



Full wwPDB EM Validation Report ⓘ

Aug 25, 2026 – 10:45 pm BST

PDB ID : 9SQR / pdb_00009sqr
EMDB ID : EMD-55116
Title : Symmetry relaxed reconstruction of Rhodospirillum rubrum encapsulin:encapsulated ferritin nanocompartment
Authors : McIver, Z.; McCorvie, T.J.; Basle, A.; Marles-Wright, J.
Deposited on : 2025-09-23
Resolution : 3.73 Å(reported)
Based on initial model : .

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:

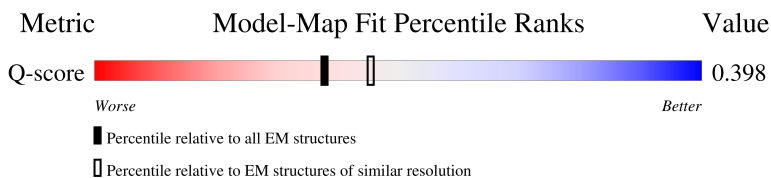
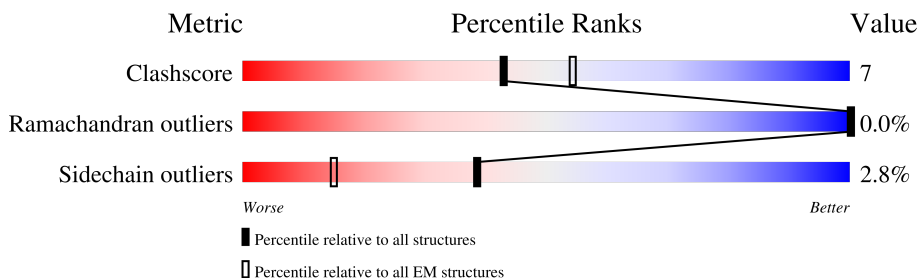
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 3.73 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	10415 (3.23 - 4.23)

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	280	7% 78% 15% • 6%
1	A0	280	6% 76% 17% • 6%
1	AA	280	8% 78% 14% • 6%
1	AB	280	8% 77% 17% 6%

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Mol	Chain	Length	Quality of chain
1	B	280	
1	BA	280	
1	BB	280	
1	C	280	
1	CA	280	
1	CB	280	
1	D	280	
1	DA	280	
1	DB	280	
1	E	280	
1	EA	280	
1	EB	280	
1	F	280	
1	FA	280	
1	FB	280	
1	G	280	
1	GA	280	
1	GB	280	
1	H	280	
1	HA	280	
1	HB	280	
1	I	280	
1	IA	280	
1	J	280	
1	JA	280	

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Mol	Chain	Length	Quality of chain
1	K	280	
1	KA	280	
1	L	280	
1	LA	280	
1	M	280	
1	MA	280	
1	N	280	
1	NA	280	
1	O	280	
1	OA	280	
1	P	280	
1	PA	280	
1	Q	280	
1	QA	280	
1	R	280	
1	RA	280	
1	S	280	
1	SA	280	
1	T	280	
1	TA	280	
1	UA	280	
1	V	280	
1	VA	280	
1	W	280	
1	WA	280	

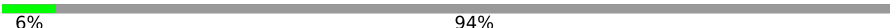
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Mol	Chain	Length	Quality of chain
1	X	280	
1	XA	280	
1	Y	280	
1	YA	280	
1	Z	280	
1	ZA	280	
2	1	140	
2	10	140	
2	11	140	
2	12	140	
2	13	140	
2	14	140	
2	15	140	
2	16	140	
2	17	140	
2	18	140	
2	19	140	
2	2	140	
2	20	140	
2	3	140	
2	4	140	
2	5	140	
2	6	140	
2	7	140	
2	8	140	

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Mol	Chain	Length	Quality of chain
2	9	140	 6% 94%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 119496 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 Type 1 encapsulin shell protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	A	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	B	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	C	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	D	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	E	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	F	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	G	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	H	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	I	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	J	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	K	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	L	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	M	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	N	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	O	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	P	262	Total 1975	C 1251	N 350	O 367	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	R	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	S	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	T	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	V	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	W	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	X	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	Y	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	Z	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	AA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	BA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	CA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	DA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	EA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	FA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	GA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	HA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	IA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	JA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	KA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	LA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	MA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	NA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	OA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	PA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	QA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	RA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	SA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	TA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	UA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	VA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	WA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	XA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	YA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	ZA	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	AB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	BB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	CB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	DB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	EB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	FB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0
1	GB	262	Total 1975	C 1251	N 350	O 367	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	HB	262	Total	C	N	O	S	0	0
			1975	1251	350	367	7		

- Molecule 2 is a protein called Encapsulated ferritin-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	8	Total	C	N	O		0	0
			48	30	8	10			
2	2	8	Total	C	N	O		0	0
			48	30	8	10			
2	3	8	Total	C	N	O		0	0
			48	30	8	10			
2	4	9	Total	C	N	O		0	0
			57	36	10	11			
2	5	8	Total	C	N	O		0	0
			48	30	8	10			
2	6	8	Total	C	N	O		0	0
			48	30	8	10			
2	7	9	Total	C	N	O		0	0
			57	36	10	11			
2	8	9	Total	C	N	O		0	0
			57	36	10	11			
2	9	8	Total	C	N	O		0	0
			48	30	8	10			
2	10	9	Total	C	N	O		0	0
			57	36	10	11			
2	11	8	Total	C	N	O		0	0
			48	30	8	10			
2	12	8	Total	C	N	O		0	0
			48	30	8	10			
2	13	8	Total	C	N	O		0	0
			48	30	8	10			
2	14	8	Total	C	N	O		0	0
			48	30	8	10			
2	15	8	Total	C	N	O		0	0
			48	30	8	10			
2	16	8	Total	C	N	O		0	0
			48	30	8	10			
2	17	8	Total	C	N	O		0	0
			48	30	8	10			
2	18	8	Total	C	N	O		0	0
			48	30	8	10			

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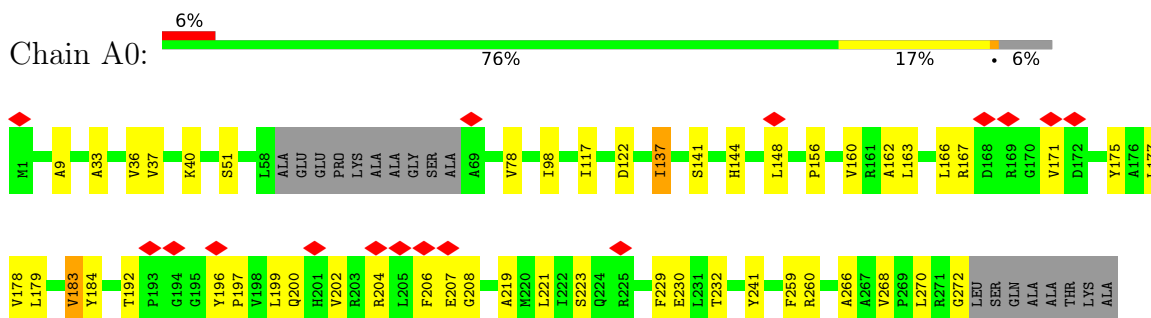
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Mol	Chain	Residues	Atoms				AltConf	Trace
2	19	8	Total	C	N	O	0	0
			48	30	8	10		
2	20	8	Total	C	N	O	0	0
			48	30	8	10		

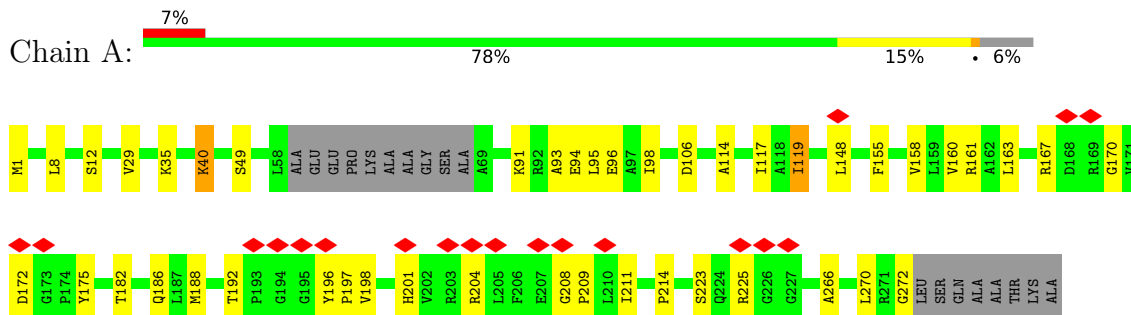
3 Residue-property plots [i](#)

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

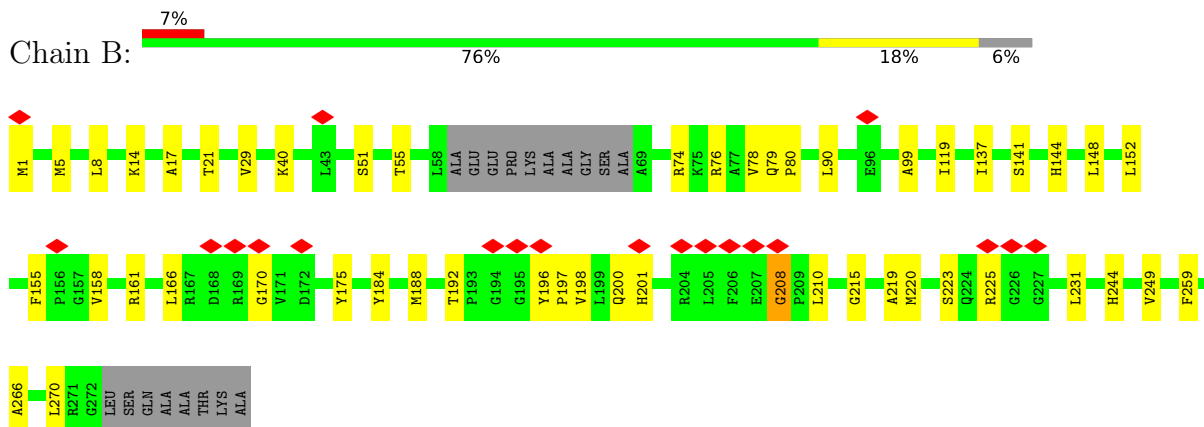
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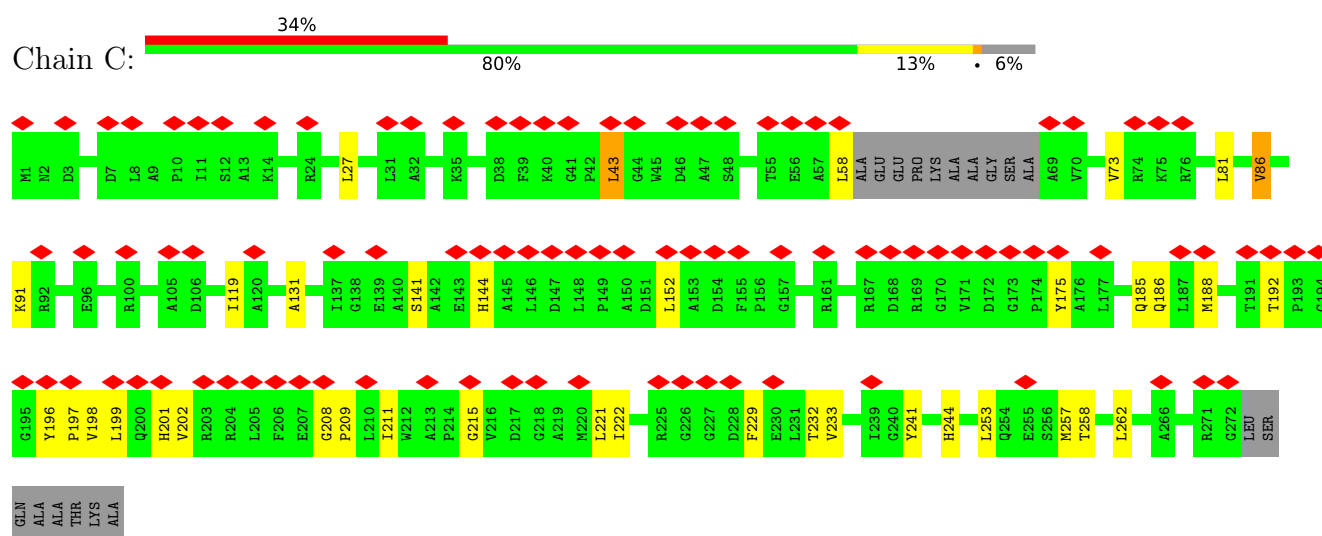
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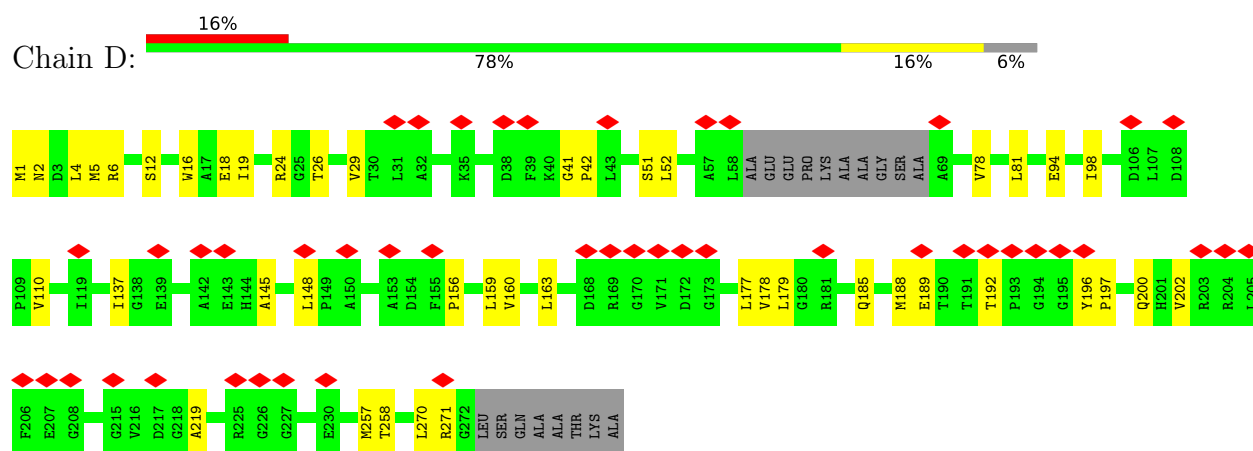
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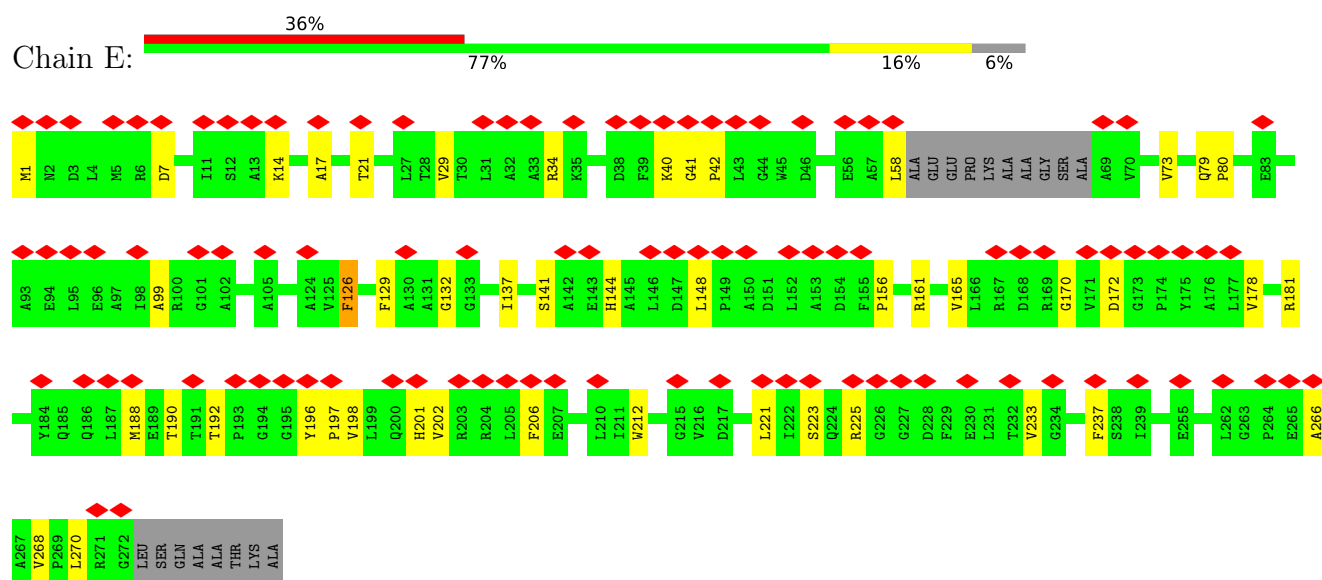
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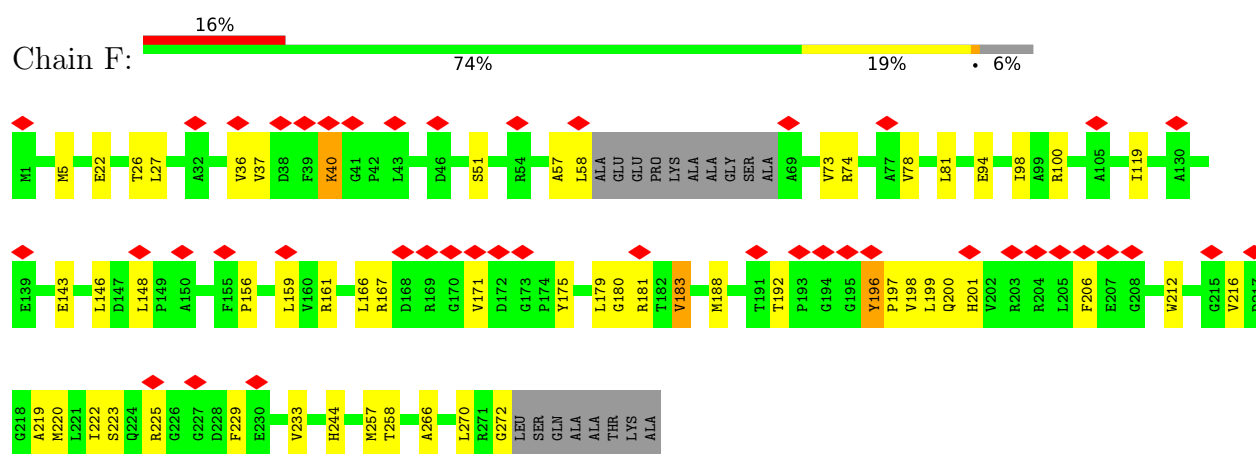
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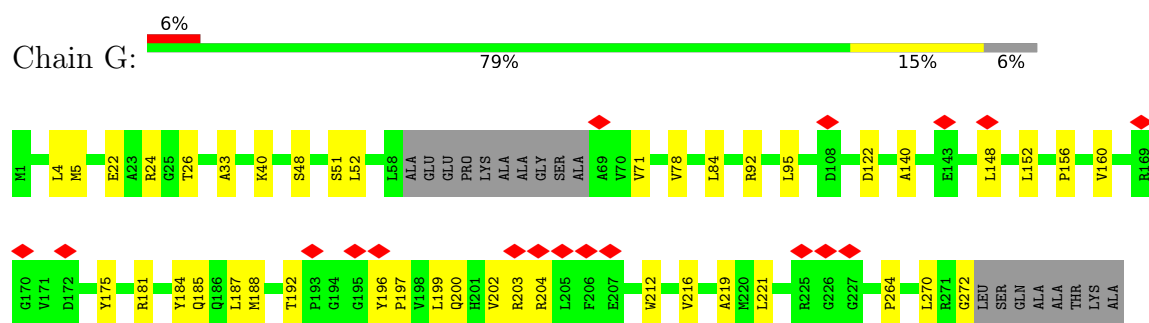
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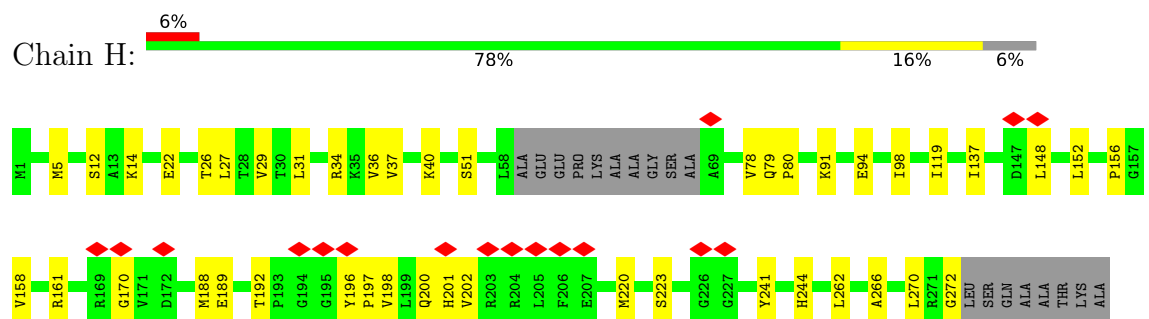
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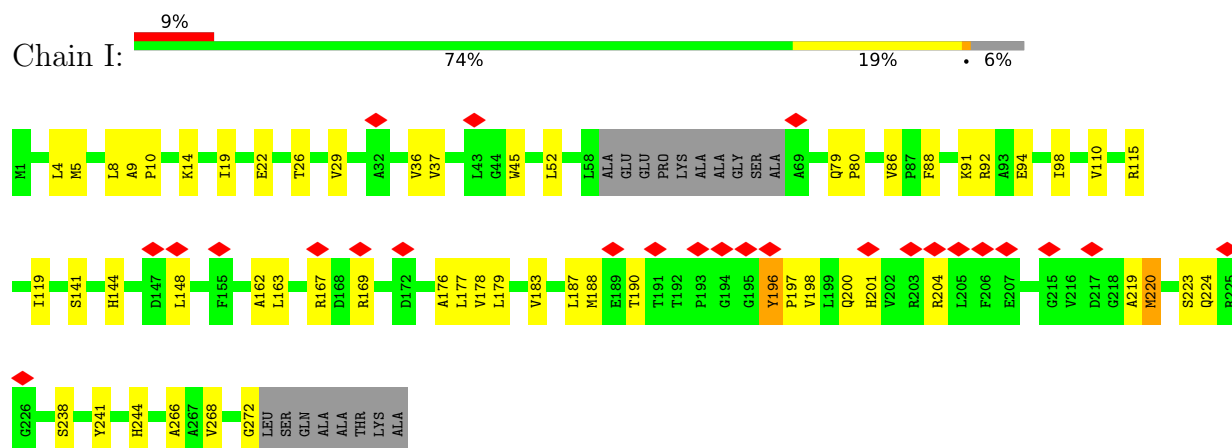
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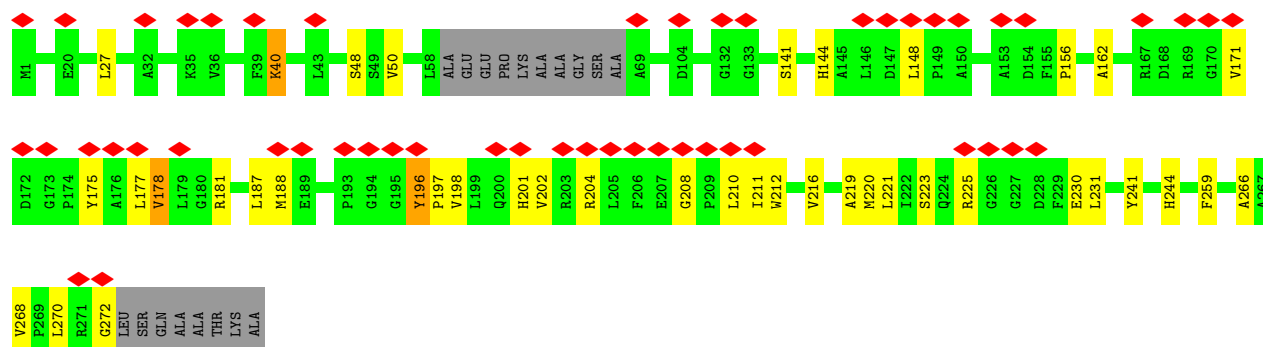
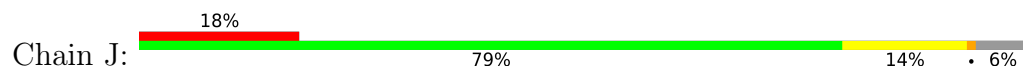
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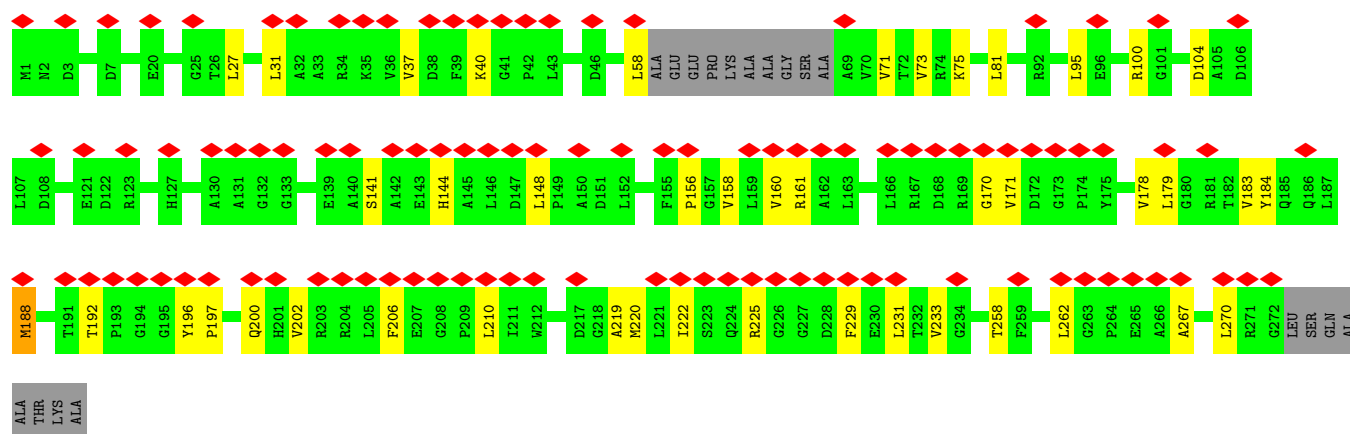
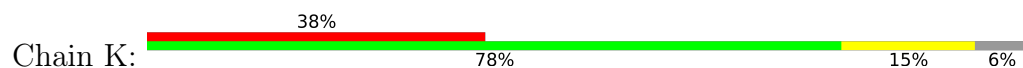
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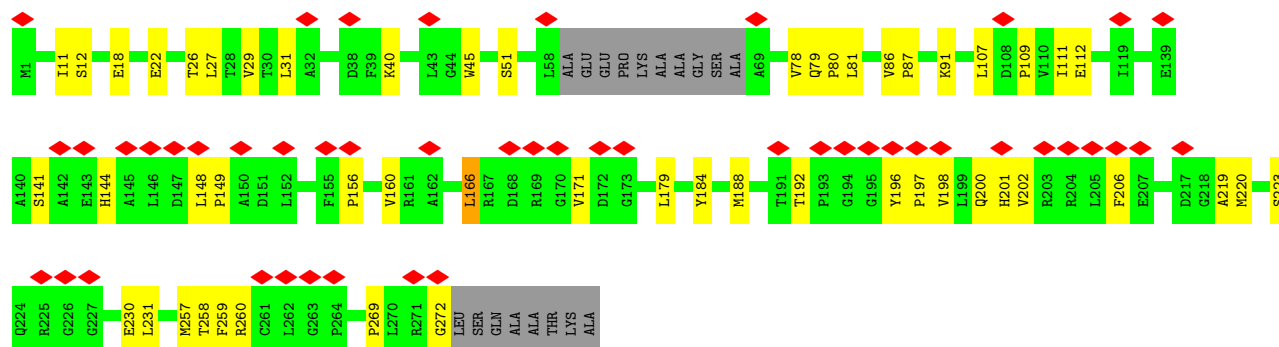
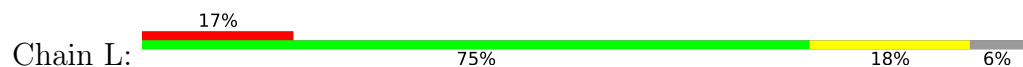
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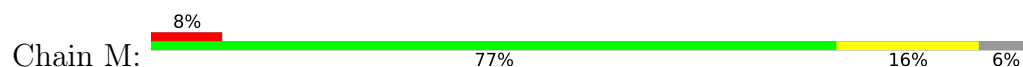
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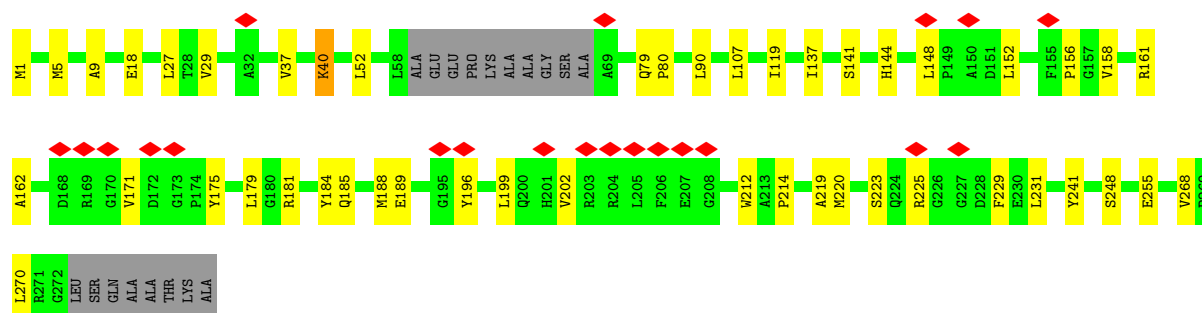


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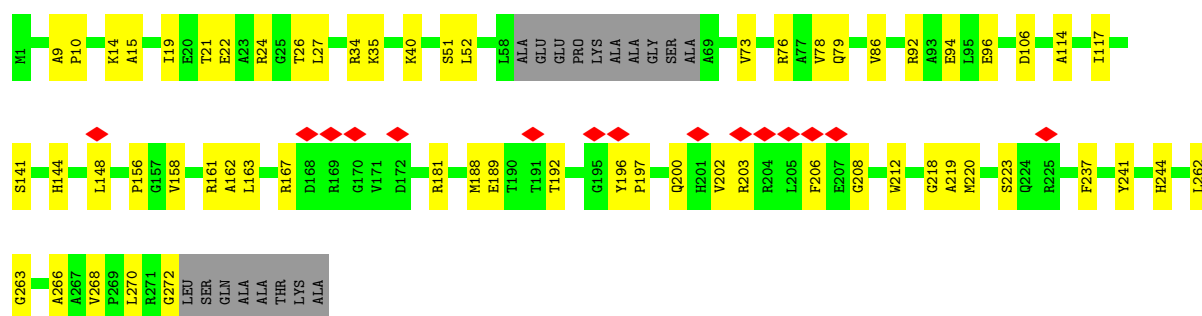
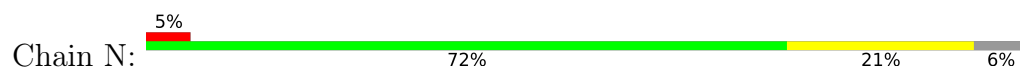


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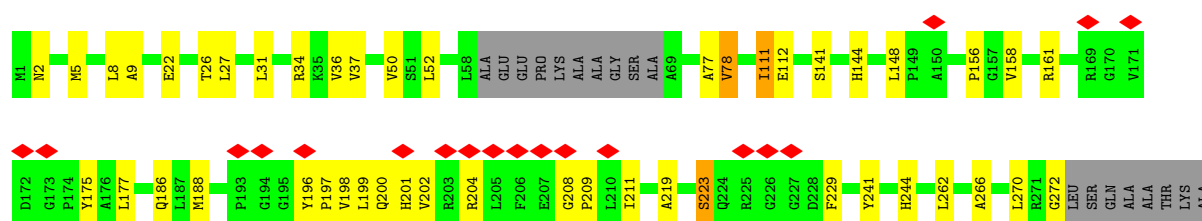
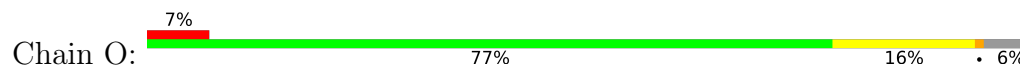




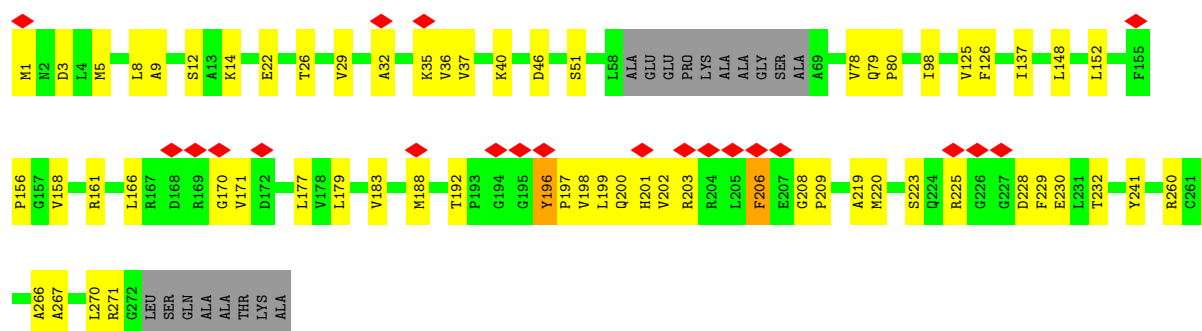
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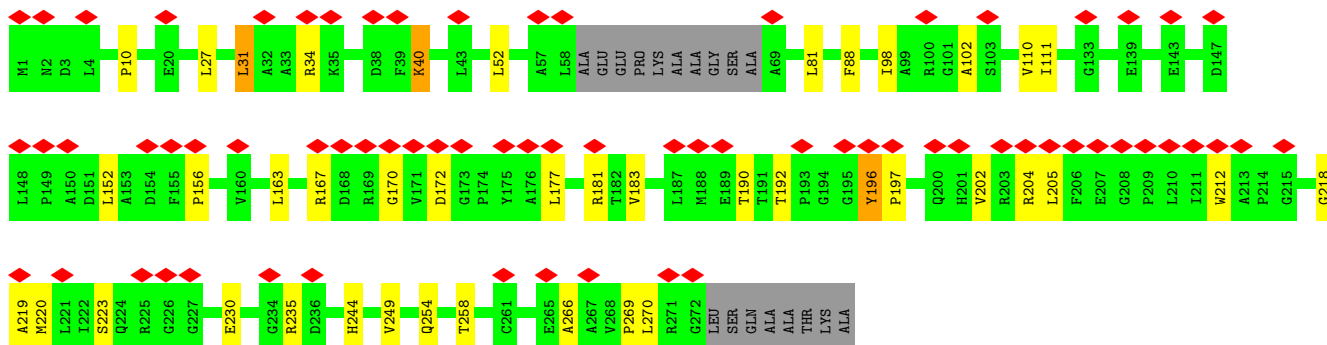
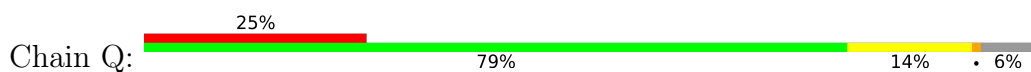
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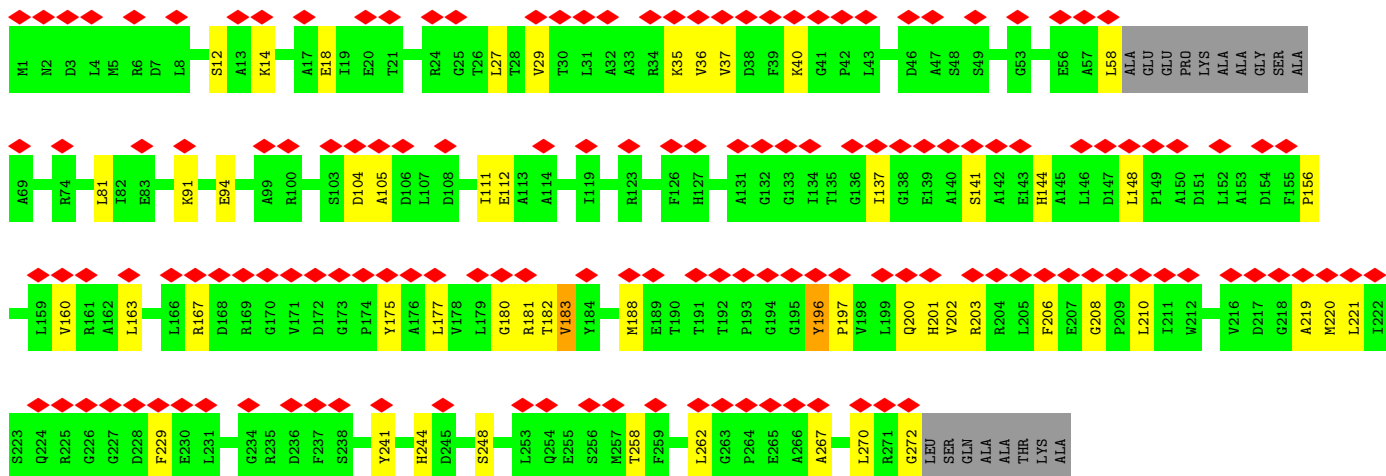
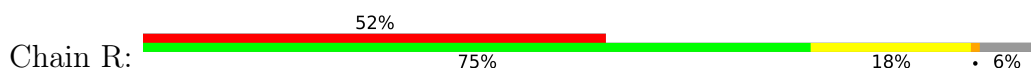
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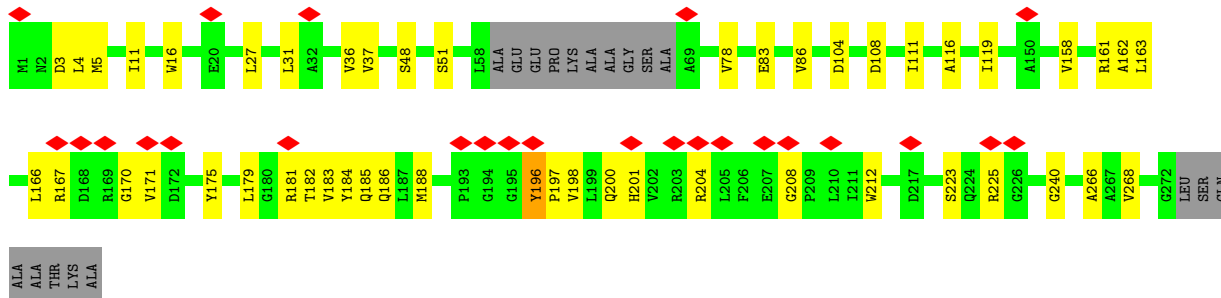
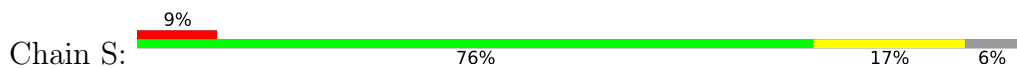
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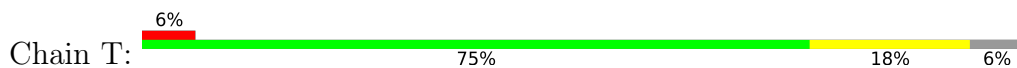
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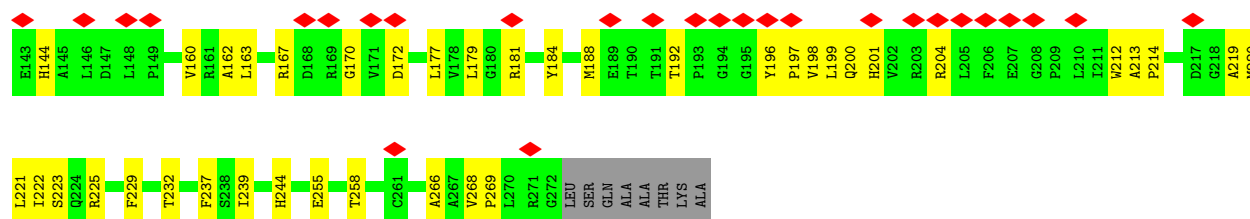


