



Full wwPDB EM Validation Report ⓘ

Apr 28, 2026 – 01:44 PM EDT

PDB ID : 9O3O / pdb_00009o3o
EMDB ID : EMD-70081
Title : Phosphonull (T175A) of stress-activating residues
Authors : Martinez-Bond, E.A.; Lopez-Ayala, I.; Qiu, L.; Garda, V.; Yu, Z.; Williams, A.H.
Deposited on : 2025-04-07
Resolution : 4.05 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:

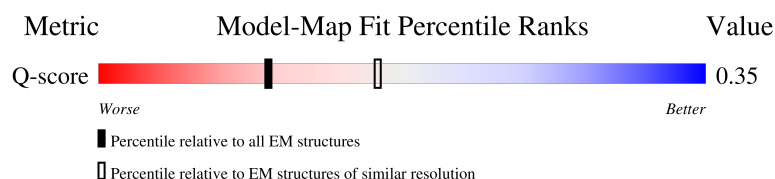
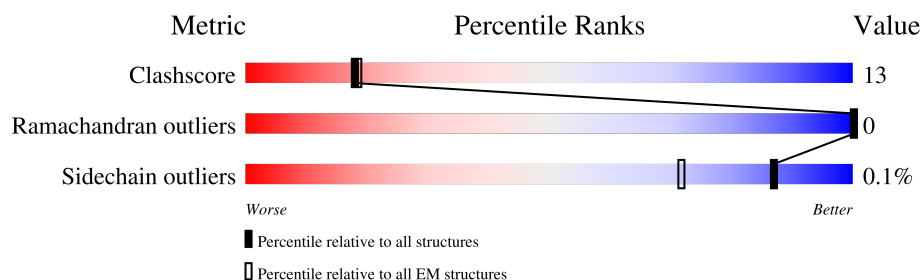
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.05 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	6569 (3.55 - 4.55)

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	278	<div> <div>9%</div> <div>37%</div> <div>10%</div> <div>53%</div> </div>
1	AB	278	<div> <div>10%</div> <div>36%</div> <div>11%</div> <div>53%</div> </div>
1	B	278	<div> <div>9%</div> <div>35%</div> <div>12%</div> <div>53%</div> </div>
1	BB	278	<div> <div>10%</div> <div>35%</div> <div>12%</div> <div>53%</div> </div>

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Mol	Chain	Length	Quality of chain
1	C	278	
1	CB	278	
1	D	278	
1	DB	278	
1	E	278	
1	EB	278	
1	F	278	
1	FB	278	
1	G	278	
1	GB	278	
1	H	278	
1	HB	278	
1	I	278	
1	IB	278	
1	J	278	
1	JB	278	
1	K	278	
1	KB	278	
1	L	278	
1	LB	278	
1	M	278	
1	MB	278	
1	N	278	
1	NB	278	
1	O	278	




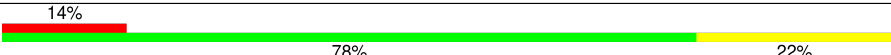
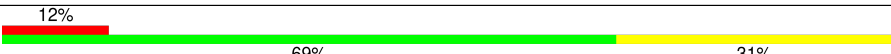
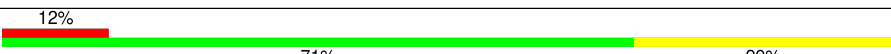
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Mol	Chain	Length	Quality of chain
1	OB	278	
1	P	278	
1	PB	278	
1	Q	278	
1	QB	278	
1	R	278	
1	RB	278	
1	S	278	
1	SB	278	
1	T	278	
1	TB	278	
2	a	118	
2	ab	118	
2	b	118	
2	bb	118	
2	c	118	
2	cb	118	
2	d	118	
2	db	118	
2	e	118	
2	eb	118	
2	f	118	
2	fb	118	
2	g	118	
2	gb	118	

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Mol	Chain	Length	Quality of chain
2	h	118	
2	hb	118	
2	i	118	
2	ib	118	
2	j	118	
2	jb	118	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 57700 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 STAS domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	AB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	B	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	BB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	C	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	CB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	D	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	DB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	E	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	EB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	F	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	FB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	G	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	GB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	H	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	HB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	I	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	IB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	J	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	JB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	K	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	KB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	L	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	LB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	M	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	MB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	N	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	NB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	O	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	OB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	P	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	PB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	Q	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	QB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	R	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	RB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	S	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	SB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		
1	TB	132	Total	C	N	O	S	0	0
			1002	637	171	188	6		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ASP	ASN	variant	UNP A0AAD2RAW1
A	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
A	278	GLY	GLU	variant	UNP A0AAD2RAW1
AB	19	ASP	ASN	variant	UNP A0AAD2RAW1
AB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
AB	278	GLY	GLU	variant	UNP A0AAD2RAW1
B	19	ASP	ASN	variant	UNP A0AAD2RAW1
B	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
B	278	GLY	GLU	variant	UNP A0AAD2RAW1
BB	19	ASP	ASN	variant	UNP A0AAD2RAW1
BB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
BB	278	GLY	GLU	variant	UNP A0AAD2RAW1
C	19	ASP	ASN	variant	UNP A0AAD2RAW1
C	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
C	278	GLY	GLU	variant	UNP A0AAD2RAW1
CB	19	ASP	ASN	variant	UNP A0AAD2RAW1
CB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
CB	278	GLY	GLU	variant	UNP A0AAD2RAW1
D	19	ASP	ASN	variant	UNP A0AAD2RAW1
D	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
D	278	GLY	GLU	variant	UNP A0AAD2RAW1
DB	19	ASP	ASN	variant	UNP A0AAD2RAW1
DB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
DB	278	GLY	GLU	variant	UNP A0AAD2RAW1
E	19	ASP	ASN	variant	UNP A0AAD2RAW1
E	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
E	278	GLY	GLU	variant	UNP A0AAD2RAW1
EB	19	ASP	ASN	variant	UNP A0AAD2RAW1
EB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
EB	278	GLY	GLU	variant	UNP A0AAD2RAW1
F	19	ASP	ASN	variant	UNP A0AAD2RAW1
F	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
F	278	GLY	GLU	variant	UNP A0AAD2RAW1
FB	19	ASP	ASN	variant	UNP A0AAD2RAW1

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Chain	Residue	Modelled	Actual	Comment	Reference
FB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
FB	278	GLY	GLU	variant	UNP A0AAD2RAW1
G	19	ASP	ASN	variant	UNP A0AAD2RAW1
G	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
G	278	GLY	GLU	variant	UNP A0AAD2RAW1
GB	19	ASP	ASN	variant	UNP A0AAD2RAW1
GB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
GB	278	GLY	GLU	variant	UNP A0AAD2RAW1
H	19	ASP	ASN	variant	UNP A0AAD2RAW1
H	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
H	278	GLY	GLU	variant	UNP A0AAD2RAW1
HB	19	ASP	ASN	variant	UNP A0AAD2RAW1
HB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
HB	278	GLY	GLU	variant	UNP A0AAD2RAW1
I	19	ASP	ASN	variant	UNP A0AAD2RAW1
I	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
I	278	GLY	GLU	variant	UNP A0AAD2RAW1
IB	19	ASP	ASN	variant	UNP A0AAD2RAW1
IB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
IB	278	GLY	GLU	variant	UNP A0AAD2RAW1
J	19	ASP	ASN	variant	UNP A0AAD2RAW1
J	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
J	278	GLY	GLU	variant	UNP A0AAD2RAW1
JB	19	ASP	ASN	variant	UNP A0AAD2RAW1
JB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
JB	278	GLY	GLU	variant	UNP A0AAD2RAW1
K	19	ASP	ASN	variant	UNP A0AAD2RAW1
K	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
K	278	GLY	GLU	variant	UNP A0AAD2RAW1
KB	19	ASP	ASN	variant	UNP A0AAD2RAW1
KB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
KB	278	GLY	GLU	variant	UNP A0AAD2RAW1
L	19	ASP	ASN	variant	UNP A0AAD2RAW1
L	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
L	278	GLY	GLU	variant	UNP A0AAD2RAW1
LB	19	ASP	ASN	variant	UNP A0AAD2RAW1
LB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
LB	278	GLY	GLU	variant	UNP A0AAD2RAW1
M	19	ASP	ASN	variant	UNP A0AAD2RAW1
M	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
M	278	GLY	GLU	variant	UNP A0AAD2RAW1
MB	19	ASP	ASN	variant	UNP A0AAD2RAW1

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Chain	Residue	Modelled	Actual	Comment	Reference
MB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
MB	278	GLY	GLU	variant	UNP A0AAD2RAW1
N	19	ASP	ASN	variant	UNP A0AAD2RAW1
N	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
N	278	GLY	GLU	variant	UNP A0AAD2RAW1
NB	19	ASP	ASN	variant	UNP A0AAD2RAW1
NB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
NB	278	GLY	GLU	variant	UNP A0AAD2RAW1
O	19	ASP	ASN	variant	UNP A0AAD2RAW1
O	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
O	278	GLY	GLU	variant	UNP A0AAD2RAW1
OB	19	ASP	ASN	variant	UNP A0AAD2RAW1
OB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
OB	278	GLY	GLU	variant	UNP A0AAD2RAW1
P	19	ASP	ASN	variant	UNP A0AAD2RAW1
P	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
P	278	GLY	GLU	variant	UNP A0AAD2RAW1
PB	19	ASP	ASN	variant	UNP A0AAD2RAW1
PB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
PB	278	GLY	GLU	variant	UNP A0AAD2RAW1
Q	19	ASP	ASN	variant	UNP A0AAD2RAW1
Q	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
Q	278	GLY	GLU	variant	UNP A0AAD2RAW1
QB	19	ASP	ASN	variant	UNP A0AAD2RAW1
QB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
QB	278	GLY	GLU	variant	UNP A0AAD2RAW1
R	19	ASP	ASN	variant	UNP A0AAD2RAW1
R	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
R	278	GLY	GLU	variant	UNP A0AAD2RAW1
RB	19	ASP	ASN	variant	UNP A0AAD2RAW1
RB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
RB	278	GLY	GLU	variant	UNP A0AAD2RAW1
S	19	ASP	ASN	variant	UNP A0AAD2RAW1
S	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
S	278	GLY	GLU	variant	UNP A0AAD2RAW1
SB	19	ASP	ASN	variant	UNP A0AAD2RAW1
SB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
SB	278	GLY	GLU	variant	UNP A0AAD2RAW1
T	19	ASP	ASN	variant	UNP A0AAD2RAW1
T	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
T	278	GLY	GLU	variant	UNP A0AAD2RAW1
TB	19	ASP	ASN	variant	UNP A0AAD2RAW1

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Chain	Residue	Modelled	Actual	Comment	Reference
TB	175	ALA	THR	engineered mutation	UNP A0AAD2RAW1
TB	278	GLY	GLU	variant	UNP A0AAD2RAW1

- Molecule 2 is a protein called RsbT antagonist protein RsbS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	ab	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	b	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	bb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	c	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	cb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	d	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	db	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	e	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	eb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	f	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	fb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	g	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	gb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	h	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	hb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	i	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	ib	118	Total	C	N	O	S	0	0
			881	565	136	175	5		

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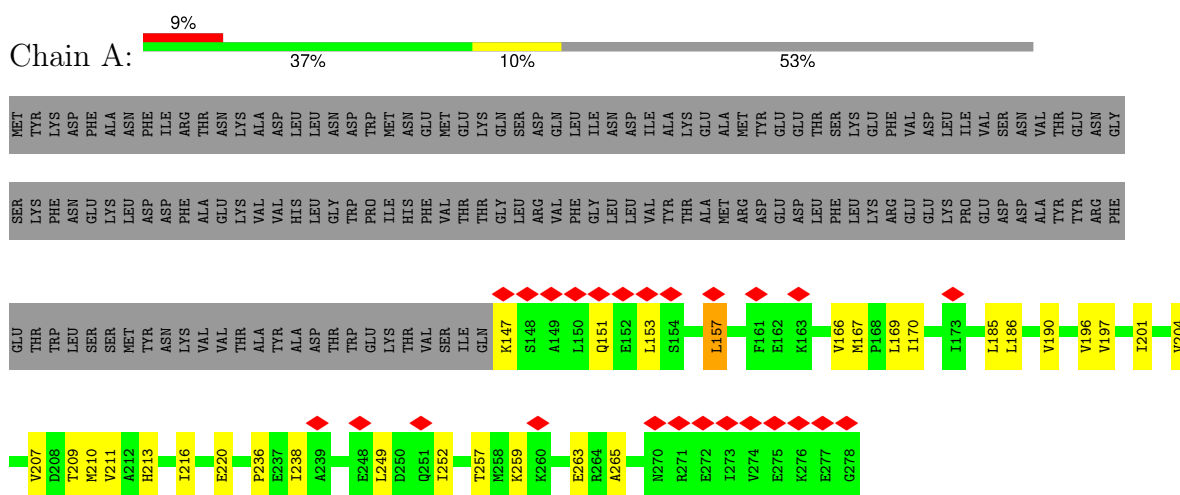
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	j	118	Total	C	N	O	S	0	0
			881	565	136	175	5		
2	jb	118	Total	C	N	O	S	0	0
			881	565	136	175	5		

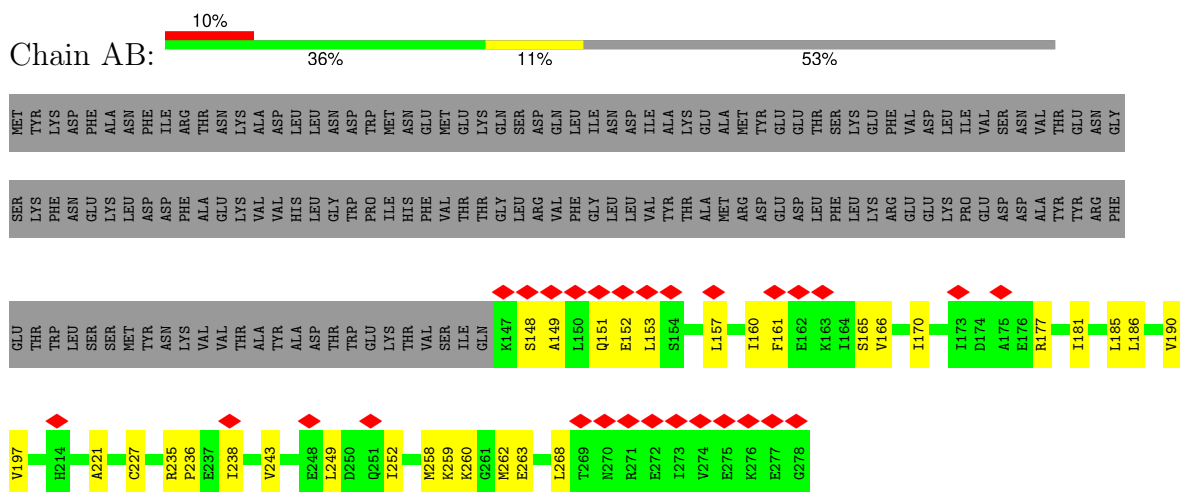
3 Residue-property plots

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.

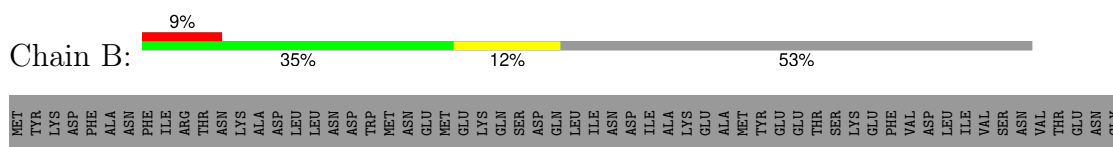
• Molecule 1: STAS domain-containing protein

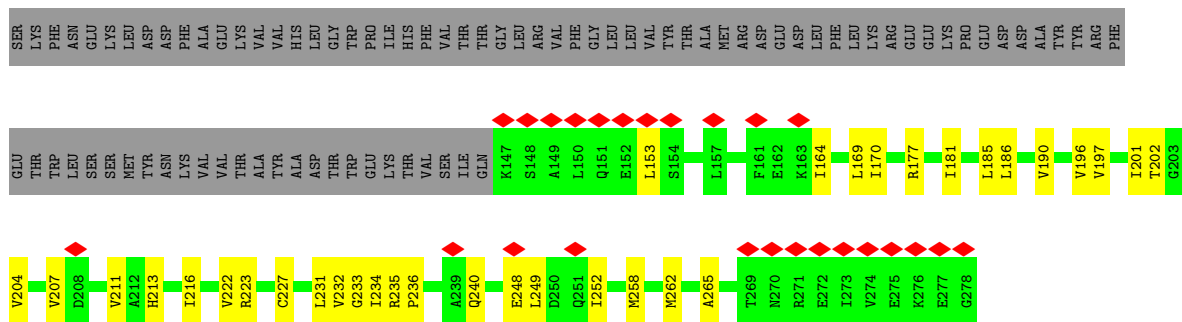


• Molecule 1: STAS domain-containing protein

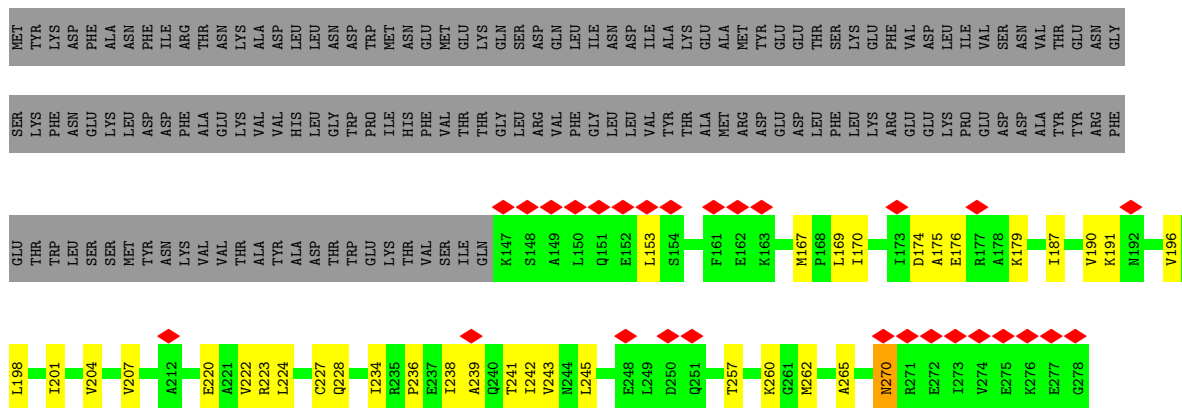
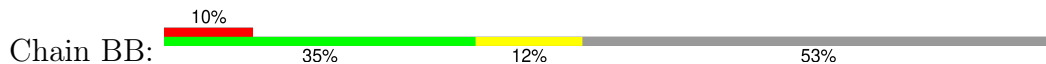


• Molecule 1: STAS domain-containing protein

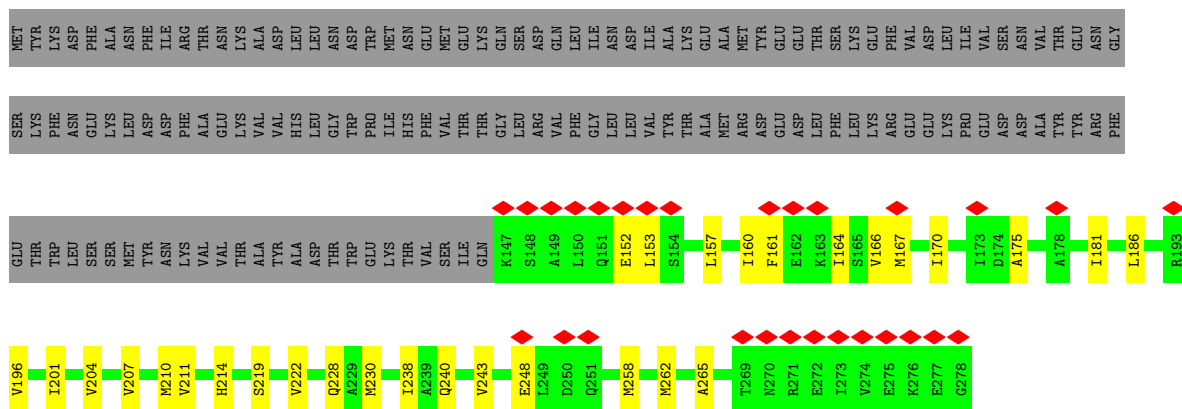
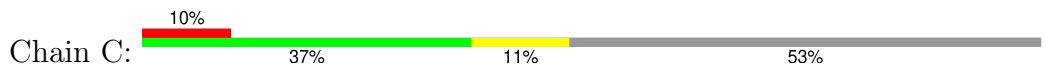




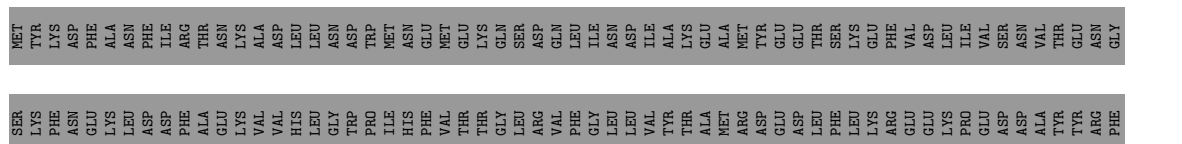
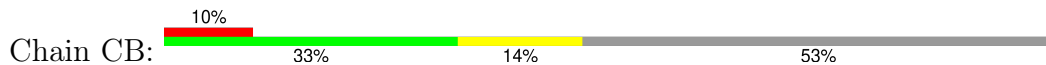
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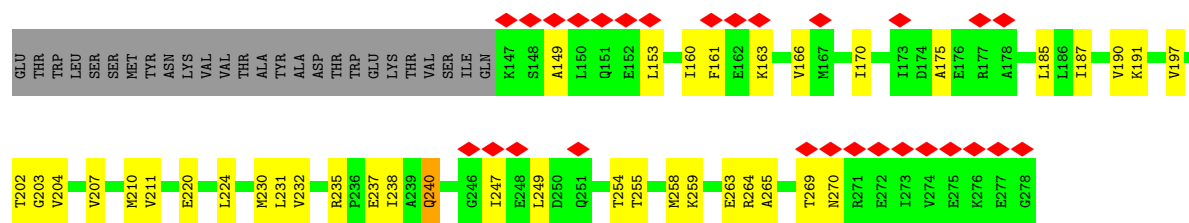


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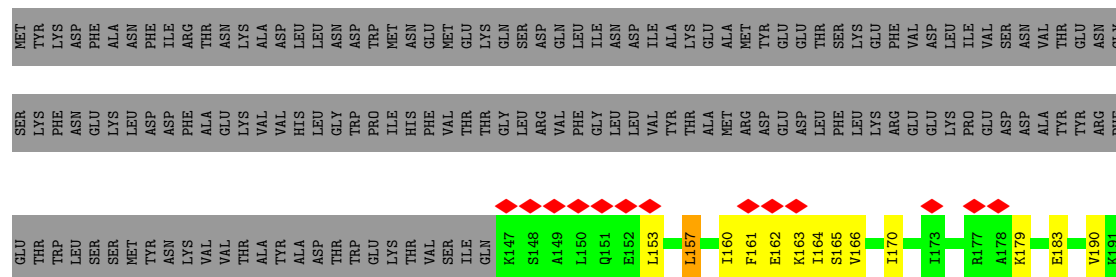
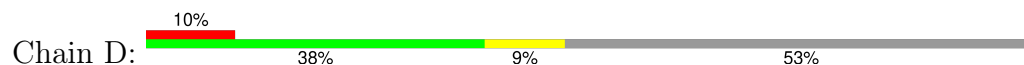


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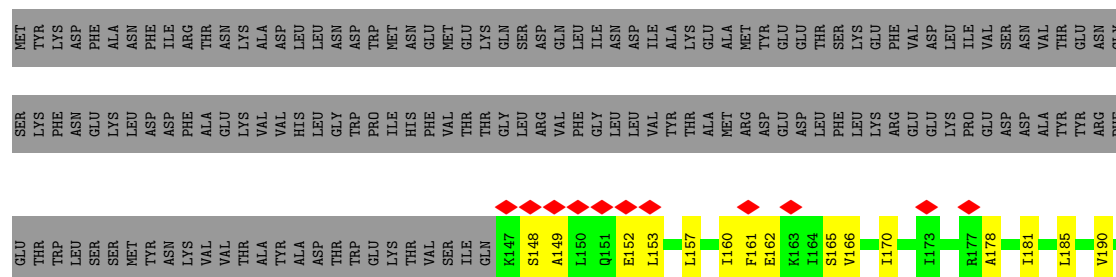
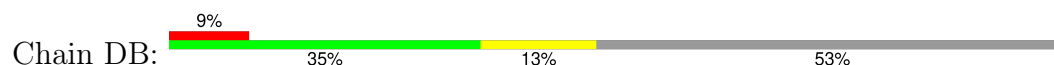




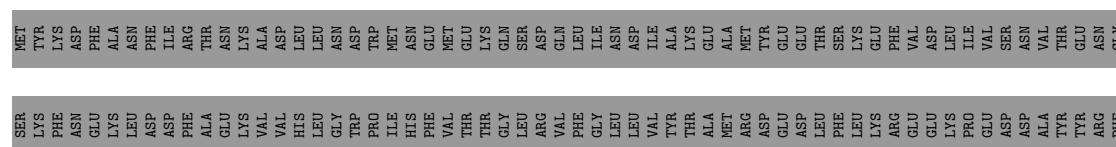
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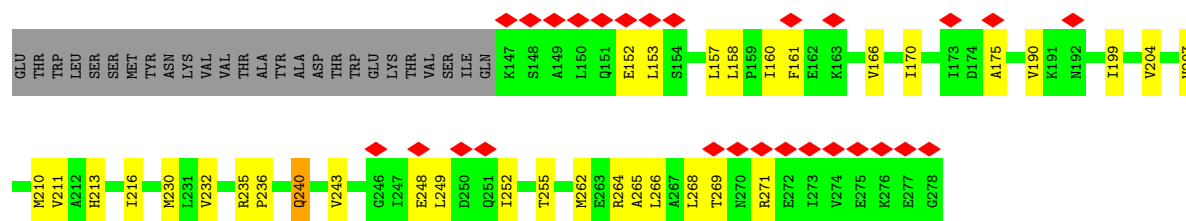


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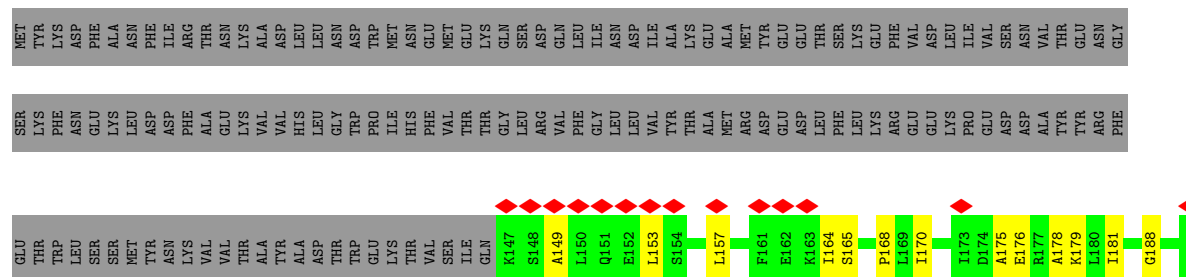
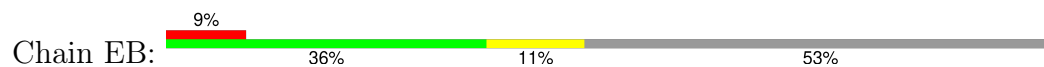


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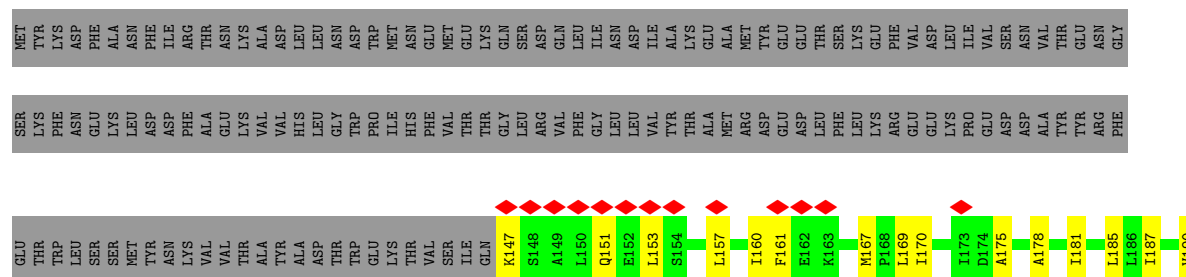
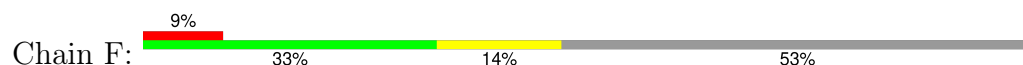




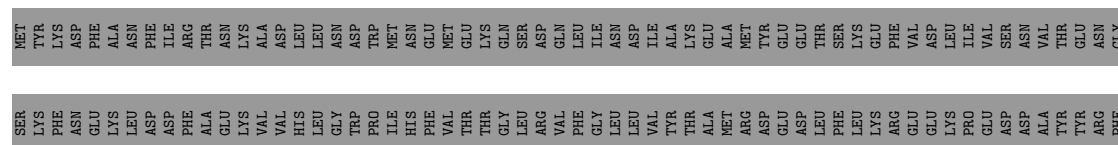
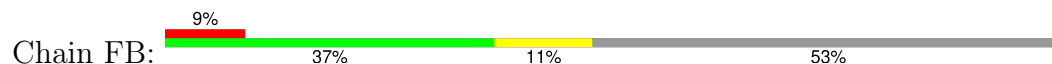
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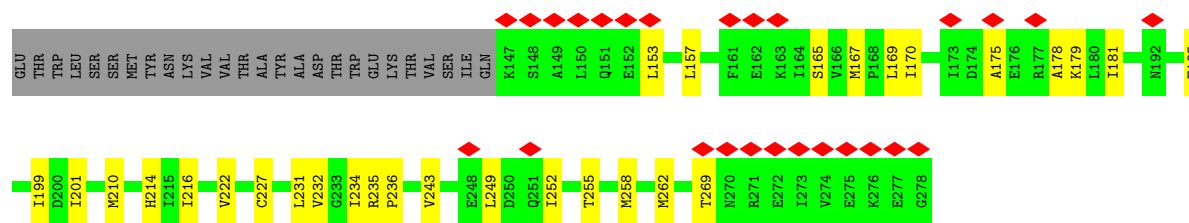


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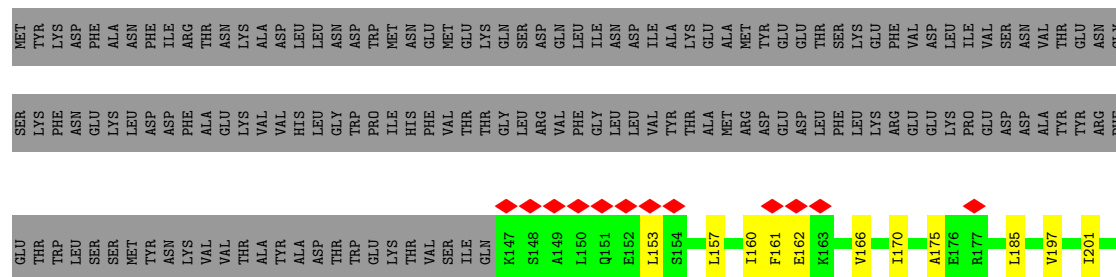
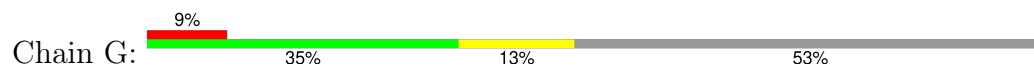


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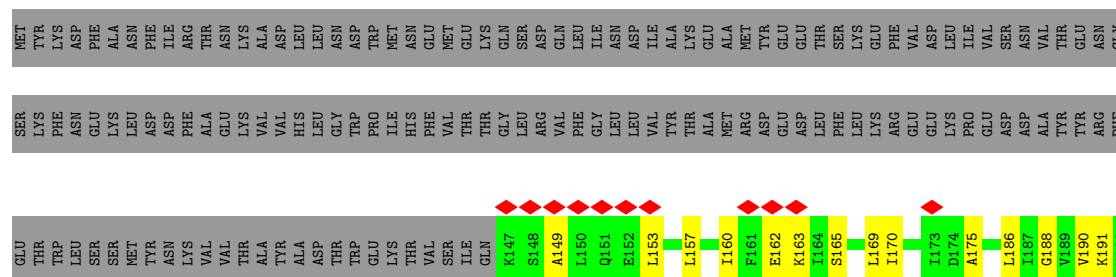
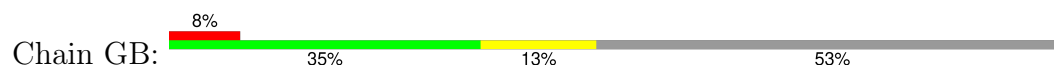




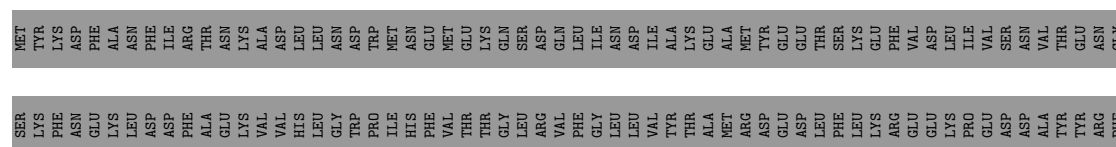
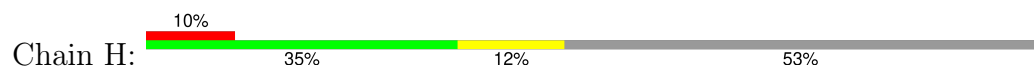
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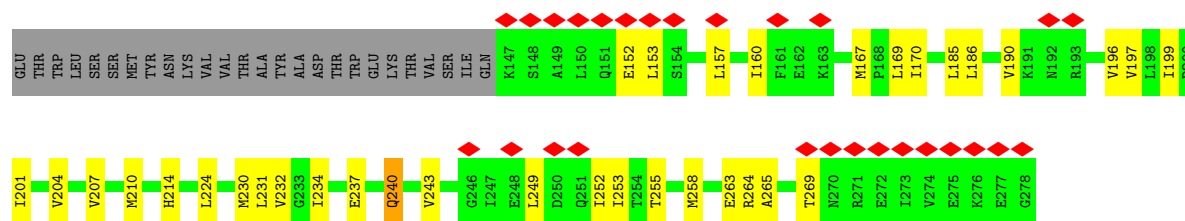


