



## Full wwPDB EM Validation Report ⓘ

May 8, 2024 – 05:29 PM JST

PDB ID : 8JYW  
EMDB ID : EMD-36732  
Title : Cryo-EM structure of the gasdermin pore from *Trichoplax adhaerens*  
Authors : Hou, Y.J.; Sun, Q.; Zeng, H.; Ding, J.  
Deposited on : 2023-07-04  
Resolution : 3.30 Å (reported)  
Based on initial model : 8JYV

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

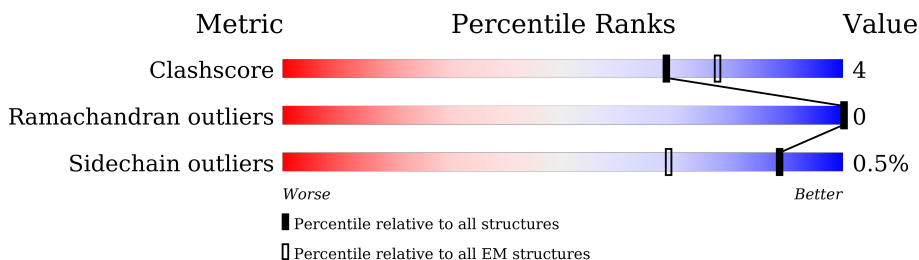
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 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 3.30 Å.

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






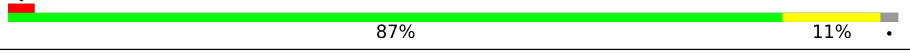
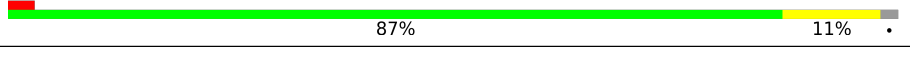



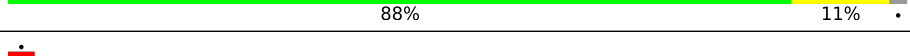
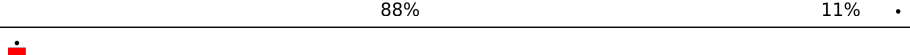
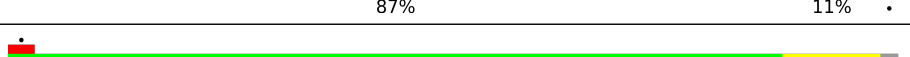
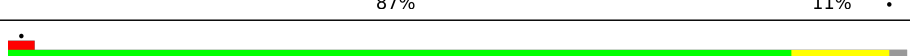

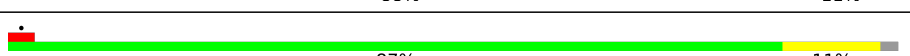
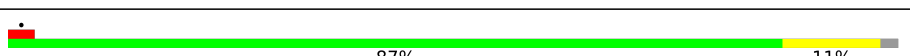
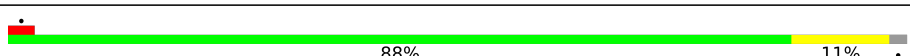





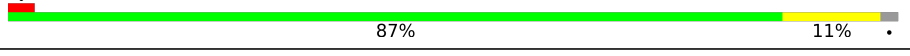



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	254	
1	AA	254	
1	AB	254	
1	AC	254	
1	B	254	
1	BA	254	
1	BB	254	
1	BC	254	




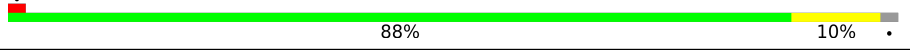
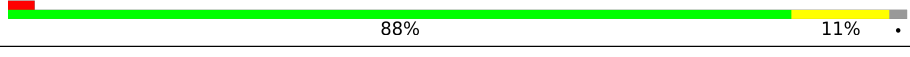



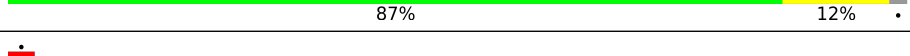
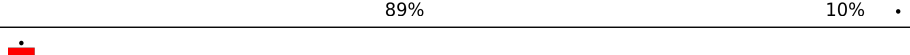
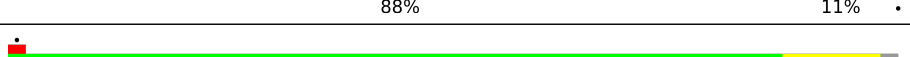
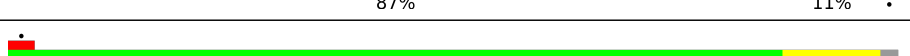

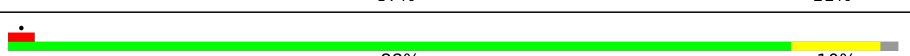
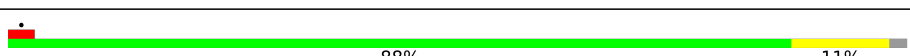
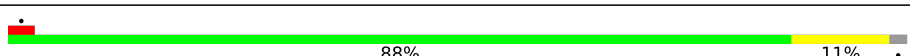





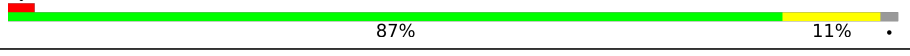



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Mol	Chain	Length	Quality of chain
1	C	254	 87% 11%
1	CA	254	 88% 11%
1	CB	254	 88% 10%
1	CC	254	 87% 11%
1	D	254	 87% 11%
1	DA	254	 88% 11%
1	DB	254	 87% 11%
1	DC	254	 87% 11%
1	E	254	 88% 11%
1	EA	254	 88% 11%
1	EB	254	 87% 11%
1	EC	254	 87% 11%
1	F	254	 88% 11%
1	FA	254	 88% 11%
1	FB	254	 87% 11%
1	FC	254	 87% 11%
1	G	254	 88% 11%
1	GA	254	 88% 11%
1	GB	254	 87% 11%
1	GC	254	 87% 11%
1	H	254	 87% 11%
1	HA	254	 88% 11%
1	HB	254	 87% 11%
1	HC	254	 88% 11%
1	I	254	 87% 11%





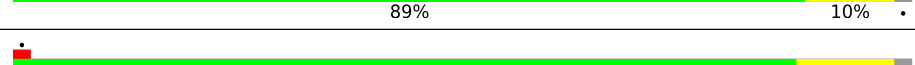
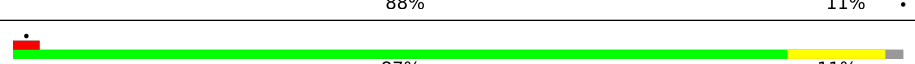
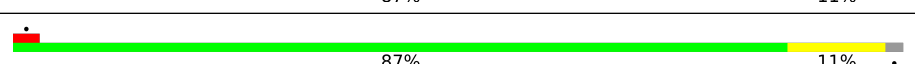
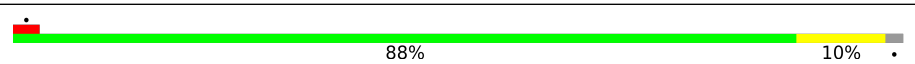


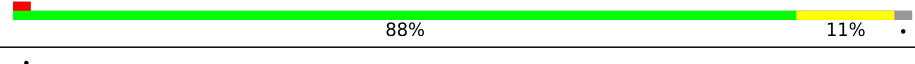
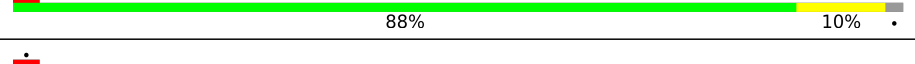

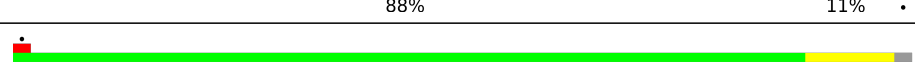
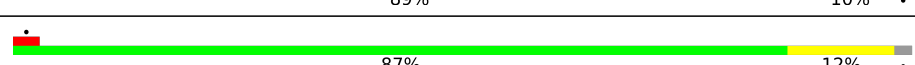



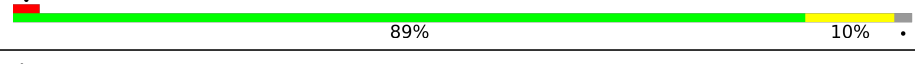






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Mol	Chain	Length	Quality of chain
1	IA	254	 88% 11%
1	IB	254	 87% 11%
1	IC	254	 88% 11%
1	J	254	 88% 10%
1	JA	254	 88% 11%
1	JB	254	 88% 11%
1	JC	254	 88% 11%
1	K	254	 87% 11%
1	KA	254	 87% 12%
1	KB	254	 89% 10%
1	KC	254	 88% 11%
1	L	254	 87% 11%
1	LA	254	 87% 11%
1	LB	254	 87% 11%
1	M	254	 88% 10%
1	MA	254	 88% 11%
1	MB	254	 88% 11%
1	N	254	 87% 11%
1	NA	254	 87% 11%
1	NB	254	 89% 10%
1	O	254	 87% 11%
1	OA	254	 87% 12%
1	OB	254	 87% 11%
1	P	254	 87% 12%
1	PA	254	 87% 11%


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Mol	Chain	Length	Quality of chain
1	PB	254	 87% 11%
1	Q	254	 88% 11%
1	QA	254	 88% 11%
1	QB	254	 88% 11%
1	R	254	 89% 10%
1	RA	254	 88% 11%
1	RB	254	 87% 11%
1	S	254	 87% 11%
1	SA	254	 88% 10%
1	SB	254	 88% 11%
1	T	254	 88% 11%
1	TA	254	 88% 11%
1	TB	254	 88% 10%
1	UA	254	 88% 11%
1	UB	254	 88% 11%
1	V	254	 89% 10%
1	VA	254	 87% 12%
1	VB	254	 87% 11%
1	W	254	 87% 12%
1	WA	254	 87% 11%
1	WB	254	 89% 10%
1	X	254	 87% 11%
1	XA	254	 87% 11%
1	XB	254	 88% 11%
1	Y	254	 87% 11%

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Mol	Chain	Length	Quality of chain
1	YA	254	 88% 11%
1	YB	254	 88% 11%
1	Z	254	 87% 11%
1	ZA	254	 88% 11%
1	ZB	254	 88% 10%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 165088 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 Gasdermin pore forming domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	250	1876	1178	323	364	11	0	0
1	B	250	1876	1178	323	364	11	0	0
1	C	250	1876	1178	323	364	11	0	0
1	D	250	1876	1178	323	364	11	0	0
1	E	250	1876	1178	323	364	11	0	0
1	F	250	1876	1178	323	364	11	0	0
1	G	250	1876	1178	323	364	11	0	0
1	H	250	1876	1178	323	364	11	0	0
1	I	250	1876	1178	323	364	11	0	0
1	J	250	1876	1178	323	364	11	0	0
1	K	250	1876	1178	323	364	11	0	0
1	L	250	1876	1178	323	364	11	0	0
1	M	250	1876	1178	323	364	11	0	0
1	N	250	1876	1178	323	364	11	0	0
1	O	250	1876	1178	323	364	11	0	0
1	P	250	1876	1178	323	364	11	0	0
1	Q	250	1876	1178	323	364	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	S	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	T	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	V	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	W	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	X	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	Y	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	Z	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	AA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	BA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	CA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	DA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	EA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	FA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	GA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	HA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	IA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	JA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	KA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	LA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	MA	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	NA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	OA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	PA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	QA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	RA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	SA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	TA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	UA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	VA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	WA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	XA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	YA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	ZA	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	AB	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	BB	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	CB	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	DB	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	EB	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	FB	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	GB	250	Total 1876	C 1178	N 323	O 364	S 11	0	0
1	HB	250	Total 1876	C 1178	N 323	O 364	S 11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	JB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	KB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	LB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	MB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	NB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	OB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	PB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	QB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	RB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	SB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	TB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	UB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	VB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	WB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	XB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	YB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	ZB	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	AC	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	BC	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		
1	CC	250	Total	C	N	O	S	0	0
			1876	1178	323	364	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	DC	250	1876	1178	323	364	11	0	0
1	EC	250	1876	1178	323	364	11	0	0
1	FC	250	1876	1178	323	364	11	0	0
1	GC	250	1876	1178	323	364	11	0	0
1	HC	250	1876	1178	323	364	11	0	0
1	IC	250	1876	1178	323	364	11	0	0
1	JC	250	1876	1178	323	364	11	0	0
1	KC	250	1876	1178	323	364	11	0	0

There are 352 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP B3RMM6
A	-2	GLY	-	expression tag	UNP B3RMM6
A	-1	ARG	-	expression tag	UNP B3RMM6
A	0	PRO	-	expression tag	UNP B3RMM6
B	-3	SER	-	expression tag	UNP B3RMM6
B	-2	GLY	-	expression tag	UNP B3RMM6
B	-1	ARG	-	expression tag	UNP B3RMM6
B	0	PRO	-	expression tag	UNP B3RMM6
C	-3	SER	-	expression tag	UNP B3RMM6
C	-2	GLY	-	expression tag	UNP B3RMM6
C	-1	ARG	-	expression tag	UNP B3RMM6
C	0	PRO	-	expression tag	UNP B3RMM6
D	-3	SER	-	expression tag	UNP B3RMM6
D	-2	GLY	-	expression tag	UNP B3RMM6
D	-1	ARG	-	expression tag	UNP B3RMM6
D	0	PRO	-	expression tag	UNP B3RMM6
E	-3	SER	-	expression tag	UNP B3RMM6
E	-2	GLY	-	expression tag	UNP B3RMM6
E	-1	ARG	-	expression tag	UNP B3RMM6
E	0	PRO	-	expression tag	UNP B3RMM6
F	-3	SER	-	expression tag	UNP B3RMM6
F	-2	GLY	-	expression tag	UNP B3RMM6
F	-1	ARG	-	expression tag	UNP B3RMM6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	PRO	-	expression tag	UNP B3RMM6
G	-3	SER	-	expression tag	UNP B3RMM6
G	-2	GLY	-	expression tag	UNP B3RMM6
G	-1	ARG	-	expression tag	UNP B3RMM6
G	0	PRO	-	expression tag	UNP B3RMM6
H	-3	SER	-	expression tag	UNP B3RMM6
H	-2	GLY	-	expression tag	UNP B3RMM6
H	-1	ARG	-	expression tag	UNP B3RMM6
H	0	PRO	-	expression tag	UNP B3RMM6
I	-3	SER	-	expression tag	UNP B3RMM6
I	-2	GLY	-	expression tag	UNP B3RMM6
I	-1	ARG	-	expression tag	UNP B3RMM6
I	0	PRO	-	expression tag	UNP B3RMM6
J	-3	SER	-	expression tag	UNP B3RMM6
J	-2	GLY	-	expression tag	UNP B3RMM6
J	-1	ARG	-	expression tag	UNP B3RMM6
J	0	PRO	-	expression tag	UNP B3RMM6
K	-3	SER	-	expression tag	UNP B3RMM6
K	-2	GLY	-	expression tag	UNP B3RMM6
K	-1	ARG	-	expression tag	UNP B3RMM6
K	0	PRO	-	expression tag	UNP B3RMM6
L	-3	SER	-	expression tag	UNP B3RMM6
L	-2	GLY	-	expression tag	UNP B3RMM6
L	-1	ARG	-	expression tag	UNP B3RMM6
L	0	PRO	-	expression tag	UNP B3RMM6
M	-3	SER	-	expression tag	UNP B3RMM6
M	-2	GLY	-	expression tag	UNP B3RMM6
M	-1	ARG	-	expression tag	UNP B3RMM6
M	0	PRO	-	expression tag	UNP B3RMM6
N	-3	SER	-	expression tag	UNP B3RMM6
N	-2	GLY	-	expression tag	UNP B3RMM6
N	-1	ARG	-	expression tag	UNP B3RMM6
N	0	PRO	-	expression tag	UNP B3RMM6
O	-3	SER	-	expression tag	UNP B3RMM6
O	-2	GLY	-	expression tag	UNP B3RMM6
O	-1	ARG	-	expression tag	UNP B3RMM6
O	0	PRO	-	expression tag	UNP B3RMM6
P	-3	SER	-	expression tag	UNP B3RMM6
P	-2	GLY	-	expression tag	UNP B3RMM6
P	-1	ARG	-	expression tag	UNP B3RMM6
P	0	PRO	-	expression tag	UNP B3RMM6
Q	-3	SER	-	expression tag	UNP B3RMM6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-2	GLY	-	expression tag	UNP B3RMM6
Q	-1	ARG	-	expression tag	UNP B3RMM6
Q	0	PRO	-	expression tag	UNP B3RMM6
R	-3	SER	-	expression tag	UNP B3RMM6
R	-2	GLY	-	expression tag	UNP B3RMM6
R	-1	ARG	-	expression tag	UNP B3RMM6
R	0	PRO	-	expression tag	UNP B3RMM6
S	-3	SER	-	expression tag	UNP B3RMM6
S	-2	GLY	-	expression tag	UNP B3RMM6
S	-1	ARG	-	expression tag	UNP B3RMM6
S	0	PRO	-	expression tag	UNP B3RMM6
T	-3	SER	-	expression tag	UNP B3RMM6
T	-2	GLY	-	expression tag	UNP B3RMM6
T	-1	ARG	-	expression tag	UNP B3RMM6
T	0	PRO	-	expression tag	UNP B3RMM6
V	-3	SER	-	expression tag	UNP B3RMM6
V	-2	GLY	-	expression tag	UNP B3RMM6
V	-1	ARG	-	expression tag	UNP B3RMM6
V	0	PRO	-	expression tag	UNP B3RMM6
W	-3	SER	-	expression tag	UNP B3RMM6
W	-2	GLY	-	expression tag	UNP B3RMM6
W	-1	ARG	-	expression tag	UNP B3RMM6
W	0	PRO	-	expression tag	UNP B3RMM6
X	-3	SER	-	expression tag	UNP B3RMM6
X	-2	GLY	-	expression tag	UNP B3RMM6
X	-1	ARG	-	expression tag	UNP B3RMM6
X	0	PRO	-	expression tag	UNP B3RMM6
Y	-3	SER	-	expression tag	UNP B3RMM6
Y	-2	GLY	-	expression tag	UNP B3RMM6
Y	-1	ARG	-	expression tag	UNP B3RMM6
Y	0	PRO	-	expression tag	UNP B3RMM6
Z	-3	SER	-	expression tag	UNP B3RMM6
Z	-2	GLY	-	expression tag	UNP B3RMM6
Z	-1	ARG	-	expression tag	UNP B3RMM6
Z	0	PRO	-	expression tag	UNP B3RMM6
AA	-3	SER	-	expression tag	UNP B3RMM6
AA	-2	GLY	-	expression tag	UNP B3RMM6
AA	-1	ARG	-	expression tag	UNP B3RMM6
AA	0	PRO	-	expression tag	UNP B3RMM6
BA	-3	SER	-	expression tag	UNP B3RMM6
BA	-2	GLY	-	expression tag	UNP B3RMM6
BA	-1	ARG	-	expression tag	UNP B3RMM6

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Chain	Residue	Modelled	Actual	Comment	Reference
BA	0	PRO	-	expression tag	UNP B3RMM6
CA	-3	SER	-	expression tag	UNP B3RMM6
CA	-2	GLY	-	expression tag	UNP B3RMM6
CA	-1	ARG	-	expression tag	UNP B3RMM6
CA	0	PRO	-	expression tag	UNP B3RMM6
DA	-3	SER	-	expression tag	UNP B3RMM6
DA	-2	GLY	-	expression tag	UNP B3RMM6
DA	-1	ARG	-	expression tag	UNP B3RMM6
DA	0	PRO	-	expression tag	UNP B3RMM6
EA	-3	SER	-	expression tag	UNP B3RMM6
EA	-2	GLY	-	expression tag	UNP B3RMM6
EA	-1	ARG	-	expression tag	UNP B3RMM6
EA	0	PRO	-	expression tag	UNP B3RMM6
FA	-3	SER	-	expression tag	UNP B3RMM6
FA	-2	GLY	-	expression tag	UNP B3RMM6
FA	-1	ARG	-	expression tag	UNP B3RMM6
FA	0	PRO	-	expression tag	UNP B3RMM6
GA	-3	SER	-	expression tag	UNP B3RMM6
GA	-2	GLY	-	expression tag	UNP B3RMM6
GA	-1	ARG	-	expression tag	UNP B3RMM6
GA	0	PRO	-	expression tag	UNP B3RMM6
HA	-3	SER	-	expression tag	UNP B3RMM6
HA	-2	GLY	-	expression tag	UNP B3RMM6
HA	-1	ARG	-	expression tag	UNP B3RMM6
HA	0	PRO	-	expression tag	UNP B3RMM6
IA	-3	SER	-	expression tag	UNP B3RMM6
IA	-2	GLY	-	expression tag	UNP B3RMM6
IA	-1	ARG	-	expression tag	UNP B3RMM6
IA	0	PRO	-	expression tag	UNP B3RMM6
JA	-3	SER	-	expression tag	UNP B3RMM6
JA	-2	GLY	-	expression tag	UNP B3RMM6
JA	-1	ARG	-	expression tag	UNP B3RMM6
JA	0	PRO	-	expression tag	UNP B3RMM6
KA	-3	SER	-	expression tag	UNP B3RMM6
KA	-2	GLY	-	expression tag	UNP B3RMM6
KA	-1	ARG	-	expression tag	UNP B3RMM6
KA	0	PRO	-	expression tag	UNP B3RMM6
LA	-3	SER	-	expression tag	UNP B3RMM6
LA	-2	GLY	-	expression tag	UNP B3RMM6
LA	-1	ARG	-	expression tag	UNP B3RMM6
LA	0	PRO	-	expression tag	UNP B3RMM6
MA	-3	SER	-	expression tag	UNP B3RMM6

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Chain	Residue	Modelled	Actual	Comment	Reference
MA	-2	GLY	-	expression tag	UNP B3RMM6
MA	-1	ARG	-	expression tag	UNP B3RMM6
MA	0	PRO	-	expression tag	UNP B3RMM6
NA	-3	SER	-	expression tag	UNP B3RMM6
NA	-2	GLY	-	expression tag	UNP B3RMM6
NA	-1	ARG	-	expression tag	UNP B3RMM6
NA	0	PRO	-	expression tag	UNP B3RMM6
OA	-3	SER	-	expression tag	UNP B3RMM6
OA	-2	GLY	-	expression tag	UNP B3RMM6
OA	-1	ARG	-	expression tag	UNP B3RMM6
OA	0	PRO	-	expression tag	UNP B3RMM6
PA	-3	SER	-	expression tag	UNP B3RMM6
PA	-2	GLY	-	expression tag	UNP B3RMM6
PA	-1	ARG	-	expression tag	UNP B3RMM6
PA	0	PRO	-	expression tag	UNP B3RMM6
QA	-3	SER	-	expression tag	UNP B3RMM6
QA	-2	GLY	-	expression tag	UNP B3RMM6
QA	-1	ARG	-	expression tag	UNP B3RMM6
QA	0	PRO	-	expression tag	UNP B3RMM6
RA	-3	SER	-	expression tag	UNP B3RMM6
RA	-2	GLY	-	expression tag	UNP B3RMM6
RA	-1	ARG	-	expression tag	UNP B3RMM6
RA	0	PRO	-	expression tag	UNP B3RMM6
SA	-3	SER	-	expression tag	UNP B3RMM6
SA	-2	GLY	-	expression tag	UNP B3RMM6
SA	-1	ARG	-	expression tag	UNP B3RMM6
SA	0	PRO	-	expression tag	UNP B3RMM6
TA	-3	SER	-	expression tag	UNP B3RMM6
TA	-2	GLY	-	expression tag	UNP B3RMM6
TA	-1	ARG	-	expression tag	UNP B3RMM6
TA	0	PRO	-	expression tag	UNP B3RMM6
UA	-3	SER	-	expression tag	UNP B3RMM6
UA	-2	GLY	-	expression tag	UNP B3RMM6
UA	-1	ARG	-	expression tag	UNP B3RMM6
UA	0	PRO	-	expression tag	UNP B3RMM6
VA	-3	SER	-	expression tag	UNP B3RMM6
VA	-2	GLY	-	expression tag	UNP B3RMM6
VA	-1	ARG	-	expression tag	UNP B3RMM6
VA	0	PRO	-	expression tag	UNP B3RMM6
WA	-3	SER	-	expression tag	UNP B3RMM6
WA	-2	GLY	-	expression tag	UNP B3RMM6
WA	-1	ARG	-	expression tag	UNP B3RMM6

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Chain	Residue	Modelled	Actual	Comment	Reference
WA	0	PRO	-	expression tag	UNP B3RMM6
XA	-3	SER	-	expression tag	UNP B3RMM6
XA	-2	GLY	-	expression tag	UNP B3RMM6
XA	-1	ARG	-	expression tag	UNP B3RMM6
XA	0	PRO	-	expression tag	UNP B3RMM6
YA	-3	SER	-	expression tag	UNP B3RMM6
YA	-2	GLY	-	expression tag	UNP B3RMM6
YA	-1	ARG	-	expression tag	UNP B3RMM6
YA	0	PRO	-	expression tag	UNP B3RMM6
ZA	-3	SER	-	expression tag	UNP B3RMM6
ZA	-2	GLY	-	expression tag	UNP B3RMM6
ZA	-1	ARG	-	expression tag	UNP B3RMM6
ZA	0	PRO	-	expression tag	UNP B3RMM6
AB	-3	SER	-	expression tag	UNP B3RMM6
AB	-2	GLY	-	expression tag	UNP B3RMM6
AB	-1	ARG	-	expression tag	UNP B3RMM6
AB	0	PRO	-	expression tag	UNP B3RMM6
BB	-3	SER	-	expression tag	UNP B3RMM6
BB	-2	GLY	-	expression tag	UNP B3RMM6
BB	-1	ARG	-	expression tag	UNP B3RMM6
BB	0	PRO	-	expression tag	UNP B3RMM6
CB	-3	SER	-	expression tag	UNP B3RMM6
CB	-2	GLY	-	expression tag	UNP B3RMM6
CB	-1	ARG	-	expression tag	UNP B3RMM6
CB	0	PRO	-	expression tag	UNP B3RMM6
DB	-3	SER	-	expression tag	UNP B3RMM6
DB	-2	GLY	-	expression tag	UNP B3RMM6
DB	-1	ARG	-	expression tag	UNP B3RMM6
DB	0	PRO	-	expression tag	UNP B3RMM6
EB	-3	SER	-	expression tag	UNP B3RMM6
EB	-2	GLY	-	expression tag	UNP B3RMM6
EB	-1	ARG	-	expression tag	UNP B3RMM6
EB	0	PRO	-	expression tag	UNP B3RMM6
FB	-3	SER	-	expression tag	UNP B3RMM6
FB	-2	GLY	-	expression tag	UNP B3RMM6
FB	-1	ARG	-	expression tag	UNP B3RMM6
FB	0	PRO	-	expression tag	UNP B3RMM6
GB	-3	SER	-	expression tag	UNP B3RMM6
GB	-2	GLY	-	expression tag	UNP B3RMM6
GB	-1	ARG	-	expression tag	UNP B3RMM6
GB	0	PRO	-	expression tag	UNP B3RMM6
HB	-3	SER	-	expression tag	UNP B3RMM6

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Chain	Residue	Modelled	Actual	Comment	Reference
HB	-2	GLY	-	expression tag	UNP B3RMM6
HB	-1	ARG	-	expression tag	UNP B3RMM6
HB	0	PRO	-	expression tag	UNP B3RMM6
IB	-3	SER	-	expression tag	UNP B3RMM6
IB	-2	GLY	-	expression tag	UNP B3RMM6
IB	-1	ARG	-	expression tag	UNP B3RMM6
IB	0	PRO	-	expression tag	UNP B3RMM6
JB	-3	SER	-	expression tag	UNP B3RMM6
JB	-2	GLY	-	expression tag	UNP B3RMM6
JB	-1	ARG	-	expression tag	UNP B3RMM6
JB	0	PRO	-	expression tag	UNP B3RMM6
KB	-3	SER	-	expression tag	UNP B3RMM6
KB	-2	GLY	-	expression tag	UNP B3RMM6
KB	-1	ARG	-	expression tag	UNP B3RMM6
KB	0	PRO	-	expression tag	UNP B3RMM6
LB	-3	SER	-	expression tag	UNP B3RMM6
LB	-2	GLY	-	expression tag	UNP B3RMM6
LB	-1	ARG	-	expression tag	UNP B3RMM6
LB	0	PRO	-	expression tag	UNP B3RMM6
MB	-3	SER	-	expression tag	UNP B3RMM6
MB	-2	GLY	-	expression tag	UNP B3RMM6
MB	-1	ARG	-	expression tag	UNP B3RMM6
MB	0	PRO	-	expression tag	UNP B3RMM6
NB	-3	SER	-	expression tag	UNP B3RMM6
NB	-2	GLY	-	expression tag	UNP B3RMM6
NB	-1	ARG	-	expression tag	UNP B3RMM6
NB	0	PRO	-	expression tag	UNP B3RMM6
OB	-3	SER	-	expression tag	UNP B3RMM6
OB	-2	GLY	-	expression tag	UNP B3RMM6
OB	-1	ARG	-	expression tag	UNP B3RMM6
OB	0	PRO	-	expression tag	UNP B3RMM6
PB	-3	SER	-	expression tag	UNP B3RMM6
PB	-2	GLY	-	expression tag	UNP B3RMM6
PB	-1	ARG	-	expression tag	UNP B3RMM6
PB	0	PRO	-	expression tag	UNP B3RMM6
QB	-3	SER	-	expression tag	UNP B3RMM6
QB	-2	GLY	-	expression tag	UNP B3RMM6
QB	-1	ARG	-	expression tag	UNP B3RMM6
QB	0	PRO	-	expression tag	UNP B3RMM6
RB	-3	SER	-	expression tag	UNP B3RMM6
RB	-2	GLY	-	expression tag	UNP B3RMM6
RB	-1	ARG	-	expression tag	UNP B3RMM6

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Chain	Residue	Modelled	Actual	Comment	Reference
RB	0	PRO	-	expression tag	UNP B3RMM6
SB	-3	SER	-	expression tag	UNP B3RMM6
SB	-2	GLY	-	expression tag	UNP B3RMM6
SB	-1	ARG	-	expression tag	UNP B3RMM6
SB	0	PRO	-	expression tag	UNP B3RMM6
TB	-3	SER	-	expression tag	UNP B3RMM6
TB	-2	GLY	-	expression tag	UNP B3RMM6
TB	-1	ARG	-	expression tag	UNP B3RMM6
TB	0	PRO	-	expression tag	UNP B3RMM6
UB	-3	SER	-	expression tag	UNP B3RMM6
UB	-2	GLY	-	expression tag	UNP B3RMM6
UB	-1	ARG	-	expression tag	UNP B3RMM6
UB	0	PRO	-	expression tag	UNP B3RMM6
VB	-3	SER	-	expression tag	UNP B3RMM6
VB	-2	GLY	-	expression tag	UNP B3RMM6
VB	-1	ARG	-	expression tag	UNP B3RMM6
VB	0	PRO	-	expression tag	UNP B3RMM6
WB	-3	SER	-	expression tag	UNP B3RMM6
WB	-2	GLY	-	expression tag	UNP B3RMM6
WB	-1	ARG	-	expression tag	UNP B3RMM6
WB	0	PRO	-	expression tag	UNP B3RMM6
XB	-3	SER	-	expression tag	UNP B3RMM6
XB	-2	GLY	-	expression tag	UNP B3RMM6
XB	-1	ARG	-	expression tag	UNP B3RMM6
XB	0	PRO	-	expression tag	UNP B3RMM6
YB	-3	SER	-	expression tag	UNP B3RMM6
YB	-2	GLY	-	expression tag	UNP B3RMM6
YB	-1	ARG	-	expression tag	UNP B3RMM6
YB	0	PRO	-	expression tag	UNP B3RMM6
ZB	-3	SER	-	expression tag	UNP B3RMM6
ZB	-2	GLY	-	expression tag	UNP B3RMM6
ZB	-1	ARG	-	expression tag	UNP B3RMM6
ZB	0	PRO	-	expression tag	UNP B3RMM6
AC	-3	SER	-	expression tag	UNP B3RMM6
AC	-2	GLY	-	expression tag	UNP B3RMM6
AC	-1	ARG	-	expression tag	UNP B3RMM6
AC	0	PRO	-	expression tag	UNP B3RMM6
BC	-3	SER	-	expression tag	UNP B3RMM6
BC	-2	GLY	-	expression tag	UNP B3RMM6
BC	-1	ARG	-	expression tag	UNP B3RMM6
BC	0	PRO	-	expression tag	UNP B3RMM6
CC	-3	SER	-	expression tag	UNP B3RMM6