- Molecule 1: Type 1 encapsulin shell protein

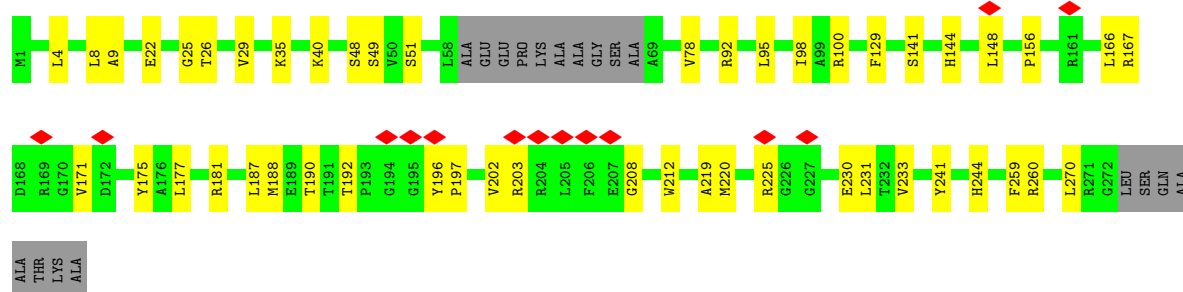
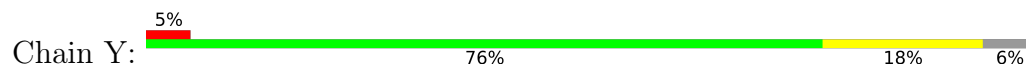


- Molecule 1: Type 1 encapsulin shell protein

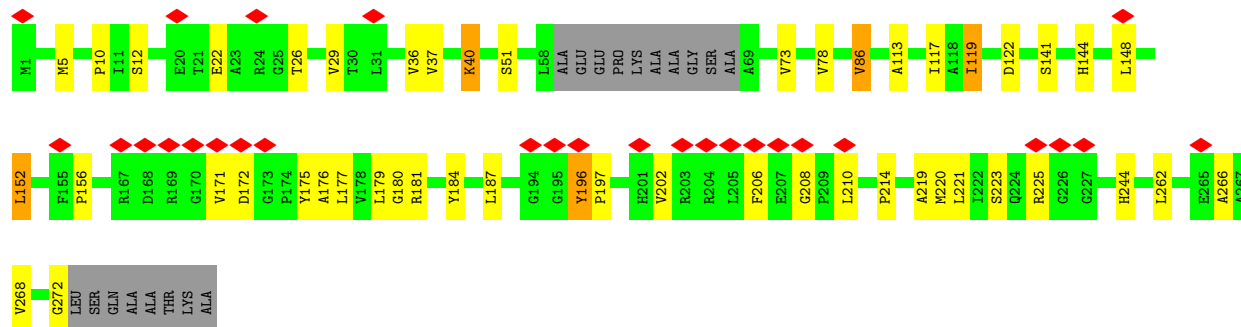




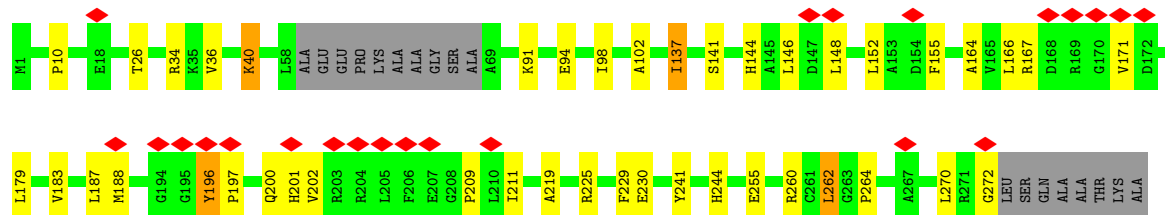
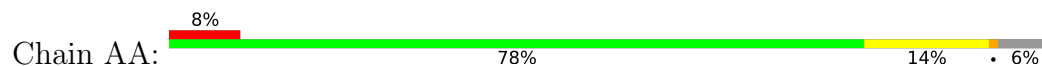
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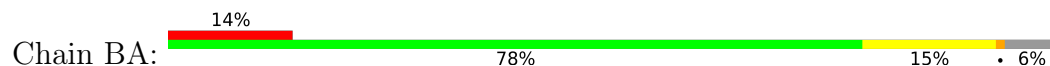
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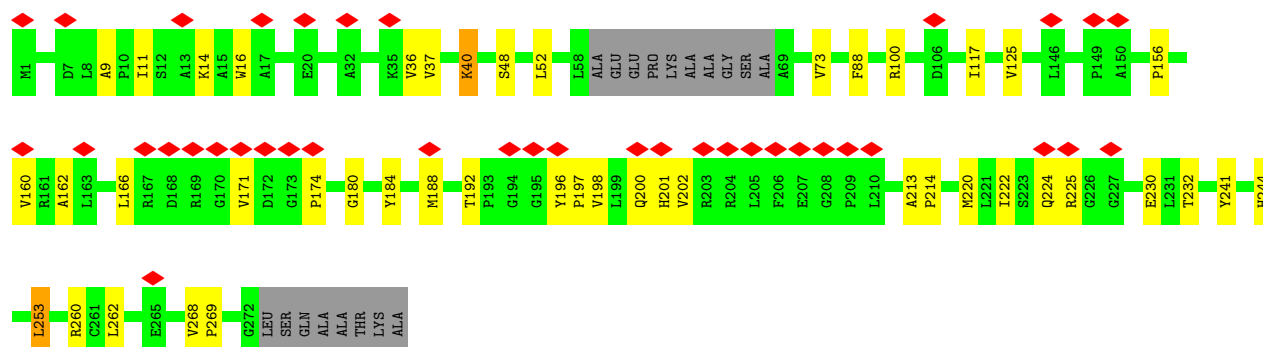


- Molecule 1: Type 1 encapsulin shell protein



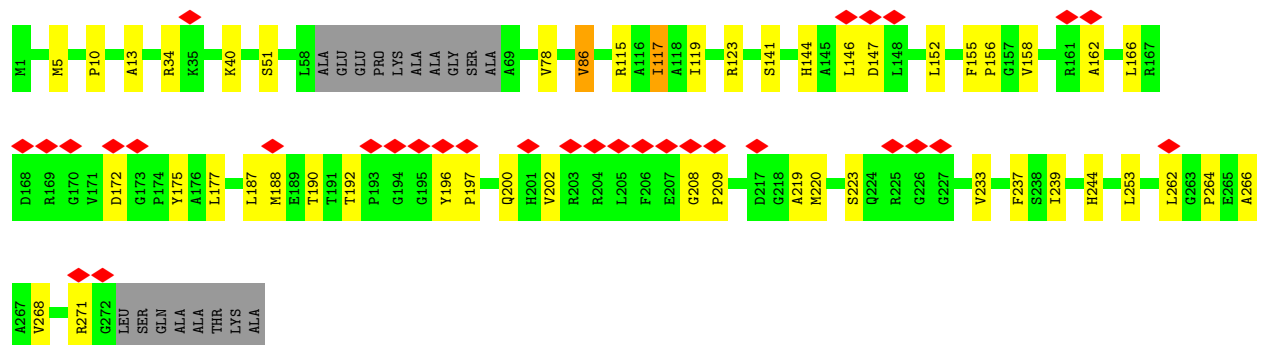
- Molecule 1: Type 1 encapsulin shell protein





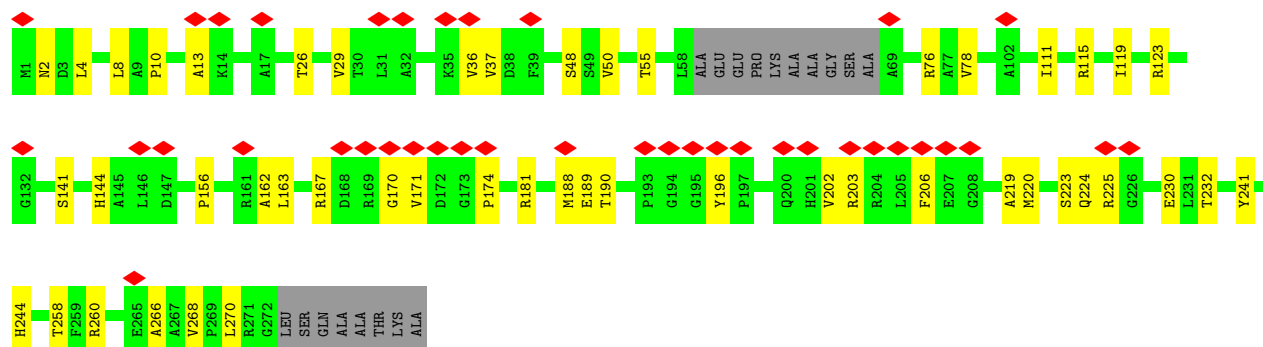
• Molecule 1: Type 1 encapsulin shell protein

Chain CA: 11% 76% 16% 6%



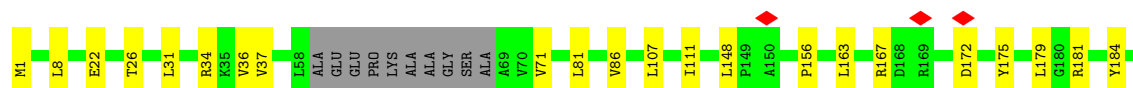
• Molecule 1: Type 1 encapsulin shell protein

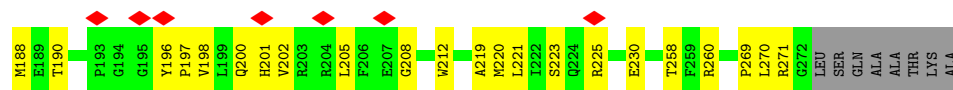
Chain DA: 14% 76% 18% 6%



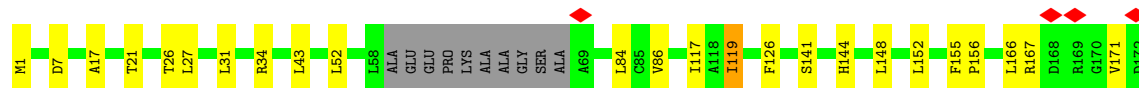
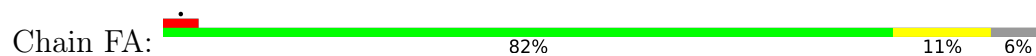
• Molecule 1: Type 1 encapsulin shell protein

Chain EA: 78% 16% 6%

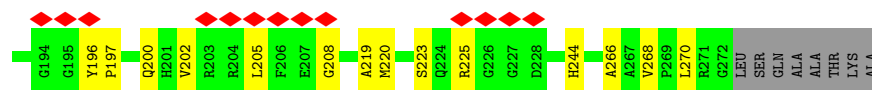
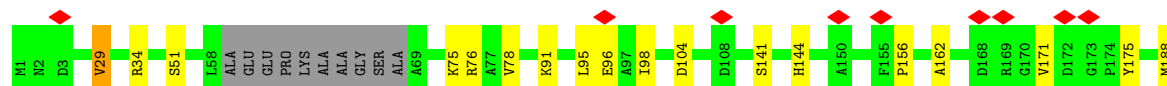
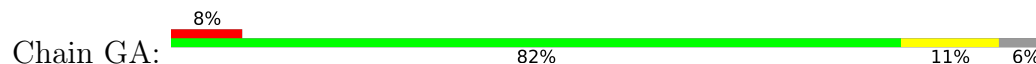




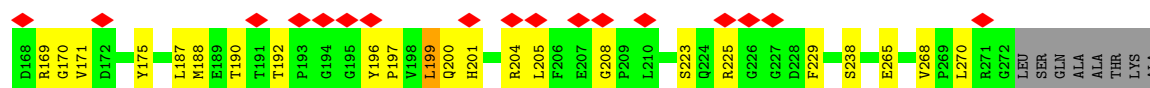
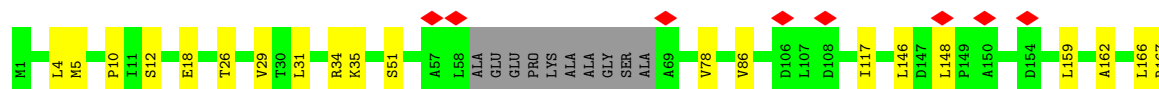
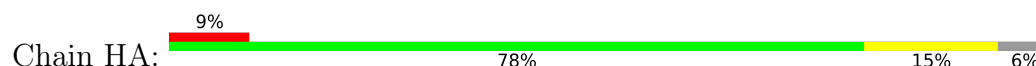
- Molecule 1: Type 1 encapsulin shell protein



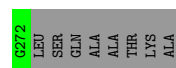
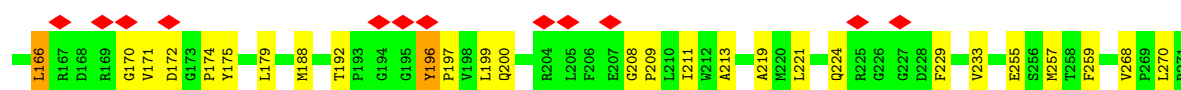
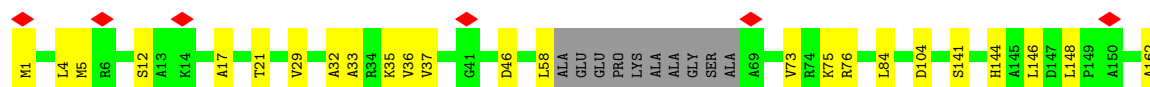
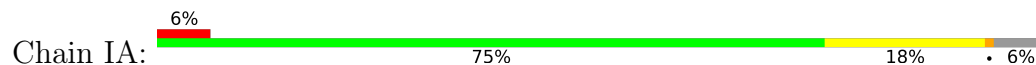
- Molecule 1: Type 1 encapsulin shell protein



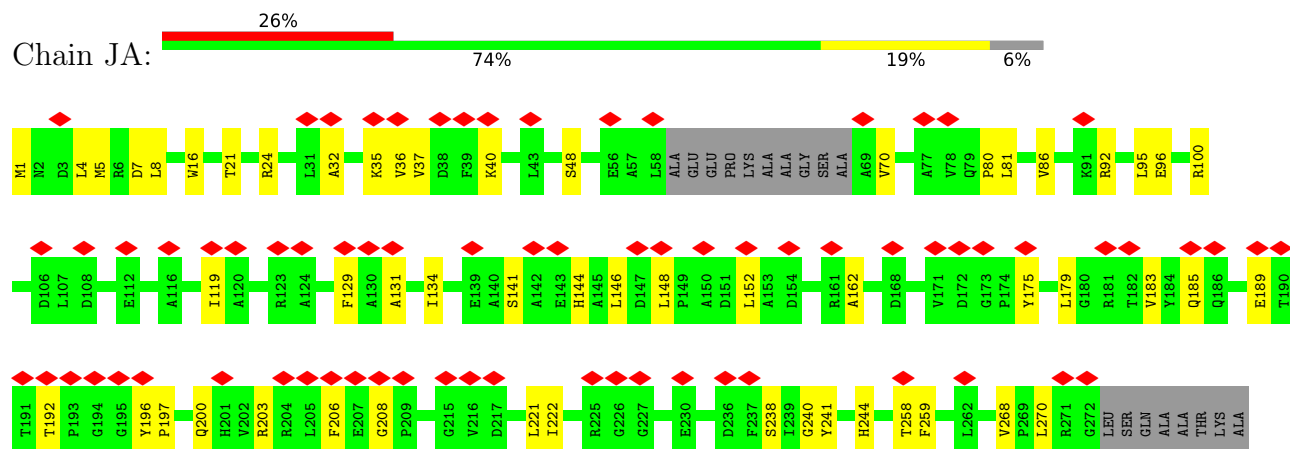
- Molecule 1: Type 1 encapsulin shell protein



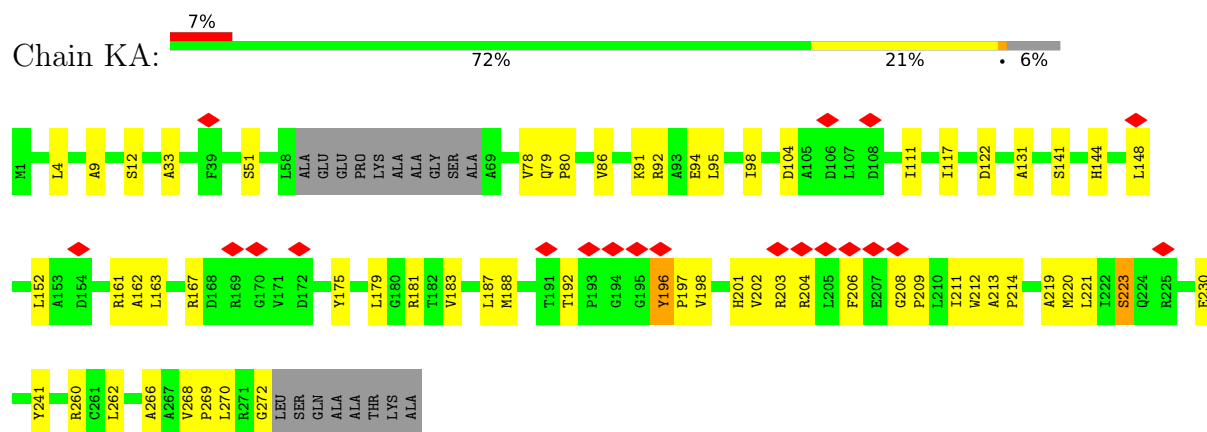
- Molecule 1: Type 1 encapsulin shell protein



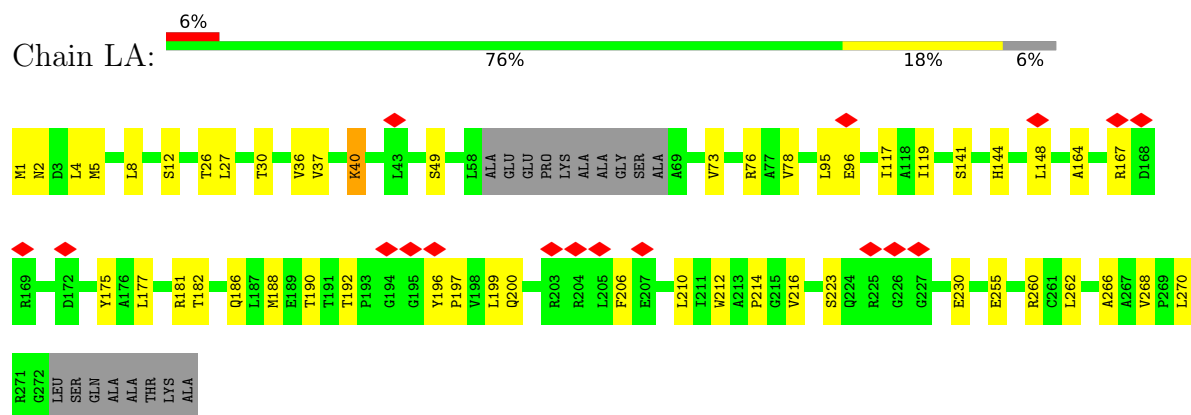
- Molecule 1: Type 1 encapsulin shell protein



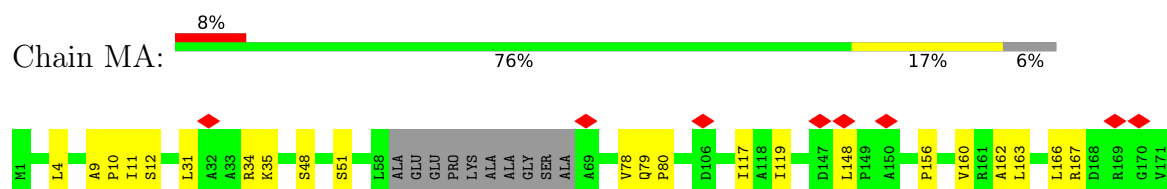
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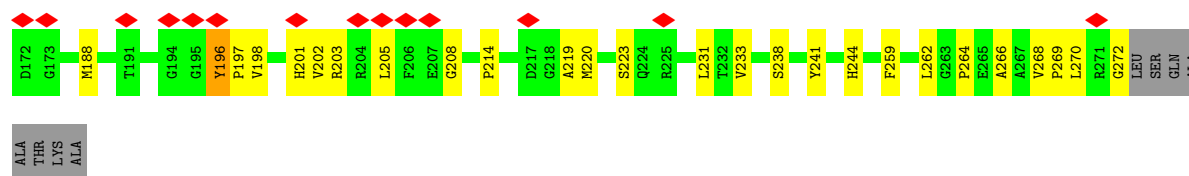


- Molecule 1: Type 1 encapsulin shell protein

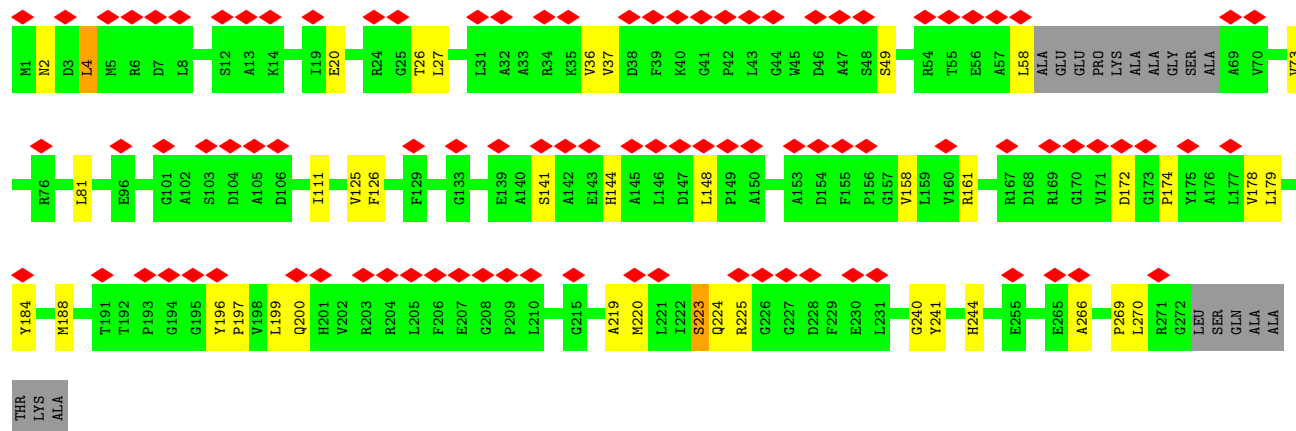
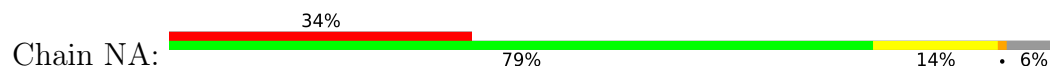


- Molecule 1: Type 1 encapsulin shell protein

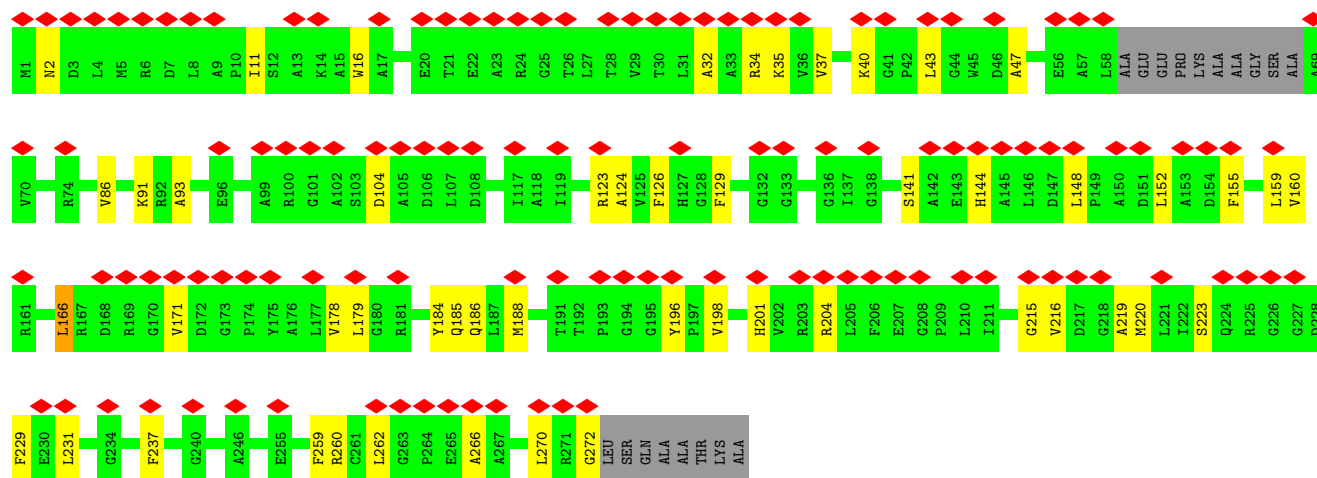




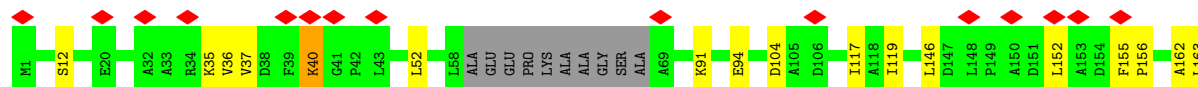
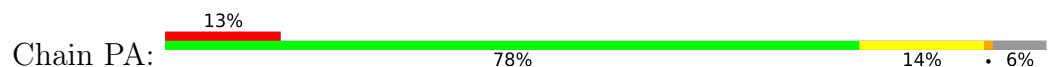
- Molecule 1: Type 1 encapsulin shell protein

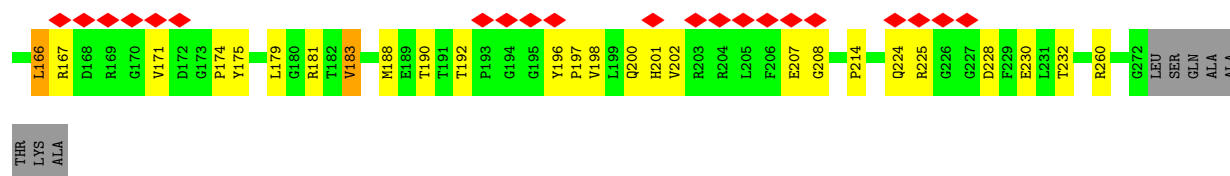


- Molecule 1: Type 1 encapsulin shell protein

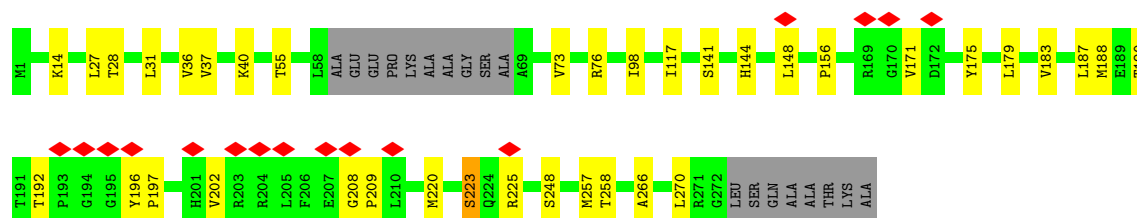
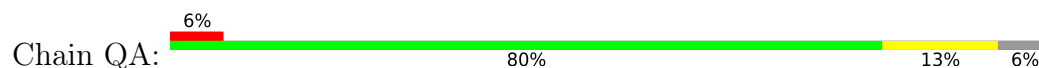


- Molecule 1: Type 1 encapsulin shell protein

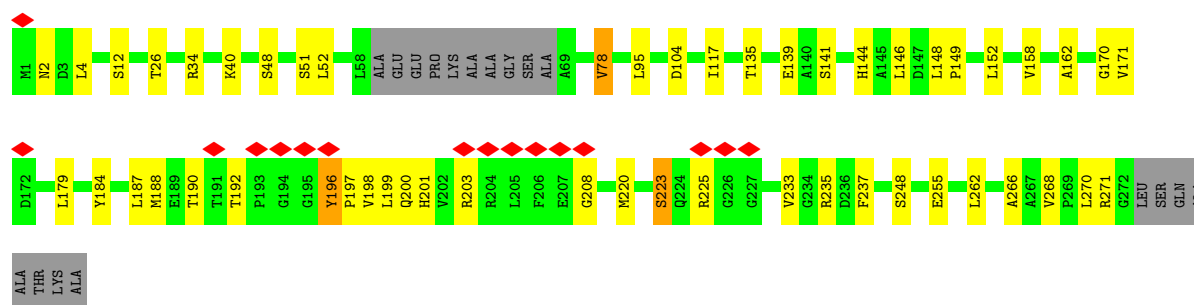
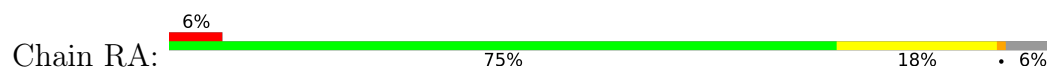




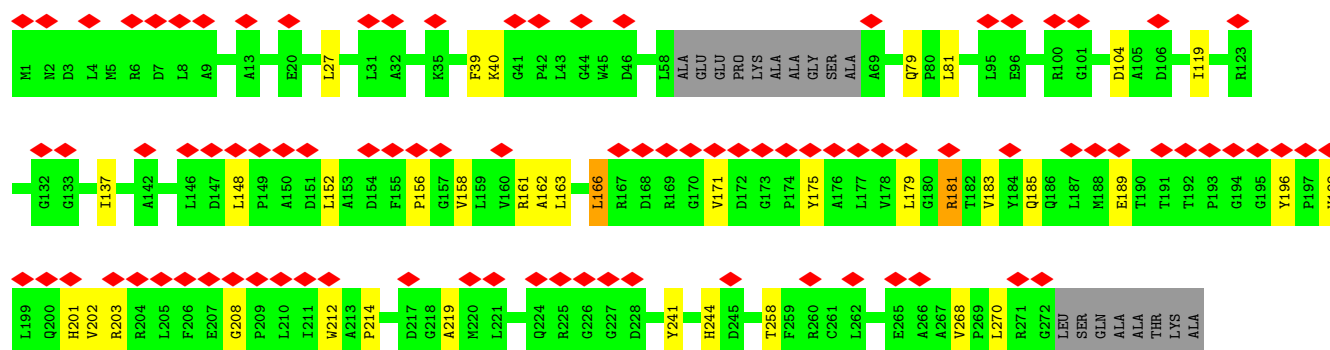
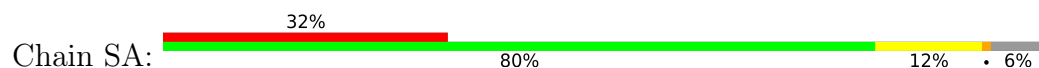
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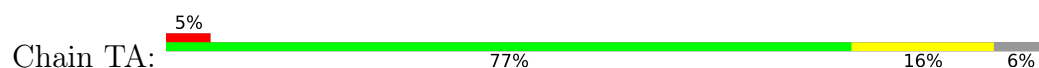
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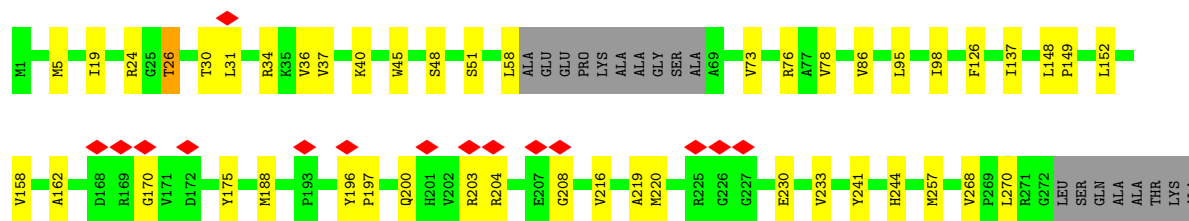


- Molecule 1: Type 1 encapsulin shell protein

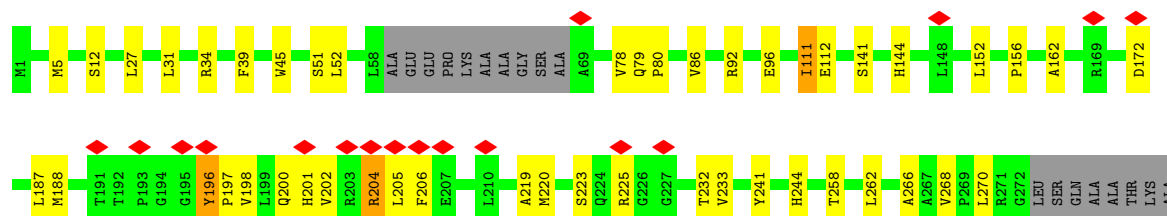
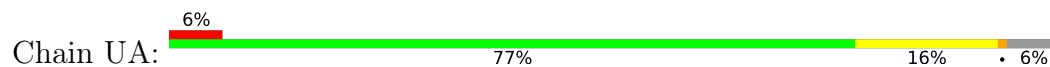


- Molecule 1: Type 1 encapsulin shell protein

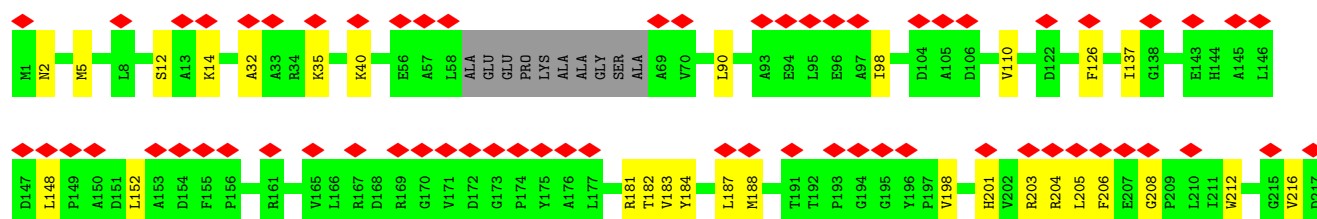
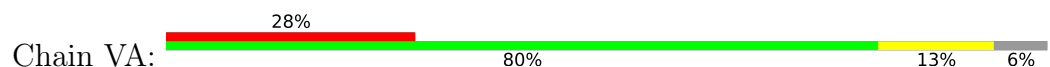




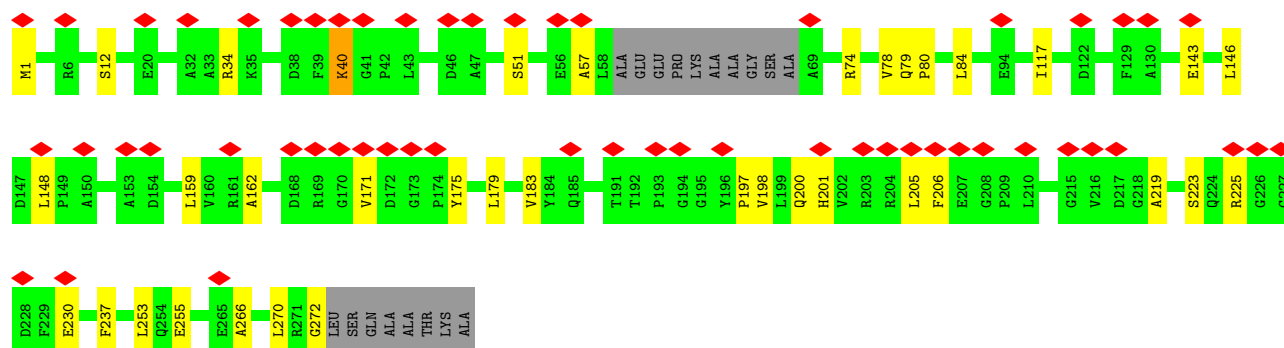
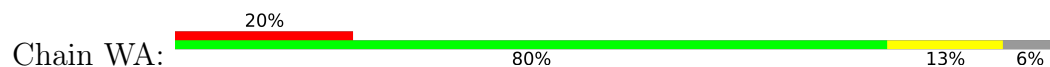
- Molecule 1: Type 1 encapsulin shell protein



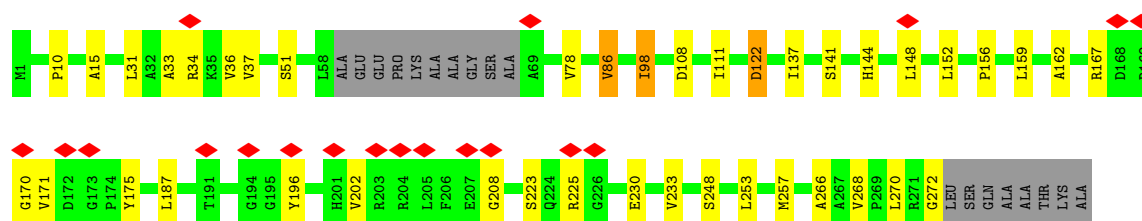
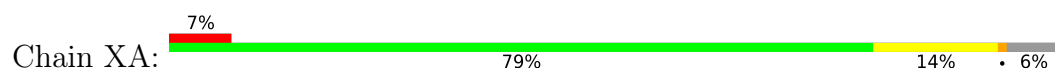
- Molecule 1: Type 1 encapsulin shell protein



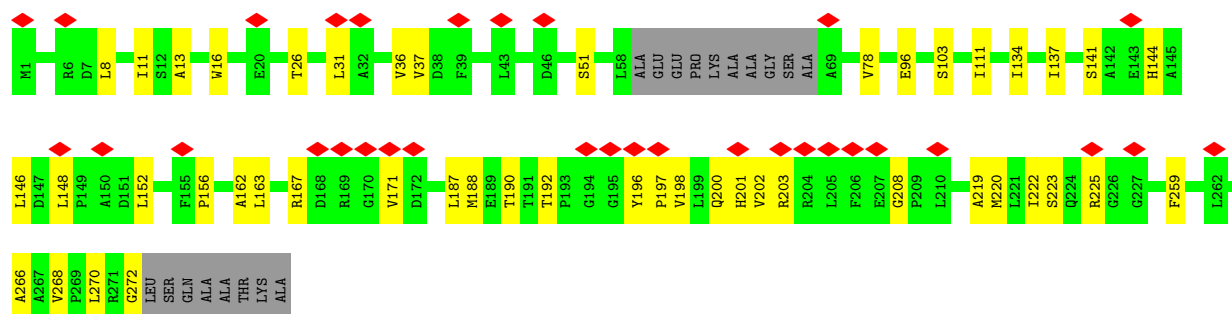
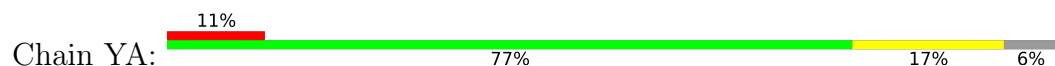
- Molecule 1: Type 1 encapsulin shell protein