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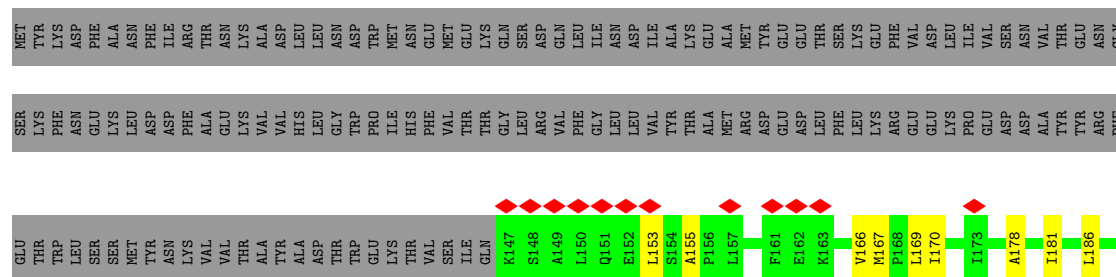
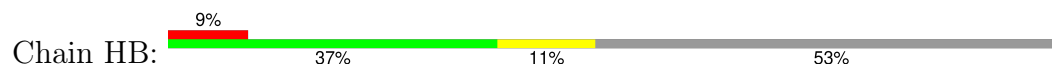


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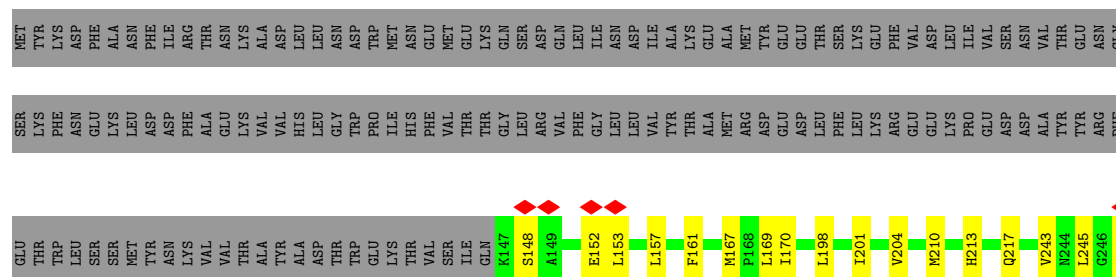
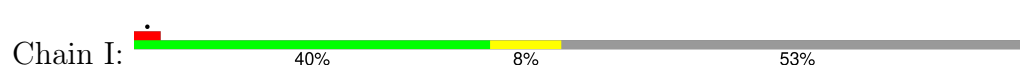




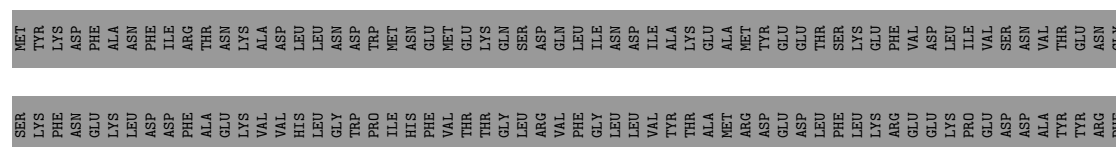
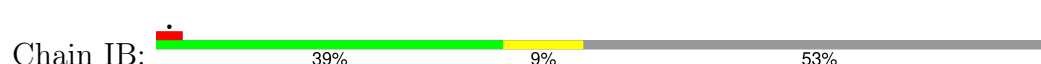
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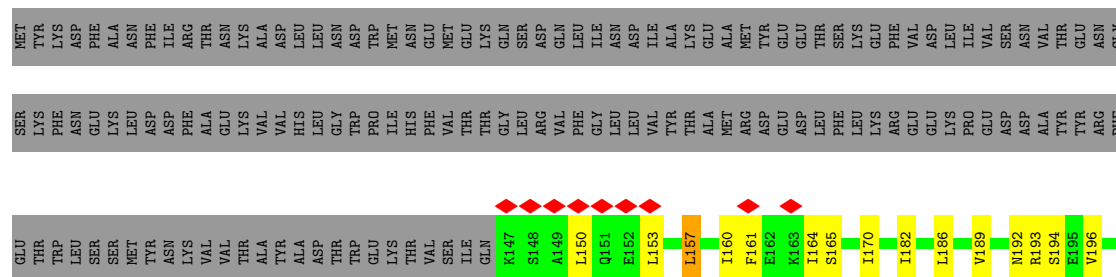
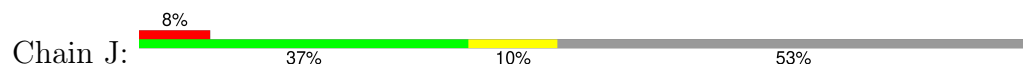
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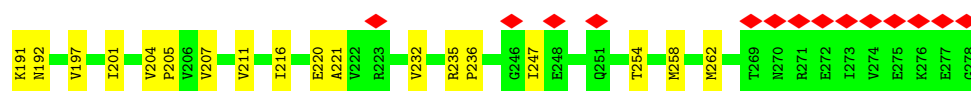
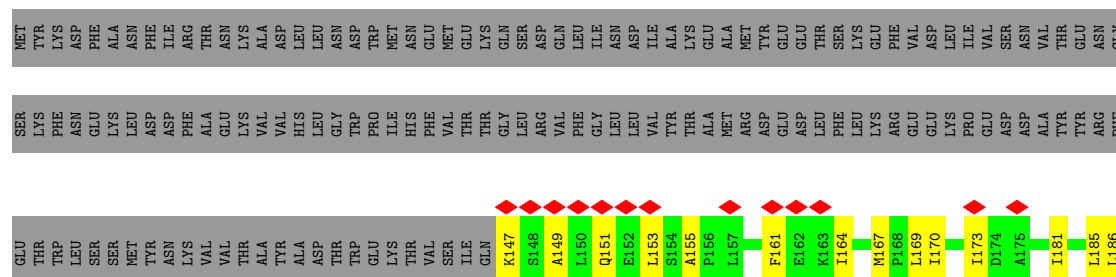
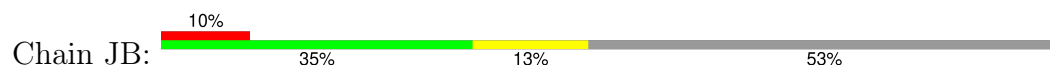
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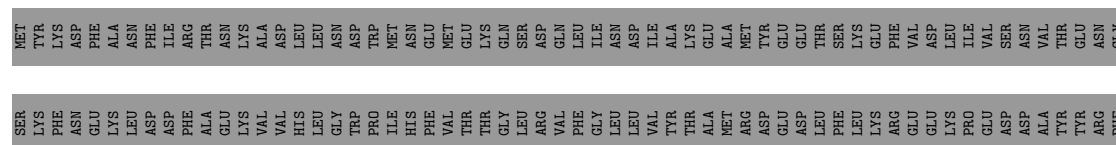
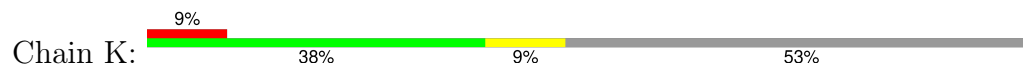
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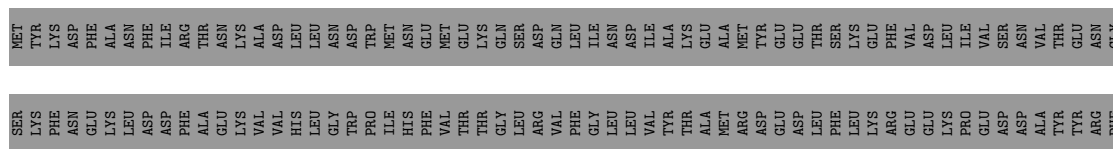


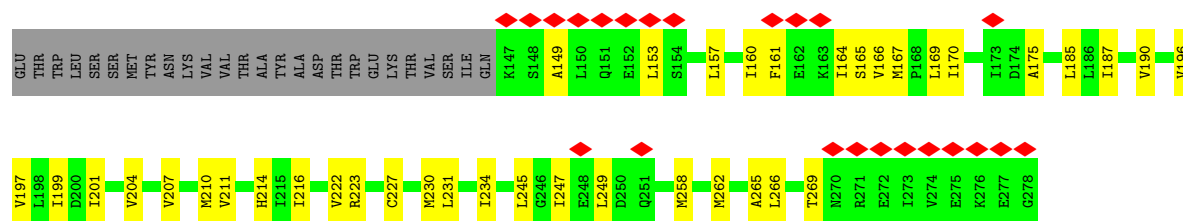
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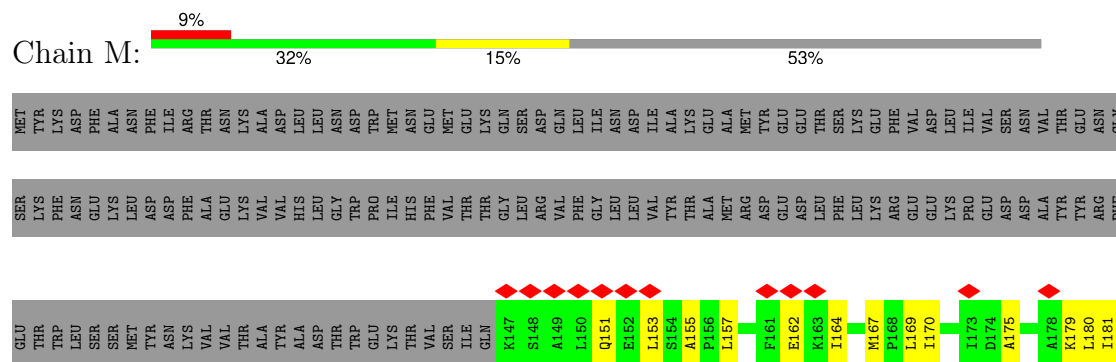
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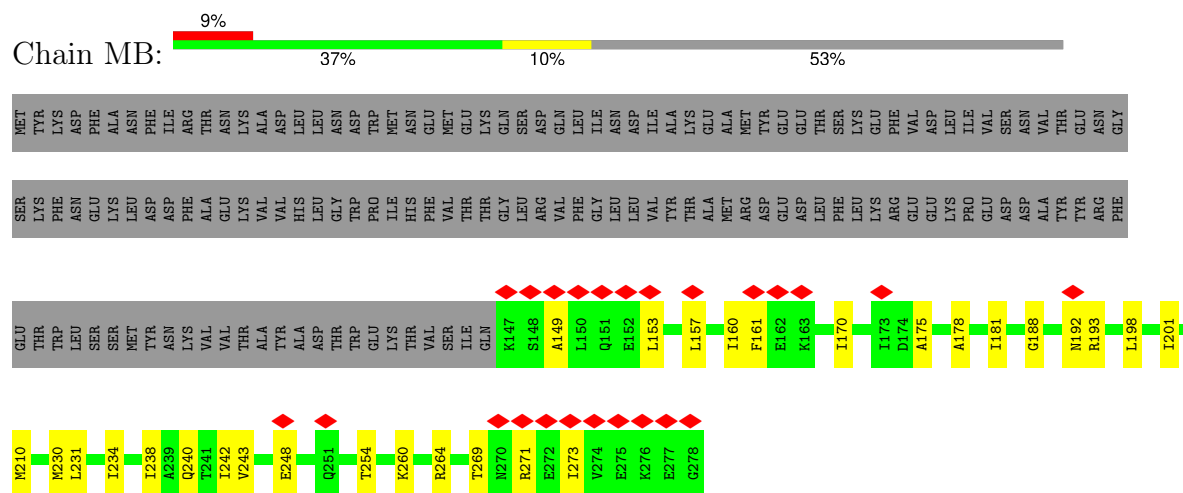




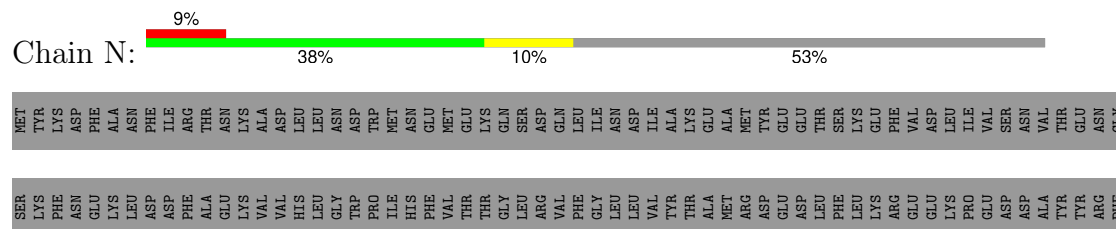
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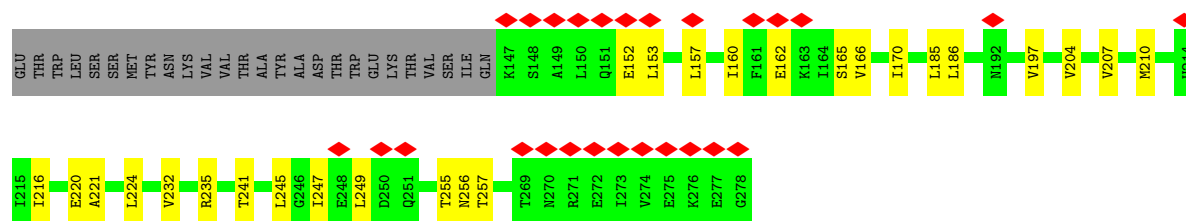


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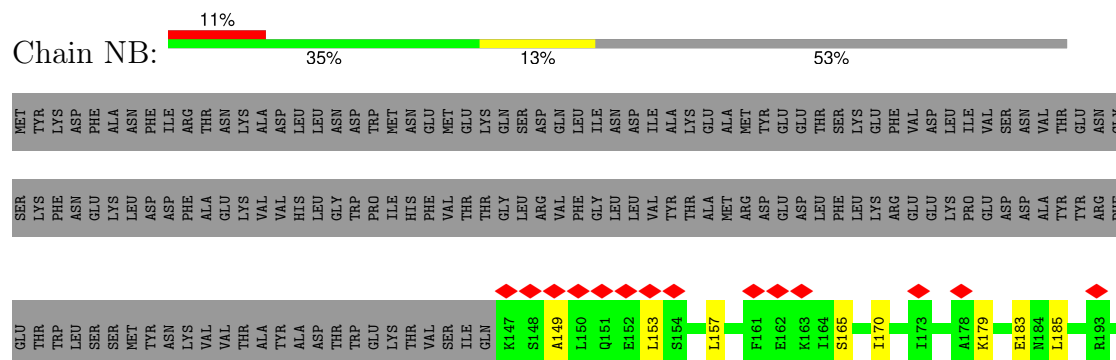


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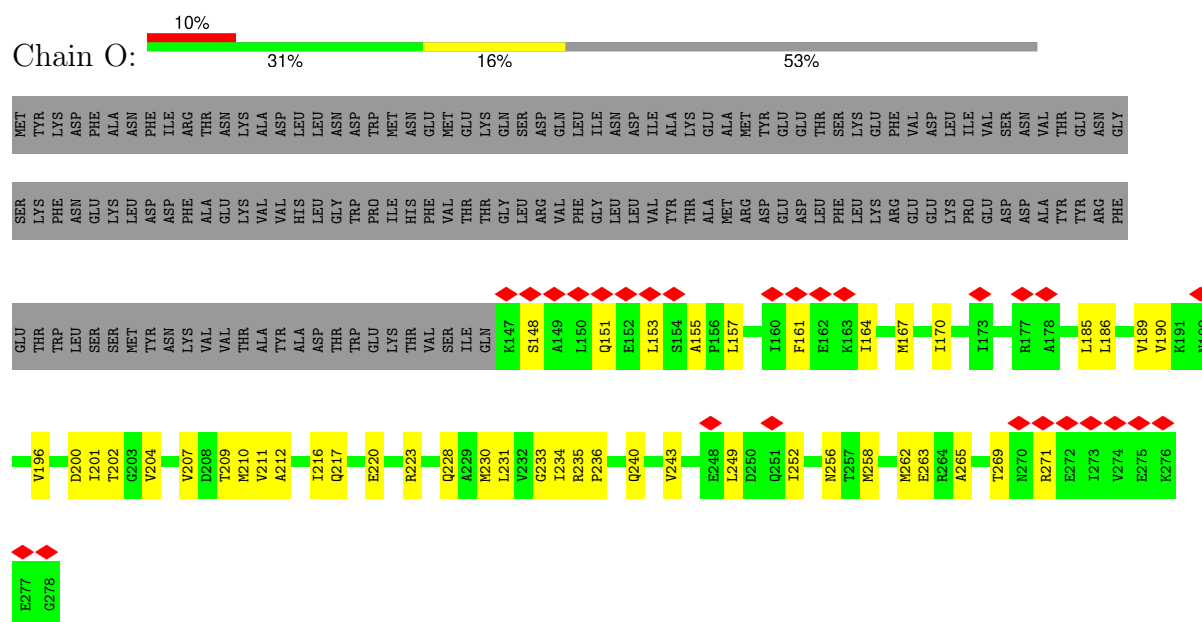




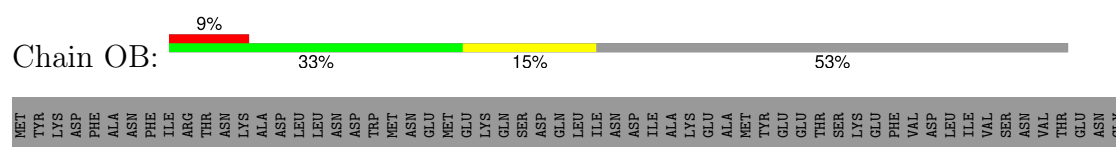
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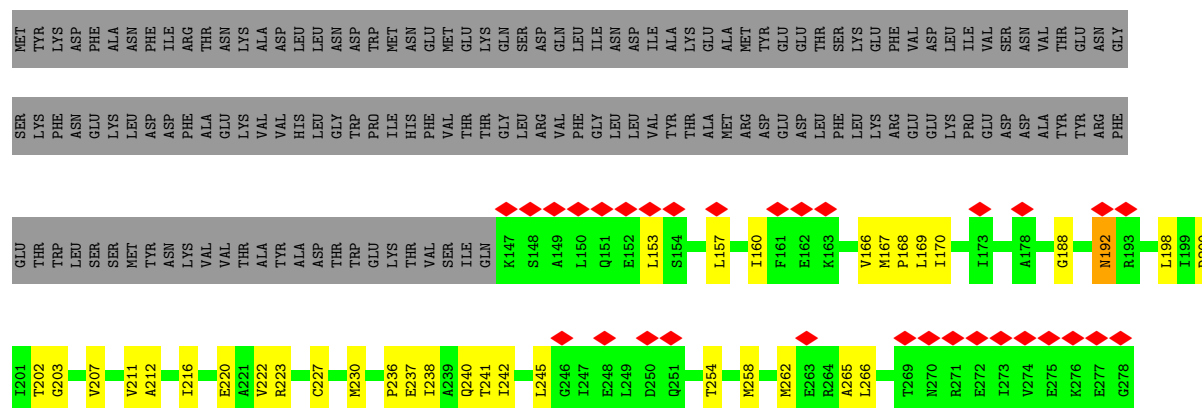
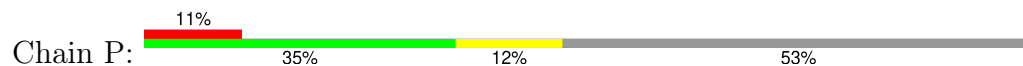
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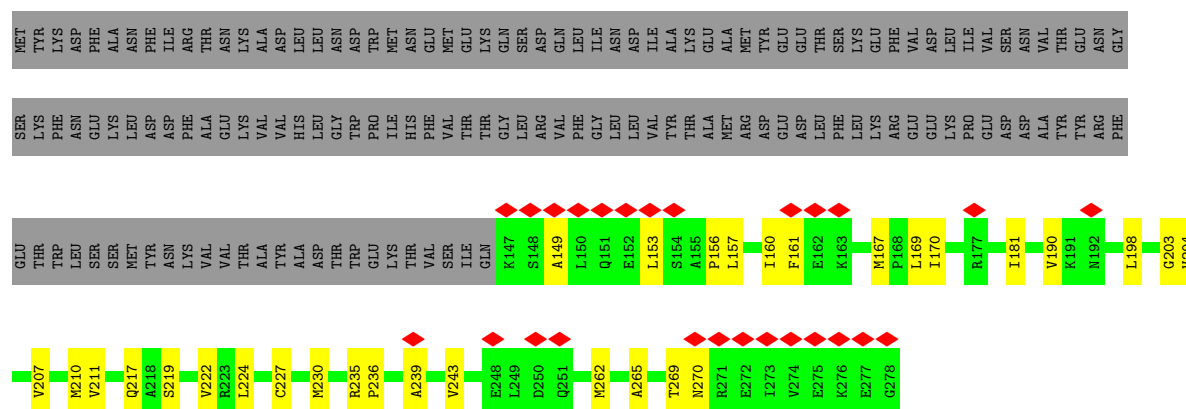
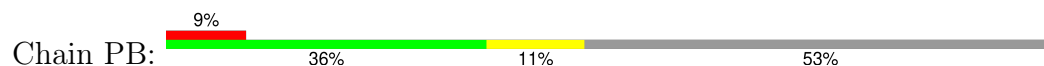
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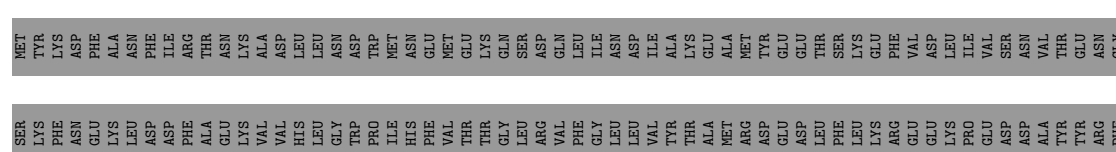
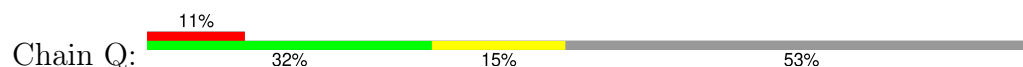
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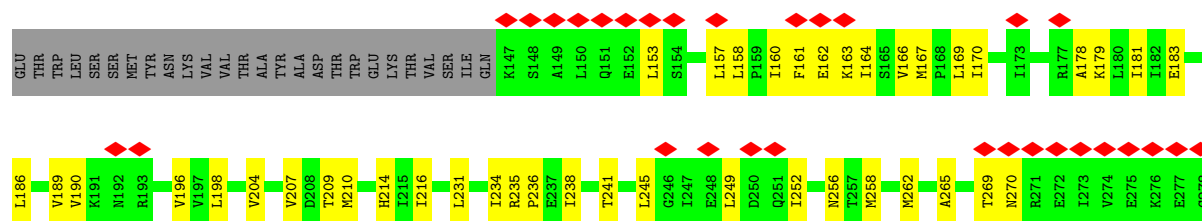


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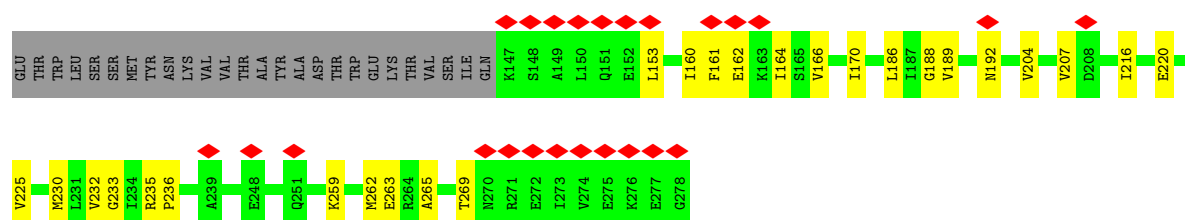
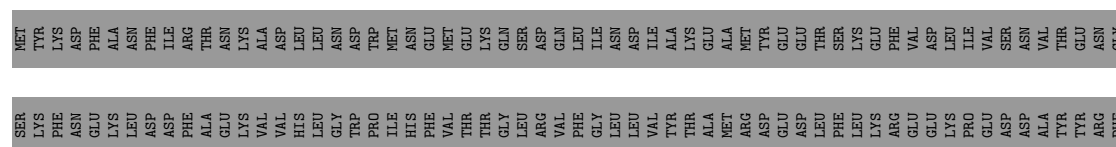
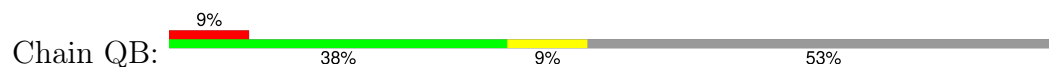


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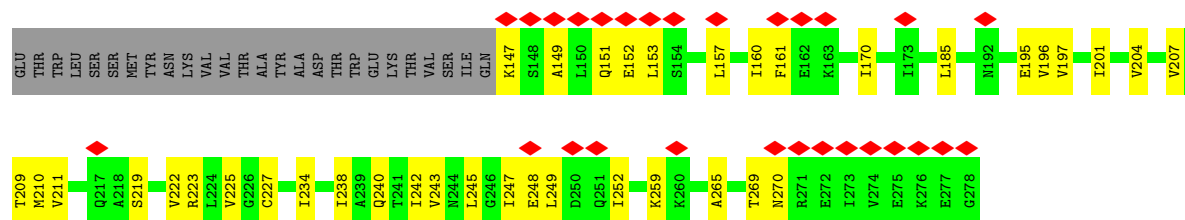
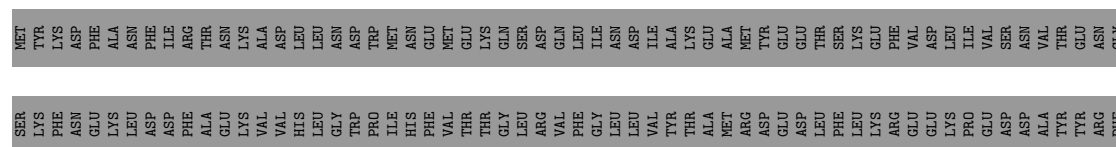
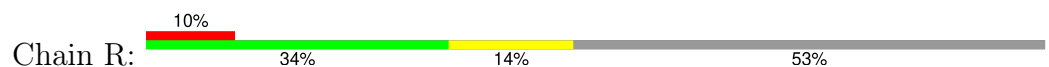




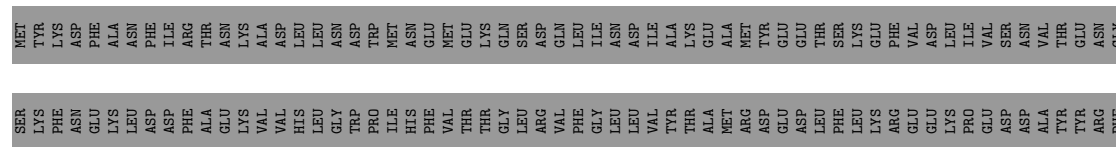
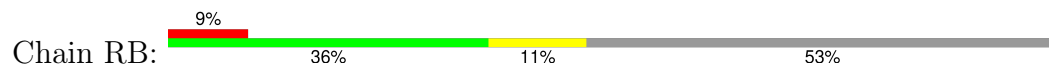
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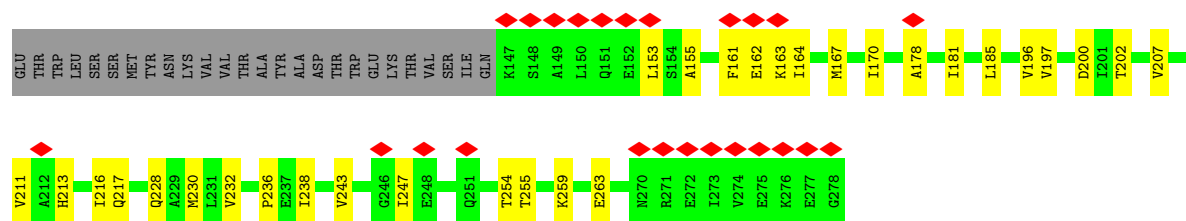


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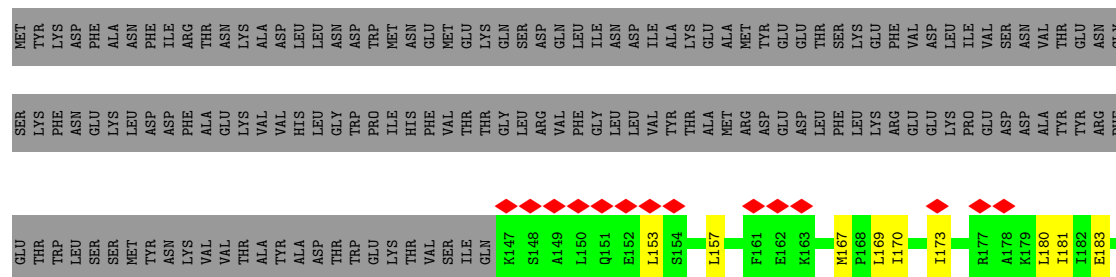
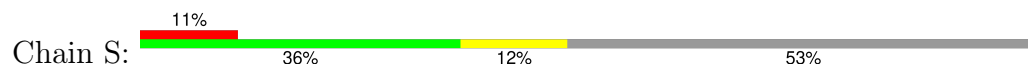


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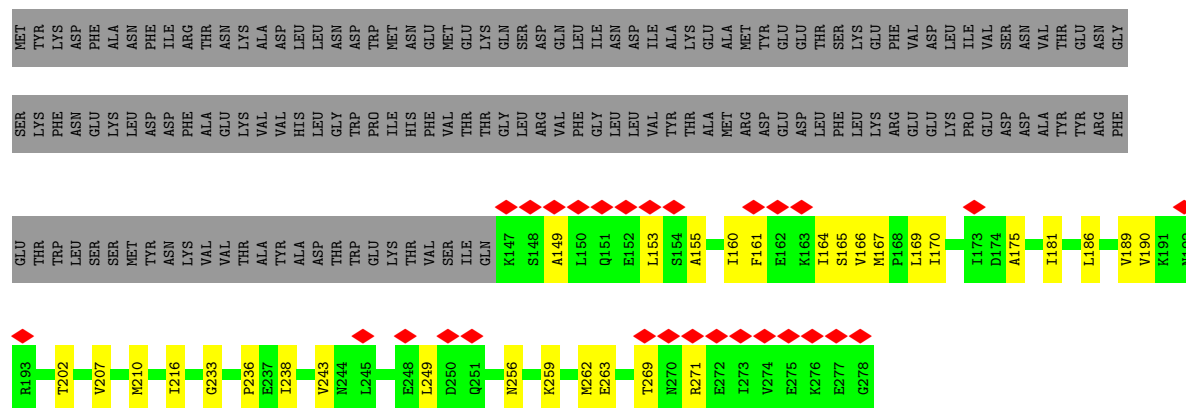
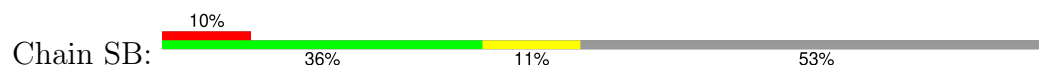




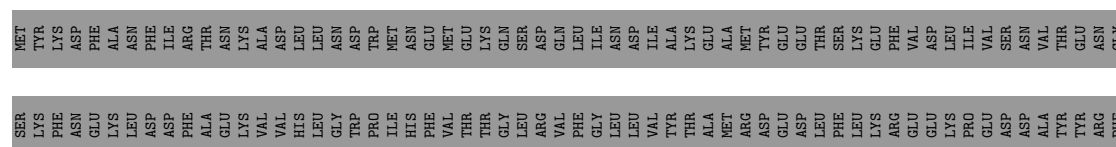
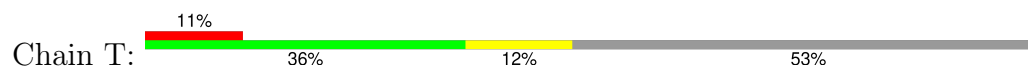
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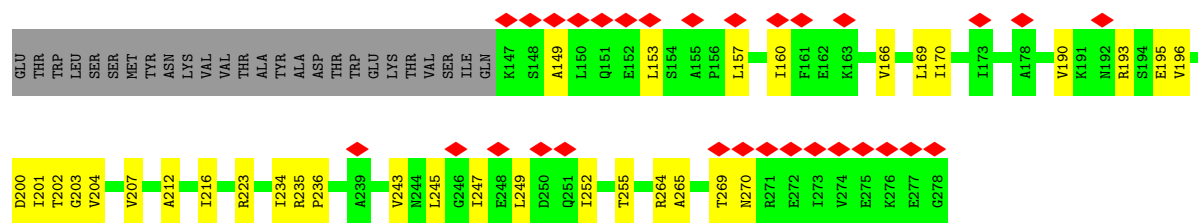


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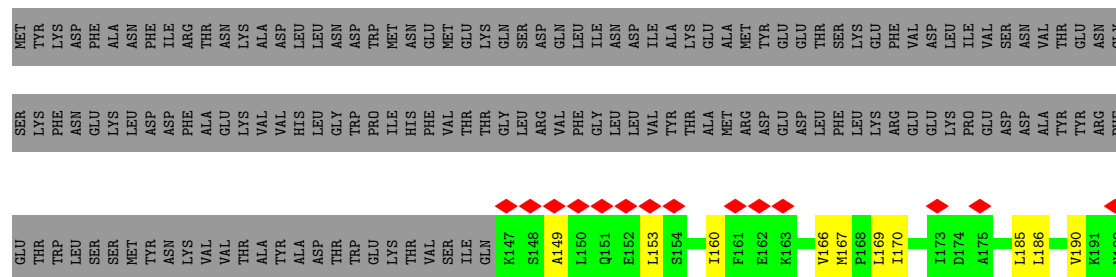
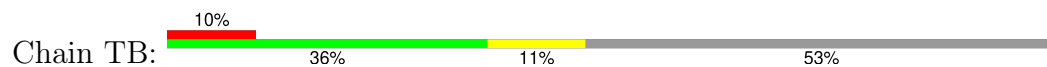


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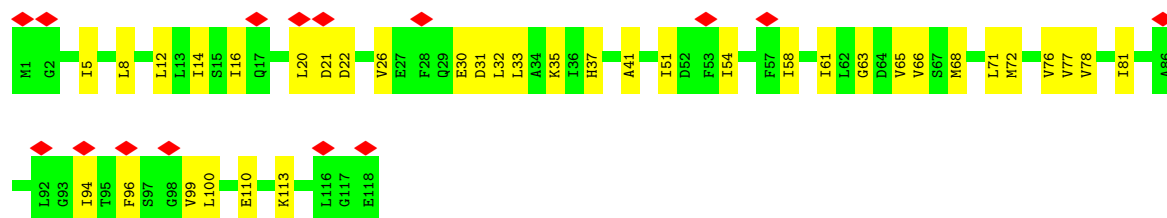