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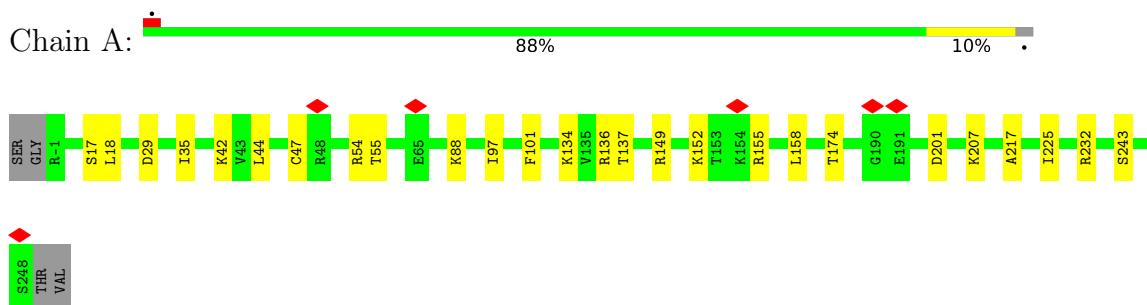
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Chain	Residue	Modelled	Actual	Comment	Reference
CC	-2	GLY	-	expression tag	UNP B3RMM6
CC	-1	ARG	-	expression tag	UNP B3RMM6
CC	0	PRO	-	expression tag	UNP B3RMM6
DC	-3	SER	-	expression tag	UNP B3RMM6
DC	-2	GLY	-	expression tag	UNP B3RMM6
DC	-1	ARG	-	expression tag	UNP B3RMM6
DC	0	PRO	-	expression tag	UNP B3RMM6
EC	-3	SER	-	expression tag	UNP B3RMM6
EC	-2	GLY	-	expression tag	UNP B3RMM6
EC	-1	ARG	-	expression tag	UNP B3RMM6
EC	0	PRO	-	expression tag	UNP B3RMM6
FC	-3	SER	-	expression tag	UNP B3RMM6
FC	-2	GLY	-	expression tag	UNP B3RMM6
FC	-1	ARG	-	expression tag	UNP B3RMM6
FC	0	PRO	-	expression tag	UNP B3RMM6
GC	-3	SER	-	expression tag	UNP B3RMM6
GC	-2	GLY	-	expression tag	UNP B3RMM6
GC	-1	ARG	-	expression tag	UNP B3RMM6
GC	0	PRO	-	expression tag	UNP B3RMM6
HC	-3	SER	-	expression tag	UNP B3RMM6
HC	-2	GLY	-	expression tag	UNP B3RMM6
HC	-1	ARG	-	expression tag	UNP B3RMM6
HC	0	PRO	-	expression tag	UNP B3RMM6
IC	-3	SER	-	expression tag	UNP B3RMM6
IC	-2	GLY	-	expression tag	UNP B3RMM6
IC	-1	ARG	-	expression tag	UNP B3RMM6
IC	0	PRO	-	expression tag	UNP B3RMM6
JC	-3	SER	-	expression tag	UNP B3RMM6
JC	-2	GLY	-	expression tag	UNP B3RMM6
JC	-1	ARG	-	expression tag	UNP B3RMM6
JC	0	PRO	-	expression tag	UNP B3RMM6
KC	-3	SER	-	expression tag	UNP B3RMM6
KC	-2	GLY	-	expression tag	UNP B3RMM6
KC	-1	ARG	-	expression tag	UNP B3RMM6
KC	0	PRO	-	expression tag	UNP B3RMM6

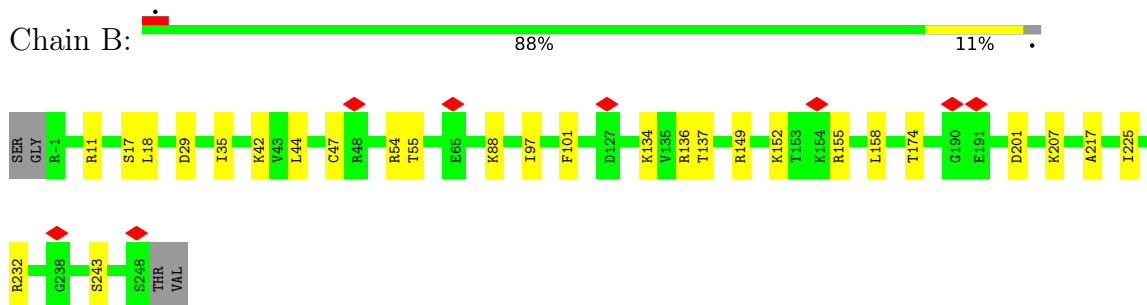
### 3 Residue-property plots [i](#)

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.

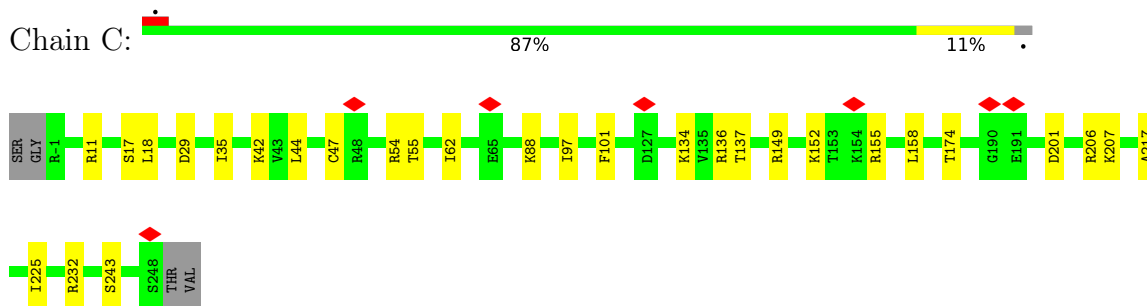
- Molecule 1: Gasdermin pore forming domain-containing protein



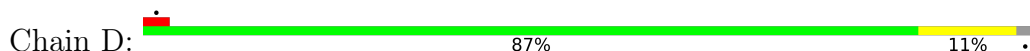
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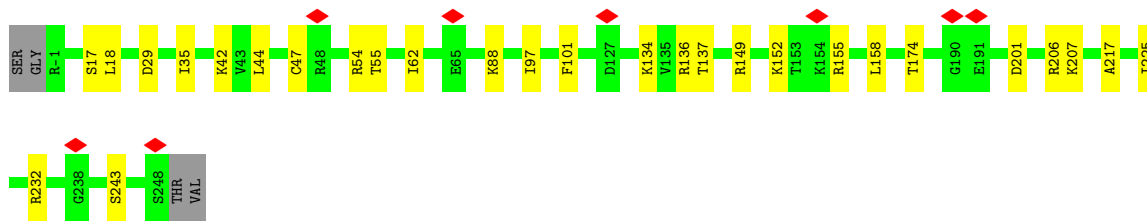


- Molecule 1: Gasdermin pore forming domain-containing protein



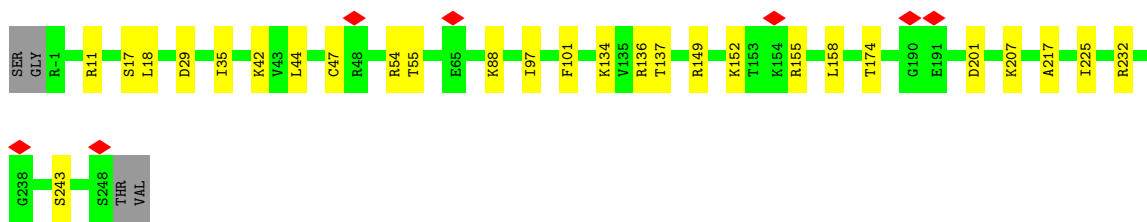
- Molecule 1: Gasdermin pore forming domain-containing protein





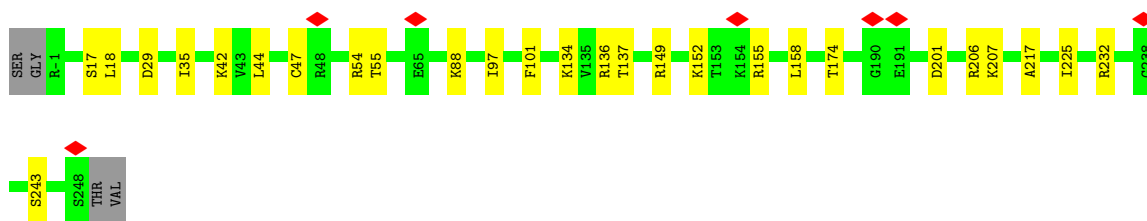
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain E: 88% 11%



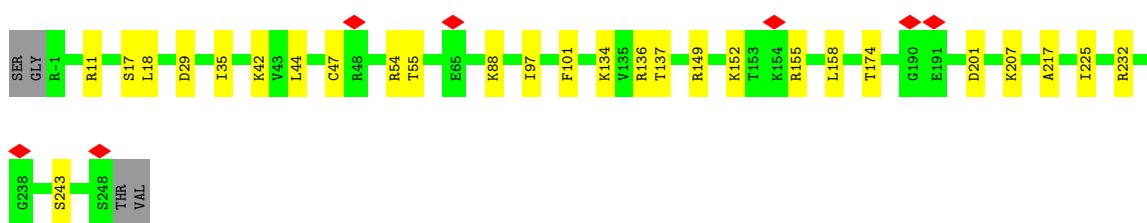
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain F: 88% 11%



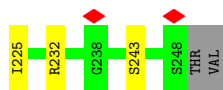
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain G: 88% 11%



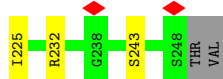
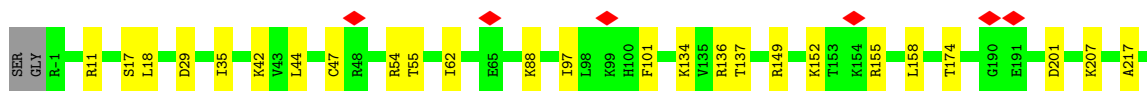
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain H: 87% 11%



- Molecule 1: Gasdermin pore forming domain-containing protein

Chain I: 87% 11%



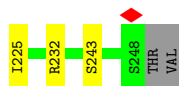
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain J: 88% 10%



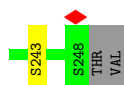
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain K: 87% 11%

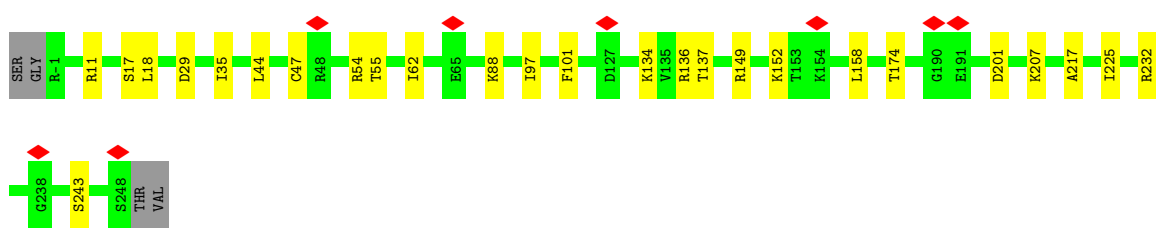
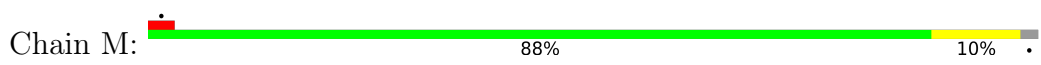


- Molecule 1: Gasdermin pore forming domain-containing protein

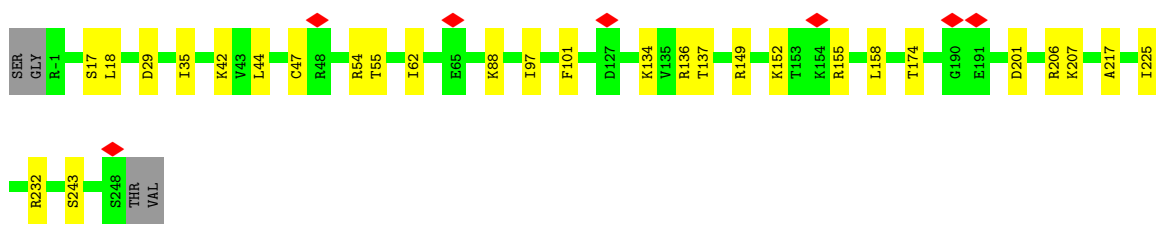
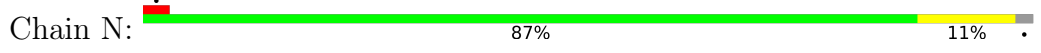
Chain L: 87% 11%



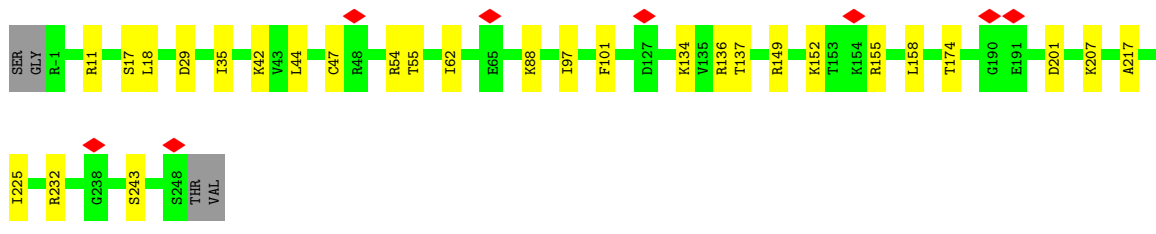
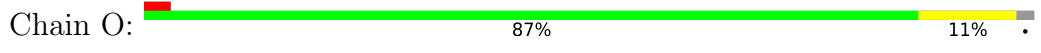
- Molecule 1: Gasdermin pore forming domain-containing protein



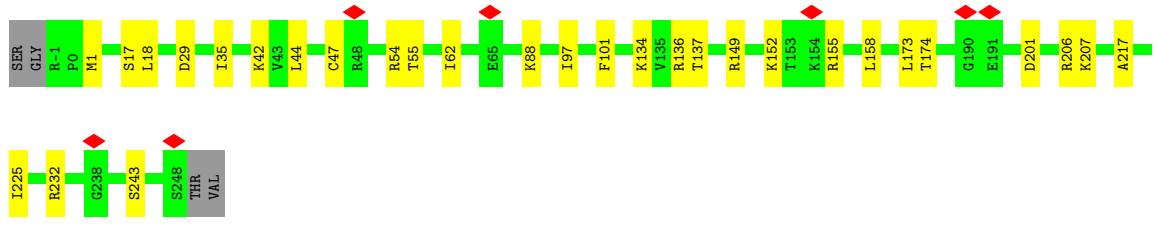
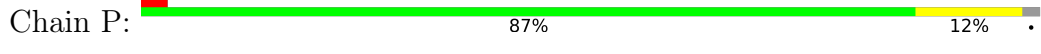
• Molecule 1: Gasdermin pore forming domain-containing protein



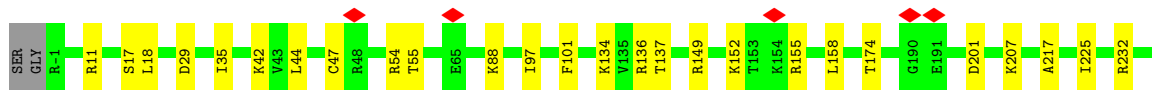
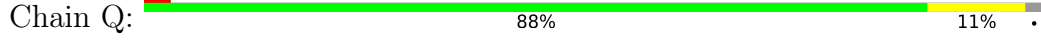
• Molecule 1: Gasdermin pore forming domain-containing protein

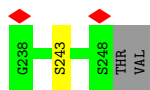


• Molecule 1: Gasdermin pore forming domain-containing protein

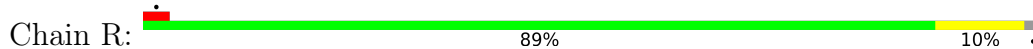


• Molecule 1: Gasdermin pore forming domain-containing protein

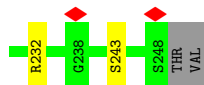
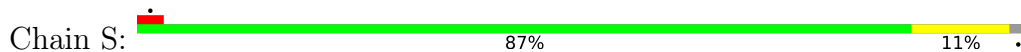




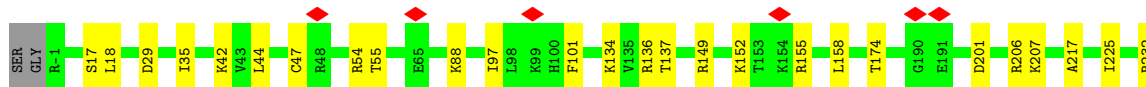
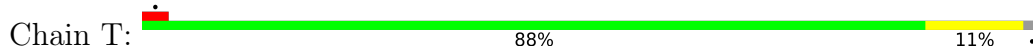
• Molecule 1: Gasdermin pore forming domain-containing protein



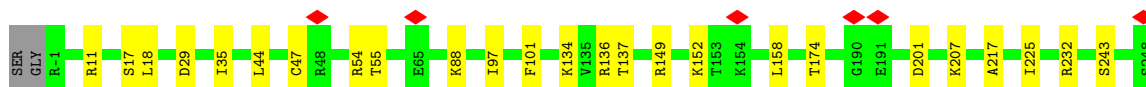
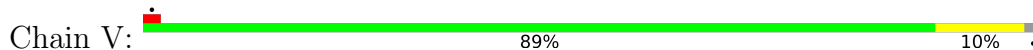
• Molecule 1: Gasdermin pore forming domain-containing protein



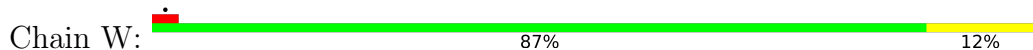
• Molecule 1: Gasdermin pore forming domain-containing protein



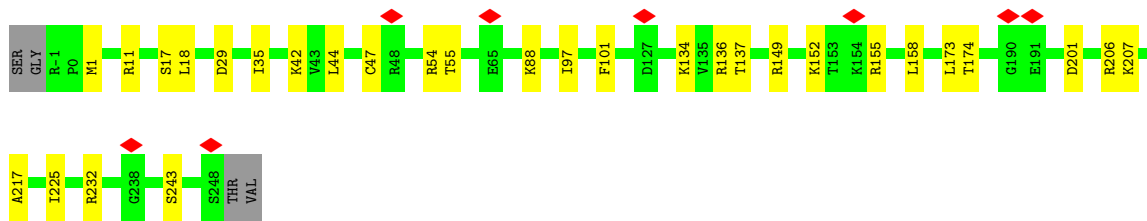
• Molecule 1: Gasdermin pore forming domain-containing protein



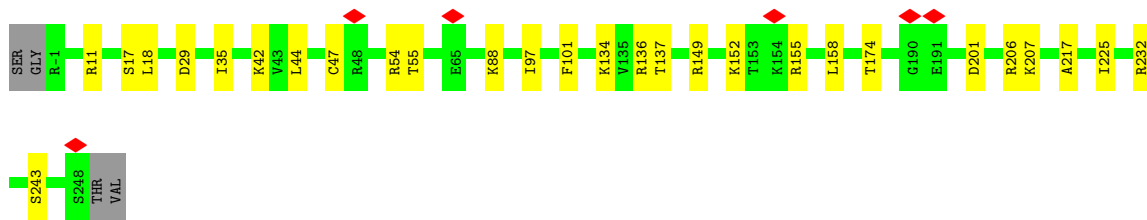
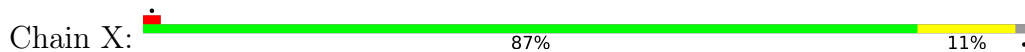
• Molecule 1: Gasdermin pore forming domain-containing protein



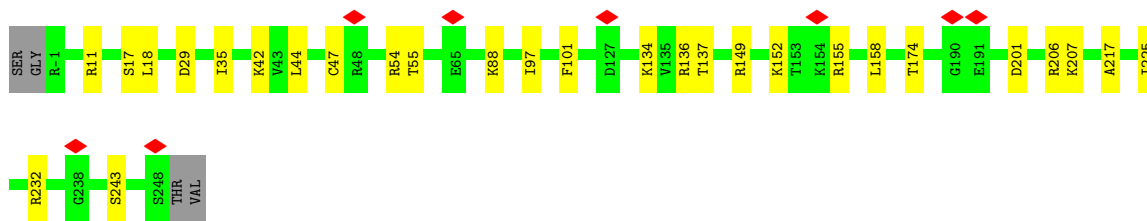
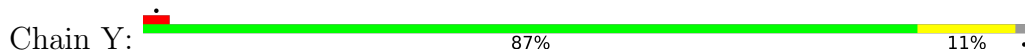




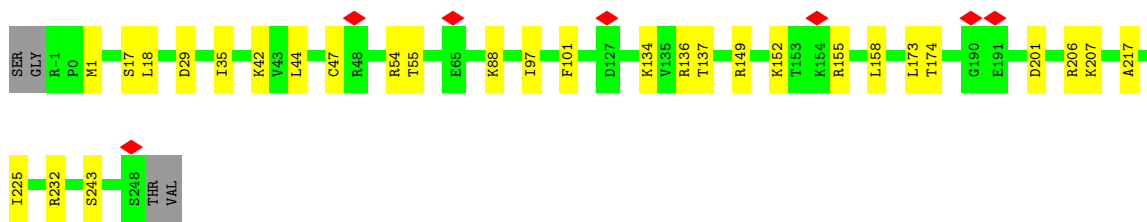
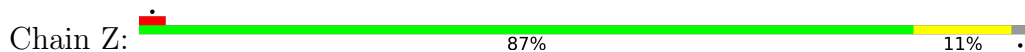
● Molecule 1: Gasdermin pore forming domain-containing protein



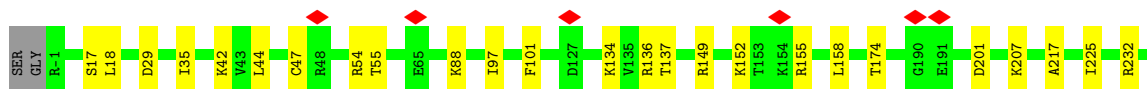
● Molecule 1: Gasdermin pore forming domain-containing protein

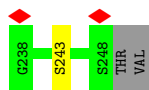


● Molecule 1: Gasdermin pore forming domain-containing protein



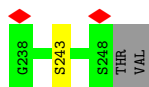
● Molecule 1: Gasdermin pore forming domain-containing protein





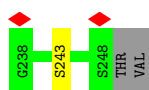
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain BA: 88% 11%



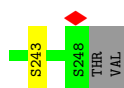
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain CA: 88% 11%



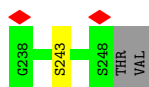
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain DA: 88% 11%

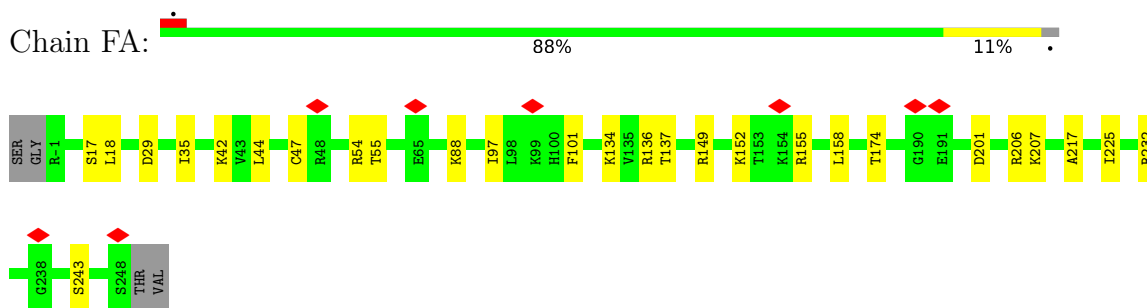


- Molecule 1: Gasdermin pore forming domain-containing protein

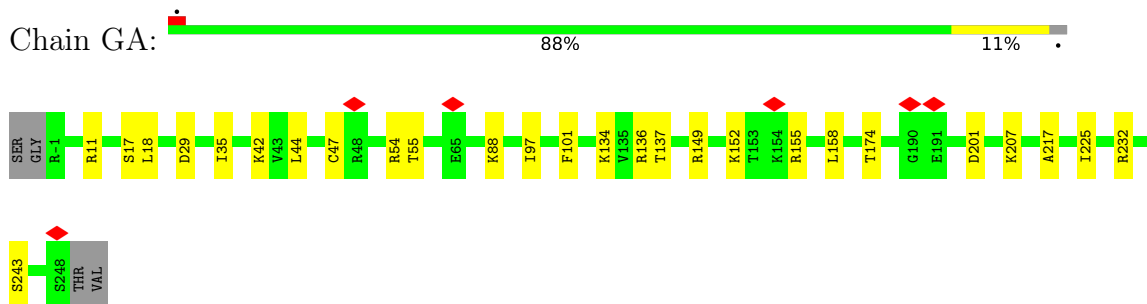
Chain EA: 88% 11%



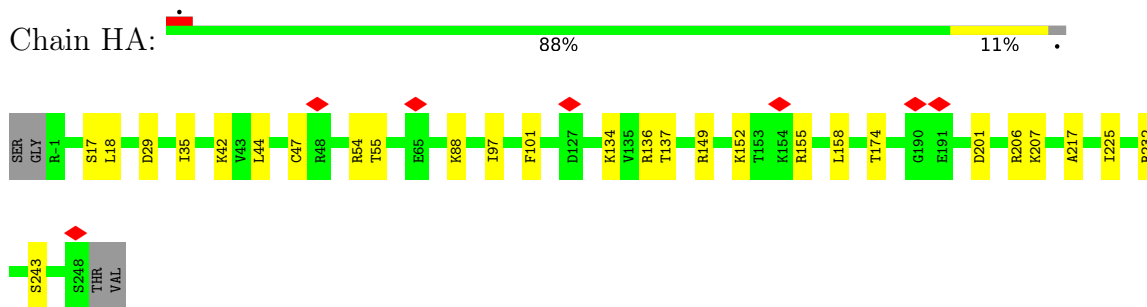
- Molecule 1: Gasdermin pore forming domain-containing protein



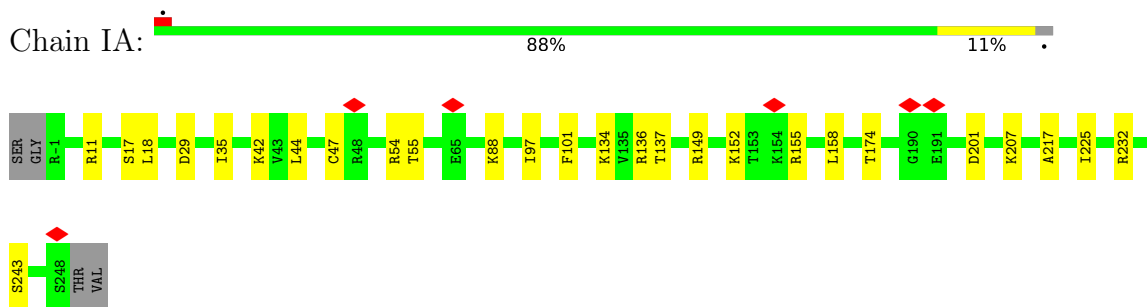
- Molecule 1: Gasdermin pore forming domain-containing protein



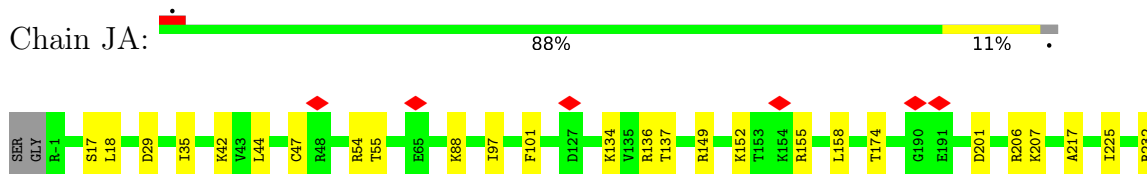
- Molecule 1: Gasdermin pore forming domain-containing protein

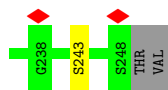


- Molecule 1: Gasdermin pore forming domain-containing protein



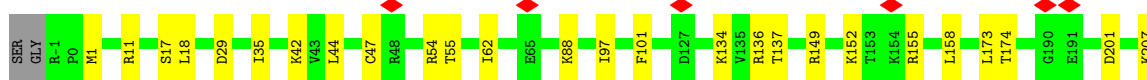
- Molecule 1: Gasdermin pore forming domain-containing protein





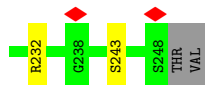
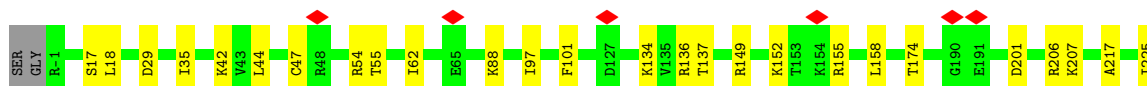
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain KA: 87% 12%



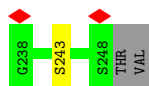
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain LA: 87% 11%



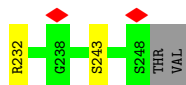
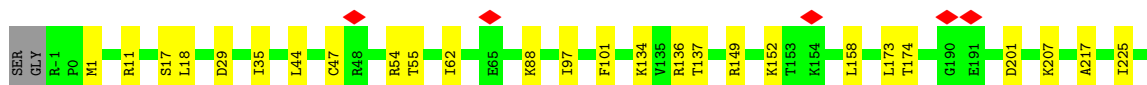
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain MA: 88% 11%



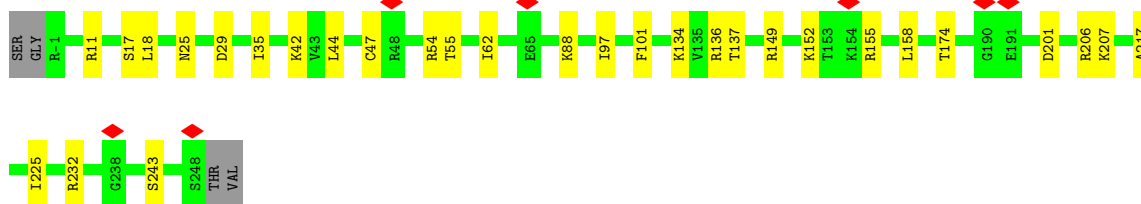
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain NA: 87% 11%




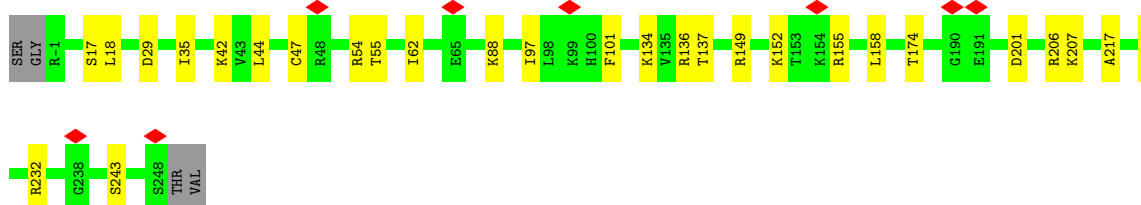
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain OA:  87% 12%




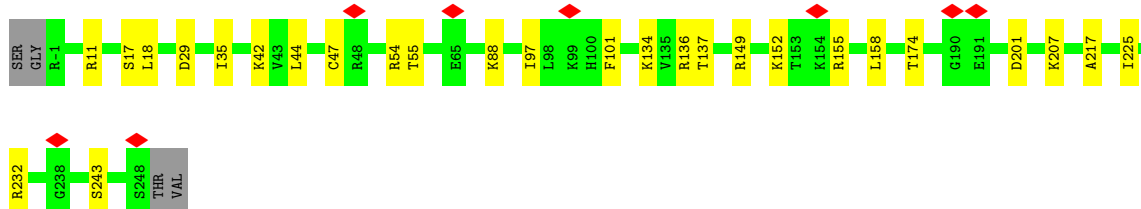
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain PA:  87% 11%