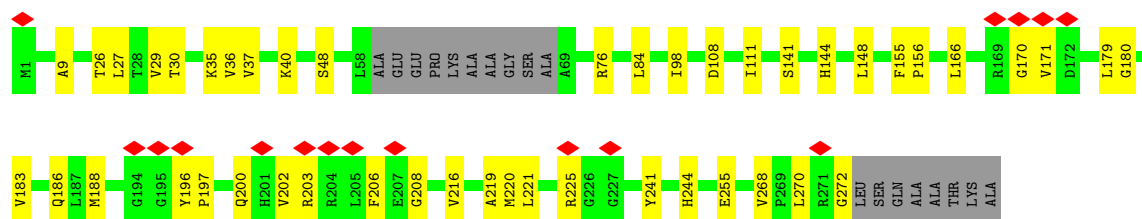
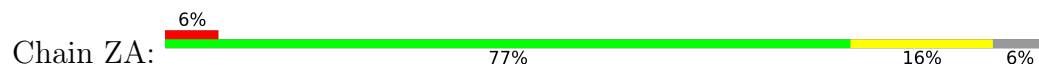
- Molecule 1: Type 1 encapsulin shell protein



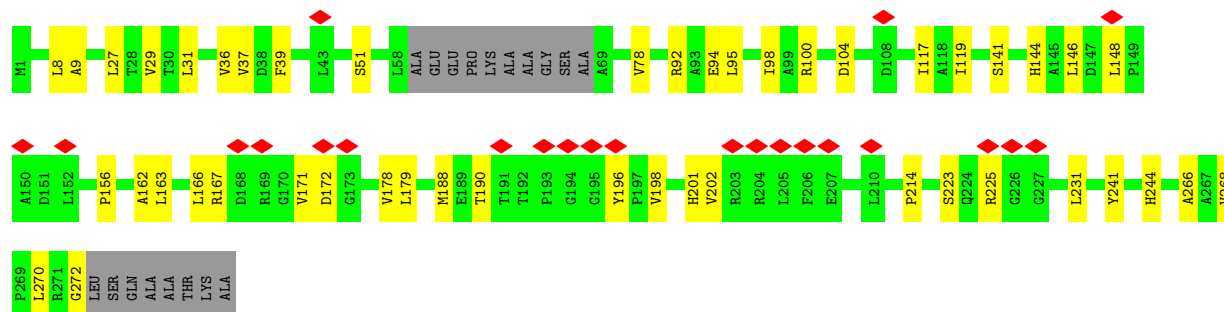
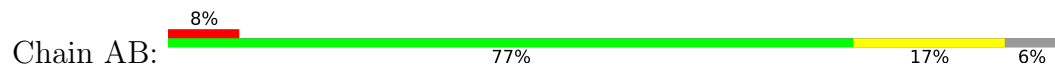
- Molecule 1: Type 1 encapsulin shell protein



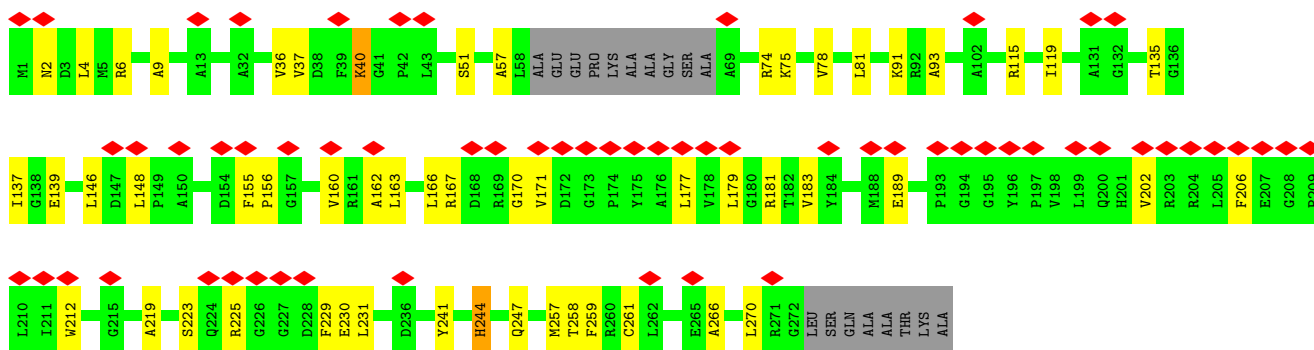
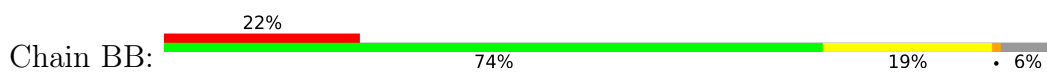
- Molecule 1: Type 1 encapsulin shell protein



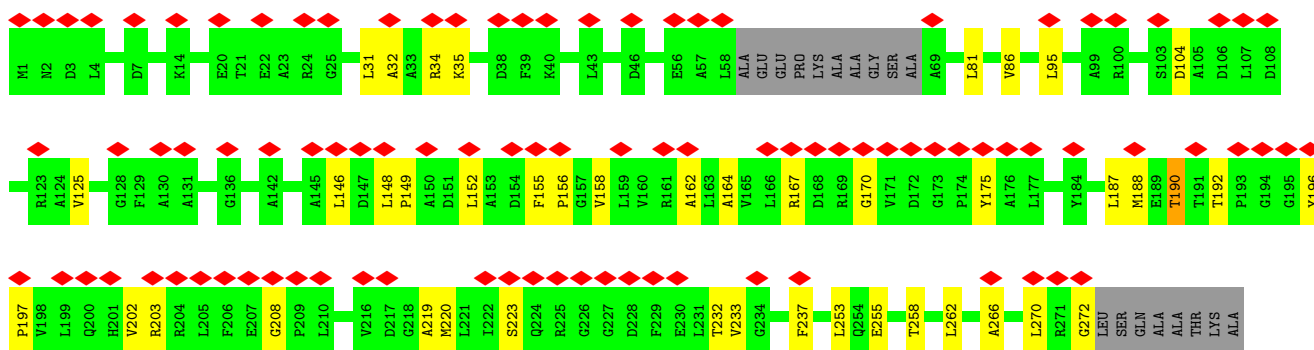
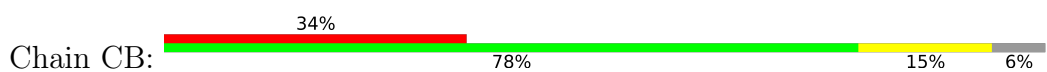
- Molecule 1: Type 1 encapsulin shell protein



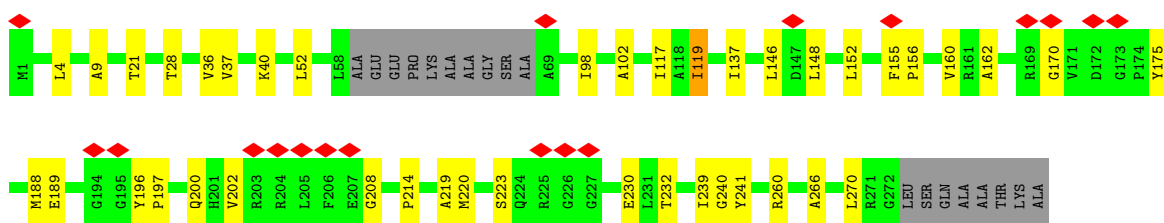
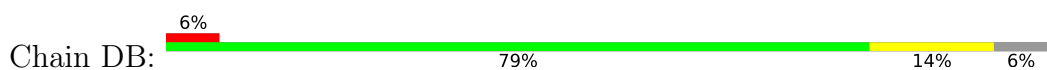
- Molecule 1: Type 1 encapsulin shell protein



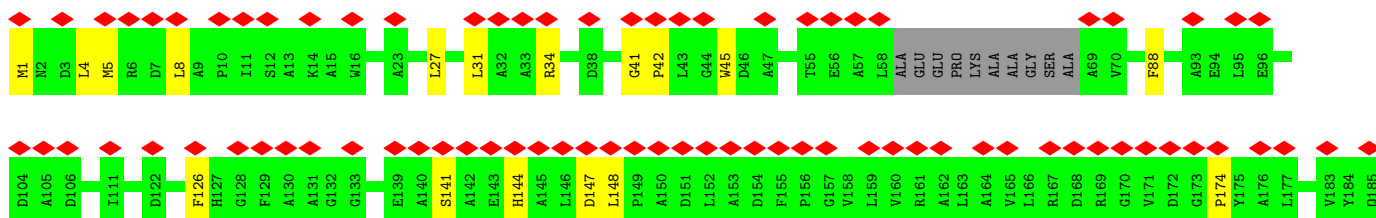
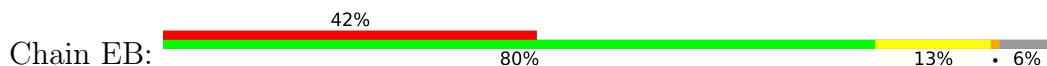
• Molecule 1: Type 1 encapsulin shell protein

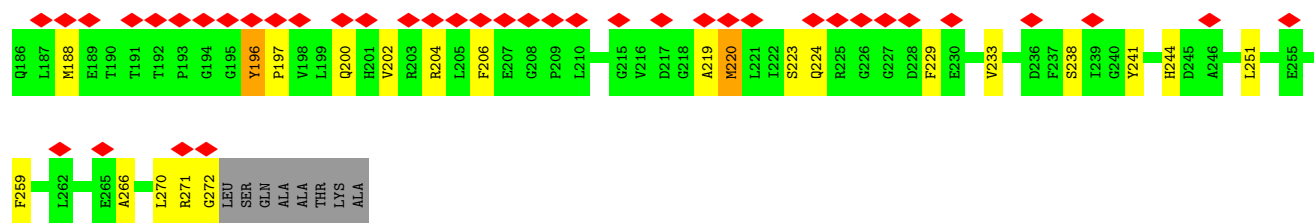


• Molecule 1: Type 1 encapsulin shell protein

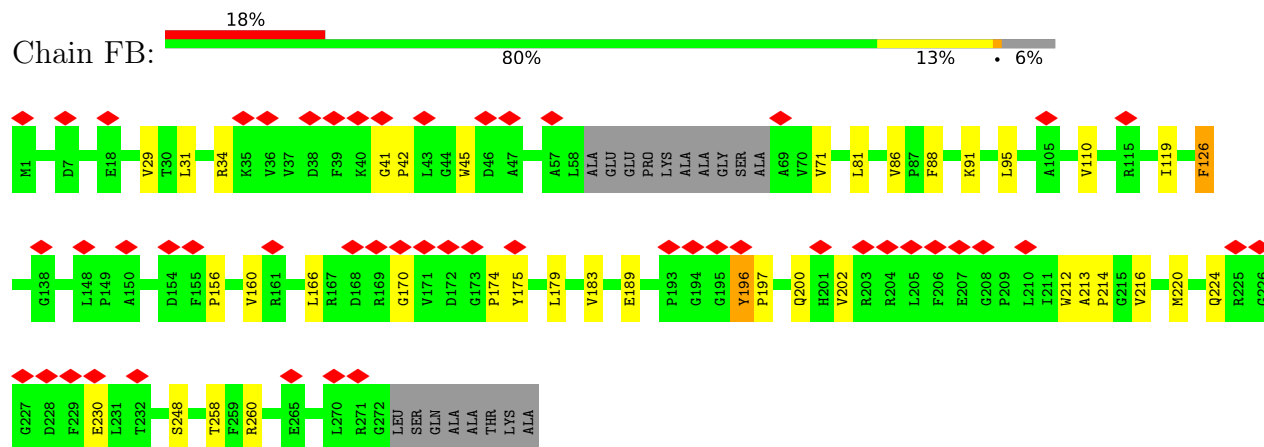


• Molecule 1: Type 1 encapsulin shell protein

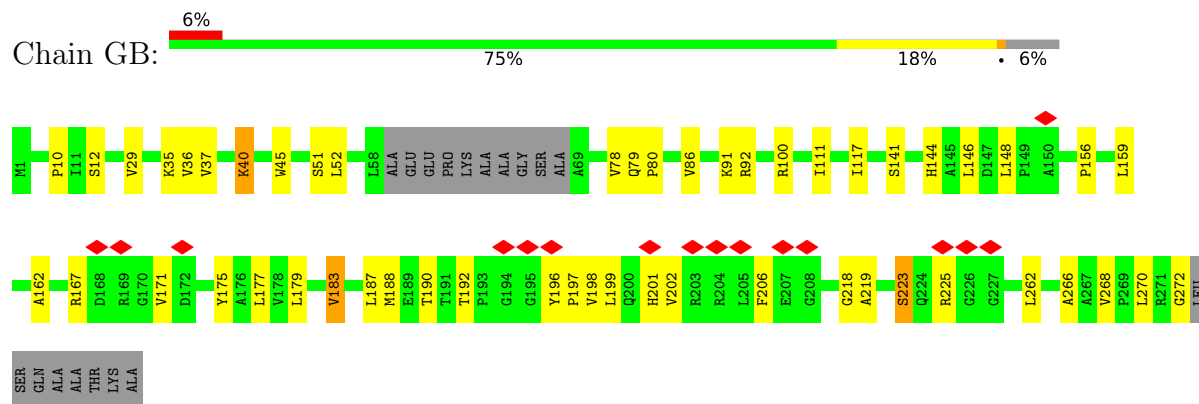




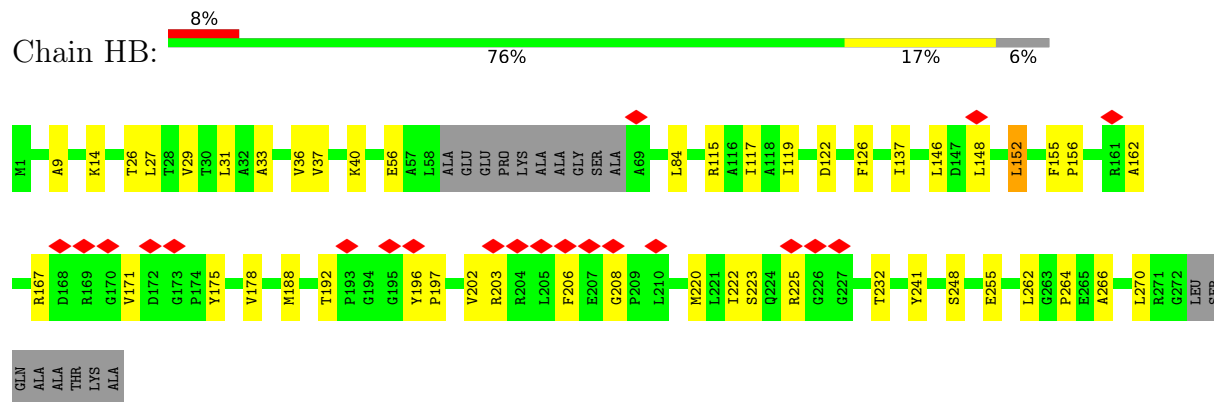
- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



- Molecule 1: Type 1 encapsulin shell protein



- Molecule 2: Encapsulated ferritin-like protein

Chain 1:  6% 94%

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

G121	G124	I125	G126	S127	L128	LYS	GLY	GLU	ALA	ALA	LEU	ALA	ARG	PRO	PRO	ARG	LEU
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- Molecule 2: Encapsulated ferritin-like protein

Chain 2:  5% 94%

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

G121	S122	L123	G124	I125	G126	S127	L128	LYS	GLY	GLU	ALA	ALA	LEU	ALA	ARG	PRO	PRO	ARG	LEU
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- Molecule 2: Encapsulated ferritin-like protein

Chain 3:  5% 94%

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

G121	S122	L123	G124	I125	L128	LYS	GLY	GLU	ALA	ALA	LEU	ALA	ARG	PRO	PRO	ARG	LEU
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- Molecule 2: Encapsulated ferritin-like protein

Chain 4:  6% 94%

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

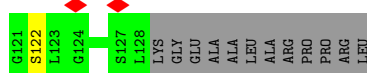
G121	S122	L123	G124	I125	G126	S127	L128	K129	GLY	GLU	ALA	ALA	LEU	ALA	ARG	PRO	PRO	ARG	LEU
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- Molecule 2: Encapsulated ferritin-like protein

Chain 5:  5% . 94%

MET ALA GLN SER SER SER THR HIS HIS PRO LEU LEU VAL LYS LYS GLU THR VAL ASN ARG HIS HIS ARG ARG ALA ILE VAL VAL SER VAL MET MET GLU GLU LEU LEU GLU

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

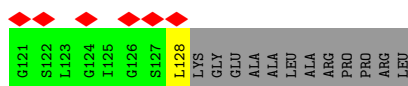
 G121 S122 L123 G124 I125 G126 S127 L128

- Molecule 2: Encapsulated ferritin-like protein

Chain 6:  5% . 94%

MET ALA GLN SER SER SER THR HIS HIS PRO LEU LEU VAL LYS LYS GLU THR VAL ASN ARG HIS HIS ARG ARG ALA ILE VAL VAL SER VAL MET MET GLU GLU LEU LEU GLU

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

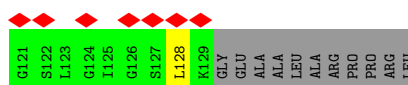
 G121 S122 L123 G124 I125 G126 S127 L128

- Molecule 2: Encapsulated ferritin-like protein

Chain 7:  5% 6% . 94%

MET ALA GLN SER SER SER THR HIS HIS PRO LEU LEU VAL LYS LYS GLU THR VAL ASN ARG HIS HIS ARG ARG ALA ILE VAL VAL SER VAL MET MET GLU GLU LEU LEU GLU

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

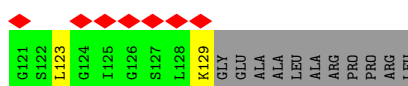
 G121 S122 L123 G124 I125 G126 S127 L128 K129

- Molecule 2: Encapsulated ferritin-like protein

Chain 8:  5% 5% . 94%

MET ALA GLN SER SER SER THR HIS HIS PRO LEU LEU VAL LYS LYS GLU THR VAL ASN ARG HIS HIS ARG ARG ALA ILE VAL VAL SER VAL MET MET GLU GLU LEU LEU GLU

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

 G121 S122 L123 G124 I125 G126 S127 L128 K129

- Molecule 2: Encapsulated ferritin-like protein

Chain 9:  6% 94%

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

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

 G121
 L128
LYS GLY ALA ALA ALA ALA ARG PRO ARG LEU

- Molecule 2: Encapsulated ferritin-like protein

Chain 10:  6% 5% 94%

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

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

 G121
 S122
 L123
 G124
 I125
 G126
 S127
 L128
 K129
GLY GLU ALA ALA LEU LEU ALA ALA PRO ARG LEU

- Molecule 2: Encapsulated ferritin-like protein

Chain 11:  5% 5% 94%

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

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

 G121
 S122
 I126
 G126
 S127
 L128
LYS GLY GLU ALA ALA LEU LEU ALA ALA PRO ARG LEU

- Molecule 2: Encapsulated ferritin-like protein

Chain 12:  5% 5% 94%

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

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

 G121
 G124
 L128
LYS GLY GLU ALA ALA LEU LEU ALA ALA PRO ARG LEU

- Molecule 2: Encapsulated ferritin-like protein

[illegible][illegible][illegible][illegible]

Chain 17:  94%

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

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

 G121  G124  S127  L128 LYS GLY GLU ALA ALA LEU ARG ARG PRO PRO ARG ARG LEU

• Molecule 2: Encapsulated ferritin-like protein

Chain 18:  94%

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

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

 G121  S122  L123  G124  I125 LYS GLY GLU ALA ALA LEU ARG ARG PRO PRO ARG ARG LEU

• Molecule 2: Encapsulated ferritin-like protein

Chain 19:  94%

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

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

 G121  S122  L123  G124  I125  S127  L128 LYS GLY GLU ALA ALA LEU ARG ARG PRO PRO ARG ARG LEU

• Molecule 2: Encapsulated ferritin-like protein

Chain 20:  94%

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

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

 G121  I125  G126  S127  L128 LYS GLY GLU ALA ALA LEU ARG ARG PRO PRO ARG ARG LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	41954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.425	Depositor
Minimum map value	-0.176	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	432.576, 432.576, 432.576	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1265, 1.1265, 1.1265	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.31	0/2013	0.71	2/2737 (0.1%)
1	A0	0.30	0/2013	0.71	2/2737 (0.1%)
1	AA	0.30	0/2013	0.72	2/2737 (0.1%)
1	AB	0.29	0/2013	0.69	2/2737 (0.1%)
1	B	0.30	0/2013	0.71	4/2737 (0.1%)
1	BA	0.30	0/2013	0.73	2/2737 (0.1%)
1	BB	0.28	0/2013	0.69	0/2737
1	C	0.29	0/2013	0.69	2/2737 (0.1%)
1	CA	0.29	0/2013	0.70	2/2737 (0.1%)
1	CB	0.28	0/2013	0.72	2/2737 (0.1%)
1	D	0.29	0/2013	0.70	2/2737 (0.1%)
1	DA	0.29	0/2013	0.71	2/2737 (0.1%)
1	DB	0.30	0/2013	0.70	2/2737 (0.1%)
1	E	0.29	0/2013	0.70	2/2737 (0.1%)
1	EA	0.29	0/2013	0.69	2/2737 (0.1%)
1	EB	0.28	0/2013	0.70	2/2737 (0.1%)
1	F	0.29	0/2013	0.70	2/2737 (0.1%)
1	FA	0.29	0/2013	0.69	2/2737 (0.1%)
1	FB	0.29	0/2013	0.70	2/2737 (0.1%)
1	G	0.30	0/2013	0.70	2/2737 (0.1%)
1	GA	0.29	0/2013	0.68	2/2737 (0.1%)
1	GB	0.30	0/2013	0.70	2/2737 (0.1%)
1	H	0.30	0/2013	0.70	2/2737 (0.1%)
1	HA	0.29	0/2013	0.72	2/2737 (0.1%)
1	HB	0.30	0/2013	0.70	2/2737 (0.1%)
1	I	0.31	0/2013	0.74	2/2737 (0.1%)
1	IA	0.30	0/2013	0.71	2/2737 (0.1%)
1	J	0.29	0/2013	0.69	2/2737 (0.1%)
1	JA	0.28	0/2013	0.69	2/2737 (0.1%)
1	K	0.29	0/2013	0.68	2/2737 (0.1%)
1	KA	0.29	0/2013	0.70	2/2737 (0.1%)
1	L	0.30	0/2013	0.69	2/2737 (0.1%)
1	LA	0.31	0/2013	0.71	2/2737 (0.1%)
1	M	0.30	0/2013	0.69	2/2737 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	MA	0.29	0/2013	0.69	2/2737 (0.1%)
1	N	0.30	0/2013	0.69	2/2737 (0.1%)
1	NA	0.29	0/2013	0.70	2/2737 (0.1%)
1	O	0.30	0/2013	0.70	2/2737 (0.1%)
1	OA	0.29	0/2013	0.70	2/2737 (0.1%)
1	P	0.29	0/2013	0.70	2/2737 (0.1%)
1	PA	0.29	0/2013	0.69	2/2737 (0.1%)
1	Q	0.29	0/2013	0.68	2/2737 (0.1%)
1	QA	0.30	0/2013	0.71	2/2737 (0.1%)
1	R	0.29	0/2013	0.70	2/2737 (0.1%)
1	RA	0.29	0/2013	0.70	2/2737 (0.1%)
1	S	0.30	0/2013	0.69	2/2737 (0.1%)
1	SA	0.29	0/2013	0.72	4/2737 (0.1%)
1	T	0.29	0/2013	0.70	2/2737 (0.1%)
1	TA	0.29	0/2013	0.71	2/2737 (0.1%)
1	UA	0.29	0/2013	0.71	2/2737 (0.1%)
1	V	0.29	0/2013	0.70	2/2737 (0.1%)
1	VA	0.29	0/2013	0.69	0/2737
1	W	0.28	0/2013	0.69	2/2737 (0.1%)
1	WA	0.28	0/2013	0.68	0/2737
1	X	0.30	0/2013	0.69	2/2737 (0.1%)
1	XA	0.29	0/2013	0.70	2/2737 (0.1%)
1	Y	0.30	0/2013	0.71	2/2737 (0.1%)
1	YA	0.30	0/2013	0.71	2/2737 (0.1%)
1	Z	0.29	0/2013	0.68	2/2737 (0.1%)
1	ZA	0.30	0/2013	0.71	2/2737 (0.1%)
2	1	0.26	0/47	0.59	0/61
2	10	0.33	0/56	0.70	0/72
2	11	0.18	0/47	0.54	0/61
2	12	0.24	0/47	0.56	0/61
2	13	0.24	0/47	0.57	0/61
2	14	0.29	0/47	0.78	0/61
2	15	0.21	0/47	0.59	0/61
2	16	0.28	0/47	0.71	0/61
2	17	0.26	0/47	0.55	0/61
2	18	0.24	0/47	0.49	0/61
2	19	0.37	0/47	0.57	0/61
2	2	0.22	0/47	0.54	0/61
2	20	0.28	0/47	0.63	0/61
2	3	0.24	0/47	0.60	0/61
2	4	0.22	0/56	0.58	0/72
2	5	0.24	0/47	0.69	0/61
2	6	0.26	0/47	0.54	0/61

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	7	0.29	0/56	0.66	0/72
2	8	0.21	0/56	0.53	0/72
2	9	0.23	0/47	0.48	0/61
All	All	0.29	0/121756	0.70	118/165484 (0.1%)