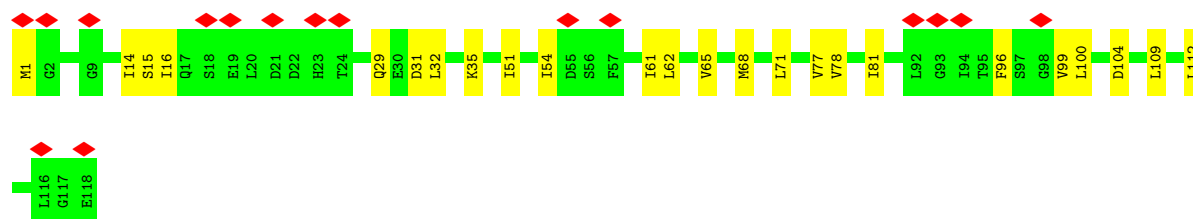
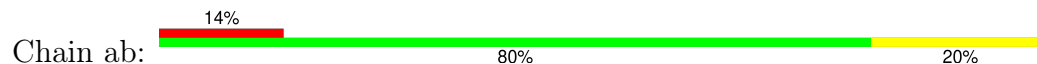
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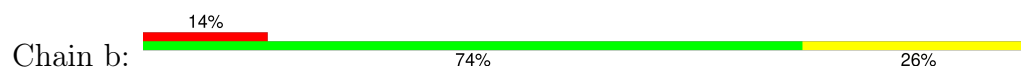
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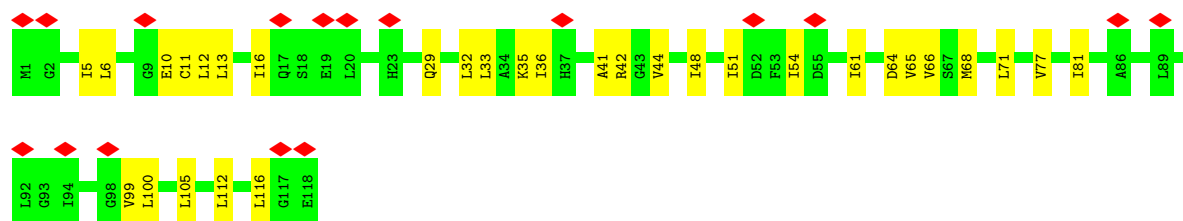


• Molecule 2: RsbT antagonist protein RsbS

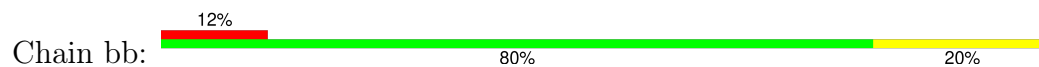


• Molecule 2: RsbT antagonist protein RsbS

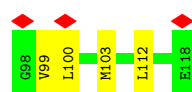
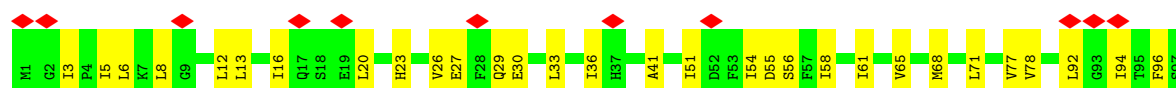




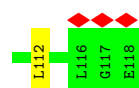
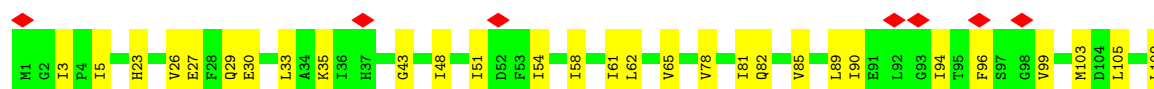
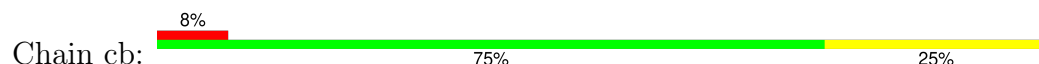
- Molecule 2: RsbT antagonist protein RsbS



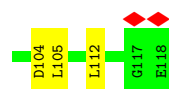
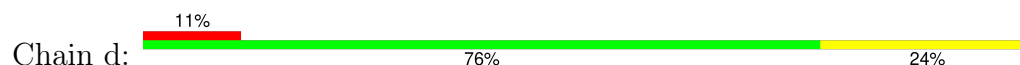
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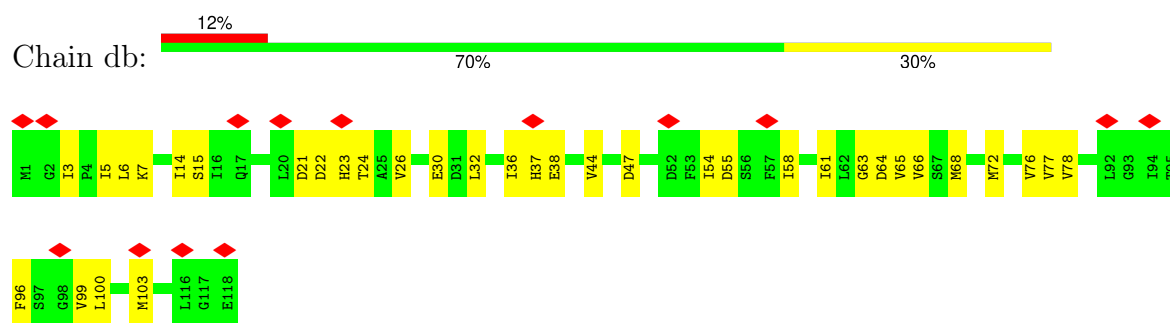
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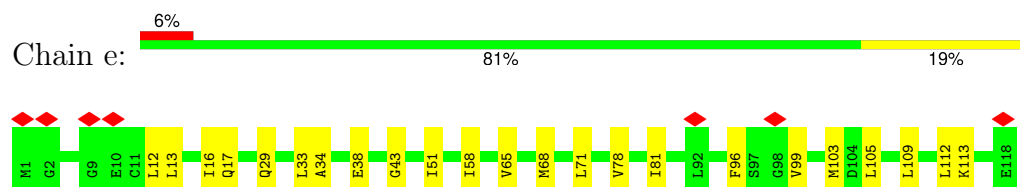
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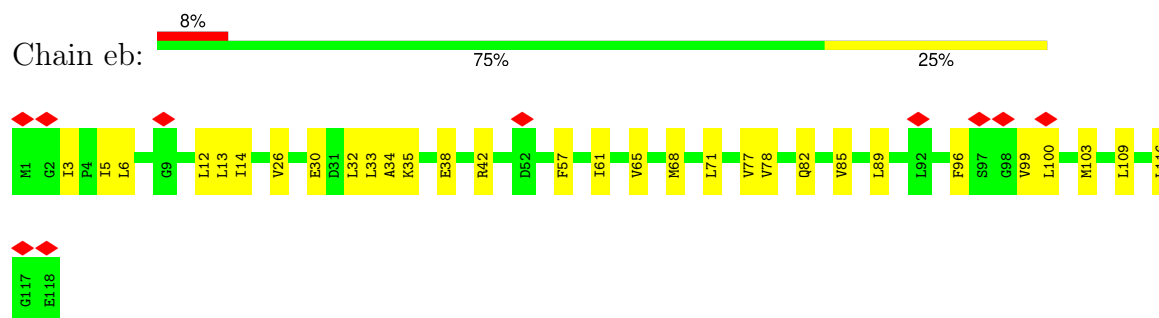
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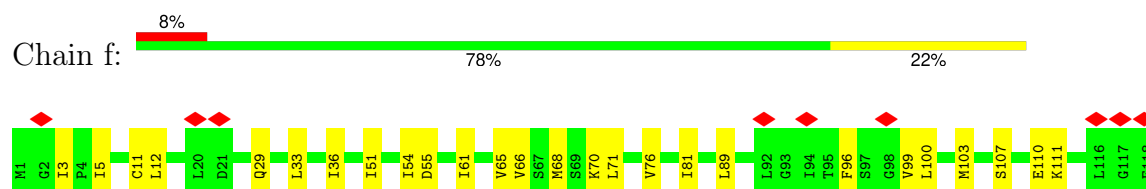
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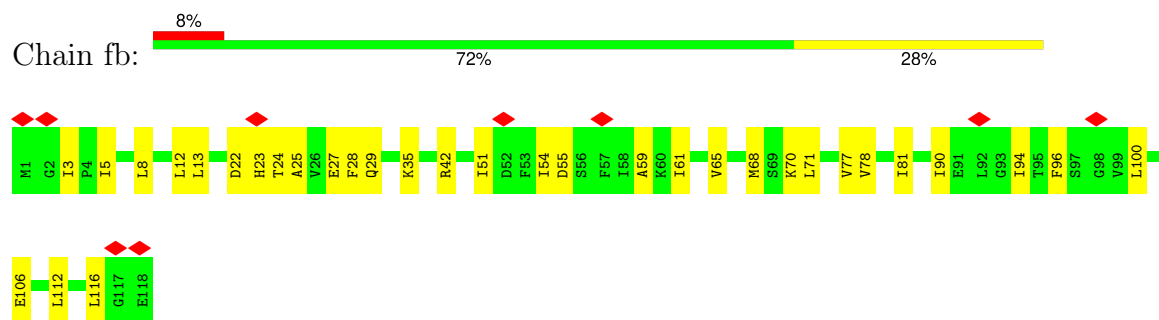
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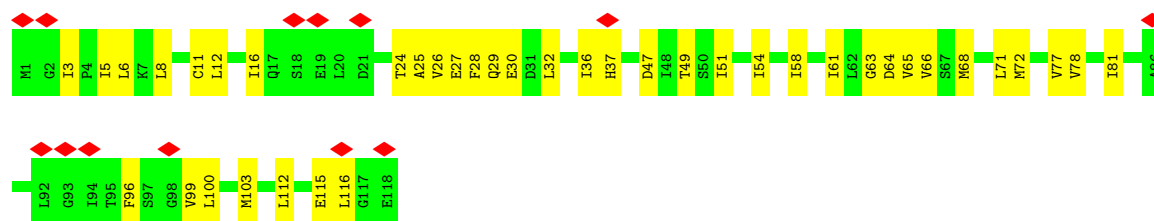


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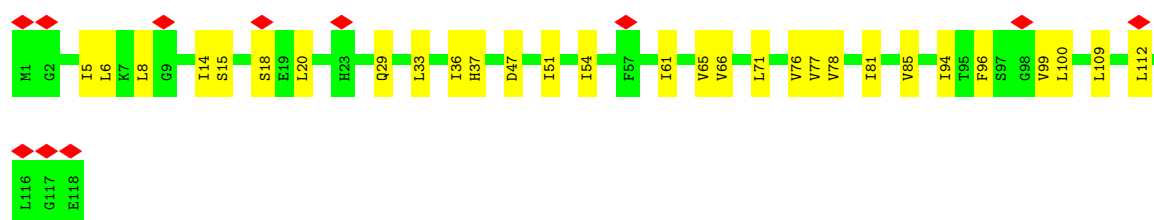
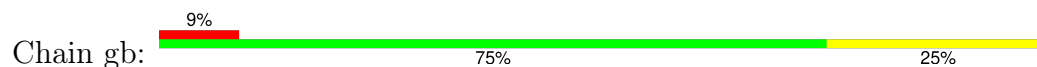


- Molecule 2: RsbT antagonist protein RsbS

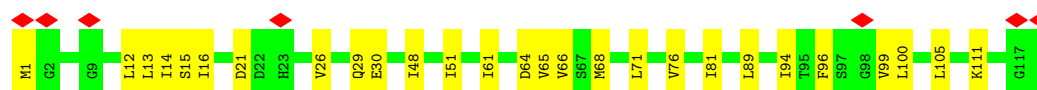
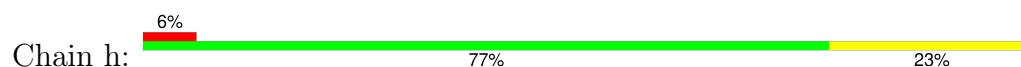




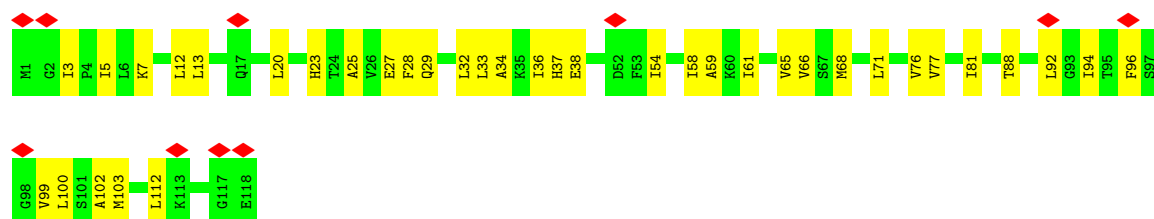
- Molecule 2: RsbT antagonist protein RsbS



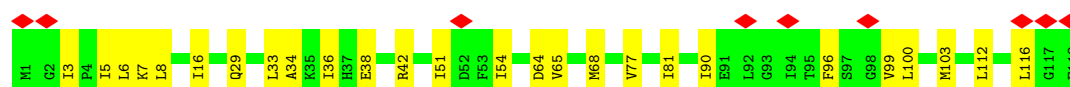
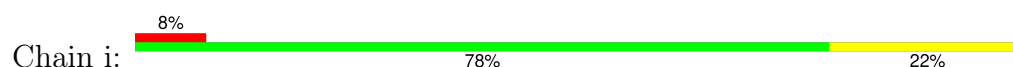
- Molecule 2: RsbT antagonist protein RsbS



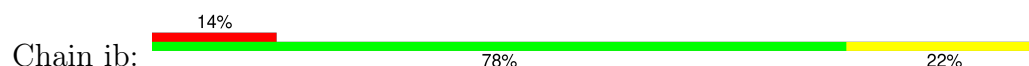
- Molecule 2: RsbT antagonist protein RsbS

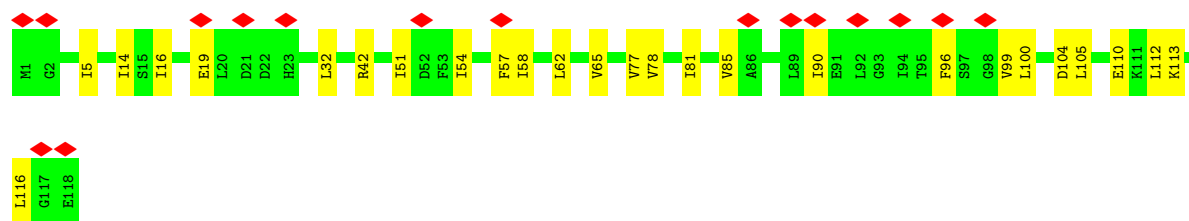


- Molecule 2: RsbT antagonist protein RsbS

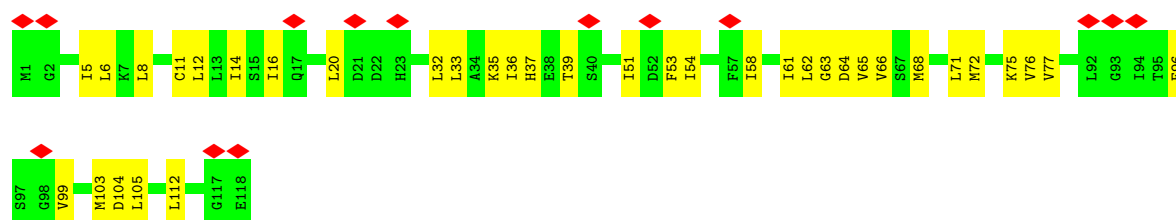


- Molecule 2: RsbT antagonist protein RsbS

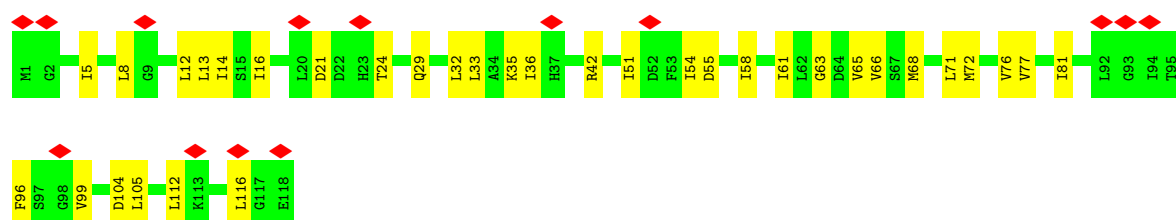
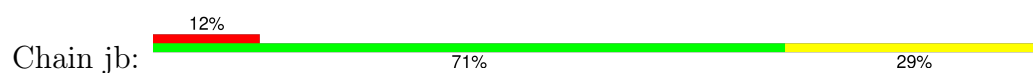




- Molecule 2: RsbT antagonist protein RsbS



- Molecule 2: RsbT antagonist protein RsbS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.325	Depositor
Minimum map value	-0.497	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.3	Depositor
Map size (\AA)	501.0, 501.0, 501.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.835, 0.835, 0.835	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	0.19	0/1009	0.45	1/1365 (0.1%)
1	AB	0.20	0/1009	0.39	0/1365
1	B	0.22	0/1009	0.46	0/1365
1	BB	0.19	0/1009	0.39	0/1365
1	C	0.20	0/1009	0.44	1/1365 (0.1%)
1	CB	0.20	0/1009	0.40	0/1365
1	D	0.20	0/1009	0.45	2/1365 (0.1%)
1	DB	0.20	0/1009	0.41	0/1365
1	E	0.20	0/1009	0.47	2/1365 (0.1%)
1	EB	0.17	0/1009	0.40	0/1365
1	F	0.29	1/1009 (0.1%)	0.50	3/1365 (0.2%)
1	FB	0.19	0/1009	0.38	0/1365
1	G	0.24	0/1009	0.49	3/1365 (0.2%)
1	GB	0.21	0/1009	0.41	0/1365
1	H	0.21	0/1009	0.46	1/1365 (0.1%)
1	HB	0.19	0/1009	0.37	0/1365
1	I	0.22	0/1009	0.44	2/1365 (0.1%)
1	IB	0.23	0/1009	0.39	0/1365
1	J	0.20	0/1009	0.47	3/1365 (0.2%)
1	JB	0.20	0/1009	0.41	0/1365
1	K	0.18	0/1009	0.46	3/1365 (0.2%)
1	KB	0.18	0/1009	0.35	0/1365
1	L	0.25	0/1009	0.50	3/1365 (0.2%)
1	LB	0.21	0/1009	0.44	0/1365
1	M	0.25	0/1009	0.47	3/1365 (0.2%)
1	MB	0.19	0/1009	0.37	0/1365
1	N	0.19	0/1009	0.42	0/1365
1	NB	0.19	0/1009	0.41	0/1365
1	O	0.21	0/1009	0.47	1/1365 (0.1%)
1	OB	0.20	0/1009	0.39	0/1365
1	P	0.21	0/1009	0.47	2/1365 (0.1%)
1	PB	0.19	0/1009	0.37	0/1365
1	Q	0.20	0/1009	0.48	3/1365 (0.2%)
1	QB	0.19	0/1009	0.41	0/1365

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	R	0.21	0/1009	0.49	2/1365 (0.1%)
1	RB	0.20	0/1009	0.43	0/1365
1	S	0.23	0/1009	0.47	2/1365 (0.1%)
1	SB	0.19	0/1009	0.37	0/1365
1	T	0.21	0/1009	0.49	2/1365 (0.1%)
1	TB	0.20	0/1009	0.39	0/1365
2	a	0.19	0/888	0.39	0/1197
2	ab	0.21	0/888	0.37	0/1197
2	b	0.19	0/888	0.37	0/1197
2	bb	0.19	0/888	0.36	0/1197
2	c	0.21	0/888	0.40	0/1197
2	cb	0.19	0/888	0.37	0/1197
2	d	0.18	0/888	0.36	0/1197
2	db	0.20	0/888	0.41	0/1197
2	e	0.20	0/888	0.36	0/1197
2	eb	0.21	0/888	0.40	0/1197
2	f	0.20	0/888	0.35	0/1197
2	fb	0.23	0/888	0.50	0/1197
2	g	0.22	0/888	0.48	0/1197
2	gb	0.18	0/888	0.34	0/1197
2	h	0.21	0/888	0.38	0/1197
2	hb	0.21	0/888	0.46	0/1197
2	i	0.20	0/888	0.37	0/1197
2	ib	0.19	0/888	0.38	0/1197
2	j	0.20	0/888	0.38	0/1197
2	jb	0.19	0/888	0.36	0/1197
All	All	0.21	1/58120 (0.0%)	0.42	39/78540 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	234	ILE	C-N	6.30	1.41	1.32