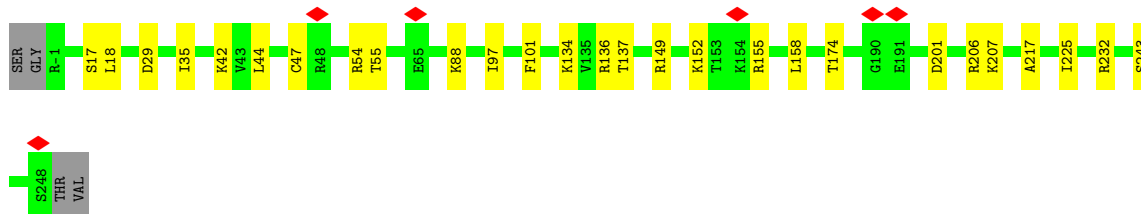
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain QA:  88% 11%




- Molecule 1: Gasdermin pore forming domain-containing protein

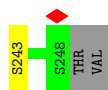
Chain RA:  88% 11%



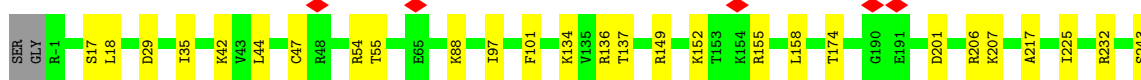
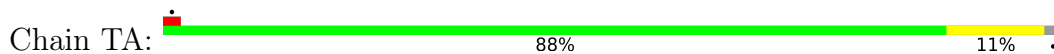
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain SA:  88% 10%

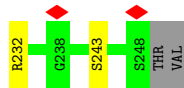
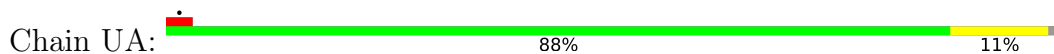




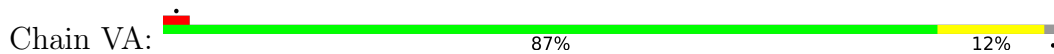
• Molecule 1: Gasdermin pore forming domain-containing protein



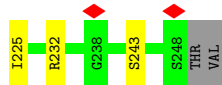
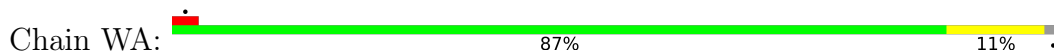
• Molecule 1: Gasdermin pore forming domain-containing protein



• Molecule 1: Gasdermin pore forming domain-containing protein

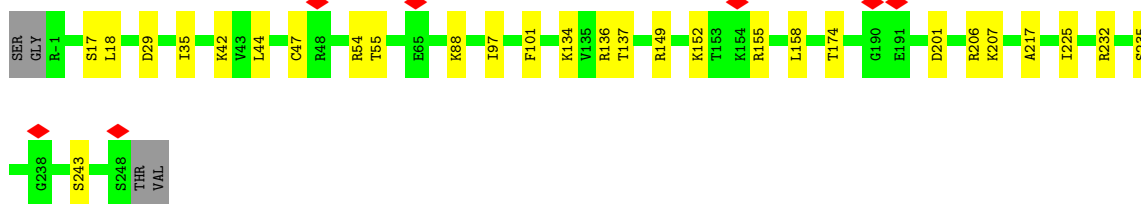


• Molecule 1: Gasdermin pore forming domain-containing protein




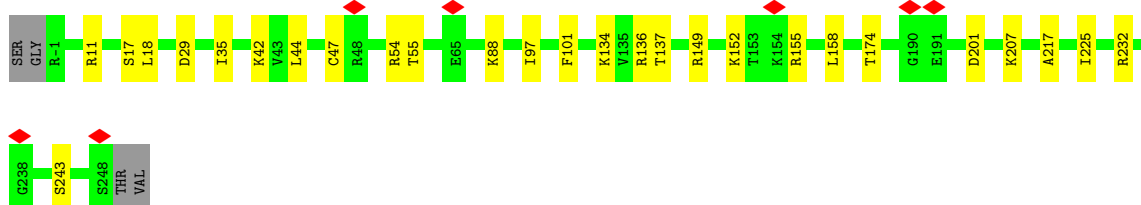
• Molecule 1: Gasdermin pore forming domain-containing protein

Chain XA:  87% 11%




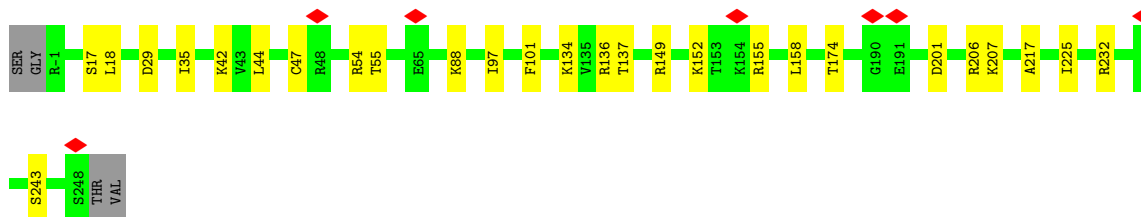
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain YA:  88% 11%




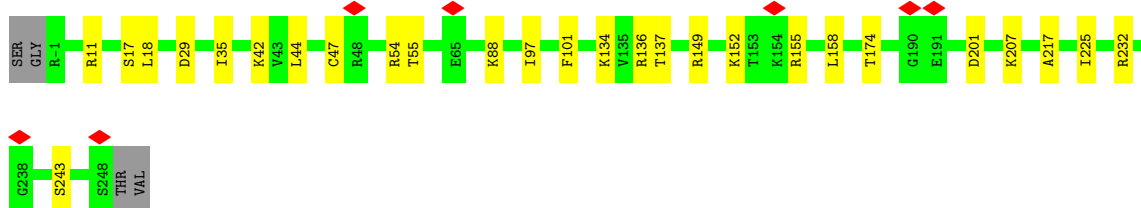
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain ZA:  88% 11%




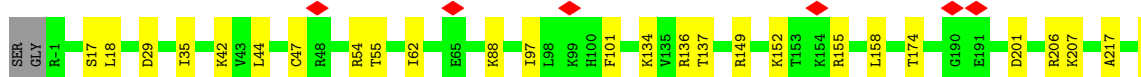
- Molecule 1: Gasdermin pore forming domain-containing protein

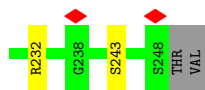
Chain AB:  88% 11%



- Molecule 1: Gasdermin pore forming domain-containing protein

Chain BB:  87% 11%





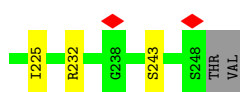
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain CB: 88% 10%



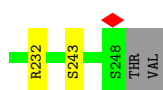
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain DB: 87% 11%



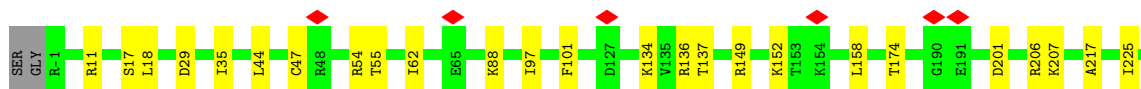
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain EB: 87% 11%



- Molecule 1: Gasdermin pore forming domain-containing protein

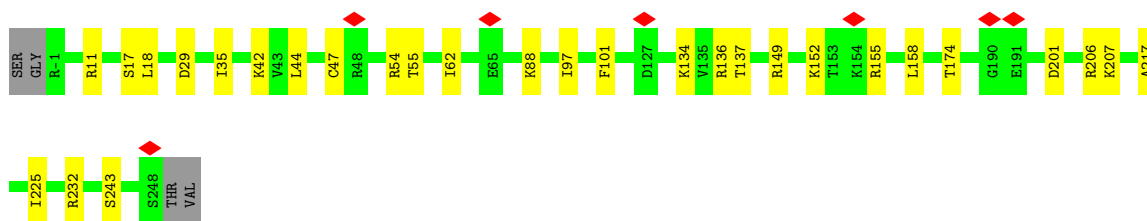
Chain FB: 87% 11%



- Molecule 1: Gasdermin pore forming domain-containing protein

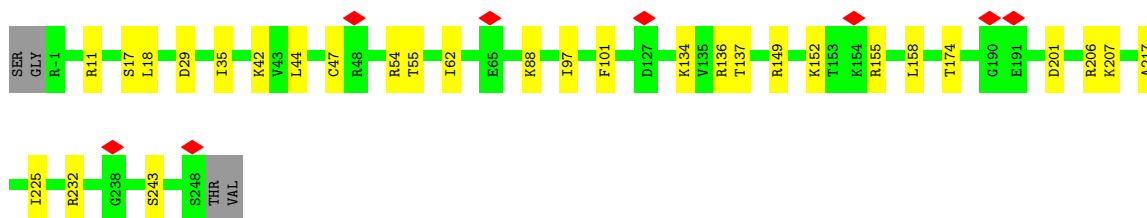


Chain GB:  87% 11%




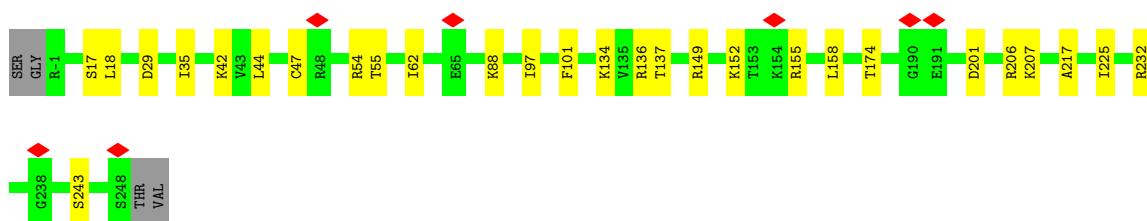
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain HB:  87% 11%




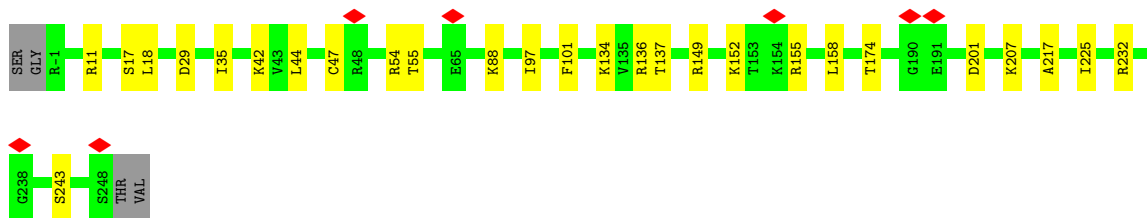
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain IB:  87% 11%




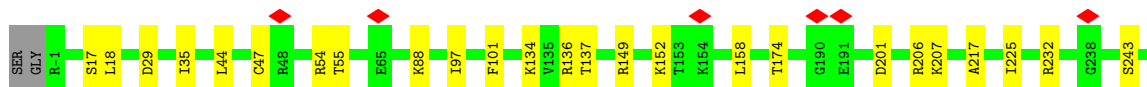
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain JB:  88% 11%



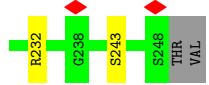
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain KB:  89% 10%

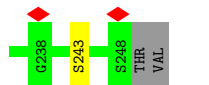
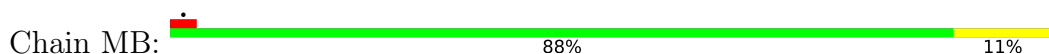




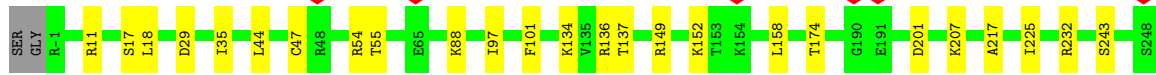
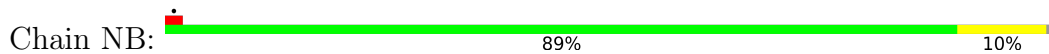
• Molecule 1: Gasdermin pore forming domain-containing protein



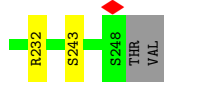
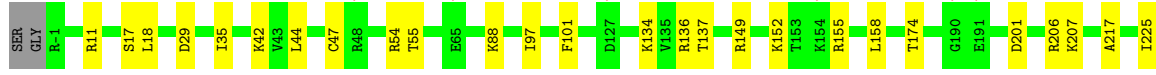
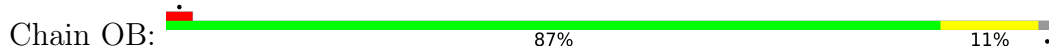
• Molecule 1: Gasdermin pore forming domain-containing protein



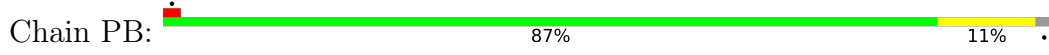
• Molecule 1: Gasdermin pore forming domain-containing protein

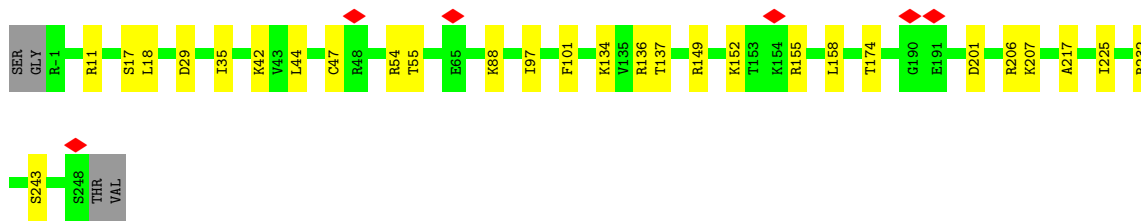


• Molecule 1: Gasdermin pore forming domain-containing protein

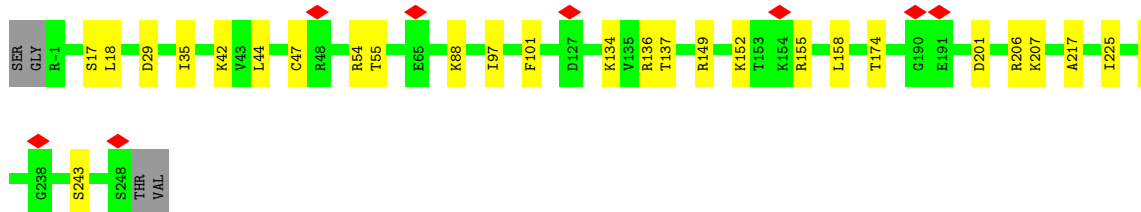
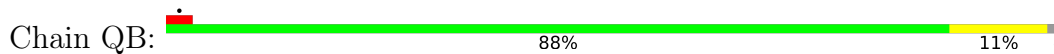


• Molecule 1: Gasdermin pore forming domain-containing protein

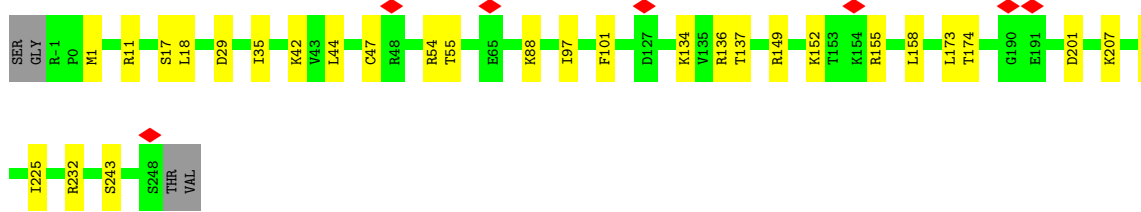
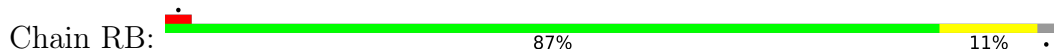




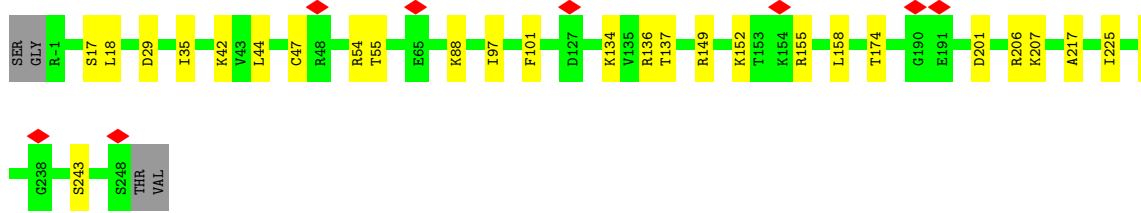
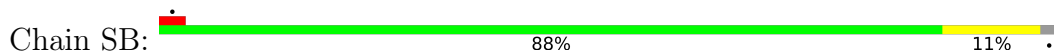
• Molecule 1: Gasdermin pore forming domain-containing protein



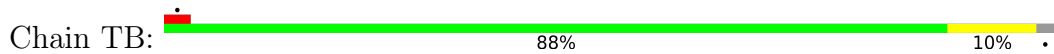
• Molecule 1: Gasdermin pore forming domain-containing protein

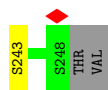


• Molecule 1: Gasdermin pore forming domain-containing protein



• Molecule 1: Gasdermin pore forming domain-containing protein





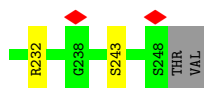
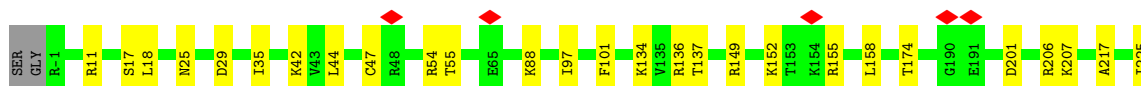
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain UB: 88% 11%



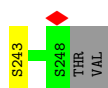
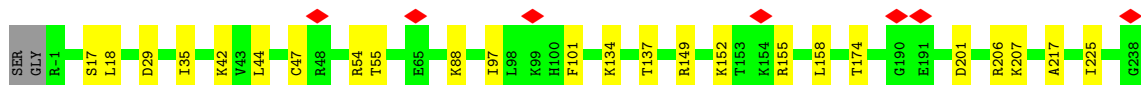
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain VB: 87% 11%



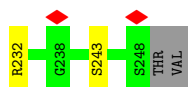
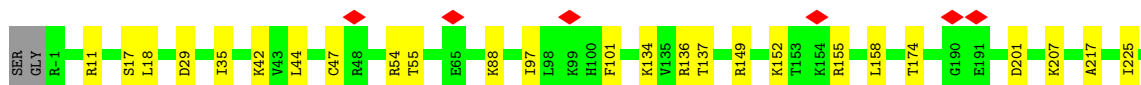
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain WB: 89% 10%

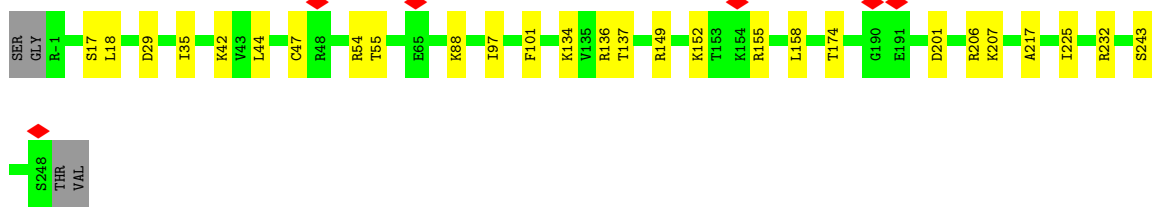
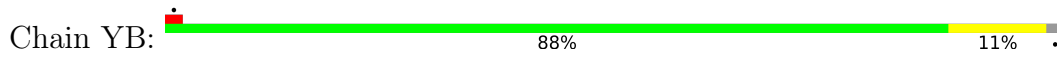


- Molecule 1: Gasdermin pore forming domain-containing protein

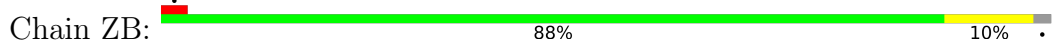
Chain XB: 88% 11%



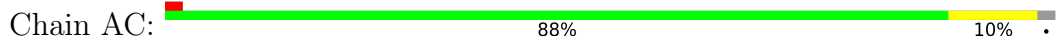
- Molecule 1: Gasdermin pore forming domain-containing protein



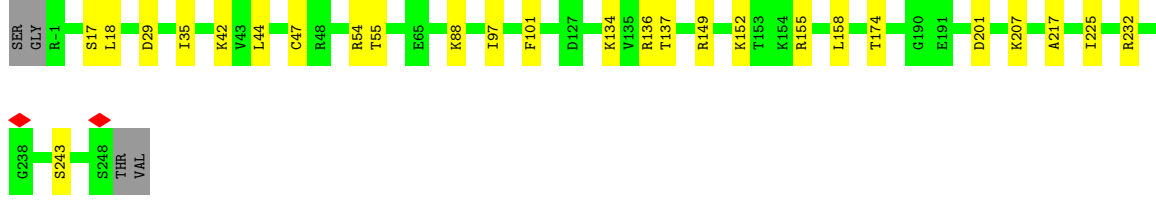
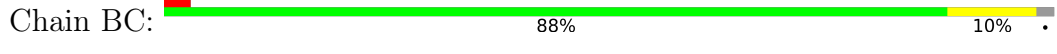
• Molecule 1: Gasdermin pore forming domain-containing protein



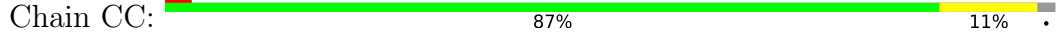
• Molecule 1: Gasdermin pore forming domain-containing protein

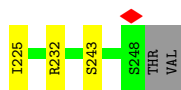


• Molecule 1: Gasdermin pore forming domain-containing protein



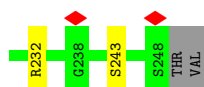
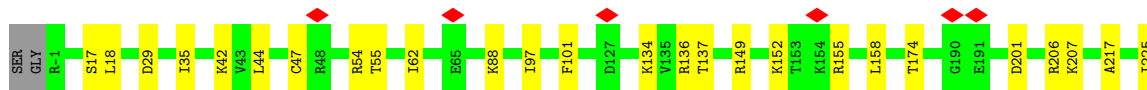
• Molecule 1: Gasdermin pore forming domain-containing protein





- Molecule 1: Gasdermin pore forming domain-containing protein

Chain DC: 87% 11%



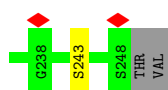
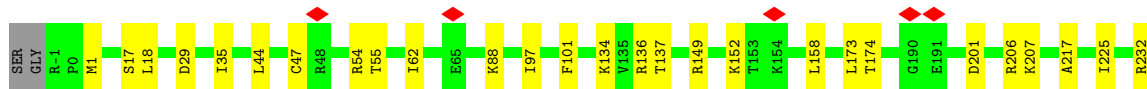
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain EC: 87% 11%



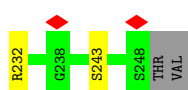
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain FC: 87% 11%




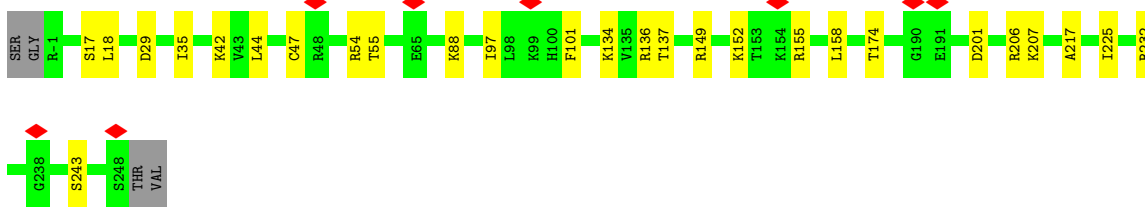
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain GC: 87% 11%




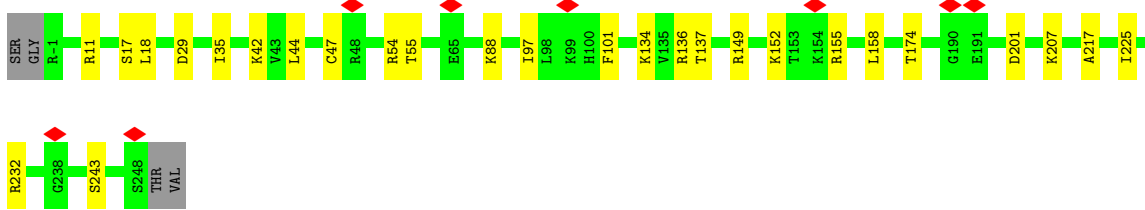
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain HC:  88% 11%




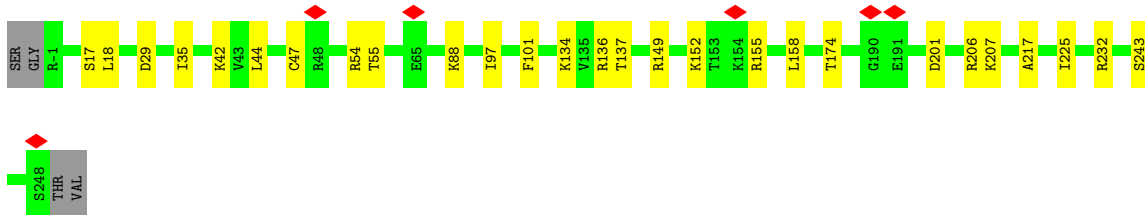
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain IC:  88% 11%




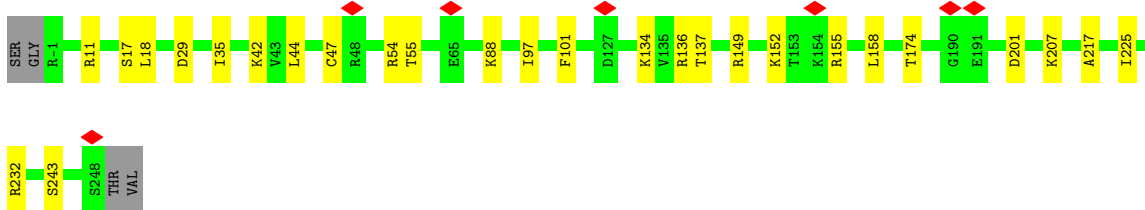
- Molecule 1: Gasdermin pore forming domain-containing protein

Chain JC:  88% 11%



- Molecule 1: Gasdermin pore forming domain-containing protein

Chain KC:  88% 11%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D44	Depositor
Number of particles used	52901	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	544.0, 544.0, 544.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor



## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/1902	0.48	0/2573
1	AA	0.25	0/1902	0.48	0/2573
1	AB	0.25	0/1902	0.48	0/2573
1	AC	0.25	0/1902	0.48	0/2573
1	B	0.25	0/1902	0.48	0/2573
1	BA	0.25	0/1902	0.48	0/2573
1	BB	0.25	0/1902	0.48	0/2573
1	BC	0.25	0/1902	0.48	0/2573
1	C	0.25	0/1902	0.48	0/2573
1	CA	0.25	0/1902	0.48	0/2573
1	CB	0.25	0/1902	0.48	0/2573
1	CC	0.25	0/1902	0.48	0/2573
1	D	0.25	0/1902	0.48	0/2573
1	DA	0.25	0/1902	0.48	0/2573
1	DB	0.25	0/1902	0.48	0/2573
1	DC	0.25	0/1902	0.48	0/2573
1	E	0.25	0/1902	0.48	0/2573
1	EA	0.25	0/1902	0.48	0/2573
1	EB	0.25	0/1902	0.48	0/2573
1	EC	0.25	0/1902	0.48	0/2573
1	F	0.25	0/1902	0.48	0/2573
1	FA	0.25	0/1902	0.48	0/2573
1	FB	0.25	0/1902	0.48	0/2573
1	FC	0.25	0/1902	0.48	0/2573
1	G	0.25	0/1902	0.48	0/2573
1	GA	0.25	0/1902	0.48	0/2573
1	GB	0.25	0/1902	0.48	0/2573
1	GC	0.25	0/1902	0.48	0/2573
1	H	0.25	0/1902	0.48	0/2573
1	HA	0.25	0/1902	0.48	0/2573
1	HB	0.25	0/1902	0.48	0/2573
1	HC	0.25	0/1902	0.48	0/2573
1	I	0.25	0/1902	0.48	0/2573
1	IA	0.25	0/1902	0.48	0/2573

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	IB	0.25	0/1902	0.48	0/2573
1	IC	0.25	0/1902	0.48	0/2573
1	J	0.25	0/1902	0.48	0/2573
1	JA	0.25	0/1902	0.48	0/2573
1	JB	0.25	0/1902	0.48	0/2573
1	JC	0.25	0/1902	0.48	0/2573
1	K	0.25	0/1902	0.48	0/2573
1	KA	0.25	0/1902	0.48	0/2573
1	KB	0.25	0/1902	0.48	0/2573
1	KC	0.25	0/1902	0.48	0/2573
1	L	0.25	0/1902	0.48	0/2573
1	LA	0.25	0/1902	0.48	0/2573
1	LB	0.25	0/1902	0.48	0/2573
1	M	0.25	0/1902	0.48	0/2573
1	MA	0.25	0/1902	0.48	0/2573
1	MB	0.25	0/1902	0.48	0/2573
1	N	0.25	0/1902	0.48	0/2573
1	NA	0.25	0/1902	0.48	0/2573
1	NB	0.25	0/1902	0.48	0/2573
1	O	0.25	0/1902	0.48	0/2573
1	OA	0.25	0/1902	0.48	0/2573
1	OB	0.25	0/1902	0.48	0/2573
1	P	0.25	0/1902	0.48	0/2573
1	PA	0.25	0/1902	0.48	0/2573
1	PB	0.25	0/1902	0.48	0/2573
1	Q	0.25	0/1902	0.48	0/2573
1	QA	0.25	0/1902	0.48	0/2573
1	QB	0.25	0/1902	0.48	0/2573
1	R	0.25	0/1902	0.48	0/2573
1	RA	0.25	0/1902	0.48	0/2573
1	RB	0.25	0/1902	0.48	0/2573
1	S	0.25	0/1902	0.48	0/2573
1	SA	0.25	0/1902	0.48	0/2573
1	SB	0.25	0/1902	0.48	0/2573
1	T	0.25	0/1902	0.48	0/2573
1	TA	0.25	0/1902	0.48	0/2573
1	TB	0.25	0/1902	0.48	0/2573
1	UA	0.25	0/1902	0.48	0/2573
1	UB	0.25	0/1902	0.48	0/2573
1	V	0.25	0/1902	0.48	0/2573
1	VA	0.25	0/1902	0.48	0/2573
1	VB	0.25	0/1902	0.48	0/2573
1	W	0.25	0/1902	0.48	0/2573

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	WA	0.25	0/1902	0.48	0/2573
1	WB	0.25	0/1902	0.48	0/2573
1	X	0.25	0/1902	0.48	0/2573
1	XA	0.25	0/1902	0.48	0/2573
1	XB	0.25	0/1902	0.48	0/2573
1	Y	0.25	0/1902	0.48	0/2573
1	YA	0.25	0/1902	0.48	0/2573
1	YB	0.25	0/1902	0.48	0/2573
1	Z	0.25	0/1902	0.48	0/2573
1	ZA	0.25	0/1902	0.48	0/2573
1	ZB	0.25	0/1902	0.48	0/2573
All	All	0.25	0/167376	0.48	0/226424

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1876	0	1938	13	0
1	AA	1876	0	1938	14	0
1	AB	1876	0	1938	14	0
1	AC	1876	0	1938	13	0
1	B	1876	0	1938	14	0
1	BA	1876	0	1938	14	0
1	BB	1876	0	1938	15	0
1	BC	1876	0	1938	13	0
1	C	1876	0	1938	16	0
1	CA	1876	0	1938	14	0
1	CB	1876	0	1938	15	0
1	CC	1876	0	1938	15	0
1	D	1876	0	1938	15	0
1	DA	1876	0	1938	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DB	1876	0	1938	16	0
1	DC	1876	0	1938	15	0
1	E	1876	0	1938	14	0
1	EA	1876	0	1938	14	0
1	EB	1876	0	1938	17	0
1	EC	1876	0	1938	15	0
1	F	1876	0	1938	14	0
1	FA	1876	0	1938	14	0
1	FB	1876	0	1938	17	0
1	FC	1876	0	1938	15	0
1	G	1876	0	1938	14	0
1	GA	1876	0	1938	14	0
1	GB	1876	0	1938	17	0
1	GC	1876	0	1938	15	0
1	H	1876	0	1938	15	0
1	HA	1876	0	1938	14	0
1	HB	1876	0	1938	17	0
1	HC	1876	0	1938	14	0
1	I	1876	0	1938	15	0
1	IA	1876	0	1938	14	0
1	IB	1876	0	1938	16	0
1	IC	1876	0	1938	14	0
1	J	1876	0	1938	15	0
1	JA	1876	0	1938	14	0
1	JB	1876	0	1938	15	0
1	JC	1876	0	1938	15	0
1	K	1876	0	1938	15	0
1	KA	1876	0	1938	16	0
1	KB	1876	0	1938	14	0
1	KC	1876	0	1938	14	0
1	L	1876	0	1938	16	0
1	LA	1876	0	1938	15	0
1	LB	1876	0	1938	16	0
1	M	1876	0	1938	15	0
1	MA	1876	0	1938	14	0
1	MB	1876	0	1938	15	0
1	N	1876	0	1938	16	0
1	NA	1876	0	1938	16	0
1	NB	1876	0	1938	14	0
1	O	1876	0	1938	16	0
1	OA	1876	0	1938	18	0
1	OB	1876	0	1938	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1876	0	1938	17	0
1	PA	1876	0	1938	15	0
1	PB	1876	0	1938	16	0
1	Q	1876	0	1938	15	0
1	QA	1876	0	1938	14	0
1	QB	1876	0	1938	15	0
1	R	1876	0	1938	14	0
1	RA	1876	0	1938	14	0
1	RB	1876	0	1938	15	0
1	S	1876	0	1938	17	0
1	SA	1876	0	1938	13	0
1	SB	1876	0	1938	14	0
1	T	1876	0	1938	15	0
1	TA	1876	0	1938	14	0
1	TB	1876	0	1938	13	0
1	UA	1876	0	1938	14	0
1	UB	1876	0	1938	16	0
1	V	1876	0	1938	14	0
1	VA	1876	0	1938	16	0
1	VB	1876	0	1938	17	0
1	W	1876	0	1938	17	0
1	WA	1876	0	1938	15	0
1	WB	1876	0	1938	13	0
1	X	1876	0	1938	16	0
1	XA	1876	0	1938	15	0
1	XB	1876	0	1938	14	0
1	Y	1876	0	1938	16	0
1	YA	1876	0	1938	15	0
1	YB	1876	0	1938	14	0
1	Z	1876	0	1938	15	0
1	ZA	1876	0	1938	14	0
1	ZB	1876	0	1938	13	0
All	All	165088	0	170544	1258	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 4.