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	196	TYR	CA-C-N	7.02	128.61	119.84
1	P	196	TYR	C-N-CA	7.02	128.61	119.84
1	J	196	TYR	CA-C-N	6.78	128.31	119.84
1	J	196	TYR	C-N-CA	6.78	128.31	119.84
1	L	196	TYR	CA-C-N	6.62	128.12	119.84
1	L	196	TYR	C-N-CA	6.62	128.12	119.84
1	R	196	TYR	CA-C-N	6.58	128.06	119.84
1	R	196	TYR	C-N-CA	6.58	128.06	119.84
1	OA	196	TYR	CA-C-N	6.54	128.02	119.84
1	OA	196	TYR	C-N-CA	6.54	128.02	119.84
1	AA	196	TYR	CA-C-N	6.44	127.89	119.84
1	AA	196	TYR	C-N-CA	6.44	127.89	119.84
1	IA	196	TYR	CA-C-N	6.43	127.88	119.84
1	IA	196	TYR	C-N-CA	6.43	127.88	119.84
1	A	196	TYR	CA-C-N	6.34	127.76	119.84
1	A	196	TYR	C-N-CA	6.34	127.76	119.84
1	MA	196	TYR	CA-C-N	6.31	127.73	119.84
1	MA	196	TYR	C-N-CA	6.31	127.73	119.84
1	I	196	TYR	CA-C-N	6.29	127.71	119.84
1	I	196	TYR	C-N-CA	6.29	127.71	119.84
1	GB	196	TYR	CA-C-N	6.23	127.63	119.84
1	GB	196	TYR	C-N-CA	6.23	127.63	119.84
1	AB	196	TYR	CA-C-N	6.20	127.59	119.84
1	AB	196	TYR	C-N-CA	6.20	127.59	119.84
1	CB	196	TYR	CA-C-N	6.20	127.59	119.84
1	CB	196	TYR	C-N-CA	6.20	127.59	119.84
1	RA	196	TYR	CA-C-N	6.19	127.57	119.84
1	RA	196	TYR	C-N-CA	6.19	127.57	119.84
1	ZA	196	TYR	CA-C-N	6.17	127.55	119.84
1	ZA	196	TYR	C-N-CA	6.17	127.55	119.84
1	EB	196	TYR	CA-C-N	6.12	127.49	119.84
1	EB	196	TYR	C-N-CA	6.12	127.49	119.84
1	DB	196	TYR	CA-C-N	6.11	127.48	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DB	196	TYR	C-N-CA	6.11	127.48	119.84
1	FB	196	TYR	CA-C-N	6.11	127.48	119.84
1	FB	196	TYR	C-N-CA	6.11	127.48	119.84
1	UA	196	TYR	CA-C-N	6.07	127.43	119.84
1	UA	196	TYR	C-N-CA	6.07	127.43	119.84
1	BA	196	TYR	CA-C-N	6.06	127.42	119.84
1	BA	196	TYR	C-N-CA	6.06	127.42	119.84
1	JA	196	TYR	CA-C-N	5.99	127.33	119.84
1	JA	196	TYR	C-N-CA	5.99	127.33	119.84
1	XA	196	TYR	CA-C-N	5.99	127.32	119.84
1	XA	196	TYR	C-N-CA	5.99	127.32	119.84
1	Y	196	TYR	CA-C-N	5.96	127.29	119.84
1	Y	196	TYR	C-N-CA	5.96	127.29	119.84
1	SA	196	TYR	CA-C-N	5.96	127.28	119.84
1	SA	196	TYR	C-N-CA	5.96	127.28	119.84
1	B	196	TYR	CA-C-N	5.95	127.28	119.84
1	B	196	TYR	C-N-CA	5.95	127.28	119.84
1	A0	196	TYR	CA-C-N	5.94	127.26	119.84
1	A0	196	TYR	C-N-CA	5.94	127.26	119.84
1	N	196	TYR	CA-C-N	5.93	127.25	119.84
1	N	196	TYR	C-N-CA	5.93	127.25	119.84
1	E	196	TYR	CA-C-N	5.92	127.24	119.84
1	E	196	TYR	C-N-CA	5.92	127.24	119.84
1	H	196	TYR	CA-C-N	5.92	127.24	119.84
1	H	196	TYR	C-N-CA	5.92	127.24	119.84
1	Q	196	TYR	CA-C-N	5.90	127.21	119.84
1	Q	196	TYR	C-N-CA	5.90	127.21	119.84
1	F	196	TYR	CA-C-N	5.83	127.13	119.84
1	F	196	TYR	C-N-CA	5.83	127.13	119.84
1	CA	196	TYR	CA-C-N	5.82	127.12	119.84
1	CA	196	TYR	C-N-CA	5.82	127.12	119.84
1	M	196	TYR	CA-C-N	5.77	127.05	119.84
1	M	196	TYR	C-N-CA	5.77	127.05	119.84
1	LA	196	TYR	CA-C-N	5.77	127.05	119.84
1	LA	196	TYR	C-N-CA	5.77	127.05	119.84
1	NA	196	TYR	CA-C-N	5.76	127.04	119.84
1	NA	196	TYR	C-N-CA	5.76	127.04	119.84
1	K	196	TYR	CA-C-N	5.74	127.02	119.84
1	K	196	TYR	C-N-CA	5.74	127.02	119.84
1	DA	196	TYR	CA-C-N	5.72	126.99	119.84
1	DA	196	TYR	C-N-CA	5.72	126.99	119.84
1	KA	196	TYR	CA-C-N	5.72	126.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	KA	196	TYR	C-N-CA	5.72	126.99	119.84
1	YA	196	TYR	CA-C-N	5.65	126.91	119.84
1	YA	196	TYR	C-N-CA	5.65	126.91	119.84
1	X	196	TYR	CA-C-N	5.59	126.82	119.84
1	X	196	TYR	C-N-CA	5.59	126.82	119.84
1	S	196	TYR	CA-C-N	5.56	126.79	119.84
1	S	196	TYR	C-N-CA	5.56	126.79	119.84
1	O	196	TYR	CA-C-N	5.55	126.78	119.84
1	O	196	TYR	C-N-CA	5.55	126.78	119.84
1	GA	196	TYR	CA-C-N	5.55	126.78	119.84
1	GA	196	TYR	C-N-CA	5.55	126.78	119.84
1	SA	79	GLN	CA-C-N	5.46	125.36	119.85
1	SA	79	GLN	C-N-CA	5.46	125.36	119.85
1	W	196	TYR	CA-C-N	5.46	126.66	119.84
1	W	196	TYR	C-N-CA	5.46	126.66	119.84
1	FA	196	TYR	CA-C-N	5.42	126.62	119.84
1	FA	196	TYR	C-N-CA	5.42	126.62	119.84
1	D	196	TYR	CA-C-N	5.41	126.60	119.84
1	D	196	TYR	C-N-CA	5.41	126.60	119.84
1	Z	196	TYR	CA-C-N	5.40	126.59	119.84
1	Z	196	TYR	C-N-CA	5.40	126.59	119.84
1	HB	196	TYR	CA-C-N	5.36	126.54	119.84
1	HB	196	TYR	C-N-CA	5.36	126.54	119.84
1	TA	196	TYR	CA-C-N	5.35	126.53	119.84
1	TA	196	TYR	C-N-CA	5.35	126.53	119.84
1	HA	196	TYR	CA-C-N	5.30	126.46	119.84
1	HA	196	TYR	C-N-CA	5.30	126.46	119.84
1	T	196	TYR	CA-C-N	5.28	126.44	119.84
1	T	196	TYR	C-N-CA	5.28	126.44	119.84
1	V	196	TYR	CA-C-N	5.24	126.39	119.84
1	V	196	TYR	C-N-CA	5.24	126.39	119.84
1	B	208	GLY	CA-C-N	5.21	125.11	119.85
1	B	208	GLY	C-N-CA	5.21	125.11	119.85
1	QA	196	TYR	CA-C-N	5.17	126.30	119.84
1	QA	196	TYR	C-N-CA	5.17	126.30	119.84
1	EA	196	TYR	CA-C-N	5.12	126.24	119.84
1	EA	196	TYR	C-N-CA	5.12	126.24	119.84
1	C	196	TYR	CA-C-N	5.07	126.18	119.84
1	C	196	TYR	C-N-CA	5.07	126.18	119.84
1	PA	196	TYR	CA-C-N	5.06	126.17	119.84
1	PA	196	TYR	C-N-CA	5.06	126.17	119.84
1	G	196	TYR	CA-C-N	5.00	126.09	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	TYR	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1975	0	1984	30	0
1	A0	1975	0	1984	30	0
1	AA	1975	0	1984	28	0
1	AB	1975	0	1984	27	0
1	B	1975	0	1984	29	0
1	BA	1975	0	1984	28	0
1	BB	1975	0	1984	35	0
1	C	1975	0	1984	24	0
1	CA	1975	0	1984	30	0
1	CB	1975	0	1984	27	0
1	D	1975	0	1984	24	0
1	DA	1975	0	1984	26	0
1	DB	1975	0	1984	23	0
1	E	1975	0	1984	29	0
1	EA	1975	0	1984	22	0
1	EB	1975	0	1984	24	0
1	F	1975	0	1984	33	0
1	FA	1975	0	1984	17	0
1	FB	1975	0	1984	21	0
1	G	1975	0	1984	24	0
1	GA	1975	0	1984	17	0
1	GB	1975	0	1984	30	0
1	H	1975	0	1984	25	0
1	HA	1975	0	1984	23	0
1	HB	1975	0	1984	27	0
1	I	1975	0	1984	40	0
1	IA	1975	0	1984	35	0
1	J	1975	0	1984	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JA	1975	0	1984	33	0
1	K	1975	0	1984	33	0
1	KA	1975	0	1984	34	0
1	L	1975	0	1984	32	0
1	LA	1975	0	1984	28	0
1	M	1975	0	1984	26	0
1	MA	1975	0	1984	28	0
1	N	1975	0	1984	38	0
1	NA	1975	0	1984	23	0
1	O	1975	0	1984	28	0
1	OA	1975	0	1984	29	0
1	P	1975	0	1984	40	0
1	PA	1975	0	1984	22	0
1	Q	1975	0	1984	22	0
1	QA	1975	0	1984	18	0
1	R	1975	0	1984	37	0
1	RA	1975	0	1984	30	0
1	S	1975	0	1984	30	0
1	SA	1975	0	1984	21	0
1	T	1975	0	1984	31	0
1	TA	1975	0	1984	26	0
1	UA	1975	0	1984	31	0
1	V	1975	0	1984	26	0
1	VA	1975	0	1984	24	0
1	W	1975	0	1984	31	0
1	WA	1975	0	1984	23	0
1	X	1975	0	1984	36	0
1	XA	1975	0	1984	20	0
1	Y	1975	0	1984	30	0
1	YA	1975	0	1984	32	0
1	Z	1975	0	1984	30	0
1	ZA	1975	0	1984	30	0
2	1	48	0	51	0	0
2	10	57	0	64	1	0
2	11	48	0	51	1	0
2	12	48	0	51	1	0
2	13	48	0	51	0	0
2	14	48	0	51	1	0
2	15	48	0	51	0	0
2	16	48	0	51	2	0
2	17	48	0	51	1	0
2	18	48	0	51	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	19	48	0	51	1	0
2	2	48	0	51	1	0
2	20	48	0	51	0	0
2	3	48	0	51	1	0
2	4	57	0	64	1	0
2	5	48	0	51	0	0
2	6	48	0	51	1	0
2	7	57	0	64	1	0
2	8	57	0	64	2	0
2	9	48	0	51	0	0
All	All	119496	0	120112	1581	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 (1581) 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:I:91:LYS:HZ2	1:I:92:ARG:H	1.24	0.81
1:HA:199:LEU:HB2	1:KA:204:ARG:HH12	1.49	0.78
1:AB:171:VAL:HG22	1:AB:225:ARG:HE	1.50	0.77
1:B:119:ILE:HD11	1:B:215:GLY:HA3	1.68	0.75
1:R:91:LYS:HE3	1:R:91:LYS:HA	1.67	0.75
1:T:171:VAL:HG22	1:T:225:ARG:HE	1.50	0.75
1:HB:40:LYS:HD2	1:HB:232:THR:HG22	1.69	0.75
1:O:5:MET:HE3	1:O:5:MET:HA	1.71	0.72
1:WA:171:VAL:HA	1:WA:225:ARG:HH21	1.54	0.72
1:ZA:171:VAL:HG22	1:ZA:225:ARG:HE	1.55	0.71
1:EB:1:MET:HE2	1:EB:5:MET:HE3	1.74	0.70
1:I:5:MET:HE2	1:I:8:LEU:HD13	1.75	0.69
1:MA:162:ALA:HB1	1:MA:268:VAL:HG11	1.75	0.69
1:ZA:203:ARG:HH12	1:ZA:208:GLY:H	1.39	0.69
1:F:233:VAL:HG23	1:F:257:MET:HB3	1.75	0.68
1:KA:92:ARG:HA	1:KA:95:LEU:HD12	1.75	0.68
1:GA:51:SER:HA	1:GA:78:VAL:HG12	1.75	0.68
1:AA:171:VAL:HG13	1:AA:225:ARG:HE	1.59	0.67
1:YA:146:LEU:HD11	1:YA:162:ALA:HB2	1.76	0.67
1:PA:225:ARG:HH12	1:PA:228:ASP:HB2	1.57	0.67
1:EB:147:ASP:HA	1:EB:271:ARG:HB2	1.77	0.67
1:N:148:LEU:HD22	1:N:272:GLY:HA2	1.77	0.67
1:HA:5:MET:HE3	1:HA:5:MET:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WA:171:VAL:HG13	1:WA:225:ARG:HE	1.59	0.67
1:W:188:MET:HE2	1:W:188:MET:HA	1.77	0.66
1:BA:40:LYS:HD2	1:BA:232:THR:HG22	1.77	0.66
1:MA:156:PRO:HG3	1:MA:202:VAL:HG12	1.76	0.66
1:SA:81:LEU:HG	1:SA:258:THR:HB	1.77	0.66
1:PA:40:LYS:HD2	1:PA:232:THR:HG22	1.76	0.66
1:L:40:LYS:HZ1	1:L:231:LEU:H	1.44	0.66
1:DA:156:PRO:HG3	1:DA:202:VAL:HG12	1.77	0.66
1:ZA:219:ALA:HB3	1:ZA:270:LEU:HD23	1.76	0.66
1:VA:32:ALA:HA	1:VA:35:LYS:HZ3	1.60	0.66
1:IA:219:ALA:HB3	1:IA:270:LEU:HD23	1.78	0.65
1:G:188:MET:HE3	1:G:188:MET:HA	1.79	0.65
1:Y:29:VAL:HG11	1:RA:170:GLY:HA2	1.78	0.65
1:B:219:ALA:HB3	1:B:270:LEU:HD23	1.79	0.65
1:G:148:LEU:HD13	1:G:272:GLY:HA2	1.76	0.65
1:Z:156:PRO:HG3	1:Z:202:VAL:HG12	1.78	0.64
1:GA:219:ALA:HB3	1:GA:270:LEU:HD23	1.78	0.64
1:BA:48:SER:HB3	1:IA:76:ARG:HH11	1.62	0.64
1:GA:171:VAL:HG22	1:GA:225:ARG:HE	1.63	0.64
1:CA:13:ALA:HB2	1:JA:1:MET:HB3	1.78	0.64
1:CA:152:LEU:HG	1:CA:187:LEU:HD12	1.80	0.64
1:KA:203:ARG:HH12	1:KA:208:GLY:H	1.46	0.64
1:A0:197:PRO:HG2	1:A0:200:GLN:HE22	1.61	0.64
1:S:167:ARG:HH22	1:FB:29:VAL:HG22	1.63	0.64
1:BA:156:PRO:HG3	1:BA:202:VAL:HG12	1.79	0.64
1:F:175:TYR:HB2	1:F:206:PHE:HE1	1.61	0.64
1:GA:156:PRO:HG3	1:GA:202:VAL:HG12	1.79	0.64
1:IA:188:MET:HE3	1:IA:188:MET:HA	1.80	0.63
1:EB:31:LEU:HD21	1:EB:34:ARG:HG3	1.79	0.63
1:A:29:VAL:HG11	1:TA:170:GLY:HA2	1.79	0.63
1:D:156:PRO:HG3	1:D:202:VAL:HG12	1.80	0.63
1:I:179:LEU:HD23	1:I:183:VAL:HG12	1.81	0.63
1:K:156:PRO:HG3	1:K:202:VAL:HG12	1.81	0.63
1:TA:51:SER:HA	1:TA:78:VAL:HG12	1.79	0.63
1:KA:51:SER:HA	1:KA:78:VAL:HG12	1.80	0.63
1:E:17:ALA:O	1:E:21:THR:HG23	1.99	0.63
1:UA:5:MET:HE3	1:UA:5:MET:HA	1.81	0.63
1:GA:162:ALA:HB1	1:GA:268:VAL:HG11	1.80	0.62
1:RA:51:SER:HA	1:RA:78:VAL:HG12	1.80	0.62
1:B:1:MET:HE1	1:B:8:LEU:HG	1.79	0.62
1:F:223:SER:HB3	1:F:266:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:148:LEU:HD22	1:L:272:GLY:HA2	1.80	0.62
1:AB:148:LEU:HD22	1:AB:272:GLY:HA2	1.79	0.62
1:DA:162:ALA:HB1	1:DA:268:VAL:HG11	1.81	0.62
1:I:19:ILE:HD11	1:I:110:VAL:HG21	1.80	0.62
1:J:156:PRO:HG3	1:J:202:VAL:HG12	1.81	0.62
1:XA:156:PRO:HG3	1:XA:202:VAL:HG12	1.81	0.62
1:DA:163:LEU:HD23	1:DA:167:ARG:HH11	1.65	0.62
1:YA:51:SER:HA	1:YA:78:VAL:HG12	1.81	0.62
1:ZA:35:LYS:HE3	1:ZA:35:LYS:HA	1.82	0.62
1:BB:156:PRO:HG3	1:BB:202:VAL:HG12	1.81	0.62
1:V:219:ALA:HB3	1:V:270:LEU:HD23	1.82	0.62
1:DA:219:ALA:HB3	1:DA:270:LEU:HD23	1.82	0.62
1:YA:188:MET:HA	1:YA:188:MET:HE3	1.82	0.62
1:LA:164:ALA:HA	1:LA:167:ARG:HE	1.65	0.62
1:GB:171:VAL:HG13	1:GB:225:ARG:HE	1.65	0.61
1:A0:40:LYS:HD2	1:A0:232:THR:HG22	1.82	0.61
1:L:197:PRO:HG2	1:L:200:GLN:HE22	1.65	0.61
1:Y:92:ARG:HA	1:Y:95:LEU:HD23	1.82	0.61
1:YA:134:ILE:HD11	1:YA:259:PHE:H	1.65	0.61
1:A0:162:ALA:HB1	1:A0:268:VAL:HG11	1.83	0.61
1:VA:35:LYS:N	1:VA:35:LYS:HD3	2.14	0.61
1:BA:192:THR:HG21	1:BA:197:PRO:HA	1.83	0.61
1:A0:51:SER:HA	1:A0:78:VAL:HG12	1.81	0.61
1:CA:223:SER:HB3	1:CA:266:ALA:HB1	1.83	0.61
1:D:51:SER:HA	1:D:78:VAL:HG12	1.82	0.61
1:GA:223:SER:HB3	1:GA:266:ALA:HB1	1.83	0.61
1:F:58:LEU:HB2	1:F:73:VAL:HG23	1.82	0.60
1:Z:119:ILE:HD11	1:Z:214:PRO:HB2	1.81	0.60
1:GA:34:ARG:HB2	2:6:128:LEU:HD23	1.83	0.60
1:RA:203:ARG:HH12	1:RA:208:GLY:H	1.50	0.60
1:YA:219:ALA:HB3	1:YA:270:LEU:HD23	1.84	0.60
1:A0:204:ARG:H	1:A0:204:ARG:HD2	1.65	0.60
1:TA:24:ARG:HG3	2:16:125:ILE:HD11	1.83	0.60
1:I:5:MET:HE3	1:I:5:MET:HA	1.83	0.60
1:R:137:ILE:HD11	1:R:220:MET:HG3	1.82	0.60
1:B:225:ARG:HH21	1:B:266:ALA:HB2	1.67	0.60
1:M:1:MET:HE3	1:M:5:MET:HG2	1.84	0.60
1:NA:49:SER:HA	1:NA:81:LEU:HD13	1.82	0.60
1:D:19:ILE:HD11	1:D:110:VAL:HG21	1.83	0.59
1:TA:48:SER:HB3	1:ZA:76:ARG:HH11	1.66	0.59
1:P:156:PRO:HG3	1:P:202:VAL:HG12	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:162:ALA:HB1	1:JA:268:VAL:HG11	1.82	0.59
1:A:198:VAL:HA	1:A:201:HIS:HB3	1.85	0.59
1:E:223:SER:HB3	1:E:266:ALA:HB1	1.83	0.59
1:N:34:ARG:HH12	1:N:237:PHE:HE2	1.49	0.59
1:Q:220:MET:HG2	1:Q:269:PRO:HA	1.85	0.59
1:EB:141:SER:HB3	1:EB:144:HIS:HE1	1.68	0.59
1:F:197:PRO:HG2	1:F:200:GLN:HE22	1.67	0.59
1:I:223:SER:HB3	1:I:266:ALA:HB1	1.82	0.59
1:Y:171:VAL:HG13	1:Y:225:ARG:HE	1.68	0.59
1:TA:31:LEU:HD21	1:TA:34:ARG:HG3	1.85	0.59
1:EB:1:MET:HE1	1:EB:8:LEU:HG	1.83	0.59
1:F:51:SER:HA	1:F:78:VAL:HG12	1.83	0.59
1:M:29:VAL:HG11	1:P:170:GLY:HA2	1.84	0.59
1:O:223:SER:HB3	1:O:266:ALA:HB1	1.85	0.59
1:HA:51:SER:HA	1:HA:78:VAL:HG12	1.84	0.59
1:M:119:ILE:HD11	1:M:214:PRO:HB2	1.84	0.59
1:S:179:LEU:HD23	1:S:183:VAL:HG23	1.84	0.59
1:LA:223:SER:HB3	1:LA:266:ALA:HB1	1.85	0.59
1:MA:31:LEU:HD21	1:MA:34:ARG:HG3	1.82	0.59
1:DB:223:SER:HB3	1:DB:266:ALA:HB1	1.84	0.59
1:FB:31:LEU:HD21	1:FB:34:ARG:HG3	1.83	0.59
1:I:91:LYS:HZ2	1:I:92:ARG:N	1.99	0.59
1:O:148:LEU:HA	1:O:270:LEU:HD11	1.84	0.59
1:R:163:LEU:HD23	1:R:167:ARG:HD2	1.85	0.59
1:V:75:LYS:HD2	1:JA:80:PRO:HB2	1.85	0.59
1:C:119:ILE:HD11	1:C:215:GLY:HA3	1.84	0.58
1:GB:156:PRO:HG3	1:GB:202:VAL:HG12	1.85	0.58
1:S:163:LEU:O	1:S:167:ARG:HG2	2.03	0.58
1:T:197:PRO:HG2	1:T:200:GLN:HE22	1.67	0.58
1:T:16:TRP:HA	1:T:19:ILE:HD12	1.83	0.58
1:EA:205:LEU:H	1:EA:205:LEU:HD23	1.68	0.58
1:SA:162:ALA:HB1	1:SA:268:VAL:HG11	1.85	0.58
1:AB:241:TYR:HE1	1:AB:244:HIS:HB3	1.68	0.58
1:CA:51:SER:HA	1:CA:78:VAL:HG12	1.86	0.58
1:P:197:PRO:HG2	1:P:200:GLN:HE22	1.68	0.58
1:JA:197:PRO:HG2	1:JA:200:GLN:HE22	1.68	0.58
1:OA:198:VAL:HA	1:OA:201:HIS:HB3	1.86	0.58
1:UA:223:SER:HB3	1:UA:266:ALA:HB1	1.85	0.58
1:GB:179:LEU:HD21	1:GB:187:LEU:HD13	1.85	0.58
1:Z:179:LEU:HD23	1:Z:184:TYR:HD1	1.68	0.58
1:T:145:ALA:HA	1:T:269:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:RA:179:LEU:HD23	1:RA:184:TYR:HD1	1.68	0.58
1:D:188:MET:HB3	1:X:160:VAL:HG21	1.84	0.58
1:G:51:SER:HA	1:G:78:VAL:HG12	1.86	0.58
1:H:188:MET:HE2	1:H:188:MET:HA	1.86	0.58
1:R:141:SER:HB3	1:R:144:HIS:HE1	1.69	0.58
1:Q:170:GLY:HA2	1:Z:29:VAL:HG11	1.86	0.58
1:I:45:TRP:HE1	1:JA:100:ARG:HG2	1.69	0.57
1:I:187:LEU:O	1:I:190:THR:HG23	2.04	0.57
1:K:37:VAL:HG12	1:K:229:PHE:HB3	1.86	0.57
1:P:198:VAL:HA	1:P:201:HIS:HB3	1.86	0.57
1:J:178:VAL:HG22	1:J:220:MET:HB2	1.86	0.57
1:T:170:GLY:HA2	1:ZA:29:VAL:HG11	1.86	0.57
1:AB:156:PRO:HG3	1:AB:202:VAL:HG12	1.86	0.57
1:X:198:VAL:HA	1:X:201:HIS:HB3	1.86	0.57
1:RA:162:ALA:HB1	1:RA:268:VAL:HG11	1.84	0.57
1:FB:126:PHE:HD2	1:FB:216:VAL:HG11	1.69	0.57
1:MA:219:ALA:HB3	1:MA:270:LEU:HD23	1.85	0.57
1:SA:179:LEU:HD23	1:SA:183:VAL:HG23	1.86	0.57
1:UA:31:LEU:HD21	1:UA:34:ARG:HG3	1.86	0.57
1:X:34:ARG:HH22	1:X:237:PHE:HE2	1.50	0.57
1:AA:164:ALA:HA	1:AA:167:ARG:HD3	1.87	0.57
1:DA:171:VAL:HG13	1:DA:225:ARG:HD3	1.86	0.57
1:TA:204:ARG:H	1:TA:204:ARG:HD2	1.69	0.57
1:G:48:SER:HB3	1:N:76:ARG:HH11	1.70	0.57
1:Z:51:SER:HA	1:Z:78:VAL:HG12	1.86	0.57
1:NA:241:TYR:HE1	1:NA:244:HIS:HB3	1.69	0.57
1:I:141:SER:HB3	1:I:144:HIS:HE1	1.69	0.57
1:AA:197:PRO:HG2	1:AA:200:GLN:HE22	1.69	0.57
1:CA:177:LEU:HD11	1:CA:219:ALA:HB1	1.87	0.57
1:B:244:HIS:HB2	1:B:249:VAL:HG12	1.87	0.57
1:V:162:ALA:HB1	1:V:268:VAL:HG11	1.86	0.57
1:PA:156:PRO:HG3	1:PA:202:VAL:HG12	1.86	0.57
1:ZA:148:LEU:HD13	1:ZA:272:GLY:HA2	1.86	0.57
1:T:1:MET:HE1	1:T:7:ASP:HB2	1.87	0.57
1:W:26:THR:HG21	1:W:111:ILE:HG22	1.87	0.57
1:AB:223:SER:HB3	1:AB:266:ALA:HB1	1.87	0.57
1:CB:146:LEU:HD11	1:CB:162:ALA:HB2	1.87	0.57
1:I:10:PRO:HA	1:CA:5:MET:HE1	1.87	0.57
1:P:37:VAL:HG12	1:P:229:PHE:HB3	1.85	0.56
1:X:179:LEU:HD22	1:X:184:TYR:HD1	1.70	0.56
1:GA:29:VAL:HG11	1:XA:170:GLY:HA2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:146:LEU:HD11	1:BB:162:ALA:HB2	1.85	0.56
1:F:188:MET:HA	1:F:188:MET:HE3	1.87	0.56
1:Z:177:LEU:HD11	1:Z:219:ALA:HB1	1.87	0.56
1:HB:156:PRO:HG3	1:HB:202:VAL:HG12	1.86	0.56
1:A:188:MET:HE2	1:A:188:MET:HA	1.86	0.56
1:N:40:LYS:HE2	1:N:40:LYS:HA	1.87	0.56
1:S:51:SER:HA	1:S:78:VAL:HG12	1.87	0.56
1:CA:192:THR:HG21	1:CA:197:PRO:HA	1.87	0.56
1:JA:175:TYR:HB2	1:JA:206:PHE:HE1	1.70	0.56
1:XA:51:SER:HA	1:XA:78:VAL:HG12	1.87	0.56
1:A0:219:ALA:HB3	1:A0:270:LEU:HD23	1.88	0.56
1:O:148:LEU:HD13	1:O:272:GLY:HA2	1.88	0.56
1:DA:8:LEU:HD22	1:DA:241:TYR:HE2	1.71	0.56
1:IA:58:LEU:HB2	1:IA:73:VAL:HG23	1.86	0.56
1:YA:148:LEU:HD22	1:YA:272:GLY:HA2	1.88	0.56
1:B:231:LEU:HD12	1:B:259:PHE:HB2	1.88	0.56
1:MA:51:SER:HA	1:MA:78:VAL:HG12	1.87	0.56
1:H:223:SER:HB3	1:H:266:ALA:HB1	1.88	0.56
1:M:188:MET:HE3	1:M:188:MET:HA	1.87	0.56
1:P:192:THR:HG21	1:P:197:PRO:HA	1.88	0.56
1:Z:262:LEU:HD12	1:PA:104:ASP:HB3	1.88	0.56
1:JA:203:ARG:HH22	1:JA:208:GLY:H	1.54	0.56
1:FB:220:MET:HE2	1:FB:220:MET:N	2.20	0.56
1:S:197:PRO:HG2	1:S:200:GLN:HE22	1.71	0.56
1:VA:241:TYR:HE1	1:VA:244:HIS:HB3	1.71	0.56
1:WA:205:LEU:HD23	1:WA:205:LEU:H	1.70	0.56
1:CB:188:MET:HE2	1:CB:188:MET:HA	1.87	0.56
1:DB:156:PRO:HG3	1:DB:202:VAL:HG12	1.88	0.56
1:F:171:VAL:HG13	1:F:225:ARG:HE	1.70	0.56
1:Z:220:MET:N	1:Z:220:MET:HE2	2.20	0.56
1:FA:223:SER:HB3	1:FA:266:ALA:HB1	1.86	0.56
1:XA:223:SER:HB3	1:XA:266:ALA:HB1	1.88	0.56
1:AB:188:MET:HE3	1:AB:188:MET:HA	1.87	0.56
1:GB:148:LEU:HA	1:GB:270:LEU:HD11	1.88	0.56
1:Q:223:SER:HB3	1:Q:266:ALA:HB1	1.88	0.55
1:CA:146:LEU:HD11	1:CA:162:ALA:HB2	1.88	0.55
1:JA:4:LEU:HD11	1:JA:238:SER:HB3	1.87	0.55
1:RA:34:ARG:HH12	1:RA:237:PHE:HE2	1.52	0.55
1:CB:149:PRO:HB3	1:CB:158:VAL:HG21	1.88	0.55
1:E:132:GLY:HA2	1:K:75:LYS:HE2	1.88	0.55
1:S:171:VAL:HG13	1:S:225:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KA:162:ALA:HB1	1:KA:268:VAL:HG11	1.88	0.55
1:P:9:ALA:HB2	1:P:241:TYR:HB2	1.86	0.55
1:WA:219:ALA:HB3	1:WA:270:LEU:HD23	1.89	0.55
1:ZA:197:PRO:HG2	1:ZA:200:GLN:HE22	1.72	0.55
1:BB:181:ARG:HA	1:BB:212:TRP:HE1	1.71	0.55
1:G:175:TYR:HB3	1:G:221:LEU:HD11	1.88	0.55
1:K:171:VAL:HG22	1:K:225:ARG:HE	1.72	0.55
1:Y:48:SER:HB3	1:LA:76:ARG:HH11	1.72	0.55
1:LA:188:MET:HE3	1:LA:188:MET:HA	1.88	0.55
1:MA:231:LEU:HD12	1:MA:259:PHE:HB2	1.88	0.55
1:E:29:VAL:HG11	1:FB:170:GLY:HA2	1.87	0.55
1:NA:220:MET:HG3	1:NA:269:PRO:HA	1.88	0.55
1:CB:156:PRO:HG3	1:CB:202:VAL:HG12	1.88	0.55
1:GB:146:LEU:HD11	1:GB:162:ALA:HB2	1.87	0.55
1:KA:219:ALA:HB3	1:KA:270:LEU:HD23	1.88	0.55
1:OA:148:LEU:HA	1:OA:270:LEU:HD11	1.89	0.55
1:F:198:VAL:HA	1:F:201:HIS:HB3	1.89	0.55
1:J:162:ALA:HB1	1:J:268:VAL:HG11	1.87	0.55
1:WA:57:ALA:HA	1:WA:74:ARG:HE	1.72	0.55
1:CB:220:MET:N	1:CB:220:MET:HE2	2.21	0.55
1:HB:223:SER:HB3	1:HB:266:ALA:HB1	1.89	0.55
1:E:221:LEU:HD12	1:E:268:VAL:HB	1.89	0.55
1:P:262:LEU:HD23	1:P:262:LEU:H	1.72	0.55
1:CA:220:MET:N	1:CA:220:MET:HE2	2.21	0.55
1:RA:104:ASP:HB3	1:UA:262:LEU:HD12	1.88	0.55
1:NA:125:VAL:HG13	1:NA:126:PHE:CD1	2.42	0.55
1:TA:220:MET:N	1:TA:220:MET:HE2	2.22	0.55
1:BB:223:SER:HB3	1:BB:266:ALA:HB1	1.88	0.55
1:K:160:VAL:HG21	1:R:188:MET:HB3	1.89	0.55
1:R:156:PRO:HG3	1:R:202:VAL:HG12	1.87	0.55
1:V:221:LEU:HB3	1:V:268:VAL:HB	1.88	0.55
1:IA:209:PRO:HB2	1:IA:211:ILE:HD11	1.89	0.55
2:7:128:LEU:HD23	2:7:128:LEU:H	1.72	0.55
1:O:156:PRO:HG3	1:O:202:VAL:HG12	1.89	0.54
1:Y:51:SER:HA	1:Y:78:VAL:HG12	1.89	0.54
1:SA:219:ALA:HB3	1:SA:270:LEU:HD23	1.89	0.54
1:A:182:THR:O	1:A:186:GLN:HG2	2.07	0.54
1:A:192:THR:HG21	1:A:197:PRO:HA	1.88	0.54
1:W:27:LEU:HD13	1:W:237:PHE:CE1	2.42	0.54
1:BA:174:PRO:HG2	1:BA:224:GLN:HB2	1.89	0.54
1:WA:51:SER:HA	1:WA:78:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:257:MET:HE2	1:BB:258:THR:N	2.22	0.54
1:IA:146:LEU:HD11	1:IA:162:ALA:HB2	1.88	0.54
1:JA:192:THR:HG21	1:JA:197:PRO:HA	1.90	0.54
1:MA:223:SER:HB3	1:MA:266:ALA:HB1	1.90	0.54
1:QA:223:SER:HB3	1:QA:266:ALA:HB1	1.90	0.54
1:UA:241:TYR:HE1	1:UA:244:HIS:HB3	1.72	0.54
1:XA:152:LEU:HD12	1:XA:187:LEU:HD12	1.88	0.54
1:I:162:ALA:HB1	1:I:268:VAL:HG11	1.87	0.54
1:FA:119:ILE:HD11	1:FA:214:PRO:HB2	1.90	0.54
1:NA:188:MET:HE3	1:NA:188:MET:HA	1.90	0.54
1:AB:51:SER:HA	1:AB:78:VAL:HG12	1.89	0.54
1:R:181:ARG:HG3	1:R:182:THR:HG23	1.88	0.54
1:HA:188:MET:HA	1:HA:188:MET:HE3	1.89	0.54
1:PA:152:LEU:HA	1:PA:155:PHE:CZ	2.42	0.54
1:BB:163:LEU:HG	1:BB:167:ARG:HH21	1.73	0.54
1:K:58:LEU:HB2	1:K:73:VAL:HG23	1.89	0.54
1:M:162:ALA:HB1	1:M:268:VAL:HG11	1.90	0.54
1:N:203:ARG:HH12	1:N:208:GLY:H	1.56	0.54
1:X:188:MET:HA	1:X:188:MET:HE2	1.89	0.54
1:PA:163:LEU:HD22	1:PA:167:ARG:HH11	1.73	0.54
1:A0:223:SER:HB3	1:A0:266:ALA:HB1	1.89	0.54
1:J:221:LEU:HB2	1:J:268:VAL:HB	1.89	0.54
1:R:94:GLU:HB2	1:R:105:ALA:HB1	1.90	0.54
1:BA:36:VAL:HG23	1:BA:37:VAL:HG13	1.88	0.54
1:OA:91:LYS:HG3	1:OA:93:ALA:H	1.73	0.54
1:BB:166:LEU:HD22	1:BB:167:ARG:NH1	2.23	0.54
1:E:58:LEU:HB2	1:E:73:VAL:HG23	1.89	0.54
1:J:219:ALA:HB3	1:J:270:LEU:HD23	1.89	0.54
1:EB:241:TYR:HE1	1:EB:244:HIS:HB3	1.73	0.54
1:DB:146:LEU:HD11	1:DB:162:ALA:HB2	1.91	0.53
1:B:197:PRO:HG2	1:B:200:GLN:HE22	1.73	0.53
1:I:29:VAL:HG11	1:HA:170:GLY:HA2	1.90	0.53
1:X:197:PRO:HG2	1:X:200:GLN:HE22	1.74	0.53
1:CA:34:ARG:HH12	1:CA:237:PHE:HE2	1.56	0.53
1:E:188:MET:HE2	1:E:188:MET:HA	1.88	0.53
1:N:219:ALA:HB3	1:N:270:LEU:HD23	1.89	0.53
1:W:4:LEU:HD21	1:W:238:SER:HB2	1.91	0.53
1:KA:175:TYR:HB3	1:KA:221:LEU:HD11	1.91	0.53
1:LA:119:ILE:HD11	1:LA:214:PRO:HB2	1.90	0.53
1:OA:259:PHE:HD1	1:OA:260:ARG:N	2.06	0.53
1:RA:188:MET:HA	1:RA:188:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:WA:179:LEU:HD23	1:WA:183:VAL:HG23	1.89	0.53
1:H:94:GLU:O	1:H:98:ILE:HG22	2.08	0.53
1:X:172:ASP:H	1:X:225:ARG:HD3	1.73	0.53
1:BA:220:MET:HE2	1:BA:220:MET:HA	1.90	0.53
1:CB:148:LEU:HD22	1:CB:272:GLY:HA2	1.90	0.53
1:E:156:PRO:HG3	1:E:202:VAL:HG12	1.90	0.53
1:IA:233:VAL:HG12	1:IA:257:MET:HB3	1.90	0.53
1:UA:162:ALA:HB1	1:UA:268:VAL:HG11	1.90	0.53
1:L:188:MET:HE3	1:L:188:MET:HA	1.89	0.53
1:O:188:MET:HE2	1:O:188:MET:HA	1.90	0.53
1:T:16:TRP:O	1:T:20:GLU:HG3	2.09	0.53
1:FA:152:LEU:HD12	1:FA:155:PHE:HD2	1.73	0.53
1:FB:179:LEU:HD23	1:FB:183:VAL:HG23	1.89	0.53
1:A:148:LEU:HA	1:A:270:LEU:HD11	1.91	0.53
1:N:220:MET:HE2	1:N:220:MET:N	2.23	0.53
1:JA:4:LEU:HD22	1:JA:240:GLY:HA3	1.90	0.53
1:CB:192:THR:HG21	1:CB:197:PRO:HA	1.91	0.53
1:I:141:SER:HB3	1:I:144:HIS:CE1	2.44	0.53
1:Q:177:LEU:HD11	1:Q:219:ALA:HB1	1.91	0.53
1:X:141:SER:HB3	1:X:144:HIS:CE1	2.44	0.53
1:BB:179:LEU:HD23	1:BB:183:VAL:HG23	1.91	0.53
1:V:76:ARG:HH11	1:JA:48:SER:HB3	1.74	0.53
1:AA:219:ALA:H	1:AA:270:LEU:HB3	1.74	0.53
1:HA:35:LYS:HE2	2:8:129:LYS:HE3	1.91	0.53
1:IA:5:MET:HE2	1:IA:5:MET:H	1.74	0.53
1:AB:9:ALA:HB2	1:AB:241:TYR:HB2	1.89	0.53
1:CB:81:LEU:HG	1:CB:258:THR:HB	1.89	0.53
1:C:43:LEU:HD11	1:C:232:THR:HG22	1.91	0.53
1:P:179:LEU:HD23	1:P:183:VAL:HG23	1.91	0.53
1:X:223:SER:HB3	1:X:266:ALA:HB1	1.90	0.53
1:Z:172:ASP:H	1:Z:225:ARG:HD3	1.73	0.53
1:DB:148:LEU:HA	1:DB:270:LEU:HD11	1.90	0.53
1:HA:4:LEU:HD21	1:HA:238:SER:HB3	1.91	0.52
1:SA:198:VAL:HA	1:SA:201:HIS:HB3	1.90	0.52
1:C:262:LEU:HB2	1:SA:104:ASP:HB3	1.91	0.52
1:HA:31:LEU:HD21	1:HA:34:ARG:HG3	1.90	0.52
1:C:81:LEU:HG	1:C:258:THR:HB	1.91	0.52
1:H:51:SER:HA	1:H:78:VAL:HG12	1.90	0.52
1:DA:48:SER:HB3	1:GA:76:ARG:HH11	1.74	0.52
1:AB:162:ALA:HB1	1:AB:268:VAL:HG11	1.91	0.52
1:BB:148:LEU:HA	1:BB:270:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:235:ARG:HD3	1:Q:254:GLN:HE22	1.75	0.52
1:DA:36:VAL:HG23	1:DA:37:VAL:HG13	1.92	0.52
1:DA:188:MET:HB3	1:BB:160:VAL:HG21	1.91	0.52
1:KA:192:THR:HG21	1:KA:197:PRO:HA	1.92	0.52
1:LA:197:PRO:HG2	1:LA:200:GLN:HE22	1.75	0.52
1:D:192:THR:HG21	1:D:197:PRO:HA	1.91	0.52
1:L:148:LEU:HD12	1:L:149:PRO:HD2	1.92	0.52
1:AA:148:LEU:HD22	1:AA:272:GLY:HA2	1.92	0.52
1:JA:81:LEU:HG	1:JA:258:THR:HB	1.92	0.52
1:OA:32:ALA:HA	1:OA:35:LYS:HZ1	1.73	0.52
1:QA:28:THR:HG23	2:14:128:LEU:HD12	1.91	0.52
1:D:81:LEU:HG	1:D:258:THR:HB	1.90	0.52
1:M:219:ALA:HB3	1:M:270:LEU:HD23	1.90	0.52
1:FA:148:LEU:HA	1:FA:270:LEU:HD11	1.92	0.52
1:I:167:ARG:HH21	1:AB:29:VAL:HG13	1.75	0.52
1:M:220:MET:N	1:M:220:MET:HE2	2.24	0.52
1:V:223:SER:HB3	1:V:266:ALA:HB1	1.90	0.52
1:W:177:LEU:HD11	1:W:219:ALA:HB1	1.92	0.52
1:Y:35:LYS:HZ1	2:19:128:LEU:HG	1.75	0.52
1:AA:179:LEU:HD23	1:AA:183:VAL:HG23	1.90	0.52
1:CA:197:PRO:HG2	1:CA:200:GLN:HE22	1.73	0.52
1:LA:192:THR:HG21	1:LA:197:PRO:HA	1.91	0.52
1:PA:36:VAL:HG23	1:PA:37:VAL:HG13	1.92	0.52
1:D:148:LEU:HA	1:D:270:LEU:HD11	1.92	0.52
1:E:1:MET:HE1	1:E:7:ASP:HB2	1.92	0.52
1:I:198:VAL:HA	1:I:201:HIS:HB3	1.92	0.52
1:J:241:TYR:HE1	1:J:244:HIS:HB3	1.75	0.52
1:L:198:VAL:HA	1:L:201:HIS:HB3	1.92	0.52
1:DA:188:MET:HA	1:DA:188:MET:HE2	1.92	0.52
1:KA:148:LEU:HB3	1:KA:272:GLY:HA2	1.91	0.52
1:BB:155:PHE:HD2	1:BB:202:VAL:HG11	1.75	0.52
1:K:179:LEU:HD22	1:K:183:VAL:HG13	1.92	0.52
1:O:111:ILE:HG13	1:O:112:GLU:N	2.24	0.52
1:HA:159:LEU:HD11	1:HA:205:LEU:HD11	1.90	0.52
1:VA:90:LEU:HD21	1:VA:110:VAL:HG23	1.92	0.52
1:XA:171:VAL:HA	1:XA:225:ARG:HH21	1.75	0.52
1:F:219:ALA:HB3	1:F:270:LEU:HD23	1.92	0.52
1:N:262:LEU:HD12	1:N:263:GLY:N	2.25	0.52
1:V:12:SER:HB3	1:V:14:LYS:HZ2	1.75	0.52
1:BB:135:THR:HG23	1:BB:139:GLU:HG3	1.91	0.52
1:B:223:SER:HB3	1:B:266:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:160:VAL:HG21	1:CB:188:MET:HB3	1.91	0.51
1:LA:190:THR:HB	1:LA:192:THR:HG23	1.92	0.51
1:NA:172:ASP:H	1:NA:225:ARG:HD3	1.74	0.51
1:G:148:LEU:HA	1:G:270:LEU:HD11	1.93	0.51
1:R:175:TYR:HB2	1:R:206:PHE:HE1	1.75	0.51
1:X:58:LEU:HD21	1:X:75:LYS:HB3	1.92	0.51
1:K:81:LEU:HG	1:K:258:THR:HB	1.92	0.51
1:K:192:THR:HG21	1:K:197:PRO:HA	1.91	0.51
1:N:148:LEU:HA	1:N:270:LEU:HD11	1.93	0.51
1:HA:162:ALA:HB1	1:HA:268:VAL:HG11	1.91	0.51
1:MA:163:LEU:O	1:MA:167:ARG:HG2	2.11	0.51
1:SA:119:ILE:HD11	1:SA:214:PRO:HB2	1.93	0.51
1:A:170:GLY:HA2	1:H:29:VAL:HG11	1.91	0.51
1:BA:14:LYS:HD2	1:BA:14:LYS:C	2.36	0.51
1:LA:177:LEU:HD23	1:LA:210:LEU:HD22	1.92	0.51
1:SA:148:LEU:HA	1:SA:270:LEU:HD11	1.91	0.51
1:DB:40:LYS:HD2	1:DB:232:THR:HG22	1.92	0.51
1:A:1:MET:HE1	1:A:8:LEU:HD23	1.93	0.51
1:N:156:PRO:HG3	1:N:202:VAL:HG12	1.93	0.51
1:JA:92:ARG:HA	1:JA:95:LEU:HD12	1.91	0.51
1:WA:148:LEU:HA	1:WA:270:LEU:HD11	1.92	0.51
1:HB:171:VAL:HG22	1:HB:225:ARG:HE	1.76	0.51
1:B:198:VAL:HA	1:B:201:HIS:HB3	1.92	0.51
1:L:166:LEU:HG	1:L:171:VAL:HB	1.91	0.51
1:V:141:SER:HB3	1:V:144:HIS:CE1	2.45	0.51
1:SA:241:TYR:HE1	1:SA:244:HIS:HB3	1.75	0.51
1:BB:219:ALA:H	1:BB:270:LEU:HB3	1.75	0.51
1:N:86:VAL:HG21	1:N:117:ILE:HB	1.93	0.51
1:V:40:LYS:HZ1	1:V:231:LEU:H	1.58	0.51
1:D:1:MET:HE2	1:D:5:MET:HA	1.92	0.51
1:K:141:SER:HB3	1:K:144:HIS:HE1	1.76	0.51
1:K:229:PHE:HZ	1:K:267:ALA:HB2	1.76	0.51
1:L:220:MET:HE2	1:L:220:MET:N	2.25	0.51
1:P:35:LYS:HD3	1:P:35:LYS:N	2.25	0.51
1:V:141:SER:HB3	1:V:144:HIS:HE1	1.76	0.51
1:W:175:TYR:HD1	1:W:223:SER:HA	1.74	0.51
1:PA:197:PRO:HG2	1:PA:200:GLN:HE22	1.76	0.51
1:ZA:148:LEU:HA	1:ZA:270:LEU:HD11	1.93	0.51
1:F:180:GLY:HA2	1:F:216:VAL:HG23	1.93	0.51
1:KA:148:LEU:HA	1:KA:270:LEU:HD11	1.93	0.51
1:RA:171:VAL:HG13	1:RA:225:ARG:HE	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ARG:HA	1:F:212:TRP:HE1	1.76	0.51
1:I:36:VAL:HG23	1:I:37:VAL:HG13	1.93	0.51
1:Y:192:THR:HG21	1:Y:197:PRO:HA	1.92	0.51
1:NA:223:SER:HB3	1:NA:266:ALA:HB1	1.93	0.51
1:OA:34:ARG:HH12	1:OA:237:PHE:HE2	1.59	0.51
1:SA:40:LYS:HD3	1:SA:40:LYS:N	2.27	0.51
1:DB:119:ILE:HD11	1:DB:214:PRO:HB2	1.93	0.51
1:GB:223:SER:HB3	1:GB:266:ALA:HB1	1.92	0.51
1:A0:199:LEU:HD12	1:A0:199:LEU:H	1.77	0.50
1:I:9:ALA:HB2	1:I:241:TYR:HB2	1.93	0.50
1:K:40:LYS:HZ1	1:K:231:LEU:H	1.59	0.50
1:R:188:MET:HE2	1:R:188:MET:HA	1.93	0.50
1:T:148:LEU:HA	1:T:270:LEU:HD11	1.92	0.50
1:OA:43:LEU:HD22	1:OA:47:ALA:HB2	1.92	0.50
1:GB:192:THR:HG21	1:GB:197:PRO:HA	1.93	0.50
1:HB:9:ALA:HB2	1:HB:241:TYR:HB2	1.92	0.50
1:H:170:GLY:HA2	1:HB:29:VAL:HG21	1.92	0.50
1:N:92:ARG:O	1:N:96:GLU:HG2	2.11	0.50
1:X:177:LEU:HD11	1:X:219:ALA:HB1	1.93	0.50
1:KA:198:VAL:HA	1:KA:201:HIS:HB3	1.93	0.50
1:GB:179:LEU:HD23	1:GB:183:VAL:HG23	1.93	0.50
1:C:222:ILE:HG23	1:C:229:PHE:HE2	1.76	0.50
1:G:92:ARG:HA	1:G:95:LEU:HD23	1.92	0.50
1:I:169:ARG:CZ	1:I:169:ARG:HA	2.42	0.50
1:LA:148:LEU:HA	1:LA:270:LEU:HD11	1.93	0.50
1:OA:37:VAL:HG12	1:OA:229:PHE:HB2	1.92	0.50
1:B:74:ARG:HB2	1:S:83:GLU:HB2	1.92	0.50
1:DA:13:ALA:HB2	1:WA:1:MET:HB3	1.92	0.50
1:JA:1:MET:HE1	1:JA:7:ASP:HB2	1.94	0.50
1:LA:175:TYR:HB2	1:LA:206:PHE:HE1	1.77	0.50
1:Z:141:SER:HB3	1:Z:144:HIS:CE1	2.46	0.50
1:DB:9:ALA:HB2	1:DB:241:TYR:HB2	1.94	0.50
1:I:204:ARG:H	1:I:204:ARG:HD2	1.76	0.50
1:P:229:PHE:HZ	1:P:267:ALA:HB2	1.77	0.50
1:X:199:LEU:HD12	1:AA:201:HIS:CE1	2.45	0.50
1:MA:220:MET:HE1	1:MA:270:LEU:H	1.77	0.50
1:QA:148:LEU:HA	1:QA:270:LEU:HD11	1.93	0.50
1:B:170:GLY:HA2	1:T:29:VAL:HG11	1.93	0.50
1:C:188:MET:HE2	1:C:188:MET:HA	1.93	0.50
1:Y:25:GLY:O	1:Y:29:VAL:HG12	2.12	0.50
1:Y:188:MET:HE3	1:Y:188:MET:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:SER:HB3	1:E:144:HIS:CE1	2.47	0.50
1:K:222:ILE:HG12	1:K:229:PHE:HE1	1.76	0.50
1:Q:181:ARG:HA	1:Q:212:TRP:HE1	1.76	0.50
1:OA:126:PHE:HD2	1:OA:216:VAL:HG11	1.77	0.50
1:SA:39:PHE:C	1:SA:40:LYS:HD3	2.36	0.50
1:C:198:VAL:HB	1:C:202:VAL:HG13	1.94	0.50
1:D:219:ALA:HB3	1:D:270:LEU:HD23	1.93	0.50
1:J:171:VAL:HG22	1:J:225:ARG:HE	1.77	0.50
1:K:148:LEU:HA	1:K:270:LEU:HD11	1.93	0.50
1:R:262:LEU:HD12	1:CB:104:ASP:HB3	1.94	0.50
1:W:219:ALA:HB3	1:W:270:LEU:HD23	1.94	0.50
1:Y:241:TYR:HE1	1:Y:244:HIS:HB3	1.77	0.50
1:Z:180:GLY:O	1:Z:184:TYR:HB2	2.12	0.50
1:MA:198:VAL:HA	1:MA:201:HIS:HB3	1.94	0.50
1:TA:188:MET:HE2	1:TA:188:MET:HA	1.93	0.50
1:P:171:VAL:HG13	1:P:225:ARG:HE	1.77	0.49
1:BB:231:LEU:HD12	1:BB:259:PHE:HB2	1.92	0.49
1:LA:1:MET:HE1	1:LA:8:LEU:HD23	1.94	0.49
1:UA:188:MET:HE3	1:UA:188:MET:HA	1.94	0.49
1:CB:148:LEU:HA	1:CB:270:LEU:HD11	1.95	0.49
1:EB:223:SER:HB3	1:EB:266:ALA:HB1	1.94	0.49
1:GB:35:LYS:HE3	1:GB:35:LYS:HA	1.94	0.49
1:B:55:THR:HG22	1:B:76:ARG:HA	1.93	0.49
1:B:220:MET:HE2	1:B:220:MET:N	2.28	0.49
1:O:9:ALA:HB2	1:O:241:TYR:HB2	1.94	0.49
1:Q:219:ALA:HB3	1:Q:270:LEU:HD23	1.94	0.49
1:NA:148:LEU:HA	1:NA:270:LEU:HD11	1.93	0.49
1:PA:188:MET:N	1:PA:188:MET:HE2	2.26	0.49
1:ZA:156:PRO:HG3	1:ZA:202:VAL:HG12	1.94	0.49
1:GB:188:MET:HE3	1:GB:199:LEU:HD22	1.94	0.49
1:H:198:VAL:HA	1:H:201:HIS:HB3	1.94	0.49
1:FA:141:SER:HB3	1:FA:144:HIS:CE1	2.47	0.49
1:IA:36:VAL:HG23	1:IA:37:VAL:HG13	1.93	0.49
1:VA:203:ARG:HH12	1:VA:208:GLY:H	1.60	0.49
1:E:14:LYS:HE2	1:E:99:ALA:HA	1.94	0.49
1:N:52:LEU:HD21	1:N:79:GLN:HB2	1.95	0.49
1:O:262:LEU:HD12	1:KA:104:ASP:HB3	1.95	0.49
1:FA:141:SER:HB3	1:FA:144:HIS:HE1	1.76	0.49
1:YA:225:ARG:NH2	1:YA:266:ALA:HB2	2.28	0.49
1:G:192:THR:HG21	1:G:197:PRO:HA	1.95	0.49
1:J:210:LEU:C	1:J:211:ILE:HD13	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:223:SER:HB3	1:J:266:ALA:HB1	1.94	0.49
1:T:221:LEU:HB2	1:T:268:VAL:HB	1.95	0.49
1:DA:174:PRO:HG2	1:DA:224:GLN:HB2	1.93	0.49
1:EA:175:TYR:HB3	1:EA:221:LEU:HD21	1.95	0.49
1:EA:198:VAL:HA	1:EA:201:HIS:HB3	1.94	0.49
1:HA:201:HIS:HA	1:HA:204:ARG:HD2	1.93	0.49
1:AB:172:ASP:H	1:AB:225:ARG:HD3	1.78	0.49
1:FB:88:PHE:HE2	1:FB:110:VAL:HG22	1.77	0.49
1:E:148:LEU:HA	1:E:270:LEU:HD11	1.94	0.49
1:I:188:MET:HA	1:I:188:MET:HE2	1.93	0.49
1:DA:220:MET:HE2	1:DA:220:MET:N	2.28	0.49
1:HA:146:LEU:HD11	1:HA:162:ALA:HB2	1.94	0.49
1:TA:233:VAL:HG12	1:TA:257:MET:HB3	1.93	0.49
1:UA:219:ALA:HB3	1:UA:270:LEU:HD23	1.94	0.49
1:WA:223:SER:HB3	1:WA:266:ALA:HB1	1.95	0.49
1:D:160:VAL:HG21	1:VA:188:MET:HB3	1.94	0.49
1:R:220:MET:N	1:R:220:MET:HE2	2.28	0.49
1:V:220:MET:HE2	1:V:220:MET:N	2.27	0.49
1:KA:209:PRO:HB2	1:KA:211:ILE:HD11	1.95	0.49
1:ZA:141:SER:HB3	1:ZA:144:HIS:CE1	2.47	0.49
1:BB:229:PHE:HZ	1:BB:266:ALA:HB3	1.78	0.49
1:CB:164:ALA:HA	1:CB:167:ARG:HE	1.78	0.49
1:X:163:LEU:O	1:X:167:ARG:HG3	2.13	0.49
1:Y:203:ARG:HH12	1:Y:208:GLY:H	1.59	0.49
1:YA:36:VAL:HG23	1:YA:37:VAL:HG13	1.95	0.49
1:EB:141:SER:HB3	1:EB:144:HIS:CE1	2.47	0.49
1:R:177:LEU:HD11	1:R:219:ALA:HB1	1.94	0.49
1:Y:181:ARG:HA	1:Y:212:TRP:HE1	1.78	0.49
1:LA:181:ARG:HA	1:LA:212:TRP:HE1	1.78	0.49
1:P:14:LYS:HZ1	1:P:98:ILE:HB	1.78	0.48
1:W:171:VAL:HG22	1:W:225:ARG:HE	1.76	0.48
1:X:192:THR:HG21	1:X:197:PRO:HB3	1.95	0.48
1:Z:36:VAL:HG23	1:Z:37:VAL:HG13	1.95	0.48
1:YA:225:ARG:HH21	1:YA:266:ALA:HB2	1.78	0.48
1:A0:156:PRO:HG3	1:A0:202:VAL:HG12	1.94	0.48
1:B:188:MET:HE3	1:B:188:MET:HA	1.95	0.48
1:J:231:LEU:HD12	1:J:259:PHE:HB2	1.95	0.48
1:K:27:LEU:O	1:K:31:LEU:HB2	2.13	0.48
1:W:152:LEU:HD22	1:W:187:LEU:HD12	1.95	0.48
1:Y:9:ALA:HB2	1:Y:241:TYR:HB2	1.95	0.48
1:FA:166:LEU:HD23	1:FA:167:ARG:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:203:ARG:NH2	1:JA:208:GLY:H	2.10	0.48
1:OA:124:ALA:HB1	1:OA:129:PHE:HB2	1.95	0.48
1:TA:203:ARG:HH22	1:TA:208:GLY:H	1.61	0.48
1:UA:51:SER:HA	1:UA:78:VAL:HG12	1.94	0.48
1:BB:171:VAL:HG22	1:BB:225:ARG:HE	1.78	0.48
1:H:156:PRO:HG3	1:H:202:VAL:HG12	1.95	0.48
1:J:198:VAL:HA	1:J:201:HIS:HB3	1.96	0.48
1:P:137:ILE:HD11	1:P:229:PHE:CZ	2.48	0.48
1:P:177:LEU:HD11	1:P:219:ALA:HB1	1.96	0.48
1:P:223:SER:HB3	1:P:266:ALA:HB1	1.95	0.48
1:MA:4:LEU:HD21	1:MA:238:SER:HB3	1.94	0.48
1:WA:80:PRO:HB2	1:BB:75:LYS:HD2	1.95	0.48
1:AB:92:ARG:HA	1:AB:95:LEU:HD23	1.95	0.48
1:EB:4:LEU:HD11	1:EB:238:SER:HB3	1.95	0.48
1:A0:206:PHE:HD1	1:A0:207:GLU:N	2.11	0.48
1:C:198:VAL:HA	1:C:201:HIS:HB3	1.95	0.48
1:P:1:MET:HE1	1:P:8:LEU:HG	1.94	0.48
1:W:262:LEU:HD12	1:OA:104:ASP:HB3	1.94	0.48
1:IA:174:PRO:HG2	1:IA:224:GLN:HB2	1.95	0.48
1:ZA:183:VAL:HA	1:ZA:186:GLN:HG2	1.94	0.48
1:DB:197:PRO:HG2	1:DB:200:GLN:HE22	1.78	0.48
1:EB:241:TYR:CE1	1:EB:244:HIS:HB3	2.48	0.48
1:P:32:ALA:HA	1:P:35:LYS:NZ	2.27	0.48
1:T:163:LEU:HD23	1:T:167:ARG:HH21	1.77	0.48
1:X:129:PHE:HD1	1:X:132:GLY:H	1.62	0.48
1:AA:10:PRO:HG3	1:AA:244:HIS:CD2	2.48	0.48
1:KA:181:ARG:HA	1:KA:212:TRP:HE1	1.78	0.48
1:YA:203:ARG:HH12	1:YA:208:GLY:H	1.60	0.48
1:AB:36:VAL:HG23	1:AB:37:VAL:HG13	1.95	0.48
1:BB:91:LYS:HG3	1:BB:93:ALA:H	1.78	0.48
1:CB:219:ALA:HB3	1:CB:270:LEU:HD23	1.95	0.48
1:EB:188:MET:HE2	1:EB:188:MET:HA	1.96	0.48
1:EB:229:PHE:HB3	1:EB:259:PHE:HE1	1.78	0.48
1:A:95:LEU:O	1:A:98:ILE:HG22	2.14	0.48
1:Y:190:THR:HB	1:Y:192:THR:HG23	1.94	0.48
1:KA:220:MET:HG3	1:KA:269:PRO:HA	1.96	0.48
1:UA:220:MET:HE2	1:UA:220:MET:N	2.29	0.48
1:BB:2:ASN:HD21	1:BB:4:LEU:HD12	1.78	0.48
1:V:188:MET:HE3	1:V:188:MET:HA	1.95	0.48
1:AA:148:LEU:HA	1:AA:270:LEU:HD11	1.96	0.48
1:TA:241:TYR:HE1	1:TA:244:HIS:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ALA:HA	1:F:74:ARG:HE	1.79	0.48
1:J:177:LEU:HD11	1:J:219:ALA:HB1	1.94	0.48
1:N:21:THR:HG23	1:N:24:ARG:HH22	1.79	0.48
1:EA:148:LEU:HA	1:EA:270:LEU:HD11	1.95	0.48
1:JA:32:ALA:HA	1:JA:35:LYS:HD2	1.96	0.48
1:WA:34:ARG:HH12	1:WA:237:PHE:HE2	1.60	0.48
1:WA:159:LEU:HD23	1:WA:159:LEU:H	1.77	0.48
1:XA:36:VAL:HG23	1:XA:37:VAL:HG13	1.96	0.48
1:YA:197:PRO:HG2	1:YA:200:GLN:HE22	1.79	0.48
1:ZA:166:LEU:HD13	1:ZA:171:VAL:HG12	1.96	0.48
1:W:220:MET:N	1:W:220:MET:HE2	2.29	0.48
1:NA:26:THR:HG21	1:NA:111:ILE:HG22	1.96	0.48
1:RA:220:MET:N	1:RA:220:MET:HE2	2.29	0.48
1:UA:92:ARG:O	1:UA:96:GLU:HG2	2.13	0.48
1:A:155:PHE:HD1	1:A:155:PHE:O	1.97	0.48
1:H:192:THR:HG21	1:H:197:PRO:HA	1.96	0.48
1:L:156:PRO:O	1:L:160:VAL:HG23	2.14	0.48
1:Z:175:TYR:HB3	1:Z:221:LEU:HD11	1.96	0.48
1:AA:40:LYS:HZ1	1:AA:230:GLU:HB2	1.78	0.48
1:PA:181:ARG:HH21	1:PA:214:PRO:HB3	1.79	0.48
1:DB:220:MET:HE2	1:DB:220:MET:N	2.29	0.48
1:F:148:LEU:HB3	1:F:272:GLY:HA2	1.96	0.47
1:G:22:GLU:O	1:G:26:THR:HG22	2.14	0.47
1:X:220:MET:HE2	1:X:220:MET:N	2.28	0.47
1:Z:141:SER:HB3	1:Z:144:HIS:HE1	1.79	0.47
1:RA:141:SER:HB3	1:RA:144:HIS:CE1	2.48	0.47
1:AB:94:GLU:O	1:AB:98:ILE:HG13	2.14	0.47
1:E:161:ARG:O	1:E:165:VAL:HG12	2.14	0.47
1:N:197:PRO:HG2	1:N:200:GLN:HE22	1.79	0.47
1:P:51:SER:HA	1:P:78:VAL:HG12	1.96	0.47
1:CA:188:MET:HA	1:CA:188:MET:HE3	1.96	0.47
1:EA:181:ARG:HA	1:EA:212:TRP:HE1	1.78	0.47
1:FB:166:LEU:HD23	1:FB:175:TYR:HE1	1.78	0.47
1:A:93:ALA:O	1:A:96:GLU:HG2	2.13	0.47
1:F:222:ILE:HG23	1:F:229:PHE:HE2	1.79	0.47
1:I:163:LEU:O	1:I:167:ARG:HG2	2.14	0.47
1:P:148:LEU:HA	1:P:270:LEU:HD11	1.94	0.47
1:Q:88:PHE:CE2	1:Q:110:VAL:HG22	2.49	0.47
1:R:111:ILE:HG13	1:R:112:GLU:N	2.29	0.47
1:Z:113:ALA:O	1:Z:117:ILE:HG22	2.14	0.47
1:CB:190:THR:HB	1:CB:192:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:LEU:HD13	1:K:184:TYR:HA	1.95	0.47
1:Q:190:THR:HB	1:Q:192:THR:HG23	1.96	0.47
1:VA:219:ALA:HB3	1:VA:270:LEU:HD23	1.96	0.47
1:AB:119:ILE:HD11	1:AB:214:PRO:HB2	1.96	0.47
1:GB:188:MET:HE3	1:GB:188:MET:HA	1.97	0.47
1:W:148:LEU:HA	1:W:270:LEU:HD11	1.95	0.47
1:Z:184:TYR:HE1	1:Z:210:LEU:HD21	1.79	0.47
1:SA:152:LEU:HD12	1:SA:152:LEU:H	1.80	0.47
1:UA:172:ASP:H	1:UA:225:ARG:HD3	1.78	0.47
1:XA:162:ALA:HB1	1:XA:268:VAL:HG11	1.96	0.47
1:DB:175:TYR:O	1:DB:208:GLY:HA3	2.14	0.47
1:A:163:LEU:O	1:A:167:ARG:HG2	2.14	0.47
1:C:86:VAL:HG23	1:C:253:LEU:HB2	1.96	0.47
1:G:187:LEU:O	1:G:199:LEU:HD21	2.15	0.47
1:H:220:MET:N	1:H:220:MET:HE2	2.30	0.47
1:M:148:LEU:HA	1:M:270:LEU:HD11	1.96	0.47
1:M:179:LEU:HD22	1:M:184:TYR:HA	1.97	0.47
1:IA:5:MET:HE2	1:IA:5:MET:N	2.29	0.47
1:YA:156:PRO:HG3	1:YA:202:VAL:HG12	1.96	0.47
1:HB:148:LEU:HA	1:HB:270:LEU:HD11	1.95	0.47
1:I:176:ALA:HB2	1:I:224:GLN:HE22	1.80	0.47
1:L:141:SER:HB3	1:L:144:HIS:HE1	1.80	0.47
1:O:197:PRO:HG2	1:O:200:GLN:HE22	1.78	0.47
1:O:198:VAL:HA	1:O:201:HIS:HB3	1.97	0.47
1:P:188:MET:HB3	1:DB:160:VAL:HG21	1.97	0.47
1:R:91:LYS:HB2	1:R:94:GLU:CD	2.40	0.47
1:W:123:ARG:HD2	1:W:127:HIS:HD2	1.80	0.47
1:X:37:VAL:HG12	1:X:229:PHE:HB2	1.96	0.47
1:X:141:SER:HB3	1:X:144:HIS:HE1	1.80	0.47
1:Y:156:PRO:HG3	1:Y:202:VAL:HG12	1.96	0.47
1:AA:241:TYR:HE1	1:AA:244:HIS:HB3	1.80	0.47
1:EA:156:PRO:HG3	1:EA:202:VAL:HG12	1.95	0.47
1:IA:148:LEU:HA	1:IA:270:LEU:HD11	1.95	0.47
1:JA:141:SER:HB3	1:JA:144:HIS:CE1	2.50	0.47
1:OA:219:ALA:HB3	1:OA:270:LEU:HD23	1.96	0.47
1:PA:166:LEU:HG	1:PA:171:VAL:HB	1.97	0.47
1:TA:76:ARG:HH11	1:ZA:48:SER:HB3	1.80	0.47
1:ZA:179:LEU:HD12	1:ZA:180:GLY:N	2.29	0.47
1:BB:36:VAL:HG23	1:BB:37:VAL:HG13	1.97	0.47
1:FB:81:LEU:HG	1:FB:258:THR:HB	1.97	0.47
1:HB:146:LEU:HD11	1:HB:162:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:192:THR:HG21	1:A0:197:PRO:HA	1.96	0.47
1:C:233:VAL:HG22	1:C:257:MET:HB3	1.97	0.47
1:E:198:VAL:HA	1:E:201:HIS:HB3	1.97	0.47
1:F:192:THR:HG21	1:F:197:PRO:HA	1.96	0.47
1:J:181:ARG:HA	1:J:212:TRP:HE1	1.80	0.47
1:K:188:MET:HB3	1:OA:160:VAL:HG21	1.97	0.47
1:X:36:VAL:HG23	1:X:37:VAL:HG13	1.96	0.47
1:KA:188:MET:HA	1:KA:188:MET:HE2	1.96	0.47
1:MA:35:LYS:N	1:MA:35:LYS:HD2	2.30	0.47
1:P:171:VAL:HG22	1:P:225:ARG:HH21	1.79	0.47
1:RA:192:THR:HG21	1:RA:197:PRO:HA	1.97	0.47
1:D:2:ASN:ND2	1:D:4:LEU:HD12	2.30	0.47
1:D:6:ARG:HD3	1:D:16:TRP:CZ3	2.50	0.47
1:L:141:SER:HB3	1:L:144:HIS:CE1	2.50	0.47
1:P:29:VAL:HG11	1:DB:170:GLY:HA2	1.98	0.47
1:S:3:ASP:O	1:S:5:MET:HE2	2.15	0.47
1:NA:219:ALA:HB3	1:NA:270:LEU:HD23	1.97	0.47
1:YA:148:LEU:HA	1:YA:270:LEU:HD11	1.97	0.47
2:18:123:LEU:HD12	2:18:123:LEU:H	1.79	0.47
1:A:91:LYS:HB2	1:A:94:GLU:OE1	2.15	0.46
1:D:197:PRO:HG2	1:D:200:GLN:HE22	1.80	0.46
1:E:188:MET:HB3	1:FB:160:VAL:HG21	1.97	0.46
1:P:40:LYS:HD3	1:P:232:THR:HG22	1.97	0.46
1:T:119:ILE:HD11	1:T:215:GLY:HA3	1.97	0.46
1:Z:223:SER:HB3	1:Z:266:ALA:HB1	1.97	0.46
1:DA:141:SER:HB3	1:DA:144:HIS:CE1	2.49	0.46
1:UA:141:SER:HB3	1:UA:144:HIS:HE1	1.80	0.46
1:AB:39:PHE:HD1	1:AB:231:LEU:HD23	1.80	0.46
1:HB:220:MET:HB2	1:HB:222:ILE:HD11	1.97	0.46
1:B:192:THR:HG21	1:B:197:PRO:HA	1.97	0.46
1:P:220:MET:N	1:P:220:MET:HE2	2.29	0.46
1:T:219:ALA:HB3	1:T:270:LEU:HD23	1.97	0.46
1:V:231:LEU:HD12	1:V:259:PHE:HB2	1.97	0.46
1:W:158:VAL:O	1:W:161:ARG:HG2	2.15	0.46
1:JA:146:LEU:HD11	1:JA:162:ALA:HB2	1.97	0.46
1:KA:141:SER:HB3	1:KA:144:HIS:CE1	2.49	0.46
1:MA:241:TYR:HE1	1:MA:244:HIS:HB3	1.80	0.46
1:YA:8:LEU:HD12	1:YA:8:LEU:O	2.15	0.46
1:ZA:188:MET:HE3	1:ZA:188:MET:HA	1.96	0.46
1:S:104:ASP:HB3	1:CA:262:LEU:HD12	1.96	0.46
1:PA:198:VAL:HA	1:PA:201:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:36:VAL:HG23	1:TA:37:VAL:HG13	1.98	0.46
1:DB:219:ALA:HB3	1:DB:270:LEU:HD23	1.98	0.46
1:B:51:SER:HA	1:B:78:VAL:HG12	1.96	0.46
1:I:4:LEU:H	1:I:4:LEU:HD12	1.81	0.46
1:V:197:PRO:HG2	1:V:200:GLN:HE22	1.80	0.46
1:W:81:LEU:HG	1:W:258:THR:HB	1.97	0.46
1:W:86:VAL:HG21	1:W:117:ILE:HB	1.98	0.46
1:AA:152:LEU:HG	1:AA:187:LEU:HD12	1.97	0.46
1:BA:188:MET:HE3	1:BA:188:MET:HA	1.98	0.46
1:KA:9:ALA:HB2	1:KA:241:TYR:HB2	1.97	0.46
1:RA:198:VAL:HA	1:RA:201:HIS:HB3	1.98	0.46
1:VA:241:TYR:CE1	1:VA:244:HIS:HB3	2.49	0.46
1:CB:203:ARG:HH22	1:CB:208:GLY:H	1.63	0.46
1:GB:162:ALA:HB1	1:GB:268:VAL:HG11	1.96	0.46
1:A0:175:TYR:HB3	1:A0:221:LEU:HD11	1.96	0.46
1:L:81:LEU:HG	1:L:258:THR:HB	1.97	0.46
1:N:162:ALA:HB1	1:N:268:VAL:HG11	1.96	0.46
1:P:202:VAL:O	1:P:206:PHE:HB2	2.15	0.46
1:BA:9:ALA:HB2	1:BA:241:TYR:HB2	1.96	0.46
1:CA:86:VAL:HG21	1:CA:117:ILE:HB	1.98	0.46
1:AB:148:LEU:HA	1:AB:270:LEU:HD11	1.97	0.46
1:A0:137:ILE:HD11	1:A0:229:PHE:CD1	2.50	0.46
1:H:27:LEU:HD23	1:H:27:LEU:HA	1.81	0.46
1:M:185:GLN:O	1:M:189:GLU:HG2	2.14	0.46
1:N:158:VAL:HA	1:N:161:ARG:NE	2.31	0.46
1:R:81:LEU:HG	1:R:258:THR:HB	1.96	0.46
1:S:36:VAL:HG23	1:S:37:VAL:HG13	1.97	0.46
1:HA:197:PRO:HG2	1:HA:200:GLN:HE22	1.80	0.46
1:IA:188:MET:HE3	1:IA:199:LEU:HD22	1.97	0.46
1:VA:198:VAL:HA	1:VA:201:HIS:HB3	1.96	0.46
1:G:84:LEU:HD23	1:N:73:VAL:HG12	1.98	0.46
1:H:148:LEU:HD22	1:H:272:GLY:HA2	1.98	0.46
1:I:241:TYR:HE1	1:I:244:HIS:HB3	1.79	0.46
1:L:27:LEU:O	1:L:31:LEU:HB2	2.15	0.46
1:L:29:VAL:HG11	1:DA:170:GLY:HA2	1.98	0.46
1:S:204:ARG:H	1:S:204:ARG:HD2	1.79	0.46
1:Y:129:PHE:HE2	1:LA:73:VAL:HG11	1.79	0.46
1:EA:1:MET:HE1	1:EA:8:LEU:HD23	1.97	0.46
