



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:35 AM UTC

PDB ID : 8RMN / pdb_00008rmn
EMDB ID : EMD-19365
Title : Cryo-EM structure of a dimer of decameric human CALHM4 in complex with synthetic nanobody SbC4
Authors : Peter, M.; Drozdzyk, K.; Dutzler, R.
Deposited on : 2024-01-08
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

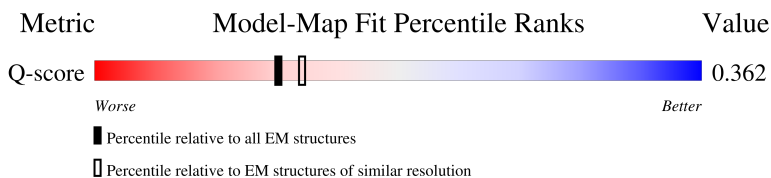
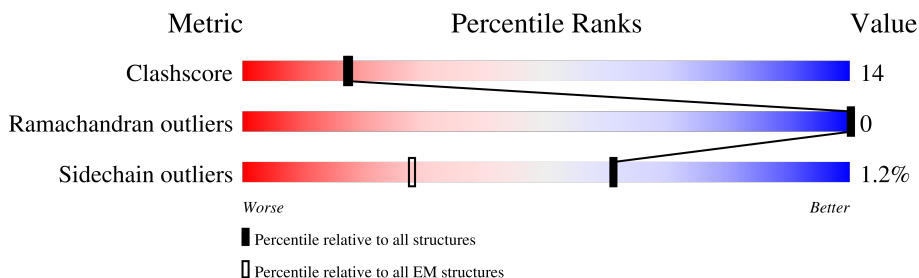
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	A	322	13% 63% 17% 19%
1	B	322	13% 63% 18% 19%
1	C	322	14% 63% 17% 19%
1	D	322	13% 62% 18% 19%

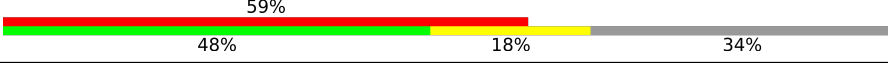
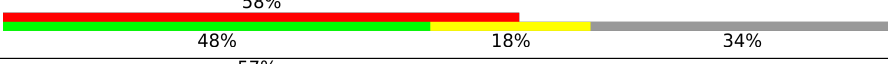
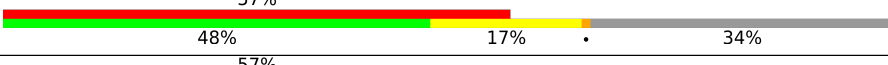
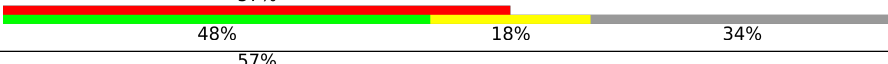
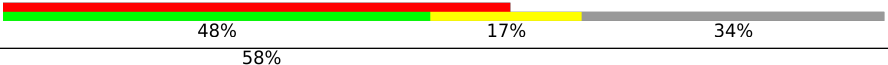
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Mol	Chain	Length	Quality of chain
1	E	322	
1	F	322	
1	G	322	
1	H	322	
1	I	322	
1	J	322	
1	K	322	
1	L	322	
1	M	322	
1	N	322	
1	O	322	
1	P	322	
1	Q	322	
1	R	322	
1	S	322	
1	T	322	
2	U	143	
2	V	143	
2	W	143	
2	X	143	
2	Y	143	
2	Z	143	
2	a	143	
2	b	143	
2	c	143	

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Mol	Chain	Length	Quality of chain
2	d	143	
2	e	143	
2	f	143	
2	g	143	
2	h	143	
2	i	143	
2	j	143	
2	k	143	
2	l	143	
2	m	143	
2	n	143	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 55440 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 Calcium homeostasis modulator protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	B	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	C	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	D	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	E	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	F	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	G	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	H	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	I	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	J	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	K	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	L	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	M	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	N	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	O	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	P	261	Total 2039	C 1313	N 343	O 364	S 19	0	0
1	Q	261	Total 2039	C 1313	N 343	O 364	S 19	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	261	Total	C	N	O	S	0	0
			2039	1313	343	364	19		
1	S	261	Total	C	N	O	S	0	0
			2039	1313	343	364	19		
1	T	261	Total	C	N	O	S	0	0
			2039	1313	343	364	19		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q5JW98
A	1	SER	-	expression tag	UNP Q5JW98
A	315	ALA	-	expression tag	UNP Q5JW98
A	316	LEU	-	expression tag	UNP Q5JW98
A	317	GLU	-	expression tag	UNP Q5JW98
A	318	VAL	-	expression tag	UNP Q5JW98
A	319	LEU	-	expression tag	UNP Q5JW98
A	320	PHE	-	expression tag	UNP Q5JW98
A	321	GLN	-	expression tag	UNP Q5JW98
B	0	MET	-	initiating methionine	UNP Q5JW98
B	1	SER	-	expression tag	UNP Q5JW98
B	315	ALA	-	expression tag	UNP Q5JW98
B	316	LEU	-	expression tag	UNP Q5JW98
B	317	GLU	-	expression tag	UNP Q5JW98
B	318	VAL	-	expression tag	UNP Q5JW98
B	319	LEU	-	expression tag	UNP Q5JW98
B	320	PHE	-	expression tag	UNP Q5JW98
B	321	GLN	-	expression tag	UNP Q5JW98
C	0	MET	-	initiating methionine	UNP Q5JW98
C	1	SER	-	expression tag	UNP Q5JW98
C	315	ALA	-	expression tag	UNP Q5JW98
C	316	LEU	-	expression tag	UNP Q5JW98
C	317	GLU	-	expression tag	UNP Q5JW98
C	318	VAL	-	expression tag	UNP Q5JW98
C	319	LEU	-	expression tag	UNP Q5JW98
C	320	PHE	-	expression tag	UNP Q5JW98
C	321	GLN	-	expression tag	UNP Q5JW98
D	0	MET	-	initiating methionine	UNP Q5JW98
D	1	SER	-	expression tag	UNP Q5JW98
D	315	ALA	-	expression tag	UNP Q5JW98
D	316	LEU	-	expression tag	UNP Q5JW98
D	317	GLU	-	expression tag	UNP Q5JW98

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Chain	Residue	Modelled	Actual	Comment	Reference
D	318	VAL	-	expression tag	UNP Q5JW98
D	319	LEU	-	expression tag	UNP Q5JW98
D	320	PHE	-	expression tag	UNP Q5JW98
D	321	GLN	-	expression tag	UNP Q5JW98
E	0	MET	-	initiating methionine	UNP Q5JW98
E	1	SER	-	expression tag	UNP Q5JW98
E	315	ALA	-	expression tag	UNP Q5JW98
E	316	LEU	-	expression tag	UNP Q5JW98
E	317	GLU	-	expression tag	UNP Q5JW98
E	318	VAL	-	expression tag	UNP Q5JW98
E	319	LEU	-	expression tag	UNP Q5JW98
E	320	PHE	-	expression tag	UNP Q5JW98
E	321	GLN	-	expression tag	UNP Q5JW98
F	0	MET	-	initiating methionine	UNP Q5JW98
F	1	SER	-	expression tag	UNP Q5JW98
F	315	ALA	-	expression tag	UNP Q5JW98
F	316	LEU	-	expression tag	UNP Q5JW98
F	317	GLU	-	expression tag	UNP Q5JW98
F	318	VAL	-	expression tag	UNP Q5JW98
F	319	LEU	-	expression tag	UNP Q5JW98
F	320	PHE	-	expression tag	UNP Q5JW98
F	321	GLN	-	expression tag	UNP Q5JW98
G	0	MET	-	initiating methionine	UNP Q5JW98
G	1	SER	-	expression tag	UNP Q5JW98
G	315	ALA	-	expression tag	UNP Q5JW98
G	316	LEU	-	expression tag	UNP Q5JW98
G	317	GLU	-	expression tag	UNP Q5JW98
G	318	VAL	-	expression tag	UNP Q5JW98
G	319	LEU	-	expression tag	UNP Q5JW98
G	320	PHE	-	expression tag	UNP Q5JW98
G	321	GLN	-	expression tag	UNP Q5JW98
H	0	MET	-	initiating methionine	UNP Q5JW98
H	1	SER	-	expression tag	UNP Q5JW98
H	315	ALA	-	expression tag	UNP Q5JW98
H	316	LEU	-	expression tag	UNP Q5JW98
H	317	GLU	-	expression tag	UNP Q5JW98
H	318	VAL	-	expression tag	UNP Q5JW98
H	319	LEU	-	expression tag	UNP Q5JW98
H	320	PHE	-	expression tag	UNP Q5JW98
H	321	GLN	-	expression tag	UNP Q5JW98
I	0	MET	-	initiating methionine	UNP Q5JW98
I	1	SER	-	expression tag	UNP Q5JW98

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Chain	Residue	Modelled	Actual	Comment	Reference
I	315	ALA	-	expression tag	UNP Q5JW98
I	316	LEU	-	expression tag	UNP Q5JW98
I	317	GLU	-	expression tag	UNP Q5JW98
I	318	VAL	-	expression tag	UNP Q5JW98
I	319	LEU	-	expression tag	UNP Q5JW98
I	320	PHE	-	expression tag	UNP Q5JW98
I	321	GLN	-	expression tag	UNP Q5JW98
J	0	MET	-	initiating methionine	UNP Q5JW98
J	1	SER	-	expression tag	UNP Q5JW98
J	315	ALA	-	expression tag	UNP Q5JW98
J	316	LEU	-	expression tag	UNP Q5JW98
J	317	GLU	-	expression tag	UNP Q5JW98
J	318	VAL	-	expression tag	UNP Q5JW98
J	319	LEU	-	expression tag	UNP Q5JW98
J	320	PHE	-	expression tag	UNP Q5JW98
J	321	GLN	-	expression tag	UNP Q5JW98
K	0	MET	-	initiating methionine	UNP Q5JW98
K	1	SER	-	expression tag	UNP Q5JW98
K	315	ALA	-	expression tag	UNP Q5JW98
K	316	LEU	-	expression tag	UNP Q5JW98
K	317	GLU	-	expression tag	UNP Q5JW98
K	318	VAL	-	expression tag	UNP Q5JW98
K	319	LEU	-	expression tag	UNP Q5JW98
K	320	PHE	-	expression tag	UNP Q5JW98
K	321	GLN	-	expression tag	UNP Q5JW98
L	0	MET	-	initiating methionine	UNP Q5JW98
L	1	SER	-	expression tag	UNP Q5JW98
L	315	ALA	-	expression tag	UNP Q5JW98
L	316	LEU	-	expression tag	UNP Q5JW98
L	317	GLU	-	expression tag	UNP Q5JW98
L	318	VAL	-	expression tag	UNP Q5JW98
L	319	LEU	-	expression tag	UNP Q5JW98
L	320	PHE	-	expression tag	UNP Q5JW98
L	321	GLN	-	expression tag	UNP Q5JW98
M	0	MET	-	initiating methionine	UNP Q5JW98
M	1	SER	-	expression tag	UNP Q5JW98
M	315	ALA	-	expression tag	UNP Q5JW98
M	316	LEU	-	expression tag	UNP Q5JW98
M	317	GLU	-	expression tag	UNP Q5JW98
M	318	VAL	-	expression tag	UNP Q5JW98
M	319	LEU	-	expression tag	UNP Q5JW98
M	320	PHE	-	expression tag	UNP Q5JW98

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Chain	Residue	Modelled	Actual	Comment	Reference
M	321	GLN	-	expression tag	UNP Q5JW98
N	0	MET	-	initiating methionine	UNP Q5JW98
N	1	SER	-	expression tag	UNP Q5JW98
N	315	ALA	-	expression tag	UNP Q5JW98
N	316	LEU	-	expression tag	UNP Q5JW98
N	317	GLU	-	expression tag	UNP Q5JW98
N	318	VAL	-	expression tag	UNP Q5JW98
N	319	LEU	-	expression tag	UNP Q5JW98
N	320	PHE	-	expression tag	UNP Q5JW98
N	321	GLN	-	expression tag	UNP Q5JW98
O	0	MET	-	initiating methionine	UNP Q5JW98
O	1	SER	-	expression tag	UNP Q5JW98
O	315	ALA	-	expression tag	UNP Q5JW98
O	316	LEU	-	expression tag	UNP Q5JW98
O	317	GLU	-	expression tag	UNP Q5JW98
O	318	VAL	-	expression tag	UNP Q5JW98
O	319	LEU	-	expression tag	UNP Q5JW98
O	320	PHE	-	expression tag	UNP Q5JW98
O	321	GLN	-	expression tag	UNP Q5JW98
P	0	MET	-	initiating methionine	UNP Q5JW98
P	1	SER	-	expression tag	UNP Q5JW98
P	315	ALA	-	expression tag	UNP Q5JW98
P	316	LEU	-	expression tag	UNP Q5JW98
P	317	GLU	-	expression tag	UNP Q5JW98
P	318	VAL	-	expression tag	UNP Q5JW98
P	319	LEU	-	expression tag	UNP Q5JW98
P	320	PHE	-	expression tag	UNP Q5JW98
P	321	GLN	-	expression tag	UNP Q5JW98
Q	0	MET	-	initiating methionine	UNP Q5JW98
Q	1	SER	-	expression tag	UNP Q5JW98
Q	315	ALA	-	expression tag	UNP Q5JW98
Q	316	LEU	-	expression tag	UNP Q5JW98
Q	317	GLU	-	expression tag	UNP Q5JW98
Q	318	VAL	-	expression tag	UNP Q5JW98
Q	319	LEU	-	expression tag	UNP Q5JW98
Q	320	PHE	-	expression tag	UNP Q5JW98
Q	321	GLN	-	expression tag	UNP Q5JW98
R	0	MET	-	initiating methionine	UNP Q5JW98
R	1	SER	-	expression tag	UNP Q5JW98
R	315	ALA	-	expression tag	UNP Q5JW98
R	316	LEU	-	expression tag	UNP Q5JW98
R	317	GLU	-	expression tag	UNP Q5JW98

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Chain	Residue	Modelled	Actual	Comment	Reference
R	318	VAL	-	expression tag	UNP Q5JW98
R	319	LEU	-	expression tag	UNP Q5JW98
R	320	PHE	-	expression tag	UNP Q5JW98
R	321	GLN	-	expression tag	UNP Q5JW98
S	0	MET	-	initiating methionine	UNP Q5JW98
S	1	SER	-	expression tag	UNP Q5JW98
S	315	ALA	-	expression tag	UNP Q5JW98
S	316	LEU	-	expression tag	UNP Q5JW98
S	317	GLU	-	expression tag	UNP Q5JW98
S	318	VAL	-	expression tag	UNP Q5JW98
S	319	LEU	-	expression tag	UNP Q5JW98
S	320	PHE	-	expression tag	UNP Q5JW98
S	321	GLN	-	expression tag	UNP Q5JW98
T	0	MET	-	initiating methionine	UNP Q5JW98
T	1	SER	-	expression tag	UNP Q5JW98
T	315	ALA	-	expression tag	UNP Q5JW98
T	316	LEU	-	expression tag	UNP Q5JW98
T	317	GLU	-	expression tag	UNP Q5JW98
T	318	VAL	-	expression tag	UNP Q5JW98
T	319	LEU	-	expression tag	UNP Q5JW98
T	320	PHE	-	expression tag	UNP Q5JW98
T	321	GLN	-	expression tag	UNP Q5JW98

- Molecule 2 is a protein called Synthetic nanobody SbC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	94	Total	C	N	O	S	0	0
			733	461	131	137	4		
2	V	94	Total	C	N	O	S	0	0
			733	461	131	137	4		
2	W	94	Total	C	N	O	S	0	0
			733	461	131	137	4		
2	X	94	Total	C	N	O	S	0	0
			733	461	131	137	4		
2	Y	94	Total	C	N	O	S	0	0
			733	461	131	137	4		
2	Z	94	Total	C	N	O	S	0	0
			733	461	131	137	4		
2	a	94	Total	C	N	O	S	0	0
			733	461	131	137	4		
2	b	94	Total	C	N	O	S	0	0
			733	461	131	137	4		

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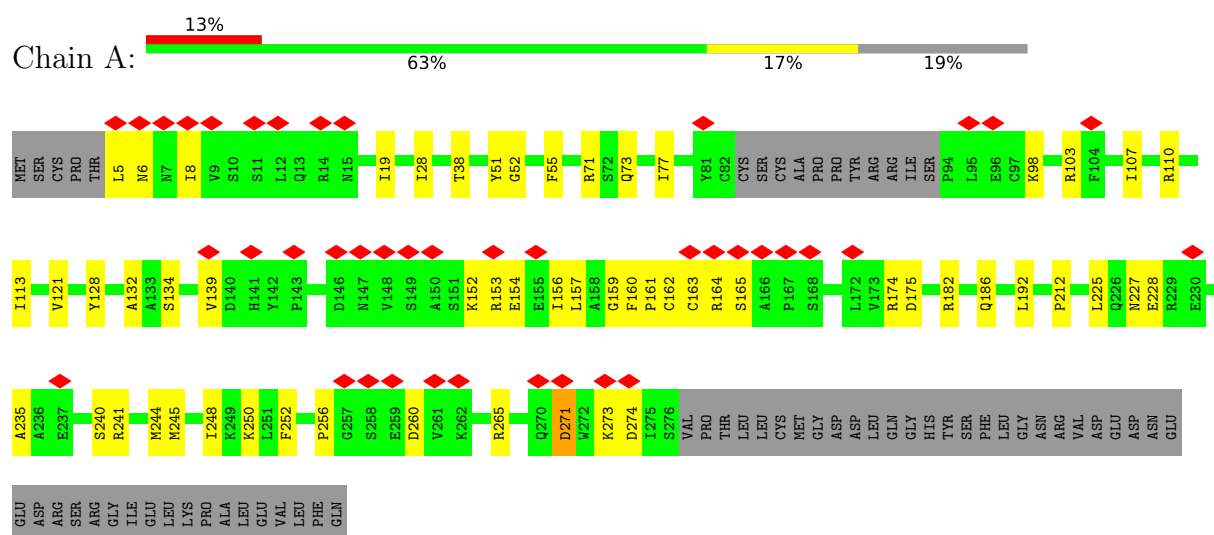
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	d	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	e	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	f	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	g	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	h	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	i	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	j	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	k	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	l	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	m	94	Total 733	C 461	N 131	O 137	S 4	0	0
2	n	94	Total 733	C 461	N 131	O 137	S 4	0	0

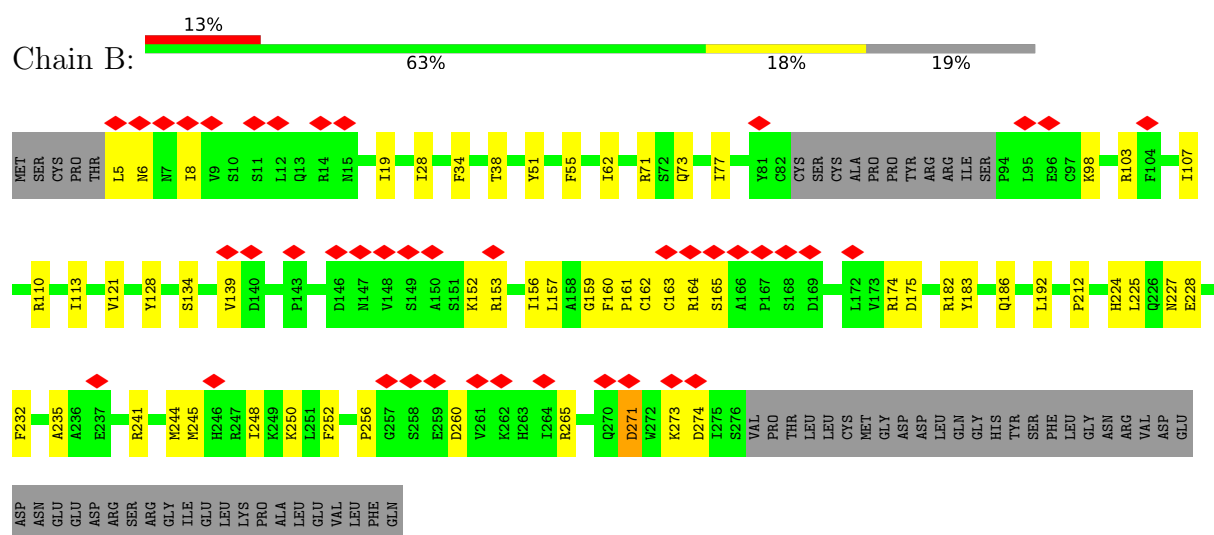
3 Residue-property plots

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

• Molecule 1: Calcium homeostasis modulator protein 4

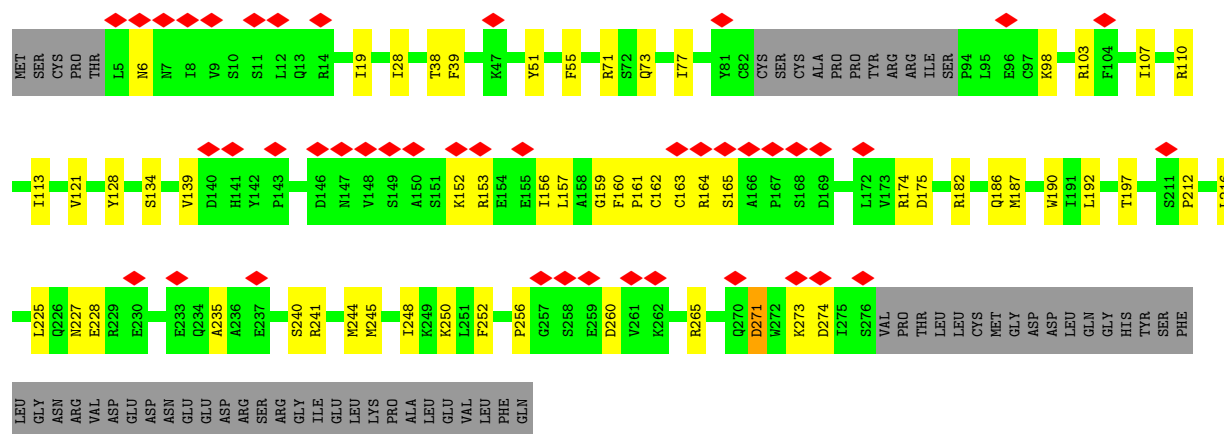


• Molecule 1: Calcium homeostasis modulator protein 4

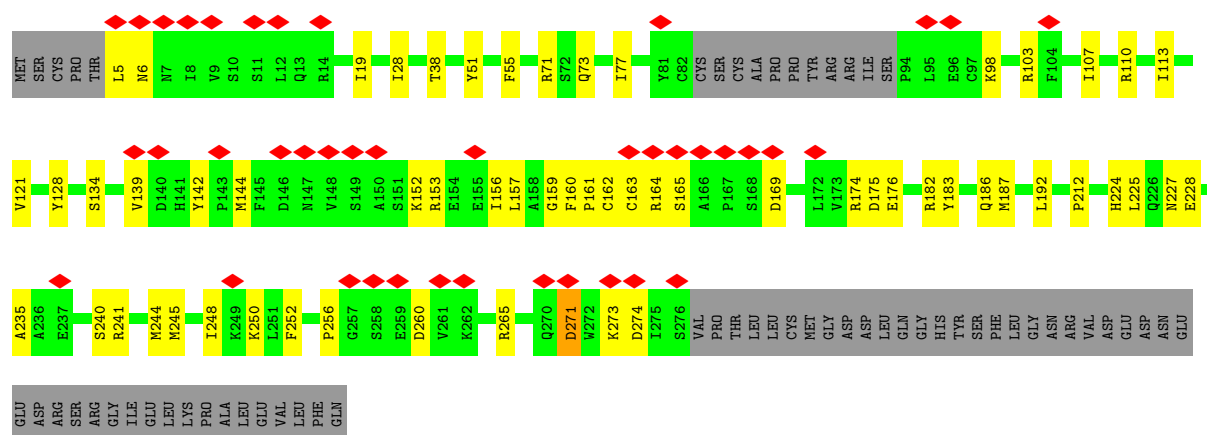


• Molecule 1: Calcium homeostasis modulator protein 4

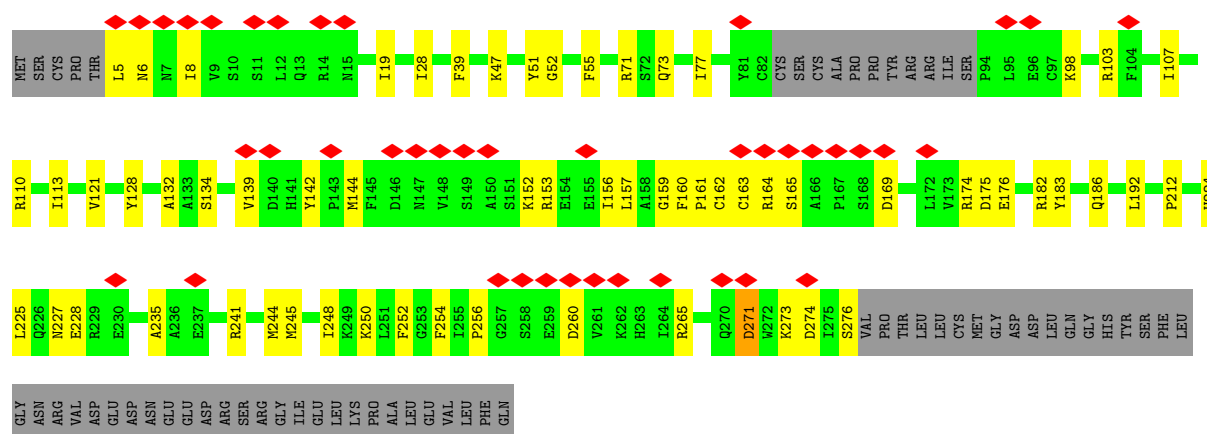




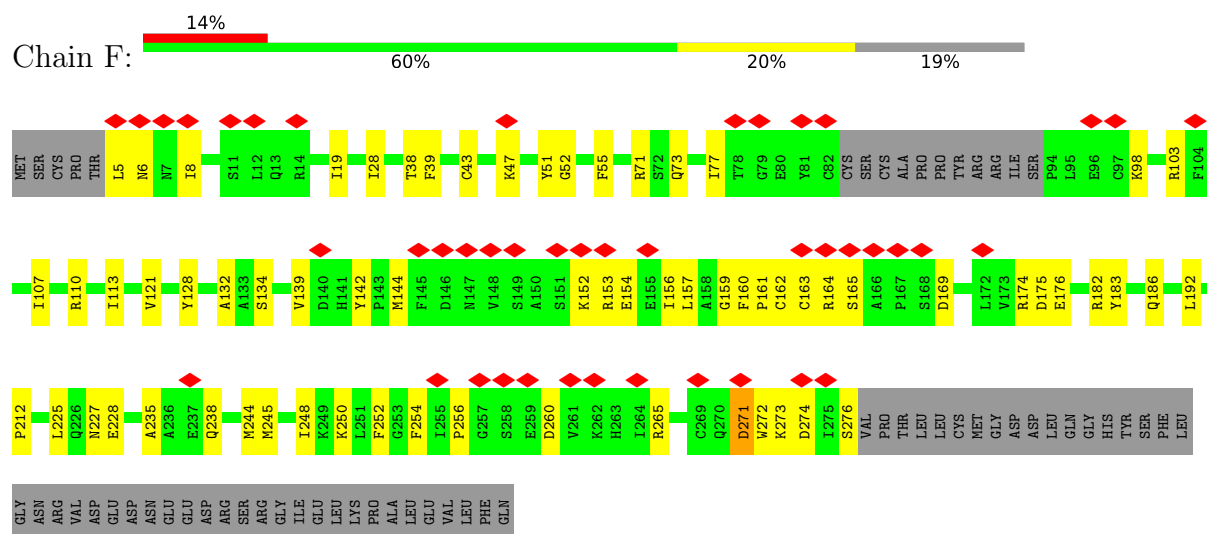
• Molecule 1: Calcium homeostasis modulator protein 4



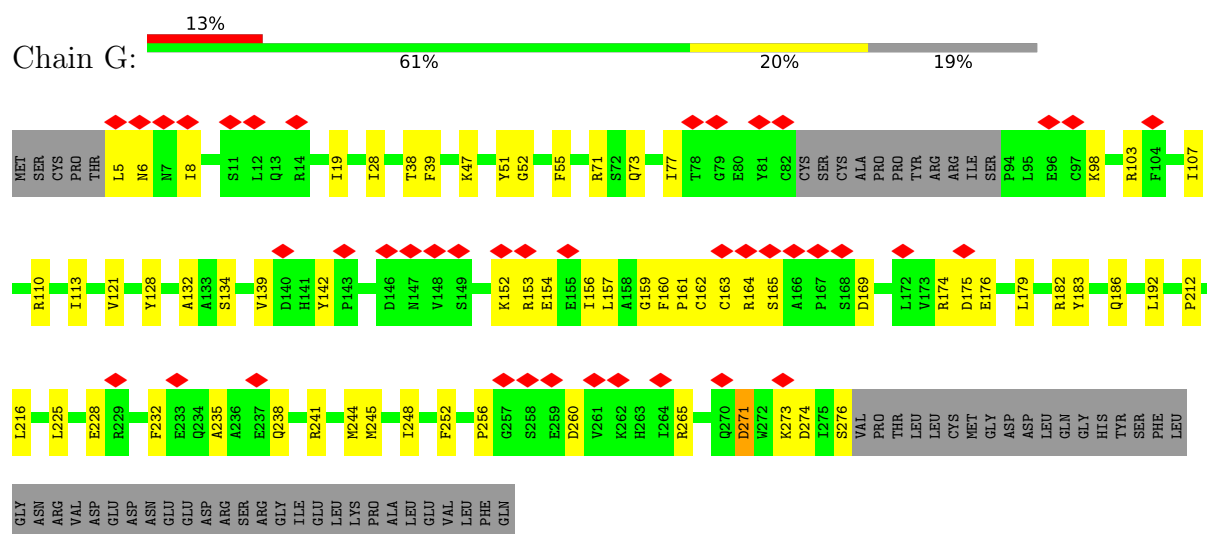
• Molecule 1: Calcium homeostasis modulator protein 4



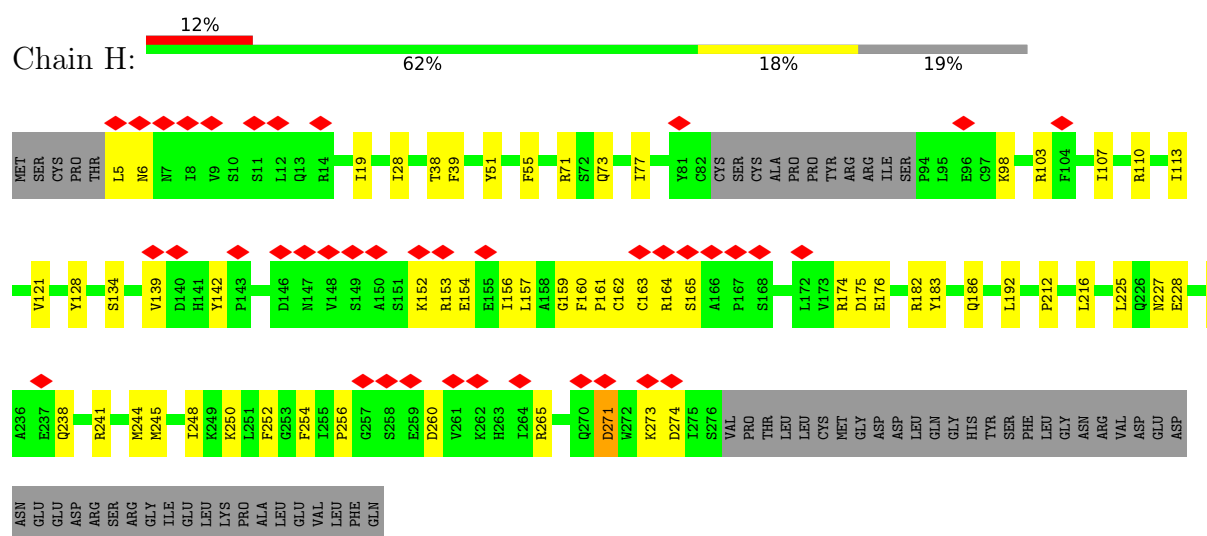
• Molecule 1: Calcium homeostasis modulator protein 4



