	THR	THR	GLY	LYS	PHE	TRP	ILE
K1678	I1573	ASN	F1385	T1254	E1151	GLY	ALA	THR	THR	GLY	LYS	GLY	GLY	LEU
D1681	K1580	LYS	GLN	I1255	PRO	THR	ALA	THR	THR	GLY	LYS	PHE	GLY	GLN
K1685	Y1581	ASN	LYS	I1256	E1154	VAL	MET	THR	THR	GLY	LYS	HIS	GLY	GLN
I1691	Y1582	LYS	ASP	H1257	N1159	ARG	LYS	THR	THR	GLY	LYS	GLY	GLY	ASN
Y1694	K1583	C1486	ILE	T1260	GLY	GLY	TTR	LYS	LYS	ASN	LYS	ARG	GLN	ARG
N1695	N1585	S1491	GLY	I1261	ASP	TTR	LYS	GLU	LYS	GLU	GLY	TYR	GLY	GLY
R1692	N1586	GLY	VAL	G1262	TRP	GLU	LYS	ARG	PHE	ASP	ILE	PRO	GLU	SER
D1697	A1587	GLN	GLY	A1263	S1163	ASP	ASN	ASP	ILE	THR	GLY	ALA	GLU	ALA
V1708	K1590	G1494	SER	C1264	K1164	GLY	D1000	LYS	ALA	ALA	LYS	ALA	ASN	SER
H1709	N1591	D1495	THR	T1269	I1177	ASN	L1004	LYS	CYS	ILE	PRO	GLN	ASN	ASN
T1713	N1592	K1496	E1399	I1272	K1178	ASN	C1005	THR	CYS	GLY	GLY	GLN	THR	THR
K1714	L1595	I1497	M1400	L1272	K1179	ASN	T1016	ILE	ALA	THR	THR	THR	GLY	GLY
Y1715	L1595	Q1498	V1401	S1281	C1180	THR	V1017	ARG	ALA	ALA	LEU	LEU	LEU	ASP
K1719	K1599	K1504	N1402	E1281	N1183	GLN	R1018	PHE	GLY	GLY	PRO	ARG	LYS	LYS
D1600	D1600	C1505	R1410	D1291	H1186	GLY	SER	SER	ILE	ILE	LEU	LEU	ASN	ASN
N1601	N1601	E1506	E1411	T1292	G1187	THR	ASN	THR	THR	THR	LEU	LEU	THR	THR
D1602	D1602	K1507	M1412	K1293	E1188	ASN	S1022	THR	PHE	PHE	LEU	LEU	LEU	LEU
W1605	W1605	K1510	W1413	L1295	E1189	K1094	D1025	GLY	LYS	GLY	ARG	GLU	TYR	GLY
K1611	K1611	E1514	I1420	I1300	I1190	C1097	F1031	ASN	PRO	ILE	THR	GLY	ASN	ASN
E1614	E1614	K1515	K1422	I1304	S1192	K1098	F1032	PRO	THR	ASP	CYS	TRP	ASN	LEU
N1615	N1615	Q1517	I1423	H1305	E1193	C1099	N1033	PRO	ILE	ILE	GLY	GLU	PRO	LYS
Q1616	Q1616	E1518	N1424	H1305	K1194	Y1100	E1036	GLY	GLY	GLY	ALA	THR	ALA	VAL
R1617	R1617	W1519	K1425	L1311	L1195	L1101	Q1037	ASN	THR	THR	GLN	ASN	TYR	LEU
S1618	S1618	D1520	I1431	K1328	K1196	W1103	W1038	THR	THR	ASP	ALA	GLY	GLY	ALA
P1625	P1625	K1521	F1432	N1334	E1199	K1106	N1039	PRO	PRO	PRO	GLN	LYS	ASN	ASN
P1626	P1626	K1525	N1433	N1334	K1203	Q1114	K1040	TTR	THR	THR	ILE	VAL	VAL	LEU
R1627	R1627	A1535	D1435	L1339	GLU	Q1114	E1041	ARG	SER	SER	ILE	THR	CYS	THR
R1628	R1628		E1436		ASN		I1042	ILE	THR	THR	ASP	TRP	GLU	ASN







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	371049	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00805	Depositor
Map size (Å)	594.0, 594.0, 594.0	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/1053	0.51	0/1442
1	B	0.25	0/1809	0.54	0/2478
1	C	0.24	0/1794	0.52	0/2457
1	D	0.25	0/1788	0.53	0/2449
1	E	0.25	0/1788	0.53	0/2449
1	F	0.25	0/1767	0.52	0/2420
1	G	0.25	0/1788	0.52	0/2449
1	H	0.25	0/1830	0.52	0/2507
1	K	0.25	0/1831	0.52	0/2506
1	L	0.25	0/1019	0.55	0/1395
2	I	0.24	0/9392	0.46	0/12593
2	M	0.25	0/9392	0.47	0/12593
3	J	0.23	0/864	0.55	0/1173
All	All	0.25	0/36115	0.49	0/48911

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1026	0	1001	33	0
1	B	1764	0	1724	61	0
1	C	1749	0	1713	48	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1743	0	1709	40	0
1	E	1743	0	1709	48	0
1	F	1723	0	1682	41	0
1	G	1743	0	1708	57	0
1	H	1785	0	1735	42	0
1	K	1786	0	1737	43	0
1	L	993	0	959	39	0
2	I	9208	0	8976	235	0
2	M	9208	0	8974	240	0
3	J	851	0	843	37	0
All	All	35322	0	34470	927	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 13.