1:IA:162:ALA:HB1	1:IA:268:VAL:HG11	1.98	0.46
1:ZA:220:MET:HE2	1:ZA:220:MET:N	2.31	0.46
1:DB:36:VAL:HG23	1:DB:37:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HB:175:TYR:O	1:HB:208:GLY:HA3	2.16	0.46
1:B:14:LYS:HE2	1:B:99:ALA:HA	1.98	0.46
1:B:141:SER:HB3	1:B:144:HIS:CE1	2.51	0.46
1:H:31:LEU:HD21	1:H:34:ARG:HG3	1.97	0.46
1:T:158:VAL:HA	1:T:161:ARG:NE	2.31	0.46
1:JA:241:TYR:HE1	1:JA:244:HIS:HB3	1.81	0.46
1:NA:197:PRO:HG2	1:NA:200:GLN:HE22	1.80	0.46
1:OA:40:LYS:HZ3	1:OA:231:LEU:C	2.23	0.46
1:QA:171:VAL:HG22	1:QA:225:ARG:HE	1.81	0.46
1:AA:34:ARG:HB2	2:3:128:LEU:HD23	1.98	0.46
1:IA:197:PRO:HG2	1:IA:200:GLN:HE22	1.80	0.46
1:SA:181:ARG:HA	1:SA:212:TRP:HE1	1.81	0.46
1:TA:148:LEU:HA	1:TA:270:LEU:HD11	1.97	0.46
1:ZA:221:LEU:HB2	1:ZA:268:VAL:HB	1.97	0.46
1:G:160:VAL:HG21	1:EA:188:MET:HB3	1.97	0.46
1:CA:10:PRO:HG3	1:CA:244:HIS:CD2	2.51	0.46
1:GA:197:PRO:HG2	1:GA:200:GLN:HE22	1.80	0.46
1:HA:169:ARG:HH11	1:HA:265:GLU:HA	1.81	0.46
1:IA:1:MET:HE3	1:IA:1:MET:HB2	1.82	0.46
1:IA:32:ALA:HB3	1:IA:213:ALA:HB2	1.97	0.46
1:QA:188:MET:HE2	1:QA:188:MET:HA	1.98	0.46
1:ZA:170:GLY:HA2	1:GB:29:VAL:HG11	1.97	0.46
1:L:230:GLU:OE2	1:L:260:ARG:HB2	2.16	0.45
1:M:18:GLU:OE1	1:M:107:LEU:HD11	2.16	0.45
1:N:192:THR:HG21	1:N:197:PRO:HA	1.97	0.45
1:P:36:VAL:HG23	1:P:37:VAL:HG13	1.97	0.45
1:T:5:MET:HE1	1:HA:10:PRO:C	2.42	0.45
1:BA:198:VAL:HA	1:BA:201:HIS:HB3	1.98	0.45
1:EA:179:LEU:HD22	1:EA:184:TYR:HD1	1.81	0.45
1:GA:141:SER:HB3	1:GA:144:HIS:CE1	2.52	0.45
1:QA:156:PRO:HG3	1:QA:202:VAL:HG12	1.97	0.45
1:BB:40:LYS:HE2	1:BB:230:GLU:HB2	1.98	0.45
1:BB:51:SER:HA	1:BB:78:VAL:HG12	1.97	0.45
1:A0:148:LEU:HD22	1:A0:272:GLY:HA2	1.98	0.45
1:A0:230:GLU:OE2	1:A0:260:ARG:HB2	2.16	0.45
1:F:188:MET:HE3	1:F:199:LEU:HD22	1.97	0.45
1:M:9:ALA:HB2	1:M:241:TYR:HB2	1.97	0.45
1:Q:31:LEU:HD21	1:Q:34:ARG:HG3	1.98	0.45
1:R:197:PRO:HG2	1:R:200:GLN:HE22	1.80	0.45
1:W:241:TYR:HE1	1:W:244:HIS:HB3	1.82	0.45
1:TA:149:PRO:HG3	1:TA:158:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:GLU:O	1:F:98:ILE:HG23	2.17	0.45
1:L:109:PRO:HA	1:L:112:GLU:HG2	1.98	0.45
1:N:181:ARG:HA	1:N:212:TRP:HE1	1.81	0.45
1:Q:163:LEU:O	1:Q:167:ARG:HG2	2.16	0.45
1:Q:244:HIS:HB2	1:Q:249:VAL:HG22	1.98	0.45
1:Z:148:LEU:HB3	1:Z:272:GLY:HA2	1.98	0.45
1:RA:262:LEU:HD23	1:RA:262:LEU:H	1.81	0.45
1:CB:34:ARG:HH12	1:CB:237:PHE:HE2	1.65	0.45
1:HB:115:ARG:O	1:HB:119:ILE:HG23	2.17	0.45
1:A:223:SER:HB3	1:A:266:ALA:HB1	1.99	0.45
1:G:185:GLN:CD	1:G:185:GLN:H	2.24	0.45
1:R:27:LEU:HD23	1:R:27:LEU:HA	1.79	0.45
1:R:177:LEU:HD23	1:R:210:LEU:HD22	1.99	0.45
1:Y:22:GLU:O	1:Y:26:THR:HG22	2.17	0.45
1:Y:231:LEU:HD12	1:Y:259:PHE:HB2	1.99	0.45
1:DA:202:VAL:HG23	1:DA:203:ARG:HH11	1.82	0.45
1:UA:232:THR:HB	1:UA:258:THR:HG22	1.99	0.45
1:VA:152:LEU:HD13	1:VA:187:LEU:HA	1.97	0.45
1:EB:126:PHE:CG	1:EB:220:MET:HE1	2.51	0.45
1:A0:166:LEU:HG	1:A0:171:VAL:HB	1.99	0.45
1:F:81:LEU:HG	1:F:258:THR:HB	1.99	0.45
1:H:14:LYS:NZ	1:H:98:ILE:HG12	2.30	0.45
1:K:197:PRO:HG2	1:K:200:GLN:HE22	1.81	0.45
1:N:9:ALA:HB2	1:N:241:TYR:HB2	1.98	0.45
1:W:141:SER:HB3	1:W:144:HIS:HE1	1.81	0.45
1:MA:11:ILE:HD13	1:MA:11:ILE:HA	1.87	0.45
1:OA:220:MET:N	1:OA:220:MET:HE2	2.32	0.45
1:OA:223:SER:HB3	1:OA:266:ALA:HB1	1.97	0.45
1:PA:175:TYR:O	1:PA:208:GLY:HA3	2.17	0.45
1:QA:141:SER:HB3	1:QA:144:HIS:CE1	2.51	0.45
1:ZA:141:SER:HB3	1:ZA:144:HIS:HE1	1.80	0.45
1:FB:174:PRO:HG2	1:FB:224:GLN:HB2	1.97	0.45
1:B:148:LEU:HA	1:B:270:LEU:HD11	1.97	0.45
1:O:31:LEU:HD21	1:O:34:ARG:HG3	1.98	0.45
1:W:175:TYR:O	1:W:208:GLY:HA3	2.16	0.45
1:AA:91:LYS:HB2	1:AA:94:GLU:CD	2.42	0.45
1:CA:86:VAL:HG23	1:CA:253:LEU:HB2	1.99	0.45
1:FA:1:MET:HE3	1:FA:7:ASP:HB3	1.99	0.45
1:NA:174:PRO:HG2	1:NA:224:GLN:HB2	1.98	0.45
1:SA:166:LEU:HG	1:SA:171:VAL:HB	1.98	0.45
1:F:22:GLU:O	1:F:26:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:262:LEU:HD23	1:H:262:LEU:H	1.82	0.45
1:J:141:SER:HB3	1:J:144:HIS:CE1	2.51	0.45
1:O:31:LEU:O	1:O:31:LEU:HD23	2.17	0.45
1:S:27:LEU:O	1:S:31:LEU:HB2	2.17	0.45
1:X:181:ARG:HA	1:X:212:TRP:HE1	1.82	0.45
1:Y:177:LEU:HD11	1:Y:219:ALA:HB1	1.99	0.45
1:AA:262:LEU:HD23	1:AA:262:LEU:H	1.82	0.45
1:EA:230:GLU:OE2	1:EA:260:ARG:HB2	2.17	0.45
1:IA:141:SER:HB3	1:IA:144:HIS:CE1	2.52	0.45
1:ZA:108:ASP:HA	1:ZA:111:ILE:HG22	1.97	0.45
1:FB:197:PRO:HG2	1:FB:200:GLN:HE22	1.82	0.45
1:K:40:LYS:HB2	1:K:40:LYS:HE2	1.82	0.45
1:O:188:MET:HE2	1:O:199:LEU:HD22	1.97	0.45
1:AA:155:PHE:HE1	1:AA:202:VAL:HG21	1.81	0.45
1:BA:162:ALA:HB1	1:BA:268:VAL:HG11	1.99	0.45
1:HA:192:THR:HG21	1:HA:197:PRO:HA	1.99	0.45
1:KA:152:LEU:HD12	1:KA:187:LEU:HD13	1.98	0.45
1:UA:111:ILE:HG13	1:UA:112:GLU:N	2.32	0.45
1:GB:198:VAL:HA	1:GB:201:HIS:HB3	1.98	0.45
1:A0:36:VAL:HG23	1:A0:37:VAL:HG13	1.99	0.45
1:B:29:VAL:HG11	1:IA:170:GLY:HA2	1.99	0.45
1:C:185:GLN:HE21	1:C:186:GLN:HE21	1.65	0.45
1:H:197:PRO:HG2	1:H:200:GLN:HE22	1.82	0.45
1:T:222:ILE:HG23	1:T:229:PHE:HE2	1.82	0.45
1:X:84:LEU:HD12	1:X:255:GLU:HB3	1.99	0.45
1:Y:141:SER:HB3	1:Y:144:HIS:CE1	2.51	0.45
1:Z:221:LEU:HB3	1:Z:268:VAL:HB	1.99	0.45
1:JA:21:THR:HA	1:JA:24:ARG:NH1	2.31	0.45
1:RA:148:LEU:HB3	1:RA:271:ARG:O	2.17	0.45
1:WA:148:LEU:HD13	1:WA:272:GLY:HA2	1.99	0.45
1:A:114:ALA:O	1:A:117:ILE:HG22	2.16	0.45
1:C:131:ALA:HB1	1:R:58:LEU:HD13	1.99	0.45
1:E:181:ARG:HA	1:E:212:TRP:HE1	1.82	0.45
1:L:51:SER:HA	1:L:78:VAL:HG13	1.99	0.45
1:N:202:VAL:O	1:N:206:PHE:HB3	2.17	0.45
1:CA:187:LEU:O	1:CA:190:THR:HG23	2.17	0.45
1:GA:188:MET:HE2	1:GA:188:MET:HA	1.99	0.45
1:JA:185:GLN:O	1:JA:189:GLU:HG2	2.17	0.45
1:AB:198:VAL:HA	1:AB:201:HIS:HB3	1.99	0.45
1:BB:241:TYR:HE1	1:BB:244:HIS:HB3	1.81	0.45
1:K:220:MET:N	1:K:220:MET:HE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:141:SER:HB3	1:O:144:HIS:CE1	2.52	0.44
1:R:91:LYS:NZ	1:R:248:SER:HB3	2.32	0.44
1:R:148:LEU:HA	1:R:270:LEU:HD11	1.99	0.44
1:R:219:ALA:HB3	1:R:270:LEU:HD23	1.99	0.44
1:Y:220:MET:N	1:Y:220:MET:HE2	2.31	0.44
1:BA:160:VAL:HG21	1:YA:188:MET:HB3	1.99	0.44
1:CA:156:PRO:HG3	1:CA:202:VAL:HG12	1.99	0.44
1:OA:141:SER:HB3	1:OA:144:HIS:CE1	2.53	0.44
1:TA:162:ALA:HB1	1:TA:268:VAL:HG11	1.99	0.44
1:BB:9:ALA:HB2	1:BB:241:TYR:HB2	2.00	0.44
1:GB:91:LYS:HZ2	1:GB:92:ARG:N	2.15	0.44
1:A0:148:LEU:HA	1:A0:270:LEU:HD11	2.00	0.44
1:A:158:VAL:O	1:A:161:ARG:HG2	2.18	0.44
1:K:202:VAL:O	1:K:206:PHE:HB3	2.17	0.44
1:L:192:THR:HG21	1:L:197:PRO:HB3	2.00	0.44
1:AA:141:SER:HB3	1:AA:144:HIS:CE1	2.52	0.44
1:DA:115:ARG:O	1:DA:119:ILE:HG12	2.17	0.44
1:JA:148:LEU:HA	1:JA:270:LEU:HD11	1.99	0.44
1:LA:36:VAL:HG23	1:LA:37:VAL:HG13	1.98	0.44
1:PA:192:THR:HG21	1:PA:197:PRO:HA	1.98	0.44
1:QA:220:MET:HE2	1:QA:220:MET:N	2.32	0.44
1:HB:126:PHE:HA	1:HB:137:ILE:HG22	1.98	0.44
1:B:5:MET:O	1:B:5:MET:HG3	2.16	0.44
1:B:141:SER:HB3	1:B:144:HIS:HE1	1.83	0.44
1:I:220:MET:HE3	1:I:220:MET:HA	1.98	0.44
1:K:171:VAL:HG13	1:K:225:ARG:HG3	2.00	0.44
1:M:156:PRO:HG3	1:M:202:VAL:HG12	1.99	0.44
1:O:22:GLU:O	1:O:26:THR:HG22	2.18	0.44
1:W:27:LEU:HA	1:W:27:LEU:HD23	1.64	0.44
1:X:201:HIS:HA	1:X:204:ARG:HD2	2.00	0.44
1:IA:192:THR:HG21	1:IA:197:PRO:HA	2.00	0.44
1:VA:205:LEU:H	1:VA:205:LEU:HD23	1.80	0.44
1:XA:141:SER:HB3	1:XA:144:HIS:CE1	2.52	0.44
1:YA:162:ALA:HB1	1:YA:268:VAL:HG11	1.99	0.44
1:CB:232:THR:HB	1:CB:258:THR:HG22	2.00	0.44
1:GB:36:VAL:HG23	1:GB:37:VAL:HG13	1.99	0.44
1:C:185:GLN:HG3	1:C:186:GLN:N	2.32	0.44
1:E:126:PHE:CD1	1:E:137:ILE:HD13	2.52	0.44
1:V:36:VAL:HG23	1:V:37:VAL:HG13	1.99	0.44
1:X:232:THR:HB	1:X:258:THR:HG22	1.99	0.44
1:DA:119:ILE:O	1:DA:123:ARG:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:18:GLU:OE1	1:HA:18:GLU:N	2.47	0.44
1:HA:35:LYS:HB3	2:8:129:LYS:HD2	1.99	0.44
1:KA:213:ALA:HA	1:KA:214:PRO:HD3	1.86	0.44
1:RA:223:SER:HB3	1:RA:266:ALA:HB1	1.99	0.44
1:UA:197:PRO:HG2	1:UA:200:GLN:HE22	1.83	0.44
1:UA:198:VAL:HA	1:UA:201:HIS:HB3	1.99	0.44
1:AB:163:LEU:O	1:AB:167:ARG:HG2	2.18	0.44
1:BB:219:ALA:HB3	1:BB:270:LEU:HD23	1.98	0.44
1:A:35:LYS:HD3	2:2:128:LEU:HD13	2.00	0.44
1:E:172:ASP:HB3	1:V:29:VAL:HG22	1.98	0.44
1:F:5:MET:HE1	1:AA:10:PRO:C	2.42	0.44
1:M:37:VAL:HG12	1:M:229:PHE:HB2	2.00	0.44
1:P:199:LEU:HD12	1:P:199:LEU:H	1.81	0.44
1:V:241:TYR:HE1	1:V:244:HIS:HB3	1.82	0.44
1:EA:175:TYR:O	1:EA:208:GLY:HA3	2.17	0.44
1:OA:11:ILE:HB	1:OA:16:TRP:NE1	2.33	0.44
1:WA:159:LEU:HA	1:WA:162:ALA:HB3	1.99	0.44
1:YA:220:MET:N	1:YA:220:MET:HE2	2.33	0.44
1:AB:141:SER:HB3	1:AB:144:HIS:HE1	1.82	0.44
1:BB:57:ALA:HA	1:BB:74:ARG:HD2	2.00	0.44
1:CB:175:TYR:O	1:CB:208:GLY:HA3	2.17	0.44
1:A0:163:LEU:O	1:A0:167:ARG:HG2	2.17	0.44
1:A:148:LEU:HD13	1:A:272:GLY:HA2	1.99	0.44
1:F:220:MET:N	1:F:220:MET:HE2	2.32	0.44
1:K:219:ALA:HB3	1:K:270:LEU:HD23	1.99	0.44
1:T:192:THR:HG21	1:T:197:PRO:HA	1.99	0.44
1:W:27:LEU:HG	1:W:114:ALA:HB1	1.99	0.44
1:W:31:LEU:HD23	1:W:31:LEU:O	2.18	0.44
1:BA:117:ILE:HD12	1:BA:117:ILE:HA	1.91	0.44
1:DA:10:PRO:HG3	1:DA:244:HIS:CD2	2.53	0.44
1:IA:175:TYR:O	1:IA:208:GLY:HA3	2.18	0.44
1:NA:241:TYR:CE1	1:NA:244:HIS:HB3	2.49	0.44
1:PA:146:LEU:HD11	1:PA:162:ALA:HB2	1.98	0.44
1:WA:175:TYR:HB2	1:WA:206:PHE:HE1	1.82	0.44
1:J:188:MET:HE3	1:J:188:MET:HA	2.00	0.44
1:K:262:LEU:HD12	1:R:104:ASP:HB3	1.98	0.44
1:M:52:LEU:HD23	1:M:52:LEU:HA	1.86	0.44
1:R:180:GLY:H	1:R:183:VAL:HG22	1.83	0.44
1:S:27:LEU:HD23	1:S:27:LEU:HA	1.81	0.44
1:S:181:ARG:HA	1:S:212:TRP:HE1	1.83	0.44
1:X:162:ALA:HB1	1:X:268:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CA:172:ASP:OD1	1:CA:172:ASP:C	2.60	0.44
1:FA:31:LEU:HD21	1:FA:34:ARG:HG3	1.99	0.44
1:IA:104:ASP:HB3	1:GB:262:LEU:HD12	1.98	0.44
1:RA:148:LEU:HA	1:RA:270:LEU:HD11	2.00	0.44
1:SA:185:GLN:O	1:SA:189:GLU:HG3	2.18	0.44
1:VA:14:LYS:HZ1	1:VA:98:ILE:HG23	1.82	0.44
1:WA:146:LEU:HD11	1:WA:162:ALA:HB2	1.99	0.44
1:A0:160:VAL:HG21	1:FA:188:MET:HG3	1.99	0.44
1:F:156:PRO:O	1:F:159:LEU:HD12	2.17	0.44
1:J:148:LEU:HA	1:J:270:LEU:HD11	2.00	0.44
1:S:158:VAL:HA	1:S:161:ARG:HE	1.82	0.44
1:S:175:TYR:O	1:S:208:GLY:HA3	2.17	0.44
1:T:233:VAL:HG23	1:T:257:MET:HB3	2.00	0.44
1:X:22:GLU:O	1:X:26:THR:HG22	2.18	0.44
1:EA:163:LEU:O	1:EA:167:ARG:HG2	2.18	0.44
1:FA:156:PRO:HG3	1:FA:202:VAL:HG12	2.00	0.44
1:IA:1:MET:N	1:YA:13:ALA:HB2	2.33	0.44
1:VA:148:LEU:HA	1:VA:270:LEU:HD11	2.00	0.44
1:YA:163:LEU:O	1:YA:167:ARG:HG2	2.18	0.44
1:AB:27:LEU:HD23	1:AB:27:LEU:HA	1.82	0.44
1:HB:33:ALA:HB2	1:HB:122:ASP:OD1	2.17	0.44
1:A0:175:TYR:O	1:A0:208:GLY:HA3	2.18	0.44
1:A:49:SER:OG	1:O:78:VAL:HG21	2.18	0.44
1:C:175:TYR:HB3	1:C:221:LEU:HD11	2.00	0.44
1:V:230:GLU:OE2	1:V:260:ARG:HB2	2.17	0.44
1:HA:148:LEU:HA	1:HA:270:LEU:HD11	2.00	0.44
1:NA:141:SER:HB3	1:NA:144:HIS:CE1	2.53	0.44
1:ZA:27:LEU:HD23	1:ZA:27:LEU:HA	1.85	0.44
1:A0:9:ALA:HB2	1:A0:241:TYR:HB2	1.98	0.43
1:A0:141:SER:HB3	1:A0:144:HIS:CE1	2.52	0.43
1:A:119:ILE:HD11	1:A:214:PRO:HB2	2.00	0.43
1:L:11:ILE:HD13	1:L:11:ILE:HA	1.87	0.43
1:N:188:MET:HB3	1:MA:160:VAL:HG21	2.00	0.43
1:T:22:GLU:O	1:T:26:THR:HG22	2.17	0.43
1:GA:171:VAL:HG13	1:GA:225:ARG:HG3	1.99	0.43
1:MA:188:MET:HA	1:MA:188:MET:HE3	1.99	0.43
1:NA:179:LEU:HB3	1:NA:184:TYR:HB2	2.00	0.43
1:TA:45:TRP:HE1	1:GB:100:ARG:HG2	1.83	0.43
1:UA:27:LEU:HD23	1:UA:27:LEU:HA	1.78	0.43
1:UA:156:PRO:HG3	1:UA:202:VAL:HG12	1.99	0.43
1:I:79:GLN:HA	1:I:80:PRO:HD3	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:223:SER:HB3	1:N:266:ALA:HB1	2.00	0.43
1:JA:40:LYS:HD2	1:JA:40:LYS:N	2.33	0.43
1:MA:9:ALA:HB2	1:MA:241:TYR:HB2	1.98	0.43
1:NA:58:LEU:HD12	1:NA:73:VAL:HG12	2.00	0.43
1:QA:208:GLY:HA2	1:QA:209:PRO:HD3	1.86	0.43
1:UA:39:PHE:CD2	2:17:127:SER:HB2	2.53	0.43
1:AB:166:LEU:HD23	1:AB:167:ARG:HD2	1.99	0.43
1:DB:4:LEU:HD12	1:DB:240:GLY:HA3	1.99	0.43
1:EB:197:PRO:HG2	1:EB:200:GLN:HE22	1.83	0.43
1:GB:148:LEU:HD22	1:GB:272:GLY:HA2	1.99	0.43
1:HB:203:ARG:HH12	1:HB:208:GLY:H	1.65	0.43
1:A0:166:LEU:HD23	1:A0:167:ARG:HD2	2.00	0.43
1:A:160:VAL:HG21	1:H:188:MET:HB3	2.00	0.43
1:B:79:GLN:HA	1:B:80:PRO:HD3	1.81	0.43
1:G:40:LYS:HE3	1:G:40:LYS:HB3	1.92	0.43
1:I:22:GLU:O	1:I:26:THR:HG22	2.19	0.43
1:W:137:ILE:HD11	1:W:229:PHE:CE1	2.53	0.43
1:X:213:ALA:HA	1:X:214:PRO:HD3	1.88	0.43
1:SA:175:TYR:O	1:SA:208:GLY:HA3	2.18	0.43
1:VA:126:PHE:HA	1:VA:137:ILE:HG22	2.01	0.43
1:M:40:LYS:NZ	1:M:231:LEU:H	2.17	0.43
1:X:222:ILE:HG23	1:X:229:PHE:HE2	1.84	0.43
1:DA:232:THR:HB	1:DA:258:THR:HG22	2.00	0.43
1:GA:75:LYS:HE3	1:GA:75:LYS:HB2	1.76	0.43
1:MA:119:ILE:HD11	1:MA:214:PRO:HB2	1.99	0.43
1:ZA:203:ARG:HD2	1:ZA:203:ARG:HA	1.80	0.43
1:EB:88:PHE:CZ	1:EB:251:LEU:HB2	2.54	0.43
1:GB:218:GLY:HA3	1:GB:270:LEU:O	2.19	0.43
1:HB:188:MET:HA	1:HB:188:MET:HE2	2.00	0.43
1:A:40:LYS:HE3	1:A:40:LYS:HB3	1.85	0.43
1:B:76:ARG:HH11	1:S:48:SER:HB3	1.84	0.43
1:F:36:VAL:HG23	1:F:37:VAL:HG13	2.00	0.43
1:G:219:ALA:HB3	1:G:270:LEU:HD23	2.00	0.43
1:P:22:GLU:O	1:P:26:THR:HG22	2.18	0.43
1:Q:40:LYS:HE3	1:Q:40:LYS:HB3	1.90	0.43
1:W:129:PHE:HD1	1:W:132:GLY:H	1.66	0.43
1:AA:262:LEU:O	1:AA:264:PRO:HD3	2.17	0.43
1:BA:230:GLU:OE2	1:BA:260:ARG:HB2	2.18	0.43
1:LA:182:THR:O	1:LA:186:GLN:HG2	2.19	0.43
1:VA:181:ARG:NH2	1:VA:182:THR:HG22	2.33	0.43
1:XA:148:LEU:HA	1:XA:270:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:141:SER:HB3	1:AB:144:HIS:CE1	2.54	0.43
2:10:125:ILE:C	2:10:125:ILE:HD12	2.43	0.43
1:C:141:SER:HB3	1:C:144:HIS:CE1	2.53	0.43
1:E:40:LYS:HE3	1:E:40:LYS:HB3	1.92	0.43
1:J:40:LYS:HZ3	1:J:231:LEU:H	1.65	0.43
1:J:175:TYR:O	1:J:208:GLY:HA3	2.19	0.43
1:M:141:SER:HB3	1:M:144:HIS:CE1	2.54	0.43
1:O:175:TYR:O	1:O:208:GLY:HA3	2.18	0.43
1:S:185:GLN:HA	1:S:188:MET:HB2	2.01	0.43
1:Y:175:TYR:O	1:Y:208:GLY:HA3	2.18	0.43
1:AA:98:ILE:HA	1:AA:102:ALA:HB3	2.01	0.43
1:CA:115:ARG:O	1:CA:119:ILE:HG12	2.19	0.43
1:DA:29:VAL:HG21	1:BB:170:GLY:HA2	2.00	0.43
1:EA:36:VAL:HG23	1:EA:37:VAL:HG13	2.00	0.43
1:LA:230:GLU:OE2	1:LA:260:ARG:HB2	2.18	0.43
1:UA:196:TYR:HA	1:UA:197:PRO:HD2	1.85	0.43
1:CB:223:SER:HB3	1:CB:266:ALA:HB1	1.99	0.43
1:E:34:ARG:HH22	1:E:237:PHE:HE1	1.65	0.43
1:E:192:THR:HG21	1:E:197:PRO:HA	2.00	0.43
1:G:71:VAL:HG13	1:N:86:VAL:HG22	2.00	0.43
1:I:94:GLU:O	1:I:98:ILE:HG23	2.19	0.43
1:I:148:LEU:HD13	1:I:272:GLY:HA2	2.01	0.43
1:J:148:LEU:HD22	1:J:272:GLY:HA2	2.00	0.43
1:O:36:VAL:HG23	1:O:37:VAL:HG13	2.00	0.43
1:R:175:TYR:HB3	1:R:221:LEU:HD11	2.01	0.43
1:T:75:LYS:HZ2	1:KA:80:PRO:HB2	1.84	0.43
1:X:81:LEU:HG	1:X:258:THR:HB	1.99	0.43
1:Z:40:LYS:HE3	1:Z:40:LYS:HB3	1.90	0.43
1:Z:152:LEU:HG	1:Z:187:LEU:HD12	2.00	0.43
1:AA:230:GLU:OE2	1:AA:260:ARG:HB2	2.18	0.43
1:BA:52:LEU:HD23	1:BA:52:LEU:HA	1.90	0.43
1:BA:73:VAL:HG12	1:IA:84:LEU:HD23	2.00	0.43
1:MA:262:LEU:O	1:MA:264:PRO:HD3	2.19	0.43
1:VA:126:PHE:HD2	1:VA:216:VAL:HG11	1.83	0.43
1:WA:198:VAL:HA	1:WA:201:HIS:HB3	2.00	0.43
1:YA:11:ILE:HB	1:YA:16:TRP:NE1	2.34	0.43
1:YA:203:ARG:HD2	1:YA:203:ARG:HA	1.86	0.43
1:H:158:VAL:HA	1:H:161:ARG:NE	2.34	0.43
1:J:196:TYR:HA	1:J:197:PRO:HD2	1.81	0.43
1:Q:10:PRO:HG3	1:Q:244:HIS:ND1	2.34	0.43
1:EA:22:GLU:HG3	1:EA:107:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FA:27:LEU:HD23	1:FA:27:LEU:HA	1.87	0.43
1:MA:148:LEU:HB3	1:MA:272:GLY:HA2	2.00	0.43
1:OA:179:LEU:HD22	1:OA:184:TYR:HA	1.99	0.43
1:QA:187:LEU:O	1:QA:190:THR:HG23	2.19	0.43
1:XA:31:LEU:HD21	1:XA:34:ARG:HG3	2.00	0.43
1:HB:220:MET:HE2	1:HB:220:MET:N	2.34	0.43
1:D:29:VAL:HG11	1:X:170:GLY:HA2	2.00	0.43
1:F:179:LEU:HD23	1:F:183:VAL:HG23	2.01	0.43
1:G:203:ARG:HA	1:G:203:ARG:HD2	1.72	0.43
1:I:88:PHE:CE2	1:I:110:VAL:HG22	2.53	0.43
1:I:115:ARG:O	1:I:119:ILE:HG12	2.19	0.43
1:W:229:PHE:N	1:W:229:PHE:CD2	2.87	0.43
1:Z:73:VAL:HG12	1:FA:84:LEU:HD23	2.01	0.43
1:BA:100:ARG:HG2	1:FB:45:TRP:HE1	1.84	0.43
1:CA:162:ALA:HB1	1:CA:268:VAL:HG11	2.01	0.43
1:EA:26:THR:HG21	1:EA:111:ILE:HG13	2.01	0.43
1:OA:166:LEU:HG	1:OA:171:VAL:HB	2.01	0.43
1:PA:230:GLU:OE2	1:PA:260:ARG:HB2	2.19	0.43
1:FB:230:GLU:OE2	1:FB:260:ARG:HB2	2.19	0.43
1:B:17:ALA:O	1:B:21:THR:HG23	2.19	0.43
1:C:192:THR:HG21	1:C:197:PRO:HA	2.01	0.43
1:I:177:LEU:HD11	1:I:219:ALA:HB1	2.00	0.43
1:R:35:LYS:HE3	1:R:35:LYS:HA	2.01	0.43
1:S:166:LEU:HG	1:S:171:VAL:HB	2.01	0.43
1:CA:262:LEU:O	1:CA:264:PRO:HD3	2.19	0.43
1:UA:152:LEU:HD12	1:UA:187:LEU:HD12	2.01	0.43
1:VA:5:MET:O	1:VA:241:TYR:HB3	2.19	0.43
1:YA:152:LEU:HG	1:YA:187:LEU:HD12	2.01	0.43
1:ZA:9:ALA:HB2	1:ZA:241:TYR:HB2	2.00	0.43
1:DB:98:ILE:HA	1:DB:102:ALA:HB3	2.00	0.43
1:EB:148:LEU:HA	1:EB:270:LEU:HD11	2.00	0.43
1:EB:219:ALA:HB3	1:EB:270:LEU:HD23	2.01	0.43
1:HB:155:PHE:CD1	1:HB:155:PHE:C	2.97	0.43
1:D:137:ILE:HD13	1:D:137:ILE:HA	1.94	0.42
1:E:129:PHE:HZ	1:K:73:VAL:HG21	1.84	0.42
1:F:100:ARG:HG2	1:UA:45:TRP:HE1	1.84	0.42
1:K:184:TYR:HE1	1:K:210:LEU:HD21	1.84	0.42
1:M:171:VAL:HG22	1:M:225:ARG:HE	1.84	0.42
1:N:22:GLU:O	1:N:26:THR:HG22	2.19	0.42
1:P:203:ARG:HH22	1:P:208:GLY:H	1.66	0.42
1:Q:52:LEU:HD23	1:Q:52:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:223:SER:HB3	1:S:266:ALA:HB1	1.99	0.42
1:T:156:PRO:HG3	1:T:202:VAL:HG12	2.01	0.42
1:Z:202:VAL:O	1:Z:206:PHE:HB3	2.19	0.42
1:GA:91:LYS:O	1:GA:95:LEU:HD23	2.19	0.42
1:IA:166:LEU:HG	1:IA:171:VAL:HB	2.00	0.42
1:LA:262:LEU:HD23	1:LA:262:LEU:H	1.84	0.42
1:RA:135:THR:HG23	1:RA:139:GLU:HG3	2.01	0.42
1:UA:201:HIS:O	1:UA:204:ARG:HD3	2.19	0.42
1:VA:2:ASN:C	1:VA:2:ASN:OD1	2.61	0.42
1:XA:33:ALA:HB2	1:XA:122:ASP:OD1	2.19	0.42
1:BB:163:LEU:HG	1:BB:167:ARG:HE	1.84	0.42
1:DB:40:LYS:HE3	1:DB:40:LYS:HB3	1.83	0.42
1:EB:41:GLY:HA2	1:EB:42:PRO:HD3	1.92	0.42
1:HB:167:ARG:HD2	1:HB:167:ARG:HA	1.78	0.42
1:C:241:TYR:HE1	1:C:244:HIS:HB3	1.85	0.42
1:I:52:LEU:HD23	1:I:52:LEU:HA	1.88	0.42
1:I:241:TYR:CE1	1:I:244:HIS:HB3	2.53	0.42
1:J:27:LEU:HD23	1:J:27:LEU:HA	1.81	0.42
1:K:27:LEU:HD23	1:K:27:LEU:HA	1.80	0.42
1:N:163:LEU:O	1:N:167:ARG:HG2	2.20	0.42
1:S:4:LEU:HD12	1:S:240:GLY:HA3	2.01	0.42
1:X:40:LYS:HE3	1:X:40:LYS:HB3	1.86	0.42
1:X:239:ILE:HD11	2:18:123:LEU:HD21	2.02	0.42
1:NA:188:MET:HE3	1:NA:199:LEU:HD22	2.01	0.42
1:VA:5:MET:HE2	1:VA:5:MET:HA	2.01	0.42
1:XA:167:ARG:HD2	1:XA:167:ARG:HA	1.77	0.42
1:YA:192:THR:HG21	1:YA:197:PRO:HB3	2.01	0.42
1:BB:167:ARG:N	1:BB:167:ARG:HD3	2.34	0.42
1:A:209:PRO:HB2	1:A:211:ILE:HD11	2.02	0.42
1:C:141:SER:HB3	1:C:144:HIS:HE1	1.84	0.42
1:BA:40:LYS:HE2	1:BA:230:GLU:HB2	2.00	0.42
1:DA:223:SER:HB3	1:DA:266:ALA:HB1	2.00	0.42
1:RA:146:LEU:HD11	1:RA:162:ALA:HB2	2.00	0.42
1:DB:52:LEU:HD23	1:DB:52:LEU:HA	1.89	0.42
1:HB:27:LEU:HD23	1:HB:27:LEU:HA	1.82	0.42
1:H:148:LEU:HA	1:H:270:LEU:HD11	2.02	0.42
1:P:32:ALA:HA	1:P:35:LYS:HZ1	1.84	0.42
1:R:229:PHE:HZ	1:R:267:ALA:HB2	1.84	0.42
1:T:213:ALA:HA	1:T:214:PRO:HD3	1.90	0.42
1:V:220:MET:SD	1:V:269:PRO:HA	2.59	0.42
1:AA:91:LYS:HE2	1:AA:91:LYS:HB3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IA:46:ASP:OD1	1:IA:46:ASP:C	2.62	0.42
1:KA:179:LEU:HD23	1:KA:183:VAL:HG13	2.01	0.42
1:KA:202:VAL:O	1:KA:206:PHE:HB3	2.19	0.42
1:KA:230:GLU:OE2	1:KA:260:ARG:HB2	2.19	0.42
1:LA:96:GLU:H	1:LA:96:GLU:HG2	1.59	0.42
1:OA:2:ASN:OD1	1:OA:2:ASN:C	2.62	0.42
1:OA:152:LEU:HD12	1:OA:155:PHE:HD2	1.84	0.42
1:PA:40:LYS:HE3	1:PA:40:LYS:HB3	1.91	0.42
1:E:79:GLN:HA	1:E:80:PRO:HD3	1.85	0.42
1:G:181:ARG:HA	1:G:212:TRP:HE1	1.84	0.42
1:H:5:MET:HE3	1:XA:10:PRO:HA	2.01	0.42
1:N:203:ARG:HA	1:N:203:ARG:HD2	1.78	0.42
1:P:148:LEU:HB3	1:P:271:ARG:O	2.19	0.42
1:R:14:LYS:NZ	1:R:18:GLU:HB2	2.35	0.42
1:T:196:TYR:HA	1:T:197:PRO:HD2	1.87	0.42
1:Y:187:LEU:O	1:Y:190:THR:HG23	2.19	0.42
1:BA:244:HIS:CD2	1:BA:244:HIS:C	2.97	0.42
1:HA:29:VAL:HG11	1:KA:167:ARG:HH12	1.84	0.42
1:UA:202:VAL:O	1:UA:206:PHE:HB3	2.19	0.42
1:DB:189:GLU:H	1:DB:189:GLU:HG3	1.64	0.42
1:HB:56:GLU:OE1	1:HB:56:GLU:N	2.53	0.42
1:C:209:PRO:HB2	1:C:211:ILE:HD11	2.01	0.42
1:D:94:GLU:O	1:D:98:ILE:HG23	2.20	0.42
1:J:40:LYS:HE3	1:J:40:LYS:HB3	1.89	0.42
1:T:180:GLY:O	1:T:184:TYR:HB2	2.19	0.42
1:W:196:TYR:HA	1:W:197:PRO:HD2	1.86	0.42
1:Y:35:LYS:HE3	1:Y:35:LYS:HA	2.01	0.42
1:LA:1:MET:HE3	1:LA:5:MET:HA	2.02	0.42
1:OA:201:HIS:HA	1:OA:204:ARG:HD2	2.00	0.42
1:UA:241:TYR:CE1	1:UA:244:HIS:HB3	2.53	0.42
1:BB:247:GLN:OE1	1:BB:247:GLN:N	2.53	0.42
1:EB:202:VAL:O	1:EB:206:PHE:HB3	2.20	0.42
1:GB:52:LEU:HD23	1:GB:52:LEU:HA	1.88	0.42
1:A0:229:PHE:HB3	1:A0:259:PHE:HE1	1.85	0.42
1:B:158:VAL:HA	1:B:161:ARG:NE	2.34	0.42
1:E:141:SER:HB3	1:E:144:HIS:HE1	1.84	0.42
1:I:197:PRO:HG2	1:I:200:GLN:HE22	1.84	0.42
1:M:175:TYR:HD1	1:M:223:SER:HA	1.85	0.42
1:P:3:ASP:O	1:P:5:MET:HE2	2.19	0.42
1:S:182:THR:O	1:S:186:GLN:HG2	2.18	0.42
1:S:198:VAL:HA	1:S:201:HIS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:40:LYS:HE3	1:T:40:LYS:HB3	1.90	0.42
1:AA:137:ILE:HD11	1:AA:229:PHE:CD1	2.55	0.42
1:HA:187:LEU:O	1:HA:190:THR:HG23	2.20	0.42
1:JA:36:VAL:HG23	1:JA:37:VAL:HG13	2.01	0.42
1:KA:163:LEU:O	1:KA:167:ARG:HG2	2.19	0.42
1:LA:27:LEU:HD23	1:LA:27:LEU:HA	1.82	0.42
1:RA:141:SER:HB3	1:RA:144:HIS:HE1	1.85	0.42
1:WA:197:PRO:HG2	1:WA:200:GLN:HE22	1.84	0.42
1:XA:15:ALA:HA	1:XA:98:ILE:HD11	2.01	0.42
1:CB:152:LEU:HA	1:CB:155:PHE:CD1	2.54	0.42
1:DB:188:MET:HE3	1:DB:188:MET:HA	2.01	0.42
1:EB:148:LEU:HB3	1:EB:272:GLY:HA2	2.02	0.42
1:B:175:TYR:O	1:B:208:GLY:HA3	2.19	0.42
1:C:43:LEU:HD12	1:C:43:LEU:H	1.84	0.42
1:D:26:THR:HA	1:D:29:VAL:HG12	2.01	0.42
1:D:145:ALA:HB3	1:D:271:ARG:NH2	2.34	0.42
1:E:170:GLY:HA2	1:V:29:VAL:HG11	2.01	0.42
1:F:146:LEU:HD13	1:F:161:ARG:HD2	2.01	0.42
1:G:140:ALA:HB1	1:G:264:PRO:HB3	2.00	0.42
1:I:14:LYS:HZ1	1:I:98:ILE:HG13	1.83	0.42
1:L:45:TRP:HE1	1:AB:100:ARG:HG2	1.84	0.42
1:L:79:GLN:HA	1:L:80:PRO:HD3	1.76	0.42
1:M:119:ILE:HD13	1:M:119:ILE:HA	1.87	0.42
1:Q:156:PRO:HG3	1:Q:202:VAL:HG12	2.02	0.42
1:S:179:LEU:HD22	1:S:184:TYR:HD1	1.85	0.42
1:X:10:PRO:HG3	1:X:244:HIS:CG	2.55	0.42
1:Y:95:LEU:HA	1:Y:98:ILE:HG22	2.01	0.42
1:BA:200:GLN:OE1	1:BA:200:GLN:N	2.52	0.42
1:QA:179:LEU:HD23	1:QA:183:VAL:HG22	2.02	0.42
1:VA:203:ARG:HA	1:VA:203:ARG:HD2	1.78	0.42
1:YA:137:ILE:HD12	1:YA:137:ILE:HA	1.91	0.42
1:AB:146:LEU:HD11	1:AB:162:ALA:HB2	2.02	0.42
1:GB:177:LEU:HD11	1:GB:219:ALA:HB1	2.01	0.42
1:D:160:VAL:O	1:D:163:LEU:HG	2.20	0.42
1:E:172:ASP:H	1:E:225:ARG:HD3	1.85	0.42
1:E:190:THR:HB	1:E:192:THR:HG23	2.02	0.42
1:M:27:LEU:HD23	2:11:125:ILE:HD12	2.02	0.42
1:N:15:ALA:O	1:N:19:ILE:HG22	2.20	0.42
1:Q:88:PHE:HE2	1:Q:110:VAL:HG22	1.83	0.42
1:BA:171:VAL:HG13	1:BA:225:ARG:HG3	2.01	0.42
1:IA:17:ALA:O	1:IA:21:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JA:179:LEU:HD23	1:JA:183:VAL:HG23	2.02	0.42
1:RA:2:ASN:OD1	1:RA:4:LEU:HB2	2.20	0.42
1:XA:175:TYR:O	1:XA:208:GLY:HA3	2.20	0.42
1:C:27:LEU:HD23	1:C:27:LEU:HA	1.86	0.42
1:C:152:LEU:HD23	1:C:152:LEU:HA	1.92	0.42
1:G:33:ALA:HB2	1:G:122:ASP:OD1	2.20	0.42
1:L:22:GLU:O	1:L:26:THR:HG22	2.20	0.42
1:M:181:ARG:HA	1:M:212:TRP:HE1	1.84	0.42
1:O:27:LEU:HD23	1:O:27:LEU:HA	1.77	0.42
1:O:158:VAL:HA	1:O:161:ARG:NE	2.35	0.42
1:S:108:ASP:O	1:S:111:ILE:HG22	2.19	0.42
1:V:76:ARG:HD2	1:JA:48:SER:HB3	2.02	0.42
1:DA:55:THR:HG22	1:DA:76:ARG:HA	2.02	0.42
1:IA:229:PHE:HB3	1:IA:259:PHE:HE1	1.85	0.42
1:JA:21:THR:HA	1:JA:24:ARG:HH12	1.84	0.42
1:LA:141:SER:HB3	1:LA:144:HIS:CE1	2.54	0.42
1:MA:196:TYR:HA	1:MA:197:PRO:HD2	1.83	0.42
1:NA:2:ASN:C	1:NA:2:ASN:OD1	2.62	0.42
1:OA:123:ARG:HH21	1:OA:215:GLY:HA2	1.85	0.42
1:WA:79:GLN:HA	1:WA:80:PRO:HD3	1.92	0.42
1:YA:134:ILE:HD11	1:YA:259:PHE:N	2.31	0.42
1:YA:141:SER:HB3	1:YA:144:HIS:CE1	2.54	0.42
1:CB:32:ALA:HA	1:CB:35:LYS:HE2	2.02	0.42
1:EB:27:LEU:HD23	1:EB:27:LEU:HA	1.83	0.42
1:EB:174:PRO:HB2	1:EB:224:GLN:HB2	2.01	0.42
1:FB:212:TRP:CZ2	1:FB:214:PRO:HG3	2.55	0.42
1:GB:79:GLN:HA	1:GB:80:PRO:HD3	1.91	0.42
1:HB:36:VAL:HG23	1:HB:37:VAL:HG13	2.01	0.42
1:K:158:VAL:HA	1:K:161:ARG:NE	2.35	0.41
1:O:209:PRO:HB2	1:O:211:ILE:HD11	2.02	0.41
1:T:162:ALA:HB1	1:T:268:VAL:HG11	2.01	0.41
1:X:221:LEU:HB3	1:X:268:VAL:HB	2.02	0.41
1:EA:172:ASP:H	1:EA:225:ARG:HD3	1.85	0.41
1:MA:79:GLN:HA	1:MA:80:PRO:HD3	1.81	0.41
1:WA:253:LEU:HD23	1:WA:253:LEU:HA	1.93	0.41
2:4:129:LYS:HE2	2:4:129:LYS:HB3	1.76	0.41
1:A0:33:ALA:HB2	1:A0:122:ASP:OD1	2.20	0.41
1:O:2:ASN:OD1	1:O:2:ASN:C	2.63	0.41
1:P:196:TYR:HA	1:P:197:PRO:HD2	1.87	0.41
1:P:228:ASP:O	1:P:229:PHE:HD1	2.02	0.41
1:R:148:LEU:HD22	1:R:272:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:218:GLY:HA3	1:T:270:LEU:O	2.20	0.41
1:W:160:VAL:HG21	1:OA:188:MET:HB3	2.02	0.41
1:CA:147:ASP:HA	1:CA:271:ARG:HD2	2.02	0.41
1:CA:155:PHE:CE2	1:CA:202:VAL:HG21	2.55	0.41
1:EA:219:ALA:HB3	1:EA:270:LEU:HD23	2.02	0.41
1:HA:175:TYR:O	1:HA:208:GLY:HA3	2.20	0.41
1:IA:35:LYS:H	1:IA:35:LYS:HG2	1.68	0.41
1:KA:111:ILE:HD13	1:KA:111:ILE:HA	1.85	0.41
1:LA:2:ASN:OD1	1:LA:4:LEU:HG	2.19	0.41
1:MA:205:LEU:HD23	1:MA:205:LEU:H	1.85	0.41
1:UA:79:GLN:HA	1:UA:80:PRO:HD3	1.90	0.41
1:VA:222:ILE:HG23	1:VA:229:PHE:HE2	1.85	0.41
1:ZA:155:PHE:CD1	1:ZA:155:PHE:C	2.98	0.41
1:ZA:206:PHE:CD1	1:ZA:206:PHE:C	2.98	0.41
1:CB:31:LEU:HD21	1:CB:34:ARG:HG3	2.02	0.41
1:A0:204:ARG:HD2	1:A0:204:ARG:N	2.33	0.41
1:A:175:TYR:O	1:A:208:GLY:HA3	2.20	0.41
1:B:90:LEU:HD23	1:B:90:LEU:HA	1.82	0.41
1:K:170:GLY:HA2	1:R:29:VAL:HG11	2.02	0.41
1:O:201:HIS:O	1:O:204:ARG:HG3	2.20	0.41
1:Q:27:LEU:HD23	1:Q:27:LEU:HA	1.83	0.41
1:V:242:HIS:HB3	1:V:250:HIS:CE1	2.55	0.41
1:Y:100:ARG:HG2	1:GB:45:TRP:HE1	1.85	0.41
1:Z:86:VAL:HG21	1:Z:117:ILE:HB	2.02	0.41
1:CA:175:TYR:O	1:CA:208:GLY:HA3	2.20	0.41
1:CA:208:GLY:HA2	1:CA:209:PRO:HD3	1.84	0.41
1:EA:81:LEU:HG	1:EA:258:THR:HB	2.02	0.41
1:KA:223:SER:HB3	1:KA:266:ALA:HB1	2.01	0.41
1:PA:179:LEU:HD23	1:PA:183:VAL:HG22	2.02	0.41
1:QA:14:LYS:NZ	1:QA:98:ILE:HG12	2.36	0.41
1:QA:192:THR:HG21	1:QA:197:PRO:HA	2.01	0.41
1:RA:52:LEU:HD23	1:RA:52:LEU:HA	1.87	0.41
1:UA:52:LEU:HD23	1:UA:52:LEU:HA	1.89	0.41
1:XA:86:VAL:HG23	1:XA:253:LEU:HB2	2.03	0.41
1:YA:220:MET:HB2	1:YA:222:ILE:HD11	2.01	0.41
1:BB:40:LYS:HZ3	1:BB:231:LEU:H	1.68	0.41
1:BB:81:LEU:HG	1:BB:258:THR:HB	2.01	0.41
1:GB:51:SER:HA	1:GB:78:VAL:HG12	2.02	0.41
1:GB:190:THR:HB	1:GB:192:THR:HG23	2.02	0.41
1:D:177:LEU:HD21	1:D:179:LEU:HD21	2.03	0.41
1:F:196:TYR:HA	1:F:197:PRO:HD2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:218:GLY:HA3	1:Q:270:LEU:O	2.21	0.41
1:V:198:VAL:HA	1:V:201:HIS:HB3	2.01	0.41
1:Z:196:TYR:HA	1:Z:197:PRO:HD2	1.86	0.41
1:EA:220:MET:HG3	1:EA:269:PRO:HA	2.02	0.41
1:HA:171:VAL:HG13	1:HA:225:ARG:HE	1.85	0.41
1:NA:158:VAL:O	1:NA:161:ARG:HG2	2.20	0.41
1:RA:203:ARG:HA	1:RA:203:ARG:HD2	1.80	0.41
1:TA:5:MET:HE1	1:GB:10:PRO:C	2.45	0.41
1:VA:201:HIS:O	1:VA:204:ARG:HD2	2.20	0.41
1:XA:108:ASP:O	1:XA:111:ILE:HG12	2.20	0.41
1:HB:202:VAL:O	1:HB:206:PHE:HB3	2.20	0.41
1:D:52:LEU:HD23	1:D:52:LEU:HA	1.94	0.41
1:F:181:ARG:HA	1:F:212:TRP:NE1	2.35	0.41
1:G:184:TYR:HB3	1:G:185:GLN:NE2	2.35	0.41
1:G:200:GLN:HB2	1:G:204:ARG:NH1	2.36	0.41
1:H:22:GLU:O	1:H:26:THR:HG22	2.20	0.41
1:J:40:LYS:NZ	1:J:231:LEU:H	2.18	0.41
1:S:11:ILE:HB	1:S:16:TRP:NE1	2.36	0.41
1:S:170:GLY:HA2	1:FB:29:VAL:HG11	2.02	0.41
1:V:52:LEU:HD23	1:V:52:LEU:HA	1.91	0.41
1:W:29:VAL:HG11	1:CB:170:GLY:HA2	2.01	0.41
1:DA:203:ARG:HH12	1:DA:206:PHE:HD2	1.67	0.41
1:FA:17:ALA:O	1:FA:21:THR:HG23	2.20	0.41
1:GA:205:LEU:H	1:GA:205:LEU:HD23	1.86	0.41
1:IA:172:ASP:OD2	1:IA:172:ASP:N	2.53	0.41
1:IA:175:TYR:HB3	1:IA:221:LEU:HD11	2.02	0.41
1:JA:4:LEU:HD23	1:JA:4:LEU:HA	1.82	0.41
1:MA:203:ARG:HA	1:MA:203:ARG:HD2	1.81	0.41
1:OA:259:PHE:C	1:OA:259:PHE:CD1	2.99	0.41
1:QA:55:THR:HG22	1:QA:76:ARG:HA	2.01	0.41
1:RA:199:LEU:HB3	1:UA:204:ARG:HH21	1.85	0.41
1:SA:27:LEU:HD23	1:SA:27:LEU:HA	1.84	0.41
1:CB:86:VAL:HG23	1:CB:253:LEU:HB2	2.02	0.41
1:FB:213:ALA:HA	1:FB:214:PRO:HD3	1.87	0.41
1:G:52:LEU:HD23	1:G:52:LEU:HA	1.89	0.41
1:L:86:VAL:HA	1:L:87:PRO:HD3	1.95	0.41
1:L:219:ALA:C	1:L:220:MET:HE2	2.45	0.41
1:R:241:TYR:HE1	1:R:244:HIS:HB3	1.85	0.41
1:Y:230:GLU:OE2	1:Y:260:ARG:HB2	2.21	0.41
1:Y:241:TYR:CE1	1:Y:244:HIS:HB3	2.55	0.41
1:BA:180:GLY:O	1:BA:184:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:268:VAL:O	1:LA:268:VAL:HG23	2.20	0.41
1:QA:175:TYR:O	1:QA:208:GLY:HA3	2.21	0.41
1:RA:196:TYR:HA	1:RA:197:PRO:HD2	1.86	0.41
1:RA:197:PRO:HG2	1:RA:200:GLN:HE22	1.85	0.41
1:WA:40:LYS:HE3	1:WA:40:LYS:HB3	1.88	0.41
1:BB:137:ILE:HD12	1:BB:261:CYS:SG	2.60	0.41
1:GB:40:LYS:HE3	1:GB:40:LYS:HB3	1.90	0.41
1:E:202:VAL:O	1:E:206:PHE:HB3	2.20	0.41
1:F:166:LEU:HG	1:F:171:VAL:HB	2.02	0.41
1:I:4:LEU:HD21	1:I:238:SER:HB3	2.02	0.41
1:K:179:LEU:HD23	1:K:179:LEU:HA	1.90	0.41
1:L:257:MET:HE2	1:L:258:THR:N	2.36	0.41
1:O:141:SER:HB3	1:O:144:HIS:HE1	1.86	0.41
1:O:241:TYR:HE1	1:O:244:HIS:HB3	1.85	0.41
1:P:208:GLY:HA2	1:P:209:PRO:HD3	1.86	0.41
1:Q:196:TYR:HA	1:Q:197:PRO:HD2	1.83	0.41
1:Z:5:MET:HE3	1:MA:10:PRO:HA	2.02	0.41
1:BA:262:LEU:HD13	1:YA:103:SER:OG	2.20	0.41
1:DA:2:ASN:OD1	1:DA:2:ASN:C	2.62	0.41
1:IA:33:ALA:O	1:IA:37:VAL:HG22	2.21	0.41
1:NA:27:LEU:HD23	1:NA:27:LEU:HA	1.81	0.41
1:QA:36:VAL:HG23	1:QA:37:VAL:HG13	2.03	0.41
1:QA:257:MET:HE2	1:QA:258:THR:N	2.36	0.41
1:SA:203:ARG:HA	1:SA:203:ARG:HD2	1.87	0.41
1:TA:19:ILE:HD11	1:TA:95:LEU:HD11	2.03	0.41
1:TA:175:TYR:O	1:TA:208:GLY:HA3	2.20	0.41
1:TA:197:PRO:HG2	1:TA:200:GLN:HE22	1.85	0.41
1:YA:171:VAL:HG22	1:YA:225:ARG:NH1	2.36	0.41
1:YA:198:VAL:HA	1:YA:201:HIS:HB3	2.03	0.41
1:ZA:171:VAL:HG22	1:ZA:225:ARG:NE	2.30	0.41
1:BB:177:LEU:HG	1:BB:206:PHE:CZ	2.56	0.41
1:FB:156:PRO:HG3	1:FB:202:VAL:HG12	2.03	0.41
1:HB:262:LEU:O	1:HB:264:PRO:HD3	2.21	0.41
1:A0:179:LEU:HD23	1:A0:183:VAL:HG22	2.03	0.41
1:C:58:LEU:HD12	1:C:73:VAL:HG12	2.03	0.41
1:F:175:TYR:HD1	1:F:223:SER:HA	1.85	0.41
1:G:156:PRO:HG3	1:G:202:VAL:HG12	2.03	0.41
1:K:95:LEU:HD13	1:K:95:LEU:HA	1.93	0.41
1:L:231:LEU:HD12	1:L:259:PHE:HB2	2.03	0.41
1:N:51:SER:HA	1:N:78:VAL:HG12	2.02	0.41
1:R:203:ARG:HH22	1:R:208:GLY:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:162:ALA:HB1	1:S:268:VAL:HG11	2.02	0.41
1:BA:11:ILE:HB	1:BA:16:TRP:NE1	2.36	0.41
1:JA:175:TYR:O	1:JA:208:GLY:HA3	2.20	0.41
1:MA:241:TYR:CE1	1:MA:244:HIS:HB3	2.56	0.41
1:YA:31:LEU:HD23	1:YA:31:LEU:HA	1.83	0.41
1:CB:148:LEU:HA	1:CB:149:PRO:HD2	1.91	0.41
1:DB:155:PHE:C	1:DB:155:PHE:CD2	2.99	0.41
1:A:172:ASP:H	1:A:225:ARG:HD3	1.86	0.41
1:B:152:LEU:O	1:B:155:PHE:HB2	2.21	0.41
1:F:40:LYS:HE3	1:F:40:LYS:HB3	1.88	0.41
1:H:36:VAL:HG23	1:H:37:VAL:HG13	2.03	0.41
1:H:241:TYR:HE1	1:H:244:HIS:HB3	1.86	0.41
1:I:196:TYR:HA	1:I:197:PRO:HD2	1.86	0.41
1:L:179:LEU:HD22	1:L:184:TYR:HA	2.03	0.41
1:M:188:MET:HE3	1:M:199:LEU:HD22	2.02	0.41
1:N:10:PRO:HG3	1:N:244:HIS:CD2	2.56	0.41
1:N:94:GLU:HG2	1:N:106:ASP:H	1.85	0.41
1:N:241:TYR:HE1	1:N:244:HIS:HB3	1.84	0.41
1:T:17:ALA:HA	1:T:20:GLU:OE2	2.21	0.41
1:T:79:GLN:HA	1:T:80:PRO:HD3	1.88	0.41
1:V:139:GLU:H	1:V:139:GLU:HG2	1.66	0.41
1:W:262:LEU:O	1:W:264:PRO:HD3	2.21	0.41
1:X:220:MET:SD	1:X:269:PRO:HA	2.61	0.41
1:Y:49:SER:OG	1:LA:78:VAL:HG21	2.21	0.41
1:Y:148:LEU:HA	1:Y:270:LEU:HD11	2.02	0.41
1:Z:22:GLU:O	1:Z:26:THR:HG22	2.20	0.41
1:Z:171:VAL:HG22	1:Z:225:ARG:HE	1.86	0.41
1:AA:241:TYR:CE1	1:AA:244:HIS:HB3	2.56	0.41
1:EA:148:LEU:HB3	1:EA:271:ARG:O	2.20	0.41
1:JA:92:ARG:O	1:JA:96:GLU:HG3	2.20	0.41
1:KA:33:ALA:HB2	1:KA:122:ASP:OD1	2.21	0.41
1:KA:91:LYS:HB2	1:KA:94:GLU:CD	2.46	0.41
1:KA:262:LEU:H	1:KA:262:LEU:HD23	1.86	0.41
1:MA:220:MET:SD	1:MA:269:PRO:HA	2.61	0.41
1:PA:91:LYS:HB2	1:PA:94:GLU:CD	2.46	0.41
1:PA:174:PRO:HG2	1:PA:224:GLN:HB2	2.02	0.41
1:QA:73:VAL:HG12	1:HB:84:LEU:HD23	2.02	0.41
1:TA:26:THR:O	1:TA:30:THR:HG22	2.21	0.41
1:TA:219:ALA:HB3	1:TA:270:LEU:HD23	2.03	0.41
1:VA:40:LYS:NZ	1:VA:230:GLU:HB3	2.36	0.41
1:XA:148:LEU:HD13	1:XA:272:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:ZA:36:VAL:HG23	1:ZA:37:VAL:HG13	2.02	0.41
1:ZA:84:LEU:HD12	1:ZA:255:GLU:OE2	2.21	0.41
1:CB:203:ARG:NH2	1:CB:208:GLY:H	2.18	0.41
1:FB:41:GLY:HA2	1:FB:42:PRO:HD3	1.85	0.41
1:HB:192:THR:HG21	1:HB:197:PRO:HA	2.03	0.41
1:HB:203:ARG:HA	1:HB:203:ARG:HD2	1.82	0.41
1:A:94:GLU:HG2	1:A:106:ASP:HB3	2.03	0.41
1:F:27:LEU:HD23	1:F:27:LEU:HA	1.81	0.41
1:K:104:ASP:HB3	1:OA:262:LEU:HD12	2.03	0.41
1:L:141:SER:O	1:L:269:PRO:HG2	2.21	0.41
1:N:141:SER:HB3	1:N:144:HIS:HE1	1.85	0.41
1:O:52:LEU:HB2	1:O:77:ALA:O	2.21	0.41
1:P:158:VAL:HA	1:P:161:ARG:NE	2.36	0.41
1:AA:146:LEU:O	1:AA:270:LEU:HD12	2.21	0.41
1:BA:88:PHE:HE1	1:BA:253:LEU:HD23	1.86	0.41
1:BA:213:ALA:HA	1:BA:214:PRO:HD3	1.88	0.41
1:GA:175:TYR:O	1:GA:208:GLY:HA3	2.21	0.41
1:OA:148:LEU:HD13	1:OA:272:GLY:HA2	2.02	0.41
1:RA:95:LEU:HD13	1:RA:95:LEU:HA	1.96	0.41
1:SA:163:LEU:HD12	1:SA:163:LEU:HA	1.86	0.41
1:TA:58:LEU:HB2	1:TA:73:VAL:HG23	2.02	0.41
1:XA:233:VAL:HG12	1:XA:257:MET:HB3	2.02	0.41
1:BB:115:ARG:O	1:BB:119:ILE:HG22	2.21	0.41
1:DB:230:GLU:OE2	1:DB:260:ARG:HB2	2.20	0.41
1:GB:141:SER:HB3	1:GB:144:HIS:CE1	2.56	0.41
1:A0:179:LEU:HD22	1:A0:184:TYR:HD1	1.85	0.40
1:A:201:HIS:O	1:A:204:ARG:HD2	2.21	0.40
1:D:185:GLN:O	1:D:189:GLU:HG2	2.21	0.40
1:E:41:GLY:HA2	1:E:42:PRO:HD3	1.94	0.40
1:K:100:ARG:HG2	1:EB:45:TRP:HE1	1.87	0.40
1:L:202:VAL:O	1:L:206:PHE:HB3	2.21	0.40
1:P:230:GLU:OE2	1:P:260:ARG:HB2	2.20	0.40
1:R:36:VAL:HG23	1:R:37:VAL:HG13	2.03	0.40
1:W:123:ARG:HD2	1:W:127:HIS:CD2	2.56	0.40
1:W:203:ARG:HH22	1:W:208:GLY:H	1.68	0.40
1:Z:176:ALA:HA	1:Z:208:GLY:HA3	2.02	0.40
1:AA:209:PRO:HB2	1:AA:211:ILE:HD11	2.03	0.40
1:EA:31:LEU:HD21	1:EA:34:ARG:HG3	2.03	0.40
1:FA:126:PHE:HD2	1:FA:216:VAL:HG11	1.86	0.40
1:FA:166:LEU:HG	1:FA:171:VAL:HB	2.02	0.40
1:TA:34:ARG:HB2	2:16:128:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:UA:141:SER:HB3	1:UA:144:HIS:CE1	2.56	0.40
1:FB:91:LYS:HE2	1:FB:91:LYS:HB3	1.88	0.40
1:GB:175:TYR:HB2	1:GB:206:PHE:HE1	1.86	0.40
1:A:172:ASP:OD1	1:A:172:ASP:N	2.54	0.40
1:C:175:TYR:O	1:C:208:GLY:HA3	2.21	0.40
1:L:18:GLU:OE1	1:L:107:LEU:HD21	2.21	0.40
1:M:79:GLN:HA	1:M:80:PRO:HD3	1.89	0.40
1:P:125:VAL:HG13	1:P:126:PHE:HD1	1.85	0.40
1:R:175:TYR:O	1:R:208:GLY:HA3	2.21	0.40
1:R:196:TYR:HA	1:R:197:PRO:HD2	1.83	0.40
1:T:58:LEU:HD13	1:KA:131:ALA:HB1	2.03	0.40
1:V:177:LEU:HD23	1:V:177:LEU:HA	1.89	0.40
1:AA:152:LEU:HG	1:AA:187:LEU:HB2	2.02	0.40
1:CA:141:SER:HB3	1:CA:144:HIS:CE1	2.56	0.40
1:CA:155:PHE:HE2	1:CA:202:VAL:HG21	1.86	0.40
1:JA:129:PHE:CZ	1:JA:131:ALA:HB3	2.57	0.40
1:JA:221:LEU:C	1:JA:222:ILE:HD12	2.46	0.40
1:LA:188:MET:HE3	1:LA:199:LEU:HD22	2.03	0.40
1:NA:4:LEU:HD13	1:NA:4:LEU:HA	1.94	0.40
1:SA:156:PRO:HG3	1:SA:202:VAL:HG12	2.02	0.40
1:VA:184:TYR:HD1	1:VA:212:TRP:CD1	2.39	0.40
1:AB:178:VAL:C	1:AB:179:LEU:HD22	2.47	0.40
1:HB:152:LEU:HD13	1:HB:152:LEU:HA	1.93	0.40
1:D:41:GLY:HA2	1:D:42:PRO:HD3	1.96	0.40
1:I:169:ARG:HA	1:I:169:ARG:NE	2.36	0.40
1:N:27:LEU:HD13	1:N:114:ALA:HB1	2.03	0.40
1:N:218:GLY:HA3	1:N:270:LEU:O	2.21	0.40
1:Q:81:LEU:HG	1:Q:258:THR:HB	2.04	0.40
1:BA:268:VAL:HA	1:BA:269:PRO:HD2	1.94	0.40
1:IA:58:LEU:HD11	1:IA:75:LYS:HB2	2.04	0.40
1:JA:134:ILE:HD13	1:JA:259:PHE:H	1.86	0.40
1:LA:26:THR:O	1:LA:30:THR:HG22	2.22	0.40
1:PA:35:LYS:HA	1:PA:35:LYS:HD3	1.97	0.40
1:RA:149:PRO:HG3	1:RA:158:VAL:HG21	2.03	0.40
1:RA:187:LEU:O	1:RA:190:THR:HG23	2.21	0.40
1:TA:126:PHE:HD2	1:TA:216:VAL:HG11	1.86	0.40
1:AB:31:LEU:HD23	1:AB:31:LEU:O	2.21	0.40
1:CB:95:LEU:HD13	1:CB:95:LEU:HA	1.98	0.40
1:FB:196:TYR:HA	1:FB:197:PRO:HD2	1.82	0.40
1:A:158:VAL:HA	1:A:161:ARG:NE	2.36	0.40
1:D:5:MET:HE3	1:Z:10:PRO:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:GLN:HA	1:H:80:PRO:HD3	1.93	0.40
1:H:91:LYS:HB2	1:H:94:GLU:CD	2.47	0.40
1:L:31:LEU:HD23	1:L:31:LEU:HA	1.93	0.40
1:L:91:LYS:HE2	1:L:91:LYS:HB3	1.89	0.40
1:M:158:VAL:HA	1:M:161:ARG:NE	2.37	0.40
1:N:35:LYS:HD3	2:12:128:LEU:HD12	2.04	0.40
1:N:52:LEU:HD23	1:N:78:VAL:HA	2.03	0.40
1:O:177:LEU:HD11	1:O:219:ALA:HB1	2.03	0.40
1:S:116:ALA:O	1:S:119:ILE:HG22	2.21	0.40
1:T:95:LEU:HD13	1:T:95:LEU:HA	1.94	0.40
1:X:95:LEU:O	1:X:98:ILE:HG22	2.21	0.40
1:AA:196:TYR:HA	1:AA:197:PRO:HD2	1.80	0.40
1:CA:155:PHE:HA	1:CA:158:VAL:HG22	2.03	0.40
1:DA:230:GLU:OE2	1:DA:260:ARG:HB2	2.21	0.40
1:FA:52:LEU:HD23	1:FA:52:LEU:HA	1.90	0.40
1:IA:1:MET:H2	1:YA:13:ALA:HB2	1.86	0.40
1:MA:203:ARG:HH12	1:MA:208:GLY:H	1.70	0.40
1:OA:185:GLN:HG3	1:OA:186:GLN:OE1	2.21	0.40
1:RA:235:ARG:O	1:RA:255:GLU:HG2	2.22	0.40
1:SA:158:VAL:HA	1:SA:161:ARG:NE	2.36	0.40
1:WA:84:LEU:HD12	1:WA:255:GLU:OE2	2.22	0.40
1:EB:196:TYR:HA	1:EB:197:PRO:HD2	1.85	0.40
1:A0:177:LEU:HD11	1:A0:219:ALA:HB1	2.02	0.40
1:A:95:LEU:HD13	1:A:95:LEU:HA	1.93	0.40
1:M:90:LEU:HD23	1:M:90:LEU:HA	1.93	0.40
1:P:79:GLN:HA	1:P:80:PRO:HD3	1.87	0.40
1:Q:98:ILE:HA	1:Q:102:ALA:HB3	2.03	0.40
1:S:196:TYR:HA	1:S:197:PRO:HD2	1.83	0.40
1:X:10:PRO:HG3	1:X:244:HIS:CD2	2.55	0.40
1:CA:239:ILE:HD12	1:CA:239:ILE:HA	1.96	0.40
1:EA:197:PRO:HG2	1:EA:200:GLN:HE22	1.87	0.40
1:IA:196:TYR:HA	1:IA:197:PRO:HD2	1.87	0.40
1:KA:79:GLN:HA	1:KA:80:PRO:HD3	1.82	0.40
1:KA:196:TYR:HA	1:KA:197:PRO:HD2	1.84	0.40
1:LA:40:LYS:HE3	1:LA:40:LYS:HB3	1.84	0.40
1:NA:4:LEU:HD12	1:NA:240:GLY:HA3	2.03	0.40
1:NA:36:VAL:HG23	1:NA:37:VAL:HG13	2.04	0.40
1:PA:52:LEU:HD23	1:PA:52:LEU:HA	1.92	0.40
1:UA:204:ARG:HG2	1:UA:205:LEU:N	2.34	0.40
1:ZA:26:THR:O	1:ZA:30:THR:HG22	2.22	0.40
1:DB:239:ILE:HD13	1:DB:239:ILE:HA	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	A0	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	AA	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	AB	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	B	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	BA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	BB	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	C	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	CA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	CB	258/280 (92%)	250 (97%)	8 (3%)	0	100	100
1	D	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	DA	258/280 (92%)	250 (97%)	8 (3%)	0	100	100
1	DB	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	E	258/280 (92%)	243 (94%)	15 (6%)	0	100	100
1	EA	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	EB	258/280 (92%)	251 (97%)	7 (3%)	0	100	100
1	F	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	FA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	FB	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	G	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	GA	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	GB	258/280 (92%)	248 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	HA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	HB	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	I	258/280 (92%)	243 (94%)	15 (6%)	0	100	100
1	IA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	J	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	JA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	K	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	KA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	L	258/280 (92%)	245 (95%)	13 (5%)	0	100	100
1	LA	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	M	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	MA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	N	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	NA	258/280 (92%)	250 (97%)	8 (3%)	0	100	100
1	O	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	OA	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	P	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	PA	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	Q	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	QA	258/280 (92%)	245 (95%)	13 (5%)	0	100	100
1	R	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	RA	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	S	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	SA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	T	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	TA	258/280 (92%)	249 (96%)	9 (4%)	0	100	100
1	UA	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	V	258/280 (92%)	246 (95%)	12 (5%)	0	100	100
1	VA	258/280 (92%)	251 (97%)	7 (3%)	0	100	100
1	W	258/280 (92%)	251 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	WA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	X	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	XA	258/280 (92%)	245 (95%)	13 (5%)	0	100	100
1	Y	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	YA	258/280 (92%)	248 (96%)	10 (4%)	0	100	100
1	Z	258/280 (92%)	244 (95%)	14 (5%)	0	100	100
1	ZA	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
2	1	6/140 (4%)	6 (100%)	0	0	100	100
2	10	7/140 (5%)	6 (86%)	1 (14%)	0	100	100
2	11	6/140 (4%)	5 (83%)	0	1 (17%)	0	2
2	12	6/140 (4%)	6 (100%)	0	0	100	100
2	13	6/140 (4%)	6 (100%)	0	0	100	100
2	14	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	15	6/140 (4%)	6 (100%)	0	0	100	100
2	16	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	17	6/140 (4%)	6 (100%)	0	0	100	100
2	18	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	19	6/140 (4%)	6 (100%)	0	0	100	100
2	2	6/140 (4%)	6 (100%)	0	0	100	100
2	20	6/140 (4%)	2 (33%)	3 (50%)	1 (17%)	0	2
2	3	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	4	7/140 (5%)	7 (100%)	0	0	100	100
2	5	6/140 (4%)	5 (83%)	1 (17%)	0	100	100
2	6	6/140 (4%)	6 (100%)	0	0	100	100
2	7	7/140 (5%)	6 (86%)	1 (14%)	0	100	100
2	8	7/140 (5%)	7 (100%)	0	0	100	100
2	9	6/140 (4%)	6 (100%)	0	0	100	100
All	All	15604/19600 (80%)	14935 (96%)	667 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	20	125	ILE