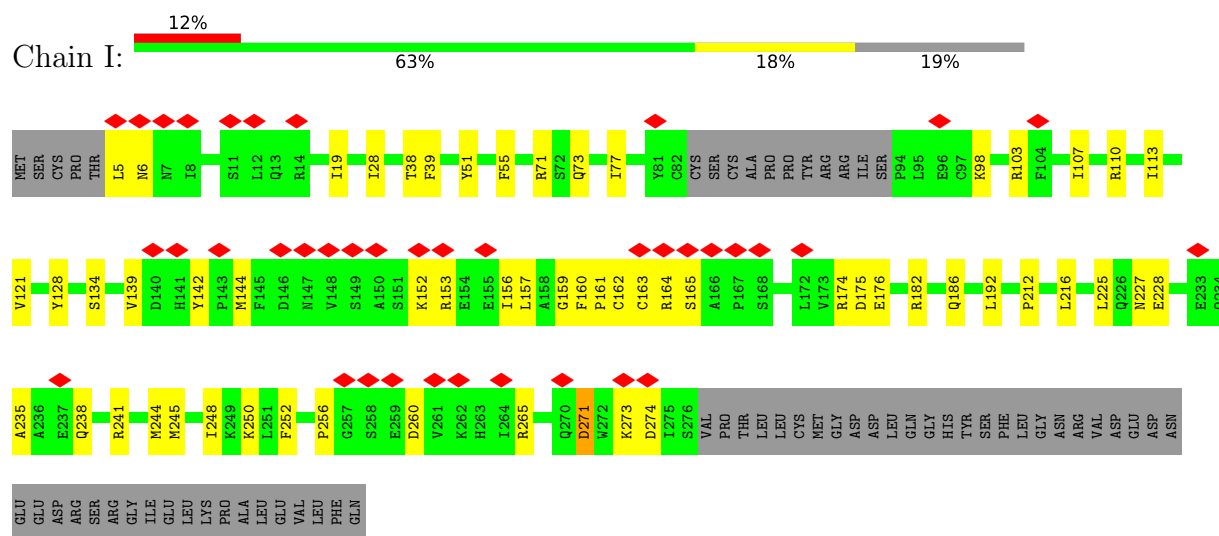
• Molecule 1: Calcium homeostasis modulator protein 4



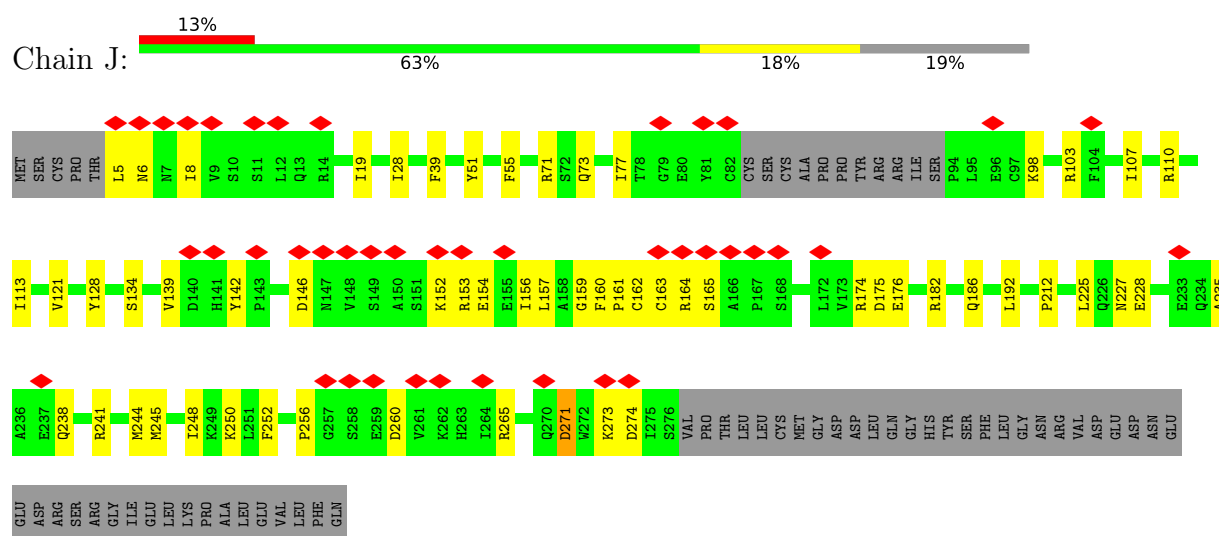
• Molecule 1: Calcium homeostasis modulator protein 4



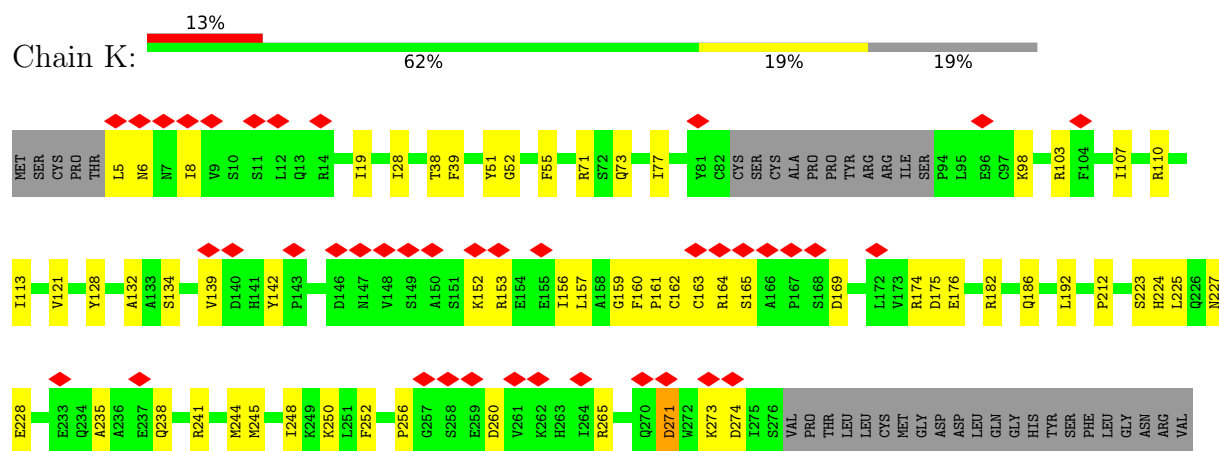
• Molecule 1: Calcium homeostasis modulator protein 4



• Molecule 1: Calcium homeostasis modulator protein 4



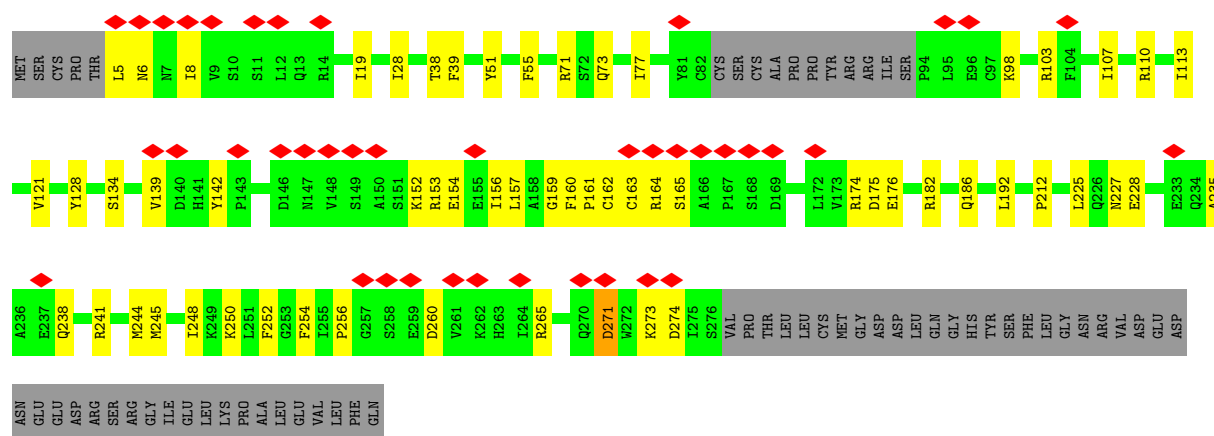
• Molecule 1: Calcium homeostasis modulator protein 4



ASP
GLU
SER
ASN
PRO
GLU
GLU
ASP
ARG
SER
ARG
GLY
ILE
GLU
LEU
LYS
PRO
ALA
LEU
GLU
PHE
GLN

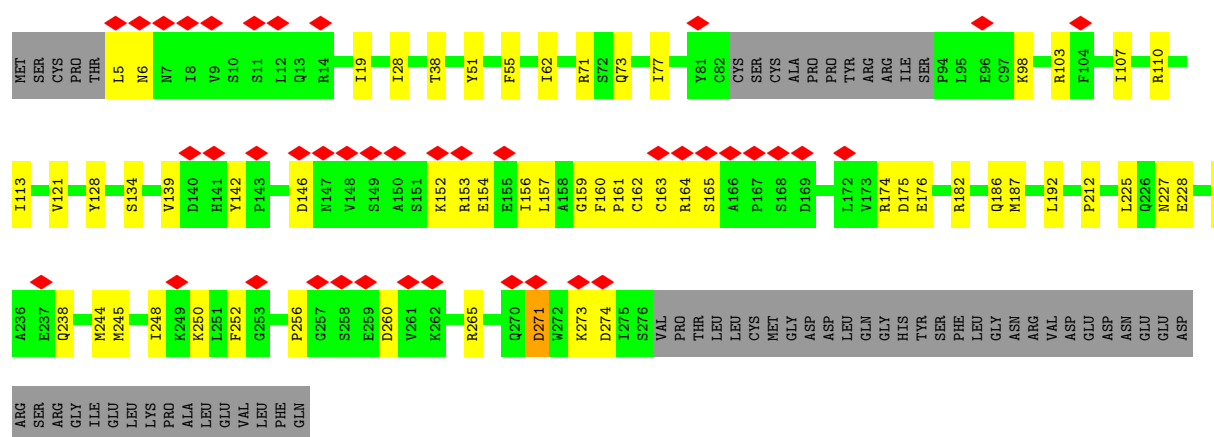
• Molecule 1: Calcium homeostasis modulator protein 4

Chain L: 13% 63% 18% 19%



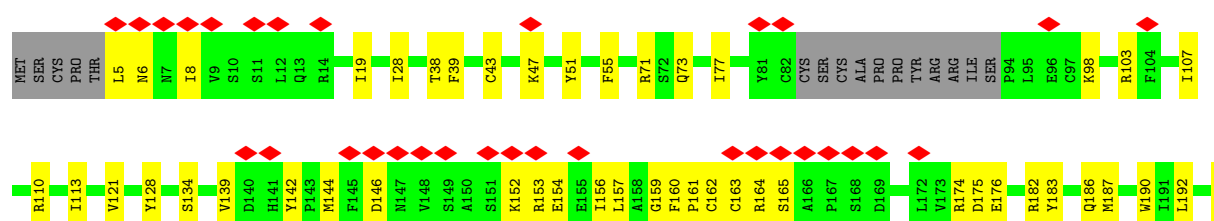
• Molecule 1: Calcium homeostasis modulator protein 4

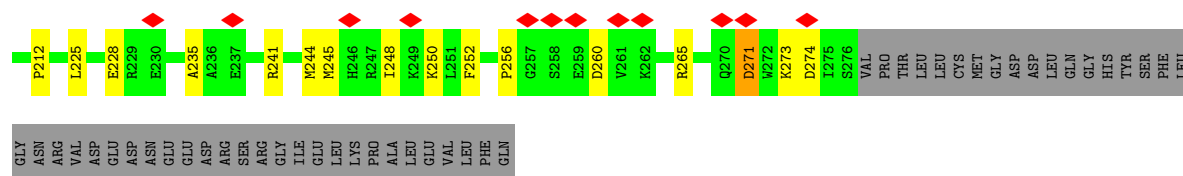
Chain M: 13% 63% 18% 19%



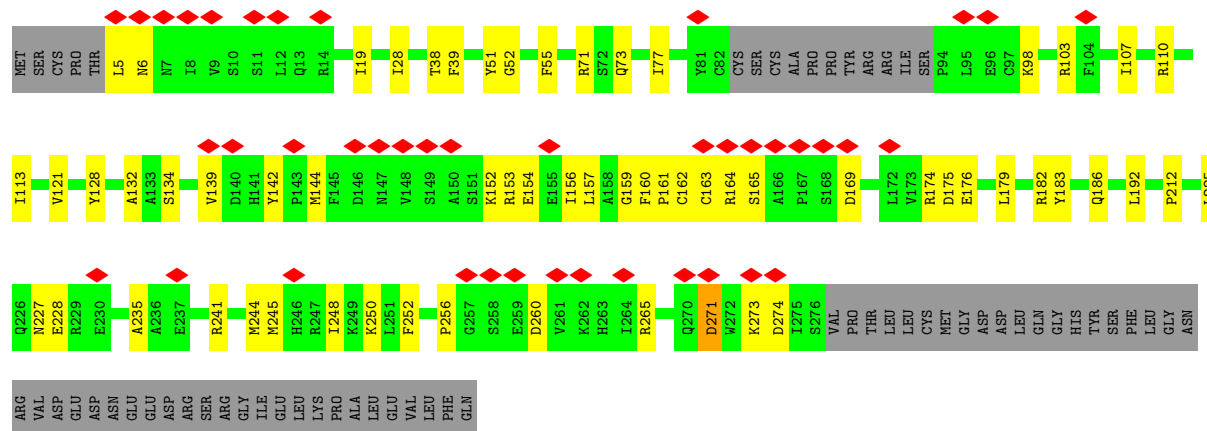
• Molecule 1: Calcium homeostasis modulator protein 4

Chain N: 14% 61% 20% 19%

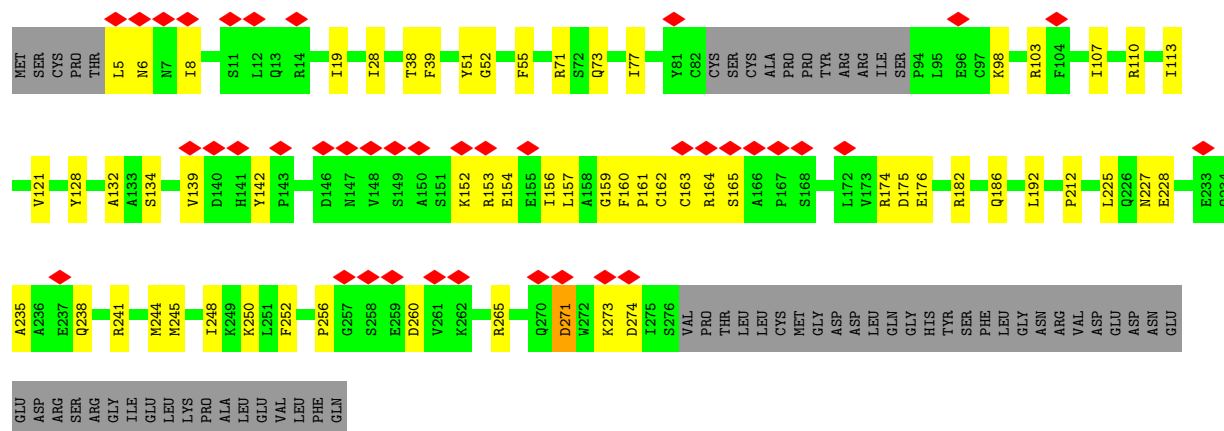




• Molecule 1: Calcium homeostasis modulator protein 4

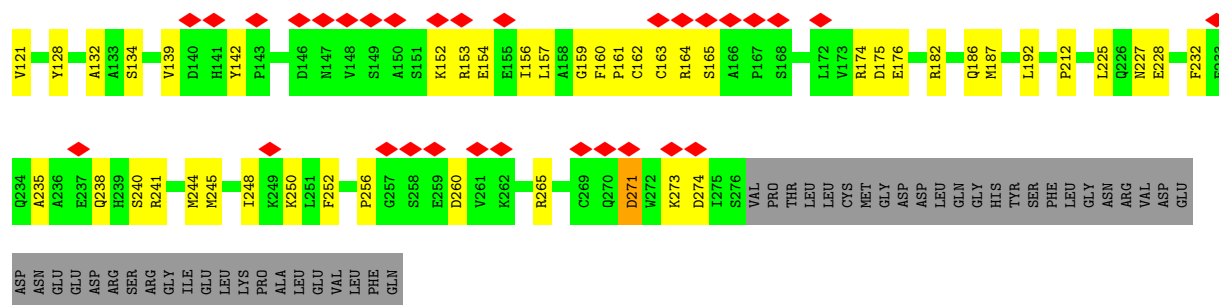


• Molecule 1: Calcium homeostasis modulator protein 4

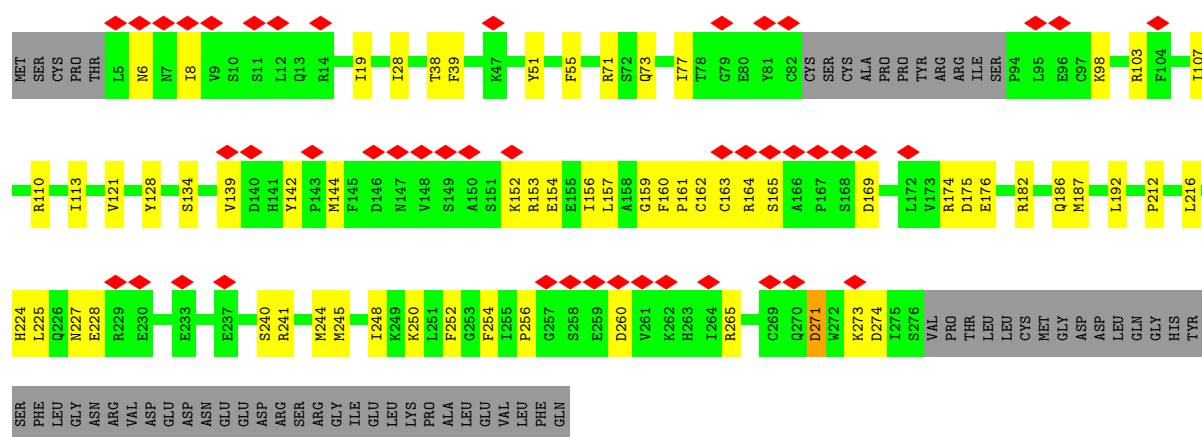


• Molecule 1: Calcium homeostasis modulator protein 4

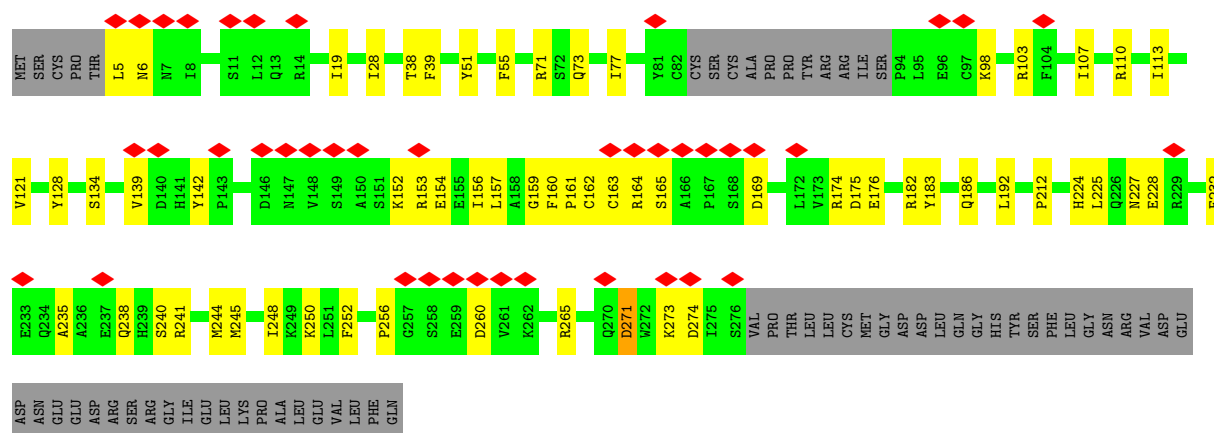




• Molecule 1: Calcium homeostasis modulator protein 4

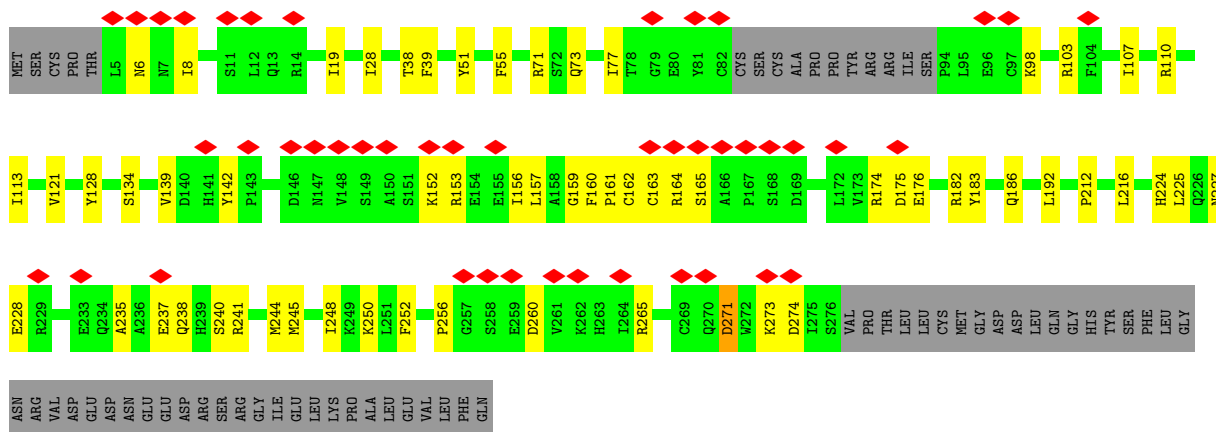


• Molecule 1: Calcium homeostasis modulator protein 4

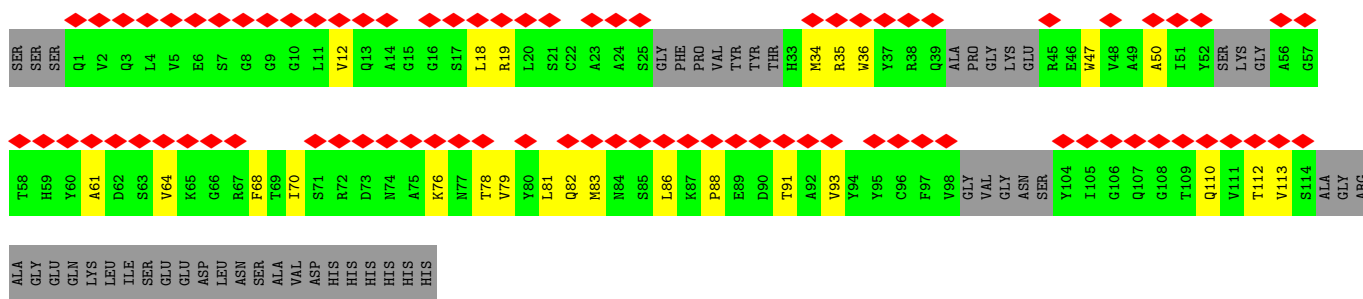


• Molecule 1: Calcium homeostasis modulator protein 4

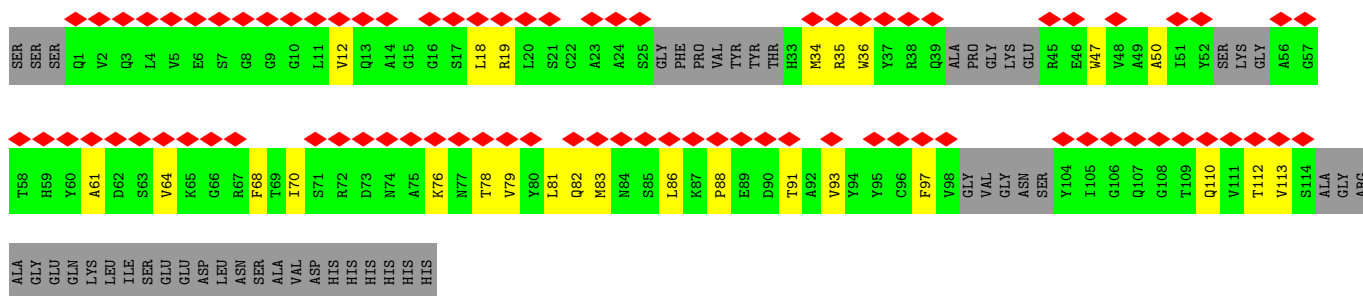




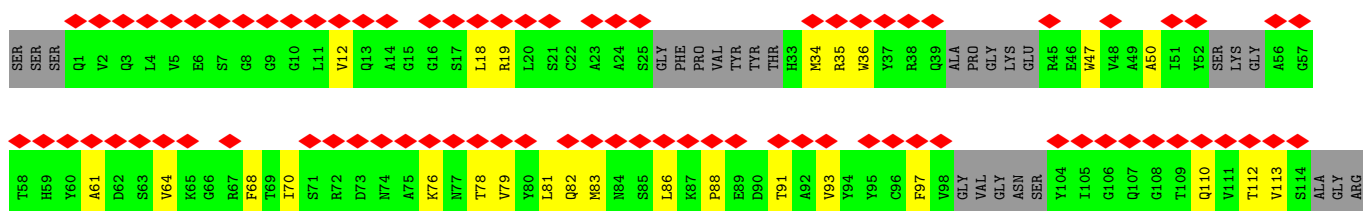
• Molecule 2: Synthetic nanobody SbC4



• Molecule 2: Synthetic nanobody SbC4

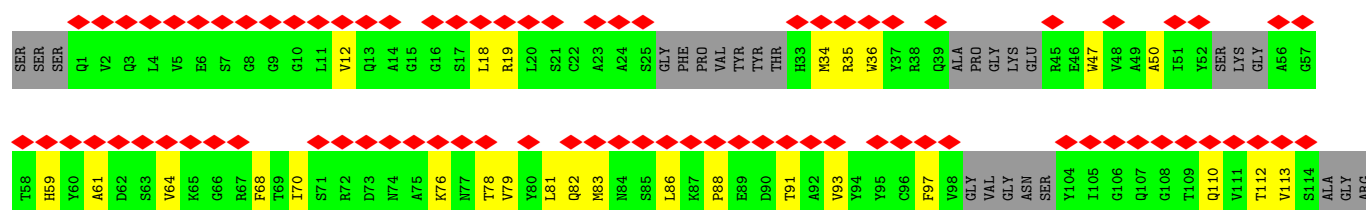


• Molecule 2: Synthetic nanobody SbC4



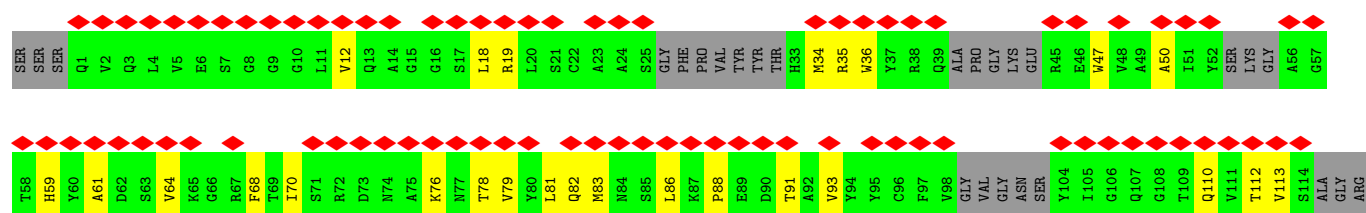
ALA
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ILE
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GLU
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SER
VAL
VAL
ASP
HIS
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HIS
HIS

• Molecule 2: Synthetic nanobody SbC4



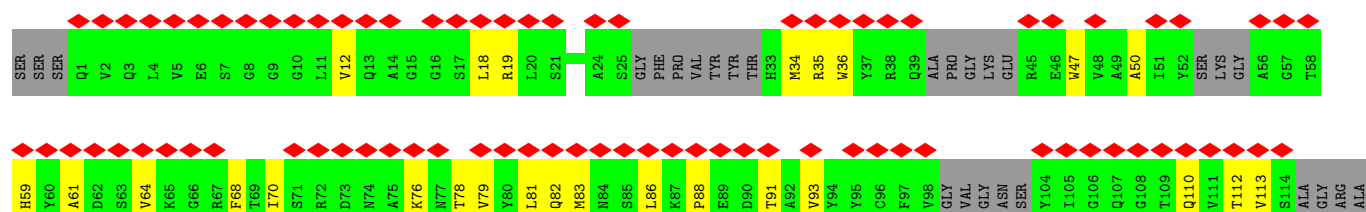
ALA
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• Molecule 2: Synthetic nanobody SbC4



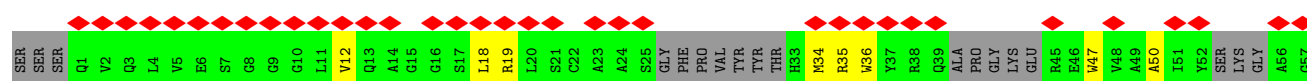
ALA
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• Molecule 2: Synthetic nanobody SbC4

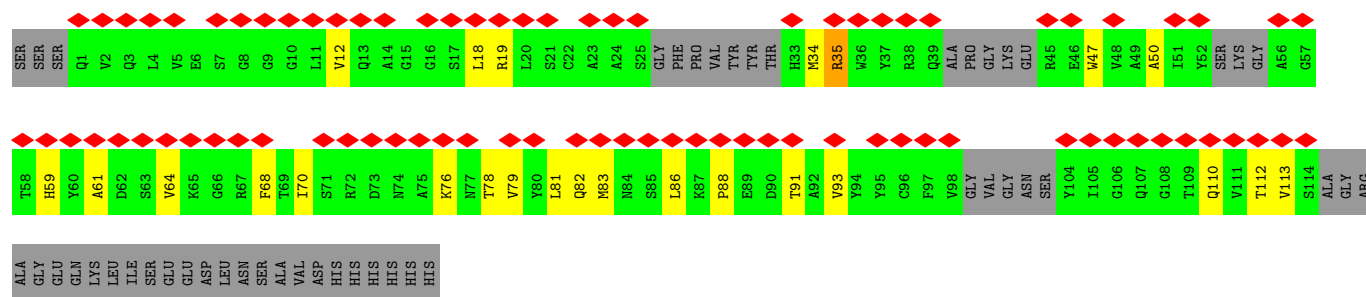


GLY
GLU
GLN
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GLU
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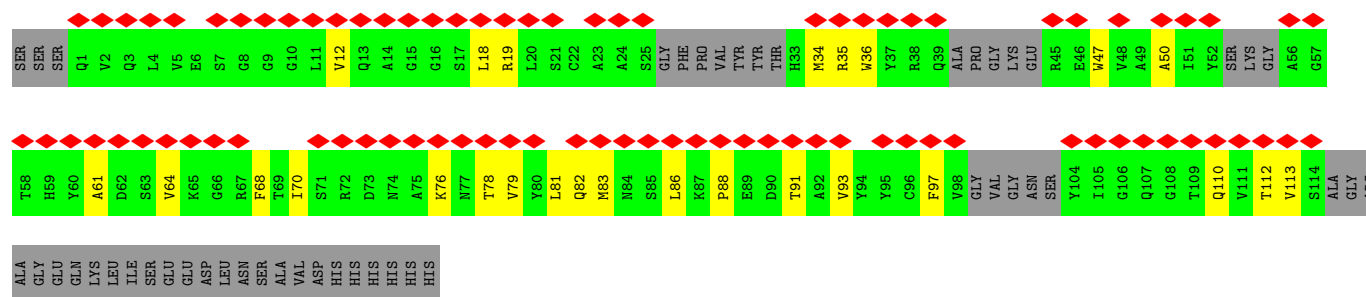
• Molecule 2: Synthetic nanobody SbC4