All (1258) 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:M:174:THR:HG22	1:M:207:LYS:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:174:THR:HG22	1:P:207:LYS:HG3	1.80	0.64
1:IB:174:THR:HG22	1:IB:207:LYS:HG3	1.80	0.64
1:WB:174:THR:HG22	1:WB:207:LYS:HG3	1.80	0.64
1:S:174:THR:HG22	1:S:207:LYS:HG3	1.80	0.64
1:BA:174:THR:HG22	1:BA:207:LYS:HG3	1.80	0.64
1:EA:174:THR:HG22	1:EA:207:LYS:HG3	1.80	0.64
1:HA:174:THR:HG22	1:HA:207:LYS:HG3	1.80	0.64
1:MA:174:THR:HG22	1:MA:207:LYS:HG3	1.80	0.64
1:FB:174:THR:HG22	1:FB:207:LYS:HG3	1.80	0.64
1:LB:174:THR:HG22	1:LB:207:LYS:HG3	1.80	0.64
1:TB:174:THR:HG22	1:TB:207:LYS:HG3	1.80	0.64
1:ZB:174:THR:HG22	1:ZB:207:LYS:HG3	1.80	0.64
1:Y:174:THR:HG22	1:Y:207:LYS:HG3	1.80	0.64
1:JA:174:THR:HG22	1:JA:207:LYS:HG3	1.80	0.64
1:PA:174:THR:HG22	1:PA:207:LYS:HG3	1.80	0.64
1:QB:174:THR:HG22	1:QB:207:LYS:HG3	1.80	0.64
1:CC:174:THR:HG22	1:CC:207:LYS:HG3	1.80	0.64
1:EC:174:THR:HG22	1:EC:207:LYS:HG3	1.80	0.64
1:HC:174:THR:HG22	1:HC:207:LYS:HG3	1.80	0.64
1:V:174:THR:HG22	1:V:207:LYS:HG3	1.80	0.64
1:KA:174:THR:HG22	1:KA:207:LYS:HG3	1.80	0.64
1:NB:174:THR:HG22	1:NB:207:LYS:HG3	1.80	0.64
1:OB:174:THR:HG22	1:OB:207:LYS:HG3	1.80	0.64
1:BC:174:THR:HG22	1:BC:207:LYS:HG3	1.80	0.64
1:H:174:THR:HG22	1:H:207:LYS:HG3	1.80	0.64
1:J:174:THR:HG22	1:J:207:LYS:HG3	1.80	0.64
1:R:174:THR:HG22	1:R:207:LYS:HG3	1.80	0.64
1:AB:174:THR:HG22	1:AB:207:LYS:HG3	1.80	0.64
1:CB:174:THR:HG22	1:CB:207:LYS:HG3	1.80	0.64
1:E:174:THR:HG22	1:E:207:LYS:HG3	1.80	0.64
1:W:174:THR:HG22	1:W:207:LYS:HG3	1.80	0.64
1:GA:174:THR:HG22	1:GA:207:LYS:HG3	1.80	0.64
1:DB:174:THR:HG22	1:DB:207:LYS:HG3	1.80	0.64
1:KB:174:THR:HG22	1:KB:207:LYS:HG3	1.80	0.64
1:B:174:THR:HG22	1:B:207:LYS:HG3	1.80	0.64
1:K:174:THR:HG22	1:K:207:LYS:HG3	1.80	0.64
1:SA:174:THR:HG22	1:SA:207:LYS:HG3	1.80	0.64
1:XA:174:THR:HG22	1:XA:207:LYS:HG3	1.80	0.64
1:RB:174:THR:HG22	1:RB:207:LYS:HG3	1.80	0.64
1:YB:174:THR:HG22	1:YB:207:LYS:HG3	1.80	0.64
1:FC:174:THR:HG22	1:FC:207:LYS:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KC:174:THR:HG22	1:KC:207:LYS:HG3	1.80	0.64
1:UA:174:THR:HG22	1:UA:207:LYS:HG3	1.80	0.64
1:GB:174:THR:HG22	1:GB:207:LYS:HG3	1.80	0.64
1:O:174:THR:HG22	1:O:207:LYS:HG3	1.80	0.63
1:Z:174:THR:HG22	1:Z:207:LYS:HG3	1.80	0.63
1:NA:174:THR:HG22	1:NA:207:LYS:HG3	1.80	0.63
1:RA:174:THR:HG22	1:RA:207:LYS:HG3	1.80	0.63
1:N:174:THR:HG22	1:N:207:LYS:HG3	1.80	0.63
1:CA:174:THR:HG22	1:CA:207:LYS:HG3	1.80	0.63
1:VA:174:THR:HG22	1:VA:207:LYS:HG3	1.80	0.63
1:HB:174:THR:HG22	1:HB:207:LYS:HG3	1.80	0.63
1:UB:174:THR:HG22	1:UB:207:LYS:HG3	1.80	0.63
1:JC:174:THR:HG22	1:JC:207:LYS:HG3	1.80	0.63
1:G:174:THR:HG22	1:G:207:LYS:HG3	1.80	0.63
1:DA:174:THR:HG22	1:DA:207:LYS:HG3	1.80	0.63
1:OA:174:THR:HG22	1:OA:207:LYS:HG3	1.80	0.63
1:VB:174:THR:HG22	1:VB:207:LYS:HG3	1.80	0.63
1:C:174:THR:HG22	1:C:207:LYS:HG3	1.80	0.63
1:ZA:174:THR:HG22	1:ZA:207:LYS:HG3	1.80	0.63
1:JB:174:THR:HG22	1:JB:207:LYS:HG3	1.80	0.63
1:XB:174:THR:HG22	1:XB:207:LYS:HG3	1.80	0.63
1:Q:174:THR:HG22	1:Q:207:LYS:HG3	1.80	0.63
1:AA:174:THR:HG22	1:AA:207:LYS:HG3	1.80	0.63
1:FA:174:THR:HG22	1:FA:207:LYS:HG3	1.80	0.63
1:GC:174:THR:HG22	1:GC:207:LYS:HG3	1.80	0.63
1:L:174:THR:HG22	1:L:207:LYS:HG3	1.80	0.63
1:YA:174:THR:HG22	1:YA:207:LYS:HG3	1.80	0.63
1:IC:174:THR:HG22	1:IC:207:LYS:HG3	1.80	0.63
1:F:174:THR:HG22	1:F:207:LYS:HG3	1.80	0.63
1:SB:174:THR:HG22	1:SB:207:LYS:HG3	1.80	0.63
1:AC:174:THR:HG22	1:AC:207:LYS:HG3	1.80	0.63
1:D:174:THR:HG22	1:D:207:LYS:HG3	1.80	0.63
1:X:174:THR:HG22	1:X:207:LYS:HG3	1.80	0.63
1:LA:174:THR:HG22	1:LA:207:LYS:HG3	1.80	0.63
1:QA:174:THR:HG22	1:QA:207:LYS:HG3	1.80	0.63
1:EB:174:THR:HG22	1:EB:207:LYS:HG3	1.80	0.63
1:MB:174:THR:HG22	1:MB:207:LYS:HG3	1.80	0.62
1:IA:174:THR:HG22	1:IA:207:LYS:HG3	1.80	0.62
1:WA:174:THR:HG22	1:WA:207:LYS:HG3	1.80	0.62
1:DC:174:THR:HG22	1:DC:207:LYS:HG3	1.80	0.62
1:PB:174:THR:HG22	1:PB:207:LYS:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:174:THR:HG22	1:BB:207:LYS:HG3	1.80	0.62
1:T:174:THR:HG22	1:T:207:LYS:HG3	1.80	0.62
1:I:174:THR:HG22	1:I:207:LYS:HG3	1.80	0.62
1:A:174:THR:HG22	1:A:207:LYS:HG3	1.80	0.62
1:TA:174:THR:HG22	1:TA:207:LYS:HG3	1.80	0.62
1:K:149:ARG:HD2	1:K:152:LYS:HE3	1.83	0.61
1:Q:149:ARG:HD2	1:Q:152:LYS:HE3	1.83	0.61
1:M:149:ARG:HD2	1:M:152:LYS:HE3	1.83	0.61
1:O:149:ARG:HD2	1:O:152:LYS:HE3	1.83	0.61
1:V:149:ARG:HD2	1:V:152:LYS:HE3	1.83	0.61
1:FB:149:ARG:HD2	1:FB:152:LYS:HE3	1.83	0.61
1:JB:149:ARG:HD2	1:JB:152:LYS:HE3	1.83	0.61
1:LB:149:ARG:HD2	1:LB:152:LYS:HE3	1.83	0.61
1:G:149:ARG:HD2	1:G:152:LYS:HE3	1.83	0.61
1:I:149:ARG:HD2	1:I:152:LYS:HE3	1.83	0.61
1:S:149:ARG:HD2	1:S:152:LYS:HE3	1.83	0.61
1:BB:149:ARG:HD2	1:BB:152:LYS:HE3	1.83	0.61
1:DB:149:ARG:HD2	1:DB:152:LYS:HE3	1.83	0.61
1:HB:149:ARG:HD2	1:HB:152:LYS:HE3	1.83	0.61
1:NB:149:ARG:HD2	1:NB:152:LYS:HE3	1.83	0.61
1:C:149:ARG:HD2	1:C:152:LYS:HE3	1.83	0.61
1:E:149:ARG:HD2	1:E:152:LYS:HE3	1.83	0.61
1:X:149:ARG:HD2	1:X:152:LYS:HE3	1.83	0.61
1:PB:149:ARG:HD2	1:PB:152:LYS:HE3	1.83	0.61
1:RB:149:ARG:HD2	1:RB:152:LYS:HE3	1.83	0.61
1:Z:149:ARG:HD2	1:Z:152:LYS:HE3	1.83	0.60
1:XA:149:ARG:HD2	1:XA:152:LYS:HE3	1.83	0.60
1:ZA:149:ARG:HD2	1:ZA:152:LYS:HE3	1.83	0.60
1:A:149:ARG:HD2	1:A:152:LYS:HE3	1.83	0.60
1:VA:149:ARG:HD2	1:VA:152:LYS:HE3	1.83	0.60
1:TB:149:ARG:HD2	1:TB:152:LYS:HE3	1.83	0.60
1:BA:149:ARG:HD2	1:BA:152:LYS:HE3	1.83	0.60
1:TA:149:ARG:HD2	1:TA:152:LYS:HE3	1.83	0.60
1:DA:149:ARG:HD2	1:DA:152:LYS:HE3	1.83	0.60
1:PA:149:ARG:HD2	1:PA:152:LYS:HE3	1.83	0.60
1:RA:149:ARG:HD2	1:RA:152:LYS:HE3	1.83	0.60
1:UA:149:ARG:HD2	1:UA:152:LYS:HE3	1.83	0.60
1:WA:149:ARG:HD2	1:WA:152:LYS:HE3	1.83	0.60
1:VB:149:ARG:HD2	1:VB:152:LYS:HE3	1.83	0.60
1:HC:149:ARG:HD2	1:HC:152:LYS:HE3	1.83	0.60
1:B:149:ARG:HD2	1:B:152:LYS:HE3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:149:ARG:HD2	1:SA:152:LYS:HE3	1.83	0.60
1:YA:149:ARG:HD2	1:YA:152:LYS:HE3	1.83	0.60
1:JC:149:ARG:HD2	1:JC:152:LYS:HE3	1.83	0.60
1:KC:149:ARG:HD2	1:KC:152:LYS:HE3	1.83	0.60
1:D:149:ARG:HD2	1:D:152:LYS:HE3	1.83	0.60
1:FA:149:ARG:HD2	1:FA:152:LYS:HE3	1.83	0.60
1:HA:149:ARG:HD2	1:HA:152:LYS:HE3	1.83	0.60
1:JA:149:ARG:HD2	1:JA:152:LYS:HE3	1.83	0.60
1:LA:149:ARG:HD2	1:LA:152:LYS:HE3	1.83	0.60
1:NA:149:ARG:HD2	1:NA:152:LYS:HE3	1.83	0.60
1:AB:149:ARG:HD2	1:AB:152:LYS:HE3	1.83	0.60
1:XB:149:ARG:HD2	1:XB:152:LYS:HE3	1.83	0.60
1:FC:149:ARG:HD2	1:FC:152:LYS:HE3	1.83	0.60
1:F:149:ARG:HD2	1:F:152:LYS:HE3	1.83	0.60
1:ZB:149:ARG:HD2	1:ZB:152:LYS:HE3	1.83	0.60
1:BC:149:ARG:HD2	1:BC:152:LYS:HE3	1.83	0.60
1:DC:149:ARG:HD2	1:DC:152:LYS:HE3	1.83	0.60
1:IC:149:ARG:HD2	1:IC:152:LYS:HE3	1.83	0.60
1:H:149:ARG:HD2	1:H:152:LYS:HE3	1.83	0.60
1:QA:149:ARG:HD2	1:QA:152:LYS:HE3	1.83	0.60
1:CB:149:ARG:HD2	1:CB:152:LYS:HE3	1.83	0.60
1:GC:149:ARG:HD2	1:GC:152:LYS:HE3	1.83	0.60
1:T:149:ARG:HD2	1:T:152:LYS:HE3	1.83	0.59
1:W:149:ARG:HD2	1:W:152:LYS:HE3	1.83	0.59
1:OA:149:ARG:HD2	1:OA:152:LYS:HE3	1.83	0.59
1:J:149:ARG:HD2	1:J:152:LYS:HE3	1.83	0.59
1:R:149:ARG:HD2	1:R:152:LYS:HE3	1.83	0.59
1:Y:149:ARG:HD2	1:Y:152:LYS:HE3	1.83	0.59
1:EB:149:ARG:HD2	1:EB:152:LYS:HE3	1.83	0.59
1:OB:149:ARG:HD2	1:OB:152:LYS:HE3	1.83	0.59
1:GB:149:ARG:HD2	1:GB:152:LYS:HE3	1.83	0.59
1:MB:149:ARG:HD2	1:MB:152:LYS:HE3	1.83	0.59
1:EC:149:ARG:HD2	1:EC:152:LYS:HE3	1.83	0.59
1:L:149:ARG:HD2	1:L:152:LYS:HE3	1.83	0.59
1:AA:149:ARG:HD2	1:AA:152:LYS:HE3	1.83	0.59
1:P:149:ARG:HD2	1:P:152:LYS:HE3	1.83	0.59
1:MA:149:ARG:HD2	1:MA:152:LYS:HE3	1.83	0.59
1:QB:149:ARG:HD2	1:QB:152:LYS:HE3	1.83	0.59
1:CC:149:ARG:HD2	1:CC:152:LYS:HE3	1.83	0.59
1:N:149:ARG:HD2	1:N:152:LYS:HE3	1.83	0.59
1:IB:149:ARG:HD2	1:IB:152:LYS:HE3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:149:ARG:HD2	1:KB:152:LYS:HE3	1.83	0.59
1:CA:149:ARG:HD2	1:CA:152:LYS:HE3	1.83	0.59
1:KA:149:ARG:HD2	1:KA:152:LYS:HE3	1.83	0.59
1:SB:149:ARG:HD2	1:SB:152:LYS:HE3	1.83	0.59
1:UB:149:ARG:HD2	1:UB:152:LYS:HE3	1.83	0.59
1:AC:149:ARG:HD2	1:AC:152:LYS:HE3	1.83	0.59
1:EA:149:ARG:HD2	1:EA:152:LYS:HE3	1.83	0.59
1:IA:149:ARG:HD2	1:IA:152:LYS:HE3	1.83	0.58
1:YB:149:ARG:HD2	1:YB:152:LYS:HE3	1.83	0.58
1:WB:149:ARG:HD2	1:WB:152:LYS:HE3	1.83	0.58
1:GA:149:ARG:HD2	1:GA:152:LYS:HE3	1.83	0.58
1:Y:17:SER:HA	1:Y:243:SER:HB2	1.86	0.57
1:QB:17:SER:HA	1:QB:243:SER:HB2	1.86	0.57
1:X:17:SER:HA	1:X:243:SER:HB2	1.87	0.57
1:Z:17:SER:HA	1:Z:243:SER:HB2	1.86	0.57
1:PB:17:SER:HA	1:PB:243:SER:HB2	1.87	0.57
1:OB:17:SER:HA	1:OB:243:SER:HB2	1.87	0.57
1:Q:17:SER:HA	1:Q:243:SER:HB2	1.86	0.57
1:W:17:SER:HA	1:W:243:SER:HB2	1.87	0.57
1:AA:17:SER:HA	1:AA:243:SER:HB2	1.87	0.57
1:BA:17:SER:HA	1:BA:243:SER:HB2	1.87	0.57
1:IB:17:SER:HA	1:IB:243:SER:HB2	1.87	0.57
1:JB:17:SER:HA	1:JB:243:SER:HB2	1.86	0.57
1:MB:17:SER:HA	1:MB:243:SER:HB2	1.86	0.57
1:NB:17:SER:HA	1:NB:243:SER:HB2	1.86	0.57
1:RB:17:SER:HA	1:RB:243:SER:HB2	1.87	0.57
1:P:17:SER:HA	1:P:243:SER:HB2	1.87	0.57
1:SB:17:SER:HA	1:SB:243:SER:HB2	1.87	0.57
1:N:17:SER:HA	1:N:243:SER:HB2	1.86	0.57
1:O:17:SER:HA	1:O:243:SER:HB2	1.87	0.57
1:R:17:SER:HA	1:R:243:SER:HB2	1.87	0.57
1:T:17:SER:HA	1:T:243:SER:HB2	1.87	0.57
1:V:17:SER:HA	1:V:243:SER:HB2	1.87	0.57
1:FA:17:SER:HA	1:FA:243:SER:HB2	1.87	0.57
1:GB:17:SER:HA	1:GB:243:SER:HB2	1.87	0.57
1:HB:17:SER:HA	1:HB:243:SER:HB2	1.87	0.57
1:KB:17:SER:HA	1:KB:243:SER:HB2	1.87	0.57
1:TB:17:SER:HA	1:TB:243:SER:HB2	1.87	0.57
1:WB:17:SER:HA	1:WB:243:SER:HB2	1.86	0.57
1:XB:17:SER:HA	1:XB:243:SER:HB2	1.87	0.57
1:YB:17:SER:HA	1:YB:243:SER:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:17:SER:HA	1:S:243:SER:HB2	1.86	0.57
1:CA:17:SER:HA	1:CA:243:SER:HB2	1.87	0.57
1:DA:17:SER:HA	1:DA:243:SER:HB2	1.86	0.57
1:EA:17:SER:HA	1:EA:243:SER:HB2	1.86	0.57
1:GA:17:SER:HA	1:GA:243:SER:HB2	1.86	0.57
1:FB:17:SER:HA	1:FB:243:SER:HB2	1.87	0.57
1:LB:17:SER:HA	1:LB:243:SER:HB2	1.86	0.57
1:VB:17:SER:HA	1:VB:243:SER:HB2	1.87	0.57
1:HA:17:SER:HA	1:HA:243:SER:HB2	1.87	0.57
1:UB:17:SER:HA	1:UB:243:SER:HB2	1.86	0.57
1:M:17:SER:HA	1:M:243:SER:HB2	1.87	0.57
1:IA:17:SER:HA	1:IA:243:SER:HB2	1.87	0.57
1:ZB:17:SER:HA	1:ZB:243:SER:HB2	1.87	0.57
1:EB:17:SER:HA	1:EB:243:SER:HB2	1.87	0.57
1:AC:17:SER:HA	1:AC:243:SER:HB2	1.87	0.57
1:L:17:SER:HA	1:L:243:SER:HB2	1.87	0.56
1:H:17:SER:HA	1:H:243:SER:HB2	1.86	0.56
1:I:17:SER:HA	1:I:243:SER:HB2	1.87	0.56
1:K:17:SER:HA	1:K:243:SER:HB2	1.87	0.56
1:JA:17:SER:HA	1:JA:243:SER:HB2	1.87	0.56
1:BB:17:SER:HA	1:BB:243:SER:HB2	1.87	0.56
1:CB:17:SER:HA	1:CB:243:SER:HB2	1.86	0.56
1:DB:17:SER:HA	1:DB:243:SER:HB2	1.87	0.56
1:BC:17:SER:HA	1:BC:243:SER:HB2	1.87	0.56
1:J:17:SER:HA	1:J:243:SER:HB2	1.87	0.56
1:KA:17:SER:HA	1:KA:243:SER:HB2	1.86	0.56
1:AB:17:SER:HA	1:AB:243:SER:HB2	1.87	0.56
1:ZA:17:SER:HA	1:ZA:243:SER:HB2	1.86	0.56
1:EC:17:SER:HA	1:EC:243:SER:HB2	1.87	0.56
1:G:17:SER:HA	1:G:243:SER:HB2	1.87	0.56
1:MA:17:SER:HA	1:MA:243:SER:HB2	1.87	0.56
1:CC:17:SER:HA	1:CC:243:SER:HB2	1.87	0.56
1:FC:17:SER:HA	1:FC:243:SER:HB2	1.86	0.56
1:F:17:SER:HA	1:F:243:SER:HB2	1.86	0.56
1:LA:17:SER:HA	1:LA:243:SER:HB2	1.87	0.56
1:NA:17:SER:HA	1:NA:243:SER:HB2	1.87	0.56
1:YA:17:SER:HA	1:YA:243:SER:HB2	1.86	0.56
1:DC:17:SER:HA	1:DC:243:SER:HB2	1.87	0.56
1:OA:17:SER:HA	1:OA:243:SER:HB2	1.87	0.56
1:PA:17:SER:HA	1:PA:243:SER:HB2	1.86	0.56
1:GC:17:SER:HA	1:GC:243:SER:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SA:17:SER:HA	1:SA:243:SER:HB2	1.87	0.56
1:B:17:SER:HA	1:B:243:SER:HB2	1.87	0.56
1:QA:17:SER:HA	1:QA:243:SER:HB2	1.87	0.56
1:HC:17:SER:HA	1:HC:243:SER:HB2	1.87	0.56
1:IC:17:SER:HA	1:IC:243:SER:HB2	1.87	0.56
1:KC:17:SER:HA	1:KC:243:SER:HB2	1.87	0.56
1:A:17:SER:HA	1:A:243:SER:HB2	1.87	0.55
1:C:17:SER:HA	1:C:243:SER:HB2	1.86	0.55
1:TA:17:SER:HA	1:TA:243:SER:HB2	1.87	0.55
1:UA:17:SER:HA	1:UA:243:SER:HB2	1.87	0.55
1:VA:17:SER:HA	1:VA:243:SER:HB2	1.86	0.55
1:XA:17:SER:HA	1:XA:243:SER:HB2	1.87	0.55
1:E:17:SER:HA	1:E:243:SER:HB2	1.87	0.55
1:C:29:ASP:OD2	1:C:54:ARG:NH1	2.40	0.55
1:D:17:SER:HA	1:D:243:SER:HB2	1.87	0.55
1:P:29:ASP:OD2	1:P:54:ARG:NH1	2.40	0.55
1:VA:29:ASP:OD2	1:VA:54:ARG:NH1	2.40	0.55
1:WA:17:SER:HA	1:WA:243:SER:HB2	1.87	0.55
1:YA:29:ASP:OD2	1:YA:54:ARG:NH1	2.40	0.55
1:IB:29:ASP:OD2	1:IB:54:ARG:NH1	2.40	0.55
1:YB:29:ASP:OD2	1:YB:54:ARG:NH1	2.40	0.55
1:FC:29:ASP:OD2	1:FC:54:ARG:NH1	2.40	0.55
1:JC:17:SER:HA	1:JC:243:SER:HB2	1.87	0.55
1:S:29:ASP:OD2	1:S:54:ARG:NH1	2.40	0.55
1:W:29:ASP:OD2	1:W:54:ARG:NH1	2.40	0.55
1:GA:29:ASP:OD2	1:GA:54:ARG:NH1	2.40	0.55
1:NA:29:ASP:OD2	1:NA:54:ARG:NH1	2.40	0.55
1:QA:29:ASP:OD2	1:QA:54:ARG:NH1	2.40	0.55
1:RA:17:SER:HA	1:RA:243:SER:HB2	1.87	0.55
1:SA:29:ASP:OD2	1:SA:54:ARG:NH1	2.40	0.55
1:FB:29:ASP:OD2	1:FB:54:ARG:NH1	2.40	0.55
1:LB:29:ASP:OD2	1:LB:54:ARG:NH1	2.40	0.55
1:OB:29:ASP:OD2	1:OB:54:ARG:NH1	2.40	0.55
1:VB:29:ASP:OD2	1:VB:54:ARG:NH1	2.40	0.55
1:IC:29:ASP:OD2	1:IC:54:ARG:NH1	2.40	0.55
1:KC:29:ASP:OD2	1:KC:54:ARG:NH1	2.40	0.55
1:F:29:ASP:OD2	1:F:54:ARG:NH1	2.40	0.55
1:L:29:ASP:OD2	1:L:54:ARG:NH1	2.40	0.55
1:M:29:ASP:OD2	1:M:54:ARG:NH1	2.40	0.55
1:Z:29:ASP:OD2	1:Z:54:ARG:NH1	2.40	0.55
1:CA:29:ASP:OD2	1:CA:54:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:29:ASP:OD2	1:DA:54:ARG:NH1	2.40	0.55
1:JA:29:ASP:OD2	1:JA:54:ARG:NH1	2.40	0.55
1:RB:29:ASP:OD2	1:RB:54:ARG:NH1	2.40	0.55
1:SB:29:ASP:OD2	1:SB:54:ARG:NH1	2.40	0.55
1:H:29:ASP:OD2	1:H:54:ARG:NH1	2.40	0.55
1:I:29:ASP:OD2	1:I:54:ARG:NH1	2.40	0.55
1:K:29:ASP:OD2	1:K:54:ARG:NH1	2.40	0.55
1:KA:29:ASP:OD2	1:KA:54:ARG:NH1	2.40	0.55
1:PA:29:ASP:OD2	1:PA:54:ARG:NH1	2.40	0.55
1:TA:29:ASP:OD2	1:TA:54:ARG:NH1	2.40	0.55
1:AB:29:ASP:OD2	1:AB:54:ARG:NH1	2.40	0.55
1:BB:29:ASP:OD2	1:BB:54:ARG:NH1	2.40	0.55
1:DB:29:ASP:OD2	1:DB:54:ARG:NH1	2.40	0.55
1:EB:29:ASP:OD2	1:EB:54:ARG:NH1	2.40	0.55
1:UB:29:ASP:OD2	1:UB:54:ARG:NH1	2.40	0.55
1:BC:29:ASP:OD2	1:BC:54:ARG:NH1	2.40	0.55
1:CC:29:ASP:OD2	1:CC:54:ARG:NH1	2.40	0.55
1:A:29:ASP:OD2	1:A:54:ARG:NH1	2.40	0.55
1:O:29:ASP:OD2	1:O:54:ARG:NH1	2.40	0.55
1:AA:29:ASP:OD2	1:AA:54:ARG:NH1	2.40	0.55
1:FA:29:ASP:OD2	1:FA:54:ARG:NH1	2.40	0.55
1:HB:29:ASP:OD2	1:HB:54:ARG:NH1	2.40	0.55
1:PB:29:ASP:OD2	1:PB:54:ARG:NH1	2.40	0.55
1:AC:29:ASP:OD2	1:AC:54:ARG:NH1	2.40	0.55
1:HC:29:ASP:OD2	1:HC:54:ARG:NH1	2.40	0.55
1:E:29:ASP:OD2	1:E:54:ARG:NH1	2.40	0.55
1:X:29:ASP:OD2	1:X:54:ARG:NH1	2.40	0.55
1:IA:29:ASP:OD2	1:IA:54:ARG:NH1	2.40	0.55
1:DC:29:ASP:OD2	1:DC:54:ARG:NH1	2.40	0.55
1:WA:29:ASP:OD2	1:WA:54:ARG:NH1	2.40	0.55
1:XA:29:ASP:OD2	1:XA:54:ARG:NH1	2.40	0.55
1:CB:29:ASP:OD2	1:CB:54:ARG:NH1	2.40	0.55
1:MB:29:ASP:OD2	1:MB:54:ARG:NH1	2.40	0.55
1:XB:29:ASP:OD2	1:XB:54:ARG:NH1	2.40	0.55
1:ZB:29:ASP:OD2	1:ZB:54:ARG:NH1	2.40	0.55
1:J:29:ASP:OD2	1:J:54:ARG:NH1	2.40	0.55
1:R:29:ASP:OD2	1:R:54:ARG:NH1	2.40	0.55
1:T:29:ASP:OD2	1:T:54:ARG:NH1	2.40	0.55
1:LA:29:ASP:OD2	1:LA:54:ARG:NH1	2.40	0.55
1:MA:29:ASP:OD2	1:MA:54:ARG:NH1	2.40	0.55
1:GB:29:ASP:OD2	1:GB:54:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:29:ASP:OD2	1:EC:54:ARG:NH1	2.40	0.55
1:B:29:ASP:OD2	1:B:54:ARG:NH1	2.40	0.54
1:D:29:ASP:OD2	1:D:54:ARG:NH1	2.40	0.54
1:N:29:ASP:OD2	1:N:54:ARG:NH1	2.40	0.54
1:Q:29:ASP:OD2	1:Q:54:ARG:NH1	2.40	0.54
1:HA:29:ASP:OD2	1:HA:54:ARG:NH1	2.40	0.54
1:JB:29:ASP:OD2	1:JB:54:ARG:NH1	2.40	0.54
1:KB:29:ASP:OD2	1:KB:54:ARG:NH1	2.40	0.54
1:UA:29:ASP:OD2	1:UA:54:ARG:NH1	2.40	0.54
1:GC:29:ASP:OD2	1:GC:54:ARG:NH1	2.40	0.54
1:OA:29:ASP:OD2	1:OA:54:ARG:NH1	2.40	0.54
1:RA:29:ASP:OD2	1:RA:54:ARG:NH1	2.40	0.54
1:WB:29:ASP:OD2	1:WB:54:ARG:NH1	2.40	0.54
1:JC:29:ASP:OD2	1:JC:54:ARG:NH1	2.40	0.54
1:V:29:ASP:OD2	1:V:54:ARG:NH1	2.40	0.54
1:NB:29:ASP:OD2	1:NB:54:ARG:NH1	2.40	0.54
1:EA:29:ASP:OD2	1:EA:54:ARG:NH1	2.40	0.54
1:ZA:29:ASP:OD2	1:ZA:54:ARG:NH1	2.40	0.54
1:G:29:ASP:OD2	1:G:54:ARG:NH1	2.40	0.54
1:Y:29:ASP:OD2	1:Y:54:ARG:NH1	2.40	0.54
1:QB:29:ASP:OD2	1:QB:54:ARG:NH1	2.40	0.54
1:TB:29:ASP:OD2	1:TB:54:ARG:NH1	2.40	0.54
1:BA:29:ASP:OD2	1:BA:54:ARG:NH1	2.40	0.54
1:K:35:ILE:O	1:K:55:THR:OG1	2.29	0.51
1:LA:35:ILE:O	1:LA:55:THR:OG1	2.29	0.51
1:QA:35:ILE:O	1:QA:55:THR:OG1	2.29	0.51
1:ZA:35:ILE:O	1:ZA:55:THR:OG1	2.29	0.51
1:DB:35:ILE:O	1:DB:55:THR:OG1	2.29	0.51
1:B:35:ILE:O	1:B:55:THR:OG1	2.29	0.51
1:F:35:ILE:O	1:F:55:THR:OG1	2.29	0.51
1:G:35:ILE:O	1:G:55:THR:OG1	2.29	0.51
1:PA:35:ILE:O	1:PA:55:THR:OG1	2.29	0.51
1:UA:35:ILE:O	1:UA:55:THR:OG1	2.29	0.51
1:DC:35:ILE:O	1:DC:55:THR:OG1	2.29	0.51
1:IC:35:ILE:O	1:IC:55:THR:OG1	2.29	0.51
1:HA:35:ILE:O	1:HA:55:THR:OG1	2.29	0.51
1:MA:35:ILE:O	1:MA:55:THR:OG1	2.29	0.51
1:VA:35:ILE:O	1:VA:55:THR:OG1	2.29	0.51
1:YA:35:ILE:O	1:YA:55:THR:OG1	2.29	0.51
1:EC:35:ILE:O	1:EC:55:THR:OG1	2.29	0.51
1:HC:35:ILE:O	1:HC:55:THR:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ILE:O	1:C:55:THR:OG1	2.29	0.51
1:J:35:ILE:O	1:J:55:THR:OG1	2.29	0.51
1:ZB:35:ILE:O	1:ZB:55:THR:OG1	2.29	0.51
1:A:35:ILE:O	1:A:55:THR:OG1	2.29	0.50
1:O:35:ILE:O	1:O:55:THR:OG1	2.29	0.50
1:CB:35:ILE:O	1:CB:55:THR:OG1	2.29	0.50
1:EB:35:ILE:O	1:EB:55:THR:OG1	2.29	0.50
1:JC:35:ILE:O	1:JC:55:THR:OG1	2.29	0.50
1:L:35:ILE:O	1:L:55:THR:OG1	2.29	0.50
1:GA:35:ILE:O	1:GA:55:THR:OG1	2.29	0.50
1:TA:35:ILE:O	1:TA:55:THR:OG1	2.29	0.50
1:AB:35:ILE:O	1:AB:55:THR:OG1	2.29	0.50
1:HB:35:ILE:O	1:HB:55:THR:OG1	2.29	0.50
1:AC:35:ILE:O	1:AC:55:THR:OG1	2.29	0.50
1:P:35:ILE:O	1:P:55:THR:OG1	2.29	0.50
1:IA:35:ILE:O	1:IA:55:THR:OG1	2.29	0.50
1:KA:35:ILE:O	1:KA:55:THR:OG1	2.29	0.50
1:RA:35:ILE:O	1:RA:55:THR:OG1	2.29	0.50
1:IB:35:ILE:O	1:IB:55:THR:OG1	2.29	0.50
1:YB:35:ILE:O	1:YB:55:THR:OG1	2.29	0.50
1:H:35:ILE:O	1:H:55:THR:OG1	2.29	0.50
1:VB:35:ILE:O	1:VB:55:THR:OG1	2.29	0.50
1:CC:35:ILE:O	1:CC:55:THR:OG1	2.29	0.50
1:E:35:ILE:O	1:E:55:THR:OG1	2.29	0.50
1:CA:35:ILE:O	1:CA:55:THR:OG1	2.29	0.50
1:DA:35:ILE:O	1:DA:55:THR:OG1	2.29	0.50
1:OA:35:ILE:O	1:OA:55:THR:OG1	2.29	0.50
1:MB:35:ILE:O	1:MB:55:THR:OG1	2.29	0.50
1:UB:35:ILE:O	1:UB:55:THR:OG1	2.29	0.50
1:FC:35:ILE:O	1:FC:55:THR:OG1	2.29	0.50
1:N:35:ILE:O	1:N:55:THR:OG1	2.29	0.50
1:S:35:ILE:O	1:S:55:THR:OG1	2.29	0.50
1:T:35:ILE:O	1:T:55:THR:OG1	2.29	0.50
1:XA:35:ILE:O	1:XA:55:THR:OG1	2.29	0.50
1:Y:35:ILE:O	1:Y:55:THR:OG1	2.29	0.50
1:NA:35:ILE:O	1:NA:55:THR:OG1	2.29	0.50
1:WA:35:ILE:O	1:WA:55:THR:OG1	2.29	0.50
1:GB:35:ILE:O	1:GB:55:THR:OG1	2.29	0.50
1:QB:35:ILE:O	1:QB:55:THR:OG1	2.29	0.50
1:GC:35:ILE:O	1:GC:55:THR:OG1	2.29	0.50
1:D:35:ILE:O	1:D:55:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:201:ASP:OD1	1:N:201:ASP:N	2.45	0.50
1:LB:35:ILE:O	1:LB:55:THR:OG1	2.29	0.50
1:RB:35:ILE:O	1:RB:55:THR:OG1	2.29	0.50
1:I:35:ILE:O	1:I:55:THR:OG1	2.29	0.50
1:J:201:ASP:N	1:J:201:ASP:OD1	2.45	0.50
1:Z:35:ILE:O	1:Z:55:THR:OG1	2.29	0.50
1:CB:201:ASP:OD1	1:CB:201:ASP:N	2.45	0.50
1:GB:201:ASP:N	1:GB:201:ASP:OD1	2.45	0.50
1:WB:35:ILE:O	1:WB:55:THR:OG1	2.29	0.50
1:Q:201:ASP:N	1:Q:201:ASP:OD1	2.45	0.49
1:R:201:ASP:OD1	1:R:201:ASP:N	2.45	0.49
1:BA:35:ILE:O	1:BA:55:THR:OG1	2.29	0.49
1:EA:35:ILE:O	1:EA:55:THR:OG1	2.29	0.49
1:SA:35:ILE:O	1:SA:55:THR:OG1	2.29	0.49
1:JB:35:ILE:O	1:JB:55:THR:OG1	2.29	0.49
1:KB:201:ASP:OD1	1:KB:201:ASP:N	2.45	0.49
1:NB:35:ILE:O	1:NB:55:THR:OG1	2.29	0.49
1:M:201:ASP:OD1	1:M:201:ASP:N	2.45	0.49
1:Q:35:ILE:O	1:Q:55:THR:OG1	2.29	0.49
1:R:35:ILE:O	1:R:55:THR:OG1	2.29	0.49
1:V:35:ILE:O	1:V:55:THR:OG1	2.29	0.49
1:FA:35:ILE:O	1:FA:55:THR:OG1	2.29	0.49
1:OA:201:ASP:N	1:OA:201:ASP:OD1	2.45	0.49
1:YA:201:ASP:OD1	1:YA:201:ASP:N	2.45	0.49
1:BB:35:ILE:O	1:BB:55:THR:OG1	2.29	0.49
1:FB:35:ILE:O	1:FB:55:THR:OG1	2.29	0.49
1:JB:201:ASP:OD1	1:JB:201:ASP:N	2.45	0.49
1:TB:35:ILE:O	1:TB:55:THR:OG1	2.29	0.49
1:BC:35:ILE:O	1:BC:55:THR:OG1	2.29	0.49
1:F:201:ASP:OD1	1:F:201:ASP:N	2.45	0.49
1:I:201:ASP:OD1	1:I:201:ASP:N	2.45	0.49
1:M:35:ILE:O	1:M:55:THR:OG1	2.29	0.49
1:V:201:ASP:N	1:V:201:ASP:OD1	2.45	0.49
1:FA:201:ASP:OD1	1:FA:201:ASP:N	2.45	0.49
1:JA:35:ILE:O	1:JA:55:THR:OG1	2.29	0.49
1:DB:201:ASP:N	1:DB:201:ASP:OD1	2.45	0.49
1:FB:201:ASP:OD1	1:FB:201:ASP:N	2.45	0.49
1:NB:201:ASP:N	1:NB:201:ASP:OD1	2.45	0.49
1:XB:35:ILE:O	1:XB:55:THR:OG1	2.29	0.49
1:XB:201:ASP:N	1:XB:201:ASP:OD1	2.45	0.49
1:KC:35:ILE:O	1:KC:55:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:201:ASP:OD1	1:K:201:ASP:N	2.45	0.49
1:W:201:ASP:OD1	1:W:201:ASP:N	2.45	0.49
1:KA:201:ASP:OD1	1:KA:201:ASP:N	2.45	0.49
1:ZA:201:ASP:OD1	1:ZA:201:ASP:N	2.45	0.49
1:KB:35:ILE:O	1:KB:55:THR:OG1	2.29	0.49
1:OB:201:ASP:OD1	1:OB:201:ASP:N	2.45	0.49