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Mol	Chain	Res	Type
2	11	125	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	A0	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	AA	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	AB	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	B	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	BA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	BB	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	C	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	CA	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	CB	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	D	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	DA	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	DB	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	E	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	EA	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	EB	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	F	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	FA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	FB	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	G	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	GA	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	GB	200/210 (95%)	191 (96%)	9 (4%)	24	49
1	H	200/210 (95%)	194 (97%)	6 (3%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HA	200/210 (95%)	191 (96%)	9 (4%)	24	49
1	HB	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	I	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	IA	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	J	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	JA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	K	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	KA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	L	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	LA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	M	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	MA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	N	200/210 (95%)	198 (99%)	2 (1%)	68	74
1	NA	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	O	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	OA	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	P	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	PA	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	Q	200/210 (95%)	191 (96%)	9 (4%)	24	49
1	QA	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	R	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	RA	200/210 (95%)	190 (95%)	10 (5%)	22	47
1	S	200/210 (95%)	199 (100%)	1 (0%)	81	80
1	SA	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	T	200/210 (95%)	197 (98%)	3 (2%)	57	68
1	TA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	UA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	V	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	VA	200/210 (95%)	196 (98%)	4 (2%)	48	64
1	W	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	WA	200/210 (95%)	195 (98%)	5 (2%)	42	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	XA	200/210 (95%)	193 (96%)	7 (4%)	32	54
1	Y	200/210 (95%)	194 (97%)	6 (3%)	36	57
1	YA	200/210 (95%)	195 (98%)	5 (2%)	42	61
1	Z	200/210 (95%)	192 (96%)	8 (4%)	28	52
1	ZA	200/210 (95%)	196 (98%)	4 (2%)	48	64
2	1	5/108 (5%)	5 (100%)	0	100	100
2	10	6/108 (6%)	5 (83%)	1 (17%)	2	14
2	11	5/108 (5%)	5 (100%)	0	100	100
2	12	5/108 (5%)	5 (100%)	0	100	100
2	13	5/108 (5%)	3 (60%)	2 (40%)	0	0
2	14	5/108 (5%)	5 (100%)	0	100	100
2	15	5/108 (5%)	5 (100%)	0	100	100
2	16	5/108 (5%)	5 (100%)	0	100	100
2	17	5/108 (5%)	5 (100%)	0	100	100
2	18	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	19	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	2	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	20	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	3	5/108 (5%)	5 (100%)	0	100	100
2	4	6/108 (6%)	5 (83%)	1 (17%)	2	14
2	5	5/108 (5%)	4 (80%)	1 (20%)	1	9
2	6	5/108 (5%)	5 (100%)	0	100	100
2	7	6/108 (6%)	6 (100%)	0	100	100
2	8	6/108 (6%)	5 (83%)	1 (17%)	2	14
2	9	5/108 (5%)	5 (100%)	0	100	100
All	All	12104/14760 (82%)	11762 (97%)	342 (3%)	38	58