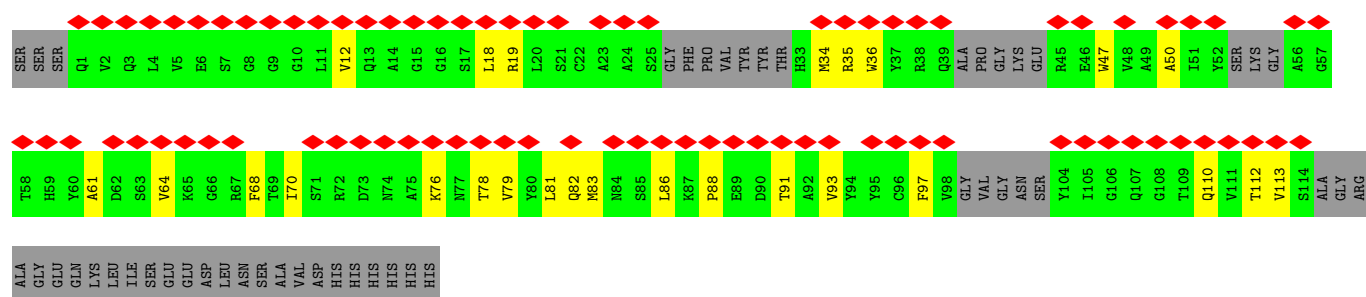




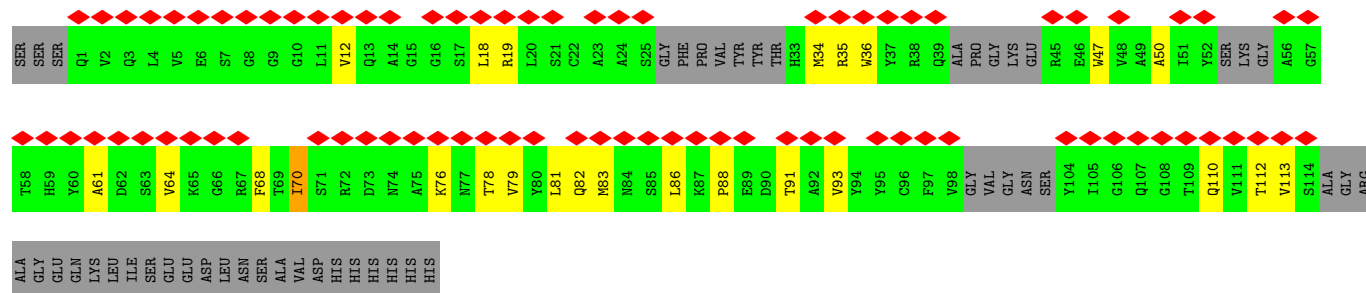
• Molecule 2: Synthetic nanobody SbC4



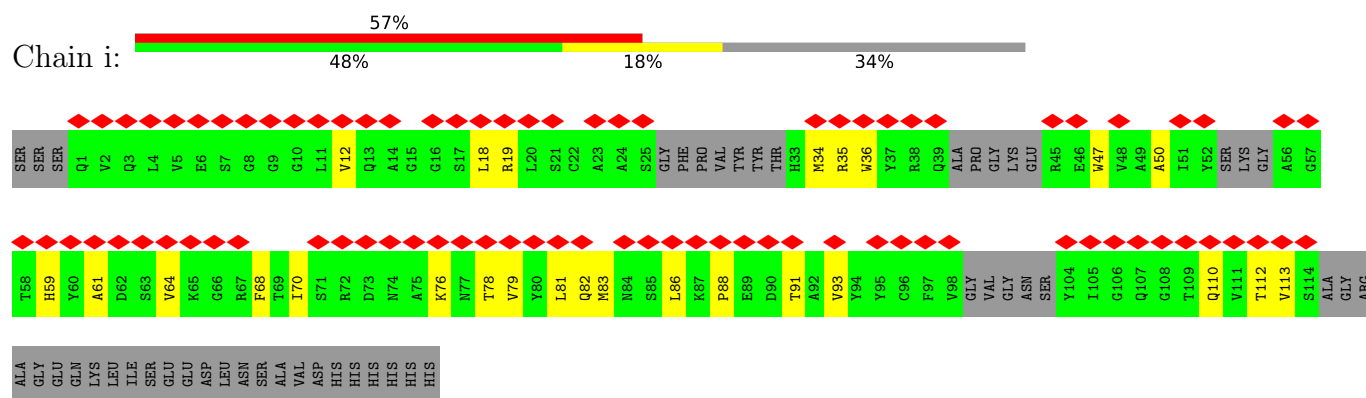
• Molecule 2: Synthetic nanobody SbC4



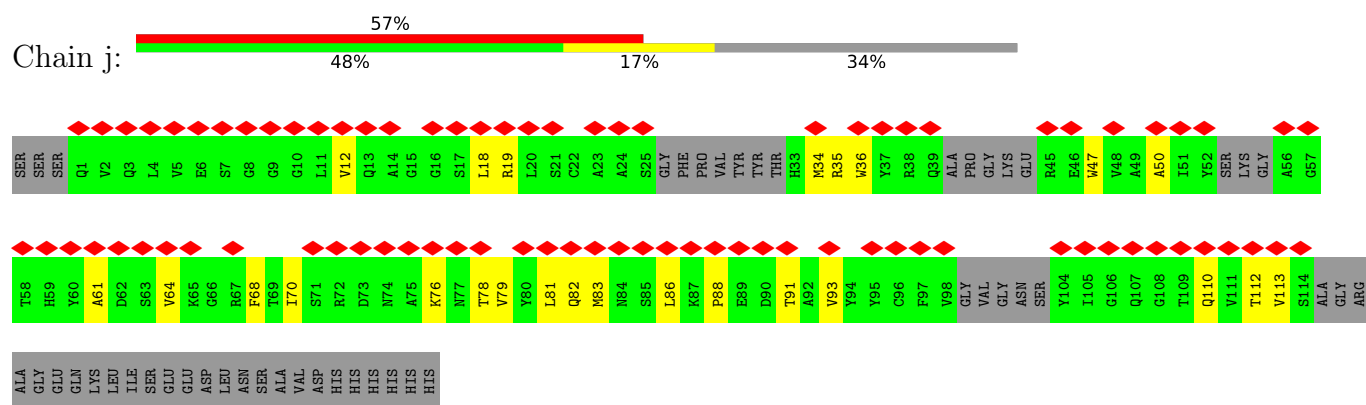
• Molecule 2: Synthetic nanobody SbC4



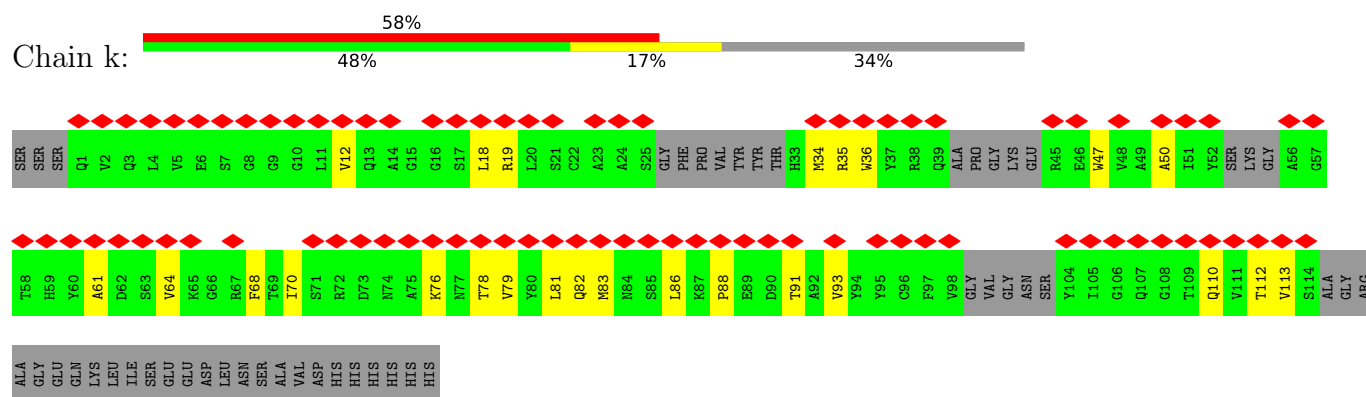
• Molecule 2: Synthetic nanobody SbC4



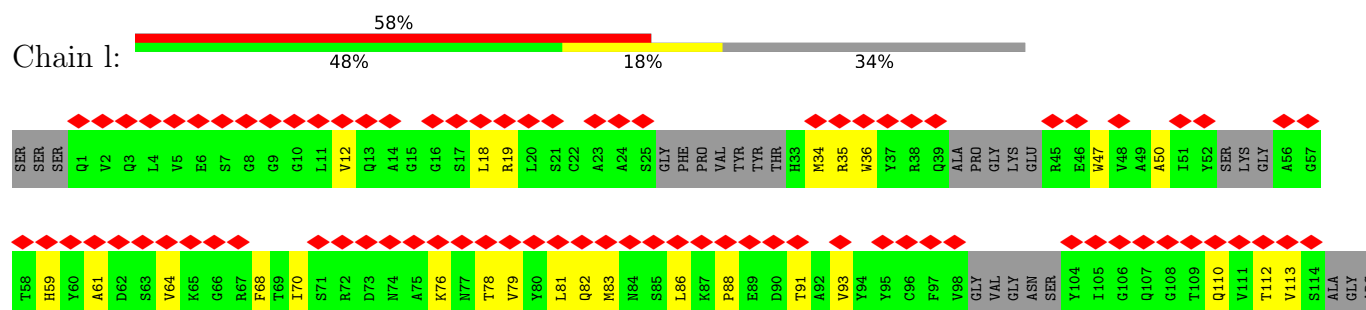
• Molecule 2: Synthetic nanobody SbC4



• Molecule 2: Synthetic nanobody SbC4



• Molecule 2: Synthetic nanobody SbC4



ALA	GLY	GLU	GLN	LYS	LEU	ILE	SER	GLU	GLU	ASP	LEU	ASN	SER	ALA	VAL	ASP	HIS	HIS	HIS	HIS	HIS	HIS
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● Molecule 2: Synthetic nanobody SbC4



SER	SER	SER	Q1	V2	Q3	L4	V5	E6	S7	G8	G9	G10	L11	V12	Q13	A14	G15	G16	S17	L18	R19	L20	S21	C22	A23	A24	S25	GLY	PHE	PRO	VAL	TYR	TYR	THR	H33	K34	R35	W36	Y37	R38	Q39	ALA	PRO	GLY	LYS	GLU	R45	E46	W47	V48	A49	A50	I51	Y52	SER	LYS	GLY	A56	G57
T58	H59	Y60	A61	D62	S63	V64	K65	G66	R67	F68	T69	I70	S71	R72	D73	N74	A75	K76	N77	T78	V79	Y80	L81	Q82	M83	N84	S85	L86	K87	P88	E89	D90	T91	A92	V93	Y94	Y95	C96	F97	V98	GLY	VAL	GLY	ASN	SER	Y104	I105	G106	Q107	G108	T109	Q110	V111	T112	V113	S114	ALA	GLY	ARG

ALA	GLY	GLU	GLN	LYS	LEU	ILE	SER	GLU	GLU	ASP	LEU	ASN	SER	ALA	VAL	ASP	HIS	HIS	HIS	HIS	HIS	HIS
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● Molecule 2: Synthetic nanobody SbC4



SER	SER	SER	Q1	V2	Q3	L4	V5	E6	S7	G8	G9	G10	L11	V12	Q13	A14	G15	G16	S17	L18	R19	L20	S21	C22	A23	A24	S25	GLY	PHE	PRO	VAL	TYR	THR	H33	K34	R35	W36	Y37	R38	Q39	ALA	PRO	GLY	LYS	GLU	R45	E46	W47	V48	A49	A50	I51	Y52	SER	LYS	GLY	A56	G57	
T58	H59	Y60	A61	D62	S63	V64	K65	G66	R67	F68	T69	I70	S71	R72	D73	N74	A75	K76	N77	T78	V79	Y80	L81	Q82	M83	N84	S85	L86	K87	P88	E89	D90	T91	A92	V93	Y94	Y95	C96	F97	V98	GLY	VAL	GLY	ASN	SER	Y104	I105	G106	Q107	G108	T109	Q110	V111	T112	V113	S114	ALA	GLY	ARG

ALA	GLY	GLU	GLN	LYS	LEU	ILE	SER	GLU	GLU	ASP	LEU	ASN	SER	ALA	VAL	ASP	HIS	HIS	HIS	HIS	HIS	HIS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D10	Depositor
Number of particles used	52248	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.014	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0058	Depositor
Map size (Å)	325.5, 325.5, 325.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.651, 0.651, 0.651	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/2086	0.42	0/2830
1	B	0.22	0/2086	0.42	0/2830
1	C	0.21	0/2086	0.41	0/2830
1	D	0.21	0/2086	0.42	0/2830
1	E	0.21	0/2086	0.41	0/2830
1	F	0.21	0/2086	0.41	0/2830
1	G	0.21	0/2086	0.41	0/2830
1	H	0.21	0/2086	0.41	0/2830
1	I	0.21	0/2086	0.41	0/2830
1	J	0.21	0/2086	0.41	0/2830
1	K	0.21	0/2086	0.41	0/2830
1	L	0.21	0/2086	0.41	0/2830
1	M	0.21	0/2086	0.42	0/2830
1	N	0.21	0/2086	0.41	0/2830
1	O	0.21	0/2086	0.41	0/2830
1	P	0.21	0/2086	0.41	0/2830
1	Q	0.21	0/2086	0.41	0/2830
1	R	0.21	0/2086	0.41	0/2830
1	S	0.21	0/2086	0.41	0/2830
1	T	0.21	0/2086	0.41	0/2830
2	U	0.13	0/744	0.31	0/1001
2	V	0.13	0/744	0.31	0/1001
2	W	0.13	0/744	0.31	0/1001
2	X	0.13	0/744	0.31	0/1001
2	Y	0.13	0/744	0.31	0/1001
2	Z	0.13	0/744	0.31	0/1001
2	a	0.13	0/744	0.31	0/1001
2	b	0.13	0/744	0.31	0/1001
2	c	0.13	0/744	0.31	0/1001
2	d	0.13	0/744	0.31	0/1001
2	e	0.23	0/744	0.36	0/1001
2	f	0.13	0/744	0.31	0/1001
2	g	0.13	0/744	0.31	0/1001
2	h	0.13	0/744	0.31	0/1001

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	i	0.13	0/744	0.31	0/1001
2	j	0.13	0/744	0.31	0/1001
2	k	0.13	0/744	0.31	0/1001
2	l	0.13	0/744	0.31	0/1001
2	m	0.13	0/744	0.31	0/1001
2	n	0.13	0/744	0.31	0/1001
All	All	0.19	0/56600	0.39	0/76620

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	e	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	e	35	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2039	0	2045	61	0
1	B	2039	0	2045	61	0
1	C	2039	0	2045	64	0
1	D	2039	0	2045	68	0
1	E	2039	0	2045	71	0
1	F	2039	0	2045	84	0
1	G	2039	0	2045	74	0
1	H	2039	0	2045	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2039	0	2045	62	0
1	J	2039	0	2045	62	0
1	K	2039	0	2045	66	0
1	L	2039	0	2045	62	0
1	M	2039	0	2045	65	0
1	N	2039	0	2045	64	0
1	O	2039	0	2045	62	0
1	P	2039	0	2045	60	0
1	Q	2039	0	2045	60	0
1	R	2039	0	2045	67	0
1	S	2039	0	2045	69	0
1	T	2039	0	2045	68	0
2	U	733	0	712	20	0
2	V	733	0	712	21	0
2	W	733	0	712	21	0
2	X	733	0	712	23	0
2	Y	733	0	712	23	0
2	Z	733	0	712	22	0
2	a	733	0	712	21	0
2	b	733	0	712	20	0
2	c	733	0	712	21	0
2	d	733	0	712	23	0
2	e	733	0	712	20	0
2	f	733	0	712	21	0
2	g	733	0	712	25	0
2	h	733	0	712	22	0
2	i	733	0	712	23	0
2	j	733	0	712	20	0
2	k	733	0	712	20	0
2	l	733	0	712	24	0
2	m	733	0	712	21	0
2	n	733	0	712	20	0
All	All	55440	0	55140	1509	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 14.