1:CC:201:ASP:OD1	1:CC:201:ASP:N	2.45	0.49
1:O:201:ASP:N	1:O:201:ASP:OD1	2.45	0.49
1:BB:201:ASP:N	1:BB:201:ASP:OD1	2.45	0.49
1:HB:201:ASP:OD1	1:HB:201:ASP:N	2.45	0.49
1:E:201:ASP:N	1:E:201:ASP:OD1	2.45	0.49
1:Z:201:ASP:OD1	1:Z:201:ASP:N	2.45	0.49
1:B:201:ASP:OD1	1:B:201:ASP:N	2.45	0.49
1:NA:134:LYS:HA	1:NA:137:THR:HG22	1.95	0.49
1:UA:201:ASP:OD1	1:UA:201:ASP:N	2.45	0.49
1:XA:201:ASP:OD1	1:XA:201:ASP:N	2.45	0.49
1:IB:201:ASP:N	1:IB:201:ASP:OD1	2.45	0.49
1:SB:35:ILE:O	1:SB:55:THR:OG1	2.29	0.49
1:FC:134:LYS:HA	1:FC:137:THR:HG22	1.95	0.49
1:P:201:ASP:OD1	1:P:201:ASP:N	2.45	0.49
1:T:201:ASP:N	1:T:201:ASP:OD1	2.45	0.49
1:AA:35:ILE:O	1:AA:55:THR:OG1	2.29	0.49
1:QA:134:LYS:HA	1:QA:137:THR:HG22	1.95	0.49
1:RB:201:ASP:OD1	1:RB:201:ASP:N	2.45	0.49
1:HC:201:ASP:OD1	1:HC:201:ASP:N	2.45	0.49
1:A:201:ASP:OD1	1:A:201:ASP:N	2.45	0.49
1:GA:201:ASP:OD1	1:GA:201:ASP:N	2.45	0.49
1:HA:134:LYS:HA	1:HA:137:THR:HG22	1.95	0.49
1:KA:134:LYS:HA	1:KA:137:THR:HG22	1.95	0.49
1:NA:201:ASP:OD1	1:NA:201:ASP:N	2.45	0.49
1:PA:201:ASP:OD1	1:PA:201:ASP:N	2.45	0.49
1:MB:201:ASP:OD1	1:MB:201:ASP:N	2.45	0.49
1:YB:201:ASP:OD1	1:YB:201:ASP:N	2.45	0.49
1:ZB:134:LYS:HA	1:ZB:137:THR:HG22	1.95	0.49
1:ZB:201:ASP:N	1:ZB:201:ASP:OD1	2.45	0.49
1:CC:134:LYS:HA	1:CC:137:THR:HG22	1.95	0.49
1:FC:201:ASP:N	1:FC:201:ASP:OD1	2.45	0.49
1:IC:134:LYS:HA	1:IC:137:THR:HG22	1.95	0.49
1:L:201:ASP:OD1	1:L:201:ASP:N	2.45	0.49
1:W:35:ILE:O	1:W:55:THR:OG1	2.29	0.49
1:BA:201:ASP:OD1	1:BA:201:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:HA:201:ASP:OD1	1:HA:201:ASP:N	2.45	0.49
1:JA:201:ASP:N	1:JA:201:ASP:OD1	2.45	0.49
1:TB:201:ASP:OD1	1:TB:201:ASP:N	2.45	0.49
1:N:18:LEU:HG	1:N:217:ALA:HB1	1.95	0.48
1:Q:18:LEU:HG	1:Q:217:ALA:HB1	1.95	0.48
1:Y:201:ASP:N	1:Y:201:ASP:OD1	2.45	0.48
1:CA:134:LYS:HA	1:CA:137:THR:HG22	1.95	0.48
1:KA:18:LEU:HG	1:KA:217:ALA:HB1	1.95	0.48
1:PA:134:LYS:HA	1:PA:137:THR:HG22	1.95	0.48
1:SA:134:LYS:HA	1:SA:137:THR:HG22	1.95	0.48
1:TA:134:LYS:HA	1:TA:137:THR:HG22	1.95	0.48
1:JB:18:LEU:HG	1:JB:217:ALA:HB1	1.95	0.48
1:OB:35:ILE:O	1:OB:55:THR:OG1	2.29	0.48
1:UB:134:LYS:HA	1:UB:137:THR:HG22	1.95	0.48
1:XB:134:LYS:HA	1:XB:137:THR:HG22	1.95	0.48
1:AC:134:LYS:HA	1:AC:137:THR:HG22	1.95	0.48
1:BC:201:ASP:OD1	1:BC:201:ASP:N	2.45	0.48
1:FC:18:LEU:HG	1:FC:217:ALA:HB1	1.95	0.48
1:GC:201:ASP:OD1	1:GC:201:ASP:N	2.45	0.48
1:A:134:LYS:HA	1:A:137:THR:HG22	1.95	0.48
1:DA:201:ASP:OD1	1:DA:201:ASP:N	2.45	0.48
1:EA:134:LYS:HA	1:EA:137:THR:HG22	1.95	0.48
1:FA:134:LYS:HA	1:FA:137:THR:HG22	1.95	0.48
1:IA:134:LYS:HA	1:IA:137:THR:HG22	1.95	0.48
1:NA:18:LEU:HG	1:NA:217:ALA:HB1	1.96	0.48
1:QA:18:LEU:HG	1:QA:217:ALA:HB1	1.96	0.48
1:EB:201:ASP:OD1	1:EB:201:ASP:N	2.45	0.48
1:GB:18:LEU:HG	1:GB:217:ALA:HB1	1.96	0.48
1:MB:18:LEU:HG	1:MB:217:ALA:HB1	1.96	0.48
1:QB:201:ASP:N	1:QB:201:ASP:OD1	2.45	0.48
1:VB:201:ASP:OD1	1:VB:201:ASP:N	2.45	0.48
1:WB:134:LYS:HA	1:WB:137:THR:HG22	1.95	0.48
1:CC:18:LEU:HG	1:CC:217:ALA:HB1	1.96	0.48
1:DC:201:ASP:N	1:DC:201:ASP:OD1	2.45	0.48
1:KC:134:LYS:HA	1:KC:137:THR:HG22	1.95	0.48
1:C:134:LYS:HA	1:C:137:THR:HG22	1.95	0.48
1:H:201:ASP:N	1:H:201:ASP:OD1	2.45	0.48
1:O:18:LEU:HG	1:O:217:ALA:HB1	1.96	0.48
1:R:18:LEU:HG	1:R:217:ALA:HB1	1.96	0.48
1:T:18:LEU:HG	1:T:217:ALA:HB1	1.96	0.48
1:V:18:LEU:HG	1:V:217:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:35:ILE:O	1:X:55:THR:OG1	2.29	0.48
1:Y:18:LEU:HG	1:Y:217:ALA:HB1	1.95	0.48
1:EA:18:LEU:HG	1:EA:217:ALA:HB1	1.95	0.48
1:LA:18:LEU:HG	1:LA:217:ALA:HB1	1.96	0.48
1:LA:201:ASP:N	1:LA:201:ASP:OD1	2.45	0.48
1:QA:201:ASP:N	1:QA:201:ASP:OD1	2.45	0.48
1:RA:18:LEU:HG	1:RA:217:ALA:HB1	1.95	0.48
1:RA:201:ASP:OD1	1:RA:201:ASP:N	2.45	0.48
1:TA:201:ASP:N	1:TA:201:ASP:OD1	2.45	0.48
1:IB:18:LEU:HG	1:IB:217:ALA:HB1	1.96	0.48
1:QB:18:LEU:HG	1:QB:217:ALA:HB1	1.95	0.48
1:EC:18:LEU:HG	1:EC:217:ALA:HB1	1.96	0.48
1:GC:18:LEU:HG	1:GC:217:ALA:HB1	1.95	0.48
1:HC:134:LYS:HA	1:HC:137:THR:HG22	1.95	0.48
1:IC:18:LEU:HG	1:IC:217:ALA:HB1	1.96	0.48
1:IC:201:ASP:N	1:IC:201:ASP:OD1	2.45	0.48
1:JC:201:ASP:OD1	1:JC:201:ASP:N	2.45	0.48
1:A:18:LEU:HG	1:A:217:ALA:HB1	1.96	0.48
1:K:18:LEU:HG	1:K:217:ALA:HB1	1.96	0.48
1:M:18:LEU:HG	1:M:217:ALA:HB1	1.96	0.48
1:S:18:LEU:HG	1:S:217:ALA:HB1	1.95	0.48
1:HA:18:LEU:HG	1:HA:217:ALA:HB1	1.96	0.48
1:JA:18:LEU:HG	1:JA:217:ALA:HB1	1.96	0.48
1:MA:18:LEU:HG	1:MA:217:ALA:HB1	1.96	0.48
1:TA:18:LEU:HG	1:TA:217:ALA:HB1	1.96	0.48
1:VA:134:LYS:HA	1:VA:137:THR:HG22	1.95	0.48
1:DB:18:LEU:HG	1:DB:217:ALA:HB1	1.96	0.48
1:FB:18:LEU:HG	1:FB:217:ALA:HB1	1.96	0.48
1:HB:18:LEU:HG	1:HB:217:ALA:HB1	1.96	0.48
1:LB:18:LEU:HG	1:LB:217:ALA:HB1	1.95	0.48
1:NB:18:LEU:HG	1:NB:217:ALA:HB1	1.96	0.48
1:PB:18:LEU:HG	1:PB:217:ALA:HB1	1.96	0.48
1:PB:35:ILE:O	1:PB:55:THR:OG1	2.29	0.48
1:RB:134:LYS:HA	1:RB:137:THR:HG22	1.95	0.48
1:SB:18:LEU:HG	1:SB:217:ALA:HB1	1.96	0.48
1:WB:18:LEU:HG	1:WB:217:ALA:HB1	1.95	0.48
1:ZB:18:LEU:HG	1:ZB:217:ALA:HB1	1.96	0.48
1:BC:18:LEU:HG	1:BC:217:ALA:HB1	1.96	0.48
1:DC:18:LEU:HG	1:DC:217:ALA:HB1	1.96	0.48
1:DC:134:LYS:HA	1:DC:137:THR:HG22	1.95	0.48
1:JC:18:LEU:HG	1:JC:217:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HG	1:B:217:ALA:HB1	1.96	0.48
1:D:18:LEU:HG	1:D:217:ALA:HB1	1.96	0.48
1:E:18:LEU:HG	1:E:217:ALA:HB1	1.96	0.48
1:F:134:LYS:HA	1:F:137:THR:HG22	1.95	0.48
1:G:18:LEU:HG	1:G:217:ALA:HB1	1.95	0.48
1:H:18:LEU:HG	1:H:217:ALA:HB1	1.96	0.48
1:J:18:LEU:HG	1:J:217:ALA:HB1	1.96	0.48
1:P:18:LEU:HG	1:P:217:ALA:HB1	1.96	0.48
1:X:18:LEU:HG	1:X:217:ALA:HB1	1.96	0.48
1:Z:134:LYS:HA	1:Z:137:THR:HG22	1.95	0.48
1:AA:18:LEU:HG	1:AA:217:ALA:HB1	1.96	0.48
1:BA:18:LEU:HG	1:BA:217:ALA:HB1	1.96	0.48
1:DA:18:LEU:HG	1:DA:217:ALA:HB1	1.95	0.48
1:GA:18:LEU:HG	1:GA:217:ALA:HB1	1.96	0.48
1:MA:134:LYS:HA	1:MA:137:THR:HG22	1.95	0.48
1:MA:201:ASP:OD1	1:MA:201:ASP:N	2.45	0.48
1:OA:18:LEU:HG	1:OA:217:ALA:HB1	1.96	0.48
1:UA:18:LEU:HG	1:UA:217:ALA:HB1	1.96	0.48
1:WA:18:LEU:HG	1:WA:217:ALA:HB1	1.96	0.48
1:XA:18:LEU:HG	1:XA:217:ALA:HB1	1.96	0.48
1:YA:134:LYS:HA	1:YA:137:THR:HG22	1.95	0.48
1:ZA:18:LEU:HG	1:ZA:217:ALA:HB1	1.96	0.48
1:AB:18:LEU:HG	1:AB:217:ALA:HB1	1.96	0.48
1:AB:201:ASP:OD1	1:AB:201:ASP:N	2.45	0.48
1:CB:18:LEU:HG	1:CB:217:ALA:HB1	1.96	0.48
1:KB:18:LEU:HG	1:KB:217:ALA:HB1	1.96	0.48
1:VB:18:LEU:HG	1:VB:217:ALA:HB1	1.96	0.48
1:WB:201:ASP:OD1	1:WB:201:ASP:N	2.45	0.48
1:HC:18:LEU:HG	1:HC:217:ALA:HB1	1.96	0.48
1:D:201:ASP:OD1	1:D:201:ASP:N	2.45	0.48
1:L:18:LEU:HG	1:L:217:ALA:HB1	1.96	0.48
1:BA:134:LYS:HA	1:BA:137:THR:HG22	1.95	0.48
1:CA:201:ASP:N	1:CA:201:ASP:OD1	2.45	0.48
1:IA:18:LEU:HG	1:IA:217:ALA:HB1	1.96	0.48
1:LA:134:LYS:HA	1:LA:137:THR:HG22	1.95	0.48
1:PA:18:LEU:HG	1:PA:217:ALA:HB1	1.96	0.48
1:WA:201:ASP:OD1	1:WA:201:ASP:N	2.45	0.48
1:OB:18:LEU:HG	1:OB:217:ALA:HB1	1.96	0.48
1:TB:18:LEU:HG	1:TB:217:ALA:HB1	1.96	0.48
1:YB:18:LEU:HG	1:YB:217:ALA:HB1	1.96	0.48
1:EC:134:LYS:HA	1:EC:137:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EC:201:ASP:OD1	1:EC:201:ASP:N	2.45	0.48
1:GC:134:LYS:HA	1:GC:137:THR:HG22	1.95	0.48
1:W:18:LEU:HG	1:W:217:ALA:HB1	1.96	0.48
1:Z:18:LEU:HG	1:Z:217:ALA:HB1	1.95	0.48
1:EA:201:ASP:N	1:EA:201:ASP:OD1	2.45	0.48
1:JA:134:LYS:HA	1:JA:137:THR:HG22	1.95	0.48
1:WA:134:LYS:HA	1:WA:137:THR:HG22	1.95	0.48
1:EB:18:LEU:HG	1:EB:217:ALA:HB1	1.96	0.48
1:UB:18:LEU:HG	1:UB:217:ALA:HB1	1.95	0.48
1:UB:201:ASP:OD1	1:UB:201:ASP:N	2.45	0.48
1:AC:18:LEU:HG	1:AC:217:ALA:HB1	1.96	0.48
1:KC:18:LEU:HG	1:KC:217:ALA:HB1	1.96	0.48
1:D:134:LYS:HA	1:D:137:THR:HG22	1.95	0.48
1:F:18:LEU:HG	1:F:217:ALA:HB1	1.95	0.48
1:CA:18:LEU:HG	1:CA:217:ALA:HB1	1.96	0.48
1:FA:18:LEU:HG	1:FA:217:ALA:HB1	1.96	0.48
1:SA:18:LEU:HG	1:SA:217:ALA:HB1	1.96	0.48
1:RB:18:LEU:HG	1:RB:217:ALA:HB1	1.96	0.48
1:XB:18:LEU:HG	1:XB:217:ALA:HB1	1.96	0.48
1:C:18:LEU:HG	1:C:217:ALA:HB1	1.96	0.48
1:I:18:LEU:HG	1:I:217:ALA:HB1	1.96	0.48
1:W:134:LYS:HA	1:W:137:THR:HG22	1.95	0.48
1:OA:134:LYS:HA	1:OA:137:THR:HG22	1.95	0.48
1:VA:18:LEU:HG	1:VA:217:ALA:HB1	1.96	0.48
1:BB:18:LEU:HG	1:BB:217:ALA:HB1	1.96	0.48
1:SB:201:ASP:N	1:SB:201:ASP:OD1	2.45	0.48
1:TB:134:LYS:HA	1:TB:137:THR:HG22	1.95	0.48
1:AC:201:ASP:N	1:AC:201:ASP:OD1	2.45	0.48
1:BC:134:LYS:HA	1:BC:137:THR:HG22	1.95	0.48
1:I:134:LYS:HA	1:I:137:THR:HG22	1.95	0.48
1:AA:201:ASP:OD1	1:AA:201:ASP:N	2.45	0.48
1:IA:201:ASP:OD1	1:IA:201:ASP:N	2.45	0.48
1:YA:18:LEU:HG	1:YA:217:ALA:HB1	1.96	0.48
1:BB:134:LYS:HA	1:BB:137:THR:HG22	1.95	0.48
1:OB:134:LYS:HA	1:OB:137:THR:HG22	1.95	0.48
1:PB:201:ASP:OD1	1:PB:201:ASP:N	2.45	0.48
1:KC:201:ASP:N	1:KC:201:ASP:OD1	2.45	0.48
1:S:201:ASP:OD1	1:S:201:ASP:N	2.45	0.47
1:SA:201:ASP:OD1	1:SA:201:ASP:N	2.45	0.47
1:PB:134:LYS:HA	1:PB:137:THR:HG22	1.95	0.47
1:SB:134:LYS:HA	1:SB:137:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JC:134:LYS:HA	1:JC:137:THR:HG22	1.95	0.47
1:C:201:ASP:N	1:C:201:ASP:OD1	2.45	0.47
1:G:201:ASP:OD1	1:G:201:ASP:N	2.45	0.47
1:H:134:LYS:HA	1:H:137:THR:HG22	1.95	0.47
1:X:201:ASP:OD1	1:X:201:ASP:N	2.45	0.47
1:GA:134:LYS:HA	1:GA:137:THR:HG22	1.95	0.47
1:E:134:LYS:HA	1:E:137:THR:HG22	1.95	0.47
1:K:134:LYS:HA	1:K:137:THR:HG22	1.95	0.47
1:Q:134:LYS:HA	1:Q:137:THR:HG22	1.95	0.47
1:T:134:LYS:HA	1:T:137:THR:HG22	1.95	0.47
1:X:134:LYS:HA	1:X:137:THR:HG22	1.95	0.47
1:AB:134:LYS:HA	1:AB:137:THR:HG22	1.95	0.47
1:LB:201:ASP:N	1:LB:201:ASP:OD1	2.45	0.47
1:MB:134:LYS:HA	1:MB:137:THR:HG22	1.95	0.47
1:B:134:LYS:HA	1:B:137:THR:HG22	1.95	0.47
1:G:134:LYS:HA	1:G:137:THR:HG22	1.95	0.47
1:N:134:LYS:HA	1:N:137:THR:HG22	1.95	0.47
1:S:134:LYS:HA	1:S:137:THR:HG22	1.95	0.47
1:AA:134:LYS:HA	1:AA:137:THR:HG22	1.95	0.47
1:RA:134:LYS:HA	1:RA:137:THR:HG22	1.95	0.47
1:VA:201:ASP:N	1:VA:201:ASP:OD1	2.45	0.47
1:XA:134:LYS:HA	1:XA:137:THR:HG22	1.95	0.47
1:ZA:134:LYS:HA	1:ZA:137:THR:HG22	1.95	0.47
1:DB:134:LYS:HA	1:DB:137:THR:HG22	1.95	0.47
1:EB:134:LYS:HA	1:EB:137:THR:HG22	1.95	0.47
1:GB:134:LYS:HA	1:GB:137:THR:HG22	1.95	0.47
1:JB:134:LYS:HA	1:JB:137:THR:HG22	1.95	0.47
1:VB:134:LYS:HA	1:VB:137:THR:HG22	1.95	0.47
1:L:134:LYS:HA	1:L:137:THR:HG22	1.95	0.47
1:DA:134:LYS:HA	1:DA:137:THR:HG22	1.95	0.47
1:LB:134:LYS:HA	1:LB:137:THR:HG22	1.95	0.47
1:YB:134:LYS:HA	1:YB:137:THR:HG22	1.95	0.47
1:Y:134:LYS:HA	1:Y:137:THR:HG22	1.95	0.47
1:UA:134:LYS:HA	1:UA:137:THR:HG22	1.95	0.47
1:O:134:LYS:HA	1:O:137:THR:HG22	1.95	0.47
1:P:134:LYS:HA	1:P:137:THR:HG22	1.95	0.47
1:R:134:LYS:HA	1:R:137:THR:HG22	1.95	0.47
1:HB:134:LYS:HA	1:HB:137:THR:HG22	1.95	0.47
1:IB:134:LYS:HA	1:IB:137:THR:HG22	1.95	0.47
1:KB:134:LYS:HA	1:KB:137:THR:HG22	1.95	0.47
1:QB:134:LYS:HA	1:QB:137:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:134:LYS:HA	1:M:137:THR:HG22	1.95	0.47
1:FB:134:LYS:HA	1:FB:137:THR:HG22	1.95	0.47
1:J:134:LYS:HA	1:J:137:THR:HG22	1.95	0.47
1:V:134:LYS:HA	1:V:137:THR:HG22	1.95	0.46
1:CB:134:LYS:HA	1:CB:137:THR:HG22	1.95	0.46
1:NB:134:LYS:HA	1:NB:137:THR:HG22	1.95	0.46
1:B:158:LEU:HD12	1:B:225:ILE:HD11	1.99	0.45
1:E:97:ILE:HB	1:E:101:PHE:HB3	1.99	0.45
1:DA:158:LEU:HD12	1:DA:225:ILE:HD11	1.99	0.45
1:XA:97:ILE:HB	1:XA:101:PHE:HB3	1.99	0.45
1:FB:97:ILE:HB	1:FB:101:PHE:HB3	1.99	0.45
1:A:97:ILE:HB	1:A:101:PHE:HB3	1.99	0.45
1:B:97:ILE:HB	1:B:101:PHE:HB3	1.99	0.45
1:D:97:ILE:HB	1:D:101:PHE:HB3	1.99	0.45
1:E:158:LEU:HD12	1:E:225:ILE:HD11	1.99	0.45
1:H:97:ILE:HB	1:H:101:PHE:HB3	1.99	0.45
1:I:97:ILE:HB	1:I:101:PHE:HB3	1.99	0.45
1:L:97:ILE:HB	1:L:101:PHE:HB3	1.99	0.45
1:M:97:ILE:HB	1:M:101:PHE:HB3	1.99	0.45
1:PA:97:ILE:HB	1:PA:101:PHE:HB3	1.99	0.45
1:QA:97:ILE:HB	1:QA:101:PHE:HB3	1.99	0.45
1:TA:97:ILE:HB	1:TA:101:PHE:HB3	1.99	0.45
1:UA:97:ILE:HB	1:UA:101:PHE:HB3	1.99	0.45
1:UA:158:LEU:HD12	1:UA:225:ILE:HD11	1.99	0.45
1:XA:158:LEU:HD12	1:XA:225:ILE:HD11	1.99	0.45
1:BB:97:ILE:HB	1:BB:101:PHE:HB3	1.99	0.45
1:EB:97:ILE:HB	1:EB:101:PHE:HB3	1.99	0.45
1:JB:97:ILE:HB	1:JB:101:PHE:HB3	1.99	0.45
1:NB:158:LEU:HD12	1:NB:225:ILE:HD11	1.99	0.45
1:QB:158:LEU:HD12	1:QB:225:ILE:HD11	1.99	0.45
1:TB:158:LEU:HD12	1:TB:225:ILE:HD11	1.99	0.45
1:HC:97:ILE:HB	1:HC:101:PHE:HB3	1.99	0.45
1:IC:97:ILE:HB	1:IC:101:PHE:HB3	1.99	0.45
1:O:97:ILE:HB	1:O:101:PHE:HB3	1.99	0.45
1:P:97:ILE:HB	1:P:101:PHE:HB3	1.99	0.45
1:Q:97:ILE:HB	1:Q:101:PHE:HB3	1.99	0.45
1:V:158:LEU:HD12	1:V:225:ILE:HD11	1.99	0.45
1:Y:158:LEU:HD12	1:Y:225:ILE:HD11	1.99	0.45
1:AA:158:LEU:HD12	1:AA:225:ILE:HD11	1.99	0.45
1:BA:158:LEU:HD12	1:BA:225:ILE:HD11	1.99	0.45
1:GA:158:LEU:HD12	1:GA:225:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LA:97:ILE:HB	1:LA:101:PHE:HB3	1.99	0.45
1:MA:97:ILE:HB	1:MA:101:PHE:HB3	1.99	0.45
1:RA:158:LEU:HD12	1:RA:225:ILE:HD11	1.99	0.45
1:SA:97:ILE:HB	1:SA:101:PHE:HB3	1.99	0.45
1:WA:97:ILE:HB	1:WA:101:PHE:HB3	1.99	0.45
1:YA:97:ILE:HB	1:YA:101:PHE:HB3	1.99	0.45
1:AB:97:ILE:HB	1:AB:101:PHE:HB3	1.99	0.45
1:AB:158:LEU:HD12	1:AB:225:ILE:HD11	1.99	0.45
1:CB:97:ILE:HB	1:CB:101:PHE:HB3	1.99	0.45
1:HB:97:ILE:HB	1:HB:101:PHE:HB3	1.99	0.45
1:IB:97:ILE:HB	1:IB:101:PHE:HB3	1.99	0.45
1:VB:158:LEU:HD12	1:VB:225:ILE:HD11	1.99	0.45
1:DC:97:ILE:HB	1:DC:101:PHE:HB3	1.99	0.45
1:EC:97:ILE:HB	1:EC:101:PHE:HB3	1.99	0.45
1:F:97:ILE:HB	1:F:101:PHE:HB3	1.99	0.45
1:G:158:LEU:HD12	1:G:225:ILE:HD11	1.99	0.45
1:J:97:ILE:HB	1:J:101:PHE:HB3	1.99	0.45
1:J:158:LEU:HD12	1:J:225:ILE:HD11	1.99	0.45
1:K:97:ILE:HB	1:K:101:PHE:HB3	1.99	0.45
1:R:158:LEU:HD12	1:R:225:ILE:HD11	1.99	0.45
1:JA:158:LEU:HD12	1:JA:225:ILE:HD11	1.99	0.45
1:OA:97:ILE:HB	1:OA:101:PHE:HB3	1.99	0.45
1:RA:97:ILE:HB	1:RA:101:PHE:HB3	1.99	0.45
1:CB:158:LEU:HD12	1:CB:225:ILE:HD11	1.99	0.45
1:GB:97:ILE:HB	1:GB:101:PHE:HB3	1.99	0.45
1:JB:11:ARG:HE	1:KB:206:ARG:HH12	1.64	0.45
1:SB:158:LEU:HD12	1:SB:225:ILE:HD11	1.99	0.45
1:YB:158:LEU:HD12	1:YB:225:ILE:HD11	1.99	0.45
1:HC:158:LEU:HD12	1:HC:225:ILE:HD11	1.99	0.45
1:JC:97:ILE:HB	1:JC:101:PHE:HB3	1.99	0.45
1:JC:158:LEU:HD12	1:JC:225:ILE:HD11	1.99	0.45
1:G:97:ILE:HB	1:G:101:PHE:HB3	1.99	0.45
1:H:158:LEU:HD12	1:H:225:ILE:HD11	1.99	0.45
1:M:158:LEU:HD12	1:M:225:ILE:HD11	1.99	0.45
1:P:158:LEU:HD12	1:P:225:ILE:HD11	1.99	0.45
1:OA:158:LEU:HD12	1:OA:225:ILE:HD11	1.99	0.45
1:PA:158:LEU:HD12	1:PA:225:ILE:HD11	1.99	0.45
1:ZA:158:LEU:HD12	1:ZA:225:ILE:HD11	1.99	0.45
1:DB:97:ILE:HB	1:DB:101:PHE:HB3	1.99	0.45
1:FB:158:LEU:HD12	1:FB:225:ILE:HD11	1.99	0.45
1:IB:158:LEU:HD12	1:IB:225:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KB:97:ILE:HB	1:KB:101:PHE:HB3	1.99	0.45
1:KB:158:LEU:HD12	1:KB:225:ILE:HD11	1.99	0.45
1:LB:158:LEU:HD12	1:LB:225:ILE:HD11	1.99	0.45
1:WB:158:LEU:HD12	1:WB:225:ILE:HD11	1.99	0.45
1:BC:158:LEU:HD12	1:BC:225:ILE:HD11	1.99	0.45
1:EC:158:LEU:HD12	1:EC:225:ILE:HD11	1.99	0.45
1:GC:97:ILE:HB	1:GC:101:PHE:HB3	1.99	0.45
1:GC:158:LEU:HD12	1:GC:225:ILE:HD11	1.99	0.45
1:KC:97:ILE:HB	1:KC:101:PHE:HB3	1.99	0.45
1:KC:158:LEU:HD12	1:KC:225:ILE:HD11	1.99	0.45
1:N:97:ILE:HB	1:N:101:PHE:HB3	1.99	0.45
1:R:97:ILE:HB	1:R:101:PHE:HB3	1.99	0.45
1:S:158:LEU:HD12	1:S:225:ILE:HD11	1.99	0.45
1:T:97:ILE:HB	1:T:101:PHE:HB3	1.99	0.45
1:V:97:ILE:HB	1:V:101:PHE:HB3	1.99	0.45
1:X:158:LEU:HD12	1:X:225:ILE:HD11	1.99	0.45
1:KA:97:ILE:HB	1:KA:101:PHE:HB3	1.99	0.45
1:MA:158:LEU:HD12	1:MA:225:ILE:HD11	1.99	0.45
1:NA:97:ILE:HB	1:NA:101:PHE:HB3	1.99	0.45
1:SA:158:LEU:HD12	1:SA:225:ILE:HD11	1.99	0.45
1:VA:97:ILE:HB	1:VA:101:PHE:HB3	1.99	0.45
1:ZA:97:ILE:HB	1:ZA:101:PHE:HB3	1.99	0.45
1:MB:97:ILE:HB	1:MB:101:PHE:HB3	1.99	0.45
1:NB:97:ILE:HB	1:NB:101:PHE:HB3	1.99	0.45
1:CC:97:ILE:HB	1:CC:101:PHE:HB3	1.99	0.45
1:FC:97:ILE:HB	1:FC:101:PHE:HB3	1.99	0.45
1:C:97:ILE:HB	1:C:101:PHE:HB3	1.99	0.45
1:D:158:LEU:HD12	1:D:225:ILE:HD11	1.99	0.45
1:O:158:LEU:HD12	1:O:225:ILE:HD11	1.99	0.45
1:S:97:ILE:HB	1:S:101:PHE:HB3	1.99	0.45
1:W:97:ILE:HB	1:W:101:PHE:HB3	1.99	0.45
1:EA:158:LEU:HD12	1:EA:225:ILE:HD11	1.99	0.45
1:LA:158:LEU:HD12	1:LA:225:ILE:HD11	1.99	0.45
1:OB:97:ILE:HB	1:OB:101:PHE:HB3	1.99	0.45
1:PB:158:LEU:HD12	1:PB:225:ILE:HD11	1.99	0.45
1:ZB:97:ILE:HB	1:ZB:101:PHE:HB3	1.99	0.45
1:HA:97:ILE:HB	1:HA:101:PHE:HB3	1.99	0.45
1:DB:158:LEU:HD12	1:DB:225:ILE:HD11	1.99	0.45
1:LB:97:ILE:HB	1:LB:101:PHE:HB3	1.99	0.45
1:YB:97:ILE:HB	1:YB:101:PHE:HB3	1.99	0.45
1:AC:97:ILE:HB	1:AC:101:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:158:LEU:HD12	1:K:225:ILE:HD11	1.99	0.44
1:GA:97:ILE:HB	1:GA:101:PHE:HB3	1.99	0.44
1:IA:97:ILE:HB	1:IA:101:PHE:HB3	1.99	0.44
1:IA:158:LEU:HD12	1:IA:225:ILE:HD11	1.99	0.44
1:JA:97:ILE:HB	1:JA:101:PHE:HB3	1.99	0.44
1:VA:158:LEU:HD12	1:VA:225:ILE:HD11	1.99	0.44
1:WA:158:LEU:HD12	1:WA:225:ILE:HD11	1.99	0.44
1:HB:158:LEU:HD12	1:HB:225:ILE:HD11	1.99	0.44
1:OB:158:LEU:HD12	1:OB:225:ILE:HD11	1.99	0.44
1:PB:97:ILE:HB	1:PB:101:PHE:HB3	1.99	0.44
1:SB:97:ILE:HB	1:SB:101:PHE:HB3	1.99	0.44
1:BC:97:ILE:HB	1:BC:101:PHE:HB3	1.99	0.44
1:DC:158:LEU:HD12	1:DC:225:ILE:HD11	1.99	0.44
1:C:158:LEU:HD12	1:C:225:ILE:HD11	1.99	0.44
1:X:97:ILE:HB	1:X:101:PHE:HB3	1.99	0.44
1:Z:97:ILE:HB	1:Z:101:PHE:HB3	1.99	0.44
1:AA:97:ILE:HB	1:AA:101:PHE:HB3	1.99	0.44
1:BA:97:ILE:HB	1:BA:101:PHE:HB3	1.99	0.44
1:EA:97:ILE:HB	1:EA:101:PHE:HB3	1.99	0.44
1:FA:97:ILE:HB	1:FA:101:PHE:HB3	1.99	0.44
1:RB:97:ILE:HB	1:RB:101:PHE:HB3	1.99	0.44
1:TB:97:ILE:HB	1:TB:101:PHE:HB3	1.99	0.44
1:UB:97:ILE:HB	1:UB:101:PHE:HB3	1.99	0.44
1:XB:97:ILE:HB	1:XB:101:PHE:HB3	1.99	0.44
1:ZB:158:LEU:HD12	1:ZB:225:ILE:HD11	1.99	0.44
1:AC:158:LEU:HD12	1:AC:225:ILE:HD11	1.99	0.44
1:A:158:LEU:HD12	1:A:225:ILE:HD11	1.99	0.44
1:W:158:LEU:HD12	1:W:225:ILE:HD11	1.99	0.44
1:Y:97:ILE:HB	1:Y:101:PHE:HB3	1.99	0.44
1:CA:97:ILE:HB	1:CA:101:PHE:HB3	1.99	0.44
1:FA:158:LEU:HD12	1:FA:225:ILE:HD11	1.99	0.44
1:HA:158:LEU:HD12	1:HA:225:ILE:HD11	1.99	0.44
1:WB:97:ILE:HB	1:WB:101:PHE:HB3	1.99	0.44
1:L:158:LEU:HD12	1:L:225:ILE:HD11	1.99	0.44
1:T:158:LEU:HD12	1:T:225:ILE:HD11	1.99	0.44
1:YA:158:LEU:HD12	1:YA:225:ILE:HD11	1.99	0.44
1:GB:158:LEU:HD12	1:GB:225:ILE:HD11	1.99	0.44
1:QB:97:ILE:HB	1:QB:101:PHE:HB3	1.99	0.44
1:CC:158:LEU:HD12	1:CC:225:ILE:HD11	1.99	0.44
1:F:158:LEU:HD12	1:F:225:ILE:HD11	1.99	0.44
1:CA:11:ARG:HE	1:DA:206:ARG:HH12	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:TA:158:LEU:HD12	1:TA:225:ILE:HD11	1.99	0.44
1:EB:158:LEU:HD12	1:EB:225:ILE:HD11	1.99	0.44
1:MB:158:LEU:HD12	1:MB:225:ILE:HD11	1.99	0.44
1:RB:1:MET:HE1	1:RB:173:LEU:HB3	2.00	0.44
1:RB:158:LEU:HD12	1:RB:225:ILE:HD11	1.99	0.44
1:VB:97:ILE:HB	1:VB:101:PHE:HB3	1.99	0.44
1:XB:158:LEU:HD12	1:XB:225:ILE:HD11	1.99	0.44
1:N:158:LEU:HD12	1:N:225:ILE:HD11	1.99	0.44
1:Z:1:MET:HE1	1:Z:173:LEU:HB3	2.00	0.44
1:CA:158:LEU:HD12	1:CA:225:ILE:HD11	1.99	0.44
1:DA:97:ILE:HB	1:DA:101:PHE:HB3	1.99	0.44
1:KA:158:LEU:HD12	1:KA:225:ILE:HD11	1.99	0.44
1:Z:158:LEU:HD12	1:Z:225:ILE:HD11	1.99	0.44
1:FC:158:LEU:HD12	1:FC:225:ILE:HD11	1.99	0.44
1:UB:158:LEU:HD12	1:UB:225:ILE:HD11	1.99	0.44
1:I:158:LEU:HD12	1:I:225:ILE:HD11	1.99	0.44
1:T:44:LEU:HB3	1:T:47:CYS:HB2	2.00	0.44
1:QA:158:LEU:HD12	1:QA:225:ILE:HD11	1.99	0.44
1:YA:11:ARG:HE	1:ZA:206:ARG:HH12	1.64	0.44
1:MB:44:LEU:HB3	1:MB:47:CYS:HB2	2.00	0.44
1:Q:44:LEU:HB3	1:Q:47:CYS:HB2	2.00	0.43
1:V:44:LEU:HB3	1:V:47:CYS:HB2	2.00	0.43
1:X:44:LEU:HB3	1:X:47:CYS:HB2	2.00	0.43
1:JB:44:LEU:HB3	1:JB:47:CYS:HB2	2.00	0.43
1:LB:44:LEU:HB3	1:LB:47:CYS:HB2	2.00	0.43
1:PB:44:LEU:HB3	1:PB:47:CYS:HB2	2.00	0.43
1:Q:158:LEU:HD12	1:Q:225:ILE:HD11	1.99	0.43
1:NA:158:LEU:HD12	1:NA:225:ILE:HD11	1.99	0.43
1:BB:158:LEU:HD12	1:BB:225:ILE:HD11	1.99	0.43
1:IB:44:LEU:HB3	1:IB:47:CYS:HB2	2.00	0.43
1:JB:158:LEU:HD12	1:JB:225:ILE:HD11	1.99	0.43
1:IC:158:LEU:HD12	1:IC:225:ILE:HD11	1.99	0.43
1:N:44:LEU:HB3	1:N:47:CYS:HB2	2.00	0.43
1:O:11:ARG:HE	1:P:206:ARG:HH12	1.66	0.43
1:R:44:LEU:HB3	1:R:47:CYS:HB2	2.00	0.43
1:S:11:ARG:HE	1:T:206:ARG:HH12	1.66	0.43
1:S:44:LEU:HB3	1:S:47:CYS:HB2	2.00	0.43
1:Y:44:LEU:HB3	1:Y:47:CYS:HB2	2.00	0.43
1:NB:44:LEU:HB3	1:NB:47:CYS:HB2	2.00	0.43
1:OB:44:LEU:HB3	1:OB:47:CYS:HB2	2.00	0.43
1:QB:44:LEU:HB3	1:QB:47:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:44:LEU:HB3	1:P:47:CYS:HB2	2.00	0.43
1:AA:44:LEU:HB3	1:AA:47:CYS:HB2	2.00	0.43
1:OA:11:ARG:HE	1:PA:206:ARG:HH12	1.65	0.43
1:FB:44:LEU:HB3	1:FB:47:CYS:HB2	2.00	0.43
1:GB:44:LEU:HB3	1:GB:47:CYS:HB2	2.00	0.43
1:KB:44:LEU:HB3	1:KB:47:CYS:HB2	2.00	0.43
1:SB:44:LEU:HB3	1:SB:47:CYS:HB2	2.00	0.43
1:G:11:ARG:HE	1:H:206:ARG:HH12	1.66	0.43
1:M:44:LEU:HB3	1:M:47:CYS:HB2	2.00	0.43
1:W:44:LEU:HB3	1:W:47:CYS:HB2	2.00	0.43