All (342) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	98	ILE
1	A0	117	ILE

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Mol	Chain	Res	Type
1	A0	137	ILE
1	A0	178	VAL
1	A0	183	VAL
1	A	12	SER
1	A	40	LYS
1	A	119	ILE
1	B	40	LYS
1	B	137	ILE
1	B	166	LEU
1	B	184	TYR
1	B	210	LEU
1	C	43	LEU
1	C	86	VAL
1	C	91	LYS
1	C	199	LEU
1	D	12	SER
1	D	18	GLU
1	D	24	ARG
1	D	159	LEU
1	D	178	VAL
1	D	257	MET
1	E	126	PHE
1	E	178	VAL
1	E	233	VAL
1	F	40	LYS
1	F	119	ILE
1	F	143	GLU
1	F	167	ARG
1	F	183	VAL
1	F	244	HIS
1	G	4	LEU
1	G	5	MET
1	G	24	ARG
1	G	152	LEU
1	G	216	VAL
1	H	12	SER
1	H	40	LYS
1	H	119	ILE
1	H	137	ILE
1	H	152	LEU
1	H	189	GLU
1	I	86	VAL

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Mol	Chain	Res	Type
1	I	178	VAL
1	I	220	MET
1	J	40	LYS
1	J	48	SER
1	J	50	VAL
1	J	178	VAL
1	J	187	LEU
1	J	204	ARG
1	J	216	VAL
1	J	230	GLU
1	K	71	VAL
1	K	178	VAL
1	K	188	MET
1	K	233	VAL
1	L	12	SER
1	L	111	ILE
1	L	166	LEU
1	L	223	SER
1	M	40	LYS
1	M	137	ILE
1	M	152	LEU
1	M	248	SER
1	M	255	GLU
1	N	14	LYS
1	N	189	GLU
1	O	8	LEU
1	O	50	VAL
1	O	78	VAL
1	O	111	ILE
1	O	186	GLN
1	O	223	SER
1	O	229	PHE
1	P	12	SER
1	P	46	ASP
1	P	152	LEU
1	P	166	LEU
1	P	206	PHE
1	Q	31	LEU
1	Q	40	LYS
1	Q	111	ILE
1	Q	152	LEU
1	Q	172	ASP

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Mol	Chain	Res	Type
1	Q	183	VAL
1	Q	204	ARG
1	Q	205	LEU
1	Q	230	GLU
1	R	12	SER
1	R	40	LYS
1	R	183	VAL
1	R	201	HIS
1	S	86	VAL
1	T	50	VAL
1	T	86	VAL
1	T	190	THR
1	V	14	LYS
1	V	40	LYS
1	V	50	VAL
1	V	95	LEU
1	W	12	SER
1	W	86	VAL
1	W	98	ILE
1	W	166	LEU
1	W	183	VAL
1	W	210	LEU
1	W	223	SER
1	W	255	GLU
1	X	4	LEU
1	X	84	LEU
1	X	86	VAL
1	X	119	ILE
1	X	122	ASP
1	X	126	PHE
1	Y	4	LEU
1	Y	8	LEU
1	Y	40	LYS
1	Y	166	LEU
1	Y	167	ARG
1	Y	233	VAL
1	Z	12	SER
1	Z	40	LYS
1	Z	86	VAL
1	Z	119	ILE
1	Z	122	ASP
1	Z	152	LEU

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Mol	Chain	Res	Type
1	Z	181	ARG
1	Z	244	HIS
1	AA	26	THR
1	AA	36	VAL
1	AA	40	LYS
1	AA	137	ILE
1	AA	166	LEU
1	AA	188	MET
1	AA	255	GLU
1	AA	262	LEU
1	BA	40	LYS
1	BA	125	VAL
1	BA	166	LEU
1	BA	222	ILE
1	BA	253	LEU
1	CA	40	LYS
1	CA	86	VAL
1	CA	117	ILE
1	CA	123	ARG
1	CA	166	LEU
1	CA	233	VAL
1	DA	4	LEU
1	DA	26	THR
1	DA	50	VAL
1	DA	78	VAL
1	DA	111	ILE
1	DA	181	ARG
1	DA	189	GLU
1	DA	190	THR
1	EA	71	VAL
1	EA	86	VAL
1	EA	190	THR
1	EA	223	SER
1	FA	26	THR
1	FA	43	LEU
1	FA	86	VAL
1	FA	117	ILE
1	FA	119	ILE
1	GA	29	VAL
1	GA	96	GLU
1	GA	98	ILE
1	GA	104	ASP

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Mol	Chain	Res	Type
1	GA	220	MET
1	GA	244	HIS
1	HA	12	SER
1	HA	26	THR
1	HA	86	VAL
1	HA	117	ILE
1	HA	166	LEU
1	HA	167	ARG
1	HA	199	LEU
1	HA	223	SER
1	HA	229	PHE
1	IA	4	LEU
1	IA	12	SER
1	IA	29	VAL
1	IA	166	LEU
1	IA	179	LEU
1	IA	255	GLU
1	JA	5	MET
1	JA	8	LEU
1	JA	16	TRP
1	JA	70	VAL
1	JA	86	VAL
1	JA	119	ILE
1	JA	152	LEU
1	KA	4	LEU
1	KA	12	SER
1	KA	86	VAL
1	KA	98	ILE
1	KA	117	ILE
1	KA	161	ARG
1	KA	223	SER
1	LA	12	SER
1	LA	40	LYS
1	LA	49	SER
1	LA	95	LEU
1	LA	117	ILE
1	LA	216	VAL
1	LA	255	GLU
1	MA	12	SER
1	MA	48	SER
1	MA	117	ILE
1	MA	166	LEU

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Mol	Chain	Res	Type
1	MA	233	VAL
1	NA	4	LEU
1	NA	20	GLU
1	NA	178	VAL
1	NA	223	SER
1	OA	86	VAL
1	OA	159	LEU
1	OA	166	LEU
1	OA	178	VAL
1	PA	12	SER
1	PA	40	LYS
1	PA	117	ILE
1	PA	119	ILE
1	PA	166	LEU
1	PA	183	VAL
1	PA	190	THR
1	PA	207	GLU
1	QA	27	LEU
1	QA	31	LEU
1	QA	40	LYS
1	QA	117	ILE
1	QA	223	SER
1	QA	248	SER
1	RA	12	SER
1	RA	26	THR
1	RA	40	LYS
1	RA	48	SER
1	RA	78	VAL
1	RA	117	ILE
1	RA	152	LEU
1	RA	223	SER
1	RA	233	VAL
1	RA	248	SER
1	SA	137	ILE
1	SA	166	LEU
1	SA	181	ARG
1	TA	26	THR
1	TA	40	LYS
1	TA	86	VAL
1	TA	98	ILE
1	TA	137	ILE
1	TA	152	LEU

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Mol	Chain	Res	Type
1	TA	230	GLU
1	UA	12	SER
1	UA	86	VAL
1	UA	111	ILE
1	UA	204	ARG
1	UA	233	VAL
1	VA	12	SER
1	VA	183	VAL
1	VA	206	PHE
1	VA	255	GLU
1	WA	12	SER
1	WA	40	LYS
1	WA	117	ILE
1	WA	143	GLU
1	WA	230	GLU
1	XA	86	VAL
1	XA	98	ILE
1	XA	122	ASP
1	XA	137	ILE
1	XA	159	LEU
1	XA	230	GLU
1	XA	248	SER
1	YA	26	THR
1	YA	96	GLU
1	YA	111	ILE
1	YA	190	THR
1	YA	223	SER
1	ZA	40	LYS
1	ZA	98	ILE
1	ZA	216	VAL
1	ZA	244	HIS
1	AB	8	LEU
1	AB	104	ASP
1	AB	117	ILE
1	AB	190	THR
1	BB	6	ARG
1	BB	40	LYS
1	BB	189	GLU
1	BB	244	HIS
1	CB	125	VAL
1	CB	187	LEU
1	CB	190	THR

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Mol	Chain	Res	Type
1	CB	233	VAL
1	CB	255	GLU
1	CB	262	LEU
1	DB	21	THR
1	DB	28	THR
1	DB	117	ILE
1	DB	119	ILE
1	DB	137	ILE
1	DB	152	LEU
1	EB	204	ARG
1	EB	220	MET
1	EB	233	VAL
1	FB	71	VAL
1	FB	86	VAL
1	FB	95	LEU
1	FB	119	ILE
1	FB	126	PHE
1	FB	189	GLU
1	FB	248	SER
1	GB	12	SER
1	GB	40	LYS
1	GB	86	VAL
1	GB	111	ILE
1	GB	117	ILE
1	GB	159	LEU
1	GB	167	ARG
1	GB	183	VAL
1	GB	223	SER
1	HB	14	LYS
1	HB	26	THR
1	HB	31	LEU
1	HB	117	ILE
1	HB	152	LEU
1	HB	178	VAL
1	HB	248	SER
1	HB	255	GLU
2	2	128	LEU
2	4	125	ILE
2	5	122	SER
2	8	123	LEU
2	10	128	LEU
2	13	123	LEU

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Mol	Chain	Res	Type
2	13	125	ILE
2	18	125	ILE
2	19	122	SER
2	20	125	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	200	GLN
1	A	254	GLN
1	C	79	GLN
1	C	144	HIS
1	C	185	GLN
1	D	186	GLN
1	E	2	ASN
1	E	79	GLN
1	E	224	GLN
1	F	186	GLN
1	F	247	GLN
1	G	186	GLN
1	G	224	GLN
1	G	247	GLN
1	H	200	GLN
1	J	224	GLN
1	J	254	GLN
1	K	144	HIS
1	K	247	GLN
1	K	254	GLN
1	M	224	GLN
1	N	200	GLN
1	O	224	GLN
1	O	254	GLN
1	R	144	HIS
1	S	79	GLN
1	T	200	GLN
1	T	224	GLN
1	T	254	GLN
1	V	224	GLN
1	V	254	GLN
1	W	144	HIS
1	W	200	GLN
1	W	224	GLN

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Mol	Chain	Res	Type
1	X	224	GLN
1	Z	247	GLN
1	AA	200	GLN
1	AA	254	GLN
1	BA	79	GLN
1	CA	200	GLN
1	CA	224	GLN
1	DA	254	GLN
1	EA	224	GLN
1	FA	144	HIS
1	FA	254	GLN
1	GA	201	HIS
1	GA	224	GLN
1	GA	254	GLN
1	IA	224	GLN
1	JA	254	GLN
1	LA	254	GLN
1	NA	200	GLN
1	OA	247	GLN
1	PA	79	GLN
1	PA	200	GLN
1	PA	254	GLN
1	QA	254	GLN
1	SA	224	GLN
1	TA	185	GLN
1	TA	254	GLN
1	UA	254	GLN
1	VA	224	GLN
1	VA	254	GLN
1	WA	79	GLN
1	WA	224	GLN
1	XA	144	HIS
1	YA	254	GLN
1	ZA	254	GLN
1	AB	200	GLN
1	BB	79	GLN
1	BB	224	GLN
1	BB	254	GLN
1	CB	2	ASN
1	CB	201	HIS
1	CB	224	GLN
1	DB	200	GLN

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Mol	Chain	Res	Type
1	EB	200	GLN
1	EB	224	GLN
1	GB	254	GLN
1	HB	254	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

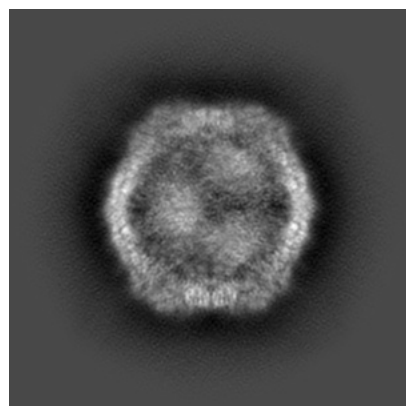
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55116. These allow visual inspection of the internal detail of the map and identification of artifacts.