All (1509) 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:F:248:ILE:HD11	1:G:235:ALA:CB	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ASN:ND2	1:F:5:LEU:HD22	1.68	1.08
1:E:248:ILE:HD11	1:F:235:ALA:HB3	1.31	1.07
1:E:6:ASN:HD22	1:F:5:LEU:HD22	0.90	1.04
1:R:248:ILE:HD11	1:S:235:ALA:HB3	1.36	1.03
1:F:248:ILE:HD11	1:G:235:ALA:HB3	1.41	1.02
1:E:248:ILE:HD11	1:F:235:ALA:CB	1.90	1.01
1:E:248:ILE:CD1	1:F:235:ALA:HB3	1.94	0.97
1:L:248:ILE:HD11	1:M:235:ALA:HB3	1.46	0.94
1:F:254:PHE:CE2	1:G:238:GLN:NE2	2.38	0.92
1:F:248:ILE:CD1	1:G:235:ALA:CB	2.48	0.91
1:F:162:CYS:SG	1:F:163:CYS:N	2.45	0.90
1:I:162:CYS:SG	1:I:163:CYS:N	2.45	0.90
1:R:162:CYS:SG	1:R:163:CYS:N	2.45	0.90
1:R:248:ILE:HD11	1:S:235:ALA:CB	2.01	0.90
1:S:162:CYS:SG	1:S:163:CYS:N	2.45	0.90
1:H:162:CYS:SG	1:H:163:CYS:N	2.45	0.90
1:G:248:ILE:HD11	1:H:235:ALA:HB3	1.51	0.90
1:P:162:CYS:SG	1:P:163:CYS:N	2.45	0.89
1:H:248:ILE:HD11	1:I:235:ALA:HB3	1.54	0.89
1:G:162:CYS:SG	1:G:163:CYS:N	2.45	0.89
1:Q:162:CYS:SG	1:Q:163:CYS:N	2.45	0.89
1:J:162:CYS:SG	1:J:163:CYS:N	2.45	0.89
1:T:162:CYS:SG	1:T:163:CYS:N	2.45	0.89
1:C:162:CYS:SG	1:C:163:CYS:N	2.45	0.89
1:M:162:CYS:SG	1:M:163:CYS:N	2.45	0.89
1:L:162:CYS:SG	1:L:163:CYS:N	2.45	0.88
1:B:162:CYS:SG	1:B:163:CYS:N	2.45	0.88
1:O:162:CYS:SG	1:O:163:CYS:N	2.45	0.88
1:E:162:CYS:SG	1:E:163:CYS:N	2.45	0.88
1:D:162:CYS:SG	1:D:163:CYS:N	2.45	0.87
1:N:162:CYS:SG	1:N:163:CYS:N	2.45	0.87
1:A:162:CYS:SG	1:A:163:CYS:N	2.45	0.87
1:K:162:CYS:SG	1:K:163:CYS:N	2.45	0.87
2:g:19:ARG:HH11	2:g:82:GLN:HB2	1.43	0.83
2:Y:19:ARG:HH11	2:Y:82:GLN:HB2	1.43	0.83
2:i:19:ARG:HH11	2:i:82:GLN:HB2	1.43	0.83
2:W:19:ARG:HH11	2:W:82:GLN:HB2	1.43	0.83
2:j:19:ARG:HH11	2:j:82:GLN:HB2	1.43	0.83
2:Z:19:ARG:HH11	2:Z:82:GLN:HB2	1.43	0.82
2:b:19:ARG:HH11	2:b:82:GLN:HB2	1.43	0.82
1:R:248:ILE:CD1	1:S:235:ALA:HB3	2.07	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:19:ARG:HH11	2:V:82:GLN:HB2	1.43	0.82
2:n:19:ARG:HH11	2:n:82:GLN:HB2	1.43	0.82
2:d:19:ARG:HH11	2:d:82:GLN:HB2	1.43	0.82
2:f:19:ARG:HH11	2:f:82:GLN:HB2	1.43	0.82
1:L:248:ILE:CD1	1:M:235:ALA:HB3	2.09	0.82
2:X:19:ARG:HH11	2:X:82:GLN:HB2	1.43	0.82
2:e:19:ARG:HH11	2:e:82:GLN:HB2	1.43	0.81
2:h:19:ARG:HH11	2:h:82:GLN:HB2	1.43	0.81
2:U:19:ARG:HH11	2:U:82:GLN:HB2	1.43	0.81
2:a:19:ARG:HH11	2:a:82:GLN:HB2	1.43	0.81
2:m:19:ARG:HH11	2:m:82:GLN:HB2	1.43	0.81
2:c:19:ARG:HH11	2:c:82:GLN:HB2	1.43	0.81
2:k:19:ARG:HH11	2:k:82:GLN:HB2	1.43	0.81
1:F:248:ILE:CD1	1:G:235:ALA:HB3	2.08	0.80
1:L:248:ILE:HD11	1:M:235:ALA:CB	2.11	0.80
1:F:47:LYS:HD3	1:G:183:TYR:OH	1.81	0.80
1:F:276:SER:HA	1:H:216:LEU:CD1	2.13	0.79
1:H:77:ILE:HD11	1:H:103:ARG:HE	1.48	0.79
1:R:77:ILE:HD11	1:R:103:ARG:HE	1.48	0.79
1:S:241:ARG:HB2	1:T:227:ASN:ND2	1.98	0.79
1:Q:77:ILE:HD11	1:Q:103:ARG:HE	1.48	0.79
1:K:77:ILE:HD11	1:K:103:ARG:HE	1.48	0.79
1:A:77:ILE:HD11	1:A:103:ARG:HE	1.48	0.78
1:G:77:ILE:HD11	1:G:103:ARG:HE	1.48	0.78
1:I:77:ILE:HD11	1:I:103:ARG:HE	1.48	0.78
1:D:77:ILE:HD11	1:D:103:ARG:HE	1.48	0.78
1:E:248:ILE:CD1	1:F:235:ALA:CB	2.58	0.78
1:B:77:ILE:HD11	1:B:103:ARG:HE	1.48	0.78
1:E:77:ILE:HD11	1:E:103:ARG:HE	1.48	0.78
1:N:77:ILE:HD11	1:N:103:ARG:HE	1.48	0.78
1:F:276:SER:HA	1:H:216:LEU:HD13	1.65	0.78
1:L:77:ILE:HD11	1:L:103:ARG:HE	1.48	0.78
1:K:235:ALA:HB3	1:T:248:ILE:HD11	1.65	0.78
1:O:248:ILE:HD11	1:P:235:ALA:HB3	1.65	0.78
1:S:77:ILE:HD11	1:S:103:ARG:HE	1.48	0.78
1:C:77:ILE:HD11	1:C:103:ARG:HE	1.48	0.78
1:L:6:ASN:HD22	1:M:5:LEU:HD22	1.49	0.78
1:O:77:ILE:HD11	1:O:103:ARG:HE	1.48	0.78
1:M:77:ILE:HD11	1:M:103:ARG:HE	1.48	0.78
1:F:248:ILE:HD11	1:G:235:ALA:HB1	1.61	0.78
1:G:248:ILE:CD1	1:H:235:ALA:HB3	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:ILE:HD11	1:I:235:ALA:CB	2.14	0.78
2:I:19:ARG:HH11	2:I:82:GLN:HB2	1.49	0.78
1:P:77:ILE:HD11	1:P:103:ARG:HE	1.48	0.77
1:F:77:ILE:HD11	1:F:103:ARG:HE	1.48	0.77
1:J:77:ILE:HD11	1:J:103:ARG:HE	1.48	0.77
1:T:77:ILE:HD11	1:T:103:ARG:HE	1.48	0.77
1:C:6:ASN:HD22	1:D:5:LEU:HD22	1.50	0.77
1:N:248:ILE:HD11	1:O:235:ALA:HB3	1.66	0.76
1:G:248:ILE:HD11	1:H:235:ALA:CB	2.14	0.76
1:P:248:ILE:HD11	1:Q:235:ALA:HB3	1.67	0.76
1:R:6:ASN:HD22	1:S:5:LEU:HD22	1.51	0.76
1:K:227:ASN:ND2	1:T:241:ARG:HB2	2.00	0.76
1:C:241:ARG:HB2	1:D:227:ASN:ND2	2.01	0.75
1:C:248:ILE:HD11	1:D:235:ALA:HB3	1.69	0.75
1:R:169:ASP:OD2	2:I:59:HIS:CE1	2.40	0.75
1:M:182:ARG:NH1	1:M:186:GLN:OE1	2.20	0.75
1:I:182:ARG:NH1	1:I:186:GLN:OE1	2.20	0.75
1:S:182:ARG:NH1	1:S:186:GLN:OE1	2.20	0.75
1:C:182:ARG:NH1	1:C:186:GLN:OE1	2.20	0.75
1:H:182:ARG:NH1	1:H:186:GLN:OE1	2.20	0.75
1:M:146:ASP:H	2:g:35:ARG:HH22	1.35	0.75
1:O:182:ARG:NH1	1:O:186:GLN:OE1	2.20	0.75
1:R:182:ARG:NH1	1:R:186:GLN:OE1	2.20	0.75
1:E:182:ARG:NH1	1:E:186:GLN:OE1	2.20	0.75
1:A:182:ARG:NH1	1:A:186:GLN:OE1	2.20	0.75
1:J:182:ARG:NH1	1:J:186:GLN:OE1	2.20	0.75
1:K:182:ARG:NH1	1:K:186:GLN:OE1	2.20	0.75
1:P:182:ARG:NH1	1:P:186:GLN:OE1	2.20	0.75
1:T:182:ARG:NH1	1:T:186:GLN:OE1	2.20	0.74
1:D:182:ARG:NH1	1:D:186:GLN:OE1	2.20	0.74
1:N:182:ARG:NH1	1:N:186:GLN:OE1	2.20	0.74
1:A:235:ALA:HB3	1:J:248:ILE:HD11	1.68	0.74
1:F:182:ARG:NH1	1:F:186:GLN:OE1	2.20	0.74
1:B:182:ARG:NH1	1:B:186:GLN:OE1	2.20	0.74
1:L:182:ARG:NH1	1:L:186:GLN:OE1	2.20	0.74
1:K:248:ILE:HD11	1:L:235:ALA:HB3	1.68	0.74
1:G:182:ARG:NH1	1:G:186:GLN:OE1	2.20	0.74
1:Q:182:ARG:NH1	1:Q:186:GLN:OE1	2.20	0.74
1:R:241:ARG:HB2	1:S:227:ASN:ND2	2.03	0.74
1:F:71:ARG:HD3	1:F:107:ILE:HG23	1.71	0.73
1:K:71:ARG:HD3	1:K:107:ILE:HG23	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:HD3	1:A:107:ILE:HG23	1.71	0.73
1:N:51:TYR:OH	1:O:186:GLN:NE2	2.21	0.73
1:D:6:ASN:HD22	1:E:5:LEU:HD22	1.52	0.73
1:E:71:ARG:HD3	1:E:107:ILE:HG23	1.71	0.73
1:T:71:ARG:HD3	1:T:107:ILE:HG23	1.71	0.73
1:O:71:ARG:HD3	1:O:107:ILE:HG23	1.71	0.73
1:J:71:ARG:HD3	1:J:107:ILE:HG23	1.71	0.73
1:P:71:ARG:HD3	1:P:107:ILE:HG23	1.71	0.73
1:S:71:ARG:HD3	1:S:107:ILE:HG23	1.71	0.72
1:B:71:ARG:HD3	1:B:107:ILE:HG23	1.71	0.72
1:D:71:ARG:HD3	1:D:107:ILE:HG23	1.71	0.72
1:L:71:ARG:HD3	1:L:107:ILE:HG23	1.71	0.72
1:N:71:ARG:HD3	1:N:107:ILE:HG23	1.71	0.72
1:G:71:ARG:HD3	1:G:107:ILE:HG23	1.71	0.72
1:I:71:ARG:HD3	1:I:107:ILE:HG23	1.71	0.72
1:K:5:LEU:HD22	1:T:6:ASN:HD22	1.55	0.72
1:N:248:ILE:HD11	1:O:235:ALA:CB	2.18	0.72
1:O:6:ASN:HD22	1:P:5:LEU:HD22	1.55	0.72
1:R:71:ARG:HD3	1:R:107:ILE:HG23	1.71	0.72
1:Q:71:ARG:HD3	1:Q:107:ILE:HG23	1.71	0.71
1:H:71:ARG:HD3	1:H:107:ILE:HG23	1.71	0.71
1:F:144:MET:O	2:Z:35:ARG:NH2	2.23	0.71
1:C:71:ARG:HD3	1:C:107:ILE:HG23	1.71	0.71
1:M:71:ARG:HD3	1:M:107:ILE:HG23	1.71	0.71
1:F:272:TRP:HZ3	1:G:232:PHE:HZ	1.37	0.71
1:O:248:ILE:HD11	1:P:235:ALA:CB	2.21	0.70
1:J:146:ASP:H	2:d:35:ARG:HH22	1.40	0.70
1:I:248:ILE:HD11	1:J:235:ALA:HB3	1.73	0.70
2:e:18:LEU:HB3	2:e:83:MET:HE2	1.74	0.69
2:U:18:LEU:HB3	2:U:83:MET:HE2	1.74	0.69
2:n:18:LEU:HB3	2:n:83:MET:HE2	1.74	0.69
2:j:18:LEU:HB3	2:j:83:MET:HE2	1.75	0.69
2:a:18:LEU:HB3	2:a:83:MET:HE2	1.74	0.69
2:c:18:LEU:HB3	2:c:83:MET:HE2	1.75	0.69
2:d:18:LEU:HB3	2:d:83:MET:HE2	1.74	0.69
1:R:260:ASP:OD2	1:S:238:GLN:NE2	2.26	0.69
2:W:18:LEU:HB3	2:W:83:MET:HE2	1.74	0.69
2:X:18:LEU:HB3	2:X:83:MET:HE2	1.75	0.69
2:h:18:LEU:HB3	2:h:83:MET:HE2	1.75	0.69
2:k:18:LEU:HB3	2:k:83:MET:HE2	1.74	0.69
2:l:18:LEU:HB3	2:l:83:MET:HE2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:18:LEU:HB3	2:f:83:MET:HE2	1.74	0.69
2:i:18:LEU:HB3	2:i:83:MET:HE2	1.75	0.69
2:m:18:LEU:HB3	2:m:83:MET:HE2	1.74	0.69
1:M:6:ASN:HD22	1:N:5:LEU:HD22	1.57	0.69
2:Z:18:LEU:HB3	2:Z:83:MET:HE2	1.74	0.69
2:g:18:LEU:HB3	2:g:83:MET:HE2	1.74	0.69
2:V:18:LEU:HB3	2:V:83:MET:HE2	1.74	0.68
2:X:91:THR:HG23	2:X:112:THR:HA	1.76	0.68
2:Y:18:LEU:HB3	2:Y:83:MET:HE2	1.74	0.68
2:b:18:LEU:HB3	2:b:83:MET:HE2	1.74	0.68
2:a:91:THR:HG23	2:a:112:THR:HA	1.76	0.68
2:b:91:THR:HG23	2:b:112:THR:HA	1.76	0.68
2:h:91:THR:HG23	2:h:112:THR:HA	1.76	0.68
2:W:91:THR:HG23	2:W:112:THR:HA	1.76	0.68
2:i:91:THR:HG23	2:i:112:THR:HA	1.76	0.68
2:k:91:THR:HG23	2:k:112:THR:HA	1.76	0.68
2:g:91:THR:HG23	2:g:112:THR:HA	1.76	0.68
2:Y:91:THR:HG23	2:Y:112:THR:HA	1.76	0.68
2:Z:91:THR:HG23	2:Z:112:THR:HA	1.76	0.68
2:e:91:THR:HG23	2:e:112:THR:HA	1.76	0.67
2:j:91:THR:HG23	2:j:112:THR:HA	1.76	0.67
2:l:91:THR:HG23	2:l:112:THR:HA	1.76	0.67
2:c:91:THR:HG23	2:c:112:THR:HA	1.76	0.67
1:E:254:PHE:CE2	1:F:238:GLN:NE2	2.63	0.67
2:V:91:THR:HG23	2:V:112:THR:HA	1.76	0.67
2:U:91:THR:HG23	2:U:112:THR:HA	1.76	0.67
2:d:91:THR:HG23	2:d:112:THR:HA	1.76	0.67
2:f:91:THR:HG23	2:f:112:THR:HA	1.76	0.67
2:m:91:THR:HG23	2:m:112:THR:HA	1.76	0.67
2:n:91:THR:HG23	2:n:112:THR:HA	1.76	0.66
1:A:186:GLN:NE2	1:J:51:TYR:OH	2.30	0.65
1:A:248:ILE:HD11	1:B:235:ALA:HB3	1.78	0.65
1:H:6:ASN:HD22	1:I:5:LEU:HD22	1.61	0.65
1:F:160:PHE:HB2	1:F:174:ARG:HH21	1.62	0.65
1:M:160:PHE:HB2	1:M:174:ARG:HH21	1.62	0.65
1:Q:232:PHE:CE2	1:R:216:LEU:HB3	2.31	0.65
1:C:160:PHE:HB2	1:C:174:ARG:HH21	1.62	0.65
1:K:142:TYR:OH	1:K:176:GLU:OE1	2.13	0.64
1:K:235:ALA:HB3	1:T:248:ILE:CD1	2.27	0.64
1:O:165:SER:HA	1:O:174:ARG:HH12	1.63	0.64
1:O:160:PHE:HB2	1:O:174:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:6:ASN:HD22	1:Q:5:LEU:HD22	1.61	0.64
1:C:165:SER:HA	1:C:174:ARG:HH12	1.63	0.64
1:E:165:SER:HA	1:E:174:ARG:HH12	1.63	0.64
1:G:165:SER:HA	1:G:174:ARG:HH12	1.63	0.64
1:G:241:ARG:HB2	1:H:227:ASN:ND2	2.12	0.64
1:P:160:PHE:HB2	1:P:174:ARG:HH21	1.62	0.64
1:Q:165:SER:HA	1:Q:174:ARG:HH12	1.63	0.64
1:C:248:ILE:CD1	1:D:235:ALA:HB3	2.27	0.64
1:M:165:SER:HA	1:M:174:ARG:HH12	1.63	0.64
1:A:160:PHE:HB2	1:A:174:ARG:HH21	1.62	0.64
1:R:165:SER:HA	1:R:174:ARG:HH12	1.63	0.64
1:S:165:SER:HA	1:S:174:ARG:HH12	1.63	0.64
1:E:160:PHE:HB2	1:E:174:ARG:HH21	1.62	0.64
1:H:165:SER:HA	1:H:174:ARG:HH12	1.63	0.64
1:F:165:SER:HA	1:F:174:ARG:HH12	1.63	0.64
1:H:160:PHE:HB2	1:H:174:ARG:HH21	1.62	0.64
1:K:160:PHE:HB2	1:K:174:ARG:HH21	1.62	0.64
1:Q:160:PHE:HB2	1:Q:174:ARG:HH21	1.62	0.64
1:R:160:PHE:HB2	1:R:174:ARG:HH21	1.62	0.64
1:F:276:SER:CA	1:H:216:LEU:HD13	2.28	0.64
1:I:165:SER:HA	1:I:174:ARG:HH12	1.63	0.64
1:J:160:PHE:HB2	1:J:174:ARG:HH21	1.62	0.64
1:R:169:ASP:OD2	2:I:59:HIS:HE1	1.78	0.63
1:T:160:PHE:HB2	1:T:174:ARG:HH21	1.62	0.63
1:T:165:SER:HA	1:T:174:ARG:HH12	1.63	0.63
1:D:160:PHE:HB2	1:D:174:ARG:HH21	1.62	0.63
1:K:165:SER:HA	1:K:174:ARG:HH12	1.63	0.63
1:N:160:PHE:HB2	1:N:174:ARG:HH21	1.62	0.63
1:P:165:SER:HA	1:P:174:ARG:HH12	1.63	0.63
1:A:165:SER:HA	1:A:174:ARG:HH12	1.63	0.63
1:J:165:SER:HA	1:J:174:ARG:HH12	1.63	0.63
1:L:241:ARG:HB2	1:M:227:ASN:ND2	2.12	0.63
1:L:160:PHE:HB2	1:L:174:ARG:HH21	1.62	0.63
1:S:160:PHE:HB2	1:S:174:ARG:HH21	1.62	0.63
1:B:160:PHE:HB2	1:B:174:ARG:HH21	1.62	0.63
1:G:160:PHE:HB2	1:G:174:ARG:HH21	1.62	0.63
1:I:160:PHE:HB2	1:I:174:ARG:HH21	1.62	0.63
1:N:165:SER:HA	1:N:174:ARG:HH12	1.63	0.63
1:B:165:SER:HA	1:B:174:ARG:HH12	1.63	0.63
1:D:165:SER:HA	1:D:174:ARG:HH12	1.63	0.63
1:S:244:MET:SD	1:T:228:GLU:HB2	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:248:ILE:HD11	1:T:235:ALA:HB3	1.80	0.63
1:L:165:SER:HA	1:L:174:ARG:HH12	1.63	0.63
1:C:256:PRO:HB3	1:D:235:ALA:HB2	1.79	0.62
1:F:51:TYR:OH	1:G:186:GLN:NE2	2.32	0.62
1:P:248:ILE:HD11	1:Q:235:ALA:CB	2.29	0.62
1:A:227:ASN:ND2	1:J:241:ARG:HB2	2.14	0.62
1:S:240:SER:OG	1:T:224:HIS:HB2	1.98	0.62
1:A:241:ARG:HB2	1:B:227:ASN:ND2	2.14	0.62
1:A:235:ALA:HB3	1:J:248:ILE:CD1	2.30	0.62
1:I:19:ILE:HG21	1:I:110:ARG:HH21	1.66	0.61
1:S:19:ILE:HG21	1:S:110:ARG:HH21	1.66	0.61
1:A:19:ILE:HG21	1:A:110:ARG:HH21	1.66	0.61
1:F:19:ILE:HG21	1:F:110:ARG:HH21	1.66	0.61
1:G:6:ASN:HD22	1:H:5:LEU:HD22	1.65	0.61
1:K:19:ILE:HG21	1:K:110:ARG:HH21	1.66	0.61
1:B:19:ILE:HG21	1:B:110:ARG:HH21	1.66	0.61
1:L:19:ILE:HG21	1:L:110:ARG:HH21	1.66	0.61
1:A:6:ASN:HD22	1:B:5:LEU:HD22	1.65	0.61
1:G:19:ILE:HG21	1:G:110:ARG:HH21	1.65	0.61
1:J:19:ILE:HG21	1:J:110:ARG:HH21	1.66	0.61
1:O:51:TYR:OH	1:P:186:GLN:NE2	2.34	0.61
1:P:19:ILE:HG21	1:P:110:ARG:HH21	1.66	0.61
1:Q:232:PHE:CD2	1:R:216:LEU:HD23	2.35	0.61
1:Q:232:PHE:CZ	1:R:216:LEU:HB3	2.36	0.61
1:T:19:ILE:HG21	1:T:110:ARG:HH21	1.66	0.61
1:O:19:ILE:HG21	1:O:110:ARG:HH21	1.65	0.60
1:O:169:ASP:OD2	2:i:59:HIS:CE1	2.54	0.60
1:D:19:ILE:HG21	1:D:110:ARG:HH21	1.66	0.60
1:E:19:ILE:HG21	1:E:110:ARG:HH21	1.66	0.60
1:I:6:ASN:HD22	1:J:5:LEU:HD22	1.66	0.60
1:R:19:ILE:HG21	1:R:110:ARG:HH21	1.66	0.60
1:N:19:ILE:HG21	1:N:110:ARG:HH21	1.66	0.60
1:Q:19:ILE:HG21	1:Q:110:ARG:HH21	1.66	0.60
1:H:19:ILE:HG21	1:H:110:ARG:HH21	1.66	0.60
1:H:248:ILE:CD1	1:I:235:ALA:HB3	2.28	0.60
1:G:39:PHE:O	1:G:51:TYR:OH	2.17	0.60
1:H:260:ASP:OD2	1:I:238:GLN:NE2	2.35	0.60
1:I:241:ARG:HB2	1:J:227:ASN:ND2	2.16	0.60
1:K:248:ILE:HD11	1:L:235:ALA:CB	2.32	0.60
1:G:142:TYR:OH	1:G:176:GLU:OE1	2.13	0.59
1:Q:39:PHE:O	1:Q:51:TYR:OH	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:PHE:O	1:J:51:TYR:OH	2.17	0.59
1:A:235:ALA:CB	1:J:248:ILE:HD11	2.31	0.59
1:M:19:ILE:HG21	1:M:110:ARG:HH21	1.66	0.59
1:D:241:ARG:HB2	1:E:227:ASN:ND2	2.18	0.59
1:T:39:PHE:O	1:T:51:TYR:OH	2.17	0.59
1:C:19:ILE:HG21	1:C:110:ARG:HH21	1.66	0.59
1:F:272:TRP:HZ3	1:G:232:PHE:CZ	2.20	0.59
1:J:103:ARG:HD3	1:J:225:LEU:HD13	1.85	0.59
1:T:103:ARG:HD3	1:T:225:LEU:HD13	1.85	0.59
1:I:71:ARG:HD3	1:I:107:ILE:HD12	1.86	0.58
1:J:71:ARG:HD3	1:J:107:ILE:HD12	1.86	0.58
1:K:241:ARG:HB2	1:L:227:ASN:ND2	2.17	0.58
1:P:241:ARG:HB2	1:Q:227:ASN:ND2	2.17	0.58
1:S:71:ARG:HD3	1:S:107:ILE:HD12	1.86	0.58
1:T:71:ARG:HD3	1:T:107:ILE:HD12	1.86	0.58
1:G:103:ARG:HD3	1:G:225:LEU:HD13	1.85	0.58
1:K:103:ARG:HD3	1:K:225:LEU:HD13	1.85	0.58
1:O:248:ILE:CD1	1:P:235:ALA:HB3	2.33	0.58
1:Q:103:ARG:HD3	1:Q:225:LEU:HD13	1.85	0.58
1:A:71:ARG:HD3	1:A:107:ILE:HD12	1.85	0.58
1:A:103:ARG:HD3	1:A:225:LEU:HD13	1.85	0.58
1:D:103:ARG:HD3	1:D:225:LEU:HD13	1.85	0.58
1:D:256:PRO:HB3	1:E:235:ALA:HB2	1.85	0.58
1:E:103:ARG:HD3	1:E:225:LEU:HD13	1.85	0.58
1:I:103:ARG:HD3	1:I:225:LEU:HD13	1.85	0.58
1:O:103:ARG:HD3	1:O:225:LEU:HD13	1.85	0.58
1:O:144:MET:O	2:i:35:ARG:NH2	2.37	0.58
1:K:71:ARG:HD3	1:K:107:ILE:HD12	1.86	0.58
1:K:235:ALA:HB2	1:T:256:PRO:HB3	1.85	0.58
1:N:103:ARG:HD3	1:N:225:LEU:HD13	1.85	0.58
1:B:244:MET:O	1:B:248:ILE:HG22	2.04	0.58
1:G:71:ARG:HD3	1:G:107:ILE:HD12	1.85	0.58
1:H:71:ARG:HD3	1:H:107:ILE:HD12	1.85	0.58
1:Q:71:ARG:HD3	1:Q:107:ILE:HD12	1.86	0.58
1:A:244:MET:O	1:A:248:ILE:HG22	2.04	0.58
1:F:244:MET:O	1:F:248:ILE:HG22	2.04	0.58
1:K:244:MET:O	1:K:248:ILE:HG22	2.04	0.58
1:D:244:MET:O	1:D:248:ILE:HG22	2.04	0.58
1:F:6:ASN:HD22	1:G:5:LEU:HD22	1.69	0.58
1:L:244:MET:O	1:L:248:ILE:HG22	2.04	0.58
1:N:244:MET:O	1:N:248:ILE:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:71:ARG:HD3	1:R:107:ILE:HD12	1.86	0.58
1:R:103:ARG:HD3	1:R:225:LEU:HD13	1.85	0.58
1:S:103:ARG:HD3	1:S:225:LEU:HD13	1.85	0.58
1:C:103:ARG:HD3	1:C:225:LEU:HD13	1.85	0.57
1:H:103:ARG:HD3	1:H:225:LEU:HD13	1.85	0.57
1:J:244:MET:O	1:J:248:ILE:HG22	2.04	0.57
1:M:51:TYR:OH	1:N:186:GLN:NE2	2.37	0.57
1:M:244:MET:O	1:M:248:ILE:HG22	2.04	0.57
1:F:71:ARG:HD3	1:F:107:ILE:HD12	1.85	0.57
1:F:103:ARG:HD3	1:F:225:LEU:HD13	1.85	0.57
1:G:51:TYR:OH	1:H:186:GLN:NE2	2.37	0.57
1:P:103:ARG:HD3	1:P:225:LEU:HD13	1.85	0.57
1:P:244:MET:O	1:P:248:ILE:HG22	2.04	0.57
1:Q:244:MET:O	1:Q:248:ILE:HG22	2.04	0.57
1:R:248:ILE:CD1	1:S:235:ALA:CB	2.75	0.57
1:S:232:PHE:CZ	1:T:216:LEU:HB3	2.39	0.57
1:S:244:MET:O	1:S:248:ILE:HG22	2.04	0.57
1:T:244:MET:O	1:T:248:ILE:HG22	2.04	0.57
2:Z:34:MET:HG3	2:Z:79:VAL:HG21	1.87	0.57
2:k:34:MET:HG3	2:k:79:VAL:HG21	1.87	0.57
1:C:244:MET:O	1:C:248:ILE:HG22	2.04	0.57
1:D:51:TYR:HD2	1:E:183:TYR:HD1	1.51	0.57
1:I:244:MET:O	1:I:248:ILE:HG22	2.04	0.57
1:Q:77:ILE:HD11	1:Q:103:ARG:NE	2.19	0.57
1:R:244:MET:O	1:R:248:ILE:HG22	2.04	0.57
2:j:34:MET:HG3	2:j:79:VAL:HG21	1.87	0.57
1:E:142:TYR:OH	1:E:176:GLU:OE1	2.13	0.57
1:H:244:MET:O	1:H:248:ILE:HG22	2.04	0.57
1:L:71:ARG:HD3	1:L:107:ILE:HD12	1.85	0.57
1:M:103:ARG:HD3	1:M:225:LEU:HD13	1.85	0.57
1:T:142:TYR:OH	1:T:176:GLU:OE1	2.13	0.57
2:a:34:MET:HG3	2:a:79:VAL:HG21	1.87	0.57
1:B:103:ARG:HD3	1:B:225:LEU:HD13	1.85	0.57
1:L:103:ARG:HD3	1:L:225:LEU:HD13	1.85	0.57
1:P:71:ARG:HD3	1:P:107:ILE:HD12	1.85	0.57
1:B:71:ARG:HD3	1:B:107:ILE:HD12	1.86	0.57
1:G:244:MET:O	1:G:248:ILE:HG22	2.04	0.57
1:P:110:ARG:HA	1:P:113:ILE:HG22	1.86	0.57
2:W:34:MET:HG3	2:W:79:VAL:HG21	1.87	0.57
1:E:71:ARG:HD3	1:E:107:ILE:HD12	1.86	0.57
1:E:77:ILE:HD11	1:E:103:ARG:NE	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:ARG:HA	1:G:113:ILE:HG22	1.86	0.57
1:M:71:ARG:HD3	1:M:107:ILE:HD12	1.85	0.57
1:N:77:ILE:HD11	1:N:103:ARG:NE	2.19	0.57
1:N:248:ILE:CD1	1:O:235:ALA:HB3	2.33	0.57
1:O:77:ILE:HD11	1:O:103:ARG:NE	2.19	0.57
1:P:39:PHE:O	1:P:51:TYR:OH	2.17	0.57
1:R:110:ARG:HA	1:R:113:ILE:HG22	1.86	0.57
2:V:34:MET:HG3	2:V:79:VAL:HG21	1.87	0.57
2:l:34:MET:HG3	2:l:79:VAL:HG21	1.87	0.57
1:D:77:ILE:HD11	1:D:103:ARG:NE	2.19	0.57
1:O:71:ARG:HD3	1:O:107:ILE:HD12	1.86	0.57
1:Q:110:ARG:HA	1:Q:113:ILE:HG22	1.86	0.57
2:i:34:MET:HG3	2:i:79:VAL:HG21	1.87	0.57
1:E:110:ARG:HA	1:E:113:ILE:HG22	1.86	0.57
1:F:110:ARG:HA	1:F:113:ILE:HG22	1.86	0.57
1:H:110:ARG:HA	1:H:113:ILE:HG22	1.86	0.57
1:J:142:TYR:OH	1:J:176:GLU:OE1	2.13	0.57
1:O:110:ARG:HA	1:O:113:ILE:HG22	1.86	0.57
1:C:71:ARG:HD3	1:C:107:ILE:HD12	1.86	0.57
1:E:39:PHE:O	1:E:51:TYR:OH	2.17	0.57
1:F:142:TYR:OH	1:F:176:GLU:OE1	2.13	0.57
1:H:77:ILE:HD11	1:H:103:ARG:NE	2.19	0.57
1:Q:240:SER:OG	1:R:224:HIS:HB2	2.05	0.57
2:f:34:MET:HG3	2:f:79:VAL:HG21	1.87	0.57
2:g:34:MET:HG3	2:g:79:VAL:HG21	1.87	0.57
2:m:34:MET:HG3	2:m:79:VAL:HG21	1.87	0.57
2:n:34:MET:HG3	2:n:79:VAL:HG21	1.86	0.57
1:A:110:ARG:HA	1:A:113:ILE:HG22	1.86	0.56
1:E:244:MET:O	1:E:248:ILE:HG22	2.04	0.56
1:K:110:ARG:HA	1:K:113:ILE:HG22	1.86	0.56
1:M:77:ILE:HD11	1:M:103:ARG:NE	2.19	0.56
1:S:110:ARG:HA	1:S:113:ILE:HG22	1.86	0.56
2:Y:34:MET:HG3	2:Y:79:VAL:HG21	1.86	0.56
2:d:35:ARG:HD3	2:d:47:TRP:HZ3	1.70	0.56
2:k:35:ARG:HD3	2:k:47:TRP:HZ3	1.70	0.56
2:n:47:TRP:CH2	2:n:50:ALA:HB2	2.40	0.56
2:U:35:ARG:HD3	2:U:47:TRP:HZ3	1.70	0.56
2:U:47:TRP:CH2	2:U:50:ALA:HB2	2.41	0.56
1:I:110:ARG:HA	1:I:113:ILE:HG22	1.86	0.56
2:V:47:TRP:CH2	2:V:50:ALA:HB2	2.40	0.56
2:a:35:ARG:HD3	2:a:47:TRP:HZ3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:34:MET:HG3	2:b:79:VAL:HG21	1.87	0.56
2:f:47:TRP:CH2	2:f:50:ALA:HB2	2.41	0.56
2:j:47:TRP:CH2	2:j:50:ALA:HB2	2.40	0.56
2:n:35:ARG:HD3	2:n:47:TRP:HZ3	1.70	0.56
1:C:77:ILE:HD11	1:C:103:ARG:NE	2.19	0.56
1:H:241:ARG:HB2	1:I:227:ASN:ND2	2.19	0.56
1:K:248:ILE:CD1	1:L:235:ALA:HB3	2.35	0.56
1:O:244:MET:O	1:O:248:ILE:HG22	2.04	0.56
1:P:77:ILE:HD11	1:P:103:ARG:NE	2.19	0.56
1:R:77:ILE:HD11	1:R:103:ARG:NE	2.19	0.56
2:Y:35:ARG:HD3	2:Y:47:TRP:HZ3	1.70	0.56
2:Z:47:TRP:CH2	2:Z:50:ALA:HB2	2.40	0.56
2:b:35:ARG:HD3	2:b:47:TRP:HZ3	1.70	0.56
2:d:34:MET:HG3	2:d:79:VAL:HG21	1.87	0.56
2:d:47:TRP:CH2	2:d:50:ALA:HB2	2.40	0.56
2:e:47:TRP:CH2	2:e:50:ALA:HB2	2.41	0.56
2:i:35:ARG:HD3	2:i:47:TRP:HZ3	1.70	0.56
2:U:34:MET:HG3	2:U:79:VAL:HG21	1.87	0.56
1:I:39:PHE:O	1:I:51:TYR:OH	2.17	0.56
1:I:142:TYR:OH	1:I:176:GLU:OE1	2.13	0.56
1:L:260:ASP:OD2	1:M:238:GLN:NE2	2.37	0.56
2:W:35:ARG:HD3	2:W:47:TRP:HZ3	1.70	0.56
2:X:34:MET:HG3	2:X:79:VAL:HG21	1.86	0.56
2:a:47:TRP:CH2	2:a:50:ALA:HB2	2.40	0.56
2:l:35:ARG:HD3	2:l:47:TRP:HZ3	1.71	0.56
1:C:51:TYR:OH	1:D:186:GLN:NE2	2.38	0.56
1:I:77:ILE:HD11	1:I:103:ARG:NE	2.19	0.56
1:L:248:ILE:CD1	1:M:235:ALA:CB	2.79	0.56
1:N:71:ARG:HD3	1:N:107:ILE:HD12	1.85	0.56
2:V:35:ARG:HD3	2:V:47:TRP:HZ3	1.70	0.56
2:Y:47:TRP:CH2	2:Y:50:ALA:HB2	2.40	0.56
2:g:35:ARG:HD3	2:g:47:TRP:HZ3	1.70	0.56
2:g:47:TRP:CH2	2:g:50:ALA:HB2	2.40	0.56
2:k:47:TRP:CH2	2:k:50:ALA:HB2	2.41	0.56
1:D:71:ARG:HD3	1:D:107:ILE:HD12	1.85	0.56
1:J:110:ARG:HA	1:J:113:ILE:HG22	1.86	0.56
1:L:39:PHE:O	1:L:51:TYR:OH	2.17	0.56
1:S:77:ILE:HD11	1:S:103:ARG:NE	2.19	0.56
2:W:47:TRP:CH2	2:W:50:ALA:HB2	2.41	0.56
2:m:47:TRP:CH2	2:m:50:ALA:HB2	2.41	0.56
1:D:110:ARG:HA	1:D:113:ILE:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:146:ASP:H	2:d:35:ARG:NH2	2.01	0.56
1:S:39:PHE:O	1:S:51:TYR:OH	2.17	0.56
2:c:34:MET:HG3	2:c:79:VAL:HG21	1.87	0.56
2:i:47:TRP:CH2	2:i:50:ALA:HB2	2.41	0.56
1:B:77:ILE:HD11	1:B:103:ARG:NE	2.19	0.56
1:N:110:ARG:HA	1:N:113:ILE:HG22	1.86	0.56
1:T:110:ARG:HA	1:T:113:ILE:HG22	1.86	0.56
2:c:47:TRP:CH2	2:c:50:ALA:HB2	2.40	0.56
2:X:47:TRP:CH2	2:X:50:ALA:HB2	2.40	0.56
2:c:35:ARG:HD3	2:c:47:TRP:HZ3	1.70	0.56
2:f:35:ARG:HD3	2:f:47:TRP:HZ3	1.70	0.56
2:k:12:VAL:HG11	2:k:86:LEU:HD12	1.88	0.56
1:B:28:ILE:HG12	1:B:121:VAL:HG21	1.88	0.56
1:C:110:ARG:HA	1:C:113:ILE:HG22	1.86	0.56
1:K:39:PHE:O	1:K:51:TYR:OH	2.17	0.56
1:L:28:ILE:HG12	1:L:121:VAL:HG21	1.88	0.56
1:L:77:ILE:HD11	1:L:103:ARG:NE	2.19	0.56
1:M:110:ARG:HA	1:M:113:ILE:HG22	1.86	0.56
1:O:39:PHE:O	1:O:51:TYR:OH	2.17	0.56
2:a:12:VAL:HG11	2:a:86:LEU:HD12	1.88	0.56
2:h:34:MET:HG3	2:h:79:VAL:HG21	1.86	0.56
2:j:35:ARG:HD3	2:j:47:TRP:HZ3	1.70	0.56
2:U:12:VAL:HG11	2:U:86:LEU:HD12	1.88	0.55
1:K:169:ASP:OD2	2:e:59:HIS:CE1	2.60	0.55
1:L:110:ARG:HA	1:L:113:ILE:HG22	1.86	0.55
1:S:260:ASP:OD2	1:T:238:GLN:NE2	2.39	0.55
2:Z:35:ARG:HD3	2:Z:47:TRP:HZ3	1.70	0.55
2:b:47:TRP:CH2	2:b:50:ALA:HB2	2.40	0.55
2:e:12:VAL:HG11	2:e:86:LEU:HD12	1.88	0.55
2:h:12:VAL:HG11	2:h:86:LEU:HD12	1.88	0.55
2:l:47:TRP:CH2	2:l:50:ALA:HB2	2.40	0.55
1:C:28:ILE:HG12	1:C:121:VAL:HG21	1.88	0.55
1:K:235:ALA:CB	1:T:248:ILE:HD11	2.35	0.55
1:B:110:ARG:HA	1:B:113:ILE:HG22	1.86	0.55
1:K:77:ILE:HD11	1:K:103:ARG:NE	2.19	0.55
1:M:28:ILE:HG12	1:M:121:VAL:HG21	1.88	0.55
2:W:12:VAL:HG11	2:W:86:LEU:HD12	1.88	0.55
2:X:12:VAL:HG11	2:X:86:LEU:HD12	1.88	0.55
2:d:12:VAL:HG11	2:d:86:LEU:HD12	1.88	0.55
2:j:12:VAL:HG11	2:j:86:LEU:HD12	1.88	0.55
2:n:12:VAL:HG11	2:n:86:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:12:VAL:HG11	2:Z:86:LEU:HD12	1.88	0.55
2:f:12:VAL:HG11	2:f:86:LEU:HD12	1.88	0.55
2:h:47:TRP:CH2	2:h:50:ALA:HB2	2.40	0.55
1:A:28:ILE:HG12	1:A:121:VAL:HG21	1.88	0.55
1:A:77:ILE:HD11	1:A:103:ARG:NE	2.19	0.55
1:F:28:ILE:HG12	1:F:121:VAL:HG21	1.88	0.55
2:V:12:VAL:HG11	2:V:86:LEU:HD12	1.88	0.55
2:g:12:VAL:HG11	2:g:86:LEU:HD12	1.88	0.55
1:K:28:ILE:HG12	1:K:121:VAL:HG21	1.88	0.55
2:h:35:ARG:HD3	2:h:47:TRP:HZ3	1.70	0.55
1:G:28:ILE:HG12	1:G:121:VAL:HG21	1.88	0.55
1:Q:28:ILE:HG12	1:Q:121:VAL:HG21	1.88	0.55
2:m:12:VAL:HG11	2:m:86:LEU:HD12	1.88	0.55
1:C:39:PHE:O	1:C:51:TYR:OH	2.17	0.55
1:D:28:ILE:HG12	1:D:121:VAL:HG21	1.88	0.55
2:c:12:VAL:HG11	2:c:86:LEU:HD12	1.88	0.55
1:R:28:ILE:HG12	1:R:121:VAL:HG21	1.88	0.55
2:X:35:ARG:HD3	2:X:47:TRP:HZ3	1.70	0.55
2:i:12:VAL:HG11	2:i:86:LEU:HD12	1.88	0.55
2:m:35:ARG:HD3	2:m:47:TRP:HZ3	1.70	0.55
1:M:260:ASP:OD1	1:M:260:ASP:N	2.40	0.55
1:N:28:ILE:HG12	1:N:121:VAL:HG21	1.88	0.55
1:B:260:ASP:OD1	1:B:260:ASP:N	2.40	0.54
1:C:260:ASP:OD1	1:C:260:ASP:N	2.40	0.54
1:H:28:ILE:HG12	1:H:121:VAL:HG21	1.88	0.54
1:J:260:ASP:OD1	1:J:260:ASP:N	2.40	0.54
1:L:260:ASP:OD1	1:L:260:ASP:N	2.40	0.54
1:P:28:ILE:HG12	1:P:121:VAL:HG21	1.88	0.54
2:b:12:VAL:HG11	2:b:86:LEU:HD12	1.88	0.54
1:R:241:ARG:HB2	1:S:227:ASN:HD21	1.70	0.54
1:T:260:ASP:OD1	1:T:260:ASP:N	2.40	0.54
2:l:12:VAL:HG11	2:l:86:LEU:HD12	1.88	0.54
1:E:28:ILE:HG12	1:E:121:VAL:HG21	1.88	0.54
1:O:28:ILE:HG12	1:O:121:VAL:HG21	1.88	0.54
1:J:28:ILE:HG12	1:J:121:VAL:HG21	1.88	0.54
1:I:260:ASP:OD1	1:I:260:ASP:N	2.40	0.54
1:N:260:ASP:OD1	1:N:260:ASP:N	2.40	0.54
1:S:260:ASP:OD1	1:S:260:ASP:N	2.40	0.54
2:Y:12:VAL:HG11	2:Y:86:LEU:HD12	1.88	0.54
1:D:260:ASP:OD1	1:D:260:ASP:N	2.40	0.54
2:Z:61:ALA:HB3	2:Z:64:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:61:ALA:HB3	2:a:64:VAL:HG22	1.90	0.54
2:m:61:ALA:HB3	2:m:64:VAL:HG22	1.90	0.54
1:K:228:GLU:HB2	1:T:244:MET:SD	2.47	0.54
1:S:28:ILE:HG12	1:S:121:VAL:HG21	1.88	0.54
1:T:28:ILE:HG12	1:T:121:VAL:HG21	1.88	0.54
2:c:61:ALA:HB3	2:c:64:VAL:HG22	1.90	0.54
2:k:61:ALA:HB3	2:k:64:VAL:HG22	1.90	0.54
2:l:61:ALA:HB3	2:l:64:VAL:HG22	1.90	0.54
1:G:77:ILE:HD11	1:G:103:ARG:NE	2.19	0.53
2:b:61:ALA:HB3	2:b:64:VAL:HG22	1.90	0.53
2:n:61:ALA:HB3	2:n:64:VAL:HG22	1.90	0.53
1:I:28:ILE:HG12	1:I:121:VAL:HG21	1.88	0.53
1:J:77:ILE:HD11	1:J:103:ARG:NE	2.19	0.53
1:S:142:TYR:OH	1:S:176:GLU:OE1	2.13	0.53
1:F:254:PHE:CZ	1:G:238:GLN:NE2	2.74	0.53
2:d:61:ALA:HB3	2:d:64:VAL:HG22	1.90	0.53
1:A:51:TYR:HD2	1:B:183:TYR:HD1	1.55	0.53
1:E:245:MET:HG3	1:E:256:PRO:HD2	1.90	0.53
1:P:245:MET:HG3	1:P:256:PRO:HD2	1.90	0.53
1:R:260:ASP:OD1	1:R:260:ASP:N	2.40	0.53
2:j:61:ALA:HB3	2:j:64:VAL:HG22	1.90	0.53
1:D:245:MET:HG3	1:D:256:PRO:HD2	1.90	0.53
1:E:260:ASP:OD2	1:F:238:GLN:NE2	2.42	0.53
1:G:248:ILE:CD1	1:H:235:ALA:CB	2.81	0.53
1:H:260:ASP:OD1	1:H:260:ASP:N	2.40	0.53
1:J:245:MET:HG3	1:J:256:PRO:HD2	1.90	0.53
1:P:248:ILE:CD1	1:Q:235:ALA:HB3	2.38	0.53
2:Z:47:TRP:HH2	2:Z:50:ALA:HB2	1.74	0.53
2:Z:83:MET:HE3	2:Z:86:LEU:HD11	1.91	0.53
2:c:47:TRP:HH2	2:c:50:ALA:HB2	1.74	0.53
1:F:77:ILE:HD11	1:F:103:ARG:NE	2.19	0.53
1:H:39:PHE:O	1:H:51:TYR:OH	2.17	0.53
1:N:245:MET:HG3	1:N:256:PRO:HD2	1.90	0.53
1:R:244:MET:SD	1:S:228:GLU:HB2	2.49	0.53
2:h:47:TRP:HH2	2:h:50:ALA:HB2	1.74	0.53
2:k:47:TRP:HH2	2:k:50:ALA:HB2	1.74	0.53
1:O:245:MET:HG3	1:O:256:PRO:HD2	1.90	0.53
1:R:254:PHE:CE2	1:S:238:GLN:NE2	2.77	0.53
1:T:77:ILE:HD11	1:T:103:ARG:NE	2.19	0.53
1:T:245:MET:HG3	1:T:256:PRO:HD2	1.90	0.53
2:X:47:TRP:HH2	2:X:50:ALA:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:83:MET:HE3	2:Y:86:LEU:HD11	1.91	0.53
2:i:83:MET:HE3	2:i:86:LEU:HD11	1.91	0.53
1:C:245:MET:HG3	1:C:256:PRO:HD2	1.90	0.53
1:I:248:ILE:HD11	1:J:235:ALA:CB	2.38	0.53
2:W:61:ALA:HB3	2:W:64:VAL:HG22	1.90	0.53
2:g:83:MET:HE3	2:g:86:LEU:HD11	1.91	0.53
2:h:83:MET:HE3	2:h:86:LEU:HD11	1.91	0.53
2:i:61:ALA:HB3	2:i:64:VAL:HG22	1.90	0.53
1:F:245:MET:HG3	1:F:256:PRO:HD2	1.90	0.53
1:K:245:MET:HG3	1:K:256:PRO:HD2	1.90	0.53
1:P:160:PHE:N	1:P:161:PRO:HD2	2.25	0.53
1:R:39:PHE:O	1:R:51:TYR:OH	2.17	0.53
1:A:245:MET:HG3	1:A:256:PRO:HD2	1.90	0.52
2:U:61:ALA:HB3	2:U:64:VAL:HG22	1.90	0.52
1:F:160:PHE:N	1:F:161:PRO:HD2	2.25	0.52
1:M:245:MET:HG3	1:M:256:PRO:HD2	1.90	0.52
1:Q:245:MET:HG3	1:Q:256:PRO:HD2	1.90	0.52
2:W:83:MET:HE3	2:W:86:LEU:HD11	1.91	0.52
2:b:47:TRP:HH2	2:b:50:ALA:HB2	1.74	0.52
1:C:160:PHE:N	1:C:161:PRO:HD2	2.25	0.52
1:K:160:PHE:N	1:K:161:PRO:HD2	2.24	0.52
2:j:47:TRP:HH2	2:j:50:ALA:HB2	1.74	0.52
2:j:83:MET:HE3	2:j:86:LEU:HD11	1.91	0.52
2:m:47:TRP:HH2	2:m:50:ALA:HB2	1.74	0.52
1:A:160:PHE:N	1:A:161:PRO:HD2	2.24	0.52
1:E:260:ASP:OD1	1:E:260:ASP:N	2.40	0.52
1:F:260:ASP:OD1	1:F:260:ASP:N	2.40	0.52
1:G:152:LYS:O	1:G:156:ILE:HG22	2.09	0.52
1:G:245:MET:HG3	1:G:256:PRO:HD2	1.90	0.52
1:H:152:LYS:O	1:H:156:ILE:HG22	2.09	0.52
1:I:245:MET:HG3	1:I:256:PRO:HD2	1.90	0.52
1:J:160:PHE:N	1:J:161:PRO:HD2	2.24	0.52
1:L:160:PHE:N	1:L:161:PRO:HD2	2.24	0.52
1:M:160:PHE:N	1:M:161:PRO:HD2	2.25	0.52
2:V:61:ALA:HB3	2:V:64:VAL:HG22	1.90	0.52
2:X:61:ALA:HB3	2:X:64:VAL:HG22	1.90	0.52
2:X:83:MET:HE3	2:X:86:LEU:HD11	1.91	0.52
1:B:160:PHE:N	1:B:161:PRO:HD2	2.25	0.52
1:S:245:MET:HG3	1:S:256:PRO:HD2	1.90	0.52
1:T:160:PHE:N	1:T:161:PRO:HD2	2.25	0.52
2:a:83:MET:HE3	2:a:86:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:61:ALA:HB3	2:g:64:VAL:HG22	1.90	0.52
1:D:160:PHE:N	1:D:161:PRO:HD2	2.25	0.52
1:L:152:LYS:O	1:L:156:ILE:HG22	2.09	0.52
1:N:160:PHE:N	1:N:161:PRO:HD2	2.24	0.52
1:O:260:ASP:OD1	1:O:260:ASP:N	2.40	0.52
1:Q:152:LYS:O	1:Q:156:ILE:HG22	2.10	0.52
1:R:152:LYS:O	1:R:156:ILE:HG22	2.09	0.52
2:V:47:TRP:HH2	2:V:50:ALA:HB2	1.74	0.52
2:Y:61:ALA:HB3	2:Y:64:VAL:HG22	1.90	0.52
2:f:47:TRP:HH2	2:f:50:ALA:HB2	1.74	0.52
2:i:47:TRP:HH2	2:i:50:ALA:HB2	1.74	0.52
2:k:83:MET:HE3	2:k:86:LEU:HD11	1.91	0.52
1:B:152:LYS:O	1:B:156:ILE:HG22	2.10	0.52
1:D:51:TYR:OH	1:E:186:GLN:NE2	2.43	0.52
1:I:152:LYS:O	1:I:156:ILE:HG22	2.09	0.52
1:L:245:MET:HG3	1:L:256:PRO:HD2	1.90	0.52
1:Q:160:PHE:N	1:Q:161:PRO:HD2	2.25	0.52
1:S:152:LYS:O	1:S:156:ILE:HG22	2.09	0.52
2:h:61:ALA:HB3	2:h:64:VAL:HG22	1.90	0.52
1:B:245:MET:HG3	1:B:256:PRO:HD2	1.90	0.52
1:H:152:LYS:O	1:H:152:LYS:HD2	2.10	0.52
1:I:160:PHE:N	1:I:161:PRO:HD2	2.25	0.52
1:N:39:PHE:O	1:N:51:TYR:OH	2.17	0.52
1:R:245:MET:HG3	1:R:256:PRO:HD2	1.90	0.52
2:e:34:MET:HG3	2:e:79:VAL:HG21	1.91	0.52
2:e:47:TRP:HH2	2:e:50:ALA:HB2	1.74	0.52
2:e:61:ALA:HB3	2:e:64:VAL:HG22	1.90	0.52
2:n:47:TRP:HH2	2:n:50:ALA:HB2	1.74	0.52
1:F:276:SER:CB	1:H:216:LEU:CD1	2.87	0.52
1:R:152:LYS:O	1:R:152:LYS:HD2	2.10	0.52
1:S:152:LYS:O	1:S:152:LYS:HD2	2.10	0.52
1:S:160:PHE:N	1:S:161:PRO:HD2	2.25	0.52
2:l:19:ARG:NH1	2:l:82:GLN:HB2	2.22	0.52
2:l:47:TRP:HH2	2:l:50:ALA:HB2	1.74	0.52
2:m:83:MET:HE3	2:m:86:LEU:HD11	1.91	0.52
2:n:83:MET:HE3	2:n:86:LEU:HD11	1.91	0.52
2:U:83:MET:HE3	2:U:86:LEU:HD11	1.91	0.52
1:F:276:SER:CA	1:H:216:LEU:CD1	2.85	0.52
1:G:160:PHE:N	1:G:161:PRO:HD2	2.24	0.52
1:H:245:MET:HG3	1:H:256:PRO:HD2	1.90	0.52
1:I:152:LYS:O	1:I:152:LYS:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:152:LYS:O	1:N:156:ILE:HG22	2.09	0.52
1:O:169:ASP:OD2	2:i:59:HIS:HE1	1.92	0.52
2:d:83:MET:HE3	2:d:86:LEU:HD11	1.91	0.52
2:f:61:ALA:HB3	2:f:64:VAL:HG22	1.90	0.52
1:D:152:LYS:O	1:D:156:ILE:HG22	2.10	0.52
1:E:160:PHE:N	1:E:161:PRO:HD2	2.24	0.52
1:E:248:ILE:HD11	1:F:235:ALA:HB1	1.87	0.52
1:G:152:LYS:O	1:G:152:LYS:HD2	2.10	0.52
1:G:260:ASP:OD1	1:G:260:ASP:N	2.40	0.52
1:T:273:LYS:HD2	1:T:273:LYS:O	2.10	0.52
2:Y:47:TRP:HH2	2:Y:50:ALA:HB2	1.74	0.52
2:a:47:TRP:HH2	2:a:50:ALA:HB2	1.74	0.52
1:C:248:ILE:HD11	1:D:235:ALA:CB	2.38	0.51
1:F:152:LYS:HD2	1:F:152:LYS:O	2.10	0.51
1:F:152:LYS:O	1:F:156:ILE:HG22	2.09	0.51
1:N:152:LYS:O	1:N:152:LYS:HD2	2.10	0.51
1:P:152:LYS:HD2	1:P:152:LYS:O	2.10	0.51
1:P:152:LYS:O	1:P:156:ILE:HG22	2.09	0.51
1:P:273:LYS:HD2	1:P:273:LYS:O	2.11	0.51
1:S:273:LYS:HD2	1:S:273:LYS:O	2.10	0.51
2:c:83:MET:HE3	2:c:86:LEU:HD11	1.91	0.51
2:d:47:TRP:HH2	2:d:50:ALA:HB2	1.74	0.51
2:U:47:TRP:HH2	2:U:50:ALA:HB2	1.74	0.51
1:D:152:LYS:O	1:D:152:LYS:HD2	2.10	0.51
1:F:273:LYS:HD2	1:F:273:LYS:O	2.10	0.51
1:I:273:LYS:HD2	1:I:273:LYS:O	2.11	0.51
1:P:260:ASP:OD1	1:P:260:ASP:N	2.40	0.51
2:V:83:MET:HE3	2:V:86:LEU:HD11	1.91	0.51
2:b:83:MET:HE3	2:b:86:LEU:HD11	1.91	0.51
2:f:83:MET:HE3	2:f:86:LEU:HD11	1.91	0.51
1:J:152:LYS:O	1:J:156:ILE:HG22	2.09	0.51
1:J:273:LYS:HD2	1:J:273:LYS:O	2.11	0.51
1:Q:152:LYS:O	1:Q:152:LYS:HD2	2.10	0.51
1:Q:260:ASP:OD1	1:Q:260:ASP:N	2.40	0.51
1:T:152:LYS:O	1:T:156:ILE:HG22	2.10	0.51
2:W:47:TRP:HH2	2:W:50:ALA:HB2	1.74	0.51
2:m:68:PHE:CD2	2:m:83:MET:HG2	2.46	0.51
1:B:248:ILE:HD11	1:C:235:ALA:HB3	1.92	0.51
1:J:152:LYS:O	1:J:152:LYS:HD2	2.10	0.51
1:T:152:LYS:O	1:T:152:LYS:HD2	2.10	0.51
2:e:83:MET:HE3	2:e:86:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:47:TRP:HH2	2:g:50:ALA:HB2	1.74	0.51
2:h:68:PHE:CD2	2:h:83:MET:HG2	2.46	0.51
2:l:83:MET:HE3	2:l:86:LEU:HD11	1.91	0.51
1:A:152:LYS:O	1:A:156:ILE:HG22	2.09	0.51
1:F:134:SER:OG	1:F:161:PRO:HG3	2.11	0.51
1:K:152:LYS:O	1:K:156:ILE:HG22	2.09	0.51
1:M:152:LYS:HD2	1:M:152:LYS:O	2.10	0.51
1:O:160:PHE:N	1:O:161:PRO:HD2	2.25	0.51
2:c:68:PHE:CD2	2:c:83:MET:HG2	2.46	0.51
1:A:152:LYS:O	1:A:152:LYS:HD2	2.10	0.51
1:C:152:LYS:HD2	1:C:152:LYS:O	2.10	0.51
1:E:134:SER:OG	1:E:161:PRO:HG3	2.11	0.51
1:E:273:LYS:HD2	1:E:273:LYS:O	2.11	0.51
1:G:134:SER:OG	1:G:161:PRO:HG3	2.11	0.51
1:H:160:PHE:N	1:H:161:PRO:HD2	2.25	0.51
1:O:134:SER:OG	1:O:161:PRO:HG3	2.11	0.51
1:O:152:LYS:HD2	1:O:152:LYS:O	2.10	0.51
1:O:152:LYS:O	1:O:156:ILE:HG22	2.09	0.51
1:P:51:TYR:OH	1:Q:186:GLN:NE2	2.44	0.51
1:P:134:SER:OG	1:P:161:PRO:HG3	2.11	0.51
1:R:160:PHE:N	1:R:161:PRO:HD2	2.24	0.51
2:X:68:PHE:CD2	2:X:83:MET:HG2	2.46	0.51
1:B:51:TYR:OH	1:C:186:GLN:NE2	2.43	0.51
1:B:273:LYS:HD2	1:B:273:LYS:O	2.11	0.51
1:C:152:LYS:O	1:C:156:ILE:HG22	2.09	0.51
1:H:134:SER:OG	1:H:161:PRO:HG3	2.11	0.51
1:K:152:LYS:O	1:K:152:LYS:HD2	2.10	0.51
1:O:273:LYS:HD2	1:O:273:LYS:O	2.10	0.51
1:R:134:SER:OG	1:R:161:PRO:HG3	2.11	0.51
2:g:68:PHE:CD2	2:g:83:MET:HG2	2.46	0.51
2:l:68:PHE:CD2	2:l:83:MET:HG2	2.46	0.51
1:C:273:LYS:HD2	1:C:273:LYS:O	2.10	0.51
1:E:152:LYS:HD2	1:E:152:LYS:O	2.10	0.51
1:H:273:LYS:HD2	1:H:273:LYS:O	2.11	0.51
1:L:134:SER:OG	1:L:161:PRO:HG3	2.11	0.51
1:L:273:LYS:HD2	1:L:273:LYS:O	2.11	0.51
1:M:152:LYS:O	1:M:156:ILE:HG22	2.09	0.51
1:M:273:LYS:HD2	1:M:273:LYS:O	2.11	0.51
1:P:260:ASP:OD2	1:Q:238:GLN:NE2	2.44	0.51
1:Q:134:SER:OG	1:Q:161:PRO:HG3	2.11	0.51
1:Q:142:TYR:OH	1:Q:176:GLU:OE1	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:68:PHE:HD2	2:W:83:MET:HG2	1.76	0.51
2:i:68:PHE:HD2	2:i:83:MET:HG2	1.76	0.51
1:A:134:SER:OG	1:A:161:PRO:HG3	2.11	0.51
2:U:68:PHE:HD2	2:U:83:MET:HG2	1.76	0.51
1:B:134:SER:OG	1:B:161:PRO:HG3	2.11	0.51
1:D:134:SER:OG	1:D:161:PRO:HG3	2.11	0.51
1:K:134:SER:OG	1:K:161:PRO:HG3	2.11	0.51
1:K:273:LYS:HD2	1:K:273:LYS:O	2.11	0.51
1:N:134:SER:OG	1:N:161:PRO:HG3	2.11	0.51
2:Y:68:PHE:CD2	2:Y:83:MET:HG2	2.46	0.51
2:e:68:PHE:HD2	2:e:83:MET:HG2	1.76	0.51
2:g:68:PHE:HD2	2:g:83:MET:HG2	1.76	0.51
2:i:68:PHE:CD2	2:i:83:MET:HG2	2.46	0.51
1:A:273:LYS:HD2	1:A:273:LYS:O	2.11	0.51
1:G:273:LYS:HD2	1:G:273:LYS:O	2.11	0.51
1:Q:273:LYS:HD2	1:Q:273:LYS:O	2.11	0.51
1:R:273:LYS:HD2	1:R:273:LYS:O	2.11	0.51
2:Y:68:PHE:HD2	2:Y:83:MET:HG2	1.76	0.51
1:D:273:LYS:HD2	1:D:273:LYS:O	2.10	0.50
1:L:152:LYS:O	1:L:152:LYS:HD2	2.10	0.50
2:W:68:PHE:CD2	2:W:83:MET:HG2	2.46	0.50
1:B:103:ARG:HD3	1:B:225:LEU:CD1	2.42	0.50
1:E:152:LYS:O	1:E:156:ILE:HG22	2.10	0.50
1:F:254:PHE:HE2	1:G:238:GLN:NE2	2.04	0.50
1:L:103:ARG:HD3	1:L:225:LEU:CD1	2.42	0.50
1:N:273:LYS:HD2	1:N:273:LYS:O	2.10	0.50
1:S:232:PHE:CD2	1:T:216:LEU:HD23	2.46	0.50
2:a:68:PHE:HD2	2:a:83:MET:HG2	1.76	0.50
1:B:152:LYS:O	1:B:152:LYS:HD2	2.10	0.50
1:C:73:GLN:HB2	1:C:107:ILE:HD11	1.93	0.50
1:C:103:ARG:HD3	1:C:225:LEU:CD1	2.42	0.50
1:M:103:ARG:HD3	1:M:225:LEU:CD1	2.42	0.50
1:M:146:ASP:H	2:g:35:ARG:NH2	2.05	0.50
1:M:146:ASP:HB2	2:g:35:ARG:NH2	2.26	0.50
1:R:103:ARG:HD3	1:R:225:LEU:CD1	2.42	0.50
2:a:68:PHE:CD2	2:a:83:MET:HG2	2.46	0.50
2:b:68:PHE:CD2	2:b:83:MET:HG2	2.46	0.50
2:d:68:PHE:CD2	2:d:83:MET:HG2	2.46	0.50
2:e:35:ARG:HB3	2:e:47:TRP:CZ3	2.44	0.50
2:k:68:PHE:HD2	2:k:83:MET:HG2	1.76	0.50
2:n:68:PHE:CD2	2:n:83:MET:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:68:PHE:CD2	2:U:83:MET:HG2	2.46	0.50
1:D:103:ARG:HD3	1:D:225:LEU:CD1	2.42	0.50
1:H:103:ARG:HD3	1:H:225:LEU:CD1	2.42	0.50
1:J:134:SER:OG	1:J:161:PRO:HG3	2.11	0.50
1:M:73:GLN:HB2	1:M:107:ILE:HD11	1.94	0.50
1:N:73:GLN:HB2	1:N:107:ILE:HD11	1.93	0.50
2:k:68:PHE:CD2	2:k:83:MET:HG2	2.46	0.50
1:A:103:ARG:HD3	1:A:225:LEU:CD1	2.42	0.50
1:D:73:GLN:HB2	1:D:107:ILE:HD11	1.93	0.50
1:M:146:ASP:N	2:g:35:ARG:HH22	2.06	0.50
1:N:103:ARG:HD3	1:N:225:LEU:CD1	2.42	0.50
1:T:134:SER:OG	1:T:161:PRO:HG3	2.11	0.50
2:f:68:PHE:CD2	2:f:83:MET:HG2	2.46	0.50
2:l:68:PHE:HD2	2:l:83:MET:HG2	1.76	0.50
1:E:157:LEU:HA	1:E:160:PHE:CE2	2.47	0.50
1:J:73:GLN:HB2	1:J:107:ILE:HD11	1.93	0.50