All (927) 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:K:369:VAL:O	1:K:406:SER:HA	1.58	1.04
2:I:1191:PHE:O	2:I:1194:LYS:HB2	1.66	0.93
3:J:4:ARG:HH22	3:J:36:ASN:H	1.23	0.87
1:B:490:GLN:HG2	1:B:491:ARG:HG2	1.60	0.83
1:C:452:PRO:HB3	1:C:479:PHE:HB3	1.61	0.81
1:H:347:VAL:HG22	1:H:369:VAL:HG12	1.64	0.80
1:B:452:PRO:HB3	1:B:479:PHE:HB3	1.62	0.79
2:M:2075:GLN:NE2	2:M:2155:ALA:O	2.16	0.79
1:B:428:VAL:O	1:B:436:PRO:HA	1.84	0.78
1:D:426:CYS:HB3	1:D:439:GLN:HB2	1.67	0.77
1:D:527:GLU:OE1	1:D:534:TYR:OH	2.02	0.77
3:J:4:ARG:HH21	3:J:18:THR:HG23	1.49	0.77
2:M:1367:GLU:CD	2:M:1368:HIS:H	1.90	0.75
2:I:2067:LYS:HA	2:I:2070:ILE:HG12	1.69	0.73
1:K:452:PRO:HB3	1:K:479:PHE:HB3	1.70	0.73
2:I:2129:ARG:NH1	2:I:2132:GLU:O	2.21	0.73
2:M:2139:LYS:HD3	2:M:2142:GLU:HB3	1.71	0.73
2:I:1900:ILE:HB	2:I:1908:SER:HB2	1.71	0.72
2:M:2125:ILE:HG22	2:M:2129:ARG:HH11	1.54	0.72
3:J:4:ARG:HH11	3:J:20:ARG:HB2	1.53	0.71
1:B:454:VAL:HG21	1:B:538:VAL:HG11	1.70	0.71
1:D:425:THR:HG22	1:D:440:THR:HG22	1.73	0.70
2:I:1626:PRO:HA	2:I:1629:GLN:HE21	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2060:LEU:HD11	2:I:2064:ASN:HA	1.73	0.70
1:F:535:THR:HG22	1:F:551:THR:HB	1.74	0.70
1:K:378:VAL:HG12	1:K:430:HIS:HD2	1.56	0.69
2:I:1293:LYS:HE3	2:I:1380:ILE:HD13	1.74	0.69
1:D:489:MET:HB3	1:D:535:THR:HG23	1.75	0.69
2:I:2213:VAL:HG12	2:I:2214:THR:HG23	1.73	0.69
1:G:467:ARG:O	2:I:2059:ASN:ND2	2.26	0.69
2:M:1365:ILE:H	2:M:1369:ILE:HD11	1.57	0.69
1:L:478:GLY:O	1:L:514:ARG:NH2	2.27	0.68
2:M:1497:ILE:HG22	2:M:1499:GLY:H	1.57	0.68
1:C:463:GLN:NE2	1:C:469:SER:O	2.27	0.68
1:D:452:PRO:HB3	1:D:479:PHE:HB3	1.74	0.68
2:I:1122:ARG:NH1	2:I:1125:GLN:O	2.27	0.68
1:C:380:ILE:HG21	1:C:407:ALA:HB1	1.76	0.68
1:A:458:PRO:HA	1:A:472:ILE:HD12	1.76	0.68
1:B:489:MET:O	1:B:535:THR:OG1	2.08	0.68
2:I:1226:TYR:HE2	2:I:1228:ARG:HH12	1.42	0.68
1:D:393:HIS:HD2	1:D:396:ILE:HD11	1.58	0.68
2:I:2029:LEU:O	2:I:2032:THR:OG1	2.11	0.68
2:M:2054:VAL:HG12	2:M:2056:GLY:H	1.59	0.67
2:I:987:CYS:HA	2:I:1005:CYS:HA	1.76	0.67
2:M:1028:ASP:OD2	2:M:1125:GLN:NE2	2.27	0.67
1:G:383:THR:HB	1:G:387:GLY:HA2	1.74	0.67
1:G:567:VAL:HB	1:H:567:VAL:HG12	1.75	0.67
1:C:384:ARG:HB2	1:C:388:GLU:HB2	1.77	0.67
1:H:369:VAL:O	1:H:406:SER:HA	1.94	0.67
1:E:454:VAL:HG22	1:E:476:VAL:HG22	1.77	0.67
1:C:347:VAL:HG22	1:C:369:VAL:HG13	1.77	0.67
1:C:347:VAL:HG13	1:C:369:VAL:HG22	1.77	0.67
2:M:1869:LYS:HD3	2:M:1874:SER:HA	1.77	0.66
2:M:978:ARG:NH2	2:M:1099:CYS:SG	2.68	0.66
1:B:382:TRP:HB3	1:B:384:ARG:HH22	1.60	0.66
1:F:357:ILE:HD13	1:F:363:THR:HB	1.77	0.66
1:F:532:GLU:HB3	1:F:534:TYR:CZ	2.31	0.66
1:D:451:ARG:HH12	1:D:544:PRO:HD3	1.61	0.66
2:M:1572:SER:O	2:M:1575:SER:N	2.26	0.66
1:G:461:ARG:O	1:G:465:ASN:ND2	2.27	0.66
2:I:1757:ARG:HA	2:I:1760:VAL:HG22	1.78	0.66
1:G:427:THR:HG22	1:G:438:LYS:HG2	1.78	0.66
2:I:2079:LYS:HD2	2:I:2094:ALA:HB1	1.78	0.66
2:M:1348:GLN:NE2	2:M:1437:CYS:SG	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1736:ARG:HH22	2:M:1740:ASP:HB3	1.60	0.66
1:B:383:THR:HB	1:B:387:GLY:HA2	1.78	0.65
1:E:465:ASN:O	1:E:467:ARG:NH1	2.29	0.65
1:G:357:ILE:HD12	1:G:363:THR:HG22	1.76	0.65
1:B:456:LEU:HD13	1:B:474:CYS:HB3	1.77	0.65
1:H:384:ARG:HG3	1:H:388:GLU:HB2	1.78	0.65
1:K:465:ASN:HA	1:K:467:ARG:HH11	1.62	0.65
1:C:379:THR:HB	1:C:429:THR:HB	1.78	0.65
2:I:1420:ILE:O	2:I:1424:ASN:ND2	2.30	0.65
2:M:1346:ALA:HA	2:M:1349:ARG:HD2	1.78	0.65
1:G:384:ARG:NH1	1:G:388:GLU:OE1	2.29	0.65
1:A:548:THR:HB	1:A:550:ARG:HH12	1.61	0.65
1:G:489:MET:HB3	1:G:535:THR:OG1	1.97	0.65
2:I:2076:SER:HB3	2:I:2158:CYS:HB2	1.79	0.64
2:I:1515:LYS:NZ	2:I:1518:GLU:OE1	2.25	0.64
2:M:1226:TYR:O	2:M:1228:ARG:NH1	2.29	0.64
1:F:426:CYS:SG	1:F:439:GLN:NE2	2.70	0.64
2:I:1348:GLN:NE2	2:I:1437:CYS:SG	2.71	0.64
2:M:1032:PHE:O	2:M:1035:PHE:HB3	1.97	0.64
2:I:1004:LEU:HA	2:I:1031:PHE:HE1	1.62	0.64
2:I:1045:GLN:OE1	2:I:1048:GLN:NE2	2.31	0.64
2:I:1964:VAL:O	2:I:1968:HIS:ND1	2.30	0.64
2:M:1669:LEU:O	2:M:1673:TYR:HB2	1.97	0.64
1:G:369:VAL:HB	1:G:407:ALA:HB3	1.80	0.63
1:A:478:GLY:HA2	1:A:514:ARG:HB3	1.80	0.63
2:M:2247:ILE:HA	2:M:2250:ARG:HE	1.63	0.63
2:I:1100:TYR:HA	2:I:1103:TRP:CD1	2.32	0.63
1:L:450:HIS:HD1	1:L:480:SER:HG	1.44	0.63
2:I:2236:TRP:HA	2:I:2239:LYS:HD2	1.81	0.63
2:I:2148:ASN:HB3	2:I:2177:THR:HB	1.81	0.63
2:M:2150:LYS:O	2:M:2154:ASN:ND2	2.31	0.63
2:M:2236:TRP:HE3	2:M:2240:ARG:HH11	1.47	0.62
2:M:2248:SER:HA	2:M:2254:TYR:HB2	1.81	0.62
1:A:544:PRO:O	1:A:546:ARG:NH1	2.32	0.62
1:C:416:ASP:OD2	1:C:417:ASP:N	2.32	0.62
2:I:2144:TRP:O	2:I:2148:ASN:ND2	2.32	0.62
1:F:374:THR:HA	1:F:405:PHE:HB2	1.81	0.62
1:F:393:HIS:HB3	1:F:410:GLU:H	1.64	0.62
1:A:493:GLN:NE2	1:A:494:PRO:O	2.33	0.62
2:I:1293:LYS:NZ	2:I:1379:ILE:O	2.32	0.62
1:L:449:LEU:N	1:L:480:SER:O	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:VAL:HG11	1:E:428:VAL:HG11	1.81	0.62
1:F:345:ILE:HD12	1:F:372:LEU:HD11	1.82	0.62
1:K:380:ILE:O	1:K:393:HIS:ND1	2.31	0.62
1:B:491:ARG:HH21	2:M:2055:ARG:CZ	2.12	0.62
1:E:380:ILE:HG12	1:E:428:VAL:HG22	1.82	0.62
2:M:2083:ASN:HB3	2:M:2086:LYS:HB3	1.80	0.61
1:C:486:VAL:HG12	1:C:538:VAL:HG23	1.81	0.61
2:M:1357:MET:HA	2:M:1363:VAL:HG21	1.81	0.61
1:H:352:PRO:HB2	1:H:357:ILE:HD11	1.81	0.61
2:I:2044:ARG:NH2	2:I:2097:ALA:O	2.33	0.61
2:M:1257:HIS:ND1	2:M:1365:ILE:O	2.33	0.61
1:B:535:THR:HB	1:B:549:GLU:OE2	2.01	0.61
1:C:398:GLU:O	1:C:406:SER:OG	2.18	0.61
1:F:484:VAL:HG23	1:F:540:HIS:HB2	1.81	0.61
2:I:1262:GLY:HA2	2:I:1525:LYS:HE2	1.83	0.61
1:A:491:ARG:NH1	1:A:533:THR:O	2.30	0.61
1:G:352:PRO:HB2	1:G:357:ILE:HD11	1.83	0.61
1:L:452:PRO:HB3	1:L:479:PHE:HB3	1.83	0.61
2:M:1857:ASN:O	2:M:1861:ASN:ND2	2.33	0.61
1:L:451:ARG:HD3	1:L:452:PRO:HD2	1.83	0.60
2:M:1142:SER:OG	2:M:1188:GLU:OE1	2.19	0.60
2:M:2029:LEU:O	2:M:2032:THR:OG1	2.19	0.60
2:M:1017:VAL:HG21	2:M:1959:MET:HG3	1.83	0.60
2:M:1121:PHE:O	2:M:1125:GLN:NE2	2.33	0.60
2:M:2249:LYS:NZ	2:M:2250:ARG:O	2.33	0.60
1:K:346:ARG:NH1	1:K:347:VAL:O	2.35	0.60
2:M:1016:THR:HG22	2:M:1026:GLY:HA2	1.83	0.60
2:M:1420:ILE:O	2:M:1424:ASN:ND2	2.35	0.60
2:M:2052:ARG:HE	2:M:2057:PRO:HG3	1.66	0.60
1:G:413:ILE:HD13	1:G:424:PHE:HE2	1.65	0.60
1:C:427:THR:HG22	1:C:438:LYS:HD3	1.83	0.60
2:M:1673:TYR:HE2	2:M:1686:LYS:HG3	1.65	0.60
1:B:442:SER:OG	1:B:445:LYS:NZ	2.35	0.60
1:E:467:ARG:NH2	2:I:1281:SER:O	2.29	0.60
1:H:382:TRP:CD2	1:H:426:CYS:HB3	2.36	0.60
3:J:14:CYS:HB2	3:J:102:THR:HG21	1.84	0.60
2:I:1093:CYS:SG	2:I:1094:LYS:N	2.73	0.60
1:L:533:THR:O	1:L:551:THR:OG1	2.19	0.60
1:G:461:ARG:HD3	1:G:465:ASN:HD21	1.67	0.59
3:J:36:ASN:ND2	1:L:563:ASN:OD1	2.35	0.59
1:L:450:HIS:ND1	1:L:480:SER:OG	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1417:ARG:NH2	2:M:1439:VAL:O	2.34	0.59
2:M:2023:GLU:OE2	2:M:2046:ARG:NH2	2.34	0.59
1:G:346:ARG:NE	1:G:370:THR:OG1	2.35	0.59
1:C:533:THR:HG1	1:C:551:THR:HG1	1.33	0.59
1:H:345:ILE:HG21	1:H:433:LEU:HD12	1.84	0.59
1:H:489:MET:O	1:H:535:THR:OG1	2.17	0.59
2:I:1516:LYS:HD2	2:I:1555:PHE:HB3	1.83	0.59
2:I:2030:ARG:HE	2:I:2031:GLY:H	1.49	0.59
1:G:374:THR:HA	1:G:405:PHE:HB2	1.84	0.59
2:M:2241:SER:HA	2:M:2244:TRP:NE1	2.18	0.59
1:B:381:SER:OG	1:B:427:THR:OG1	2.19	0.59
1:K:443:ARG:HH12	1:K:445:LYS:HD3	1.68	0.59
1:L:496:SER:OG	1:L:498:GLU:OE1	2.20	0.59
1:F:452:PRO:HB3	1:F:479:PHE:HB3	1.84	0.59
2:I:1514:GLU:O	2:I:1517:GLN:NE2	2.36	0.59
2:I:2107:ASP:HB2	2:I:2112:THR:HB	1.83	0.59
2:M:1413:TRP:NE1	2:M:1439:VAL:O	2.33	0.59
1:G:553:ASP:OD1	1:G:556:THR:OG1	2.17	0.59
2:I:2147:THR:HG23	2:I:2150:LYS:HE2	1.85	0.59
1:D:383:THR:HB	1:D:387:GLY:HA2	1.85	0.59
2:M:2076:SER:HB3	2:M:2158:CYS:HB2	1.85	0.58
2:I:1334:ASN:ND2	2:I:1339:LEU:O	2.36	0.58
1:A:547:VAL:HG11	3:J:113:VAL:HG21	1.85	0.58
1:C:419:ASN:O	1:C:443:ARG:NH2	2.35	0.58
1:F:457:LEU:HB2	1:F:473:THR:HB	1.85	0.58
3:J:103:TYR:HB2	1:L:574:THR:HA	1.84	0.58
2:M:1100:TYR:HA	2:M:1103:TRP:HD1	1.68	0.58
2:M:1724:PHE:HD2	2:M:1738:ARG:HG2	1.69	0.58
2:I:2055:ARG:NH2	2:I:2059:ASN:OD1	2.36	0.58
1:H:370:THR:HG22	1:H:406:SER:HB2	1.85	0.58
1:H:391:LYS:NZ	1:H:392:THR:O	2.34	0.58
2:M:1702:ILE:O	2:M:1738:ARG:NH1	2.37	0.58
1:G:384:ARG:NE	1:G:386:ASN:OD1	2.36	0.58
1:L:562:TYR:HB3	1:L:564:VAL:HG23	1.86	0.58
1:G:459:PRO:HG2	1:G:464:LEU:HD11	1.86	0.58
2:I:2041:ILE:O	2:I:2046:ARG:NH2	2.37	0.58
2:M:981:TYR:HE2	2:M:1099:CYS:HB3	1.68	0.58
1:C:381:SER:HA	1:C:393:HIS:HE1	1.68	0.58
1:C:491:ARG:NH2	1:C:532:GLU:OE1	2.36	0.58
2:M:2075:GLN:HE22	2:M:2156:MET:HA	1.69	0.58
1:B:549:GLU:O	1:B:550:ARG:NH1	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:GLU:O	1:G:406:SER:OG	2.21	0.57
2:I:2029:LEU:HD22	2:I:2115:LEU:HD12	1.85	0.57
2:I:2015:LYS:HB3	2:I:2078:GLY:HA2	1.87	0.57
1:K:454:VAL:HG21	1:K:538:VAL:HG11	1.86	0.57
2:I:1305:HIS:HE1	2:I:1422:LYS:HD2	1.69	0.57
2:M:1038:TRP:O	2:M:1041:GLU:HG3	2.03	0.57
2:I:1033:ASN:HB3	2:I:1949:LYS:HD2	1.86	0.57
2:M:1036:GLU:O	2:M:1039:ASN:HB3	2.03	0.57
2:M:2143:ASP:OD1	2:M:2144:TRP:N	2.38	0.57
2:M:2145:TRP:HE1	2:M:2178:THR:HA	1.68	0.57
1:F:393:HIS:ND1	1:F:408:VAL:O	2.38	0.57
2:I:1799:LEU:HD13	2:I:1859:MET:HG3	1.87	0.57
2:M:1219:CYS:N	2:M:1418:CYS:SG	2.78	0.57
1:A:500:TYR:HB3	1:A:521:LEU:HD13	1.87	0.57
1:B:450:HIS:CE1	1:B:514:ARG:HH21	2.23	0.57
3:J:129:THR:OG1	3:J:133:CYS:SG	2.59	0.57
1:L:558:LYS:HZ3	1:L:560:THR:HA	1.69	0.57
1:A:451:ARG:NH2	1:A:542:ALA:O	2.38	0.57
1:F:454:VAL:HG22	1:F:476:VAL:HG22	1.86	0.57
2:M:1293:LYS:NZ	2:M:1379:ILE:O	2.36	0.57
2:M:1757:ARG:HA	2:M:1760:VAL:HG22	1.87	0.56
2:M:2026:ASP:OD2	2:M:2030:ARG:NH2	2.37	0.56
1:D:527:GLU:O	1:D:530:THR:OG1	2.18	0.56
1:E:399:SER:HA	1:E:405:PHE:HA	1.86	0.56
2:I:1356:ASN:HD22	2:I:1449:GLN:HG2	1.69	0.56
2:I:2024:TRP:CD1	2:I:2043:PRO:HD3	2.40	0.56
2:M:1113:LYS:O	2:M:1117:ASN:ND2	2.38	0.56
1:E:452:PRO:HB3	1:E:479:PHE:HB3	1.86	0.56
1:H:536:CYS:N	1:H:549:GLU:OE2	2.37	0.56
2:I:1452:SER:O	2:I:1456:GLU:HG2	2.05	0.56
3:J:33:VAL:HB	1:L:559:PRO:HA	1.85	0.56
1:G:430:HIS:HB3	1:G:433:LEU:HD13	1.87	0.56
1:H:452:PRO:HB3	1:H:479:PHE:HB3	1.88	0.56
2:M:2200:GLN:HA	2:M:2203:LYS:HZ3	1.71	0.56
2:I:2181:PRO:HB3	2:I:2185:LEU:HD22	1.86	0.56
2:I:2024:TRP:HD1	2:I:2042:PRO:HA	1.70	0.56
2:M:2077:GLU:HA	2:M:2080:PHE:HB3	1.86	0.56
2:M:2236:TRP:O	2:M:2240:ARG:NH1	2.39	0.56
1:C:565:SER:O	1:C:567:VAL:HG23	2.06	0.56
1:E:383:THR:HA	1:E:389:ALA:HA	1.87	0.56
1:E:416:ASP:OD1	1:E:417:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1599:LYS:O	2:I:1672:GLN:NE2	2.39	0.56
2:I:1856:TRP:HA	2:I:1859:MET:SD	2.46	0.56
2:M:1043:GLN:O	2:M:1046:ILE:HG22	2.06	0.56
2:I:1122:ARG:NH1	2:I:1125:GLN:OE1	2.39	0.56
1:D:423:ARG:HA	1:D:442:SER:HB3	1.88	0.55
1:G:382:TRP:HB2	1:G:390:VAL:HG21	1.87	0.55
1:G:486:VAL:HG12	1:G:538:VAL:HG23	1.88	0.55
1:K:391:LYS:NZ	1:K:392:THR:O	2.35	0.55
2:M:2213:VAL:HG12	2:M:2214:THR:HG23	1.88	0.55
2:M:1122:ARG:NH1	2:M:1139:VAL:O	2.39	0.55
2:M:1151:GLU:HA	2:M:1154:ILE:HG22	1.88	0.55
2:M:1100:TYR:HA	2:M:1103:TRP:CD1	2.41	0.55
1:E:459:PRO:HD3	1:E:472:ILE:HG13	1.87	0.55
3:J:4:ARG:NH2	3:J:18:THR:O	2.40	0.55
2:M:1421:THR:HA	2:M:1424:ASN:HD21	1.72	0.55
2:M:2075:GLN:HA	2:M:2079:LYS:H	1.72	0.55
2:M:2125:ILE:HG22	2:M:2129:ARG:NH1	2.22	0.55
2:M:2142:GLU:O	2:M:2146:LYS:N	2.34	0.55
2:I:1644:GLU:OE2	2:I:1719:LYS:NZ	2.39	0.55
2:M:1850:ASN:HD22	2:M:1853:ARG:HH12	1.55	0.55
2:I:978:ARG:NH2	2:I:1099:CYS:SG	2.72	0.55
2:M:1701:ILE:HG22	2:M:1706:ASP:HB2	1.88	0.55
2:I:1154:ILE:HG21	2:I:1164:LYS:HE2	1.89	0.55
1:K:465:ASN:HA	1:K:467:ARG:NH1	2.22	0.55
1:D:383:THR:OG1	1:D:425:THR:OG1	2.25	0.55
1:D:402:ASN:OD1	1:D:404:THR:OG1	2.21	0.55
1:H:503:SER:OG	1:H:504:ALA:N	2.40	0.55
2:M:2095:LEU:HD22	2:M:2172:TRP:HD1	1.72	0.55
1:C:369:VAL:HG11	1:C:428:VAL:HG21	1.88	0.54
2:M:1871:ASN:ND2	2:M:1877:GLY:O	2.38	0.54
2:I:1041:GLU:O	2:I:1045:GLN:N	2.38	0.54
1:K:374:THR:HA	1:K:405:PHE:HB2	1.89	0.54
2:M:1421:THR:HG22	2:M:1433:ASN:HA	1.89	0.54
1:C:400:HIS:CD2	1:C:406:SER:HB3	2.42	0.54
1:C:567:VAL:HG12	1:C:567:VAL:O	2.07	0.54
1:F:489:MET:HB3	1:F:535:THR:OG1	2.08	0.54
2:M:1821:CYS:O	2:M:1957:HIS:NE2	2.40	0.54
2:M:2036:HIS:CE1	2:M:2250:ARG:HH22	2.25	0.54
2:M:2107:ASP:HB3	2:M:2112:THR:HB	1.88	0.54
2:I:1151:GLU:HA	2:I:1154:ILE:HG22	1.89	0.54
1:K:353:SER:O	1:K:357:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2015:LYS:HB3	2:M:2078:GLY:HA2	1.88	0.54
1:A:459:PRO:HG3	1:A:470:ALA:HB1	1.89	0.54
3:J:57:ARG:NH2	3:J:59:ARG:O	2.40	0.54
2:M:1719:LYS:O	2:M:1723:ILE:HG12	2.06	0.54
2:I:1183:ASN:HB2	2:I:1186:HIS:HB3	1.90	0.54
2:M:1473:ARG:O	2:M:1477:THR:OG1	2.19	0.54
2:I:971:ASN:OD1	2:I:974:THR:OG1	2.26	0.54
2:I:1792:LYS:O	2:I:1797:ARG:NH1	2.41	0.54
2:M:1227:ILE:HD11	2:M:1302:ASN:HB3	1.90	0.54
2:M:2016:THR:HG21	2:M:2081:LEU:HD22	1.90	0.54
1:E:489:MET:HB3	1:E:535:THR:OG1	2.08	0.54
2:I:1605:TRP:CE2	2:I:1626:PRO:HD3	2.43	0.54
2:M:978:ARG:HH12	2:M:1095:GLU:HB2	1.73	0.54
1:E:393:HIS:HB3	1:E:410:GLU:H	1.73	0.54
1:H:393:HIS:HB2	1:H:410:GLU:HG3	1.88	0.54
2:I:1895:ARG:NH2	2:I:1904:TYR:O	2.40	0.53
2:M:1985:LEU:HB2	2:M:2149:LYS:HE3	1.90	0.53
2:I:1349:ARG:NH1	2:I:1456:GLU:OE1	2.41	0.53
2:M:1955:SER:HA	2:M:1958:LYS:HD3	1.89	0.53
1:B:535:THR:HG22	1:B:551:THR:HG23	1.89	0.53
1:H:345:ILE:N	1:H:371:ASP:O	2.42	0.53
2:I:2044:ARG:HH12	2:I:2100:ASN:HB2	1.72	0.53
2:I:2241:SER:HA	2:I:2244:TRP:CH2	2.44	0.53
1:L:503:SER:OG	1:L:504:ALA:N	2.41	0.53
2:M:1786:GLU:OE2	2:M:1787:HIS:ND1	2.41	0.53
1:B:383:THR:OG1	1:B:425:THR:OG1	2.26	0.53
2:I:1399:GLU:HG2	2:I:1401:VAL:HG22	1.89	0.53
2:I:2025:ASN:HA	2:I:2040:LEU:HD22	1.91	0.53
1:A:499:LYS:NZ	1:A:522:THR:O	2.41	0.53
1:D:380:ILE:HD13	1:D:407:ALA:HB1	1.89	0.53
1:D:433:LEU:HD21	1:D:437:LEU:HB2	1.90	0.53
2:I:1114:GLN:HA	2:I:1117:ASN:HD21	1.73	0.53
1:E:524:SER:OG	1:E:526:GLU:OE1	2.26	0.53
1:F:347:VAL:HG22	1:F:369:VAL:HG13	1.91	0.53
1:H:543:LEU:HD13	1:H:548:THR:HG23	1.91	0.53
2:I:2064:ASN:HB3	2:I:2067:LYS:HE3	1.90	0.53
3:J:46:ARG:NH1	3:J:51:ASP:O	2.30	0.53
1:K:480:SER:HB3	1:K:514:ARG:HE	1.74	0.53
1:B:380:ILE:HG23	1:B:428:VAL:HG12	1.91	0.53
2:M:1853:ARG:HE	2:M:1948:ASN:HA	1.72	0.53
1:C:450:HIS:HB2	1:C:480:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:ILE:HG21	1:F:409:GLY:HA3	1.90	0.53
2:I:1345:HIS:C	2:I:1349:ARG:HE	2.13	0.53
2:I:1497:ILE:O	2:I:1498:GLN:NE2	2.34	0.53