1:BA:44:LEU:HB3	1:BA:47:CYS:HB2	2.00	0.43
1:NA:1:MET:HE1	1:NA:173:LEU:HB3	2.00	0.43
1:OA:44:LEU:HB3	1:OA:47:CYS:HB2	2.00	0.43
1:RB:44:LEU:HB3	1:RB:47:CYS:HB2	2.00	0.43
1:GC:44:LEU:HB3	1:GC:47:CYS:HB2	2.00	0.43
1:JC:44:LEU:HB3	1:JC:47:CYS:HB2	2.00	0.43
1:K:44:LEU:HB3	1:K:47:CYS:HB2	2.00	0.43
1:O:44:LEU:HB3	1:O:47:CYS:HB2	2.00	0.43
1:Q:11:ARG:HE	1:R:206:ARG:HH12	1.66	0.43
1:Z:44:LEU:HB3	1:Z:47:CYS:HB2	2.00	0.43
1:RA:44:LEU:HB3	1:RA:47:CYS:HB2	2.00	0.43
1:DB:44:LEU:HB3	1:DB:47:CYS:HB2	2.00	0.43
1:HB:44:LEU:HB3	1:HB:47:CYS:HB2	2.00	0.43
1:TB:44:LEU:HB3	1:TB:47:CYS:HB2	2.00	0.43
1:DC:44:LEU:HB3	1:DC:47:CYS:HB2	2.00	0.43
1:A:44:LEU:HB3	1:A:47:CYS:HB2	2.00	0.43
1:CA:44:LEU:HB3	1:CA:47:CYS:HB2	2.00	0.43
1:LA:44:LEU:HB3	1:LA:47:CYS:HB2	2.00	0.43
1:QA:44:LEU:HB3	1:QA:47:CYS:HB2	2.00	0.43
1:TA:44:LEU:HB3	1:TA:47:CYS:HB2	2.00	0.43
1:CB:44:LEU:HB3	1:CB:47:CYS:HB2	2.00	0.43
1:VB:11:ARG:HE	1:WB:206:ARG:HH12	1.65	0.43
1:E:11:ARG:HE	1:F:206:ARG:HH12	1.66	0.43
1:I:62:ILE:HD12	1:I:62:ILE:HA	1.94	0.43
1:J:44:LEU:HB3	1:J:47:CYS:HB2	2.00	0.43
1:LB:11:ARG:HE	1:MB:206:ARG:HH12	1.65	0.43
1:VB:44:LEU:HB3	1:VB:47:CYS:HB2	2.00	0.43
1:B:44:LEU:HB3	1:B:47:CYS:HB2	2.00	0.43
1:C:62:ILE:HD12	1:C:62:ILE:HA	1.94	0.43
1:D:44:LEU:HB3	1:D:47:CYS:HB2	2.00	0.43
1:L:44:LEU:HB3	1:L:47:CYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DA:44:LEU:HB3	1:DA:47:CYS:HB2	2.00	0.43
1:EA:44:LEU:HB3	1:EA:47:CYS:HB2	2.00	0.43
1:UA:44:LEU:HB3	1:UA:47:CYS:HB2	2.00	0.43
1:WA:44:LEU:HB3	1:WA:47:CYS:HB2	2.00	0.43
1:EB:44:LEU:HB3	1:EB:47:CYS:HB2	2.00	0.43
1:UB:44:LEU:HB3	1:UB:47:CYS:HB2	2.00	0.43
1:WB:44:LEU:HB3	1:WB:47:CYS:HB2	2.00	0.43
1:IC:44:LEU:HB3	1:IC:47:CYS:HB2	2.00	0.43
1:NA:44:LEU:HB3	1:NA:47:CYS:HB2	2.00	0.43
1:BB:62:ILE:HD12	1:BB:62:ILE:HA	1.94	0.43
1:H:44:LEU:HB3	1:H:47:CYS:HB2	2.00	0.42
1:EA:11:ARG:HE	1:FA:206:ARG:HH12	1.65	0.42
1:IA:44:LEU:HB3	1:IA:47:CYS:HB2	2.00	0.42
1:AB:44:LEU:HB3	1:AB:47:CYS:HB2	2.00	0.42
1:AC:44:LEU:HB3	1:AC:47:CYS:HB2	2.00	0.42
1:FC:44:LEU:HB3	1:FC:47:CYS:HB2	2.00	0.42
1:VA:62:ILE:HD12	1:VA:62:ILE:HA	1.94	0.42
1:EC:44:LEU:HB3	1:EC:47:CYS:HB2	2.00	0.42
1:I:44:LEU:HB3	1:I:47:CYS:HB2	2.00	0.42
1:M:11:ARG:HE	1:N:206:ARG:HH12	1.67	0.42
1:FA:44:LEU:HB3	1:FA:47:CYS:HB2	2.00	0.42
1:KA:11:ARG:HE	1:LA:206:ARG:HH12	1.66	0.42
1:MA:44:LEU:HB3	1:MA:47:CYS:HB2	2.00	0.42
1:ZA:44:LEU:HB3	1:ZA:47:CYS:HB2	2.00	0.42
1:AB:11:ARG:HE	1:BB:206:ARG:HH12	1.66	0.42
1:BB:44:LEU:HB3	1:BB:47:CYS:HB2	2.00	0.42
1:YB:44:LEU:HB3	1:YB:47:CYS:HB2	2.00	0.42
1:BC:44:LEU:HB3	1:BC:47:CYS:HB2	2.00	0.42
1:G:44:LEU:HB3	1:G:47:CYS:HB2	2.00	0.42
1:I:11:ARG:HE	1:J:206:ARG:HH12	1.67	0.42
1:GA:44:LEU:HB3	1:GA:47:CYS:HB2	2.00	0.42
1:HA:44:LEU:HB3	1:HA:47:CYS:HB2	2.00	0.42
1:JA:44:LEU:HB3	1:JA:47:CYS:HB2	2.00	0.42
1:XA:44:LEU:HB3	1:XA:47:CYS:HB2	2.00	0.42
1:FB:62:ILE:HD12	1:FB:62:ILE:HA	1.94	0.42
1:XB:44:LEU:HB3	1:XB:47:CYS:HB2	2.00	0.42
1:HC:44:LEU:HB3	1:HC:47:CYS:HB2	2.00	0.42
1:E:44:LEU:HB3	1:E:47:CYS:HB2	2.00	0.42
1:K:11:ARG:HE	1:L:206:ARG:HH12	1.68	0.42
1:M:62:ILE:HD12	1:M:62:ILE:HA	1.94	0.42
1:WA:11:ARG:HE	1:XA:206:ARG:HH12	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:62:ILE:HD12	1:N:62:ILE:HA	1.94	0.42
1:MA:62:ILE:HD12	1:MA:62:ILE:HA	1.94	0.42
1:PA:44:LEU:HB3	1:PA:47:CYS:HB2	2.00	0.42
1:GB:62:ILE:HD12	1:GB:62:ILE:HA	1.94	0.42
1:ZB:44:LEU:HB3	1:ZB:47:CYS:HB2	2.00	0.42
1:EC:11:ARG:HE	1:FC:206:ARG:HH12	1.66	0.42
1:GC:11:ARG:HE	1:HC:206:ARG:HH12	1.66	0.42
1:KA:44:LEU:HB3	1:KA:47:CYS:HB2	2.00	0.42
1:EC:62:ILE:HD12	1:EC:62:ILE:HA	1.94	0.42
1:NA:62:ILE:HD12	1:NA:62:ILE:HA	1.94	0.42
1:YA:44:LEU:HB3	1:YA:47:CYS:HB2	2.00	0.42
1:EB:62:ILE:HD12	1:EB:62:ILE:HA	1.94	0.42
1:F:44:LEU:HB3	1:F:47:CYS:HB2	2.00	0.42
1:S:1:MET:HE1	1:S:173:LEU:HB3	2.02	0.42
1:LA:62:ILE:HD12	1:LA:62:ILE:HA	1.94	0.42
1:CC:44:LEU:HB3	1:CC:47:CYS:HB2	2.00	0.42
1:FC:1:MET:HE1	1:FC:173:LEU:HB3	2.01	0.42
1:FC:62:ILE:HD12	1:FC:62:ILE:HA	1.94	0.42
1:KC:44:LEU:HB3	1:KC:47:CYS:HB2	2.00	0.42
1:C:44:LEU:HB3	1:C:47:CYS:HB2	2.00	0.42
1:P:1:MET:HE1	1:P:173:LEU:HB3	2.02	0.42
1:R:18:LEU:HD12	1:R:18:LEU:HA	1.95	0.42
1:KB:18:LEU:HD12	1:KB:18:LEU:HA	1.95	0.42
1:DC:62:ILE:HD12	1:DC:62:ILE:HA	1.94	0.42
1:L:62:ILE:HD12	1:L:62:ILE:HA	1.94	0.41
1:O:62:ILE:HD12	1:O:62:ILE:HA	1.94	0.41
1:SA:44:LEU:HB3	1:SA:47:CYS:HB2	2.00	0.41
1:VA:44:LEU:HB3	1:VA:47:CYS:HB2	2.00	0.41
1:GA:136:ARG:NH2	1:GA:232:ARG:HD2	2.36	0.41
1:FB:11:ARG:HE	1:GB:206:ARG:HH12	1.68	0.41
1:HB:18:LEU:HD12	1:HB:18:LEU:HA	1.95	0.41
1:RB:11:ARG:HE	1:SB:206:ARG:HH12	1.66	0.41
1:J:62:ILE:HD12	1:J:62:ILE:HA	1.94	0.41
1:O:18:LEU:HD12	1:O:18:LEU:HA	1.95	0.41
1:P:18:LEU:HD12	1:P:18:LEU:HA	1.95	0.41
1:S:136:ARG:NH2	1:S:232:ARG:HD2	2.36	0.41
1:V:11:ARG:HE	1:W:206:ARG:HH12	1.67	0.41
1:V:18:LEU:HD12	1:V:18:LEU:HA	1.95	0.41
1:DB:11:ARG:HE	1:EB:206:ARG:HH12	1.68	0.41
1:IB:18:LEU:HD12	1:IB:18:LEU:HA	1.95	0.41
1:LB:136:ARG:NH2	1:LB:232:ARG:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NB:18:LEU:HD12	1:NB:18:LEU:HA	1.95	0.41
1:UB:136:ARG:NH2	1:UB:232:ARG:HD2	2.36	0.41
1:YB:136:ARG:NH2	1:YB:232:ARG:HD2	2.36	0.41
1:O:136:ARG:NH2	1:O:232:ARG:HD2	2.36	0.41
1:S:18:LEU:HD12	1:S:18:LEU:HA	1.95	0.41
1:X:136:ARG:NH2	1:X:232:ARG:HD2	2.36	0.41
1:Y:136:ARG:NH2	1:Y:232:ARG:HD2	2.36	0.41
1:CA:136:ARG:NH2	1:CA:232:ARG:HD2	2.36	0.41
1:KA:136:ARG:NH2	1:KA:232:ARG:HD2	2.36	0.41
1:OA:62:ILE:HD12	1:OA:62:ILE:HA	1.94	0.41
1:EB:11:ARG:HE	1:FB:206:ARG:HH12	1.67	0.41
1:HB:62:ILE:HD12	1:HB:62:ILE:HA	1.94	0.41
1:HB:136:ARG:NH2	1:HB:232:ARG:HD2	2.36	0.41
1:LB:18:LEU:HD12	1:LB:18:LEU:HA	1.95	0.41
1:MB:136:ARG:NH2	1:MB:232:ARG:HD2	2.36	0.41
1:QB:136:ARG:NH2	1:QB:232:ARG:HD2	2.36	0.41
1:CC:136:ARG:NH2	1:CC:232:ARG:HD2	2.36	0.41
1:T:136:ARG:NH2	1:T:232:ARG:HD2	2.36	0.41
1:W:11:ARG:HE	1:X:206:ARG:HH12	1.68	0.41
1:Y:11:ARG:HE	1:Z:206:ARG:HH12	1.68	0.41
1:BA:136:ARG:NH2	1:BA:232:ARG:HD2	2.36	0.41
1:FA:136:ARG:NH2	1:FA:232:ARG:HD2	2.36	0.41
1:UA:11:ARG:HE	1:VA:206:ARG:HH12	1.67	0.41
1:VA:1:MET:HE1	1:VA:173:LEU:HB3	2.02	0.41
1:AB:136:ARG:NH2	1:AB:232:ARG:HD2	2.36	0.41
1:PB:136:ARG:NH2	1:PB:232:ARG:HD2	2.36	0.41
1:A:136:ARG:NH2	1:A:232:ARG:HD2	2.36	0.41
1:C:136:ARG:NH2	1:C:232:ARG:HD2	2.36	0.41
1:F:136:ARG:NH2	1:F:232:ARG:HD2	2.36	0.41
1:H:136:ARG:NH2	1:H:232:ARG:HD2	2.36	0.41
1:M:18:LEU:HD12	1:M:18:LEU:HA	1.95	0.41
1:IA:11:ARG:HE	1:JA:206:ARG:HH12	1.67	0.41
1:JA:136:ARG:NH2	1:JA:232:ARG:HD2	2.36	0.41
1:TA:136:ARG:NH2	1:TA:232:ARG:HD2	2.36	0.41
1:YA:136:ARG:NH2	1:YA:232:ARG:HD2	2.36	0.41
1:IB:136:ARG:NH2	1:IB:232:ARG:HD2	2.36	0.41
1:TB:136:ARG:NH2	1:TB:232:ARG:HD2	2.36	0.41
1:DC:136:ARG:NH2	1:DC:232:ARG:HD2	2.36	0.41
1:GC:62:ILE:HD12	1:GC:62:ILE:HA	1.94	0.41
1:C:11:ARG:HE	1:D:206:ARG:HH12	1.68	0.41
1:D:42:LYS:HD2	1:D:155:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ILE:HD12	1:D:62:ILE:HA	1.94	0.41
1:I:42:LYS:HD2	1:I:155:ARG:CZ	2.51	0.41
1:P:136:ARG:NH2	1:P:232:ARG:HD2	2.36	0.41
1:W:42:LYS:HD2	1:W:155:ARG:CZ	2.51	0.41
1:BA:42:LYS:HD2	1:BA:155:ARG:CZ	2.51	0.41
1:FA:42:LYS:HD2	1:FA:155:ARG:CZ	2.51	0.41
1:GA:11:ARG:HE	1:HA:206:ARG:HH12	1.67	0.41
1:IA:42:LYS:HD2	1:IA:155:ARG:CZ	2.51	0.41
1:LA:136:ARG:NH2	1:LA:232:ARG:HD2	2.36	0.41
1:OA:136:ARG:NH2	1:OA:232:ARG:HD2	2.36	0.41
1:SA:42:LYS:HD2	1:SA:155:ARG:CZ	2.51	0.41
1:VA:136:ARG:NH2	1:VA:232:ARG:HD2	2.36	0.41
1:WA:42:LYS:HD2	1:WA:155:ARG:CZ	2.51	0.41
1:YA:42:LYS:HD2	1:YA:155:ARG:CZ	2.51	0.41
1:FB:18:LEU:HD12	1:FB:18:LEU:HA	1.95	0.41
1:OB:42:LYS:HD2	1:OB:155:ARG:CZ	2.51	0.41
1:TB:42:LYS:HD2	1:TB:155:ARG:CZ	2.51	0.41
1:XB:42:LYS:HD2	1:XB:155:ARG:CZ	2.51	0.41
1:XB:136:ARG:NH2	1:XB:232:ARG:HD2	2.36	0.41
1:ZB:136:ARG:NH2	1:ZB:232:ARG:HD2	2.36	0.41
1:AC:42:LYS:HD2	1:AC:155:ARG:CZ	2.51	0.41
1:BC:136:ARG:NH2	1:BC:232:ARG:HD2	2.36	0.41
1:CC:62:ILE:HD12	1:CC:62:ILE:HA	1.94	0.41
1:GC:136:ARG:NH2	1:GC:232:ARG:HD2	2.36	0.41
1:HC:136:ARG:NH2	1:HC:232:ARG:HD2	2.36	0.41
1:KC:42:LYS:HD2	1:KC:155:ARG:CZ	2.51	0.41
1:F:42:LYS:HD2	1:F:155:ARG:CZ	2.51	0.41
1:J:136:ARG:NH2	1:J:232:ARG:HD2	2.36	0.41
1:K:136:ARG:NH2	1:K:232:ARG:HD2	2.36	0.41
1:Z:42:LYS:HD2	1:Z:155:ARG:CZ	2.51	0.41
1:HA:136:ARG:NH2	1:HA:232:ARG:HD2	2.36	0.41
1:LA:42:LYS:HD2	1:LA:155:ARG:CZ	2.51	0.41
1:PA:42:LYS:HD2	1:PA:155:ARG:CZ	2.51	0.41
1:PA:136:ARG:NH2	1:PA:232:ARG:HD2	2.36	0.41
1:TA:206:ARG:HH12	1:KC:11:ARG:HE	1.68	0.41
1:BB:42:LYS:HD2	1:BB:155:ARG:CZ	2.51	0.41
1:CB:11:ARG:HE	1:DB:206:ARG:HH12	1.67	0.41
1:CB:62:ILE:HD12	1:CB:62:ILE:HA	1.94	0.41
1:DB:62:ILE:HD12	1:DB:62:ILE:HA	1.94	0.41
1:DB:136:ARG:NH2	1:DB:232:ARG:HD2	2.36	0.41
1:JB:18:LEU:HD12	1:JB:18:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:MB:18:LEU:HD12	1:MB:18:LEU:HA	1.95	0.41
1:WB:42:LYS:HD2	1:WB:155:ARG:CZ	2.51	0.41
1:DC:42:LYS:HD2	1:DC:155:ARG:CZ	2.51	0.41
1:HC:42:LYS:HD2	1:HC:155:ARG:CZ	2.51	0.41
1:JC:136:ARG:NH2	1:JC:232:ARG:HD2	2.36	0.41
1:A:42:LYS:HD2	1:A:155:ARG:CZ	2.51	0.41
1:C:42:LYS:HD2	1:C:155:ARG:CZ	2.51	0.41
1:E:136:ARG:NH2	1:E:232:ARG:HD2	2.36	0.41
1:G:42:LYS:HD2	1:G:155:ARG:CZ	2.51	0.41
1:H:42:LYS:HD2	1:H:155:ARG:CZ	2.51	0.41
1:K:42:LYS:HD2	1:K:155:ARG:CZ	2.51	0.41
1:L:18:LEU:HD12	1:L:18:LEU:HA	1.95	0.41
1:M:136:ARG:NH2	1:M:232:ARG:HD2	2.36	0.41
1:N:42:LYS:HD2	1:N:155:ARG:CZ	2.51	0.41
1:N:136:ARG:NH2	1:N:232:ARG:HD2	2.36	0.41
1:Q:18:LEU:HD12	1:Q:18:LEU:HA	1.95	0.41
1:Q:42:LYS:HD2	1:Q:155:ARG:CZ	2.51	0.41
1:R:136:ARG:NH2	1:R:232:ARG:HD2	2.36	0.41
1:S:42:LYS:HD2	1:S:155:ARG:CZ	2.51	0.41
1:T:18:LEU:HD12	1:T:18:LEU:HA	1.95	0.41
1:W:18:LEU:HD12	1:W:18:LEU:HA	1.95	0.41
1:W:136:ARG:NH2	1:W:232:ARG:HD2	2.36	0.41
1:X:11:ARG:HE	1:Y:206:ARG:HH12	1.67	0.41
1:X:42:LYS:HD2	1:X:155:ARG:CZ	2.51	0.41
1:Y:42:LYS:HD2	1:Y:155:ARG:CZ	2.51	0.41
1:CA:42:LYS:HD2	1:CA:155:ARG:CZ	2.51	0.41
1:EA:42:LYS:HD2	1:EA:155:ARG:CZ	2.51	0.41
1:KA:1:MET:HE1	1:KA:173:LEU:HB3	2.02	0.41
1:KA:62:ILE:HD12	1:KA:62:ILE:HA	1.94	0.41
1:MA:42:LYS:HD2	1:MA:155:ARG:CZ	2.51	0.41
1:QA:11:ARG:HE	1:RA:206:ARG:HH12	1.67	0.41
1:QA:136:ARG:NH2	1:QA:232:ARG:HD2	2.36	0.41
1:RA:136:ARG:NH2	1:RA:232:ARG:HD2	2.36	0.41
1:TA:42:LYS:HD2	1:TA:155:ARG:CZ	2.51	0.41
1:VA:42:LYS:HD2	1:VA:155:ARG:CZ	2.51	0.41
1:WA:62:ILE:HD12	1:WA:62:ILE:HA	1.94	0.41
1:WA:136:ARG:NH2	1:WA:232:ARG:HD2	2.36	0.41
1:XA:235:SER:O	1:YA:149:ARG:NH1	2.51	0.41
1:ZA:42:LYS:HD2	1:ZA:155:ARG:CZ	2.51	0.41
1:AB:42:LYS:HD2	1:AB:155:ARG:CZ	2.51	0.41
1:CB:136:ARG:NH2	1:CB:232:ARG:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:42:LYS:HD2	1:DB:155:ARG:CZ	2.51	0.41
1:EB:18:LEU:HD12	1:EB:18:LEU:HA	1.95	0.41
1:FB:136:ARG:NH2	1:FB:232:ARG:HD2	2.36	0.41
1:GB:11:ARG:HE	1:HB:206:ARG:HH12	1.68	0.41
1:GB:42:LYS:HD2	1:GB:155:ARG:CZ	2.51	0.41
1:GB:136:ARG:NH2	1:GB:232:ARG:HD2	2.36	0.41
1:JB:42:LYS:HD2	1:JB:155:ARG:CZ	2.51	0.41
1:KB:136:ARG:NH2	1:KB:232:ARG:HD2	2.36	0.41
1:LB:42:LYS:HD2	1:LB:155:ARG:CZ	2.51	0.41
1:NB:11:ARG:HE	1:OB:206:ARG:HH12	1.67	0.41
1:OB:18:LEU:HD12	1:OB:18:LEU:HA	1.95	0.41
1:PB:42:LYS:HD2	1:PB:155:ARG:CZ	2.51	0.41
1:QB:42:LYS:HD2	1:QB:155:ARG:CZ	2.51	0.41
1:RB:42:LYS:HD2	1:RB:155:ARG:CZ	2.51	0.41
1:SB:136:ARG:NH2	1:SB:232:ARG:HD2	2.36	0.41
1:UB:18:LEU:HD13	1:VB:25:ASN:ND2	2.36	0.41
1:UB:42:LYS:HD2	1:UB:155:ARG:CZ	2.51	0.41
1:VB:136:ARG:NH2	1:VB:232:ARG:HD2	2.36	0.41
1:CC:11:ARG:HE	1:DC:206:ARG:HH12	1.68	0.41
1:EC:42:LYS:HD2	1:EC:155:ARG:CZ	2.51	0.41
1:GC:42:LYS:HD2	1:GC:155:ARG:CZ	2.51	0.41
1:IC:11:ARG:HE	1:JC:206:ARG:HH12	1.67	0.41
1:D:136:ARG:NH2	1:D:232:ARG:HD2	2.36	0.41
1:K:62:ILE:HD12	1:K:62:ILE:HA	1.94	0.41
1:L:42:LYS:HD2	1:L:155:ARG:CZ	2.51	0.41
1:T:42:LYS:HD2	1:T:155:ARG:CZ	2.51	0.41
1:Y:18:LEU:HD12	1:Y:18:LEU:HA	1.95	0.41
1:AA:136:ARG:NH2	1:AA:232:ARG:HD2	2.36	0.41
1:DA:42:LYS:HD2	1:DA:155:ARG:CZ	2.51	0.41
1:DA:136:ARG:NH2	1:DA:232:ARG:HD2	2.36	0.41
1:JA:42:LYS:HD2	1:JA:155:ARG:CZ	2.51	0.41
1:NA:18:LEU:HD13	1:OA:25:ASN:ND2	2.36	0.41
1:NA:136:ARG:NH2	1:NA:232:ARG:HD2	2.36	0.41
1:OA:42:LYS:HD2	1:OA:155:ARG:CZ	2.51	0.41
1:XA:136:ARG:NH2	1:XA:232:ARG:HD2	2.36	0.41
1:HB:42:LYS:HD2	1:HB:155:ARG:CZ	2.51	0.41
1:LB:1:MET:HE1	1:LB:173:LEU:HB3	2.03	0.41
1:MB:42:LYS:HD2	1:MB:155:ARG:CZ	2.51	0.41
1:QB:18:LEU:HD12	1:QB:18:LEU:HA	1.95	0.41
1:RB:136:ARG:NH2	1:RB:232:ARG:HD2	2.36	0.41
1:VB:42:LYS:HD2	1:VB:155:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XB:11:ARG:HE	1:YB:206:ARG:HH12	1.67	0.41
1:BC:42:LYS:HD2	1:BC:155:ARG:CZ	2.51	0.41
1:EC:136:ARG:NH2	1:EC:232:ARG:HD2	2.36	0.41
1:IC:136:ARG:NH2	1:IC:232:ARG:HD2	2.36	0.41
1:JC:42:LYS:HD2	1:JC:155:ARG:CZ	2.51	0.41
1:B:42:LYS:HD2	1:B:155:ARG:CZ	2.51	0.40
1:H:1:MET:HE1	1:H:173:LEU:HB3	2.03	0.40
1:O:42:LYS:HD2	1:O:155:ARG:CZ	2.51	0.40
1:P:42:LYS:HD2	1:P:155:ARG:CZ	2.51	0.40
1:GA:42:LYS:HD2	1:GA:155:ARG:CZ	2.51	0.40
1:MA:136:ARG:NH2	1:MA:232:ARG:HD2	2.36	0.40
1:NA:11:ARG:HE	1:OA:206:ARG:HH12	1.68	0.40
1:RA:42:LYS:HD2	1:RA:155:ARG:CZ	2.51	0.40
1:EB:42:LYS:HD2	1:EB:155:ARG:CZ	2.51	0.40
1:EB:136:ARG:NH2	1:EB:232:ARG:HD2	2.36	0.40
1:NB:136:ARG:NH2	1:NB:232:ARG:HD2	2.36	0.40
1:PB:18:LEU:HD12	1:PB:18:LEU:HA	1.95	0.40
1:SB:42:LYS:HD2	1:SB:155:ARG:CZ	2.51	0.40
1:YB:42:LYS:HD2	1:YB:155:ARG:CZ	2.51	0.40
1:ZB:42:LYS:HD2	1:ZB:155:ARG:CZ	2.51	0.40
1:E:42:LYS:HD2	1:E:155:ARG:CZ	2.51	0.40
1:L:136:ARG:NH2	1:L:232:ARG:HD2	2.36	0.40
1:P:62:ILE:HD12	1:P:62:ILE:HA	1.94	0.40
1:S:207:LYS:HE3	1:S:207:LYS:HB2	1.88	0.40
1:V:136:ARG:NH2	1:V:232:ARG:HD2	2.36	0.40
1:W:1:MET:HE1	1:W:173:LEU:HB3	2.03	0.40
1:X:18:LEU:HD12	1:X:18:LEU:HA	1.95	0.40
1:Z:136:ARG:NH2	1:Z:232:ARG:HD2	2.36	0.40
1:AA:42:LYS:HD2	1:AA:155:ARG:CZ	2.51	0.40
1:HA:42:LYS:HD2	1:HA:155:ARG:CZ	2.51	0.40
1:QA:42:LYS:HD2	1:QA:155:ARG:CZ	2.51	0.40
1:UA:42:LYS:HD2	1:UA:155:ARG:CZ	2.51	0.40
1:UA:136:ARG:NH2	1:UA:232:ARG:HD2	2.36	0.40
1:GB:18:LEU:HD12	1:GB:18:LEU:HA	1.95	0.40
1:HB:11:ARG:HE	1:IB:206:ARG:HH12	1.69	0.40
1:IB:42:LYS:HD2	1:IB:155:ARG:CZ	2.51	0.40
1:OB:136:ARG:NH2	1:OB:232:ARG:HD2	2.36	0.40
1:PB:11:ARG:HE	1:QB:206:ARG:HH12	1.67	0.40
1:B:136:ARG:NH2	1:B:232:ARG:HD2	2.36	0.40
1:J:18:LEU:HD12	1:J:18:LEU:HA	1.95	0.40
1:SA:136:ARG:NH2	1:SA:232:ARG:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:42:LYS:HD2	1:XA:155:ARG:CZ	2.51	0.40
1:ZA:136:ARG:NH2	1:ZA:232:ARG:HD2	2.36	0.40
1:CB:18:LEU:HD12	1:CB:18:LEU:HA	1.95	0.40
1:IB:62:ILE:HD12	1:IB:62:ILE:HA	1.94	0.40
1:JB:136:ARG:NH2	1:JB:232:ARG:HD2	2.36	0.40
1:OB:11:ARG:HE	1:PB:206:ARG:HH12	1.69	0.40
1:FC:136:ARG:NH2	1:FC:232:ARG:HD2	2.36	0.40
1:IC:42:LYS:HD2	1:IC:155:ARG:CZ	2.51	0.40
1:G:136:ARG:NH2	1:G:232:ARG:HD2	2.36	0.40
1:N:18:LEU:HD12	1:N:18:LEU:HA	1.95	0.40
1:AA:18:LEU:HD13	1:BA:25:ASN:ND2	2.37	0.40
1:EA:136:ARG:NH2	1:EA:232:ARG:HD2	2.36	0.40
1:FB:229:ARG:HD3	1:FB:229:ARG:HA	1.94	0.40
1:UB:17:SER:HB2	1:VB:54:ARG:HH21	1.87	0.40
1:JC:158:LEU:HD23	1:JC:158:LEU:HA	1.94	0.40
1:KC:136:ARG:NH2	1:KC:232:ARG:HD2	2.36	0.40
1:B:11:ARG:HE	1:C:206:ARG:HH12	1.69	0.40
1:I:136:ARG:NH2	1:I:232:ARG:HD2	2.36	0.40
1:Q:136:ARG:NH2	1:Q:232:ARG:HD2	2.36	0.40
1:IA:136:ARG:NH2	1:IA:232:ARG:HD2	2.36	0.40
1:KA:42:LYS:HD2	1:KA:155:ARG:CZ	2.51	0.40
1:OA:158:LEU:HD23	1:OA:158:LEU:HA	1.94	0.40
1:PA:62:ILE:HD12	1:PA:62:ILE:HA	1.94	0.40
1:BB:136:ARG:NH2	1:BB:232:ARG:HD2	2.36	0.40
1:UB:11:ARG:HE	1:VB:206:ARG:HH12	1.68	0.40
1:AC:136:ARG:NH2	1:AC:232:ARG:HD2	2.36	0.40
1:CC:42:LYS:HD2	1:CC:155:ARG:CZ	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	AA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	AB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	AC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	B	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	BA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	BB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	BC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	C	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	CA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	CB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	CC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	D	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	DA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	DB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	DC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	E	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	EA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	EB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	EC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	F	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	FA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	FB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	FC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	G	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	GA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	GB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	GC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	H	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	HA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	HB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	HC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	IA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	IB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	IC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	J	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	JA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	JB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	JC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	K	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	KA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	KB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	KC	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	L	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	LA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	LB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	M	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	MA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	MB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	N	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	NA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	NB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	O	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	OA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	OB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	P	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	PA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	PB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	Q	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	QA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	QB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	R	248/254 (98%)	246 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	RA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	RB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	S	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	SA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	SB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	T	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	TA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	TB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	UA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	UB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	V	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	VA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	VB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	W	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	WA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	WB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	X	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	XA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	XB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	Y	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	YA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	YB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	Z	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	ZA	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
1	ZB	248/254 (98%)	246 (99%)	2 (1%)	0	100	100
All	All	21824/22352 (98%)	21648 (99%)	176 (1%)	0	100	100