1:K:103:ARG:HD3	1:K:225:LEU:CD1	2.42	0.50
1:O:157:LEU:HA	1:O:160:PHE:CE2	2.47	0.50
2:V:68:PHE:CD2	2:V:83:MET:HG2	2.46	0.50
2:Z:36:TRP:CD2	2:Z:81:LEU:HD12	2.47	0.50
2:m:36:TRP:CD2	2:m:81:LEU:HD12	2.47	0.50
1:A:73:GLN:HB2	1:A:107:ILE:HD11	1.93	0.50
1:C:134:SER:OG	1:C:161:PRO:HG3	2.11	0.50
1:O:103:ARG:HD3	1:O:225:LEU:CD1	2.42	0.50
1:T:73:GLN:HB2	1:T:107:ILE:HD11	1.93	0.50
2:b:68:PHE:HD2	2:b:83:MET:HG2	1.77	0.50
2:i:36:TRP:CD2	2:i:81:LEU:HD12	2.47	0.50
2:j:68:PHE:CD2	2:j:83:MET:HG2	2.45	0.50
1:D:157:LEU:HA	1:D:160:PHE:CE2	2.47	0.50
1:I:51:TYR:OH	1:J:186:GLN:NE2	2.45	0.50
1:K:73:GLN:HB2	1:K:107:ILE:HD11	1.93	0.50
1:N:157:LEU:HA	1:N:160:PHE:CE2	2.47	0.50
1:S:134:SER:OG	1:S:161:PRO:HG3	2.11	0.50
2:d:68:PHE:HD2	2:d:83:MET:HG2	1.76	0.50
1:G:157:LEU:HA	1:G:160:PHE:CE2	2.47	0.50
1:M:134:SER:OG	1:M:161:PRO:HG3	2.11	0.50
2:Y:36:TRP:CD2	2:Y:81:LEU:HD12	2.47	0.50
2:c:36:TRP:CD2	2:c:81:LEU:HD12	2.47	0.50
2:e:68:PHE:CD2	2:e:83:MET:HG2	2.46	0.50
2:j:36:TRP:CD2	2:j:81:LEU:HD12	2.47	0.50
1:E:103:ARG:HD3	1:E:225:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:TYR:OH	1:I:186:GLN:NE2	2.45	0.49
2:Z:68:PHE:CD2	2:Z:83:MET:HG2	2.46	0.49
2:d:36:TRP:CD2	2:d:81:LEU:HD12	2.47	0.49
2:h:36:TRP:CD2	2:h:81:LEU:HD12	2.47	0.49
2:n:36:TRP:CD2	2:n:81:LEU:HD12	2.47	0.49
2:n:68:PHE:HD2	2:n:83:MET:HG2	1.76	0.49
1:I:134:SER:OG	1:I:161:PRO:HG3	2.11	0.49
1:J:103:ARG:HD3	1:J:225:LEU:CD1	2.42	0.49
1:M:157:LEU:HA	1:M:160:PHE:CE2	2.47	0.49
1:P:157:LEU:HA	1:P:160:PHE:CE2	2.47	0.49
2:a:36:TRP:CD2	2:a:81:LEU:HD12	2.47	0.49
1:A:51:TYR:OH	1:B:186:GLN:NE2	2.45	0.49
1:B:73:GLN:HB2	1:B:107:ILE:HD11	1.93	0.49
1:C:157:LEU:HA	1:C:160:PHE:CE2	2.47	0.49
1:F:157:LEU:HA	1:F:160:PHE:CE2	2.47	0.49
1:G:73:GLN:HB2	1:G:107:ILE:HD11	1.93	0.49
1:L:38:THR:O	1:L:38:THR:OG1	2.30	0.49
1:L:73:GLN:HB2	1:L:107:ILE:HD11	1.93	0.49
1:L:157:LEU:HA	1:L:160:PHE:CE2	2.47	0.49
2:j:68:PHE:HD2	2:j:83:MET:HG2	1.76	0.49
1:B:38:THR:O	1:B:38:THR:OG1	2.30	0.49
1:H:157:LEU:HA	1:H:160:PHE:CE2	2.47	0.49
1:M:6:ASN:HD21	1:N:8:ILE:HG13	1.78	0.49
1:Q:157:LEU:HA	1:Q:160:PHE:CE2	2.47	0.49
2:k:36:TRP:CD2	2:k:81:LEU:HD12	2.47	0.49
1:B:157:LEU:HA	1:B:160:PHE:CE2	2.47	0.49
1:I:73:GLN:HB2	1:I:107:ILE:HD11	1.94	0.49
1:N:6:ASN:HD22	1:O:5:LEU:HD22	1.75	0.49
2:V:68:PHE:HD2	2:V:83:MET:HG2	1.76	0.49
2:U:36:TRP:CD2	2:U:81:LEU:HD12	2.47	0.49
1:D:144:MET:O	2:X:35:ARG:NH2	2.45	0.49
1:F:73:GLN:HB2	1:F:107:ILE:HD11	1.93	0.49
1:R:157:LEU:HA	1:R:160:PHE:CE2	2.47	0.49
1:S:73:GLN:HB2	1:S:107:ILE:HD11	1.93	0.49
1:T:103:ARG:HD3	1:T:225:LEU:CD1	2.42	0.49
2:Z:68:PHE:HD2	2:Z:83:MET:HG2	1.76	0.49
2:f:68:PHE:HD2	2:f:83:MET:HG2	1.76	0.49
2:m:68:PHE:HD2	2:m:83:MET:HG2	1.76	0.49
1:O:73:GLN:HB2	1:O:107:ILE:HD11	1.94	0.49
1:Q:73:GLN:HB2	1:Q:107:ILE:HD11	1.93	0.49
1:S:103:ARG:HD3	1:S:225:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:36:TRP:CD2	2:W:81:LEU:HD12	2.47	0.49
2:l:36:TRP:CD2	2:l:81:LEU:HD12	2.47	0.49
1:A:157:LEU:HA	1:A:160:PHE:CE2	2.47	0.49
1:G:103:ARG:HD3	1:G:225:LEU:CD1	2.42	0.49
1:P:73:GLN:HB2	1:P:107:ILE:HD11	1.93	0.49
1:Q:103:ARG:HD3	1:Q:225:LEU:CD1	2.42	0.49
1:S:244:MET:HG2	1:T:228:GLU:HA	1.95	0.49
2:X:36:TRP:CD2	2:X:81:LEU:HD12	2.47	0.49
2:b:36:TRP:CD2	2:b:81:LEU:HD12	2.47	0.49
2:c:68:PHE:HD2	2:c:83:MET:HG2	1.76	0.49
2:g:36:TRP:CD2	2:g:81:LEU:HD12	2.47	0.49
2:h:68:PHE:HD2	2:h:83:MET:HG2	1.76	0.49
1:M:38:THR:O	1:M:38:THR:OG1	2.30	0.49
1:P:103:ARG:HD3	1:P:225:LEU:CD1	2.42	0.49
1:R:51:TYR:OH	1:S:186:GLN:NE2	2.46	0.49
2:X:68:PHE:HD2	2:X:83:MET:HG2	1.76	0.49
1:F:103:ARG:HD3	1:F:225:LEU:CD1	2.42	0.49
1:H:73:GLN:HB2	1:H:107:ILE:HD11	1.93	0.49
1:I:157:LEU:HA	1:I:160:PHE:CE2	2.47	0.49
1:K:157:LEU:HA	1:K:160:PHE:CE2	2.47	0.49
2:V:36:TRP:CD2	2:V:81:LEU:HD12	2.47	0.49
1:C:38:THR:O	1:C:38:THR:OG1	2.30	0.48
1:E:73:GLN:HB2	1:E:107:ILE:HD11	1.93	0.48
1:R:73:GLN:HB2	1:R:107:ILE:HD11	1.93	0.48
1:S:157:LEU:HA	1:S:160:PHE:CE2	2.47	0.48
1:T:271:ASP:HA	1:T:274:ASP:OD2	2.13	0.48
1:I:103:ARG:HD3	1:I:225:LEU:CD1	2.42	0.48
1:J:271:ASP:HA	1:J:274:ASP:OD2	2.13	0.48
1:J:157:LEU:HA	1:J:160:PHE:CE2	2.47	0.48
1:S:271:ASP:HA	1:S:274:ASP:OD2	2.13	0.48
1:T:157:LEU:HA	1:T:160:PHE:CE2	2.47	0.48
1:A:271:ASP:HA	1:A:274:ASP:OD2	2.13	0.48
1:E:169:ASP:OD2	2:Y:59:HIS:CE1	2.66	0.48
1:G:38:THR:O	1:G:38:THR:OG1	2.30	0.48
1:I:271:ASP:HA	1:I:274:ASP:OD2	2.13	0.48
1:K:271:ASP:HA	1:K:274:ASP:OD2	2.13	0.48
2:f:36:TRP:CD2	2:f:81:LEU:HD12	2.47	0.48
1:D:6:ASN:HD21	1:E:8:ILE:HG13	1.78	0.48
1:D:271:ASP:HA	1:D:274:ASP:OD2	2.13	0.48
1:J:146:ASP:N	2:d:35:ARG:HH22	2.07	0.48
1:Q:241:ARG:HB2	1:R:227:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:38:THR:O	1:H:38:THR:OG1	2.30	0.48
1:F:43:CYS:SG	1:G:179:LEU:HD13	2.53	0.48
1:H:271:ASP:HA	1:H:274:ASP:OD2	2.13	0.48
1:N:146:ASP:H	2:h:35:ARG:HH22	1.61	0.48
1:N:271:ASP:HA	1:N:274:ASP:OD2	2.13	0.48
1:D:142:TYR:OH	1:D:176:GLU:OE1	2.13	0.48
1:G:47:LYS:HD3	1:H:183:TYR:OH	2.14	0.48
1:P:38:THR:O	1:P:38:THR:OG1	2.30	0.48
1:R:38:THR:O	1:R:38:THR:OG1	2.30	0.48
1:R:271:ASP:HA	1:R:274:ASP:OD2	2.13	0.48
1:M:62:ILE:HD12	1:N:197:THR:HG21	1.94	0.48
1:O:271:ASP:HA	1:O:274:ASP:OD2	2.13	0.48
1:B:271:ASP:HA	1:B:274:ASP:OD2	2.13	0.47
1:L:271:ASP:HA	1:L:274:ASP:OD2	2.13	0.47
1:C:244:MET:SD	1:D:228:GLU:HB2	2.54	0.47
1:I:38:THR:O	1:I:38:THR:OG1	2.30	0.47
1:N:142:TYR:OH	1:N:176:GLU:OE1	2.13	0.47
1:P:142:TYR:OH	1:P:176:GLU:OE1	2.13	0.47
1:R:142:TYR:OH	1:R:176:GLU:OE1	2.13	0.47
1:R:144:MET:O	2:l:35:ARG:NH2	2.46	0.47
1:E:271:ASP:HA	1:E:274:ASP:OD2	2.13	0.47
1:F:39:PHE:O	1:F:51:TYR:OH	2.17	0.47
1:N:38:THR:O	1:N:38:THR:OG1	2.30	0.47
1:Q:51:TYR:OH	1:R:186:GLN:NE2	2.48	0.47
1:C:271:ASP:HA	1:C:274:ASP:OD2	2.13	0.47
1:K:224:HIS:HB2	1:T:240:SER:OG	2.14	0.47
1:R:240:SER:OG	1:S:224:HIS:HA	2.14	0.47
1:S:232:PHE:CE2	1:T:216:LEU:HB3	2.49	0.47
1:A:260:ASP:OD1	1:A:260:ASP:N	2.40	0.47
1:F:271:ASP:HA	1:F:274:ASP:OD2	2.13	0.47
1:K:260:ASP:OD1	1:K:260:ASP:N	2.40	0.47
1:D:38:THR:O	1:D:38:THR:OG1	2.30	0.47
1:K:51:TYR:OH	1:L:186:GLN:NE2	2.48	0.47
1:M:271:ASP:HA	1:M:274:ASP:OD2	2.13	0.47
1:A:5:LEU:HD22	1:J:6:ASN:HD22	1.80	0.47
1:A:248:ILE:CD1	1:B:235:ALA:HB3	2.44	0.47
1:N:47:LYS:HD3	1:O:183:TYR:OH	2.15	0.47
1:Q:271:ASP:HA	1:Q:274:ASP:OD2	2.13	0.47
1:S:38:THR:O	1:S:38:THR:OG1	2.30	0.47
2:d:64:VAL:HB	2:d:68:PHE:CE1	2.50	0.47
2:f:64:VAL:HB	2:f:68:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:64:VAL:HB	2:j:68:PHE:CE1	2.50	0.47
2:l:64:VAL:HB	2:l:68:PHE:CE1	2.50	0.47
2:n:64:VAL:HB	2:n:68:PHE:CE1	2.50	0.47
1:C:252:PHE:C	1:C:265:ARG:HB2	2.40	0.47
1:N:252:PHE:C	1:N:265:ARG:HB2	2.40	0.47
1:D:252:PHE:C	1:D:265:ARG:HB2	2.40	0.47
1:P:271:ASP:HA	1:P:274:ASP:OD2	2.13	0.47
2:V:64:VAL:HB	2:V:68:PHE:CE1	2.50	0.47
2:b:64:VAL:HB	2:b:68:PHE:CE1	2.50	0.47
1:B:252:PHE:C	1:B:265:ARG:HB2	2.40	0.47
1:E:51:TYR:OH	1:F:186:GLN:NE2	2.48	0.47
1:G:271:ASP:HA	1:G:274:ASP:OD2	2.13	0.47
1:H:142:TYR:OH	1:H:176:GLU:OE1	2.13	0.47
1:L:252:PHE:C	1:L:265:ARG:HB2	2.40	0.47
1:M:252:PHE:C	1:M:265:ARG:HB2	2.40	0.47
1:O:142:TYR:OH	1:O:176:GLU:OE1	2.13	0.47
2:c:64:VAL:HB	2:c:68:PHE:CE1	2.50	0.47
1:G:252:PHE:C	1:G:265:ARG:HB2	2.40	0.46
1:H:252:PHE:C	1:H:265:ARG:HB2	2.40	0.46
1:L:254:PHE:CE2	1:M:238:GLN:NE2	2.83	0.46
1:M:142:TYR:OH	1:M:176:GLU:OE1	2.13	0.46
1:Q:252:PHE:C	1:Q:265:ARG:HB2	2.40	0.46
1:T:38:THR:O	1:T:38:THR:OG1	2.30	0.46
2:W:64:VAL:HB	2:W:68:PHE:CE1	2.50	0.46
2:Z:64:VAL:HB	2:Z:68:PHE:CE1	2.50	0.46
1:A:252:PHE:C	1:A:265:ARG:HB2	2.40	0.46
1:I:252:PHE:C	1:I:265:ARG:HB2	2.40	0.46
1:K:252:PHE:C	1:K:265:ARG:HB2	2.40	0.46
1:G:159:GLY:C	1:G:161:PRO:HD2	2.41	0.46
1:R:252:PHE:C	1:R:265:ARG:HB2	2.40	0.46
1:S:252:PHE:C	1:S:265:ARG:HB2	2.40	0.46
2:a:64:VAL:HB	2:a:68:PHE:CE1	2.50	0.46
1:F:260:ASP:OD2	1:G:238:GLN:NE2	2.49	0.46
2:e:64:VAL:HB	2:e:68:PHE:CE1	2.50	0.46
2:h:64:VAL:HB	2:h:68:PHE:CE1	2.50	0.46
1:O:241:ARG:HB2	1:P:227:ASN:ND2	2.30	0.46
1:P:252:PHE:C	1:P:265:ARG:HB2	2.40	0.46
1:Q:159:GLY:C	1:Q:161:PRO:HD2	2.41	0.46
1:T:252:PHE:C	1:T:265:ARG:HB2	2.40	0.46
2:g:64:VAL:HB	2:g:68:PHE:CE1	2.50	0.46
2:U:64:VAL:HB	2:U:68:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:PHE:C	1:E:265:ARG:HB2	2.40	0.46
1:F:159:GLY:C	1:F:161:PRO:HD2	2.41	0.46
1:I:159:GLY:C	1:I:161:PRO:HD2	2.41	0.46
1:M:159:GLY:C	1:M:161:PRO:HD2	2.41	0.46
1:O:260:ASP:OD2	1:P:238:GLN:NE2	2.49	0.46
1:Q:6:ASN:HD21	1:R:8:ILE:HG13	1.80	0.46
2:k:64:VAL:HB	2:k:68:PHE:CE1	2.50	0.46
1:A:38:THR:O	1:A:38:THR:OG1	2.30	0.46
1:D:240:SER:OG	1:E:224:HIS:HB2	2.15	0.46
1:F:248:ILE:CD1	1:G:235:ALA:HB2	2.41	0.46
1:J:252:PHE:C	1:J:265:ARG:HB2	2.40	0.46
1:R:159:GLY:C	1:R:161:PRO:HD2	2.41	0.46
2:X:64:VAL:HB	2:X:68:PHE:CE1	2.50	0.46
2:i:64:VAL:HB	2:i:68:PHE:CE1	2.50	0.46
1:A:248:ILE:HD11	1:B:235:ALA:CB	2.44	0.46
1:C:159:GLY:C	1:C:161:PRO:HD2	2.41	0.46
1:C:256:PRO:CB	1:D:235:ALA:HB2	2.45	0.46
1:F:252:PHE:C	1:F:265:ARG:HB2	2.40	0.46
1:H:159:GLY:C	1:H:161:PRO:HD2	2.41	0.46
1:K:38:THR:O	1:K:38:THR:OG1	2.30	0.46
1:N:159:GLY:C	1:N:161:PRO:HD2	2.41	0.46
1:S:159:GLY:C	1:S:161:PRO:HD2	2.41	0.46
2:m:64:VAL:HB	2:m:68:PHE:CE1	2.50	0.46
1:A:8:ILE:HG13	1:J:6:ASN:HD21	1.81	0.46
1:D:159:GLY:C	1:D:161:PRO:HD2	2.41	0.46
1:H:248:ILE:CD1	1:I:235:ALA:CB	2.90	0.46
1:N:43:CYS:SG	1:O:179:LEU:HD13	2.56	0.46
1:O:252:PHE:C	1:O:265:ARG:HB2	2.40	0.46
1:T:159:GLY:C	1:T:161:PRO:HD2	2.41	0.46
2:Y:64:VAL:HB	2:Y:68:PHE:CE1	2.50	0.46
1:B:34:PHE:HZ	1:C:190:TRP:CZ2	2.34	0.45
1:J:159:GLY:C	1:J:161:PRO:HD2	2.41	0.45
1:K:186:GLN:NE2	1:T:51:TYR:OH	2.48	0.45
1:L:142:TYR:OH	1:L:176:GLU:OE1	2.13	0.45
1:O:159:GLY:C	1:O:161:PRO:HD2	2.41	0.45
1:P:159:GLY:C	1:P:161:PRO:HD2	2.41	0.45
2:i:88:PRO:HA	2:i:113:VAL:HB	1.98	0.45
1:B:159:GLY:C	1:B:161:PRO:HD2	2.41	0.45
1:E:159:GLY:C	1:E:161:PRO:HD2	2.41	0.45
1:M:248:ILE:HD11	1:N:235:ALA:HB3	1.98	0.45
2:Y:88:PRO:HA	2:Y:113:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:SER:HA	1:H:216:LEU:HD11	1.95	0.45
1:P:103:ARG:HH11	1:P:225:LEU:HD11	1.82	0.45
2:X:88:PRO:HA	2:X:113:VAL:HB	1.99	0.45
2:h:88:PRO:HA	2:h:113:VAL:HB	1.98	0.45
1:L:159:GLY:C	1:L:161:PRO:HD2	2.41	0.45
2:Z:88:PRO:HA	2:Z:113:VAL:HB	1.98	0.45
2:g:88:PRO:HA	2:g:113:VAL:HB	1.98	0.45
1:A:159:GLY:C	1:A:161:PRO:HD2	2.41	0.45
1:E:103:ARG:HH11	1:E:225:LEU:HD11	1.82	0.45
1:I:260:ASP:OD2	1:J:238:GLN:NE2	2.50	0.45
1:K:159:GLY:C	1:K:161:PRO:HD2	2.41	0.45
2:i:70:ILE:CG2	2:i:81:LEU:HG	2.47	0.45
2:j:88:PRO:HA	2:j:113:VAL:HB	1.98	0.45
1:D:103:ARG:HH11	1:D:225:LEU:HD11	1.82	0.45
1:F:103:ARG:HH11	1:F:225:LEU:HD11	1.82	0.45
1:M:103:ARG:HH11	1:M:225:LEU:HD11	1.82	0.45
1:O:103:ARG:HH11	1:O:225:LEU:HD11	1.82	0.45
1:T:8:ILE:HD13	1:T:8:ILE:HA	1.83	0.45
1:C:103:ARG:HH11	1:C:225:LEU:HD11	1.82	0.45
1:E:241:ARG:HB2	1:F:227:ASN:ND2	2.31	0.45
1:F:110:ARG:HA	1:F:113:ILE:CG2	2.47	0.45
1:N:103:ARG:HH11	1:N:225:LEU:HD11	1.82	0.45
1:Q:103:ARG:HH11	1:Q:225:LEU:HD11	1.82	0.45
2:W:88:PRO:HA	2:W:113:VAL:HB	1.98	0.45
1:B:103:ARG:HH11	1:B:225:LEU:HD11	1.82	0.45
1:G:98:LYS:HD3	1:G:212:PRO:HD3	1.99	0.45
1:K:103:ARG:HH11	1:K:225:LEU:HD11	1.82	0.45
1:L:103:ARG:HH11	1:L:225:LEU:HD11	1.82	0.45
1:P:110:ARG:HA	1:P:113:ILE:CG2	2.47	0.45
1:R:110:ARG:HA	1:R:113:ILE:CG2	2.47	0.45
2:Y:70:ILE:CG2	2:Y:81:LEU:HG	2.47	0.45
2:j:70:ILE:CG2	2:j:81:LEU:HG	2.47	0.45
1:A:103:ARG:HH11	1:A:225:LEU:HD11	1.82	0.45
2:U:70:ILE:CG2	2:U:81:LEU:HG	2.47	0.45
1:D:51:TYR:CD2	1:E:183:TYR:HD1	2.32	0.45
1:G:103:ARG:HH11	1:G:225:LEU:HD11	1.82	0.45
1:H:110:ARG:HA	1:H:113:ILE:CG2	2.47	0.45
1:I:110:ARG:HA	1:I:113:ILE:CG2	2.47	0.45
1:J:8:ILE:HD13	1:J:8:ILE:HA	1.83	0.45
1:M:51:TYR:CD2	1:N:183:TYR:HD1	2.34	0.45
1:Q:98:LYS:HD3	1:Q:212:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:93:VAL:HG23	2:b:110:GLN:HA	1.99	0.45
1:B:34:PHE:CZ	1:C:190:TRP:CZ2	3.04	0.44
1:F:276:SER:CB	1:H:216:LEU:HD13	2.47	0.44
2:a:88:PRO:HA	2:a:113:VAL:HB	1.98	0.44
2:c:93:VAL:HG23	2:c:110:GLN:HA	1.99	0.44
2:k:88:PRO:HA	2:k:113:VAL:HB	1.98	0.44
2:m:93:VAL:HG23	2:m:110:GLN:HA	1.99	0.44
1:C:256:PRO:CG	1:D:235:ALA:HB2	2.47	0.44
1:F:169:ASP:OD2	2:Z:59:HIS:CE1	2.70	0.44
1:G:260:ASP:OD2	1:H:238:GLN:NE2	2.50	0.44
1:I:244:MET:SD	1:J:228:GLU:HB2	2.58	0.44
1:K:6:ASN:HD22	1:L:5:LEU:HD22	1.82	0.44
1:K:110:ARG:HA	1:K:113:ILE:CG2	2.47	0.44
1:O:38:THR:O	1:O:38:THR:OG1	2.30	0.44
1:P:98:LYS:HD3	1:P:212:PRO:HD3	1.99	0.44
1:S:110:ARG:HA	1:S:113:ILE:CG2	2.47	0.44
2:l:93:VAL:HG23	2:l:110:GLN:HA	1.99	0.44
2:n:88:PRO:HA	2:n:113:VAL:HB	1.98	0.44
1:A:98:LYS:HD3	1:A:212:PRO:HD3	1.99	0.44
1:A:110:ARG:HA	1:A:113:ILE:CG2	2.47	0.44
1:E:47:LYS:HD3	1:F:183:TYR:OH	2.17	0.44
1:F:98:LYS:HD3	1:F:212:PRO:HD3	1.99	0.44
1:J:103:ARG:HH11	1:J:225:LEU:HD11	1.82	0.44
1:K:98:LYS:HD3	1:K:212:PRO:HD3	1.99	0.44
1:R:103:ARG:HH11	1:R:225:LEU:HD11	1.82	0.44
2:e:70:ILE:CG2	2:e:81:LEU:HG	2.47	0.44
2:m:35:ARG:HD3	2:m:47:TRP:CZ3	2.52	0.44
2:m:70:ILE:CG2	2:m:81:LEU:HG	2.47	0.44
1:H:98:LYS:HD3	1:H:212:PRO:HD3	1.99	0.44
1:O:110:ARG:HA	1:O:113:ILE:CG2	2.47	0.44
2:Z:70:ILE:CG2	2:Z:81:LEU:HG	2.47	0.44
2:b:70:ILE:CG2	2:b:81:LEU:HG	2.47	0.44
2:n:70:ILE:CG2	2:n:81:LEU:HG	2.47	0.44
1:D:169:ASP:OD2	2:X:59:HIS:CE1	2.71	0.44
1:E:110:ARG:HA	1:E:113:ILE:CG2	2.47	0.44
1:K:228:GLU:HA	1:T:244:MET:HG2	1.99	0.44
1:P:55:PHE:HB3	1:P:128:TYR:CE2	2.53	0.44
1:T:98:LYS:HD3	1:T:212:PRO:HD3	1.99	0.44
2:V:88:PRO:HA	2:V:113:VAL:HB	1.98	0.44
2:W:70:ILE:CG2	2:W:81:LEU:HG	2.47	0.44
2:c:35:ARG:HD3	2:c:47:TRP:CZ3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:88:PRO:HA	2:e:113:VAL:HB	1.98	0.44
2:g:70:ILE:CG2	2:g:81:LEU:HG	2.47	0.44
2:l:70:ILE:CG2	2:l:81:LEU:HG	2.47	0.44
1:B:110:ARG:HA	1:B:113:ILE:CG2	2.47	0.44
1:H:103:ARG:HH11	1:H:225:LEU:HD11	1.82	0.44
1:R:98:LYS:HD3	1:R:212:PRO:HD3	1.99	0.44
2:a:93:VAL:HG23	2:a:110:GLN:HA	1.99	0.44
2:l:88:PRO:HA	2:l:113:VAL:HB	1.98	0.44
2:U:88:PRO:HA	2:U:113:VAL:HB	1.98	0.44
1:D:55:PHE:HB3	1:D:128:TYR:CE2	2.53	0.44
1:E:164:ARG:NE	1:E:164:ARG:HA	2.33	0.44
1:G:8:ILE:HD13	1:G:8:ILE:HA	1.83	0.44
1:J:98:LYS:HD3	1:J:212:PRO:HD3	1.99	0.44
1:L:110:ARG:HA	1:L:113:ILE:CG2	2.47	0.44
1:M:51:TYR:HD2	1:N:183:TYR:HD1	1.65	0.44
1:Q:55:PHE:HB3	1:Q:128:TYR:CE2	2.53	0.44
1:Q:73:GLN:O	1:Q:77:ILE:HG12	2.18	0.44
1:S:73:GLN:O	1:S:77:ILE:HG12	2.18	0.44
1:S:241:ARG:HB2	1:T:227:ASN:HD22	1.79	0.44
1:T:103:ARG:HH11	1:T:225:LEU:HD11	1.82	0.44
2:X:93:VAL:HG23	2:X:110:GLN:HA	1.99	0.44
2:b:88:PRO:HA	2:b:113:VAL:HB	1.98	0.44
2:c:70:ILE:CG2	2:c:81:LEU:HG	2.47	0.44
2:d:70:ILE:CG2	2:d:81:LEU:HG	2.47	0.44
2:d:88:PRO:HA	2:d:113:VAL:HB	1.98	0.44
2:f:88:PRO:HA	2:f:113:VAL:HB	1.98	0.44
2:h:70:ILE:CG2	2:h:81:LEU:HG	2.47	0.44
2:k:93:VAL:HG23	2:k:110:GLN:HA	1.99	0.44
1:A:164:ARG:HA	1:A:164:ARG:NE	2.33	0.44
1:D:73:GLN:O	1:D:77:ILE:HG12	2.18	0.44
1:H:73:GLN:O	1:H:77:ILE:HG12	2.18	0.44
1:I:73:GLN:O	1:I:77:ILE:HG12	2.18	0.44
1:N:73:GLN:O	1:N:77:ILE:HG12	2.18	0.44
1:O:55:PHE:HB3	1:O:128:TYR:CE2	2.53	0.44
1:S:241:ARG:HB2	1:T:227:ASN:HD21	1.81	0.44
1:T:110:ARG:HA	1:T:113:ILE:CG2	2.47	0.44
1:T:164:ARG:NE	1:T:164:ARG:HA	2.33	0.44
2:V:70:ILE:CG2	2:V:81:LEU:HG	2.47	0.44
2:f:70:ILE:CG2	2:f:81:LEU:HG	2.47	0.44
2:g:93:VAL:HG23	2:g:110:GLN:HA	1.99	0.44
2:h:93:VAL:HG23	2:h:110:GLN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:83:MET:CE	2:l:86:LEU:HD11	2.48	0.44
2:n:93:VAL:HG23	2:n:110:GLN:HA	1.99	0.44
1:A:8:ILE:HD13	1:A:8:ILE:HA	1.83	0.44
1:B:98:LYS:HD3	1:B:212:PRO:HD3	1.99	0.44
1:E:55:PHE:HB3	1:E:128:TYR:CE2	2.53	0.44
1:G:73:GLN:O	1:G:77:ILE:HG12	2.18	0.44
1:J:110:ARG:HA	1:J:113:ILE:CG2	2.47	0.44
1:K:164:ARG:NE	1:K:164:ARG:HA	2.33	0.44
1:L:73:GLN:O	1:L:77:ILE:HG12	2.18	0.44
1:L:98:LYS:HD3	1:L:212:PRO:HD3	1.99	0.44
1:N:55:PHE:HB3	1:N:128:TYR:CE2	2.53	0.44
1:O:164:ARG:NE	1:O:164:ARG:HA	2.33	0.44
1:R:73:GLN:O	1:R:77:ILE:HG12	2.18	0.44
2:n:35:ARG:HD3	2:n:47:TRP:CZ3	2.52	0.44
1:B:55:PHE:CE2	1:C:190:TRP:NE1	2.80	0.43
1:B:164:ARG:HA	1:B:164:ARG:NE	2.33	0.43
1:C:110:ARG:HA	1:C:113:ILE:CG2	2.47	0.43
1:F:73:GLN:O	1:F:77:ILE:HG12	2.18	0.43
1:F:164:ARG:HA	1:F:164:ARG:NE	2.33	0.43
1:J:73:GLN:O	1:J:77:ILE:HG12	2.18	0.43
1:L:164:ARG:NE	1:L:164:ARG:HA	2.33	0.43
2:V:93:VAL:HG23	2:V:110:GLN:HA	1.99	0.43
2:Z:93:VAL:HG23	2:Z:110:GLN:HA	1.99	0.43
2:b:83:MET:CE	2:b:86:LEU:HD11	2.48	0.43
2:d:35:ARG:HD3	2:d:47:TRP:CZ3	2.52	0.43
2:d:83:MET:CE	2:d:86:LEU:HD11	2.48	0.43
2:d:93:VAL:HG23	2:d:110:GLN:HA	1.99	0.43
1:A:244:MET:SD	1:B:228:GLU:HB2	2.58	0.43
1:B:73:GLN:O	1:B:77:ILE:HG12	2.18	0.43
1:G:55:PHE:HB3	1:G:128:TYR:CE2	2.53	0.43
1:H:164:ARG:HA	1:H:164:ARG:NE	2.33	0.43
1:I:248:ILE:CD1	1:J:235:ALA:HB3	2.44	0.43
1:M:55:PHE:HB3	1:M:128:TYR:CE2	2.53	0.43
1:P:73:GLN:O	1:P:77:ILE:HG12	2.18	0.43
1:R:164:ARG:HA	1:R:164:ARG:NE	2.33	0.43
1:S:103:ARG:HH11	1:S:225:LEU:HD11	1.82	0.43
1:T:73:GLN:O	1:T:77:ILE:HG12	2.18	0.43
2:c:88:PRO:HA	2:c:113:VAL:HB	1.98	0.43
2:f:93:VAL:HG23	2:f:110:GLN:HA	1.99	0.43
2:k:35:ARG:HD3	2:k:47:TRP:CZ3	2.52	0.43
2:n:83:MET:CE	2:n:86:LEU:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:PHE:HB3	1:C:128:TYR:CE2	2.53	0.43
1:C:164:ARG:HA	1:C:164:ARG:NE	2.33	0.43
1:E:98:LYS:HD3	1:E:212:PRO:HD3	1.99	0.43
1:F:55:PHE:HB3	1:F:128:TYR:CE2	2.53	0.43
1:I:55:PHE:HB3	1:I:128:TYR:CE2	2.53	0.43
1:I:98:LYS:HD3	1:I:212:PRO:HD3	1.99	0.43
1:J:55:PHE:HB3	1:J:128:TYR:CE2	2.53	0.43
1:O:98:LYS:HD3	1:O:212:PRO:HD3	1.99	0.43
1:T:55:PHE:HB3	1:T:128:TYR:CE2	2.53	0.43
2:V:83:MET:CE	2:V:86:LEU:HD11	2.48	0.43
2:W:93:VAL:HG23	2:W:110:GLN:HA	1.99	0.43
2:h:83:MET:CE	2:h:86:LEU:HD11	2.48	0.43
1:D:164:ARG:HA	1:D:164:ARG:NE	2.33	0.43
1:H:55:PHE:HB3	1:H:128:TYR:CE2	2.53	0.43
1:K:8:ILE:HD13	1:K:8:ILE:HA	1.83	0.43
1:M:110:ARG:HA	1:M:113:ILE:CG2	2.47	0.43
1:M:164:ARG:HA	1:M:164:ARG:NE	2.33	0.43
1:O:73:GLN:O	1:O:77:ILE:HG12	2.18	0.43
1:R:55:PHE:HB3	1:R:128:TYR:CE2	2.53	0.43
1:S:55:PHE:HB3	1:S:128:TYR:CE2	2.53	0.43
1:S:98:LYS:HD3	1:S:212:PRO:HD3	1.99	0.43
2:Y:93:VAL:HG23	2:Y:110:GLN:HA	1.99	0.43
2:a:70:ILE:CG2	2:a:81:LEU:HG	2.47	0.43
2:k:70:ILE:CG2	2:k:81:LEU:HG	2.47	0.43
1:A:174:ARG:HG2	1:A:175:ASP:N	2.34	0.43
1:G:169:ASP:OD2	2:a:59:HIS:CE1	2.72	0.43
1:I:164:ARG:NE	1:I:164:ARG:HA	2.33	0.43
1:K:73:GLN:O	1:K:77:ILE:HG12	2.18	0.43
1:N:164:ARG:HA	1:N:164:ARG:NE	2.33	0.43
1:Q:110:ARG:HA	1:Q:113:ILE:CG2	2.47	0.43
1:R:51:TYR:HD1	1:S:183:TYR:HD1	1.66	0.43
1:S:164:ARG:NE	1:S:164:ARG:HA	2.33	0.43
2:X:35:ARG:N	2:X:97:PHE:O	2.47	0.43
2:X:70:ILE:CG2	2:X:81:LEU:HG	2.47	0.43
2:a:35:ARG:HD3	2:a:47:TRP:CZ3	2.52	0.43
2:f:83:MET:CE	2:f:86:LEU:HD11	2.48	0.43
2:m:88:PRO:HA	2:m:113:VAL:HB	1.98	0.43
1:A:73:GLN:O	1:A:77:ILE:HG12	2.18	0.43
2:U:83:MET:CE	2:U:86:LEU:HD11	2.48	0.43
1:B:232:PHE:CE2	1:C:216:LEU:HB3	2.54	0.43
1:H:225:LEU:O	1:H:228:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:103:ARG:HH11	1:I:225:LEU:HD11	1.82	0.43
1:K:174:ARG:HG2	1:K:175:ASP:N	2.34	0.43
1:M:77:ILE:HD13	1:M:77:ILE:N	2.34	0.43
1:R:225:LEU:O	1:R:228:GLU:HG3	2.19	0.43
2:W:35:ARG:HD3	2:W:47:TRP:CZ3	2.52	0.43
2:g:35:ARG:HD3	2:g:47:TRP:CZ3	2.52	0.43
2:j:83:MET:CE	2:j:86:LEU:HD11	2.48	0.43
2:U:35:ARG:HD3	2:U:47:TRP:CZ3	2.52	0.43
1:C:77:ILE:HD13	1:C:77:ILE:N	2.34	0.43
1:F:38:THR:O	1:F:38:THR:OG1	2.30	0.43
1:K:55:PHE:HB3	1:K:128:TYR:CE2	2.53	0.43
1:L:55:PHE:HB3	1:L:128:TYR:CE2	2.53	0.43
1:M:98:LYS:HD3	1:M:212:PRO:HD3	1.99	0.43
1:N:110:ARG:HA	1:N:113:ILE:CG2	2.47	0.43
2:X:83:MET:CE	2:X:86:LEU:HD11	2.48	0.43
2:i:93:VAL:HG23	2:i:110:GLN:HA	1.99	0.43
1:A:55:PHE:HB3	1:A:128:TYR:CE2	2.53	0.43
1:B:55:PHE:HB3	1:B:128:TYR:CE2	2.53	0.43
1:B:174:ARG:HG2	1:B:175:ASP:N	2.34	0.43
1:C:98:LYS:HD3	1:C:212:PRO:HD3	1.99	0.43
1:D:110:ARG:HA	1:D:113:ILE:CG2	2.47	0.43
1:E:73:GLN:O	1:E:77:ILE:HG12	2.18	0.43
1:E:103:ARG:NH1	1:E:225:LEU:HD11	2.34	0.43
1:F:103:ARG:NH1	1:F:225:LEU:HD11	2.34	0.43
1:H:103:ARG:NH1	1:H:225:LEU:HD11	2.34	0.43
1:P:103:ARG:NH1	1:P:225:LEU:HD11	2.34	0.43
1:Q:164:ARG:NE	1:Q:164:ARG:HA	2.33	0.43
2:e:93:VAL:HG23	2:e:110:GLN:HA	1.99	0.43
1:A:225:LEU:O	1:A:228:GLU:HG3	2.19	0.43
1:A:256:PRO:HB3	1:B:235:ALA:HB2	2.01	0.43
2:U:93:VAL:HG23	2:U:110:GLN:HA	1.99	0.43
1:C:187:MET:HE3	1:C:187:MET:HB3	1.89	0.43
1:J:77:ILE:N	1:J:77:ILE:HD13	2.34	0.43
1:J:225:LEU:O	1:J:228:GLU:HG3	2.19	0.43
1:L:174:ARG:HG2	1:L:175:ASP:N	2.34	0.43
1:N:241:ARG:HB2	1:O:227:ASN:ND2	2.34	0.43
1:O:103:ARG:NH1	1:O:225:LEU:HD11	2.34	0.43
1:P:164:ARG:HA	1:P:164:ARG:NE	2.33	0.43
1:T:225:LEU:O	1:T:228:GLU:HG3	2.19	0.43
2:c:83:MET:CE	2:c:86:LEU:HD11	2.48	0.43
2:m:83:MET:CE	2:m:86:LEU:HD11	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LYS:HD3	1:D:212:PRO:HD3	1.99	0.43
1:D:103:ARG:NH1	1:D:225:LEU:HD11	2.34	0.43
1:F:225:LEU:O	1:F:228:GLU:HG3	2.19	0.43
1:G:110:ARG:HA	1:G:113:ILE:CG2	2.47	0.43
1:J:103:ARG:NH1	1:J:225:LEU:HD11	2.34	0.43
1:J:164:ARG:NE	1:J:164:ARG:HA	2.33	0.43
1:K:103:ARG:NH1	1:K:225:LEU:HD11	2.34	0.43
1:K:224:HIS:HA	1:T:240:SER:OG	2.18	0.43
1:K:225:LEU:O	1:K:228:GLU:HG3	2.19	0.43
1:K:260:ASP:OD2	1:L:238:GLN:NE2	2.52	0.43
1:M:187:MET:HE3	1:M:187:MET:HB3	1.89	0.43
1:N:103:ARG:NH1	1:N:225:LEU:HD11	2.34	0.43
1:R:103:ARG:NH1	1:R:225:LEU:HD11	2.34	0.43
1:S:103:ARG:NH1	1:S:225:LEU:HD11	2.34	0.43
2:Y:83:MET:CE	2:Y:86:LEU:HD11	2.48	0.43
2:Z:83:MET:CE	2:Z:86:LEU:HD11	2.48	0.43
1:A:77:ILE:N	1:A:77:ILE:HD13	2.34	0.42
1:A:103:ARG:NH1	1:A:225:LEU:HD11	2.34	0.42
1:C:73:GLN:O	1:C:77:ILE:HG12	2.18	0.42
1:I:174:ARG:HG2	1:I:175:ASP:N	2.34	0.42
1:L:8:ILE:HD13	1:L:8:ILE:HA	1.83	0.42
1:P:77:ILE:N	1:P:77:ILE:HD13	2.34	0.42
1:P:225:LEU:O	1:P:228:GLU:HG3	2.19	0.42
2:W:35:ARG:N	2:W:97:PHE:O	2.47	0.42
2:a:83:MET:CE	2:a:86:LEU:HD11	2.48	0.42
2:e:83:MET:CE	2:e:86:LEU:HD11	2.48	0.42
2:h:76:LYS:HB2	2:h:78:THR:HG22	2.01	0.42
2:i:83:MET:CE	2:i:86:LEU:HD11	2.48	0.42
1:B:139:VAL:HG11	1:B:153:ARG:HD2	2.02	0.42
1:G:276:SER:HA	1:I:216:LEU:CD1	2.48	0.42
1:H:174:ARG:HG2	1:H:175:ASP:N	2.34	0.42
1:L:51:TYR:OH	1:M:186:GLN:NE2	2.52	0.42
1:M:73:GLN:O	1:M:77:ILE:HG12	2.18	0.42
1:N:98:LYS:HD3	1:N:212:PRO:HD3	1.99	0.42
1:R:174:ARG:HG2	1:R:175:ASP:N	2.34	0.42
1:S:169:ASP:OD2	2:m:59:HIS:CE1	2.72	0.42
1:T:77:ILE:N	1:T:77:ILE:HD13	2.34	0.42
2:a:76:LYS:HB2	2:a:78:THR:HG22	2.01	0.42
2:j:93:VAL:HG23	2:j:110:GLN:HA	1.99	0.42
2:k:76:LYS:HB2	2:k:78:THR:HG22	2.01	0.42
1:B:225:LEU:O	1:B:228:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:LEU:O	1:E:228:GLU:HG3	2.19	0.42
1:F:8:ILE:HD13	1:F:8:ILE:HA	1.83	0.42
1:I:103:ARG:NH1	1:I:225:LEU:HD11	2.34	0.42
1:K:77:ILE:N	1:K:77:ILE:HD13	2.34	0.42
1:L:139:VAL:HG11	1:L:153:ARG:HD2	2.02	0.42
1:L:225:LEU:O	1:L:228:GLU:HG3	2.19	0.42
1:N:225:LEU:HD23	1:N:225:LEU:HA	1.89	0.42
1:O:225:LEU:O	1:O:228:GLU:HG3	2.19	0.42
1:Q:103:ARG:NH1	1:Q:225:LEU:HD11	2.34	0.42
1:S:174:ARG:HG2	1:S:175:ASP:N	2.34	0.42
1:T:103:ARG:NH1	1:T:225:LEU:HD11	2.34	0.42
2:j:35:ARG:HD3	2:j:47:TRP:CZ3	2.52	0.42
2:j:76:LYS:HB2	2:j:78:THR:HG22	2.01	0.42
1:B:62:ILE:HD12	1:C:197:THR:HG21	2.01	0.42
1:B:103:ARG:NH1	1:B:225:LEU:HD11	2.34	0.42
1:D:77:ILE:N	1:D:77:ILE:HD13	2.34	0.42
1:D:174:ARG:HG2	1:D:175:ASP:N	2.34	0.42
1:D:225:LEU:HD23	1:D:225:LEU:HA	1.89	0.42
1:E:256:PRO:HG3	1:F:235:ALA:HB2	2.01	0.42
1:G:164:ARG:HA	1:G:164:ARG:NE	2.33	0.42
1:G:225:LEU:O	1:G:228:GLU:HG3	2.19	0.42
1:N:174:ARG:HG2	1:N:175:ASP:N	2.34	0.42
1:Q:225:LEU:O	1:Q:228:GLU:HG3	2.19	0.42
2:V:35:ARG:HD3	2:V:47:TRP:CZ3	2.52	0.42
2:W:83:MET:CE	2:W:86:LEU:HD11	2.48	0.42
2:b:76:LYS:HB2	2:b:78:THR:HG22	2.01	0.42
2:h:35:ARG:HD3	2:h:47:TRP:CZ3	2.52	0.42
2:k:83:MET:CE	2:k:86:LEU:HD11	2.48	0.42
2:n:76:LYS:HB2	2:n:78:THR:HG22	2.01	0.42
2:U:76:LYS:HB2	2:U:78:THR:HG22	2.01	0.42
1:E:254:PHE:HE2	1:F:238:GLN:NE2	2.16	0.42
1:K:244:MET:SD	1:L:228:GLU:HB2	2.60	0.42
1:L:103:ARG:NH1	1:L:225:LEU:HD11	2.34	0.42
2:g:83:MET:CE	2:g:86:LEU:HD11	2.48	0.42
1:A:139:VAL:HG11	1:A:153:ARG:HD2	2.02	0.42
1:I:225:LEU:O	1:I:228:GLU:HG3	2.19	0.42
2:V:76:LYS:HB2	2:V:78:THR:HG22	2.01	0.42
2:X:76:LYS:HB2	2:X:78:THR:HG22	2.01	0.42
2:f:76:LYS:HB2	2:f:78:THR:HG22	2.01	0.42
1:A:51:TYR:CD2	1:B:183:TYR:HD1	2.35	0.42
1:C:103:ARG:NH1	1:C:225:LEU:HD11	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LEU:O	1:C:228:GLU:HG3	2.19	0.42
1:K:139:VAL:HG11	1:K:153:ARG:HD2	2.02	0.42
1:L:256:PRO:HG3	1:M:235:ALA:HB2	2.01	0.42
1:N:77:ILE:N	1:N:77:ILE:HD13	2.34	0.42
1:N:225:LEU:O	1:N:228:GLU:HG3	2.19	0.42
1:O:139:VAL:HG11	1:O:153:ARG:HD2	2.02	0.42
1:S:225:LEU:O	1:S:228:GLU:HG3	2.19	0.42
2:d:76:LYS:HB2	2:d:78:THR:HG22	2.01	0.42
2:f:35:ARG:HD3	2:f:47:TRP:CZ3	2.52	0.42
2:g:76:LYS:HB2	2:g:78:THR:HG22	2.01	0.42
1:B:8:ILE:HD13	1:B:8:ILE:HA	1.83	0.42
1:B:77:ILE:N	1:B:77:ILE:HD13	2.34	0.42
1:C:139:VAL:HG11	1:C:153:ARG:HD2	2.02	0.42
1:D:225:LEU:O	1:D:228:GLU:HG3	2.19	0.42
1:L:77:ILE:N	1:L:77:ILE:HD13	2.34	0.42
1:M:103:ARG:NH1	1:M:225:LEU:HD11	2.34	0.42
1:M:139:VAL:HG11	1:M:153:ARG:HD2	2.02	0.42
1:M:225:LEU:O	1:M:228:GLU:HG3	2.19	0.42
2:W:76:LYS:HB2	2:W:78:THR:HG22	2.01	0.42
2:Z:76:LYS:HB2	2:Z:78:THR:HG22	2.01	0.42
2:f:35:ARG:N	2:f:97:PHE:O	2.47	0.42
1:E:77:ILE:N	1:E:77:ILE:HD13	2.34	0.42
1:E:139:VAL:HG11	1:E:153:ARG:HD2	2.02	0.42
1:O:174:ARG:HG2	1:O:175:ASP:N	2.34	0.42
2:Y:76:LYS:HB2	2:Y:78:THR:HG22	2.01	0.42
2:g:35:ARG:N	2:g:97:PHE:O	2.47	0.42
2:m:76:LYS:HB2	2:m:78:THR:HG22	2.01	0.42
1:A:240:SER:OG	1:B:224:HIS:HB2	2.20	0.42
1:E:144:MET:O	2:Y:35:ARG:NH2	2.52	0.42
1:E:174:ARG:HG2	1:E:175:ASP:N	2.34	0.42
1:G:103:ARG:NH1	1:G:225:LEU:HD11	2.34	0.42
1:G:244:MET:SD	1:H:228:GLU:HB2	2.60	0.42
1:H:244:MET:SD	1:I:228:GLU:HB2	2.60	0.42
1:M:55:PHE:CE2	1:N:190:TRP:NE1	2.71	0.42
1:F:174:ARG:HG2	1:F:175:ASP:N	2.34	0.41
2:V:35:ARG:N	2:V:97:PHE:O	2.47	0.41
2:e:76:LYS:HB2	2:e:78:THR:HG22	2.01	0.41
2:i:76:LYS:HB2	2:i:78:THR:HG22	2.01	0.41
1:F:248:ILE:HD11	1:G:235:ALA:HB2	1.83	0.41
1:P:139:VAL:HG11	1:P:153:ARG:HD2	2.02	0.41
2:X:35:ARG:HD3	2:X:47:TRP:CZ3	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:35:ARG:HD3	2:Z:47:TRP:CZ3	2.52	0.41
2:l:76:LYS:HB2	2:l:78:THR:HG22	2.01	0.41
1:H:77:ILE:N	1:H:77:ILE:HD13	2.34	0.41
1:M:174:ARG:HG2	1:M:175:ASP:N	2.34	0.41
1:O:77:ILE:N	1:O:77:ILE:HD13	2.34	0.41
1:C:174:ARG:HG2	1:C:175:ASP:N	2.34	0.41
1:F:6:ASN:OD1	1:F:6:ASN:C	2.64	0.41
1:J:174:ARG:HG2	1:J:175:ASP:N	2.34	0.41
1:R:77:ILE:N	1:R:77:ILE:HD13	2.34	0.41
1:S:6:ASN:OD1	1:S:6:ASN:C	2.64	0.41
1:H:254:PHE:CE2	1:I:238:GLN:NE2	2.89	0.41
1:I:6:ASN:OD1	1:I:6:ASN:C	2.64	0.41
1:N:248:ILE:CD1	1:O:235:ALA:CB	2.92	0.41
1:P:8:ILE:HD13	1:P:8:ILE:HA	1.83	0.41
1:Q:77:ILE:HD13	1:Q:77:ILE:N	2.34	0.41
2:c:76:LYS:HB2	2:c:78:THR:HG22	2.01	0.41
2:e:35:ARG:HB3	2:e:47:TRP:HZ3	1.84	0.41
1:D:6:ASN:OD1	1:D:6:ASN:C	2.64	0.41
1:D:51:TYR:HD2	1:E:183:TYR:CD1	2.36	0.41
1:D:139:VAL:HG11	1:D:153:ARG:HD2	2.02	0.41
1:D:187:MET:HE3	1:D:187:MET:HB3	1.89	0.41
1:F:139:VAL:HG11	1:F:153:ARG:HD2	2.02	0.41
1:N:144:MET:O	2:h:35:ARG:NH2	2.54	0.41
1:P:6:ASN:OD1	1:P:6:ASN:C	2.64	0.41
1:R:244:MET:HG2	1:S:228:GLU:HA	2.02	0.41
1:A:235:ALA:HB2	1:J:256:PRO:HB3	2.03	0.41
1:C:240:SER:OG	1:D:224:HIS:HB2	2.21	0.41
1:I:144:MET:O	2:c:35:ARG:NH2	2.54	0.41
1:N:6:ASN:OD1	1:N:6:ASN:C	2.64	0.41
1:P:244:MET:SD	1:Q:228:GLU:HB2	2.61	0.41
1:T:174:ARG:HG2	1:T:175:ASP:N	2.34	0.41
1:E:160:PHE:HA	1:E:164:ARG:HB2	2.03	0.41
1:F:77:ILE:N	1:F:77:ILE:HD13	2.34	0.41
1:H:6:ASN:OD1	1:H:6:ASN:C	2.64	0.41
1:I:77:ILE:N	1:I:77:ILE:HD13	2.34	0.41
1:K:238:GLN:NE2	1:T:260:ASP:OD2	2.54	0.41
1:L:244:MET:SD	1:M:228:GLU:HB2	2.61	0.41
1:N:139:VAL:HG11	1:N:153:ARG:HD2	2.02	0.41
1:Q:6:ASN:OD1	1:Q:6:ASN:C	2.64	0.41
1:Q:139:VAL:HG11	1:Q:153:ARG:HD2	2.02	0.41
1:Q:174:ARG:HG2	1:Q:175:ASP:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASN:C	1:A:6:ASN:OD1	2.64	0.41
1:C:51:TYR:HD1	1:D:183:TYR:HD1	1.68	0.41
1:D:273:LYS:HD2	1:D:273:LYS:C	2.46	0.41
1:E:169:ASP:OD2	2:Y:59:HIS:HE1	2.04	0.41
1:G:77:ILE:HD13	1:G:77:ILE:N	2.34	0.41
1:G:139:VAL:HG11	1:G:153:ARG:HD2	2.02	0.41
1:G:273:LYS:HD2	1:G:273:LYS:C	2.46	0.41
1:H:139:VAL:HG11	1:H:153:ARG:HD2	2.02	0.41
1:J:273:LYS:HD2	1:J:273:LYS:C	2.46	0.41
1:K:6:ASN:OD1	1:K:6:ASN:C	2.64	0.41
1:N:187:MET:HE3	1:N:187:MET:HB3	1.89	0.41
1:N:273:LYS:HD2	1:N:273:LYS:C	2.46	0.41
1:O:160:PHE:HA	1:O:164:ARG:HB2	2.03	0.41
1:P:52:GLY:HA3	1:P:132:ALA:HB2	2.03	0.41
1:Q:187:MET:HE3	1:Q:187:MET:HB3	1.89	0.41
1:R:6:ASN:OD1	1:R:6:ASN:C	2.64	0.41
1:T:273:LYS:HD2	1:T:273:LYS:C	2.46	0.41
2:Y:35:ARG:HD3	2:Y:47:TRP:CZ3	2.52	0.41
2:i:35:ARG:HD3	2:i:47:TRP:CZ3	2.52	0.41
1:C:256:PRO:HG3	1:D:235:ALA:HB2	2.03	0.41
1:D:160:PHE:HA	1:D:164:ARG:HB2	2.03	0.41
1:G:174:ARG:HG2	1:G:175:ASP:N	2.34	0.41
1:H:273:LYS:HD2	1:H:273:LYS:C	2.46	0.41
1:J:139:VAL:HG11	1:J:153:ARG:HD2	2.02	0.41
1:M:273:LYS:HD2	1:M:273:LYS:C	2.46	0.41
1:P:160:PHE:HA	1:P:164:ARG:HB2	2.03	0.41
1:P:273:LYS:HD2	1:P:273:LYS:C	2.46	0.41
1:Q:225:LEU:HD23	1:Q:225:LEU:HA	1.89	0.41
1:R:273:LYS:HD2	1:R:273:LYS:C	2.46	0.41
1:S:77:ILE:HD13	1:S:77:ILE:N	2.34	0.41
1:T:139:VAL:HG11	1:T:153:ARG:HD2	2.02	0.41
2:b:35:ARG:HD3	2:b:47:TRP:CZ3	2.52	0.41
2:l:35:ARG:HD3	2:l:47:TRP:CZ3	2.52	0.41
1:A:273:LYS:HD2	1:A:273:LYS:C	2.46	0.40
1:C:273:LYS:HD2	1:C:273:LYS:C	2.46	0.40
1:G:6:ASN:OD1	1:G:6:ASN:C	2.64	0.40
1:I:160:PHE:HA	1:I:164:ARG:HB2	2.03	0.40
1:J:160:PHE:HA	1:J:164:ARG:HB2	2.03	0.40
1:K:223:SER:OG	1:T:237:GLU:HA	2.21	0.40
1:L:6:ASN:OD1	1:L:6:ASN:C	2.64	0.40
1:O:6:ASN:OD1	1:O:6:ASN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:139:VAL:HG11	1:R:153:ARG:HD2	2.02	0.40
1:B:6:ASN:OD1	1:B:6:ASN:C	2.64	0.40
1:E:52:GLY:HA3	1:E:132:ALA:HB2	2.03	0.40
1:E:276:SER:HB2	1:G:216:LEU:CD1	2.51	0.40
1:F:52:GLY:HA3	1:F:132:ALA:HB2	2.03	0.40
1:G:52:GLY:HA3	1:G:132:ALA:HB2	2.03	0.40
1:I:139:VAL:HG11	1:I:153:ARG:HD2	2.02	0.40
1:K:273:LYS:HD2	1:K:273:LYS:C	2.46	0.40
1:L:273:LYS:HD2	1:L:273:LYS:C	2.46	0.40
1:N:160:PHE:HA	1:N:164:ARG:HB2	2.03	0.40
1:O:52:GLY:HA3	1:O:132:ALA:HB2	2.03	0.40
1:P:174:ARG:HG2	1:P:175:ASP:N	2.34	0.40
1:R:187:MET:HE3	1:R:187:MET:HB3	1.89	0.40
1:S:51:TYR:HD1	1:T:183:TYR:HD1	1.69	0.40
1:S:139:VAL:HG11	1:S:153:ARG:HD2	2.02	0.40
1:T:160:PHE:HA	1:T:164:ARG:HB2	2.03	0.40
1:B:34:PHE:CZ	1:C:190:TRP:CH2	3.09	0.40
1:B:273:LYS:HD2	1:B:273:LYS:C	2.46	0.40
1:E:248:ILE:HD13	1:E:248:ILE:HG21	1.89	0.40
1:Q:52:GLY:HA3	1:Q:132:ALA:HB2	2.03	0.40
1:Q:273:LYS:HD2	1:Q:273:LYS:C	2.46	0.40
1:S:160:PHE:HA	1:S:164:ARG:HB2	2.03	0.40
1:B:241:ARG:HB2	1:C:227:ASN:ND2	2.35	0.40
1:C:6:ASN:OD1	1:C:6:ASN:C	2.64	0.40
1:E:273:LYS:HD2	1:E:273:LYS:C	2.46	0.40
1:F:273:LYS:HD2	1:F:273:LYS:C	2.46	0.40
1:K:52:GLY:HA3	1:K:132:ALA:HB2	2.03	0.40
1:M:6:ASN:OD1	1:M:6:ASN:C	2.64	0.40
1:A:52:GLY:HA3	1:A:132:ALA:HB2	2.03	0.40
1:E:6:ASN:OD1	1:E:6:ASN:C	2.64	0.40
1:J:6:ASN:OD1	1:J:6:ASN:C	2.64	0.40
1:Q:160:PHE:HA	1:Q:164:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	B	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	C	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	D	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	E	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	F	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	G	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	H	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	I	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	J	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	K	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	L	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	M	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	N	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	O	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	P	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	Q	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	R	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	S	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
1	T	257/322 (80%)	244 (95%)	13 (5%)	0	100	100
2	U	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	V	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	W	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	X	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	Y	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	Z	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	a	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	b	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	c	84/143 (59%)	82 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	d	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	e	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	f	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	g	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	h	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	i	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	j	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	k	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	l	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	m	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
2	n	84/143 (59%)	82 (98%)	2 (2%)	0	100	100
All	All	6820/9300 (73%)	6520 (96%)	300 (4%)	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	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	B	225/280 (80%)	222 (99%)	3 (1%)	61	71
1	C	225/280 (80%)	222 (99%)	3 (1%)	61	71
1	D	225/280 (80%)	222 (99%)	3 (1%)	61	71
1	E	225/280 (80%)	222 (99%)	3 (1%)	61	71
1	F	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	G	225/280 (80%)	222 (99%)	3 (1%)	61	71
1	H	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	I	225/280 (80%)	222 (99%)	3 (1%)	61	71
1	J	225/280 (80%)	221 (98%)	4 (2%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	225/280 (80%)	222 (99%)	3 (1%)	61	71
1	L	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	M	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	N	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	O	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	P	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	Q	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	R	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	S	225/280 (80%)	221 (98%)	4 (2%)	51	67
1	T	225/280 (80%)	222 (99%)	3 (1%)	61	71
2	U	76/114 (67%)	76 (100%)	0	100	100
2	V	76/114 (67%)	76 (100%)	0	100	100
2	W	76/114 (67%)	76 (100%)	0	100	100
2	X	76/114 (67%)	76 (100%)	0	100	100
2	Y	76/114 (67%)	76 (100%)	0	100	100
2	Z	76/114 (67%)	76 (100%)	0	100	100
2	a	76/114 (67%)	76 (100%)	0	100	100
2	b	76/114 (67%)	76 (100%)	0	100	100
2	c	76/114 (67%)	76 (100%)	0	100	100
2	d	76/114 (67%)	76 (100%)	0	100	100
2	e	76/114 (67%)	76 (100%)	0	100	100
2	f	76/114 (67%)	76 (100%)	0	100	100
2	g	76/114 (67%)	76 (100%)	0	100	100
2	h	76/114 (67%)	75 (99%)	1 (1%)	61	71
2	i	76/114 (67%)	76 (100%)	0	100	100
2	j	76/114 (67%)	76 (100%)	0	100	100
2	k	76/114 (67%)	76 (100%)	0	100	100
2	l	76/114 (67%)	76 (100%)	0	100	100
2	m	76/114 (67%)	76 (100%)	0	100	100
2	n	76/114 (67%)	76 (100%)	0	100	100
All	All	6020/7880 (76%)	5947 (99%)	73 (1%)	61	72