2:I:2134:GLU:HG2	2:I:2136:ASN:H	1.74	0.53
3:J:4:ARG:HE	3:J:18:THR:HG23	1.74	0.53
1:B:532:GLU:HB3	1:B:534:TYR:CZ	2.44	0.53
1:H:393:HIS:HB3	1:H:410:GLU:H	1.73	0.53
2:I:1143:ASN:HB3	2:I:1973:LEU:HD21	1.91	0.53
2:I:1425:LYS:HA	2:I:1431:ILE:HG12	1.91	0.53
1:B:543:LEU:HB2	1:B:546:ARG:HA	1.91	0.52
2:I:2233:TYR:HA	2:I:2236:TRP:NE1	2.24	0.52
1:K:489:MET:HB3	1:K:535:THR:OG1	2.08	0.52
2:M:1143:ASN:HB3	2:M:1973:LEU:HD11	1.91	0.52
2:M:1681:ASP:OD1	2:M:1682:ASP:N	2.40	0.52
1:E:396:ILE:HG23	1:E:407:ALA:HA	1.91	0.52
1:G:503:SER:OG	1:G:504:ALA:N	2.42	0.52
2:I:1580:LYS:O	2:I:1590:LYS:NZ	2.42	0.52
2:M:1154:ILE:HG21	2:M:1164:LYS:HE2	1.91	0.52
2:M:1740:ASP:OD1	2:M:1741:TRP:N	2.42	0.52
2:M:2247:ILE:HA	2:M:2250:ARG:NE	2.24	0.52
1:E:398:GLU:O	1:E:406:SER:OG	2.23	0.52
2:I:2137:ASN:OD1	2:I:2139:LYS:NZ	2.42	0.52
3:J:4:ARG:NH2	3:J:36:ASN:HB2	2.24	0.52
1:B:503:SER:HG	1:B:518:HIS:H	1.58	0.52
2:M:2017:LYS:HE3	2:M:2047:GLN:HB3	1.92	0.52
1:G:365:LEU:HB2	1:G:411:ALA:HB3	1.92	0.52
1:K:463:GLN:NE2	1:K:469:SER:O	2.43	0.52
2:M:1147:PHE:CE1	2:M:1969:VAL:HG22	2.44	0.52
2:M:1193:GLU:O	2:M:1197:ASN:ND2	2.42	0.52
2:M:1572:SER:OG	2:M:1573:ILE:N	2.41	0.52
1:C:393:HIS:CD2	1:C:409:GLY:HA2	2.45	0.52
1:D:475:LEU:HD12	1:D:518:HIS:HE2	1.75	0.52
1:F:347:VAL:HG13	1:F:369:VAL:HG22	1.92	0.52
2:I:1681:ASP:O	2:I:1685:LYS:HG2	2.10	0.52
1:H:383:THR:HB	1:H:387:GLY:HA2	1.92	0.52
2:I:1639:ILE:O	2:I:1643:ASN:ND2	2.43	0.52
2:I:1655:LEU:HD12	2:I:1658:LEU:HD11	1.91	0.52
2:M:1354:TYR:O	2:M:1358:ILE:HG23	2.09	0.52
1:F:530:THR:OG1	2:M:1238:LYS:NZ	2.41	0.51
2:I:2015:LYS:HG3	2:I:2077:GLU:HB3	1.91	0.51
2:M:1356:ASN:HD22	2:M:1449:GLN:HG2	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2060:LEU:HB2	2:I:2127:LEU:HD12	1.92	0.51
2:I:2095:LEU:HD13	2:I:2172:TRP:CD1	2.44	0.51
2:M:1381:GLU:OE1	2:M:1400:ASN:ND2	2.44	0.51
2:I:1627:ARG:NH1	2:I:1697:ASP:OD2	2.43	0.51
1:H:569:SER:OG	1:H:569:SER:O	2.29	0.51
2:I:1399:GLU:N	2:I:1402:ASN:OD1	2.44	0.51
2:M:2080:PHE:HB2	2:M:2162:LYS:HG3	1.93	0.51
2:M:2175:ILE:HD12	2:M:2176:PRO:HD2	1.92	0.51
1:L:488:TRP:HB3	1:L:495:LEU:HD12	1.93	0.51
2:M:1710:ASP:OD1	2:M:1713:THR:OG1	2.27	0.51
1:C:367:CYS:HB2	1:C:382:TRP:CZ2	2.46	0.51
1:D:503:SER:OG	1:D:504:ALA:N	2.43	0.51
2:I:1421:THR:HA	2:I:1424:ASN:HD21	1.76	0.51
2:I:1457:TRP:NE1	2:I:1518:GLU:OE1	2.36	0.51
2:I:2118:ILE:HA	2:I:2121:LYS:HZ3	1.74	0.51
2:I:2129:ARG:NH2	2:I:2135:THR:HG22	2.25	0.51
2:M:2244:TRP:O	2:M:2247:ILE:HG22	2.11	0.51
1:G:416:ASP:OD1	1:G:417:ASP:N	2.44	0.51
1:G:466:LEU:HD11	2:I:2056:GLY:HA3	1.92	0.51
3:J:4:ARG:NH2	3:J:18:THR:HG23	2.21	0.51
3:J:29:ASN:HD22	1:L:529:ASN:HD22	1.57	0.51
1:C:346:ARG:NE	1:C:370:THR:OG1	2.42	0.51
1:C:489:MET:HB3	1:C:535:THR:HG23	1.92	0.51
2:I:1147:PHE:CE2	2:I:1969:VAL:HG22	2.46	0.51
2:I:1975:GLU:HA	2:I:1978:ASN:HD21	1.75	0.51
1:B:486:VAL:HG12	1:B:538:VAL:HG23	1.92	0.51
1:K:568:MET:HA	1:L:568:MET:SD	2.51	0.51
2:M:1443:THR:OG1	2:M:1445:ASN:OD1	2.20	0.51
1:A:467:ARG:HD2	1:A:525:GLU:HG3	1.92	0.51
1:E:384:ARG:HD2	1:E:388:GLU:HB2	1.93	0.51
1:H:380:ILE:HG13	1:H:428:VAL:HG22	1.92	0.51
1:K:563:ASN:HB3	1:L:563:ASN:HA	1.93	0.51
1:K:383:THR:HG22	1:K:390:VAL:HG11	1.93	0.50
2:M:1582:TYR:HB2	2:M:1590:LYS:HD3	1.92	0.50
1:G:467:ARG:HA	1:G:525:GLU:HG3	1.93	0.50
2:I:1305:HIS:CE1	2:I:1422:LYS:HD2	2.46	0.50
2:I:1249:TRP:HB3	2:I:1264:CYS:HB3	1.92	0.50
1:K:352:PRO:HB2	1:K:357:ILE:HD11	1.92	0.50
2:M:1723:ILE:HG13	2:M:1724:PHE:N	2.27	0.50
2:M:2169:ASP:OD1	2:M:2169:ASP:N	2.44	0.50
1:A:459:PRO:HB3	1:A:471:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2015:LYS:HE2	2:I:2077:GLU:HB2	1.92	0.50
1:A:553:ASP:H	1:A:556:THR:HG22	1.77	0.50
1:F:467:ARG:HB2	1:F:467:ARG:NH1	2.25	0.50
1:G:484:VAL:HG12	1:G:540:HIS:CD2	2.47	0.50
2:I:1772:VAL:HG13	2:I:1777:GLU:HG3	1.94	0.50
1:K:496:SER:HB3	1:K:499:LYS:HD3	1.93	0.50
2:M:1723:ILE:HG13	2:M:1724:PHE:H	1.77	0.50
2:I:1671:LYS:HD3	2:I:1775:LYS:HE2	1.94	0.50
2:I:2169:ASP:N	2:I:2169:ASP:OD1	2.44	0.50
2:M:1452:SER:O	2:M:1456:GLU:HG2	2.11	0.50
2:M:2123:ILE:O	2:M:2127:LEU:HD23	2.12	0.50
1:E:443:ARG:O	1:E:445:LYS:NZ	2.45	0.50
2:I:1839:LYS:HB2	2:I:1964:VAL:HG21	1.93	0.50
1:D:384:ARG:HG2	1:D:385:GLN:H	1.75	0.50
2:I:1097:CYS:SG	2:I:1101:LYS:NZ	2.84	0.50
2:M:2183:GLN:HA	2:M:2186:ARG:HB3	1.92	0.50
1:D:382:TRP:HB2	1:D:390:VAL:HG21	1.94	0.50
1:K:465:ASN:OD1	1:K:466:LEU:HD12	2.11	0.50
2:M:1838:CYS:SG	2:M:1960:LYS:NZ	2.82	0.50
1:B:491:ARG:NH2	2:M:2055:ARG:HG2	2.27	0.49
1:D:466:LEU:HG	1:D:468:GLU:OE1	2.12	0.49
1:G:347:VAL:HG23	1:G:369:VAL:HG22	1.94	0.49
2:I:1768:VAL:O	2:I:1772:VAL:HG23	2.12	0.49
2:I:2188:ILE:O	2:I:2192:GLY:N	2.41	0.49
1:K:553:ASP:O	1:K:556:THR:OG1	2.26	0.49
2:M:2222:GLU:HG3	2:M:2224:ASN:H	1.77	0.49
1:F:454:VAL:HG21	1:F:538:VAL:HG11	1.92	0.49
2:I:1570:TYR:C	2:I:1572:SER:H	2.15	0.49
1:K:378:VAL:HG12	1:K:430:HIS:CD2	2.41	0.49
2:M:1349:ARG:NE	2:M:1456:GLU:OE2	2.45	0.49
1:G:457:LEU:HB2	1:G:473:THR:OG1	2.13	0.49
2:I:1896:CYS:O	2:I:1907:CYS:HB2	2.13	0.49
1:K:484:VAL:HG12	1:K:540:HIS:CD2	2.47	0.49
2:M:2186:ARG:NH1	2:M:2190:GLU:HB2	2.28	0.49
1:B:463:GLN:NE2	1:B:469:SER:O	2.46	0.49
2:I:1177:ILE:HD11	2:I:1980:ILE:HD11	1.93	0.49
2:I:1411:GLU:N	2:I:1411:GLU:OE1	2.41	0.49
1:K:461:ARG:NH1	1:K:465:ASN:HB3	2.28	0.49
1:E:345:ILE:HG13	1:E:372:LEU:HG	1.95	0.49
2:M:1345:HIS:HB3	2:M:1349:ARG:CZ	2.43	0.49
2:M:2152:ILE:HG12	2:M:2175:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:454:VAL:HG21	1:H:538:VAL:HG11	1.95	0.49
2:I:1365:ILE:HG13	2:I:1366:TYR:N	2.28	0.49
2:I:1457:TRP:CH2	2:I:1519:TRP:HB2	2.48	0.49
2:M:1497:ILE:HB	2:M:1502:LYS:HB3	1.95	0.49
1:F:416:ASP:N	1:F:416:ASP:OD1	2.46	0.49
1:L:485:PHE:HB2	1:L:539:ALA:HB3	1.93	0.49
2:M:2188:ILE:O	2:M:2192:GLY:N	2.42	0.49
1:F:430:HIS:CD2	1:F:432:ASP:H	2.31	0.49
2:I:2076:SER:OG	2:I:2077:GLU:N	2.46	0.49
1:L:540:HIS:H	1:L:543:LEU:HD12	1.77	0.49
2:M:1045:GLN:HB3	2:M:1049:TYR:CE2	2.47	0.49
2:I:2075:GLN:NE2	2:I:2155:ALA:O	2.46	0.49
2:I:2126:LYS:NZ	2:I:2130:LEU:HD11	2.27	0.49
2:I:2196:CYS:O	2:I:2199:LYS:HG2	2.13	0.49
1:C:503:SER:OG	1:C:504:ALA:N	2.46	0.49
1:G:490:GLN:HE22	1:G:534:TYR:HE1	1.58	0.49
2:I:1601:ASN:OD1	2:I:1672:GLN:NE2	2.45	0.49
2:M:1444:GLY:HA2	2:M:1447:GLU:HG3	1.95	0.49
2:M:2193:THR:HA	2:M:2196:CYS:SG	2.53	0.49
1:A:452:PRO:HD3	1:A:542:ALA:HB3	1.95	0.48
2:I:1572:SER:OG	2:I:1573:ILE:N	2.32	0.48
1:L:488:TRP:CZ3	1:L:536:CYS:HB3	2.47	0.48
1:D:491:ARG:HH21	1:D:532:GLU:HG2	1.78	0.48
1:H:382:TRP:HB2	1:H:390:VAL:HG21	1.94	0.48
2:I:1681:ASP:N	2:I:1681:ASP:OD1	2.44	0.48
2:I:2049:CYS:O	2:I:2070:ILE:HD12	2.14	0.48
2:M:1981:LYS:HD3	2:M:1984:LYS:HZ3	1.77	0.48
2:M:2064:ASN:HB3	2:M:2067:LYS:HD3	1.95	0.48
2:I:1193:GLU:O	2:I:1196:LYS:HB2	2.13	0.48
1:L:491:ARG:NH1	1:L:532:GLU:O	2.46	0.48
2:M:2251:TYR:O	2:M:2252:LYS:HE2	2.13	0.48
1:H:357:ILE:HG12	1:H:363:THR:HB	1.96	0.48
2:M:1972:GLN:O	2:M:1975:GLU:HG3	2.13	0.48
1:E:475:LEU:HD13	1:E:518:HIS:CD2	2.49	0.48
1:H:560:THR:HG22	1:K:559:PRO:HA	1.95	0.48
2:I:1114:GLN:HA	2:I:1117:ASN:ND2	2.29	0.48
2:I:2210:CYS:HB3	2:I:2226:CYS:HB3	1.71	0.48
3:J:43:LEU:HD22	1:L:570:ASP:HB2	1.94	0.48
1:L:532:GLU:O	1:L:533:THR:HG22	2.14	0.48
2:M:1182:ASN:HB3	2:M:1186:HIS:HE1	1.77	0.48
2:M:1977:ASP:HA	2:M:1980:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG21	1:A:481:PRO:HB3	1.96	0.48
1:E:425:THR:OG1	1:E:440:THR:HG22	2.13	0.48
1:G:381:SER:HA	1:G:393:HIS:HE1	1.77	0.48
2:I:1658:LEU:HA	2:I:1661:VAL:HG12	1.96	0.48
2:I:1735:LYS:HE2	2:I:1738:ARG:HD3	1.95	0.48
2:I:2132:GLU:HG2	2:I:2138:THR:HA	1.95	0.48
2:M:1029:VAL:O	2:M:1032:PHE:HB3	2.14	0.48
2:M:1154:ILE:HD12	2:M:1158:PHE:HD2	1.79	0.48
2:I:1356:ASN:ND2	2:I:1449:GLN:HG2	2.29	0.48
2:M:2103:TYR:HB3	2:M:2186:ARG:HE	1.77	0.48
1:B:525:GLU:O	1:B:529:ASN:ND2	2.46	0.48
1:G:429:THR:HG23	1:G:436:PRO:HG3	1.95	0.48
2:I:2213:VAL:O	2:I:2214:THR:OG1	2.31	0.48
3:J:43:LEU:HB3	1:L:570:ASP:HA	1.95	0.48
3:J:106:ASN:OD1	3:J:107:LYS:N	2.47	0.48
1:K:415:GLU:O	1:K:419:ASN:ND2	2.47	0.48
2:M:1254:THR:OG1	2:M:1258:GLY:O	2.25	0.48
2:M:1611:LYS:HB3	2:M:1709:HIS:CG	2.48	0.48
1:B:382:TRP:CZ2	1:B:426:CYS:HB2	2.49	0.47
1:D:379:THR:HB	1:D:429:THR:HB	1.96	0.47
1:E:461:ARG:O	1:E:461:ARG:NH1	2.46	0.47
2:I:1102:LEU:HD23	2:I:1106:LYS:HD3	1.95	0.47
2:I:1269:THR:O	2:I:1272:LEU:HB2	2.14	0.47
2:M:1844:ASN:HA	2:M:1847:ASN:HD21	1.79	0.47
2:M:1853:ARG:NE	2:M:1947:LEU:O	2.47	0.47
1:B:425:THR:HG22	1:B:440:THR:HG22	1.96	0.47
1:C:467:ARG:HA	1:C:525:GLU:OE2	2.14	0.47
1:E:348:PHE:O	1:E:367:CYS:HA	2.14	0.47
1:G:413:ILE:HD12	1:G:417:ASP:HB2	1.95	0.47
2:M:2124:LYS:NZ	2:M:2125:ILE:HG12	2.28	0.47
2:I:1506:GLU:HB3	2:I:1510:LYS:NZ	2.29	0.47
1:K:393:HIS:CD2	1:K:396:ILE:HD11	2.50	0.47
2:M:2079:LYS:NZ	2:M:2098:MET:SD	2.88	0.47
1:E:391:LYS:NZ	1:E:392:THR:O	2.36	0.47
1:G:400:HIS:HB2	1:G:404:THR:HB	1.96	0.47
2:M:1590:LYS:HB2	2:M:1664:ARG:HH22	1.79	0.47
1:B:423:ARG:HA	1:B:441:ILE:O	2.14	0.47
1:G:466:LEU:HD12	2:I:2058:ALA:H	1.79	0.47
2:I:1602:ASP:N	2:I:1602:ASP:OD1	2.48	0.47
1:G:552:VAL:HG23	1:G:556:THR:HG21	1.97	0.47
2:I:1381:GLU:O	2:I:1382:LYS:NZ	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1581:TYR:HB2	2:I:1660:ILE:HD11	1.97	0.47
2:I:2232:LYS:O	2:I:2235:GLU:HG2	2.15	0.47
2:M:1292:THR:H	2:M:1295:LEU:HD12	1.80	0.47
2:M:1843:ALA:O	2:M:1847:ASN:ND2	2.48	0.47
2:M:2063:LEU:HB2	2:M:2065:GLU:OE2	2.15	0.47
1:B:449:LEU:HD22	1:B:481:PRO:HD3	1.97	0.47
1:B:514:ARG:HD3	1:B:514:ARG:HA	1.71	0.47
1:B:518:HIS:HD2	1:B:520:ILE:HD11	1.80	0.47
1:F:384:ARG:NH1	1:F:388:GLU:OE1	2.47	0.47
1:G:413:ILE:HD13	1:G:424:PHE:CE2	2.49	0.47
2:I:1977:ASP:OD1	2:I:1978:ASN:N	2.48	0.47
2:M:1639:ILE:HD13	2:M:1657:THR:HG21	1.96	0.47
1:E:496:SER:OG	1:E:498:GLU:OE1	2.26	0.47
2:I:1504:LYS:HA	2:I:1507:LYS:HD2	1.97	0.47
3:J:113:VAL:HG13	3:J:126:THR:HG21	1.97	0.47
2:M:1497:ILE:HD13	2:M:1501:CYS:HB3	1.97	0.47
2:M:2240:ARG:HA	2:M:2243:GLN:HG3	1.96	0.47
1:B:417:ASP:O	1:B:420:SER:OG	2.33	0.47
1:C:466:LEU:HB2	1:C:468:GLU:OE1	2.14	0.47
1:F:456:LEU:HD11	1:F:536:CYS:SG	2.55	0.47
1:H:456:LEU:HD13	1:H:550:ARG:HB2	1.97	0.47
1:D:457:LEU:HB2	1:D:473:THR:OG1	2.15	0.47
1:F:417:ASP:OD1	1:F:418:TRP:N	2.47	0.47
2:M:1868:ARG:HA	2:M:1881:SER:HA	1.97	0.47
1:K:379:THR:HB	1:K:429:THR:OG1	2.15	0.46
1:H:345:ILE:HG12	1:H:372:LEU:HD23	1.97	0.46
2:I:1592:ASN:HB3	2:I:1595:LEU:HB2	1.97	0.46
2:M:2066:PHE:CE2	2:M:2070:ILE:HD11	2.50	0.46
1:E:356:SER:O	1:E:360:THR:OG1	2.25	0.46
2:I:2205:TYR:OH	2:I:2229:GLU:OE1	2.33	0.46
2:M:1960:LYS:O	2:M:1963:GLU:HG3	2.15	0.46
1:A:451:ARG:HH22	1:A:544:PRO:HD3	1.80	0.46
1:F:419:ASN:O	1:F:443:ARG:NH2	2.43	0.46
2:I:1260:THR:HG22	2:I:1262:GLY:H	1.81	0.46
2:I:2041:ILE:HD12	2:I:2042:PRO:HD2	1.98	0.46
1:K:383:THR:N	1:K:425:THR:O	2.42	0.46
2:M:987:CYS:HA	2:M:1005:CYS:HA	1.98	0.46
2:M:1556:ASN:ND2	2:M:1561:TYR:HB3	2.30	0.46
2:M:2045:ARG:NE	2:M:2113:ASP:OD2	2.48	0.46
1:B:512:PRO:O	1:B:514:ARG:N	2.39	0.46
1:D:541:GLU:OE1	1:D:541:GLU:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:423:ARG:HA	1:E:442:SER:HB3	1.97	0.46
1:F:456:LEU:HD23	1:F:552:VAL:HG12	1.96	0.46
2:M:1506:GLU:HB3	2:M:1510:LYS:NZ	2.31	0.46
1:E:457:LEU:HB2	1:E:473:THR:OG1	2.15	0.46
2:I:1291:ASP:OD1	2:I:1292:THR:N	2.48	0.46
1:L:462:GLU:HA	1:L:465:ASN:ND2	2.31	0.46
2:M:1278:TRP:HB2	2:M:1372:LEU:HD21	1.97	0.46
1:B:375:TYR:HE2	1:B:431:THR:HB	1.81	0.46
1:C:384:ARG:HH21	1:C:386:ASN:HB2	1.79	0.46
1:H:366:THR:HG23	1:H:410:GLU:HB3	1.97	0.46
2:I:1038:TRP:O	2:I:1041:GLU:HG3	2.15	0.46
2:I:1971:GLU:OE1	2:I:1972:GLN:NE2	2.46	0.46
1:L:552:VAL:HG13	1:L:556:THR:HB	1.97	0.46
2:I:970:THR:OG1	2:I:971:ASN:N	2.49	0.46
1:B:525:GLU:HA	1:B:528:TRP:HB3	1.97	0.46
1:D:465:ASN:O	1:D:467:ARG:HG3	2.16	0.46
2:M:1420:ILE:HA	2:M:1423:ILE:HG22	1.98	0.46
2:M:2189:LYS:O	2:M:2193:THR:N	2.32	0.46
1:G:418:TRP:O	1:G:443:ARG:HD3	2.16	0.45
2:I:1559:ILE:O	2:I:1563:THR:HG22	2.16	0.45
2:M:1664:ARG:HD2	2:M:1668:TYR:CZ	2.51	0.45
1:B:348:PHE:HD2	1:B:368:LEU:HD11	1.81	0.45
2:M:2202:HIS:HA	2:M:2205:TYR:CD2	2.50	0.45
1:B:378:VAL:HG22	1:B:430:HIS:ND1	2.31	0.45
1:C:490:GLN:HB2	1:C:495:LEU:HD11	1.97	0.45
1:G:450:HIS:CD2	1:G:514:ARG:HH21	2.34	0.45
2:I:1189:GLU:O	2:I:1192:SER:HB3	2.17	0.45
2:I:1346:ALA:N	2:I:1349:ARG:HH21	2.14	0.45
2:I:1420:ILE:HA	2:I:1423:ILE:HG22	1.98	0.45
2:I:2114:MET:SD	2:I:2114:MET:N	2.87	0.45
3:J:46:ARG:CZ	3:J:52:PRO:HA	2.47	0.45
1:A:538:VAL:HG12	1:A:548:THR:H	1.82	0.45
2:I:2193:THR:HA	2:I:2196:CYS:SG	2.56	0.45
1:A:449:LEU:HB3	1:A:542:ALA:HA	1.98	0.45
1:F:348:PHE:HE1	1:F:370:THR:HG22	1.82	0.45
1:H:421:GLY:HA2	1:H:443:ARG:HD2	1.97	0.45
2:I:1349:ARG:HH11	2:I:1456:GLU:HG3	1.82	0.45
2:I:1691:ILE:HD11	2:I:1783:MET:HG3	1.98	0.45
2:I:1715:TYR:O	2:I:1719:LYS:HG2	2.17	0.45
3:J:57:ARG:HB3	3:J:60:PHE:CE2	2.51	0.45
2:M:1376:ILE:HA	2:M:1379:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2181:PRO:HB2	2:M:2186:ARG:HB2	1.98	0.45
1:A:549:GLU:O	1:A:550:ARG:NH1	2.43	0.45
1:C:484:VAL:HG12	1:C:540:HIS:CD2	2.51	0.45
1:F:364:LYS:NZ	1:F:412:SER:OG	2.35	0.45
1:G:400:HIS:NE2	1:G:406:SER:HB3	2.32	0.45
2:I:2129:ARG:HH22	2:I:2135:THR:HG22	1.82	0.45
2:M:1027:ASN:O	2:M:1030:THR:OG1	2.28	0.45
2:M:1039:ASN:OD1	2:M:1043:GLN:NE2	2.46	0.45
2:M:1949:LYS:HB2	2:M:1954:TYR:CE2	2.51	0.45
1:C:399:SER:HA	1:C:405:PHE:HA	1.97	0.45
1:D:378:VAL:HG22	1:D:430:HIS:CE1	2.51	0.45
1:D:530:THR:OG1	1:D:532:GLU:OE2	2.34	0.45
1:G:384:ARG:HB2	1:G:422:GLU:HG2	1.99	0.45
1:H:466:LEU:HD23	1:H:466:LEU:H	1.82	0.45
2:M:2051:SER:OG	2:M:2052:ARG:NH1	2.50	0.45
1:A:535:THR:OG1	1:A:549:GLU:OE1	2.22	0.45
1:B:347:VAL:HG22	1:B:369:VAL:HG13	1.99	0.45
1:C:400:HIS:N	1:C:404:THR:O	2.50	0.45
1:D:456:LEU:HD23	1:D:550:ARG:HB2	1.99	0.45
1:D:535:THR:HB	1:D:551:THR:HG22	1.99	0.45
1:G:549:GLU:OE1	1:G:549:GLU:N	2.50	0.45
2:I:1039:ASN:O	2:I:1043:GLN:NE2	2.50	0.45
2:I:1583:LYS:HG3	2:I:1584:TYR:H	1.82	0.45
2:M:1514:GLU:HG2	2:M:1515:LYS:N	2.32	0.45
2:M:1965:TYR:O	2:M:1969:VAL:HG23	2.17	0.45
1:D:568:MET:SD	1:D:568:MET:N	2.86	0.45
1:E:535:THR:HG22	1:E:551:THR:HB	1.98	0.45
3:J:134:TYR:HD1	3:J:135:PRO:HD2	1.81	0.45
1:B:384:ARG:HA	1:B:424:PHE:HD1	1.83	0.45
1:E:423:ARG:HB3	1:E:440:THR:HB	1.98	0.45
1:E:509:PRO:HD3	1:F:501:VAL:HG21	1.99	0.45
2:I:1544:PRO:HA	2:I:1547:ILE:HD11	1.99	0.45