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	157	LEU	CB-CA-C	6.02	120.82	110.77
1	R	157	LEU	N-CA-CB	5.95	118.91	110.46
1	J	157	LEU	N-CA-C	5.90	117.82	108.67
1	F	157	LEU	N-CA-CB	5.81	118.67	110.24
1	L	157	LEU	CB-CA-C	5.77	120.11	110.88
1	S	157	LEU	N-CA-CB	5.76	118.64	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	157	LEU	N-CA-CB	5.72	118.58	110.46
1	Q	157	LEU	N-CA-CB	5.64	118.42	110.24
1	D	157	LEU	N-CA-CB	5.63	118.46	110.46
1	P	157	LEU	N-CA-CB	5.63	118.46	110.46
1	T	157	LEU	N-CA-CB	5.60	118.41	110.46
1	E	157	LEU	N-CA-CB	5.58	118.38	110.46
1	L	157	LEU	N-CA-C	5.54	117.49	108.63
1	M	157	LEU	N-CA-CB	5.52	118.30	110.46
1	J	157	LEU	N-CA-CB	5.51	118.76	109.94
1	S	157	LEU	CB-CA-C	5.51	120.50	111.41
1	R	157	LEU	CB-CA-C	5.50	120.48	111.41
1	K	157	LEU	CB-CA-C	5.50	120.48	111.41
1	O	157	LEU	N-CA-CB	5.47	118.22	110.46
1	G	157	LEU	N-CA-CB	5.46	118.22	110.46
1	T	157	LEU	CB-CA-C	5.46	120.41	111.41
1	L	157	LEU	N-CA-CB	5.44	118.48	109.88
1	F	157	LEU	CB-CA-C	5.44	120.24	111.05
1	P	157	LEU	CB-CA-C	5.44	120.38	111.41
1	F	157	LEU	N-CA-C	5.41	117.53	108.23
1	H	157	LEU	N-CA-CB	5.40	118.13	110.46
1	I	157	LEU	CB-CA-C	5.37	120.53	111.41
1	A	157	LEU	N-CA-CB	5.35	118.41	110.49
1	D	157	LEU	CB-CA-C	5.31	120.18	111.41
1	M	157	LEU	CB-CA-C	5.31	120.17	111.41
1	G	157	LEU	CB-CA-C	5.30	120.15	111.41
1	Q	157	LEU	CB-CA-C	5.29	120.00	111.05
1	E	157	LEU	CB-CA-C	5.29	120.14	111.41
1	Q	157	LEU	N-CA-C	5.19	117.16	108.23
1	G	157	LEU	N-CA-C	5.18	117.75	108.17
1	M	157	LEU	N-CA-C	5.09	117.59	108.17
1	I	157	LEU	N-CA-C	5.02	117.55	107.41
1	K	157	LEU	N-CA-C	5.00	117.42	108.17
1	C	157	LEU	N-CA-CB	5.00	118.94	110.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1002	0	1083	26	0
1	AB	1002	0	1083	34	0
1	B	1002	0	1083	27	0
1	BB	1002	0	1083	33	0
1	C	1002	0	1083	31	0
1	CB	1002	0	1083	43	0
1	D	1002	0	1083	31	0
1	DB	1002	0	1083	40	0
1	E	1002	0	1083	31	0
1	EB	1002	0	1083	31	0
1	F	1002	0	1083	35	0
1	FB	1002	0	1083	33	0
1	G	1002	0	1083	32	0
1	GB	1002	0	1083	36	0
1	H	1002	0	1083	31	0
1	HB	1002	0	1083	30	0
1	I	1002	0	1083	22	0
1	IB	1002	0	1083	25	0
1	J	1002	0	1083	26	0
1	JB	1002	0	1083	34	0
1	K	1002	0	1083	25	0
1	KB	1002	0	1083	29	0
1	L	1002	0	1083	31	0
1	LB	1002	0	1083	38	0
1	M	1002	0	1083	40	0
1	MB	1002	0	1083	29	0
1	N	1002	0	1083	25	0
1	NB	1002	0	1083	33	0
1	O	1002	0	1083	45	0
1	OB	1002	0	1083	42	0
1	P	1002	0	1083	33	0
1	PB	1002	0	1083	35	0
1	Q	1002	0	1083	42	0
1	QB	1002	0	1083	23	0
1	R	1002	0	1083	34	0
1	RB	1002	0	1083	29	0
1	S	1002	0	1083	29	0
1	SB	1002	0	1083	30	0
1	T	1002	0	1083	38	0
1	TB	1002	0	1083	33	0
2	a	881	0	928	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	ab	881	0	928	25	0
2	b	881	0	928	23	0
2	bb	881	0	928	17	0
2	c	881	0	928	36	0
2	cb	881	0	928	26	0
2	d	881	0	928	19	0
2	db	881	0	928	28	0
2	e	881	0	928	24	0
2	eb	881	0	928	30	0
2	f	881	0	928	23	0
2	fb	881	0	928	30	0
2	g	881	0	928	30	0
2	gb	881	0	928	26	0
2	h	881	0	928	21	0
2	hb	881	0	928	31	0
2	i	881	0	928	19	0
2	ib	881	0	928	22	0
2	j	881	0	928	30	0
2	jb	881	0	928	30	0
All	All	57700	0	61880	1588	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1588) 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:O:249:LEU:HD22	1:O:252:ILE:HD11	1.41	0.99
1:HB:201:ILE:HD11	1:HB:234:ILE:HD13	1.46	0.98
1:IB:245:LEU:HD23	1:IB:247:ILE:HD11	1.48	0.94
1:DB:201:ILE:HD11	1:DB:234:ILE:HD13	1.47	0.93
2:f:51:ILE:HG21	2:f:54:ILE:HD11	1.52	0.92
1:E:153:LEU:HD22	1:EB:170:ILE:CG2	2.01	0.91
2:fb:51:ILE:HG21	2:fb:54:ILE:HD11	1.54	0.90
1:Q:167:MET:HE1	1:Q:181:ILE:HD11	1.52	0.90
1:I:249:LEU:HD22	1:I:252:ILE:HD11	1.54	0.89
1:S:249:LEU:HD22	1:S:252:ILE:HD11	1.54	0.88
1:T:153:LEU:HD22	1:TB:170:ILE:CG2	2.05	0.87
1:LB:245:LEU:HD23	1:LB:247:ILE:HD11	1.58	0.85
1:P:153:LEU:HD22	1:PB:170:ILE:HG21	1.58	0.85
2:c:61:ILE:O	2:c:65:VAL:HG23	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HD22	1:BB:170:ILE:CG2	2.07	0.85
1:IB:167:MET:HE1	1:IB:181:ILE:HG23	1.61	0.83
2:jb:77:VAL:HG23	2:jb:112:LEU:HD21	1.60	0.83
1:G:249:LEU:HD13	1:G:252:ILE:HD11	1.61	0.83
1:P:160:ILE:HD11	1:P:166:VAL:HG22	1.61	0.83
1:O:153:LEU:HD22	1:OB:170:ILE:CG2	2.10	0.82
1:M:230:MET:HE1	1:M:265:ALA:HB2	1.62	0.81
1:B:153:LEU:HD22	1:BB:170:ILE:HG21	1.61	0.81
1:P:167:MET:HE1	1:P:169:LEU:HD21	1.63	0.81
1:I:245:LEU:HD23	1:I:247:ILE:HD11	1.63	0.80
2:ab:77:VAL:HG13	2:ab:112:LEU:HD21	1.63	0.80
1:T:249:LEU:HD23	1:T:252:ILE:HD11	1.62	0.80
1:H:201:ILE:HD11	1:H:234:ILE:HD13	1.63	0.79
1:PB:167:MET:HE1	1:PB:181:ILE:HG23	1.64	0.78
1:DB:231:LEU:HD13	1:DB:234:ILE:HD11	1.64	0.78
1:E:153:LEU:HD22	1:EB:170:ILE:HG21	1.63	0.78
1:J:153:LEU:HD22	1:JB:170:ILE:CG2	2.13	0.77
1:OB:175:ALA:HB2	1:OB:210:MET:HE1	1.65	0.77
1:B:240:GLN:HA	2:b:68:MET:HE3	1.65	0.77
1:K:153:LEU:HD22	1:KB:170:ILE:CG2	2.15	0.77
1:GB:190:VAL:HG13	1:GB:191:LYS:HD3	1.67	0.76
1:HB:249:LEU:HD12	2:gb:71:LEU:HD13	1.67	0.76
1:F:167:MET:HE1	1:F:181:ILE:HD11	1.67	0.76
1:I:170:ILE:CG2	1:IB:153:LEU:HD22	2.16	0.76
2:d:61:ILE:O	2:d:65:VAL:HG23	1.86	0.75
1:AB:249:LEU:HD12	1:CB:224:LEU:HD22	1.67	0.75
1:L:170:ILE:CG2	1:LB:153:LEU:HD22	2.15	0.75
2:ib:77:VAL:HG13	2:ib:112:LEU:HD21	1.67	0.74
2:j:14:ILE:HD11	2:j:32:LEU:HD13	1.69	0.74
1:T:170:ILE:CG2	1:TB:153:LEU:HD22	2.18	0.74
2:g:47:ASP:OD1	2:g:49:THR:HG23	1.86	0.74
2:f:61:ILE:O	2:f:65:VAL:HG23	1.88	0.74
1:G:153:LEU:HD13	1:GB:170:ILE:HG22	1.69	0.74
1:M:236:PRO:HG3	1:O:190:VAL:HG21	1.69	0.73
1:F:175:ALA:HB2	1:F:210:MET:HE1	1.70	0.73
1:G:230:MET:HE1	1:G:265:ALA:HB2	1.69	0.73
1:M:153:LEU:HD13	1:MB:170:ILE:HG22	1.71	0.73
1:LB:196:VAL:HG11	1:LB:265:ALA:CB	2.19	0.73
2:i:51:ILE:HG21	2:i:54:ILE:HD11	1.71	0.73
1:BB:201:ILE:HD11	1:BB:234:ILE:HD13	1.70	0.72
1:C:160:ILE:HG22	1:C:161:PHE:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:gb:77:VAL:HG23	2:gb:112:LEU:HD21	1.71	0.72
2:i:77:VAL:HG13	2:i:112:LEU:HD21	1.70	0.72
1:A:170:ILE:CG2	1:AB:153:LEU:HD22	2.20	0.72
1:TB:270:ASN:O	1:TB:270:ASN:ND2	2.21	0.72
1:F:153:LEU:HD13	1:FB:170:ILE:HG22	1.71	0.71
1:M:170:ILE:HD11	1:MB:153:LEU:HD22	1.72	0.71
1:L:196:VAL:HG11	1:L:265:ALA:CB	2.19	0.71
1:LB:175:ALA:HB2	1:LB:210:MET:HE1	1.70	0.71
1:LB:207:VAL:HG13	1:LB:211:VAL:HG23	1.71	0.71
1:M:162:GLU:O	1:M:164:ILE:HD12	1.91	0.71
1:C:153:LEU:HD13	1:CB:170:ILE:HG22	1.73	0.71
1:J:160:ILE:HG22	1:J:161:PHE:HD1	1.56	0.71
1:EB:175:ALA:HA	1:EB:210:MET:HE1	1.73	0.71
1:G:170:ILE:CG2	1:GB:153:LEU:HD22	2.20	0.71
1:K:234:ILE:HD12	1:K:234:ILE:H	1.56	0.70
1:KB:157:LEU:HD11	1:KB:165:SER:HB3	1.71	0.70
2:hb:77:VAL:HG22	2:hb:100:LEU:HB2	1.74	0.70
1:K:256:ASN:OD1	1:K:257:THR:HG23	1.90	0.70
2:a:51:ILE:HG21	2:a:54:ILE:HD11	1.71	0.70
1:P:153:LEU:HD22	1:PB:170:ILE:CG2	2.20	0.70
1:D:170:ILE:CG2	1:DB:153:LEU:HD22	2.22	0.70
2:g:81:ILE:H	2:g:81:ILE:HD12	1.56	0.70
1:PB:230:MET:HE1	1:PB:265:ALA:HA	1.74	0.70
1:HB:249:LEU:HD13	1:HB:252:ILE:HD11	1.73	0.70
1:I:249:LEU:HD22	1:I:252:ILE:CD1	2.20	0.70
1:S:249:LEU:HD22	1:S:252:ILE:CD1	2.21	0.70
1:T:153:LEU:HD22	1:TB:170:ILE:HG21	1.74	0.69
1:BB:270:ASN:O	1:BB:270:ASN:ND2	2.23	0.69
1:KB:151:GLN:OE1	1:KB:180:LEU:HD12	1.92	0.69
1:LB:216:ILE:HD11	1:LB:249:LEU:HD11	1.74	0.69
1:F:160:ILE:HG22	1:F:161:PHE:CD2	2.28	0.69
1:S:187:ILE:HG23	1:S:191:LYS:NZ	2.08	0.69
1:G:207:VAL:HG13	1:G:211:VAL:HG23	1.75	0.69
1:Q:153:LEU:HD22	1:QB:170:ILE:CG2	2.23	0.69
2:bb:77:VAL:HG23	2:bb:112:LEU:HD21	1.75	0.69
1:C:170:ILE:CG2	1:CB:153:LEU:HD22	2.23	0.68
1:HB:167:MET:CE	1:HB:181:ILE:HD11	2.24	0.68
1:OB:216:ILE:HD11	1:OB:249:LEU:HD11	1.75	0.68
1:CB:240:GLN:HA	2:ab:68:MET:HE3	1.75	0.68
1:S:170:ILE:CG2	1:SB:153:LEU:HD22	2.23	0.68
1:L:153:LEU:HD13	1:LB:170:ILE:HG22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:ILE:CG2	1:FB:153:LEU:HD22	2.24	0.68
2:fb:12:LEU:C	2:fb:13:LEU:HD12	2.18	0.68
2:fb:61:ILE:O	2:fb:65:VAL:HG23	1.94	0.67
2:gb:94:ILE:HG23	2:gb:94:ILE:O	1.94	0.67
1:NB:185:LEU:HD11	1:NB:197:VAL:HG21	1.76	0.67
2:ib:54:ILE:HD13	2:ib:85:VAL:HG13	1.77	0.67
1:CB:207:VAL:HG13	1:CB:211:VAL:HG23	1.74	0.67
1:FB:201:ILE:HD11	1:FB:234:ILE:HD13	1.76	0.67
1:J:170:ILE:HD11	1:JB:153:LEU:HD22	1.75	0.67
2:c:94:ILE:HG23	2:c:94:ILE:O	1.95	0.67
1:K:170:ILE:HG21	1:KB:153:LEU:HD22	1.77	0.67
1:L:175:ALA:HB2	1:L:210:MET:HE1	1.76	0.67
1:Q:234:ILE:H	1:Q:234:ILE:HD12	1.59	0.67
2:gb:61:ILE:O	2:gb:65:VAL:HG23	1.94	0.67
1:PB:207:VAL:HG13	1:PB:211:VAL:HG23	1.77	0.67
2:eb:14:ILE:HD11	2:eb:32:LEU:HD13	1.77	0.67
1:HB:167:MET:HE1	1:HB:181:ILE:HD11	1.76	0.66
1:R:201:ILE:HD11	1:R:234:ILE:HD13	1.75	0.66
1:B:232:VAL:HG11	1:B:258:MET:HA	1.77	0.66
1:LB:196:VAL:HG11	1:LB:265:ALA:HB1	1.75	0.66
1:Q:153:LEU:HD22	1:QB:170:ILE:HG21	1.77	0.66
1:GB:204:VAL:HG13	1:GB:235:ARG:HH22	1.58	0.66
2:b:77:VAL:HG13	2:b:112:LEU:HD21	1.76	0.66
1:D:153:LEU:HD13	1:DB:170:ILE:HG22	1.77	0.66
1:H:170:ILE:HD11	1:HB:153:LEU:HD22	1.78	0.66
2:a:94:ILE:HG23	2:a:94:ILE:O	1.95	0.66
2:j:75:LYS:HE3	2:j:75:LYS:HA	1.78	0.66
1:DB:224:LEU:O	1:G:254:THR:HG21	1.96	0.66
1:K:170:ILE:CG2	1:KB:153:LEU:HD22	2.26	0.66
2:a:33:LEU:HD11	2:a:68:MET:CE	2.26	0.66
1:J:160:ILE:HG22	1:J:161:PHE:CD1	2.31	0.66
1:P:170:ILE:CG2	1:PB:153:LEU:HD22	2.26	0.66
1:T:234:ILE:HD12	1:T:234:ILE:H	1.60	0.65
2:fb:78:VAL:HG21	2:fb:96:PHE:HE1	1.61	0.65
1:BB:167:MET:HE3	1:BB:167:MET:O	1.96	0.65
1:GB:269:THR:HG22	1:GB:269:THR:O	1.96	0.65
1:IB:247:ILE:HG22	1:IB:249:LEU:HD12	1.77	0.65
1:M:230:MET:CE	1:M:265:ALA:HB2	2.26	0.65
1:OB:269:THR:O	1:OB:269:THR:HG22	1.97	0.65
2:g:25:ALA:HA	2:g:28:PHE:CE1	2.32	0.65
1:QB:216:ILE:O	1:QB:220:GLU:OE1	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:170:ILE:CG2	1:NB:153:LEU:HD22	2.25	0.65
1:I:161:PHE:CE1	1:IB:273:ILE:HD11	2.31	0.65
1:Q:210:MET:HE3	1:Q:210:MET:HA	1.78	0.65
1:R:170:ILE:CG2	1:RB:153:LEU:HD22	2.26	0.65
2:ib:42:ARG:NH1	2:ib:116:LEU:HD22	2.12	0.65
1:QB:220:GLU:HG2	2:ib:90:ILE:HD13	1.78	0.65
2:hb:12:LEU:C	2:hb:13:LEU:HD12	2.22	0.65
2:d:29:GLN:HG2	2:d:65:VAL:HG22	1.78	0.65
1:IB:167:MET:HE2	1:IB:169:LEU:HD21	1.78	0.65
1:H:249:LEU:HD22	1:H:252:ILE:HD11	1.79	0.64
2:cb:43:GLY:HA3	2:cb:112:LEU:HD21	1.79	0.64
2:f:103:MET:HE3	2:f:103:MET:HA	1.78	0.64
1:E:269:THR:HG22	1:E:269:THR:O	1.96	0.64
1:G:225:VAL:O	2:hb:103:MET:HE1	1.98	0.64
1:L:160:ILE:HD12	1:L:166:VAL:HG21	1.78	0.64
1:TB:210:MET:HE3	1:TB:214:HIS:CE1	2.33	0.64
2:ab:14:ILE:HD11	2:ab:32:LEU:HD13	1.79	0.64
2:c:8:LEU:HD21	2:cb:105:LEU:CD2	2.28	0.64
1:DB:231:LEU:HD23	1:DB:252:ILE:HD13	1.78	0.64
1:R:153:LEU:HD22	1:RB:170:ILE:CG2	2.27	0.64
1:D:164:ILE:HD13	1:D:262:MET:HE1	1.80	0.64
1:L:196:VAL:HG11	1:L:265:ALA:HB1	1.79	0.64
1:BB:190:VAL:HG21	1:SB:236:PRO:HG3	1.80	0.64
1:CB:160:ILE:HG22	1:CB:161:PHE:HD1	1.61	0.64
2:c:51:ILE:HG21	2:c:54:ILE:HD11	1.79	0.64
1:A:249:LEU:HD12	1:D:224:LEU:HD22	1.80	0.64
1:E:170:ILE:CG2	1:EB:153:LEU:HD22	2.27	0.64
1:EB:262:MET:HA	1:EB:262:MET:HE2	1.80	0.64
2:eb:12:LEU:C	2:eb:13:LEU:HD12	2.22	0.64
1:H:231:LEU:HD21	1:H:234:ILE:HD11	1.79	0.63
2:cb:61:ILE:O	2:cb:65:VAL:HG23	1.98	0.63
1:DB:231:LEU:HD12	1:DB:231:LEU:O	1.97	0.63
1:KB:216:ILE:HD13	1:KB:249:LEU:HD23	1.79	0.63
2:a:77:VAL:HG12	2:a:100:LEU:HB2	1.79	0.63
1:CB:175:ALA:HB2	1:CB:210:MET:HE2	1.80	0.63
1:MB:260:LYS:HE3	1:MB:260:LYS:HA	1.81	0.63
1:SB:269:THR:HG22	1:SB:269:THR:O	1.99	0.63
2:a:51:ILE:HG21	2:a:54:ILE:CD1	2.29	0.63
2:h:94:ILE:HG23	2:h:94:ILE:O	1.98	0.63
2:hb:34:ALA:O	2:hb:38:GLU:OE1	2.17	0.63
1:M:271:ARG:HH21	1:MB:273:ILE:HG23	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:170:ILE:CG2	1:QB:153:LEU:HD22	2.28	0.63
1:RB:243:VAL:HG21	2:j:68:MET:HG3	1.81	0.63
2:jb:5:ILE:HG21	2:jb:35:LYS:HG2	1.79	0.63
2:b:77:VAL:HG12	2:b:100:LEU:HB2	1.81	0.63
1:TB:185:LEU:HD11	1:TB:197:VAL:HG21	1.81	0.63
1:N:247:ILE:HG22	1:N:249:LEU:HD12	1.79	0.63
1:Q:269:THR:HG22	1:Q:269:THR:O	1.99	0.63
1:R:245:LEU:HD23	1:R:247:ILE:HD11	1.80	0.63
1:MB:269:THR:O	1:MB:269:THR:HG22	1.97	0.63
1:BB:236:PRO:HG3	1:Q:190:VAL:HG21	1.80	0.62
1:E:232:VAL:HG23	1:E:255:THR:OG1	1.99	0.62
1:H:253:ILE:HG21	1:H:264:ARG:CD	2.28	0.62
1:CB:175:ALA:HB2	1:CB:210:MET:CE	2.28	0.62
1:H:269:THR:HG22	1:H:269:THR:O	1.99	0.62
1:A:201:ILE:O	1:A:204:VAL:HG12	1.99	0.62
1:C:230:MET:HE1	1:C:265:ALA:HB2	1.81	0.62
2:c:20:LEU:O	2:c:58:ILE:HD11	1.99	0.62
1:AB:148:SER:O	1:AB:152:GLU:OE1	2.18	0.62
1:C:175:ALA:CA	1:C:210:MET:HE1	2.29	0.62
1:I:170:ILE:HG21	1:IB:153:LEU:HD22	1.80	0.62
1:F:160:ILE:HG22	1:F:161:PHE:HD2	1.64	0.62
1:H:153:LEU:HD13	1:HB:170:ILE:HG22	1.82	0.62
1:J:153:LEU:HD22	1:JB:170:ILE:HG21	1.79	0.62
2:d:78:VAL:HG21	2:d:96:PHE:HE1	1.64	0.62
1:G:185:LEU:HD11	1:G:197:VAL:HG21	1.80	0.61
1:G:201:ILE:O	1:G:204:VAL:HG12	1.99	0.61
1:LB:269:THR:HG22	1:LB:269:THR:O	1.98	0.61
1:O:153:LEU:HD22	1:OB:170:ILE:HG22	1.81	0.61
2:b:51:ILE:HG21	2:b:54:ILE:HD11	1.82	0.61
1:E:230:MET:HE1	1:E:265:ALA:HA	1.82	0.61
1:J:153:LEU:HD13	1:JB:170:ILE:HG22	1.81	0.61
1:K:173:ILE:HD13	1:K:177:ARG:HH21	1.65	0.61
2:d:48:ILE:HD11	2:d:81:ILE:HG13	1.81	0.61
1:P:160:ILE:HD11	1:P:166:VAL:CG2	2.30	0.61
2:a:61:ILE:O	2:a:65:VAL:HG23	2.00	0.61
1:EB:175:ALA:CA	1:EB:210:MET:HE1	2.30	0.61
1:T:196:VAL:HG11	1:T:265:ALA:CB	2.31	0.61
1:F:185:LEU:HD11	1:F:197:VAL:HG21	1.82	0.61
1:G:216:ILE:O	1:G:220:GLU:OE1	2.18	0.61
1:Q:167:MET:CE	1:Q:181:ILE:HD11	2.29	0.61
2:eb:26:VAL:O	2:eb:30:GLU:OE1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:VAL:HG21	1:Q:236:PRO:HG3	1.82	0.61
1:NB:269:THR:HG22	1:NB:269:THR:O	2.00	0.61
1:DB:185:LEU:HD11	1:DB:197:VAL:HG21	1.83	0.61
1:NB:262:MET:HA	1:NB:262:MET:HE2	1.83	0.60
2:jb:66:VAL:HG23	2:jb:76:VAL:HG11	1.81	0.60
1:E:249:LEU:HD13	1:E:252:ILE:HD11	1.82	0.60
2:e:16:ILE:HG22	2:e:51:ILE:HD11	1.83	0.60
2:i:34:ALA:O	2:i:38:GLU:OE1	2.18	0.60
1:FB:216:ILE:HD11	1:FB:249:LEU:HD11	1.82	0.60
1:N:153:LEU:HD13	1:NB:170:ILE:HG22	1.83	0.60
2:g:61:ILE:O	2:g:65:VAL:HG23	2.02	0.60
1:R:153:LEU:HD22	1:RB:170:ILE:HG22	1.81	0.60
2:hb:54:ILE:HD11	2:hb:58:ILE:CG2	2.32	0.60
2:ab:16:ILE:HG22	2:ab:51:ILE:HD11	1.83	0.60
1:C:175:ALA:HA	1:C:210:MET:HE1	1.83	0.60
1:DB:190:VAL:HG21	1:G:236:PRO:HG3	1.84	0.60
1:L:170:ILE:HG22	1:LB:153:LEU:HD22	1.83	0.60
1:GB:193:ARG:HA	2:i:103:MET:HE2	1.83	0.60
1:N:153:LEU:HD22	1:NB:170:ILE:CG2	2.31	0.60
1:QB:269:THR:HG22	1:QB:269:THR:O	2.02	0.60
2:ab:78:VAL:HG21	2:ab:96:PHE:HE2	1.66	0.60
1:M:151:GLN:NE2	1:M:180:LEU:HD12	2.17	0.60
1:G:269:THR:HG22	1:G:269:THR:O	2.00	0.60
1:SB:167:MET:HE1	1:SB:181:ILE:HG23	1.82	0.60
2:hb:20:LEU:HD13	2:hb:28:PHE:CE1	2.37	0.60
1:HB:249:LEU:HD12	2:gb:71:LEU:CD1	2.31	0.60
1:P:188:GLY:O	1:P:192:ASN:ND2	2.31	0.60
1:FB:231:LEU:HD12	1:FB:231:LEU:O	2.02	0.59
1:K:153:LEU:HD22	1:KB:170:ILE:HG21	1.84	0.59
1:S:269:THR:O	1:S:269:THR:HG22	2.00	0.59
1:AB:235:ARG:NH2	1:CB:190:VAL:HG21	2.17	0.59
1:D:207:VAL:HB	1:D:238:ILE:HG23	1.83	0.59
1:Q:179:LYS:O	1:Q:183:GLU:OE1	2.20	0.59
1:S:180:LEU:HD23	1:S:183:GLU:OE2	2.02	0.59
1:MB:175:ALA:HB2	1:MB:210:MET:HE1	1.83	0.59
1:L:196:VAL:HG11	1:L:265:ALA:HB2	1.83	0.59
2:a:33:LEU:HD11	2:a:68:MET:HE3	1.85	0.59
2:eb:14:ILE:CD1	2:eb:32:LEU:HD13	2.32	0.59
2:fb:78:VAL:HG21	2:fb:96:PHE:CE1	2.37	0.59
1:K:153:LEU:HD13	1:KB:170:ILE:HG22	1.85	0.59
2:hb:103:MET:HE2	2:hb:103:MET:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:GLU:HG3	1:C:153:LEU:HD23	1.84	0.59
1:PB:222:VAL:HG22	1:PB:227:CYS:HB3	1.85	0.59
2:hb:25:ALA:HA	2:hb:28:PHE:CE1	2.37	0.59
1:R:243:VAL:HG11	2:fb:68:MET:CG	2.33	0.59
1:RB:259:LYS:O	1:RB:263:GLU:OE1	2.21	0.59
1:T:255:THR:HG22	1:T:264:ARG:NH1	2.18	0.59
1:AB:249:LEU:HD13	1:AB:252:ILE:HD11	1.85	0.59
1:BB:239:ALA:O	1:BB:243:VAL:HG22	2.02	0.59
2:bb:61:ILE:O	2:bb:65:VAL:HG23	2.03	0.59
1:L:160:ILE:HD12	1:L:166:VAL:CG2	2.33	0.58
1:R:210:MET:N	1:R:210:MET:HE2	2.17	0.58
1:T:216:ILE:HD11	1:T:247:ILE:HD13	1.85	0.58
2:b:16:ILE:HG22	2:b:51:ILE:HD11	1.84	0.58
2:g:115:GLU:OE1	2:g:116:LEU:HD22	2.03	0.58
1:D:157:LEU:HD11	1:D:165:SER:CB	2.33	0.58
1:TB:186:LEU:HD21	1:TB:221:ALA:HB1	1.85	0.58
1:TB:196:VAL:HG11	1:TB:265:ALA:HB1	1.85	0.58
1:C:207:VAL:HG13	1:C:211:VAL:HG23	1.84	0.58
1:FB:210:MET:HG2	1:FB:214:HIS:CE1	2.38	0.58
1:IB:167:MET:CE	1:IB:169:LEU:HD21	2.34	0.58
1:FB:157:LEU:HD11	1:FB:165:SER:CB	2.33	0.58
1:G:170:ILE:HG22	1:GB:153:LEU:HD22	1.84	0.58
1:QB:160:ILE:HD12	1:QB:166:VAL:HG21	1.84	0.58
2:c:29:GLN:OE1	2:c:65:VAL:HG22	2.04	0.58
1:M:170:ILE:CD1	1:MB:153:LEU:HD22	2.33	0.58
1:OB:232:VAL:HG21	1:OB:258:MET:HA	1.86	0.58
1:RB:228:GLN:N	1:RB:228:GLN:OE1	2.37	0.58
2:jb:72:MET:HE3	2:jb:72:MET:O	2.04	0.58
1:AB:185:LEU:HD11	1:AB:197:VAL:HG21	1.86	0.58
1:F:167:MET:CE	1:F:181:ILE:HD11	2.34	0.58
1:A:153:LEU:HD22	1:AB:170:ILE:CG2	2.34	0.58
2:e:78:VAL:HG21	2:e:96:PHE:CE1	2.39	0.58
2:f:29:GLN:HG3	2:f:65:VAL:HG22	1.85	0.58
2:j:61:ILE:O	2:j:65:VAL:HG23	2.04	0.58
1:B:207:VAL:HG13	1:B:211:VAL:HG23	1.86	0.58
1:M:210:MET:HE2	1:M:210:MET:HA	1.86	0.58
2:g:26:VAL:O	2:g:30:GLU:OE1	2.22	0.58
2:jb:54:ILE:HG23	2:jb:58:ILE:HG23	1.86	0.58
1:D:157:LEU:HD11	1:D:165:SER:HB3	1.86	0.58
1:J:170:ILE:CD1	1:JB:153:LEU:HD22	2.34	0.58
1:PB:239:ALA:O	1:PB:243:VAL:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:bb:81:ILE:H	2:bb:81:ILE:HD12	1.68	0.58
1:HB:241:THR:O	1:HB:245:LEU:HD23	2.04	0.57
1:NB:179:LYS:O	1:NB:183:GLU:OE1	2.21	0.57
1:S:232:VAL:HG12	1:S:255:THR:CG2	2.34	0.57
1:F:236:PRO:HG3	1:PB:190:VAL:HG21	1.85	0.57
1:M:271:ARG:NH2	1:MB:273:ILE:HG23	2.20	0.57
2:hb:61:ILE:O	2:hb:65:VAL:HG23	2.04	0.57
2:ib:42:ARG:HH11	2:ib:116:LEU:HD22	1.70	0.57
1:FB:201:ILE:HD11	1:FB:234:ILE:CD1	2.33	0.57
2:cb:78:VAL:HG21	2:cb:96:PHE:HE1	1.69	0.57
1:E:190:VAL:HG21	1:J:236:PRO:HG3	1.84	0.57
2:g:71:LEU:O	2:g:71:LEU:HD23	2.05	0.57
1:B:196:VAL:HG11	1:B:265:ALA:CB	2.35	0.57
1:P:170:ILE:HG22	1:PB:153:LEU:HD22	1.86	0.57
2:g:54:ILE:HD11	2:g:58:ILE:CG2	2.34	0.57
2:j:20:LEU:O	2:j:58:ILE:HD11	2.05	0.57
1:G:228:GLN:N	1:G:228:GLN:OE1	2.37	0.57
1:I:210:MET:HE2	1:I:210:MET:HA	1.86	0.57
2:jb:55:ASP:OD1	2:jb:58:ILE:HG22	2.05	0.57
1:EB:201:ILE:HD11	1:EB:234:ILE:CD1	2.34	0.57
1:KB:157:LEU:HD11	1:KB:165:SER:CB	2.34	0.57
2:ab:14:ILE:CD1	2:ab:32:LEU:HD13	2.34	0.57
1:C:160:ILE:HG22	1:C:161:PHE:HD2	1.66	0.57
1:CB:160:ILE:HG22	1:CB:161:PHE:CD1	2.40	0.57
1:CB:259:LYS:O	1:CB:263:GLU:OE1	2.23	0.57
1:L:235:ARG:HB3	1:L:236:PRO:CD	2.35	0.57
2:b:48:ILE:HD11	2:b:81:ILE:HG12	1.87	0.57
2:eb:34:ALA:O	2:eb:38:GLU:OE1	2.22	0.57
1:JB:169:LEU:C	1:JB:169:LEU:HD23	2.30	0.57
1:S:273:ILE:HD13	1:SB:161:PHE:CE1	2.40	0.57
1:GB:196:VAL:HG11	1:GB:265:ALA:HB1	1.85	0.56
2:f:51:ILE:HG21	2:f:54:ILE:CD1	2.30	0.56
2:g:3:ILE:O	2:g:5:ILE:HD12	2.04	0.56
2:j:64:ASP:O	2:j:68:MET:HE3	2.05	0.56
2:jb:33:LEU:HD11	2:jb:68:MET:HE1	1.86	0.56
1:A:236:PRO:HG3	1:D:190:VAL:HG21	1.88	0.56
1:IB:201:ILE:HD11	1:IB:234:ILE:HG12	1.86	0.56
1:NB:243:VAL:HG11	1:TB:220:GLU:CD	2.30	0.56
1:O:201:ILE:O	1:O:204:VAL:HG12	2.04	0.56
2:cb:103:MET:HE3	2:cb:103:MET:HA	1.86	0.56
2:hb:81:ILE:HD12	2:hb:81:ILE:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:jb:12:LEU:C	2:jb:13:LEU:HD12	2.30	0.56
1:GB:196:VAL:HG11	1:GB:265:ALA:CB	2.36	0.56
1:H:224:LEU:HD22	1:O:249:LEU:HD12	1.86	0.56
1:JB:190:VAL:HG13	1:JB:191:LYS:HD2	1.86	0.56
1:NB:210:MET:N	1:NB:210:MET:HE2	2.20	0.56
1:A:249:LEU:HD13	1:A:252:ILE:HD11	1.86	0.56
1:R:195:GLU:N	1:R:195:GLU:OE1	2.39	0.56
2:cb:78:VAL:HG21	2:cb:96:PHE:CE1	2.41	0.56
2:f:81:ILE:HD12	2:f:81:ILE:H	1.70	0.56
2:hb:23:HIS:O	2:hb:27:GLU:OE1	2.23	0.56
2:hb:29:GLN:HG3	2:hb:65:VAL:HG22	1.87	0.56
1:K:262:MET:HE2	1:K:262:MET:HA	1.87	0.56
1:T:196:VAL:HG11	1:T:265:ALA:HB1	1.87	0.56
2:c:71:LEU:HD23	2:c:71:LEU:O	2.05	0.56
2:hb:66:VAL:HG23	2:hb:76:VAL:HG11	1.88	0.56
1:JB:207:VAL:HG13	1:JB:211:VAL:HG23	1.87	0.56
1:F:230:MET:HE1	1:F:265:ALA:HB2	1.88	0.56
2:e:109:LEU:HD21	2:e:113:LYS:HE3	1.88	0.56
1:AB:186:LEU:HD21	1:AB:221:ALA:HB1	1.88	0.56
1:G:160:ILE:HD12	1:G:166:VAL:CG2	2.35	0.56
1:I:167:MET:HE2	1:I:169:LEU:HD21	1.86	0.56
1:SB:259:LYS:O	1:SB:263:GLU:OE1	2.23	0.56
1:D:160:ILE:HG22	1:D:161:PHE:HD2	1.71	0.56
2:ab:71:LEU:HD23	2:ab:71:LEU:O	2.05	0.56
1:CB:232:VAL:HG23	1:CB:255:THR:OG1	2.06	0.55
2:d:5:ILE:HG23	2:d:14:ILE:HD11	1.89	0.55
1:M:167:MET:HE2	1:M:169:LEU:HD21	1.87	0.55
1:T:160:ILE:HD12	1:T:166:VAL:CG2	2.37	0.55
2:b:10:GLU:N	2:b:10:GLU:OE1	2.39	0.55
2:eb:85:VAL:O	2:eb:89:LEU:HD13	2.06	0.55
2:fb:51:ILE:HG21	2:fb:54:ILE:CD1	2.30	0.55
2:fb:77:VAL:HG13	2:fb:112:LEU:HD21	1.86	0.55
2:h:16:ILE:HG22	2:h:51:ILE:HD11	1.89	0.55
1:TB:196:VAL:HG11	1:TB:265:ALA:CB	2.35	0.55
1:GB:217:GLN:OE1	2:i:90:ILE:HG21	2.06	0.55
1:J:231:LEU:HD23	1:J:234:ILE:HD11	1.89	0.55
1:TB:230:MET:HE1	1:TB:261:GLY:O	2.06	0.55
2:e:12:LEU:C	2:e:13:LEU:HD12	2.31	0.55
2:g:29:GLN:HG2	2:g:65:VAL:HG22	1.88	0.55
1:D:179:LYS:O	1:D:183:GLU:OE1	2.24	0.55
1:G:160:ILE:HD12	1:G:166:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:175:ALA:HB1	1:M:179:LYS:NZ	2.21	0.55
1:NB:243:VAL:HG23	1:TB:224:LEU:HD11	1.89	0.55
2:c:77:VAL:HG12	2:c:100:LEU:HB2	1.89	0.55
2:i:42:ARG:NH1	2:i:116:LEU:HD22	2.22	0.55
2:ib:78:VAL:HG21	2:ib:96:PHE:HE1	1.71	0.55
1:B:196:VAL:HG11	1:B:265:ALA:HB1	1.89	0.55
1:DB:160:ILE:HD12	1:DB:166:VAL:CG2	2.37	0.55
1:O:196:VAL:HG11	1:O:265:ALA:CB	2.36	0.55
1:O:234:ILE:H	1:O:234:ILE:HD12	1.72	0.55
1:P:167:MET:HE1	1:P:169:LEU:CD2	2.36	0.55
1:S:153:LEU:HD13	1:SB:170:ILE:HG22	1.88	0.55
2:e:103:MET:HE3	2:e:103:MET:HA	1.88	0.55
1:N:152:GLU:OE1	1:N:153:LEU:HD23	2.05	0.55
1:P:167:MET:O	1:P:167:MET:SD	2.64	0.55
1:QB:225:VAL:HG12	1:QB:225:VAL:O	2.07	0.55
2:b:5:ILE:HG21	2:b:35:LYS:HG2	1.88	0.55
2:c:6:LEU:HD23	2:cb:105:LEU:HD13	1.89	0.55
1:A:207:VAL:HG13	1:A:211:VAL:HG23	1.88	0.55
1:NB:236:PRO:HD3	1:TB:190:VAL:HG21	1.88	0.55
2:a:16:ILE:HG22	2:a:51:ILE:HD11	1.88	0.55
1:C:167:MET:HE1	1:C:181:ILE:HG23	1.89	0.55
1:EB:201:ILE:HD11	1:EB:234:ILE:HD12	1.89	0.55
1:L:222:VAL:HG22	1:L:227:CYS:HB3	1.89	0.55
1:LB:234:ILE:HD12	1:LB:234:ILE:H	1.72	0.55
2:eb:61:ILE:O	2:eb:65:VAL:HG23	2.07	0.55
1:DB:185:LEU:CD1	1:DB:197:VAL:HG21	2.37	0.55
1:IB:167:MET:CE	1:IB:181:ILE:HG23	2.36	0.55
1:QB:160:ILE:HD12	1:QB:166:VAL:CG2	2.37	0.55
1:BB:241:THR:O	1:BB:245:LEU:HD23	2.07	0.54
1:E:235:ARG:NH2	1:M:190:VAL:HG21	2.22	0.54
1:K:232:VAL:HG21	1:K:258:MET:HA	1.90	0.54
1:L:225:VAL:HG12	1:L:225:VAL:O	2.07	0.54
2:c:77:VAL:HG13	2:c:112:LEU:HD21	1.88	0.54
1:N:216:ILE:HD11	1:N:247:ILE:HG21	1.88	0.54
2:b:71:LEU:O	2:b:71:LEU:HD23	2.07	0.54
1:B:222:VAL:HG22	1:B:227:CYS:HB3	1.90	0.54
1:F:222:VAL:HG22	1:F:227:CYS:HB2	1.89	0.54
1:MB:234:ILE:HD13	2:f:71:LEU:HD21	1.89	0.54
1:SB:160:ILE:HD12	1:SB:166:VAL:CG2	2.37	0.54
1:DB:269:THR:HG22	1:DB:269:THR:O	2.08	0.54
1:FB:269:THR:O	1:FB:269:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:207:VAL:HG13	1:M:211:VAL:HG23	1.89	0.54
2:e:43:GLY:HA3	2:e:112:LEU:HD21	1.89	0.54
2:jb:61:ILE:O	2:jb:65:VAL:HG23	2.08	0.54
1:E:235:ARG:HH22	1:M:190:VAL:HG21	1.73	0.54
1:OB:207:VAL:HB	1:OB:238:ILE:HG23	1.90	0.54
1:SB:155:ALA:HB1	1:SB:167:MET:HE2	1.89	0.54
2:gb:51:ILE:HG21	2:gb:54:ILE:HD11	1.90	0.54
2:gb:78:VAL:HG21	2:gb:96:PHE:HE1	1.72	0.54
1:K:260:LYS:HE2	1:K:260:LYS:HA	1.90	0.54
1:TB:167:MET:HE1	1:TB:169:LEU:HD21	1.90	0.54
2:jb:29:GLN:HG3	2:jb:65:VAL:HG22	1.89	0.54
1:JB:187:ILE:HG23	1:JB:191:LYS:NZ	2.22	0.54
2:a:71:LEU:HD23	2:a:71:LEU:O	2.08	0.54
1:FB:210:MET:CG	1:FB:214:HIS:HE1	2.20	0.54
1:P:241:THR:O	1:P:245:LEU:HD23	2.07	0.54
1:Q:169:LEU:HD23	1:Q:169:LEU:C	2.33	0.54
2:bb:12:LEU:C	2:bb:13:LEU:HD22	2.32	0.54
1:A:185:LEU:HD11	1:A:197:VAL:HG21	1.90	0.54
1:O:249:LEU:HD22	1:O:252:ILE:CD1	2.28	0.54
1:R:170:ILE:HG22	1:RB:153:LEU:HD22	1.89	0.54
2:c:3:ILE:O	2:c:5:ILE:HD12	2.08	0.54
2:db:78:VAL:HG21	2:db:96:PHE:CE1	2.43	0.54
2:jb:81:ILE:HD12	2:jb:81:ILE:H	1.73	0.54
1:JB:169:LEU:HD21	1:JB:173:ILE:HD11	1.90	0.54
2:h:61:ILE:O	2:h:65:VAL:HG23	2.08	0.54
1:K:160:ILE:HD12	1:K:166:VAL:HG11	1.89	0.53
1:LB:175:ALA:CB	1:LB:210:MET:HE1	2.38	0.53
1:N:210:MET:HE2	1:N:210:MET:HA	1.89	0.53
1:IB:207:VAL:HG13	1:IB:211:VAL:HG23	1.89	0.53
1:J:170:ILE:CG1	1:JB:153:LEU:HD22	2.38	0.53
2:hb:54:ILE:HD11	2:hb:58:ILE:HG22	1.91	0.53
1:JB:147:LYS:O	1:JB:151:GLN:OE1	2.25	0.53
1:M:195:GLU:N	1:M:195:GLU:OE1	2.40	0.53
1:OB:225:VAL:HG12	1:OB:225:VAL:O	2.09	0.53
1:PB:210:MET:HE2	1:PB:210:MET:HA	1.89	0.53
2:c:103:MET:HE3	2:c:103:MET:HA	1.90	0.53
2:db:72:MET:HA	2:db:72:MET:HE2	1.90	0.53
1:AB:249:LEU:HD22	1:AB:252:ILE:HD11	1.90	0.53
1:D:230:MET:HE1	1:D:265:ALA:HA	1.89	0.53
1:MB:240:GLN:HA	2:f:68:MET:HE3	1.89	0.53
1:TB:160:ILE:HD12	1:TB:166:VAL:CG2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:103:MET:HE3	2:j:103:MET:HA	1.89	0.53
1:H:253:ILE:HG21	1:H:264:ARG:HD3	1.91	0.53
1:LB:169:LEU:C	1:LB:169:LEU:HD23	2.33	0.53
2:c:26:VAL:O	2:c:30:GLU:OE1	2.26	0.53
2:e:33:LEU:HD11	2:e:68:MET:HE2	1.89	0.53
1:FB:195:GLU:N	1:FB:195:GLU:OE2	2.42	0.53
1:O:230:MET:HE1	1:O:265:ALA:HB2	1.91	0.53
1:TB:200:ASP:OD2	1:TB:202:THR:HG22	2.08	0.53
2:j:16:ILE:HG22	2:j:51:ILE:HD11	1.90	0.53
1:B:177:ARG:O	1:B:181:ILE:HG12	2.09	0.53
1:FB:231:LEU:HD13	1:FB:234:ILE:HD11	1.91	0.53
1:G:269:THR:HG21	1:G:271:ARG:NH2	2.24	0.53
1:PB:170:ILE:HG23	1:PB:203:GLY:HA3	1.91	0.53
2:jb:21:ASP:OD1	2:jb:24:THR:HG23	2.09	0.53
1:C:170:ILE:HG22	1:CB:153:LEU:HD22	1.91	0.53
2:c:54:ILE:HG22	2:c:55:ASP:O	2.08	0.53
2:eb:103:MET:HA	2:eb:103:MET:HE2	1.90	0.53
1:D:207:VAL:HG13	1:D:211:VAL:HG23	1.89	0.53
1:M:198:LEU:HD22	1:M:262:MET:HE2	1.91	0.53
2:c:8:LEU:HD12	2:c:13:LEU:HD11	1.90	0.53
1:O:231:LEU:HG	1:O:252:ILE:HD12	1.91	0.53
2:e:109:LEU:C	2:e:109:LEU:HD23	2.34	0.53
2:fb:77:VAL:HG12	2:fb:100:LEU:HB2	1.90	0.53
1:D:170:ILE:HG21	1:DB:153:LEU:HD22	1.91	0.52
1:E:213:HIS:O	1:E:216:ILE:HG22	2.08	0.52
1:F:147:LYS:O	1:F:151:GLN:OE1	2.26	0.52
1:T:170:ILE:HG21	1:TB:153:LEU:HD22	1.89	0.52
2:fb:81:ILE:HD12	2:fb:81:ILE:H	1.73	0.52
1:J:192:ASN:CG	1:J:194:SER:HG	2.16	0.52
1:N:170:ILE:HG21	1:NB:153:LEU:HD22	1.90	0.52
1:N:256:ASN:OD1	1:N:257:THR:HG23	2.08	0.52
1:PB:160:ILE:HG22	1:PB:161:PHE:CD2	2.45	0.52
2:db:64:ASP:HB3	2:db:68:MET:HE3	1.91	0.52
1:A:147:LYS:O	1:A:151:GLN:OE1	2.27	0.52
1:S:170:ILE:HG21	1:SB:153:LEU:HD22	1.91	0.52
1:S:198:LEU:HD11	1:S:262:MET:HE2	1.91	0.52
2:bb:77:VAL:HG22	2:bb:100:LEU:HB2	1.91	0.52
2:fb:25:ALA:HA	2:fb:28:PHE:CE1	2.44	0.52
2:j:62:LEU:C	2:j:62:LEU:HD23	2.35	0.52
1:RB:216:ILE:HD11	1:RB:247:ILE:HG21	1.92	0.52
2:i:33:LEU:O	2:i:36:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD12	1:D:224:LEU:CD2	2.38	0.52
1:BB:223:ARG:HD2	1:BB:223:ARG:O	2.10	0.52
1:MB:157:LEU:HD22	1:MB:188:GLY:HA3	1.92	0.52
1:O:196:VAL:HG11	1:O:265:ALA:HB1	1.90	0.52
1:P:220:GLU:OE1	1:P:220:GLU:HA	2.09	0.52
2:eb:109:LEU:HD23	2:eb:109:LEU:O	2.08	0.52
1:A:170:ILE:HG22	1:AB:153:LEU:HD22	1.92	0.52
1:FB:157:LEU:HD11	1:FB:165:SER:HB2	1.90	0.52
1:HB:169:LEU:HD23	1:HB:169:LEU:C	2.35	0.52
1:I:243:VAL:HG11	2:e:68:MET:CG	2.39	0.52
1:Q:170:ILE:HG21	1:QB:153:LEU:HD22	1.92	0.52
2:db:78:VAL:HG21	2:db:96:PHE:HE1	1.75	0.52
2:e:81:ILE:HD12	2:e:81:ILE:H	1.75	0.52
2:j:35:LYS:HE2	2:j:39:THR:HG21	1.91	0.52
2:jb:12:LEU:HD11	2:jb:35:LYS:HE3	1.92	0.52
1:B:249:LEU:HD22	1:B:252:ILE:HD11	1.92	0.52
1:GB:201:ILE:O	1:GB:204:VAL:HG12	2.09	0.52
1:LB:196:VAL:HG11	1:LB:265:ALA:HB2	1.90	0.52
1:O:164:ILE:HG21	1:O:262:MET:HE1	1.92	0.52
1:OB:231:LEU:HD23	1:OB:234:ILE:HD11	1.91	0.52
2:a:26:VAL:O	2:a:30:GLU:OE1	2.27	0.52
2:fb:29:GLN:HG3	2:fb:65:VAL:HG22	1.92	0.52
1:CB:204:VAL:HG11	1:CB:207:VAL:HG23	1.91	0.52
1:O:262:MET:HA	1:O:262:MET:HE2	1.91	0.52
2:eb:5:ILE:HG21	2:eb:35:LYS:HG2	1.92	0.52
2:g:64:ASP:HB3	2:g:68:MET:HE3	1.91	0.52
1:BB:196:VAL:HG11	1:BB:265:ALA:HB1	1.92	0.52
1:OB:186:LEU:HD21	1:OB:221:ALA:HB1	1.92	0.52
1:T:153:LEU:HD22	1:TB:170:ILE:HG22	1.89	0.52
2:e:78:VAL:HG21	2:e:96:PHE:HE1	1.73	0.52
2:fb:24:THR:O	2:fb:27:GLU:HG3	2.09	0.52
2:fb:59:ALA:HB1	2:fb:94:ILE:CD1	2.40	0.52
1:B:169:LEU:HD23	1:B:169:LEU:C	2.36	0.52
1:PB:207:VAL:CG1	1:PB:211:VAL:HG23	2.40	0.52
2:h:105:LEU:HD23	2:h:105:LEU:C	2.35	0.52
1:AB:151:GLN:C	1:AB:151:GLN:OE1	2.53	0.51
1:B:231:LEU:HD23	1:B:234:ILE:HD11	1.92	0.51
1:P:254:THR:HG21	2:eb:71:LEU:O	2.09	0.51
2:i:51:ILE:HG21	2:i:54:ILE:CD1	2.39	0.51
1:FB:262:MET:HE2	1:FB:262:MET:HA	1.92	0.51
1:LB:207:VAL:CG1	1:LB:211:VAL:HG23	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:170:ILE:HG12	1:OB:153:LEU:HD22	1.92	0.51
1:QB:235:ARG:HG2	1:QB:236:PRO:HD2	1.92	0.51
1:RB:217:GLN:OE1	1:RB:217:GLN:HA	2.10	0.51
2:cb:26:VAL:O	2:cb:30:GLU:OE1	2.27	0.51
2:e:34:ALA:O	2:e:38:GLU:OE1	2.28	0.51
2:h:29:GLN:HG3	2:h:65:VAL:HG22	1.92	0.51
1:CB:264:ARG:NH1	1:CB:264:ARG:HB2	2.25	0.51
1:CB:269:THR:O	1:CB:270:ASN:OD1	2.28	0.51
1:JB:188:GLY:O	1:JB:192:ASN:ND2	2.40	0.51
1:KB:213:HIS:O	1:KB:216:ILE:HG22	2.11	0.51
1:TB:269:THR:O	1:TB:269:THR:HG22	2.10	0.51
2:db:26:VAL:O	2:db:30:GLU:OE1	2.28	0.51
2:ib:32:LEU:HD23	2:ib:65:VAL:HG21	1.91	0.51
1:AB:160:ILE:HD12	1:AB:166:VAL:CG2	2.41	0.51
1:K:216:ILE:O	1:K:220:GLU:OE1	2.29	0.51
1:O:207:VAL:HG13	1:O:211:VAL:HG23	1.90	0.51
1:S:262:MET:O	1:S:266:LEU:HD23	2.11	0.51
2:d:11:CYS:O	2:d:12:LEU:HD12	2.09	0.51
1:AB:177:ARG:O	1:AB:181:ILE:HG12	2.10	0.51
1:R:207:VAL:HG13	1:R:211:VAL:HG23	1.92	0.51
2:jb:71:LEU:HD23	2:jb:71:LEU:O	2.11	0.51
1:GB:204:VAL:O	1:GB:235:ARG:NH2	2.43	0.51
1:I:254:THR:HG21	2:e:71:LEU:O	2.11	0.51
1:OB:232:VAL:HG23	1:OB:255:THR:OG1	2.10	0.51
1:P:207:VAL:HG13	1:P:211:VAL:HG23	1.92	0.51
1:RB:161:PHE:HB2	1:RB:164:ILE:HD12	1.92	0.51
2:a:14:ILE:CD1	2:a:32:LEU:HD12	2.41	0.51
2:eb:96:PHE:HB3	2:eb:99:VAL:HB	1.93	0.51
2:fb:71:LEU:HD23	2:fb:71:LEU:O	2.11	0.51
1:BB:196:VAL:HG23	1:BB:228:GLN:O	2.09	0.51
1:F:204:VAL:HG11	1:F:207:VAL:HG23	1.93	0.51
1:I:169:LEU:O	1:I:170:ILE:HD13	2.11	0.51
1:J:193:ARG:HD2	1:J:193:ARG:O	2.11	0.51
1:LB:247:ILE:HG22	1:LB:249:LEU:HD12	1.92	0.51
1:M:175:ALA:HB1	1:M:179:LYS:HZ1	1.76	0.51
1:MB:240:GLN:CA	2:f:68:MET:HE3	2.41	0.51
1:RB:200:ASP:OD1	1:RB:202:THR:HG23	2.10	0.51
2:j:64:ASP:C	2:j:68:MET:HE3	2.35	0.51
1:LB:210:MET:HE2	1:LB:214:HIS:NE2	2.25	0.51
1:O:200:ASP:OD1	1:O:202:THR:HG23	2.11	0.51
1:P:258:MET:HE1	1:PB:160:ILE:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PB:204:VAL:HG11	1:PB:207:VAL:HG22	1.92	0.51
1:R:225:VAL:HG12	1:R:225:VAL:O	2.10	0.51
1:T:245:LEU:HD23	1:T:247:ILE:HD11	1.93	0.51
1:RB:155:ALA:HB1	1:RB:181:ILE:HD12	1.92	0.51
2:fb:42:ARG:CZ	2:fb:116:LEU:HD12	2.41	0.51
2:jb:14:ILE:HD11	2:jb:32:LEU:HD13	1.93	0.51
2:db:21:ASP:OD1	2:db:24:THR:HG23	2.11	0.51
2:gb:77:VAL:CG2	2:gb:112:LEU:HD21	2.41	0.51
1:A:170:ILE:HG21	1:AB:153:LEU:HD22	1.92	0.50
1:G:262:MET:HE2	1:G:262:MET:HA	1.92	0.50
1:H:196:VAL:HG11	1:H:265:ALA:HB1	1.94	0.50
1:N:235:ARG:CZ	1:N:235:ARG:HA	2.41	0.50
1:Q:216:ILE:HD11	1:Q:249:LEU:HD11	1.93	0.50
2:d:54:ILE:HD11	2:d:58:ILE:CG2	2.42	0.50
2:ib:105:LEU:C	2:ib:105:LEU:HD23	2.36	0.50
1:G:230:MET:HE1	1:G:265:ALA:CB	2.39	0.50
1:H:170:ILE:CD1	1:HB:153:LEU:HD22	2.40	0.50
1:KB:231:LEU:HD23	1:KB:231:LEU:C	2.36	0.50
1:KB:235:ARG:HH22	1:T:190:VAL:HG13	1.75	0.50
1:LB:164:ILE:HG21	1:LB:262:MET:HE1	1.93	0.50
1:NB:207:VAL:HG13	1:NB:211:VAL:HG23	1.93	0.50
1:PB:236:PRO:HB3	1:SB:186:LEU:HB3	1.93	0.50
1:TB:223:ARG:HE	1:TB:223:ARG:C	2.20	0.50
2:ab:29:GLN:OE1	2:ab:65:VAL:HG22	2.11	0.50
1:F:169:LEU:HD12	1:F:181:ILE:CD1	2.41	0.50
2:d:16:ILE:HG22	2:d:51:ILE:HD11	1.94	0.50
2:eb:3:ILE:O	2:eb:5:ILE:HD12	2.12	0.50
2:hb:96:PHE:HB3	2:hb:99:VAL:HB	1.93	0.50
2:ib:19:GLU:OE1	2:ib:19:GLU:N	2.44	0.50
1:C:175:ALA:HB2	1:C:210:MET:HE1	1.92	0.50
1:DB:216:ILE:HD11	1:DB:247:ILE:HG21	1.92	0.50
1:FB:231:LEU:HD23	1:FB:252:ILE:HD13	1.94	0.50
1:S:187:ILE:HG23	1:S:191:LYS:HZ2	1.77	0.50
2:d:104:ASP:OD2	2:d:104:ASP:C	2.55	0.50
1:F:196:VAL:CG2	1:F:230:MET:HE2	2.42	0.50
2:fb:70:LYS:HD3	2:fb:70:LYS:C	2.36	0.50
2:h:48:ILE:HD11	2:h:81:ILE:HG13	1.92	0.50
2:j:104:ASP:C	2:j:104:ASP:OD2	2.54	0.50
1:FB:235:ARG:HB2	1:FB:236:PRO:HD2	1.93	0.50
1:GB:175:ALA:HB2	1:GB:210:MET:HE1	1.94	0.50
1:N:162:GLU:HA	1:N:162:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:247:ILE:HG22	1:R:249:LEU:HD22	1.94	0.50
2:h:16:ILE:HG22	2:h:16:ILE:O	2.09	0.50
1:CB:237:GLU:O	1:CB:240:GLN:HG3	2.12	0.50
1:GB:157:LEU:HD11	1:GB:165:SER:CB	2.42	0.50
1:H:230:MET:HE1	1:H:265:ALA:HA	1.93	0.50
2:c:51:ILE:HG21	2:c:54:ILE:CD1	2.42	0.50
2:db:61:ILE:O	2:db:65:VAL:HG23	2.12	0.50
2:hb:7:LYS:HD3	2:hb:7:LYS:C	2.37	0.50
2:ib:78:VAL:HG21	2:ib:96:PHE:CE1	2.46	0.50
1:B:170:ILE:HD12	1:BB:153:LEU:HB3	1.93	0.50
1:B:186:LEU:O	1:B:190:VAL:HG23	2.12	0.50
1:SB:164:ILE:HD11	1:SB:271:ARG:NH2	2.27	0.50
1:T:200:ASP:OD2	1:T:202:THR:HG22	2.12	0.50
1:TB:169:LEU:O	1:TB:204:VAL:HG23	2.12	0.50
2:jb:105:LEU:HD23	2:jb:105:LEU:C	2.36	0.50
1:D:258:MET:HE2	1:DB:160:ILE:HA	1.93	0.50
1:H:186:LEU:HB3	1:O:236:PRO:HB3	1.94	0.50
1:HB:178:ALA:O	1:HB:181:ILE:HG22	2.12	0.50
1:J:230:MET:HE1	1:J:265:ALA:HA	1.93	0.50
1:R:196:VAL:HG11	1:R:265:ALA:HB1	1.92	0.50
1:RB:167:MET:HE2	1:RB:181:ILE:HD11	1.93	0.50
1:T:195:GLU:N	1:T:195:GLU:OE2	2.45	0.50
2:ab:81:ILE:HD12	2:ab:81:ILE:H	1.76	0.50
2:d:78:VAL:HG21	2:d:96:PHE:CE1	2.45	0.50
1:H:152:GLU:HG3	1:H:153:LEU:HD23	1.94	0.49
1:DB:228:GLN:N	1:DB:228:GLN:OE1	2.44	0.49
1:E:160:ILE:HD12	1:E:166:VAL:CG2	2.43	0.49
1:H:231:LEU:CD2	1:H:234:ILE:HD11	2.42	0.49
1:M:247:ILE:HG22	1:M:249:LEU:HD12	1.94	0.49
2:fb:59:ALA:HB1	2:fb:94:ILE:HD12	1.95	0.49
2:h:21:ASP:OD2	2:h:21:ASP:C	2.55	0.49
2:h:100:LEU:HD12	2:h:111:LYS:NZ	2.27	0.49
1:AB:157:LEU:HD11	1:AB:165:SER:HB2	1.94	0.49
1:C:207:VAL:HB	1:C:238:ILE:HG23	1.94	0.49
1:EB:175:ALA:HA	1:EB:210:MET:CE	2.42	0.49
1:EB:196:VAL:HG21	1:EB:265:ALA:HB1	1.93	0.49
1:MB:269:THR:HG21	1:MB:271:ARG:NH2	2.27	0.49
1:OB:220:GLU:OE1	1:OB:220:GLU:HA	2.13	0.49
1:PB:160:ILE:HG22	1:PB:161:PHE:CE2	2.48	0.49
1:QB:259:LYS:O	1:QB:263:GLU:HG2	2.12	0.49
2:ab:109:LEU:C	2:ab:109:LEU:HD23	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:IB:216:ILE:HD11	1:IB:247:ILE:HD13	1.94	0.49
1:K:186:LEU:O	1:K:190:VAL:HG23	2.13	0.49
1:M:167:MET:CE	1:M:169:LEU:HD21	2.43	0.49
1:Q:161:PHE:HB2	1:Q:164:ILE:HD12	1.95	0.49
1:R:248:GLU:OE2	1:R:248:GLU:N	2.45	0.49
1:S:232:VAL:HG12	1:S:255:THR:HG22	1.93	0.49
2:g:25:ALA:HA	2:g:28:PHE:HE1	1.76	0.49
1:B:213:HIS:O	1:B:216:ILE:HG22	2.12	0.49
1:BB:201:ILE:HD11	1:BB:234:ILE:CD1	2.42	0.49
1:EB:228:GLN:OE1	1:EB:228:GLN:N	2.45	0.49
1:F:195:GLU:OE2	1:F:195:GLU:N	2.45	0.49
1:G:175:ALA:HB2	1:G:210:MET:HE1	1.95	0.49
1:GB:199:ILE:HG23	1:GB:199:ILE:O	2.11	0.49
1:RB:196:VAL:HG21	1:RB:230:MET:HE1	1.95	0.49
1:S:187:ILE:HG23	1:S:191:LYS:HZ3	1.76	0.49
1:DB:160:ILE:HD12	1:DB:166:VAL:HG21	1.94	0.49
1:GB:207:VAL:HG13	1:GB:211:VAL:HG23	1.94	0.49
1:HB:254:THR:HG21	2:gb:71:LEU:O	2.13	0.49
1:L:207:VAL:HG13	1:L:211:VAL:HG23	1.95	0.49
1:M:198:LEU:HD22	1:M:262:MET:CE	2.41	0.49
1:SB:160:ILE:HG22	1:SB:161:PHE:HD2	1.77	0.49
2:ab:61:ILE:O	2:ab:65:VAL:HG23	2.12	0.49
2:eb:89:LEU:HD23	2:eb:96:PHE:CE2	2.48	0.49
2:fb:3:ILE:O	2:fb:5:ILE:HD12	2.13	0.49
2:h:89:LEU:HD22	2:h:94:ILE:HG21	1.94	0.49
2:jb:63:GLY:O	2:jb:66:VAL:HG12	2.12	0.49
1:FB:157:LEU:HD11	1:FB:165:SER:HB3	1.94	0.49
1:S:209:THR:HG22	1:S:245:LEU:HD21	1.95	0.49
2:db:63:GLY:O	2:db:66:VAL:HG12	2.12	0.49
1:E:204:VAL:HG11	1:E:207:VAL:CG2	2.43	0.49
1:GB:209:THR:HG23	1:GB:210:MET:N	2.27	0.49
1:R:185:LEU:HD11	1:R:197:VAL:HG21	1.94	0.49
2:e:105:LEU:HD23	2:e:105:LEU:O	2.13	0.49
2:h:81:ILE:HD12	2:h:81:ILE:H	1.76	0.49
1:A:196:VAL:HG11	1:A:265:ALA:HB1	1.95	0.49
1:P:160:ILE:HD13	1:P:166:VAL:HG13	1.94	0.49
1:P:222:VAL:HG22	1:P:227:CYS:HB3	1.94	0.49
1:R:153:LEU:HD13	1:RB:170:ILE:HG22	1.95	0.49
1:D:237:GLU:H	1:D:237:GLU:CD	2.20	0.49
1:MB:157:LEU:HD23	1:MB:192:ASN:OD1	2.13	0.49
1:O:216:ILE:HD11	1:O:249:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DB:269:THR:HG21	1:DB:271:ARG:NH2	2.27	0.48
1:GB:186:LEU:O	1:GB:190:VAL:HG12	2.12	0.48
1:OB:253:ILE:HG21	1:OB:264:ARG:CD	2.43	0.48
1:S:204:VAL:HG11	1:S:207:VAL:HG22	1.94	0.48
1:S:207:VAL:HG13	1:S:211:VAL:HG23	1.94	0.48
2:a:63:GLY:CA	2:a:94:ILE:HD11	2.43	0.48
2:eb:71:LEU:O	2:eb:71:LEU:HD23	2.13	0.48
1:A:213:HIS:O	1:A:216:ILE:HG22	2.12	0.48
1:EB:223:ARG:HD2	1:EB:223:ARG:O	2.12	0.48
1:FB:232:VAL:HG21	1:FB:258:MET:HA	1.95	0.48
1:IB:168:PRO:HB2	1:IB:170:ILE:HD11	1.95	0.48
1:L:230:MET:HE1	1:L:265:ALA:HB2	1.95	0.48
1:N:204:VAL:HG11	1:N:207:VAL:HG22	1.94	0.48
1:O:170:ILE:HD11	1:OB:153:LEU:HD22	1.95	0.48
1:O:212:ALA:O	1:O:216:ILE:HG12	2.12	0.48
1:Q:153:LEU:HD22	1:QB:170:ILE:HG22	1.95	0.48
1:RB:185:LEU:HD11	1:RB:197:VAL:HG21	1.95	0.48
2:f:3:ILE:O	2:f:5:ILE:HD12	2.13	0.48
1:S:259:LYS:HZ1	1:SB:161:PHE:C	2.21	0.48
2:a:81:ILE:HD12	2:a:81:ILE:H	1.78	0.48
2:gb:5:ILE:C	2:gb:6:LEU:HD12	2.38	0.48
1:C:243:VAL:HG21	2:c:68:MET:CG	2.43	0.48
1:C:258:MET:HE1	1:CB:160:ILE:HA	1.96	0.48
1:F:238:ILE:HD12	1:F:238:ILE:H	1.79	0.48
1:GB:235:ARG:HB3	1:GB:236:PRO:HD2	1.94	0.48
1:JB:254:THR:HG21	2:a:71:LEU:O	2.14	0.48
1:L:160:ILE:HA	1:LB:258:MET:HE2	1.94	0.48
1:M:192:ASN:O	1:M:193:ARG:HG2	2.13	0.48
1:OB:254:THR:HG21	2:hb:71:LEU:O	2.12	0.48
1:PB:149:ALA:O	1:PB:153:LEU:HG	2.13	0.48
1:RB:243:VAL:HG21	2:j:68:MET:CG	2.44	0.48
1:RB:254:THR:HG21	2:j:71:LEU:O	2.13	0.48
2:eb:82:GLN:HA	2:eb:82:GLN:OE1	2.13	0.48
2:ib:54:ILE:HG23	2:ib:58:ILE:HB	1.95	0.48
1:BB:174:ASP:CG	1:BB:175:ALA:H	2.20	0.48
1:FB:199:ILE:HG13	1:FB:199:ILE:O	2.12	0.48
1:FB:232:VAL:HG23	1:FB:255:THR:OG1	2.13	0.48
1:I:210:MET:HE2	1:I:210:MET:CA	2.43	0.48
1:LB:222:VAL:HG22	1:LB:227:CYS:HB3	1.94	0.48
1:TB:216:ILE:HD11	1:TB:247:ILE:CG2	2.44	0.48
2:c:8:LEU:HD12	2:c:13:LEU:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:cb:48:ILE:O	2:cb:51:ILE:HG22	2.13	0.48
2:e:105:LEU:HD23	2:e:105:LEU:C	2.39	0.48
2:i:81:ILE:HD12	2:i:81:ILE:H	1.77	0.48
1:F:196:VAL:HG21	1:F:230:MET:HE2	1.96	0.48
1:F:249:LEU:HD13	1:F:252:ILE:HD11	1.95	0.48
1:H:160:ILE:HA	1:HB:258:MET:HE2	1.95	0.48
1:L:167:MET:HE2	1:L:181:ILE:HG23	1.94	0.48
1:RB:196:VAL:CG2	1:RB:230:MET:HE1	2.43	0.48
2:e:33:LEU:HD11	2:e:68:MET:CE	2.43	0.48
1:DB:241:THR:O	1:DB:245:LEU:HD23	2.14	0.48
1:EB:157:LEU:HD11	1:EB:165:SER:CB	2.43	0.48
1:Q:198:LEU:N	1:Q:198:LEU:HD12	2.29	0.48
2:g:11:CYS:O	2:g:12:LEU:HD12	2.14	0.48
2:jb:33:LEU:HD11	2:jb:68:MET:CE	2.43	0.48
1:AB:243:VAL:HG23	1:CB:224:LEU:HD12	1.95	0.48
1:BB:222:VAL:HG22	1:BB:227:CYS:HB3	1.96	0.48
1:C:175:ALA:CB	1:C:210:MET:HE1	2.44	0.48
1:E:153:LEU:HD13	1:EB:170:ILE:HG22	1.95	0.48
1:FB:179:LYS:C	1:FB:179:LYS:HD2	2.38	0.48
1:MB:178:ALA:O	1:MB:181:ILE:HG22	2.13	0.48
1:R:240:GLN:CA	2:fb:68:MET:HE3	2.44	0.48
1:R:269:THR:O	1:R:270:ASN:OD1	2.32	0.48
1:RB:232:VAL:HG23	1:RB:255:THR:OG1	2.14	0.48
2:b:12:LEU:C	2:b:13:LEU:HD12	2.38	0.48
1:J:164:ILE:HG21	1:J:262:MET:HE1	1.96	0.48
1:S:205:PRO:HA	1:S:235:ARG:HH12	1.78	0.48
2:ab:104:ASP:OD2	2:ab:104:ASP:C	2.57	0.48
2:cb:81:ILE:HD12	2:cb:81:ILE:H	1.79	0.48
2:cb:96:PHE:HB3	2:cb:99:VAL:HB	1.96	0.48
2:eb:77:VAL:HG12	2:eb:100:LEU:HB2	1.96	0.48
2:hb:34:ALA:O	2:hb:37:HIS:HB3	2.14	0.48
1:CB:232:VAL:HG21	1:CB:258:MET:HA	1.96	0.48
1:GB:175:ALA:CB	1:GB:210:MET:HE1	2.44	0.48
1:J:170:ILE:HG12	1:JB:153:LEU:HD22	1.96	0.48
1:O:240:GLN:HA	1:O:243:VAL:HG12	1.95	0.48
1:PB:262:MET:HE2	1:PB:262:MET:HA	1.96	0.48
2:c:33:LEU:O	2:c:36:ILE:HG22	2.14	0.48
1:J:182:ILE:O	1:J:186:LEU:HD23	2.14	0.47
1:KB:186:LEU:HD21	1:KB:221:ALA:HB1	1.96	0.47
1:KB:255:THR:HG22	1:KB:264:ARG:NH2	2.28	0.47
1:R:222:VAL:HG22	1:R:227:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:269:THR:C	1:T:270:ASN:OD1	2.57	0.47
2:db:55:ASP:OD2	2:db:55:ASP:C	2.57	0.47
2:hb:20:LEU:HD13	2:hb:28:PHE:HE1	1.79	0.47
2:hb:102:ALA:C	2:hb:103:MET:HE2	2.39	0.47
2:j:105:LEU:HD23	2:j:105:LEU:O	2.14	0.47
1:C:230:MET:CE	1:C:265:ALA:HB2	2.44	0.47
1:F:269:THR:O	1:F:270:ASN:OD1	2.32	0.47
1:FB:210:MET:CG	1:FB:214:HIS:CE1	2.96	0.47
1:GB:210:MET:HE2	1:GB:214:HIS:NE2	2.28	0.47
1:J:160:ILE:HA	1:JB:258:MET:HE1	1.95	0.47
1:NB:241:THR:O	1:NB:245:LEU:HD23	2.14	0.47
1:OB:207:VAL:HG13	1:OB:211:VAL:HG23	1.95	0.47
2:bb:96:PHE:HB3	2:bb:99:VAL:HB	1.96	0.47
2:ib:110:GLU:HA	2:ib:113:LYS:HE3	1.96	0.47
1:LB:201:ILE:O	1:LB:204:VAL:HG12	2.15	0.47
2:c:71:LEU:HD23	2:c:71:LEU:C	2.39	0.47
2:i:6:LEU:HD22	2:ib:105:LEU:HD13	1.96	0.47
1:H:269:THR:O	1:H:269:THR:CG2	2.63	0.47
1:M:258:MET:SD	1:M:258:MET:C	2.98	0.47
2:ab:32:LEU:HD23	2:ab:65:VAL:HG13	1.96	0.47
2:db:64:ASP:O	2:db:68:MET:HG3	2.15	0.47
2:f:54:ILE:HG22	2:f:55:ASP:O	2.14	0.47
2:g:78:VAL:HG21	2:g:96:PHE:CE1	2.49	0.47
2:jb:105:LEU:HD23	2:jb:105:LEU:O	2.15	0.47
1:AB:262:MET:HE2	1:AB:262:MET:HA	1.96	0.47
1:E:240:GLN:HA	1:E:243:VAL:HG12	1.96	0.47
1:E:262:MET:O	1:E:266:LEU:HD23	2.14	0.47
1:JB:232:VAL:HG11	1:JB:258:MET:HA	1.95	0.47
1:LB:185:LEU:HD11	1:LB:197:VAL:HG21	1.96	0.47
1:N:185:LEU:HD11	1:N:197:VAL:HG21	1.96	0.47
1:NB:228:GLN:N	1:NB:228:GLN:OE1	2.47	0.47
1:T:170:ILE:HG22	1:TB:153:LEU:HD22	1.92	0.47
2:b:61:ILE:O	2:b:65:VAL:HG23	2.13	0.47