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
1	A	192	LEU
1	A	250	LYS
1	A	271	ASP
1	B	192	LEU
1	B	250	LYS
1	B	271	ASP
1	C	192	LEU
1	C	250	LYS
1	C	271	ASP
1	D	192	LEU
1	D	250	LYS
1	D	271	ASP
1	E	192	LEU
1	E	250	LYS
1	E	271	ASP
1	F	154	GLU
1	F	192	LEU
1	F	250	LYS
1	F	271	ASP
1	G	154	GLU
1	G	192	LEU
1	G	271	ASP
1	H	154	GLU
1	H	192	LEU
1	H	250	LYS
1	H	271	ASP
1	I	192	LEU
1	I	250	LYS
1	I	271	ASP
1	J	154	GLU
1	J	192	LEU
1	J	250	LYS
1	J	271	ASP
1	K	192	LEU
1	K	250	LYS
1	K	271	ASP
1	L	154	GLU
1	L	192	LEU
1	L	250	LYS
1	L	271	ASP
1	M	154	GLU

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Mol	Chain	Res	Type
1	M	192	LEU
1	M	250	LYS
1	M	271	ASP
1	N	154	GLU
1	N	192	LEU
1	N	250	LYS
1	N	271	ASP
1	O	154	GLU
1	O	192	LEU
1	O	250	LYS
1	O	271	ASP
1	P	154	GLU
1	P	192	LEU
1	P	250	LYS
1	P	271	ASP
1	Q	154	GLU
1	Q	192	LEU
1	Q	250	LYS
1	Q	271	ASP
1	R	154	GLU
1	R	192	LEU
1	R	250	LYS
1	R	271	ASP
1	S	154	GLU
1	S	192	LEU
1	S	250	LYS
1	S	271	ASP
1	T	192	LEU
1	T	250	LYS
1	T	271	ASP
2	h	70	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
2	U	39	GLN
2	U	110	GLN
1	C	6	ASN
1	C	238	GLN
1	D	6	ASN
1	E	6	ASN