1:K:478:GLY:HA2	1:K:514:ARG:HB3	1.99	0.45
2:M:1100:TYR:OH	2:M:1198:ALA:O	2.29	0.45
2:M:1783:MET:O	2:M:1783:MET:HG2	2.17	0.45
1:B:382:TRP:HB3	1:B:384:ARG:NH2	2.28	0.44
1:C:523:VAL:HG11	1:C:534:TYR:CE2	2.52	0.44
2:I:979:LYS:HD3	2:I:1865:LYS:HD2	1.98	0.44
2:M:1352:ILE:HD11	2:M:1442:PRO:HB2	1.98	0.44
2:M:1515:LYS:HA	2:M:1518:GLU:HG3	1.99	0.44
2:M:1515:LYS:HD2	2:M:1518:GLU:OE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:2035:LYS:HG3	2:M:2036:HIS:H	1.82	0.44
1:A:467:ARG:HH12	1:A:529:ASN:HD21	1.64	0.44
1:D:393:HIS:HA	1:D:410:GLU:HG2	1.98	0.44
1:D:491:ARG:HA	1:D:533:THR:HG21	2.00	0.44
1:E:374:THR:OG1	1:E:403:ALA:O	2.35	0.44
2:I:1692:ARG:NH1	2:I:1902:GLY:O	2.51	0.44
2:I:1843:ALA:O	2:I:1847:ASN:ND2	2.50	0.44
1:L:566:LEU:HD23	1:L:566:LEU:H	1.82	0.44
2:I:1611:LYS:HD2	2:I:1709:HIS:HE1	1.82	0.44
2:I:2054:VAL:HG23	2:I:2123:ILE:HD12	1.98	0.44
2:M:1362:SER:O	2:M:1362:SER:OG	2.33	0.44
2:M:1516:LYS:NZ	2:M:1555:PHE:O	2.35	0.44
2:M:1570:TYR:C	2:M:1572:SER:H	2.20	0.44
2:M:2124:LYS:HG3	2:M:2125:ILE:N	2.32	0.44
1:B:345:ILE:HA	1:B:371:ASP:HB3	2.00	0.44
1:B:433:LEU:O	1:B:433:LEU:HD12	2.18	0.44
2:I:1367:GLU:OE1	2:I:1368:HIS:ND1	2.51	0.44
2:I:1742:TRP:CE2	2:I:1757:ARG:HB3	2.52	0.44
1:K:558:LYS:HE2	1:K:558:LYS:HA	1.99	0.44
2:M:1454:PHE:HD1	2:M:1522:GLN:HG2	1.82	0.44
2:M:1813:TYR:O	2:M:1817:MET:HG2	2.18	0.44
2:M:1853:ARG:HH22	2:M:1949:LYS:HZ1	1.65	0.44
2:M:2233:TYR:HA	2:M:2236:TRP:CD1	2.52	0.44
1:B:491:ARG:NH1	1:B:532:GLU:OE2	2.51	0.44
1:H:382:TRP:CE2	1:H:426:CYS:HB3	2.52	0.44
2:I:2030:ARG:NE	2:I:2031:GLY:H	2.14	0.44
1:B:372:LEU:HD23	1:B:372:LEU:HA	1.88	0.44
1:C:383:THR:HG22	1:C:389:ALA:HA	2.00	0.44
1:E:385:GLN:HB3	1:E:422:GLU:HG3	1.99	0.44
1:E:512:PRO:HD2	2:M:1226:TYR:CZ	2.53	0.44
1:E:553:ASP:OD1	1:E:556:THR:OG1	2.29	0.44
1:G:415:GLU:HG3	1:G:419:ASN:HD22	1.83	0.44
2:I:1291:ASP:OD1	2:I:1295:LEU:HB2	2.17	0.44
2:I:1625:PRO:HG3	2:I:1798:TRP:CD1	2.52	0.44
2:I:2185:LEU:HA	2:I:2188:ILE:HG12	1.99	0.44
2:M:1583:LYS:HG2	2:M:1584:TYR:H	1.82	0.44
2:M:2124:LYS:HB2	2:M:2124:LYS:HE2	1.80	0.44
1:G:353:SER:O	1:G:357:ILE:HG12	2.17	0.44
1:H:365:LEU:HD22	1:H:413:ILE:HG12	2.00	0.44
1:L:531:GLY:C	1:L:533:THR:H	2.20	0.44
2:M:1194:LYS:HA	2:M:1197:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1544:PRO:HA	2:M:1547:ILE:HD11	2.00	0.44
1:A:455:TYR:CE2	1:B:463:GLN:HB2	2.52	0.44
1:E:400:HIS:CD2	1:E:406:SER:HB3	2.53	0.44
1:E:531:GLY:C	1:E:533:THR:H	2.20	0.44
2:I:1708:VAL:HG23	2:I:1713:THR:HG21	1.99	0.44
2:M:1041:GLU:OE1	2:M:1045:GLN:NE2	2.51	0.44
2:M:1365:ILE:HG13	2:M:1366:TYR:N	2.32	0.44
2:M:1561:TYR:O	2:M:1565:TYR:HB2	2.18	0.44
2:M:2062:SER:O	2:M:2131:LEU:HD11	2.18	0.44
3:J:19:SER:HB2	3:J:35:ARG:HD2	2.00	0.44
1:L:490:GLN:HG2	1:L:491:ARG:HG2	1.99	0.44
1:B:468:GLU:OE1	1:B:468:GLU:N	2.51	0.43
1:F:469:SER:OG	1:F:470:ALA:N	2.51	0.43
2:I:1901:ASN:HD21	2:I:1903:ASN:HB2	1.83	0.43
2:I:2207:LYS:HD3	2:I:2207:LYS:HA	1.70	0.43
3:J:102:THR:HG21	1:L:575:CYS:HB2	1.99	0.43
2:M:2170:PRO:O	2:M:2174:THR:N	2.51	0.43
1:A:567:VAL:HG12	3:J:61:VAL:HA	2.00	0.43
1:C:461:ARG:HD2	1:C:462:GLU:N	2.34	0.43
1:E:484:VAL:HG23	1:E:540:HIS:HB2	1.99	0.43
1:G:456:LEU:HD23	1:G:550:ARG:HB2	1.99	0.43
2:I:1605:TRP:CH2	2:I:1802:TRP:HB2	2.54	0.43
2:I:1646:GLY:HA3	2:I:1649:LYS:HE3	1.99	0.43
2:M:1046:ILE:O	2:M:1050:MET:HG2	2.18	0.43
2:M:1740:ASP:O	2:M:1744:ASN:N	2.52	0.43
2:M:2236:TRP:O	2:M:2240:ARG:HG2	2.18	0.43
1:E:529:ASN:HA	1:E:554:LYS:HD2	1.99	0.43
1:F:552:VAL:HG23	1:F:556:THR:HG21	1.99	0.43
1:K:506:MET:SD	1:K:507:PRO:HD2	2.59	0.43
2:M:1365:ILE:HG13	2:M:1366:TYR:H	1.82	0.43
2:I:2237:SER:O	2:I:2241:SER:N	2.48	0.43
2:M:1853:ARG:HG2	2:M:1947:LEU:HB3	2.01	0.43
1:C:345:ILE:HG12	1:C:372:LEU:HD23	2.00	0.43
1:C:418:TRP:O	1:C:443:ARG:NH1	2.52	0.43
1:C:443:ARG:O	1:C:445:LYS:NZ	2.46	0.43
1:G:490:GLN:HB2	1:G:495:LEU:HD11	2.00	0.43
2:I:1382:LYS:HA	2:I:1382:LYS:HD3	1.79	0.43
2:I:2090:ASP:HB3	2:I:2093:LYS:HD3	2.00	0.43
1:B:568:MET:HB3	1:C:568:MET:HG2	2.00	0.43
1:E:421:GLY:HA3	1:E:445:LYS:HD3	2.01	0.43
1:G:453:ASP:OD2	1:G:455:TYR:OH	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2247:ILE:O	2:I:2254:TYR:HB2	2.18	0.43
1:K:490:GLN:HG3	1:K:491:ARG:HG2	1.99	0.43
2:M:1506:GLU:HB3	2:M:1510:LYS:HZ1	1.84	0.43
2:M:1514:GLU:HA	2:M:1517:GLN:NE2	2.34	0.43
2:M:1671:LYS:HD3	2:M:1775:LYS:HZ1	1.83	0.43
2:M:2028:ASP:N	2:M:2028:ASP:OD1	2.51	0.43
2:M:2139:LYS:HD2	2:M:2139:LYS:O	2.19	0.43
2:M:2144:TRP:O	2:M:2148:ASN:ND2	2.52	0.43
1:B:354:PHE:HA	1:B:357:ILE:HD12	2.00	0.43
1:C:365:LEU:HD23	1:C:365:LEU:H	1.84	0.43
1:C:567:VAL:HG13	1:D:567:VAL:HG13	2.00	0.43
1:H:425:THR:HG21	1:H:438:LYS:HD3	2.01	0.43
2:I:1413:TRP:CG	2:I:1441:PRO:HD3	2.54	0.43
1:L:497:PRO:HA	1:L:500:TYR:CZ	2.54	0.43
1:A:485:PHE:HB3	1:A:539:ALA:HB3	2.00	0.43
1:E:419:ASN:HA	1:E:443:ARG:NE	2.33	0.43
1:H:543:LEU:HB2	1:H:546:ARG:HA	2.01	0.43
2:I:1272:LEU:HD11	2:I:1354:TYR:CE1	2.54	0.43
2:I:1808:GLU:HG3	2:I:1809:LYS:HE2	2.00	0.43
2:I:2064:ASN:CB	2:I:2067:LYS:HE3	2.49	0.43
2:M:1227:ILE:HG23	2:M:1276:GLU:OE2	2.19	0.43
2:M:2125:ILE:HA	2:M:2128:ASP:OD2	2.18	0.43
1:A:568:MET:HB3	1:B:568:MET:SD	2.58	0.43
1:B:469:SER:HA	1:B:524:SER:HA	1.99	0.43
2:I:1899:GLU:HG3	2:I:1901:ASN:H	1.84	0.43
2:I:1639:ILE:HG21	2:I:1657:THR:HG21	2.01	0.43
2:I:1660:ILE:O	2:I:1664:ARG:HG2	2.19	0.43
2:I:1844:ASN:HA	2:I:1847:ASN:HD21	1.84	0.43
3:J:4:ARG:HD2	3:J:20:ARG:HB2	2.01	0.43
2:M:1265:ILE:HG12	2:M:1365:ILE:HG21	2.01	0.43
1:A:495:LEU:HD23	1:A:495:LEU:HA	1.84	0.42
1:C:508:GLU:OE2	1:C:511:ALA:HB3	2.19	0.42
1:D:372:LEU:HD23	1:D:430:HIS:CD2	2.54	0.42
2:I:1454:PHE:HE2	2:I:1535:ALA:HB1	1.83	0.42
2:I:2236:TRP:O	2:I:2240:ARG:N	2.46	0.42
2:M:1309:GLU:HG2	2:M:1423:ILE:HD12	2.01	0.42
2:M:1458:GLY:HA3	2:M:1539:LEU:HD11	2.01	0.42
2:M:1719:LYS:O	2:M:1722:GLU:HG3	2.19	0.42
2:M:2075:GLN:NE2	2:M:2156:MET:HA	2.33	0.42
2:M:2182:PRO:O	2:M:2186:ARG:N	2.31	0.42
1:B:419:ASN:O	1:B:443:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLN:HG3	1:B:464:LEU:HD12	2.01	0.42
1:E:346:ARG:HD2	1:E:348:PHE:CZ	2.54	0.42
1:F:459:PRO:HD3	1:F:472:ILE:HG12	2.01	0.42
1:H:382:TRP:HA	1:H:426:CYS:HA	2.01	0.42
2:I:1142:SER:HB3	2:I:1187:GLY:HA2	2.01	0.42
1:L:533:THR:HA	1:L:553:ASP:HA	2.01	0.42
2:M:1240:PHE:CD1	2:M:1241:PRO:HA	2.54	0.42
2:M:1600:ASP:N	2:M:1630:GLN:OE1	2.52	0.42
2:M:1698:LEU:HA	2:M:1701:ILE:HG12	2.00	0.42
2:M:2148:ASN:HA	2:M:2151:SER:HB3	2.02	0.42
1:C:418:TRP:CZ2	1:C:443:ARG:HB3	2.54	0.42
1:F:400:HIS:NE2	1:F:406:SER:OG	2.46	0.42
2:I:1462:CYS:HB3	2:I:1546:CYS:HB3	1.85	0.42
2:M:2107:ASP:OD2	2:M:2187:TRP:NE1	2.52	0.42
1:G:417:ASP:O	1:G:420:SER:OG	2.36	0.42
2:I:1903:ASN:O	2:I:1905:ILE:N	2.49	0.42
2:I:2063:LEU:HB3	2:I:2065:GLU:HG3	1.99	0.42
3:J:25:SER:O	3:J:27:ASP:N	2.52	0.42
1:K:490:GLN:HB2	1:K:495:LEU:HD11	2.02	0.42
2:M:1357:MET:O	2:M:1373:GLN:NE2	2.49	0.42
2:M:2024:TRP:HB2	2:M:2040:LEU:HD13	2.01	0.42
1:A:539:ALA:HB2	3:J:115:LEU:HD11	2.01	0.42
1:C:511:ALA:HB1	1:C:512:PRO:HD2	2.01	0.42
2:I:2202:HIS:CE1	2:I:2233:TYR:HB3	2.54	0.42
2:M:2225:ASN:ND2	2:M:2229:GLU:OE2	2.52	0.42
2:I:1617:ARG:NH1	2:I:1875:GLU:OE1	2.53	0.42
2:I:1731:ASP:O	2:I:1735:LYS:HG2	2.19	0.42
2:I:2080:PHE:O	2:I:2083:ASN:N	2.52	0.42
1:L:543:LEU:HB2	1:L:546:ARG:HA	2.02	0.42
2:M:2035:LYS:HG3	2:M:2036:HIS:CD2	2.55	0.42
1:A:466:LEU:H	1:A:466:LEU:HD23	1.83	0.42
1:D:549:GLU:N	1:D:549:GLU:OE1	2.53	0.42
1:E:419:ASN:HA	1:E:443:ARG:HE	1.85	0.42
2:I:1311:LEU:HD23	2:I:1311:LEU:HA	1.85	0.42
2:M:1025:ASP:OD1	2:M:1025:ASP:N	2.50	0.42
2:M:1029:VAL:HA	2:M:1032:PHE:HB3	2.00	0.42
2:M:1114:GLN:HA	2:M:1117:ASN:HD21	1.84	0.42
1:G:498:GLU:OE1	1:G:498:GLU:N	2.53	0.42
2:I:1042:ILE:HD13	2:I:1042:ILE:HA	1.90	0.42
2:I:1252:LYS:HD3	2:I:1521:LYS:HG2	2.01	0.42
2:I:1974:ASN:HA	2:I:1977:ASP:OD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2162:LYS:HD3	2:I:2162:LYS:HA	1.86	0.42
2:M:1626:PRO:O	2:M:1630:GLN:HG2	2.19	0.42
1:B:419:ASN:HA	1:B:443:ARG:NH1	2.35	0.42
1:E:396:ILE:HA	1:E:408:VAL:HG22	2.02	0.42
1:E:473:THR:HG22	1:E:520:ILE:HG22	2.02	0.42
1:F:384:ARG:HB2	1:F:388:GLU:HB2	2.01	0.42
1:G:419:ASN:O	1:G:445:LYS:NZ	2.44	0.42
2:I:1410:ARG:HD2	2:I:1410:ARG:HA	1.86	0.42
2:I:1765:GLN:HA	2:I:1768:VAL:HG12	2.01	0.42
1:K:475:LEU:HD13	1:K:518:HIS:CE1	2.55	0.42
2:M:2119:GLU:OE1	2:M:2124:LYS:HB3	2.20	0.42
1:A:455:TYR:CZ	1:B:463:GLN:HB2	2.55	0.42
1:D:373:THR:HG23	1:D:375:TYR:HB3	2.01	0.42
1:E:378:VAL:HG22	1:E:430:HIS:CD2	2.55	0.42
1:G:384:ARG:HE	1:G:386:ASN:CG	2.20	0.42
1:H:569:SER:N	1:K:569:SER:HB2	2.35	0.42
2:I:1036:GLU:O	2:I:1040:LYS:HG2	2.19	0.42
2:I:2143:ASP:OD1	2:I:2144:TRP:N	2.52	0.42
3:J:17:ILE:HD11	3:J:35:ARG:HH21	1.83	0.42
2:M:1146:PHE:HA	2:M:1149:CYS:SG	2.60	0.42
2:M:1944:ASN:OD1	2:M:1945:GLU:N	2.52	0.42
1:D:419:ASN:O	1:D:443:ARG:NE	2.53	0.41
1:H:428:VAL:HB	1:H:437:LEU:HB2	2.01	0.41
2:I:1457:TRP:HZ2	2:I:1515:LYS:HD2	1.85	0.41
2:I:2197:ILE:HD12	2:I:2197:ILE:HA	1.94	0.41
3:J:49:ILE:HG13	3:J:103:TYR:CE1	2.55	0.41
1:L:463:GLN:HE22	1:L:471:THR:HG23	1.85	0.41
1:L:558:LYS:HZ3	1:L:560:THR:HG22	1.84	0.41
1:B:490:GLN:OE1	1:B:495:LEU:HD21	2.20	0.41
1:B:491:ARG:HH12	2:M:2054:VAL:HG13	1.85	0.41
1:D:475:LEU:HD12	1:D:518:HIS:NE2	2.34	0.41
1:E:364:LYS:HE3	1:E:364:LYS:HB3	1.92	0.41
1:F:475:LEU:HD13	1:F:518:HIS:CD2	2.55	0.41
1:G:364:LYS:HD3	1:G:412:SER:HA	2.02	0.41
3:J:69:LYS:NZ	3:J:98:GLU:OE2	2.39	0.41
1:A:562:TYR:HB2	1:B:562:TYR:HD1	1.85	0.41
1:H:350:ILE:O	1:H:350:ILE:HG13	2.20	0.41
2:I:1328:LYS:HD2	2:I:1328:LYS:O	2.20	0.41
1:K:543:LEU:HD13	1:K:548:THR:HG23	2.01	0.41
2:M:1381:GLU:O	2:M:1382:LYS:HE2	2.19	0.41
2:M:1963:GLU:O	2:M:1966:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:THR:OG1	1:C:551:THR:OG1	2.14	0.41
2:I:1444:GLY:HA2	2:I:1447:GLU:HG3	2.01	0.41
2:I:1561:TYR:O	2:I:1565:TYR:HB2	2.20	0.41
2:I:2020:GLU:HG3	2:I:2024:TRP:HZ2	1.84	0.41
2:I:2041:ILE:HG23	2:I:2046:ARG:HH21	1.85	0.41
1:K:527:GLU:OE1	1:K:534:TYR:OH	2.34	0.41
2:M:1356:ASN:ND2	2:M:1449:GLN:HG2	2.35	0.41
2:M:1669:LEU:O	2:M:1673:TYR:CB	2.68	0.41
2:M:2247:ILE:O	2:M:2250:ARG:HG2	2.20	0.41
1:C:479:PHE:CE1	1:C:515:TYR:HB2	2.55	0.41
1:F:382:TRP:CD2	1:F:426:CYS:HB3	2.55	0.41
2:I:2187:TRP:O	2:I:2190:GLU:HG3	2.20	0.41
2:M:1272:LEU:HD12	2:M:1272:LEU:O	2.20	0.41
2:M:1497:ILE:HG21	2:M:1501:CYS:HB3	2.03	0.41
2:M:1529:LYS:HG3	2:M:1530:TYR:HD1	1.85	0.41
2:M:2089:LYS:HD3	2:M:2089:LYS:HA	1.77	0.41
1:B:368:LEU:HB3	1:B:408:VAL:HA	2.02	0.41
1:G:518:HIS:CE1	1:H:520:ILE:HD11	2.56	0.41
1:G:488:TRP:HE1	1:G:519:SER:HG	1.68	0.41
2:I:1272:LEU:O	2:I:1272:LEU:HD12	2.21	0.41
2:I:1300:ILE:O	2:I:1304:ILE:HG12	2.20	0.41
2:I:1368:HIS:CD2	2:I:1371:LYS:HB2	2.56	0.41
2:I:1558:ASN:HB3	2:I:1561:TYR:HD2	1.86	0.41
3:J:41:VAL:HG12	1:L:568:MET:HB2	2.02	0.41
1:G:543:LEU:HB2	1:G:546:ARG:HA	2.02	0.41
1:H:526:GLU:HG2	1:H:527:GLU:N	2.36	0.41
2:I:981:TYR:CE2	2:I:1099:CYS:HB3	2.55	0.41
2:I:1179:LYS:HG2	2:I:1180:CYS:SG	2.61	0.41
2:I:1611:LYS:HD2	2:I:1709:HIS:CE1	2.56	0.41
2:I:2142:GLU:O	2:I:2146:LYS:N	2.37	0.41
1:A:451:ARG:HH12	1:A:544:PRO:HD2	1.86	0.41
1:A:456:LEU:HD23	1:A:550:ARG:HG3	2.01	0.41
1:B:352:PRO:HD3	1:B:365:LEU:HB3	2.03	0.41
1:B:372:LEU:O	1:B:404:THR:HA	2.21	0.41
1:E:443:ARG:HA	1:E:444:PRO:HD3	1.93	0.41
1:F:364:LYS:HE3	1:F:364:LYS:HB3	1.77	0.41
1:F:529:ASN:HA	1:F:554:LYS:HD3	2.02	0.41
1:H:374:THR:HA	1:H:405:PHE:HB2	2.03	0.41
2:I:1025:ASP:OD1	2:I:1025:ASP:N	2.53	0.41
2:I:1195:LEU:O	2:I:1199:GLU:N	2.54	0.41
2:I:1742:TRP:CZ2	2:I:1757:ARG:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1891:TYR:O	2:I:1895:ARG:HB2	2.21	0.41
2:I:1975:GLU:HA	2:I:1978:ASN:ND2	2.34	0.41
2:I:2089:LYS:HD3	2:I:2089:LYS:HA	1.77	0.41
3:J:4:ARG:HH11	3:J:20:ARG:CB	2.29	0.41
2:M:1662:ALA:O	2:M:1665:GLU:HG3	2.20	0.41
2:M:1717:ASP:OD1	2:M:1718:SER:N	2.54	0.41
2:M:1874:SER:OG	2:M:1876:ASP:O	2.36	0.41
2:M:2018:LEU:HD21	2:M:2021:LEU:HD13	2.02	0.41
2:M:2071:LEU:HD11	2:M:2154:ASN:OD1	2.21	0.41
1:C:456:LEU:HD13	1:C:550:ARG:HB2	2.03	0.41
1:E:532:GLU:OE2	2:I:1238:LYS:NZ	2.51	0.41
1:H:562:TYR:HB2	1:K:562:TYR:HB2	2.03	0.41
2:I:1042:ILE:O	2:I:1045:GLN:HB3	2.21	0.41
2:I:1515:LYS:HD3	2:I:1515:LYS:HA	1.83	0.41
3:J:59:ARG:HD2	3:J:60:PHE:N	2.36	0.41
1:K:509:PRO:HG2	1:K:510:GLN:OE1	2.21	0.41
2:M:1613:LEU:HD11	2:M:1617:ARG:HG3	2.03	0.41
2:M:1724:PHE:CD2	2:M:1738:ARG:HG2	2.53	0.41
1:G:396:ILE:HD11	1:G:407:ALA:HA	2.03	0.40
2:I:1899:GLU:O	2:I:1905:ILE:HG12	2.20	0.40
1:D:345:ILE:HD12	1:D:372:LEU:HG	2.02	0.40
1:D:454:VAL:HG21	1:D:538:VAL:HG11	2.03	0.40
1:F:511:ALA:HB3	1:F:514:ARG:HB2	2.03	0.40
1:H:398:GLU:HG2	1:H:399:SER:H	1.87	0.40
3:J:106:ASN:OD1	3:J:107:LYS:HG3	2.21	0.40
1:K:382:TRP:CE2	1:K:426:CYS:HB2	2.57	0.40
2:M:1868:ARG:NH2	2:M:1884:MET:SD	2.94	0.40
1:F:508:GLU:OE1	1:F:510:GLN:N	2.54	0.40
1:G:364:LYS:HE2	1:G:364:LYS:HB2	1.90	0.40
2:I:1433:ASN:C	2:I:1435:ASP:H	2.25	0.40
2:I:2043:PRO:HA	2:I:2046:ARG:NE	2.36	0.40
1:K:457:LEU:HB2	1:K:473:THR:CG2	2.52	0.40
1:L:471:THR:HB	1:L:520:ILE:HD11	2.03	0.40
1:L:496:SER:H	1:L:499:LYS:HZ2	1.70	0.40
1:B:357:ILE:HG12	1:B:363:THR:HG22	2.03	0.40
1:B:568:MET:HB3	1:C:568:MET:CG	2.52	0.40
1:F:514:ARG:NH1	2:I:1226:TYR:OH	2.55	0.40
2:I:1461:PHE:O	2:I:1464:GLU:HG3	2.21	0.40
2:I:1889:ILE:HD12	2:I:1892:LEU:HD11	2.02	0.40
3:J:12:CYS:SG	3:J:13:LYS:N	2.94	0.40
1:D:459:PRO:HG2	1:D:464:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1178:LYS:HB3	2:I:1178:LYS:HE2	1.86	0.40
2:I:1364:ASN:N	2:I:1364:ASN:OD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/453 (29%)	123 (95%)	7 (5%)	0	100	100
1	B	225/453 (50%)	206 (92%)	19 (8%)	0	100	100
1	C	223/453 (49%)	195 (87%)	28 (13%)	0	100	100
1	D	222/453 (49%)	204 (92%)	18 (8%)	0	100	100
1	E	222/453 (49%)	206 (93%)	16 (7%)	0	100	100
1	F	217/453 (48%)	198 (91%)	19 (9%)	0	100	100
1	G	222/453 (49%)	203 (91%)	19 (9%)	0	100	100
1	H	226/453 (50%)	206 (91%)	20 (9%)	0	100	100
1	K	226/453 (50%)	206 (91%)	20 (9%)	0	100	100
1	L	123/453 (27%)	112 (91%)	11 (9%)	0	100	100
2	I	1085/2680 (40%)	991 (91%)	94 (9%)	0	100	100
2	M	1085/2680 (40%)	976 (90%)	108 (10%)	1 (0%)	48	79
3	J	102/136 (75%)	89 (87%)	13 (13%)	0	100	100
All	All	4308/10026 (43%)	3915 (91%)	392 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	1367	GLU