2:d:12:LEU:HD13	2:d:41:ALA:CB	2.44	0.47
2:f:89:LEU:HD22	2:f:96:PHE:HE2	1.78	0.47
1:CB:163:LYS:HE3	1:CB:163:LYS:HA	1.96	0.47
1:E:248:GLU:N	1:E:248:GLU:OE1	2.47	0.47
1:MB:175:ALA:HA	1:MB:210:MET:CE	2.44	0.47
1:PB:210:MET:HE2	1:PB:210:MET:CA	2.45	0.47
2:a:20:LEU:O	2:a:58:ILE:HD11	2.15	0.47
2:ib:81:ILE:H	2:ib:81:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:HB3	2:cb:90:ILE:HD12	1.95	0.47
1:B:185:LEU:HD11	1:B:197:VAL:HG21	1.96	0.47
1:D:160:ILE:HA	1:DB:258:MET:HE1	1.97	0.47
1:K:153:LEU:HD22	1:KB:170:ILE:HG22	1.94	0.47
1:K:160:ILE:HD12	1:K:166:VAL:CG1	2.45	0.47
1:LB:199:ILE:O	1:LB:231:LEU:HD12	2.15	0.47
1:NB:210:MET:HE2	1:NB:210:MET:CA	2.45	0.47
1:Q:210:MET:HE2	1:Q:214:HIS:CE1	2.50	0.47
1:Q:258:MET:SD	1:Q:258:MET:C	2.97	0.47
2:ab:1:MET:HA	2:ab:1:MET:HE2	1.96	0.47
2:eb:42:ARG:CZ	2:eb:116:LEU:HD12	2.45	0.47
2:g:112:LEU:O	2:g:116:LEU:HD23	2.15	0.47
2:hb:32:LEU:O	2:hb:36:ILE:HG22	2.15	0.47
2:j:6:LEU:HD23	2:jb:105:LEU:CD1	2.45	0.47
2:j:96:PHE:HB3	2:j:99:VAL:HB	1.97	0.47
1:C:248:GLU:OE2	1:C:248:GLU:N	2.47	0.47
1:H:232:VAL:HG12	1:H:255:THR:OG1	2.15	0.47
1:NB:157:LEU:HD11	1:NB:165:SER:CB	2.45	0.47
2:b:6:LEU:HD12	2:b:6:LEU:N	2.29	0.47
2:gb:6:LEU:HD12	2:gb:6:LEU:N	2.30	0.47
2:i:16:ILE:HG22	2:i:51:ILE:HD11	1.97	0.47
1:H:258:MET:C	1:H:258:MET:SD	2.97	0.47
1:NB:232:VAL:HG21	1:NB:258:MET:HA	1.97	0.47
1:OB:225:VAL:HG12	2:g:103:MET:SD	2.54	0.47
1:RB:178:ALA:O	1:RB:181:ILE:HG22	2.14	0.47
2:a:78:VAL:HG21	2:a:96:PHE:CE1	2.50	0.47
2:d:43:GLY:HA3	2:d:112:LEU:HD21	1.97	0.47
1:KB:234:ILE:HD11	1:KB:238:ILE:HG22	1.96	0.47
1:RB:207:VAL:HB	1:RB:238:ILE:HG23	1.96	0.47
2:db:72:MET:SD	2:db:72:MET:O	2.73	0.47
2:g:16:ILE:HG22	2:g:51:ILE:HD11	1.96	0.47
2:i:3:ILE:O	2:i:5:ILE:HD12	2.14	0.47
1:D:153:LEU:HD22	1:DB:170:ILE:CG2	2.45	0.46
1:D:160:ILE:HD12	1:D:166:VAL:CG2	2.45	0.46
1:OB:260:LYS:HE2	1:OB:260:LYS:HA	1.96	0.46
2:c:8:LEU:HD21	2:cb:105:LEU:HD22	1.97	0.46
2:c:12:LEU:HD13	2:c:41:ALA:CB	2.45	0.46
2:h:66:VAL:HG23	2:h:76:VAL:HG11	1.97	0.46
1:CB:185:LEU:HD11	1:CB:197:VAL:HG11	1.98	0.46
1:DB:222:VAL:HG22	1:DB:227:CYS:HB3	1.97	0.46
1:G:258:MET:HE1	1:GB:160:ILE:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:249:LEU:CD2	1:T:252:ILE:HD11	2.41	0.46
2:c:78:VAL:HG21	2:c:96:PHE:HE1	1.79	0.46
2:cb:58:ILE:O	2:cb:62:LEU:HD23	2.14	0.46
1:C:186:LEU:HB3	1:K:236:PRO:HB3	1.96	0.46
1:HB:217:GLN:OE1	1:HB:217:GLN:C	2.59	0.46
1:I:213:HIS:O	1:I:217:GLN:OE1	2.33	0.46
1:M:162:GLU:N	1:M:162:GLU:OE1	2.49	0.46
1:O:153:LEU:HD13	1:OB:170:ILE:HG22	1.96	0.46
1:O:167:MET:SD	1:O:185:LEU:HD13	2.55	0.46
1:OB:157:LEU:HD13	1:OB:167:MET:HE2	1.96	0.46
1:S:249:LEU:CD2	1:S:252:ILE:HD11	2.38	0.46
1:DB:220:GLU:OE1	1:DB:220:GLU:HA	2.16	0.46
1:EB:230:MET:HE1	1:EB:261:GLY:O	2.15	0.46
1:J:269:THR:O	1:J:270:ASN:OD1	2.33	0.46
1:MB:231:LEU:HD23	1:MB:234:ILE:HD11	1.96	0.46
1:OB:168:PRO:O	1:OB:169:LEU:HD12	2.15	0.46
1:OB:175:ALA:HB2	1:OB:210:MET:CE	2.39	0.46
1:Q:204:VAL:HG11	1:Q:207:VAL:CG2	2.45	0.46
2:c:6:LEU:HD23	2:cb:105:LEU:CD1	2.44	0.46
2:f:70:LYS:HD3	2:f:70:LYS:C	2.40	0.46
2:fb:112:LEU:O	2:fb:116:LEU:HD23	2.15	0.46
1:B:248:GLU:N	1:B:248:GLU:OE2	2.49	0.46
1:D:160:ILE:HD12	1:D:166:VAL:HG21	1.98	0.46
1:E:170:ILE:HG22	1:EB:153:LEU:HD22	1.95	0.46
1:EB:264:ARG:O	1:EB:268:LEU:HD23	2.16	0.46
1:FB:178:ALA:O	1:FB:181:ILE:HG22	2.16	0.46
1:I:198:LEU:HD12	1:I:198:LEU:N	2.31	0.46
1:KB:160:ILE:HG22	1:KB:161:PHE:CD1	2.51	0.46
1:M:155:ALA:HB1	1:M:167:MET:HE3	1.97	0.46
1:N:186:LEU:HD21	1:N:221:ALA:HB1	1.98	0.46
1:O:256:ASN:OD1	1:O:256:ASN:C	2.59	0.46
1:T:204:VAL:HG11	1:T:207:VAL:CG2	2.45	0.46
2:c:29:GLN:HE22	2:c:65:VAL:HG22	1.80	0.46
1:A:209:THR:HG23	1:A:210:MET:N	2.31	0.46
1:LB:157:LEU:HD11	1:LB:165:SER:CB	2.45	0.46
1:M:223:ARG:HA	1:M:227:CYS:O	2.15	0.46
1:P:230:MET:HE1	1:P:265:ALA:HA	1.97	0.46
2:g:77:VAL:HG12	2:g:100:LEU:HB2	1.97	0.46
2:i:96:PHE:HB3	2:i:99:VAL:HB	1.97	0.46
1:AB:268:LEU:C	1:AB:268:LEU:HD23	2.40	0.46
1:HB:237:GLU:CD	1:HB:237:GLU:H	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:196:VAL:HG23	1:J:228:GLN:O	2.15	0.46
1:M:198:LEU:HD13	1:M:262:MET:HE1	1.98	0.46
1:O:153:LEU:HD22	1:OB:170:ILE:HG21	1.93	0.46
2:c:56:SER:HA	2:c:92:LEU:HD22	1.97	0.46
2:db:100:LEU:N	2:db:100:LEU:HD12	2.31	0.46
1:AB:186:LEU:O	1:AB:190:VAL:HG23	2.15	0.46
1:KB:196:VAL:HG11	1:KB:265:ALA:HB1	1.97	0.46
1:OB:262:MET:O	1:OB:266:LEU:HD23	2.16	0.46
2:e:29:GLN:HG3	2:e:65:VAL:HG22	1.98	0.46
2:i:29:GLN:HG3	2:i:65:VAL:HG22	1.97	0.46
2:i:64:ASP:HB3	2:i:68:MET:HE3	1.98	0.46
2:ib:62:LEU:O	2:ib:65:VAL:HG12	2.16	0.46
1:A:153:LEU:HD13	1:AB:170:ILE:HG22	1.98	0.46
1:C:262:MET:HA	1:C:262:MET:HE2	1.98	0.46
1:CB:254:THR:HG21	2:ab:71:LEU:O	2.16	0.46
1:GB:269:THR:O	1:GB:269:THR:CG2	2.63	0.46
1:JB:201:ILE:O	1:JB:204:VAL:HG12	2.16	0.46
1:KB:198:LEU:N	1:KB:198:LEU:HD12	2.31	0.46
1:LB:258:MET:SD	1:LB:258:MET:C	2.99	0.46
1:OB:258:MET:SD	1:OB:258:MET:C	2.99	0.46
1:R:147:LYS:O	1:R:151:GLN:OE1	2.34	0.46
1:TB:167:MET:C	1:TB:167:MET:SD	2.99	0.46
2:db:38:GLU:OE2	2:db:38:GLU:C	2.58	0.46
2:f:96:PHE:HB3	2:f:99:VAL:HB	1.98	0.46
2:ib:77:VAL:CG1	2:ib:112:LEU:HD21	2.41	0.46
1:IB:256:ASN:OD1	1:IB:256:ASN:C	2.58	0.46
2:a:96:PHE:HB3	2:a:99:VAL:HB	1.98	0.46
2:c:78:VAL:HG21	2:c:96:PHE:CE1	2.51	0.46
1:C:153:LEU:HD22	1:CB:170:ILE:CG2	2.46	0.45
1:GB:191:LYS:HD3	1:GB:191:LYS:N	2.31	0.45
1:HB:204:VAL:HG13	1:HB:204:VAL:O	2.17	0.45
1:HB:207:VAL:HG13	1:HB:211:VAL:HG23	1.98	0.45
1:HB:236:PRO:HG3	2:gb:37:HIS:HB2	1.97	0.45
1:N:153:LEU:HD22	1:NB:170:ILE:HG22	1.97	0.45
1:R:204:VAL:HG11	1:R:207:VAL:HG22	1.98	0.45
1:R:242:ILE:HG23	1:R:247:ILE:HD12	1.97	0.45
1:TB:241:THR:O	1:TB:245:LEU:HD23	2.16	0.45
2:db:6:LEU:HD23	2:db:7:LYS:N	2.31	0.45
1:CB:187:ILE:O	1:CB:191:LYS:HG2	2.16	0.45
1:CB:204:VAL:HG11	1:CB:207:VAL:CG2	2.46	0.45
1:CB:240:GLN:CB	2:ab:68:MET:HE3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:207:VAL:HG13	1:EB:211:VAL:HG23	1.98	0.45
1:FB:222:VAL:HG22	1:FB:227:CYS:HB3	1.98	0.45
1:HB:198:LEU:HD12	1:HB:198:LEU:N	2.31	0.45
1:IB:249:LEU:HD22	2:h:71:LEU:HD13	1.97	0.45
1:J:157:LEU:HD21	1:J:165:SER:HB3	1.98	0.45
1:O:228:GLN:OE1	1:O:228:GLN:N	2.49	0.45
1:PB:169:LEU:C	1:PB:169:LEU:HD23	2.42	0.45
1:SB:262:MET:HA	1:SB:262:MET:HE2	1.97	0.45
1:T:201:ILE:HD11	1:T:234:ILE:HG13	1.98	0.45
2:ib:104:ASP:OD1	2:ib:104:ASP:C	2.59	0.45
1:BB:167:MET:O	1:BB:167:MET:CE	2.64	0.45
1:CB:258:MET:O	1:CB:258:MET:SD	2.74	0.45
1:DB:148:SER:O	1:DB:152:GLU:HG2	2.15	0.45
1:E:152:GLU:HG3	1:E:153:LEU:HG	1.99	0.45
1:FB:175:ALA:HB2	1:FB:210:MET:SD	2.57	0.45
1:IB:149:ALA:O	1:IB:153:LEU:HG	2.17	0.45
1:IB:249:LEU:HD22	2:h:71:LEU:CD1	2.46	0.45
1:L:262:MET:O	1:L:266:LEU:HD23	2.15	0.45
1:NB:239:ALA:HB1	1:TB:224:LEU:HD12	1.97	0.45
1:P:238:ILE:O	1:P:242:ILE:HG12	2.16	0.45
1:QB:188:GLY:O	1:QB:192:ASN:ND2	2.43	0.45
1:SB:175:ALA:HB2	1:SB:210:MET:SD	2.56	0.45
2:c:23:HIS:O	2:c:27:GLU:OE1	2.34	0.45
2:gb:33:LEU:O	2:gb:36:ILE:HG22	2.16	0.45
2:hb:66:VAL:HG23	2:hb:76:VAL:CG1	2.46	0.45
1:A:169:LEU:C	1:A:169:LEU:HD23	2.41	0.45
1:AB:157:LEU:HD11	1:AB:165:SER:CB	2.47	0.45
1:DB:160:ILE:HG22	1:DB:161:PHE:CD2	2.51	0.45
1:F:178:ALA:O	1:F:181:ILE:HG22	2.16	0.45
1:F:204:VAL:HG11	1:F:207:VAL:CG2	2.46	0.45
1:G:237:GLU:CD	1:G:237:GLU:H	2.25	0.45
1:GB:157:LEU:HD11	1:GB:165:SER:HB2	1.97	0.45
1:O:258:MET:HE1	1:OB:160:ILE:HD13	1.98	0.45
1:PB:219:SER:O	1:PB:222:VAL:HG12	2.17	0.45
1:QB:232:VAL:HG22	1:QB:233:GLY:N	2.31	0.45
1:RB:207:VAL:HG13	1:RB:211:VAL:HG23	1.98	0.45
2:d:105:LEU:H	2:d:105:LEU:HD12	1.81	0.45
2:h:96:PHE:HB3	2:h:99:VAL:HB	1.98	0.45
1:A:204:VAL:O	1:A:204:VAL:HG13	2.17	0.45
1:GB:157:LEU:HD22	1:GB:188:GLY:HA3	1.98	0.45
1:LB:149:ALA:O	1:LB:153:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:157:LEU:HD11	1:N:165:SER:CB	2.47	0.45
1:NB:216:ILE:HD11	1:NB:247:ILE:CG2	2.47	0.45
1:NB:243:VAL:HG11	1:TB:220:GLU:CG	2.46	0.45
2:eb:6:LEU:O	2:eb:12:LEU:HD13	2.17	0.45
2:eb:78:VAL:HG21	2:eb:96:PHE:HE1	1.81	0.45
2:g:32:LEU:HD11	2:g:36:ILE:HD11	1.99	0.45
2:gb:29:GLN:HG3	2:gb:65:VAL:HG22	1.97	0.45
2:hb:3:ILE:O	2:hb:5:ILE:HD12	2.16	0.45
1:AB:235:ARG:HH22	1:CB:190:VAL:HG21	1.82	0.45
1:F:196:VAL:HG11	1:F:265:ALA:HB1	1.99	0.45
1:GB:263:GLU:OE1	1:GB:263:GLU:HA	2.17	0.45
1:T:153:LEU:HD13	1:TB:170:ILE:HG22	1.98	0.45
1:TB:216:ILE:HD11	1:TB:247:ILE:HG23	1.99	0.45
2:bb:6:LEU:HD12	2:bb:6:LEU:N	2.32	0.45
2:c:29:GLN:NE2	2:c:65:VAL:HG22	2.31	0.45
2:eb:100:LEU:HD12	2:eb:100:LEU:H	1.82	0.45
2:f:33:LEU:O	2:f:36:ILE:HG22	2.16	0.45
2:h:14:ILE:HG22	2:h:15:SER:N	2.31	0.45
1:H:237:GLU:O	1:H:240:GLN:HG3	2.17	0.45
1:H:258:MET:SD	1:H:258:MET:O	2.74	0.45
1:HB:201:ILE:O	1:HB:204:VAL:HG12	2.17	0.45
1:O:217:GLN:C	1:O:217:GLN:OE1	2.59	0.45
2:cb:23:HIS:O	2:cb:27:GLU:OE1	2.34	0.45
2:db:47:ASP:C	2:db:47:ASP:OD1	2.60	0.45
2:gb:100:LEU:HD12	2:gb:100:LEU:H	1.80	0.45
2:i:77:VAL:HG12	2:i:100:LEU:HB2	1.98	0.45
1:B:153:LEU:HD22	1:BB:170:ILE:HG22	1.93	0.45
1:D:170:ILE:HG22	1:DB:153:LEU:HD22	1.96	0.45
1:E:264:ARG:O	1:E:268:LEU:HD23	2.17	0.45
1:KB:200:ASP:OD2	1:KB:202:THR:HG22	2.16	0.45
1:Q:160:ILE:HD11	1:Q:166:VAL:HB	1.98	0.45
1:BB:190:VAL:CG2	1:SB:236:PRO:HG3	2.46	0.45
1:GB:149:ALA:O	1:GB:153:LEU:HG	2.17	0.45
1:H:185:LEU:HD11	1:H:197:VAL:HG21	1.99	0.45
1:JB:262:MET:HE2	1:JB:262:MET:HA	1.99	0.45
1:L:231:LEU:HD23	1:L:231:LEU:C	2.42	0.45
1:C:240:GLN:HA	2:c:68:MET:SD	2.56	0.45
1:FB:210:MET:HG2	1:FB:214:HIS:HE1	1.79	0.45
1:J:153:LEU:HD22	1:JB:170:ILE:HG22	1.98	0.45
1:K:231:LEU:HG	1:K:234:ILE:HD11	1.97	0.45
1:OB:149:ALA:O	1:OB:153:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:236:PRO:HB3	2:eb:33:LEU:HB3	1.98	0.45
1:TB:256:ASN:OD1	1:TB:256:ASN:C	2.60	0.45
2:e:17:GLN:OE1	2:e:17:GLN:N	2.50	0.45
1:A:186:LEU:O	1:A:190:VAL:HG23	2.17	0.44
1:G:170:ILE:HG21	1:GB:153:LEU:HD22	1.96	0.44
1:H:240:GLN:HA	1:H:243:VAL:HG12	1.99	0.44
1:JB:185:LEU:HD11	1:JB:197:VAL:HG21	1.99	0.44
1:K:258:MET:SD	1:K:258:MET:C	3.00	0.44
1:L:156:PRO:HB2	1:L:158:LEU:HD21	1.98	0.44
1:LB:160:ILE:HD12	1:LB:166:VAL:CG2	2.46	0.44
1:M:188:GLY:O	1:M:192:ASN:ND2	2.50	0.44
1:MB:230:MET:HE1	1:MB:264:ARG:HB3	1.98	0.44
1:NB:210:MET:HE2	1:NB:210:MET:HA	1.98	0.44
1:O:170:ILE:CD1	1:OB:153:LEU:HD22	2.46	0.44
2:bb:12:LEU:HD13	2:bb:41:ALA:CB	2.48	0.44
2:db:66:VAL:HG23	2:db:76:VAL:HG11	1.97	0.44
2:hb:33:LEU:HD21	2:hb:68:MET:HG2	1.98	0.44
1:A:238:ILE:HD12	1:A:238:ILE:H	1.82	0.44
1:E:269:THR:HG21	1:E:271:ARG:NH2	2.32	0.44
1:H:210:MET:O	1:H:214:HIS:CD2	2.70	0.44
1:JB:161:PHE:HB2	1:JB:164:ILE:HD12	2.00	0.44
1:P:166:VAL:HG12	1:P:198:LEU:HB2	1.98	0.44
1:Q:204:VAL:HG11	1:Q:207:VAL:HG23	1.98	0.44
2:eb:71:LEU:HD23	2:eb:71:LEU:C	2.41	0.44
2:fb:55:ASP:OD1	2:fb:55:ASP:C	2.60	0.44
1:AB:235:ARG:HB2	1:AB:238:ILE:HD12	1.98	0.44
1:EB:263:GLU:OE1	1:EB:263:GLU:HA	2.18	0.44
1:G:231:LEU:HD23	1:G:231:LEU:C	2.42	0.44
1:KB:241:THR:O	1:KB:245:LEU:HD23	2.18	0.44
1:L:259:LYS:NZ	1:LB:161:PHE:HA	2.32	0.44
1:PB:236:PRO:HG3	1:SB:190:VAL:HG21	1.98	0.44
1:RB:162:GLU:O	1:RB:163:LYS:HB2	2.17	0.44
2:c:96:PHE:HB3	2:c:99:VAL:HB	1.98	0.44
2:eb:96:PHE:HD1	2:eb:99:VAL:HG11	1.82	0.44
2:f:71:LEU:HD23	2:f:71:LEU:O	2.17	0.44
2:jb:104:ASP:C	2:jb:104:ASP:OD1	2.60	0.44
1:I:201:ILE:O	1:I:204:VAL:HG12	2.17	0.44
1:J:256:ASN:OD1	1:J:257:THR:HG23	2.18	0.44
1:JB:216:ILE:HG22	1:JB:220:GLU:OE1	2.17	0.44
1:L:235:ARG:HB3	1:L:236:PRO:HD2	1.98	0.44
1:N:157:LEU:HD11	1:N:165:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:153:LEU:HD13	1:PB:170:ILE:HG22	1.99	0.44
2:fb:5:ILE:HG21	2:fb:35:LYS:HD2	2.00	0.44
2:fb:71:LEU:HD23	2:fb:71:LEU:C	2.43	0.44
1:E:269:THR:O	1:E:269:THR:CG2	2.66	0.44
1:G:161:PHE:CD1	1:G:162:GLU:N	2.85	0.44
1:M:170:ILE:CG1	1:MB:153:LEU:HD22	2.46	0.44
1:MB:243:VAL:HG11	2:f:68:MET:CG	2.47	0.44
1:Q:209:THR:HG23	1:Q:210:MET:N	2.33	0.44
1:Q:235:ARG:HG2	1:Q:238:ILE:HD12	1.98	0.44
1:R:210:MET:HE2	1:R:210:MET:CA	2.46	0.44
1:S:240:GLN:HA	2:jb:68:MET:HE3	2.00	0.44
2:ab:71:LEU:HD23	2:ab:71:LEU:C	2.43	0.44
2:c:8:LEU:HD21	2:cb:105:LEU:HD23	2.00	0.44
2:db:103:MET:HE2	2:db:103:MET:HA	2.00	0.44
2:j:105:LEU:HD23	2:j:105:LEU:C	2.41	0.44
1:B:223:ARG:HD2	1:B:223:ARG:O	2.17	0.44
1:BB:220:GLU:HA	1:BB:220:GLU:OE1	2.18	0.44
1:IB:182:ILE:HG12	1:IB:218:ALA:HB2	2.00	0.44
1:LB:230:MET:HE1	1:LB:265:ALA:HB2	2.00	0.44
1:O:235:ARG:HG2	1:O:236:PRO:HD2	2.00	0.44
1:O:258:MET:HE1	1:OB:160:ILE:HA	1.99	0.44
1:P:262:MET:O	1:P:266:LEU:HD23	2.16	0.44
2:g:5:ILE:C	2:g:6:LEU:HD12	2.43	0.44
2:hb:59:ALA:HB1	2:hb:94:ILE:HD12	1.99	0.44
1:EB:157:LEU:HD11	1:EB:165:SER:HB3	1.99	0.44
1:K:262:MET:O	1:K:266:LEU:HD23	2.17	0.44
1:LB:187:ILE:O	1:LB:190:VAL:HG12	2.17	0.44
1:MB:160:ILE:HG22	1:MB:161:PHE:HD2	1.82	0.44
1:R:152:GLU:OE1	1:R:153:LEU:HD23	2.18	0.44
2:ab:96:PHE:HB3	2:ab:99:VAL:HB	1.99	0.44
2:db:22:ASP:OD1	2:db:23:HIS:N	2.51	0.44
2:fb:25:ALA:HA	2:fb:28:PHE:CD1	2.53	0.44
2:g:29:GLN:C	2:g:29:GLN:OE1	2.60	0.44
1:B:236:PRO:HB3	2:b:33:LEU:HB3	2.00	0.44
1:EB:217:GLN:OE1	2:fb:90:ILE:HG21	2.17	0.44
1:M:204:VAL:HG21	1:M:207:VAL:HG22	2.00	0.44
2:b:29:GLN:NE2	2:b:65:VAL:HG22	2.31	0.44
2:bb:58:ILE:H	2:bb:58:ILE:HD12	1.82	0.44
2:d:26:VAL:O	2:d:30:GLU:OE1	2.35	0.44
2:g:8:LEU:HD11	2:gb:109:LEU:HD23	1.99	0.44
1:A:259:LYS:HZ2	1:AB:161:PHE:C	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PHE:HB2	1:C:164:ILE:HD12	2.00	0.44
1:CB:240:GLN:CA	2:ab:68:MET:HE3	2.45	0.44
1:DB:198:LEU:N	1:DB:198:LEU:HD12	2.33	0.44
1:P:237:GLU:O	1:P:240:GLN:HG3	2.17	0.44
1:T:160:ILE:HD12	1:T:166:VAL:HG21	1.99	0.44
2:a:5:ILE:HD13	2:a:14:ILE:HD11	2.00	0.44
2:cb:29:GLN:OE1	2:cb:33:LEU:HD11	2.18	0.44
2:db:36:ILE:HD11	2:db:44:VAL:CG2	2.47	0.44
2:db:36:ILE:HD11	2:db:44:VAL:HG22	1.99	0.44
1:E:160:ILE:HD12	1:E:166:VAL:HG21	2.00	0.43
1:JB:205:PRO:HA	1:JB:235:ARG:HH12	1.83	0.43
1:M:241:THR:O	1:M:245:LEU:HD23	2.18	0.43
1:MB:238:ILE:O	1:MB:242:ILE:HG12	2.17	0.43
1:OB:259:LYS:HE2	1:OB:259:LYS:HA	1.99	0.43
1:QB:162:GLU:OE1	1:QB:162:GLU:HA	2.19	0.43
1:T:169:LEU:C	1:T:169:LEU:HD23	2.43	0.43
2:bb:29:GLN:OE1	2:bb:65:VAL:HG22	2.18	0.43
2:bb:63:GLY:O	2:bb:66:VAL:HG12	2.18	0.43
2:ib:77:VAL:HG12	2:ib:100:LEU:HB2	1.99	0.43
1:AB:249:LEU:HD12	1:CB:224:LEU:CD2	2.44	0.43
1:E:199:ILE:HG13	1:E:199:ILE:O	2.17	0.43
1:KB:168:PRO:O	1:KB:169:LEU:HD12	2.18	0.43
1:M:201:ILE:O	1:M:204:VAL:HG12	2.18	0.43
1:O:170:ILE:CG1	1:OB:153:LEU:HD22	2.47	0.43
1:Q:241:THR:O	1:Q:245:LEU:HD23	2.19	0.43
1:R:259:LYS:HZ3	1:RB:161:PHE:HA	1.83	0.43
2:cb:29:GLN:NE2	2:cb:65:VAL:HG22	2.33	0.43
2:d:21:ASP:OD1	2:d:21:ASP:C	2.61	0.43
2:eb:109:LEU:HD23	2:eb:109:LEU:C	2.43	0.43
2:g:96:PHE:HB3	2:g:99:VAL:HB	2.00	0.43
2:h:12:LEU:O	2:h:13:LEU:HD23	2.18	0.43
1:A:157:LEU:HD13	1:A:167:MET:HB2	2.01	0.43
1:AB:149:ALA:O	1:AB:153:LEU:HG	2.18	0.43
1:D:238:ILE:O	1:D:242:ILE:HG12	2.18	0.43
1:EB:164:ILE:HG21	1:EB:262:MET:HE1	2.00	0.43
1:EB:178:ALA:O	1:EB:181:ILE:HG22	2.18	0.43
1:F:230:MET:CE	1:F:265:ALA:HB2	2.46	0.43
1:HB:219:SER:O	1:HB:222:VAL:HG22	2.18	0.43
1:JB:155:ALA:HB2	1:JB:181:ILE:HD13	2.00	0.43
1:N:241:THR:O	1:N:245:LEU:HD23	2.18	0.43
1:NB:149:ALA:O	1:NB:153:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:SB:202:THR:HG23	1:SB:233:GLY:HA3	2.00	0.43
2:cb:54:ILE:HG13	2:cb:58:ILE:HB	2.00	0.43
2:db:77:VAL:HG22	2:db:100:LEU:HB2	2.01	0.43
2:eb:57:PHE:CE2	2:eb:61:ILE:HD11	2.53	0.43
2:f:66:VAL:HG23	2:f:76:VAL:HB	2.00	0.43
2:ib:5:ILE:HD12	2:ib:14:ILE:HD11	1.98	0.43
1:C:219:SER:O	1:C:222:VAL:HG22	2.18	0.43
1:D:164:ILE:HG21	1:D:262:MET:HE1	1.99	0.43
1:E:236:PRO:HB3	1:M:186:LEU:HB3	2.01	0.43
1:OB:253:ILE:HG21	1:OB:264:ARG:HD2	1.99	0.43
1:PB:198:LEU:N	1:PB:198:LEU:HD12	2.33	0.43
1:R:240:GLN:HA	2:fb:68:MET:HE3	2.00	0.43
1:S:262:MET:HE2	1:S:262:MET:HA	2.01	0.43
2:d:81:ILE:HD12	2:d:81:ILE:H	1.84	0.43
2:eb:89:LEU:HD23	2:eb:96:PHE:HE2	1.83	0.43
1:BB:236:PRO:HB3	1:Q:186:LEU:HB3	2.01	0.43
1:CB:149:ALA:O	1:CB:153:LEU:HG	2.18	0.43
1:H:167:MET:SD	1:H:185:LEU:HD13	2.58	0.43
1:L:170:ILE:HG21	1:LB:153:LEU:HD22	1.98	0.43
1:M:167:MET:HE1	1:M:181:ILE:HG23	2.01	0.43
1:MB:198:LEU:HD23	1:MB:230:MET:HB2	2.00	0.43
1:N:256:ASN:OD1	1:N:256:ASN:C	2.62	0.43
1:Q:256:ASN:OD1	1:Q:256:ASN:C	2.61	0.43
1:SB:186:LEU:O	1:SB:189:VAL:HG12	2.18	0.43
1:T:269:THR:HG22	1:T:269:THR:O	2.17	0.43
2:a:12:LEU:HD13	2:a:41:ALA:CB	2.48	0.43
2:ab:77:VAL:CG1	2:ab:112:LEU:HD21	2.41	0.43
2:f:96:PHE:HD1	2:f:99:VAL:HG11	1.82	0.43
2:fb:106:GLU:C	2:fb:106:GLU:OE1	2.61	0.43
2:gb:66:VAL:HG23	2:gb:76:VAL:HG11	1.98	0.43
2:gb:78:VAL:HG21	2:gb:96:PHE:CE1	2.52	0.43
1:BB:257:THR:HG22	1:BB:260:LYS:HD3	1.99	0.43
1:G:204:VAL:HG13	1:G:204:VAL:O	2.18	0.43
1:IB:212:ALA:HB1	1:IB:242:ILE:CD1	2.49	0.43
1:J:150:LEU:HD13	1:J:153:LEU:HD12	2.01	0.43
1:KB:202:THR:HG23	1:KB:203:GLY:N	2.34	0.43
1:NB:201:ILE:HD11	1:NB:234:ILE:HG12	1.99	0.43
1:R:209:THR:HG23	1:R:245:LEU:HD22	2.01	0.43
1:S:183:GLU:O	1:S:187:ILE:HG13	2.18	0.43
2:cb:89:LEU:HD23	2:cb:94:ILE:HG21	2.01	0.43
1:C:160:ILE:HD11	1:C:166:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CB:247:ILE:HG22	1:CB:249:LEU:HD22	2.00	0.43
1:EB:204:VAL:HG11	1:EB:207:VAL:HG22	2.00	0.43
1:FB:167:MET:SD	1:FB:167:MET:C	3.02	0.43
1:HB:204:VAL:HG21	1:HB:207:VAL:HG22	2.01	0.43
1:J:193:ARG:O	1:J:193:ARG:CG	2.66	0.43
1:N:216:ILE:HD11	1:N:247:ILE:CG2	2.48	0.43
1:PB:207:VAL:HG13	1:PB:211:VAL:CG2	2.47	0.43
1:Q:269:THR:O	1:Q:270:ASN:OD1	2.37	0.43
1:RB:162:GLU:O	1:RB:164:ILE:HG13	2.19	0.43
1:SB:256:ASN:C	1:SB:256:ASN:OD1	2.62	0.43
1:T:212:ALA:O	1:T:216:ILE:HD12	2.18	0.43
1:T:223:ARG:HD2	1:T:223:ARG:O	2.19	0.43
2:gb:94:ILE:O	2:gb:94:ILE:CG2	2.64	0.43
1:KB:237:GLU:O	1:KB:240:GLN:HG3	2.18	0.43
1:LB:216:ILE:HG13	1:LB:247:ILE:HG21	2.01	0.43
1:M:238:ILE:O	1:M:242:ILE:HG12	2.19	0.43
1:MB:254:THR:HG21	2:f:71:LEU:O	2.19	0.43
2:c:29:GLN:CD	2:c:65:VAL:HG22	2.43	0.43
2:c:94:ILE:O	2:c:94:ILE:CG2	2.66	0.43
2:ib:16:ILE:HG22	2:ib:51:ILE:HD11	2.00	0.43
1:D:204:VAL:HG11	1:D:207:VAL:HG22	2.01	0.43
1:IB:207:VAL:CG1	1:IB:211:VAL:HG23	2.49	0.43
1:P:223:ARG:O	1:P:223:ARG:NE	2.49	0.43
1:PB:156:PRO:C	1:PB:157:LEU:HD22	2.44	0.43
1:R:249:LEU:HD12	1:R:252:ILE:HG21	2.00	0.43
1:SB:160:ILE:HD12	1:SB:166:VAL:HG23	2.00	0.43
2:g:63:GLY:O	2:g:66:VAL:HG12	2.18	0.43
2:gb:96:PHE:HB3	2:gb:99:VAL:HB	2.01	0.43
2:hb:77:VAL:HG23	2:hb:112:LEU:HD21	2.00	0.43
1:AB:258:MET:SD	1:AB:258:MET:C	3.02	0.43
1:GB:220:GLU:HA	1:GB:220:GLU:OE1	2.19	0.43
1:GB:232:VAL:HG11	1:GB:258:MET:HA	2.01	0.43
1:I:210:MET:HE2	1:I:210:MET:N	2.32	0.43
1:O:186:LEU:O	1:O:189:VAL:HG22	2.19	0.43
1:Q:262:MET:HE2	1:QB:161:PHE:CE1	2.54	0.43
1:R:219:SER:O	1:R:222:VAL:HG12	2.19	0.43
1:E:158:LEU:HD21	1:EB:168:PRO:HB3	2.01	0.42
1:JB:149:ALA:O	1:JB:153:LEU:HG	2.19	0.42
1:LB:167:MET:SD	1:LB:167:MET:C	3.02	0.42
1:Q:160:ILE:HD13	1:Q:166:VAL:HG23	2.00	0.42
1:Q:231:LEU:HG	1:Q:252:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QB:230:MET:HE1	1:QB:265:ALA:HB2	2.00	0.42
1:S:238:ILE:O	1:S:242:ILE:HG12	2.19	0.42
2:b:42:ARG:HE	2:b:116:LEU:HD12	1.83	0.42
2:c:16:ILE:HG22	2:c:51:ILE:HD11	2.00	0.42
2:e:58:ILE:H	2:e:58:ILE:HD12	1.83	0.42
2:g:25:ALA:HA	2:g:28:PHE:CD1	2.53	0.42
2:h:1:MET:HE2	2:h:1:MET:HA	2.01	0.42
2:jb:77:VAL:CG2	2:jb:112:LEU:HD21	2.40	0.42
1:AB:197:VAL:HG12	1:AB:227:CYS:SG	2.59	0.42
1:C:196:VAL:HG23	1:C:228:GLN:O	2.19	0.42
1:G:160:ILE:CD1	1:G:166:VAL:HG21	2.49	0.42
1:H:263:GLU:OE2	1:H:263:GLU:HA	2.19	0.42
1:JB:167:MET:HE3	1:JB:167:MET:O	2.19	0.42
1:M:194:SER:O	1:M:227:CYS:SG	2.76	0.42
1:OB:208:ASP:OD1	1:OB:210:MET:HG2	2.19	0.42
1:S:167:MET:HE2	1:S:181:ILE:HG23	2.01	0.42
2:b:32:LEU:HD23	2:b:65:VAL:HG13	2.02	0.42
2:d:33:LEU:O	2:d:36:ILE:HG22	2.20	0.42
2:e:96:PHE:HB3	2:e:99:VAL:HB	2.01	0.42
2:jb:96:PHE:HB3	2:jb:99:VAL:HB	2.00	0.42
1:AB:235:ARG:CZ	1:CB:190:VAL:HG21	2.48	0.42
1:AB:259:LYS:HA	1:AB:259:LYS:HE3	2.01	0.42
1:DB:201:ILE:HD11	1:DB:234:ILE:CD1	2.33	0.42
1:E:204:VAL:HG11	1:E:207:VAL:HG23	2.01	0.42
1:E:210:MET:HG3	1:E:211:VAL:N	2.35	0.42
1:F:249:LEU:HD12	1:PB:224:LEU:HD22	2.01	0.42
1:G:253:ILE:HG22	1:G:254:THR:N	2.34	0.42
1:I:148:SER:O	1:I:152:GLU:OE1	2.38	0.42
1:IB:198:LEU:N	1:IB:198:LEU:HD12	2.33	0.42
1:JB:167:MET:SD	1:JB:167:MET:C	3.02	0.42
1:NB:235:ARG:HB3	1:NB:236:PRO:HD2	2.01	0.42
1:QB:204:VAL:HG11	1:QB:207:VAL:HG22	2.01	0.42
1:SB:149:ALA:O	1:SB:153:LEU:HG	2.19	0.42
2:eb:5:ILE:CG2	2:eb:12:LEU:HD12	2.49	0.42
2:f:107:SER:O	2:f:110:GLU:HG3	2.19	0.42
2:jb:33:LEU:O	2:jb:36:ILE:HG22	2.19	0.42
1:B:232:VAL:HG12	1:B:233:GLY:N	2.35	0.42
1:DB:149:ALA:O	1:DB:153:LEU:HG	2.20	0.42
1:T:236:PRO:CG	2:db:37:HIS:HB2	2.48	0.42
2:ab:14:ILE:HG22	2:ab:15:SER:N	2.35	0.42
2:b:66:VAL:HG21	2:b:99:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:100:LEU:HD12	2:h:111:LYS:HE2	2.02	0.42
1:AB:260:LYS:HA	1:AB:263:GLU:HG2	2.01	0.42
1:C:170:ILE:HG21	1:CB:153:LEU:HD22	1.99	0.42
1:C:201:ILE:O	1:C:204:VAL:HG12	2.19	0.42
1:F:212:ALA:O	1:F:216:ILE:HD12	2.19	0.42
1:MB:201:ILE:HD11	1:MB:234:ILE:HG12	2.02	0.42
1:PB:210:MET:HE2	1:PB:210:MET:N	2.34	0.42
1:PB:236:PRO:CG	1:SB:190:VAL:HG21	2.49	0.42
1:Q:158:LEU:O	1:Q:160:ILE:HD12	2.19	0.42
1:Q:186:LEU:O	1:Q:189:VAL:HG12	2.20	0.42
1:QB:186:LEU:O	1:QB:189:VAL:HG12	2.20	0.42
2:b:105:LEU:C	2:b:105:LEU:HD23	2.45	0.42
2:db:54:ILE:HD11	2:db:58:ILE:HG22	2.02	0.42
2:h:26:VAL:O	2:h:30:GLU:OE1	2.37	0.42
2:j:6:LEU:HD23	2:jb:105:LEU:HD13	2.02	0.42
2:j:77:VAL:HG23	2:j:112:LEU:HD13	2.02	0.42
1:A:157:LEU:HD12	1:A:166:VAL:O	2.19	0.42
1:B:204:VAL:O	1:B:204:VAL:HG13	2.20	0.42
1:CB:230:MET:HE1	1:CB:265:ALA:HB2	2.02	0.42
1:D:160:ILE:HG22	1:D:161:PHE:CD2	2.54	0.42
1:D:196:VAL:HB	1:D:230:MET:HE3	2.00	0.42
1:HB:155:ALA:HB1	1:HB:181:ILE:HD12	2.02	0.42
1:KB:167:MET:SD	1:KB:185:LEU:HD13	2.59	0.42
1:MB:149:ALA:O	1:MB:153:LEU:HG	2.20	0.42
1:O:209:THR:HG23	1:O:210:MET:N	2.35	0.42
1:QB:164:ILE:HG21	1:QB:262:MET:HE1	2.00	0.42
2:ab:29:GLN:OE1	2:ab:65:VAL:CG2	2.68	0.42
2:ab:54:ILE:CD1	2:ab:62:LEU:HD12	2.49	0.42
2:hb:103:MET:HE2	2:hb:103:MET:CA	2.49	0.42
1:K:201:ILE:HD11	1:K:234:ILE:HG13	1.99	0.42
1:NB:238:ILE:O	1:NB:242:ILE:HG12	2.20	0.42
1:O:220:GLU:O	1:O:223:ARG:HB3	2.20	0.42
2:e:71:LEU:C	2:e:71:LEU:HD23	2.45	0.42
2:g:24:THR:HA	2:g:27:GLU:CG	2.50	0.42
2:i:7:LYS:HD3	2:i:7:LYS:C	2.45	0.42
2:ib:96:PHE:HB3	2:ib:99:VAL:HB	2.02	0.42
1:AB:160:ILE:HD12	1:AB:166:VAL:HG23	2.01	0.42
1:I:153:LEU:HD13	1:IB:170:ILE:HG22	2.01	0.42
1:JB:216:ILE:HD11	1:JB:247:ILE:HG21	2.02	0.42
1:LB:262:MET:HE3	1:LB:266:LEU:HD21	2.02	0.42
1:O:155:ALA:HB1	1:O:167:MET:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:168:PRO:O	1:P:169:LEU:HD23	2.20	0.42
1:RB:167:MET:CE	1:RB:181:ILE:HD11	2.50	0.42
1:T:269:THR:O	1:T:270:ASN:OD1	2.37	0.42
2:ab:31:ASP:O	2:ab:35:LYS:HG2	2.19	0.42
2:cb:82:GLN:O	2:cb:85:VAL:HG12	2.20	0.42
2:e:78:VAL:HG12	2:e:81:ILE:HD11	2.02	0.42
2:gb:47:ASP:OD1	2:gb:47:ASP:C	2.62	0.42
2:jb:54:ILE:HG23	2:jb:58:ILE:CG2	2.50	0.42
1:N:170:ILE:HG22	1:NB:153:LEU:HD13	2.02	0.42
2:g:24:THR:O	2:g:27:GLU:HG3	2.20	0.42
2:hb:88:THR:O	2:hb:92:LEU:HD23	2.20	0.42
2:j:54:ILE:HG13	2:j:58:ILE:HB	2.02	0.42
2:j:63:GLY:O	2:j:66:VAL:HG12	2.19	0.42
1:BB:167:MET:SD	1:BB:167:MET:C	3.03	0.42
1:D:160:ILE:HA	1:DB:258:MET:CE	2.50	0.42
1:D:193:ARG:HH11	1:D:193:ARG:HA	1.85	0.42
1:DB:258:MET:O	1:DB:258:MET:SD	2.78	0.42
1:EB:196:VAL:HG21	1:EB:265:ALA:CB	2.50	0.42
1:FB:231:LEU:HD12	1:FB:231:LEU:C	2.44	0.42
1:HB:236:PRO:HB3	2:gb:33:LEU:HB3	2.01	0.42
1:L:149:ALA:O	1:L:153:LEU:HG	2.20	0.42
1:L:198:LEU:N	1:L:198:LEU:HD12	2.35	0.42
1:LB:204:VAL:O	1:LB:204:VAL:HG13	2.20	0.42
1:P:192:ASN:ND2	1:P:192:ASN:N	2.68	0.42
1:Q:169:LEU:HD12	1:Q:181:ILE:CD1	2.50	0.42
1:Q:258:MET:SD	1:Q:258:MET:O	2.78	0.42
1:S:273:ILE:HD13	1:SB:161:PHE:CZ	2.55	0.42
1:SB:169:LEU:C	1:SB:170:ILE:HD12	2.44	0.42
1:T:193:ARG:HD3	1:T:193:ARG:N	2.34	0.42
2:a:31:ASP:O	2:a:35:LYS:HG2	2.20	0.42
2:a:72:MET:O	2:a:72:MET:SD	2.78	0.42
2:ab:77:VAL:HG12	2:ab:100:LEU:HB2	2.02	0.42
2:bb:32:LEU:HD23	2:bb:65:VAL:CG1	2.50	0.42
2:bb:55:ASP:OD2	2:bb:56:SER:N	2.52	0.42
2:db:66:VAL:HG21	2:db:99:VAL:HG11	2.01	0.42
2:fb:22:ASP:OD1	2:fb:23:HIS:N	2.53	0.42
1:B:204:VAL:HG21	1:B:207:VAL:HG22	2.01	0.41
1:BB:238:ILE:O	1:BB:242:ILE:HG12	2.19	0.41
1:D:258:MET:O	1:D:258:MET:SD	2.78	0.41
1:DB:162:GLU:N	1:DB:162:GLU:OE1	2.51	0.41
1:E:160:ILE:HG22	1:E:161:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FB:169:LEU:C	1:FB:170:ILE:HD12	2.45	0.41
1:H:167:MET:HE2	1:H:169:LEU:HD11	2.02	0.41
1:L:223:ARG:O	1:L:223:ARG:NH1	2.53	0.41
1:MB:248:GLU:CD	1:MB:248:GLU:N	2.78	0.41
1:N:232:VAL:HG12	1:N:255:THR:OG1	2.19	0.41
1:NB:157:LEU:HD11	1:NB:165:SER:HB2	2.01	0.41
1:NB:264:ARG:O	1:NB:268:LEU:HD23	2.20	0.41
1:OB:247:ILE:HG22	1:OB:249:LEU:CD1	2.50	0.41
1:Q:162:GLU:O	1:Q:163:LYS:HB2	2.20	0.41
1:Q:196:VAL:HG11	1:Q:265:ALA:HB1	2.01	0.41
1:T:169:LEU:HD23	1:T:169:LEU:O	2.20	0.41
2:cb:3:ILE:O	2:cb:5:ILE:HD12	2.20	0.41
2:e:16:ILE:CG2	2:e:51:ILE:HD11	2.50	0.41
2:j:11:CYS:O	2:j:12:LEU:HD12	2.19	0.41
1:A:263:GLU:OE1	1:A:263:GLU:C	2.63	0.41
1:C:175:ALA:HA	1:C:210:MET:CE	2.48	0.41
1:G:253:ILE:HG21	1:G:264:ARG:HD3	2.01	0.41
1:HB:231:LEU:CD2	1:HB:234:ILE:HD11	2.50	0.41
1:I:245:LEU:HD23	1:I:247:ILE:CD1	2.44	0.41
1:JB:236:PRO:HB3	2:a:33:LEU:HB3	2.02	0.41
1:KB:237:GLU:HG2	1:KB:238:ILE:N	2.36	0.41
1:N:160:ILE:HD12	1:N:166:VAL:CG2	2.50	0.41
1:P:160:ILE:CD1	1:P:166:VAL:HG22	2.41	0.41
1:T:149:ALA:O	1:T:153:LEU:CD1	2.68	0.41
2:a:66:VAL:HG23	2:a:76:VAL:HG11	2.01	0.41
2:bb:48:ILE:HD11	2:bb:81:ILE:HG13	2.01	0.41
2:j:5:ILE:O	2:j:5:ILE:HG23	2.20	0.41
1:B:153:LEU:HD13	1:BB:170:ILE:HG22	2.03	0.41
1:E:175:ALA:N	1:E:210:MET:HE1	2.35	0.41
1:EB:258:MET:O	1:EB:258:MET:SD	2.78	0.41
1:F:241:THR:O	1:F:245:LEU:HD23	2.21	0.41
1:GB:231:LEU:CD2	1:GB:234:ILE:HD11	2.51	0.41
1:GB:231:LEU:HD21	1:GB:234:ILE:HD11	2.02	0.41
1:KB:230:MET:HE1	1:KB:265:ALA:HB2	2.03	0.41
1:OB:186:LEU:HD21	1:OB:221:ALA:CB	2.49	0.41
1:P:200:ASP:C	1:P:200:ASP:OD1	2.63	0.41
1:SB:164:ILE:HG22	1:SB:165:SER:N	2.36	0.41
1:T:247:ILE:HG22	1:T:249:LEU:HD12	2.02	0.41
2:cb:109:LEU:HD23	2:cb:109:LEU:C	2.45	0.41
2:jb:8:LEU:HD23	2:jb:8:LEU:C	2.44	0.41
2:jb:42:ARG:NH1	2:jb:116:LEU:HD22	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ILE:O	1:B:204:VAL:HG12	2.19	0.41
1:B:202:THR:C	1:B:235:ARG:HH22	2.28	0.41
1:C:210:MET:HE3	1:C:214:HIS:CD2	2.55	0.41
1:CB:207:VAL:HB	1:CB:238:ILE:HG23	2.03	0.41
1:F:170:ILE:HG22	1:FB:153:LEU:HD22	2.01	0.41
1:L:204:VAL:O	1:L:204:VAL:HG13	2.21	0.41
1:NB:230:MET:HE1	1:NB:265:ALA:HB2	2.01	0.41
1:OB:223:ARG:O	1:OB:223:ARG:NH1	2.53	0.41
1:T:235:ARG:HH11	1:T:235:ARG:HG3	1.85	0.41
2:bb:16:ILE:HG22	2:bb:51:ILE:HD11	2.03	0.41
2:db:14:ILE:HG22	2:db:15:SER:N	2.35	0.41
2:g:71:LEU:HD23	2:g:71:LEU:C	2.45	0.41
2:gb:14:ILE:HG22	2:gb:15:SER:N	2.35	0.41
2:hb:81:ILE:HD12	2:hb:81:ILE:N	2.34	0.41
2:j:53:PHE:CD1	2:j:53:PHE:C	2.97	0.41
1:AB:249:LEU:O	1:AB:252:ILE:HG12	2.20	0.41
1:CB:237:GLU:H	1:CB:237:GLU:CD	2.28	0.41
1:IB:156:PRO:O	1:IB:157:LEU:HD22	2.20	0.41
1:JB:155:ALA:CB	1:JB:181:ILE:HD13	2.50	0.41
1:JB:204:VAL:O	1:JB:204:VAL:HG13	2.21	0.41
1:KB:240:GLN:HA	1:KB:243:VAL:HG12	2.02	0.41
1:L:207:VAL:HB	1:L:238:ILE:HG23	2.02	0.41
1:P:240:GLN:HA	2:eb:68:MET:HE2	2.02	0.41
2:a:110:GLU:O	2:a:113:LYS:HG2	2.20	0.41
1:DB:157:LEU:HD11	1:DB:165:SER:CB	2.50	0.41
1:DB:157:LEU:HD11	1:DB:165:SER:HB3	2.02	0.41
1:DB:231:LEU:HD13	1:DB:234:ILE:CD1	2.43	0.41
1:O:148:SER:HA	1:O:151:GLN:HG2	2.03	0.41
1:O:161:PHE:CD2	1:OB:259:LYS:NZ	2.89	0.41
1:O:249:LEU:CD2	1:O:252:ILE:HD11	2.30	0.41
1:R:207:VAL:HB	1:R:238:ILE:HG23	2.02	0.41
1:SB:216:ILE:HG22	1:SB:249:LEU:HD21	2.03	0.41
2:g:78:VAL:HG21	2:g:96:PHE:HE1	1.84	0.41
2:j:66:VAL:HG23	2:j:76:VAL:HG11	2.03	0.41
1:AB:235:ARG:HE	1:AB:236:PRO:HD2	1.86	0.41
1:BB:169:LEU:C	1:BB:169:LEU:HD23	2.45	0.41
1:F:169:LEU:HD12	1:F:181:ILE:HD13	2.01	0.41
1:F:224:LEU:HD22	1:Q:249:LEU:HD22	2.02	0.41
1:G:230:MET:CE	1:G:265:ALA:HB2	2.45	0.41
1:H:170:ILE:CG1	1:HB:153:LEU:HD22	2.51	0.41
1:IB:245:LEU:HD23	1:IB:247:ILE:CD1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OB:260:LYS:O	1:OB:263:GLU:HG2	2.20	0.41
1:SB:207:VAL:HB	1:SB:238:ILE:HG23	2.03	0.41
1:T:216:ILE:HD11	1:T:247:ILE:HG21	2.02	0.41
2:gb:8:LEU:C	2:gb:8:LEU:HD23	2.45	0.41
2:gb:18:SER:O	2:gb:20:LEU:HD22	2.21	0.41
2:j:8:LEU:C	2:j:8:LEU:HD23	2.45	0.41
1:A:257:THR:HG21	1:D:193:ARG:HE	1.85	0.41
1:BB:198:LEU:N	1:BB:198:LEU:HD12	2.35	0.41
1:BB:204:VAL:HG11	1:BB:207:VAL:HG22	2.03	0.41
1:CB:160:ILE:HD11	1:CB:166:VAL:CG1	2.51	0.41
1:CB:202:THR:O	1:CB:235:ARG:CZ	2.69	0.41
1:DB:160:ILE:CD1	1:DB:166:VAL:HG21	2.51	0.41
1:DB:178:ALA:HA	1:DB:181:ILE:HG22	2.03	0.41
1:EB:149:ALA:O	1:EB:153:LEU:HG	2.20	0.41
1:FB:258:MET:SD	1:FB:258:MET:C	3.03	0.41
1:LB:230:MET:HE1	1:LB:265:ALA:N	2.36	0.41
1:OB:147:LYS:O	1:OB:151:GLN:OE1	2.39	0.41
1:OB:196:VAL:HG12	1:OB:197:VAL:N	2.36	0.41
2:a:5:ILE:CD1	2:a:14:ILE:HD11	2.51	0.41
2:b:11:CYS:C	2:b:12:LEU:HD12	2.46	0.41
2:b:64:ASP:O	2:b:68:MET:HG3	2.21	0.41
2:g:37:HIS:HB2	2:g:72:MET:HE1	2.02	0.41
2:j:72:MET:HE2	2:j:72:MET:HB3	1.90	0.41
2:jb:16:ILE:HG22	2:jb:51:ILE:HD11	2.03	0.41
1:BB:187:ILE:O	1:BB:191:LYS:HG2	2.21	0.41
1:EB:176:GLU:O	1:EB:179:LYS:HG2	2.21	0.41
1:F:238:ILE:O	1:F:242:ILE:HG12	2.21	0.41
1:H:199:ILE:HG22	1:H:201:ILE:HG23	2.03	0.41
1:I:170:ILE:HG22	1:IB:153:LEU:HD13	2.02	0.41
1:I:245:LEU:O	1:I:245:LEU:HG	2.21	0.41
1:J:189:VAL:HG13	1:J:227:CYS:SG	2.61	0.41
1:JB:186:LEU:HD21	1:JB:221:ALA:HB1	2.02	0.41
1:L:248:GLU:OE1	1:L:248:GLU:HA	2.21	0.41
1:LB:157:LEU:HD11	1:LB:165:SER:HB2	2.01	0.41
1:M:273:ILE:HD13	1:MB:161:PHE:CE1	2.56	0.41
1:NB:207:VAL:HB	1:NB:238:ILE:HG23	2.03	0.41
1:PB:169:LEU:HD23	1:PB:169:LEU:O	2.20	0.41
1:PB:204:VAL:N	1:PB:235:ARG:HH22	2.19	0.41
1:RB:213:HIS:CE1	1:RB:217:GLN:HE21	2.39	0.41
1:TB:149:ALA:O	1:TB:153:LEU:HG	2.21	0.41
2:b:11:CYS:O	2:b:12:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:db:32:LEU:HD23	2:db:65:VAL:CG1	2.51	0.41
2:eb:32:LEU:HD23	2:eb:65:VAL:CG1	2.51	0.41
1:C:204:VAL:O	1:C:204:VAL:HG13	2.20	0.41
1:CB:220:GLU:HA	1:CB:220:GLU:OE2	2.21	0.41
1:DB:178:ALA:O	1:DB:181:ILE:HG22	2.21	0.41
1:E:170:ILE:HG21	1:EB:153:LEU:HD22	2.00	0.41
1:F:207:VAL:HB	1:F:238:ILE:HG23	2.03	0.41
1:FB:243:VAL:HG11	2:i:68:MET:HG3	2.03	0.41
1:GB:163:LYS:HD3	1:GB:195:GLU:OE1	2.21	0.41
1:K:213:HIS:O	1:K:217:GLN:HG2	2.21	0.41
1:L:197:VAL:C	1:L:198:LEU:HD12	2.45	0.41
1:L:205:PRO:HA	1:L:235:ARG:HH22	1.85	0.41
1:P:202:THR:HG23	1:P:203:GLY:N	2.36	0.41
1:TB:202:THR:HG23	1:TB:203:GLY:N	2.35	0.41
1:BB:224:LEU:HD12	1:SB:243:VAL:HG23	2.03	0.40
1:D:162:GLU:O	1:D:163:LYS:HB2	2.21	0.40
1:F:153:LEU:HD22	1:FB:170:ILE:CG2	2.51	0.40
1:F:187:ILE:O	1:F:191:LYS:HG2	2.21	0.40
1:G:219:SER:O	1:G:222:VAL:HG22	2.21	0.40
1:G:253:ILE:HG21	1:G:264:ARG:CD	2.51	0.40
1:GB:162:GLU:O	1:GB:163:LYS:HB2	2.22	0.40
1:HB:166:VAL:HG22	1:HB:198:LEU:HB2	2.03	0.40
1:I:257:THR:HG23	1:I:260:LYS:H	1.85	0.40
1:MB:193:ARG:N	1:MB:193:ARG:HD3	2.36	0.40
1:O:202:THR:HG22	1:O:233:GLY:HA3	2.03	0.40
1:OB:269:THR:HG21	1:OB:271:ARG:NH2	2.36	0.40
1:P:212:ALA:O	1:P:216:ILE:HG12	2.20	0.40
1:R:149:ALA:O	1:R:153:LEU:HG	2.22	0.40
1:R:210:MET:HE2	1:R:210:MET:HA	2.02	0.40
1:R:223:ARG:NH1	1:R:223:ARG:O	2.54	0.40
1:S:169:LEU:HD11	1:S:173:ILE:HD11	2.03	0.40
2:b:36:ILE:HD11	2:b:44:VAL:CG2	2.51	0.40
2:c:29:GLN:NE2	2:c:68:MET:CE	2.85	0.40
2:cb:81:ILE:HG23	2:cb:85:VAL:HG13	2.02	0.40
2:f:11:CYS:C	2:f:12:LEU:HD12	2.45	0.40
2:fb:8:LEU:C	2:fb:8:LEU:HD23	2.47	0.40
2:j:33:LEU:O	2:j:36:ILE:HG22	2.22	0.40
1:B:164:ILE:HG21	1:B:262:MET:HE1	2.04	0.40
1:BB:262:MET:HA	1:BB:262:MET:HE2	2.03	0.40
1:H:190:VAL:HG21	1:O:236:PRO:CG	2.51	0.40
1:HB:186:LEU:O	1:HB:189:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JB:236:PRO:CG	2:a:37:HIS:HB2	2.50	0.40
1:L:160:ILE:CD1	1:L:166:VAL:HG21	2.47	0.40
1:LB:223:ARG:O	1:LB:223:ARG:NH1	2.55	0.40
1:M:198:LEU:HD12	1:M:198:LEU:N	2.36	0.40
1:NB:219:SER:O	1:NB:222:VAL:HG22	2.21	0.40
1:Q:231:LEU:HB3	1:Q:234:ILE:HD11	2.02	0.40
1:S:186:LEU:O	1:S:190:VAL:HG23	2.21	0.40
1:T:243:VAL:HB	2:db:68:MET:HG2	2.02	0.40
2:a:21:ASP:OD2	2:a:22:ASP:OD2	2.40	0.40
2:bb:95:THR:HG23	2:bb:95:THR:O	2.20	0.40
2:d:1:MET:HE3	2:d:1:MET:O	2.22	0.40
2:d:66:VAL:HG23	2:d:76:VAL:HG11	2.03	0.40
2:hb:25:ALA:HB1	2:hb:61:ILE:HD13	2.03	0.40
1:CB:202:THR:HG23	1:CB:203:GLY:N	2.37	0.40
1:J:237:GLU:HG2	1:J:238:ILE:N	2.36	0.40
1:KB:199:ILE:HG22	1:KB:201:ILE:HG23	2.03	0.40
1:PB:269:THR:O	1:PB:270:ASN:OD1	2.40	0.40
1:Q:178:ALA:O	1:Q:181:ILE:HG22	2.20	0.40
1:R:160:ILE:HG22	1:R:161:PHE:CE2	2.56	0.40
1:TB:160:ILE:HD12	1:TB:166:VAL:HG23	2.03	0.40
2:cb:5:ILE:HG21	2:cb:35:LYS:HG2	2.04	0.40
2:h:64:ASP:HB3	2:h:68:MET:HE3	2.03	0.40
2:hb:68:MET:O	2:hb:71:LEU:HB3	2.22	0.40
2:i:8:LEU:HD23	2:i:8:LEU:C	2.46	0.40
1:BB:176:GLU:O	1:BB:179:LYS:HG2	2.21	0.40
1:DB:212:ALA:O	1:DB:216:ILE:HD12	2.21	0.40
1:DB:219:SER:O	1:DB:222:VAL:HG12	2.21	0.40
1:EB:157:LEU:HD22	1:EB:188:GLY:HA3	2.04	0.40
1:GB:169:LEU:C	1:GB:169:LEU:HD23	2.46	0.40
1:K:230:MET:HE1	1:K:265:ALA:HB2	2.04	0.40
1:K:258:MET:SD	1:K:258:MET:O	2.80	0.40
1:M:201:ILE:HD11	1:M:231:LEU:HD21	2.02	0.40
1:N:204:VAL:HG11	1:N:207:VAL:CG2	2.52	0.40
1:O:161:PHE:HB2	1:O:164:ILE:HB	2.03	0.40
1:O:263:GLU:OE1	1:O:263:GLU:HA	2.21	0.40
1:O:269:THR:HG21	1:O:271:ARG:HH21	1.87	0.40
1:P:160:ILE:HD12	1:P:160:ILE:H	1.87	0.40
1:PB:217:GLN:C	1:PB:217:GLN:OE1	2.64	0.40
1:Q:262:MET:HE2	1:QB:161:PHE:HE1	1.87	0.40
2:b:12:LEU:HD13	2:b:41:ALA:CB	2.51	0.40
2:db:3:ILE:O	2:db:5:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BB:167:MET:HE1	1:BB:169:LEU:HB2	2.04	0.40
1:CB:231:LEU:HD12	1:CB:231:LEU:O	2.21	0.40
1:H:204:VAL:HG11	1:H:207:VAL:CG2	2.52	0.40
1:HB:209:THR:HG23	1:HB:210:MET:N	2.36	0.40
1:K:160:ILE:CD1	1:K:166:VAL:HG11	2.52	0.40
1:N:220:GLU:O	1:N:224:LEU:HD23	2.21	0.40
1:Q:153:LEU:HD13	1:QB:170:ILE:HG22	2.03	0.40
1:RB:236:PRO:HD3	2:j:37:HIS:ND1	2.36	0.40
1:T:196:VAL:HG11	1:T:265:ALA:HB2	2.03	0.40
1:T:202:THR:HG23	1:T:203:GLY:N	2.36	0.40
2:a:8:LEU:C	2:a:8:LEU:HD23	2.46	0.40
2:bb:7:LYS:HD2	2:bb:7:LYS:C	2.47	0.40
2:e:81:ILE:HD12	2:e:81:ILE:N	2.37	0.40
2:f:100:LEU:HD12	2:f:111:LYS:HE2	2.04	0.40
2:gb:81:ILE:HG23	2:gb:85:VAL:HG23	2.04	0.40
2:ib:57:PHE:CD1	2:ib:57:PHE:C	2.99	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	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	AB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	B	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	BB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	C	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	CB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	D	130/278 (47%)	124 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	E	130/278 (47%)	122 (94%)	8 (6%)	0	100	100
1	EB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	F	130/278 (47%)	121 (93%)	9 (7%)	0	100	100
1	FB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	G	130/278 (47%)	121 (93%)	9 (7%)	0	100	100
1	GB	130/278 (47%)	119 (92%)	11 (8%)	0	100	100
1	H	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	HB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	I	130/278 (47%)	122 (94%)	8 (6%)	0	100	100
1	IB	130/278 (47%)	122 (94%)	8 (6%)	0	100	100
1	J	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	JB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	K	130/278 (47%)	128 (98%)	2 (2%)	0	100	100
1	KB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	L	130/278 (47%)	121 (93%)	9 (7%)	0	100	100
1	LB	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	M	130/278 (47%)	121 (93%)	9 (7%)	0	100	100
1	MB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	N	130/278 (47%)	124 (95%)	6 (5%)	0	100	100
1	NB	130/278 (47%)	125 (96%)	5 (4%)	0	100	100
1	O	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	OB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	P	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	PB	130/278 (47%)	129 (99%)	1 (1%)	0	100	100
1	Q	130/278 (47%)	122 (94%)	8 (6%)	0	100	100
1	QB	130/278 (47%)	122 (94%)	8 (6%)	0	100	100
1	R	130/278 (47%)	121 (93%)	9 (7%)	0	100	100
1	RB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
1	S	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	SB	130/278 (47%)	124 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	130/278 (47%)	123 (95%)	7 (5%)	0	100	100
1	TB	130/278 (47%)	126 (97%)	4 (3%)	0	100	100
2	a	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	ab	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
2	b	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	bb	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
2	c	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	cb	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	d	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	db	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
2	e	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
2	eb	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	f	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
2	fb	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	g	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	gb	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
2	h	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
2	hb	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
2	i	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
2	ib	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
2	j	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
2	jb	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
All	All	7520/13480 (56%)	7193 (96%)	327 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/246 (46%)	113 (100%)	0	100	100
1	AB	113/246 (46%)	113 (100%)	0	100	100
1	B	113/246 (46%)	113 (100%)	0	100	100
1	BB	113/246 (46%)	112 (99%)	1 (1%)	70	77
1	C	113/246 (46%)	113 (100%)	0	100	100
1	CB	113/246 (46%)	112 (99%)	1 (1%)	70	77
1	D	113/246 (46%)	113 (100%)	0	100	100
1	DB	113/246 (46%)	113 (100%)	0	100	100
1	E	113/246 (46%)	112 (99%)	1 (1%)	70	77
1	EB	113/246 (46%)	113 (100%)	0	100	100
1	F	113/246 (46%)	113 (100%)	0	100	100
1	FB	113/246 (46%)	113 (100%)	0	100	100
1	G	113/246 (46%)	113 (100%)	0	100	100
1	GB	113/246 (46%)	113 (100%)	0	100	100
1	H	113/246 (46%)	112 (99%)	1 (1%)	70	77
1	HB	113/246 (46%)	113 (100%)	0	100	100
1	I	113/246 (46%)	113 (100%)	0	100	100
1	IB	113/246 (46%)	113 (100%)	0	100	100
1	J	113/246 (46%)	113 (100%)	0	100	100
1	JB	113/246 (46%)	113 (100%)	0	100	100
1	K	113/246 (46%)	113 (100%)	0	100	100
1	KB	113/246 (46%)	113 (100%)	0	100	100
1	L	113/246 (46%)	113 (100%)	0	100	100
1	LB	113/246 (46%)	113 (100%)	0	100	100
1	M	113/246 (46%)	113 (100%)	0	100	100
1	MB	113/246 (46%)	113 (100%)	0	100	100
1	N	113/246 (46%)	113 (100%)	0	100	100
1	NB	113/246 (46%)	113 (100%)	0	100	100
1	O	113/246 (46%)	113 (100%)	0	100	100
1	OB	113/246 (46%)	113 (100%)	0	100	100
1	P	113/246 (46%)	112 (99%)	1 (1%)	70	77
1	PB	113/246 (46%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	113/246 (46%)	113 (100%)	0	100	100
1	QB	113/246 (46%)	113 (100%)	0	100	100
1	R	113/246 (46%)	113 (100%)	0	100	100
1	RB	113/246 (46%)	113 (100%)	0	100	100
1	S	113/246 (46%)	113 (100%)	0	100	100
1	SB	113/246 (46%)	113 (100%)	0	100	100
1	T	113/246 (46%)	113 (100%)	0	100	100
1	TB	113/246 (46%)	112 (99%)	1 (1%)	70	77
2	a	100/100 (100%)	100 (100%)	0	100	100
2	ab	100/100 (100%)	100 (100%)	0	100	100
2	b	100/100 (100%)	100 (100%)	0	100	100
2	bb	100/100 (100%)	100 (100%)	0	100	100
2	c	100/100 (100%)	100 (100%)	0	100	100
2	cb	100/100 (100%)	100 (100%)	0	100	100
2	d	100/100 (100%)	100 (100%)	0	100	100
2	db	100/100 (100%)	100 (100%)	0	100	100
2	e	100/100 (100%)	100 (100%)	0	100	100
2	eb	100/100 (100%)	100 (100%)	0	100	100
2	f	100/100 (100%)	100 (100%)	0	100	100
2	fb	100/100 (100%)	100 (100%)	0	100	100
2	g	100/100 (100%)	100 (100%)	0	100	100
2	gb	100/100 (100%)	100 (100%)	0	100	100
2	h	100/100 (100%)	100 (100%)	0	100	100
2	hb	100/100 (100%)	100 (100%)	0	100	100
2	i	100/100 (100%)	100 (100%)	0	100	100
2	ib	100/100 (100%)	100 (100%)	0	100	100
2	j	100/100 (100%)	100 (100%)	0	100	100
2	jb	100/100 (100%)	100 (100%)	0	100	100
All	All	6520/11840 (55%)	6514 (100%)	6 (0%)	87	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BB	270	ASN
1	CB	240	GLN
1	E	240	GLN
1	H	240	GLN
1	P	192	ASN
1	TB	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	AB	251	GLN
1	B	192	ASN
1	BB	192	ASN
1	BB	214	HIS
1	CB	192	ASN
1	CB	213	HIS
1	DB	192	ASN
1	DB	213	HIS
1	DB	214	HIS
1	E	213	HIS
1	E	217	GLN
1	E	228	GLN
1	E	240	GLN
1	G	251	GLN
1	GB	213	HIS
1	H	192	ASN
1	H	214	HIS
1	H	217	GLN
1	H	240	GLN
1	I	192	ASN
1	IB	213	HIS
1	IB	240	GLN
1	J	228	GLN
1	JB	213	HIS
1	JB	217	GLN
1	K	192	ASN
1	K	213	HIS
1	KB	192	ASN
1	L	251	GLN
1	LB	213	HIS
1	LB	228	GLN
1	M	151	GLN