There are no Ramachandran outliers to report.

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

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	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	AA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	AB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	AC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	B	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	BA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	BB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	BC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	C	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	CA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	CB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	CC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	D	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	DA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	DB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	DC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	E	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	EA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	EB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	EC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	F	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	FA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	FB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	FC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	G	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	GA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	GB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	GC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	H	211/215 (98%)	210 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	HA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	HB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	HC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	I	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	IA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	IB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	IC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	J	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	JA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	JB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	JC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	K	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	KA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	KB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	KC	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	L	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	LA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	LB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	M	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	MA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	MB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	N	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	NA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	NB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	O	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	OA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	OB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	P	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	PA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	PB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	Q	211/215 (98%)	210 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	QA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	QB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	R	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	RA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	RB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	S	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	SA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	SB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	T	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	TA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	TB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	UA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	UB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	V	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	VA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	VB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	W	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	WA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	WB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	X	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	XA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	XB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	Y	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	YA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	YB	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	Z	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	ZA	211/215 (98%)	210 (100%)	1 (0%)	88	93
1	ZB	211/215 (98%)	210 (100%)	1 (0%)	88	93
All	All	18568/18920 (98%)	18480 (100%)	88 (0%)	89	93

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
1	B	88	LYS
1	C	88	LYS
1	D	88	LYS
1	E	88	LYS
1	F	88	LYS
1	G	88	LYS
1	H	88	LYS
1	I	88	LYS
1	J	88	LYS
1	K	88	LYS
1	L	88	LYS
1	M	88	LYS
1	N	88	LYS
1	O	88	LYS
1	P	88	LYS
1	Q	88	LYS
1	R	88	LYS
1	S	88	LYS
1	T	88	LYS
1	V	88	LYS
1	W	88	LYS
1	X	88	LYS
1	Y	88	LYS
1	Z	88	LYS
1	AA	88	LYS
1	BA	88	LYS
1	CA	88	LYS
1	DA	88	LYS
1	EA	88	LYS
1	FA	88	LYS
1	GA	88	LYS
1	HA	88	LYS
1	IA	88	LYS
1	JA	88	LYS
1	KA	88	LYS
1	LA	88	LYS
1	MA	88	LYS
1	NA	88	LYS
1	OA	88	LYS
1	PA	88	LYS
1	QA	88	LYS
1	RA	88	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	SA	88	LYS
1	TA	88	LYS
1	UA	88	LYS
1	VA	88	LYS
1	WA	88	LYS
1	XA	88	LYS
1	YA	88	LYS
1	ZA	88	LYS
1	AB	88	LYS
1	BB	88	LYS
1	CB	88	LYS
1	DB	88	LYS
1	EB	88	LYS
1	FB	88	LYS
1	GB	88	LYS
1	HB	88	LYS
1	IB	88	LYS
1	JB	88	LYS
1	KB	88	LYS
1	LB	88	LYS
1	MB	88	LYS
1	NB	88	LYS
1	OB	88	LYS
1	PB	88	LYS
1	QB	88	LYS
1	RB	88	LYS
1	SB	88	LYS
1	TB	88	LYS
1	UB	88	LYS
1	VB	88	LYS
1	WB	88	LYS
1	XB	88	LYS
1	YB	88	LYS
1	ZB	88	LYS
1	AC	88	LYS
1	BC	88	LYS
1	CC	88	LYS
1	DC	88	LYS
1	EC	88	LYS
1	FC	88	LYS
1	GC	88	LYS
1	HC	88	LYS

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Mol	Chain	Res	Type
1	IC	88	LYS
1	JC	88	LYS
1	KC	88	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	25	ASN
1	M	25	ASN
1	O	25	ASN
1	Q	25	ASN
1	S	25	ASN
1	V	25	ASN
1	X	25	ASN
1	Z	25	ASN
1	BA	25	ASN
1	CA	25	ASN
1	DA	25	ASN
1	FA	25	ASN
1	HA	25	ASN
1	IA	25	ASN
1	JA	25	ASN
1	KA	25	ASN
1	MA	25	ASN
1	OA	25	ASN
1	QA	25	ASN
1	SA	25	ASN
1	AB	25	ASN
1	CB	25	ASN
1	GB	25	ASN
1	IB	25	ASN
1	JB	25	ASN
1	MB	25	ASN
1	NB	25	ASN
1	OB	25	ASN
1	PB	25	ASN
1	QB	25	ASN
1	RB	25	ASN
1	TB	25	ASN
1	VB	25	ASN
1	XB	25	ASN
1	ZB	25	ASN

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Mol	Chain	Res	Type
1	AC	25	ASN
1	BC	25	ASN
1	CC	25	ASN
1	GC	25	ASN

### 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 monosaccharides 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.

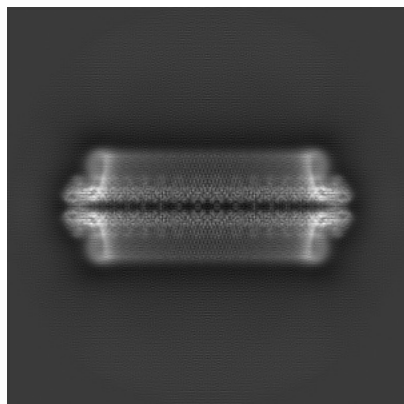
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36732. These allow visual inspection of the internal detail of the map and identification of artifacts.

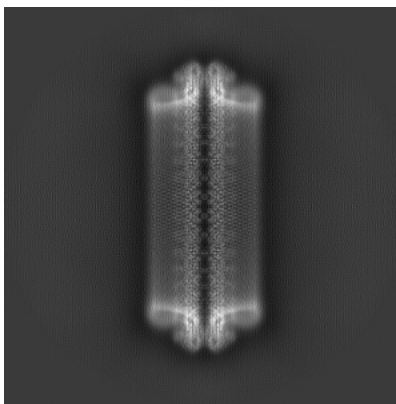
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

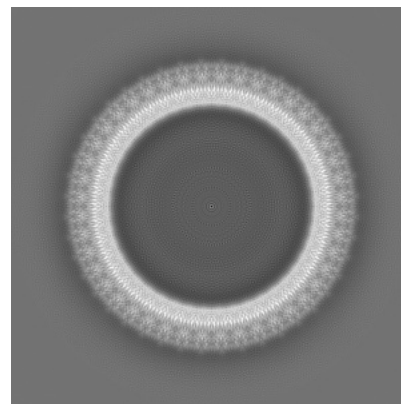
#### 6.1.1 Primary map



X

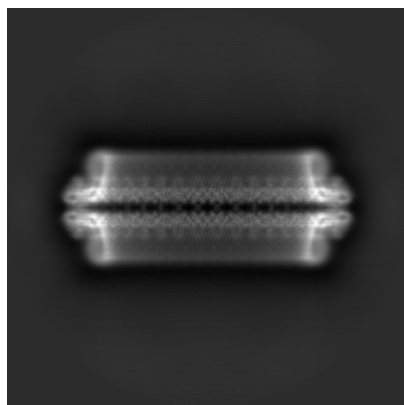


Y

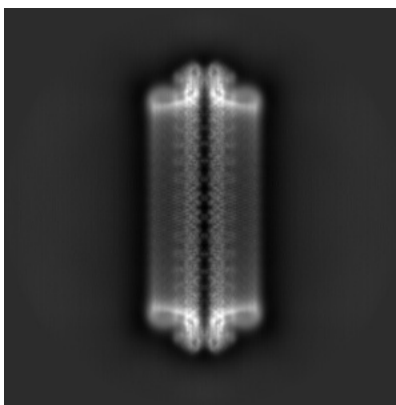


Z

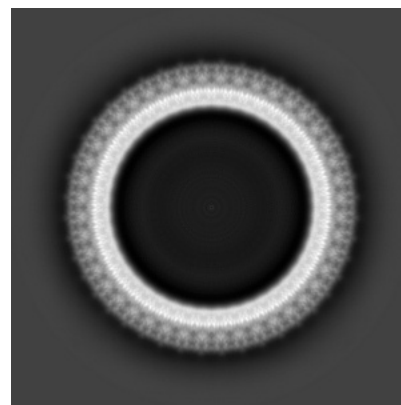
#### 6.1.2 Raw map



X



Y

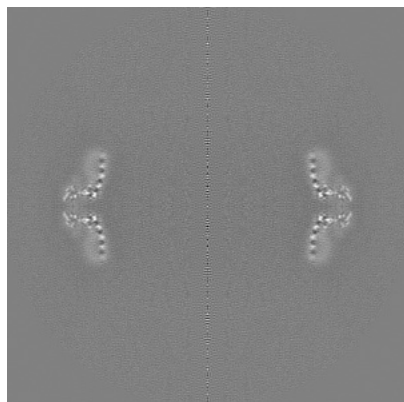


Z

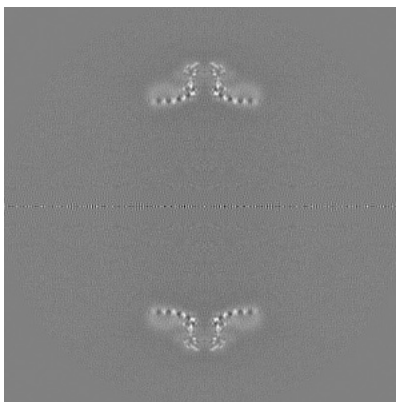
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

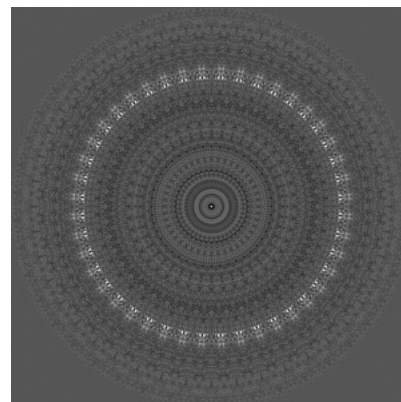
### 6.2.1 Primary map



X Index: 200

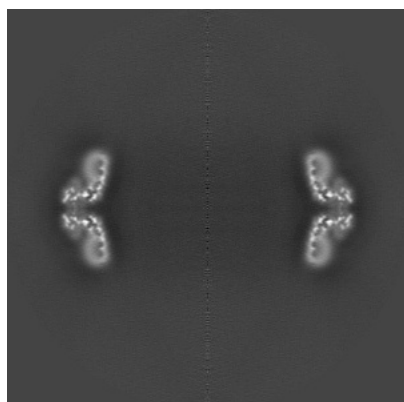


Y Index: 200

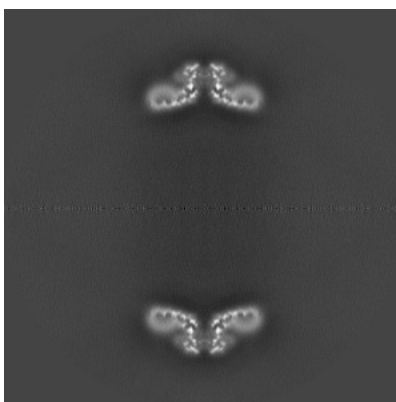


Z Index: 200

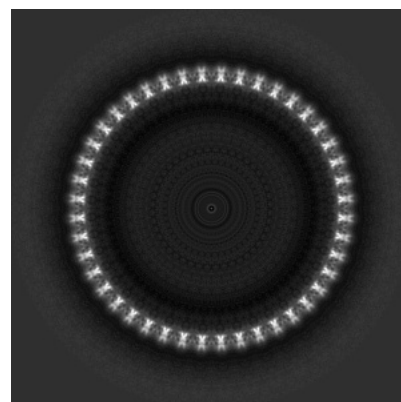
### 6.2.2 Raw map



X Index: 200



Y Index: 200



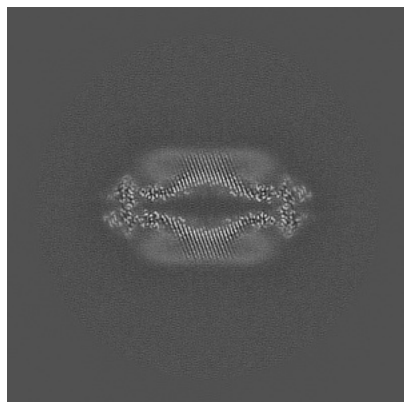
Z Index: 200

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

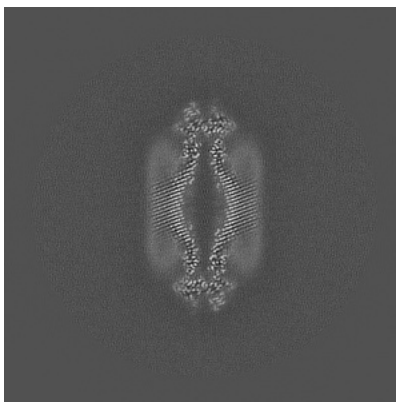


## 6.3 Largest variance slices [i](#)

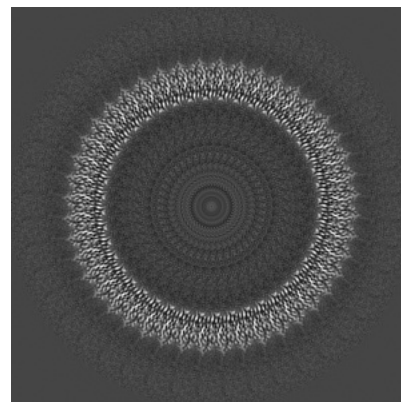
### 6.3.1 Primary map



X Index: 95

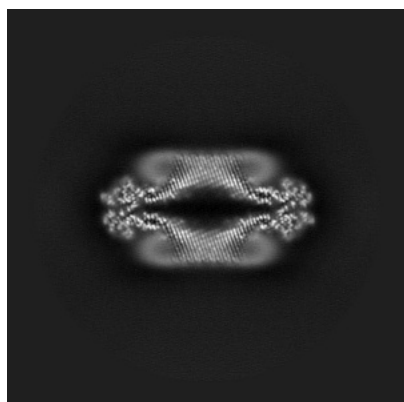


Y Index: 95

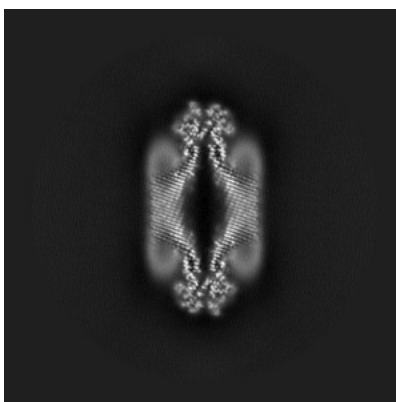


Z Index: 214

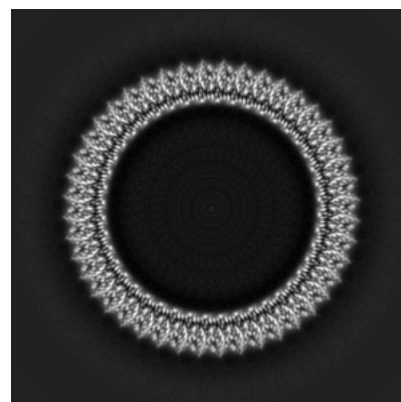
### 6.3.2 Raw map



X Index: 97



Y Index: 303

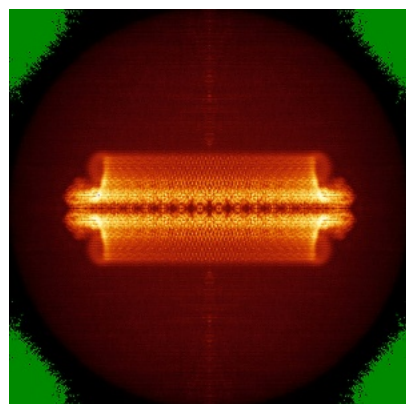


Z Index: 186

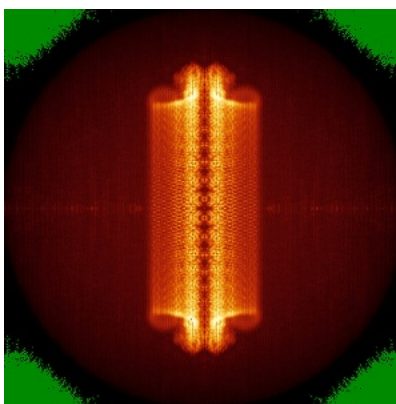
The images above show the largest variance slices of the map in three orthogonal directions.