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	115/399 (29%)	114 (99%)	1 (1%)	75	87
1	B	203/399 (51%)	203 (100%)	0	100	100
1	C	201/399 (50%)	201 (100%)	0	100	100
1	D	200/399 (50%)	199 (100%)	1 (0%)	86	93
1	E	200/399 (50%)	200 (100%)	0	100	100
1	F	198/399 (50%)	198 (100%)	0	100	100
1	G	200/399 (50%)	198 (99%)	2 (1%)	73	85
1	H	205/399 (51%)	204 (100%)	1 (0%)	86	93
1	K	205/399 (51%)	203 (99%)	2 (1%)	73	85
1	L	112/399 (28%)	112 (100%)	0	100	100
2	I	1013/2431 (42%)	1004 (99%)	9 (1%)	75	87
2	M	1013/2431 (42%)	1009 (100%)	4 (0%)	89	95
3	J	100/128 (78%)	100 (100%)	0	100	100
All	All	3965/8980 (44%)	3945 (100%)	20 (0%)	85	93

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	ARG
1	D	391	LYS
1	G	461	ARG
1	G	467	ARG
1	H	443	ARG
2	I	1328	LYS
2	I	1349	ARG
2	I	1496	LYS
2	I	1628	ARG
2	I	1649	LYS
2	I	1853	ARG
2	I	2017	LYS