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Mol	Chain	Res	Type
1	MB	244	ASN
1	N	213	HIS
1	N	217	GLN
1	N	251	GLN
1	OB	251	GLN
1	P	184	ASN
1	PB	217	GLN
1	R	192	ASN
1	R	228	GLN
1	RB	213	HIS
1	RB	214	HIS
1	RB	251	GLN
1	SB	228	GLN
1	T	192	ASN
1	T	213	HIS
1	T	217	GLN
1	T	251	GLN
1	TB	192	ASN
1	TB	214	HIS
2	cb	37	HIS
2	db	23	HIS
2	db	37	HIS
2	e	29	GLN
2	e	37	HIS
2	eb	29	GLN
2	fb	37	HIS
2	hb	23	HIS
2	hb	37	HIS
2	i	29	GLN
2	jb	37	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

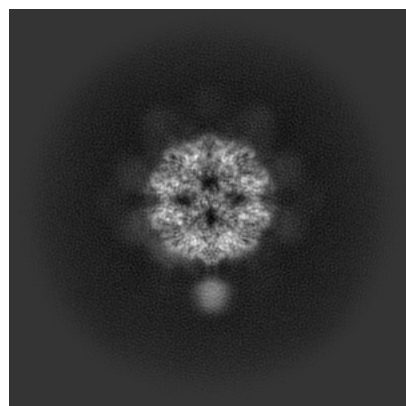
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70081. These allow visual inspection of the internal detail of the map and identification of artifacts.