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

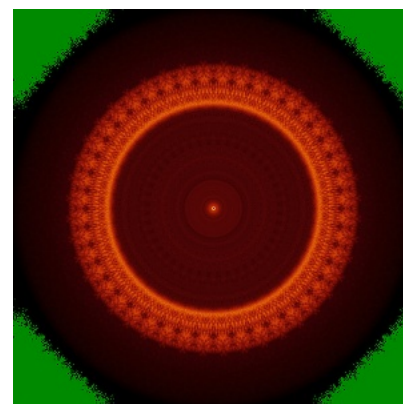
### 6.4.1 Primary map



X

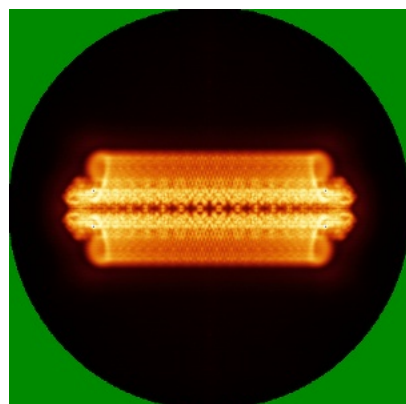


Y

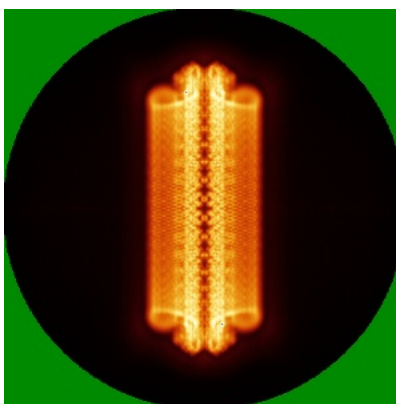


Z

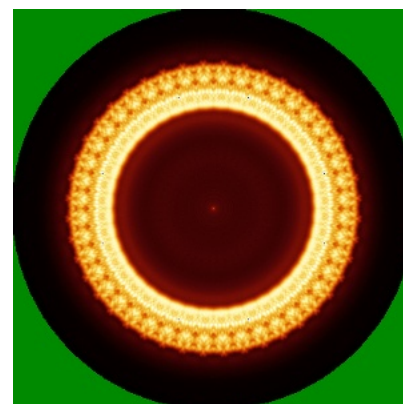
### 6.4.2 Raw map



X



Y

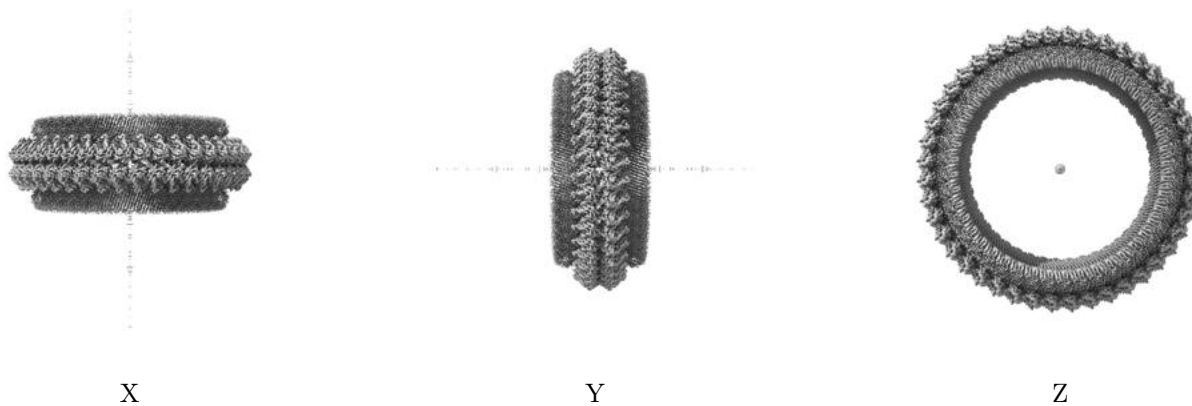


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

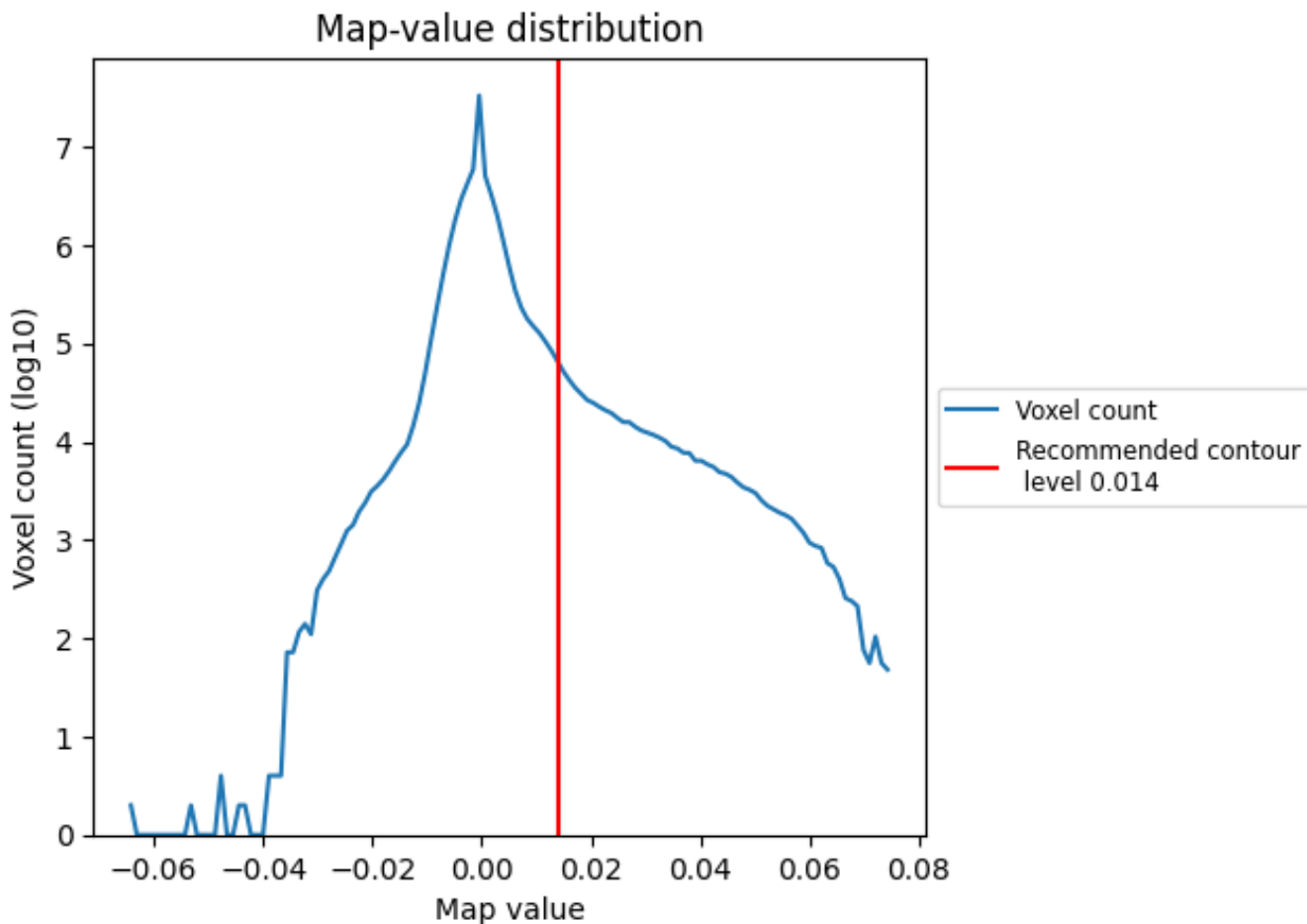
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

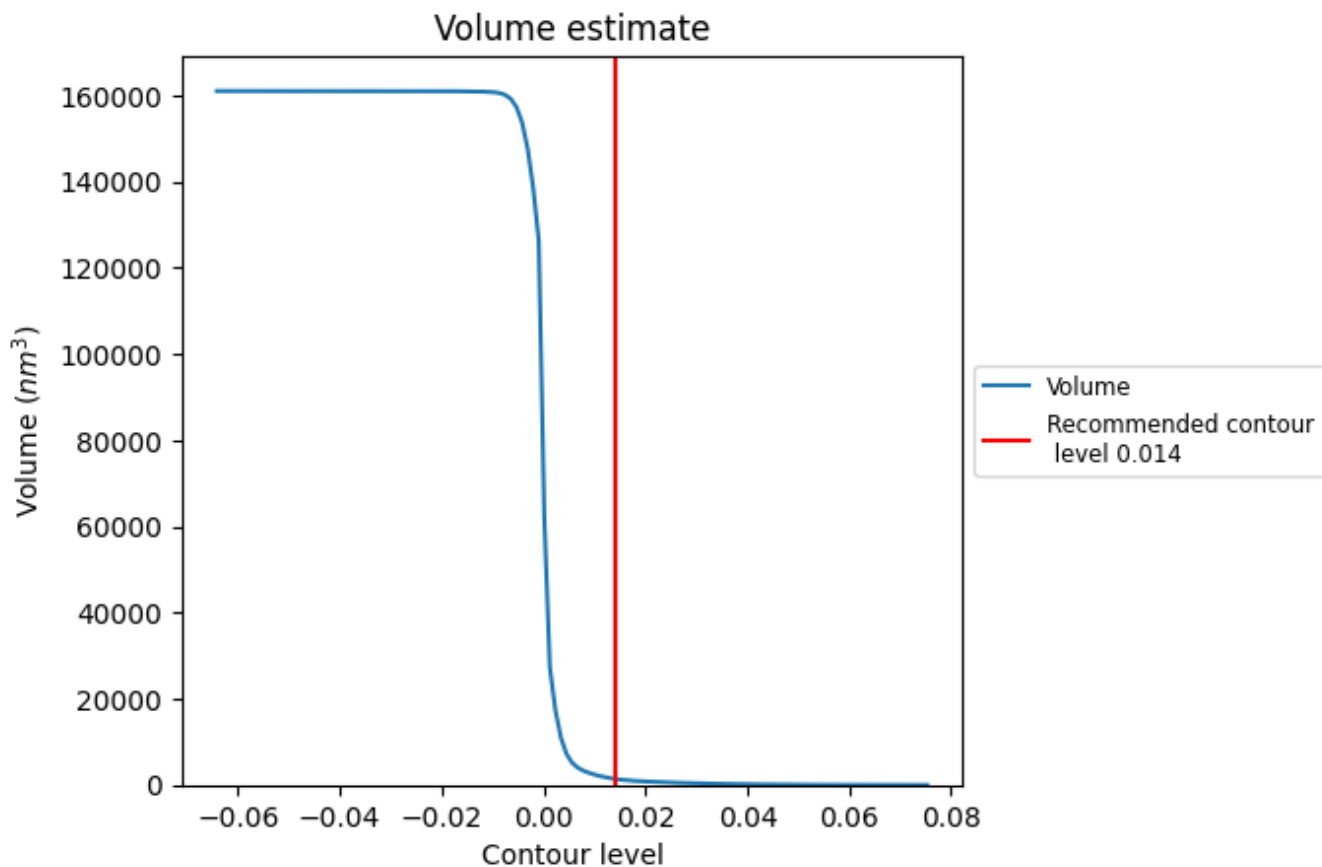
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

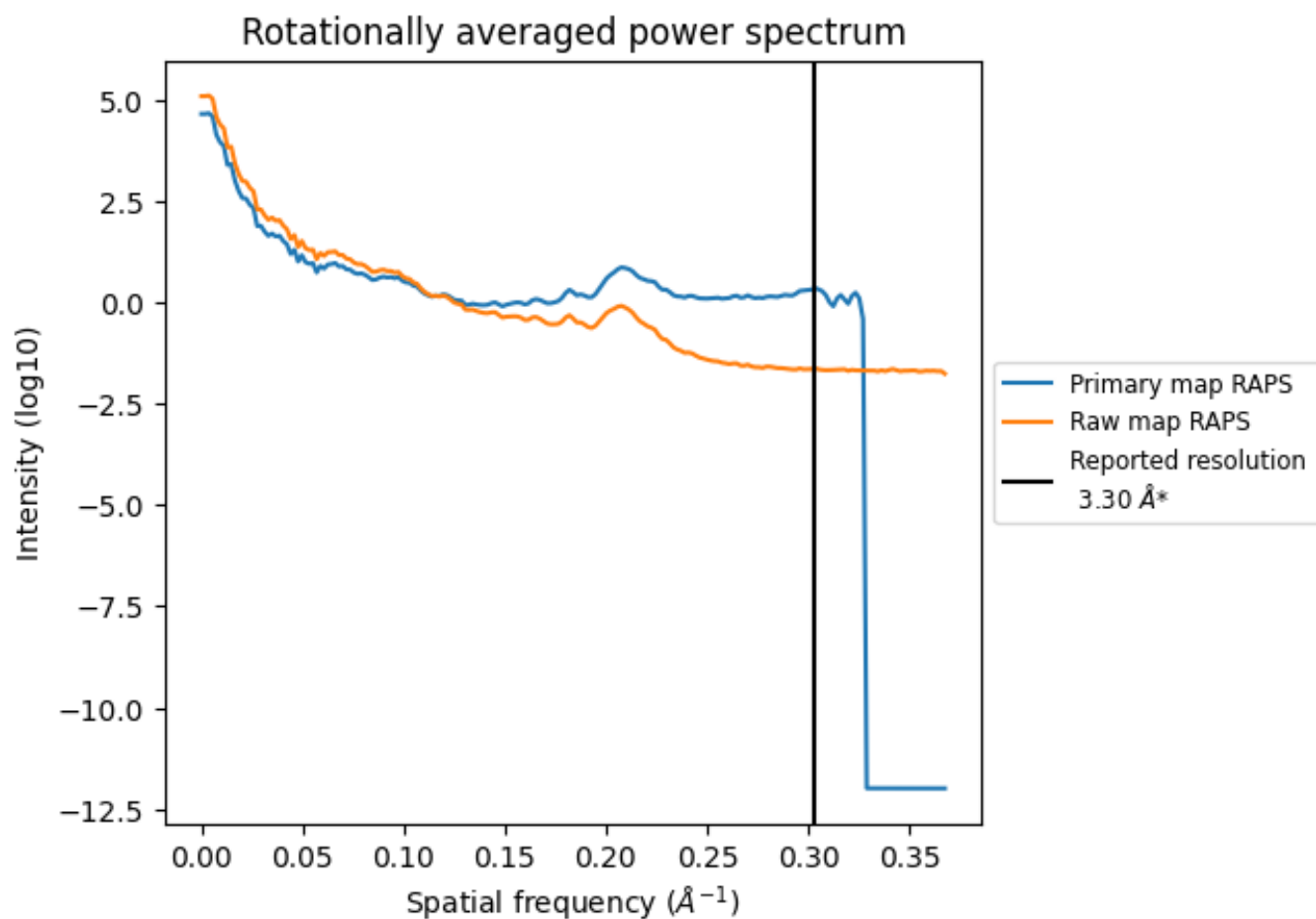
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1404 nm<sup>3</sup>; this corresponds to an approximate mass of 1268 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

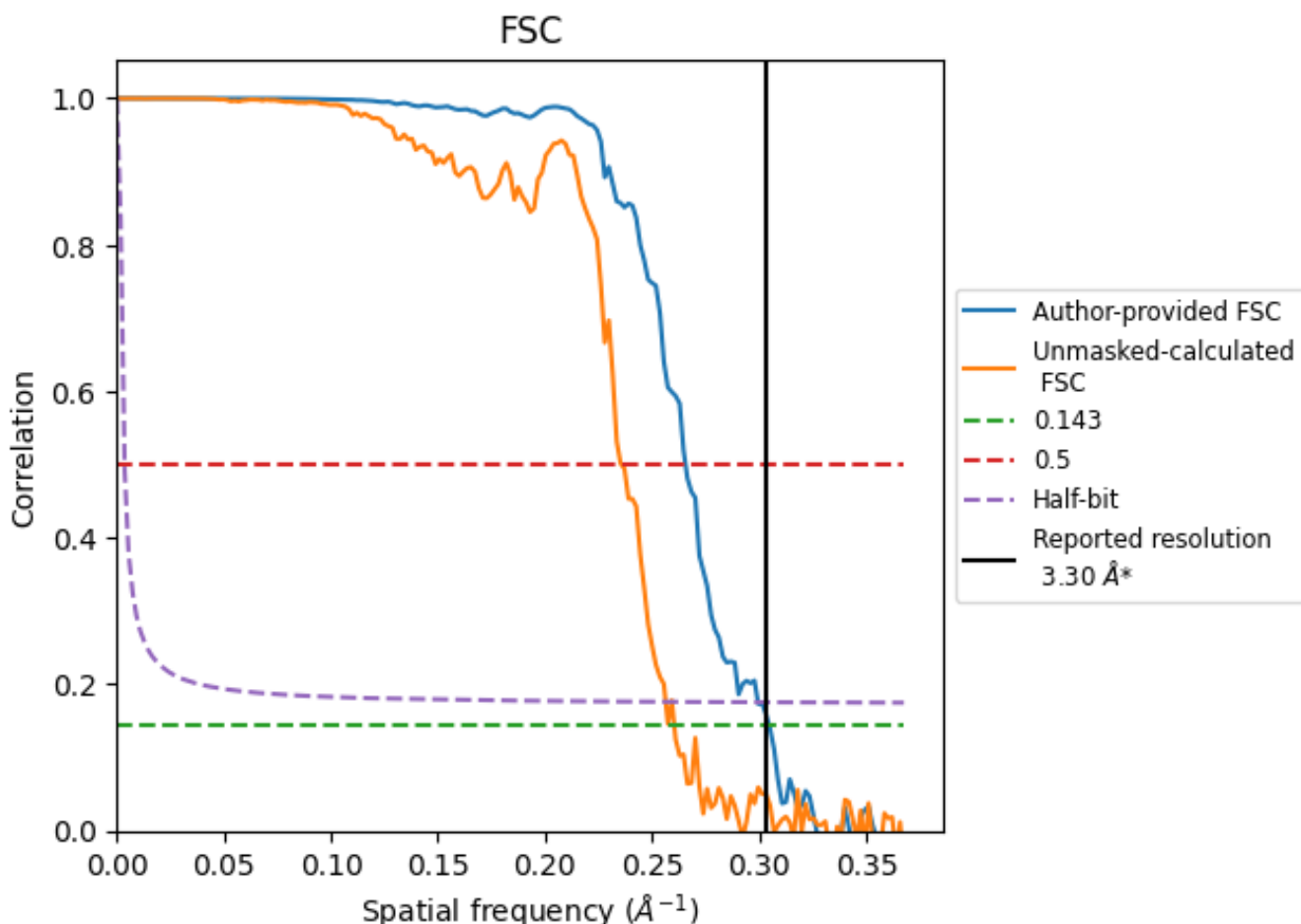


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	3.77	3.34
Unmasked-calculated*	3.84	4.24	3.90

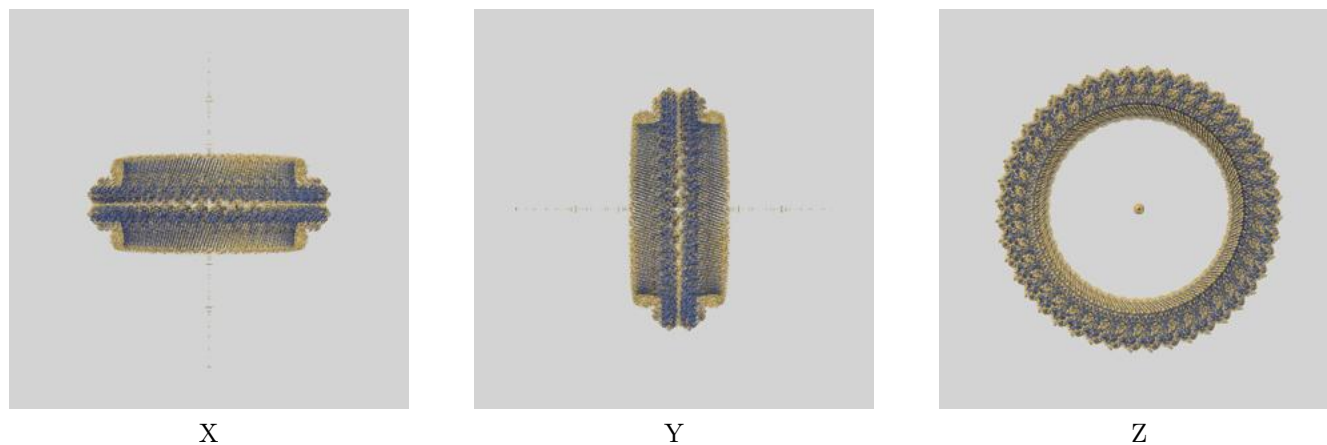
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 3.3 by more than 10 %



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

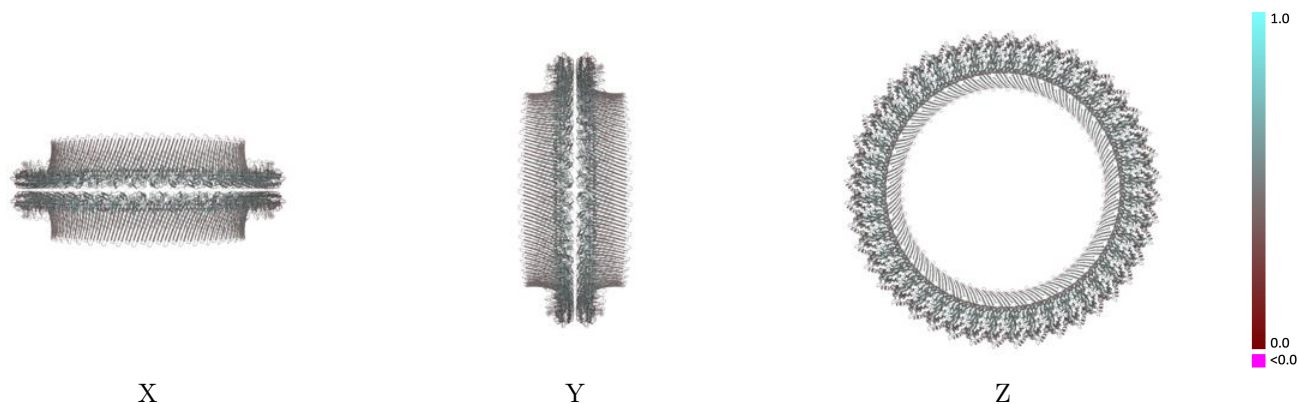
This section contains information regarding the fit between EMDB map EMD-36732 and PDB model 8JYW. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



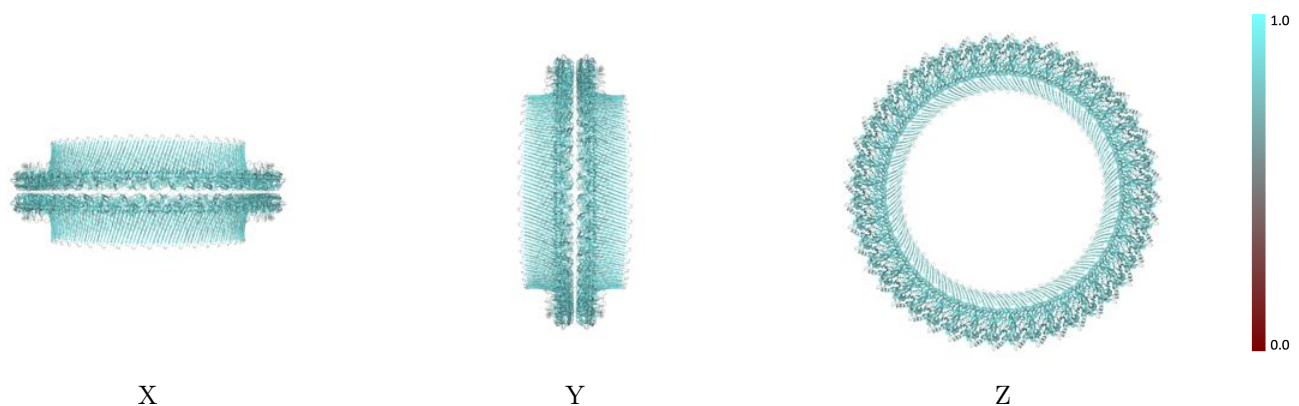
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



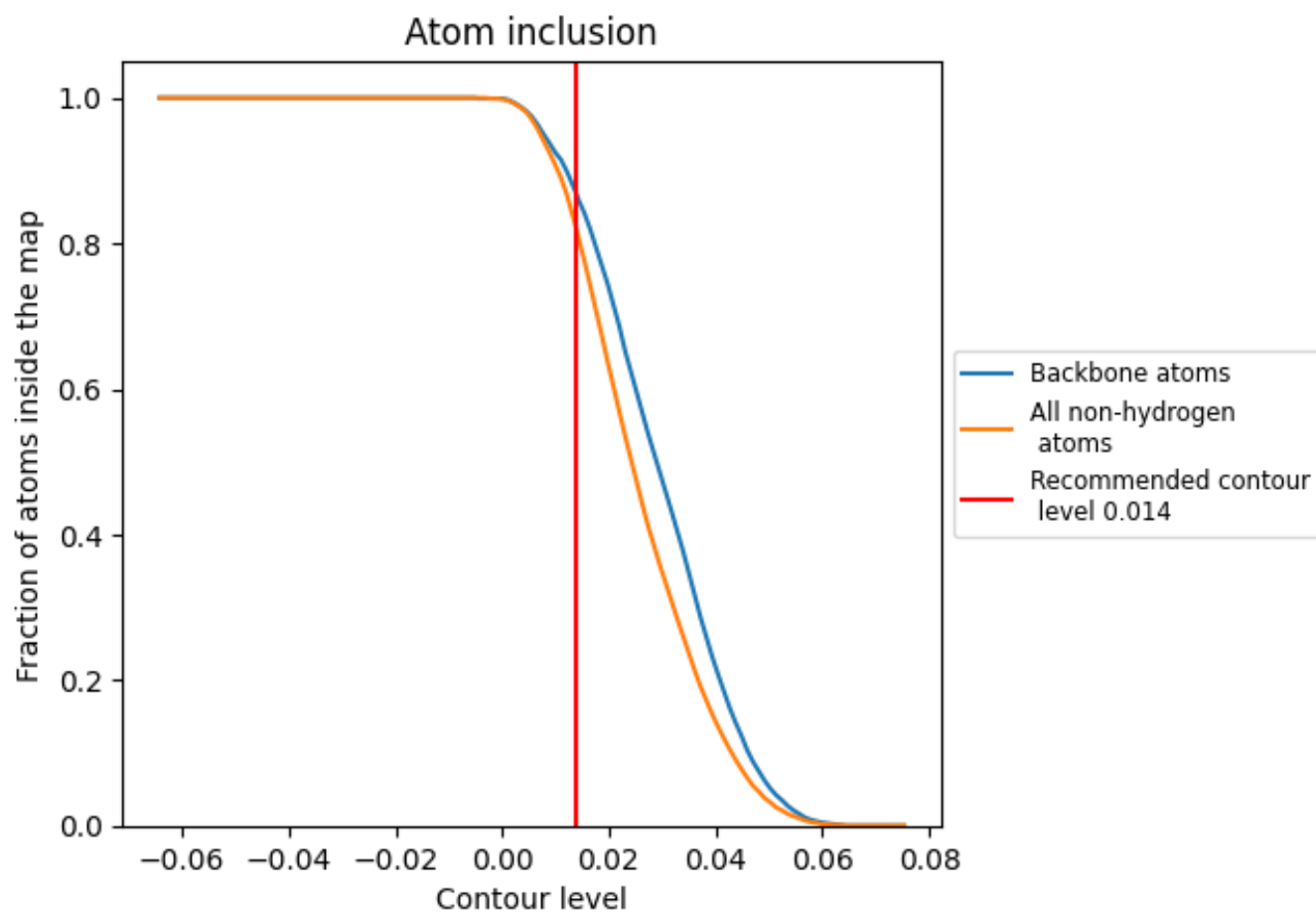
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8180	 0.4750
A	 0.8190	 0.4770
AA	 0.8150	 0.4740
AB	 0.8200	 0.4760
AC	 0.8190	 0.4760
B	 0.8190	 0.4760
BA	 0.8200	 0.4750
BB	 0.8160	 0.4760
BC	 0.8190	 0.4760
C	 0.8200	 0.4760
CA	 0.8230	 0.4750
CB	 0.8190	 0.4760
CC	 0.8200	 0.4750
D	 0.8160	 0.4740
DA	 0.8180	 0.4740
DB	 0.8170	 0.4760
DC	 0.8160	 0.4730
E	 0.8190	 0.4740
EA	 0.8170	 0.4760
EB	 0.8190	 0.4770
EC	 0.8190	 0.4730
F	 0.8210	 0.4740
FA	 0.8160	 0.4760
FB	 0.8190	 0.4760
FC	 0.8210	 0.4740
G	 0.8200	 0.4740
GA	 0.8160	 0.4780
GB	 0.8200	 0.4770
GC	 0.8200	 0.4720
H	 0.8190	 0.4770
HA	 0.8170	 0.4790
HB	 0.8150	 0.4750
HC	 0.8190	 0.4730
I	 0.8170	 0.4750
IA	 0.8190	 0.4800



























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Chain	Atom inclusion	Q-score
IB	 0.8190	 0.4750
IC	 0.8180	 0.4720
J	 0.8170	 0.4750
JA	 0.8170	 0.4790
JB	 0.8230	 0.4750
JC	 0.8170	 0.4730
K	 0.8160	 0.4750
KA	 0.8200	 0.4770
KB	 0.8170	 0.4760
KC	 0.8170	 0.4750
L	 0.8190	 0.4760
LA	 0.8170	 0.4740
LB	 0.8170	 0.4780
M	 0.8180	 0.4750
MA	 0.8190	 0.4740
MB	 0.8160	 0.4780
N	 0.8210	 0.4760
NA	 0.8210	 0.4740
NB	 0.8160	 0.4780
O	 0.8160	 0.4730
OA	 0.8200	 0.4740
OB	 0.8170	 0.4780
P	 0.8190	 0.4720
PA	 0.8150	 0.4770
PB	 0.8190	 0.4790
Q	 0.8220	 0.4730
QA	 0.8170	 0.4770
QB	 0.8170	 0.4780
R	 0.8170	 0.4720
RA	 0.8160	 0.4780
RB	 0.8200	 0.4780
S	 0.8200	 0.4730
SA	 0.8160	 0.4760
SB	 0.8170	 0.4760
T	 0.8160	 0.4730
TA	 0.8190	 0.4760
TB	 0.8190	 0.4750
UA	 0.8180	 0.4760
UB	 0.8210	 0.4750
V	 0.8190	 0.4750
VA	 0.8210	 0.4760
VB	 0.8200	 0.4730

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Chain	Atom inclusion	Q-score
W	 0.8170	 0.4770
WA	 0.8160	 0.4720
WB	 0.8150	 0.4760
X	 0.8190	 0.4780
XA	 0.8190	 0.4730
XB	 0.8170	 0.4750
Y	 0.8190	 0.4770
YA	 0.8220	 0.4740
YB	 0.8160	 0.4760
Z	 0.8200	 0.4770
ZA	 0.8170	 0.4740
ZB	 0.8160	 0.4750