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Mol	Chain	Res	Type
2	I	2055	ARG
2	I	2114	MET
1	K	346	ARG
1	K	443	ARG
2	M	1628	ARG
2	M	1840	LYS
2	M	2139	LYS
2	M	2186	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	ASN
1	B	529	ASN
1	D	393	HIS
1	D	430	HIS
1	G	465	ASN
1	H	490	GLN
2	I	1117	ASN
2	I	1305	HIS
2	I	1629	GLN
2	I	2148	ASN
2	M	1197	ASN
2	M	1400	ASN
2	M	1850	ASN
2	M	2036	HIS
2	M	2075	GLN
2	M	2148	ASN

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

There are no ligands in this entry.

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.

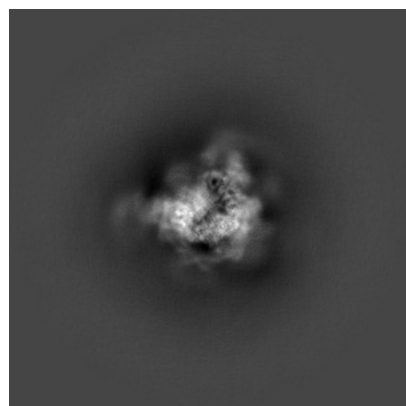
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34399. These allow visual inspection of the internal detail of the map and identification of artifacts.

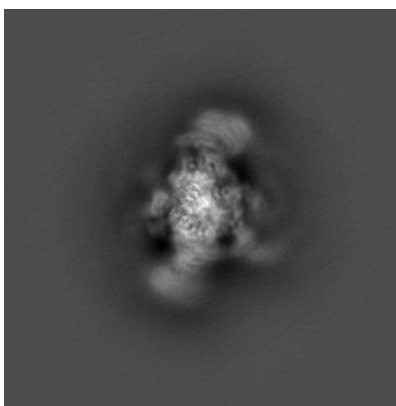
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

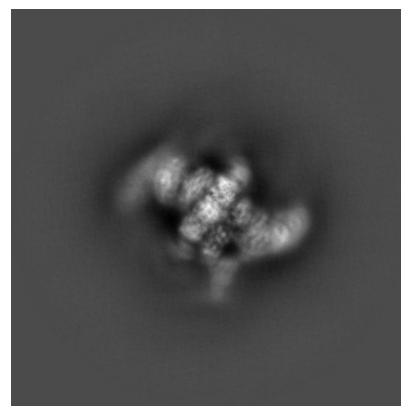
6.1.1 Primary map



X

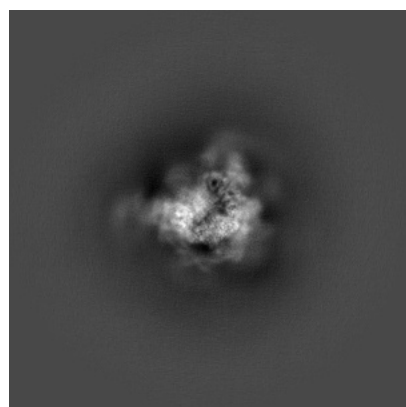


Y

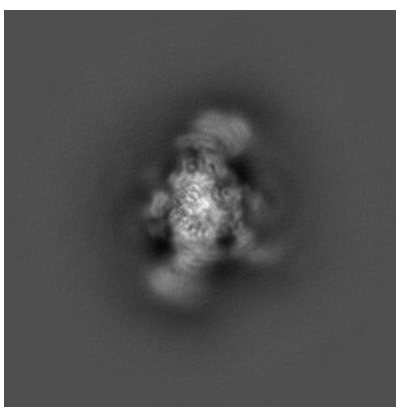


Z

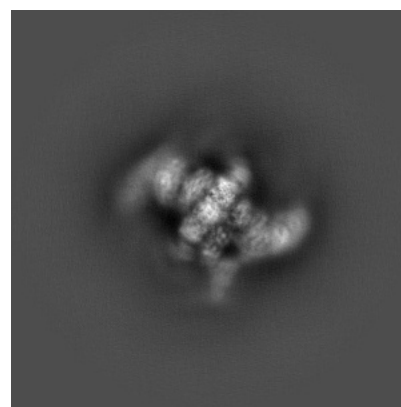
6.1.2 Raw map



X



Y

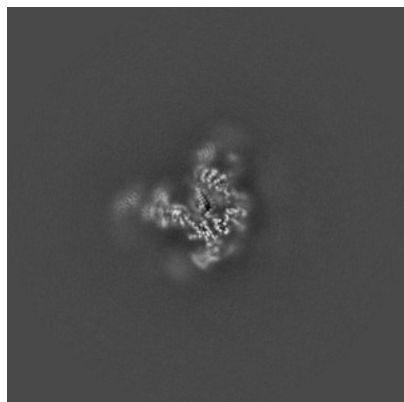


Z

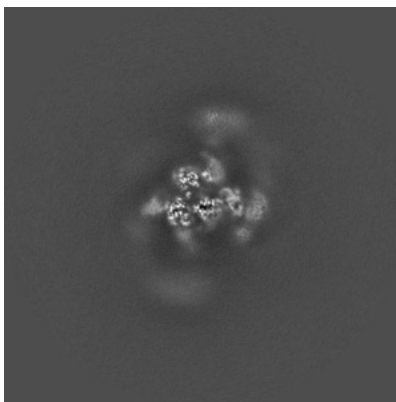
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

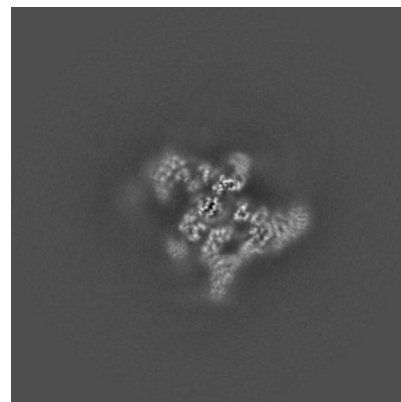
6.2.1 Primary map



X Index: 270

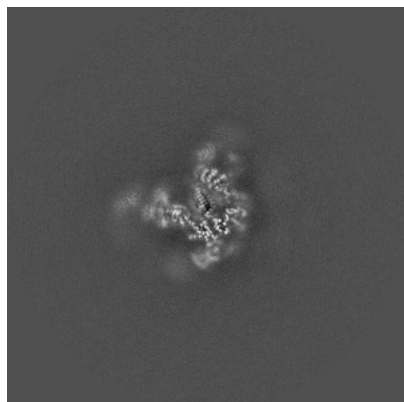


Y Index: 270

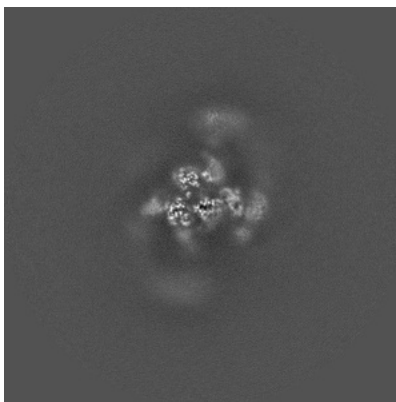


Z Index: 270

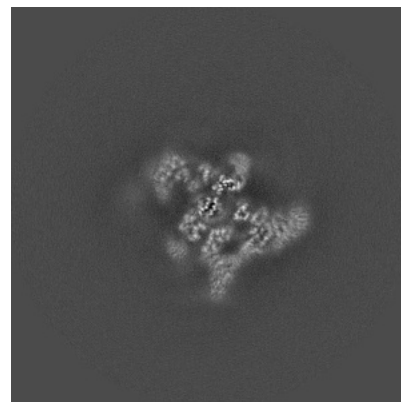
6.2.2 Raw map



X Index: 270



Y Index: 270

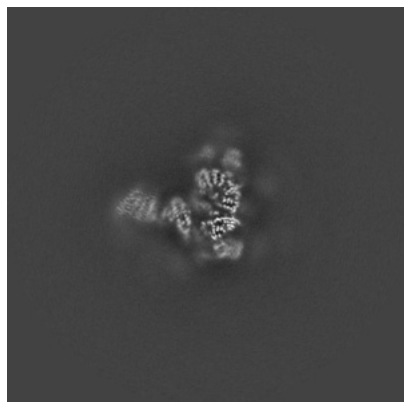


Z Index: 270

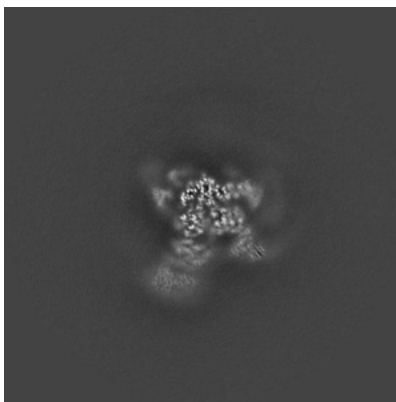
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

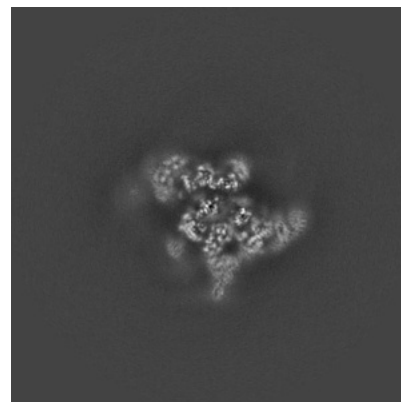
6.3.1 Primary map



X Index: 283

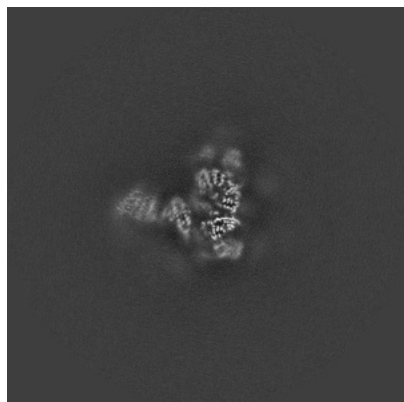


Y Index: 301

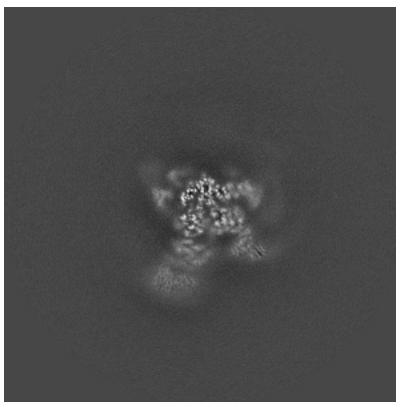


Z Index: 265

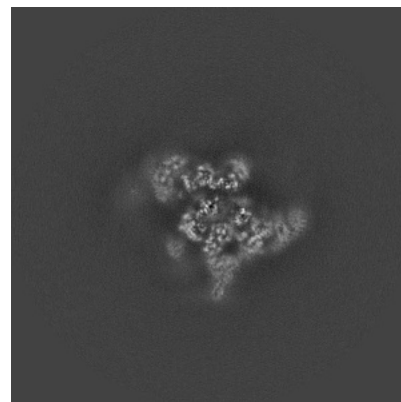
6.3.2 Raw map



X Index: 283



Y Index: 301

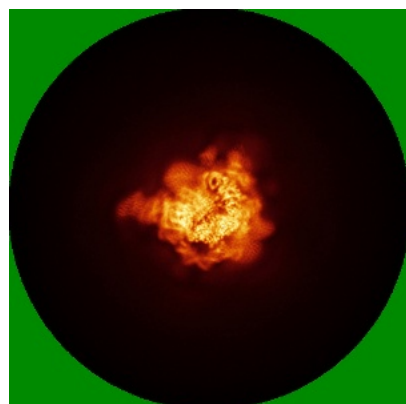


Z Index: 265

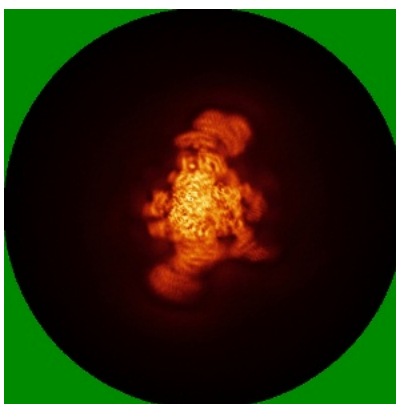
The images above show the largest variance slices of the map in three orthogonal directions.