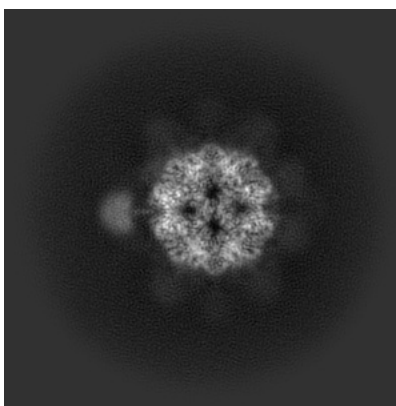
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

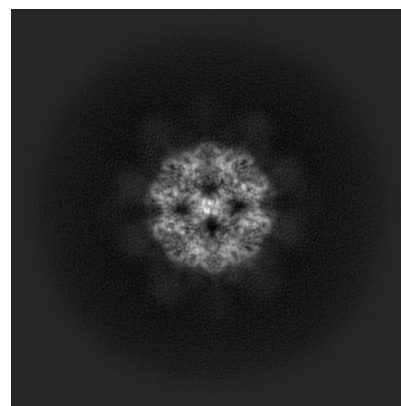
6.1.1 Primary map



X

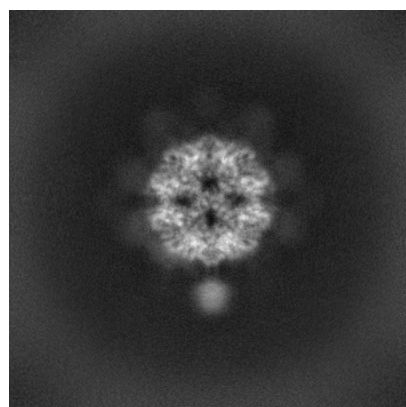


Y

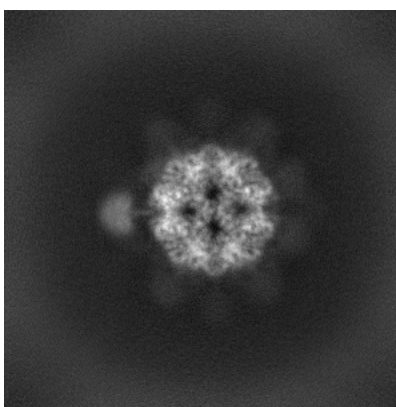


Z

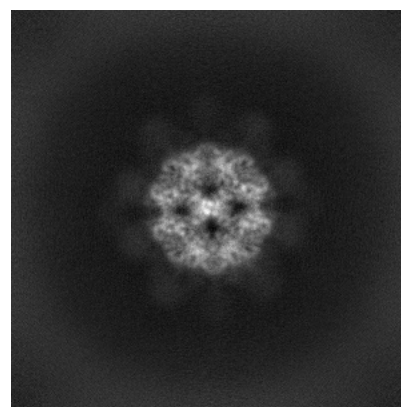
6.1.2 Raw map



X



Y

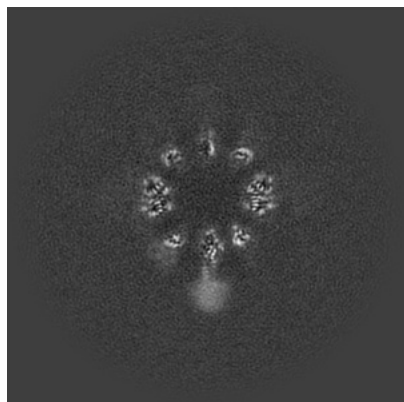


Z

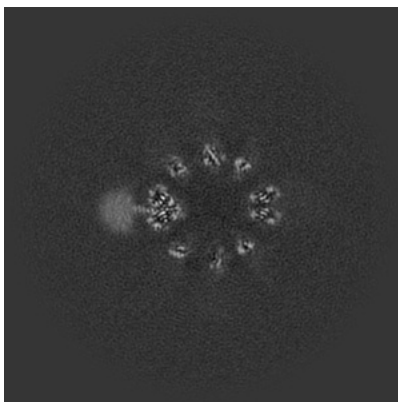
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

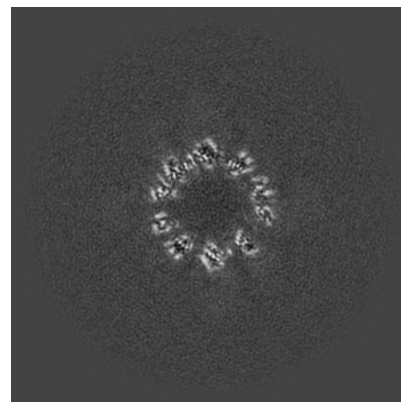
6.2.1 Primary map



X Index: 300

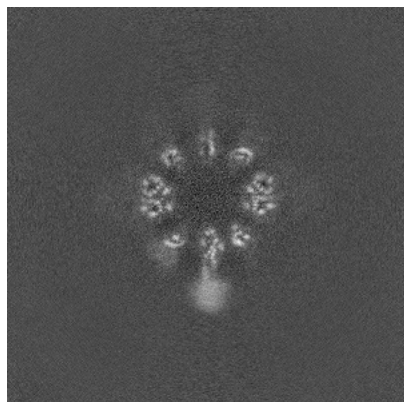


Y Index: 300

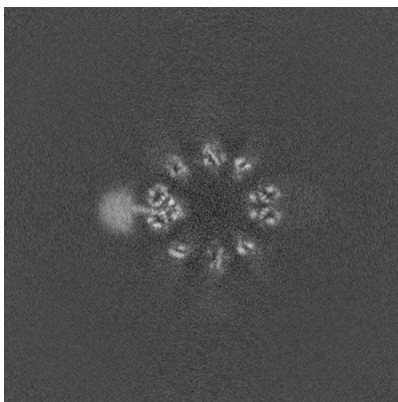


Z Index: 300

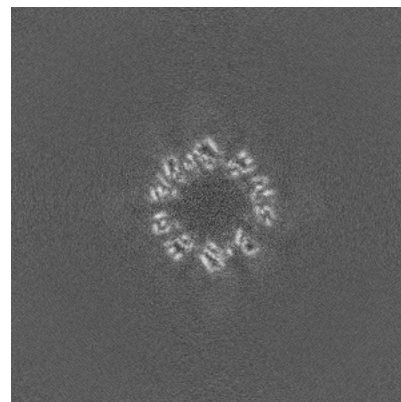
6.2.2 Raw map



X Index: 300



Y Index: 300

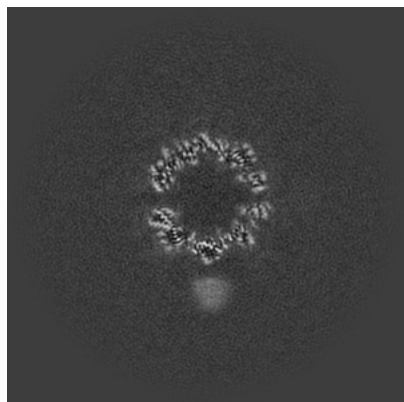


Z Index: 300

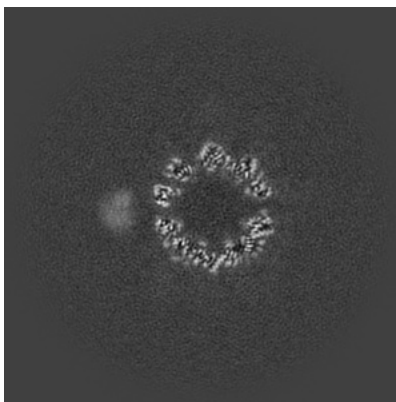
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

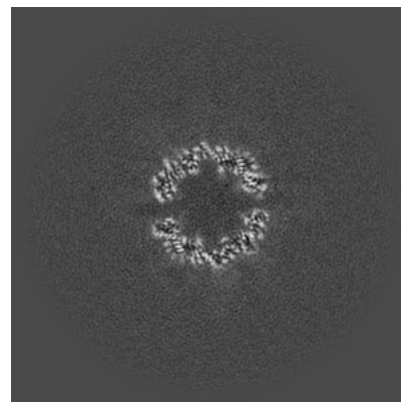
6.3.1 Primary map



X Index: 279

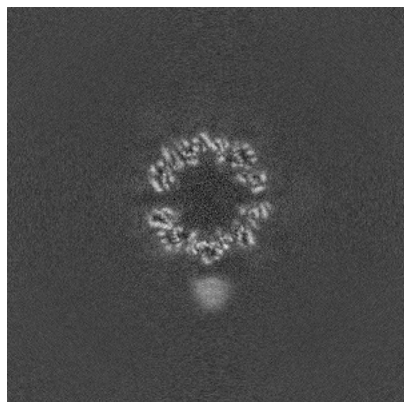


Y Index: 320

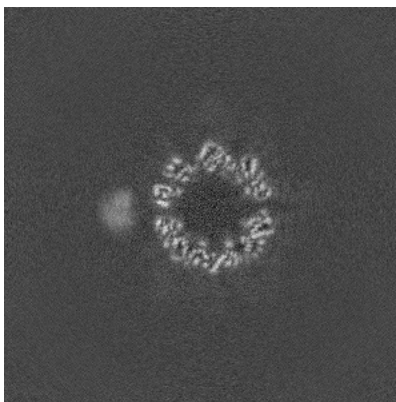


Z Index: 290

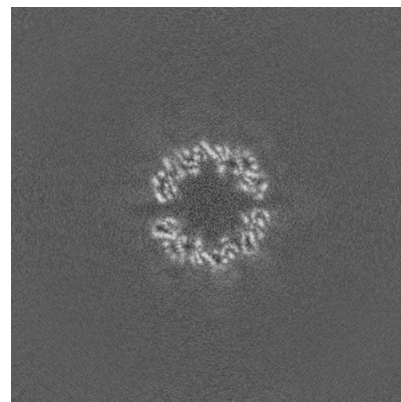
6.3.2 Raw map



X Index: 278



Y Index: 320

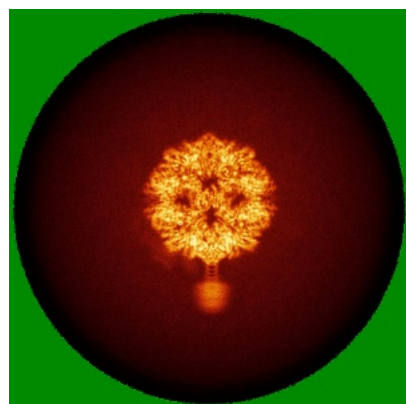


Z Index: 291

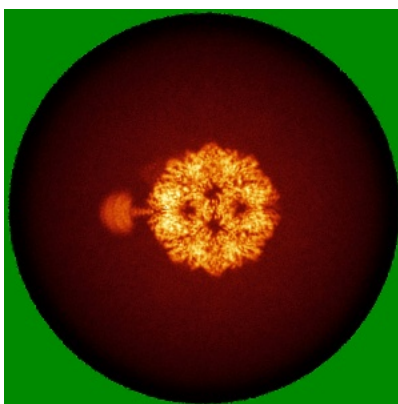
The images above show the largest variance slices of the map in three orthogonal directions.