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Mol	Chain	Res	Type
1	E	239	HIS
1	F	6	ASN
1	G	6	ASN
1	G	238	GLN
1	I	6	ASN
1	I	238	GLN
1	J	6	ASN
1	J	238	GLN
1	K	6	ASN
1	L	6	ASN
1	L	238	GLN
1	M	6	ASN
1	N	6	ASN
1	N	186	GLN
1	O	6	ASN
1	O	238	GLN
1	P	6	ASN
1	Q	6	ASN
1	Q	238	GLN
1	R	6	ASN
1	T	6	ASN
2	V	59	HIS
2	V	110	GLN
2	W	39	GLN
2	W	110	GLN
2	X	39	GLN
2	X	59	HIS
2	X	110	GLN
2	Y	59	HIS
2	Y	110	GLN
2	Z	39	GLN
2	Z	59	HIS
2	Z	110	GLN
2	a	59	HIS
2	a	110	GLN
2	b	39	GLN
2	b	110	GLN
2	c	59	HIS
2	c	110	GLN
2	d	110	GLN
2	e	39	GLN
2	e	59	HIS

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Mol	Chain	Res	Type
2	e	110	GLN
2	f	39	GLN
2	f	59	HIS
2	f	110	GLN
2	g	110	GLN
2	h	110	GLN
2	i	59	HIS
2	i	110	GLN
2	j	110	GLN
2	k	110	GLN
2	l	39	GLN
2	l	59	HIS
2	l	110	GLN
2	m	39	GLN
2	m	59	HIS
2	m	110	GLN
2	n	110	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

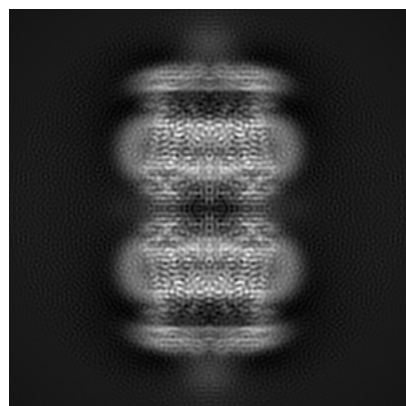
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19365. These allow visual inspection of the internal detail of the map and identification of artifacts.

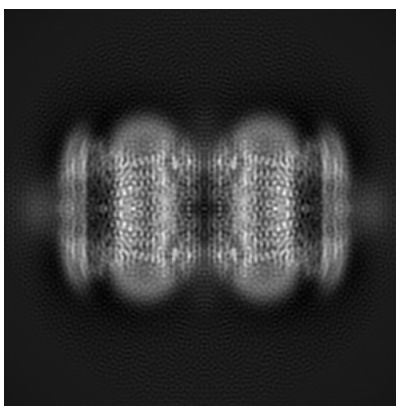
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

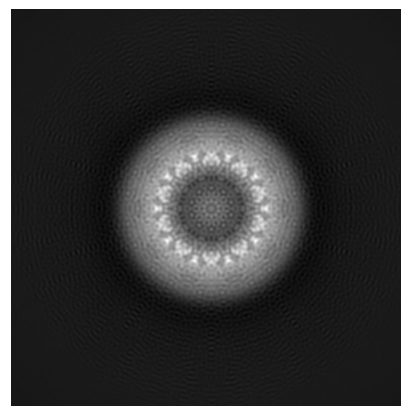
6.1.1 Primary map



X

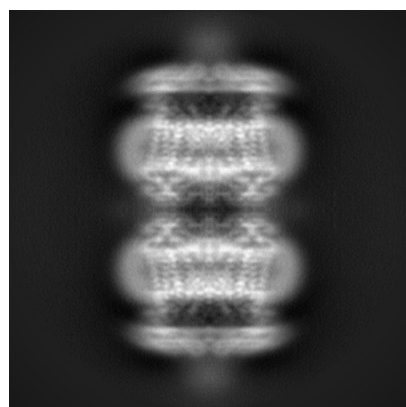


Y

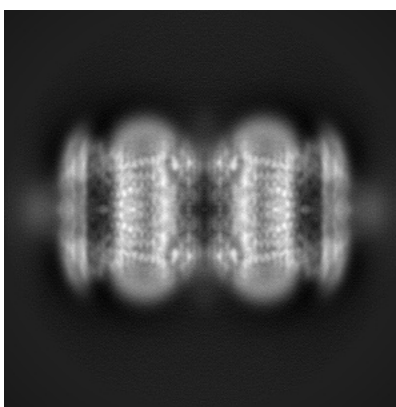


Z

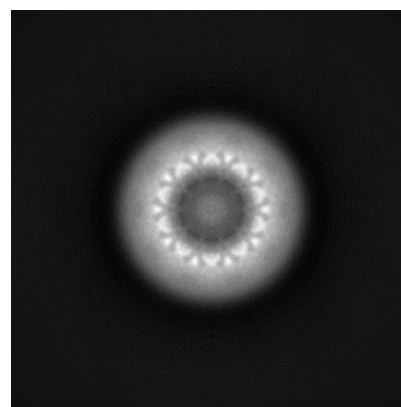
6.1.2 Raw map



X



Y

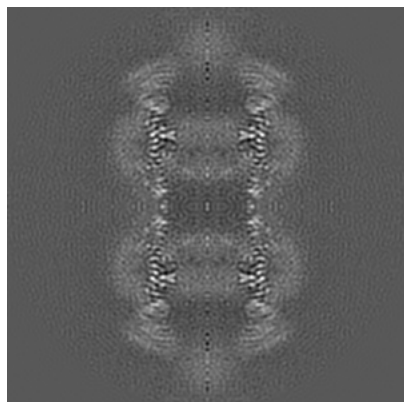


Z

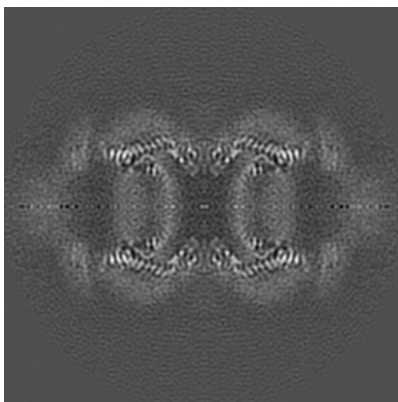
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

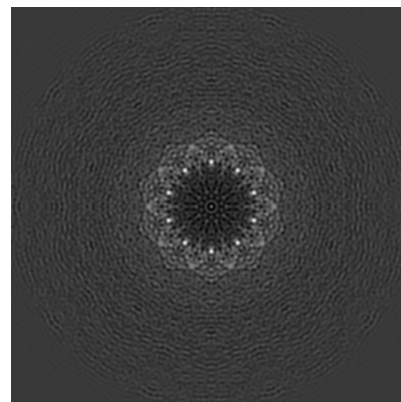
6.2.1 Primary map



X Index: 250

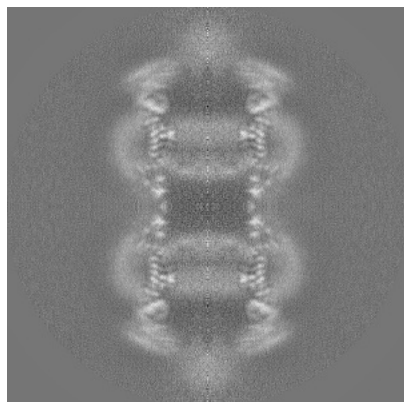


Y Index: 250

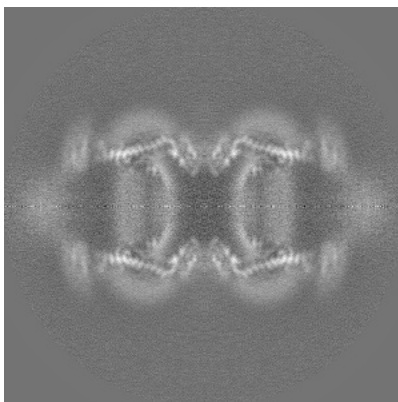


Z Index: 250

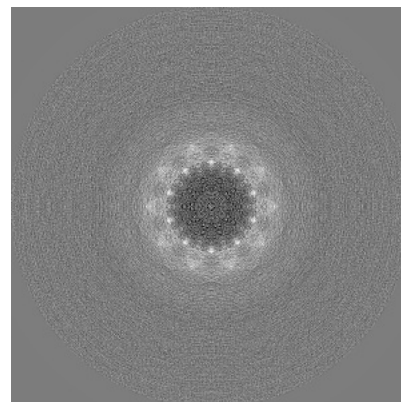
6.2.2 Raw map



X Index: 250



Y Index: 250

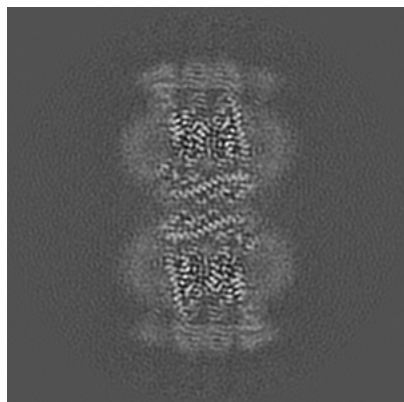


Z Index: 250

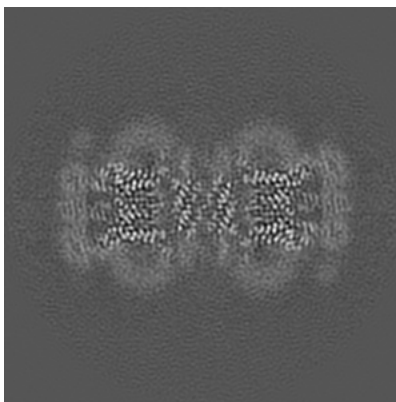
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