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

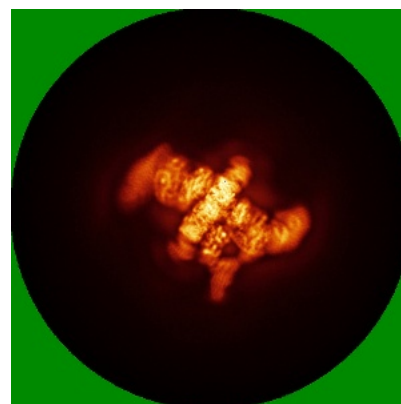
6.4.1 Primary map



X

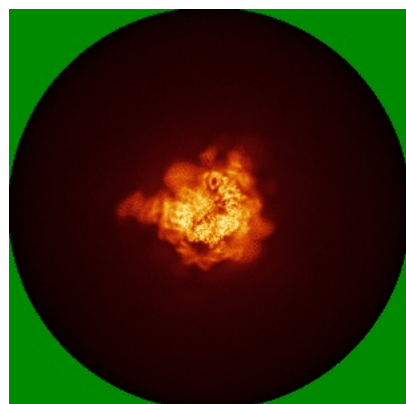


Y

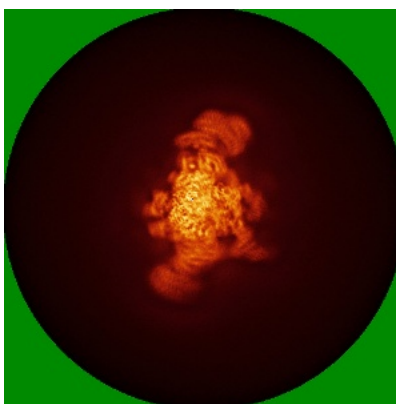


Z

6.4.2 Raw map



X



Y

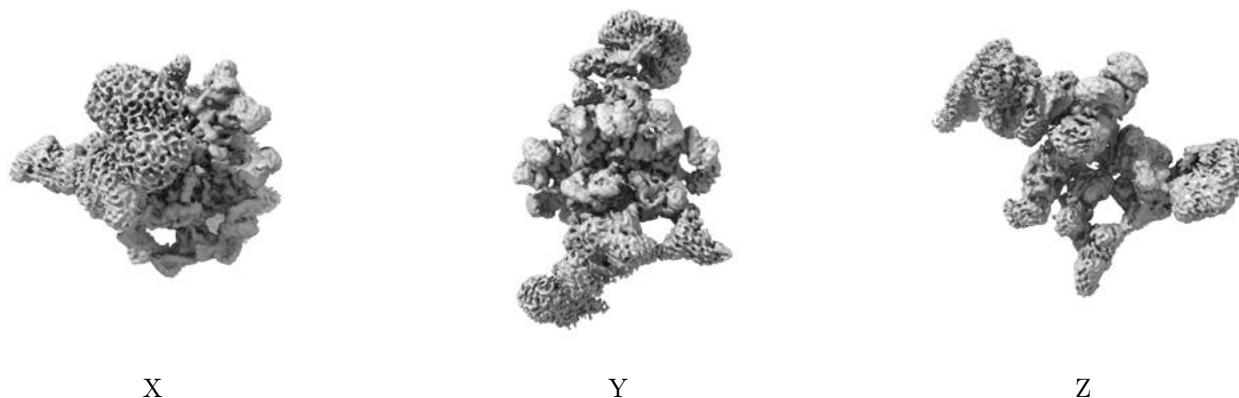


Z

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.

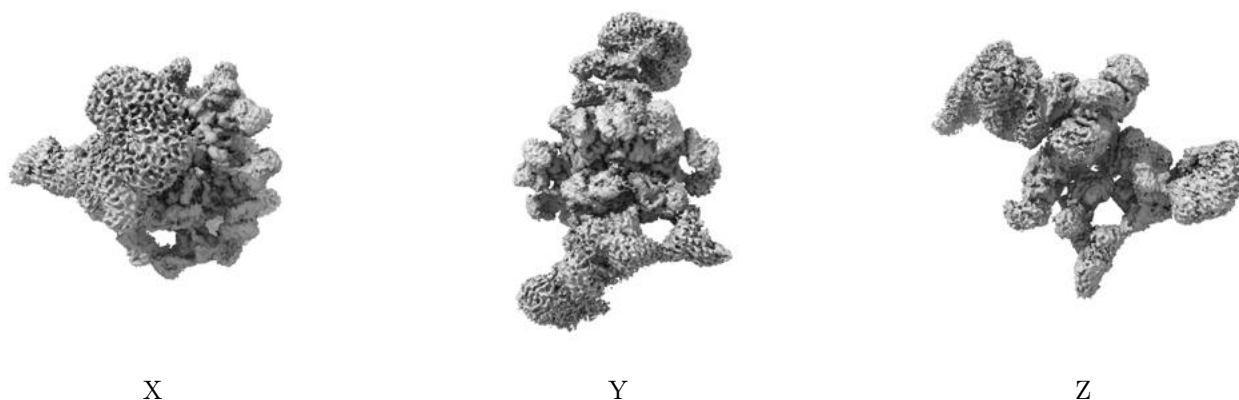
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00805. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

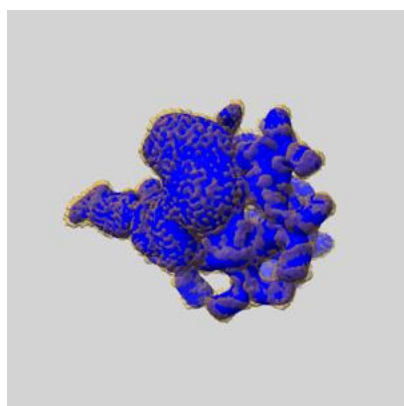
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

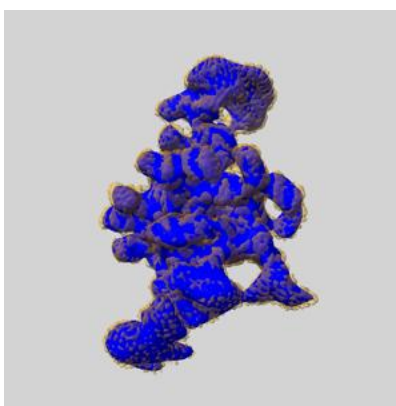
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

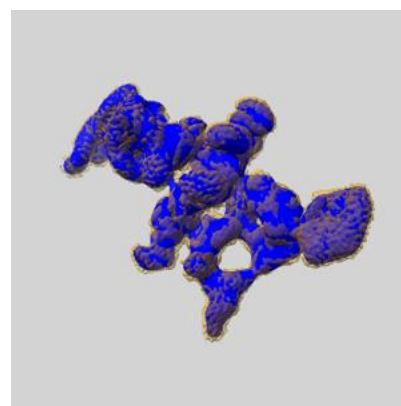
6.6.1 emd_34399_msk_1.map [i](#)



X



Y

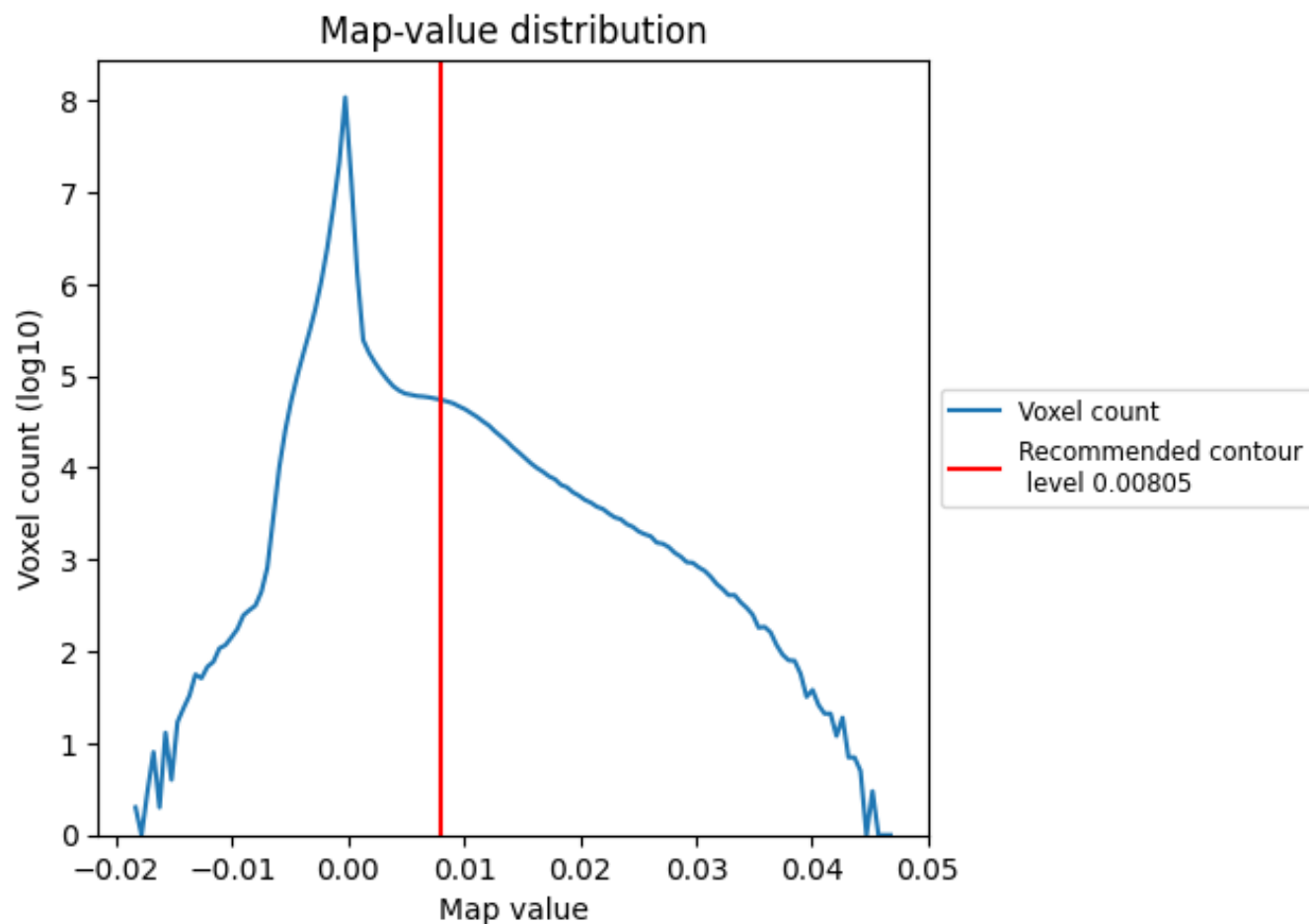


Z

7 Map analysis [i](#)

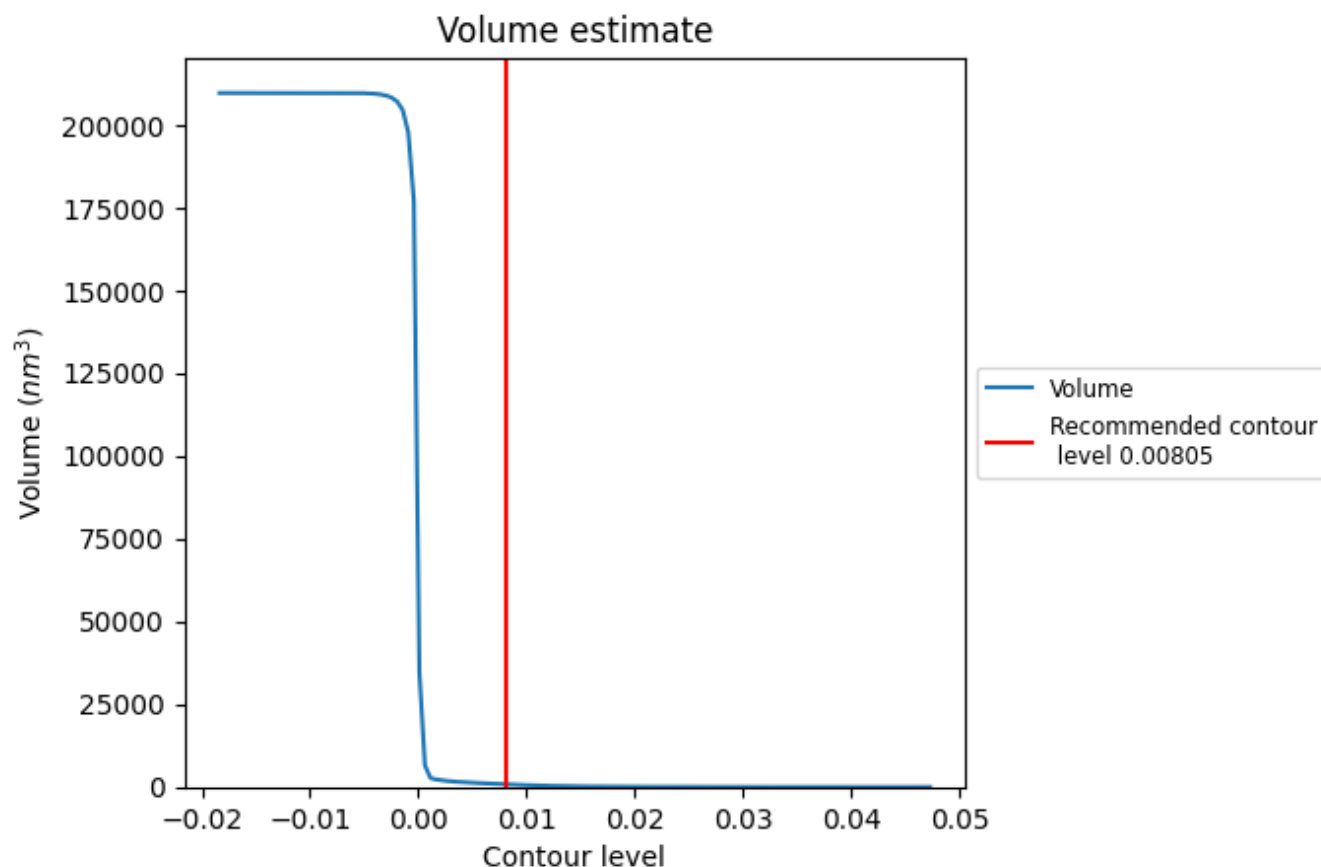
This section contains the results of statistical analysis of the map.

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.