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

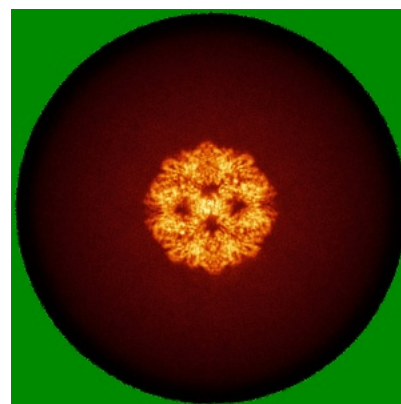
6.4.1 Primary map



X

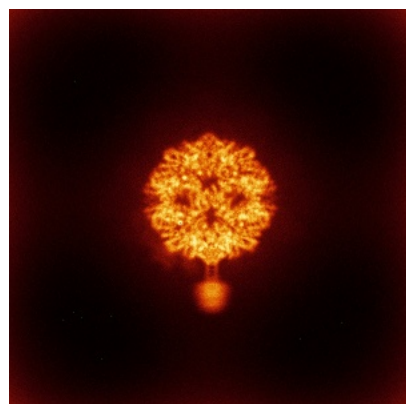


Y

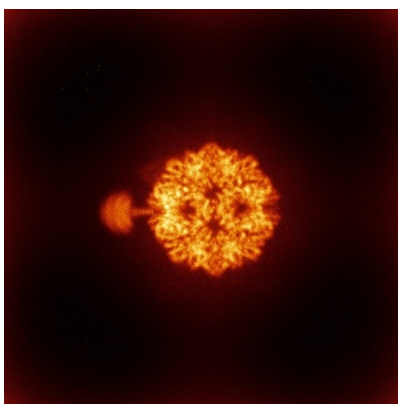


Z

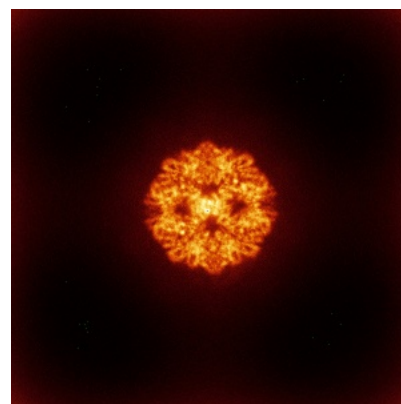
6.4.2 Raw map



X



Y

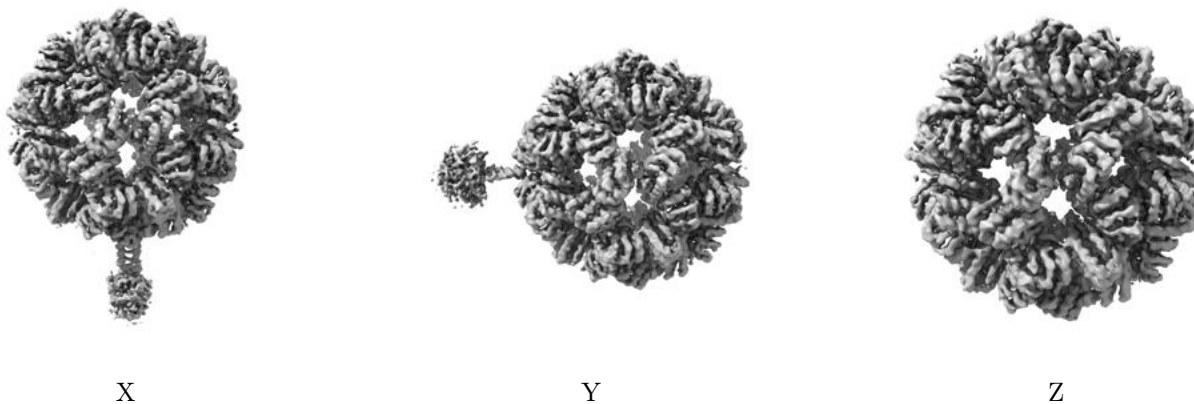


Z

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

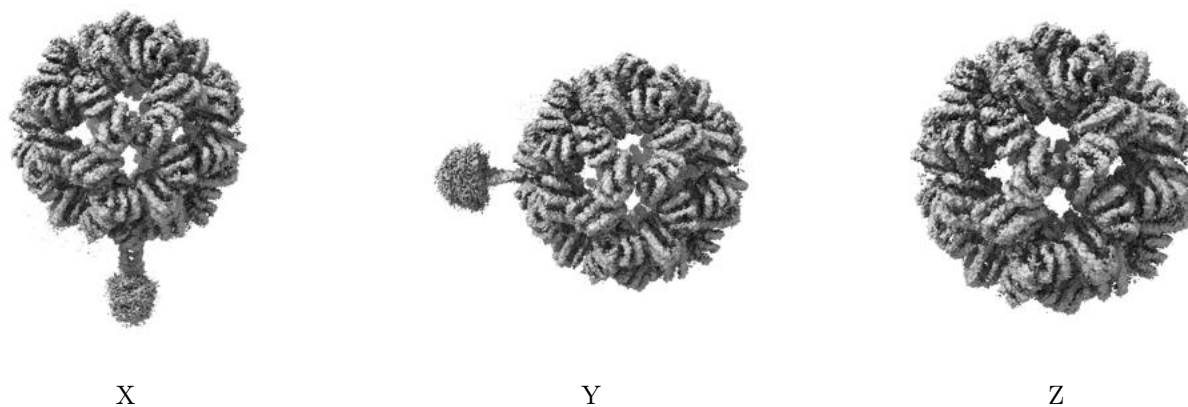
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

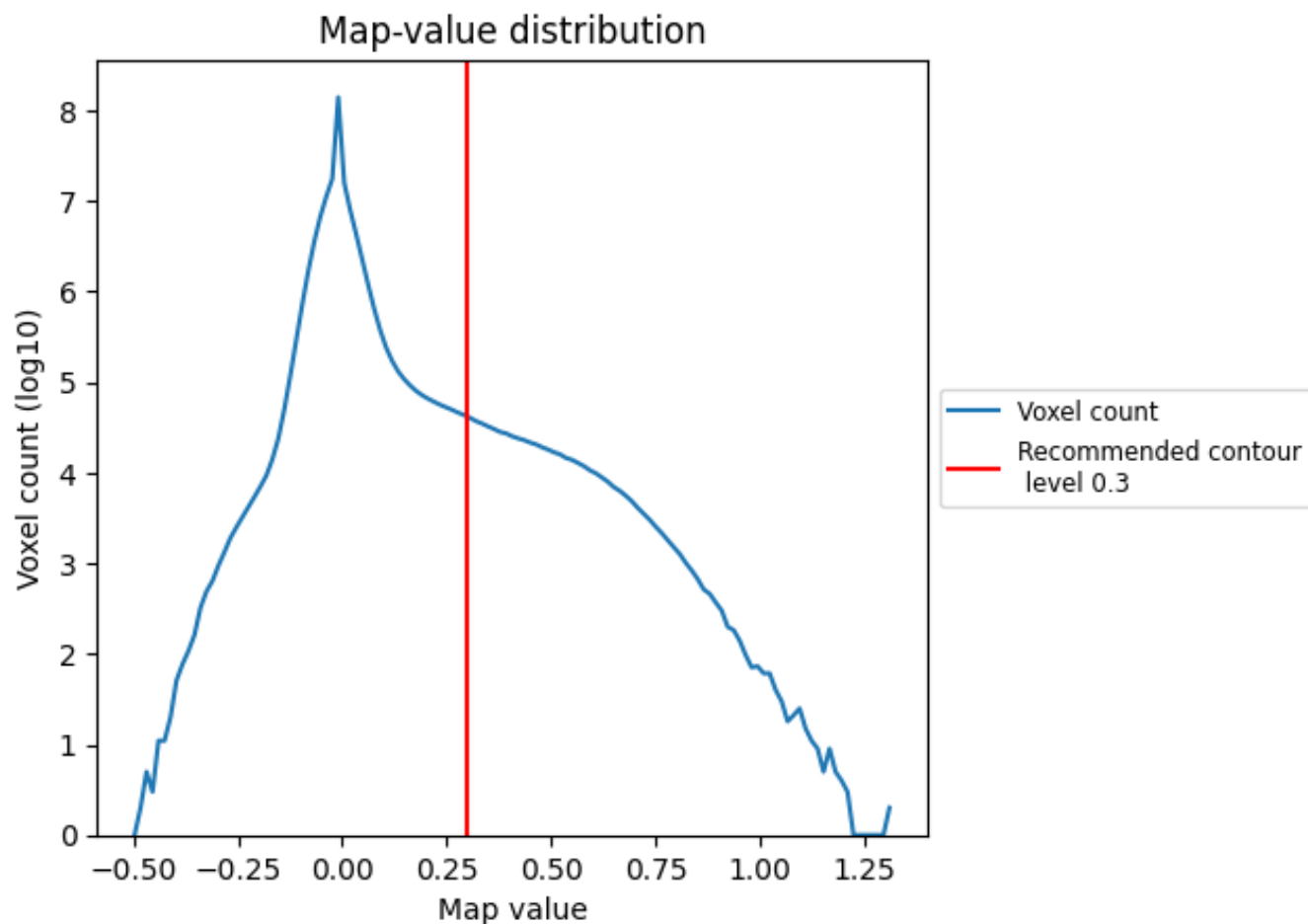
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

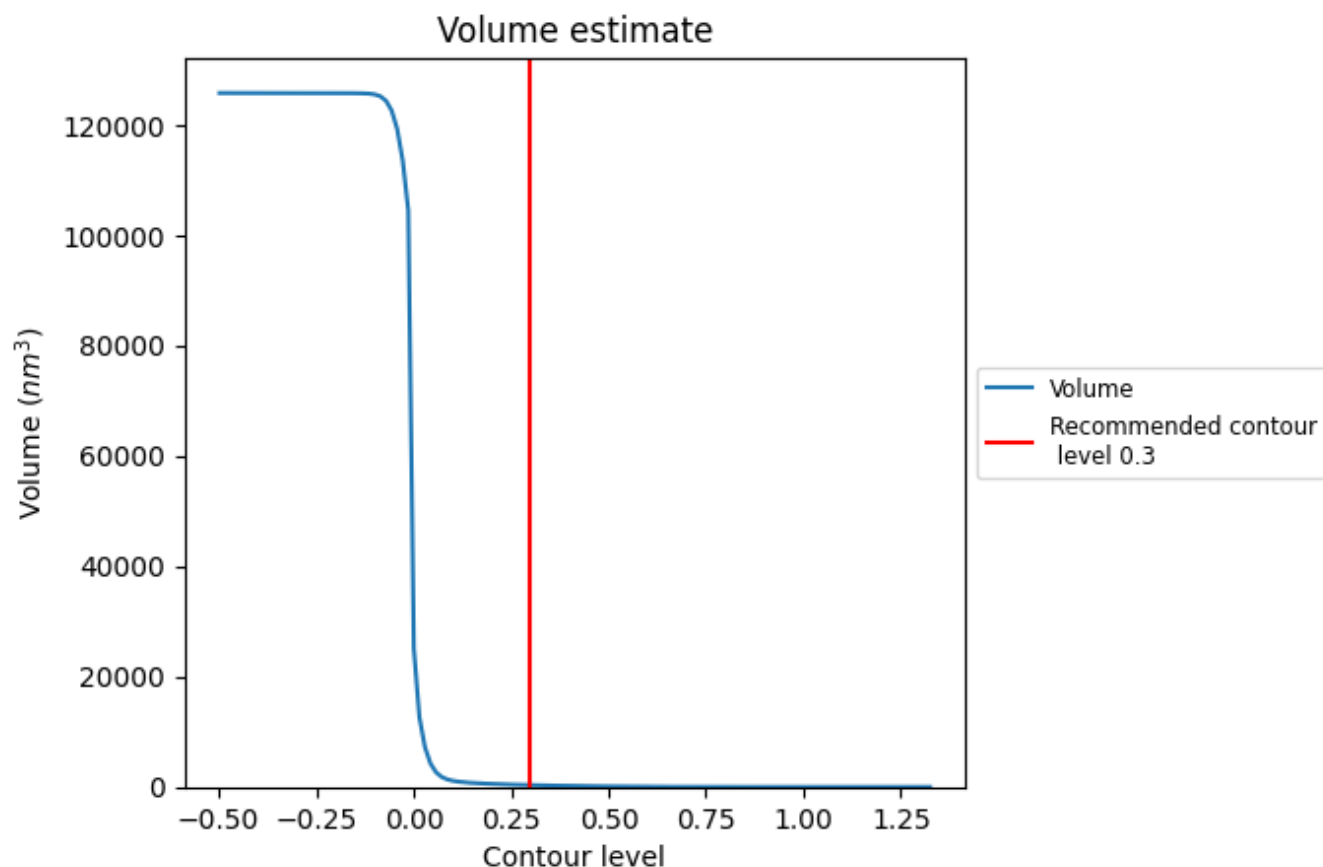
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

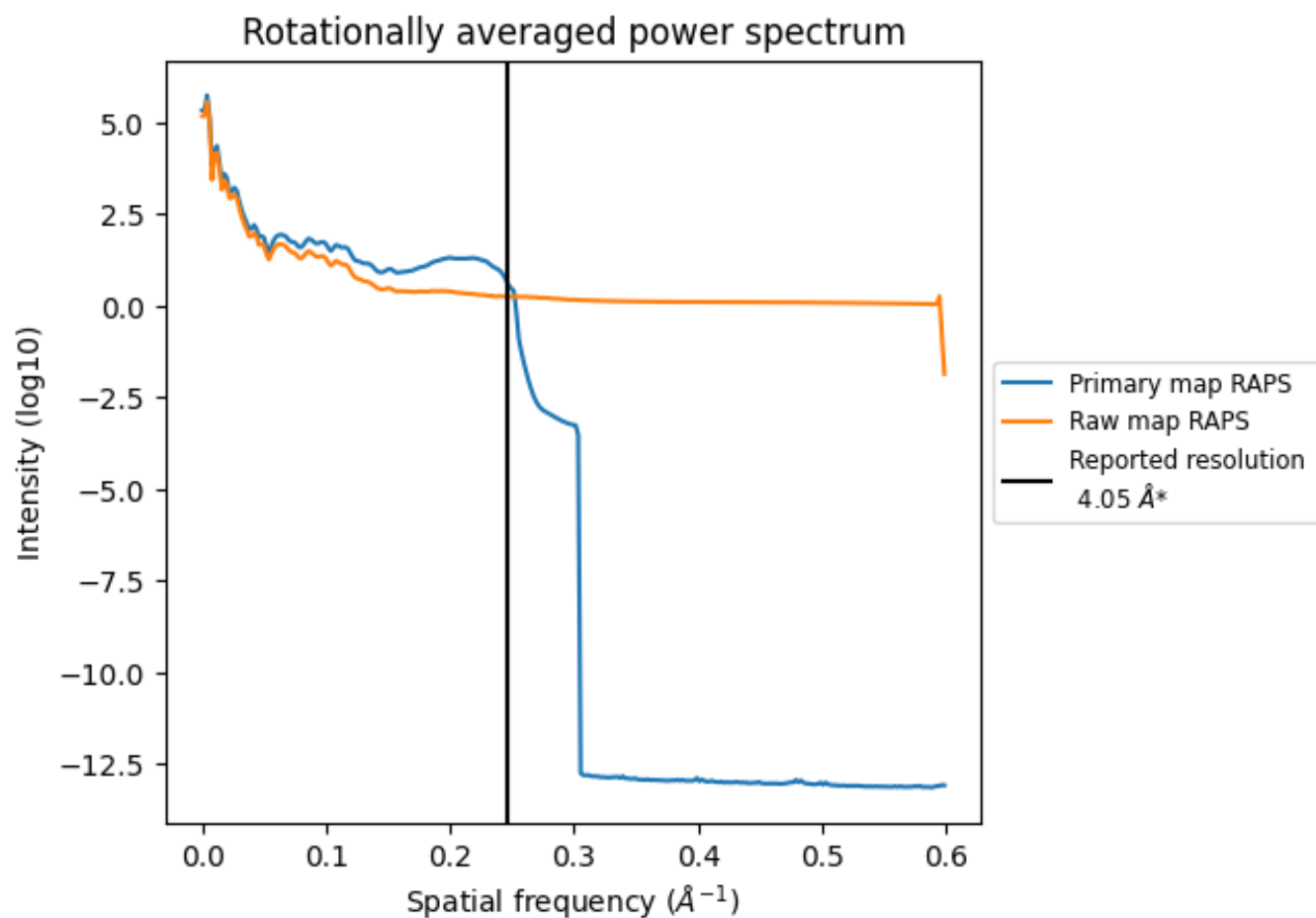
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 333 nm³; this corresponds to an approximate mass of 301 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 ⓘ

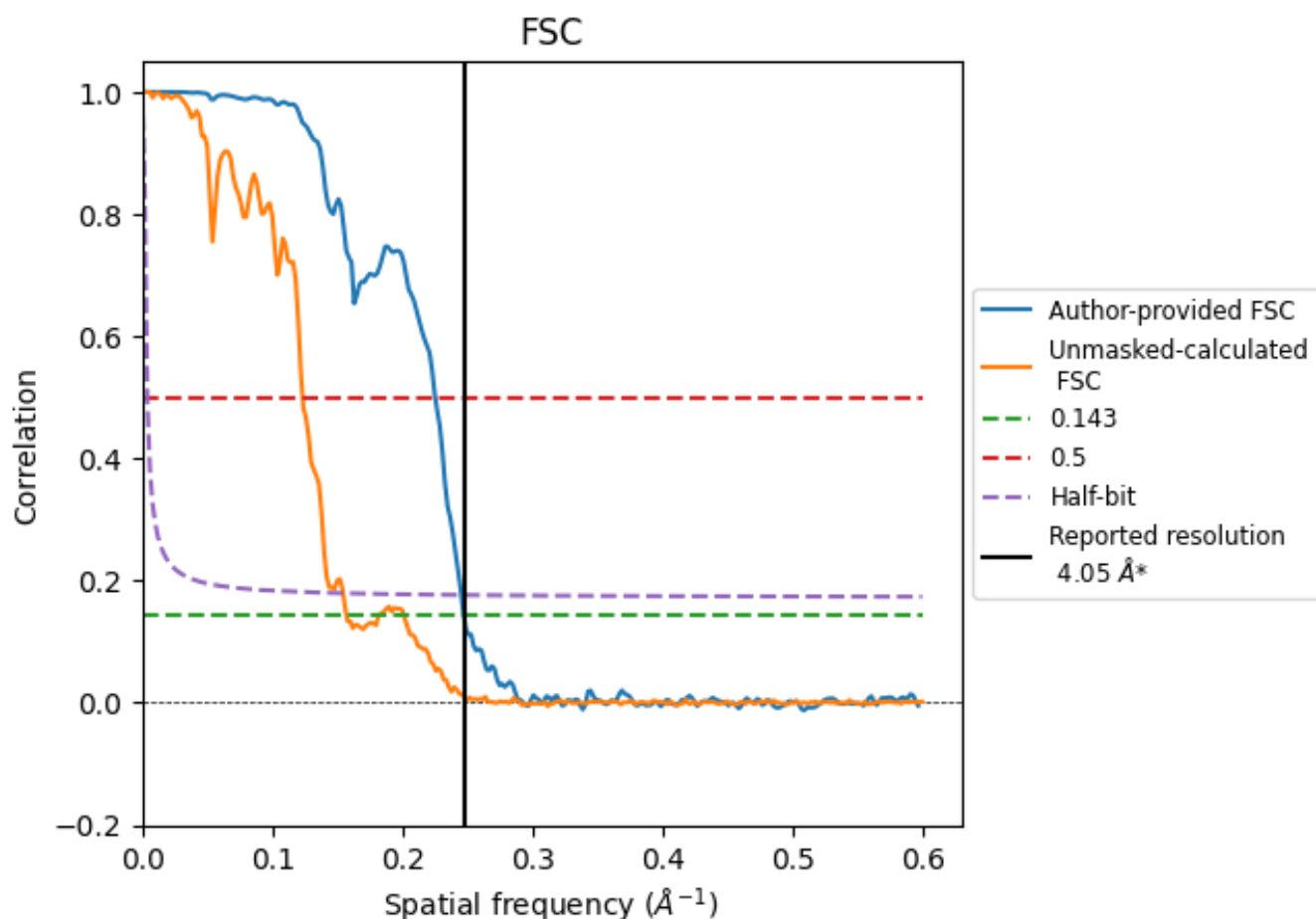


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

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 0.247 \AA^{-1}

8.2 Resolution estimates [i](#)

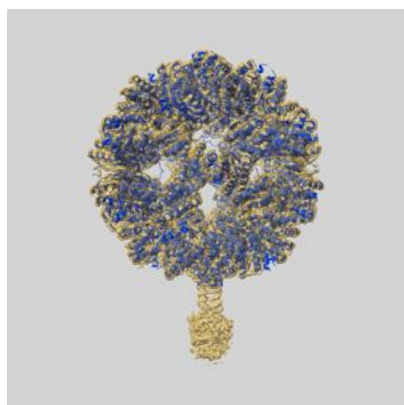
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.05	4.45	4.08
Unmasked-calculated*	6.37	8.12	6.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.37 differs from the reported value 4.05 by more than 10 %

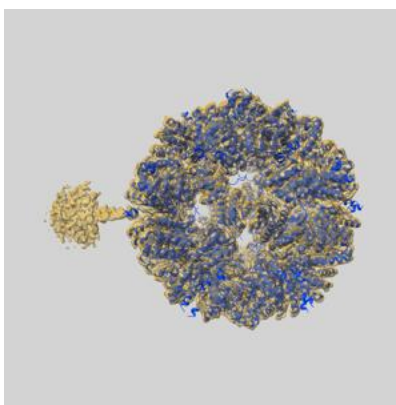
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70081 and PDB model 9O3O. Per-residue inclusion information can be found in section 3 on page 13.

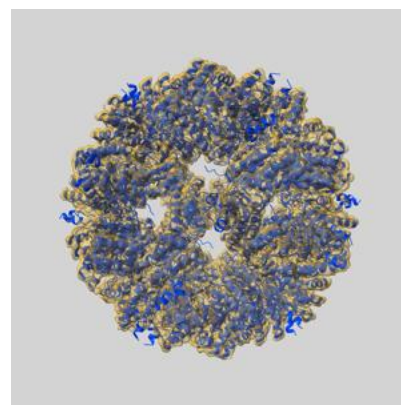
9.1 Map-model overlay [i](#)



X



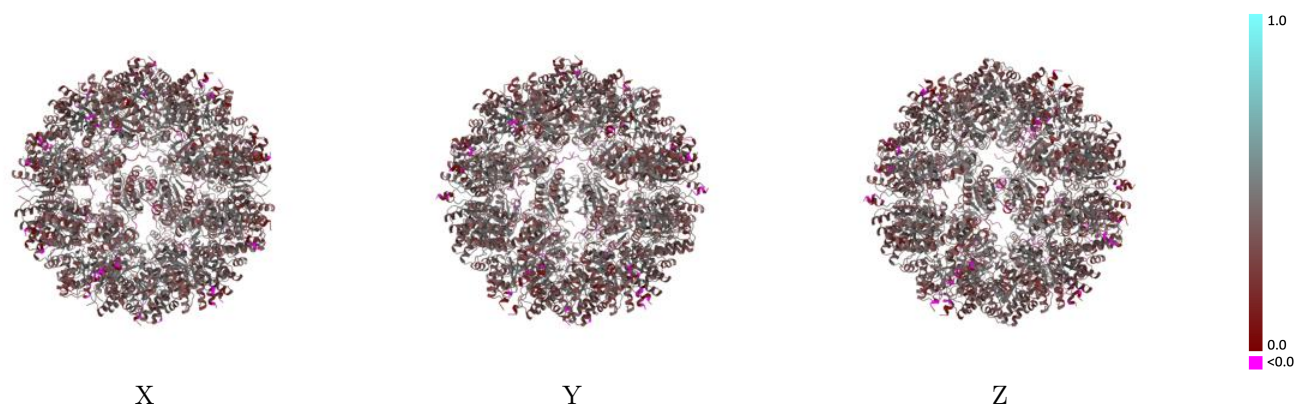
Y



Z

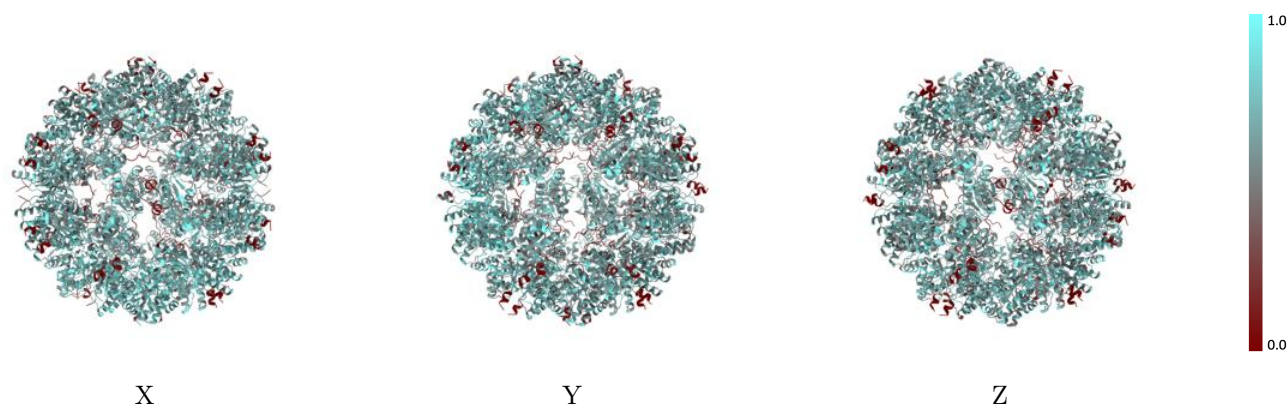
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



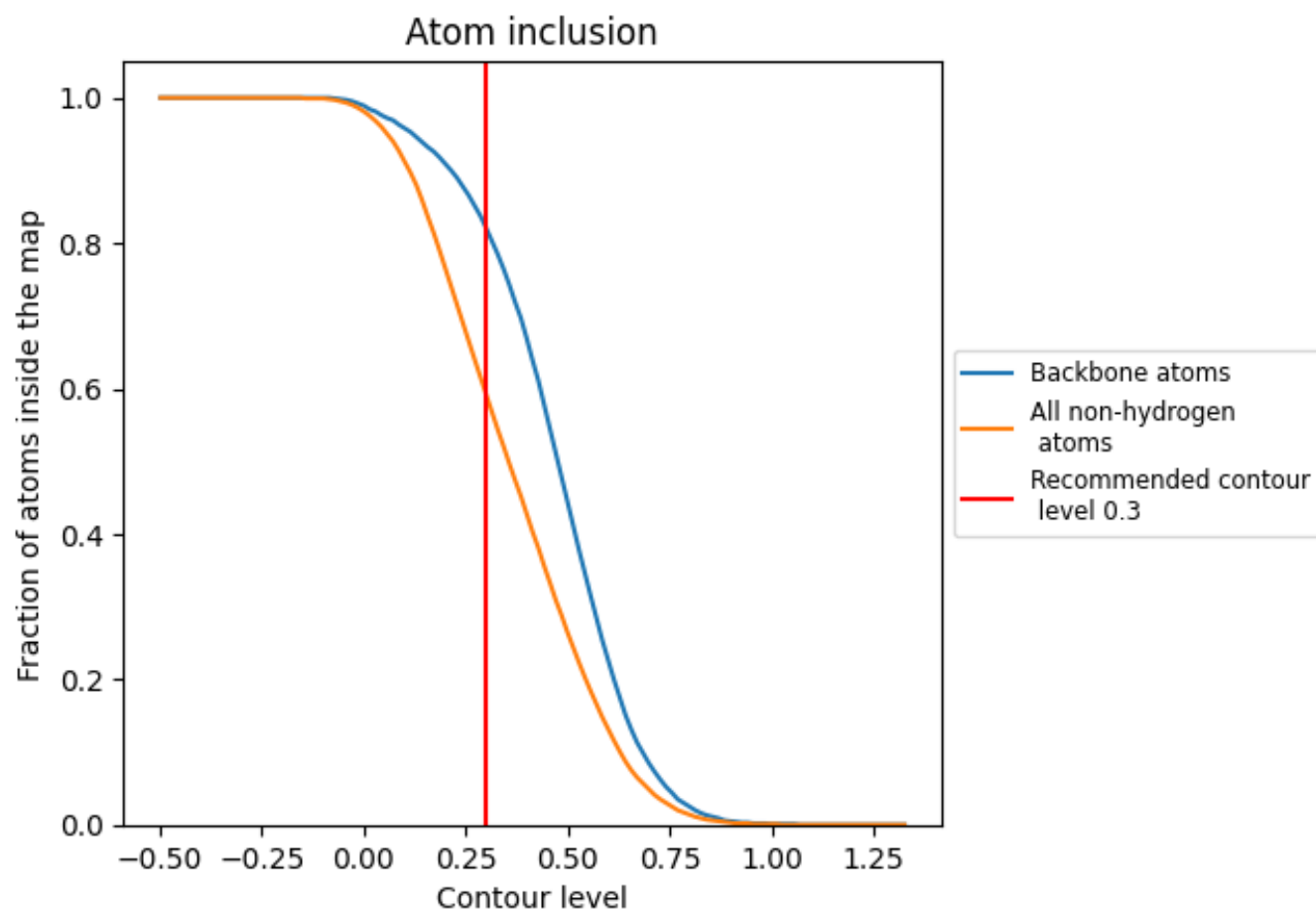
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 59% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5920	 0.3500
A	 0.5640	 0.3310
AB	 0.5530	 0.3380
B	 0.5470	 0.3450
BB	 0.5450	 0.3370
C	 0.5460	 0.3230
CB	 0.5440	 0.3270
D	 0.5670	 0.3370
DB	 0.5800	 0.3580
E	 0.5590	 0.3360
EB	 0.5600	 0.3400
F	 0.5840	 0.3500
FB	 0.5580	 0.3320
G	 0.6140	 0.3180
GB	 0.6170	 0.3240
H	 0.5620	 0.3350
HB	 0.5490	 0.3370
I	 0.7600	 0.4050
IB	 0.7530	 0.4010
J	 0.5620	 0.3380
JB	 0.5400	 0.3230
K	 0.5460	 0.3360
KB	 0.5430	 0.3340
L	 0.6150	 0.3330
LB	 0.6050	 0.3260
M	 0.5680	 0.3360
MB	 0.5610	 0.3370
N	 0.5660	 0.3430
NB	 0.5490	 0.3340
O	 0.5410	 0.3150
OB	 0.5530	 0.3250
P	 0.5440	 0.3270
PB	 0.5570	 0.3340
Q	 0.5520	 0.3280
QB	 0.5460	 0.3310



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Chain	Atom inclusion	Q-score
R	 0.5660	 0.3430
RB	 0.5760	 0.3330
S	 0.5450	 0.3210
SB	 0.5430	 0.3230
T	 0.5360	 0.3190
TB	 0.5440	 0.3380
a	 0.6160	 0.3820
ab	 0.6090	 0.3790
b	 0.6100	 0.3910
bb	 0.6220	 0.3800
c	 0.6270	 0.3800
cb	 0.6210	 0.3800
d	 0.6110	 0.3760
db	 0.6280	 0.3810
e	 0.6990	 0.4050
eb	 0.6590	 0.3780
f	 0.6630	 0.3890
fb	 0.6680	 0.3770
g	 0.6270	 0.3790
gb	 0.6440	 0.3870
h	 0.6970	 0.3970
hb	 0.6790	 0.3750
i	 0.6520	 0.3890
ib	 0.6260	 0.3770
j	 0.6350	 0.3760
jb	 0.6250	 0.3760