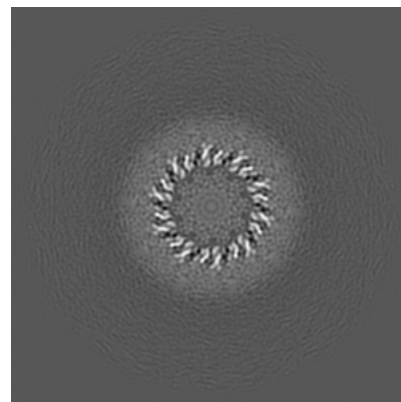
6.3.1 Primary map



X Index: 306

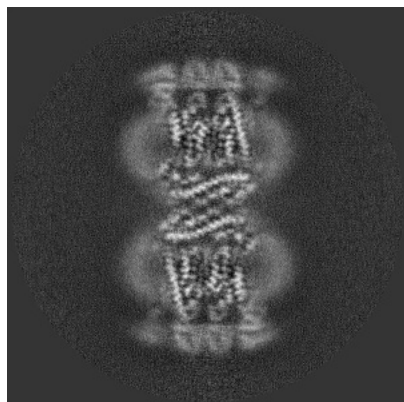


Y Index: 195

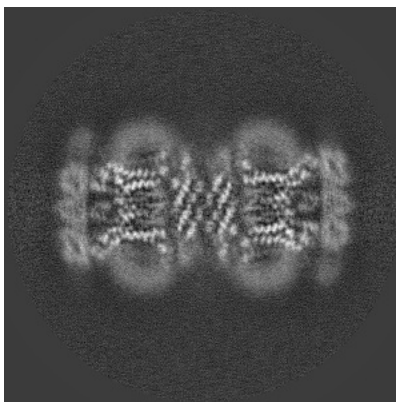


Z Index: 146

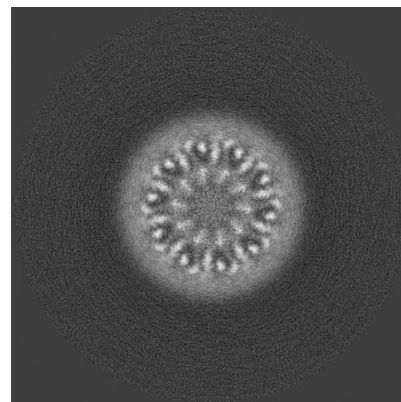
6.3.2 Raw map



X Index: 194



Y Index: 304

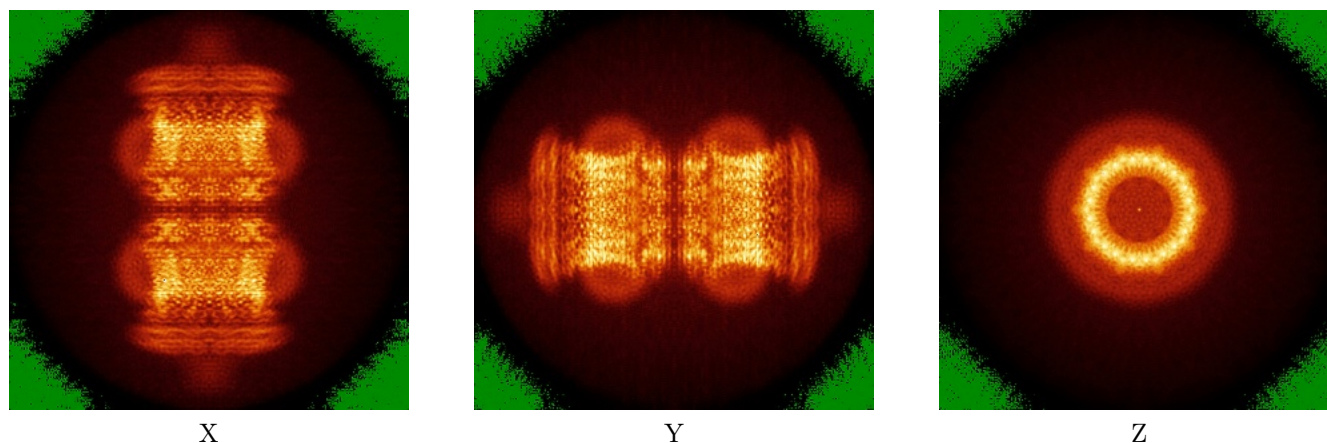


Z Index: 199

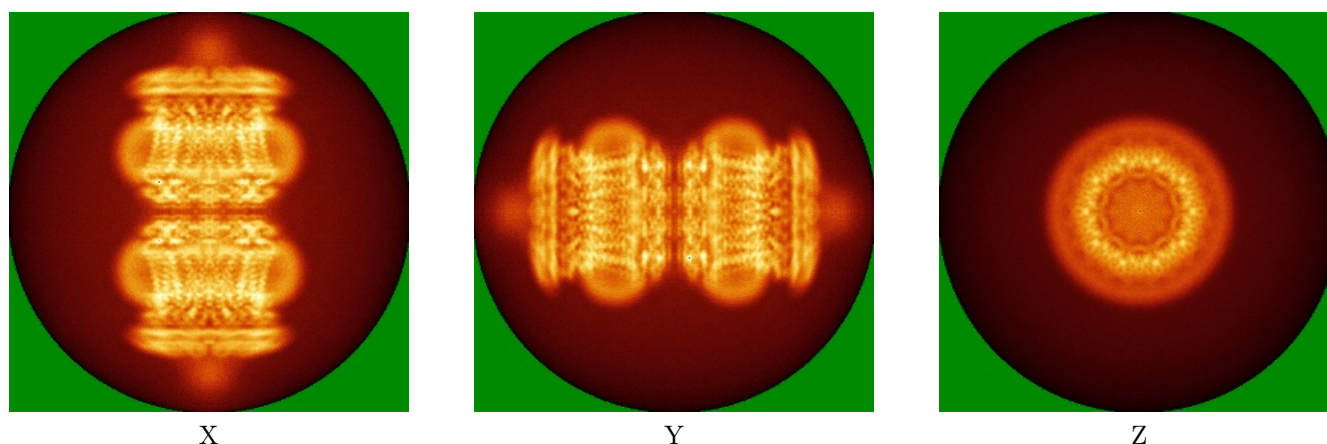
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

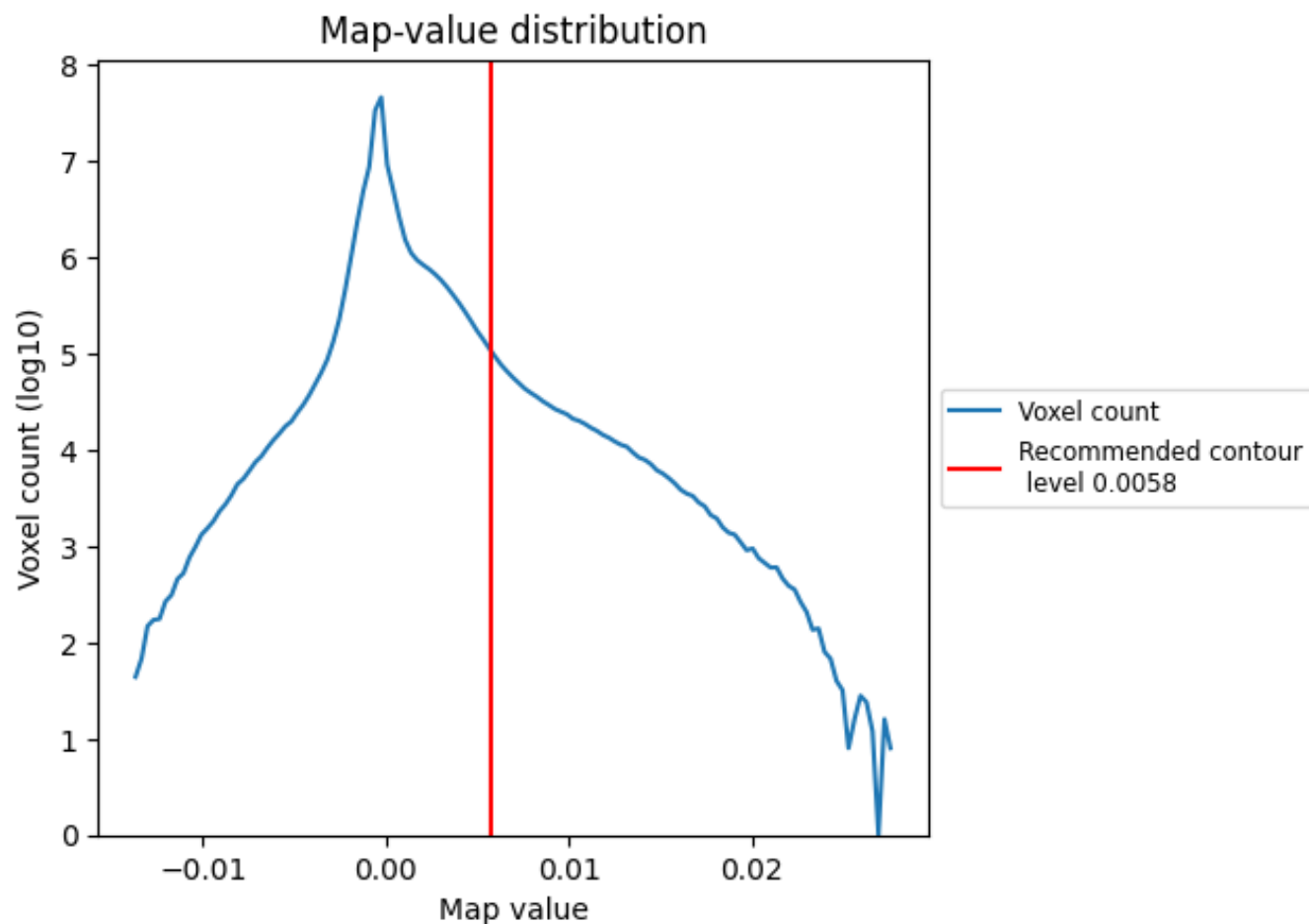
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

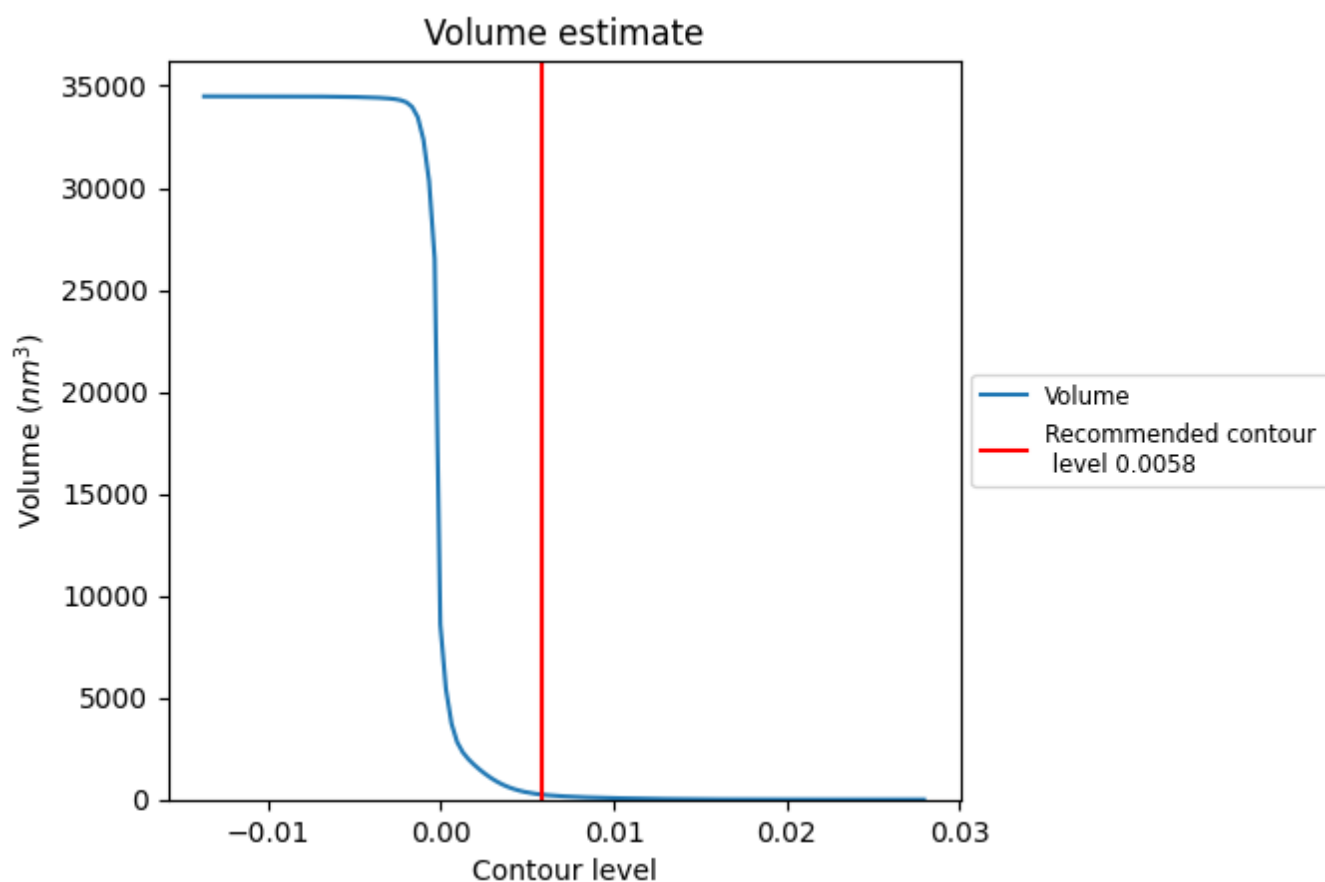
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

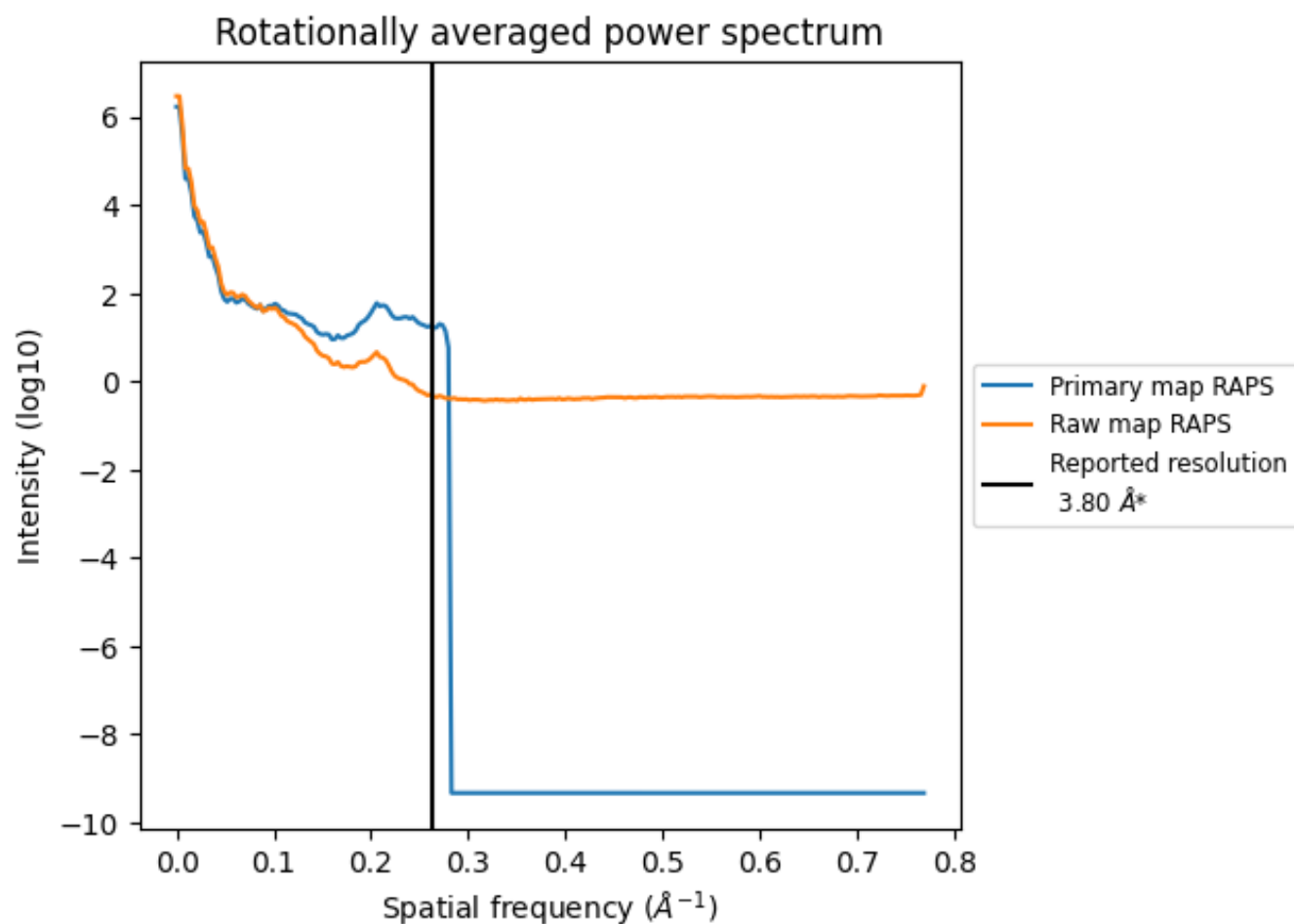
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 248 nm³; this corresponds to an approximate mass of 224 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

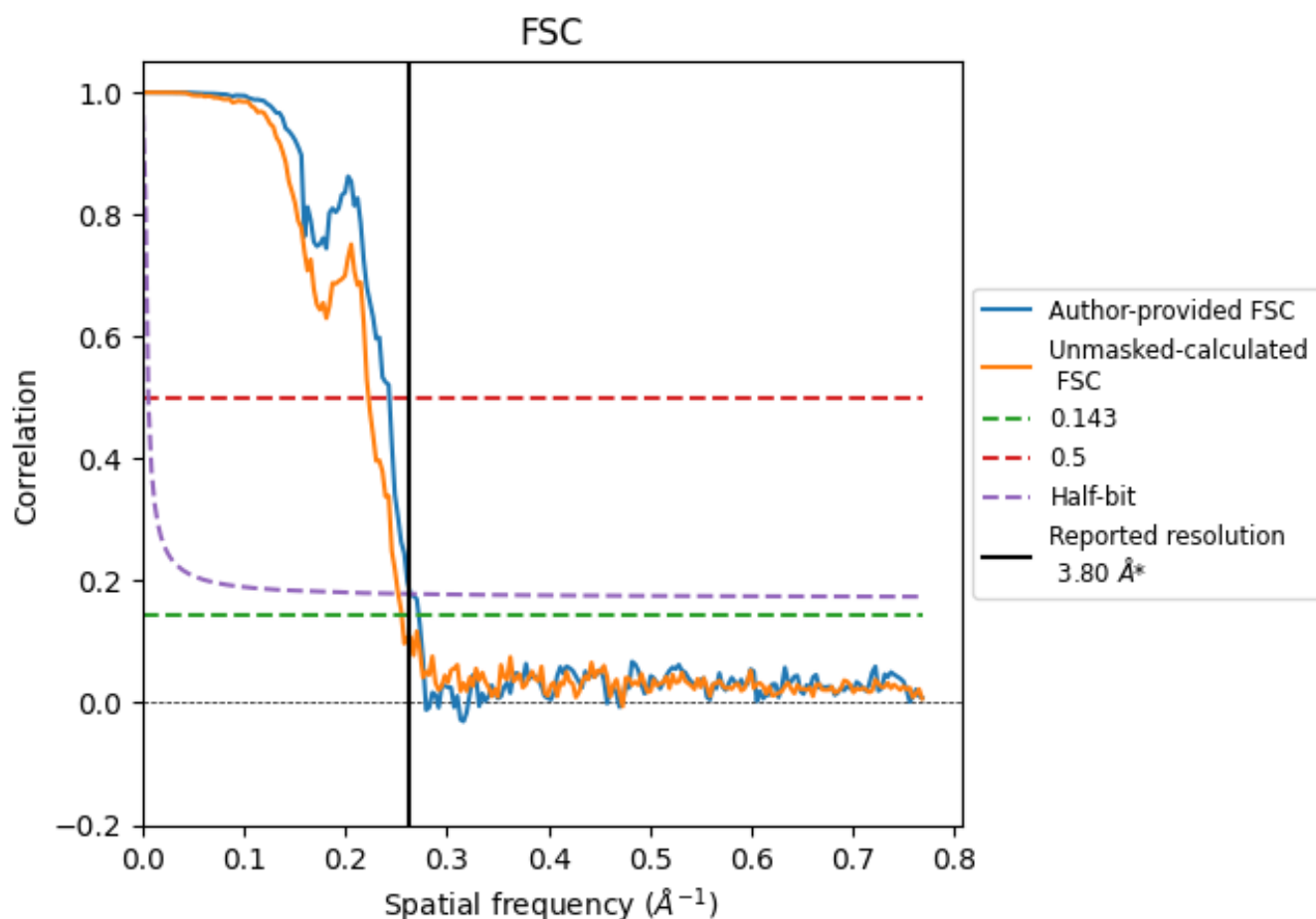


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.263 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

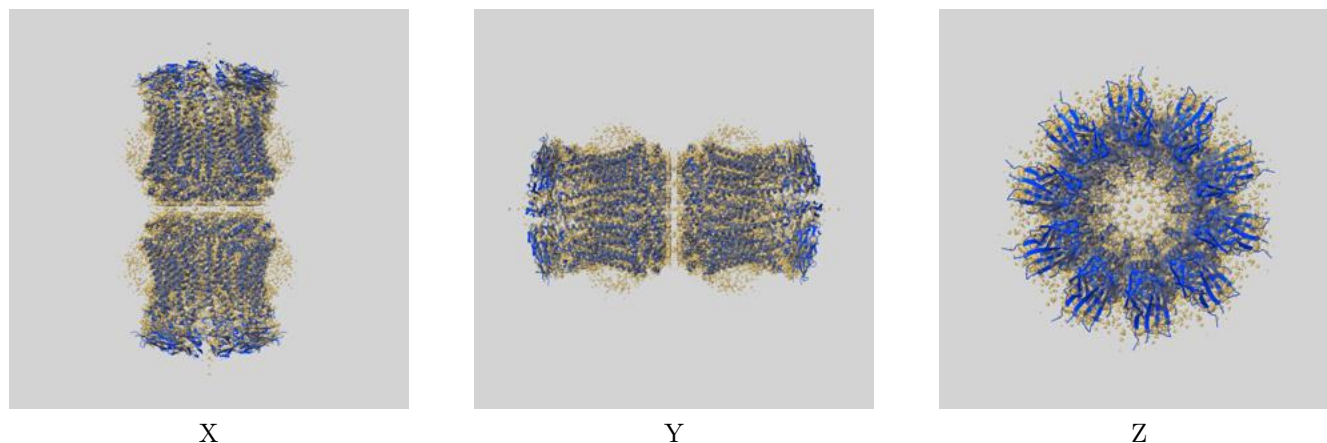
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.67	4.11	3.79
Unmasked-calculated*	3.91	4.49	3.97

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

9 Map-model fit [i](#)

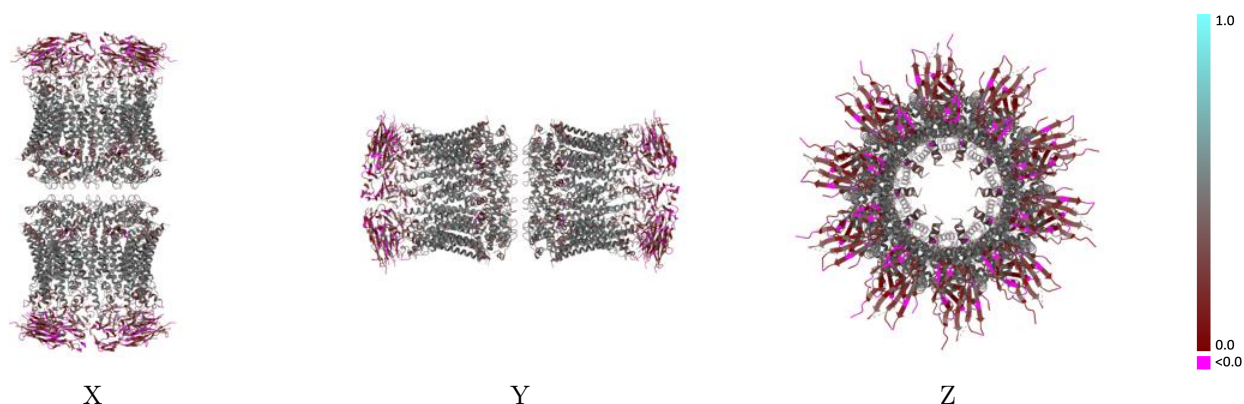
This section contains information regarding the fit between EMDB map EMD-19365 and PDB model 8RMN. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



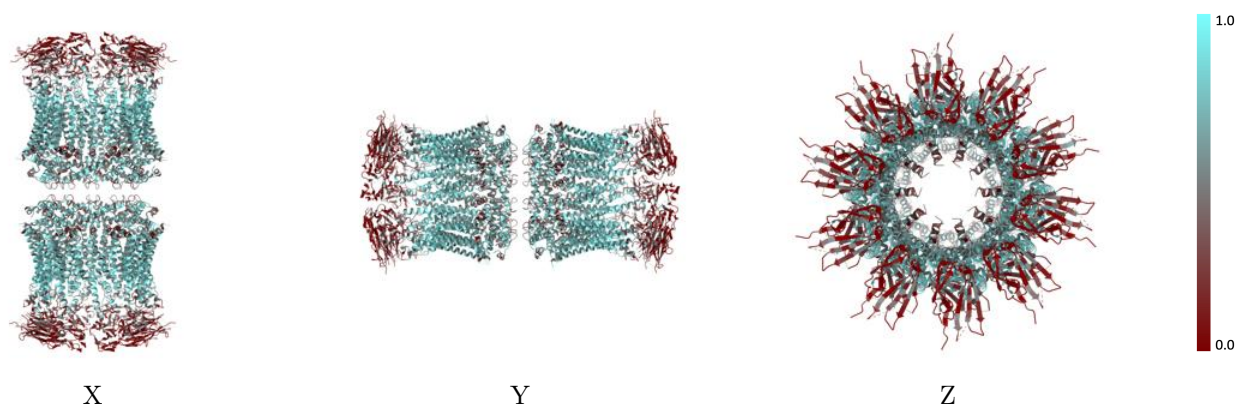
The images above show the 3D surface view of the map at the recommended contour level 0.0058 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



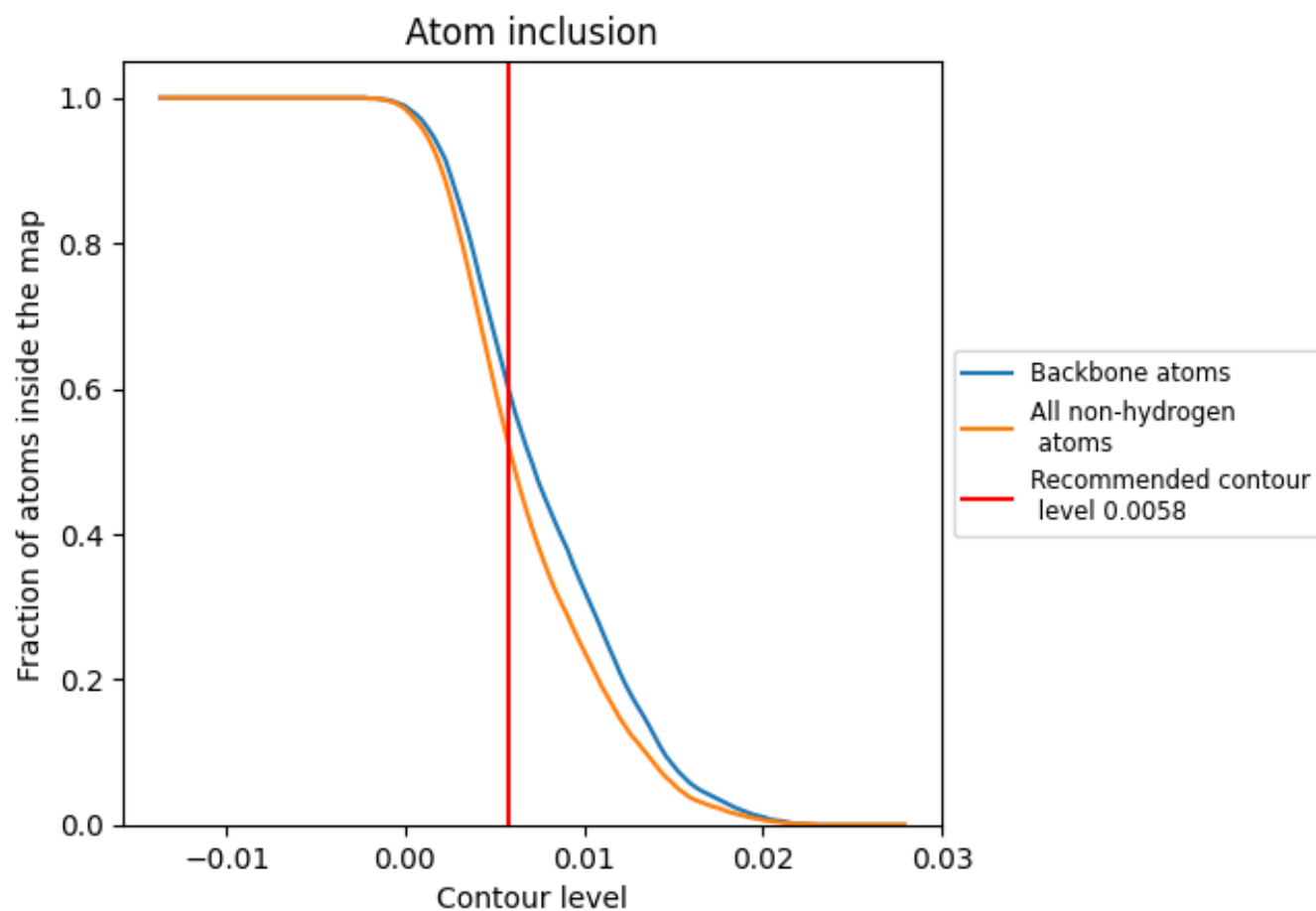
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0058).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 52% 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 (0.0058) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5190	 0.3620
A	 0.6440	 0.4320
B	 0.6440	 0.4310
C	 0.6430	 0.4260
D	 0.6450	 0.4310
E	 0.6390	 0.4270
F	 0.6250	 0.4140
G	 0.6400	 0.4250
H	 0.6480	 0.4330
I	 0.6420	 0.4300
J	 0.6440	 0.4320
K	 0.6430	 0.4340
L	 0.6450	 0.4310
M	 0.6380	 0.4270
N	 0.6340	 0.4250
O	 0.6460	 0.4310
P	 0.6450	 0.4300
Q	 0.6430	 0.4290
R	 0.6430	 0.4220
S	 0.6350	 0.4200
T	 0.6340	 0.4280
U	 0.1780	 0.1820
V	 0.1740	 0.1830
W	 0.1810	 0.1760
X	 0.1830	 0.1810
Y	 0.1740	 0.1800
Z	 0.1800	 0.1880
a	 0.1760	 0.1850
b	 0.1800	 0.1860
c	 0.1770	 0.1890
d	 0.1850	 0.1790
e	 0.1840	 0.1950
f	 0.1810	 0.1830
g	 0.1740	 0.1620
h	 0.1810	 0.1760



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Chain	Atom inclusion	Q-score
i	 0.1740	 0.1780
j	 0.1740	 0.1650
k	 0.1670	 0.1680
l	 0.1700	 0.1740
m	 0.1800	 0.1820
n	 0.1730	 0.1740