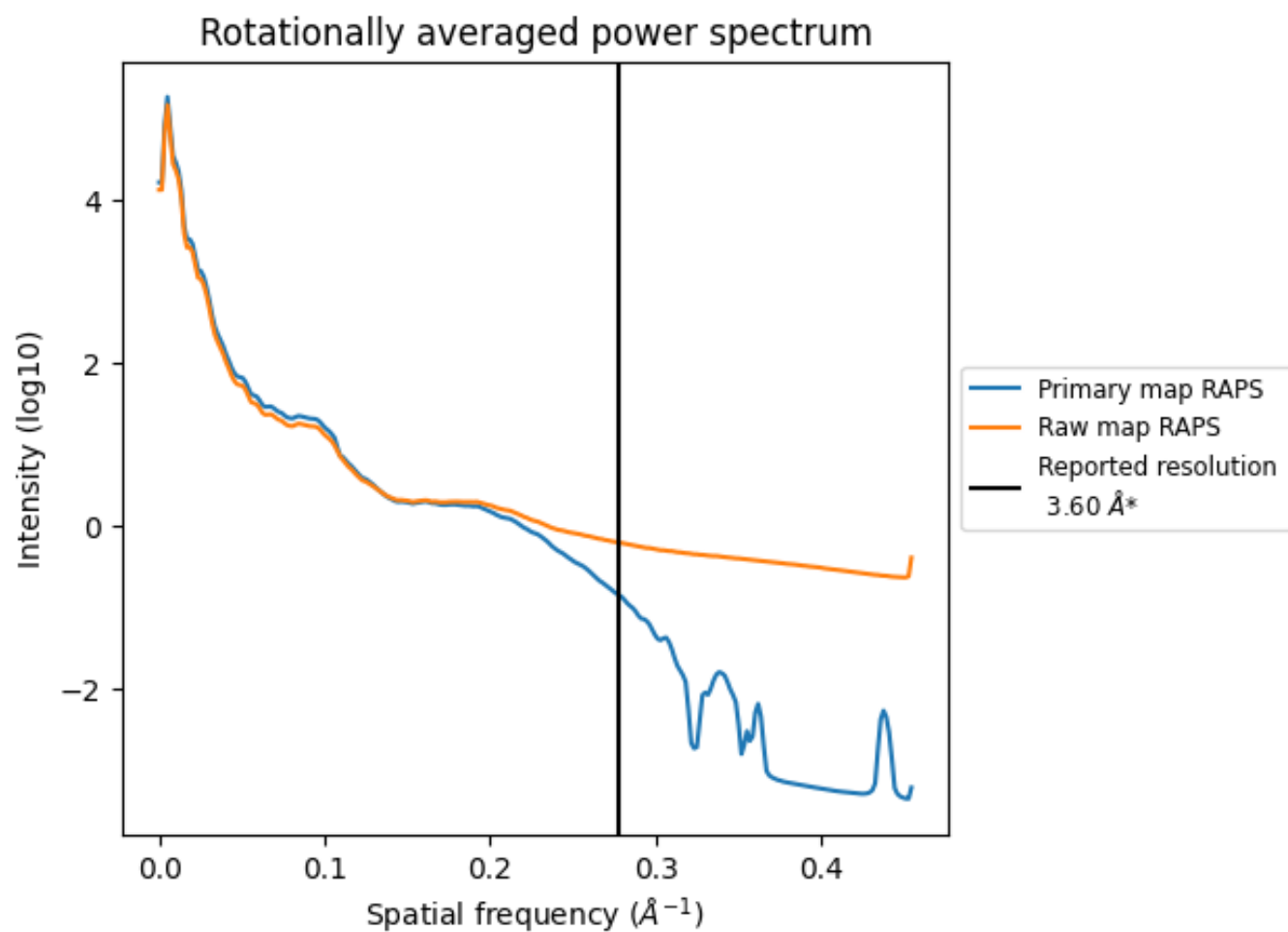
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 809 nm^3 ; this corresponds to an approximate mass of 731 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 ⓘ

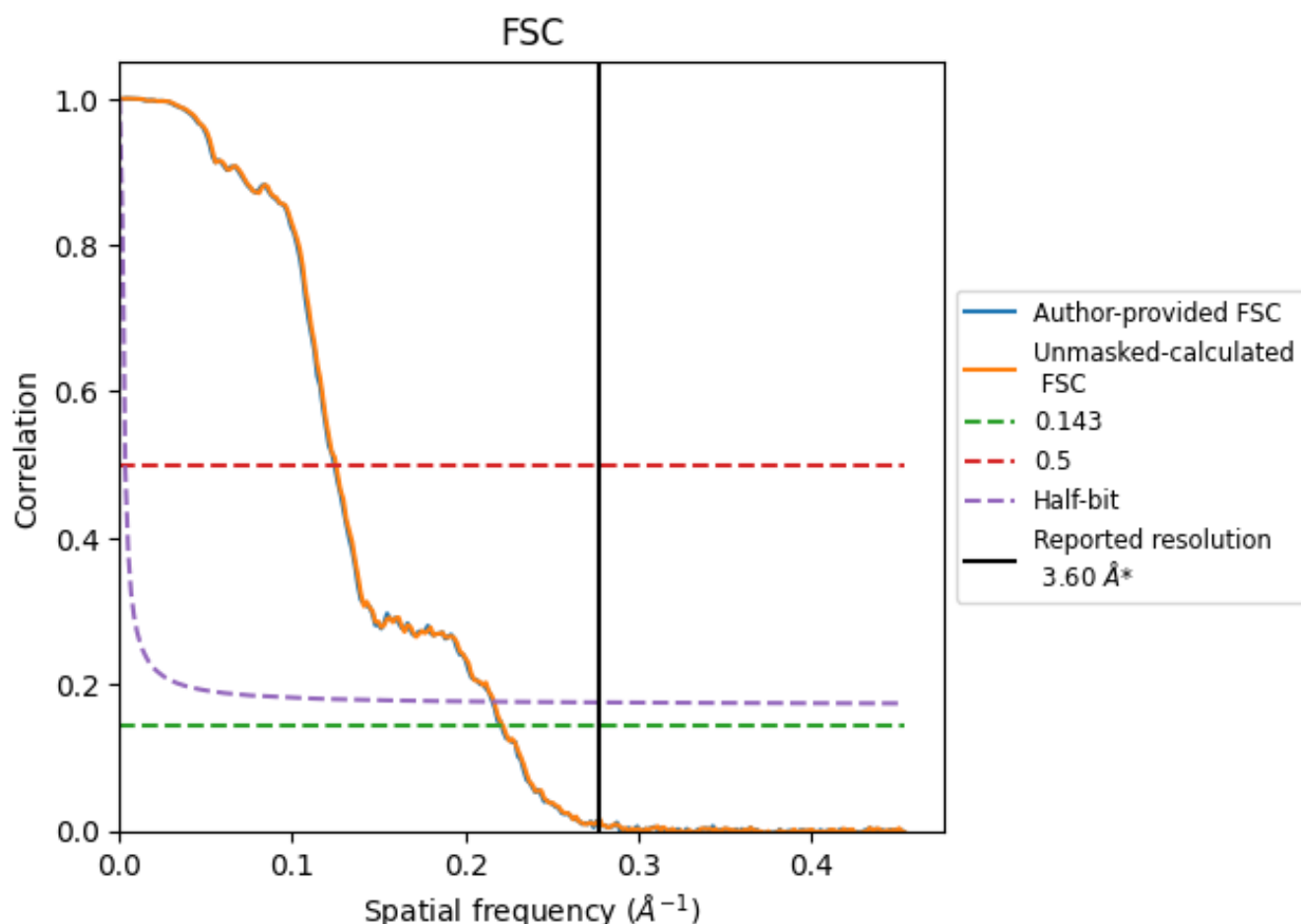


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	4.52	8.05	4.63
Unmasked-calculated*	4.50	7.98	4.61

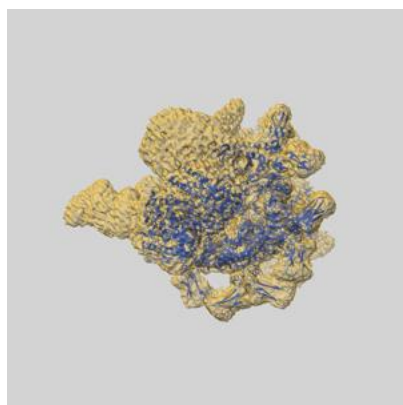
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.52 differs from the reported value 3.6 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.6 by more than 10 %

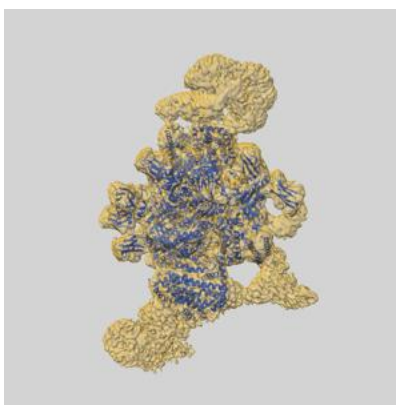
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34399 and PDB model 8GZN. Per-residue inclusion information can be found in section 3 on page 5.

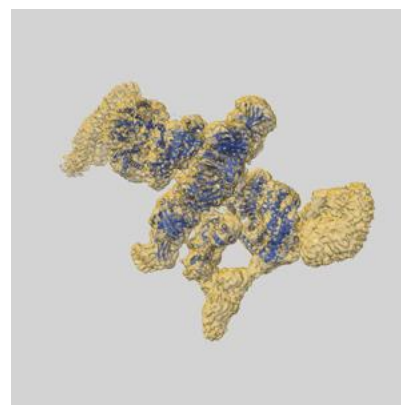
9.1 Map-model overlay [i](#)



X



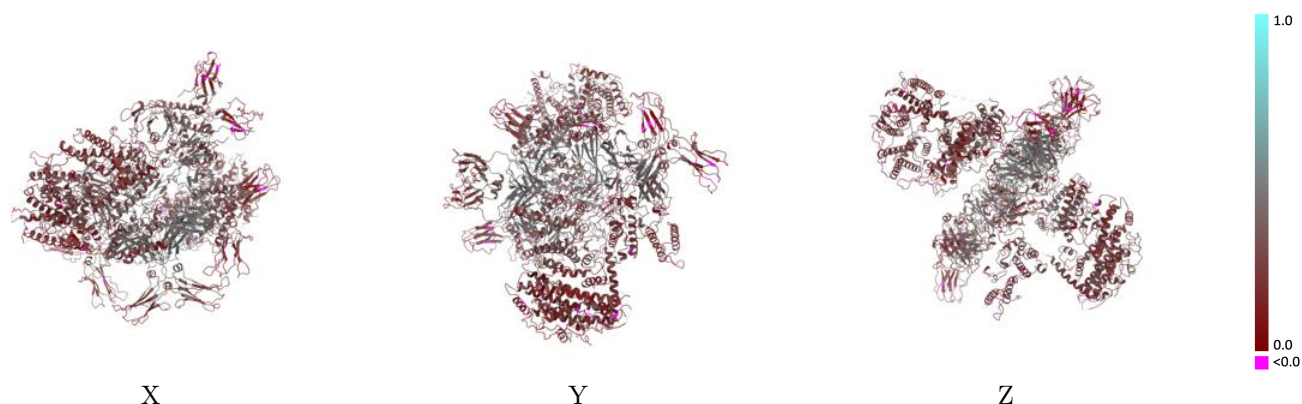
Y



Z

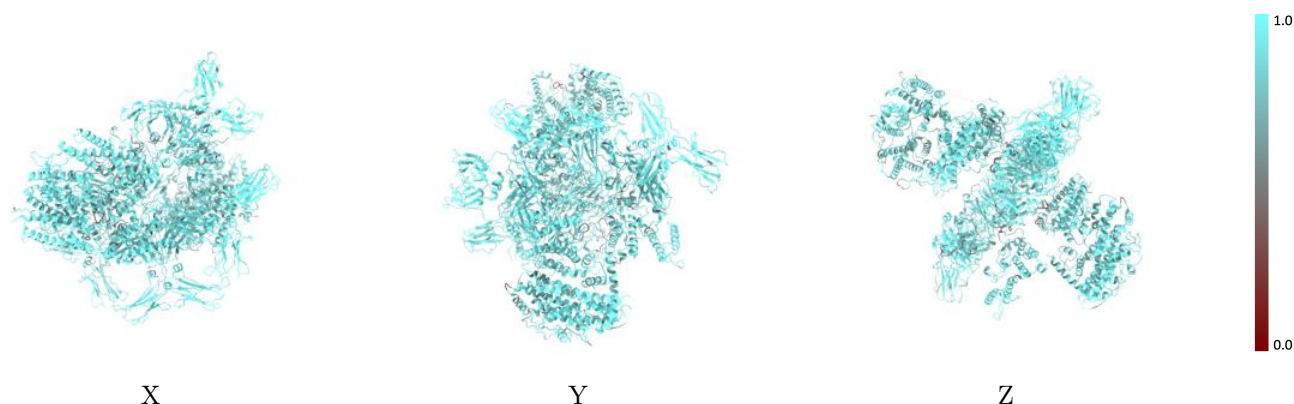
The images above show the 3D surface view of the map at the recommended contour level 0.00805 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



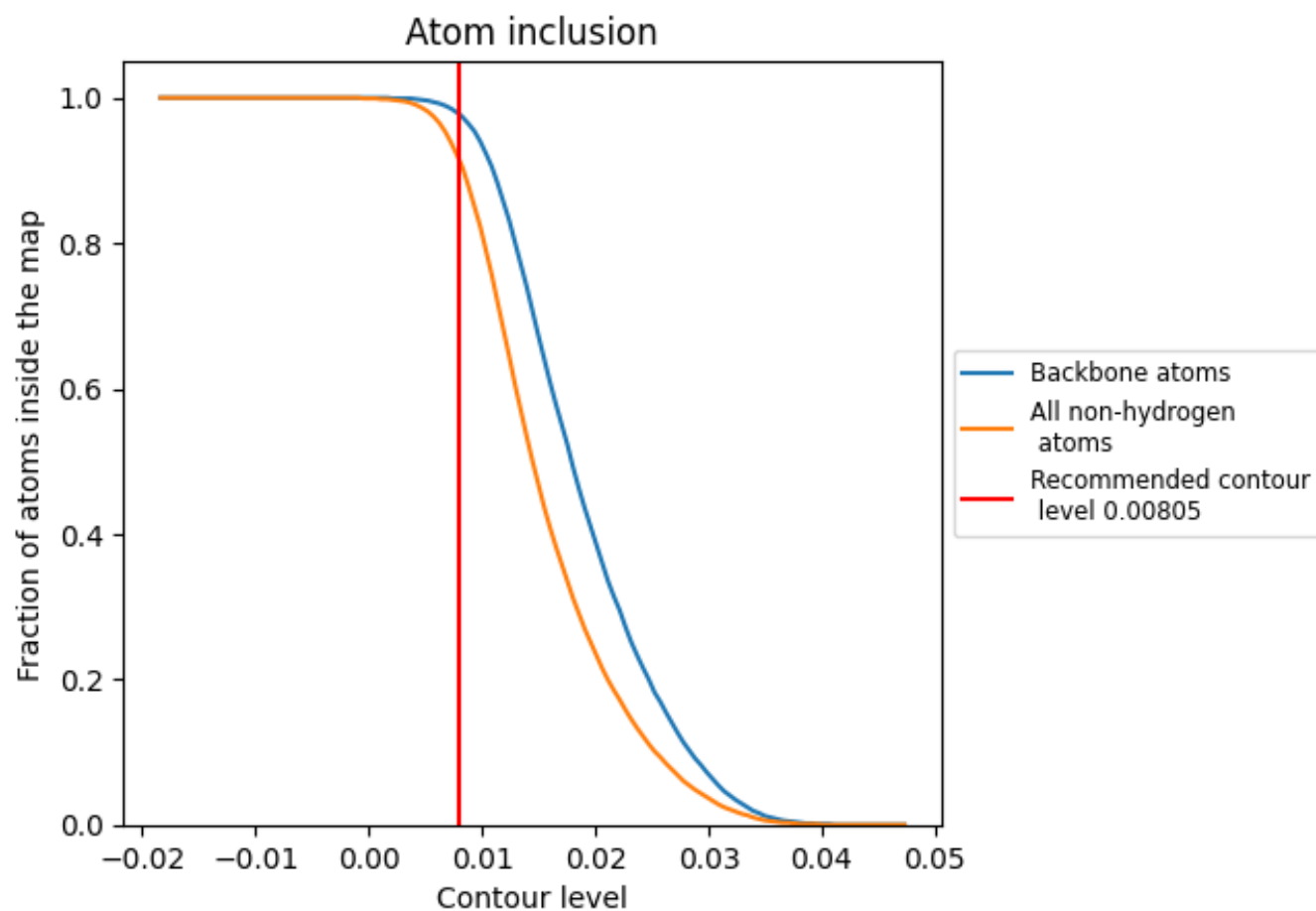
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00805).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00805) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.3040
A	 0.9120	 0.3280
B	 0.9120	 0.3300
C	 0.9560	 0.3410
D	 0.9550	 0.3630
E	 0.9590	 0.3830
F	 0.9510	 0.3730
G	 0.9400	 0.3620
H	 0.9450	 0.3300
I	 0.8870	 0.2540
J	 0.7250	 0.2720
K	 0.9210	 0.3080
L	 0.9550	 0.3170
M	 0.9070	 0.2840