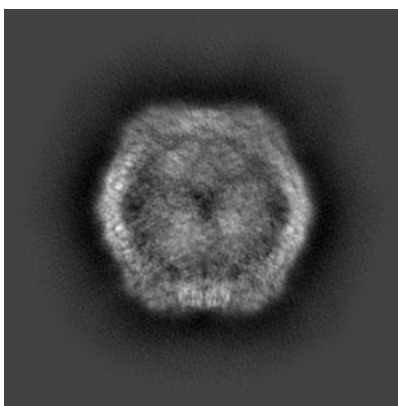
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

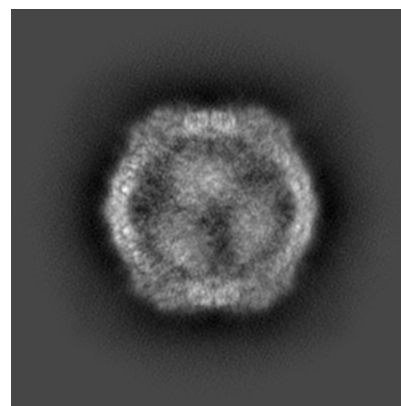
6.1.1 Primary map



X

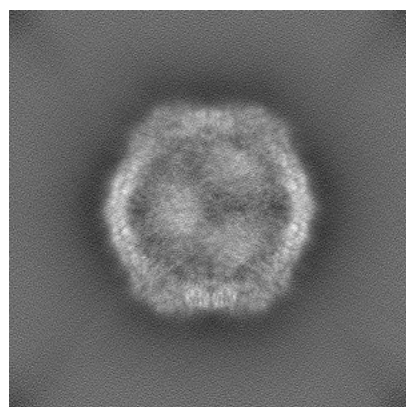


Y

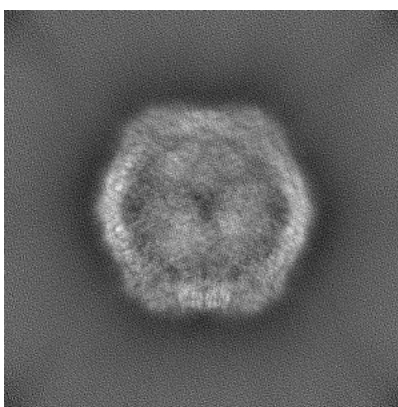


Z

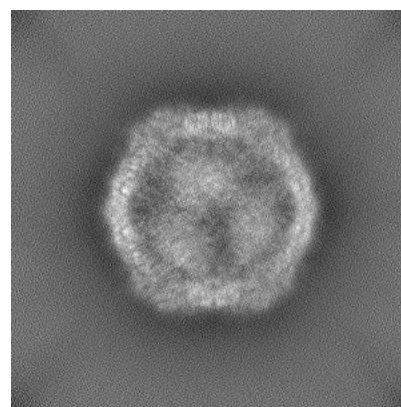
6.1.2 Raw map



X



Y

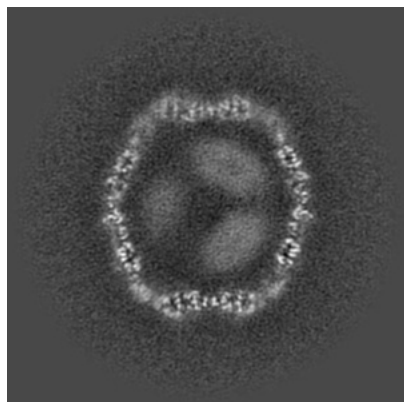


Z

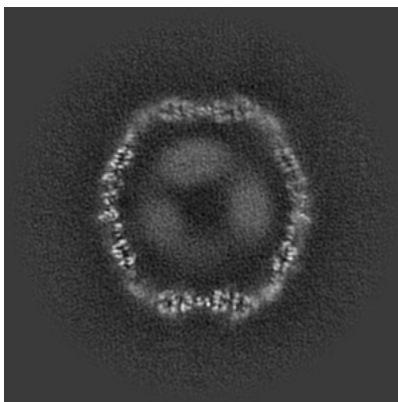
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

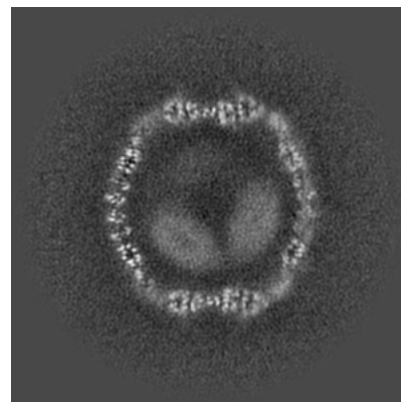
6.2.1 Primary map



X Index: 192

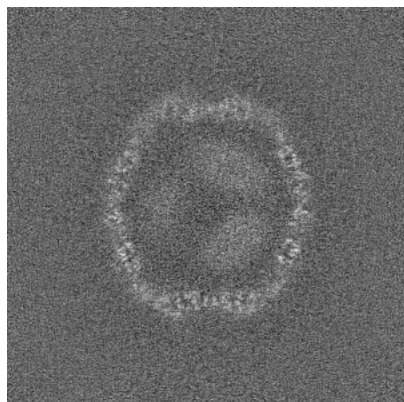


Y Index: 192

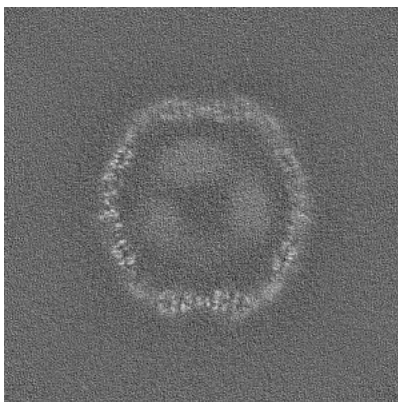


Z Index: 192

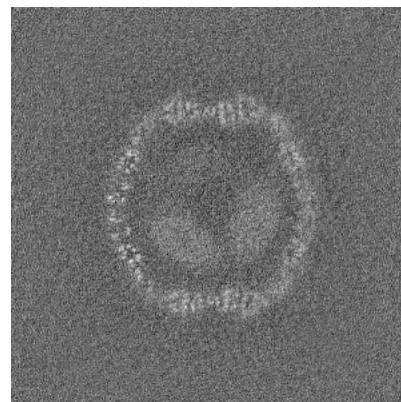
6.2.2 Raw map



X Index: 192



Y Index: 192

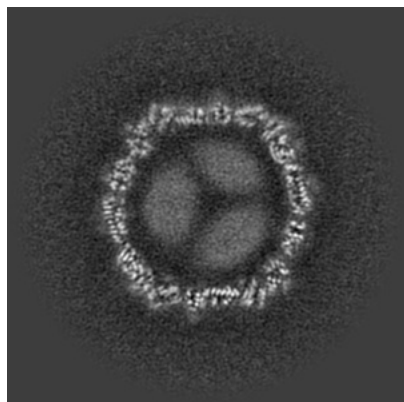


Z Index: 192

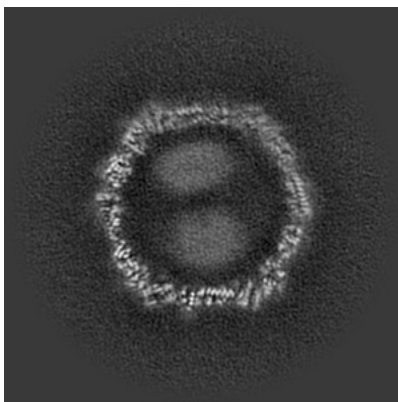
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

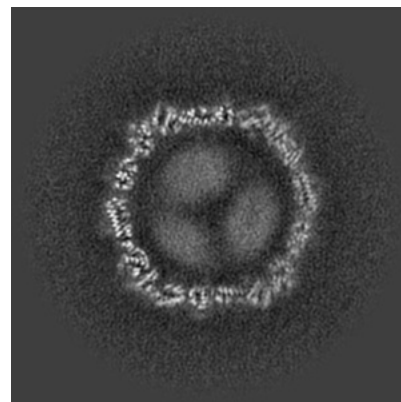
6.3.1 Primary map



X Index: 173

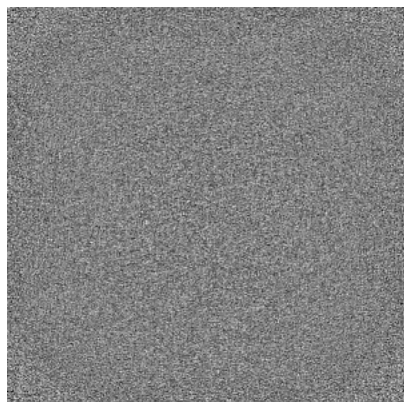


Y Index: 171

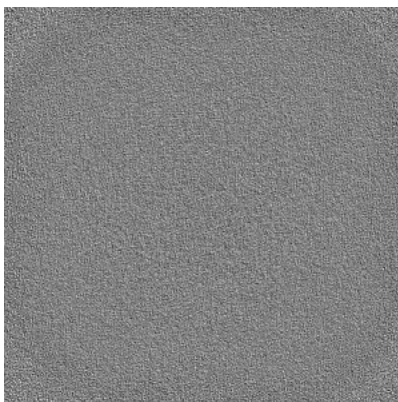


Z Index: 173

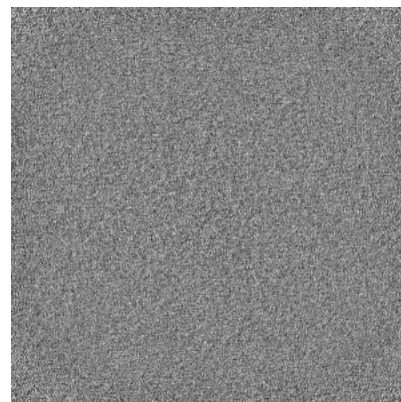
6.3.2 Raw map



X Index: 0



Y Index: 0

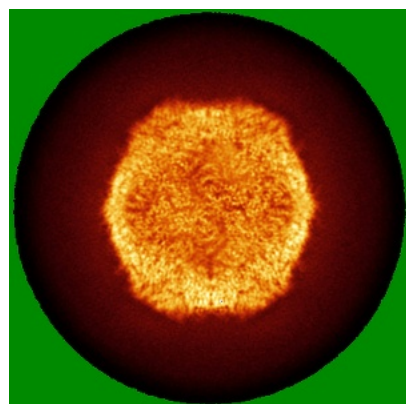


Z Index: 0

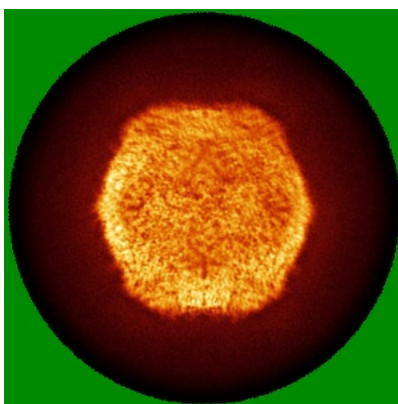
The images above show the largest variance slices of the map in three orthogonal directions.

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

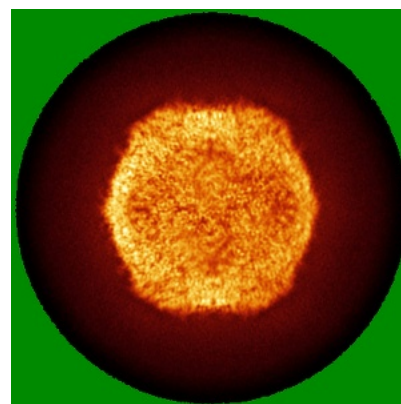
6.4.1 Primary map



X

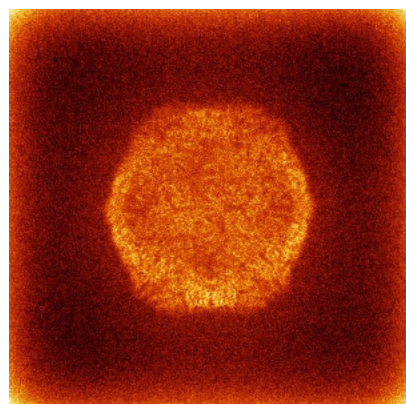


Y

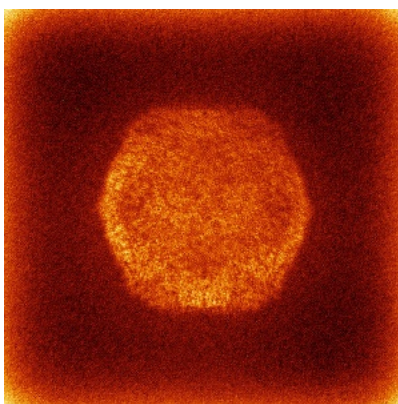


Z

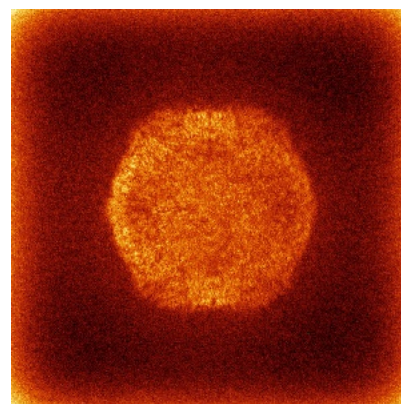
6.4.2 Raw map



X



Y

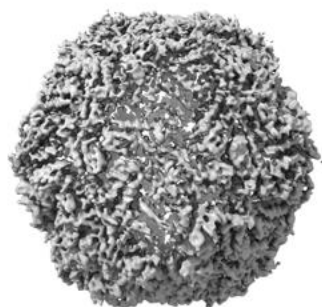


Z

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](#)

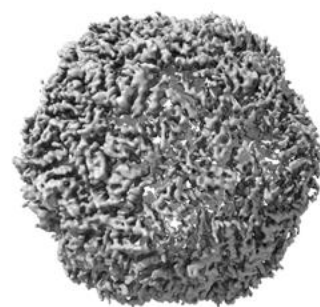
6.5.1 Primary map



X



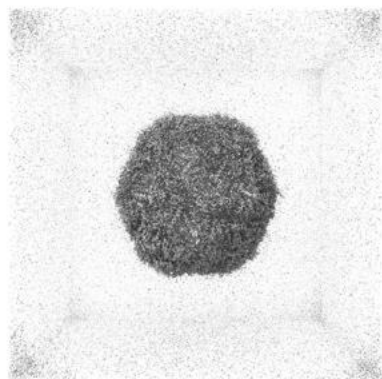
Y



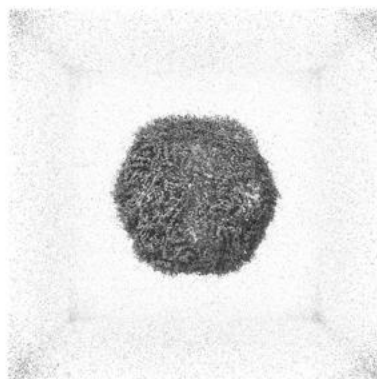
Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

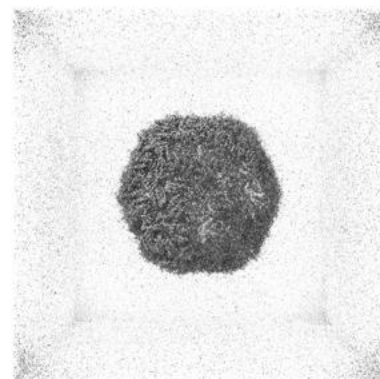
6.5.2 Raw map



X



Y



Z

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.

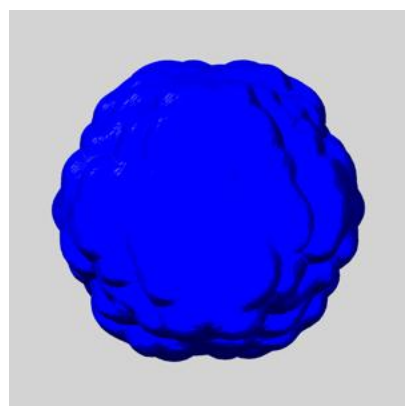
6.6 Mask visualisation [i](#)

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

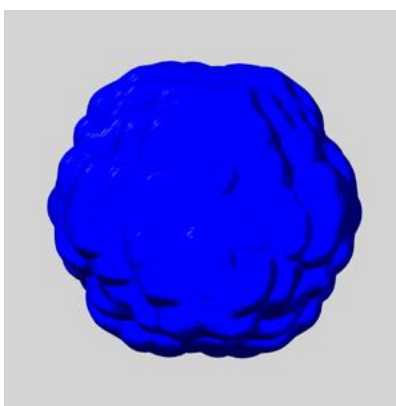
A mask typically either:

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

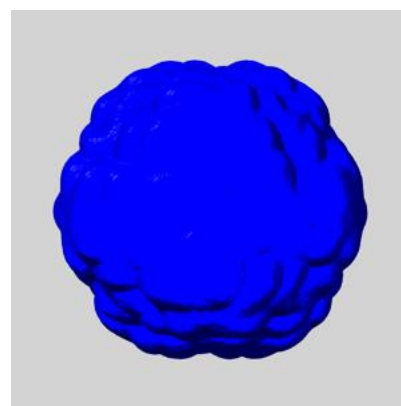
6.6.1 emd_55116_msk_1.map [i](#)



X



Y

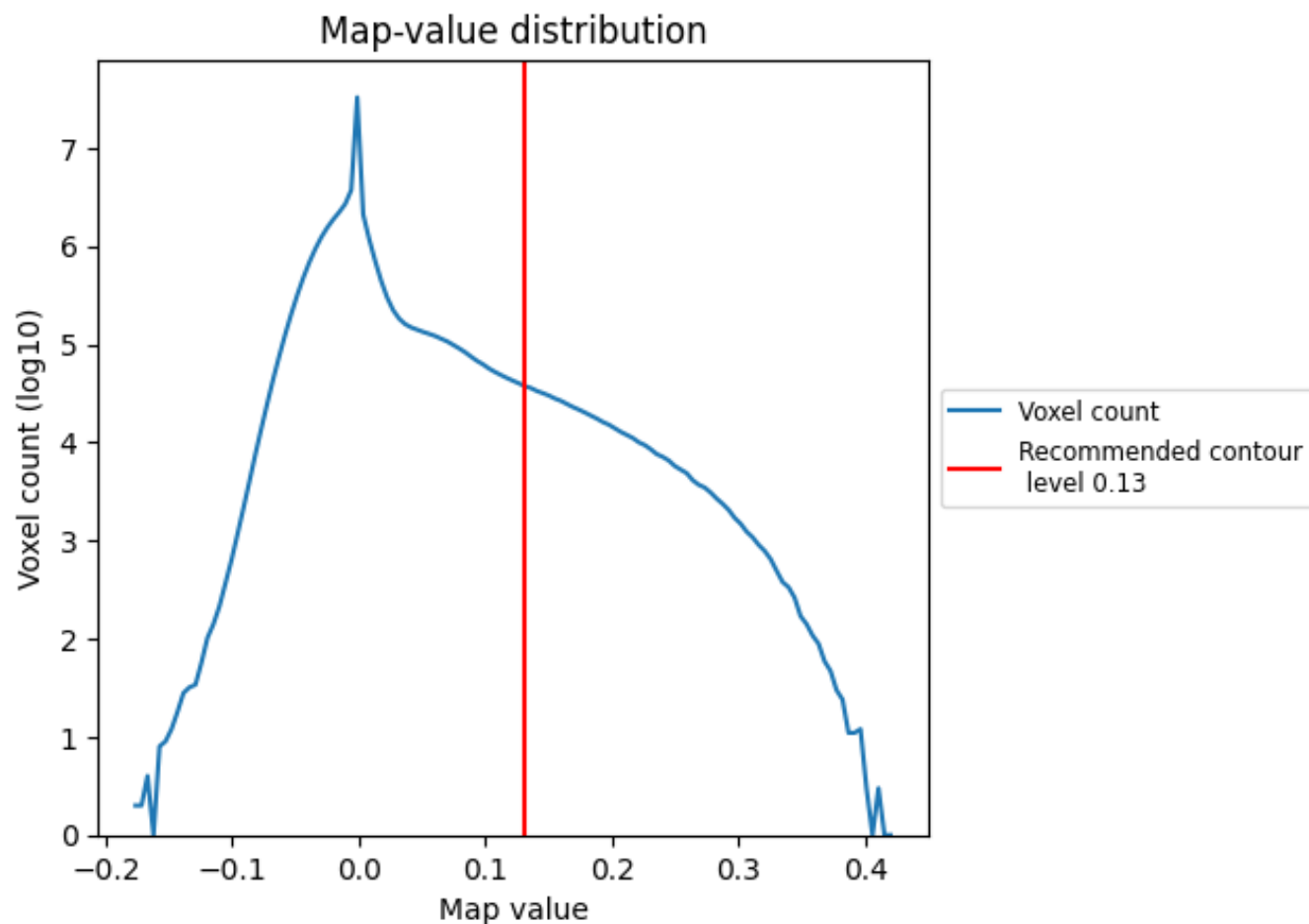


Z

7 Map analysis [i](#)

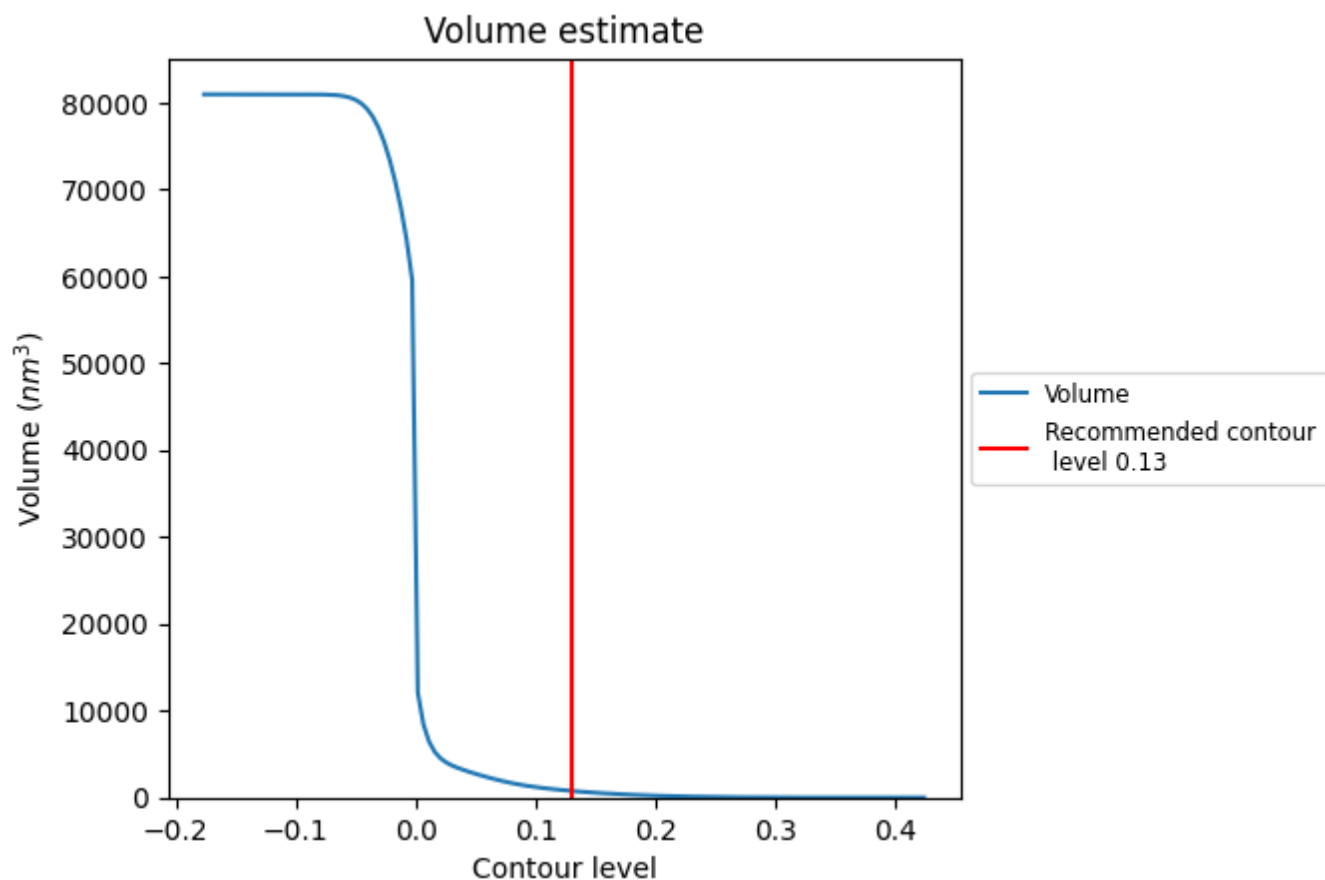
This section contains the results of statistical analysis of the map.

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.

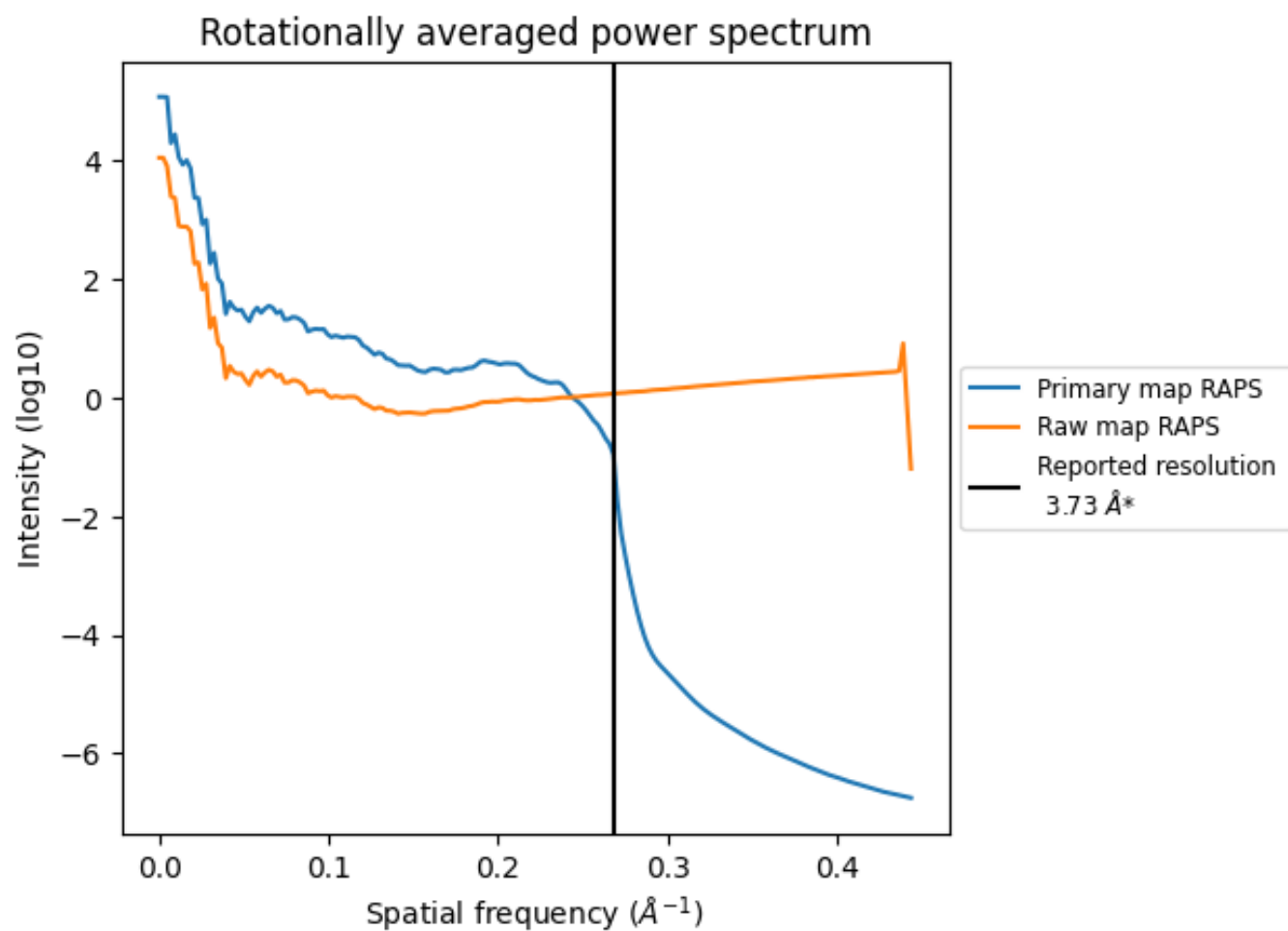
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 768 nm³; this corresponds to an approximate mass of 694 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

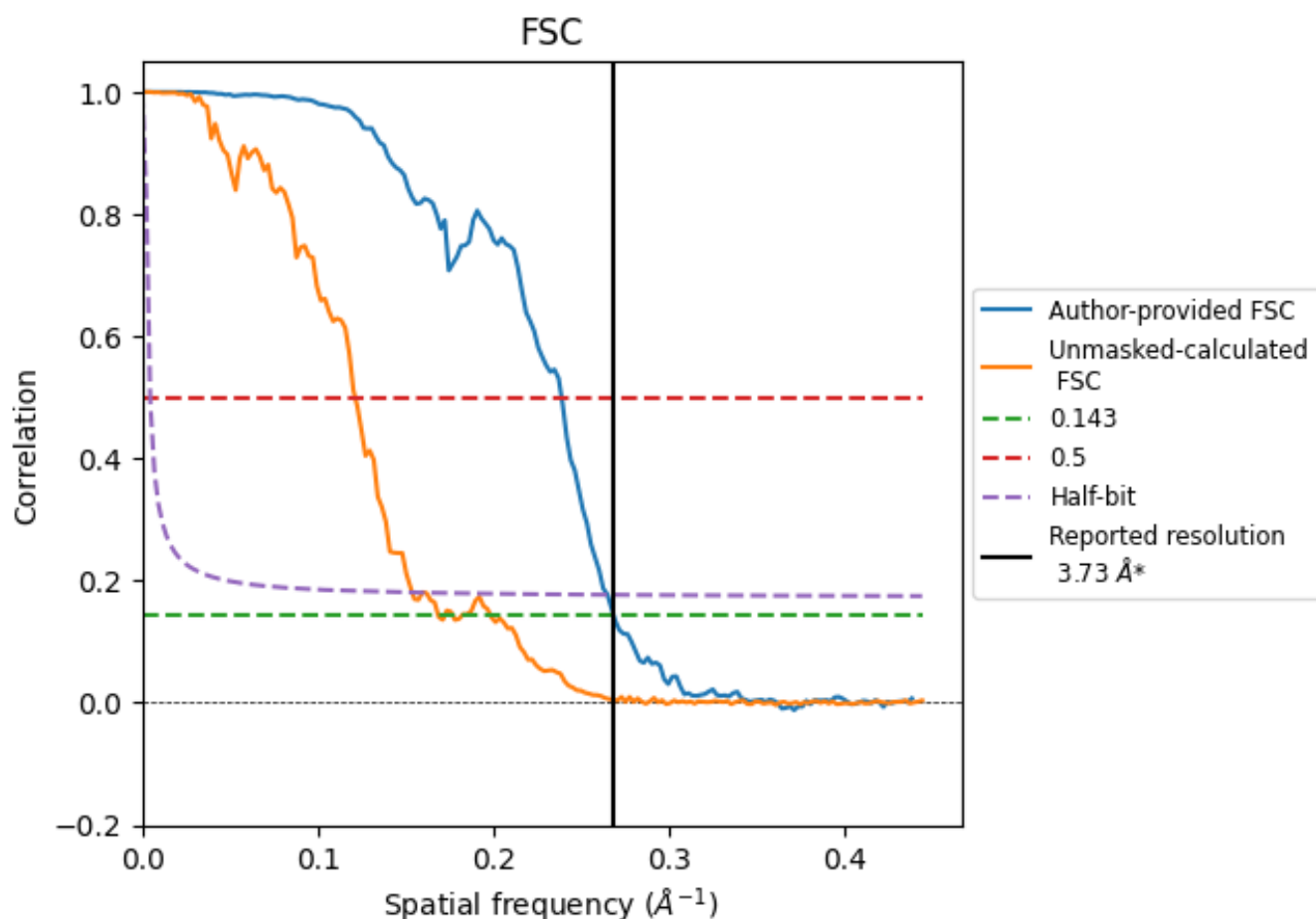


*Reported resolution corresponds to spatial frequency of 0.268 $\text{\AA}^{-1}$

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 0.268 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

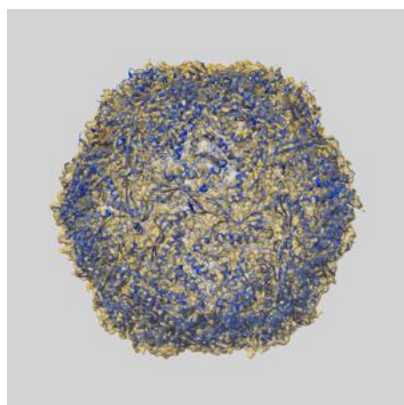
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	3.73	4.19	3.78
Unmasked-calculated*	5.93	8.25	6.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.93 differs from the reported value 3.73 by more than 10 %

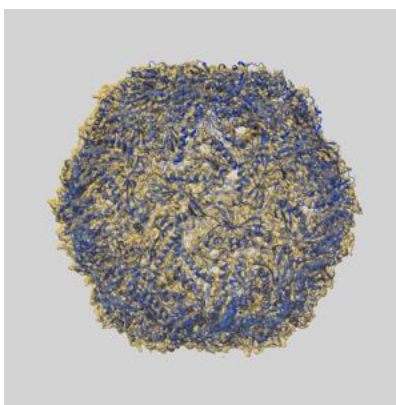
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55116 and PDB model 9SQR. Per-residue inclusion information can be found in section 3 on page 12.

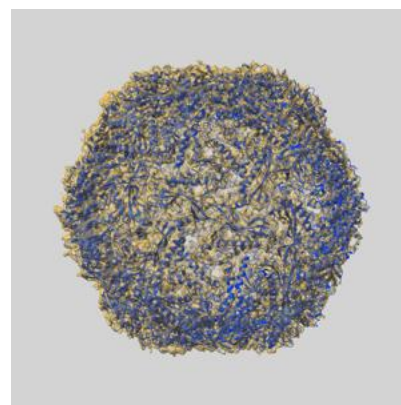
9.1 Map-model overlay [i](#)



X



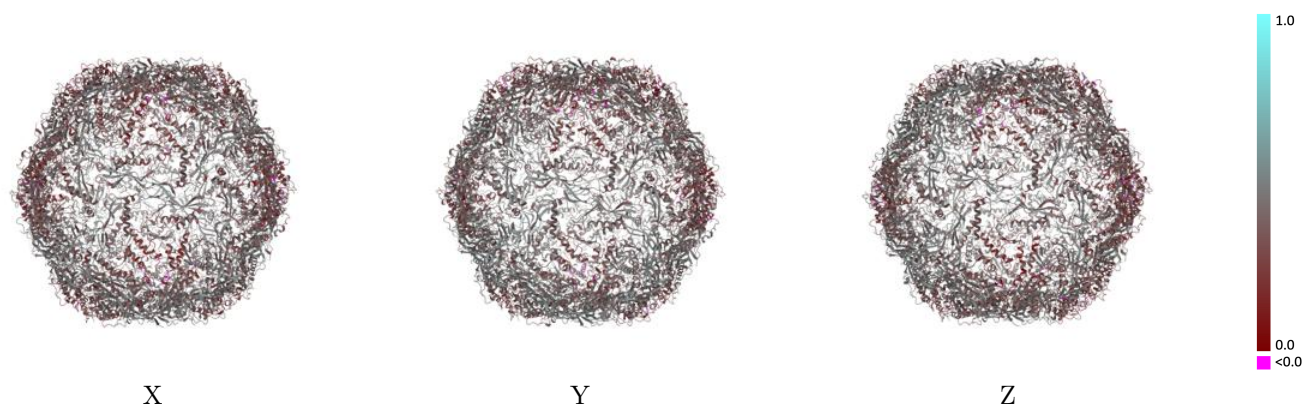
Y



Z

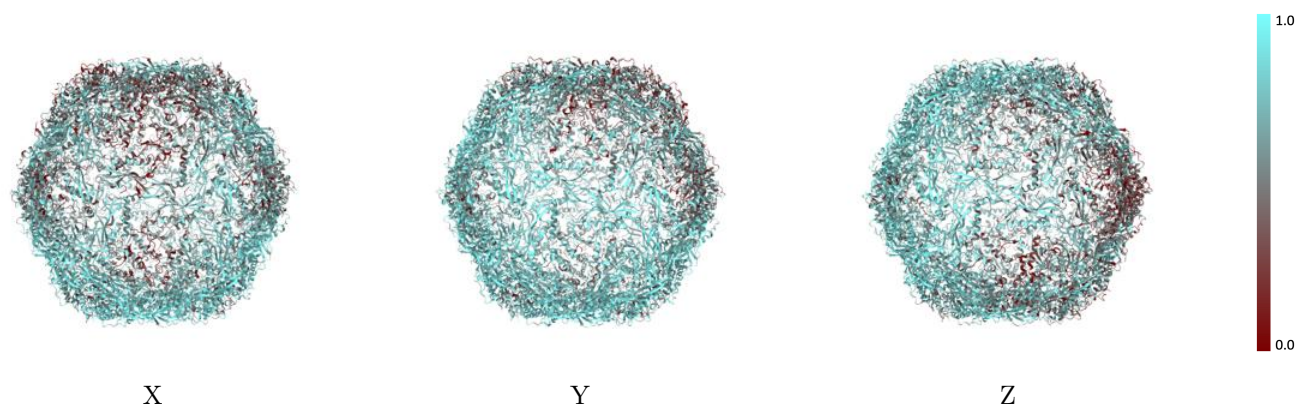
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



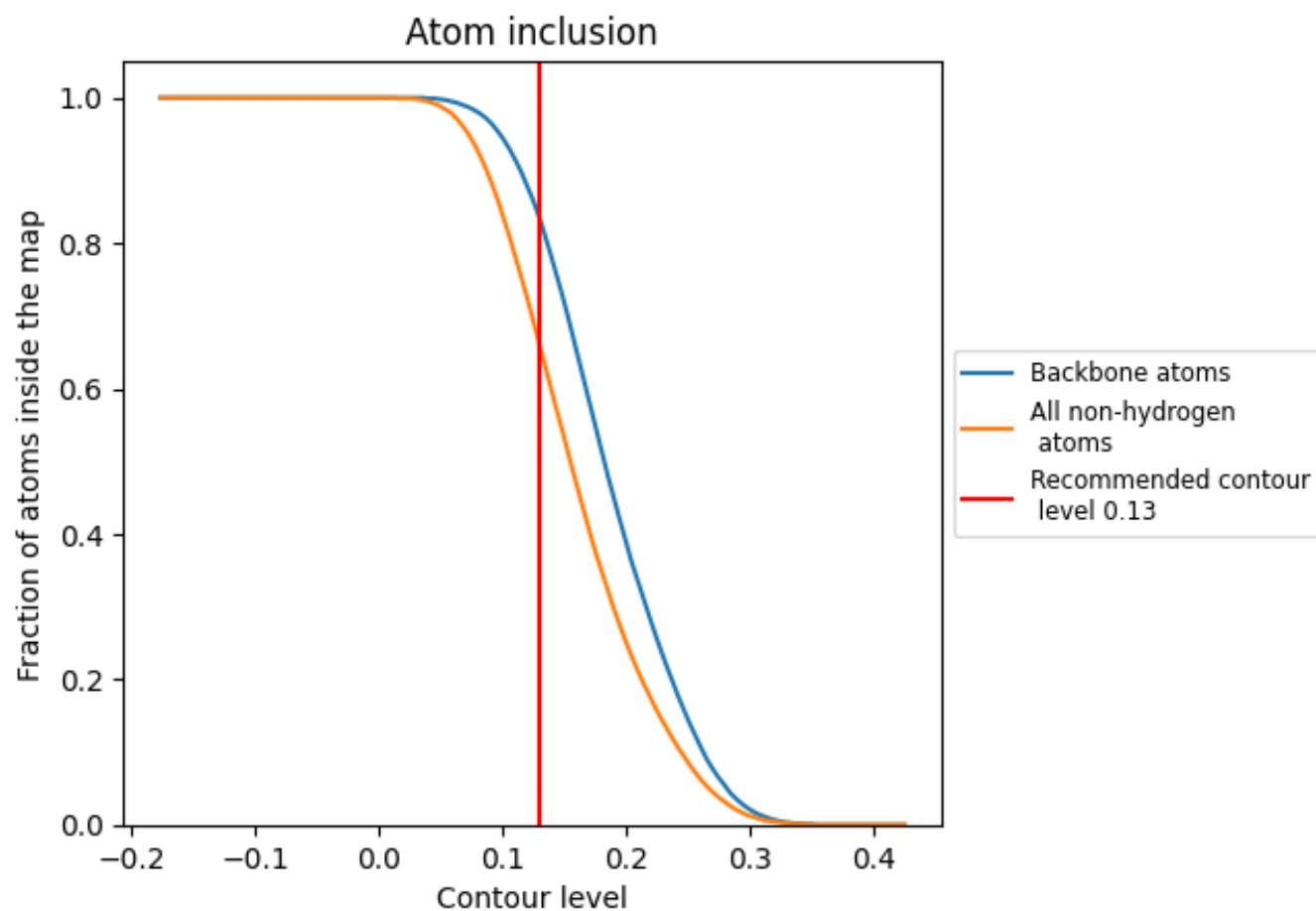
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 66% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6600	 0.3980
1	 0.5210	 0.4900
10	 0.1750	 0.4070
11	 0.5210	 0.4750
12	 0.5620	 0.4990
13	 0.3960	 0.4520
14	 0.3120	 0.4410
15	 0.4580	 0.4370
16	 0.5000	 0.4670
17	 0.4790	 0.4570
18	 0.5000	 0.4350
19	 0.2710	 0.4120
2	 0.3750	 0.4640
20	 0.5620	 0.4960
3	 0.4380	 0.4490
4	 0.1930	 0.3730
5	 0.4580	 0.4460
6	 0.3330	 0.4550
7	 0.3680	 0.4280
8	 0.2810	 0.4420
9	 0.5830	 0.4710
A	 0.7420	 0.4210
A0	 0.7610	 0.4270
AA	 0.7180	 0.3960
AB	 0.7250	 0.4250
B	 0.7360	 0.3940
BA	 0.6880	 0.3770
BB	 0.5670	 0.3620
C	 0.4910	 0.3760
CA	 0.6910	 0.3940
CB	 0.4850	 0.3690
D	 0.6320	 0.3890
DA	 0.6790	 0.3850
DB	 0.7420	 0.4070
E	 0.4930	 0.3750



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Chain	Atom inclusion	Q-score
EA	 0.7620	 0.4170
EB	 0.4340	 0.3730
F	 0.6320	 0.3770
FA	 0.7690	 0.4200
FB	 0.6050	 0.3940
G	 0.7340	 0.4220
GA	 0.7410	 0.4100
GB	 0.7560	 0.4150
H	 0.7490	 0.4220
HA	 0.7240	 0.4130
HB	 0.7370	 0.4280
I	 0.6980	 0.3980
IA	 0.7720	 0.4070
J	 0.6130	 0.3600
JA	 0.5750	 0.3820
K	 0.4660	 0.3580
KA	 0.7490	 0.4250
L	 0.6410	 0.3870
LA	 0.7540	 0.4290
M	 0.7360	 0.4160
MA	 0.7240	 0.4050
N	 0.7520	 0.4110
NA	 0.4840	 0.3780
O	 0.7320	 0.4260
OA	 0.4240	 0.3620
P	 0.7470	 0.4070
PA	 0.6850	 0.4020
Q	 0.5780	 0.3660
QA	 0.7570	 0.4270
R	 0.3730	 0.3700
RA	 0.7660	 0.4220
S	 0.6860	 0.3980
SA	 0.5120	 0.3660
T	 0.7560	 0.4080
TA	 0.7630	 0.4280
UA	 0.7430	 0.4130
V	 0.5720	 0.3530
VA	 0.5300	 0.3730
W	 0.4100	 0.3730
WA	 0.6170	 0.3840
X	 0.6880	 0.3990
XA	 0.7220	 0.4140

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Chain	Atom inclusion	Q-score
Y	 0.7540	 0.4220
YA	 0.7030	 0.3970
Z	 0.6960	 0.3850
ZA	 0.7640	 0.4190